| 별책부록 |

페닐화합물류 노출에 의한 랫드와 마우스의 성별·장기별 발암성 고찰

OSHRI

산업재해예방
안전보건공단
산업안전보건연구원

연구보고서 별책부록

페닐화합물류 노출에 의한 랫드와 마우스의 성별·장기별 발암성 고찰

임경택

산업재해예방
안전보건공단
산업안전보건연구원

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
(-)-Adrenalin hydrochloride	51-31-2	C1=CC(=C(C=C1)C(O)CNC)O)O.Cl	-	-	-	Mouse	Female	B6C3F1	Inhalation	104	107	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				stomach kidney thyroid gland lung	stomach thyroid gland stomach	kidney thyroid gland stomach	-	-
(-)-Aflatoxin B1	1162-65-8	C3=C(C1=C(OC(C2=C1)C(C2=O)=O)C(4=C3O)C(=@)[O]C@H]C@H]C=CO5)[H])[H]OC	경구 독성(분말) : 구분4 생식독성 : 구분2	-	-	Cynomolgus monkey	Mixed	Not specified	Multiple routes	960	960	Positive	Bile duct	Carcinoma - spindle cell	CYP1A CYP2A13 CYP1A2 CYP3A4 CYP1A1	PLCG2 GPLD1 ACOT2 SLC41A3 OCLN	KIAA0247 MT1B BIRC5 RFP36|RC ENC1	hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (2) hsa1553 K17685 CYP2A13; cytochrome P450 family 2 subfamily A member 13 hsa1576 K17686 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (2) hsa1553 K17685 CYP2A13; cytochrome P450 family 2 subfamily A member 13 hsa1576 K17686 CYP3A4; cytochrome P450 family 3 subfamily A member 4	kidney liver large intestine vascular system	liver	-	vascular system	Carcinoma, Hepatocellular Lung Neoplasms Cell Transformation, Neoplastic Precancerous Conditions Liver Neoplasms Adenoma, Liver Cell Liver Neoplasms, Experimental Kidney Neoplasm Carcinoma, Hepatocellular
(-)-Aflatoxin B1	1162-65-8					Mouse	Female	C57BL/6N	Intraperitoneal	52	92	Negative	Liver	Multiple tumour types									
(-)-Aflatoxin B1	1162-65-8					Mouse	Male	C57BL/6N	Intraperitoneal	52	92	Negative	Liver	Tumour - benign									
(-)-Aflatoxin B1	1162-65-8					Rat	Male	Buffalo	Diet	65	65	Positive	Liver	Carcinoma - hepatocellular									
(-)-Aflatoxin B1	1162-65-8					Rat	Male	Buffalo	Diet	26	52	Positive	Liver	Carcinoma - hepatocellular									
(-)-Aflatoxin B1	1162-65-8					Rat	Female	Fischer 344	Diet	104	104	Positive	Liver	Hepatoma									
(-)-Aflatoxin B1	1162-65-8					Rat	Female	Fischer 344	Diet	75	75	Positive	Colon	Multiple tumour types									
(-)-Aflatoxin B1	1162-65-8					Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Carcinoma - hepatocellular									
(-)-Aflatoxin B1	1162-65-8					Rat	Male	Fischer 344	Diet	104	104	Positive	Liver	Hepatoma									
(-)-Aflatoxin B1	1162-65-8					Rat	Male	Fischer 344	Diet	52	104	Positive	Kidney	Adenocarcinoma									
(-)-delta 9-Tetrahydrocannabinol	1972-08-3	CC2(C)OC=1C=C(C=C(O)C=1)[C@H](C[C@H](C)CCC)=C3C(CCCCC	-	7, 14, 19, 21, 23, **25**, **28**, **30**, 41, 46, 52, 53, 57, 64, 66, 67, 71, 111, 112, 117, 122, 132, 133, 135, 150, 163, **165**, **167**, 187, **200**, 214, **307**, 310, 318	-	Mouse	Female	B6C3F1	Gavage	105	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma	CNR1 MAPK1 MAPK3 CNR2	PPIH SEC16A HSPA5 SEDH1 DHER	EIF3CS4 ALDOA PPP1CB DNAJB14 CKB	hsa05133 Pertussis - Homo sapiens (human) (2) hsa5594 K04371 MAPK1; mitogen-activated protein kinase 1 hsa5595 K04371 MAPK3; mitogen-activated protein kinase 3 hsa05166 Human T-cell leukemia virus 1 infection - Homo sapiens (human) (2) hsa5594 K04371 MAPK1; mitogen-activated protein kinase 1 hsa5595 K04371 MAPK3; mitogen-activated protein kinase 3 hsa01522 Endocrine resistance - Homo sapiens (human) (2) hsa5594 K04371 MAPK1; mitogen-activated protein kinase 1 hsa5595 K04371 MAPK3; mitogen-activated protein kinase 3	-	-	-	-	Colonic Neoplasm
(-)-delta 9-Tetrahydrocannabinol	1972-08-3					Mouse	Male	B6C3F1	Gavage	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
(-)-delta 9-Tetrahydrocannabinol	1972-08-3					Rat	Female	Fischer 344	Gavage	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
(-)-delta 9-Tetrahydrocannabinol	1972-08-3					Rat	Male	Fischer 344	Gavage	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
(-)-Demecolcine	477-30-5	CN[C@H](CCC1=CC(=O)C(=C1C=a2C2=CC(C)(OC)=CC=3)=O)(OC)OC)OC	-	19, 23, **29**, **30**, 46, 52, 53, 67, 111, 112, 117, **165**, **167**, 187, **200**, 307	-	Rat	Male	BR 46	Intravenous	52	104	Negative	Multiple sites	Multiple tumour types	CASP3 ABCB1 CYP1A1 U25LIRP ZNG307	TAGLN ACOT2 DSPP HEATR3 TBC1D9	ASAH1 BACSAAP1 GBS2 PHYH TMIP12	hsa05206 MicroRNAs in cancer - Homo sapiens (human) (2) hsa1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa5243 K05658 ABCB1; ATP binding cassette subfamily B member 1 hsa05226 Gastric cancer - Homo sapiens (human) (2) hsa1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa5243 K05658 ABCB1; ATP binding cassette subfamily B member 1	-	ear Zymbals gland	urinary bladder thyroid gland	-	-
(-)-Emetine hydrochloride	316-42-7	O(C1=c(OC(C=c2C)=c1C)CN[C@]2C]2@H](C)[C@H]3C]=c(COC)c1c(OC)c=CC(OC)=c(OC)c1)C(OC)=O)[C@H](C)C(C)[H]) C.Cl.Cl	-	7, 14, 19, 23, 25, 27, **29**, **30**, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, **165**, **167**, 187, **200**, 204, 207, 318	-	Mouse	Female	B6C3F1	Intraperitoneal	40	78	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				vascular system skin all tumor bearing animals	vascular system	urinary bladder	-	-
(-)-Emetine hydrochloride	316-42-7					Mouse	Male	B6C3F1	Intraperitoneal	44	78	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Emetine hydrochloride	316-42-7					Rat	Female	SD	Intraperitoneal	52	83	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Emetine hydrochloride	316-42-7					Rat	Male	SD	Intraperitoneal	52	83	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Ephedrine sulphate	134-72-5	C1=CC=CC(=C1)[C@H](C)[C@H](C)NC)O.O5O2)(=O)=O.C2=CC=CC=C2)[C@H](C)[C@H](C)NC)O	피부 과민성 : 구분1(A/1B) 특정표적장기 독성(반복 노출) : 구분2		-	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				-	-	-	-	-
(-)-Ephedrine sulphate	134-72-5					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Ephedrine sulphate	134-72-5					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Ephedrine sulphate	134-72-5					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Epigallocatechin 3-O-gallate	989-51-5	O(C.=4C2)C(=@H)[C@H](C=1C.=2C(=)=C(C.=2)O)O)O)C(C3=)=C(=)=C(O)=C3)O)O)=O)=C(C.=4)O)O	-	19, 23, **29**, **30**, 52, 53, 61, 67, 111, 112, 117, 122, 123, 150, **165**, 167, 187, **200**, 220, 307	-	Mouse	Male	C3H/HeN	Drinking water	58	58	Negative	Liver	Multiple tumour types	IL1B CAT CASP3 PTGS2 TNF	CXORF48 GSS ITGAV TSPM SLC38A1	HIVEP1 RGL1 SLC29A4 NOTCH1 SLC20A1	hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (3) hsa5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa836 K02187 CASP3; caspase 3 hsa847 K03781 CAT; catalase	stomach	stomach	stomach	-	Breast Neoplasm
(-)-Phenylephrine hydrochloride	61-76-7	C1=CC=CC(=C1)[C@H](C)NC)O.Cl	경구 독성(분말) : 구분4 생식독성 : 구분2	8, 11, 60	Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic					stomach kidney all tumor bearing animals	stomach	kidney thyroid gland	-	-
(-)-Phenylephrine hydrochloride	61-76-7					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Phenylephrine hydrochloride	61-76-7					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Phenylephrine hydrochloride	61-76-7					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Reserpine	50-55-5	C1=c(C(=c(C)=C1)OC)OC)OC)C(O[C@H](C)[C@]3[C@H](C[C@H](C[C@H](C[C@H]3O)C)C)=O)[C]C@@]6[C]=O)C=4C=N6)=c(C)=CC=4OC)C)CN[C]3[H])[H])[H]=O	경구 독성(분말) : 구분4 피부 부식성/자극 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(A/B) 생식독성 : 구분1B 특정표적장기 독성(반복 노출) : 구분2	Cancer slope factor: 0.0031 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: predicted to be genotoxic		Mouse	Female	B6C3F1	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	TH NPY PDNK FOS SLC18A2	ITGAV	AURKA CYP2A4	hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (2) hsa4852 K05232 NPY; neuropeptide Y hsa5179 K18852 PDNK; pyruvate/pyruvate hsa04024 cAMP signaling pathway - Homo sapiens (human) (2) hsa2353 K04379 FOS; fos proto-oncogene, AP-1 transcription factor subunit hsa4852 K05232 NPY; neuropeptide Y	vascular system	-	-	Breast Neoplasm Mammary Neoplasms, Experimental Pheochromocytoma Neoplasms, Experimental
(-)-Reserpine	50-55-5					Mouse	Male	B6C3F1	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Reserpine	50-55-5					Mouse	Female	C3H (MTV+)	Diet	104	104	Not specified	Mammary gland	Adenocarcinoma									
(-)-Reserpine	50-55-5					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Reserpine	50-55-5					Rat	Male	Fischer 344	Diet	103	104	Positive	Adrenal gland	Pheochromocytoma | Pheochromocytoma - malignant									
(-)-Reserpine	50-55-5					Rat	Female	Wistar	Diet	75	75	Negative	Mammary gland	Fibroadenoma									
(-)-Reserpine	50-55-5					Rat	Male	Wistar	Diet	75	75	Negative	Pituitary gland	Adenoma									
(-)-Rotenone	83-79-4	C2=4C[C@]1(C3=c(OC)C)[C@]1(O2)[H])C=1C(=)=C(C)=C3)O(OC)OC)[H])=O)=CC=CC=3C=4C)[H])O)C(=)=C	경구 독성(분말) : 구분1 경구 독성(캡슐) : 구분2 피부 부식성/자극 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(A/B) 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분1 경口 수생환경 유해성 : 구분1 무機 수생환경 유해성 : 구분1	7, 8, 14, 19, 23, 25, **27**, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 59, 60, 61, 62, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 125, 146, 150, 153, 163, **165**, **167**, 187, **200**, 214, 220, 307, 318	Carcinogenicity data available: EPA OPP-Group E Evidence of Non-carcinogenicity for Humans	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	CASP3 SNCA TNF BCL2 NOS2 IL1B	GSS	CDKSR MDURD CHEK1 ITGAV	hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (4) hsa4843 K13241 NOS2; nitric oxide synthase 2 hsa596 K02161 BCL2; BCL2 apoptosis regulator hsa6622 K04528 SNCA; synuclein alpha hsa7124 K03156 TNF; tumor necrosis factor	vascular system	-	stomach	-	Pancreatic Neoplasm
(-)-Rotenone	83-79-4					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(-)-Rotenone	83-79-4					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(-)-Rotenone	83-79-4					Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Rotenone	83-79-4					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Multiple tumour types									
(-)-Rotenone	83-79-4					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Rotenone	83-79-4					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(-)-Rotenone	83-79-4					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(+)-Hematoxylin	517-28-2	C1=C(C)=CC2=C1C(C@@](O)[C@]2(C4=O)OC)O)=C)C=O(O)O)O)O	심한 눈 손상성/눈 자극성 : 구분2A(A/B)	-	Genotoxicity Data: predicted to be genotoxic	Rat	Mixed	Wistar	Diet	78	78	Positive	Abdomen	Lymphoma - malignant	-	ZBTB10 TBC1D9 HEATR3 NOPS6 MBNL2	AURKA CHEK1 BLM IERS1 MFT		-	small intestine	stomach	pituitary gland hematopoietic system	-
(+)-Vinblastine	865-21-4	O(C.@)(4CC(CN7CCC8=c(C)c(C@@](C=JC.=C1[C@@]34[C@@]1N(C1=CC=JOC)C)[C@@]2[C@@](C[C@]5[C@@]5(N)C=4)C=C5[H])C)C)OC.)=O)O)C)=O)OC)[H])C)=O)OC)[C@@H](C)=O)C=C[C@@H](C)C7N(.=)C.8=.C=.C=.C=.H	-	-	-	Rat	Male	BR 46	Intravenous	52	104	Negative	Multiple sites	Multiple tumour types	ABCB1 ABCC2 SOD2 FGA8	NGF	AURKA	hsa04213 longevity regulating pathway - multiple species - Homo sapiens (human) (1) hsa6648 K04564 SOD2; superoxide dismutase 2 hsa02010 ABC transporters - Homo sapiens (human) (1) hsa1244 K05666 ABCC2; ATP binding cassette subfamily C member 2 hsa04976 Bile secretion - Homo sapiens (human) (1) hsa1244 K05666 ABCC2; ATP binding cassette subfamily C member 2	vascular system	-	-	-	Myelitis, Transverse Urinary Bladder Neoplasm Carcinoma, Transitional Cell Testicular Neoplasm

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
(±)-1-Phenylethanol	98-85-1	C1=CC=CC=C1C(O)C	경련 독성(반복) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A/2B 생식세포 변이원성 : 구분2	-	Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	PHUM_PHUM225140 PHUM_PHUM218810	SRSRI3 TOB1 ALDH18A1 RNF12 PPP1CA	PLAGL6 CA2 SDC1 SPAG6 POLR2A		kidney stomach lung Malignant head cancers spleen nasal cavity vascular system thyroid gland	nasal cavity	vascular system	pituitary gland thyroid gland ovary	-
(±)-1-Phenylethanol	98-85-1					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-1-Phenylethanol	98-85-1					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-1-Phenylethanol	98-85-1					Rat	Male	Fischer 344	Gavage	103	104	Positive	Adrenal gland medulla	Pheochromocytoma | Pheochromocytoma- malignant									
(±)-alpha-Tocopherol	10191-41-0	C[C@H](CCC[C@H](C)CCC[C@H](C)CCCC(C)C)CCc1c(C)c(O)c(C)c(C)c1O	피부 부식성/피부 자극성 : 구분2 피부 과민성 : 구분1(1A/1B) 특정표적장기 독성(반복 노출) : 구분2	-	Genotoxicity Data: predicted to be genotoxic	Rat	Female	Fischer 344/DuCr	Diet	54	54	Negative	Colon	Multiple tumour types	TNF CASP3 CAT	SMARCC1 NADK MAGT4 MSH3 TBLR1	ALDOA ERCC6 ABHD2 PCK OS9	hsa05014 Amyotrophic lateral sclerosis - Homo sapiens (human) (1) hsa836 402187 CASP2; caspase 2 hsa04623 Cytosolic DNA-sensing pathway - Homo sapiens (human) (1) hsa836 402187 CASP2; caspase 2 hsa05132 Salmonella infection - Homo sapiens (human) (1) hsa836 402187 CASP2; caspase 2	-	-	liver	-	**Lung Neoplasm** Cell Transformation, Neoplastic **Liver Neoplasms**
(±)-alpha-Tocopherol	10191-41-0					Rat	Male	Fischer 344/DuCr	Diet	52	52	Negative	Forestomach	Multiple tumour types									
(±)-Amphetamine sulphate	60-13-9	C1=CC=CC(=C1)C(CN(C,O)O)(=O)=O.C2=CC=CC(=C2)C(CN)C			-	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				-	-	-	-	-
(±)-Amphetamine sulphate	60-13-9					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-Amphetamine sulphate	60-13-9					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-Amphetamine sulphate	60-13-9					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-Benzoin	119-53-9	C1=CC=CC(=C1)C(C)C(=O)C=CC=CC=C2C(=O)=O	피부염증	8, 11, 60	Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				stomach lung kidney	-	vascular system	pituitary gland ovary	-
(±)-Benzoin	119-53-9					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-Benzoin	119-53-9					Rat	Female	Fischer 344	Diet	104	103	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-Benzoin	119-53-9					Rat	Male	Fischer 344	Diet	104	103	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-Chlorpheniramine maleate	113-92-8	C1(=CC=CC=C1C(N(C)C)CCN(C)C)C2=NC=CC=C2C(=O)C(C)=O.C(=C/C(=O)O)\C(=O)=O	경련 독성(반복) : 구분4 생식독성 : 구분2	8, 11, **29**, **30**, 43, 52, 53, 60, 67, 91, 93, 94, 96, 97, 98, 112, **165**, **167**, 195, 197, **198**, 203, 204	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	HRH1 KCNH2 SLC22A2	-	-		-	-	-	-	-
(±)-Chlorpheniramine maleate	113-92-8					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Adrenal capsule	Adenoma									
(±)-Chlorpheniramine maleate	113-92-8					Rat	Female	Fischer 344	Diet	106	128	Negative	Liver	Nodule- neoplastic									
(±)-Chlorpheniramine maleate	113-92-8					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Carcinoma- hepatocellular | Noduleneoplastic | Adenoma- hepatocellular									
(±)-Chlorpheniramine maleate	113-92-8					Rat	Male	Fischer 344	Diet	106	128	Negative	Liver	Nodule- neoplastic									
(±)-Chlorpheniramine maleate	113-92-8					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
(±)-Ciprofibrate	52214-84-3	C2C(3)(C)C(C1=CC=C(C=C1)OC(C)(C)C(O)=O)CC2	-	6, 8, 11, 18, 34, 36, 37, 51, 58, 60, 61, 72, 163, 166, 318	-	Mouse	Male	C57BL/6N	Diet	78	78	Positive	Liver	Adenoma- hepatocellular	PPARA NR1I3 ACOX1 CYP4A1	APOA1 NAPTL1 TNFC2 GSNRM RPS19	PPARA CPT1A NR1H2 CYP4A11 PPARD	hsa0171,2 fatty acid metabolism - Homo sapiens (human) (1) hsa.51 630.32 ACOX1; acyl-CoA oxidase 1 hsa00592 alpha-Linolenic acid metabolism - Homo sapiens (human) (1) hsa.51 630.32 ACOX1; acyl-CoA oxidase 1 hsa01200 Carbon metabolism - Homo sapiens (human) (1) hsa.51 630.32 ACOX1; acyl-CoA oxidase 1	stomach liver	stomach liver	liver	liver	Carcinoma, Hepatocellular **Liver Neoplasm** **Lung Neoplasm** Neoplasm Metastasis Precancerous Conditions
(±)-Ciprofibrate	52214-84-3					Mouse	Male	C57BL/6N	Diet	89	91	Positive	Liver	Adenoma- hepatocellular									
(±)-Ciprofibrate	52214-84-3					Rat	Female	Fischer 344	Diet	104	104	Positive	Stomach - glandular	Carcinoma- hepatocellular									
(±)-Ciprofibrate	52214-84-3					Rat	Male	Fischer 344	Diet	60	60	Positive	Liver	Carcinoma- hepatocellular									
(±)-Ciprofibrate	52214-84-3					Rat	Male	Fischer 344	Diet	104	104	Positive	Stomach - glandular	Carcinoma- hepatocellular									
(±)-Ciprofibrate	52214-84-3					Rat	Male	Fischer 344	Diet	95	95	Positive	Liver	Multiple tumour types									
(±)-Ciprofibrate	52214-84-3					Rat	Male	Fischer 344	Diet	60	60	Positive	Liver	Carcinoma- hepatocellular									
(±)-Ciprofibrate	52214-84-3					Rat	Male	Fischer 344	Diet	60	60	Positive	Liver	Carcinoma- hepatocellular									
(±)-Dichlorprop	120-36-5	C1=C(C=CC(=C1Cl)OC(C)C(O)=O)Cl	경련 독성(반복) : 구분4 경련 독성(급성) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A/2B **발암성 : 구분2** 경로 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 34, 36, 57, 58, 60, 72, 122, 123, 150, 163, 220	Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Angioma	-				-	-	kidney liver vascular system	-	-
(±)-Dichlorprop	120-36-5					Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Dichlorprop	120-36-5					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Dichlorprop	120-36-5					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Dichlorprop	120-36-5					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Dichlorprop	120-36-5					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Dichlorprop	120-36-5					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Dichlorprop	120-36-5					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Dopa	63-84-3	C1=C(C(=CC(=C1)C(CC(O)=O)N)O)O	-	-	-	Rat	Male	Fischer 344/DuCr	Diet	51	52	Not specified	Forestomach	Multiple tumour types	FOYN FOSB COMT	SOD1 SHC1 ITGAV TBRAP AKRIC2	SOD3 AKR1B10 NQO1 TPI1 OS9	hsa05031 Amphetamine addiction - Homo sapiens (human) (1) hsa2354 #209029 FOSB; FosB proto-oncogene, AP-1 transcription factor subunit hsa05034 Alcoholism - Homo sapiens (human) (1) hsa2354 #209029 FOSB; FosB proto-oncogene, AP-1 transcription factor subunit hsa04380 Osteoclast differentiation - Homo sapiens (human) (1) hsa2354 #209029 FOSB; FosB proto-oncogene, AP-1 transcription factor subunit	kidney stomach urinary bladder skin	kidney stomach	kidney lung stomach	lung	Neoplasm Bile Duct Neoplasm Melanoma
(±)-Etodolac	41340-25-4	C(C)(C)(C)c-2NC1=C(C=CC=C1C=a2CCO)C(C)(C)(O)=O	-	34, 36, 58, 61, 72, 163	-	Mouse	Female	CD1	Diet	78	78	Negative	Liver	Adenoma- hepatocellular	PTGS2 **Bcl2** **BIRC5** **BIRC2** **CASP3** CASP9	NGF NAPTL1 TOB1	-	hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa.320 #16060 BIRC2; baculoviral IAP repeat-containing 2 hsa.332 #08713 BIRC5; baculoviral IAP repeat-containing 5 hsa.596 #02161 BCL2; BCL2 apoptosis regulator hsa.836 #02187 CASP2; caspase 2 hsa04215 Apoptosis - multiple species - Homo sapiens (human) (4) hsa.320 #16060 BIRC2; baculoviral IAP repeat-containing 2 hsa.332 #08713 BIRC5; baculoviral IAP repeat-containing 5 hsa.596 #02161 BCL2; BCL2 apoptosis regulator hsa.836 #02187 CASP2; caspase 2 hsa04210 Apoptosis - Homo sapiens (human) (4) hsa.320 #16060 BIRC2; baculoviral IAP repeat-containing 2 hsa.332 #08713 BIRC5; baculoviral IAP repeat-containing 5 hsa.596 #02161 BCL2; BCL2 apoptosis regulator hsa.836 #02187 CASP2; caspase 2	-	-	-	-	Neoplasm Metastasis Colonic Neoplasm Colorectal Neoplasm **Liver Neoplasms**
(±)-Etodolac	41340-25-4					Mouse	Male	CD1	Diet	78	78	Negative	Liver	Adenoma- hepatocellular									
(±)-Etodolac	41340-25-4					Rat	Female	SD	Diet	104	104	Negative	Liver	Carcinoma- hepatocellular									
(±)-Etodolac	41340-25-4					Rat	Male	SD	Diet	104	104	Negative	Liver	Carcinoma- hepatocellular									
(±)-Fenoprop	93-72-1	C1(=C(C=C(C)=C1)OC(C)(C)(=O)C)C(=O)C)Cl	경련 독성(반복) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A/2B **발암성 : 구분2** 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2 경로 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	34, 36, 58, 72, 163	Carcinogenicity data available EPA OPP-Group D Not Classifiable as to Human Carcinogenicity	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	GSTA3 GSTM2	MEAP4 FABP4 BIBA4P MYBL1 TMSB15A	FTL GCLC PPARA BEL FTCD1		-	-	kidney	-	-
(±)-Fenoprop	93-72-1					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Fenoprop	93-72-1					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(±)-Fenoprop	93-72-1					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
(+)-Reserpine acetate	54143-56-5	C(C)(C)NC1(C)C(C)C(=C(C=C(C)C(C)(C)(C)C(C)(C)(C)C)C=C)C	-	-	-	Mouse	Female	CD1	Diet	78	78	Negative	Liver	Adenoma									
(+)-Reserpine acetate	54143-56-5					Mouse	Male	CD1	Diet	78	78	Negative	Liver	Adenoma									
(+)-Reserpine acetate	54143-56-5					Rat	Female	CrlCD(SD)IGS	Diet	104	104	Negative	Liver	Adenoma									
(+)-Reserpine acetate	54143-56-5					Rat	Male	CrlCD(SD)IGS	Diet	104	104	Negative	Liver	Adenoma									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
(+)-Ketoprofen	22071-15-4	C[C@H](c1ccc(C(=O)c2ccccc2)c2ccccc12)C(=O)O	급성 독성(경구) - 구분3	34, 36, 58, 72, 163	-	Rat	Male	Fischer 344	Diet	54	54	Not specified	Colon	Multiple tumour types	UGT2B7 ALB DHRS11	BACE1 FABP4 NEF TOR1 AFOA1	GCLC GCLM TPI1 HPGD TBN11	hsa04918: Thyroid hormone synthesis - Homo sapiens (human) (1) hsa-miR-21-5p: ALB; albumin	-	liver	vascular system	liver	-
(±)-Methadone hydrochloride	1095-90-5	C[C@]1(c2ccccc2)CC[C]1c1ccccc1C[C@]1c1ccccc1C(=O)CC[N]1(C)C.Cl	-	8, 11, 33, 34, 46, 57, 58, 60, 61, 62, 91, 93, 94, 96, 97, 98, 126, 131, 165, 192, 200, 204	-	Mouse	Female	B6C3F1	Diet	106	106	Negative	Liver	Adenoma - hepatocellular	-				all tumor bearing animals	uterus thyroid gland hematopoietic system brain	kidney thyroid gland	lung	-
(±)-Methadone hydrochloride	1095-90-5					Mouse	Male	B6C3F1	Diet	106	106	Negative	Liver	Adenoma - hepatocellular									
(±)-Methadone hydrochloride	1095-90-5					Rat	Female	Fischer 344	Diet	106	106	Negative	Liver	Neuroma - neoplastic									
(±)-Methadone hydrochloride	1095-90-5					Rat	Male	Fischer 344	Diet	106	106	Negative	Liver	Carcinoma - hepatocellular									
(±)-Oxazepam	604-75-1	N2C(C)(N=c(c1ccccc1)c1cc(Cl)ccc12)C(=O)c1ccc(Cl)cc1O	발암성 - 구분2 특정표적장기 독성(반복 노출) - 구분2	19, 23, 29, 30, 34, 36, 52, 53, 58, 61, 62, 67, 72, 111, 112, 117, 165, 166, 167, 187, 200, 207	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	98	105	Positive	Liver	Adenoma - hepatocellular	CYP2B10 GADD45B GSTM1 UGT2B7	VTN TGFBR3 TNC PCDGC32 FABP4	SP1 SCD5 BEL CYP2B1 AHR8	hsa05224: Breast cancer - Homo sapiens (human) (1) hsa-miR-6-3p: GADD45B; growth arrest and DNA damage inducible beta hsa05210: Colorectal cancer - Homo sapiens (human) (1) hsa-miR-6-3p: GADD45B; growth arrest and DNA damage inducible beta hsa00040: Pentose and glucuronate interconversions - Homo sapiens (human) (1) hsa-miR-6-3p: GADD45B; UGT2B15; LYZL6; cob-n-cornucopia/cobinamide kinase; Pseudo 3; xenobiotic 8/15	-	all tumor bearing animals	liver	thyroid gland liver	Liver Neoplasms Adenoma, Liver Cell Liver Neoplasms, Experimental Carcinoma, Hepatocellular
(+)-Oxazepam	604-75-1					Mouse	Male	B6C3F1	Diet	99	104	Positive	Liver	Adenoma - hepatocellular									
(+)-Oxazepam	604-75-1					Mouse	Female	Swiss Webster	Diet	57	57	Positive	Liver	Adenoma - hepatocellular									
(+)-Oxazepam	604-75-1					Mouse	Male	Swiss Webster	Diet	57	57	Positive	Liver	Adenoma - hepatocellular									
(+)-Oxazepam	604-75-1					Rat	Female	Fischer 344	Diet	26	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma									
(+)-Oxazepam	604-75-1					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma									
(+)-Oxazepam	604-75-1					Rat	Male	Fischer 344	Diet	26	103	Not specified	Kidney	Adenoma - tubular									
(+)-Oxazepam	604-75-1					Rat	Male	Fischer 344	Diet	101	101	Not specified	Kidney	Adenoma - tubular									
(+)-Phenipiprazine hydrochloride	66-05-7	N(N)(CCc1c1c=cc=cc=1)(C.C)	-	-	-	Mouse	Female	Swiss	Drinking water	119	127	Negative	Liver	Hepatoma	-				all tumor bearing animals	kidney hematopoietic system mammary gland uterus	lung kidney liver stomach	lung hematopoietic system liver	-
(+)-Phenipiprazine hydrochloride	66-05-7					Mouse	Male	Swiss	Drinking water	100	112	Negative	Liver	Hepatoma									
(+)-Praziquantel	55268-74-1					Syrian hamster	Female	Not specified	Gavage	80	80	Negative	Multiple sites	Multiple tumour types									
(+)-Praziquantel	55268-74-1					Syrian hamster	Male	Not specified	Gavage	80	80	Negative	Multiple sites	Multiple tumour types									
(+)-Praziquantel	55268-74-1	C1[C]N(C(C)N)CCC2=c2c=c=c=c(C2)C(=O)C4CCCCC4)=O	-	8, 11, 29, 30, 52, 53, 60, 67, 112, 165, 167, 200	-	Rat	Female	SD	Gavage	104	130	Negative	Multiple sites	Multiple tumour types	TRPM8 VEGFA AKR7A3	NEF ALDH18A1 SLC16A1 TOR1 MFBL1	SLC2A4 TMEM41B C10ORF118 HMGCS1 PLINA2	hsa04926: Relaxin signaling pathway - Homo sapiens (human) (1) hsa-miR-7422: 435448; VEGFA; vascular endothelial growth factor A hsa05208: Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa-miR-7422: 435448; VEGFA; vascular endothelial growth factor A hsa05323: Rheumatoid arthritis - Homo sapiens (human) (1) hsa-miR-7422: 435448; VEGFA; vascular endothelial growth factor A	vascular system	-	-	-	-
(+)-Praziquantel	55268-74-1					Rat	Male	SD	Gavage	104	130	Negative	Multiple sites	Multiple tumour types									
(+)-Prorenalol	54-80-8	C1(c)CC=2C(C=c1(c)=c(C=c(C=2)C(O)NC)C)CO	-	19, 23, 111, 112, 187, 207		Mouse	Female	Not specified	Diet	64	64	Not specified	Thymus gland	Multiple tumour types					all tumor bearing animals	-	-	-	-
(+)-Prorenalol	54-80-8					Mouse	Male	Not specified	Diet	64	64	Not specified	Thymus gland	Multiple tumour types									
(+)-Prorenalol hydrochloride	51-02-5	C1(c)CC=2C(C=c1(c)=c(C=c(C=2)C(O)NC)C)CO.Cl	급성 독성(경구) - 구분4	-	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	CF-1	Diet	78	78	Negative	Liver	Multiple tumour types	-				all tumor bearing animals	-	-	-	-
(+)-Prorenalol hydrochloride	51-02-5					Mouse	Male	CF-1	Diet	78	78	Negative	Liver	Adenoma									
(+)-Temazepam	846-50-4	N2C(C)(N=c(C=1C=c(C=c(Cl)c1)c2c(c=c(C)=c(C)C)(O)c)=O)C	급성 독성(경구) - 구분4 만성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	14, 19, 23, 29, 30, 52, 53, 64, 66, 67, 71, 111, 112, 117, 165, 167, 187, 200, 204, 207, 318	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be clastogenic	Mouse	Female	CD1	Diet	78	78	Negative	Liver	Adenoma - hepatocellular	CYP3A4	VTN TGFBR3 TNC MFBL1 ALDH18A1	SP1 LST1 BEL SCD5 HPN	hsa01100: Metabolic pathways - Homo sapiens (human) (1) hsa-1576: 617689; CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa00983: Drug metabolism - other enzymes - Homo sapiens (human) (1) hsa-1576: 617689; CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa05207: Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa-1576: 617689; CYP3A4; cytochrome P450 family 3 subfamily A member 4	-	ear Zymbals gland	liver	thyroid gland liver	-
(+)-Temazepam	846-50-4					Mouse	Male	CD1	Diet	78	78	Negative	Liver	Adenoma - hepatocellular									
(+)-Terbutaline	23031-25-6	C=1(C=1C(C=1C=1)O)O)C(O)CNC(C)(C)C	-	-	-	Rat	Female	SD	Diet	104	104	Positive	Mesovarium	Leiomyoma	ADRB2 TNF	CBR4 ALDH18A1 WWP2 ZFAND5 HRPD	SYTB CA2 TCF12 OGG1 CSF72		stomach	-	-	pituitary gland	-
(+)-Tryptophan	54-12-6	C=2c(C(C)(C)O)c=0(N)C=1C=c(C=c(N)C=1)N)C=c2	심한 눈 손상/눈 자극성 - 구분2A(GB)	21, 41, 51, 131, 193, 203	Genotoxicity Data: predicted to be clastogenic	Rat	Male	Fischer 344	Diet	98	98	Negative	Liver	Multiple tumour types					skin		kidney	lung	
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7	C1=c(C=c(C(=c(C1)C)C2=c(C=c(C(=c(C)C)OC)=O	피부 과민성 - 구분1(1A/1B) 만성 수생환경 유해성 - 구분1	8, 11, 21, 26, 30, 34, 36, 41, 52, 53, 57, 58, 60, 61, 67, 72, 107, 132, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 210	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	92	91	Not specified			ESR1 AR PPARG	ITGB8 SERPINB1 HTR7 CXORF48 NSE4	TEF1 GA6A GCLM MGST1 KIAA0247	hsa05207: Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa-367: 408557; AR; androgen receptor hsa05200: Pathways in cancer - Homo sapiens (human) (1) hsa-367: 408557; AR; androgen receptor hsa04114: Oocyte meiosis - Homo sapiens (human) (1) hsa-367: 408557; AR; androgen receptor	stomach urinary bladder liver kidney nasal cavity	urinary bladder stomach hematopoietic system	stomach vascular system kidney urinary bladder	liver urinary bladder pituitary gland	-
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7					Mouse	Female	B6C3F1	Dermal	92	91	Not specified											
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7					Mouse	Male	B6C3F1	Diet	13	13	Not specified											
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7					Mouse	Male	B6C3F1	Dermal	13	13	Not specified											
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7					Rat	Female	Fischer 344	Diet	95 d	91 d	Not specified											
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7					Rat	Female	Fischer 344	Dermal	95 d	91 d	Not specified											
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7					Rat	Male	Fischer 344	Diet	95 d	91 d	Not specified											
(2-Hydroxy-4-methoxyphenyl)phenylmethanone	131-57-7					Rat	Male	Fischer 344	Dermal	95 d	91 d	Not specified											
(2-Nitromethyl)benzene	102-96-5	C1=c(C=c(C(=c(C1)C=c(N+)[O-])=O	-	7, 8, 11, 14, 19, 23, 25, 27, 28, 29, 30, 34, 36, 43, 46, 52, 53, 57, 58, 59, 60, 61, 62, 64, 66, 67, 71, 72, 100, 101, 102, 103, 111, 112, 117, 122, 123, 148, 153, 163, 165, 167, 177, 187, 200, 214, 307, 318	Genotoxicity Data: predicted to be genotoxic	Rat	Female	Fischer 344	Gavage	108	104	Not specified	Adrenal gland	Pheochromocytoma	E6	SPAST ADAR1 HSPB11 IFJ2 RNF12	ITGA6 MGST1 SAT AKR1B10 SOD3	hsa05143: African trypanosomiasis - Homo sapiens (human) (1) hsa-3569: 835435; IL6; interleukin 6 hsa04060: Cytokine-cytokine receptor interaction - Homo sapiens (human) (1) hsa-3569: 835435; IL6; interleukin 6 hsa04621: NOD-like receptor signaling pathway - Homo sapiens (human) (1) hsa-3569: 835435; IL6; interleukin 6	spleen ear Zymbals gland Mallorci head cancers thyroid gland	clitoral gland	lung vascular system urinary bladder	ovary stomach lung urinary bladder	-
(2-Nitromethyl)benzene	102-96-5					Rat	Male	Fischer 344	Gavage	108	104	Not specified	Abdominal cavity	Mesothelioma									
(3R,5S,6E)-ret-7-(3-(4-Fluorophenyl)-1-(1-methylethyl)-1H-indol-2-yl)-3,5-dihydroxy-6-heptenoic acid	93957-54-1	C(C(C)N(C=3C=(C=c(C=c(C(C1=c(C=c(C=c(F)=c(C=2)C=c(C)H)(C)C)O)=O)H)(C)C)O)=C)H)O	-	7, 8, 11, 14, 19, 21, 23, 25, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 150, 153, 163, 165, 167, 187, 200, 214, 307, 318, 318	-	Rat	Male	SD	Gavage	104	104	Not specified	Liver	Adenoma - hepatocellular	SLCO1B1 TRRC HMGCR ABCC2 F2	SRSRF2 NAPT11	CYP2B6 PON1 PPARD SP1 PPARA		thyroid gland	-	-	-	Neoplasm Invasiveness Cell Transformation, Neoplastic Multiple Myeloma
(3R,5S,6E)-ret-7-(3-(4-Fluorophenyl)-1-(1-methylethyl)-1H-indol-2-yl)-3,5-dihydroxy-6-heptenoic acid	93957-54-1					Rat	Male	SD	Gavage	104	104	Positive	Liver	Adenoma - hepatocellular									
(4-Ethoxyphenyl)urea	150-69-6	C1=c(C)=c(C=c(N(C)=O)N)OCC	급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	29, 30, 52, 53, 67, 112, 165, 167, 200	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Rat	Mixed	Osborne-Mendel	Diet	104	104	Positive	Liver	Multiple tumour types	GNAT3	ALDH18A1 TYMP4 ADAM19 CCNC TEF1	CSF72 PON LST1 CYTH1 CDH5I	hsa04742: Taste transduction - Homo sapiens (human) (1) hsa-246542: 619729; GNAT3; G protein subunit alpha transducin 3 hsa04973: Carbohydrate digestion and absorption - Homo sapiens (human) (1) hsa-246542: 619729; GNAT3; G protein subunit alpha transducin 3	kidney stomach urinary bladder large intestine skin	ear Zymbals gland urinary bladder small intestine stomach hematopoietic system mammary gland uterus brain	kidney thyroid gland urinary bladder	urinary bladder	-
(E)-(3-p-Anisoyl-2-bromoacrylic acid) sodium salt	21739-91-3	C(=c(C)(C1=cC=c(C=c1C(=O)C=c)O)B)C(O=[S(=O)=O].[Na+]	-	7, 8, 11, 14, 19, 23, 25, 27, 28, 29, 30, 34, 36, 43, 46, 52, 53, 57, 58, 59, 60, 61, 62, 64, 66, 67, 71, 72, 100, 101, 102, 103, 111, 112, 117, 122, 123, 148, 153, 163, 165, 167, 177, 187, 200, 214, 307, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Intraperitoneal	105	104	Not specified	Adrenal gland	Pheochromocytoma	-					-	-	-	Carcinoma, Squamous Cell Lung Neoplasms Ovarian Neoplasm
(E)-(3-p-Anisoyl-2-bromoacrylic acid) sodium salt	21739-91-3					Mouse	Male	B6C3F1	Intraperitoneal	2 yrs	2 yrs	Not specified	Abdomen	Fibrosarcoma									
(E)-(3-p-Anisoyl-2-bromoacrylic acid) sodium salt	21739-91-3					Rat	Female	Fischer 344	Intraperitoneal	2 yrs	2 yrs	Not specified	Abdominal cavity	Sarcoma									
(E)-(3-p-Anisoyl-2-bromoacrylic acid) sodium salt	21739-91-3					Rat	Male	Fischer 344	Intraperitoneal	105	104	Not specified	Abdomen	Sarcoma									
(E)-4-Phenyl-3-buten-2-one	1896-62-4																						
(E)-4-Phenyl-3-buten-2-one	1896-62-4																						
(E)-4-Phenyl-3-buten-2-one	1896-62-4	C=1(C=c(C(C)=O)C=c(C=c(C=c(C=1	심한 눈 손상/눈 자극성 - 구분2A(GB) 만성 수생환경 유해성 - 구분3	6, 8, 11, 18, 34, 36, 37, 51, 58, 60, 61, 72, 122, 123, 150, 163, 166, 220, 318	-	Mouse	Female	B6C3F1/N	Dermal	92 d	91 d	Not specified	Uterus	Polyp - stromal cell	-				thyroid gland nasal cavity kidney oral cavity large intestine stomach skin Mallorci head cancers lung spleen	stomach uterus vascular system nasal cavity thyroid gland lung liver oral cavity	stomach lung vascular system urinary bladder	ovary stomach urinary bladder thyroid gland pituitary gland lung	-
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Mouse	Female	B6C3F1/N	Diet	92 d	91 d	Not specified											
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Mouse	Female	B6C3F1/N	Dermal	192 d	190 d	Not specified	Adrenal gland capsule	Adenoma									
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Mouse	Male	B6C3F1/N	Dermal	92 d	91 d	Not specified											
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Mouse	Male	B6C3F1/N	Dermal	2 yrs	2 yrs	Not specified	Adrenal gland capsule	Adenoma									
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Rat	Female	Fischer 344	Dermal	93 d	91 d	Not specified											
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Rat	Female	Fischer 344	Diet	92 d	91 d	Not specified											
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Rat	Female	Fischer 344	Dermal	193 d	190 d	Not specified	Adrenal gland cortex	Adenoma									
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Rat	Male	Fischer 344	Dermal	92 d	91 d	Not specified											
(E)-4-Phenyl-3-buten-2-one	1896-62-4					Rat	Male	Fischer 344	Dermal	191 d	190 d	Not specified	Adrenal gland cortex	Adenoma									
(E)-Anethole	4180-23-8	C(=c(C(=1C=c(C(c)=c(C=1)O(C	급성 독성(흡입: 증기) - 구분3 피부 과민성 - 구분1(1A/1B) 생식독성 - 구분1A	57, 131	Genotoxicity Data: non-clastogenic	Rat	Female	SD	Diet	119	119	Not specified	Liver	Adenoma - hepatocellular	-				kidney stomach ear Zymbals gland skin vascular system nasal cavity hematopoietic system	stomach hematopoietic system urinary bladder nasal cavity	stomach urinary bladder vascular system lung	urinary bladder stomach	-
(E)-Anethole	4180-23-8					Rat	Male	SD	Diet	119	119	Not specified	Liver	Adenoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
(E)-Cinnamaldehyde	14371-10-9	C1=CC=CC(=C1)C=CC=O	-	8, 11, **29**, 30, 34, 36, 52, 53, 58, 60, 61, 67, 72, 112, 163, **165**, **167**, **200**	-	Mouse	Female	B6C3F1	Diet	105	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma					kidney Maltoni head cancers spleen ear Zymbals gland	-	stomach lung	stomach **ovary** peritoneal cavity urinary bladder	-
(E)-Cinnamaldehyde	14371-10-9					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
(E)-Cinnamaldehyde	14371-10-9					Rat	Female	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
(E)-Cinnamaldehyde	14371-10-9					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
(E)-Diethylstilbestrol	56-53-1	C/C(=C/C=C/C=C\C)C(=C(C)c2ccc(O)cc2)c2ccc(O)cc2CCC	피부 과민성 - 구분1(1A/1B) **발암성 - 구분1A** 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분3	2, 8, 11, 14, 16, 23, 25, 27, 28, 30, 33, 34, 36, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 113, 120, 123, 133, 136, 153, 163, 164, **165**, **167**, 187, **200**, 214, 220, 307, 318	Cancer slope factor: 0.1 (kg/mld)-1 (carcinogenicity, inhalation) Carcinogenicity data available: NTP 8DC-Known Human Carcinogen	Mouse	Female	(C57BL/6 x BALB/c)F1	Diet	148	161	Positive	Cervix	Carcinoma - squamous cell	**ESR1** **ESR2** **PR,**	WNT7A SAT RAM120B CCBP2 RAB20	IL4R ADAMTS9 NATN CDC20 EPHA1L2	hsa05200 Pathways in cancer - Homo sapiens (human) (1) : hsa:2100 KEGG: 1.5.1.2; estrogen receptor 2 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) : hsa:2100 KEGG: 1.5.1.2; estrogen receptor 2 hsa01522 Endocrine resistance - Homo sapiens (human) (1) : hsa:2100 KEGG: 1.5.1.2; estrogen receptor 2	stomach **urinary bladder** nasal cavity hematopoietic system kidney	liver hematopoietic system **urinary bladder** stomach thyroid gland	thyroid gland kidney stomach	**ovary** thyroid gland pituitary gland stomach	Neoplasm Metastasis Mammary Neoplasm, Experimental Mammary Neoplasm, Animal Carcinoma, Squamous Cell Ovarian Neoplasm Urinary Bladder Neoplasm
(E)-Diethylstilbestrol	56-53-1					Mouse	Male	(C57BL/6 x BALB/c)F1	Diet	150	169	Positive		Mortality									
(E)-Diethylstilbestrol	56-53-1					Mouse	Female	BALB/c(Sc/HEC)HEN(F)	Diet	122	133	Positive	Cervix	Adenoacanthoma									
(E)-Diethylstilbestrol	56-53-1					Mouse	Male	BALB/c(Sc/HEC)HEN(F)	Diet	121	126	Positive		Mortality									
(E)-Diethylstilbestrol	56-53-1					Rat	Female	SD	Diet	91	104	Negative	Liver	Hepatoma									
(E)-Diethylstilbestrol	56-53-1					Rat	Female	SD	Gavage	52	52	Positive	Liver	Adenoma - hepatocellular									
(E)-Diethylstilbestrol	56-53-1					Rat	Male	SD	Diet	91	104	Negative	Liver	Multiple tumour types									
(E)-Diethylstilbestrol	56-53-1					Rat	Male	SD	Diet	66	66	Positive	Adrenal gland	Adenoma - cortical									
(R,R)-Labetalol hydrochloride	75659-08-9	C1=c(C(=O)Nc2ccc(C(C)NC[C@H](O)[C@H](C)Cc3ccccc3)ccc2)ccc(c1)NC)			-	Rat	Female	SD	Diet	104	104	Negative	Heart	Sarcoma - endocardial	-				stomach all tumor bearing animals		kidney		
(R,R)-Labetalol hydrochloride	75659-08-9					Rat	Male	SD	Diet	104	104	Negative	Heart	Sarcoma - endocardial									
(S)-Zearalenone	17924-92-4	C1(C)(CCCc(C)c2c(C)C(C@H](C(=O)C)c(O)c(CC)c(=C)c2)O)O)=O	-	2, 8, 11, 14, 16, 23, 25, 27, 28, 30, 34, 36, 46, 52, 53, 58, 60, 61, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 153, 163, **165**, **167**, 187, **200**, 214, 307, 318	-	Mouse	Female	B6C3F1	Diet	104	105	Positive	Liver	Adenoma - hepatocellular	**ESR1** CASP3 IL1B TNF	CIC0E4B GAUS2 MSCH1 MFG18 EBP27	MYKEP1 CORO1C TTPA1 CUTA#1 CHAC2	hsa04022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) : hsa:3553 KO4519 IL1B; interleukin 1 beta : hsa:836 KO2187 CASP3; caspase 3 hsa05163 Human cytomegalovirus infection - Homo sapiens (human) (2) : hsa:3553 KO4519 IL1B; interleukin 1 beta : hsa:836 KO2187 CASP3; caspase 3 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (2) : hsa:3553 KO4519 IL1B; interleukin 1 beta : hsa:836 KO2187 CASP3; caspase 3	kidney urinary bladder	-	kidney	pituitary gland liver	-
(S)-Zearalenone	17924-92-4					Mouse	Male	B6C3F1	Diet	104	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(S)-Zearalenone	17924-92-4					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(S)-Zearalenone	17924-92-4					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
(Trichloromethyl)benzene	98-07-7	C1=c(C(=c(C(=c1)C)Cl)Cl)Cl	급성 독성(경구) - 구분4 급성 독성(흡입) - 분류 - 구분2 만성 눈 손상/자극성 - 구분1 피부 과민성 - 구분1(1A/1B) **발암성 - 구분1A** 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	8, 11, **29**, 30, 52, 53, 60, 67, 112, **165**, **167**, **200**	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	ICR	Gavage	25	78	Positive	Forestomach	Carcinoma - squamous cell	**ERK5**	SIX7 MAND1 TGFB2 TRF1 WDR67	ADAMTS9 DLC1 MLPH HK2 AND1	**hsa04725 Cholinergic synapse - Homo sapiens (human) (1)** **: hsa:3845 K07827 KRAS; KRAS proto-oncogene, GTPase** **hsa04933 AGE-RAGE signaling pathway in diabetic complications - Homo sapiens (human) (1)** **: hsa:3845 K07827 KRAS; KRAS proto-oncogene, GTPase** **hsa05216 Thyroid cancer - Homo sapiens (human) (1)** **: hsa:3845 K07827 KRAS; KRAS proto-oncogene, GTPase**	spleen oral cavity Maltoni head cancers thyroid gland ear Zymbals gland nasal cavity	thyroid gland **uterus** kidney clitoral gland nasal cavity hematopoietic system	**lung** vascular system small intestine urinary bladder	hematopoietic system **lung** stomach thyroid gland urinary bladder **ovary** peritoneal cavity pituitary gland vascular system small intestine	Lymphoma Adenoma Lung Neoplasms Skin Neoplasm
[1,1'-Biphenyl]-3,3',4,4'-tetraniline tetrahydrochloride	7411-48-4	C=2(C=1C=C(C(=C(C=1)N)N)C=C(C=1)N)N(NCl.Cl.Cl.Cl)	만성 눈 손상/자극성 - 구분2A(2B) 만성 수생환경 유해성 - 구분1 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분1	7, 19, 25, 33, 25, 36, 41, 46, 57, 61, 111, 117, 122, 123, 133, 150, 187, 207, 210	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	CD-1 Hsd(ICR)	Diet	77	98	Negative	Liver	Multiple tumour types	-				ear Zymbals gland spleen urinary bladder thyroid gland	urinary bladder ear Zymbals gland **uterus** thyroid gland clitoral gland hematopoietic system liver mammary gland lung stomach kidney nasal cavity	urinary bladder thyroid gland liver vascular system lung	liver urinary bladder thyroid gland vascular system hematopoietic system stomach **ovary** pituitary gland lung	-
[1,1'-Biphenyl]-3,3',4,4'-tetraniline tetrahydrochloride	7411-48-4					Mouse	Male	CD-1 Hsd(ICR)	Diet	77	94	Positive	Liver	Multiple tumour types									
[1,1'-Biphenyl]-3,3',4,4'-tetraniline tetrahydrochloride	7411-48-4					Rat	Male	SD	Diet	77	107	Positive	Liver	Hepatoma									
[1,1'-Biphenyl]-4-ol	92-69-3	C2(C=1C=CC=CC=1)=CC=C(C=C2)O	피부 부식성/피부 자극성 - 구분2 만성 눈 손상/자극성 - 구분2A(2B) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분3	8, 19, 23, 27, **29**, **30**, 34, 36, 52, 53, 57, 58, 61, 67, 72, 107, 111, 112, 117, 120, 123, 148, 150, 163, **165**, **167**, 187, 200, 220, 307	Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	**ESR1** **AR** UGT2B15 ESR2 UGT2B1 CYP19A1 NCOA2 PPARG	HEATR3 IFIH1 MTTH RNF12 COG5	VASN GGH STMN1 ADAMTS9 GNAI1	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) : hsa:2100 KO8551 ESR2; estrogen receptor 2 : hsa:367 KO8557 AR; androgen receptor : hsa:7364 KO0699 UGT2B15; UDP glucuronosyltransferase family 2 member B15 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (2) : hsa:1588 KO7434 CYP19A1; cytochrome P450 family 19 subfamily A member 1 : hsa:7364 KO0699 UGT2B15; UDP glucuronosyltransferase family 2 member B15 hsa01100 Metabolic pathways - Homo sapiens (human) (2) : hsa:1588 KO7434 CYP19A1; cytochrome P450 family 19 subfamily A member 1 : hsa:7364 KO0699 UGT2B15; UDP glucuronosyltransferase family 2 member B15	kidney urinary bladder stomach nasal cavity hematopoietic system thyroid gland ear Zymbals gland Maltoni head cancers large intestine oral cavity spleen	hematopoietic system urinary bladder stomach nasal cavity liver kidney clitoral gland **uterus** thyroid gland small intestine	thyroid gland kidney stomach urinary bladder liver lung vascular system	**ovary** thyroid gland stomach pituitary gland urinary bladder vascular system hematopoietic system liver	-
[1,1'-Biphenyl]-4-ol	92-69-3					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
[1,1'-Biphenyl]-4-ol	92-69-3					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
[1,1'-Biphenyl]-4-ol	92-69-3					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
1-(Phenylsulphonyl)-3-thiosemicarbazide	5351-66-5	O=S(=O)(C=1C=CC=CC=1)NNC(N)=S			-	Mouse	Female	Swiss	Gavage	50	60	Not specified	Liver	Tumour- liver cell	-				spleen		thyroid gland	thyroid gland	-
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7	C1=c(C(=c(C(=c1)Cl)Cl)Cl)C=2(C=(C(=c(C(=c2)Cl)Cl)Cl)Cl)Cl	급성 독성(경구) - 구분1 **발암성 - 구분2** 생식독성 - 구분1B 만성 수생환경 유해성 - 구분4	-	Cancer slope factor: 38 (kg/mld)-1 (carcinogenicity, inhalation) Carcinogenicity data available: IRIS 82 (Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals)	Mouse	Female	B6C3F1	Gavage	106	104	Not specified	Adrenal gland	Pheochromocytoma	CYP1A1 **AHR** CYP1B1	ARNT CADPS2 CCDC49 FNBP2 GCA	RAM171A1 HSPA12A LIM2 MAP3K7IP3 NRXN1	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) : hsa:196 K09083 AHR; aryl hydrocarbon receptor hsa04934 Cushing syndrome - Homo sapiens (human) (1) : hsa:196 K09083 AHR; aryl hydrocarbon receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) : hsa:196 K09083 AHR; aryl hydrocarbon receptor	thyroid gland oral cavity	liver lung kidney	liver vascular system	liver thyroid gland urinary bladder vascular system peritoneal cavity	-
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7					Mouse	Male	B6C3F1	Gavage	106	104	Not specified	Adrenal gland	Carcinoma- alveolar/bronchiolar/metastatic									
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7					Mouse	Female	Swiss Webster	Dermal	2 yrs	2 yrs	Not specified	Abdominal cavity	Lipoma									
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7					Mouse	Male	Swiss Webster	Dermal	110	104	Not specified	Adrenal gland	Pheochromocytoma									
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7					Rat	Female	Osborne-Mendel	Gavage	110	104	Not specified	Abdomen- subcutaneous tissue	Rhabdomyosarcoma									
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7					Rat	Male	Osborne-Mendel	Gavage	110	104	Not specified	Abdominal cavity	Tumour- mixed cell- malignant									
1,2,3-Benzotriazole	95-14-7	N1=NC2=C(N(C)=C=C=C2	급성 독성(경구) - 구분4 급성 독성(흡입) 분진/미스트 - 구분4 만성 눈 손상/자극성 - 구분2A(2B) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	21, **29**, **30**, 36, 41, 46, 52, 53, 57, 67, 112, 131, 150, **165**, **167**, **200**, 210	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	104	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				spleen ear Zymbals gland thyroid gland oral cavity hematopoietic system urinary bladder vascular system kidney nasal cavity skin Maltoni head cancers	kidney **uterus** hematopoietic system all tumor bearing animals	thyroid gland vascular system urinary bladder lung stomach small intestine liver preputial gland	**ovary** thyroid gland stomach urinary bladder vascular system pituitary gland liver lung peritoneal cavity small intestine	-
1,2,3-Benzotriazole	95-14-7					Mouse	Male	B6C3F1	Diet	104	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2,3-Benzotriazole	95-14-7					Rat	Female	Fischer 344	Diet	78	105	Not specified	Brain	Glioma									
1,2,3-Benzotriazole	95-14-7					Rat	Male	Fischer 344	Diet	78	104	Not specified	Brain	Glioma | Oligodendroglioma									
1,2,4,5-Tetrachloro-3-methoxy-6-nitrobenzene	2438-88-2	C1(=c(C(=c(C(=c1Cl)Cl)OC)Cl)[N+](O-])=O	-	-	-	Mouse	Female	B6C3F1	Diet	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				ear Zymbals gland hematopoietic system kidney nasal cavity urinary bladder stomach skin	hematopoietic system kidney urinary bladder **uterus** stomach clitoral gland	vascular system liver urinary bladder	vascular system urinary bladder liver	-
1,2,4,5-Tetrachloro-3-methoxy-6-nitrobenzene	2438-88-2					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2,4,5-Tetrachloro-3-methoxy-6-nitrobenzene	2438-88-2					Rat	Female	Fischer 344	Diet	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2,4,5-Tetrachloro-3-methoxy-6-nitrobenzene	2438-88-2					Rat	Male	Fischer 344	Diet	104	105	Not specified	Liver	Nodule - neoplastic | Adenoma|hepatocellular | Carcinoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
1,2,4,5-Tetrachlorobenzene	95-94-3	C1=1Cl=CC=CC=1Cl|Cl|Cl|Cl	급성 독성(경구) - 구분4 생식독성 - 구분2 생식독성 - 수유독성 특정표적장기 독성(반복 노출) - 구분1(혈액계통) 특정표적장기 독성(반복 노출) - 구분1 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	29, 30, 52, 53, 57, 61, 67, 112, 165, 167, 200	Carcinogenicity data available: PPRTV (ORNL) - Inadequate for an assessment of carcinogenic potential Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Diet	93	91	Not specified		CYP1A2 CYP2B1 CYP2B2 FOS	DABP4 AIRN7 CADPH2 CCDC40 FNIP2	BEL DAM1TIA1 HSPA12A LRA2 MAP2K7IP2	hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (1) hsa1571 K07415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa04932 Non-alcoholic fatty liver disease - Homo sapiens (human) (1) hsa1571 K07415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (1) hsa1571 K07415 CYP2E1; cytochrome P450 family 2 subfamily E member 1	thyroid gland oral cavity hematopoietic system kidney ear Zymbals gland nasal cavity Mallorn head cancers liver lung spleen	liver kidney thyroid gland lung hematopoietic system uterus nasal cavity urinary bladder clitoral gland oral cavity	liver vascular system lung small intestine	thyroid gland liver ovary peritoneal cavity vascular system pituitary gland stomach small intestine	Liver Neoplasm
1,2,4,5-Tetrachlorobenzene	95-94-3					Mouse	Male	B6C3F1	Diet	94	91	Not specified											
1,2,4,5-Tetrachlorobenzene	95-94-3					Rat	Female	Fischer 344	Diet	88 d	91 d	Not specified											
1,2,4,5-Tetrachlorobenzene	95-94-3					Rat	Male	Fischer 344	Diet	91 d	91 d	Not specified											
1,2,4-Trimethylbenzene	95-63-6	C1=1C(C=C(C(=C1)C)C)C	인화성 액체 - 구분3 급성 독성(흡입: 증기) - 구분4 피부 부식성/피부 자극성 - 구분2 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분2	8, 11, 60	Carcinogenicity data available: IRIS -Inadequate information to assess carcinogenic potential Genotoxicity Data: non-genotoxic	Rat	Female	SD	Gavage	104	123	Not specified	Multiple sites	Multiple tumour types	PTGS2 ACAA2 ACADVL ACAT1	CTSD IRS2 KLF10 CEBPG RNF12	BCL2A1 MAP3K8 DDN6GA 2CCHC2 NFATS	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa10449 K07508 ACAA2; acetyl-CoA acyltransferase 2 hsa37 K08479 ACADVL; acyl-CoA dehydrogenase very long chain hsa01212 Fatty acid metabolism - Homo sapiens (human) (2) hsa10449 K07508 ACAA2; acetyl-CoA acyltransferase 2 hsa37 K08479 ACADVL; acyl-CoA dehydrogenase very long chain hsa00071 Fatty acid degradation - Homo sapiens (human) (2) hsa10449 K07508 ACAA2; acetyl-CoA acyltransferase 2 hsa37 K08479 ACADVL; acyl-CoA dehydrogenase very long chain	oral cavity Mallorn head cancers spleen liver nasal cavity vascular system ear Zymbals gland urinary bladder thyroid gland lung hematopoietic system	liver lung oral cavity clitoral gland nasal cavity urinary bladder thyroid gland uterus	urinary bladder vascular system thyroid gland lung kidney small intestine	urinary bladder pituitary gland thyroid gland liver vascular system ovary peritoneal cavity stomach small intestine	-
1,2,4-Trimethylbenzene	95-63-6					Rat	Male	SD	Gavage	104	123	Positive	Ear canal	Carcinoma									
1,2-Benzenediamine dihydrochloride	615-28-1	C1=1C(=C(C(=C1)N)N).Cl.Cl	급성 독성(경구) - 구분4 급성 독성(흡입): 분진/미스트 - 구분4 심한 눈 손상/눈 자극성 - 구분2A(사) 피부 과민성 - 구분1(사/하) 생식세포 변이원성 - 구분2 발암성 - 구분2 특정표적장기 독성(1회 노출) - 구분1 특정표적장기 독성(반복 노출) - 구분2 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	19, 21, 23, 27, 29, 30, 41, 46, 52, 53, 57, 61, 67, 111, 112, 117, 151, 152, 165, 167, 187, 200, 207, 310	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	CD-1 HsMUCR	Diet	77	90	Positive	Liver	Hepatoma	-				spleen urinary bladder ear Zymbals gland thyroid gland all tumor bearing animals	urinary gland uterus ear Zymbals gland thyroid gland hematopoietic system stomach kidney clitoral gland lung liver mammary gland nasal cavity small intestine	thyroid gland urinary bladder liver vascular system lung stomach small intestine	liver thyroid gland urinary bladder vascular system hematopoietic system stomach lung pituitary gland peritoneal cavity small intestine	-
1,2-Benzenediamine dihydrochloride	615-28-1					Mouse	Male	CD-1 HsMUCR	Diet	77	86	Positive	Liver	Hepatoma									
1,2-Benzenediamine dihydrochloride	615-28-1					Rat	Male	SD	Diet	77	107	Positive	Liver	Hepatoma									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0	O(C(CCCCCC)C)C(C(=O)c1c(C(=O)O)cccc1)C(C)=O	자료없음	8, 11, 19, 23, 29, 30, 52, 53, 60, 67, 111, 112, 117, 165, 167, 187, 200, 307	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	78	104	Positive	Liver	Carcinoma - hepatocellular	-				kidney hematopoietic system liver	hematopoietic system liver	liver	liver lung hematopoietic system	-
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Mouse	Female	B6C3F1	Diet	79	79	Not specified	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Mouse	Female	B6C3F1	Diet	104	104	Not specified	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Mouse	Male	B6C3F1	Diet	78	104	Not specified	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Mouse	Male	B6C3F1	Diet	79	79	Not specified	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Mouse	Male	B6C3F1	Diet	104	104	Positive	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Multiple tumour types									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Female	Fischer 344	Diet	78	104	Positive	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Female	Fischer 344	Diet	79	79	Not specified	Liver	Adenoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Female	Fischer 344	Diet	104	104	Positive	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Multiple tumour types									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Male	Fischer 344	Diet	78	104	Positive	Liver	Carcinoma - tubular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Male	Fischer 344	Diet	79	79	Not specified	Liver	Carcinoma - hepatocellular									
1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich.	68515-48-0					Rat	Male	Fischer 344	Diet	104	104	Positive	Kidney	Carcinoma - tubular									
1,2-Dichlorobenzene	95-50-1	C1=1C(Cl)C=CC=C1Cl	인화성 액체 - 구분3 급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상/눈 자극성 - 구분2A(사) 피부 과민성 - 구분1(사/하) 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	29, 30, 52, 53, 57, 67, 112, 165, 167, 200	Carcinogenicity data available: Health Canada - Group V: CEPA (probably not carcinogenic to humans) Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	CYP2E1 GLUD1 CAT CARS1 CYP2D2 GSTP1 UBE	-	-	hsa01100 Metabolic pathways - Homo sapiens (human) (4) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa2746 K00261 GLUD1; glutamate dehydrogenase 1 hsa2950 K23790 GSTP1; glutathione S-transferase pi 1 hsa847 K03781 CAT; catalase hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa847 K03781 CAT; catalase	thyroid gland oral cavity kidney hematopoietic system liver ear Zymbals gland nasal cavity spleen Mallorn head cancers urinary bladder lung	liver kidney lung thyroid gland hematopoietic system uterus urinary bladder nasal cavity clitoral gland oral cavity	liver vascular system lung small intestine kidney	thyroid gland liver urinary bladder vascular system ovary peritoneal cavity stomach pituitary gland small intestine	Neuroectodermal Tumors, Primitive
1,2-Dichlorobenzene	95-50-1					Mouse	Male	B6C3F1	Gavage	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2-Dichlorobenzene	95-50-1					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2-Dichlorobenzene	95-50-1					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2-Dihydro-2,2,4-trimethylquinoline	147-47-7	CC1(NC2=CC=C1)C(C=CC=C2			Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Dermal	95 d	91 d	Not specified							spleen	all tumor bearing animals	urinary bladder vascular system thyroid gland	thyroid gland vascular system urinary bladder	
1,2-Dihydro-2,2,4-trimethylquinoline	147-47-7					Mouse	Female	B6C3F1	Dermal	66	104	Not specified	Adrenal gland capsule	Lymphoma - malignant|mixed| NOS									
1,2-Diphenylhydrazine	122-66-7	C1=1C(=C(C(=C1)NNC2=C(C=C(C=C2	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상/눈 자극성 - 구분2A(사) 발암성 - 구분1B 특정표적장기 독성(1회 노출) - 구분3 특정표적장기 독성(반복 노출) - 구분2(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분1 급성 수생환경 유해성 - 구분1	28, 29, 30, 34, 36, 46, 52, 53, 57, 58, 61, 63, 67, 72, 100, 101, 102, 103, 112, 131, 162, 165, 167, 177, 200	Cancer slope factor: 0.00022 (ug/m3)-1 carcinogenicity.) Carcinogenicity data available: IRIS -B2 (Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals) Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	95	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	-				ear Zymbals gland spleen liver thyroid gland	mammary gland liver hematopoietic system uterus kidney ear Zymbals gland thyroid gland urinary bladder clitoral gland small intestine lung	vascular system lung urinary bladder thyroid gland small intestine	liver ovary vascular system thyroid gland lung hematopoietic system urinary bladder stomach pituitary gland peritoneal cavity small intestine	-
1,2-Diphenylhydrazine	122-66-7					Mouse	Male	B6C3F1	Diet	78	95	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2-Diphenylhydrazine	122-66-7					Rat	Female	Fischer 344	Diet	78	106	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1,2-Diphenylhydrazine	122-66-7					Rat	Male	Fischer 344	Diet	78	106	Positive	Adrenal gland	Pheochromocytoma									
1,3,5-Trinitrobenzene	99-35-4	C1=1C(=C(C=C(C=1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-])=O	폭발성 물질 - 등급1 급성 독성(경구) - 구분3 심한 눈 손상/눈 자극성 - 구분1 특정표적장기 독성(반복 노출) - 구분2 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	-	Rat	Female	Fischer 344	Diet	52	52	Negative	Liver	Multiple tumour types	IL1B IFNG NOS2 TNF	DSE PDGFRB CCR6 CCR7 CYP11A1	EHHADH MGST1 CCR5 SOD3 AKR1B10	hsa05145 Toxoplasmosis - Homo sapiens (human) (2) hsa3458 K04687 IFNG; interferon gamma hsa4843 K13241 NOS2; nitric oxide synthase 2 hsa04066 HIF-1 signaling pathway - Homo sapiens (human) (2) hsa3458 K04687 IFNG; interferon gamma hsa4843 K13241 NOS2; nitric oxide synthase 2 hsa05146 Amoebiasis - Homo sapiens (human) (2) hsa3458 K04687 IFNG; interferon gamma hsa4843 K13241 NOS2; nitric oxide synthase 2	kidney ear Zymbals gland thyroid gland skin spleen urinary bladder hematopoietic system liver lung oral cavity Mallorn head cancers large intestine nasal cavity stomach	uterus hematopoietic system clitoral gland kidney lung mammary gland urinary bladder liver all tumor bearing animals thyroid gland stomach small intestine ear Zymbals gland nasal cavity	thyroid gland vascular system kidney liver lung urinary bladder small intestine	ovary vascular system liver hematopoietic system stomach urinary bladder thyroid gland peritoneal cavity pituitary gland small intestine	-
1,3,5-Trinitrobenzene	99-35-4					Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Multiple tumour types									
1,3,5-Trinitrobenzene	99-35-4					Rat	Male	Fischer 344	Diet	104	104	Negative	Liver	Multiple tumour types									
1,3-Benzenediamine dihydrochloride	541-69-5	C=1C(N)=CC=CC=1N.Cl.Cl	급성 독성(경구) - 구분3 급성 독성(흡입): 분진/미스트 - 구분3 심한 눈 손상/눈 자극성 - 구분2A(사) 피부 과민성 - 구분1(사/하) 생식세포 변이원성 - 구분2 특정표적장기 독성(1회 노출) - 구분1 특정표적장기 독성(반복 노출) - 구분1 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	21, 41, 57, 61, 131, 150, 310	-	Mouse	Female	CD-1 HsMUCR	Diet	64	77	Negative	Liver	Multiple tumour types	-				spleen ear Zymbals gland thyroid gland urinary bladder	urinary bladder uterus ear Zymbals gland thyroid gland hematopoietic system clitoral gland lung liver kidney mammary gland nasal cavity	thyroid gland urinary bladder liver vascular system lung	thyroid gland liver urinary bladder vascular system ovary hematopoietic system stomach peritoneal cavity	-
1,3-Benzenediamine dihydrochloride	541-69-5					Mouse	Male	CD-1 HsMUCR	Diet	64	77	Negative	Liver	Multiple tumour types									
1,3-Benzenediamine dihydrochloride	541-69-5					Rat	Male	SD	Diet	77	107	Negative	Liver	Multiple tumour types									
1,3-Benzodioxol-5-ol	533-31-3	C1=1C(=)=CC2=C1OCO2O	-	19, 23, 29, 30, 52, 53, 62, 111, 112, 117, 165, 167, 187, 200, 307	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	96	96	Positive	Forestomach	Carcinoma - squamous cell	TNF CASP3 CASP9 HMGB1	TBCTD8 PCDLCE2 AIM1 CTTORF75 COG6	CDYS1 ELOVL1 GALE51 GCCM1 KATZ8	hsa05010 Alzheimer disease - Homo sapiens (human) (2) hsa836 K02187 CASP3; caspase 3 hsa842 K04399 CASP9; caspase 9 hsa05145 Toxoplasmosis - Homo sapiens (human) (2) hsa836 K02187 CASP3; caspase 3 hsa842 K04399 CASP9; caspase 9 hsa05020 Prion disease - Homo sapiens (human) (2) hsa836 K02187 CASP3; caspase 3 hsa842 K04399 CASP9; caspase 9	stomach liver urinary bladder kidney	stomach urinary bladder small intestine hematopoietic system liver	stomach liver vascular system kidney thyroid gland	stomach thyroid gland ovary pituitary gland liver lung	-
1,3-Benzodioxol-5-ol	533-31-3					Mouse	Male	B6C3F1	Diet	96	96	Positive	Forestomach	Carcinoma - squamous cell									
1,3-Benzodioxol-5-ol	533-31-3					Rat	Female	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell									
1,3-Benzodioxol-5-ol	533-31-3					Rat	Male	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
1,3-Benzodioxol-5-ol	533-31-3					Rat	Male	Fischer 344/DuCr	Diet	60	60	Positive	Forestomach	Carcinoma - squamous cell									
1,4-Benzenediamine, N,N'-mixed Ph. and tolyl deriv.	68953-84-4	C1=CC=CC(=C1)NC2=CC=CC=C2NC3=CC=CC=C3	심한 눈 손상/눈 자극성 - 구분2A(R) 경로 수용한은 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	-	Rat	Female	Fischer 344	Diet	52	52	Negative	Liver	Multiple tumour types	-				-	-	-	-	-
1,4-Benzenediamine, N,N'-mixed Ph. and tolyl deriv.	68953-84-4					Rat	Female	Fischer 344	Diet	52	64	Negative	Liver	Multiple tumour types									
1,4-Benzenediamine, N,N'-mixed Ph. and tolyl deriv.	68953-84-4					Rat	Male	Fischer 344	Diet	52	52	Negative	Liver	Multiple tumour types									
1,4-Benzenediamine, N,N'-mixed Ph. and tolyl deriv.	68953-84-4					Rat	Male	Fischer 344	Diet	52	64	Negative	Liver	Multiple tumour types									
1,4-Bis(2-(3,5-dichloropyridyloxy)benzene	76150-91-9	C1(=NC=C(C=C1Cl)Cl)OC2=CC=C(C=C2)OC=C3C=C(C=CC=C3)Cl	-	8, 11, 21, 24, 26, 45, 57, 58, 60, 61, 72, 131, 150, 162, 210	-	Rat	Male	Fischer 344	Diet	72	72	Not specified	Liver	Adenoma - hepatocellular	NR1I3 CYP2B10 CTNNB1	PCDLCE2 INFU PAQR3 GPC1 RNF11	CYP1A2 CYP2B6 EPSR1 GAPC ABHD2						Carcinoma, Hepatocellular Liver Neoplasm, Experimental Adenoma, Liver Cell
1,4-Bis[(Chloromethoxy)methyl]benzene	56894-91-8	C1=CC=CC(=C1)COCCl)COCCl	만성 수생환경 유해성 - 구분2	-	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	Hsd/ICR	Intraperitoneal	77	77	Positive	Abdomen	Sarcoma	-				vascular system	-	stomach vascular system	peritoneal cavity stomach thyroid gland pituitary gland	-
1,4-Dichlorobenzene	106-46-7	C1(Cl)=CC=C(Cl)C=C1	심한 눈 손상/눈 자극성 - 구분2A(R) 발암성 - 구분2 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	21, 27, 28, 57, 61, 62, 100, 101, 102, 103, 122, 123, 130, 220	Cancer slope factor: 1.1e-05 (ug/m3)-1 (inhalation-chr) Carcinogenicity data available: Health Canada - Group III: CBPA (possibly carcinogenic to humans) Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular	**CYP2E1** SMCP1 MRM240 **Genes** PPARA	FABP4 IEG7 MANSC1 MYC5C AIRN7	BEL ADAMTS9 EICC2 SAT LRP6	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa-let-7 KO0510 HMOX1; heme oxygenase 1 hsa-miR-6958-3B NFE2L2 NFE2 like bZIP transcription factor 2 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa-let-7 KO0510 HMOX1; heme oxygenase 1 hsa-miR-6958-3B NFE2L2; NFE2 like bZIP transcription factor 2 hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (2) hsa-let-7 KO0510 HMOX1; heme oxygenase 1 hsa-miR-6958-3B NFE2L2; NFE2 like bZIP transcription factor 2	thyroid gland **kidney** oral cavity hematopoietic system liver ear Zymbals gland nasal cavity Maltoni head cancers urinary bladder lung spleen	**kidney** thyroid gland liver urinary bladder hematopoietic system **uterus** lung nasal cavity clitoral gland oral cavity	liver vascular system **kidney** lung small intestine	thyroid gland liver urinary bladder vascular system **ovary** peritoneal cavity pituitary gland hematopoietic system stomach lung small intestine	Liver Neoplasm, Experimental Liver Neoplasm Carcinoma, Hepatocellular Carcinoma Adenoma Kidney Neoplasm
1,4-Dichlorobenzene	106-46-7					Mouse	Male	B6C3F1	Gavage	103	104	Positive	Adrenal gland medulla	Pheochromocytoma | Pheochromocytoma - malignant									
1,4-Dimethyl-5H-pyridot[4,3-b]indol-3-amine acetate	75104-43-7	C(C)(C)=CC=C2C3C=4C=C(C)C=2C(C)=NC(=C)C=2N3)C)NC				Mouse	Female	CD1	Diet	88	88	Positive	Liver	Carcinoma - hepatocellular									
1,4-Dimethyl-5H-pyridot[4,3-b]indol-3-amine acetate	75104-43-7					Mouse	Male	CD1	Diet	88	88	Positive	Liver	Carcinoma - hepatocellular									
1,4-Dimethyl-5H-pyridot[4,3-b]indol-3-amine acetate	75104-43-7					Rat	Female	Fischer 344/DuCr	Diet	52	52	Positive	Liver	Carcinoma - hepatocellular									
1,4-Dimethyl-5H-pyridot[4,3-b]indol-3-amine acetate	75104-43-7					Rat	Male	Fischer 344/DuCr	Diet	52	52	Positive	Liver	Carcinoma - hepatocellular									
1,5-Naphthalenediamine	2243-62-1	C1=2C(C)N)=CC=C(1)=CC=CC=2)N	급성 독성(경구) - 구분4 발암성 - 구분2 만성 수생환경 유해성 - 구분2	14, 21, 27, 28, 30, 38, 44, 49, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 91, 93, 94, 96, 112, 151, 155, 160, 167, 197, 200, 214, 216, 218, 318	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Diet	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	ACSM1 CD51 **Genes** NR1I3	CCR6 DRAM2 AMH R2 TEP1 OAS1	HTATSF2 BCL2A1 SAT CCR5 CXCL11	hsa04976 Bile secretion - Homo sapiens (human) (1) hsa-let-7 KO1253 EPHX1; epoxide hydrolase 1 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (5) hsa-let-7 KO1253 EPHX1; epoxide hydrolase 1 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (1) hsa-let-7 KO1253 EPHX1; epoxide hydrolase 1	spleen ear Zymbals gland urinary bladder thyroid gland all tumor bearing animals liver hematopoietic system kidney large intestine **lung** skin Maltoni head cancers oral cavity vascular system nasal cavity	urinary bladder **uterus** ear Zymbals gland clitoral gland hematopoietic system thyroid gland **lung** liver kidney mammary gland nasal cavity	thyroid gland urinary bladder liver vascular system **lung** stomach	thyroid gland liver urinary bladder **ovary** **lung** vascular system hematopoietic system stomach	Lung Neoplasm Carcinoma, Hepatocellular Adenoma, Liver Cell
1,5-Naphthalenediamine	2243-62-1					Mouse	Male	B6C3F1	Diet	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic Adenoma | Carcinoma									
1,5-Naphthalenediamine	2243-62-1					Rat	Female	Fischer 344	Diet	103	106	Positive	Mouse gland	Adenoma - hepatocellular | Carcinoma|hepatocellular									
1,5-Naphthalenediamine	2243-62-1					Rat	Male	Fischer 344	Diet	103	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
1-Acetoxyasfrole	34627-78-6	C1=CC(=CC2=C1OCO2)C(C=C)OCC=O)C	-	-	-	Mouse	Male	CD1	Diet	56	69	Not specified	Liver	Carcinoma	-				stomach liver	stomach	stomach vascular system liver	stomach liver lung	Liver Neoplasm, Experimental
1-Acetoxyasfrole	34627-78-6					Mouse	Male	CD1	Diet	20	69	Not specified	Liver	Carcinoma									
1-Acetoxyasfrole	34627-78-6					Rat	Male	SD	Diet	47	69	Positive	Forestomach	Papilloma									
1-Acetoxyasfrole	34627-78-6					Rat	Male	SD	Diet	26	52	Positive	Forestomach	Papilloma									
1-Acetyl-2-phenylhydrazine	114-83-0	CC(=O)NNC1=CC=CC=C1	급성 독성(경구) - 구분3 생식독성 - 구분2 만성 수생환경 유해성 - 구분1	14, 29, 30, 52, 53, 64, 66, 67, 71, 152, 165, 167, 200, 214, 318	Genotoxicity Data: genotoxic	Mouse	Female	Swiss	Drinking water	111	111	Positive	Blood vessel	Angioma	-				spleen all tumor bearing animals	ear Zymbals gland **uterus** hematopoietic system mammary gland small intestine kidney	vascular system lung urinary bladder kidney thyroid gland	vascular system lung urinary bladder **ovary** hematopoietic system	-
1-Acetyl-2-phenylhydrazine	114-83-0					Mouse	Male	Swiss	Drinking water	106	106	Positive	Blood vessel	Angioma									
1-Acetylaminofluorene	28314-03-8	C1=CC(=C2C(=C1)C3=C(C2)C=CC=C3)NC(=O)C	-	-	-	Rat	Female	Buffalo	Diet	47	88	Not specified	Adrenal gland	Carcinoma	-				kidney skin stomach liver spleen urinary bladder	ear Zymbals gland mammary gland liver urinary bladder **uterus** lung small intestine	urinary bladder thyroid gland kidney	urinary bladder stomach **ovary** liver	-
1-Amino-2,5-dimethylbenzene hydrochloride	51786-53-9	C=1(C)=CC=C(C=1)C)NH.Cl	-	-	-	Mouse	Female	CD-1 HsMs/ICR	Diet	68	94	Positive	Liver	Hepatoma	-				spleen urinary bladder liver lung clitoral gland thyroid gland ear Zymbals gland **uterus** mammary gland nasal cavity	urinary bladder liver clitoral gland thyroid gland ear Zymbals gland **uterus** mammary gland nasal cavity	urinary bladder thyroid gland vascular system liver kidney	liver urinary bladder vascular system thyroid gland	-
1-Amino-2,5-dimethylbenzene hydrochloride	51786-53-9					Mouse	Male	CD-1 HsMs/ICR	Diet	68	94	Positive	Liver	Multiple tumour types									
1-Amino-2,5-dimethylbenzene hydrochloride	51786-53-9					Rat	Male	SD	Diet	77	103	Positive	Liver	Multiple tumour types									
1-Benzoyl-2,6-dimethyl-4-nitrosopiperazine	61604-40-0	C1=CC=CC(=C1C(N)C(N)C)NC(C)C(N=O)C(=O	-	-	-	Rat	Female	Fischer 344	Drinking water	50	125	Positive	Forestomach	Carcinoma - basal cell	-				all tumor bearing animals	stomach nasal cavity vascular system all tumor bearing animals	stomach	-	-
1H-Indole-3-acetic acid	87-51-4	C(CC=2C=1C=CC=CC=1NC=2)(=O)O	피부염증	8, 11, 21, 29, 30, 34, 36, 41, 52, 53, 57, 58, 60, 61, 62, 72, 112, 135, 150, 163, 165, 167, 200, 210	Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	F2 **Genes** NFKB1	SRSBF2 TOB1 NAPI11 FABP4 SLC16A1	TMS B4X MPGD PPARD PPARA CYSORT1B	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (9) hsa-let-7 KO0903 AHR; aryl hydrocarbon receptor hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa-let-7 KO0903 AHR; aryl hydrocarbon receptor hsa04659 Th17 cell differentiation - Homo sapiens (human) (1) hsa-let-7 KO0903 AHR; aryl hydrocarbon receptor	-	all tumor bearing animals ear Zymbals gland	stomach urinary bladder	thyroid gland lung	-
1H-Indole-3-acetic acid	87-51-4					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
1H-Indole-3-acetic acid	87-51-4					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
1H-Indole-3-acetic acid	87-51-4					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
1-Hydroxyanthraquinone	129-43-1	C1(C3=C(C)C2=C1C=CC=C2C(=O)C=C(C=C3)O)=O	발암성 - 구분2 만성 수생환경 유해성 - 구분2	-	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Rat	Male	ACI/n	Diet	68	68	Positive	Caecum	Adenocarcinoma	-				urinary bladder kidney stomach large intestine liver vascular system nasal cavity	urinary bladder kidney liver ear Zymbal gland small intestine	stomach liver thyroid gland kidney vascular system	**ovary** thyroid gland pituitary gland vascular system hematopoietic system stomach liver urinary bladder	-
1-Hydroxyanthraquinone	129-43-1					Rat	Male	Fischer 344	Diet	78	78	Positive	Caecum	Adenocarcinoma									
1'-Hydroxyestragole	51410-64-7	C1=CC=CC(=C1)C(C=C)COC	-	-	-	Mouse	Female	CD1	Diet	51	86	Positive	Liver	Hepatoma	HSD17B2	TOB1 EJF5 ITGB8 H1F0 TIMM	SOD3 TNNI3K AKR1B10 ITGA6 FECH	hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa-let-7 KO3268 HSD17B2; hydroxysteroid 17-beta dehydrogenase 2 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (1) hsa-let-7 KO3268 HSD17B2; hydroxysteroid 17-beta dehydrogenase 2 hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa-let-7 KO3268 HSD17B2; hydroxysteroid 17-beta dehydrogenase 2	stomach kidney liver nasal cavity hematopoietic system large intestine	stomach nasal cavity	vascular system stomach	liver **ovary**	Liver Neoplasm Liver Neoplasm, Experimental Neoplasm
1'-Hydroxyasfrole	5208-87-7	C1=C(C=C2C(=C1)OCO2)C(=C)O	-	-	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F2 br	Diet	52	69	Not specified	Liver	Hepatoma	CYP2D6	MYBL1 TFAM AIRN7 CASP12 CCDC41	CASP2 PLK3 SYBAH FAM171A1 HSPA12A	hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (1) hsa-let-7 K17712 CYP2D6; cytochrome P450 family 2 subfamily D member 6 hsa00982 Drug metabolism - cytochrome P450 - Homo sapiens (human) (1) hsa-let-7 K17712 CYP2D6; cytochrome P450 family 2 subfamily D member 6 hsa01522 Endocrine resistance - Homo sapiens (human) (1) hsa-let-7 K17712 CYP2D6; cytochrome P450 family 2 subfamily D member 6	stomach liver	stomach	vascular system stomach liver	liver lung stomach	Liver Neoplasm, Experimental
1'-Hydroxyasfrole	5208-87-7					Mouse	Female	B6C.H2 pfb	Diet	52	69	Positive	Liver	Hepatoma									
1'-Hydroxyasfrole	5208-87-7					Mouse	Female	CD1	Diet	51	73	Positive	Liver	Carcinoma - hepatocellular									
1'-Hydroxyasfrole	5208-87-7					Mouse	Female	CD1	Diet	52	69	Positive	Liver	Hepatoma									
1'-Hydroxyasfrole	5208-87-7					Mouse	Male	CD1	Diet	51	73	Not specified	Liver	Carcinoma									
1'-Hydroxyasfrole	5208-87-7					Mouse	Male	CD1	Diet	36	69	Positive	Intestinum	Adenocarcinoma									
1'-Hydroxyasfrole	5208-87-7					Rat	Male	SD	Diet	58	95	Positive	Liver	Carcinoma - hepatocellular									
1'-Hydroxyasfrole	5208-87-7					Rat	Male	SD	Diet	49	69	Positive	Forestomach	Papilloma									
1'-Hydroxyasfrole	5208-87-7					Rat	Male	SD	Diet	36	52	Positive	Forestomach	Papilloma									
1-Methylnaphthalene	90-12-0	C1=CC=C2C(=C1)C(=CC=C2	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상/눈 자극성 - 구분2A(R) 흡입기 과민성 - 구분1(A/St) 특정표적장기 독성(1회 노출) - 구분3(마취졸림) 특정표적장기 독성(반복 노출) - 구분2	10, 29, 30, 52, 53, 67, 112, 165, 167, 200	Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Diet	81	81	Not specified	Liver	Adenoma - hepatocellular	AHR CYP1A2	SRSBF2 CTSD RNF12 TACR3 WDR67	ENC1 TK1 APOC1 IIT1 EIF3S C4		spleen Maltoni head cancers oral cavity ear Zymbals gland nasal cavity thyroid gland hematopoietic system urinary bladder kidney liver	clitoral gland nasal cavity urinary bladder **uterus** mammary gland liver hematopoietic system oral cavity	urinary bladder thyroid gland vascular system lung kidney small intestine	vascular system urinary bladder pituitary gland thyroid gland **ovary** stomach peritoneal cavity small intestine	-
1-Methylnaphthalene	90-12-0					Mouse	Male	B6C3F1	Diet	81	81	Not specified	Liver	Adenoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
1-Naphthalenamine	134-32-7	C1=CC=C2C(=C1N)C=CC=C2	경구 독성(분말) : 구분4 경피 독성(토끼) : 구분1 경성 독성(흰쥐 흡입(먼지/미스트)) : 구분2 **발암성 : 구분1** 만성 수생환경 유해성 : 구분3	7, 8, 11, 14, 21, 25, 28, 34, 41, 57, 58, 60, 61, 62, 62, 64, 66, 71, 100, 101, 102, 103, 122, 123, 131, 148, 150, 153, 177, 214, 220, 310, 318	Cancer slope factor: 0.00051 ug/m3-1 (carcinogenicity, oral) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Male	ICR/Ussl	Diet	52	52	Positive	Liver	Hepatoma	SLC6A4 PARP1 CNR1 CNR2 CASP3	CCR6 DNAJC2 AMH R2 TEP1 CIA51	HTATIP2 BCL2A1 SAT CCR5 MGST1	hsa04080: Neuroactive ligand-receptor interaction - Homo sapiens (human) (2) hsa:1268 404077: CNR1; cannabinoid receptor 1 hsa:1269 404078: CNR2; cannabinoid receptor 2	ear Zymbals gland spleen urinary bladder thyroid gland all tumor bearing animals hematopoietic system	urinary bladder **uterus** clitoral gland ear Zymbals gland hematopoietic system thyroid gland **lung** liver mammary gland kidney nasal cavity	thyroid gland urinary bladder liver vascular system **lung**	thyroid gland liver urinary bladder **ovary** lung vascular system stomach hematopoietic system	**Lung Neoplasm** Carcinoma, Hepatocellular Adenoma, Liver Cell
1-Naphthalenecarbonitrile	86-86-2	C1=CC=C2C(=C1C(=C)C=C2)C(C)=O)N	경성 독성(분진) : 구분4	-	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma	-				spleen	**uterus** ear Zymbals gland	urinary bladder thyroid gland stomach	urinary bladder **ovary** vascular system thyroid gland stomach liver	-
1-Naphthalenecarbonitrile	86-86-2					Mouse	Male	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
1-Naphthalenecarbonitrile	86-86-2					Mouse	Female	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
1-Naphthalenecarbonitrile	86-86-2					Mouse	Male	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
1-Naphthaleneacetic acid	86-87-3	C1=CC=C2C(=C1C(=C)C=C2)C(C)=O)O	변속부식성 물질 : 구분1 경성 독성(흰쥐) : 구분4 피부 부식성/피부 자극성 : 구분1(A/1B/1C) 심한 눈 손상성/눈 자극성 : 구분1 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 만성 수생환경 유해성 : 구분3	34, 36, 58, 72, 163	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Angioma	CES2C IFNG SJ INSRA Tnf	SRBEP2 NAPTL1 TOB1 ASAH1 MAFAKA	HPGD POU62A PPARD SPAG6 NQO1	hsa04060: Cytokine-cytokine receptor interaction - Homo sapiens (human) (2) hsa:3458 404687: IFNG; interferon gamma hsa:3558 405429: IL2; interleukin 2 hsa05200: Pathways in cancer - Homo sapiens (human) (2) hsa:3458 404687: IFNG; interferon gamma hsa:3558 405429: IL2; interleukin 2 hsa04940: Type I diabetes mellitus - Homo sapiens (human) (2) hsa:3458 404687: IFNG; interferon gamma hsa:3558 405429: IL2; interleukin 2	hematopoietic system	-	kidney lung stomach	lung pituitary gland vascular system **ovary** stomach	-
1-Naphthaleneacetic acid	86-87-3					Mouse	Male	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
1-Naphthaleneacetic acid	86-87-3					Mouse	Female	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
1-Naphthaleneacetic acid	86-87-3					Mouse	Male	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
1-Nitronaphthalene	86-57-7	[N+](=[O-])c1c2ccccc2ccc1	인화성 고체 : 구분2 경성 독성(흰쥐) : 구분3 만성 수생환경 유해성 : 구분3	8, 11, 21, 28, **29**, **30**, 34, 36, 41, 43, 46, 52, 53, 57, 60, 61, 63, 67, 72, 97, 98, 100, 101, 102, 103, 107, 112, 121, 148, 150, 163, **165**, **167**, 177, 195, **200**, 203, 204, 310	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	96	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	ACTB ACTG1 AIB ALDH2	CCR6 PDGFRA CIA51 RAB20 PLEKHB1	SERPINB8 ARTJH BCL2A1 SH3BP5 MLPH	hsa04810: Regulation of actin cytoskeleton - Homo sapiens (human) (1) hsa:71 635692: ACTG1; actin gamma 1 hsa04670: Leukocyte transendothelial migration - Homo sapiens (human) (1) hsa:71 635692: ACTG1; actin gamma 1 hsa05014: Amyotrophic lateral sclerosis - Homo sapiens (human) (1) hsa:71 635692: ACTG1; actin gamma 1	ear Zymbals gland spleen thyroid gland kidney hematopoietic system lung urinary bladder skin liver	hematopoietic system ear Zymbals gland clitoral gland **uterus** mammary gland lung urinary bladder kidney liver	thyroid gland urinary bladder kidney vascular system liver lung	**ovary** liver vascular system urinary bladder thyroid gland stomach lung hematopoietic system	-
1-Nitronaphthalene	86-57-7					Mouse	Male	B6C3F1	Diet	78	96	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
1-Nitronaphthalene	86-57-7					Rat	Female	Fischer 344	Diet	78	107	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
1-Nitronaphthalene	86-57-7					Rat	Male	Fischer 344	Diet	78	107	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
1-Nitropyrene	5522-43-0	[N+](=O)(=O)c1ccc2c3c1ccc1cccc(c3ccc(c1)c(c2)[N+](=O)[O-])=O	생식세포 변이원성 : 구분2 **발암성 : 구분1B** 경구 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	14, 15, 22, **29**, **30**, 34, 36, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 163, **165**, **167**, **187**, **200**, 214, 307, 318	Cancer slope factor: 0.00011 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Female	Fischer 344/N	Gavage	55	104	Positive	Clitoral gland	Adenocarcinoma	TP53 CXCL8 ATG7 CYP1A1	CCR6 PDGFRA CIA51 RAB20 PLEKHB1	SERPINB8 ARTJH BCL2A1 SH3BP5 MLPH	hsa05200: Pathways in cancer - Homo sapiens (human) (1) hsa:3576 410830: CXCL8; C-X-C motif chemokine ligand 8 hsa05164: Influenza A - Homo sapiens (human) (1) hsa:3576 410830: CXCL8; C-X-C motif chemokine ligand 8 hsa04061: Viral protein interaction with cytokine and cytokine receptor - Homo sapiens (human) (1) hsa:3576 410830: CXCL8; C-X-C motif chemokine ligand 8	ear Zymbals gland spleen thyroid gland **lung** urinary bladder kidney skin hematopoietic system	hematopoietic system ear Zymbals gland clitoral gland **uterus** **lung** urinary bladder kidney **liver**	thyroid gland urinary bladder kidney vascular system **liver**	**ovary** **liver** stomach vascular system urinary bladder thyroid gland **lung**	Carcinoma, Hepatocellular **Lung Neoplasm** Carcinoma, Squamous Cell Cell Transformation, Neoplastic Carcinoma, Squamous Cell Adenocarcinoma **Liver Neoplasm, Experimental**
1-Nitroso-2,2,4-trimethyl-1,2-dihydroquinoline polymer	29509-77-9	CC[C]1=CC=CC=C(N(C)[C]C)C[C]C[C]C[C]C=CC=C(N(C)[C]C)C[C]N(=O)N=O)O[R]		-	-	Rat	Male	CR	Intraperitoneal	26	100	Positive	Peritoneal cavity	Sarcoma	-				spleen all tumor bearing animals	all tumor bearing animals	-	-	-
1-O-Hexyl-2,3,5-trimethylhydroquinone	148081-72-5	C1(=O)C(=C(C)=C(O)CCCCCC)C(O)C	-	7, 8, 11, 19, 21, 22, 23, 27, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 67, 72, 107, 111, 112, 117, 122, 123, 131, 150, 153, 163, **165**, **167**, **187**, **200**, 207, 210	-	Rat	Female	Fischer 344/DuCr	Diet	52	52	Not specified	Liver	Multiple tumour types	CYP1A2 MPO	ZFAND5 SEC16A NADK MAPK8 PPIH	EIF3S5C4 FTL AUDC4 CIS9 HSPCB		stomach urinary bladder	stomach urinary bladder	liver kidney thyroid gland	liver	Colonic Neoplasm **Liver Neoplasm**
1'-Oxoaflavone	304818-53-2	C1=CC(=CC2=C1OCCD2)C(=C)=O	-	-	-	Rat	Male	SD	Diet	73	95	Negative	Liver	Carcinoma	-				stomach liver	stomach	stomach vascular system liver	stomach lung liver	-
1-Phenylazo-2-naphthalenol	842-07-9	C1(=C(C=CC=C2C=1C=CC=Z0)N=NC3=CC=CC=C3	심한 눈 손상성/눈 자극성 : 구분2A(/2B) 피부 과민성 : 구분1(1A/1B) 생식세포 변이원성 : 구분2 **발암성 : 구분2** 만성 수생환경 유해성 : 구분4	8, 11, 14, 21, 27, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 107, 112, 122, 123, 130, 150, 163, 168, **167**, **200**, 214, 220, 310, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	CYP1A1 CYBEA CYP1A2 NQO1	MTTH HEATR3 COG5 DNAAK2 FARP1	CYORF62 TFF1 YAON RNF12 BUB2	hsa00980: Tryptophan metabolism - Homo sapiens (human) (1) hsa:1544 407409: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa00982: Drug metabolism - cytochrome P450 - Homo sapiens (human) (1) hsa:1544 407409: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa05207: Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa:1544 407409: CYP1A2; cytochrome P450 family 1 subfamily A member 2	spleen liver urinary bladder vascular system nasal cavity	liver urinary bladder hematopoietic system clitoral gland	thyroid gland kidney urinary bladder	**ovary** thyroid gland liver pituitary gland urinary bladder vascular system	**Liver Neoplasm, Experimental** Precancerous Conditions
1-Phenylazo-2-naphthalenol	842-07-9					Mouse	Male	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
1-Phenylazo-2-naphthalenol	842-07-9					Mouse	Female	CBA	Diet	52	104	Negative	Liver	Hepatoma									
1-Phenylazo-2-naphthalenol	842-07-9					Mouse	Male	CBA	Diet	52	104	Negative	Liver	Hepatoma									
1-Phenylazo-2-naphthalenol	842-07-9					Rat	Female	Fischer 344	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
1-Phenylazo-2-naphthalenol	842-07-9					Rat	Male	Fischer 344	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-(4-Amino-2-nitrophenyl)amino)ethanol	2871-01-4	C1=C(C=C(C)=C1)NCCO)[N+](=O)=O)N	피부염증	21, 34, 41, 57, 58, 61, 131, 150, 310	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	104	105	Inadequate test	Forestomach	Papilloma - squamous cell	-				skin urinary bladder spleen large intestine ear Zymbals gland thyroid gland	lung **uterus**	thyroid gland kidney urinary bladder liver vascular system	liver hematopoietic system	-
2-(4-Amino-2-nitrophenyl)amino)ethanol	2871-01-4					Mouse	Male	B6C3F1	Gavage	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular									
2-(4-Amino-2-nitrophenyl)amino)ethanol	2871-01-4					Rat	Female	Fischer 344	Gavage	105	106	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-(4-Amino-2-nitrophenyl)amino)ethanol	2871-01-4					Rat	Male	Fischer 344	Gavage	105	106	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-(1,3-Dioxethylidyl)-4,6-dioxino-phenol methanesulphonate	29110-68-7	O1=S(=O)(O[C=1C(N=)]O-)=O)=CC(N=)]O-)=O)=CC=1C(C)C)C)C	-		-	Rat	Female	SD	Diet	52	52	Not specified	Liver	Multiple tumour types	-				-	-	thyroid gland	-	-
2-(1,3-Dioxethylidyl)-4,6-dioxino-phenol methanesulphonate	29110-68-7					Rat	Male	SD	Diet	52	52	Not specified	Liver	Multiple tumour types									
2-(1,1-Dimethylethyl)-4-methylphenol	2409-55-4	C=1(C)=CC=C(C=1)C(C)(C)C)C	피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(/2B) 만성 수생환경 유해성 : 구분2	7, 8, 11, 19, 21, 25, 27, **29**, **30**, 34, 46, 52, 53, 58, 60, 61, 62, 67, 111, 112, 117, 122, 123, 148, 153, **165**, **167**, **187**, **200**, 307	Genotoxicity Data: predicted to be genotoxic	Rat	Male	Fischer 344/DuCr	Diet	51	52	Not specified	Forestomach	Multiple tumour types	CASP3 CAT SOD2	CCDC50 STATIA GABT PTPRO HSPA6	GCLM FOXO1 ABHD12 CIS9 NQO1	hsa00630: Glyoxylate and dicarboxylate metabolism - Homo sapiens (human) (1) hsa:847 403781: CAT; catalase hsa05022: Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (1) hsa:847 403781: CAT; catalase hsa04211: Longevity regulating pathway - Homo sapiens (human) (1) hsa:847 403781: CAT; catalase	**stomach** Malteni head cancers **urinary bladder** oral cavity spleen	**stomach**	kidney **stomach** thyroid gland **lung** liver **urinary bladder**	pituitary gland thyroid gland	Urinary Bladder Neoplasm Papilloma Adenoma **Lung Neoplasm**
2-(1-Methylheptyl)-4,6-dinitrophenyl crotonate	6119-92-2	C(C=1C(=CC(=C(C=1)[N+](O-)=O)[N+](=O)[O-]=O)[O-]=O)(C=CC)=O)(CCCCCC)C,C)(=CC(=CC(=CC(=C(C)(CCCCCC)C)C)=C)[N+](=O)[O-])[N+](O-)=O	-	-	-	Mouse	Female	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma	-							-	-
2-(1-Methylheptyl)-4,6-dinitrophenyl crotonate	6119-92-2					Mouse	Male	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2-(1-Methylheptyl)-4,6-dinitrophenyl crotonate	6119-92-2					Mouse	Female	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2-(1-Methylheptyl)-4,6-dinitrophenyl crotonate	6119-92-2					Mouse	Male	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2-(2,5-Dichlorophenoxy)propionic acid	6965-71-5	C1=C(C)=CC(=C1C)(OC)C(O)=O)Cl	-	8, 11, 60	-	Mouse	Female	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma	-				-	-	kidney liver	-	-
2-(2,5-Dichlorophenoxy)propionic acid	6965-71-5					Mouse	Male	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2-(2,5-Dichlorophenoxy)propionic acid	6965-71-5					Mouse	Female	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2-(2,5-Dichlorophenoxy)propionic acid	6965-71-5					Mouse	Male	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2-(4-Aminophenyl)-6-methyl-7-benzothiazolesulphonic acid	130-17-6	C12c=C(SC(=N1)C2)c(C)c=C(N(C(SO)(=O)=O)=C)C=c2C	천연 및 순천연(수 까지만 - 구연2A/2B) 인체 수생환경 유해성 - 구분4	19, 23, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 61, 67, 72, 111, 112, 117, 131, 150, 163, 165, 167, 187, 200, 207, 208	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	96 d	91 d	Not specified			-								
2-(4-Aminophenyl)-6-methyl-7-benzothiazolesulphonic acid	130-17-6					Mouse	Male	B6C3F1	Diet	96 d	91 d	Not specified											
2-(4-Aminophenyl)-6-methyl-7-benzothiazolesulphonic acid	130-17-6					Rat	Female	Fischer 344	Diet	97 d	91 d	Not specified											
2-(4-Aminophenyl)-6-methyl-7-benzothiazolesulphonic acid	130-17-6					Rat	Male	Fischer 344	Diet	97 d	91 d	Not specified											
2,2'-((4-Aminophenyl)imino)bisethanol sulphate	54381-16-7	C1=c(C=c(C(=N(NCCO)CCO)=C=C)=C)=S(=O)(=O)	-		Genotoxicity Data: genotoxic	Rat	Female	Fischer 344/DuCrl	Diet	104	104	Negative	Liver	Adenoma - hepatocellular	-				-	-	-	-	-
2,2'-((4-Aminophenyl)imino)bisethanol sulphate	54381-16-7					Rat	Male	Fischer 344/DuCrl	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
2,2',4,4',5,5'-Hexabromobiphenyl	67774-32-7	C2C=1(C=c(C)c(=C(C=1Br)Br)Br)=c(C)=c(C=c2Br)Br)Br	발암성 - 구분2	-	-	Mouse	Female	B6C3F1	Gavage	26	131	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				Liver large intestine kidney urinary bladder Maltoni head cancers oral cavity thyroid gland	Liver kidney urinary bladder thyroid gland	Liver stomach lung	Liver stomach lung peritoneal cavity thyroid gland urinary bladder	-
2,2',4,4',5,5'-Hexabromobiphenyl	67774-32-7					Mouse	Female	B6C3F1	Diet	105	105	Positive	Liver	Adenoma - hepatocellular									
2,2',4,4',5,5'-Hexabromobiphenyl	67774-32-7					Mouse	Male	B6C3F1	Gavage	26	131	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
2,2',4,4',5,5'-Hexabromobiphenyl	67774-32-7					Mouse	Male	B6C3F1	Diet	105	105	Positive	Liver	Adenoma - hepatocellular									
2,2',4,4'-Tetrabromodiphenyl ether	5436-43-1	C1(c=c(C)=c(C)c=C1)(OC2=c(C)=c(C)=c(C)=c2Br)Br)Br)Br	피부염증	19, 23, 27, 29, 30, 52, 53, 61, 67, 111, 112, 117, 165, 167, 187, 200, 207	Carcinogenicity data available: IRIS-Inadequate information to assess carcinogenic potential Genotoxicity Data: predicted to be clastogenic	Mouse	Female	BALB/c(by)	Gavage	-	Not specified	Not specified			TTR ESR1 CASP3 CYP1A1 PPARG	CDKN2B ERNA1 RBM13 BAGAT5 SRGAP1	CYP1A2 CTED2 STAGA1 C1ORF60 CTTN	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:2099 KEGG:5101 ESRT; estrogen receptor 1 hsa:836 KEGG:4021B7 CASP3; caspase 3 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (2) hsa:1543 KEGG:1536B CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:836 KEGG:4021B7 CASP3; caspase 3 hsa05205 Proteoglycans in cancer - Homo sapiens (human) (2) hsa:2099 KEGG:5101 ESRT; estrogen receptor 1 hsa:836 KEGG:4021B7 CASP3; caspase 3	liver kidney large intestine urinary bladder thyroid gland oral cavity	kidney liver urinary bladder thyroid gland	stomach liver lung kidney	liver stomach thyroid gland urinary bladder lung pituitary gland **ovary** peritoneal cavity	-
2,2',5,5'-Tetrachlorobenzidine	15721-02-5	C2C=1(C=c(C)=c(C)=c1)C1(NC3)=C(C=c(C)=c(C)=c2C)C3)NC)	경증 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 14, 15, 23, 23, 26, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 148, 150, 152, 163, 165, 167, 187, 200, 214, 217, 219, 218	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	dd	Diet	104	104	Not specified	Multiple sites	Lymphoma - malignant	-				ear Zymbals gland thyroid gland hematopoietic system spleen vascular system liver urinary bladder	liver lung thyroid gland mammary gland urinary bladder **uterus** kidney	liver vascular system urinary bladder thyroid gland	liver thyroid gland urinary bladder vascular system	-
2,2',5,5'-Tetrachlorobenzidine	15721-02-5					Rat	Female	Wistar	Diet	104	104	Not specified	Liver	Hepatoma									
2,2',5,5'-Tetrachlorobenzidine	15721-02-5					Rat	Male	Wistar	Diet	104	104	Not specified	Liver	Multiple tumour types									
2,2',6,6'-Tetrabromobisphenol A	79-94-7	C(C)(C)=1C=c(C)=c(C)=c1Br)C)Br)C2=c(C)=c(C)=c(C)Br)C)Br	경미독성 - 구분1B 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	6, 7, 8, 10, 11, 14, 18, 19, 23, 25, 27, 29, 30, 34, 36, 37, 46, 51, 52, 53, 58, 59, 60, 61, 62, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 148, 150, 153, 163, 165, 166, 167, 187, 200, 214, 220, 307, 318	Carcinogenicity data available: IARC-Group 2A - Probably carcinogenic to humans Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1/N	Gavage	93	91	Not specified	Adrenal gland cortex	Lymphoma - malignant	PPARG THRB THRA	CCDC50 STAT5A GART YPEL5 PTPRO	OSS CREB3L1 RNASE6 CGH HSPC8	hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (1) hsa:7068 KEGG:4382 THRB; thyroid hormone receptor beta hsa04919 Thyroid hormone signaling pathway - Homo sapiens (human) (1) hsa:7068 KEGG:4382 THRB; thyroid hormone receptor beta	urinary bladder large intestine kidney stomach hematopoietic system nasal cavity thyroid gland	urinary bladder kidney thyroid gland **liver**	stomach kidney lung **liver** thyroid gland	pituitary gland stomach thyroid gland **ovary** **liver** lung	Carcinoma Uterine Cervical Neoplasm Neoplasm, Experimental Uterine Neoplasm
2,2',6,6'-Tetrabromobisphenol A	79-94-7					Mouse	Female	B6C3F1/N	Gavage	2 yrs	2 yrs	Not specified											
2,2'-[2-(2-Thienyl)-4-quinazolinylimino]bisethanol	58189-47-2	C=1(C=c(C=c1C=2N(=C(C=N)=2)CC=c(C=c)N)CCO)CCO				Rat	Female	SD	Diet	46	66	Not specified	Multiple sites	Multiple tumour types				hsa04650 Natural killer cell mediated cytotoxicity - Homo sapiens (human) (1) hsa:3458 KEGG:4347 IFNG; interferon gamma hsa05160 Hepatitis C - Homo sapiens (human) (1) hsa:3458 KEGG:4347 IFNG; interferon gamma hsa05146 Amoebiasis - Homo sapiens (human) (1) hsa:3458 KEGG:4347 IFNG; interferon gamma	large intestine	all tumor bearing animals	thyroid gland	-	-
2,2'-Dithiobisbenzothiazole	120-78-5	C1=c(C=c(C2=c(SC)=N(S(SC3=NC4=C(S)C=c(C=c(C4	피부 과민성 - 구분1(1A/1B) 만성 수생환경 유해성 - 구분2	61	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	AGB GSR IFNG G4	CRH PDZK1 SNAI1 TRAM	CCR5 GCLC SCD5L PVRIG CYP26B1		hematopoietic system spleen	all tumor bearing animals	-	thyroid gland	-
2,2'-Dithiobisbenzothiazole	120-78-5					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2,2'-Dithiobisbenzothiazole	120-78-5					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2,2'-Dithiobisbenzothiazole	120-78-5					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2,2'-Methylenebis[6-tert-butyl-p-cresol]	119-47-1	C1=c(C)=c(C=c1C)C2=c(C)=c(C=c(C)c(C)c)C2=c(C)=c(C)=c(C)c(C)c)C)C	천연 및 순천연(수 까지만 - 구연2A/2B)	7, 8, 11, 14, 19, 23, 23, 27, 29, 30, 34, 36, 46, 52, 53, 58, 60, 61, 62, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 148, 150, 153, 163, 165, 167, 187, 200, 214, 220, 307, 318	Genotoxicity Data: non-genotoxic	Rat	Female	Wistar	Diet	52	52	Negative	Liver	Multiple tumour types	IYD	PTPRO PPIN SEC16A ZFAND5 NOPS6	OSS HSPC8 ABCA1 AUDDA FOXO1	hsa04918 Thyroid hormone synthesis - Homo sapiens (human) (1) hsa:38634 KEGG:6372D1 IYD; iodotyrosine deiodinase	vascular system stomach Maltoni head cancers	stomach	kidney lung thyroid gland	pituitary gland	-
2,2'-Methylenebis[6-tert-butyl-p-cresol]	119-47-1					Rat	Female	Wistar	Diet	78	78	Negative	Liver	Multiple tumour types									
2,2'-Methylenebis[6-tert-butyl-p-cresol]	119-47-1					Rat	Male	Wistar	Diet	52	52	Negative	Liver	Multiple tumour types									
2,2'-Methylenebis[6-tert-butyl-p-cresol]	119-47-1					Rat	Male	Wistar	Diet	78	78	Negative	Liver	Adenoma - hepatocellular									
2,2',4,4',5-Pentachlorobiphenyl	31508-00-6	C1=c(C)=c(C=c1C)C2=c(C)=c(C=c(C)c(C)c)C)c	경미 독성(경구) - 구분4 경미 독성(경피) - 구분3 피부 부식성/피부 자극성 - 구분2 천연 및 순천연(수 까지만 - 구연2A/2B) 피부 과민성 - 구분1(1A/1B) 생식세포 변이원성 - 구분2 발암성 - 구분1A 생식독성 - 구분2 생식독성 - 수유독성 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분1 경로 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	Cancer slope factor: 0.0011 (ug/m3)-1 (carcinogenicity, inhalation) Genotoxicity Data: predicted to be non-genotoxic	Rat	Female	Harlan	Gavage	733 d	730 d	Not specified	Adrenal gland cortex	Adenoma	CYP1A1 AHR	FABP4 ARNT CASP12 CCDC49 INAP2 GCA	BEL CYP1B2 IL1RN FAM171A1 HSPA12A LIM2 MAPK7CP3		thyroid gland hematopoietic system ear Zymbals gland oral cavity liver	liver	liver vascular system	thyroid gland urinary bladder liver vascular system	**Lung Neoplasms** Cholangiocarcinoma Colorectal Neoplasm Neoplasm Metastasis Brain Neoplasm **Adenoma, Liver Cell** Uterine Neoplasm
2,3,4,7,8-Pentachlorodibenzo[b,d]furan	57117-31-4	C1=c(C)=c(C2=c(Cl)C=3C(=3C2=c(C)=c(C)=c3Cl)Cl)c(Cl)c1Cl	급성 독성(경구) - 구분1 발암성 - 구분1A 생식독성 - 구분1A 특정표적장기 독성(반복 노출) - 구분2 경로 수생환경 유해성 - 구분1	-	Cancer slope factor: 11 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: IARC-Group 1 - Carcinogenic to humans	Mouse	Female	IVRcNr hemizygous	Dermal	182 d	182 d	Not specified	Application site	Carcinoma- spindle cell	CYP1A1 AHR CYP1B1 CYP1A2	ARNT CASP12 CCDC49 INAP2 GCA	CYP1A2 FAM171A1 HSPA12A LIM2 MAPK7CP3	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa:1545 KEGG:1536D CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa:196 KEGG:3066 AHR; aryl hydrocarbon receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:1545 KEGG:1536D CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa:196 KEGG:3066 AHR; aryl hydrocarbon receptor hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (1) hsa:1545 KEGG:1536D CYP1B1; cytochrome P450 family 1 subfamily B member 1	thyroid gland all tumor bearing animals	liver lung	liver urinary bladder	liver thyroid gland vascular system	**Liver Neoplasm, Experimental**
2,3,4,7,8-Pentachlorodibenzo[b,d]furan	57117-31-4					Rat	Female	Harlan	Gavage	2 yrs	2 yrs	Not specified	Adrenal gland cortex	Adenoma									
2,3,4-Trichloro-1,5-dinitrobenzene	6279-46-0	C1[N(=)[O-])c(Cl)c(Cl)c(C[N+][O-])c1Cl	-	-	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma	-				thyroid gland kidney ear Zymbals gland liver hematopoietic system lung urinary	kidney lung liver hematopoietic system **uterus** clitoral gland	liver vascular system thyroid gland kidney	vascular system liver **ovary** urinary bladder thyroid gland	-
2,3,4-Trichloro-1,5-dinitrobenzene	6279-46-0					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
2,3,4-Trichloro-1,5-dinitrobenzene	6279-46-0					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
2,3,4-Trichloro-1,5-dinitrobenzene	6279-46-0					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
2,3-Dihydro-2-(5-nitro-2-thienyl)-4(1H)-quinazolinone	33889-33-2	C1[N(=)c(=O)[O-])ccC=c(S1)C2N(C(=)C(N2)=c(C=c(C=)c)=O	-	-	-	Rat	Female	SD	Diet	46	66	Positive	Mammary gland	Adenocarcinoma	-				-	all tumor bearing animals	urinary bladder thyroid gland	-	-
2,4,5,2',4',5'-Hexachlorobiphenyl	35065-27-1	C1(c(C=c(C)=c(C)c)C2=c(C)=c(C)=c(C)=c2Cl)Cl)C3Cl)C3Cl)Cl	-	Genotoxicity Data predicted to be non-genotoxic		Rat	Female	Harlan	Gavage	731 d	730 d	Not specified	Adrenal gland cortex	Adenoma	NR1I2 NR1I3 CYP1A1 CASP3	FABP4 ARNT CASP12 CCDC49 INAP2	BEL FAM171A1 HSPA12A LIM2 MAPK7CP3	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:1543 KEGG:1536C CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:9970 KEGG:8365 NR1I3; nuclear receptor subfamily 1 group I member 3 hsa00380 Tryptophan metabolism - Homo sapiens (human) (1) hsa:1543 KEGG:1536C CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (1)	thyroid gland oral cavity hematopoietic system ear Zymbals gland **liver** Maltoni head cancers nasal cavity kidney	**liver** kidney thyroid gland lung	**liver** vascular system small intestine	thyroid gland **liver** urinary bladder peritoneal cavity vascular system small intestine stomach	Breast Neoplasm Neoplasm Metastasis **Liver Neoplasm** Neoplasm
2,4,5,6-Tetrafluoro-1,3-benzenediamine dihydrochloride	63886-77-7	C1(=c(C)=c(C)=c(C)=c1F)N(H)(H)H.N(C).Cl	-	-	-	Mouse	Female	CD-1 HaMLICR	Diet	77	94	Not specified	Liver	Multiple tumour types	-				thyroid gland spleen kidney ear Zymbals gland liver	ear Zymbals gland **uterus** thyroid gland urinary bladder lung hematopoietic system kidney clitoral gland nasal cavity	urinary bladder thyroid gland liver lung vascular system	liver hematopoietic system thyroid gland lung urinary bladder vascular system stomach **ovary** pituitary gland peritoneal cavity	-
2,4,5,6-Tetrafluoro-1,3-benzenediamine dihydrochloride	63886-77-7					Mouse	Male	CD-1 HaMLICR	Diet	77	94	Positive	Liver	Hepatoma									
2,4,5,6-Tetrafluoro-1,3-benzenediamine dihydrochloride	63886-77-7					Rat	Male	SD	Diet	77	98	Negative	Liver	Multiple tumour types									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2,4,5-T	93-76-5	C1=C(Cl)C(=C(C=C1Cl)OCC(O)=O)Cl(Cl)Cl	-	28, 34, 36, 58, 61, 63, 72, 100, 101, 102, 103, 163, 177	Genotoxicity Data: clastogenic	Mouse	Male	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma	ABCC2 GCLC ABCA7 ABCB4 ACAP2	FABP4 MYBL1 MRAP4 CYP11A1 MTTH	ITL GCLC REL GATA1 IL10RB	hsa02010 ABC transporters - Homo sapiens (human) (2) hsa10347 405645 ABCA7; ATP binding cassette subfamily A member 7 hsa5244 405659 ABCB4; ATP binding cassette subfamily B member 4 hsa04216 Ferroptosis - Homo sapiens (human) (1) hsa2729 K11204 GCLC; glutamate-cysteine ligase catalytic subunit hsa00480 Glutathione metabolism - Homo sapiens (human) (1) hsa2729 K11204 GCLC; glutamate-cysteine ligase catalytic subunit	hematopoietic system thyroid gland	-	kidney liver vascular system	-	Prostatic Neoplasm
2,4,5-T	93-76-5					Mouse	Male	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4,5-T	93-76-5					Mouse	Female	B6C3F1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4,5-T	93-76-5					Mouse	Male	B6C3F1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4,5-Trimethylaniline	137-17-7	C=1(C=C(C)=CC=1C)CCN	급성 독성(경구) - 구분2 급성 독성(피부) - 구분2 급성 독성(흡입) (증기) - 구분3 생식세포 변이원성 - 구분2 **발암성 - 구분1B** 만성 수생환경 유해성 - 구분2	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Diet	101	101	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				liver spleen urinary bladder Mattoni head cancers ear Zymbals gland skin oral cavity	liver lung urinary bladder clitoral gland thyroid gland **uterus** ear Zymbals gland mammary gland	urinary bladder thyroid gland vascular system liver	liver vascular system urinary bladder thyroid gland	-
2,4,5-Trimethylaniline	137-17-7					Mouse	Male	B6C3F1	Diet	101	101	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4,5-Trimethylaniline	137-17-7					Rat	Female	Fischer 344	Diet	101	101	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4,5-Trimethylaniline	137-17-7					Rat	Male	Fischer 344	Diet	101	101	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4,5-Trimethylaniline hydrochloride	21436-97-5	C1=C(C)=C(C=C1C)N(C)C.Cl	**발암성 - 구분1B** 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	-	Mouse	Female	CD-1 HsMx(ICR)	Diet	77	98	Positive	Liver	Hepatoma	-				liver spleen urinary bladder Mattoni head cancers ear Zymbals gland skin oral cavity	liver lung urinary bladder clitoral gland thyroid gland **uterus** ear Zymbals gland mammary gland	urinary bladder thyroid gland vascular system liver	liver vascular system urinary bladder thyroid gland	-
2,4,5-Trimethylaniline hydrochloride	21436-97-5					Mouse	Male	CD-1 HsMx(ICR)	Diet	77	98	Positive	Liver	Hepatoma									
2,4,5-Trimethylaniline hydrochloride	21436-97-5					Rat	Male	SD	Diet	77	98	Positive	Liver	Hepatoma									
2,4,6-Trichloroaniline	634-93-5	C1=C(C=C(C=C1Cl)Cl)CN	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(OB) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	Carcinogenicity data available: PPRTV (ORNL) - Suggestive evidence of carcinogenic potential	Mouse	Female	CD-1 HsMx(ICR)	Diet	68	77	Negative	Liver	Multiple tumour types	-				thyroid gland ear Zymbals gland hematopoietic system spleen all tumors bearing animals	thyroid gland lung urinary bladder **uterus** liver kidney clitoral gland ear Zymbals gland	liver vascular system urinary bladder thyroid gland	liver thyroid gland urinary bladder vascular system	-
2,4,6-Trichloroaniline	634-93-5					Mouse	Male	CD-1 HsMx(ICR)	Diet	68	77	Positive	Liver	Hepatoma									
2,4,6-Trichloroaniline	634-93-5					Rat	Male	SD	Diet	77	116	Negative	Liver	Multiple tumour types									
2,4,6-Trichlorophenol	88-06-2	C1=C(C=C(C=C1Cl)Cl)O	급성 독성(경구) - 구분4 급성 독성(피부) - 구분4 **발암성 - 구분1B** 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	6, 8, 11, 18, 21, **29**, **30**, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 67, 72, 112, 132, 133, 135, 146, 150, 163, **165**, **166**, **167**, **200**, 220, 233, 238	Cancer slope factor: 3.1e-06 ug/m3-1 (carcinogenicity, oral) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (pmewearing) than diet	76	76	Not specified	Liver	Hepatoma	CYP1A TNRB CYP11A1 CYP7BA1	CYP11A1 FABP4 MAPK5C1 MYD5C PLSC34	ERCC2 PCB REL VAGN ABHD2	hsa04919 Thyroid hormone signaling pathway - Homo sapiens (human) (1) hsa7068 K08362 THRB; thyroid hormone receptor beta hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa1583 K00496 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa04925 Aldosterone synthesis and secretion - Homo sapiens (human) (1) hsa1583 K00496 CYP11A1; cytochrome P450 family 11 subfamily A member 1	hematopoietic system thyroid gland nasal cavity kidney oral cavity urinary bladder	liver thyroid gland kidney hematopoietic system urinary bladder	liver vascular system kidney	liver thyroid gland vascular system **ovary** pituitary gland urinary bladder	-
2,4,6-Trichlorophenol	88-06-2					Mouse	Male	B6AKF1	Gavage (pmewearing) than diet	76	76	Not specified	Liver	Hepatoma									
2,4,6-Trichlorophenol	88-06-2					Mouse	Female	B6C3F1	Gavage (pmewearing) than diet	76	76	Not specified	Liver	Hepatoma									
2,4,6-Trichlorophenol	88-06-2					Mouse	Female	B6C3F1	Diet	105	105	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4,6-Tinitro-1,3,5-dimethyl-1-tert-butylbenzene	81-15-2	[N+](=O)([O-])C1=C(C)N(=[O])=C(C)=C(C)C(=[N+](=O)[O-])C(C)(C)C	인화성 고체 - 구분2 급성 독성(경구) - 구분4 **발암성 - 구분2** 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, **29**, **30**, 34, 36, 52, 53, 58, 60, 72, 72, 112, 163, **165**, **167**, **200**	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Diet	80	90	Positive	Harderian gland	Multiple tumour types	CYP3B1 CYP1A2 CYP2A5 CYP2A2 CYP3A2	CYP11A1 PDGFRL PCDLCE2 INFU PAQR3	PGR CYP19A1 ABHD2 SIGMR1 REL	hsa00830 Retinol metabolism - Homo sapiens (human) (2) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (2) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2	spleen skin lung Mattoni head cancers ear Zymbals gland	stomach clitoral gland lung	**liver** thyroid gland vascular system	**liver** vascular system **ovary** urinary bladder	liver Neoplasm
2,4,6-Tinitro-1,3,5-dimethyl-1-tert-butylbenzene	81-15-2					Mouse	Male	B6C3F1	Diet	80	90	Positive	Harderian gland	Adenoma									
2,4,6-Tri-tert-butylphenol	732-26-3	C1=C(C)=C(C=C1C)C(C)(C)C)C(C)(C)C)C(C)(C)C	급성 독성(경구) - 구분4 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 25, 27, **29**, **30**, 34, 46, 52, 53, 57, 58, 60, 61, 62, 67, 112, 132, 133, 137, 148, 152, **165**, **167**, **200**	Genotoxicity Data: predicted to be non-genotoxic	Rat	Female	Wistar	Diet	52	52	Negative	Liver	Multiple tumour types	-					stomach Mattoni head cancers	stomach	lung stomach **liver** kidney thyroid gland	pituitary gland thyroid gland **ovary**	-
2,4,6-Tri-tert-butylphenol	732-26-3					Rat	Female	Wistar	Diet	78	78	Negative	Liver	Multiple tumour types									
2,4,6-Tri-tert-butylphenol	732-26-3					Rat	Female	Wistar	Diet	104	104	Negative	Liver	Multiple tumour types									
2,4,6-Tri-tert-butylphenol	732-26-3					Rat	Male	Wistar	Diet	52	52	Negative	Liver	Multiple tumour types									
2,4,6-Tri-tert-butylphenol	732-26-3					Rat	Male	Wistar	Diet	78	78	Negative	Liver	Multiple tumour types									
2,4,6-Tri-tert-butylphenol	732-26-3					Rat	Male	Wistar	Diet	104	104	Negative	Liver	Multiple tumour types									
2,4,7-Trinitrofluorenone	129-79-3	C1=C(C)=C(C)=C1)C(C)=C(C=C(C=C(C)[N+](=O)[O-])=O)=O)[N+](=O)[O-])=O)[N+](=O)[O-])=O	생식세포 변이원성 - 구분1B 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1		-	Mouse	Female	B6C3F1	Diet	93 d	91 d	Not specified			-				kidney liver ear Zymbals gland skin urinary bladder large intestine stomach spleen	ear Zymbals gland mammary gland liver urinary bladder clitoral gland **uterus** lung	thyroid gland urinary bladder vascular system liver kidney	vascular system liver hematopoietic system **ovary** urinary bladder stomach	-
2,4-D	94-75-7	OC(C)COC1=C(C=C(C=C1)Cl)CC(=O)O	급성 독성(경구) - 구분4 급성 독성(피부) - 구분4 심한 눈 손상성/눈 자극성 - 구분1 피부 과민성 - 구분1A/1B **발암성 - 구분2** 특정표적장기 독성(반복 노출) - 구분2 급성 수생환경 유해성 - 구분1	27, 34, 36, 46, 57, 58, 68, 72, 131, 162	Carcinogenicity data available: EPA OPP Group D Not Classifiable as to Human Carcinogenicity Genotoxicity Data: clastogenic	Mouse	Female	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma	APAF1 CD6b IL1B IL1B ITGB1	CYP11A1 MYBL1 FABP4 MRAP4 TCR1	ITL REL CYP4A11 GCLC NBYH2	hsa05164 Influenza A - Homo sapiens (human) (3) hsa1021 K02091 CDK6; cyclin dependent kinase 6 hsa3553 K04519 IL1B; interleukin 1 beta hsa3606 K05482 IL18; interleukin 18 hsa05144 Malaria - Homo sapiens (human) (2) hsa3553 K04519 IL1B; interleukin 1 beta hsa3606 K05482 IL18; interleukin 18 hsa05152 Tuberculosis - Homo sapiens (human) (2) hsa3553 K04519 IL1B; interleukin 1 beta hsa3606 K05482 IL18; interleukin 18	hematopoietic system thyroid gland	-	kidney liver vascular system	-	Colonic Neoplasm Lymphoma, Non-Hodgkin prostatic Neoplasm
2,4-D	94-75-7					Mouse	Male	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-D	94-75-7					Mouse	Female	B6C3F1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-D	94-75-7					Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Adenoma- hepatocellular									
2,4-D isooctyl ester	25168-26-7	C1=C(C)=CC=C1OC(C)(O)CCCCCC(C)C)C(C)	-		-	Mouse	Female	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma	-				hematopoietic system	-	liver	liver hematopoietic system	-
2,4-D isooctyl ester	25168-26-7					Mouse	Male	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-D isooctyl ester	25168-26-7					Mouse	Female	B6C3F1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-D isooctyl ester	25168-26-7					Mouse	Male	B6C3F1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-D n-butyl ester	94-80-4	C=1(C=C(C=CC=1)OCC(=O)OCCCC(C)C)Cl	급성 독성(경구) - 구분4 생식독성 - 구분1A 특정표적장기 독성(반복 노출) - 구분2 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	**29**, **30**, 52, 53, 67, 112, **165**, **167**, **200**	-	Mouse	Female	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma	CNP	CYP11A1 LAMP3 AIRN72 FABP4 MRAP4	ITL REL CYP4A11 GCLC GATA1		hematopoietic system	-	liver vascular system kidney	liver	-
2,4-D n-butyl ester	94-80-4					Mouse	Male	B6AKF1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-D n-butyl ester	94-80-4					Mouse	Female	B6C3F1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-D n-butyl ester	94-80-4					Mouse	Male	B6C3F1	Gavage (pmewearing) than diet	76	76	Negative	Liver	Hepatoma									
2,4-Diaminoanisole sulphate	39156-41-7	C1=C(C=C(C=C1)N)NNOC.OS(O)(=O)=O	생식세포 변이원성 - 구분2 **발암성 - 구분1B**	7, 14, 15, 21, 22, 25, 27, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 132, 133, 135, 150, 152, 163, **165**, **167**, **187**, **200**, 214, 217, 232, 238	Cancer slope factor: 3.7e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: non-clastogenic	Mouse	Female	B6C3F1	Diet	78	96	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-					-	-	-	-	-
2,4-Diaminoanisole sulphate	39156-41-7					Mouse	Male	B6C3F1	Diet	78	96	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2,4-Diaminoanisole sulphate	39156-41-7					Rat	Female	Fischer 344	Diet	83	86	Positive	Clitoral gland	Carcinoma- squamous cellsebaceous									
2,4-Diaminoanisole sulphate	39156-41-7					Rat	Female	Fischer 344	Diet	78	107	Positive	Clitoral gland	Adenoma	Carcinoma	Carcinomasquamous cell	Cytadenoma	Papillomasquamous cell									
2,4-Diaminoanisole sulphate	39156-41-7					Rat	Male	Fischer 344	Diet	78	107	Positive		Ear	Carcinoma- squamous cell	Ear canal	Adenocarcinoma - sebaceous	Carcinoma - squamous cell	Preputial gland	Adenoma	Adenoma- papillary	Carcinoma	Cytadenoma	Skin	Adenocarcinoma- sebaceous	Carcinomabasal cell	Thyroid gland	Adenocarcinoma	Adenocarcinoma- papillary	Carcinoma - follicular cell	Cytadenocarcinomapapillary	Zymbal's gland	Adenocarcinoma- sebaceous									
2,4-Diaminoanisole sulphate	39156-41-7					Rat	Male	Fischer 344/DuCrl	Diet	52	52	Not specified	Liver	Multiple tumour types									
2,4-Diaminophenol dihydrochloride	137-09-7	C1=C(C=C(C(=C1)O)N)N.Cl.Cl	경성 독성(경구) : 구분2 장기 또는 순환계를 위한 유독성 : 구분2A(오래) 흡흡기 과민성 : 구분1(1A/1B) 피부 과민성 : 구분1(1A/1B)	19, 21, 23, 29, 30, 41, 52, 53, 57, 61, 62, 111, 112, 117, 131, 132 **143**, **167**, 187, **200**, 207, 210	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-					urinary bladder ear Zymbals gland kidney spleen liver thyroid gland skin	urinary bladder thyroid gland ear Zymbals gland hematopoietic system **uterus** clitoral gland liver stomach lung	thyroid gland urinary bladder kidney liver vascular system	thyroid gland liver urinary bladder vascular system **ovary** hematopoietic system pituitary gland	-
2,4-Diaminophenol dihydrochloride	137-09-7					Mouse	Male	B6C3F1	Gavage	103	104	Positive	Kidney	Adenoma- tubular									
2,4-Diaminophenol dihydrochloride	137-09-7					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Diaminophenol dihydrochloride	137-09-7					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Diaminotoluene	95-80-7	C=1(C=C(N)C=CC=1C)N	경성 독성(경구) : 구분2 경성 독성(경피) : 구분4 장기 또는 순환계를 위한 유독성 : 구분2(A/B) 피부 과민성 : 구분1(1A/1B) 생식독성 : 구분1B 발암성 : 구분2 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분2	21, 29, **30**, 32, 34, 41, 46, 52, 53, 57, 58, 60, 61, 67, 112, 118, 132, 143, **167**, **200**, 210	Cancer slope factor: 0.0011 ug/m3-1 (carcinogenicity: oral) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	101	101	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	TK1 AnkB BTG2 **CYP1A2** CYP1A1	DNAH2 CCR6 AMH2 TEP1 WIPD	HTATIP2 SOD3 TNNB2 RCL1IN1 CYTIP	Hsa04934 Cushing syndrome - Homo sapiens (human) (2) hsa:1026 KO6625 CDKN1A; cyclin-dependent kinase inhibitor 1A hsa:196 K09363 AHR; aryl hydrocarbon receptor hsa05202 Transcriptional misregulation in cancer - Homo sapiens (human) (1) hsa:1026 K06625 CDKN1A; cyclin-dependent kinase inhibitor 1A hsa05226 Gastric cancer - Homo sapiens (human) (1) hsa:1026 K06625 CDKN1A; cyclin-dependent kinase inhibitor 1A	spleen liver urinary bladder ear Zymbals gland skin all tumor bearing animals	urinary bladder liver lung ear Zymbals gland thyroid gland clitoral gland **uterus** mammary gland	thyroid gland vascular system urinary bladder liver kidney	liver vascular system thyroid gland urinary bladder hematopoietic system	Breast Neoplasm Mammary Neoplasm, Experimental Liver Neoplasms
2,4-Diaminotoluene	95-80-7					Mouse	Male	B6C3F1	Diet	101	101	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Diaminotoluene	95-80-7					Rat	Female	Fischer 344	Diet	93	103	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Diaminotoluene	95-80-7					Rat	Male	Fischer 344	Diet	91	103	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Diaminotoluene dihydrochloride	636-23-7	C1(=CC(N)=CC=C1C)N.Cl.Cl	-	-	-	Mouse	Female	CD-1 HsMLICR	Diet	77	90	Positive	Liver	Hepatoma	-				spleen liver urinary bladder ear Zymbals gland skin all tumor bearing animals	urinary bladder liver lung ear Zymbals gland thyroid gland clitoral gland **uterus** mammary gland	thyroid gland vascular system urinary bladder liver kidney	liver vascular system thyroid gland urinary bladder hematopoietic system	-
2,4-Diaminotoluene dihydrochloride	636-23-7					Mouse	Male	CD-1 HsMLICR	Diet	77	90	Positive	Liver	Hepatoma									
2,4-Diaminotoluene dihydrochloride	636-23-7					Rat	Male	SD	Diet	84	73	Positive	Liver	Hepatoma									
2,4-Dichlorophenol	120-83-2	C1=C(C=C(C=C1Cl)Cl)O	경성 독성(경피) : 구분3 경성 독성(흡입) 분진/미스트 : 구분3 피부 부식성/피부 자극성 : 구분1(1A/1B/1C) 발암성 : 구분2 만성 수생환경 유해성 : 구분2	8, 11, **29**, **30**, 52, 53, 60, 61, 67, 112, 131, **165**, **167**, 200	Carcinogenicity data available: PPRTV (ORNL): Inadequate for an assessment of carcinogenic potential Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	HSPA5 DDIT3 AR ERS1 XBP1	FABP4 CYP11A1 MAMDC1 PLSCR4 MAPK12	ERCC3 REL SLC22A1 HIVEP1 LRRK2	hsa05012 Parkinson disease - Homo sapiens (human) (2) hsa:1649 K04452 DDIT3; DNA damage inducible transcript 3 hsa:1965 K03237 EIF2S1; eukaryotic translation initiation factor 2 subunit alpha hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa:1649 K04452 DDIT3; DNA damage inducible transcript 3 hsa:1965 K03237 EIF2S1; eukaryotic translation initiation factor 2 subunit alpha hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (2) hsa:1649 K04452 DDIT3; DNA damage inducible transcript 3 hsa:1965 K03237 EIF2S1; eukaryotic translation initiation factor 2 subunit alpha	thyroid gland hematopoietic system kidney stomach urinary bladder nasal cavity	urinary bladder liver stomach	liver kidney vascular system	thyroid gland vascular system liver urinary bladder pituitary gland **ovary**	-
2,4-Dichlorophenol	120-83-2					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Forestomach	Carcinoma- squamous cell | Papilloma- squamous cell									
2,4-Dichlorophenol	120-83-2					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Dichlorophenol	120-83-2					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Dichlorophenol benzenesulphonate	97-16-5	O=S(=O)(OC=1C=CC(=CC=1Cl)C)C2=CC=CC=C2	-	8, 11, 19, 21, 23, 27, **29**, **30**, 34, 46, 41, 52, 53, 57, 58, 60, 61, 67, 72, 107, 111, 112, 117, 131, 150, 163, **165**, **167**, **187**, **200**, 207, 210	-	Mouse	Female	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma	-				vascular system spleen hematopoietic system thyroid gland	vascular system	-	thyroid gland urinary bladder	-
2,4-Dichlorophenol benzenesulphonate	97-16-5					Mouse	Male	B6AKF1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2,4-Dichlorophenol benzenesulphonate	97-16-5					Mouse	Female	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2,4-Dichlorophenol benzenesulphonate	97-16-5					Mouse	Male	B6C3F1	Gavage (pretreating) then diet	76	76	Negative	Liver	Hepatoma									
2,4-Dimethoxyaniline hydrochloride	54150-60-5	C1(=C(C(=CC=C1N)OC)OC.Cl	-	-	-	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				urinary bladder ear Zymbals gland kidney skin stomach hematopoietic system spleen nasal cavity large intestine liver vascular system	urinary bladder ear Zymbals gland hematopoietic system **uterus** stomach clitoral gland nasal cavity kidney thyroid gland	urinary bladder thyroid gland stomach vascular system liver	urinary bladder liver thyroid gland vascular system	-
2,4-Dimethoxyaniline hydrochloride	54150-60-5					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Dimethoxyaniline hydrochloride	54150-60-5					Rat	Female	Fischer 344	Diet	104	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Dimethoxyaniline hydrochloride	54150-60-5					Rat	Male	Fischer 344	Diet	104	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Dimethylaniline hydrochloride	21436-96-4	C1=C(C=C(C=C1C)C)N.Cl	-	21, 41, 57, 131, 150, 210	-	Mouse	Female	CD-1 HsMLICR	Diet	77	90	Positive	Liver	Multiple tumour types	-				spleen liver urinary bladder ear Zymbals gland oral cavity Maltoni head cancers skin all tumor bearing animals	urinary bladder liver lung clitoral gland ear Zymbals gland thyroid gland **uterus** mammary gland	urinary bladder thyroid gland vascular system liver kidney	vascular system liver urinary bladder thyroid gland	-
2,4-Dimethylaniline hydrochloride	21436-96-4					Mouse	Male	CD-1 HsMLICR	Diet	77	90	Negative	Liver	Multiple tumour types									
2,4-Dimethylaniline hydrochloride	21436-96-4					Rat	Male	SD	Diet	77	98	Negative	Liver	Multiple tumour types									
2,4-Dinitrochlorobenzene	97-00-7	C1(=C(C=C(C(=C1)[N+](=O)[O-])=O)[N+](=O)[O-])	경성 독성(경구) : 구분4 경성 독성(경피) : 구분2 피부 부식성/피부 자극성 : 구분2 장기 또는 순환계를 위한 유독성 : 구분2 흡흡기 과민성 : 구분1(1A/1B) 생식세포 변이원성 : 구분2 특정표적장기 독성(1회 노출) : 구분3(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분1 특정표적장기 독성(반복 노출) : 구분1 만성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 14, 19, 23, 25, 27, **29**, **30**, 34, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 132, 133, 153, 163, **165**, **167**, **187**, **200**, 204, 207, 210	Genotoxicity Data: genotoxic	Mouse	Female	CD-1 HsMLICR	Diet	77	94	Negative	Liver	Multiple tumour types	GSTP1 **CYB5** **CYC1B** **ZFR2**	DSE CCR7 CYP11A1 DAS1 PDGFRL	EHHADH MAGE1 AKR1B10 CCR6 SOD3	Hsa05323 Rheumatoid arthritis - Homo sapiens (human) (2) hsa:3576 K10850 CXCL8; C-X-C motif chemokine ligand 8 hsa:942 K05413 CD86; CD86 molecule hsa05202 Transcriptional misregulation in cancer - Homo sapiens (human) (2) hsa:3576 K10850 CXCL8; C-X-C motif chemokine ligand 8 hsa:942 K05413 CD86; CD86 molecule hsa05167 Kaposi sarcoma-associated herpesvirus infection - Homo sapiens (human) (2) hsa:3576 K10850 CXCL8; C-X-C motif chemokine ligand 8 hsa:942 K05413 CD86; CD86 molecule	thyroid gland ear Zymbals gland kidney liver spleen hematopoietic system lung skin	lung liver **uterus** clitoral gland mammary gland hematopoietic system kidney urinary bladder	vascular system liver thyroid gland kidney	liver vascular system urinary bladder thyroid gland hematopoietic system **ovary**	Melanoma
2,4-Dinitrochlorobenzene	97-00-7					Mouse	Male	CD-1 HsMLICR	Diet	77	94	Negative	Liver	Multiple tumour types									
2,4-Dinitrochlorobenzene	97-00-7					Rat	Male	SD	Diet	77	103	Negative	Liver	Multiple tumour types									
2,4-Dinitrophenol	51-28-5	C1(=C(C=C(C(=C1[N+](=O)[O-])=O)[N+](=O)[O-])=O	폭발성 물질 : 등급1.1 경성 독성(경구) : 구분2 경성 독성(경피) : 구분1 경성 독성(흡입) 분진/미스트 : 구분2 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	19, 21, 23, 27, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 67, 72, 111, 112, 117, 122, 123, 131, 150, 162, **165**, **167**, **187**, **200**, 220, 307, 310	Carcinogenicity data available: PPRTV (ORNL): Inadequate for an assessment of carcinogenic potential Genotoxicity Data: predicted to be genotoxic	Mouse	Mixed	C57BL	Diet	73	73	Not specified	Pituitary gland	Adenoma	CYP1A1 APP CYP1A2 EPAS1 KCNH11	CYP11A1 DAS1 DSE CCR6 PDGFRL	MGST1 SOD3 TNNB2 AKR1B10 CYTIP	hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (1) hsa:351 K04520 APP; amyloid beta precursor protein hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa00591 Linoleic acid metabolism - Homo sapiens (human) (1) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2	kidney urinary bladder thyroid gland hematopoietic system ear Zymbals gland skin large intestine stomach spleen liver	hematopoietic system urinary bladder kidney clitoral gland liver **uterus** stomach lung	thyroid gland kidney vascular system liver	**ovary** vascular system liver thyroid gland hematopoietic system pituitary gland	-

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2,4-Dinitrotoluene	121-14-2	[N+](=O)[C-]1C=C([N+](=O)[O-])=CC(C)=C1[C](O)[O-]=O	경口 독성(경구) : 구분2 경口 독성(위장) : 구분1 경皮 독성(흡입 : 증기) : 구분2 피부 과민성 : 구분1(A/1B) 생식세포 변이원성 : 구분2 발암성 : 구분1B 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1(마취계통) 특정표적장기 독성(반복 노출) : 구분2 경口 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	16, 57, 131, 281, 312	Cancer slope factor: 8.8e-05 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	93	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	FAF1 CASP3/CASP8 PPARA PPARG BPTGR4	DSE CYP11A1 CCR7 OAS1 CCR6	SOD3 TXNRD2 EHHADH ITL CYP3F	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa1647 604602 GADD45A; growth arrest and DNA damage inducible alpha hsa5468 608530 PPARG; peroxisome proliferator activated receptor gamma hsa05200 Transcriptional misregulation in cancer - Homo sapiens (human) (2) hsa1647 604602 GADD45A; growth arrest and DNA damage inducible alpha hsa5468 608530 PPARG; peroxisome proliferator activated receptor gamma hsa04932 Non-alcoholic fatty liver disease - Homo sapiens (human) (2) hsa5465 603734 PPARA; peroxisome proliferator activated receptor alpha hsa5468 608530 PPARG; peroxisome proliferator activated receptor gamma	skin spleen liver **kidney** ear Zymbals gland **urinary bladder** lung thyroid gland Maltoni head cancers	liver mammary gland clitoral gland lung **uterus** **urinary bladder** ear Zymbals gland	vascular system thyroid gland **kidney** **urinary bladder** liver	vascular system liver **ovary** **urinary bladder** hematopoietic system stomach	Carcinoma Urinary Bladder Neoplasm Urologic Neoplasm Kidney Neoplasm
2,4-Dinitrotoluene	121-14-2					Mouse	Male	B6C3F1	Diet	78	92	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,4-Dinitrotoluene	121-14-2					Mouse	Female	CD1	Diet	52	52	Not specified	Kidney	Tumour- tubular									
2,4-Dinitrotoluene	121-14-2					Mouse	Female	CD1	Diet	69	104	Not specified	Kidney	Tumour- tubular									
2,4-Dinitrotoluene	121-14-2					Mouse	Male	CD1	Diet	52	52	Not specified	Kidney	Tumour- tubular									
2,6-Dichloro-4-nitroaniline	99-30-9	C1[c:c](C:c(C(=C1N)[N+](=O)[O-])=O)Cl.N	특부 과민성 : 구분1(1A/1B)	8, 11, 14, 19, 21, 23, 25, 29, 30, 32, 34, 36, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 97, 98, 111, 113, 117, 122, 123, 131, 148, 150, 163, 165, 167, 187, 195, 199, 200, 204, 214, 220, 307, 318	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma	AR PPARG ESR1 NFH2 THRA THRB	DSE CCR7 CCR6 OAS1 AMH R2	MGST1 CYP3F SOD3 CCR5 AKR1B10	hsa04919 Thyroid hormone signaling pathway - Homo sapiens (human) (2) hsa2099 608560 ESR1; estrogen receptor 1 hsa7067 603541 THRA; thyroid hormone receptor alpha hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2099 608560 ESR1; estrogen receptor 1 hsa5468 608530 PPARG; peroxisome proliferator activated receptor gamma hsa04961 Endocrine and other factor-regulated calcium reabsorption - Homo sapiens (human) (1) hsa2099 608560 ESR1; estrogen receptor 1	ear Zymbals gland thyroid gland spleen kidney hematopoietic system urinary bladder	**uterus** lung urinary bladder clitoral bladder kidney mammary gland hematopoietic system	vascular system liver thyroid gland urinary bladder	liver vascular system thyroid gland urinary bladder hematopoietic system	-
2,6-Dichloro-4-nitroaniline	99-30-9					Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
2,6-Dichloro-4-nitroaniline	99-30-9					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
2,6-Dichloro-4-nitroaniline	99-30-9					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
2,6-Dichloro-p-phenylenediamine	609-20-1	InChI=1/C6H6Cl2N2/c7-4-1-3(9)2-5(8)6(4)10/h1-2H,9-10H2	경口 독성(경구) : 구분4 경皮 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 8, 11, 19, 21, 23, 25, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 67, 72, 111, 113, 117, 122, 123, 131, 150, 153, 163, 165, 167, 187, 200, 207, 210	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	111	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular	-				ear Zymbals gland spleen thyroid gland all tumor bearing animals	urinary bladder thyroid gland **uterus** lung ear Zymbals gland kidney hematopoietic system liver clitoral gland	liver vascular system urinary bladder thyroid gland	liver thyroid gland urinary bladder vascular system hematopoietic system	-
2,6-Dichloro-p-phenylenediamine	609-20-1					Mouse	Male	B6C3F1	Diet	103	111	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,6-Dichloro-p-phenylenediamine	609-20-1					Rat	Female	Fischer 344	Diet	103	111	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,6-Dichloro-p-phenylenediamine	609-20-1					Rat	Male	Fischer 344	Diet	103	111	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,6-Dimethylaniline	87-62-7	C1=C(C=C(C)=C1C)N.C	경口 독성(경구) : 구분4 경皮 독성(흡입 : 증기) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 발암성 : 구분2 특정표적장기 독성(1회 노출) : 구분3(호흡기 자극) 만성 수생환경 유해성 : 구분2	19, 21, 24, 36, 57, 58, 72, 111, 117, 131, 143, 187, 307	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Male	Fischer 344/Du,Cr	Diet	53	53	Not specified	Nasal cavity	Multiple tumour types	CYP2E1 MPO	DNAJC2 AMH R2 TSF1 CCR6 SREBF2	HTATSF2 BCL2A1 IRT1 PCR SOD3	hsa04726 Serotonin - Homo sapiens (human) (1) hsa2180 601897 ACSL1; acyl-CoA synthetase long chain family member 1 hsa00061 Fatty acid biosynthesis - Homo sapiens (human) (1) hsa2180 601897 ACSL1; acyl-CoA synthetase long chain family member 1 hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa2180 601897 ACSL1; acyl-CoA synthetase long chain family member 1	spleen ear Zymbals gland urinary bladder liver skin thyroid gland kidney Maltoni head cancers oral cavity	urinary bladder ear Zymbals gland clitoral gland liver **uterus** lung thyroid gland mammary gland small intestine kidney	thyroid gland urinary bladder vascular system liver kidney lung	vascular system thyroid gland urinary bladder liver hematopoietic system stomach pituitary gland **ovary**	Urinary Bladder Neoplasm Adenoma Carcinoma Cell Transformation, Neoplastic Nose Neoplasm
2,6-Dinitrotoluene	606-20-2	[N+](=O)[C-]1C=C(N+](=O)[O-])=CC(=C1C)[C](O)[O-]=O	경口 독성(경구) : 구분2 경口 독성(위장) : 구분1 경皮 독성(흡입 : 증기,미스트) : 구분2 피부 과민성 : 구분1(1A/1B) 생식세포 변이원성 : 구분2 발암성 : 구분1B 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분2 특정표적장기 독성(반복 노출) : 구분1 경口 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 14, 60, 281, 312	Cancer slope factor: 0.013 (mg/kg)-1 (carcinogenicity, inhalation) Carcinogenicity data available: PPRTV (ORNL)-Suggestive evidence of carcinogenicity in humans Genotoxicity Data: genotoxic	Rat	Male	Fischer 344	Diet	52	52	Positive	Liver	Adenocarcinoma - hepatocellular	ACACA ACSL1 AUI ALCAM	OAS1 CCR6 DSE FOSFBL CCR7	IGF1R SERPINB8 BCL2A1 EIF2A SOD3	hsa04726 Serotonin - Homo sapiens (human) (1) hsa2180 601897 ACSL1; acyl-CoA synthetase long chain family member 1 hsa00061 Fatty acid biosynthesis - Homo sapiens (human) (1) hsa2180 601897 ACSL1; acyl-CoA synthetase long chain family member 1 hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa2180 601897 ACSL1; acyl-CoA synthetase long chain family member 1	liver spleen skin ear Zymbals gland kidney thyroid gland urinary bladder lung Maltoni head cancers	clitoral gland **uterus** liver mammary gland urinary bladder hematopoietic system lung ear Zymbals gland kidney	thyroid gland vascular system kidney urinary bladder liver stomach	vascular system **ovary** liver urinary bladder stomach thyroid gland hematopoietic system	
2,6-Dinitrotoluene	606-20-2					Rat	Male	Fischer 344	Diet	52	52	Positive	Liver	Carcinoma - hepatocellular									
2,6-Dinitrotoluene	606-20-2					Rat	Male	Fischer 344	Diet	52	52	Negative	Liver	Multiple tumour types									
2,6-Dinitrotoluene	606-20-2					Rat	Male	Fischer 344	Diet	52	52	Negative	Liver	Multiple tumour types									
2,6-Di-t-butyl-4-hydroxytoluene	128-37-0	C1(=C(C=c(C(=C1O)C(C)(C)C)C)C)O	특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 경皮 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 8, 11, 14, 19, 23, 25, 29, 30, 34, 52, 53, 58, 60, 61, 62, 64, 66, 67, 71, 111, 112, 117, 122, 123, 148, 150, 160, 167, 187, 200, 204, 207, 218	Carcinogenicity data available: PPRTV (ORNL)-Suggestive evidence of carcinogenicity in humans Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	96	104	Negative	Liver	Carcinoma - hepatocellular	Tnf FOXM1 CASP3 PPARG AKCA	SEC16A PTPN9 ZFAND5 NOP56 RPS11	CD5 HSPCB ALDOA FOXO1 AMH2	hsa04932 Non-alcoholic fatty liver disease - Homo sapiens (human) (2) hsa5468 608530 PPARG; peroxisome proliferator activated receptor gamma hsa836 602187 CASP3; caspase 3 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (2) hsa5468 608530 PPARG; peroxisome proliferator activated receptor gamma hsa836 602187 CASP3; caspase 3 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa5468 608530 PPARG; peroxisome proliferator activated receptor gamma hsa836 602187 CASP3; caspase 3	stomach Maltoni head cancers oral cavity	stomach oral cavity	lung kidney **thyroid gland** stomach liver	pituitary gland **thyroid gland**	Carcinoma Lung Neoplasm Thyroid Neoplasm Colonic Neoplasm Urinary Bladder Neoplasm
2,6-Di-t-butyl-4-hydroxytoluene	128-37-0					Mouse	Female	B6C3F1	Diet	104	120	Not specified	Liver	Adenoma- hepatocellular									
2,6-Di-t-butyl-4-hydroxytoluene	128-37-0					Mouse	Female	B6C3F1	Diet	107	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,6-Di-t-butyl-4-hydroxytoluene	128-37-0					Mouse	Male	B6C3F1	Diet	96	104	Negative	Liver	Carcinoma - hepatocellular									
2,6-Di-t-butyl-4-hydroxytoluene	128-37-0					Mouse	Male	B6C3F1	Diet	104	120	Positive	Liver	Adenoma- hepatocellular									
2,7-Dichlorodibenzo[illegible]	33857-26-0	O1C3=C(OC2=C1C=c(Cl)=C(Cl)C=c(C)2)C(Cl)=C(C)=C3Cl	-	-	-	Mouse	Female	B6C3F1	Diet	90	91	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	CSK AHR AIPA1	AIRN7 CASP12 CCDC40 ZNF2 GCA	BEL FAM171A1 HSPA12A LIM2 MAFG/CEF3	hsa04904 Cushing syndrome - Homo sapiens (human) (1) hsa196 600653 AHR; aryl hydrocarbon receptor hsa04659 Th17 cell differentiation - Homo sapiens (human) (1) hsa196 600653 AHR; aryl hydrocarbon receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa196 600653 AHR; aryl hydrocarbon receptor	thyroid gland oral cavity kidney liver ear Zymbals gland urinary bladder stomach hematopoietic system	liver lung urinary bladder kidney stomach thyroid gland	liver urinary bladder vascular system stomach peritoneal cavity	thyroid gland liver urinary bladder vascular system stomach	-
2,7-Dichlorodibenzodioxin	33857-26-0					Mouse	Male	B6C3F1	Diet	90	92	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
2,7-Dichlorodibenzodioxin	33857-26-0					Rat	Female	Osborne-Mendel	Diet	110	110	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2,7-Dichlorodibenzodioxin	33857-26-0					Rat	Male	Osborne-Mendel	Diet	110	110	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-(2-Methoxy-4-(methylsulphinyl)phenyl)-1H-imidazo[4,5-c]pyridine	86315-52-8	C=1N(c=C(C=c1N)c=C(C=1N)c=C(C=c(C=C2S(C)=O)OC)N2	-	-	-	Rat	Female	Fischer 344	Diet	104	104	Positive	Adrenal gland medulla	Multiple tumour types	-			-	ear Zymbals gland	urinary bladder	-	-
2-(2-Methoxy-4-(methylsulphinyl)phenyl)-1H-imidazo[4,5-c]pyridine	86315-52-8					Rat	Male	Fischer 344	Diet	104	104	Positive	Adrenal gland medulla	Multiple tumour types									
2-Acetylaminofluorene-9-one	3096-58-2	C1=c(C)=c(C=c1)C=c1(C=a2c=c(C)=c(C=a2C3=O)NC(C)=O	-	-	-	Rat	Female	Buffalo	Diet	86	86	Positive	Ear canal	Carcinoma - squamous cell	-				kidney urinary bladder liver stomach skin	urinary bladder ear Zymbals gland liver mammary gland small intestine	urinary bladder thyroid gland kidney liver nasal cavity	urinary bladder stomach vascular system liver hematopoietic system	-
2-Acetylaminofluorene	53-96-3	C1=c(C)=c(C=c1)C=a2c=c(C)=c(C=a2C3(N)C)=O	생식세포 변이원성 : 구분2 경皮 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	14, 15, 21, 23, 29, 30, 45, 52, 53, 57, 61, 64, 66, 67, 71, 111, 112, 117, 131, 150, 160, 163, 167, 187, 200, 214, 307, 210, 318	Cancer slope factor: 0.0913 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Hamster	Male	Not specified	Diet	32	56	Positive	Liver	Carcinoma - bile duct	TEP53 GSTP1 TAT CDKN1A ABCB1B	HEATR3 ALDH18A1 TBC1D9 SEC16A CYOB5B1	RNFT2 PCR SMPD1 ECT2 CEP72	hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (2) hsa1026 604625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa2950 602700 GSTP1; glutathione S-transferase pi 1 hsa7157 604451 TP53; tumor protein p53 hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa1026 604625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa2950 602700 GSTP1; glutathione S-transferase pi 1 hsa7157 604451 TP53; tumor protein p53 hsa05215 Prostate cancer - Homo sapiens (human) (3) hsa1026 604625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa2950 602700 GSTP1; glutathione S-transferase pi 1 hsa7157 604451 TP53; tumor protein p53	kidney liver skin stomach urinary bladder nasal cavity spleen	ear Zymbals gland liver mammary gland urinary bladder **uterus** lung small intestine nasal cavity	urinary bladder thyroid gland kidney liver	urinary bladder stomach liver **ovary**	Carcinoma, Hepatocellular Cell Transformation, Neoplastic Lung Neoplasm Urinary Bladder Neoplasm Liver Neoplasm, Experimental Acute Myeloblastic
2-Acetylaminofluorene	53-96-3					Hamster	Male	Not specified	Intraperitoneal	24	69	Not specified	Forestomach	Papilloma									
2-Acetylaminofluorene	53-96-3					Mouse	Female	AL/WFC,B6N(W)x A/J(WFC,B6N)	Diet	130	130	Positive	Liver	Adenoma- hepatocellular									
2-Acetylaminofluorene	53-96-3					Mouse	Male	AL/WFC,B6N(W)x A/J(WFC,B6N)F1	Diet	130	130	Positive	Liver	Adenoma- hepatocellular									
2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine hydrochloride	-	C1(=c(C=c(C=c1)C(2=c(N(=C2C)c(N2)N)C)C)	-	-	-	Mouse	Female	CDF1	Diet	82	82	Positive	Multiple sites	Lymphoma	-				-	-	-	-	-
2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine hydrochloride	-					Mouse	Male	CDF1	Diet	82	82	Positive	Multiple sites	Lymphoma									
2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine hydrochloride	-					Rat	Male	Fischer 344	Diet	52	52	Positive	Colon	Multiple tumour types									
2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine hydrochloride	-					Rat	Female	Fischer 344/Du,Cr	Diet	52	52	Positive	Colon	Adenocarcinoma									

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2-Amino-3,4-dimethylimidazo[4,5-f]quinoline	77094-11-2	NC3=NC1=CC(=CC=2CC1=CC=CN=2)C2N3C	발암성 - 구분1B		Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	C57BL/6NCrl	Diet	85	85	Positive	Cancer	Adenocarcinoma	CYP1A2 CYP1A1 **HDAC1** TBPL1	SLC15A1 HNF0 FHIT TRAFPC3 BCAS2	CDKN1A ADIPOQ LIF1 CDK13 CNTN1	hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (2) hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa2065 KEGG: HRAS; HRas proto-oncogene, GTPase hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa2065 KEGG: HRAS; HRas proto-oncogene, GTPase hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa2065 KEGG: HRAS; HRas proto-oncogene, GTPase	skin oral cavity ear Zymbals gland large intestine **liver**	clitoral gland ear Zymbals gland small intestine **liver** oral cavity mammary gland	stomach lung **liver** urinary bladder	**liver** stomach lung	Carcinoma, Hepatocellular Breast Neoplasm Oral Neoplasm **Brain Neoplasms** Carcinoma, Squamous Cell
2-Amino-3,4-dimethylimidazo[4,5-f]quinoline	77094-11-2					Mouse	Female	CDF1	Diet	91	91	Positive	Forestomach	Carcinoma - squamous cell									
2-Amino-3,4-dimethylimidazo[4,5-f]quinoline	77094-11-2					Mouse	Male	CDF1	Diet	91	91	Positive	Forestomach	Carcinoma - squamous cell									
2-Amino-1,8-dimethylimidazo[4,5-f]quinoline	77500-04-0	CC1=CC=3C(C2=C1N(C)=N2)NC(=NC=3)N=3C	생식세포 변이원성 - 구분2 발암성 - 구분1B	-	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	CDF1	Diet	84	84	Positive	Liver	Adenoma - hepatocellular	CYP1A2 **NAT2** CYP1A1 AHR	SLC15A1 HBP0 RNF186 FHIT TRAFPC3	DNMT3A CDK12 LIF1 AHR8	hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (3) hsa10 KEGG: NAT2; N-acetyltransferase 2 hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1545 KEGG: CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa10 KEGG: NAT2; N-acetyltransferase 2 hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1545 KEGG: CYP1B1; cytochrome P450 family 1 subfamily B member 1	skin ear Zymbals gland **liver** oral cavity large intestine	**liver** ear Zymbals gland clitoral gland small intestine mammary gland oral cavity	**liver** stomach **lung**	**liver** **lung** stomach	Carcinoma, Hepatocellular Prostatic Neoplasm Colorectal Neoplasm **Lung Neoplasms** Colonic Neoplasm Carcinoma, Squamous Cell
2-Amino-1,8-dimethylimidazo[4,5-f]quinoline	77500-04-0					Mouse	Male	CDF1	Diet	84	84	Positive	Liver	Adenoma - hepatocellular									
2-Amino-1,8-dimethylimidazo[4,5-f]quinoline	77500-04-0					Rat	Female	Fischer 344/DuCrl	Diet	61	61	Positive	Clitoral gland	Carcinoma - squamous cell									
2-Amino-1,8-dimethylimidazo[4,5-f]quinoline	77500-04-0					Rat	Male	Fischer 344/DuCrl	Diet	61	61	Positive	Liver	Carcinoma - hepatocellular									
2-Amino-1,8-dimethylimidazo[4,5-f]quinoline	77500-04-0					Rat	Male	Fischer 344/DuCrl	Diet	56	56	Positive	Liver	Adenoma - hepatocellular									
2-Amino-3-methyl-9H-pyrido[2,3-b]indole acetate	117831-29-6	CC1=C(N)C2=C(C=CC=C2)N=3C=CC=CC=C2N3N(C)=CO1				Mouse	Female	CDF1	Diet	84	84	Positive	Blood vessel	Sarcoma - haemangioendothelial									
2-Amino-3-methyl-9H-pyrido[2,3-b]indole acetate	117831-29-6					Mouse	Male	CDF1	Diet	72	72	Positive	Blood vessel	Sarcoma - haemangioendothelial									
2-Amino-3-methyl-9H-pyrido[2,3-b]indole acetate	117831-29-6					Rat	Male	Fischer 344/DuCrl	Diet	100	100	Positive	Liver	Carcinoma - hepatocellular									
2-Amino-3-methylimidazo[4,5-f]quinoline hydrochloride	-	C1=CC=N(C2=CC=1C=3C=CC=C2)NC(=N3)NC(C)				Rat	Female	SD	Gavage	31	52	Positive	Liver	Carcinoma - hepatocellular									
2-Amino-4-(p-nitrophenyl)thiazole	2104-08-8	C=2N(SC=C(C=1C=CC(=CC=1)[N+]=O))O=[N+]=2	-	21, 29, 30, 41, 52, 53, 57, 67, 112, 131, 150, 166, 167, 200, 210	-	Mouse	Female	Swiss	Diet	46	66	Positive	Liver	Multiple tumour types	-				spleen urinary bladder	urinary bladder mammary gland kidney hematopoietic system stomach ear Zymbals gland small intestine lung clitoral gland **uterus**	urinary bladder thyroid gland	hematopoietic system stomach urinary bladder	-
2-Amino-4-chlorotoluene	95-79-4	C1=CC=C(C)=C1C(N)Cl	급성 독성(경구) - 구분4 특정표적장기 독성(반복 노출) - 구분1 만성 수생환경 유해성 - 구분2	-	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	91	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular	-				spleen liver urinary bladder thyroid gland kidney ear Zymbals gland	urinary bladder liver lung clitoral gland thyroid gland mammary gland	vascular system liver urinary bladder thyroid gland kidney	vascular system liver thyroid gland urinary bladder	-
2-Amino-4-chlorotoluene	95-79-4					Mouse	Male	B6C3F1	Diet	78	91	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
2-Amino-4-chlorotoluene	95-79-4					Rat	Female	Fischer 344	Diet	78	103	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Amino-4-chlorotoluene	95-79-4					Rat	Male	Fischer 344	Diet	78	103	Not specified	Adrenal gland	Pheochromocytoma									
2-Amino-4-nitrophenol	99-57-0	[N+](=O)[O-]\c1=C\C=1C=C(C=1C=C(C=1)[N+]=O)N=O	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(구와 만성 수생환경 유해성 - 구분2A(구와	21, 41, 57, 61, 131, 150, 210	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				urinary bladder kidney ear Zymbals gland skin thyroid gland spleen liver stomach large intestine	urinary bladder clitoral gland **uterus** hematopoietic system ear Zymbals gland liver stomach lung mammary gland small intestine kidney thyroid gland	thyroid gland kidney urinary bladder vascular system liver	**ovary** vascular system liver thyroid gland urinary bladder hematopoietic system	Kidney Neoplasm
2-Amino-4-nitrophenol	99-57-0					Mouse	Male	B6C3F1	Gavage	103	105	Not specified		Abdominal cavity : Haemangioma Liver : Haemangiosarcoma Lymph node- mesenteric : Haemangiosarcoma Pancreas : Haemangioma Skin- subcutaneous tissue : Haemangioma Spleen : Haemangiosarcoma									
2-Amino-4-nitrophenol	99-57-0					Rat	Female	Fischer 344	Gavage	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Amino-4-nitrophenol	99-57-0					Rat	Male	Fischer 344	Gavage	103	105	Not specified	Kidney- cortex	Adenoma									
2-Amino-6-nitrotoluene	99-55-8	C1=C(C=C(C)=C1[N+](=O)[O-])=O\C\N	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(구와 만성 수생환경 유해성 - 구분2 특정표적장기 독성(1회 노출) - 구분2(호흡기 자극)	8, 10, 11, 21, 22, 32, 34, 41, 57, 58, 60, 131, 150, 210	Carcinogenicity data available: PPRTV (ORNL) - Suggestive evidence of carcinogenic potential Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	96	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				spleen liver urinary bladder kidney ear Zymbals gland skin thyroid gland lung large intestine	liver clitoral gland urinary bladder lung **uterus** mammary gland ear Zymbals gland small intestine	vascular system thyroid gland urinary bladder kidney liver	vascular system liver urinary bladder hematopoietic system thyroid gland **ovary**	-
2-Amino-6-nitrotoluene	99-55-8					Mouse	Male	B6C3F1	Diet	78	95	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Amino-6-nitrotoluene	99-55-8					Rat	Female	Fischer 344	Diet	78	108	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Amino-6-nitrotoluene	99-55-8					Rat	Male	Fischer 344	Diet	78	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Amino-5-nitrophenol	121-88-0	[N+](C1=CC(=C(C=C1C)N)O)[O-]=O	심한 눈 손상성/눈 자극성 - 구분2A(구와 만성 수생환경 유해성 - 구분2	21, 28, 29, 30, 41, 52, 53, 57, 61, 63, 67, 100, 101, 102, 103, 112, 122, 123, 131, 150, 166, 167, 177, 200, 220, 210	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	MMP9	CCR6 CHK1 PDGFRb DNI ITGA3	SOD3 MGST1 CYP3P TIMP3 CCR5	hsa05219 Bladder cancer - Homo sapiens (human) (1) hsa4318 KEGG: MMP9; matrix metallopeptidase 9 hsa05161 Hepatitis B - Homo sapiens (human) (1) hsa4318 KEGG: MMP9; matrix metallopeptidase 9 hsa04657 IL-17 signaling pathway - Homo sapiens (human) (1) hsa4318 KEGG: MMP9; matrix metallopeptidase 9	urinary bladder kidney ear Zymbals gland spleen thyroid gland skin liver large intestine stomach	urinary bladder **uterus** clitoral gland ear Zymbals gland hematopoietic system thyroid gland lung stomach mammary gland liver kidney small intestine thyroid gland	thyroid gland urinary bladder kidney vascular system	**ovary** vascular system liver thyroid gland urinary bladder hematopoietic system	Neoplasm Invasiveness
2-Amino-5-nitrophenol	121-88-0					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Amino-5-nitrophenol	121-88-0					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Amino-5-nitrophenol	121-88-0					Rat	Male	Fischer 344	Gavage	103	104	Positive	Adrenal gland medulla	Pheochromocytoma | Pheochromocytoma- malignant									
2-Amino-9H-pyrido[2,3-b]indole	26148-68-5	C1=C(N=C2C(=C1)C3=CN(C=C3)C=CC=2)N	발암성 - 구분2 특정표적장기 독성(1회 노출) - 구분2	-	Cancer slope factor: 0.00011429 (ug/mb)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	CDF1	Diet	97	97	Positive	Blood vessel	Sarcoma- haemangioendothelial	CYP1A2 SLC22A8 **NAT2** CYP1A1	EVC2 CCNC KIF11 IL1R1 SNA1	EAM111A SAT CYP2E1 ADIPOQ CYTH1	hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa10 KEGG: NAT2; N-acetyltransferase 2 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (1) hsa10 KEGG: NAT2; N-acetyltransferase 2 hsa00232 Caffeine metabolism - Homo sapiens (human) (1) hsa10 KEGG: NAT2; N-acetyltransferase 2	ear Zymbals gland **large intestine** spleen	ear Zymbals gland **small intestine** all tumor bearing animals clitoral gland	vascular system **liver** urinary bladder stomach thyroid gland	**liver** vascular system thyroid gland	Carcinoma, Hepatocellular Neoplasm Intestinal Neoplasm
2-Amino-9H-pyrido[2,3-b]indole	26148-68-5					Mouse	Male	CDF1	Diet	97	97	Positive	Blood vessel	Multiple tumour types									
2-Aminoanthraquinone	117-79-3	C1=2C(C3=O)C(C1=CC=C(C=2N)=O)C=CC=C3)=O	발암성 - 구분1B 특정표적장기 독성(1회 노출) - 구분2 만성 수생환경 유해성 - 구분4	8, 11, 14, 21, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 112, 131, 150, 162, 166, 167, 200, 214, 215, 210	Cancer slope factor: 9.4e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	79	94	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	**ESR1**	CCR6 AMH R2 DNMT3 BGLAP TBP1	ATATAV2 BCL2A1 NGD7 CCR5 CYSP	**hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1)** **hsa2099 KOBESS: ESR1; estrogen receptor 1** **hsa04919 Thyroid hormone signaling pathway - Homo sapiens (human) (1)** **hsa2099 KOBESS: ESR1; estrogen receptor 1** **hsa01522 Endocrine resistance - Homo sapiens (human) (1)** **hsa2099 KOBESS: ESR1; estrogen receptor 1**	urinary bladder **liver** spleen kidney ear Zymbals gland	urinary bladder ear Zymbals gland **liver** **uterus** thyroid gland kidney clitoral gland mammary gland	urinary bladder thyroid gland liver vascular system stomach lung	thyroid gland **liver** urinary bladder vascular system hematopoietic system stomach **ovary** lung	Carcinoma, Hepatocellular Lymphoma
2-Aminoanthraquinone	117-79-3					Mouse	Male	B6C3F1	Diet	79	93	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
2-Aminoanthraquinone	117-79-3					Rat	Female	Fischer 344	Diet	78	109	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Aminoanthraquinone	117-79-3					Rat	Male	Fischer 344	Diet	78	106	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2-Aminodibenzofuran	3693-22-9	C=1(C)=CC=CC=1C3=C(O2)C=CC=C3)N	-	-	-	Mouse	Female	(C57 x B6F1	Diet	52	58	Positive	Liver	Hepatoma- malignant	-				ear Zymbals gland urinary bladder kidney	urinary bladder ear Zymbals gland mammary gland **uterus** liver small intestine thyroid gland lung kidney clitoral gland hematopoietic system	urinary bladder liver thyroid gland vascular system stomach	liver thyroid gland urinary bladder vascular system hematopoietic system stomach	-
2-Aminodibenzofuran	3693-22-9					Mouse	Male	(C57 x B6F1	Diet	52	67	Positive	Liver	Hepatoma- malignant									
2-Benzimidazolethiol	583-39-1	C1(=NC2=CNF)C=CC=C2S	경성 독성(경구) : 구분3 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 만성 수생환경 유해성 : 구분2	21, 28, **29**, **30**, 41, 52, 53, 57, 62, 67, 100, 101, 102, 103, 112, 131, 150, **163**, **165**, 167, 177, **200**, 210	Genotoxicity Data: non-genotoxic	Mouse	**Female**	B6C3F1	Inhalation	97 d	91 d	Not specified			CYP1A1	SLC15A1 HBPD	ABCA1 SCSDL CYP1A2 CCR5	hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (1) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1	thyroid gland stomach spleen	stomach thyroid gland ear Zymbals gland **uterus** urinary bladder kidney	thyroid gland liver urinary bladder vascular system	thyroid gland liver pituitary gland urinary bladder **ovary** vascular system	Cell Transformation, Neoplastic
2-Biphenylamine hydrochloride	2185-92-4	C=1(C)N)=CC=CC=1)C2=CC=CC=C2C)	-	-	-	Mouse	Female	B6C3F1	Diet	103	104	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				ear Zymbals gland spleen urinary bladder thyroid gland	urinary bladder **uterus** clitoris gland ear Zymbals gland hematopoietic system thyroid gland lung liver mammary gland kidney nasal cavity	thyroid gland urinary bladder liver vascular system lung	thyroid gland liver urinary bladder **ovary** lung vascular system stomach hematopoietic system	-
2-Biphenylamine hydrochloride	2185-92-4					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Biphenylamine hydrochloride	2185-92-4					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Biphenylamine hydrochloride	2185-92-4					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Butenoic acid, 3-bromo-4-(4-methoxyphenyl)-4-oxo-, sodium salt	16170-75-5	C1=CC=CC=C1)C(C)=CC(O-)=O)Br=O)OC.[Na+]				Mouse	Female	B6C3F1	Intraperitoneal	104	104	Not specified	Liver	Adenoma- hepatocellular	-				-	-	-	-	-
2-Butenoic acid, 3-bromo-4-(4-methoxyphenyl)-4-oxo-, sodium salt	16170-75-5					Mouse	Male	B6C3F1	Intraperitoneal	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Butenoic acid, 3-bromo-4-(4-methoxyphenyl)-4-oxo-, sodium salt	16170-75-5					Rat	Female	Fischer 344	Intraperitoneal	104	104	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Butenoic acid, 3-bromo-4-(4-methoxyphenyl)-4-oxo-, sodium salt	16170-75-5					Rat	Male	Fischer 344	Intraperitoneal	104	104	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chloro p-phenylenediamine sulphate	61702-44-1	C1=CC(=C(C=C1N)C)N)O)O)=O)=O		7, 8, 11, 19, 21, 23, 25, 27, 29, 30, 34, 36, 41, 43, 46, 52, 53, 57, 58, 60, 61, 62, 67, 72, 107, 111, 112, 117, 122, 123, 131, 148, 150, 152, 162, **163**, **167**, 187, **200**, 201, 210	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	96	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				-	-	-	-	-
2-Chloro p-phenylenediamine sulphate	61702-44-1					Mouse	Male	B6C3F1	Diet	95	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chloro p-phenylenediamine sulphate	61702-44-1					Rat	Female	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chloro p-phenylenediamine sulphate	61702-44-1					Rat	Male	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chloroacetophenone	532-27-4	C1(=CC=CC=C1)C(=O)CCl	경성 독성(경구) : 구분3 경성 독성(경피) : 구분4 피부 부식성/자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분1 피부 과민성 : 구분1(1A/1B) 특정표적장기 독성(1회 노출) : 구분3 특정표적장기 독성(반복 노출) : 구분2	6, 7, 8, 11, 14, 18, 19, 21, 23, 25, **29**, **30**, 34, 36, 37, 41, 43, 46, 51, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 150, 153, 163, **165**, 166, 167, 187, **200**, 204, 207, 210, 318	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Inhalation	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	CALCA CYBSA TAC1 TAC2	BAGAL7S IFI27 CHST15 TEP1 SNAG1B	SAT IGKC SLC14A1 LRP6 FGMDS	hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (1) hsa6863 K05230 TAC1; tachykinin precursor 1	oral cavity kidney nasal cavity ear Zymbals gland stomach Mallotri head cancers spleen	ear Zymbals gland kidney thyroid gland stomach nasal cavity clitoral gland **uterus** oral cavity	stomach kidney lung liver	stomach thyroid gland urinary bladder hematopoietic system lung peritoneal cavity	-
2-Chloroacetophenone	532-27-4					Mouse	Male	B6C3F1	Inhalation	103	106	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chloroacetophenone	532-27-4					Rat	Female	Fischer 344	Inhalation	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chloroacetophenone	532-27-4					Rat	Male	Fischer 344	Inhalation	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chloroaniline	95-51-2	C1=CC=C(C)=C1)C(C)N	경성 독성(경구) : 구분3 경성 독성(경피) : 구분3 경성 독성(흡입) (분진/미스트) : 구분4 심한 눈 손상성/눈 자극성 : 구분2A(개정) 생식세포 변이원성 : 구분2 특정표적장기 독성(반복 노출) : 구분1 경성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	-	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Gavage	93 d	91 d	Not specified			MPO Anlil	AMH1R2 TBP1 MHCSC DSG DNMG2	MGST1 SOD3 CCR5 ABXR1R0 CYTIP		ear Zymbals gland thyroid gland spleen hematopoietic system liver vascular system	liver urinary bladder lung thyroid gland **uterus** mammary gland ear Zymbals gland kidney clitoral gland	vascular system liver urinary bladder thyroid gland	liver thyroid gland urinary bladder vascular system hematopoietic system	-
2-Chlorobenzylidenemalononitrile	2698-41-1	C1=CC=CC(=C1C)C=C(C#N)C#N)	경성 독성(경구) : 구분3 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2	-	Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Inhalation	105	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				-	-	-	-	-
2-Chlorobenzylidenemalononitrile	2698-41-1					Mouse	Male	B6C3F1	Inhalation	105	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chlorobenzylidenemalononitrile	2698-41-1					Rat	Female	Fischer 344	Inhalation	105	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Chlorobenzylidenemalononitrile	2698-41-1					Rat	Male	Fischer 344	Inhalation	105	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
2-Hydrazino-4-(p-aminophenyl)thiazole	26049-71-8	N)N(C=1SC=C)N=1)C=2C=CC)=CC=2)N	-	19, 21, 23, 27, 34, 36, 41, 57, 58, 61, 72, 111, 112, 131, 150, 163, 187, 207, 210	-	Mouse	Female	Swiss	Diet	46	66	Positive	Liver	Multiple tumour types	-				spleen	hematopoietic system mammary gland kidney ear Zymbals gland small intestine urinary bladder **stomach**	urinary bladder thyroid gland	hematopoietic system stomach urinary bladder lung thyroid gland	-
2-Hydrazino-4-(p-aminophenyl)thiazole	26049-71-8					Rat	Female	SD	Diet	46	75	Positive	Liver	Multiple tumour types									
2-Hydrazino-4-(p-nitrophenyl)thiazole	26049-70-7		-	7, 19, 29, 33, 35, **27**, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 61, 67, 72, 111, 112, 117, 122, 123, 131, 150, 152, 163, **165**, **167**, 187, **200**, 207, 210	-	Mouse	Female	Swiss	Diet	46	66	Positive	Liver	Multiple tumour types	-				-	hematopoietic system mammary gland kidney small intestine ear Zymbals gland **stomach**	urinary bladder	hematopoietic system stomach lung urinary bladder	-
2-Hydrazino-4-(p-nitrophenyl)thiazole	26049-70-7					Rat	Female	SD	Diet	45	52	Positive	Liver	Multiple tumour types									
2-Hydrazino-4-(p-nitrophenyl)thiazole	26049-70-7					Rat	Female	SD	Diet	46	75	Positive	Forestomach	Papilloma - squamous cell									
2-Hydrazino-4-phenylthiazole	34176-52-8	C=2)NN)SC=C)C1=CC=CC=C1)N=2	-	14, 19, 21, 23, 27, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 120, 150, 163, **165**, **167**, 187, **200**, 204, 207, 210, 318	-	Rat	Female	SD	Diet	46	66	Not specified	Liver	Multiple tumour types	-				-	hematopoietic system mammary gland kidney small intestine ear Zymbals gland stomach	urinary bladder	hematopoietic system stomach lung urinary bladder	-
2-Hydroxyacetylaminofluorene	53-95-2	N)C(C)=O)O)C3=CC=CC=1C=CC=CC=3)C2=C3	-	-	-	Hamster	Male	Not specified	Diet	32	56	Positive	Forestomach	Multiple tumour types	ABCB16 NAT1 CAT NAT2 SULT2A1	AKR1C3 HEATR3 COL5A2 SEC16A CAPRIN1	BNIP2 ICT2 SAT VAIN TMEM38B	hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa10 K00622 NAT2; N-acetyltransferase 2 hsa847 K03781 CAT; catalase hsa10 K00622 NAT1; N-acetyltransferase 1 hsa00983 Drug metabolism - other enzymes - Homo sapiens (human) (2) hsa10 K00622 NAT2; N-acetyltransferase 2 hsa10 K00622 NAT1; N-acetyltransferase 1 hsa00232 Caffeine metabolism - Homo sapiens (human) (2) hsa10 K00622 NAT2; N-acetyltransferase 2 hsa10 K00622 NAT1; N-acetyltransferase 1	liver skin	liver ear Zymbals gland mammary gland	urinary bladder	urinary bladder liver stomach	**Liver Neoplasm** Carcinoma, Squamous Cell Liver Neoplasm, Experimental Ear Neoplasm
2-Hydroxyacetylaminofluorene	53-95-2					Hamster	Male	Not specified	Intraperitoneal	24	69	Not specified	Forestomach	Papilloma									
2-Hydroxyacetylaminofluorene	53-95-2					Mouse	Female	DDD	Diet	30	76	Positive	Forestomach	Multiple benign types									
2-Hydroxyacetylaminofluorene	53-95-2					Rat	Female	NBR	Diet	64	64	Positive	Liver	Cholangioma									
2-Hydroxyacetylaminofluorene	53-95-2					Rat	Male	NBR	Diet	64	64	Positive	Liver	Cholangioma									
2-Hydroxybenzoic acid	69-72-7	C1=CC=C(C)=C1)C(O)=O)O	경성 독성(경구) : 구분4 심한 눈 손상성/눈 자극성 : 구분2A(개정) 생식독성 : 구분2	19, 23, 111, 117, 187, 307	Genotoxicity Data: genotoxic	Mouse	Female	SKH-1 Hairless	Dermal	1 yr	1 yr	Not specified	Application site	Carcinoma- in situ	Tnf PTGS1 PTGS2 RELA CASP3	SERPINB1 SDC4 TOB1 TGFI SUMO1	PTGR1 AKR1B10 POLR2A PLAGL2 FTL	hsa04625 C-type lectin receptor signaling pathway - Homo sapiens (human) (2) hsa5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa04064 NF-kappa B signaling pathway - Homo sapiens (human) (2) hsa5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa05010 Alzheimer disease - Homo sapiens (human) (2) hsa5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit	urinary bladder kidney stomach	urinary bladder kidney clitoral gland stomach	kidney stomach thyroid gland liver	**ovary** pituitary gland thyroid gland liver stomach	Leukemia, Myeloid, Acute
2-Hydroxybenzoic acid	69-72-7					Mouse	Male	SKH-1 Hairless	Dermal	1 yr	1 yr	Not specified	Application site	Carcinoma- basal cell									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2-Mercaptobenzothiazole	149-30-4	C1(=NC2=CC(S)(C=CC=C2)S	피부 과민성 : 구분1(1A/1B) 발암성 : 구분2 생식 수행한전 유해성 : 구분1 한정 수행한전 유해성 : 구분1	6, 8, 11, 18, 19, 21, 23, 28, 29, 30, 32, 33, 34, 36, 37, 41, 51, 52, 53, 57, 58, 60, 61, 62, 63, 67, 72, 100, 109, 162, 163, 171, 152, 117, 131, 146, 150, 163, 165, 166, 167, 177, 187, 200, 207, 210, 318	Carcinogenicity data available EPA CPPT Group C Possible Human Carcinogen Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	CXCL8 TP53 H2AX AKR1C2 AKR1C3 CXCL14	-	CCR5 GCLC	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa3162 630510 HMOX1; heme oxygenase 1 hsa7173 630421 TPO; thyroid peroxidase hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1646 630089 AKR1C2; aldo-keto reductase family 1 member C2 hsa3162 630510 HMOX1; heme oxygenase 1 hsa04918 Thyroid hormone synthesis - Homo sapiens (human) (1) hsa7173 630421 TPO; thyroid peroxidase	hematopoietic system thyroid gland spleen ear Zymbals gland	thyroid gland uterus ear Zymbals gland urinary bladder	thyroid gland urinary bladder	thyroid gland urinary bladder	Neoplasm Involveness
2-Mercaptobenzothiazole	149-30-4					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2-Mercaptobenzothiazole	149-30-4					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2-Mercaptobenzothiazole	149-30-4					Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular									
2-Methoxy-3-dibenzofuranamine	5824-17-3	C1=C(C)(=CC=C1)C=2C=1C(=C(C=2O)N)NOC	-	19, 21, 23, 29, 30, 41, 46, 52, 53, 57, 67, 111, 112, 117, 131, 150, 165, 167, 187, 200, 207, 310	-	Rat	Female	Fischer 344	Diet	75	75	Positive	Ear canal- external	Carcinoma - squamous cell					urinary bladder kidney ear Zymbals gland	urinary bladder ear Zymbals gland hematopoietic system uterus mammary gland clitoral gland small intestine kidney	urinary bladder thyroid gland liver stomach vascular system	urinary bladder liver thyroid gland vascular system	-
2-Methoxy-3-dibenzofuranamine	5824-17-3					Rat	Male	Fischer 344	Diet	75	75	Positive	Ear canal- external	Carcinoma - squamous cell									
2-Methoxy-3-dibenzofuranamine	5824-17-3					Rat	Female	SD	Diet	75	75	Positive	Ear canal- external	Carcinoma - squamous cell									
2-Methoxy-3-dibenzofuranamine	5824-17-3					Rat	Male	SD	Diet	75	75	Positive	Kidney	Carcinoma - squamous cell									
2-Methoxy-4-nitroaniline	97-52-9	C1=C(C=C(C)(=C1)N(OC)[N+]))[O-])=O	급성 독성(경구) : 구분4 심한 눈 손상성/눈 자극성 : 구분2A(2B) 만성 수생환경 유해성 : 구분2	29, 30, 52, 53, 67, 112, 163, 167, 200	Genotoxicity Data: non-clastogenic	Mouse	Female	B6C3F1/N	Diet	15 d	14 d	Not specified			-				urinary bladder ear Zymbals gland kidney skin hematopoietic system spleen large intestine stomach liver thyroid gland	urinary bladder uterus clitoral gland hematopoietic system ear Zymbals gland kidney stomach mammary gland	thyroid gland urinary bladder vascular system liver	urinary bladder liver vascular system	-
2-Methoxy-4-nitroaniline	97-52-9					Mouse	Male	B6C3F1/N	Diet	15 d	14 d	Not specified											
2-Methoxyaniline hydrochloride	134-29-2	C1=CC=CC(=C1N)OC.Cl	발암성 : 구분1B	8, 11, 21, 28, 41, 46, 57, 60, 63, 100, 105, 152, 163, 171, 150, 177, 210	Cancer slope factor: 3.1e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic	-				urinary bladder ear Zymbals gland kidney hematopoietic system skin spleen large intestine stomach nasal cavity liver vascular system	urinary bladder hematopoietic system ear Zymbals gland uterus clitoral gland kidney nasal cavity stomach thyroid gland mammary gland	urinary bladder thyroid gland vascular system stomach liver	urinary bladder liver thyroid gland vascular system	-
2-Methoxyaniline hydrochloride	134-29-2					Mouse	Male	B6C3F1	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methoxyaniline hydrochloride	134-29-2					Rat	Female	Fischer 344	Diet	93	104	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methoxyaniline hydrochloride	134-29-2					Rat	Male	Fischer 344	Diet	95	104	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methyl-1-nitroanthraquinone	129-15-7	[N+](=O)[O-])c1cc2c(c(c1)C)C(=O)c1ccccc1C(=O)c1ccccc1C2=O	발암성 : 구분2 특정표적장기 독성(반복 노출) : 구분2	19, 21, 23, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 61, 67, 72, 111, 112, 117, 131, 150, 162, 165, 167, 187, 200, 207, 310	Cancer slope factor: 0.0012 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	49	49	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic	-				liver kidney urinary bladder spleen large intestine skin	liver urinary bladder kidney ear Zymbals gland clitoral gland mammary gland lung	vascular system thyroid gland stomach urinary bladder liver kidney	vascular system liver hematopoietic system stomach ovary urinary bladder	-
2-Methyl-1-nitroanthraquinone	129-15-7					Mouse	Male	B6C3F1	Diet	46	46	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methyl-1-nitroanthraquinone	129-15-7					Rat	Female	Fischer 344	Diet	78	109	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methyl-1-nitroanthraquinone	129-15-7					Rat	Male	Fischer 344	Diet	78	109	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methylaniline hydrochloride	636-21-5	C=1(C(C)=CC=CC=1)N.Cl	급성 독성(경구) : 구분4 심한 눈 손상성/눈 자극성 : 구분2A(2B) 발암성 : 구분1A 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분2	21, 29, 30, 41, 52, 53, 57, 67, 152, 131, 150, 165, 167, 200, 210	Cancer slope factor: 3.7e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: inconclusive	Mouse	Female	B6C3F1	Diet	102	102	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular	-				spleen urinary bladder liver ear Zymbals gland kidney skin thyroid gland	urinary bladder liver lung ear Zymbals gland clitoral gland uterus thyroid gland mammary gland	vascular system thyroid gland urinary bladder liver kidney	vascular system liver thyroid gland urinary bladder hematopoietic system ovary	-
2-Methylaniline hydrochloride	636-21-5					Mouse	Male	B6C3F1	Diet	102	102	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methylaniline hydrochloride	636-21-5					Mouse	Female	CD-1 Inb(ICR)	Diet	68	90	Positive	Liver	Multiple tumour types									
2-Methylaniline hydrochloride	636-21-5					Mouse	Male	CD-1 Inb(ICR)	Diet	68	90	Positive	Liver	Multiple tumour types									
2-Methylnaphthalene	91-57-6	C=12C=C(C=CC=1)C=CC=C2)C	급성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분2	-	Carcinogenicity data available: IRIS-Data are inadequate for an assessment of human carcinogenic potential Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Diet	81	81	Not specified	Liver	Adenoma - hepatocellular	AHR CYP1A CYP1A2	CTSD TACR2 DHFR SREBF2 CEBPG	BCL2A1 IRT1 MAP3K8 ZC3H12 CYP2E1		spleen oral cavity Malteni head cancers nasal cavity ear Zymbals gland urinary bladder liver thyroid gland hematopoietic system kidney vascular system	clitoral gland urinary bladder nasal cavity liver oral cavity uterus hematopoietic system	urinary bladder thyroid gland vascular system kidney lung small intestine	urinary bladder vascular system pituitary gland thyroid gland ovary stomach liver perforeal cavity small intestine	-
2-Methylnaphthalene	91-57-6					Mouse	Male	B6C3F1	Diet	81	81	Not specified	Liver	Adenoma - hepatocellular									
2-Methylphenol	95-48-7	C1(=C(C)C=CC=C1)O	급성 독성(경구) : 구분3 급성 독성(경피) : 구분4 피부 부식성/피부 자극성 : 구분1A/1B/1C 심한 눈 손상성/눈 자극성 : 구분1 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극)	27, 57, 61, 148	Carcinogenicity data available: IRIS-C (Possible human carcinogen) Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	92 d	91 d	Not specified			PTGS2 AKT1 JUN JUND PPARG PRKCA	RNFT2 WDR67 CTSD SEC16A ZFAND5	FTL POR ABHD2 ERO1C4 PLA2G6		urinary bladder stomach spleen kidney Malteni head cancers nasal cavity oral cavity vascular system liver hematopoietic system	urinary bladder stomach kidney clitoral gland hematopoietic system nasal cavity liver	kidney thyroid gland stomach vascular system urinary bladder liver	ovary thyroid gland pituitary gland vascular system urinary bladder hematopoietic system liver stomach	-
2-Methyl-p-hydroquinone	95-71-6	C=1(C)=CC=C(C=1)O)OC	피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 급성 수생환경 유해성 : 구분1	7, 19, 21, 23, 25, 29, 30, 41, 52, 53, 57, 61, 67, 111, 112, 117, 122, 123, 131, 150, 152, 163, 167, 187, 200, 207, 210	Genotoxicity Data: predicted to be genotoxic	Rat	Male	Fischer 344/DuCr	Diet	51	52	Not specified	Forestomach	Multiple tumour types	-				urinary bladder stomach kidney nasal cavity spleen Malteni head cancers	stomach urinary bladder hematopoietic system	kidney stomach thyroid gland liver	ovary thyroid gland pituitary gland vascular system stomach liver urinary bladder hematopoietic system	-
2-Methyl-p-phenylenediamine sulphate	6369-59-1	C=1(C)=CC=C(C=1)N(N)C.O5O(3)(=O)=O	급성 독성(경구) : 구분3 급성 독성(경피) : 구분4 급성 독성(흡입 분진/미스트) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 피부 과민성 : 구분1(1A/1B) 만성 수생환경 유해성 : 구분2	-	Carcinogenicity data available: PPRTV (ORNL)-Suggestive evidence of carcinogenic potential Genotoxicity Data: inconclusive	Mouse	Female	B6C3F1	Diet	78	94	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic	-				-	-	-	-	-
2-Methyl-p-phenylenediamine sulphate	6369-59-1					Mouse	Male	B6C3F1	Diet	78	94	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methyl-p-phenylenediamine sulphate	6369-59-1					Rat	Female	Fischer 344	Diet	78	107	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methyl-p-phenylenediamine sulphate	6369-59-1					Rat	Male	Fischer 344	Diet	78	106	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule - neoplastic									
2-Methyl-propanoic acid, 4-(2-(methylamino)ethyl)-1,2-phenylene ester, hydrochloride	75011-65-0	C(=O)(C=C)O(C=C1O(C(=O)C(C)C)OC(C)C)=O)CCNC.Cl	-	-	-	Rat	Female	SD	Gavage	104	104	Negative	Adrenal gland	Adenoma - cortical	-				stomach	-	stomach lung	lung hematopoietic system	-
2-Methyl-propanoic acid, 4-(2-(methylamino)ethyl)-1,2-phenylene ester, hydrochloride	75011-65-0					Rat	Male	SD	Gavage	104	104	Negative	Adrenal gland	Adenoma - cortical									
2-Naphthylamine	91-59-8	C=12C=C(N)C=CC=1C=CC=C2	급성 독성(경구) : 구분4 발암성 : 구분1A 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	14, 21, 28, 29, 30, 34, 41, 52, 53, 57, 58, 61, 63, 64, 66, 67, 71, 100, 105, 150, 155, 152, 131, 150, 165, 167, 200, 214, 310, 318	Cancer slope factor: 0.0855 ug/m3-1 (carcinogenicity, oral) Carcinogenicity data available: NTP IEDC-Known Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	BALB/c	Diet	40	55	Positive	Liver	Adenoma	-				spleen ear Zymbals gland thyroid gland liver urinary bladder	urinary bladder ear Zymbals gland uterus thyroid gland hematopoietic system clitoral gland liver mammary gland lung kidney nasal cavity	urinary bladder thyroid gland liver vascular system lung	urinary bladder thyroid gland liver vascular system hematopoietic system stomach ovary lung	Urinary Bladder Neoplasm
2-Naphthylamine	91-59-8					Mouse	Mixed	C3A	Gavage	79	79	Positive	Liver	Hepatoma									
2-Naphthylamine	91-59-8					Mouse	Male	ICR/Ha	Diet	52	52	Positive	Liver	Hepatoma									
2-Naphthylamine	91-59-8					Rat	Mixed	Albino	Diet	104	104	Not specified	Urinary bladder	Papilloma									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2-Naphthylamine-1-sulphonic acid	81-16-3	O=S(=O)([C-2]C1=CC=CC=C1C=CC=2N)O	특정표적장기 독성(1회 노출) : 구분3(호흡기 자극) 변이 유발성은 유해성 : 구분4 **발암성 : 구분1A** 특정표적장기 독성(반복 노출) : 구분2	21, 29, 30, 41, 52, 53, 57, 61, 67, 112, 131, 150, 165, **167**, **200**, 210	Genotoxicity Data: predicted to be clastogenic	Mouse	Female	BALB/c(albino)	Diet	66	140	Negative	Liver	Multiple tumour types	-				-	thyroid gland urinary bladder	urinary bladder thyroid gland	-
2-Naphthylamine-1-sulphonic acid	81-16-3					Mouse	Male	BALB/c(albino)	Diet	66	140	Negative	Liver	Multiple tumour types									
2-Nitroaniline	91-23-6	C1=CC=C(C(=C1)[O][N+]))O-])=O	경성 독성(흡구) : 구분4 생식세포 변이원성 : 구분2 **발암성 : 구분1B** 특정표적장기 독성(반복 노출) : 구분2	8, 11, 60	Carcinogenicity data available: CaEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	104	Positive	Liver	Adenoma - hepatocellular	CYP1A1 **CYP2E1** CYP2B6 CYP1A2 ALDH1A1	OAS1 ACOT2 FDGFRL BGLAP CCR6	SOD3 TNNRD2 MGST1 CCR5 SERPINB8	hsa00982: Drug metabolism - cytochrome P450 - Homo sapiens (human) (3) hsa:1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1555 KO7709 CYP2B6; cytochrome P450 family 2 subfamily B member 6 hsa:1571 KO7415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa01100: Metabolic pathways - Homo sapiens (human) (2) hsa:1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1555 KO7709 CYP2B6; cytochrome P450 family 2 subfamily B member 6 hsa:1571 KO7415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa00980: Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa:1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1555 KO7709 CYP2B6; cytochrome P450 family 2 subfamily B member 6 hsa:1571 KO7415 CYP2E1; cytochrome P450 family 2 subfamily E member 1	urinary bladder kidney ear Zymbals gland hematopoietic system skin large intestine stomach spleen nasal cavity thyroid gland liver vascular system	urinary bladder hematopoietic system kidney **uterus** clitoral gland stomach ear Zymbals gland nasal cavity mammary gland	urinary bladder thyroid gland vascular system stomach liver kidney	urinary bladder **ovary** liver vascular system	Urinary Bladder Neoplasm
2-Nitroaniline	91-23-6					Mouse	Male	B6C3F1	Diet	103	104	Positive	Liver	Adenoma - hepatocellular									
2-Nitroaniline	91-23-6					Rat	Female	Fischer 344	Diet	27	104	Positive	Lobe	Adenomatous polyp									
2-Nitroaniline	91-23-6					Rat	Female	Fischer 344	Diet	103	104	Positive	Forestomach	Carcinoma - squamous cell | Papilloma - squamous cell									
2-Nitroaniline	91-23-6					Rat	Male	Fischer 344	Diet	27	104	Positive	Caecum	Adenomatous polyp									
2-Nitroaniline	91-23-6					Rat	Male	Fischer 344	Diet	103	104	Positive	Adrenal gland medulla	Pheochromocytoma|benign | Pheochromocytoma - benign - bilateral									
2-Nitrochlorobenzene	88-73-3	[N+]([O-])(c1cC(c1C=CC=C1Cl)=O)	경성 독성(흡구) : 구분2 경성 독성(경피) : 구분3 경성 독성(흡입) 분진/미스트 : 구분4 피부 과민성 : 구분1(1A/1B) **발암성 : 구분2** 특정표적장기 독성(반복 노출) : 구분1 만성 수생환경 유해성 : 구분3	-	Carcinogenicity data available: PPRTV (ORNL)-Likely to be carcinogenic to humans Genotoxicity Data: genotoxic	Mouse	Female	CD-1 Hsd(ICR)	Diet	77	98	Positive	Liver	Hepatoma	-				thyroid gland ear Zymbals gland kidney spleen hematopoietic system liver lung vascular system urinary bladder	kidney lung **uterus** hematopoietic system liver urinary bladder clitoral gland mammary gland	vascular system liver thyroid gland kidney urinary bladder	liver vascular system **ovary** urinary bladder thyroid gland hematopoietic system stomach	-
2-Nitrochlorobenzene	88-73-3					Mouse	Male	CD-1 Hsd(ICR)	Diet	73	81	Positive	Liver	Hepatoma									
2-Nitrochlorobenzene	88-73-3					Rat	Male	SD	Diet	77	98	Not specified	Liver	Multiple tumour types									
2-Nitrofluorene	607-57-8	C=1C=CC=C2C=4C3=C(C=CC=C3)[N+]([O-])=O)C=C2	생식세포 변이원성 : 구분2 **발암성 : 구분2**	21, 29, 30, 41, 52, 53, 57, 61, 67, 112, 131, 150, 165, **167**, **200**, 210	Cancer slope factor: 1.1e-05 (ug/m3)-1 (carcinogenicity: inhalation) Carcinogenicity data available: CaEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Male	Wistar	Diet	47	104	Positive	Forestomach	Carcinoma - squamous cell	BAX CCNE1 CYP1A1 CAV1 MYH14 MGMT MBD1	CCR6 DSG FDGFRL OAS1 CCR7	CCR5 KRT34 SERPINB8 BCL2A1 SHARP1	hsa04115: p53 signaling pathway - Homo sapiens (human) (2) hsa:1026 KO6625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa:4193 KO6643 MDM2; MDM2 proto-oncogene hsa:900 KO1145 CCNG1; cyclin G1 hsa05206: MicroRNAs in cancer - Homo sapiens (human) (3) hsa:1026 KO6625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa:4193 KO6643 MDM2; MDM2 proto-oncogene hsa:900 KO1145 CCNG1; cyclin G1 hsa05202: Transcriptional misregulation in cancer - Homo sapiens (human) (2) hsa:1026 KO6625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa:4193 KO6643 MDM2; MDM2 proto-oncogene	kidney **liver** ear Zymbals gland skin stomach spleen thyroid gland lung	ear Zymbals gland **liver** mammary gland **uterus** clitoral gland hematopoietic system lung urinary bladder	urinary bladder thyroid gland vascular system **liver** lung kidney	**ovary** urinary bladder stomach **liver** vascular system hematopoietic system	**Liver Neoplasm**
2-Nitro-p-phenylenediamine	5307-14-2	C1=1C=CC=C(C=C1C(=N+]))O-])=O)NNN	경성 독성(흡구) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A 경성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	21, 29, 30, 41, 52, 53, 57, 61, 67, 112, 131, 150, 165, **167**, **200**, 210	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	90	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	ABCB1B ACMSD ACSL3 AIN AKR7A3 ALDH1A1 ALDH1A4	CCR6 DNAJB2 AMHR2 DSG CCR7	MGST1 AKR1B10 SOD3 FBCH PTGR1	hsa01100: Metabolic pathways - Homo sapiens (human) (3) hsa:130013 KO3392 ACMSD; aminocarboxymuconate semialdehyde decarboxylase hsa:216 KO7249 ALDH1A1; aldehyde dehydrogenase 1 family member A1 hsa:2181 KO1897 ACSL3; acyl-CoA synthetase long chain family member 3 hsa00830: Retinol metabolism - Homo sapiens (human) (1) hsa:216 KO7249 ALDH1A1; aldehyde dehydrogenase 1 family member A1 hsa00071: Fatty acid degradation - Homo sapiens (human) (1) hsa:2181 KO1897 ACSL3; acyl-CoA synthetase long chain family member 3	spleen ear Zymbals gland urinary bladder thyroid gland skin	urinary bladder **uterus** lung clitoral gland ear Zymbals gland hematopoietic system thyroid gland liver mammary gland stomach kidney	thyroid gland urinary bladder vascular system kidney	liver vascular system thyroid gland urinary bladder **ovary** hematopoietic system stomach	-
2-Nitro-p-phenylenediamine	5307-14-2					Mouse	Male	B6C3F1	Diet	78	90	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
2-Nitro-p-phenylenediamine	5307-14-2					Rat	Female	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
2-Nitro-p-phenylenediamine	5307-14-2					Rat	Male	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
2-Nitrostolueme	611-23-4	N(C=1C(C)=CC=CC=1)=O	-	29, 30, 52, 53, 61, 67, 112, **165**, **167**, **200**	Genotoxicity Data: predicted to be genotoxic	Rat	Male	Fischer 344	Diet	72	93	Positive	Liver	Hepatoma	-				spleen urinary bladder liver Maltoni head cancers skin oral cavity ear Zymbals gland lung	urinary bladder clitoral gland lung	vascular system urinary bladder liver thyroid gland kidney	vascular system urinary bladder thyroid gland	-
2-Nitrotoluene	88-72-2	C1=CC=C(C(=C1)[N+]))O-])=O)C	경성 독성(흡구) : 구분4 생식세포 변이원성 : 구분1B 발암성 : 구분1B 생식독성 : 구분2 만성 수생환경 유해성 : 구분2	7, 11, 21, 25, 27, 191, 612, 122, 123, 152, 187, 207	Carcinogenicity data available: CaEPA-Likely Human Carcinogen Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	104	104	Positive	Caecum	Carcinoma	CDKN1A FHIT WWOX ACTG2 ACTN1 ACTN4	OAS1 DSG CCR6 FDGFRL CCR7	KRT34 BCL2A1 SERPINB8 SOD3 EVX2A	hsa04510: focal adhesion - Homo sapiens (human) (1) hsa:87 K05699 ACTN1; actinin alpha 1 hsa04810: Regulation of actin cytoskeleton - Homo sapiens (human) (1) hsa:87 K05699 ACTN1; actinin alpha 1 hsa05222: Small cell lung cancer - Homo sapiens (human) (1) hsa:2273 K01522 FHIT; fragile histidine triad diadenosine triphosphatase	spleen liver skin kidney urinary bladder ear Zymbals gland **lung** thyroid gland Maltoni head cancers oral cavity large intestine hematopoietic system	liver mammary gland clitoral gland urinary bladder **lung** **uterus** hematopoietic system ear Zymbals gland kidney	vascular system thyroid gland kidney urinary bladder stomach liver	vascular system **ovary** liver urinary bladder stomach hematopoietic system thyroid gland	**Lung Neoplasm** Mesothelioma Carcinoma, Hepatocellular Breast Neoplasm Hemangiosarcoma
2-Nitrotoluene	88-72-2					Mouse	Male	B6C3F1	Diet	95	104	Positive	Caecum	Carcinoma									
2-Nitrotoluene	88-72-2					Rat	Female	Fischer 344	Diet	104	104	Positive	Liver	Adenoma - hepatocellular									
2-Nitrotoluene	88-72-2					Rat	Male	Fischer 344	Diet	14	104	Positive	Bone	Osteosarcoma									
2-Nitrotoluene	88-72-2					Rat	Male	Fischer 344	Diet	103	104	Positive	Adrenal gland medulla	Pheochromocytoma|benign									
2-Phenylphenol	90-43-7	C1=CC=C(C(=C1)C)c2c=CC=CC=C2)O	피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 경성 수생환경 유해성 : 구분1	7, 8, 11, 25, 28, 29, 30, 52, 53, 60, 61, 63, 67, 91, 93, 94, 96, 100, 101, 102, 103, 112, 122, 123, 148, 150, 153, 165, 167, 177, 187, 200, 220	Carcinogenicity data available: CaEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	**AR** **ESR1** **HRAS** **TP53** CAD	CTSD HEATR3 IRH1 COG5 DNAAF2	BACSGAP1 TBP1L2 GGH STMN1 CKN1	hsa05224: Breast cancer - Homo sapiens (human) (3) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:3265 K08833 HRAS; HRas proto-oncogene, GTPase hsa:7157 K04451 TP53; tumor protein p53 hsa04919: Thyroid hormone signaling pathway - Homo sapiens (human) (3) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:3265 K08833 HRAS; HRas proto-oncogene, GTPase hsa:7157 K04451 TP53; tumor protein p53 hsa05205: Proteoglycans in cancer - Homo sapiens (human) (3) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:3265 K08833 HRAS; HRas proto-oncogene, GTPase hsa:7157 K04451 TP53; tumor protein p53	**urinary bladder** kidney stomach nasal cavity large intestine hematopoietic system liver thyroid gland vascular system	**urinary bladder** hematopoietic system kidney nasal cavity liver stomach small intestine clitoral gland **uterus** thyroid gland	thyroid gland kidney stomach liver **urinary bladder** vascular system lung	**ovary** thyroid gland pituitary gland stomach vascular system **urinary bladder** liver hematopoietic system	Urinary Bladder Neoplasm
2-Phenylphenol	90-43-7					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2-Phenylphenol	90-43-7					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2-Phenylphenol	90-43-7					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
2-Phenylphenol	90-43-7					Mouse	Male	B6C3F1	Diet	52	52	Negative	Kidney	Multiple tumour types									
2-Phenylphenol	90-43-7					Rat	Male	Fischer 344/DuCrl	Diet	91	91	Positive	Not applicable	Mortality									
2-Phenylphenol	90-43-7					Rat	Male	Fischer 344/DuCrl	Diet	104	104	Negative	Urinary bladder	Multiple tumour types									
2-Phenylpropene	98-83-9	C(C1=CC=CC=C1)=C)C	인화성 액체 : 구분2 **발암성 : 구분2** 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 흡인 유해성 : 구분1 만성 수생환경 유해성 : 구분2	-	Carcinogenicity data available: CaEPA-Likely Human Carcinogen Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1/N	Inhalation	96 d	91 d	Not specified	**Ovary**	Teratoma - benign	**EGR1** PGR	IFI27 EAM12B WNT7A RNF72 CCBP2	IL4R CCR5B NDUFB2 ATP7I CKS1B		kidney oral cavity spleen nasal cavity Maltoni head cancers hematopoietic system stomach lung thyroid gland	**uterus** nasal cavity liver oral cavity thyroid gland	thyroid gland lung stomach vascular system urinary bladder	**ovary** thyroid gland pituitary gland stomach urinary bladder lung peritoneal cavity	-
2-Phenylpropene	98-83-9					Mouse	Female	B6C3F1/N	Inhalation	732 d	730 d	Not specified	Adrenal gland cortex	Adenoma									
2-Phenylpropene	98-83-9					Mouse	Male	B6C3F1/N	Inhalation	91 d	91 d	Not specified											
2-tert-Butylhydroquinone	1948-33-0	C1=1C(O)=C(C=C1O)(C)(C)C)O	경성 독성(흡구) : 구분4 피부 과민성 : 구분1(1A/1B) 경성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 8, 11, 14, 19, 21, 23, 25, 27, 28, 29, 30, 34, 36, 49, 52, 53, 57, 58, 60, 61, 63, 64, 66, 67, 71, 72, 100, 105, 108, 109, 111, 112, 117, 122, 123, 131, 148, 150, 152, 162, 165, 167, 177, 187, 200, 214, 217, 218, 219, 218	Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	105	105	Not specified	Harderian gland	Adenoma	NFE2L2 PARP1 NQO1 GPX1 CYP1A1	HTFX RNF72 ZFAND5 ITGB8 GTF3A	NQO1 GCLM PLAGL6 UPP2 ABHD2	hsa01100: Metabolic pathways - Homo sapiens (human) (3) hsa:728 K00515 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:2729 K11204 GCLC; glutamate-cysteine ligase catalytic subunit hsa:2162 K00510 HMOX1; heme oxygenase 1 hsa05418: fluid shear stress and atherosclerosis - Homo sapiens (human) (2) hsa:728 K00515 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:2162 K00510 HMOX1; heme oxygenase 1 hsa05225: Hepatocellular carcinoma - Homo sapiens (human) (2) hsa:728 K00515 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:2162 K00510 HMOX1; heme oxygenase 1	stomach urinary bladder kidney	stomach urinary bladder	stomach kidney thyroid gland **liver** lung	**ovary** pituitary gland thyroid gland	**Liver Neoplasm** Neoplasm
2-tert-Butylhydroquinone	1948-33-0					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
3-(Cyclopentylloxy-N-(3,5-dichloro-4-pyridyl)- 4-methoxybenzamide	144035-83-6	C1(C)CCC1(OC=,)C=)CC=CC()NC2=)C(=NC=C2Cl)C)=O)C=)OC				Rat	Female	Icr/ptr/CRA	Inhalation; aerosol	102	102	Positive	Nasal cavity: Bowman's gland	Adenocarcinoma					nasal cavity	nasal cavity	urinary bladder	-	-
3-(Cyclopentylloxy-N-(3,5-dichloro-4-pyridyl)- 4-methoxybenzamide	144035-83-6					Rat	Male	Icr/ptr/CRA	Inhalation; aerosol	104	104	Positive	Nasal cavity: Bowman's gland	Adenocarcinoma									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
3,3',4,4'-Tetrachloroazoxybenzene	21232-47-3	[N+](=N\C1=CC(=C(C=C1)Cl)Cl)([C-2]C=1C(=C(C=C(C=1)Cl)Cl)O-)[N+](=N\C3=CC(=C(C=C3)Cl)Cl)([C-4]C=1C(=C(C=C(C=1)Cl)Cl)O-)	-	-	-	Mouse	Female	B6C3F1	Gavage	92 d	91 d	Not specified			CYP1A1 CYP1A2	-	-		spleen vascular system thyroid gland liver nasal cavity oral cavity urinary bladder skin	liver urinary bladder lung kidney **uterus** thyroid gland	liver vascular system	thyroid gland liver vascular system urinary bladder	-
3,3'-Dichlorobenzidine	91-94-1	C=1(C=C(C=C(C=1)Cl)C=1)N(C3)C=C(C)=C(C=1)N(C)	의무 경인성 : 구분1(1A/1B) 생식세포 변이원성 : 구분2 발암성 : 구분1B 경구 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 14, 19, 21, 23, 25, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 128, 131, 150, 153, 163, 165, 167, 187, 200, 214, 307, 310, 318	Cancer slope factor: 0.00034 (µg/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Female	SD	Diet	65	65	Positive	Liver	Multiple tumour types	AR AHR CYP4B1 BAX BCL2	AMH/B2 TEF1 MYOSC DNAJC2 PCDX1	MGST1 CCR5 SAT ANXB10 HTATIP2	hsa04934 Cushing syndrome - Homo sapiens (human) (1) hsa196 409083 AHR; aryl hydrocarbon receptor hsa04071 Sphingolipid signaling pathway - Homo sapiens (human) (1) hsa581 403159 BAX; BCL2 associated X, apoptosis regulator hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (1) hsa581 403159 BAX; BCL2 associated X, apoptosis regulator	ear Zymbals gland hematopoietic system thyroid gland spleen liver vascular system	liver **uterus** lung urinary bladder thyroid gland mammary gland clitoral gland ear Zymbals gland	urinary bladder liver vascular system thyroid gland	thyroid gland liver vascular system urinary bladder vascular system	Neoplasm, Experimental
3,3'-Dichlorobenzidine	91-94-1					Rat	Female	SD	Diet	65	65	Positive	Liver	Multiple tumour types									
3,3'-Dichlorobenzidine	91-94-1					Rat	Male	SD	Diet	65	65	Positive	Liver	Multiple tumour types									
3,3'-Dichlorobenzidine dihydrochloride	612-83-9	C2(C1=CC(=C(C=C1)N)Cl)=CC(=C(C=C2)N)Cl.Cl.Cl	심한 눈 손상성/눈 자극성 : 구분2A(2B) 발암성 : 구분2 만성 수생환경 유해성 : 구분2	7, 8, 11, 14, 19, 20, 21, 23, 25, 27, 28, 29, 30, 34, 36, 41, 43, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 100, 101, 102, 103, 107, 111, 112, 117, 122, 123, 128, 150, 153, 163, 165, 167, 177, 187, 200, 214, 307, 310, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Male	ICR/Ict	Diet	52	52	Positive	Liver	Hepatoma	-				ear Zymbals gland hematopoietic system thyroid gland spleen liver vascular system	liver **uterus** lung urinary bladder thyroid gland mammary gland clitoral gland ear Zymbals gland	urinary bladder liver vascular system thyroid gland	thyroid gland liver urinary bladder vascular system	-
3,3'-Dihydroxybenzidine.2HCl	1502-36-5	C1=1(C(=CC(=C(C=C1)O)C)=C(C)C=C(C=C2)N(O)O)N.Cl.Cl	-	-	-	Mouse	Male	ICR/Ict	Diet	65	65	Positive	Liver	Hepatoma	-				urinary bladder kidney ear Zymbals gland spleen hematopoietic system thyroid gland liver skin	liver ear Zymbals gland **uterus** hematopoietic system clitoral gland thyroid gland liver small intestine mammary gland	thyroid gland urinary bladder kidney liver vascular system stomach	thyroid gland urinary bladder liver **ovary** vascular system pituitary gland hematopoietic system stomach	-
3,3-Dimethyl-1-phenylhiazene	7327-91-0	N(=NC=1C=CC=CC=1)N(C)C	-	8, 11, 21, 29, 30, 41, 46, 52, 53, 57, 60, 61, 67, 112, 131, 150, 165, 167, 200, 310	-	Rat	Mixed	BD	Gavage	104	104	Positive	Brain	Multiple tumour types	-				spleen vascular system	**uterus** hematopoietic system mammary gland	vascular system lung jejunum gland	hematopoietic system lung vascular system	-
3,3'-Dimethyl-4,4'-diaminobiphenyl dihydrochloride	612-82-8	C2(C1=CC(=C(C=C1)N)N(C)=CC(=C(C=C2)N)C).Cl.Cl	발암성 : 구분1A 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극)	8, 11, 14, 19, 21, 23, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 117, 131, 150, 163, 165, 167, 187, 200, 214, 307, 310, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: predicted to be genotoxic	Mouse	Female	BALB/cSc-HFC3 H(Nctr	Drinking water	52	52	Not specified	Lung	Adenocarcinoma	-				spleen urinary bladder liver ear Zymbals gland skin thyroid gland kidney	urinary bladder liver **uterus** clitoral gland lung ear Zymbals gland mammary gland thyroid gland	liver urinary bladder thyroid gland vascular system liver	vascular system urinary bladder vascular system liver thyroid gland	-
3,3'-Dimethyl-4,4'-diaminobiphenyl dihydrochloride	612-82-8					Mouse	Female	BALB/cSc-HFC3 H(Nctr	Drinking water	78	78	Not specified	Lung	Adenocarcinoma									
3,3'-Dimethyl-4,4'-diaminobiphenyl dihydrochloride	612-82-8					Mouse	Female	BALB/cSc-HFC3 H(Nctr	Drinking water	112	112	Not specified	Lung	Adenocarcinoma									
3,3'-Dimethyl-4,4'-diaminobiphenyl dihydrochloride	612-82-8					Mouse	Male	BALB/cSc-HFC3 H(Nctr	Drinking water	52	52	Not specified	Lung	Adenocarcinoma									
3,4,4'-Triaminodiphenyl ether	6264-66-0	C1=1(C=CC(=C(C=1)N)O)C2=CC=C(C)=C2)N)NN	-	19, 21, 23, 29, 30, 34, 36, 41, 52, 53, 57, 58, 61, 67, 72, 111, 112, 117, 131, 150, 163, 165, 167, 187, 200, 307, 310	-	Mouse	Male	ICR/Ict	Diet	52	52	Positive	Liver	Hepatoma	-				thyroid gland spleen ear Zymbals gland urinary bladder	urinary bladder thyroid gland **uterus** ear Zymbals gland hematopoietic system liver stomach clitoral gland lung	liver thyroid gland urinary bladder vascular system stomach	thyroid gland liver urinary bladder vascular system stomach **ovary** hematopoietic system	-
3,4,5,2',4'-Pentachlorobiphenyl	57465-28-8	C1(=C(C=C(C=C1)Cl)C2=C(C=C(C)=C2Cl)Cl)Cl	발암성 : 구분1A	-	Cancer slope factor: 34 (µg/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: IARC-Group 1 - Carcinogenic to humans Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	FVB/N hemizygous	Dermal	183 d	182 d	Not specified	Application site	Carcinoma - squamous cell	AHR CYP1A1 CYP1A2 CYP1A3 CYP1A4	FABP4 PPL AIRN7 CADPS2 CCDC49	MGST1 IBSL MCCC1 FAM171A1 HSPA12A	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1543 837408; CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 837409; CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 837410; CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (2) hsa1543 837408; CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 837409; CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 837410; CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (2) hsa1543 837408; CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 837409; CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 837410; CYP1B1; cytochrome P450 family 1 subfamily B member 1	thyroid gland liver oral cavity hematopoietic system ear Zymbals gland	liver kidney lung hematopoietic system **uterus** thyroid gland nasal cavity	liver vascular system urinary bladder small intestine	thyroid gland liver urinary bladder vascular system pituitary gland peritoneal cavity small intestine	Neoplasm Metastasis Precancerous Conditions Cholangiocarcinoma Neoplasm
3,4,5,2',4'-Pentachlorobiphenyl	57465-28-8					Rat	Female	Harlan	Gavage	107 d	730 d	Not specified	Adrenal gland cortex	Adenoma									
3,4',5,7-Tetrahydroxyflavone	520-18-3	C=1(C(=3C(OC=1C=2C=C(C)=C(C)=C(O)=C)=C(=C(O)C)=C)=O)	심한 눈 손상성/눈 자극성 : 구분2A(2B) 생식세포 변이원성 : 구분2	7, 14, 19, 21, 23, 25, 29, 30, 34, 36, 41, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 128, 150, 153, 163, 165, 167, 187, 200, 214, 307, 310, 318	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Rat	Female	ACI	Diet	77	77	Negative	Multiple sites	Multiple tumour types	CYP1A1 TNF EGR1 NOS2 AHR IL18	IFIH1 CCDC3 DNAAF2 FABP1 FCHSD2	GNAI1 UPH PITPNM1 KHNYN GOSR	hsa05010 Alzheimer disease - Homo sapiens (human) (2) hsa4843 K13241 NOS2; nitric oxide synthase 2 hsa7124 K03156 TNF; tumor necrosis factor hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa4843 K13241 NOS2; nitric oxide synthase 2 hsa7124 K03156 TNF; tumor necrosis factor hsa05152 Tuberculosis - Homo sapiens (human) (2) hsa4843 K13241 NOS2; nitric oxide synthase 2 hsa7124 K03156 TNF; tumor necrosis factor	urinary bladder kidney vascular system	urinary bladder small intestine	stomach urinary bladder thyroid gland	pituitary gland thyroid gland vascular system stomach	Leukemia Breast Neoplasm Carcinoma, Hepatocellular Cell Transformation, Neoplastic
3,4',5,7-Tetrahydroxyflavone	520-18-3					Rat	Male	ACI	Diet	77	77	Negative	Adrenal gland	Adenoma - cortical									
3',4'-Dichloro-2-methylacylanilide	2164-08-2	C1=1(C(=CC(=C(C=C1)N(C)(C(C)=C)=O)Cl)Cl)	-	6, 8, 11, 18, 19, 20, 23, 27, 29, 30, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 67, 72, 107, 111, 112, 117, 131, 150, 163, 165, 166, 167, 187, 200, 207, 310, 318	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				-	ear Zymbals gland	urinary bladder kidney liver vascular system thyroid gland	urinary bladder liver	-
3',4'-Dichloro-2-methylacylanilide	2164-08-2					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
3',4'-Dichloro-2-methylacylanilide	2164-08-2					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
3',4'-Dichloro-2-methylacylanilide	2164-08-2					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
3,4-Dihydrocoumarin	119-84-6	C1=1(C(=CC2=2)C(C)(C)O2)=O	경성 독성(흡연) : 구분4 피부 부식성/자극성 자극성 : 구분2 발암성 : 구분1B		Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular	DDIT3 DNAJA2 EGF EPHA1 HSD17B4	PLCG2 GRID1 AKRIC3 NOP56 ACOT2	RPIP8/H4C ENC1 BIM/E1 KIAA0247 MTIL	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1950 404057 EGF; epidermal growth factor hsa2052 435253 EPHA1; epoxide hydrolase 1 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa1950 404057 EGF; epidermal growth factor hsa2052 435253 EPHA1; epoxide hydrolase 1 hsa01521 EGFR tyrosine kinase inhibitor resistance - Homo sapiens (human) (1) hsa1950 404057 EGF; epidermal growth factor	kidney ear Zymbals gland liver large intestine	ear Zymbals gland	urinary bladder stomach lung	**ovary** liver lung stomach pituitary gland urinary bladder	-
3,4-Dihydrocoumarin	119-84-6					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma(Hepatocellular | Hepatoblastoma									
3,4-Dihydrocoumarin	119-84-6					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Adrenal gland medulla	Pheochromocytoma(benign | Pheochromocytoma - benign - bilateral									
3,4-Dihydrocoumarin	119-84-6					Rat	Male	Fischer 344	Gavage	64	104	Not specified	Kidney	Adenoma - tubular									
3,4-Dihydrocoumarin	119-84-6					Rat	Male	Fischer 344	Gavage	28	104	Not specified	Kidney	Adenoma - tubular									
3,4-Dihydrocoumarin	119-84-6					Rat	Male	Fischer 344	Gavage	103	104	Positive	Kidney	Adenoma - tubular									
3,4-Dihydroxycinnamic acid	331-39-5	C1(=C(C=CC(=C1)C=CC(O)=O)O)O	발암성 : 구분2	19, 23, 111, 112, 187, 307	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	96	96	Positive	Forestomach	Carcinoma - squamous cell	ALOX5 ALOX15 CAT MPO TNF GSR	NOP56 CCDC93 STX1A DIX TBL1XR1	ITL NQO1 PTGR1 OGG1 VASP	hsa04217 Necroptosis - Homo sapiens (human) (2) hsa246 400460 ALOX15; arachidonate 15-lipoxygenase hsa7124 K03156 TNF; tumor necrosis factor hsa05014 Amyotrophic lateral sclerosis - Homo sapiens (human) (2) hsa7124 K03156 TNF; tumor necrosis factor hsa847 K07781 CAT; catalase hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa246 400460 ALOX15; arachidonate 15-lipoxygenase hsa847 K07781 CAT; catalase	kidney stomach	stomach	stomach lung kidney	stomach **ovary** pituitary gland	Melanoma
3,4-Dihydroxycinnamic acid	331-39-5					Mouse	Male	B6C3F1	Diet	96	96	Positive	Forestomach	Carcinoma - squamous cell									
3,4-Dihydroxycinnamic acid	331-39-5					Rat	Female	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell									
3,4-Dihydroxycinnamic acid	331-39-5					Rat	Male	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell									
3,4-Dihydroxycinnamic acid	331-39-5					Rat	Male	Fischer 344/DuCr	Diet	51	52	Positive	Forestomach	Papilloma - squamous cell									
3,4-Dihydroxycinnamic acid	331-39-5					Rat	Male	Fischer 344/DuCr	Diet	60	60	Positive	Forestomach	Carcinoma - squamous cell									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
2,5-Di-tert-butyl-4-hydroxybenzyl alcohol	88-26-6	C1=C(C(=CC(=C1CO)C(C)(C)C)O)C(C)(C)C	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(Ai) 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 14, 19, 23, 25, 27, 29, 30, 52, 53, 61, 64, 66, 67, 71, 111, 112, 117, 122, 123, 153, 165, 167, 187, 200, 214, 307, 318	Genotoxicity Data: predicted to be non-genotoxic	Rat	Female	NZBW	Diet	104	104	Not specified	Liver	Multiple tumour types	AR	MAPK8 SDC4 PTPN3 MRAP4 STMP6	OSS EID1 CAPZ3 KDELC1 PGM2	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa:367 KDEG7 AR; androgen receptor hsa04114 Oocyte meiosis - Homo sapiens (human) (1) hsa:367 KDEG7 AR; androgen receptor hsa05200 Pathways in cancer - Homo sapiens (human) (1) hsa:367 KDEG7 AR; androgen receptor	stomach	stomach	lung stomach kidney thyroid gland liver	pituitary gland thyroid gland	-
2,5-Di-tert-butyl-4-hydroxybenzyl alcohol	88-26-6					Rat	Male	NZBW	Diet	104	104	Not specified	Liver	Multiple tumour types									
3-Amino-4-ethoxyacetanilide	17026-81-2	C1=C(C(=CC(=C1N(C)C)=O)N)OCC	-	21, 41, 57, 131, 150, 210	-	Mouse	Female	B6C3F1	Diet	78	93	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				urinary bladder kidney nasal cavity skin stomach spleen	urinary bladder ear Zymbals gland mammary gland nasal cavity small intestine	thyroid gland urinary bladder kidney liver	urinary bladder liver	-
3-Amino-4-ethoxyacetanilide	17026-81-2					Mouse	Male	B6C3F1	Diet	78	93	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Amino-4-ethoxyacetanilide	17026-81-2					Rat	Female	Fischer 344	Diet	78	106	Not specified	Adrenal gland	Adenoma- cortical | Carcinomacortical									
3-Amino-4-ethoxyacetanilide	17026-81-2					Rat	Male	Fischer 344	Diet	78	106	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Amino-4-methoxynitrobenzene	99-59-2	[N+](=O)[O-]c1cc(C(=C)C=C)c(C)c1N(C)C	현탁 눈 손상성/눈 자극성 - 구분2A(Ai) 생식세포 변이원성 - 구분2 만성 수생환경 유해성 - 구분2	21, 28, 29, 30, 41, 52, 53, 57, 61, 67, 100, 101, 102, 103, 112, 131, 150, 165, 167, 177, 200, 210	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	96	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				urinary bladder kidney ear Zymbals gland skin hematopoietic system liver spleen large intestine stomach thyroid gland	urinary bladder clitoral gland uterus hematopoietic system ear Zymbals gland kidney stomach mammary gland lung	thyroid gland urinary bladder vascular system liver stomach	urinary bladder liver vascular system thyroid gland	-
3-Amino-4-methoxynitrobenzene	99-59-2					Mouse	Male	B6C3F1	Diet	78	95	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
3-Amino-4-methoxynitrobenzene	99-59-2					Rat	Female	Fischer 344	Diet	78	106	Positive	Clitoral gland	Adenoma | Adenoma- papillary | Carcinoma | Carcinoma- squamous cell									
3-Amino-4-methoxynitrobenzene	99-59-2					Rat	Male	Fischer 344	Diet	78	106	Positive	Adrenal gland	Adenoma- cortical | Carcinomacortical									
3-Amino-4-methoxytoluene	120-71-8	C1(=CC(=C(C)C=C1)N)NOCC	경口 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(Ai) 발암성 - 구분2 특정표적장기 독성(1회 노출) - 구분2	8, 11, 21, 28, 32, 41, 57, 60, 63, 100, 101, 102, 103, 122, 123, 131, 150, 177, 200, 210	Cancer slope factor: 4.3e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	97	97	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular	AKR1B10 AKR1C2 ALDH1A1 ASF1A CDH4	BGLAP ACOT2 ADAM18 SERPINB8 ITGB8	SOD3 TNNI3K2 CASP2 C9rf21 BCL2A1	hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa:216 KEGG7249 ALDH1A1; aldehyde dehydrogenase 1 family member A1 hsa00830 Retinol metabolism - Homo sapiens (human) (1) hsa:216 KEGG7249 ALDH1A1; aldehyde dehydrogenase 1 family member A1 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (1) hsa:1646 KEGG80 AKR1C2; aldo-keto reductase family 1 member C2	urinary bladder ear Zymbals gland kidney liver spleen skin nasal cavity stomach large intestine hematopoietic system vascular system	urinary bladder clitoral gland ear Zymbals gland nasal cavity stomach hematopoietic system uterus kidney	urinary bladder thyroid gland vascular system liver stomach	urinary bladder liver thyroid gland vascular system	Urinary Bladder Neoplasm Nose Neoplasm
3-Amino-4-methoxytoluene	120-71-8					Mouse	Male	B6C3F1	Diet	97	97	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Amino-4-methoxytoluene	120-71-8					Rat	Female	Fischer 344	Diet	104	105	Positive	Adrenal gland	Adenoma- cortical									
3-Amino-4-methoxytoluene	120-71-8					Rat	Male	Fischer 344	Diet	104	105	Positive		Brain- Glioma Brain stem- Glioma									
3-Amino-9-ethylcarbazole	132-32-1	C1(=CC=C2C(=C1)C3=C(N2)C(=CC=C3)N	경口 독성(경구) - 구분2 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(Ai) 발암성 - 구분1B 만성 수생환경 유해성 - 구분2	7, 8, 11, 19, 21, 23, 25, 27, 28, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 62, 63, 67, 72, 97, 98, 100, 101, 102, 103, 107, 111, 112, 117, 122, 123, 131, 150, 152, 163, 165, 167, 177, 187, 195, 200, 203, 204, 207, 210	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	95	104	Not specified	Adrenal gland	Pheochromocytoma	-				skin ear Zymbals gland liver spleen thyroid gland	ear Zymbals gland clitoral gland uterus urinary bladder thyroid gland mammary gland	liver urinary bladder thyroid gland vascular system stomach	liver thyroid gland urinary bladder hematopoietic system vascular system	-
3-Amino-9-ethylcarbazole	132-32-1					Mouse	Male	B6C3F1	Diet	102	104	Not specified	Gall bladder	Polyp- administrative									
3-Amino-9-ethylcarbazole	132-32-1					Rat	Female	Fischer 344	Diet	113	104	Not specified	Adrenal gland	Pheochromocytoma									
3-Amino-9-ethylcarbazole	132-32-1					Rat	Male	Fischer 344	Diet	113	104	Not specified	Adrenal gland	Adenocarcinoma- metastatic									
3-Amino-9-ethylcarbazole hydrochloride	6109-97-3	N2C(C(=c1C=CC(=CC=1)C=1C=3C2=CC=C3)N(C)C)C=CC=C3)N(C)	-	7, 19, 21, 23, 25, 27, 41, 46, 57, 61, 111, 117, 122, 123, 131, 150, 153, 187, 207, 210	Cancer slope factor: 2.2e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	78	95	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				skin ear Zymbals gland liver spleen thyroid gland	ear Zymbals gland clitoral gland uterus urinary bladder thyroid gland mammary gland	liver urinary bladder thyroid gland vascular system stomach	liver thyroid gland urinary bladder hematopoietic system vascular system	-
3-Amino-9-ethylcarbazole hydrochloride	6109-97-3					Mouse	Male	B6C3F1	Diet	78	95	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
3-Amino-9-ethylcarbazole hydrochloride	6109-97-3					Rat	Female	Fischer 344	Diet	78	107	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Amino-9-ethylcarbazole hydrochloride	6109-97-3					Rat	Male	Fischer 344	Diet	78	106	Positive	Liver	Carcinoma- hepatocellular | Nodule- neoplastic									
3-Amino-9-ethylcarbazole mixture	-	C1(=CC=C2C(=C1)C3=C(N2)C(=CC=C3)N(C)C)C=CC=C3)N(C)C=C3C(=C4C(=C(NC(C)C)C=C)C=C4)N.Cl	-	-	-	Mouse	Female	B6C3F1	Diet	78	95	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				-	-	-	-	-
3-Amino-9-ethylcarbazole mixture	-					Mouse	Male	B6C3F1	Diet	78	94	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Amino-9-ethylcarbazole mixture	-					Rat	Female	Fischer 344	Diet	78	105	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Amino-9-ethylcarbazole mixture	-					Rat	Male	Fischer 344	Diet	78	105	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Aminodibenzofuran	4106-66-5	C=1C=2C(=c3C=1C=C(O)C=C3)C=CC=C2N	-	-	-	Rat	Male	Wistar	Diet	89	89	Positive	Liver	Hepatoma	-				urinary bladder ear Zymbals gland	urinary bladder ear Zymbals gland mammary gland uterus small intestine thyroid gland lung kidney clitoral gland hematopoietic system liver	urinary bladder thyroid gland liver vascular system stomach	thyroid gland liver urinary bladder vascular system hematopoietic system stomach	-
3-Benzylidenone-4-acetamide	14504-15-5	Na.1O[C(=c2[N(m-]c1C(=2)C=C(C=C2)C(C)N.c(O)O-)				Mouse	Female	DDD	Drinking water	52	52	Positive	Liver	Adenoma- hepatocellular					liver	[illegible]	[illegible]	liver	-
3-Benzylidenone-4-acetamide	14504-15-5					Rat	Male	Dorsey	Drinking water	41	91	Positive	Liver	Carcinoma- hepatocellular									
3-Benzylidenone-4-acetamide	14504-15-5					Rat	Male	Dorsey	Diet	104	104	Negative	Liver	Multiple tumour types									
3-Chloro-4-methylaniline	95-74-9	C1=C(C(=CC(=C1N)C)Cl)N	경口 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(Ai) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 경口 수생환경 유해성 - 구분1	21, 29, 30, 41, 52, 53, 57, 67, 152, 191, 150, 165, 167, 200, 210	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	78	90	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				spleen ear Zymbals gland thyroid gland liver urinary bladder	urinary bladder thyroid gland ear Zymbals gland clitoral gland uterus liver lung	vascular system urinary bladder liver thyroid gland	thyroid gland vascular system urinary bladder liver hematopoietic system	-
3-Chloro-4-methylaniline	95-74-9					Mouse	Male	B6C3F1	Diet	78	90	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Chloro-4-methylaniline	95-74-9					Rat	Female	Fischer 344	Diet	78	102	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Chloro-4-methylaniline	95-74-9					Rat	Male	Fischer 344	Diet	78	102	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
3-Chloroaniline	108-42-9	C1=C(N)C=CC=C1Cl	경口 독성(경구) - 구분3 경口 독성(경피) - 구분3 경口 독성(흡입: 분진/미스트) - 구분3 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	93 d	91 d	Not specified		MPO	AMHR2 DNAH12 CCR6 TEP1 MPO5C	MGST1 SOD3 CYP1F CCR6 TNNI3K2	hsa04613 Neutrophil extracellular trap formation - Homo sapiens (human) (1) hsa:4353 K10789 MPO; myeloperoxidase hsa00983 Drug metabolism - other enzymes - Homo sapiens (human) (1) hsa:4353 K10789 MPO; myeloperoxidase hsa04145 Phagosome - Homo sapiens (human) (1) hsa:4353 K10789 MPO; myeloperoxidase	-	urinary bladder thyroid gland uterus ear Zymbals gland liver clitoral gland lung hematopoietic system stomach kidney	liver vascular system urinary bladder thyroid gland	thyroid gland liver urinary bladder vascular system hematopoietic system	-
3-Diazotyramine hydrochloride	-	C1=C(C=CC(=C1[O-])[N+]#N)CCN.Cl				Rat	Male	Fischer 344/DuCr	Drinking water	116	116	Positive	Oral cavity	Carcinoma- squamous cell	-				-				-
3-Hydroxy-4-aminobiphenyl	4363-08-5	C=1(C=CC(=CC=1)N)C(C=2)=CC=CC=C2	-	-	-	Rat	Female	Not specified	Diet	43	65	Negative	Liver	Multiple tumour types	-				urinary bladder kidney ear Zymbals gland spleen hematopoietic system thyroid gland liver skin	urinary bladder ear Zymbals gland uterus hematopoietic system clitoral gland liver thyroid gland small intestine mammary gland	thyroid gland urinary bladder kidney vascular system liver stomach	thyroid gland urinary bladder liver ovary vascular system pituitary gland hematopoietic system	-
3-Hydroisoquinoxaline	65701-07-2	C1(N(=C(C(=CN(C)C)C)C=C)C=C)=NC=3C=C(O)C=CC=C3=O				Mouse	Female	CD1	Diet	86	86	Negative	Liver	Haemangioma							urinary bladder	hematopoietic system	
3-Hydroisoquinoxaline	65701-07-2					Mouse	Male	CD1	Diet	86	86	Negative	Liver	Haemangioma									
3-Hydroisoquinoxaline	65701-07-2					Rat	Female	Sprague	Diet	108	108	Negative	Liver	Carcinoma- hepatocellular									
3-Hydroisoquinoxaline	65701-07-2					Rat	Male	Sprague	Diet	104	104	Negative	Adrenal gland	Tumour- malignant									
3-Methoxy-1,2-benzenediol	934-00-9	C1(=CC=CC(=C1O)O)C)O	-	7, 19, 21, 23, 25, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 61, 67, 72, 111, 112, 117, 122, 123, 131, 150, 153, 163, 165, 167, 187, 200, 207, 210	-	Rat	Male	Fischer 344/DuCr	Diet	51	51	Positive	Forestomach	Carcinoma- squamous cell	COMT	HTRX SERPINB1 CAORF48 NBK4 CXCL2	MGST1 SOD3 SRR2 PTGR1 TNNI3K2	hsa04728 Dopaminergic synapse - Homo sapiens (human) (1) hsa:1312 K00545 COMT; catechol-O-methyltransferase hsa00350 Tyrosine metabolism - Homo sapiens (human) (1) hsa:1312 K00545 COMT; catechol-O-methyltransferase hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa:1312 K00545 COMT; catechol-O-methyltransferase	stomach kidney urinary bladder hematopoietic system nasal cavity ear Zymbals gland vascular system large intestine	stomach urinary bladder hematopoietic system nasal cavity kidney	stomach urinary bladder vascular system kidney thyroid gland	ovary urinary bladder thyroid gland pituitary gland stomach	-

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
3-Methoxy-4-aminoazobenzene	3544-23-8	N_{1}=NC$_{1}$=CC=CC=C1)C=2C=2(C)=CC=2)NH2C	-	-	-	Mouse	Female	B6C3F1	Diet	56	56	Positive	Liver	Adenoma - hepatocellular	CYP1A2 CYP1A1	BGLAP ACOT2 AMHR2 NR1K4 ADAM19	CASP2 TNNRD2 SCO1 CCR5 MGST1		urinary bladder spleen ear Zymbals gland vascular system skin kidney liver hematopoietic system large intestine nasal cavity stomach	urinary bladder **uterus** ear Zymbals gland hematopoietic system kidney clitoral gland stomach	urinary bladder thyroid gland vascular system liver	urinary bladder liver thyroid gland vascular system	-
3-Methoxy-4-aminoazobenzene	3544-23-8					Mouse	Male	B6C3F1	Diet	56	56	Negative	Liver	Multiple tumour types									
3-Methyl-3H-imidazo[4,5-f]quinolin-2-amine	76180-96-6	C_{1}=CN=C2C$_{2}$=C1)C=2C=2C=C(N)C$_{2}$=NS)NC		19, 21, 23, 41, 52, 115, 117, 131, 150, 187, 207, 210	Cancer slope factor: 0.0004 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Cynomolgus monkey	Mixed	Not specified	Gavage	485	485	Positive	Liver	Carcinoma - hepatocellular	CYP1A2 CYB5R3 NAT2 GSS CYP1A1	SLC15A1 HRP3 IHH7 RNF186 TRAFPC3	DNPH2 CYP1A2 CDK12 LST1 CNTN1	hsa05165 Human papillomavirus infection - Homo sapiens (human) (2) hsa1499 KS2105 CTNNB1; catenin beta 1 hsa324 KS2085 APC; APC regulator of WNT signaling pathway hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa1499 KS2105 CTNNB1; catenin beta 1 hsa324 KS2085 APC; APC regulator of WNT signaling pathway hsa05213 Endometrial cancer - Homo sapiens (human) (2) hsa1499 KS2105 CTNNB1; catenin beta 1 hsa324 KS2085 APC; APC regulator of WNT signaling pathway	ear Zymbals gland skin oral cavity large intestine liver	clitoral gland ear Zymbals gland small intestine liver oral cavity mammary gland	**stomach** **lung** liver urinary bladder	liver **stomach** **lung**	Breast Neoplasm Stomach Neoplasm Carcinoma, Hepatocellular **Lung Neoplasms** Carcinoma, Squamous Cell
3-Methyl-3H-imidazo[4,5-f]quinolin-2-amine	76180-96-6					Mouse	Female	CD1	Diet	96	96	Positive	Forestomach	Multiple tumour types									
3-Methyl-3H-imidazo[4,5-f]quinolin-2-amine	76180-96-6					Mouse	Male	CD1	Diet	96	96	Positive	Forestomach	Carcinoma - squamous cell									
3-Methyl-3H-imidazo[4,5-f]quinolin-2-amine	76180-96-6					Rat	Female	Fischer 344	Diet	52	78	Positive	Liver	Carcinoma - hepatocellular									
3-Methylaniline hydrochloride	638-03-9	C$_{1}$=C(N)=CC=CC=1C.Cl	-	21, 41, 57, 131, 150, 310	-	Mouse	Female	CD-1 HaMcICR	Diet	77	81	Negative	Liver	Multiple tumour types	-				spleen liver urinary bladder ear Zymbals gland thyroid gland	urinary bladder ear Zymbals gland clitoral gland liver **uterus** thyroid gland lung nasal cavity mammary gland	thyroid gland urinary bladder vascular system liver kidney lung	urinary bladder thyroid gland liver vascular system hematopoietic system stomach	-
3-Methylaniline hydrochloride	638-03-9					Mouse	Female	CD-1 HaMcICR	Diet	77	90	Negative	Liver	Multiple tumour types									
3-Methylaniline hydrochloride	638-03-9					Mouse	Male	CD-1 HaMcICR	Diet	77	90	Positive	Liver	Hepatoma									
3-Methylaniline hydrochloride	638-03-9					Rat	Male	SD	Diet	77	98	Negative	Liver	Multiple tumour types									
3-Methylcholanthrene	56-49-5	C^{1}=CC=3C=2C1=c(C=CC=2C=c4C=3C=CC=5C4=CC=CC=5)C	-	7, 21, 25, 29, 30, 41, 52, 52, 57, 64, 67, 112, 122, 131, 150, 152, 165, 167, 200, 210	Cancer slope factor: 0.0063 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Cynomolgus monkey	Mixed	Not specified	Diet	258	1384	Not specified	Multiple sites	Tumour - malignant	Ank6 CYP1A1 CYP1A2 AHR AGC1	DEBB2 BCAS3 PLCG2 FRH HEATR3	FCN1 ENC1 UGT2B7 AHR6 NEDD9	hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (3) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 KO7410 CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (3) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 KO7410 CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa00380 Tryptophan metabolism - Homo sapiens (human) (3) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 KO7410 CYP1B1; cytochrome P450 family 1 subfamily B member 1	ear Zymbals gland spleen kidney Maltoni head cancers	mammary gland ear Zymbals gland clitoral gland	urinary bladder	stomach urinary bladder thyroid gland **ovary** pituitary gland vascular system	Breast Neoplasm **Lung Neoplasm** Carcinoma Carcinoma, Squamous Cell Urinary Bladder Neoplasm
3-Methylcholanthrene	56-49-5					Rat	Male	Leeds	Diet	26	65	Negative	Liver	Multiple tumour types									
3-Methylcholanthrene	56-49-5					Rat	Male	Leeds	Diet	39	65	Negative	Liver	Multiple tumour types									
3-Methylcholanthrene	56-49-5					Rat	Male	Leeds	Diet	65	65	Negative	Liver	Multiple tumour types									
3-Methylcholanthrene	56-49-5					Rat	Female	Not specified	Gavage	52	52	Positive	Mammary tissue	Multiple tumour types									
3-Nitrobenzoic acid	121-92-6	C^{1}(=CC=CC(=C1)[O])=O)[N+](O-])=O	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(사) 피부 과민성 - 구분1(사1B) 생식독성 - 구분2	29, 30, 52, 53, 67, 112, 165, 167, 200	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	92 d	91 d	Not specified			-				kidney urinary bladder spleen thyroid gland liver skin ear Zymbals gland	clitoral gland urinary bladder kidney **uterus**	thyroid gland kidney vascular system urinary bladder	**ovary** liver vascular system stomach hematopoietic system	-
3-Nitrophenacetin	1777-84-0	[N+](C1=CC(NC(=O)C)=CC=C1OCC)([O-])=O	-	-	-	Mouse	Female	B6C3F1	Diet	78	97	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic	-				urinary bladder kidney skin nasal cavity stomach large intestine	urinary bladder ear Zymbals gland mammary gland hematopoietic system nasal cavity small intestine kidney stomach lung	thyroid gland kidney urinary bladder liver	urinary bladder liver	-
3-Nitrophenacetin	1777-84-0					Mouse	Male	B6C3F1	Diet	78	98	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular									
3-Nitrophenacetin	1777-84-0					Rat	Female	Fischer 344	Diet	78	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
3-Nitrophenacetin	1777-84-0					Rat	Male	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
3-Nitrotoluene	99-08-1	C^{1}(=CC=CC(=C1[N+](=O)[O-])=O)C	경성 독성(경구) - 구분4 경성 독성(경피) - 구분4 만성 수생환경 유해성 - 구분2	29, 30, 52, 53, 57, 67, 112, 131, 165, 167, 200	Carcinogenicity data available: IRIRTV (OEHL)-Inadequate for an assessment of carcinogenic potential Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	93 d	91 d	Not specified			-				spleen liver urinary bladder kidney ear Zymbals gland thyroid gland skin Maltoni head cancers oral cavity lung vascular system stomach nasal cavity	clitoral gland urinary bladder liver **uterus** lung kidney mammary gland ear Zymbals gland stomach hematopoietic system	thyroid gland urinary bladder vascular system kidney liver lung	vascular system urinary bladder **ovary** liver hematopoietic system stomach thyroid gland	-
2-Phenylpropyl isothiocyanate	2627-27-2	C[N]=C=S)CCC1=CC=CC=C1		-	-	Rat	Male	Fischer 344	Diet	89	89	Not specified	Testes	Tumour - interstitial cell					Maltoni head cancers	ear Zymbals gland		thyroid gland	
4-(1-Cyanoethyl)-1,2,3,4-tetrahydro-1-naphthalenecarbodithioate	179664-39-3	C(C(=N)C1CCC(C2=2=CC=CC=CC=C12)C#N)				Rat	Female	Fischer 344	Diet	44 d	49 d	Not specified							kidney	kidney		**ovary**	-
4-(2-Benzothiazolylthio)morpholine	102-77-2	N1(CCOCC1)[C3=NC=2C=CC=CC=2S3	경성 독성(경구) - 구분4 심한 눈 손상성/눈 자극성 - 구분2A(사9) 피부 과민성 - 구분1(사1A/1B) 수생 유해성 유해성 - 구분2	19, 21, 22, 29, 30, 41, 52, 53, 57, 67, 111, 112, 117, 121, 150, 165, 167, 187, 200, 207, 210	Genotoxicity Data: non-clastogenic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				hematopoietic system	kidney vascular system urinary bladder	-	-	-
4-(2-Benzothiazolylthio)morpholine	102-77-2					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-(2-Benzothiazolylthio)morpholine	102-77-2					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-(2-Benzothiazolylthio)morpholine	102-77-2					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-(4-Chlorophenoxy)aniline	101-79-1	O[C$_{1}$=1C=CC(C)=CC=1)C=1)C=3C=CC(N)=CC=2	-	2, 14, 19, 21, 25, 29, 30, 52, 53, 61, 64, 66, 67, 71, 111, 112, 117, 122, 123, 153, 166, 167, 187, 200, 204, 207, 210	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	CD-1 HaMcICR	Diet	68	86	Positive	Liver	Multiple tumour types					thyroid gland liver spleen ear Zymbals gland	thyroid gland liver urinary bladder ear Zymbals gland **uterus**	liver vascular system urinary bladder thyroid gland stomach	thyroid gland urinary bladder liver vascular system hematopoietic system	-
4-(4-Chlorophenoxy)aniline	101-79-1					Mouse	Male	CD-1 HaMcICR	Diet	51	55	Negative	Liver	Multiple tumour types									
4-(4-Chlorophenoxy)aniline	101-79-1					Rat	Male	SD	Diet	77	98	Positive	Liver	Hepatoma									
4-(6-Methyl-2-benzothiazolyl)benzenamine	92-36-4	C^{1}(=CC=CC=C1[C+]2SC3=C(N=2)C=CC(=C3)C)N	-	-	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	93	91	Not specified			-				spleen ear Zymbals gland large intestine urinary bladder thyroid gland hematopoietic system	ear Zymbals gland clitoral gland urinary bladder	thyroid gland urinary bladder vascular system liver	thyroid gland urinary bladder vascular system liver hematopoietic system	-
4-(Dimethylamino)-3,5-dimethylphenol	6120-10-1	C$_{1}$=1([O])=C)C=C)C=1)O)C(N)C)C	-	-	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				spleen urinary bladder liver stomach kidney	liver urinary bladder thyroid gland stomach	kidney vascular system thyroid gland	vascular system liver pituitary gland thyroid gland	-
4-(Dimethylamino)-3,5-dimethylphenol	6120-10-1					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-(Dimethylamino)-3,5-dimethylphenol	6120-10-1					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-(Dimethylamino)-3,5-dimethylphenol	6120-10-1					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-(Ethylsulphonyl)naphthalene-1-sulphonamide	840-60-2	C$_{1}$=1)[C(C)]=CS(=O)=O)C=CC(NN)=S(=O)=O)C$_{2}$=NC=CC=C2				Mouse	Female	A x F	Diet	100	100	Positive	Lung	Adenoma					spleen			thyroid gland	urinary bladder
4-(Ethylsulphonyl)naphthalene-1-sulphonamide	840-60-2					Mouse	Female	B x C57	Diet	92	92	Positive	Urinary bladder	Carcinoma									
4-(p-Fluorophenyl)aniline	326-60-6	C$_{2}$C=3C=CC(N)=CC=1)=CC=1)=CC=CC=CC2F		8, 11, 19, 21, 23, 29, 30, 41, 52, 53, 57, 60, 67, 111, 112, 117, 121, 150, 165, 166, 167, 187, 200, 207, 210	-	Mouse	Female	CBA	Gavage	26	114	Positive	Liver	Hepatoma					thyroid gland spleen kidney ear Zymbals gland liver	**uterus** ear Zymbals gland urinary bladder thyroid gland clitoral gland	urinary bladder thyroid gland liver lung vascular system	liver thyroid gland urinary bladder vascular system lung	-
4-(p-Fluorophenyl)aniline	326-60-6					Mouse	Male	CBA	Gavage	26	104	Positive	Liver	Hepatoma									
4-(Phenylazo)-benzenamine	60-11-7					Rhesus monkey	Mixed	Not specified	Diet	258	1019	Not specified	Lung	Carcinoma - alveolar/bronchiolar									
4-(Phenylazo)-N,N-dimethylaniline	60-11-7	C^{1}(=CC=CC=C1)N=NC$_{2}$=CC=C(C=C2)N(C)C	경성 독성(경구) - 구분2 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(사9) 생식세포 변이원성 - 구분2 **발암성 - 구분1B** 경성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 19, 21, 23, 25, 29, 30, 41, 52, 53, 57, 61, 67, 111, 112, 117, 122, 123, 131, 150, 153, 165, 167, 187, 200, 207, 210	Cancer slope factor: 0.0013 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Female	Wistar	Diet	33	56	Positive	Liver	Carcinoma - liver cell	TAT CAT GSTP1	CTPS1 RPRM INCENP CCNC BCC2	SRRP1 ENC1 SAT ITGAM FOXY4	hsa00630 Glyoxylate and dicarboxylate metabolism - Homo sapiens (human) (1) hsa847 KO3781 CAT; catalase hsa04211 Longevity regulating pathway - Homo sapiens (human) (1) hsa847 KO3781 CAT; catalase hsa01200 Carbon metabolism - Homo sapiens (human) (1) hsa847 KO3781 CAT; catalase	spleen liver thyroid gland vascular system	liver thyroid gland **uterus** urinary bladder kidney lung ear Zymbals gland	thyroid gland vascular system lung kidney	liver peritoneal cavity vascular system urinary bladder	**Liver Neoplasm, Experimental** Carcinoma, Hepatocellular

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
4,4'-Azodianiline	538-41-0	N(c)NC=1C=CC(N)=CC=1)(C2=CC=C(N)C=C2	-	19, 23, 61, 111, 117, 187, 307	-	Mouse	Female	BALB/cLac/+[N]	Diet	60	132	Negative	Liver	Multiple tumour types	-				spleen vascular system liver ear Zymbals gland urinary bladder thyroid gland	urinary bladder **uterus** thyroid gland ear Zymbals gland kidney liver hematopoietic system lung clitoral gland mammary gland	thyroid gland urinary bladder liver vascular system lung	thyroid gland liver urinary bladder vascular system **ovary** hematopoietic system stomach	-
4,4'-Azodianiline	538-41-0					Mouse	Male	BALB/cLac/+[N]	Diet	60	132	Negative	Liver	Multiple tumour types									
4,4'-Diaminobenzanilide	785-30-8	C(NC=1C=CC(N)=CC=1)(C=2C=CC(N)=CC=2)=O	원핀 는 순위정는 자격성 : 구분2A(GB)	-	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	BALB/cLac/+[N]	Diet	60	132	Negative	Liver	Multiple tumour types	-				spleen	**uterus** ear Zymbals gland urinary bladder thyroid gland	urinary bladder thyroid gland liver vascular system	urinary bladder thyroid gland hematopoietic system liver vascular system lung	-
4,4'-Diaminobenzanilide	785-30-8					Mouse	Male	BALB/cLac/+[N]	Diet	60	132	Negative	Liver	Multiple tumour types									
4,4'-Diisocyanato-3,3'-dimethoxybiphenyl	91-93-0	C1=CC(=C(C=1)C(=C1)C2=CC=C(C(=C2)OC)N=C=O)OC)N=C=O	피부 과민성 : 구분1(1A/1B) 흡인 유해성 : 구분2 만성 수생환경 유해성 : 구분4	21, 41, 57, 131, 150, 203	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans.	Mouse	Female	B6C3F1	Diet	78	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-					skin hematopoietic system ear Zymbals gland urinary bladder large intestine	hematopoietic system **uterus** mammary gland urinary bladder ear Zymbals gland liver clitoral gland	urinary bladder	liver urinary bladder vascular system	-
4,4'-Diisocyanato-3,3'-dimethoxybiphenyl	91-93-0					Mouse	Male	B6C3F1	Diet	78	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4,4'-Diisocyanato-3,3'-dimethoxybiphenyl	91-93-0					Rat	Female	Fischer 344	Gavage (preweaning) then diet	78	104	Positive		Ear : Adenocarcinoma - sebaceous | Carcinomasquamous cell | Trichoepithelioma Zymbal's gland : Adenocarcinoma - sebaceous | Carcinoma - squamous cell | Trichoepithelioma									
4,4'-Diisocyanato-3,3'-dimethoxybiphenyl	91-93-0					Rat	Male	Fischer 344	Gavage (preweaning) then diet	78	104	Positive		Ear : Carcinoma - squamous cell Zymbal's gland : Carcinoma - squamous cell									
4,4'-Methylenebis(2-chloroaniline)	101-14-4	C1(=C(C=CC(=C1)C(CC2=CC(=C(C=C2)N)Cl)N)Cl	급성 독성(경구) : 구분4 생식세포 변이원성 : 구분2 **발암성 : 구분1A** 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 14, 19, 23, 25, 27, **29**, **30**, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, **166**, **167**, 187, **200**, 204, 307, 318	Cancer slope factor: 0.00043 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Dog	Female	Beagle	Diet	469	469	Positive	Liver	Nodule - hyperplastic	CYP1A4 NAT2 AKR1B10 AUB	AMH|R2 CCNC AKR1C3 TEP1 DNAJG2	SOD3 POR TNNI3K2 MGST1 CYTIP	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa10 630622 NAT2; N-acetyltransferase 2 hsa57016 630011 AKR1B10; aldo-keto reductase family 1 member B10 hsa00983 Drug metabolism - other enzymes - Homo sapiens (human) (1) hsa10 630622 NAT2; N-acetyltransferase 2 hsa00051 Fructose and mannose metabolism - Homo sapiens (human) (1) hsa57016 630011 AKR1B10; aldo-keto reductase family 1 member B10	ear Zymbals gland liver vascular system thyroid gland spleen **lung** hematopoietic system	liver **lung** thyroid gland mammary gland	kidney vascular system urinary bladder liver thyroid gland	liver thyroid gland urinary bladder vascular system	Breast Neoplasm Urinary Bladder Neoplasm **Lung Neoplasm** Adenocarcinoma Carcinoma **Liver Neoplasm**
4,4'-Methylenebis(2-chloroaniline)	101-14-4					Rat	Female	SD	Diet	67	67	Positive	Liver	Adenoma - hepatocellular									
4,4'-Methylenebis(2-chloroaniline)	101-14-4					Rat	Female	SD	Diet	102	102	Positive	Liver	Adenoma - hepatocellular									
4,4'-Methylenebis(2-chloroaniline)	101-14-4					Rat	Male	SD	Diet	78	104	Positive	Liver	Carcinoma - hepatocellular									
4,4'-Methylenebis(2-methylaniline)	838-88-0	C1=1(C(=CC=C(C=1)C(=2C=C(C)(=CC)=CC=2)N)C)N)C	급성 독성(경구) : 구분4 원핀 는 순위정는 자격성 : 구분2A(GB) 피부 과민성 : 구분1(1A/1B) **발암성 : 구분1B** 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	19, 23, 27, **29**, **30**, 34, 36, 52, 53, 57, 58, 61, 62, 67, 72, 111, 112, 117, 120, 163, **166**, **167**, 187, **200**, 307	Cancer slope factor: 0.00026 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Female	SD	Diet	82	82	Positive	Liver	Adenoma - hepatocellular	-					liver spleen ear Zymbals gland vascular system thyroid gland urinary bladder lung Malloni head cancers skin	liver lung thyroid gland urinary bladder mammary gland clitoral gland ear Zymbals gland	kidney vascular system urinary bladder thyroid gland liver	liver vascular system thyroid gland urinary bladder	Neoplasm, Experimental
4,4'-Methylenebis(2-methylaniline)	838-88-0					Rat	Male	SD	Diet	68	68	Positive	Liver	Adenoma - hepatocellular									
4,4'-Methylenebis(2-chloroaniline); monohydrochloride	64091-29-2	C1=1(C(=CC(=C(C=1)C(C2=CC(=C(C=C2)N)Cl)N)Cl				Mouse	Female	CD-1 HsMcCR	Diet	77	90	Positive	Liver	Hepatoma									-
4,4'-Methylenebis(2-chloroaniline); monohydrochloride	64091-29-2					Mouse	Male	CD-1 HsMcCR	Diet	77	94	Not specified	Liver	Multiple tumour types									
4,4'-Methylenebis(2-chloroaniline); monohydrochloride	64091-29-2					Rat	Male	SD	Diet	77	98	Not specified	Liver	Multiple tumour types									
4,4'-Methylenedianilinium dichloride	13552-44-8	C=2(N)C=CC(CC1=CC=C(N)C=C1)=CC=2Cl.Cl	**발암성 : 구분1B** 특정표적장기 독성(반복 노출) : 구분2	-	Cancer slope factor: 0.00046 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Drinking water	103	104	Positive	Liver	Adenoma - hepatocellular					ear Zymbald gland thyroid gland spleen liver vascular system	thyroid gland liver lung **uterus** ear Zymbals gland urinary bladder mammary gland clitoral gland hematopoietic system	thyroid gland urinary bladder kidney vascular system liver	liver thyroid gland urinary bladder vascular system hematopoietic system **ovary**	-
4,4'-Methylenedianilinium dichloride	13552-44-8					Mouse	Male	B6C3F1	Drinking water	103	104	Positive	Adrenal gland	Pheochromocytoma									
4,4'-Methylenedianilinium dichloride	13552-44-8					Rat	Female	Fischer 344	Drinking water	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4,4'-Methylenedianilinium dichloride	13552-44-8					Rat	Male	Fischer 344	Drinking water	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4,4'-Oxydianiline	101-80-4	O(C1=CC=C(N)C=C1)C2=CC=C(N)C=C2	급성 독성(경구) : 구분3 급성 독성(흡입) : 구분3 급성 독성(흡입: 분진/미스트) : 구분3 생식세포 변이원성 : 구분1B **발암성 : 구분1B** 생식독성 : 구분2 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분2	6, 7, 18, 21, 23, **29**, **30**, 36, 37, 41, 51, 52, 53, 57, 58, 61, 67, 112, 122, 123, 131, 150, 153, 163, **166**, **167**, **200**, 310, 318	Cancer slope factor: 4e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Positive	Harderian gland	Adenoma	TPO	CCR6 AMH|R2 DNAJG2 ADAM19 SYNPK	HTATIP2 MGST1 SOD3 TNNI3K2 CYTIP	hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa2173 630431 TPO; thyroid peroxidase hsa04918 Thyroid hormone synthesis - Homo sapiens (human) (1) hsa2173 630431 TPO; thyroid peroxidase hsa05320 Autoimmune thyroid disease - Homo sapiens (human) (1) hsa2173 630431 TPO; thyroid peroxidase	thyroid gland spleen ear Zymbals gland **liver** urinary bladder	thyroid gland urinary bladder **uterus** ear Zymbals gland **liver** hematopoietic system clitoral gland lung kidney stomach	thyroid gland urinary bladder **liver** vascular system stomach	thyroid gland urinary bladder **liver** vascular system stomach **ovary** hematopoietic system pituitary gland	**Liver Neoplasm, Experimental** Thyroid Neoplasm
4,4'-Oxydianiline	101-80-4					Mouse	Male	B6C3F1	Diet	103	105	Positive	Harderian gland	Adenoma									
4,4'-Oxydianiline	101-80-4					Rat	Female	Fischer 344	Diet	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4,4'-Oxydianiline	101-80-4					Rat	Male	Fischer 344	Diet	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4,4'-Thiodianiline	139-65-1	S(C1=CC=C(N)C=C1)C2=CC=C(N)C=C2	급성 독성(경구) : 구분4 생식세포 변이원성 : 구분2 **발암성 : 구분1B** 생식독성 : 구분2	8, 11, 21, **29**, **30**, 34, 36, 41, 52, 53, 57, 58, 60, 61, 67, 72, 107, 112, 122, 123, 131, 150, 163, **166**, **167**, **200**, 220, 310	Cancer slope factor: 0.00043 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	78	91	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-					thyroid gland spleen ear Zymbals gland large intestine liver	thyroid gland ear Zymbals gland **uterus** urinary bladder hematopoietic system kidney **lung** clitoral gland	thyroid gland urinary bladder liver vascular system	thyroid gland liver urinary bladder vascular system hematopoietic system	Adenocarcinoma Adenoma Carcinoma, Hepatocellular **Lung Neoplasm** Thyroid Neoplasm
4,4'-Thiodianiline	139-65-1					Mouse	Male	B6C3F1	Diet	78	91	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular									
4,4'-Thiodianiline	139-65-1					Rat	Female	Fischer 344	Diet	70	104	Positive	Ear canal	Carcinoma - squamous cell | Papillomasquamous cell									
4,4'-Thiodianiline	139-65-1					Rat	Male	Fischer 344	Diet	68	104	Positive	Colon	Adenocarcinoma									
4,4'-Thiodianiline	139-65-1					Rat	Male	Fischer 344/DuCr[]	Diet	52	52	Positive	Liver	Carcinoma - hepatocellular									
4-(2-Hydroxyethylamino)-2-(5-nitro-2-thienyl)quinazoline	33389-36-5	C1[N]=[c]=[C](C[]=[]=CC=CS1)C=2N=CC=3C(N=2)=CC=CC=3)NCCO		-	-	Rat	Female	SD	Diet	46	66	Positive	Intestine	Leiomyosarcoma	-				large intestine	all tumor bearing animals	thyroid gland	-	-
4-(2-Hydroxy-3-[(isopropyl)amino]propoxy)phenylacetamide hydrochloride	51706-40-2	C1=1(C(=CC(=C1)C(N)=O)OCC(ON)C)C)O)Cl	-	-	-	Rat	Female	Fischer 344	Gavage	89	91	Negative	Liver	Multiple tumour types	-				all tumor bearing animals	stomach	kidney	-	-
4-(2-Hydroxy-3-[(isopropyl)amino]propoxy)phenylacetamide hydrochloride	51706-40-2					Rat	Male	Fischer 344	Gavage	89	91	Negative	Liver	Multiple tumour types									
4-(p-(Methylnitrosamino)styryl)quinoline	16499-10-8	C1(=CC=NC=2C1=CC=CC=2)C=4C=CC=3(C=CC(=C(N)N=O)C	-	-	-	Rat	Female	Fischer 344	Diet	34	52	Positive	Liver	Nodule - hyperplastic	-				liver ear Zymbals gland skin esophagus large intestine stomach	liver small intestine all tumor bearing animals	lung stomach	lung	-
4-(p-(Methylnitrosamino)styryl)quinoline	16499-10-8					Rat	Male	Fischer 344	Diet	34	52	Positive	Liver	Carcinoma									
4-Acetylaminofluorene	28322-03-3	N(C(C)=O)C1=CC=C2=C1C=2(C=CC=C2)=C	-	-	-	Rat	Female	Buffalo	Diet	62	97	Not specified	Mammary gland	Adenofibroma	FAS ABCB18 ACMSD ACSL1 AGN	HEATR3 ALDH1B1 TBC1D9 CXORF41 WWP2	RNF12 ECT2 RACGAP1 CSF72 TMEM38B	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1300 13 KEGG02 ACMSD; aminocarboxymuconate semialdehyde decarboxylase hsa2181 631857 ACSL3; acyl-CoA synthetase long chain family member 3 hsa00071 Fatty acid degradation - Homo sapiens (human) (1) hsa2181 631857 ACSL3; acyl-CoA synthetase long chain family member 3 hsa04146 Peroxisome - Homo sapiens (human) (1) hsa2181 631857 ACSL3; acyl-CoA synthetase long chain family member 3	kidney skin stomach liver spleen urinary bladder	ear Zymbals gland mammary gland liver urinary bladder **uterus** lung small intestine	urinary bladder thyroid gland kidney	urinary bladder stomach **ovary** liver	-
4-Acetylaminosphenylacetic acid	18699-02-0	C1=1(C(=CC(=C1)C(O)(O)=O)N)C)=O	-	**29**, **30**, 52, 53, 67, 112, **165**, **167**, **200**	-	Mouse	Female	B6C3F1	Diet	78	78	Negative	Liver	Adenoma - hepatocellular	-				kidney urinary bladder skin stomach nasal cavity	ear Zymbals gland urinary bladder mammary gland kidney small intestine	kidney thyroid gland urinary bladder lung	urinary bladder lung liver	-
4-Acetylaminosphenylacetic acid	18699-02-0					Mouse	Male	B6C3F1	Diet	78	78	Negative	Liver	Adenoma - hepatocellular									
4-Acetylaminosphenylacetic acid	18699-02-0					Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Multiple tumour types									
4-Acetylaminosphenylacetic acid	18699-02-0					Rat	Male	Fischer 344	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
4-Allylanisole	140-67-0	C1=1(C=CC(=C1)C(O)(C)C)=C	급성 독성(경구) : 구분4 피부 부식성/자극성 자격성 : 구분2 피부 과민성 : 구분1(1A/1B) 생식세포 변이원성 : 구분2 특정표적장기 독성(반복 노출) : 구분2	**29**, **30**, 52, 53, 67, 112, **165**, **167**, **200**	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: clastogenic	Mouse	Female	CD1	Diet	51	86	Positive	Liver	Hepatoma	CYP1A2 CCNB1 CCNE1 PCNA AnkB	EJPS TRAM SOD1 ITGB8 CCL5	AKR1B10 SOD3 MGST1 TNNI3K2 ITGA6	hsa04110 Cell cycle - Homo sapiens (human) (3) hsa5111 KO4802 PCNA; proliferating cell nuclear antigen hsa891 KO5868 CCNB1; cyclin B1 hsa898 KO4624 CCNE1; cyclin E1 hsa04115 p53 signaling pathway - Homo sapiens (human) (2) hsa891 KO5868 CCNB1; cyclin B1 hsa898 KO4624 CCNE1; cyclin E1 hsa04114 Oocyte meiosis - Homo sapiens (human) (2) hsa891 KO5868 CCNB1; cyclin B1 hsa898 KO4624 CCNE1; cyclin E1	stomach kidney nasal cavity hematopoietic system liver large intestine	stomach nasal cavity liver	stomach liver urinary bladder lung vascular system	liver **ovary** urinary bladder stomach	Liver Neoplasm, Experimental Carcinoma, Hepatocellular **Liver Neoplasm**

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
4-Amino-2-nitrophenol	119-34-6	[N+]([C-]1C=CN(C=CC=1O)[O-])=O	경구 독성(분진) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(자) 만성 수생환경 유해성 : 구분3	21, 41, 57, 61, 131, 150, 210	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	ALDH1A1 CD86 KRT14	CCR6 CIAS1 PDGFRL RAB20 DSE	MGST1 SOD3 TINN02 AKR1B10 CYP3F	hsa05206 MicroRNAs in cancer - Homo sapiens (human) (1) hsa960 KEA256 CD48 CD48 molecule (Indian blood group) hsa04512 ECM-receptor interaction - Homo sapiens (human) (1) hsa960 KEA256 CD48 CD48 molecule (Indian blood group) hsa05160 Epstein-Barr virus infection - Homo sapiens (human) (1) hsa960 KEA256 CD48 CD48 molecule (Indian blood group)	urinary bladder kidney spleen ear Zymbals gland thyroid gland large intestine skin liver hematopoietic system stomach	urinary bladder hematopoietic system **uterus** ear Zymbals gland kidney clitoral gland liver stomach lung thyroid gland mammary gland small intestine	thyroid gland kidney vascular system liver urinary bladder hematopoietic system	**ovary** thyroid gland vascular system liver urinary bladder hematopoietic system	-
4-Amino-2-nitrophenol	119-34-6					Mouse	Male	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Amino-2-nitrophenol	119-34-6					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Amino-2-nitrophenol	119-34-6					Rat	Male	Fischer 344	Diet	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Biphenylamine	92-67-1	C=2(C1=CC=CC=C1)C=CC=CC=C2N	경구 독성(분진) : 구분4 생식세포 변이원성 : 구분2 **발암성 : 구분1A**	21, 29, 30, 41, 52, 53, 57, 67, 152, 171, 150, **165**, **167**, **200**, 210	Cancer slope factor: 0.006 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: NTP ROC Known Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	(C57 x B5F1	Gavage	50	70	Positive	Liver	Hepatoma - malignant	TP53 NAT2 NAT1 Tnnc2 PARP11 H2AX	CCR6 DNAG2 AMH R2 TIP1 MHC5C	HTATIP2 MGST1 CCR5 BCL2A1 AKR1B10	hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (4) hsa10 K00622 NAT2; N-acetyltransferase 2 hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1571 K07415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa9 K00622 NAT1; N-acetyltransferase 1 hsa01100 Metabolic pathways - Homo sapiens (human) (4) hsa10 K00622 NAT2; N-acetyltransferase 2 hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1571 K07415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa9 K00622 NAT1; N-acetyltransferase 1 hsa00232 Caffeine metabolism - Homo sapiens (human) (2) hsa10 K00622 NAT2; N-acetyltransferase 2 hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa9 K00622 NAT1; N-acetyltransferase 1	spleen ear Zymbals gland thyroid gland **urinary bladder**	**urinary bladder** **uterus** ear Zymbals gland hematopoietic system thyroid gland clitoral gland liver **lung** kidney mammary gland nasal cavity	thyroid gland **urinary bladder** liver vascular system stomach **lung** stomach	thyroid gland **urinary bladder** liver vascular system **ovary** hematopoietic system stomach **lung** pituitary gland	Breast Neoplasms Cell Transformation, Neoplastic **Lung Neoplasms** Colorectal Neoplasms Urinary Bladder Neoplasms **Liver Neoplasms, Experimental**
4-Biphenylamine	92-67-1					Mouse	Male	(C57 x B5F1	Gavage	50	70	Positive	Liver	Hepatoma - malignant									
4-Biphenylamine	92-67-1					Mouse	Female	Ala x B	Gavage	20	94	Positive	Liver	Hepatoma									
4-Biphenylamine	92-67-1					Mouse	Male	Ala x B	Gavage	20	94	Positive	Liver	Hepatoma									
4-Bis(2-Hydroxyethyl)amino-2-(5-nitro-2-thiazolyl)azoanisole	33972-39-3	C1[N+](=O)[O-]c(S)n(c=1)N=C(C2=CC=CC=C2N)-3)N(CC)(C)CO		-		Rat	Male	SD	Diet	50	52	Positive	Mammary gland	Adenocarcinoma	-								
4-Chloro-2-methylaniline hydrochloride	3165-93-3	C1=CC(=CC=C1C)N.Cl	생식세포 변이원성 : 구분2 발암성 : 구분1B 특정표적장기 독성(1회 노출) : 구분1 특정표적기기 독성(반복 노출) : 구분1	8, 11, 21, 41, 57, 60, 61, 131, 150, 210	Carcinogenicity data available NTP ROC - Reasonably Anticipated To Be Human Carcinogen	Mouse	Female	B6C3F1	Diet	95	99	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-								
4-Chloro-2-methylaniline hydrochloride	3165-93-3					Mouse	Male	B6C3F1	Diet	99	99	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chloro-2-methylaniline hydrochloride	3165-93-3					Mouse	Female	CD-1 HaMcRCR	Diet	51	60	Positive	Liver	Multiple tumour types									
4-Chloro-2-methylaniline hydrochloride	3165-93-3					Mouse	Male	CD-1 HaMcRCR	Diet	55	60	Positive	Liver	Multiple tumour types									
4-Chloro-2-methylaniline hydrochloride	3165-93-3					Rat	Female	Fischer 344	Diet	107	107	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chloro-2-methylaniline hydrochloride	3165-93-3					Rat	Male	Fischer 344	Diet	107	107	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chloro-2-methylaniline hydrochloride	3165-93-3					Rat	Male	SD	Diet	77	98	Negative	Liver	Multiple tumour types									
4-Chloro-2-methylphenoxyacetic acid	94-74-6	C1(=CC=C(C(=C1C)OCC(O)=O)Cl	경구 독성(분진) : 구분4 경구 독성(물질 분진/미스트) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2 **발암성 : 구분2** 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분3 특정표적장기 독성(1회 노출) : 구분3(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분1 경성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 16, 21, 27, 34, 36, 57, 58, 60, 72, 102, 111, 117, 121, 163, 187, 207	Carcinogenicity data available SPA CPP-Not Likely to Be Carcinogenic in Humans Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6C3F1	Diet	52	52	Negative	Liver	Multiple tumour types	CLCN1 CGB3 CLCNKA FGB Tnf AJM	-	-	hsa05171 Coronavirus disease - COVID-19 - Homo sapiens (human) (2) hsa2244 K03904 FGB; fibrinogen beta chain hsa7124 K03156 TNF; tumor necrosis factor hsa05140 Leishmaniasis - Homo sapiens (human) (1) hsa7124 K03156 TNF; tumor necrosis factor hsa05132 Salmonella infection - Homo sapiens (human) (1) hsa7124 K03156 TNF; tumor necrosis factor	vascular system kidney stomach	-	kidney liver vascular system	liver	Lymphoma, Non-Hodgkin
4-Chloro-2-methylphenoxyacetic acid	94-74-6					Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
4-Chloro-2-methylphenoxyacetic acid	94-74-6					Mouse	Male	B6C3F1	Diet	52	52	Negative	Liver	Multiple tumour types									
4-Chloro-2-methylphenoxyacetic acid	94-74-6					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular									
4-Chloro-3-phenylenediamine	5131-60-2	C1=CC(=CC(=C1C)N)N	만성 수생환경 유해성 : 구분2	21, 29, 30, 36, 41, 52, 53, 57, 67, 152, 131, 150, **165**, **167**, **200**, 210	Carcinogenicity data available IRAC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	95	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	-				ear Zymbals gland thyroid gland spleen liver hematopoietic system vascular system	liver thyroid gland lung urinary bladder **uterus** mammary gland ear Zymbals gland clitoral gland	liver thyroid gland vascular system urinary bladder	liver thyroid gland urinary bladder vascular system hematopoietic system	-
4-Chloro-3-phenylenediamine	5131-60-2					Mouse	Male	B6C3F1	Diet	78	94	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chloro-3-phenylenediamine	5131-60-2					Rat	Female	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic | Pituitary tumours - benign									
4-Chloro-3-phenylenediamine	5131-60-2					Rat	Male	Fischer 344	Diet	78	104	Positive	Adrenal gland	Pheochromocytoma									
4-Chloro-alpha-ethyl-alpha-phenyl-benzenemethanol carbamate	10473-70-8	[O](C(PC)(C1=CC=CC=C1)C2=CC=CC=C2)C(=O)N)=O		-		Rat	Male	Harlan	Diet	72	94	Positive	Brain	Multiple tumour types	-				-		liver	-	-
4-Chloroaniline	106-47-8	C1(N)=CC=C(Cl)C=C1	경구 독성(분진) : 구분3 경구 독성(물질 분진/미스트) : 구분4 경구 독성(물질 분진/미스트) : 구분3(TA/1B) 피부 과민성 : 구분1(TA/1B) 생식세포 변이원성 : 구분2 **발암성 : 구분1B** 특정표적장기 독성(1회 노출) : 구분1 특정표적장기 독성(반복 노출) : 구분1 경성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	21, 29, 30, 41, 52, 53, 57, 67, 152, 131, 150, **165**, **167**, **200**, 210	Carcinogenicity data available CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	NRS1 NAT2 H2AX HGFTOL	AMH R2 CCR6 DNAG2 TIP1 MHC5C	MGST1 SOD3 CYP3F CCR5 TINN02	hsa05204 Alcoholism - Homo sapiens (human) (1) hsa3014 K11251 H2AX; H2A.X variant histone hsa5204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (1) hsa10 K00622 NAT2; N-acetyltransferase 2 hsa04613 Neutrophil extracellular trap formation - Homo sapiens (human) (1) hsa3014 K11251 H2AX; H2A.X variant histone	thyroid gland spleen ear Zymbals gland liver kidney urinary bladder	urinary bladder thyroid gland **uterus** liver ear Zymbals gland lung hematopoietic system kidney clitoral gland	liver vascular system urinary bladder thyroid gland lung	thyroid gland liver urinary bladder vascular system hematopoietic system lung	Hemangiosarcoma
4-Chloroaniline	106-47-8					Mouse	Male	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chloroaniline	106-47-8					Rat	Female	Fischer 344	Diet	78	102	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chloroaniline	106-47-8					Rat	Male	Fischer 344	Diet	78	102	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chlorobenzotrifluoride	98-56-6	C1=C(C=CC(=C1C(F)(F)F)C)	인화성 액체 : 구분2 경구 독성(분진) : 구분4 특정표적장기 독성(반복 노출) : 구분2	29, 30, 52, 53, 67, 152, **165**, **167**, **200**	Cancer slope factor: 8.6e-06 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: IRIS/TX (ORNL)-inadequate for an assessment of carcinogenic potential Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1/N	Inhalation	96 d	90 d	Not specified		IFNG	CYP11A1 IRF7 MANSC1 TAGLN WDR67		ERBB2 BEL TMSB4X ASAH1 NEFH2	hsa05205 PD-L1 expression and PD-1 checkpoint pathway in cancer - Homo sapiens (human) (1) hsa3458 K04687 IFNG; interferon gamma hsa04066 HIF-1 signaling pathway - Homo sapiens (human) (1) hsa3458 K04687 IFNG; interferon gamma hsa04612 Antigen processing and presentation - Homo sapiens (human) (1) hsa3458 K04687 IFNG; interferon gamma	thyroid gland nasal cavity oral cavity Multiori head cancers	liver	stomach liver vascular system	liver stomach lung thyroid gland urinary bladder vascular system peritoneal cavity	-
4-Chloronitrobenzene	100-00-5	C1=C(C=CC(=C1C)N+[O][O-])=O(Cl)	경구 독성(분진) : 구분4 경구 독성(분진) : 구분4 생식세포 변이원성 : 구분2 생식독성 : 구분2 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분2	21, 28, 57, 63, 100, 101, 102, 103	Carcinogenicity data available CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	CD-1 HaMcRCR	Diet	73	90	Positive	Liver	Multiple tumour types	CLTA1 ASNS GSTM2 ALDH	DSE CYP11A1 CCR7 CIAS1 PDGFRL	MGST1 SOD3 CCR5 CYP3F TINN02	hsa00480 Glutathione metabolism - Homo sapiens (human) (2) hsa2938 K00799 GSTA2; glutathione S-transferase alpha 2 hsa2946 K00799 GSTM2; glutathione S-transferase mu 2 hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa2938 K00799 GSTA2; glutathione S-transferase alpha 2 hsa2946 K00799 GSTM2; glutathione S-transferase mu 2 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2938 K00799 GSTA2; glutathione S-transferase alpha 2 hsa2946 K00799 GSTM2; glutathione S-transferase mu 2	thyroid gland kidney liver ear Zymbals gland hematopoietic system spleen urinary bladder lung skin stomach	liver **uterus** urinary bladder kidney hematopoietic system lung clitoral gland mammary gland stomach thyroid gland	vascular system liver thyroid gland kidney lung urinary bladder	vascular system liver urinary bladder thyroid gland hematopoietic system **ovary** stomach	-
4-Chloronitrobenzene	100-00-5					Mouse	Male	CD-1 HaMcRCR	Diet	73	86	Positive	Liver	Hepatoma									
4-Chloronitrobenzene	100-00-5					Rat	Male	SD	Diet	77	98	Negative	Liver	Multiple tumour types									
4-Chloro-o-phenylenediamine	95-83-0	C1=C(C=C(C=C1C)N)N	생식세포 변이원성 : 구분2 **발암성 : 구분2**	7, 8, 11, 19, 21, 23, 25, 27, 28, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 63, 67, 72, 100, 101, 102, 103, 111, 112, 117, 122, 123, 139, 148, 150, 152, 163, **165**, **167**, 177, 187, **200**, 203, 207, 210	Cancer slope factor: 4.6e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	95	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	F10 OLFML2A PCSK1N TUC1	AMH R2 TIP1 MHC5C DNAG2 MANSC1	MGST1 SOD3 TINN02 CYP3F AKR1B10		urinary bladder thyroid gland stomach **uterus** liver lung clitoral gland ear Zymbals gland kidney	liver vascular system urinary bladder thyroid gland	liver thyroid gland vascular system urinary bladder hematopoietic system	-
4-Chloro-o-phenylenediamine	95-83-0					Mouse	Male	B6C3F1	Diet	78	95	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular									
4-Chloro-o-phenylenediamine	95-83-0					Rat	Female	Fischer 344	Diet	78	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Chloro-o-phenylenediamine	95-83-0					Rat	Male	Fischer 344	Diet	78	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
4-Hexylresorcinol	136-77-6	C1=C(C=C(C(=C1)C(CCCCCC)O)O)	자료없음	2, 8, 11, 14, 16, 20, 22, 25, 27, 28, 29, 30, 33, 34, 36, 46, 52, 53, 57, 58, 60, 61, 63, 64, 66, 67, 71, 72, 100, 101, 102, 103, 111, 112, 117, 122, 123, 131, 148, 150, 153, 163, 165, 167, 177, 187, 200, 214, 220, 307, 318	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Gavage	102	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	TGM2 AR CAT ESR1 GSR	LAMP3 ZFANOS EECTA6 HSPA6 ENO2	EGR3 FGR EKOSC4 ALDOA OS9	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:2099 KEGG:5241; estrogen receptor 1 hsa:367 KEGG:7; AR; androgen receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:2099 KEGG:5241; estrogen receptor 1 hsa:367 KEGG:7; AR; androgen receptor hsa01200 Carbon metabolism - Homo sapiens (human) (1) hsa:847 KEGG:1; CAT; catalase	urinary bladder stomach hematopoietic system nasal cavity	stomach urinary bladder hematopoietic system ear Zymbals gland	kidney stomach thyroid gland liver	pituitary gland thyroid gland **ovary** liver	-
4-Hexylresorcinol	136-77-6					Mouse	Male	B6C3F1	Gavage	102	104	Not specified	Adrenal gland medulla	Pheochromocytoma									
4-Hexylresorcinol	136-77-6					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Hexylresorcinol	136-77-6					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Hydroxybenzoic acid	619-67-0	C1=C(C=CC(=C1)C(=O)=O)NN	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(구) 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	Swiss	Gavage	40	55	Negative	lung	Multiple tumour types	-				spleen	kidney hematopoietic system mammary gland clitoral gland	lung vascular system	hematopoietic system lung stomach liver	-
4-Hydroxyphenyl retinoamide	65646-68-6	C(=O)(CCCCC)c1ccc(cc1)c(c)c(c)c(c)=O)NC2=CC=C(C=C2)O)C)C)C	-	7, 14, 16, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 200, 214, 307, 318	-	Mouse	Female	MMTV/NEU (Tg/Nk)	Diet	26	26	Not specified			TNF HMOX1 PARP1 CASP3 NRAS PIAAP1	IGFBP5 BARD1 CD58 GART CCDC50	IL10RB PCR UBE2C STAGA1 PGD	hsa05206 MicroRNAs in cancer - Homo sapiens (human) (2) hsa:3162 KEGG:10; HMOX1; heme oxygenase 1 hsa:836 KEGG:187; CASP3; caspase 3 hsa04010 MAPK signaling pathway - Homo sapiens (human) (2) hsa:3164 KEGG:4893; NRAS; nuclear receptor subfamily 4 group A member 1 hsa:836 KEGG:187; CASP3; caspase 3 hsa04210 Apoptosis - Homo sapiens (human) (2) hsa:142 KEGG:10; PARP1; poly(ADP-ribose) polymerase 1 hsa:836 KEGG:187; CASP3; caspase 3	-	-	kidney thyroid gland urinary bladder	-	Hemangiosarcoma Leukemia Prostatic Neoplasm Carcinoma, Hepatocellular Breast Neoplasm
4-Isopropoxy-N-phenylaniline	101-73-5	C1=C(C=CC(=C1)N(C2=CC=CC=C2)OC)C)C	-	-	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Angioma	-				stomach spleen liver	nasal cavity stomach	urinary bladder kidney liver thyroid gland	urinary bladder thyroid gland	-
4-Isopropoxy-N-phenylaniline	101-73-5					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-Isopropoxy-N-phenylaniline	101-73-5					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-Isopropoxy-N-phenylaniline	101-73-5					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
4-Methoxy-2-methylaniline	102-50-1	C1=C(C)=CC=C1OC)N)C	피부 부식성/피부 자극성 - 구분2 만성 수생환경 유해성 - 구분2	8, 11, 29, 30, 52, 53, 58, 60, 61, 67, 107, 112, 165, 167, 200	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	53	93	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	-				urinary bladder kidney ear Zymbals gland spleen liver stomach skin large intestine vascular system nasal cavity hematopoietic system	urinary bladder stomach ear Zymbals gland clitoral gland liver **uterus** mammary gland hematopoietic system nasal cavity	urinary bladder vascular system stomach liver thyroid gland	urinary bladder liver vascular system thyroid gland	-
4-Methoxy-2-methylaniline	102-50-1					Mouse	Male	B6C3F1	Gavage	53	93	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Methoxy-2-methylaniline	102-50-1					Rat	Female	Fischer 344	Gavage	77	109	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Methoxy-2-methylaniline	102-50-1					Rat	Male	Fischer 344	Gavage	77	109	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Methoxyaniline hydrochloride	20265-97-8	C1=C(C)=CC=C1OC)N.Cl		8, 11, 21, 29, 30, 41, 52, 53, 57, 60, 67, 112, 131, 150, 165, 167, 200, 310	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				urinary bladder ear Zymbals gland spleen kidney stomach hematopoietic system skin large intestine liver thyroid gland	urinary bladder hematopoietic system **uterus** ear Zymbals gland stomach thyroid gland clitoral gland kidney nasal cavity mammary gland	urinary bladder thyroid gland vascular system liver stomach	urinary bladder thyroid gland liver vascular system hematopoietic system	-
4-Methoxyaniline hydrochloride	20265-97-8					Mouse	Male	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Methoxyaniline hydrochloride	20265-97-8					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Methoxyaniline hydrochloride	20265-97-8					Rat	Male	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Methoxyphenol	150-76-5	C1=C(C)=CC=C1OC)O	급성 독성(경구) - 구분4 심한 눈 손상성/눈 자극성 - 구분2A(구) 피부 과민성 - 구분1(1A/1B) 생식독성 - 구분2	61	Genotoxicity Data: non-genotoxic	Rat	Female	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell					urinary bladder stomach kidney hematopoietic system nasal cavity ear Zymbals gland vascular system large intestine skin	urinary bladder stomach hematopoietic system nasal cavity kidney **uterus**	stomach kidney urinary bladder thyroid gland	**ovary** thyroid gland pituitary gland urinary bladder	-
4-Methoxyphenol	150-76-5					Rat	Male	Fischer 344/DuCr	Diet	51	52	Not specified	Forestomach	Papilloma									
4-Methoxyphenol	150-76-5					Rat	Male	Fischer 344/DuCr	Diet	51	52	Negative	Forestomach	Multiple tumour types									
4-Methoxyphenol	150-76-5					Rat	Male	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell									
4-Methylaniline hydrochloride	540-23-8	C=1)N(C)=CC(=C=1)C.Cl	급성 독성(경구) - 구분3 급성 독성(경피) - 구분3 급성 독성(흡입) 분진/미스트 - 구분3 심한 눈 손상성/눈 자극성 - 구분2A(구) 피부 과민성 - 구분1(1A/1B) 생식세포 변이원성 - 구분2 **발암성 - 구분2** 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분1	21, 29, 30, 41, 52, 53, 57, 67, 112, 131, 150, 165, 167, 200, 310	-	Mouse	Female	CD-1 HsM/ICR	Diet	77	98	Positive	Liver	Hepatoma	-				spleen ear Zymbals gland liver urinary bladder thyroid gland	urinary bladder ear Zymbals gland thyroid gland clitoral gland **uterus** liver lung mammary gland hematopoietic system stomach nasal cavity small intestine	thyroid gland urinary bladder vascular system liver lung kidney	thyroid gland urinary bladder vascular system liver hematopoietic system pituitary gland **ovary**	-
4-Methylaniline hydrochloride	540-23-8					Mouse	Male	CD-1 HsM/ICR	Diet	77	98	Positive	Liver	Hepatoma									
4-Methylaniline hydrochloride	540-23-8					Rat	Male	SD	Diet	77	98	Negative	Liver	Multiple tumour types									
4-Methylphenylurea	622-51-5	C1(=C(C=C(C=C1)C)NC(N)=O	-	-	-	Mouse	Female	C57BL/6	Diet	52	69	Negative	Liver	Carcinoma - hepatocellular	-				spleen kidney stomach skin large intestine ear Zymbals gland lung urinary bladder thyroid gland	**uterus** small intestine ear Zymbals gland mammary gland hematopoietic system lung stomach urinary bladder	urinary bladder kidney	urinary bladder **ovary** hematopoietic system thyroid gland	-
4-Methylphenylurea	622-51-5					Mouse	Male	C57BL/6	Diet	52	69	Positive	Liver	Carcinoma - hepatocellular									
4-Methylphenylurea	622-51-5					Rat	Female	Fischer 344	Diet	52	69	Negative	Liver	Multiple tumour types									
4-Methylphenylurea	622-51-5					Rat	Male	Fischer 344	Diet	52	69	Negative	Liver	Carcinoma - hepatocellular									
4-Methylpyrocatechol	452-86-8	C1(=C(C=C(C=C1)C)O)O	-	7, 14, 15, 21, 23, 25, 27, 29, 30, 36, 41, 46, 52, 53, 57, 61, 64, 66, 67, 71, 111, 112, 117, 122, 123, 131, 150, 153, 165, 167, 187, 200, 214, 307, 310, 318	-	Rat	Female	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell	BTC COMT INS1 NOS2 TNF	TRAM CTSD HYRX NCPP16 RNF12	FOXO1 EP300 OGG1 PLAG16 HIVEP1	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa:1312 KEGG:45; COMT; catechol-O-methyltransferase hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa04421 Apelin signaling pathway - Homo sapiens (human) (1) hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa00220 Arginine biosynthesis - Homo sapiens (human) (1) hsa:4843 K13241 NOS2; nitric oxide synthase 2	stomach urinary bladder kidney nasal cavity Malt0ns head-cancers spleen oral cavity vascular system liver	stomach urinary bladder nasal cavity clitoral gland small intestine liver	stomach kidney thyroid gland urinary bladder lung vascular system	**ovary** pituitary gland thyroid gland stomach vascular system urinary bladder	-
4-Methylpyrocatechol	452-86-8					Rat	Male	Fischer 344/DuCr	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell									
4-Methylstyrene	622-97-9	C1=C(C=CC(=C1)C=C)C	인화성 액체 - 구분3 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(구) 생식세포 변이원성 - 구분2 특정표적장기 독성(1회 노출) - 구분2(마취졸림) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	8, 11, 16, 23, 60, 111, 112, 187, 307	Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	Swiss	Gavage	78	83	Negative	Liver	Hepatoma	-				oral cavity spleen Malt0ns head-cancers stomach nasal cavity kidney ear Zymbals gland vascular system	mammary gland stomach nasal cavity oral cavity clitoral gland	lung stomach vascular system urinary bladder	**ovary** lung urinary bladder stomach pituitary gland	-
4-Methylstyrene	622-97-9					Mouse	Male	Swiss	Gavage	78	83	Negative	Liver	Hepatoma									
4-Morpholino-2-(5-nitro-2-thiosulpuoxazoline	58139-48-3	[Na+].[O-]S(=O)(=O)CCSC1=C(N=C(C=C)[N+](=O)[O-])=CC=C1NMCCOCCN=O				Rat	Female	SD	Diet	46	66	Positive	Multiple sites	Multiple tumour types						all tumor bearing animals			
4-Nitro-1,2-benzenediamine	99-56-9	C1(=C(C=C(C)=C1)N(N)N(=O)[O-])=O	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(구) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	21, 29, 30, 41, 52, 53, 57, 61, 67, 112, 131, 150, 165, 167, 200, 310	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	102	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	ABCB18 ACMSD ACSL1 AIN AKR1B10	CCR6 DSG CCR7 CAK1 DNAJG2	MGST1 AKR1B10 SOD3 FECH CYYIP	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa:130013 KEGG:82; aminocarboxymuconate semialdehyde decarboxylase hsa:2181 K01897 ACSL3; acyl-CoA synthetase long chain family member 3 hsa04714 Thermogenesis - Homo sapiens (human) (1) hsa:2181 K01897 ACSL3; acyl-CoA synthetase long chain family member 3 hsa04216 Ferroptosis - Homo sapiens (human) (1) hsa:2181 K01897 ACSL3; acyl-CoA synthetase long chain family member 3	ear Zymbals gland urinary bladder spleen thyroid gland kidney skin liver stomach	urinary bladder **uterus** clitoral gland lung hematopoietic system ear Zymbals gland kidney stomach mammary gland thyroid gland liver small intestine	thyroid gland vascular system urinary bladder liver kidney	liver vascular system **ovary** urinary bladder thyroid gland hematopoietic system stomach	-
4-Nitro-1,2-benzenediamine	99-56-9					Mouse	Male	B6C3F1	Diet	102	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
4-Nitro-1,2-benzenediamine	99-56-9					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitro-1,2-benzenediamine	99-56-9					Rat	Male	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitroaniline	100-01-6	[N+](=O)(C1=CC=C(N)C=C1)[O-]=O	경성 독성(분구) - 구분3 경성 독성(피부) - 구분2 특정표적장기 독성(반복 노출) - 구분2	**29**, **30**, 52, 53, 57, 67, 112, 131, **165**, **167**, **200**	Carcinogenicity data available: PPRTV (ORNL)- Suggestive evidence of carcinogenic potential Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	DPP7 CYP1A2 CASP3 CYP1A1 DPP4	CCR6 DNMT3J AMH R2 DSE CCR7	MGST1 CYYR CCR5 ARFRP1 SOD3	hsa00140: Steroid hormone biosynthesis - Homo sapiens (human) (2) hsa1543 607408: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 607409: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa00980: Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (2) hsa1543 607408: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 607409: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa05417: Lipid and atherosclerosis - Homo sapiens (human) (2) hsa1543 607408: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa836: 602187: CASP2; caspase 2	thyroid gland ear Zymbals gland spleen kidney urinary bladder skin liver	**uterus** urinary bladder clitoral gland ear Zymbals gland hematopoietic system lung thyroid gland kidney mammary gland liver small intestine stomach	thyroid gland urinary bladder vascular system liver lung kidney	liver vascular system thyroid gland urinary bladder **ovary** hematopoietic system stomach	Hemangiosarcoma
4-Nitroaniline	100-01-6					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitroaniline	100-01-6					Rat	Female	SD	Gavage	104	104	Negative	Liver	Carcinoma - hepatocellular									
4-Nitroaniline	100-01-6					Rat	Male	SD	Gavage	104	104	Negative	Liver	Carcinoma - hepatocellular									
4-Nitroanthranilic acid	619-17-0	C1(=CC=C(C=C1N(=O)=O)C(=O)O)O	-	8, 11, 21, **29**, **30**, 41, 52, 53, 57, 60, 61, 67, 112, 131, 150, **165**, **167**, **200**, 310	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	93	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				kidney urinary bladder spleen ear Zymbals gland skin liver thyroid gland	clitoral gland urinary bladder **uterus** lung mammary gland liver ear Zymbals gland	thyroid gland vascular system liver urinary bladder kidney stomach	liver vascular system hematopoietic system **ovary**	-
4-Nitroanthranilic acid	619-17-0					Mouse	Male	B6C3F1	Diet	78	93	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitroanthranilic acid	619-17-0					Rat	Female	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitroanthranilic acid	619-17-0					Rat	Male	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitrobenzoic acid	62-23-7	C1(=CC=C(C=C1[N+](=O)[O-])C(=O)O)O	경성 독성(분구) - 구분4	10	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	MAOB	CCDC93 STXT1A STAT3A TGF1 CAPRIN1	AKR1B10 TECH PTGR1 ITL PGD	hsa00340: Histidine metabolism - Homo sapiens (human) (1) hsa4129 600274: MAOB; monoamine oxidase B hsa05030: Cocaine addiction - Homo sapiens (human) (1) hsa4129 600274: MAOB; monoamine oxidase B hsa00330: Arginine and proline metabolism - Homo sapiens (human) (1) hsa4129 600274: MAOB; monoamine oxidase B	kidney thyroid gland spleen skin urinary bladder ear Zymbals gland hematopoietic system	clitoral gland kidney urinary bladder **uterus** hematopoietic system	thyroid gland kidney vascular system liver	**ovary** vascular system liver hematopoietic system stomach	-
4-Nitrobenzoic acid	62-23-7					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitrobenzoic acid	62-23-7					Rat	Female	Fischer 344	Diet	103	104	Positive	Clitoral gland	Adenoma - Adenoma - Adenoma									
4-Nitrobenzoic acid	62-23-7					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
4-Nitrophenol	100-02-7	[N+](C1=CC=C(C=C1)O)([O-])=O	경성 독성(분구) - 구분3 경성 독성(피부) - 구분4 경성 독성(흡입) 분진/미스트 - 구분4 피부 부식성/피부 자극성 - 구분2(A/B/C) 심한 눈 손상성/눈 자극성 - 구분1 피부 과민성 - 구분1(A/B) 특정표적장기 독성(1회 노출) - 구분1 특정표적장기 독성(반복 노출) - 구분1	19, 23, 57, 111, 117, 187, 307	Carcinogenicity data available: EPA OPP Group D Not Classifiable as to Human Carcinogenicity Genotoxicity Data: genotoxic	Mouse	Female	Swiss Webster	Dermal	522 d	730 d	Not specified	Adrenal gland cortex	Leukaemia - lymphocytic	**CYP2E1** SULT1A1	OAS1 CYP11A1 CCR6 PDGFRL RAB20	MGST1 CORO1C SOD1 PTGR1 TINNSG2		kidney urinary bladder thyroid gland stomach ear Zymbals gland hematopoietic system skin spleen liver	hematopoietic system urinary bladder stomach **uterus** kidney clitoral gland liver small intestine	thyroid gland kidney vascular system stomach liver urinary bladder	**ovary** thyroid gland vascular system hematopoietic system stomach pituitary gland liver urinary bladder	-
4-Nitrophenol	100-02-7					Mouse	Male	Swiss Webster	Dermal	76	104	Not specified	Adrenal gland cortex	Adenoma									
4-Nitroso-N-phenylaniline	156-10-5	C1=CC=CC(=C1N(C)=CC=CC=C2)N=O	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분3	7, 8, 14, 18, 22, 23, 27, 28, 30, 34, 36, 41, 51, 52, 53, 58, 61, 62, 64, 66, 67, 71, 72, 102, 111, 112, 117, 122, 123, 148, 150, 153, 163, 166, 167, 187, 200, 214, 220, 307, 318	Cancer slope factor: 6.3e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	53	92	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	CPN2S FUT7 LRC-00007 SFDN1 ZEICANS	MHCSC OAS1 TEF1 CTDSPL PIZDK1	KRT34 VAGN HTATIP2 SAT CASP2	hsa00230: Purine metabolism - Homo sapiens (human) (1) hsa2272 601532: FHIT; fragile histidine triad diadenosine triphosphatase hsa05222: Small cell lung cancer - Homo sapiens (human) (1) hsa2272 601532: FHIT; fragile histidine triad diadenosine triphosphatase hsa05223: Non-small cell lung cancer - Homo sapiens (human) (1) hsa2272 601532: FHIT; fragile histidine triad diadenosine triphosphatase	spleen liver urinary bladder all tumor bearing animals thyroid gland	urinary bladder **uterus** thyroid gland	liver urinary bladder thyroid gland	urinary bladder thyroid gland **ovary**	-
4-Nitroso-N-phenylaniline	156-10-5					Mouse	Male	B6C3F1	Diet	53	92	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular									
4-Nitroso-N-phenylaniline	156-10-5					Rat	Female	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitroso-N-phenylaniline	156-10-5					Rat	Male	Fischer 344	Diet	78	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitrotoluene	99-99-0	C1=C(C=CC(=C1)[N+](=O)[O-])C	경성 독성(흡입) - 구분3 경성 독성(피부) - 구분2(A/B) 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분3	8, 11, 57, 60	Carcinogenicity data available: PPRTV (ORNL)- Likely to be carcinogenic to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	CSN1 **GAS6** EGR1 **CYP2** JUNBA	CYP11A1 DSE OAS1 CCR7 CCR6	BCL2A1 EVGN SOD3 KRT34 TINNSG2	hsa04928: Parathyroid hormone synthesis, secretion and action - Homo sapiens (human) (2) hsa1956 604261: EGFR; epidermal growth factor receptor hsa1958 605003: EGR1; early growth response 1 hsa05224: Breast cancer - Homo sapiens (human) (2) hsa1956 604261: EGFR; epidermal growth factor receptor hsa2100 428851: ESR2; estrogen receptor 2 hsa05207: Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa1956 604261: EGFR; epidermal growth factor receptor hsa2100 428851: ESR2; estrogen receptor 2	spleen kidney liver ear Zymbals gland thyroid gland **skin** urinary bladder Maltoni head cancers oral cavity **lung** stomach vascular system hematopoietic system	clitoral gland **uterus** urinary bladder liver **lung** hematopoietic system mammary gland stomach ear Zymbals gland kidney vascular system	thyroid gland vascular system kidney urinary bladder **lung** liver	vascular system **ovary** urinary bladder liver hematopoietic system thyroid gland stomach	**Lung Neoplasms** Skin Neoplasms
4-Nitrotoluene	99-99-0					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-Nitrotoluene	99-99-0					Rat	Female	Fischer 344	Diet	105	105	Positive	Clitoral gland	Adenoma - Carcinoma									
4-Nitrotoluene	99-99-0					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
4-tert-Butylcatechol	98-29-3	C1=C(C(=CC(=C1O)O)C(C)C)C	경성 독성(흡입) - 구분4 피부 부식성/피부 자극성 - 구분1(A/B/C) 심한 눈 손상성/눈 자극성 - 구분1 피부 과민성 - 구분1(A/B) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분3	4, 7, 8, 11, 14, 18, 19, 21, 22, 23, 27, 28, 29, 30, 34, 36, 37, 41, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 100, 101, 102, 103, 107, 111, 112, 117, 122, 123, 131, 150, 153, 163, 166, 166, 167, 177, 187, 200, 214, 220, 307, 310, 318	Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	92 d	91 d	Not specified			CASP3 CASP9	HTRX RNF72 ITGB8 MANEC1 ZFAND5	PLAA5A HIVEP1 EP300 LPPR2 OGG1		stomach urinary bladder kidney nasal cavity	stomach urinary bladder thyroid gland	stomach kidney lung thyroid gland liver	pituitary gland **ovary** thyroid gland stomach	-
4-tert-Butylphenol	98-54-4	C1=C(C=CC(=C1C)C)C(C)(C)C	심한 눈 손상성/눈 자극성 - 구분2(2A/2B) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	6, 8, 11, 18, 29, 30, 34, 37, 51, 52, 53, 58, 60, 61, 67, 107, 112, 148, 166, 166, **167**, **200**, 214, 220, 307, 310, 318	Genotoxicity Data: non-genotoxic	Rat	Male	Fischer 344/DuCr	Diet	51	52	Not specified	Forestomach	Papilloma	**ESR1** PIGR1 **AR** IL1A TNF	WDR67 HYRX RNF72 ZFAND5 ITGB8	ABHD2 EDI1 GGH STMN1 GIRA1	hsa05164: Influenza A - Homo sapiens (human) (2) hsa3552 604283: IL1A; interleukin 1 alpha hsa5295 602649: PIKR1; phosphoinositide-3-kinase regulatory subunit 1 hsa04933: AGE-RAGE signaling pathway in diabetic complications - Homo sapiens (human) (2) hsa3552 604283: IL1A; interleukin 1 alpha hsa5295 602649: PIKR1; phosphoinositide-3-kinase regulatory subunit 1 hsa04380: Osteoclast differentiation - Homo sapiens (human) (2) hsa3552 604283: IL1A; interleukin 1 alpha hsa5295 602649: PIKR1; phosphoinositide-3-kinase regulatory subunit 1	stomach urinary bladder kidney nasal cavity Maltoni head cancers	stomach hematopoietic system thyroid gland urinary bladder	stomach urinary bladder liver lung	**ovary** pituitary gland thyroid gland stomach liver	-
4-Toluenesulphonamide	70-55-3	O=S(=O)(C=1C=CC(=CC=1)C)N	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	-	Genotoxicity Data: inconclusive	Mouse	Female	B6C3F1/N	Diet	15 d	14 d	Not specified			-				spleen Maltoni head cancers	urinary bladder	thyroid gland urinary bladder	urinary bladder thyroid gland	-
5,6-Dichloro-2-benzothiazolamine	24072-75-1	C1=C(C(=CC2=C1SC(=N2)N)C)Cl	만성 수생환경 유해성 - 구분2	-	-	Mouse	Female	B6C3F1	Diet	93 d	91 d	Not specified			-				thyroid gland spleen	stomach kidney lung urinary bladder mammary gland thyroid gland ear Zymbals gland	urinary bladder thyroid gland	thyroid gland hematopoietic system urinary bladder stomach	-
5,6-Dimethoxybergamottin/cytetin	65176-75-2	C3=C(C1=C(OC2=C(C1=O)C(=C(C=C2)OC(/C(C4=C3)O)C(C4=C3)O)C@@H]5)C@H]C=C(5)[H])H)OC	-	-	-	Rat	Male	ACI/n	Diet	38	80	Positive	Bone	Osteosarcoma	-				kidney liver vascular system large intestine	-	stomach	vascular system	-
5,7-Dibromoquinoline	34522-69-1	C1=C(C(=C2C(=C1)N=CC=C2)Br)Br	-	-	-	Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic	-				large intestine liver ear Zymbals gland oral cavity urinary bladder skin	liver kidney urinary bladder ear Zymbals gland small intestine clitoral gland	stomach lung liver	stomach lung liver	-
5,7-Dibromoquinoline	34522-69-1					Rat	Male	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic									
5,7-Dimethoxycyclopentene[c]coumarin	1146-71-0	C1=C(C=C2C(=C1OC)C3=C(C(O2)=O)CCC3)OC	-	-	-	Rat	Male	Fischer 344	Gavage	52	87	Negative	Liver	Multiple tumour types	-				kidney liver large intestine vascular system ear Zymbals gland	-	stomach urinary bladder	pituitary gland	-
5,7-Dimethoxycyclopentenone[2,3-c]coumarin	1150-62-1	C1=C(C=C2C(=C1OC)C3=C(C(O2)=O)CCC3)OC	-	-	-	Rat	Male	Fischer 344	Gavage	52	87	Negative	Liver	Multiple tumour types	-				stomach kidney liver large intestine vascular system urinary bladder	liver	urinary bladder	pituitary gland liver	-

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
5,7-Dimethoxycyclopentenone[12-c]coumarin	1150-37-4	C1=CC(=C2C(=C1)OC(CC3=C(C(O)2)=O)CCC3=O)OC	-	-	-	Rat	Male	Fischer 344	Gavage	52	74	Negative	Liver	Multiple tumour types	-				kidney liver large intestine vascular system	-	urinary bladder	pituitary gland	-
5-Amino-2-methylphenol	2835-95-2	C1(=CC=C(C)=C1)O)C)N	피부 과민성 : 구분1(1A/1B) 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분2	6, 8, 11, 18, 19, 20, 23, 27, 34, 36, 37, 41, 43, 51, 57, 58, 60, 61, 113, 117, 120, 150, 166, 187, 197, 203, 218	Genotoxicity Data: inconclusive	Mouse	Female	B6C3F1/N	Dermal	93 d	91 d	Not specified	Ovary	Teratoma - benign					spleen urinary bladder ear Zymbals gland stomach all tumor bearing animals	urinary bladder ear Zymbals gland thyroid gland stomach clitoral gland	thyroid gland urinary bladder liver kidney vascular system stomach	thyroid gland vascular system liver urinary bladder hematopoietic system pituitary gland Ovary	-
5-Amino-2-methylphenol	2835-95-2					Mouse	Male	B6C3F1/N	Dermal	93 d	91 d	Not specified											
5-Chloro-2,3-dihydro-2,2-dimethyl-N-[(2-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]-7-benzofuranecarboxamide, (2E)-2-butenedioate (1:1)	123482-23-5	CC2(C)OC=1C(=CC()=CC=1)C2C()C(N)C@@H]3C(C@@H]4NC()C@H]5C(C4)=O.C(=C/C()O)=O)C(O)=O	-	-	-	Rat	Female	Fischer 344	Gavage	52	52	Not specified	Liver	Multiple tumour types	-					-	-	-	-
5-Chloro-2,3-dihydro-2,2-dimethyl-N-[(2-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]-7-benzofuranecarboxamide, (2E)-2-butenedioate (1:1)	123482-23-5					Rat	Male	Fischer 344	Gavage	52	52	Not specified	Liver	Multiple tumour types									
5-Nitroacenaphthene	602-87-9	[N+](=O)([O-])C1C2=C(C=C1)CCC=1C3=C(C=CC=1)3	발암성 : 구분1B 특정표적장기 독성(반복 노출) : 구분2	8, 11, 19, 21, 23, 28, 34, 36, 41, 57, 58, 60, 61, 63, 72, 87, 98, 100, 108, 109, 150, 151, 152, 155, 156, 159, 160, 161, 162, 163, 164, 165, 166, 177, 187, 190, 203, 204, 207, 210	Cancer slope factor: 3.7e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	96	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	CYP1A AHR AHR1B AHR2	CCR6 PDGFRL CIAS1 RAB20 CCR7	SERPINB8 MLPH RNF34 BCL2A1 SH2B3	hsa04934 Cushing syndrome - Homo sapiens (human) (1) hsa196 409363 AHR; aryl hydrocarbon receptor hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa196 409363 AHR; aryl hydrocarbon receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa196 409363 AHR; aryl hydrocarbon receptor	ear Zymbals gland kidney lung spleen liver skin thyroid gland	ear Zymbals gland clitoral gland mammary gland hematopoietic system lung uterus liver	thyroid gland urinary bladder vascular system kidney	ovary stomach Liver urinary bladder hematopoietic system vascular system thyroid gland	Breast Neoplasms Carcinoma, Hepatocellular Carcinoma, Squamous Cell Lung Neoplasms Ovarian Neoplasm
5-Nitroacenaphthene	602-87-9					Syrian hamster	Female	Not specified	Diet	26	71	Not specified	Bile duct	Cholangioma									
5-Nitroacenaphthene	602-87-9					Mouse	Male	B6C3F1	Diet	78	95	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
5-Nitroacenaphthene	602-87-9					Rat	Female	Fischer 344	Diet	78	101	Positive	Clitoral gland	Carcinoma									
5-Nitroacenaphthene	602-87-9					Rat	Male	Fischer 344	Diet	74	101	Positive	Ear canal	Carcinoma - squamous									
5-Nitrobenzimidazole	94-52-0	C1=CC(=CC2=C1NC=N2)[N+](O-)=O	만성 수생환경 유해성 : 구분2	46	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	95	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular	-				skin ear Zymbals gland spleen	uterus ear Zymbals gland hematopoietic system	liver vascular system thyroid gland urinary bladder lung	liver vascular system hematopoietic system lung	-
5-Nitrobenzimidazole	94-52-0					Mouse	Male	B6C3F1	Diet	78	95	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular									
5-Nitrobenzimidazole	94-52-0					Rat	Female	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
5-Nitrobenzimidazole	94-52-0					Rat	Male	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
5-Propyl-1,3-benzodioxole	94-58-6	C1=C(C=CC2=C1OCO2)CCC	발암성 : 구분2 특정표적장기 독성(1회 노출) : 구분1(마취영향) 특정표적장기 독성(반복 노출) : 구분2	-	Cancer slope factor: 1.3e-05 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: inconclusive	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	81	81	Not specified	Liver	Angioma	-				stomach liver Maltoni head cancers	stomach liver	liver stomach vascular system	lung liver stomach thyroid gland	-
5-Propyl-1,3-benzodioxole	94-58-6					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	81	81	Positive	Liver	Hepatoma									
5-Propyl-1,3-benzodioxole	94-58-6					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	81	81	Positive	Liver	Hepatoma									
5-Propyl-1,3-benzodioxole	94-58-6					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	81	81	Positive	Liver	Hepatoma									
5-Propyl-1,3-benzodioxole	94-58-6					Rat	Mixed	Osborne-Mendel	Diet	104	104	Positive	Oesophagus	Multiple tumour types									
5-tert-Butyl-4-hydroxy-2-methylphenyl sulphide	96-69-5	C=1(C=C(C)=CC=1O)C(SC=2C(C)=CC(O)=CC=2)C(C)(C)C(C)(C)C	전반 눈 손상/눈 자극성 : 구분2A(2A/2B) 피부 과민성 : 구분1(1A/1B) 경口 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 40, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 200, 204, 207, 218	Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma	-				stomach large intestine spleen	stomach	thyroid gland stomach kidney	thyroid gland	-
5-tert-Butyl-4-hydroxy-2-methylphenyl sulphide	96-69-5					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
5-tert-Butyl-4-hydroxy-2-methylphenyl sulphide	96-69-5					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
5-tert-Butyl-4-hydroxy-2-methylphenyl sulphide	96-69-5					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
6-Methoxy-2-benzothiazolamine	1747-60-0	C1=NC2=C(S)C(=C(C=C2)OC)N	생식세포 변이원성 : 구분2	21, 28, 29, 30, 41, 52, 53, 57, 61, 63, 63, 64, 108, 109, 150, 153, 112, 129, 150, 160, 167, 177, 200, 210	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	92 d	91 d	Not specified			-				ear Zymbals gland hematopoietic system urinary bladder large intestine spleen stomach	urinary bladder stomach kidney ear Zymbals gland mammary gland hematopoietic system small intestine	urinary bladder thyroid gland	urinary bladder hematopoietic system thyroid gland stomach	-
6-Methylquinoline	91-62-3	C1=CNc(C2C)=CH)C=CC=C2C	경口 독성(흡入) : 구분4 피부 부식성/피부 자극성 : 구분2 전반 눈 손상/눈 자극성 : 구분2A(2B) 만성 수생환경 유해성 : 구분3	57, 62, 121	Genotoxicity Data: genotoxic	Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic	ESR1	HEATR3 FTSD1 GUF1 CROBP-AS SLC38A1	ALDOA HK1 ADIPOQ IDT1 EPSB L3	hsa05205 Proteoglycans in cancer - Homo sapiens (human) (1) hsa:2099 KOBS50 ESR1; estrogen receptor 1 hsa05224 Breast cancer - Homo sapiens (human) (1) hsa:2099 KOBS50 ESR1; estrogen receptor 1 hsa01522 Endocrine resistance - Homo sapiens (human) (1) hsa:2099 KOBS50 ESR1; estrogen receptor 1	oral cavity ear Zymbals gland large intestine skin spleen liver Maltoni head cancers stomach	clitoral gland ear Zymbals gland small intestine oral cavity stomach liver mammary gland	stomach urinary bladder lung vascular system	thyroid gland stomach lung vascular system urinary bladder liver	-
6-Methylquinoline	91-62-3					Rat	Male	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic									
6-Nitroquinoline	613-50-3	C1=CC=C2C(=C1)C=CC=N2)[N+](O-)=O	-	-	-	Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic	-				ear Zymbals gland skin liver large intestine stomach oral cavity thyroid gland spleen	clitoral gland ear Zymbals gland small intestine liver mammary gland	urinary bladder stomach vascular system liver lung	stomach liver vascular system hematopoietic system lung thyroid gland urinary bladder	-
6-Nitroquinoline	613-50-3					Rat	Male	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic									
6-Phenylhexyl isothiocyanate	132920-06-6	C1=CC=CC(=C1)CCCCCCN=C=S	-	-	-	Rat	Male	Fischer 344	Diet	112	112	Negative	Liver	Adenoma - hepatocellular	CYP2A6 CYP2E1	NIDS1 TRAJA HSPA6 DHFR WDR4	GCLC NQO1 GCLM PPP1CB EIF3GA		hematopoietic system	ear Zymbals gland	lung	lung	-
6-Phenylhexyl isothiocyanate	132920-06-6					Rat	Male	Fischer 344	Diet	15	15	Negative	Colon	Multiple tumour types									
7,12-Dimethylbenz[a]anthracene	57-97-6	C=1C=CC=2C(C=1)=CC=3C(C=2)C=CC=4C=3C=CC=C4C	경口 독성(흡入) : 구분4 발암성 : 구분1A 만성 수생환경 유해성 : 구분4	6, 7, 2, 11, 14, 18, 19, 21, 23, 25, 27, 28, 29, 30, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 63, 64, 66, 67, 71, 72, 108, 109, 150, 169, 197, 111, 112, 117, 122, 123, 131, 146, 150, 153, 163, 165, 166, 167, 177, 187, 200, 214, 240, 307, 310, 318	Cancer slope factor: 0.071 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	Albino	Diet	60	60	Positive	Forestomach	Papilloma	CYP1B1 CYP1A1 AHR Blood Tumor CAT	SRSRF2 CTSD TACR3 GJA1 HEATR3	CYP1A2 ENC1 EKOC6 APOC1 IL6	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (4) hsa1543 407406 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa196 409363 AHR; aryl hydrocarbon receptor hsa596 402161 BCL2; BCL2 apoptosis regulator hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1543 407406 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa5743 411087 PTGS2; prostaglandin-endoperoxide synthase 2 hsa05206 MicroRNAs in cancer - Homo sapiens (human) (2) hsa5743 411087 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:406141 miR-21-5p (-1 SNV mature); miR-21	spleen Maltoni head cancers oral cavity ear Zymbals gland nasal cavity thyroid gland	clitoral gland ear Zymbals gland nasal cavity uterus urinary bladder	urinary bladder vascular system thyroid gland lung	vascular system urinary bladder pituitary gland thyroid gland stomach ovary	Carcinoma Mammary Neoplasms, Animal Mammary Neoplasm, Experimental Prostatic Neoplasm Breast Neoplasm Lung Neoplasm
8-Methoxypsoralen	298-81-7	C=1C(C(=2)C(=1)=CC3=C(C=2)OC)OC=C3)=O	경口 독성(흡入) : 구분4 생식세포 변이원성 : 구분2 발암성 : 구분1A 특정표적장기 독성(1회 노출) : 구분2 특정표적장기 독성(반복 노출) : 구분2	8, 11, 34, 58, 60, 61, 62, 107	Carcinogenicity data available NTP RCC: Known Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	HRA/Skh	Diet	52	80	Positive	Skin	Carcinoma - squamous cell	CYP2A6 CYP1A1 ABCB1 ABCC2 ABCG2	HIG2 PLCG2 GPD1 TACR3 CD74	PPP1R14C ENC1 KIAA0247 MFMR MLPH	hsa05170 ABC transporters - Homo sapiens (human) (2) hsa:1244 835666 ABCC2; ATP binding cassette subfamily C member 2 hsa:5243 835658 ABCB1; ATP binding cassette subfamily B member 1 hsa04976 Bile secretion - Homo sapiens (human) (2) hsa:1244 835666 ABCC2; ATP binding cassette subfamily C member 2 hsa:5243 835658 ABCB1; ATP binding cassette subfamily B member 1 hsa05206 MicroRNAs in cancer - Homo sapiens (human) (1) hsa:5243 835658 ABCB1; ATP binding cassette subfamily B member 1	Kidney ear Zymbals gland liver large intestine vascular system	kidney	stomach lung urinary bladder	lung liver stomach	Lung Neoplasms Lymphoma, T-Cell, Cutaneous Mycosis Fungoides
8-Methoxypsoralen	298-81-7					Mouse	Male	HRA/Skh	Diet	52	80	Negative	Skin	Carcinoma - squamous cell									
8-Methoxypsoralen	298-81-7					Rat	Female	Fischer 344	Gavage	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
8-Methoxypsoralen	298-81-7					Rat	Male	Fischer 344	Gavage	103	105	Positive	Kidney	Adenocarcinoma - tubular									
8-Methylquinoline	611-32-5	C1=CNc(C2)=CH)C=CC=C2C	-	-	Genotoxicity Data: genotoxic	Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic	ESR1 CYP1A	HEATR3 CROBP-AS FTSD1 GUF1 HIG2	ADIPOQ ALDOA HK1 EPSB L3 GIPC		oral cavity ear Zymbals gland spleen liver large intestine skin Maltoni head cancers stomach	ear Zymbals gland clitoral gland small intestine mammary gland liver stomach oral cavity	stomach urinary bladder vascular system lung	stomach thyroid gland vascular system liver urinary bladder lung	-
8-Methylquinoline	611-32-5					Rat	Male	Fischer 344	Diet	104	104	Negative	Liver	Nodule - hyperplastic									
8-Nitroquinoline	607-35-2	C1=CC(=C2C(=C1)C=CC=N2)[N+](O-)=O	-	21, 41, 57, 61, 121, 150, 210	-	Rat	Female	Fischer 344	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell	-				stomach ear Zymbals gland skin large intestine spleen lung thyroid gland oral cavity esophagus	stomach clitoral gland ear Zymbals gland small intestine mammary gland kidney urinary bladder hematopoietic system uterus	urinary bladder vascular system thyroid gland stomach lung liver	stomach vascular system thyroid gland ovary hematopoietic system lung liver urinary bladder	-
8-Nitroquinoline	607-35-2					Rat	Male	Fischer 344	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
8-Quinolinol	148-24-3	C1=CN=C2C(=C1)C=CC=C2O	경성 독성(경구) - 구분4	7, 8, 11, 14, 19, 23, 25, 27, 29, 30, 36, 46, 52, 53, 60, 61, 64, 66, 67, 71, 111, 112, 117, 122, 123, 131, 153, 166, 167, 187, 200, 204, 307, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	APP EGFR ATP5A2 MAPK1 MAPK3	CSORF41 HEATR3 FTSJD1 CLIP1 INTU	GCKR EPSB.3 GABPC AKR1B10 ALDOA	hsa05225 PD-L1 expression and PD-1 checkpoint pathway in cancer - Homo sapiens (human) (2) hsa:1956 KO4361 EGFR; epidermal growth factor receptor hsa:5594 KO4371 MAPK1; mitogen-activated protein kinase 1 hsa04810 Regulation of actin cytoskeleton - Homo sapiens (human) (2) hsa:1956 KO4361 EGFR; epidermal growth factor receptor hsa:5594 KO4371 MAPK1; mitogen-activated protein kinase 1 hsa04072 Phosphoinositide D signaling pathway - Homo sapiens (human) (2) hsa:1956 KO4361 EGFR; epidermal growth factor receptor hsa:5594 KO4371 MAPK1; mitogen-activated protein kinase 1	stomach ear Zymbals gland large intestine urinary bladder oral cavity skin	ear Zymbals gland stomach small intestine clitoral gland urinary bladder	stomach urinary bladder thyroid gland lung	thyroid gland stomach **ovary** vascular system lung hematopoietic system liver	Breast Neoplasm Prostatic Neoplasm Leukemia, Myeloid, Acute Hematologic Neoplasm
8-Quinolinol	148-24-3					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
8-Quinolinol	148-24-3					Rat	Female	Fischer 344	Diet	104	104	Negative	Liver	Nodule- hyperplastic									
8-Quinolinol	148-24-3					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
9-Aminoacridine hydrochloride	134-32-9	C1=CC=C2C(=C1)C(=C3C(=N2)C=CC=C3)N(C)	-	-	-	Mouse	Female	B6C3F1	Diet	92 d	91 d	Not specified		-					ear Zymbals gland spleen thyroid gland large intestine urinary bladder oral cavity skin	ear Zymbals gland stomach clitoral gland **uterus** small intestine urinary bladder	liver urinary bladder thyroid gland stomach vascular system lung	liver thyroid gland urinary bladder stomach vascular system lung hematopoietic system **ovary**	-
9H-Carbazole	86-74-8	C12=C(C=CC=C1)N(C=3C2=CC=CC=3)	생식세포 변이원성 - 구분2 **발암성 - 구분1A** 만성 수생환경 유해성 - 구분3	8, 11, 21, 41, 46, 57, 60, 131, 150, 210	Cancer slope factor: 0.00857 (mg/kt-1 (carcinogenicity, inhalation) Carcinogenicity data available: PRRTV (ORNL): Inadequate for an assessment of carcinogenic potential Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	96	104	Positive	Forestomach	Multiple tumour types	CYP1A **AHR** ARNT AHR1B AHR2	PCDC1 IL1R1 IGF2 CD86 MDB4	AHRR CYP3A1 SAT PCXR BIK	hsa04934 Cushing syndrome - Homo sapiens (human) (1) hsa:196 K09363 AHR; aryl hydrocarbon receptor hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa:196 K09363 AHR; aryl hydrocarbon receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa:196 K09363 AHR; aryl hydrocarbon receptor	thyroid gland ear Zymbals gland spleen all tumor bearing animals oral cavity skin Malloni head cancers urinary bladder	ear Zymbals gland all tumor bearing animals uterus thyroid gland hematopoietic system clitoral gland urinary bladder **kidney**	**stomach** **liver** vascular system urinary bladder thyroid gland	thyroid gland **stomach** **liver** vascular system **ovary** urinary bladder pituitary gland	**Kidney Neoplasm** **Liver Neoplasm, Experimental**
9H-Carbazole	86-74-8					Mouse	Male	B6C3F1	Diet	96	104	Positive	Forestomach	Carcinoma- squamous cell									
Acediprone	77-46-3	O=S(=O)(C1=CC=CC)=CC=1)N(C)=O)C2=CC=C(C=C2)N(C)=O	-	-	-	Rat	Female	Buffalo	Diet	43	92	Positive	Mammary gland	Adenocarcinoma	-				spleen urinary bladder	**ear Zymbals gland** **mammary gland** urinary bladder **uterus**	thyroid gland urinary bladder kidney	urinary bladder thyroid gland	-
Acetohexamide	968-81-0	O=S(=O)(C1=CC=C(C=C1)C(=O)CN(C)N(C)CCCCC2)=O	-	8, 11, 21, 34, 36, 41, 57, 58, 60, 72, 121, 150, 163, 210	-	Mouse	Female	B6C3F1	Diet	103	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	AGE DHRS11 DDIT3 DHRS2	CTPS1 INCENP KIAA1	INS IGKC	hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (1) hsa:79154 K22070 DHRS11; dehydrogenase/reductase 11 hsa04010 MAPK signalling pathway - Homo sapiens (human) (1) hsa:1649 K04452 DDIT3; DNA damage inducible transcript 3 hsa04932 Non-alcoholic fatty liver disease - Homo sapiens (human) (1) hsa:1649 K04452 DDIT3; DNA damage inducible transcript 3	spleen	-	thyroid gland	-	-
Acetohexamide	968-81-0					Mouse	Male	B6C3F1	Diet	103	107	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acetohexamide	968-81-0					Rat	Female	Fischer 344	Diet	103	106	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acetohexamide	968-81-0					Rat	Male	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acid Green 2	4680-78-8	C1=CC(=CC=CC)[N+](C)=C/C=C/C(=O)/C=C/C=1/C(C)=C(C)C3=CC=C(C=C2N(CC4=CC(S(O)[O-])=O)=O)=CC=4)C(C)=C3[O-]=O)=CC=6)C(C)=CC=5)[Na+]	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(유) 자우 과민성 - 구분1(사각)	8, 11, 21, 34, 36, 41, 57, 58, 60, 61, 72, 122, 123, 131, 150, 162, 220, 310	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	C3H/He/Fat	Diet	104	104	Negative	Liver	Multiple tumour types	-				-	-	-	-	-
Acid Green 2	4680-78-8					Mouse	Male	C3H/He/Fat	Diet	104	104	Not specified	Liver	Multiple tumour types									
Acid Green 3	4680-78-8					Rat	Female	Osborne-Mendel	Diet	104	104	Positive	Liver	Multiple tumour types									
Acid Green 3	4680-78-8					Rat	Male	Osborne-Mendel	Diet	104	104	Positive	Liver	Multiple tumour types									
Acid Green 3	4680-78-8					Rat	Mixed	Wistar	Diet	93	93	Positive	Abdomen	Lymphoma- malignant									
Acid Green 5, disodium salt	5141-20-8	[Na+].[Na+].[O-]S(=O)(C1=5C=C(C[N+]=)=C1)C=CC(C=C1)=C(C2=CC=C(S(=O)=O)[O-])C=C2)C3=CC=C(C=C3)N(CC4=CC(S(=O)=O)[O-])=O)=CC=6)C(C)=CC=5)N(CC4=CC(S=O)=O)[O-])=CC=6)C(C)=CC=5)[O-]	생식독성 - 구분2 만성 수생환경 유해성 - 구분4	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: non-genotoxic	Mouse	Female	C3H/He/Fat	Diet	104	104	Not specified	Liver	Multiple tumour types	-				-	-	-	-	-
Acid Green 5, disodium salt	5141-20-8					Mouse	Male	C3H/He/Fat	Diet	104	104	Not specified	Liver	Multiple tumour types									
Acid Green 5, disodium salt	5141-20-8					Rat	Male	Not specified	Diet	65	65	Not specified	Liver	Multiple tumour types									
Acid Green 5, disodium salt	5141-20-8					Rat	Female	Osborne-Mendel	Diet	104	104	Negative	Liver	Multiple tumour types									
Acid Green 5, disodium salt	5141-20-8					Rat	Male	Osborne-Mendel	Diet	104	104	Negative	Liver	Adenoma- hepatocellular									
Acid Green 5, disodium salt	5141-20-8					Rat	Mixed	Wistar	Diet	95	95	Positive	Caecum	Lymphoma- malignant									
Acid Orange 3	6373-74-6	C=2C(N(C=1C=CC=C=1)=CC=1C=C(C=2)NC3=C(C=C(C=C3)N(=)[O-])=O)[N+](=O)[O-])=O)[N+](=O)[O-])=O)=O)[O-])=O)=O)[Na+]	심한 눈 손상성/눈 자극성 - 구분2A(유)	8, 11, 21, 29, 30, 34, 36, 41, 52, 53, 57, 58, 60, 61, 62, 72, 112, 123, 131, 150, 163, 165, 167, 200, 220, 310	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									-
Acid Orange 3	6373-74-6					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acid Orange 3	6373-74-6					Rat	Female	Fischer 344	Gavage	103	104	Positive	Kidney	Carcinoma- transitional cell									
Acid Orange 3	6373-74-6					Rat	Male	Fischer 344	Gavage	100	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acid Red 114	6459-94-5	O=S(=O)(C5=CC6=C(C=C)N=NC1=CC=(C=1)C(=C)N=NC1=CC=(C=1)C(=O)[O-])=CC=1C=CC=C2)C(=4C=3C=CC=C4)C(O)[O-])=CC=1)C=4C(=3C=CC=C4)C(O)[O-])	**발암성 - 구분2** 특정표적장기 독성(반복 노출) - 구분2	7, 8, 11, 14, 19, 21, 23, 25, 29, 30, 34, 36, 41, 52, 53, 57, 58, 60, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 150, 153, 163, 165, 167, 187, 200, 214, 307, 312, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Female	Fischer 344	Drinking water	98	104	Positive	Adrenal gland medulla	Pheochromocytomabenign	IYD	-	-	hsa04918 Thyroid hormone synthesis - Homo sapiens (human) (1) hsa:38434 K17231 IYD; iodotyrosine deiodinase					Adenocarcinoma Adrenal Gland Neoplasm Breast Neoplasm Colonic Neoplasm Intestinal Neoplasm Leukemia **Liver Neoplasm**
Acid Red 114	6459-94-5					Rat	Male	Fischer 344	Drinking water	104	104	Positive	Adrenal gland medulla	Pheochromocytomabenign									
Acid Red 14	3567-69-9	[Na+].[Na+].[O-]S(=O)(C=3C=C(N=NC=1C=CC(S(=O)=O)[O-])=CC(=1C=CC=C2)C(=4C=3C=CC=C4)C(O)[O-])	만성 수생환경 유해성 - 구분3	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	ASH-CS1	Diet	80	80	Negative	Liver	Multiple tumour types	-				-	-	-	-	-
Acid Red 14	3567-69-9					Mouse	Male	ASH-CS1	Diet	80	80	Negative	Liver	Adenoma									
Acid Red 14	3567-69-9					Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acid Red 14	3567-69-9					Mouse	Male	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acid Red 14	3567-69-9					Rat	Female	Fischer 344	Diet	103	104	Not specified	Clitoral gland	Adenoma- sebaceous									
Acid Red 14	3567-69-9					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acid Red 18	2611-82-7	[Na+].[Na+].[Na+].[O-]S(=O)(C=3C=CC(N=NC=2C1=CC(S(=O)=O)[O-])=CC(S(=O)=O)[O-])=C1C(C=C(S(=O)=O)[O-])=CC=3)C(=O)[O-]	심한 눈 손상성/눈 자극성 - 구분2A(유) 만성 수생환경 유해성 - 구분3		Genotoxicity Data: predicted to be clastogenic	Rat	Mixed	Non-inbred	Diet	143	143	Positive	Liver	Multiple tumour types									
Acid Red 18	2611-82-7					Rat	Female	Not specified	Diet	64	64	Negative	Liver	Multiple tumour types									
Acid Red 18	2611-82-7					Rat	Male	Not specified	Diet	64	64	Negative	Liver	Multiple tumour types									
Acid Red 18	2611-82-7					Rat	Female	Sprague-Dawley	Diet	52	52	Negative	Liver	Multiple tumour types									
Acid Red 18	2611-82-7					Rat	Male	Sprague-Dawley	Diet	52	52	Negative	Liver	Multiple tumour types									
Acid Red 26	3761-53-3	[Na+].[Na+].[O-]S(=O)(C=2C(=CN=NC1=CC=(C=1)C)C=C1C(C(=3C(C=2)=CC(S(=O)=O)[O-])=CC=3O)C(=O)[O-])	생식세포 변이원성 - 구분2 **발암성 - 구분2**	-	Cancer slope factor: 1.3e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: micronucleus	Mouse	Female	D2B	Diet	81	81	Positive	Liver	Adenoma- hepatocellular					-	-	-	-	-
Acid Red 26	3761-53-3					Mouse	Male	D2B	Diet	81	81	Positive	Liver	Adenoma- hepatocellular									
Acid Red 26	3761-53-3					Rat	Female	C3B	Diet	104	104	Not specified	Liver	Nodular hyperplasia									
Acid Red 26	3761-53-3					Rat	Male	C3B	Diet	104	104	Not specified	Liver	Nodular hyperplasia									
Acid Red 26	3761-53-3					Rat	Female	Wistar	Diet	52	91	Positive	Liver	Carcinoma- hepatocellular									
Acid Red 26	3761-53-3					Rat	Female	Wistar	Diet	91	91	Positive	Liver	Carcinoma- hepatocellular									
Acid Red 26	3761-53-3					Rat	Male	Wistar	Diet	65	65	Positive	Liver	Adenoma- islet cell									
Acid Red 27	915-67-3	O=S(=O)(C=3C=CC(N=NC=1C(=CC(S(=O)=O)[O-])=C2C=C(C=1C=CC(S(=O)=O)[O-])=C2O)=CC=3C=CC=C4)C(O)[Na+].[Na+].[Na+]	생식세포 변이원성 - 구분2 특정표적장기 독성(반복 노출) - 구분2	19, 23, 29, 30, 52, 53, 67, 111, 112, 117, 165, 167, 187, 200, 307	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: non-genotoxic	Rat	Mixed	Mongrel	Diet	108	108	Positive	Liver	Multiple tumour types	GRIN2A CHRNA4 CHRNB2 CYP3A4	-	-	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:1137 K04806 CHRNA4; cholinergic receptor nicotinic alpha 4 subunit hsa:1141 K04813 CHRNB2; cholinergic receptor nicotinic beta 2 subunit hsa04725 Cholinergic synapse - Homo sapiens (human) (2) hsa:1137 K04806 CHRNA4; cholinergic receptor nicotinic alpha 4 subunit hsa:1141 K04813 CHRNB2; cholinergic receptor nicotinic beta 2 subunit hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (2) hsa:1137 K04806 CHRNA4; cholinergic receptor nicotinic alpha 4 subunit hsa:1141 K04813 CHRNB2; cholinergic receptor nicotinic beta 2 subunit	-	-	-	-	-
Acid Red 27	915-67-3					Rat	Mixed	Non-inbred	Diet	143	143	Positive	Liver	Hepatoma									
Acid Red 27	915-67-3					Rat	Female	Not specified	Diet	64	64	Negative	Liver	Multiple tumour types									
Acid Red 27	915-67-3					Rat	Male	Not specified	Diet	64	64	Negative	Liver	Multiple tumour types									
Acid Red 27	915-67-3					Rat	Female	SD	Diet	52	52	Negative	Liver	Multiple tumour types									
Acid Red 27	915-67-3					Rat	Mixed	Wistar	Diet	91	91	Positive	Abdomen	Lymphoma- malignant									
Acid Red 52	3520-42-1	[Na+].[O-]S(=O)(C4=CC(S(=O)=O)=C(O)C=C1C=C(C=C(C=C1)=C3)N(CC(=O)[O-])C=C3)=CC(=C(C)C=C4)[O-]	자료없음	7, 19, 23, 29, 30, 52, 53, 67, 111, 112, 117, 122, 123, 150, 163, 167, 187, 200, 307	-	Rat	Female	Fischer 344/DuCr	Diet	106	106	Negative	Liver	Multiple tumour types	-				-	-	-	-	-
Acid Red 52	3520-42-1					Rat	Male	Fischer 344/DuCr	Diet	106	106	Negative	Liver	Nodule- neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Acifluorfen	50594-66-6	C1(=C(C=CC(=C1)[O]C2=CC=C(C=C2Cl)[C](F)(F)[F])N+][O-])=O)C(=O)O	-	7, 8, 11, 18, 23, 25, 27, 28, 30, 34, 36, 46, 52, 53, 57, 58, 60, 62, 72, 111, 112, 117, 122, 123, 153, 163, 166, 167, 187, 200, 207	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	78	78	Positive	Liver	Adenoma- hepatocellular	PPOX CYP2B10 MBD3 Abcc4 BCL2L1	CYP11A1	ERBB2 TNFSF4K	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:596 402161 BCL2, BCL2 apoptosis regulator hsa:9970 838041 NR1I3, nuclear receptor subfamily 1 group I member 3 hsa01521 EGFR tyrosine kinase inhibitor resistance - Homo sapiens (human) (1) hsa:596 402161 BCL2, BCL2 apoptosis regulator hsa04722 Neurotrophin signaling pathway - Homo sapiens (human) (1) hsa:596 402161 BCL2, BCL2 apoptosis regulator	-	-	stomach liver kidney vascular system	liver stomach	Liver Neoplasm Colorectal Neoplasm Neoplasm, Experimental
Acifluorfen	50594-66-6					Mouse	Male	B6C3F1	Diet	78	78	Positive	Liver	Adenoma- hepatocellular									
Acifluorfen	50594-66-6					Mouse	Female	CD1	Diet	104	104	Positive	Liver	Adenoma- hepatocellular									
Acifluorfen	50594-66-6					Mouse	Male	CD1	Diet	104	104	Positive	Liver	Adenoma- hepatocellular									
Acromycine	7008-42-6	C(C4O[C@]2(c(C(=O)C(C)(C)C)c(O)cc(O)c2C)[C@H]3[C@H](C)[C@H](O)[C@H]4[C@H](O)c5c(O)cccc(O)c5C(=O)C(=C(N)[C@]34O)C(=O)N)=O				Mouse	Female	B6C3F1	Intraperitoneal	48	78	Inadequate test	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic					vascular system large intestine	mammary gland ear Zymbals gland	urinary bladder	-	
Acromycine	7008-42-6					Mouse	Male	B6C3F1	Intraperitoneal	66	78	Inadequate test	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acromycine	7008-42-6					Rat	Female	SD	Intraperitoneal	52	80	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Acromycine	7008-42-6					Rat	Male	SD	Intraperitoneal	51	80	Positive	Adrenal gland	Adenoma- cortical									
Actinomycin D	50-76-0	N(C3=C(C(NC(C)(NC(C(C(C)C)=O)NC(C)=O)N(C)C)=O)C(C)C)C(=O)c(C)c(C)c=O)c(C)c(C)c=O)c(C)c(C)c

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Aniline	62-53-3	C1=CC=CC=C1[N]	경구 독성(분말) - 구분3 경피 독성(분말) - 구분3 경口 독성(액체) - 구분3 심한 눈 손상/심한 자극성 - 구분1 피부 과민성 - 구분1(1A/1B) 생식세포 변이원성 - 구분2 **발암성 - 구분2** 특정표적장기 독성(반복 노출) - 구분1 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	Cancer slope factor: 1.6e-06 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: IRIS-B2 (Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals) Genotoxicity Data: clastogenic	Rat	Male	Wistar	Drinking water	80	80	Negative	Forestomach	Papilloma	**CYP2E1** RELA CYP1A2 IL1A Il6	CCR6 DNAJB2 AMH R2 TEP1 MYOSC	HTATIP2 MGST1 B2LBA1 CCR5 AKR1B10	hsa05164 Influenza A - Homo sapiens (human) (2) hsa:3552 K04083 IL1A; interleukin 1 alpha hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa04010 MAPK signaling pathway - Homo sapiens (human) (2) hsa:3552 K04083 IL1A; interleukin 1 alpha hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa05152 Tuberculosis - Homo sapiens (human) (2) hsa:3552 K04083 IL1A; interleukin 1 alpha hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit	spleen ear Zymbals gland thyroid gland urinary bladder	urinary bladder **uterus** ear Zymbals gland thyroid gland hematopoietic system kidney clitoral gland lung liver mammary gland nasal cavity small intestine stomach	thyroid gland urinary bladder liver vascular system lung stomach small intestine	thyroid gland liver urinary bladder vascular system stomach lung pituitary gland peritoneal cavity small intestine	Sarcoma
Aniline hydrochloride	142-04-1	C1=CC=CC(=C1)N.Cl	경구 독성(분말) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상/심한 자극성 - 구분2A/2B 생식세포 변이원성 - 구분2 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2	6, 18, **29, 30**, 36, 37, 51, 52, 53, 58, 61, 67, 112, **165**, 166, **167, 200**, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	107	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				spleen ear Zymbals gland thyroid gland urinary bladder	urinary bladder **uterus** ear Zymbals gland thyroid gland hematopoietic system kidney clitoral gland lung liver mammary gland nasal cavity small intestine stomach	thyroid gland urinary bladder liver vascular system lung stomach small intestine	thyroid gland liver urinary bladder vascular system **ovary** hematopoietic system stomach lung pituitary gland peritoneal cavity small intestine	-
Aniline hydrochloride	142-04-1					Mouse	Male	B6C3F1	Diet	103	107	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Aniline hydrochloride	142-04-1					Rat	Female	Fischer 344	Diet	103	107	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Aniline hydrochloride	142-04-1					Rat	Male	Fischer 344	Diet	103	107	Positive	Adrenal gland	Pheochromocytoma | Pheochromocytoma - malignant									
Anthranilic acid	118-92-3	C1(C(=O)O)=CC=CC=C1N	생식독성 - 구분2	-	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	IFNG AKR1B10 AKR1C1 IDO1 IL12A IL12B IL18	TRAF5 STAT5B TGFI CCDC50 STAT1A	FECH AKR1B10 POLR2A PGD PTGR1	hsa05143 African trypanosomiasis - Homo sapiens (human) (3) hsa:3592 K05406 IL12A; interleukin 12A hsa:3593 K05415 IL12B; interleukin 12B hsa:3620 K03463 IDO1; indoleamine 2,3-dioxygenase 1 hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa:1645 K00212 AKR1C1; aldo-keto reductase family 1 member C1 hsa:3620 K03463 IDO1; indoleamine 2,3-dioxygenase 1 hsa:57016 K00011 AKR1B10; aldo-keto reductase family 1 member B10 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (2) hsa:3592 K05406 IL12A; interleukin 12A hsa:3593 K05415 IL12B; interleukin 12B	kidney spleen urinary bladder ear Zymbals gland liver thyroid gland	urinary bladder clitoral gland thyroid gland **uterus** ear Zymbals gland kidney	thyroid gland urinary bladder liver vascular system stomach	liver thyroid gland vascular system urinary bladder stomach **ovary**	**Liver Neoplasm, Experimental**
Anthranilic acid	118-92-3					Mouse	Male	B6C3F1	Diet	78	105	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Anthranilic acid	118-92-3					Rat	Female	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Anthranilic acid	118-92-3					Rat	Male	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Anthraquinone	84-65-1	C1(C(=O)C(C2=C(C=CC=C2)O)C=CC=C2)=O	**발암성 - 구분2** 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분1 급성 수생환경 유해성 - 구분1	**29, 30**, 52, 53, 67, 112, **165, 167, 200**	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6AKR1	Gavage (preweaning) then diet	78	76	Negative	Liver	Hepatoma	BAX BCL2 CASP3 PTGS2	CTSD TACR3 NOS3 SERPINB1 SRSF2	BAG3AP1 TBP1L AURKA LRP6 PBK	hsa05132 Salmonella infection - Homo sapiens (human) (2) hsa:596 K02161 BCL2; BCL2 apoptosis regulator hsa:836 K02187 CASP3; caspase 3 hsa05222 Small cell lung cancer - Homo sapiens (human) (2) hsa:596 K02161 BCL2; BCL2 apoptosis regulator hsa:836 K02187 CASP3; caspase 3 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (2) hsa:596 K02161 BCL2; BCL2 apoptosis regulator hsa:836 K02187 CASP3; caspase 3	kidney urinary bladder liver large intestine	urinary bladder kidney ear Zymbals gland liver **uterus** hematopoietic system clitoral gland thyroid gland nasal cavity lung	stomach vascular system lung liver urinary bladder thyroid gland small intestine	**ovary** stomach hematopoietic system thyroid gland vascular system urinary bladder pituitary gland liver lung peritoneal cavity small intestine	-
Anthraquinone	84-65-1					Mouse	Male	B6AKR1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Anthraquinone	84-65-1					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Anthraquinone	84-65-1					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
ANTU	86-88-4	C1=CC=C2C(=C1C(=C(C=C2)N(C)=S)N)	경구 독성(분말) - 구분2 **발암성 - 구분2**	-	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6AKR1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	NOS3 MDM4 MAP2 FGF7	TEP1 CCR6 TMBIM1MA PHF14 CAK1	C1ORF63 RNF12 HTATIP2 SAT VAV3N	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:1956 K04561 EGFR; epidermal growth factor receptor hsa:7422 K05448 VEGFA; vascular endothelial growth factor A hsa05206 MicroRNAs in cancer - Homo sapiens (human) (2) hsa:1956 K04561 EGFR; epidermal growth factor receptor hsa:7422 K05448 VEGFA; vascular endothelial growth factor A hsa05219 Bladder cancer - Homo sapiens (human) (2) hsa:1956 K04561 EGFR; epidermal growth factor receptor hsa:7422 K05448 VEGFA; vascular endothelial growth factor A	thyroid gland spleen ear Zymbals gland	**uterus** ear Zymbals gland hematopoietic system thyroid gland mammary gland	thyroid gland urinary bladder	thyroid gland urinary bladder	-
ANTU	86-88-4					Mouse	Male	B6AKR1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
ANTU	86-88-4					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
ANTU	86-88-4					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Aramite	140-57-8	S(OC(CO[C+]1C=CC(=CC=1)C)C)OCCCl)=O	피부 부식성/피부 자극성 - 구분2 심한 눈 손상/심한 자극성 - 구분2A/2B **발암성 - 구분2** 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	**29, 30**, 52, 53, 67, 112, **165, 167, 200**	Cancer slope factor: 7.1e-06 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6AKR1	Gavage (preweaning) then diet	80	80	Not specified	Liver	Hepatoma	-				all tumor bearing animals	stomach	liver kidney	-	-
Aramite	140-57-8					Mouse	Male	B6AKR1	Gavage (preweaning) then diet	77	77	Not specified	Liver	Hepatoma									
Aramite	140-57-8					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	77	77	Not specified	Liver	Hepatoma									
Aramite	140-57-8					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	80	80	Positive	Liver	Hepatoma									
Aramite	140-57-8					Rat	Mixed	CRN	Diet	104	104	Positive	Bile duct	Adenoma									
Aroclor 1016	12674-11-2	C1(=CC=CC(=C1)Cl)C2=C(C=CC(=C2Cl)Cl)Cl	-	**29, 30**, 52, 53, 67, 112, **165, 167, 200**	Cancer slope factor: 2e-05 (ug/m3)-1 (carcinogenicity)	Rat	Female	SD	Diet	104	104	Positive	Liver	Adenoma - hepatocellular	SLC6A3	FABP4 MAN2C1 GJA1 PPL SNHG8	BEL IL10Rb CYP1B2 CYP1B1 GALNT6	hsa05034 Alcoholism - Homo sapiens (human) (1) hsa:6531 K05036 SLC6A3; solute carrier family 6 member 3 hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (1) hsa:6531 K05036 SLC6A3; solute carrier family 6 member 3 hsa04728 Dopaminergic synapse - Homo sapiens (human) (1) hsa:6531 K05036 SLC6A3; solute carrier family 6 member 3	thyroid gland hematopoietic system ear Zymbals gland kidney liver oral cavity nasal cavity Maltoni head cancers spleen	liver urinary bladder **uterus** clitoral gland	liver vascular system urinary bladder lung small intestine	thyroid gland urinary bladder vascular system liver small intestine peritoneal cavity pituitary gland	Adenoma, Liver Cell
Aroclor 1016	12674-11-2					Rat	Male	SD	Diet	104	104	Not specified	Liver	Multiple tumour types									
Aroclor 1242	11104-28-2	C1(=CC=CC(=C1)Cl)C2=C(C=CC(=C2Cl)Cl)Cl			Cancer slope factor: 000057 (ug/m3)-1 (carcinogenicity)	Rat	Female	SD	Diet	104	104	Positive	Liver	Adenoma - hepatocellular	-				-	-	-	-
Aroclor 1242	11104-28-2					Rat	Male	SD	Diet	104	104	Positive	Liver	Multiple tumour types									
Aroclor 1254	11097-69-1	C1(=C(C=C(C(=C1Cl)Cl)Cl)Cl)C2=C(C=C(C(=C2Cl)Cl)Cl)Cl	경구 독성(분말) - 구분4 경피 독성(분말) - 구분3 **발암성 - 구분2** 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	Cancer slope factor: 000057 (ug/m3)-1 (carcinogenicity)	Mouse	Male	BALB/cJ	Diet	26	47	Not specified	Liver	Hepatoma	CYP1A1 CYP1A2 CAT CYP11A1 CYP1A	FABP4 AIRN7 CASP12 CCDC49 RNF2	BEL CYP11B2 IL10Rb IRAK1TA1 HGFA12A	hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1583 K04846 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa:847 K03781 CAT; catalase hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:847 K03781 CAT; catalase hsa00380 Tryptophan metabolism - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:847 K03781 CAT; catalase	thyroid gland liver oral cavity kidney nasal cavity ear Zymbals gland Maltoni head cancers spleen	liver kidney	liver vascular system small intestine	thyroid gland urinary bladder vascular system liver small intestine peritoneal cavity	Carcinoma, Hepatocellular **Liver Neoplasm, Experimental** Cholangiocarcinoma Adenoma, Liver Cell
Aroclor 1254	11097-69-1					Mouse	Male	BALB/cJ	Diet	47	47	Positive	Liver	Hepatoma									
Aroclor 1254	11097-69-1					Rat	Female	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma									
Aroclor 1254	11097-69-1					Rat	Male	Fischer 344	Diet	105	105	Not specified		Cancer: | Adenocarcinoma Injunct: | Adenocarcinoma Stomach: | Adenocarcinoma									
Aroclor 1254	11097-69-1					Rat	Female	SD	Diet	104	104	Positive	Liver	Adenoma - hepatocellular									
Aroclor 1254	11097-69-1					Rat	Male	SD	Diet	104	104	Positive	Liver	Multiple tumour types									
Aroclor 1260	11096-82-5	C1(C=C(C=C(C(=C1Cl)Cl)Cl)Cl)C2=C(C=C(C(=C2Cl)Cl)Cl)	-	27, 46, 61	Cancer slope factor: 000057 (ug/m3)-1 (carcinogenicity)	Rat	Female	Sherman COBS	Diet	89	95	Positive	Liver	Carcinoma - hepatocellular	EGF NBN2 CYP2B10 G6PC CD36	FABP4 AIRN7 CASP12 CCDC49 RNF2	BEL IRAK1TA1 HGFA12A LIM2 MAP3K7IP2	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa:9970 K08541 NR1I2; nuclear receptor subfamily 1 group I member 2	thyroid gland liver oral cavity kidney nasal cavity ear Zymbals gland Maltoni head cancers	liver kidney lung thyroid gland	liver vascular system small intestine	thyroid gland urinary bladder vascular system liver peritoneal cavity small intestine	Carcinoma, Hepatocellular Adenoma, Liver Cell
Aroclor 1260	11096-82-5					Rat	Female	SD	Diet	104	104	Positive	Liver	Adenoma - hepatocellular									
Aroclor 1260	11096-82-5					Rat	Male	SD	Diet	104	104	Positive	Liver	Adenoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADRs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Anaclor 1260	11096-82-5					Rat	Male	Wistar	Diet	116	116	Positive	Liver	Carcinoma - hepatocellular									
Aspartame	22839-47-0	C(C)(C)(=O)[N]([C@H](C)C(=O)N[C@H](C(OC)=O)CC1=CC=CC=C1)=O|N(O)(O)=O	생식독성 변이원성 - 구분2	29, 30, 52, 53, 67, 112, 165, 167, 200	Genotoxicity Data: clastogenic	Rat	Female	Sic-Wistar	Diet	52	52	Not specified	Brain	Multiple tumour types	ACHE BAX TAS1R1 TAS1R2 TAS1R3	SHC1 TRRAP ALDH18A1 AKRC13 NADK	TPI1 CYBORF11B AKR1B10 OSS NQO1	hsa04742 Taste transduction - Homo sapiens (human) (2) hsa:80824 K04625 TAS1R2; taste 1 receptor member 2 hsa:80835 K04624 TAS1R1; taste 1 receptor member 1 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (1) hsa:581 K02159 BAX; BCL2 associated X, apoptosis regulator hsa04933 AGE-RAGE signaling pathway in diabetic complications - Homo sapiens (human) (1) hsa:581 K02159 BAX; BCL2 associated X, apoptosis regulator	skin	-	kidney	-	Neoplasm
Aspartame	22839-47-0					Rat	Female	Sic-Wistar	Diet	104	104	Negative	Brain	Multiple tumour types									
Aspartame	22839-47-0					Rat	Male	Sic-Wistar	Diet	52	52	Not specified	Brain	Multiple tumour types									
Aspartame	22839-47-0					Rat	Male	Sic-Wistar	Diet	104	104	Negative	Brain	Multiple tumour types									
Aspartame	22839-47-0					Rat	Female	SD	Diet	104	104	Negative	Brain	Multiple tumour types									
Aspartame	22839-47-0					Rat	Male	SD	Diet	104	104	Negative	Brain	Multiple tumour types									
Aspirin	50-78-2	C1=CC=C(C(=C1)C(O)=O)OC(=O)C	경口 독성(준각) - 구분4	8, 11, 27, 34, 36, 57, 58, 60, 61, 72, 131, 163	Genotoxicity Data: inconclusive	Mouse	Female	C57BL/6	Diet	77	77	Negative	Liver	Multiple tumour types	PTGS2 TNF IL1B PTGS1 CASP3	SERPINB1 SDC4 STAT5B SUMO1 TOB1	PCKER SPAGE PLA2G6 PCDH17 AURKA	hsa05321 Inflammatory bowel disease - Homo sapiens (human) (2) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:7124 K03156 TNF; tumor necrosis factor hsa04940 Type I diabetes mellitus - Homo sapiens (human) (2) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:7124 K03156 TNF; tumor necrosis factor hsa05171 Coronavirus disease - COVID-19 - Homo sapiens (human) (2) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:7124 K03156 TNF; tumor necrosis factor	skin **kidney** hematopoietic system urinary bladder	urinary bladder	stomach liver **kidney**	pituitary gland stomach liver	Adenocarcinoma Carcinoma, Renal Cell Kidney Neoplasms Carcinoma, Transitional Cell Ureteral Neoplasm
Aspirin	50-78-2					Mouse	Male	C57BL/6	Diet	77	77	Negative	Liver	Multiple tumour types									
Aspirin	50-78-2					Rat	Mixed	Albino	Gavage	78	78	Negative	Duodenum	Multiple tumour types									
Aspirin	50-78-2					Rat	Male	Fischer 344	Diet	68	68	Not specified	Liver	Multiple tumour types									
Aspirin	50-78-2					Rat	Male	Fischer 344	Diet	56	56	Negative	Colon	Multiple tumour types									
Aspirin	50-78-2					Rat	Male	Wistar	Diet	52	52	Negative	Liver	Multiple tumour types									
Astemizole	68844-77-9	C1=CC=C2C(=C1)N(=C(N2CCC3=CC=C(C=C3)F)NC4CN(CC4)CCCS=CC=CC=C5)OC	특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분4	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 57, 58, 61, 62, 64, 66, 67, 71, 72, 91, 93, 94, 96, 97, 98, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 195, 197, 200, 203, 204, 214, 307, 318	-	Mouse	Female	Swiss	Diet	78	78	Negative	Liver	Adenoma-hepatocellular	KCNN2 KCNH1 CYP22 HRH1	SLC15A1 MYBL1 HBPD CRH TAGLN	HMGCR SCD5 SLC2A4	hsa04750 Inflammatory mediator regulation of TRP channels - Homo sapiens (human) (1) hsa:1573 K07418 CYP2J2; cytochrome P450 family 2 subfamily J member 2 hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa:1573 K07418 CYP2J2; cytochrome P450 family 2 subfamily J member 2 hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa:1573 K07418 CYP2J2; cytochrome P450 family 2 subfamily J member 2	skin	ear Zymbals gland	-	-	Melanoma
Astemizole	68844-77-9					Mouse	Male	Swiss	Diet	78	78	Negative	Liver	Adenoma-hepatocellular									
Astemizole	68844-77-9					Rat	Female	Crl:CD(SD)IGS	Diet	105	105	Negative	Liver	Nodule -neoplastic									
Astemizole	68844-77-9					Rat	Male	Crl:CD(SD)IGS	Diet	105	105	Negative	Liver	Nodule -neoplastic									
Atropine	51-55-8	C(CO)(C)(=O)C(C=CC=C1)C(=O)OC@@H]2C[@H](C[C@H]3CC)C@@H]1C2N3C	경口 독성(준각) - 구분4 특정표적장기 독성(1회 노출) - 구분1		Genotoxicity Data: predicted to be genotoxic	Rat	Female	SD	Intraperitoneal	104	104	Negative	Multiple sites	Tumour- malignant	ACHE ACHE CHRM1 CRH PTGS2	NGF SSAR1 BACE1 MYBL1 DHFR	TMEM41B CNTN1 LST1 FAM49A PLXNA2	hsa04024 cAMP signaling pathway - Homo sapiens (human) (2) hsa:1128 K04129 CHRM1; cholinergic receptor muscarinic 1 hsa:1392 K05256 CRH; corticotropin releasing hormone hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (2) hsa:1128 K04129 CHRM1; cholinergic receptor muscarinic 1 hsa:1392 K05256 CRH; corticotropin releasing hormone hsa04750 Long-term depression - Homo sapiens (human) (1) hsa:1392 K05256 CRH; corticotropin releasing hormone	vascular system	vascular system	-	hematopoietic system lung	Breast Neoplasm Myasthenia Gravis
Atropine	51-55-8					Rat	Male	SD	Intraperitoneal	104	104	Not specified	Liver	Haemangioendothelioma									
Azelnidipine	123524-52-7	N1(CC(C1)(OC)C=2C(C)=C(NC=2)NC(C)(C)C)C(C)=C3=CC=CC(=C3[N]([N+]([O-])=O)=O)C(C)(C)C		7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 200, 204, 207, 218	-	Mouse	Female	B6C3F1	Gavage	78	78	Negative	Liver	Adenoma - hepatocellular	CYP22 AR	TAGLN	ASAH1 WIPI1 PNDC4 GDF03 HPN	-	-	-	-	-
Azelnidipine	123524-52-7					Mouse	Male	B6C3F1	Gavage	78	78	Negative	Liver	Adenoma - hepatocellular									
Azelnidipine	123524-52-7					Rat	Female	Fischer 344/DuCrl	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular									
Azelnidipine	123524-52-7					Rat	Male	Fischer 344/DuCrl	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular									
Azinphos-methyl	86-50-0	CP(P(OC)(OC)N=N[C+]1C=CC=CC=1)C2=C3=CC=CC=C2	경口 독성(준각) - 구분2 경口 독성(흡입) - 구분3 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 생식세포 변이원성 - 구분2 발암성 - 구분1B 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분1	7, 8, 10, 11, 14, 15, 22, 23, 27, 29, 30, 32, 34, 36, 42, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 135, 148, 153, 163, 165, 167, 187, 188, 200, 214, 307, 318	Carcinogenicity data available: EPA OPP: Not Likely to Be Carcinogenic in Humans	Mouse	Female	B6C3F1	Diet	80	92	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic	ACHE AR ESR1 PTGS PPARG	-	NR1I2 CYP3B6 CYP1A2	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:367 K08557 AR; androgen receptor hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:367 K08557 AR; androgen receptor hsa01522 Endocrine resistance - Homo sapiens (human) (1) hsa:2099 K08550 ESR1; estrogen receptor 1	all tumor bearing animals	liver	-	-	-
Azinphos-methyl	86-50-0					Mouse	Male	B6C3F1	Diet	80	92	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Azinphos-methyl	86-50-0					Rat	Female	Osborne-Mendel	Diet	80	115	Not specified	Adrenal gland	Adenoma - cortical									
Azinphos-methyl	86-50-0					Rat	Male	Osborne-Mendel	Diet	80	115	Not specified	Adrenal gland	Adenocarcinoma									
Azobenzene	103-33-3	C1=CC=CC=C1N=NC=1C=CC=CC=1	경口 독성(준각) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 생식세포 변이원성 - 구분2 발암성 - 구분1A 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분1	10, 21, 23, 29, 30, 34, 36, 41, 52, 53, 57, 58, 61, 67, 72, 111, 112, 117, 120, 135, 150, 163, 165, 167, 187, 200, 207, 210	Cancer dose factor: 3.1e-05 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6A6F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma	NR1I2	MT1H MYOCD CTDSPL FGD6Y DNAJC2	KIF3A HTATIP2 SAT VASN C1ORF63	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa:9970 K08541 NR1I2; nuclear receptor subfamily 1 group I member 2	spleen vascular system liver thyroid gland urinary bladder ear Zymbals gland hematopoietic system nasal cavity Mutation head-cancers oral cavity kidney	urinary bladder kidney **uterus** liver hematopoietic system thyroid gland lung clitoral gland nasal cavity	thyroid gland urinary bladder kidney vascular system lung small intestine preputial gland liver	**ovary** thyroid gland urinary bladder liver vascular system stomach pituitary gland peritoneal cavity small intestine	-
Azobenzene	103-33-3					Mouse	Male	B6A6F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Azobenzene	103-33-3					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Azobenzene	103-33-3					Mouse	Female	B6C3F1	Diet	105	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Basic Blue 9 trihydrate	7220-79-3	C=12[S+]=[c-]C(C)=NC=1C=CC(=C2N(C)C)C=CC(=C3N(C)C.O.O.O)[Cl-]	생식독성 - 구분2	7, 11, 21, 23, 25, 27, 29, 30, 45, 46, 52, 53, 57, 61, 62, 111, 112, 117, 122, 123, 131, 150, 153, 160, 167, 187, 200, 207, 210	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Gavage	30 d	28 d	Not specified			-				-	-	-	-	-
Basic fuchsin	632-99-5					Syrian hamster	Female	Not specified	Gavage	88	88	Not specified	Liver	Multiple tumour types									
Basic fuchsin	632-99-5					Syrian hamster	Male	Not specified	Gavage	84	84	Not specified	Liver	Multiple tumour types									
Basic fuchsin	632-99-5	C=1(C(=C(C=C(C=1C)N)N(C=2C=C(C)N)=CC=2)C)C=C(C)=CC=3)N)Cl	발암성 - 구분2	7, 19, 23, 25, 29, 30, 34, 36, 46, 52, 53, 58, 61, 67, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 188, 207	Carcinogenicity data available: IARC Group 2B - Possibly carcinogenic to humans Genotoxicity Data: predicted to be genotoxic	Rat	Female	SD	Gavage	107	107	Not specified	Liver	Multiple tumour types	-				spleen ear Zymbals gland liver urinary bladder skin	urinary bladder ear Zymbals gland thyroid gland lung liver clitoral gland **uterus** mammary gland	urinary bladder thyroid gland vascular system liver	thyroid gland urinary bladder vascular system liver	-
Basic fuchsin	632-99-5					Rat	Male	SD	Gavage	111	111	Not specified	Liver	Multiple tumour types									
Basic Green 4	569-64-2	C1=CC(=CC=C1C(C)=C(C=2C=CC=CC=2)N(C)C)=C2N(C)C=C3C=CC(=C(C)=C3)=[N+]=2C)C.O[-]	경口 독성(준각) - 구분2 피부 부식성/피부 자극성 - 구분1(A/1B/1C) 심한 눈 손상성/눈 자극성 - 구분1 생식독성 - 구분2 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 29, 30, 34, 36, 43, 52, 53, 57, 58, 59, 60, 61, 67, 72, 91, 93, 94, 96, 112, 120, 123, 148, 150, 163, 165, 167, 197, 200, 220	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	C57BL/6N x C3H/HeN MTV-	Diet	727 d	730 d	Not specified	Adrenal gland cortex	Adenoma	-				-	-	-	-	-
Basic Green 4	569-64-2					Rat	Female	Fischer 344	Diet	3 yrs	3 yrs	Not specified	Abdomen	Leukaemia- mononuclear cell									
Basic Red 1	989-38-8	C2(=[C(-]C(=C(OC)C=1)[C(C)]=C(C=1)[C]3=C2C4=C(C=C(C)[C]=C(OC)C(C)=)N(C)N(C)C.Cl	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 생식세포 변이원성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분1	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 62, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 200, 214, 307, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic	ACHE	TMEM194A	CASP2 TNNT1	hsa00564 Glycerophospholipid metabolism - Homo sapiens (human) (1) hsa:43 K01046 ACHE; acetylcholinesterase (Cartwright blood group) hsa04725 Cholinergic synapse - Homo sapiens (human) (1) hsa:43 K01046 ACHE; acetylcholinesterase (Cartwright blood group)	-	-	-	-	-
Basic Red 1	989-38-8					Mouse	Male	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Basic Red 1	989-38-8					Rat	Female	Fischer 344	Diet	103	105	Not specified	Adrenal gland medulla	Phaeochromocytoma|benign | Phaeochromocytoma - malignant									
Basic Red 1	989-38-8					Rat	Male	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Basic Red 9	569-61-9	C2(=)C(C1=CC=C(N(C=C1)C)C=CC=C(N(C=)C2C=)C(C=)=N(C=)C=C3Cl	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 생식세포 변이원성 - 구분2 발암성 - 구분1B 특정표적장기 독성(1회 노출) - 구분2(위장관염) 특정표적장기 독성(반복 노출) - 구분2	7, 8, 11, 19, 21, 23, 25, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 59, 60, 61, 62, 72, 111, 112, 117, 122, 123, 131, 148, 150, 153, 163, 165, 167, 187, 200, 203, 207, 210	Cancer dose factor: 7.1e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Positive	Adrenal gland	Pheochromocytoma | Pheochromocytoma - malignant	-				spleen ear Zymbals gland thyroid gland	thyroid gland **uterus** urinary bladder ear Zymbals gland clitoral gland hematopoietic system lung kidney stomach liver	thyroid gland urinary bladder liver vascular system lung stomach	thyroid gland urinary bladder vascular system liver hematopoietic system **ovary** peritoneal cavity	-
Basic Red 9	569-61-9					Mouse	Male	B6C3F1	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Basic Red 9	569-61-9					Rat	Female	Fischer 344	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Basic Red 9	569-61-9					Rat	Male	Fischer 344	Diet	103	104	Positive		Body cavities - Mesothelioma | Multiple tumour sites - Mesothelioma | Tunica vaginalis - Mesothelioma | Mesothelioma/malignant									
Basic Violet 3	548-62-9	C1=CC(C=CC1=C(C2=CC=C(C=C2)N(C)C)C3=CC=C(C=C3)N(C)C)=[N+](C)C)-[]	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분1 **발암성 - 구분2** 생식 수행한 유해성 - 구분1 만성 수생환경 유해성 - 구분1	6, 7, 8, 10, 11, 14, 16, 18, 19, 21, 25, 27, 29, 30, 33, 34, 36, 37, 43, 46, 51, 52, 53, 57, 58, 59, 60, 61, 64, 66, 67, 71, 72, 91, 93, 94, 95, 96, 97, 98, 104, 111, 112, 117, 122, 123, 126, 131, 148, 150, 153, 163, 164, 165, 166, 167, 187, 195, 197, 200, 203, 204, 214, 220, 281, 307, 312, 318	Genotoxicity Data: inconclusive	Mouse	Female	B6C3F1	Diet	52	52	Negative	Liver	Multiple tumour types	TP53 BRCA BAX CASP3 CDKN1A SOX13	-	-	hsa05210 Colorectal cancer - Homo sapiens (human) (4) hsa1026 4366625: CDKN1A; cyclin dependent kinase inhibitor 1A hsa2113 4101532 BBC3; BCL2 binding component 3 hsa581 4021559 BAX; BCL2 associated X, apoptosis regulator hsa836 4021877 CASP3; caspase 3 hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa1026 4366625: CDKN1A; cyclin dependent kinase inhibitor 1A hsa2113 4101532 BBC3; BCL2 binding component 3 hsa581 4021559 BAX; BCL2 associated X, apoptosis regulator hsa836 4021877 CASP3; caspase 3 hsa01524 Platinum drug resistance - Homo sapiens (human) (4) hsa1026 4366625: CDKN1A; cyclin dependent kinase inhibitor 1A hsa2113 4101532 BBC3; BCL2 binding component 3 hsa581 4021559 BAX; BCL2 associated X, apoptosis regulator hsa836 4021877 CASP3; caspase 3	-	-	-	-	Melanoma
Basic Violet 3	548-62-9					Mouse	Female	B6C3F1	Diet	78	78	Positive	Liver	Adenoma - hepatocellular									
Basic Violet 3	548-62-9					Mouse	Female	B6C3F1	Diet	107	107	Positive	Harderian gland	Adenoma									
Basic Violet 3	548-62-9					Mouse	Male	B6C3F1	Diet	52	52	Negative	Liver	Adenoma - hepatocellular									
Basic Yellow 2	2465-27-2	C1(C=1C=CC(N(CC)CC)=CC=1)(C=2C=CC(N(CC)CC)=CC=2)=NCl	급성 독성(경구) - 구분4 급성 독성(흡입:먼지) - 구분2 **발암성 - 구분2** 특정표적장기 독성(반복 노출) - 구분2	6, 7, 8, 10, 19, 21, 23, 25, 27, 29, 30, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 59, 60, 61, 67, 72, 107, 111, 112, 117, 122, 123, 126, 148, 150, 153, 163, 164, 165, 166, 167, 187, 200, 220, 307, 318, 319	Genotoxicity Data: genotoxic	Mouse	Female	Albino	Diet	52	79	Positive	Liver	Hepatoma	ALDH1A3 MAP1LC3B ANO6 ADM2 ATP4A2	CTPS1 RPA4 INCENP DHFR CCNC	SAT SRRF1 ENC1 ITGAM FOXY4	hsa04932 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa369 4088845: ARAF; A-Raf proto-oncogene, serine/threonine kinase hsa8943 4103455: MAP1LC3B; microtubule associated protein 1 light chain 3 beta hsa05223 Non-small cell lung cancer - Homo sapiens (human) (1) hsa369 4088845: ARAF; A-Raf proto-oncogene, serine/threonine kinase hsa05214 Glioma - Homo sapiens (human) (1) hsa369 4088845: ARAF; A-Raf proto-oncogene, serine/threonine kinase	-	thyroid gland liver ear Zymbals gland **uterus** clitoral gland lung	thyroid gland liver vascular system thyroid gland lung urinary bladder stomach	stomach liver peritoneal cavity thyroid gland vascular system urinary bladder	-
Basic Yellow 2	2465-27-2					Mouse	Male	Albino	Diet	52	79	Positive	Liver	Hepatoma									
Basic Yellow 2	2465-27-2					Mouse	Female	CBA	Diet	52	78	Positive	Liver	Hepatoma									
Basic Yellow 2	2465-27-2					Mouse	Male	CBA	Diet	52	79	Positive	Liver	Hepatoma									
Basic Yellow 2	2465-27-2					Rat	Male	Wilmslow Wistar	Diet	87	125	Positive	Liver	Hepatoma									
Benfotiazine	88132-11-2	C1(=NC(=)C(C=2N(1N=CN=2)CCOCC)C3=CC=CC=C3)N			-	Rat	Female	SD	Diet	97	105	Positive	Liver	Adenoma - hepatocellular	PCB TNF TSC2201	SLC15A1 HBP1 ALDH1B1	LZT1 SRRP1 SQLE CASP2	hsa04060 Cytokine-cytokine receptor interaction - Homo sapiens (human) (1) hsa5617 4035439 PRL; prolactin hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (1) hsa5617 4035439 PRL; prolactin hsa04917 Prolactin signaling pathway - Homo sapiens (human) (1) hsa5617 4035439 PRL; prolactin	liver	liver mammary gland ear Zymbals gland small intestine	-	-	Mammary Neoplasm, Experimental Cell Transformation, Neoplastic **Liver Neoplasm, Experimental** Thyroid Neoplasm
Benfotiazine	88132-11-2					Rat	Male	SD	Diet	97	105	Positive	Liver	Adenoma - hepatocellular									
Benzolazine	64896-26-0	C1=C(C)=CC(=C1)N=NC2=CC=CC=C2C=C2C(O)=O)C(=O)O)O	-		-	Mouse	Female	NMRI	Diet	107	107	Negative	Liver	Adenoma - hepatocellular	-				urinary bladder vascular system	kidney	kidney thyroid gland	liver **ovary**	-
Benzolazine	64896-26-0					Mouse	Male	NMRI	Diet	120	120	Negative	Liver	Adenoma - hepatocellular									
Benzolazine	64896-26-0					Rat	Female	SD	Diet	119	119	Negative	Liver	Tumour - hepatocellular									
Benzolazine	64896-26-0					Rat	Male	SD	Diet	118	118	Not specified	Liver	Adenoma - hepatocellular									
Benzaldehyde	100-52-7	C1=CC=CC(=C1)C=O	인화성 액체 - 구분4 급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(사) 생식세포 변이원성 - 구분1A 특정표적장기 독성(1회 노출) - 구분3(마취졸림) 특정표적장기 독성(1회 노출) - 구분2(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2 특정표적장기 독성(반복 노출) - 구분1		Carcinogenicity data available: PPRTV (ORNL): suggestive evidence of carcinogenic potential for oral exposure. Inadequate information for inhalation. Genotoxicity Data: clastogenic	Mouse	Male	B6C3F1	Gavage	103	105	Positive	Forestomach	Papilloma - squamous cell	ALDH3A1 CYP1A1 ALDH1A1 ALDH2 SLC28A1	IRF2 SNAI2B DSE IRDR6 ABCA13	GCLC GCLM HTATIP2 SLC14A1 KRT34	hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa1548 4176683: CYP2A6; cytochrome P450 family 2 subfamily A member 6 hsa216 4072349: ALDH1A1; aldehyde dehydrogenase 1 family member A1 hsa217 4001028: ALDH2; aldehyde dehydrogenase 2 family member hsa00830 Retinol metabolism - Homo sapiens (human) (2) hsa1548 4176683: CYP2A6; cytochrome P450 family 2 subfamily A member 6 hsa216 4072349: ALDH1A1; aldehyde dehydrogenase 1 family member A1 hsa5204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (1) hsa1548 4176683: CYP2A6; cytochrome P450 family 2 subfamily A member 6	spleen Mallorcs head cancers oral cavity ear Zymbals gland hematopoietic system thyroid gland	lung kidney thyroid gland **uterus** clitoral gland	stomach thyroid gland vascular system urinary bladder small intestine lung	stomach thyroid gland **ovary** urinary bladder pituitary gland peritoneal cavity vascular system	-
Benzaldehyde	100-52-7					Mouse	Male	B6C3F1	Gavage	104	106	Positive	Forestomach	Papilloma - squamous cell									
Benzaldehyde	100-52-7					Rat	Female	Fischer 344	Gavage	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Benzaldehyde	100-52-7					Rat	Male	Fischer 344	Gavage	103	105	Not specified	Adrenal gland medulla	Pheochromocytoma/benign | Pheochromocytoma - benign- bilateral | Pheochromocytoma - malignant									
Benzenamine, 3-methoxy-4-(phenylazo)-	80830-39-3	C1=C(C=C(C)=C1)N=NC2=CC=CC=C2)OC)N	-	-	-	Mouse	Female	B6C3F1	Diet	56	56	Negative	Liver	Multiple tumour types	-				spleen urinary bladder ear Zymbals gland liver vascular system skin large intestine	urinary bladder **uterus** hematopoietic system ear Zymbals gland kidney clitoral gland	urinary bladder thyroid gland liver vascular system	urinary bladder liver thyroid gland vascular system	-
Benzenamine, 3-methoxy-4-(phenylazo)-	80830-39-3					Mouse	Male	B6C3F1	Diet	56	56	Negative	Liver	Multiple tumour types									
Benzene	71-43-2	C1=CC=CC=C1	인화성 액체 - 구분2 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2 생식세포 변이원성 - 구분1A 발암성 - **구분1A** 특정표적장기 독성(1회 노출) - 구분1 특정표적장기 독성(반복 노출) - 구분1 흡인 유해성 - 구분1 만성 수생환경 유해성 - 구분3	-	Cancer slope factor: 7.8e-06 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: IRIS: Known/Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Male	A/J(R)	Inhalation	72	72	Negative	Multiple sites	Lymphoma - malignant	**CYP2E1** TNFSF13 NQO1	IRF2 ARNT CASP12 CCDC49 FNIP2	PPP1CB CISH IL48 BCL2A1 CYP2E1		spleen oral cavity kidney thyroid gland hematopoietic system ear Zymbals gland nasal cavity	kidney **uterus** hematopoietic system thyroid gland urinary bladder ear Zymbals gland nasal cavity **lung**	thyroid gland stomach urinary bladder **lung** vascular system liver kidney small intestine preputial gland	**ovary** thyroid gland stomach urinary bladder pituitary gland peritoneal cavity vascular system hematopoietic system **lung** liver small intestine	Breast Neoplasm **Lung Neoplasm** Stomach Neoplasm Cell Transformation, Neoplastic Carcinoma, Squamous Cell **Liver Neoplasm, Experimental** Leukemia, Myeloid, Acute
Benzene	71-43-2					Mouse	Female	B6C3F1	Gavage	103	104	Positive	Harderian gland	Adenoma | Carcinoma									
Benzene	71-43-2					Mouse	Male	B6C3F1	Gavage	103	103	Positive	Adrenal gland	Pheochromocytoma									
Benzene	71-43-2					Mouse	Male	C57BL/6J	Inhalation	60	60	Positive	Multiple sites	Lymphoma - lymphocytic									
Benzene	71-43-2					Mouse	Female	Swiss	Gavage	78	104	Positive	Liver	Hepatoma									
Benzenediazonium sulphate	6411-38-9	C1=CC=CC=C1N=[N+]([O-])S(=O)(=O)[O-]				Mouse	Female	Swiss	Gavage	52	141	Positive	Liver	Hepatoma									
Benzenediazonium sulphate	6411-38-9					Mouse	Male	Swiss	Gavage	52	129	Positive	Liver	Hepatoma									
Benzenediazonium tetrafluoroborate	369-27-3	[N+]#NC1=CC=CC=C1F[B-](F)(F)F				Syrian hamster	Female	Not specified	Gavage	60	60	Not specified	Liver	Cholangioma									
Benzenediazonium tetrafluoroborate	369-57-3					Syrian hamster	Male	Not specified	Gavage	90	90	Not specified	Liver	Haemangioma									
Benzenepropanamine, N-methyl-gamma-(4-(trifluoromethyl)phenoxy)-, hydrochloride	59333-67-4	C1=CC(=CC(=C1)C(F)(F)F)OC(CCNC)C2=CC=CC=C2)Cl	-	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 200, 204, 207, 218	-	Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Multiple tumour types	-				stomach	-	stomach	lung stomach liver	-
Benzenepropanamine, N-methyl-gamma-(4-(trifluoromethyl)phenoxy)-, hydrochloride	59333-67-4					Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Multiple tumour types									
Benzenepropanamine, N-methyl-gamma-(4-(trifluoromethyl)phenoxy)-, hydrochloride	59333-67-4					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Multiple tumour types									
Benzenepropanamine, N-methyl-gamma-(4-(trifluoromethyl)phenoxy)-, hydrochloride	59333-67-4					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Multiple tumour types									
Benzethonium chloride	121-54-0	CC(C)(C)c2ccC(c1ccccC(N(C)C)c1)cc2	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(사) 만성 수생환경 유해성 - 구분2		Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Dermal	92 d	91 d	Not specified			ECM42 CXCL8	-	-						
Benzethonium chloride	121-54-0					Mouse	Female	B6C3F1	Dermal	599 d	590 d	Not specified	Adrenal gland cortex	Carcoma - histocytic									
Benzidine	92-87-5	C2C(=CC=C(N)C=C1)=CC=C(N)C=C2	급성 독성(경구) - 구분4 **발암성 - 구분1A** 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 21, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 67, 72, 112, 131, 148, 150, 163, 165, 167, 200, 350	Cancer slope factor: 0.067 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: NTP RoC: Known Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Male	ICR/Ot1	Diet	60	60	Positive	Liver	Hepatoma	LPO NAT1 SAR1 PTGS1 PTGS2 TP53	-	-	hsa01100 Metabolic pathways - Homo sapiens (human) (4) hsa10 430602: NAT2; N-acetyltransferase 2 hsa5742 4305509: PTGS1; prostaglandin-endoperoxide synthase 1 hsa5743 4115887: PTGS2; prostaglandin-endoperoxide synthase 2 hsa9 4306022: NAT1; N-acetyltransferase 1 hsa5204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (3) hsa10 4306022: NAT2; N-acetyltransferase 2 hsa5742 4115887: PTGS2; prostaglandin-endoperoxide synthase 2 hsa9 4306022 NAT1; N-acetyltransferase 1 hsa04726 Serotonergic synapse - Homo sapiens (human) (2) hsa5742 4305509: PTGS1; prostaglandin-endoperoxide synthase 1 hsa5743 4115887: PTGS2; prostaglandin-endoperoxide synthase 2	spleen ear Zymbals gland thyroid gland urinary bladder	**urinary bladder** **uterus** ear Zymbals gland thyroid gland hematopoietic system clitoral gland	thyroid gland **urinary bladder** liver vascular system lung	thyroid gland urinary bladder liver vascular system **ovary** hematopoietic system stomach	Urinary Bladder Neoplasm
Benzidine	92-87-5					Rat	Mixed	Albino	Inhalation	86	121	Positive	Liver	Hepatoma									
Benzidine dihydrochloride	531-85-1	C=2C(=1C=CC(N)=CC=1)C(=C(N)=CC=2Cl)Cl	급성 독성(경구) - 구분4 **발암성 - 구분1A** 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 25, 123, 123, 153	-	Mouse	Female	C57BL/6JC3H/Nctr x BALB/cSLc8C3H/Ncnr	Drinking water	143	143	Positive	Harderian gland	Adenoma	-				urinary bladder **uterus** ear Zymbals gland thyroid gland hematopoietic system clitoral gland liver lung kidney mammary gland oral cavity	thyroid gland urinary bladder liver vascular system lung	thyroid gland urinary bladder liver vascular system **ovary** hematopoietic system stomach pituitary gland lung	-
Benzidine dihydrochloride	531-85-1					Mouse	Female	C57BL/6JC3H/Nctr x BALB/cSLc8C3H/Ncnr	Drinking water	60	60	Positive	Liver	Adenoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Benzidine dihydrochloride	531-85-1					Mouse	Female	C57BL/6JC3H/Nctr x BALB/cSnCrlC3H/HsNctr	Drinking water	79	80	Positive	Liver	Adenoma- hepatocellular									
Benzidine dihydrochloride	531-85-1					Mouse	Male	C57BL/6JC3H/Nctr x BALB/cSnCrlC3H/HsNctr	Drinking water	143	143	Positive	Harderian gland	Adenoma									
Benzo(a)pyrene	50-32-8	C1=CC=CS(C)=C1C=4C1=CC=3C=CC=c2C=CC(C)=4C2=3)=CS	경성 독성(경구) : 구분3 피부 과민성 : 구분1(1A/1B) 생식세포 변이원성 : 구분1B 발암성 : 구분1A 생식독성 : 구분2B 경로 수용한정 유해성 : 구분1 만성 수용한정 유해성 : 구분1	14, 15, 21, 22, 27, 28, 30, 34, 36, 41, 46, 52, 53, 57, 58, 61, 64, 67, 71, 72, 111, 112, 131, 132, 133, 150, 163, 165, 167, 187, 200, 214, 207, 210, 219	Cancer slope factor: 0.0006 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: Health Canada Group 6: CEPA (probably carcinogenic to humans) Genotoxicity Data: genotoxic	Mouse	Female	Albino	Diet	60	60	Not specified	Forestomach	Papilloma	AHR CYP1A1 CYP1A2 CYP1B1 TP53	AIRN7 CASP12 CCDC49 FMF2 GCA	IMM177A1 HGFA12A LIM2 MRPS6TP2 NKAIN7	hsa05208: Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (3) hsa1543 K07408: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 K07409: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 K07410: CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa00980: Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa1543 K07408: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 K07409: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 K07410: CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa00140: Steroid hormone biosynthesis - Homo sapiens (human) (3) hsa1543 K07408: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 K07409: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1545 K07410: CYP1B1; cytochrome P450 family 1 subfamily B member 1	ear Zymbals gland kidney thyroid gland spleen Malttoni head cancers nasal cavity	ear Zymbals gland mammary gland hematopoietic system **uterus** clitoral gland nasal cavity	urinary bladder lung thyroid gland vascular system small intestine	**stomach** **ovary** urinary bladder thyroid gland vascular system pituitary gland	Prostatic Neoplasm Carcinoma, Hepatocellular Breast Neoplasm Stomach Neoplasm Mammary Neoplasm, Animal Carcinoma
Benzo(a)pyrene	50-32-8					Mouse	Female	B6C3F1	Diet	94	104	Positive	Forestomach	Carcinoma- squamous cell									
Benzo(a)pyrene	50-32-8					Mouse	Female	C57BL/6V	Gavage	52	92	Negative	Liver	Multiple tumour types									
Benzo(a)pyrene	50-32-8					Mouse	Male	C57BL/6V	Gavage	52	92	Negative	Liver	Tumour- benign									
Benzocyclohexane	110-64-2	C=12C(=CC=CC=1)CCCC2	인화성 액체 : 구분4 피부 부식성/피부 자극성 : 구분2 만성 수용한정 유해성 : 구분1	-	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Inhalation	18 d	14 d	Not specified		-	**EGR1** EGR2	-	-	-	kidney oral cavity ear Zymbals gland liver nasal cavity Malttoni head cancers	ear Zymbals gland liver **uterus** clitoral gland lung nasal cavity	stomach urinary bladder lung vascular system small intestine liver	**ovary** stomach urinary bladder pituitary gland thyroid gland lung liver hematopoietic system	-
Benzofuran	271-89-6	C=1OC2=CC=CC=1(C=CC=CC=2)	인화성 액체 : 구분3 발암성 : 구분2 특정표적장기 독성(반복 노출) : 구분2	8, 11, 15, 21, 22, 41, 57, 60, 111, 112, 130, 150, 187, 202, 210	Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Positive	Forestomach	Carcinoma- squamous cell | Papilloma- squamous cell	ACSM1 CES1 SPHK1 MTOR PPARA	HIC2 TACR3 DCLN CDA2AN2 VRILS	PFP1B14C ENC1 RNF12 ADAMTS9 MCM6	hsa05208: Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa2052 K01252: EPHX1; epoxide hydrolase 1 hsa4350 K04148: NFE2L2; NFE2 like bZIP transcription factor 2 hsa05207: Chemical carcinogenesis - receptor activation - Homo sapiens (human) (5) hsa2052 K01252: EPHX1; epoxide hydrolase 1 hsa04976: Bile secretion - Homo sapiens (human) (1) hsa2052 K01252: EPHX1; epoxide hydrolase 1	kidney ear Zymbals gland all tumor bearing animals	kidney small intestine urinary bladder	stomach **lung** liver urinary bladder thyroid gland	**stomach** liver **lung** thyroid gland vascular system urinary bladder **ovary**	Lung Neoplasms Adenoma, Liver Cell Stomach Neoplasm
Benzofuran	271-89-6					Mouse	Male	B6C3F1	Gavage	103	104	Positive	Forestomach	Carcinoma- squamous cell									
Benzofuran	271-89-6					Rat	Female	Fischer 344	Gavage	103	104	Positive	Kidney	Adenocarcinoma- tubular									
Benzofuran	271-89-6					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma-hepatocellular | Nodule- neoplastic									
Benzoguanimine	91-76-9	N1=C(N=C(N)N=C1N)N(C2=CC=CC=C2		21, 29, 30, 41, 52, 53, 57, 67, 91, 92, 94, 96, 112, 131, 150, 165, 167, 197, 200, 202	Genotoxicity Data: inconclusive	Mouse	Female	CD-1 HsMcCB	Diet	77	94	Negative	Liver	Multiple tumour types	-				urinary bladder ear Zymbals gland spleen large intestine oral cavity	ear Zymbals gland **uterus** mammary gland clitoral gland small intestine kidney hematopoietic system	urinary bladder thyroid gland stomach vascular system lung	thyroid gland hematopoietic system urinary bladder liver stomach vascular system	-
Benzoguanimine	91-76-9					Mouse	Male	CD-1 HsMcCB	Diet	72	94	Negative	Liver	Multiple tumour types									
Benzoguanimine	91-76-9					Rat	Male	SD	Diet	77	94	Negative	Liver	Multiple tumour types									
Benzoic acid	65-85-0	C1(=CC=CC=C1C(=O)O)	경성 독성(경구) : 구분4 경성 독성(흡입 분진/미스트) : 구분1 심한 눈 손상성/눈 자극성 : 구분2A(2B) 특정표적장기 독성(1회 노출) : 구분2A(2B) 특정표적장기 독성(1회 노출) : 구분3 특정표적장기 독성(반복 노출) : 구분2	29, 30, 52, 53, 57, 67, 112, 165, 167, 200	Carcinogenicity data available: IRIS D (Not classifiable as to human carcinogenicity) Genotoxicity Data: clastogenic	Rat	Male	Fischer 344/DuCr	Diet	52	52	Not specified	Forestomach	Multiple tumour types	SLC16A1 STAT3 CAT TNF	CCDC50 STX1A STAT5B TRAF5 SUMO1	AKR1B10 PTGES FECH POLR2A ITIL	hsa04068: FoxO signaling pathway - Homo sapiens (human) (2) hsa6774 K04692: STAT3; signal transducer and activator of transcription 3 hsa847 K03781: CAT; catalase hsa05212: Pancreatic cancer - Homo sapiens (human) (1) hsa6774 K04692: STAT3; signal transducer and activator of transcription 3 hsa00630: Glyoxylate and dicarboxylate metabolism - Homo sapiens (human) (1) hsa847 K03781: CAT; catalase	kidney hematopoietic system urinary bladder spleen Malttoni head cancers thyroid gland oral cavity	clitoral gland kidney urinary bladder hematopoietic system thyroid gland **uterus**	stomach kidney vascular system	**ovary** pituitary gland stomach thyroid gland liver urinary bladder vascular system	-
Benzoic acid, hydrazide	613-94-5	C1=CC=C(C=1)C=4C=CC=CC=1)NN	-	21, 29, 30, 41, 52, 53, 57, 67, 112, 131, 150, 165, 167, 200, 210	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	Swiss	Gavage	40	55	Not specified	lung	Multiple tumour types	MPO HR2	TEP1 TMV5 CAPRIN1 CCDC50 STX1A	SAT C1QBP43 LST1 IFIT1 VNN1	-	all tumor bearing animals lung liver spleen	mammary gland all tumor bearing animals hematopoietic system kidney **uterus**	lung liver vascular system urinary bladder	lung hematopoietic system liver **ovary** stomach vascular system	-
Benzoic acid, hydrazide	613-94-5					Mouse	Female	Swiss	Drinking water	110	110	Positive	Liver	Multiple tumour types									
Benzoic acid, hydrazide	613-94-5					Mouse	Male	Swiss	Drinking water	50	50	Positive	Liver	Hepatocytoma									
Benzophenone	119-61-9	C1=CC(C(=O)C2=CC=CC=C2)=CC=CC=C2	피부 부식성/피부 자극성 : 구분2 발암성 : 구분2 생식독성 : 구분2 만성 수용한정 유해성 : 구분2	8, 11, 27, 29, 30, 46, 52, 53, 57, 60, 61, 67, 112, 165, 167, 200	Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	92	91	Not specified			ESR2 CYP2B1 **EGR1** TP53 MPO SMAD3	IEG7 TEP1 SNAI1B NPM1 RNF12	TNNT1 MAGE1 GPNCS GAS6 GLC2A4	hsa05207: Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa2099 K08510: ESR1; estrogen receptor 1 hsa2252 K04079: FOS; fos proto-oncogene, AP-1 transcription factor subunit hsa05224: Breast cancer - Homo sapiens (human) (2) hsa2099 K08510: ESR1; estrogen receptor 1 hsa2252 K04079: FOS; fos proto-oncogene, AP-1 transcription factor subunit hsa05200: Pathways in cancer - Homo sapiens (human) (2) hsa2099 K08510: ESR1; estrogen receptor 1 hsa2252 K04079: FOS; fos proto-oncogene, AP-1 transcription factor subunit	liver spleen oral cavity thyroid gland Malttoni head cancers ear Zymbals gland nasal cavity kidney	liver thyroid gland **uterus** kidney hematopoietic system urinary bladder clitoral gland nasal cavity lung	vascular system urinary bladder thyroid gland lung small intestine stomach	liver **ovary** thyroid gland urinary bladder pituitary gland stomach peritoneal cavity vascular system small intestine	-
Benzoyl peroxide	94-36-0		유기과산화물 : 형식8 심한 눈 손상성/눈 자극성 : 구분2A(2B) 피부 과민성 : 구분1(1A/1B) 경성 수용한정 유해성 : 구분1 만성 수용한정 유해성 : 구분1	46	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Mixed	Albino	Diet	80	80	Not specified	Liver	Hepatoma	CAT CDC1 GSR CRX2	NAP1L1 TRIAP GSMM IEG7 SERPINB1	ILAR TNNT1 SERPINB8 HSPA1L PLXNA2	hsa00480: Glutathione metabolism - Homo sapiens (human) (2) hsa2936 K00383: GSR; glutathione-disulfide reductase hsa4952 K01581: CDC1; ornithine decarboxylase 1 hsa04915: Diabetic cardiomyopathy - Homo sapiens (human) (1) hsa2936 K00383: GSR; glutathione-disulfide reductase	spleen Malttoni head cancers oral cavity thyroid gland hematopoietic system	clitoral gland thyroid gland hematopoietic system **uterus**	vascular system small intestine	**ovary** pituitary gland urinary bladder thyroid gland peritoneal cavity stomach small intestine	Skin Neoplasm Papilloma Mouth Neoplasm Neoplasm
Benzoyl peroxide	94-36-0					Rat	Mixed	Albino	Diet	120	120	Negative	Liver	Hepatoma- malignant									
Benzyl acetate	140-11-4	CC(=O)OC1=CC=CC=C1)=O	인화성 액체 : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 특정표적장기 독성(1회 노출) : 구분1(마취졸림) 특정표적장기 독성(1회 노출) : 구분3 특정표적장기 독성(반복 노출) : 구분1		Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	105	Positive	Forestomach	Papilloma- squamous cell	ENPP2 MMP9 PPP5CA	SDC4 SERPINB1 TOB1 IEG7 LAMP2	SPAG6 POLR2A PLAAG6 PCDH17 AKR1B10	hsa4215: Protein digestion in cancer - Homo sapiens (human) (1) hsa4318 K01403: MMP9; matrix metallopeptidase 9 hsa05202: Transcriptional misregulation in cancer - Homo sapiens (human) (1) hsa4318 K01403: MMP9; matrix metallopeptidase 9 hsa04670: Leukocyte transendothelial migration - Homo sapiens (human) (1) hsa4318 K01403: MMP9; matrix metallopeptidase 9	vascular system skin hematopoietic system stomach Malttoni head cancers	hematopoietic system vascular system	stomach liver lung vascular system	stomach liver peritoneal cavity liver thyroid gland	Pancreatic Neoplasm Neoplasm Invasiveness Liver Neoplasms Stomach Neoplasm
Benzyl acetate	140-11-4					Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma-hepatocellular | Neuroblastoma									
Benzyl acetate	140-11-4					Mouse	Male	B6C3F1	Gavage	103	105	Positive	Forestomach	Carcinoma- squamous cell | Papilloma- squamous cell									
Benzyl acetate	140-11-4					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma-hepatocellular | Neuroblastoma									
Benzyl acetate	140-11-4					Rat	Female	Fischer 344	Gavage	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma-hepatocellular | Nodule- neoplastic									
Benzyl alcohol	100-51-6	C1=CC=CC(=C1)CO	경성 독성(경구) : 구분4 경성 독성(흡입) : 구분4 경성 독성(흡입 분진/미스트) : 구분3 심한 눈 손상성/눈 자극성 : 구분2A(2B) 피부 과민성 : 구분1(1A/1B) 생식독성 : 구분2	21, 28, 57, 63, 100, 101, 102, 103	Carcinogenicity data available: PPRTV (ORNL): Inadequate for an assessment of carcinogenic potential Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma-hepatocellular | Nodule- neoplastic	AKR1B1 AKR1B8 CYP2A6 CYP2B1 CYP2E2 **CYP2C11**	SDC4 ABCA13 ABCC13 TMEM59L DMBL1	EID1 EP300 SAT TCF12 ACIR1A	hsa00982: Drug metabolism - cytochrome P450 - Homo sapiens (human) (1) hsa1548 K17683: CYP2A6; cytochrome P450 family 2 subfamily A member 6 hsa00830: Retinol metabolism - Homo sapiens (human) (1) hsa1548 K17683: CYP2A6; cytochrome P450 family 2 subfamily A member 6 hsa05417: Lipid and atherosclerosis - Homo sapiens (human) (1) hsa1548 K17683: CYP2A6; cytochrome P450 family 2 subfamily A member 6	hematopoietic system thyroid gland vascular system nasal cavity oral cavity spleen Malttoni head cancers kidney stomach lung ear Zymbals gland	kidney hematopoietic system nasal cavity thyroid gland	lung vascular system thyroid gland kidney stomach	thyroid gland lung vascular system pituitary gland hematopoietic system **ovary** stomach peritoneal cavity urinary bladder	-
Benzyl alcohol	100-51-6					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Adrenal gland	Adenoma- cortical									
Benzyl alcohol	100-51-6					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma-hepatocellular | Nodule- neoplastic									
Benzyl alcohol	100-51-6					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma-hepatocellular | Nodule- neoplastic									
Benzyl chloride	100-44-7	C1=CC=CC(=C1)CCl	인화성 액체 : 구분4 생식세포 변이원성 : 구분1 경성 독성(경구) : 구분4 경성 독성(흡입) : 구분4 경성 독성(흡입 분진/미스트) : 구분3 경성 독성(흡입 증기) : 구분1 경성 독성(흡입 분진/미스트) : 구분3 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분1 피부 과민성 : 구분1(1A/1B) 발암성 : 구분1B 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2 만성 수용한정 유해성 : 구분1	-	Cancer slope factor: 4.9e-05 ug/m3-1 (carcinogenicity oral) Carcinogenicity data available: IRIS B2 (Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals) Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	104	107	Positive	Forestomach	Carcinoma	-				oral cavity	kidney thyroid gland **uterus** clitoral gland nasal cavity oral cavity	stomach liver vascular system lung small intestine	stomach thyroid gland urinary bladder peritoneal cavity liver **ovary** pituitary gland small intestine vascular system	Skin Neoplasm
Benzyl chloride	100-44-7					Mouse	Male	B6C3F1	Gavage	104	107	Positive	Forestomach	Carcinoma									
Benzyl chloride	100-44-7					Rat	Female	Fischer 344	Gavage	104	107	Not specified	Liver	Nodule- neoplastic									
Benzyl chloride	100-44-7					Rat	Male	Fischer 344	Gavage	104	107	Not specified	Liver	Nodule- neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Benzyl isothiocyanate	622-78-6	C1=CC=CC=C1CN=C=S	-	19, 23, 27, 34, 46, 61, 111, 117, 187, 307	Genotoxicity Data: predicted to be genotoxic	Rat	Male	ACI/n	Diet	53	53	Not specified	Liver	Multiple tumour types	NFE2L2 GSTP1 DNMT1 ALDH6A1 JUN MAPK1 MAPK3	ACSL3 DNAJB2 IFI27 PPP1CA PNP14	VNN1 C1ORF63 IFIT1 NQO1 TINM22	hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa:2950 K22790 GSTP1; glutathione S-transferase pi 1 hsa:2562 K00510 HMOX1; heme oxygenase 1 hsa:3725 K04448 JUN; Jun proto-oncogene, AP-1 transcription factor subunit hsa:5594 K04371 MAPK1; mitogen-activated protein kinase 1 hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (3) hsa:2950 K22790 GSTP1; glutathione S-transferase pi 1 hsa:2562 K00510 HMOX1; heme oxygenase 1 hsa:5594 K04371 MAPK1; mitogen-activated protein kinase 1 hsa05418 Fluid shear stress and atherosclerosis - Homo sapiens (human) (3) hsa:2950 K22790 GSTP1; glutathione S-transferase pi 1 hsa:2562 K00510 HMOX1; heme oxygenase 1 hsa:3725 K04448 JUN; Jun proto-oncogene, AP-1 transcription factor subunit	all tumor bearing animals Mattoni head cancers spleen	-	-	thyroid gland	-
Benzylhydrazine dihydrochloride	20570-96-1	C=1(C(NN)C=CC=CC=1Cl).Cl	-	21, 29, 30, 41, 52, 53, 57, 61, 67, 112, 131, 150, 165, 167, 200, 310	-	Mouse	Female	Swiss	Drinking water	121	121	Positive	Liver	Angiosarcoma	-				-	kidney hematopoietic system mammary gland **uterus**	lung stomach vascular system	lung hematopoietic system **ovary** stomach vascular system thyroid gland	-
Benzylhydrazine dihydrochloride	20570-96-1					Mouse	Male	Swiss	Drinking water	100	100	Not specified	Liver	Multiple tumour types									
Benzylthiocyanate	3012-37-1	C1=CC=CC=C1CSCN	연속무작위 혼합 - 구분1	19, 23, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 67, 72, 111, 112, 117, 163, 165, 167, 187, 200, 307	Genotoxicity Data: predicted to be genotoxic	Rat	Male	ACI/n	Diet	53	53	Not specified	Liver	Multiple tumour types						Mattoni head cancers spleen	-	-	urinary bladder	-
Bifenthrin	82657-04-3	[C@H]1[C@H]([C@H](C)C)C(OC(=O)C=C(Cl)C(F)(F)F)C(C)(C)[C@H]1C=C(Cl)Cl	급성 독성(경구) - 구분2 급성 독성(경피) - 구분3 급성 독성(흡입: 분진/미스트) - 구분3 피부 과민성 - 구분1(1A/1B) **발암성 - 구분2** 특정표적장기 독성(1회 노출) - 구분1 특정표적장기 독성(반복 노출) - 구분1 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 19, 23, 27, 29, 30, 52, 53, 57, 58, 60, 61, 67, 107, 111, 112, 117, 131, 165, 167, 187, 200, 307	Carcinogenicity data available: EPA CPP-Group C Possible Human Carcinogen	Mouse	Female	Swiss Webster	Diet	92	92	Not specified	Urinary bladder	Neoplasm- mesenchymal	CGA CAT PTGS2 TNF JUN NFKB1 RELA	-	CYP3A4 TIF1 CYP3B6 FGR WNT10B	hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (4) hsa:3569 K05405 IL6; interleukin 6 hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa:847 K03781 CAT; catalase hsa05010 Alzheimer disease - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:4780 K03628 NFE2L2; NFE2 like bZIP transcription factor 2 hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2	-	-	-	-	-
Bifenthrin	82657-04-3					Mouse	Male	Swiss Webster	Diet	86	86	Not specified	Urinary bladder	Neoplasm- mesenchymal									
Biphenyl	92-52-4	C2C(C1=CC=CC=C1)=CC=CC=CC=C2	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	29, 30, 52, 53, 57, 61, 67, 112, 131, 165, 167, 200	Carcinogenicity data available: PPRTV (ORNL) - Suggestive evidence of carcinogenic potential Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	CYP1A2 CYP3A13 CYP1A1 CYP2J5 ESR1 NPH3	AIRN7 CADPS2 CCDC49 FNIP2 GCA	FAM171A1 H2AX12A LIM2 MAFIK3FS NKAIN1	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (3) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:1545 K07410 CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa:2099 K08550 ESR1; estrogen receptor 1 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa:1543 K07408,CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:1545 K07410,CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa:1553 K17683,CYP2A13; cytochrome P450 family 2 subfamily A member 13 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (3) hsa:1543 K07408,CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:1545 K07410,CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa:1553 K17683,CYP2A13; cytochrome P450 family 2 subfamily A member 13	thyroid gland spleen kidney oral cavity hematopoietic system nasal cavity **urinary bladder** Mattoni head cancers	hematopoietic system **uterus** **urinary bladder** kidney nasal cavity thyroid gland clitoral gland ear Zymbals gland liver	**urinary bladder** thyroid gland lung stomach vascular system liver kidney small intestine preputial gland	**ovary** thyroid gland **urinary bladder** stomach pituitary gland vascular system lung liver peritoneal cavity small intestine hematopoietic system	Carcinoma Urinary Bladder Neoplasm Papilloma
Biphenyl	92-52-4					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Biphenyl	92-52-4					Mouse	Female	B6CF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Biphenyl	92-52-4					Mouse	Male	B6CF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Biphenyl-2,5-diyl-bis(2,2-dimethyl-5-oxopentanoic acid)	79520-77-7	C(C)(C)CCC(=O)Oc1ccc(-c2c-c(C)c(C)c(C)c2)cc(c1C)OCCCC(C)(C)CO)o-OC2=CC=CC=C2N(C)O)o-O	-	-	-	Mouse	Female	B6CF1	Diet	104	104	Positive	Liver	Adenoma - hepatocellular	-				liver urinary bladder stomach	urinary bladder	liver kidney	liver	Adenoma, Liver Cell Carcinoma, Hepatocellular
Biphenyl-2,5-diyl-bis(2,2-dimethyl-5-oxopentanoic acid)	79520-77-7					Mouse	Male	B6CF1	Diet	104	104	Positive	Liver	Adenoma - hepatocellular									
bis(3,4-Dichlorophenyl)-diazene	14047-09-7	N(=N(C=1C=c(Cl)c(Cl=1)Cl)Cl)=c(Cl)c(Cl)Cl	**발암성 - 구분1B** 만성 수생환경 유해성 - 구분1	-	Carcinogenicity data available: CalEPA Likely Human Carcinogen	Mouse	Female	B6CF1	Gavage	92 d	91 d	Not specified			CYP1A1 CYP1A2 **AHR** **AR** ESR1 ESR2 **KRAS**	CCNC AIM1 CTCORF75 COG6 MITD1	BEL CDS51 ELOVL1 GAUS31 GCOM1	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (5) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:196 K09063 AHR; aryl hydrocarbon receptor hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2 hsa:367 K08557 AR; androgen receptor hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2 hsa:367 K08557 AR; androgen receptor hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:196 K09063 AHR; aryl hydrocarbon receptor	spleen thyroid gland vascular system liver urinary bladder oral cavity ear Zymbals gland	liver urinary bladder kidney **lung** thyroid gland **uterus**	liver vascular system kidney thyroid gland	thyroid gland liver vascular system urinary bladder	**Lung Neoplasm** Urethal Neoplasm
bis(p-Chlorophenyl) sulphone	80-07-9	O=S(=O)(C1=CC=C(C=C1)Cl)C2=CC=C(C=C2)Cl	연성 수생환경 유해성 - 구분1	8, 11, 19, 23, 29, 30, 34, 36, 52, 53, 58, 60, 61, 67, 72, 111, 112, 117, 163, 165, 167, 187, 200, 307	Carcinogenicity data available: PPRTV (ORNL) - Inadequate for an assessment of carcinogenic potential Genotoxicity Data: non-genotoxic	Mouse	Female	B6CF1	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Hepatoblastoma	AR ESR1 NPH3 TP4PC AKL	FABP4 IFI27 MANSC1 TFAM SNAG8	BEL SAT IL1RN CCR5 TMEM4K	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:5468 K08530 PPARG; peroxisome proliferator-activated receptor gamma hsa05224 Breast cancer - Homo sapiens (human) (1) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (1) hsa:5468 K08530 PPARG; peroxisome proliferator-activated receptor gamma	spleen thyroid gland	thyroid gland mammary gland	vascular system	thyroid gland urinary bladder	-
bis(p-Chlorophenyl) sulphone	80-07-9					Mouse	Male	B6CF1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Hepatoblastoma									
bis(p-Chlorophenyl) sulphone	80-07-9					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Hepatoblastoma									
bis(p-Chlorophenyl) sulphone	80-07-9					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Hepatoblastoma									
bis(Pentabromophenyl) ether	1163-19-5	C1(=C(C(=C(C(=C1Br)Br)O)C2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	생식세포 변이원성 - 구분2 특정표적장기 독성(반복 노출) - 구분2		Carcinogenicity data available: IRIS-Suggestive evidence of carcinogenic potential Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6CF1	Diet	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	CYP1A1 TIF1 **AHR** CAT CYP2J5 TNRA CYP17A1	EFNA3 CCNN2B BAGAL7S RBM13 SRGAP1	CYP1A2 CYP3A4 DIO1 CTORF63 STXGA11	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (3) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:196 K09063 AHR; aryl hydrocarbon receptor hsa:847 K03781 CAT; catalase hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:196 K09063 AHR; aryl hydrocarbon receptor hsa00100 Metabolic pathways - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:847 K03781 CAT; catalase	liver large intestine **thyroid gland** urinary bladder kidney oral cavity hematopoietic system	liver kidney **thyroid gland** urinary bladder	liver stomach lung	liver stomach **thyroid gland** urinary bladder pituitary gland peritoneal cavity **ovary**	Thyroid Cancer, Papillary Adenoma
bis(Pentabromophenyl) ether	1163-19-5					Mouse	Male	B6CF1	Diet	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
bis(Pentabromophenyl) ether	1163-19-5					Rat	Female	Fischer 344	Diet	103	104	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
bis(Pentabromophenyl) ether	1163-19-5					Rat	Male	Fischer 344	Diet	103	104	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
bis[4-Dimethylamino]phenyl]methanone	90-94-8	C(C1=CC=C(N(C)C)C=C1)(C2=CC=C(N(C)C)C=C2)=O	생식세포 변이원성 - 구분2 **발암성 - 구분2B** 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	8, 11, 19, 23, 27, 28, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 63, 67, 72, 100, 101, 102, 103, 111, 112, 117, 128, 150, 163, 165, 167, 177, 187, 200, 307, 310	Cancer slope factor: 0.00025 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6CF1	Diet	78	91	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular	-				**liver** thyroid gland	**liver** thyroid gland ear Zymbals gland	vascular system thyroid gland	**liver** peritoneal cavity	Liver Neoplasm, Experimental
bis[4-Dimethylamino]phenyl]methanone	90-94-8					Mouse	Male	B6CF1	Diet	78	91	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
bis[4-Dimethylamino]phenyl]methanone	90-94-8					Rat	Female	Fischer 344	Diet	78	107	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
bis[4-Dimethylamino]phenyl]methanone	90-94-8					Rat	Male	Fischer 344	Diet	78	106	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Bisphenol A	80-05-7	C[C](C)(C)=[C]C=[C]C=[C]C[C]=[C]C=[C]C=[C]O	천연 눈 손상성/눈 자극성 - 구분1 피부 과민성 - 구분1(1A/1B) 생식독성 - 구분1B 특정표적장기 독성(반복 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분1	6, 8, 11, 14, 18, 19, 21, 23, 27, 29, 30, 33, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 91, 93, 94, 96, 107, 111, 112, 117, 121, 150, 163, 165, 166, 167, 187, 197, 200, 214, 217, 310, 318	Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6C3F1	Diet	103	107	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	INS ESR1 ESR2 HAVCR1 AR NAPRT1	CCDC50 STX1A GART SEC16A YPEL5	CGB BAG3|AIP1 CREB3L1 RNA5SL HSPC8	hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa:2099 KEGG:5501; estrogen receptor 1 hsa:2100 KEGG:5502; estrogen receptor 2 hsa:367 KEGG:7; AR; androgen receptor hsa:5594 KEGG:7; MAPK1; mitogen-activated protein kinase 1 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (4) hsa:2099 KEGG:5501; estrogen receptor 1 hsa:2100 KEGG:5502; estrogen receptor 2 hsa:367 KEGG:7; AR; androgen receptor hsa:5594 KEGG:7; MAPK1; mitogen-activated protein kinase 1 hsa05224 Breast cancer - Homo sapiens (human) (3) hsa:2099 KEGG:5501; estrogen receptor 1 hsa:2100 KEGG:5502; estrogen receptor 2 hsa:5594 KEGG:7; MAPK1; mitogen-activated protein kinase 1	stomach urinary bladder kidney nasal cavity Malttoni head cancers	stomach hematopoietic system thyroid gland urinary bladder	kidney thyroid gland stomach	**ovary** pituitary gland thyroid gland stomach	Prostatic Neoplasm Colorectal Neoplasm Breast Neoplasm Mammary Neoplasms, Animal Neoplasm
Bisphenol A	80-05-7					Mouse	Male	B6C3F1	Diet	103	107	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Bisphenol A	80-05-7					Rat	Female	Fischer 344	Diet	103	108	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Bisphenol A	80-05-7					Rat	Male	Fischer 344	Diet	103	108	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Bithionol	97-18-7	C1(=C(C(=C(C(=C1O)SC=3C(O)(O)=C(C=C(C=2)Cl)Cl)Cl)Cl)Cl	급성 독성(경구) - 구분2 만성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분3	6, 7, 8, 11, 14, 18, 19, 23, 26, 27, 29, 30, 33, 34, 36, 37, 43, 46, 51, 52, 53, 58, 60, 61, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 146, 153, 163, 165, 166, 167, 187, 200, 214, 307, 318	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma	FYD SLC22A2 THRA THRB	FABP4 TRAM CYP11A1 MAMDC1 PLSCR4	IBS POR VAGN ABHD2 ERCC2	hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (1) hsa:7067 KEGG:47; THRA; thyroid hormone receptor alpha hsa05231 Choline metabolism in cancer - Homo sapiens (human) (1) hsa:6582 KEGG:9; SLC22A2; solute carrier family 22 member 2 hsa04919 Thyroid hormone signaling pathway - Homo sapiens (human) (1) hsa:7067 KEGG:47; THRA; thyroid hormone receptor alpha	thyroid gland hematopoietic system	thyroid gland	thyroid gland liver vascular system	thyroid gland liver	-
Bithionol	97-18-7					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Bithionol	97-18-7					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Bithionol	97-18-7					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Angioma									
Bromobenzene	108-86-1	C1=C(C=CC(=C1)Br	인화성 액체 - 구분2 피부 부식성/피부 자극성 - 구분2 천연 눈 손상성/눈 자극성 - 구분2A/2B 특정표적장기 독성(반복 노출) - 구분2 특정표적장기 독성(반복 노출) - 구분2 흡인 유해성 - 구분1 만성 수생환경 유해성 - 구분2	-	Carcinogenicity data available: IRIS-Inadequate information to assess carcinogenic potential Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Inhalation	94 d	91 d	Not specified			HMOX1 AIAD NQO1	CKBN2B BAGAL7S RBM13 EPNA3 SRGAP1	CYP1A2 C1ORF43 STEAP4 CTEC2 CTTN	hsa00860 Porphyrin metabolism - Homo sapiens (human) (1) hsa:210 KEGG:88; ALAD; aminolevulinate dehydratase hsa01240 Biosynthesis of cofactors - Homo sapiens (human) (1) hsa:210 KEGG:88; ALAD; aminolevulinate dehydratase hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa:210 KEGG:88; ALAD; aminolevulinate dehydratase	kidney large intestine oral cavity urinary bladder thyroid gland liver spleen ear Zymbals gland	kidney urinary bladder liver thyroid gland uterus nasal cavity oral cavity	stomach lung liver small intestine vascular system kidney	stomach lung liver thyroid gland **ovary** urinary bladder pituitary gland peritoneal cavity	-
Bromocriptine mesylate	22260-51-1	N1(C)=C(C2=C(C=C(C=C(C(=O)N(C)C)C@@H]1C)N(C)C@@H]2C=4)C(N(C@@(C)(O)[C@@H](C)=O)N4)C@]5(CC(C)(H)[C@]6(C)(C)C)C7=C(O)C(C)C)=O)C(H)(H)H)OS(O)(=O)=O	급성 수생환경 유해성 - 구분1	-	-	Mouse	Female	CrF1	Diet	74	74	Negative	Liver	Nodule - neoplastic	-								-
Bromocriptine mesylate	22260-51-1					Mouse	Male	CrF1	Diet	74	74	Negative	Liver	Nodule - neoplastic									
Bromocriptine mesylate	22260-51-1					Rat	Female	CrlA	Diet	103	103	Positive	Liver	Tumour - hepatocellular									
Bromocriptine mesylate	22260-51-1					Rat	Male	CrlA	Diet	103	103	Not specified	Liver	Tumour - hepatocellular									
Bromoindosteyrene	7166-19-0	[N+](C)=1C(C1=CC(=CC=C(C1)Br)[C]=1=O	급성 수생환경 유해성 - 구분1	-	-	Mouse	Female	B6C3F1	Gavage	26 d	28 d	Not specified			-				kidney ear Zymbals gland thyroid gland liver spleen oral cavity stomach skin hematopoietic system Malttoni head cancers nasal cavity lung large intestine urinary bladder	kidney stomach mammary gland hematopoietic system uterus thyroid gland liver	stomach lung kidney vascular system thyroid gland urinary bladder liver small intestine	**ovary** stomach lung hematopoietic system urinary bladder thyroid gland vascular system peritoneal cavity pituitary gland liver small intestine	-
Bucetin	1983-57-4	C1(=CC=CC=C1[N](C)C(C)(O)=O)OCC	천연 눈 손상성/눈 자극성 - 구분2A/2B 급성 수생환경 유해성 - 구분1	-	-	Mouse	Female	B6C3F1	Diet	72	84	Not specified	Liver	Adenoma - hepatocellular	-				nasal cavity urinary bladder stomach skin	nasal cavity ear Zymbals gland urinary bladder stomach mammary gland	kidney thyroid gland urinary bladder	urinary bladder	-
Bucetin	1983-57-4					Mouse	Male	B6C3F1	Diet	70	84	Positive	Kidney	Adenoma - renal cell									
Butyl benzyl phthalate	85-68-7	C(C1=C(C)(OCCC)=O)(C=CC=C1)(O)OCC2=CC=CC=C2)=O	생식세포 변이원성 - 구분2 생식독성 - 구분1B 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 29, 30, 34, 36, 46, 52, 53, 57, 58, 60, 61, 67, 72, 112, 122, 123, 131, 150, 163, 165, 167, 200, 220	Carcinogenicity data available: IRIS-C (Possible human carcinogen) Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	INS ESR1 CGA HMMR AHR NEDD4	LAMP3 AIRN72 PAPSS1	ABXB10 FTL WNT10B FBCN PCDH17	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:2099 KEGG:5501; estrogen receptor 1 hsa:5468 KEGG:30; PPARG; peroxisome proliferator-activated receptor gamma hsa04917 Prolactin signaling pathway - Homo sapiens (human) (2) hsa:1081 KEGG:22; CGA; glycoprotein hormones, alpha polypeptide hsa:2099 KEGG:5501; estrogen receptor 1 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:196 KEGG:3; AHR; aryl hydrocarbon receptor hsa:2099 KEGG:5501; estrogen receptor 1	hematopoietic system liver kidney	hematopoietic system liver	liver stomach vascular system	liver stomach	Neoplasm Metastasis Mammary Neoplasm, Animal
Butyl benzyl phthalate	85-68-7					Mouse	Male	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Butyl benzyl phthalate	85-68-7					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Butyl benzyl phthalate	85-68-7					Rat	Female	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
Butyl paraben	94-26-8	C1=C(C=CC(=C1O)C(O)OCCCC)=O	피부 부식성/피부 자극성 - 구분2 천연 눈 손상성/눈 자극성 - 구분2A/2B 피부 과민성 - 구분1(1A/1B) 특정표적장기 독성(반복 노출) - 구분1(호흡기 자극)	8, 10, 11, 16, 21, 23, 28, 29, 30, 33, 34, 36, 37, 38, 52, 53, 58, 60, 61, 63, 67, 72, 100, 105, 160, 163, 167, 193, 112, 117, 121, 122, 145, 167, 187, 200, 307	Genotoxicity Data: clastogenic	Mouse	Female	ICR/Ztd	Diet	102	106	Negative	Liver	Multiple tumour types	ESR1 PPARG NR0B2 CYP2C9 PGR CYP19A1	LAMP3 AIRN72 PAPSS1 ZFAND5 CCDC50	PTGR1 ABXB10 FBCN FTL FGD	hsa04932 Non-alcoholic fatty liver disease - Homo sapiens (human) (2) hsa:1050 KEGG:1; CEBPA; CCAAT enhancer binding protein alpha hsa:5468 KEGG:30; PPARG; peroxisome proliferator-activated receptor gamma hsa05203 Transcriptional misregulation in cancer - Homo sapiens (human) (2) hsa:1050 KEGG:1; CEBPA; CCAAT enhancer binding protein alpha hsa:5468 KEGG:30; PPARG; peroxisome proliferator-activated receptor gamma hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:1050 KEGG:1; CEBPA; CCAAT enhancer binding protein alpha hsa:5468 KEGG:30; PPARG; peroxisome proliferator-activated receptor gamma	hematopoietic system kidney urinary bladder stomach	hematopoietic system urinary bladder liver stomach	kidney liver thyroid gland stomach	pituitary gland liver **ovary** stomach thyroid gland	-
Butyl paraben	94-26-8					Mouse	Male	ICR/Ztd	Diet	102	106	Negative	Liver	Multiple tumour types									
C.I. Food Black 1	2519-30-4	[Na+].[Na+].[Na+].O=S(=O)([C-]1C=C(C(=C(C=C1)C(=C(C1=CC=C(N(=NC3=CC=C(S(=O)(=O)[O-])C=C3)N)C4=C(S(=O)(=O)[O-])C=C(N)C=C4)C5=C(C=C(C=C5)S(=O)(=O)[O-])C=C1)N)C6=C(C=CC(=C6)S(=O)(=O)[O-])C=C2)[O-].[Na+]	피폭경로		-			Mouse	Female	CFW	Diet	80	80	Negative	Liver	Multiple tumour types	-								
C.I. Food Black 1	2519-30-4					Mouse	Male	CFW	Diet	80	80	Negative	Liver	Multiple tumour types									
C.I. Food Black 1	2519-30-4					Rat	Female	CRL	Diet	104	104	Negative	Liver	Multiple tumour types									
C.I. Food Black 1	2519-30-4					Rat	Male	CRL	Diet	104	104	Negative	Liver	Multiple tumour types									
C.I. Food Brown 3	4553-88-3	O.[S](=O)(=O)=C(N)=NC1=C(C(=C(C(=C1O)C(O)N=NC1=2C=CC(S)=C(C=1)C(=C(C=C(C=C(C

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
C.I. Food Yellow 3	2783-94-0					Mouse	Male	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
C.I. Food Yellow 3	2783-94-0					Mouse	Female	SD	Diet	80	80	Negative	Liver	Multiple tumour types									
C.I. Food Yellow 3	2783-94-0					Mouse	Male	SD	Diet	80	80	Negative	Liver	Multiple tumour types									
C.I. Pigment Red 23	6471-48-4	[N+](=O)[O-]\c1cc(C4N=C(N)C(=Z\C(=C/Cl)\c2ccc(N=NC1=c(C)c(C)c(C)N=)c(C)c2)c(N=)[O-]c1c(C)c(C)N[O-])	특정표적장기 독성(1회 노출) : 구분3(호흡기 자극)	-	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				urinary bladder skin spleen	mammary gland	thyroid gland kidney urinary bladder	liver	-
C.I. Pigment Red 23	6471-48-4					Mouse	Male	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
C.I. Pigment Red 23	6471-48-4					Rat	Female	Fischer 344	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
C.I. Pigment Red 23	6471-48-4					Rat	Male	Fischer 344	Diet	103	104	Not specified	Kidney	Adenoma - tubular | Carcinoma - tubular									
C.I. Pigment Red 3	2425-85-6	[N+](C1=C(N=NC1=c(C2C)c(CC=C(C=C1)Cl)c=CC=C(Cl)c=CC=C2)Cl)c(C)c(C)c(C)c(C)[O-])=O	자료없음	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				spleen liver urinary bladder vascular system	liver clitoral gland urinary bladder	thyroid gland kidney urinary bladder	ovary liver vascular system	-
C.I. Pigment Red 3	2425-85-6					Mouse	Male	B6C3F1	Diet	103	104	Positive	Kidney - cortex	Adenoma									
C.I. Pigment Red 3	2425-85-6					Rat	Female	Fischer 344	Diet	103	104	Positive	Liver	Adenoma - hepatocellular									
C.I. Pigment Red 3	2425-85-6					Rat	Male	Fischer 344	Diet	103	104	Positive	Adrenal gland medulla	Pheochromocytoma benign									
C.I. Pigment Red 49	1248-18-6	S(C(=)C1=c(C(=c(C1(=c(C(=2Na(=NC=)c(C(=c(C4C=)c(=)c(C(=c(4O)(=)[O-])(=O)Na+)]	경구 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	-	Genotoxicity Data: non-genotoxic	Rat	Female	Osborne-Mendel	Diet	105	105	Negative	Liver	Adenoma	-				-	-	-	-	-
C.I. Pigment Red 49	1248-18-6					Rat	Male	Osborne-Mendel	Diet	105	105	Negative	Liver	Adenoma - hepatocellular									
C.I. Pigment Red 52:1	5160-02-1	[Ba+2].O=S(=O)([O-])c1N=NC=2C1=c(C=c(C=c(C1=c(C=c(C(=c(C(=c(C(C)C)[O-]C(=c(C(C)C)[O-]O=S(=O)([O-])c(N=NC=)c(C4=c(C=c(C=c(C=c(C(=c(C(C)C)[O-])c(C)c(C)c(C)[O-])c(C)c(C)c(C)[O-])c(C)c(C)c(

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Carbazoline	244-63-3	C1=NC=C2C(=C1)C3=C(N2)C=CC=C3	-	21, 41, 46, 57, 131, 150, 310	-	Rat	Male	Wistar	Diet	80	80	Negative	Forestomach	Papilloma	CYP1A1 **AHR** MAOB SLC22A1 SLC22A2 SLC22A3	SNA1 IL1R1 DNAH12 ANHX2 KIT1	AHRR CYP3B6 ADIPOQ TMEM4F02 CYSOR11B	hsa05231 Choline metabolism in cancer - Homo sapiens (human) (2) hsa6580 KSR1 SLC22A1; solute carrier family 22 member 1 hsa6582 KSR1 SLC22A2; solute carrier family 22 member 2 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa196 KR003 AHR; aryl hydrocarbon receptor hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa196 KR003 AHR; aryl hydrocarbon receptor	ear Zymbals gland thyroid gland	ear Zymbals gland all tumor bearing animals clitoral gland	stomach urinary bladder vascular system liver urinary bladder	stomach thyroid gland vascular system liver urinary bladder	-
Carbofuran	1563-66-2	CC2(C)OC1=C(OC(=O)NC)C=CC=C1C2	급성 독성(경구) : 구분2 급성 독성(흡입) : 구분2 급성 독성(경피) : 구분4 생식세포 변이원성 : 구분2 특정표적장기 독성(1회 노출) : 구분1 특정표적장기 독성(반복 노출) : 구분1 경구 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 16, 27, **29**, **30**, 52, 53, 57, 60, 67, 112, **165**, **167**, **200**, 281, 312	Carcinogenicity data available SPA OFP-Not Likely to Be Carcinogenic in Humans Genotoxicity Data: non-genotoxic	Mouse	Female	ICR	Drinking water	52	78	Negative	lung	Adenoma	ACHE CAT CYP1A4 GPT	NADK NCPR4	CYP2B6 CYP3A4 NR1I2 CSS HSPC8	hsa00100 Metabolic pathways - Homo sapiens (human) (2) hsa1576 K17689 CYP1A4; cytochrome P450 family 1 subfamily A member 4 hsa847 K03781 CAT; catalase hsa04068 FoxO signaling pathway - Homo sapiens (human) (1) hsa847 K03781 CAT; catalase hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (1) hsa1576 K17689 CYP1A4; cytochrome P450 family 1 subfamily A member 4	all tumor bearing animals	-	-	-	Prostatic Neoplasm Colonic Neoplasm
Carbofuran	1563-66-2					Mouse	Male	ICR	Drinking water	52	78	Negative	lung	Adenoma									
Catechol	120-80-9	C1(=C(C(=CC=C1)O)O)	급성 독성(경구) : 구분3 급성 독성(경피) : 구분2 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2 생식세포 변이원성 : 구분2 **발암성 : 구분2**	6, 7, 18, 19, 21, 23, 25, 27, **29**, **30**, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 67, 72, 111, 112, 117, 122, 125, 131, 150, 153, 163, **165**, 166, **167**, **187**, **200**, 220, 307, 310, 318	Carcinogenicity data available CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	96	96	Positive	Forestomach	Papilloma	COMT HMBS HBB ALAS2 MYB	HEATR3 CKS2RI4 IFIH1 COG5 DNAAF2	GNAI1 LIPH PITPNM1 CIP72 TCF12	hsa01240 Biosynthesis of cofactors - Homo sapiens (human) (2) hsa212 K00643 ALAS2; 5'-aminolevulinate synthase 2 hsa2145 K01749 HMBS; hydroxymethylbilane synthase hsa00860 Porphyrin metabolism - Homo sapiens (human) (2) hsa212 K00643 ALAS2; 5'-aminolevulinate synthase 2 hsa2145 K01749 HMBS; hydroxymethylbilane synthase hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa212 K00643 ALAS2; 5'-aminolevulinate synthase 2 hsa2145 K01749 HMBS; hydroxymethylbilane synthase	stomach kidney urinary bladder hematopoietic system nasal cavity thyroid gland oral cavity vascular system ear Zymbals gland Mammary head cancers large intestine spleen lung	stomach urinary bladder hematopoietic system kidney thyroid gland small intestine nasal cavity **uterus** liver clitoral gland lung	stomach thyroid gland kidney lung vascular system urinary bladder small intestine	**ovary** thyroid gland stomach pituitary gland urinary bladder vascular system hematopoietic system peritoneal cavity small intestine	Stomach Neoplasm
Catechol	120-80-9					Mouse	Male	B6C3F1	Diet	96	96	Positive	Forestomach	Papilloma									
Catechol	120-80-9					Rat	Male	CD(SD)IGS	Diet	104	104	Positive	Forestomach	Carcinoma, squamous cell									
Catechol	120-80-9					Rat	Male	Fischer 344	Drinking water	78	78	Negative	Pancreas	Carcinoma, in situ									
Catechol	120-80-9					Rat	Female	Fischer 344/DuCrl	Diet	104	104	Positive	Liver	Nodule- hyperplastic									
Celecoxib	169590-42-5	N1=C(C=C(N1C=2C=CC(S(=O)(=O)N)=CC=2)C3=CC=C(C=C3)C(F)(F)F	-	7, 8, 11, 14, 16, 21, 23, 25, 28, 29, **30**, 34, 36, 46, 52, 53, 57, 58, 60, 61, 63, 64, 66, 67, 71, 72, 100, 101, 160, 163, 111, 112, 117, 122, 123, 131, 150, 153, 163, **165**, **167**, **187**, **200**, 214, 220, 307, 318	-	Rat	Male	Fischer 344	Diet	53	53	Negative	Colon	Multiple tumour types	-				spleen	-	thyroid gland	urinary bladder	-
Celecoxib	169590-42-5					Rat	Male	Fischer 344	Diet	53	53	Negative	Colon	Multiple tumour types									
Celiprolol	56980-93-9	C1(=CC=C(C=C1C(C)=O)NC2N(CCOC(=O)OC(C)(N)C)C)CO	-	-	-	Mouse	Female	CD1	Diet	104	104	Negative	Lung	Multiple tumour types	ACT DYNLL1 NOS2 NPPB	FKBP5	STP8 TNNT1	hsa05010 Alzheimer disease - Homo sapiens (human) (1) hsa4843 K12241 NOS2; nitric oxide synthase 2 hsa05146 Amoebiasis - Homo sapiens (human) (1) hsa4843 K12241 NOS2; nitric oxide synthase 2 hsa05145 Toxoplasmosis - Homo sapiens (human) (1) hsa4843 K12241 NOS2; nitric oxide synthase 2	skin	-	kidney	-	-
Celiprolol	56980-93-9					Mouse	Male	CD1	Diet	104	104	Negative	Lung	Multiple tumour types									
Celiprolol	56980-93-9					Rat	Female	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Celiprolol	56980-93-9					Rat	Male	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Chloramben	133-90-4	C1(=C(C(=CC(=C1)Cl)N(C)C)C(=O)O	피부감염	57, 131	-	Mouse	Female	B6C3F1	Diet	80	91	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	-				vascular system urinary bladder ear Zymbals gland spleen liver	urinary bladder clitoral gland	liver vascular system kidney	liver thyroid gland vascular system	-
Chloramben	133-90-4					Mouse	Male	B6C3F1	Diet	80	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chloramben	133-90-4					Rat	Female	Osborne-Mendel	Diet	80	113	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chloramben	133-90-4					Rat	Male	Osborne-Mendel	Diet	80	112	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chlorambucil	305-03-3	C1(=C(=C(C=C1)N(CCCl)CCCl)CCCC(=O)=O	급성 독성(경구) : 구분3 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(사)(A) 생식세포 변이원성 : 구분2 **발암성 : 구분1A** 생식독성 : 구분1A 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극)	43, 46, 57, 61	Cancer slope factor: 0.0023 (mg/kg-day)-1 (carcinogenicity, oral) Carcinogenicity data available NTP RCC-Known Human Carcinogen	Mouse	Female	Swiss	Intraperitoneal	26	78	Positive	Liver	Lymphosarcoma	AKC1 BTNL2 GSTA1 ATP7B Bcl2 GSDA3	TRA2A NDE1 WDR4	PCKLR2k MT1L KATS ITGA6	hsa05418 fluid shear stress and atherosclerosis - Homo sapiens (human) (4) hsa2938 K00799 GSTA1; glutathione S-transferase alpha 1 hsa2950 K23790 GSTP1; glutathione S-transferase pi 1 hsa4780 K09428 NFE2L2; NFE2 like bZIP transcription factor 2 hsa596 K02161 BCL2; BCL2 apoptosis regulator hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa2938 K00799 GSTA1; glutathione S-transferase alpha 1 hsa2950 K23790 GSTP1; glutathione S-transferase pi 1 hsa4780 K09428 NFE2L2; NFE2 like bZIP transcription factor 2 hsa596 K02161 BCL2; BCL2 apoptosis regulator hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (3) hsa2938 K00799 GSTA1; glutathione S-transferase alpha 1 hsa2950 K23790 GSTP1; glutathione S-transferase pi 1 hsa4780 K09428 NFE2L2; NFE2 like bZIP transcription factor 2	hematopoietic system all tumor bearing animals liver kidney	ear Zymbals gland kidney mammary gland **uterus**	**lung** kidney stomach liver	**lung** hematopoietic system liver stomach	Lung Neoplasm Lymphoma, Large B-Cell, Diffuse Adenocarcinoma Cell Transformation, Neoplastic Carcinoma, Squamous Cell Urinary Bladder Neoplasm
Chlorambucil	305-03-3					Mouse	Male	Swiss	Intraperitoneal	26	78	Positive	Liver	Multiple tumour types									
Chlorambucil	305-03-3					Rat	Female	SD	Gavage	78	104	Positive	Ear canal, external	Carcinoma, squamous cell									
Chlorambucil	305-03-3					Rat	Male	SD	Intraperitoneal	26	78	Positive	Liver	Multiple tumour types									
Chlorfenson	80-33-1	O=S(=O)(C1=1C=CC(=CC=1)Cl)OC2=CC=C(C=C2)Cl	급성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 경미 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2 경미 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	-	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				vascular system spleen thyroid gland	vascular system	-	thyroid gland urinary bladder	-
Chlorfenson	80-33-1					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Chlorfenson	80-33-1					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Chlorfenson	80-33-1					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Chlormadinone acetate, Medroxyl mixture	8065-99-6	C[C@]34[C@H]([C@H]1[C@]([C@@]([C@]1(C)CC(=O)C=C2)(C)C)O[C@@](C)(C(=O)CO[C@@](C)(C(=O)C)O[C@@H]3[C@H]4C)=O)[C@H]4[C@H]5[C@H]6[C@H](C=C(C)C(=O)[C@]6(C)C=C[C@]5(C)[C@H]4C)[C@H]3C					Mouse	Female	B6C3F1 (MTV-1+)	Diet	104	104	Not specified	Mammary gland	Multiple tumour types	-				-		-	-	-
Chlormadinone acetate, Medroxyl mixture	8065-99-6					Mouse	Male	B6C3F1 (MTV-1+)	Diet	104	104	Not specified	Mammary tissue	Multiple tumour types									
Chlormadinone acetate, Medroxyl mixture	8065-99-6					Mouse	Female	C3H (MTV-1+)	Diet	104	104	Not specified	Mammary tissue	Multiple tumour types									
Chlormadinone acetate, Medroxyl mixture	8065-99-6					Mouse	Female	B10 (MTV-1+)	Diet	104	104	Not specified	Mammary tissue	Multiple tumour types									
Chlorobenzene	108-90-7	C1=CC=CC(=C1)Cl	인화성 액체 : 구분3 급성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2 경미 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	-	Carcinogenicity data available IRIS-D (Not classifiable as to human carcinogenicity) Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	CCL2 **CYP2E1** ABCC1 CXCL8 SERPE1 CCNA2 SOD1	IRF7 MANSC1 MYCN2 GJA1 SNHG3	BEL ADAMTS9 GAT LBP6 SLC02A3	hsa01100 Metabolic pathways - Homo sapiens (human) (4) hsa1571 K07415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa2950 K23790 GSTP1; glutathione S-transferase pi 1 hsa2162 K00510 HMOX1; heme oxygenase 1 hsa5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa2950 K23790 GSTP1; glutathione S-transferase pi 1 hsa2162 K00510 HMOX1; heme oxygenase 1 hsa3976 K18830 CXCL8; C-X-C motif chemokine ligand 8 hsa5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (3) hsa1571 K07415 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa2950 K23790 GSTP1; glutathione S-transferase pi 1 hsa5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2	thyroid gland kidney oral cavity hematopoietic system liver ear Zymbals gland nasal cavity spleen Mammary head cancers urinary bladder lung	kidney liver urinary bladder thyroid gland hematopoietic system **uterus** lung nasal cavity clitoral gland oral cavity	liver vascular system lung kidney small intestine	thyroid gland urinary bladder liver vascular system **ovary** peritoneal cavity stomach hematopoietic system lung pituitary gland small intestine	-
Chlorobenzene	108-90-7					Mouse	Male	B6C3F1	Gavage	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chlorobenzene	108-90-7					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chlorobenzene	108-90-7					Rat	Male	Fischer 344	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chlorobenzylate	510-15-6	C[C](C1=CC=C(C=C1)Cl)(C(=O)OC(C)(C)C)=C(C=C(C=C2)Cl)O	급성 독성(경구) : 구분4 경미 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 8, 11, 14, 16, 21, 23, 25, 27, **29**, **30**, 34, 36, 41, 43, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 150, 152, 153, 163, 165, 167, **200**, 214, 307, 310, 318	Cancer slope factor: 3.1e-05 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available CalEPA-Likely Human Carcinogen	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	82	82	Not specified	Liver	Hepatoma	**AR** ESR1 NR1I2 PPARG ARL1	MYBL1 DSG IRF7 SOD1 MRAP4	CYP4A11 BEL ITL CASP2 GATA1	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2099 K08532 ESR1; estrogen receptor 1 hsa5468 K08530 PPARG; peroxisome proliferator activated receptor gamma hsa04211 Longevity regulating pathway - Homo sapiens (human) (1) hsa5468 K08530 PPARG; peroxisome proliferator activated receptor gamma hsa05205 Proteoglycans in cancer - Homo sapiens (human) (1) hsa2099 K08532 ESR1; estrogen receptor 1	stomach	stomach	liver kidney	liver	Liver Neoplasm, Experimental
Chlorobenzylate	510-15-6					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	82	82	Positive	Liver	Hepatoma									

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Chlorobenzylate	510-15-6					Mouse	Female	B6C3F1	Gavage (preweaning) : then diet	82	82	Not specified	Liver	Hepatoma									
Chlorobenzylate	510-15-6					Mouse	Female	B6C3F1	Diet	78	90	Positive	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chlorobenzylate	510-15-6					Mouse	Male	B6C3F1	Gavage (preweaning) : then diet	82	82	Positive	Liver	Hepatoma									
Chlorothalonil	1897-45-6	C1(=C(C(=C(C(=C1Cl)Cl)C#N)Cl)C#N	경련 독성(흡입) 분진/미스트) : 구분2 심한 눈 손상/눈자극 자극성 : 구분1 피부 과민성 : 구분1(1A/1B) 발암성 : 구분2 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분3(호흡기 자극) 경口 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 8, 11, 14, 16, 23, 25, 27, 29, 30, 34, 36, 43, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 97, 98, 107, 111, 112, 117, 122, 123, 130, 150, 153, 163, 166, 167, 187, 195, 200, 203, 204, 214, 220, 307, 318	Cancer slope factor: 8.9e-07 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Diet	80	91	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	BAX BCL2 CASP2 CASP9 MUEL RIPK1 RIPK3	BARD1 CCNC MTTH IRF7 TAGLN	TNFSF40 TNFSF15 ABCA1 CDYD3 LRP6	hsa05170 Human immunodeficiency virus 1 infection - Homo sapiens (human) (4) hsa596 402161 BCL2; BCL2 apoptosis regulator hsa836 402187 CASP2; caspase 2 hsa842 404389 CASP9; caspase 9 hsa8737 402861 RIPK1; receptor interacting serine/threonine kinase 1 hsa05169 Epstein-Barr virus infection - Homo sapiens (human) (4) hsa596 402161 BCL2; BCL2 apoptosis regulator hsa836 402187 CASP2; caspase 2 hsa842 404389 CASP9; caspase 9 hsa8737 402861 RIPK1; receptor interacting serine/threonine kinase 1 hsa05132 Salmonella infection - Homo sapiens (human) (4) hsa197238 408849 MLKL; mixed lineage kinase domain like pseudokinase hsa596 402161 BCL2; BCL2 apoptosis regulator hsa836 402187 CASP2; caspase 2 hsa8737 402861 RIPK1; receptor interacting serine/threonine kinase 1	kidney thyroid gland	kidney	-	thyroid gland	Kidney Neoplasm
Chlorothalonil	1897-45-6					Mouse	Male	B6C3F1	Diet	80	91	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chlorothalonil	1897-45-6					Rat	Female	Osborne-Mendel	Diet	80	110	Positive	Kidney	Adenoma | Adenoma- tubular									
Chlorothalonil	1897-45-6					Rat	Male	Osborne-Mendel	Diet	80	110	Positive	Kidney	Adenocarcinoma | Adenocarcinoma/tubular | Carcinoma									
Chlorotrianiene	569-57-3	C1=CC(=CC=C(C=C1)OCC)C2=CC=C(C=C2)OCC)C3=CC=C(C=C3)OCC	발암성 : 구분1A 특정표적장기 독성(1회 노출) : 구분2 만성 수생환경 유해성 : 구분4	7, 8, 11, 16, 23, 26, 27, 29, 30, 52, 53, 60, 61, 67, 111, 112, 117, 122, 123, 163, 166, 167, 187, 200, 307	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Rat	Female	SD	Diet	104	104	Negative	Liver	Multiple tumour types	CCER1 SERPINC1	NR4A ITGB8 SERPINB1 CASP8AP ACN9	SOD3 CYP4A11 UBE2C TNNI3K2 MGST1	stomach ear Zymbals gland nasal cavity	stomach urinary bladder	urinary bladder stomach vascular system	urinary bladder liver	Prostatic Neoplasm Adenocarcinoma
Chlorotrianiene	569-57-3					Rat	Male	SD	Diet	104	104	Negative	Liver	Multiple tumour types									
Chloropropamide	94-20-2	O=S(=O)(NC(NCCC)=O)C1=CC=C(C=C1)Cl	인한 눈 손상/자극 자극성 : 구분2A(GB) 생식세포 변이원성 : 구분1B 경口 수생환경 유해성 : 구분1	8, 11, 60	-	Mouse	Female	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	INS AVP ABCC8 ACE2 FOS KCNH11	CTPS1	INS REL	hsa05171 Coronavirus disease - COVID-19 - Homo sapiens (human) (2) hsa2353 404379 FOS; Fos proto-oncogene, AP-1 transcription factor subunit hsa59272 439708 ACE2; angiotensin converting enzyme 2 hsa05142 Chagas disease - Homo sapiens (human) (1) hsa2353 404379 FOS; Fos proto-oncogene, AP-1 transcription factor subunit hsa05418 Fluid shear stress and atherosclerosis - Homo sapiens (human) (1) hsa2353 404379 FOS; Fos proto-oncogene, AP-1 transcription factor subunit	-	-	thyroid gland	thyroid gland	-
Chloropropamide	94-20-2					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chloropropamide	94-20-2					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chloropropamide	94-20-2					Rat	Male	Fischer 344	Diet	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Chlorpropham	101-21-3	C(NC1)=CC(Cl)=CC=C1)=O)OCC)C	경련 독성(흡입) : 구분4 발암성 : 구분2 생식독성 : 구분1B 특정표적장기 독성(1회 노출) : 구분2 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분2	8, 15, 16, 23, 27, 34, 36, 57, 58, 60, 61, 72, 107, 111, 117, 146, 163, 187, 200, 307	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6AKF1	Gavage (preweaning) : then diet	76	76	Negative	Liver	Hepatoma	AR NRH2 ABCC1 AnkB CGB3 CYP3A4 FOXO3	IKBKAP AKRIC3 ABM1 CT70R75 COG6	CYP2B6 TGF21 POB CDH13 KLOW21	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa1576 417686 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa196 409363 AHR; aryl hydrocarbon receptor hsa00982 Drug metabolism - cytochrome P450 - Homo sapiens (human) (1) hsa1576 417686 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa04977 Vitamin digestion and absorption - Homo sapiens (human) (1) hsa1482 405865 ABCC1; ATP binding cassette subfamily C member 1	-	-	liver stomach urinary bladder kidney	urinary bladder liver	-
Chlorpropham	101-21-3					Mouse	Male	B6AKF1	Gavage (preweaning) : then diet	76	76	Negative	Liver	Hepatoma									
Chlorpropham	101-21-3					Mouse	Female	B6C3F1	Gavage (preweaning) : then diet	76	76	Negative	Liver	Hepatoma									
Chlorpropham	101-21-3					Mouse	Male	B6C3F1	Gavage (preweaning) : then diet	76	76	Negative	Liver	Hepatoma									
Chlorpropham	101-21-3					Mouse	Mixed	Swiss	Diet	116	116	Not specified	Liver	Multiple tumour types									
Cinnamyl anthranilate	87-29-6	C1=CC=C(C(=C1)C(OCC=CC2=CC=CC=C2)=O)N	경련 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	19, 21, 23, 27, 29, 30, 40, 52, 53, 57, 61, 67, 111, 112, 117, 131, 150, 163, 166, 167, 187, 200, 207, 310	Cancer slope factor: 1.3e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	103	105	Positive	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular	ENPP2 MMP9	TRAF5 CAPRIN1	AKR1B10 FECH FTCD1 FTL PGD		kidney spleen hematopoietic system	-	liver stomach urinary bladder thyroid gland	liver urinary bladder	Neoplasm Invasiveness Liver Neoplasms
Cinnamyl anthranilate	87-29-6					Mouse	Male	B6C3F1	Diet	103	105	Positive	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular									
Cinnamyl anthranilate	87-29-6					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Cinnamyl anthranilate	87-29-6					Rat	Male	Fischer 344	Diet	103	105	Positive	Abdominal cavity	Mesothelioma- malignant | Peritoneum- Mesothelioma- malignant									
Clofibrate®	22464-47-9	C(C(C)(OC2=CC=C(C=1C=CC(=CC=C1)Cl)C(OCC)=O	-	-	-	Mouse	Female	C57BL/10	Diet	78	78	Not specified	Liver	Carcinoma - hepatocellular	-				vascular system liver	-	liver kidney vascular system	liver	-
Clofibrate®	22464-47-9					Mouse	Male	C57BL/10	Diet	78	78	Positive	Liver	Adenoma- hepatocellular									
Clofibrate®	22464-47-9					Rat	Female	Alpk:APFD	Diet	104	104	Not specified	Liver	Multiple tumour types									
Clofibrate®	22464-47-9					Rat	Male	Alpk:APFD	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular									
Clofibrate	637-07-0	C(C(C)(OC=1C=CC(=CC=1)Cl)C(OCC)=O	경련 독성(흡입) : 구분4 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분2	6, 10, 18, 21, 28, 36, 37, 51, 57, 58, 60, 61, 62, 63, 100, 101, 102, 103, 131, 166, 218	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	Alderly Park	Diet	78	78	Negative	Liver	Adenoma- hepatocellular	PPARA CAT CYP4A1 ACOX1 CYP4A14 EHHADH	APOA1 SOD1 MYBL1 IRF7 TUBGCP3	CYP4A11 CPT1A NR1H2 ABCA1 PPARD	hsa04146 Peroxisome - Homo sapiens (human) (2) hsa51 408232 ACOX1; acyl-CoA oxidase 1 hsa847 403781 CAT; catalase hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa51 408232 ACOX1; acyl-CoA oxidase 1 hsa847 403781 CAT; catalase hsa01200 Carbon metabolism - Homo sapiens (human) (2) hsa51 408232 ACOX1; acyl-CoA oxidase 1 hsa847 403781 CAT; catalase	liver stomach vascular system	stomach liver	liver kidney stomach	liver urinary bladder	Carcinoma, Hepatocellular Pancreatic Neoplasm Precancerous Conditions Liver Neoplasms Urinary Bladder Neoplasm Gastrointestinal Neoplasm
Clofibrate	637-07-0					Mouse	Male	Alderly Park	Diet	78	78	Negative	Liver	Adenoma- hepatocellular									
Clofibrate	637-07-0					Mouse	Female	C57BL/10	Diet	78	78	Negative	Liver	Adenoma- hepatocellular									
Clofibrate	637-07-0					Mouse	Male	C57BL/10	Diet	78	78	Negative	Liver	Adenoma- hepatocellular									
Clofibrate	637-07-0					Rat	Male	Fischer 344	Diet	121	121	Positive	Liver	Carcinoma - hepatocellular									
Clomiphene citrate	50-41-9	C1=C(C=CC(=C1)C(C(C2=CC=CC=C2)=C(C1=CC=C(OCCN(CC)CC)C=C1)C=C(C)C)C(OC(C(=O)O)(C(C(=O)O)(C(C(O)=O)C(C(O)=O)=O	생식독성 : 구분1B	7, 8, 11, 14, 16, 23, 25, 27, 28, 29, 30, 33, 34, 36, 43, 46, 52, 53, 57, 58, 60, 61, 62, 63, 64, 66, 67, 71, 72, 91, 93, 94, 95, 96, 97, 98, 100, 101, 102, 103, 104, 107, 111, 112, 117, 122, 123, 126, 128, 148, 153, 163, 164, 165, 167, 177, 187, 190, 197, 200, 203, 204, 214, 302, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	C57Lv/Ae x 129/Ev x C3H/HeDi/Ce x SWR/Jcr	Gavage	69	69	Negative	Lung	Multiple tumour types	ESR1 AR FRL [illegible] NR1I2 APOV1 LHB	-	-	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa2100 408551 ESR2; estrogen receptor 2 hsa367 408017 AR; androgen receptor hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2100 408551 ESR2; estrogen receptor 2 hsa367 408017 AR; androgen receptor hsa04917 Prolactin signaling pathway - Homo sapiens (human) (2) hsa2100 408551 ESR2; estrogen receptor 2 hsa4217 409439 FRS; oncogene	-	-	-	-	Breast Neoplasm Adenocarcinoma Ovarian Neoplasm Polycystic Ovary Syndrome Liver Neoplasm, Experimental
Clomiphene citrate	50-41-9					Mouse	Female	C57Lv/Ae x 129/Ev x C3H/HeDi/Ce x SWR/Jcr	Gavage	69	69	Negative	Multiple sites	Multiple tumour types									
Cloistralid	1420-04-8	C1=CC=C(C)=C1C(NC2=CC=C(C=C2)S(=O)(=O)N(C2=CC=CC=C2)N=)(O-)(=O)C(=O)=N(O)C(=C)COUN	-		-	Mouse	Female	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	-				-	-	-	-
Cloistralid	1420-04-8					Mouse	Male	B6C3F1	Diet	78	91	Inadequate test	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	-								
Cloistralid	1420-04-8					Rat	Female	Osborne-Mendel	Diet	78	110	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	-								
Cloistralid	1420-04-8					Rat	Male	Osborne-Mendel	Diet	78	110	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	-								
Clorophene	120-32-1	C1(=C(C=CC(=C1Cl)Cl)CC2=CC=CC=C2	경련 수생환경 유해성 : 구분1	6, 7, 8, 11, 14, 16, 20-22, 25, 27, 28, 29, 30, 33, 34, 36, 37, 46, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 91, 93, 94, 96, 100, 105, 160, 163, 187, 191, 192, 123, 148, 153, 163, 166, 167, 177, 187, 190, 200, 214, 307, 318	Carcinogenicity data available: EPA- OPP-Group C - Possible Human Carcinogen Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Gavage	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma	AR ESR1 NR1I2 PPARG THRB	TRAM MAMLC1 GAUS2 MBCH1 RAYGB	POB MYEF1 SLCO2A1 CABLES1 CoAC2	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2099 408550 ESR1; estrogen receptor 1 hsa5468 408530 PPARG; peroxisome proliferator activated receptor gamma hsa05205 Proteoglycans in cancer - Homo sapiens (human) (1) hsa2099 408550 ESR1; estrogen receptor 1 hsa04380 Osteoclast differentiation - Homo sapiens (human) (1) hsa5468 408530 PPARG; peroxisome proliferator activated receptor gamma	vascular system thyroid gland liver ear Zymbals gland	liver thyroid gland	kidney liver stomach	thyroid gland liver vascular system	Adenoma
Clorophene	120-32-1					Mouse	Male	B6C3F1	Gavage	103	103	Positive	Kidney	Adenocarcinoma- renal tubule | Adenoma- tubular									
Clorophene	120-32-1					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Adrenal gland medulla	Pheochromocytoma/benign									
Clorophene	120-32-1					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma									

Chemical Name	CAS No.	SMILES	GHS Classific	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Coco diethanolamides	68603-42-9	C[N+](C)(=O)C=C1(C)C1(O)CCCO)=O)CNC.C)CC(O)C)C1)=O)C(O)C)C)	인한 눈 손상성/눈 자극성 - 구분2A(Xi) **발암성 - 구분2**	-	Carcinogenicity data available EPA OPP Likely to be Carcinogenic to Humans	Mouse	Female	B6C3F1	Dermal	93	91	Not specified	-	-	-	-	-	-	-	-	-	-
Codeine	76-57-3	C1=2(C)@@(2)(C)@@H)OC1=C)C=CC=3(C)@H)(C)@@)(C=C)C)@@H)O)H)NCCS(C)OC)H)	-	19, 23, 61, 115, 117, 187, 207	-	Mouse	Female	B6C3F1	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Hepatoblastoma	CYP2D6 CYP3A4 DPP8/9 CES2 CYP2B2 CYP2D2	NGF SOAT1 DHFR CCNI GSS	CNTN1 TMEM41B GAS6	hsa00983 Drug metabolism - other enzymes - Homo sapiens (human) (2) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa8824 K03827 CES2; carboxylesterase 2 hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4	vascular system	-	-	-	Carcinoma, Transitional Cell Kidney Neoplasm Neoplasm
Codeine	76-57-3					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Hepatoblastoma									
Codeine	76-57-3					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Hepatoblastoma									
Codeine	76-57-3					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Hepatoblastoma									
Copper oxine	10380-28-6	C1=CC(=CZC)=C1)C=CC=N2O)[Ca]OC=3C=CC=C4C=3N=CC=C4	경성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	Carcinogenicity data available IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	ACHE ALCAMA CAT DLL4 EGR2A GAPA3	HEATR3 CXORF41 INTU FAQR3 QPCT	GCK6 EFGB.3 GABPC AKR1B10 ALDOA	hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa847 K03781 CAT; catalase hsa01200 Carbon metabolism - Homo sapiens (human) (1) hsa847 K03781 CAT; catalase hsa04330 Notch signaling pathway - Homo sapiens (human) (1) hsa54567 K06051 DLL4; delta like canonical Notch ligand 4	-	-	-	-	-
Copper oxine	10380-28-6					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Copper oxine	10380-28-6					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Copper oxine	10380-28-6					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Coumaphos	56-72-4	O(P)(OC)(OC)=C1=CC=C2C)=C1)OC2(=C2)OC)=O)=S)CC	피부 부식성/피부 자극성 - 구분2 경성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 19, 21, 23, 27, 29, 30, 41, 52, 53, 57, 60, 61, 62, 111, 112, 117, 121, 150, 165, 167, 187, 200, 207, 210	Carcinogenicity data available SPA OPP-Not Likely to Be Carcinogenic in Humans	Mouse	Female	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic	ACHE AR NR1I2 PPARG ACHE-2 AEL	ABNT CASP12 CCDC49 FNIP2 GCA	CYP1A2 CYP3B6 CYP3A4 NR1I3 CYP2C19	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa367 K08557 AR; androgen receptor hsa5468 K08530 PPARG; peroxisome proliferator-activated receptor gamma hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (1) hsa5468 K08530 PPARG; peroxisome proliferator-activated receptor gamma hsa05216 Thyroid cancer - Homo sapiens (human) (1) hsa5468 K08530 PPARG; peroxisome proliferator-activated receptor gamma	-	-	-	-	Prostatic Neoplasm
Coumaphos	56-72-4					Mouse	Male	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic									
Coumaphos	56-72-4					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic									
Coumaphos	56-72-4					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic									
Coumarin	91-64-5	C1=CC=C2C(=C1)C=CC(O)O=O	경성 독성(흡구) - 구분3 피부 과민성 - 구분1(1A/1B)	57	Carcinogenicity data available IARC Group 2 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Positive	Forestomach	Carcinoma- squamous cell | Papilloma- squamous cell	CYP2A6 PNPLPE18 CYP2A13 CYP1A2 GSTT1 RABP1	AIRNT CASP12 CCDC49 FNIP2 GCA	SLC26A3 SGK2 PPP1R14C BAAT1A1 HSPA13A	hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (3) hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1553 K17685 CYP2A13; cytochrome P450 family 2 subfamily A member 13 hsa2952 K00799 GSTT1; glutathione S-transferase theta 1 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1553 K17685 CYP2A13; cytochrome P450 family 2 subfamily A member 13 hsa2952 K00799 GSTT1; glutathione S-transferase theta 1 hsa00982 Drug metabolism - cytochrome P450 - Homo sapiens (human) (2) hsa1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa2952 K00799 GSTT1; glutathione S-transferase theta 1	kidney ear Zymbals gland liver	liver kidney small intestine urinary bladder hematopoietic system	lung stomach urinary bladder vascular system	liver lung stomach ovary urinary bladder pituitary gland thyroid gland	Liver Neoplasm
Coumarin	91-64-5					Mouse	Male	B6C3F1	Gavage	103	104	Positive	Forestomach	Carcinoma- squamous cell | Papilloma- squamous cell									
Coumarin	91-64-5					Mouse	Female	CD1	Diet	109	109	Negative	Liver	Multiple tumour types									
Coumarin	91-64-5					Mouse	Male	CD1	Diet	101	101	Negative	Liver	Multiple tumour types									
Coumarin	91-64-5					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Kidney	Adenoma- tubular									
Coumarin	91-64-5					Rat	Male	Fischer 344	Gavage	60	104	Not specified	Kidney	Adenoma- tubular									
Cumene	98-82-8	C1=CC(=CC=C)C)C	인화성 액체 - 구분3 **발암성 - 구분2** 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 흡인 유해성 - 구분1 만성 수생환경 유해성 - 구분2	7, 26, 123, 123, 153	Carcinogenicity data available Health Canada - Group D: IRIS (not classifiable as to human carcinogenicity) Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1/N	Inhalation	18 d	14 d	Not specified			KRAS	BACE1 IRGT RNF13 Gstm6a ALDH1BA1	TP1 PPP1CB GLUA Gdf6 GCLC	**hsa04664 Fc epsilon RI signaling pathway - Homo sapiens (human) (1)** **hsa3845 K07827 KRAS; KRAS proto-oncogene, GTPase** **hsa04916 Melanogenesis - Homo sapiens (human) (1)** **hsa3845 K07827 KRAS; KRAS proto-oncogene, GTPase** **hsa05221 Acute myeloid leukemia - Homo sapiens (human) (1)** hsa3845 K07827 KRAS; KRAS proto-oncogene, GTPase	spleen Maltoni head cancers oral cavity thyroid gland ear Zymbals gland nasal cavity **lung**	**uterus** thyroid gland liver	**lung** vascular system urinary bladder small intestine	**ovary** pituitary gland thyroid gland urinary bladder vascular system peritoneal cavity	Carcinoma Lung Neoplasm
Cyanobenzene	100-47-0	C1=CC=CC(=C1)C#N	경성 독성(흡구) - 구분4 경성 독성(경口) - 구분4 경성 독성(흡입) 증가) - 구분3 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(Xi) 특정표적장기 독성(1회 노출) - 구분3 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분1	29, 30, 52, 53, 67, 112, 165, 167, 200	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1/N	Gavage	92 d	91 d	Not specified			-				kidney spleen Maltoni head cancers oral cavity thyroid gland ear Zymbals gland nasal cavity hematopoietic system	**uterus** thyroid gland clitoral gland nasal cavity hematopoietic system	vascular system urinary bladder small intestine	**ovary** thyroid gland urinary bladder pituitary gland peritoneal cavity stomach vascular system small intestine	-
Cyclochlorotine	12663-46-6	C1(C)NC(C(C)NC)C)NC)C)NC)=O)C2N)C(C)C)C)=O)CO)=O)C3)=CC=CC)=C3)=C)O)=O	경성 독성(흡구) - 구분1 만성 수생환경 유해성 - 구분2	-	Carcinogenicity data available IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Male	ddN	Diet	160	160	Positive	Liver	Adenoma- liver cell	-			-	-	liver	-	-
D-(-)-Chloramphenicol	56-75-7	[N+](C1=CC=C2)C@@H)(C@@H)NC(C)(C)Cl)=O)CO)O)C=C1)([O-])	경성 독성(흡구) - 구분4 생식세포 변이원성 - 구분1B **발암성 - 구분1B** 생식독성 - 구분2 특정표적장기 독성(반복 노출) - 구분1 경성 수생환경 유해성 - 구분1	8, 11, 43, 60	Carcinogenicity data available NTP RDC-Reasonably Anticipated To Be Human Carcinogen Genotoxicity Data: clastogenic	Rat	Female	SD	Diet	66	75	Negative	Liver	Hepatoma	MMP13 CDKN1A ABCG2 JUN SLC7A2	ALDH1BA1	-	hsa05161 Hepatitis B - Homo sapiens (human) (2) hsa1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa3725 K04448 JUN; Jun proto-oncogene, AP-1 transcription factor subunit hsa04921 Oxytocin signaling pathway - Homo sapiens (human) (2) hsa1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa3725 K04448 JUN; Jun proto-oncogene, AP-1 transcription factor subunit hsa05210 Colorectal cancer - Homo sapiens (human) (2) hsa1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa3725 K04448 JUN; Jun proto-oncogene, AP-1 transcription factor subunit	kidney stomach lung skin	-	vascular system kidney thyroid gland	hematopoietic system	Neoplasm Metastasis Precursor Cell Lymphoblastic Leukemia-Lymphoma Leukemia, Myeloid
Daintron	117-10-2	C1(C)=O)=C(C)=2C1=C(O)C=CC=2)=O)C=CC=CC)O)=O	**발암성 - 구분1B** 경성 수생환경 유해성 - 구분1	29, 30, 52, 53, 61, 62, 112, 165, 167, 200	Cancer slope factor: 2.2e-05 (ug/m3)-1 (potencyequiv. inhalation) Carcinogenicity data available CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Male	C3H/HeN	Diet	77	77	Positive	Liver	Adenoma- hepatocellular	CASP3 CASP8 CCL26 KIRR3 IFNB1 BNIP3L	CTSD TACR3 CSORF48 SERPINB MAPK	FOXO1 BACGAP1 TRIP13 UBE2C GGH	hsa04210 Apoptosis - Homo sapiens (human) (4) hsa598 K04370 BCL2L1; BCL2 like 1 hsa841 K04388 CASP8; caspase 8 hsa842 K04389 CASP9; caspase 9 hsa9131 K04727 ARMT1; apoptosis-inducing factor mitochondria associated 1 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (3) hsa598 K04370 BCL2L1; BCL2 like 1 hsa841 K04388 CASP8; caspase 8 hsa842 K04389 CASP9; caspase 9 hsa05168 Herpes simplex virus 1 infection - Homo sapiens (human) (3) hsa598 K04370 BCL2L1; BCL2 like 1 hsa841 K04388 CASP8; caspase 8 hsa842 K04389 CASP9; caspase 9	urinary bladder kidney stomach liver vascular system nasal cavity	urinary bladder kidney liver ear Zymbals gland small intestine	stomach liver thyroid gland vascular system	**ovary** thyroid gland pituitary gland vascular system hematopoietic system stomach liver urinary bladder	-
Daintron	117-10-2					Rat	Male	ACI	Diet	60	60	Positive	Large intestine	Multiple tumour types									
Dapsone	80-08-0	O=S(=O)(C)C(=CC=C)C=C1)N)C2=CC=C)C=C2)N	경성 독성(흡구) - 구분4 심한 눈 손상성/눈 자극성 - 구분2A(Xi) 호흡기 과민성 - 구분1(1A/1B)	29, 30, 52, 53, 57, 67, 112, 165, 167, 200	Carcinogenicity data available IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	78	107	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic	CYP2C9 CYC1B CYP2A6 CAT GSR NAT2 NOS4	CCR6 DNAJB2 AMH42 FABP4 BARD1	CCR5 HTATIP2 SAT CYP3F TNNB2	hsa00190 Oxidative phosphorylation - Homo sapiens (human) (4) hsa10 K06642 NAT2; N-acetyltransferase 2 hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa2936 K00383 GSR; glutathione disulfide reductase hsa847 K03781 CAT; catalase hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (2) hsa10 K06642 NAT2; N-acetyltransferase 2 hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa00983 Drug metabolism - other enzymes - Homo sapiens (human) (2) hsa10 K06642 NAT2; N-acetyltransferase 2 hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4	spleen ear Zymbals gland thyroid gland	**uterus** thyroid gland ear Zymbals gland urinary bladder mammary gland	thyroid gland urinary bladder	thyroid gland urinary bladder liver vascular system	Prostatic Neoplasm Breast Neoplasm
Dapsone	80-08-0					Mouse	Male	B6C3F1	Diet	78	107	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic									
Dapsone	80-08-0					Rat	Female	Fischer 344	Diet	78	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic									
Dapsone	80-08-0					Rat	Male	Fischer 344	Diet	78	104	Positive	Liver	Adenoma- hepatocellular | Carcinoma hepatocellular | Nodule- neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
DDE	72-55-9	Cl/C(Cl)C(c1ccc(Cl)cc1)C(c1ccc(Cl)cc1)Cl|Cl/C=C/C=C/Cl|C/C=C/C=C/Cl|	경구 독성(분진) : 구분4 경구 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	6, 8, 11, 18, 19, 22, 27, 28, 30, 34, 36, 37, 43, 46, 51, 52, 53, 57, 58, 60, 61, 62, 67, 70, 102, 111, 122, 123, 148, 150, 165, 166, 167, 187, 200, 208, 301, 318	Cancer slope factor: 9.7e-05 (ug/m3)-1 (carcinogenicity, oral) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	78	92	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic	AR ESR1 NFE2 CYP1A1 NR1I3 CYP1B1	IEG7 MANEC1 MDN1 RNF144A SNHG8	FGB TIF1 CYP2B6 CYP2A4 BEL	hsa05205 Proteoglycans in cancer - Homo sapiens (human) (2) hsa2099 ESR1, estrogen receptor 1 hsa836 ID2187 CASP3, caspase 3 hsa5207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa2099 ESR1, estrogen receptor 1 hsa9370 ID2854 NR1I3, nuclear receptor subfamily 1 group I member 3 hsa5200 Pathways in cancer - Homo sapiens (human) (2) hsa2099 ESR1, estrogen receptor 1 hsa836 ID2187 CASP3, caspase 3	kidney hematopoietic system thyroid gland oral cavity Multiple head cancers	kidney	liver vascular system	liver urinary bladder vascular system peritoneal cavity	Prostate Neoplasm Breast Neoplasm Colorectal Neoplasm
DDE	72-55-9					Mouse	Male	B6C3F1	Diet	78	92	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
DDE	72-55-9					Mouse	Female	CF-1	Diet	108	108	Positive	Liver	Hepatoma									
DDE	72-55-9					Mouse	Male	CF-1	Diet	108	108	Positive	Liver	Hepatoma									
DDT	50-29-3	C(C(c1ccccc1)c1ccc(Cl)cc1)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1|C(Cl)(Cl)Cl	경구 독성(분진) : 구분3 경구 독성(경피) : 구분4 **발암성 : 구분2** 특정표적장기 독성(반복 노출) : 구분1 만성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 14, 19, 20, 22, 27, 28, 30, 34, 43, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 102, 111, 112, 137, 148, 165, 167, 187, 200, 204, 207, 318	Cancer slope factor: 9.7e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: **CalEPA-Likely Human Carcinogen** Genotoxicity Data: clastogenic	Cynomolgus monkey	Mixed	Not specified	Diet	559	1307	Not specified	Liver	Carcinoma - hepatocellular	ESR1 AR NFE2 CYP1A1 LDLR PGR	TGFB2 MANEC1 GALR2 MEOX1 MRGEB	ADAMTS9 DKC1 HES2 MLPH ANO1	hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa2100 ID8551 ESR2, estrogen receptor 2 hsa367 ID8557 AR, androgen receptor hsa5743 ID1987 PTGS2, prostaglandin-endoperoxide synthase 2 hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (2) hsa1588 ID7434 CYP19A1, cytochrome P450 family 19 subfamily A member 1 hsa5743 ID1987 PTGS2, prostaglandin-endoperoxide synthase 2 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa2100 ID8551 ESR2, estrogen receptor 2 hsa367 ID8557 AR, androgen receptor	liver thyroid gland	liver	liver lung vascular system	hematopoietic system liver lung thyroid gland urinary bladder vascular system	Prostate Neoplasm Breast Neoplasm Carcinoma, Hepatocellular Colonic Neoplasm Liver Neoplasm
DDT	50-29-3					Hamster	Female	Not specified	Diet	78	78	Negative	Liver	Multiple tumour types									
DDT	50-29-3					Hamster	Male	Not specified	Diet	78	78	Negative	Liver	Multiple tumour types									
DDT	50-29-3					Mouse	Female	B6AKF1	Gavage (pretreating) than diet	80	80	Positive	Liver	Hepatoma									
DDT	50-29-3					Mouse	Male	B6AKF1	Gavage (pretreating) than diet	80	80	Positive	Liver	Hepatoma									
DDT	50-29-3					Mouse	Female	B6C3F1	Gavage (pretreating) than diet	80	80	Not specified	Liver	Hepatoma									
DDT	50-29-3					Mouse	Female	B6C3F1	Diet	78	92	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
DDT	50-29-3					Mouse	Male	B6C3F1	Gavage (pretreating) than diet	80	80	Positive	Liver	Hepatoma									
DDT	50-29-3					Mouse	Male	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
DDT	50-29-3					Mouse	Female	BALB/c	Diet	125	125	Positive	Liver	Tumour- liver cell									
Deltamethrin	52918-63-5	[C@@H](C[C@@H](C1c1ccc(-c2ccccc2)cc1)Oc1ccccc1)(C[C@@H](Cl)Cl)C1C(C)(C)C1C=C(Br)Br|C(=O)C=C(C)C=C|C(=O)[C@@H](C)[C@@H](C[C@@H](C[C@@H](C

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Dibenzo-p-dioxin	262-12-4	C1=CC=CC2=C1OC3=C(O2)C=CC=C3	-	8, 11, 21, **29**, **30**, 41, 46, 52, 53, 57, 60, 61, 67, 112, 131, 150, **165**, **167**, **200**, 310	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Diet	90	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic	CYP1A1	ARNT CASP12 CCDC49 FABP2 GCA	FAM171A1 HGFA12A LIM2 MAFK(CNF) NKAIN1	hsa00380 Tryptophan metabolism - Homo sapiens (human) (1) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa00830 Retinol metabolism - Homo sapiens (human) (1) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (1) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1	oral cavity kidney thyroid gland	urinary bladder stomach kidney lung hematopoietic system small intestine ear Zymbals gland liver **uterus** thyroid gland	urinary bladder stomach liver vascular system lung small intestine thyroid gland	thyroid gland stomach **ovary** liver urinary bladder pituitary gland vascular system peritoneal cavity lung small intestine	-
Dibenzo-p-dioxin	262-12-4					Mouse	Male	B6C3F1	Diet	88	92	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dibenzo-p-dioxin	262-12-4					Rat	Female	Osborne-Mendel	Diet	110	111	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dibenzo-p-dioxin	262-12-4					Rat	Male	Osborne-Mendel	Diet	110	110	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dibenzothiamine hydrochloride	35682-60-7	N1=C(N=CC2)=C1N(C(N)C)(C)=CCCOC(C2=CC=CC=C2)=OSC(C)=CC=CC=C3)=O(C=O)C.Cl	-		-	Rat	Female	SD	Diet	105	105	Negative	Liver	Haemangioiosarcoma - anaplastic	-				large intestine	ear Zymbals gland small intestine stomach mammary gland	urinary bladder	lung hematopoietic system liver	-
Dibenzothiamine hydrochloride	35682-60-7					Rat	Male	SD	Diet	105	105	Negative	Liver	Tumour - liver cell - benign									
Dibromoacetonitrilquinone	81-49-2	C1=,3(C)(C2=C(C1=O)C=CC=C2)=O)=C(C)=CC=3Br(Br)N	발암성 - 구분2 만성 수생환경 유해성 - 구분4	21, 41, 57, 61, 121, 150, 310	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	104	104	Positive	Forestomach	Carcinoma - squamous cell	**EGR1** **KRAS** ~~TP53~~ **Tumor** NRF2	BAGAL75 BGLAP BBM12 ASMR12 CCB6	CYORF52 CASP2 HTATIP2 ETV(ALA1 CYP1A2	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa3265 KO2833 HRAS; Hras proto-oncogene, GTPase hsa4780 KO5638 NFE2L2; NFE2 like bZIP transcription factor 2 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa3265 KO2833 HRAS; Hras proto-oncogene, GTPase hsa4780 KO5638 NFE2L2; NFE2 like bZIP transcription factor 2 hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (2) hsa3265 KO2833 HRAS; Hras proto-oncogene, GTPase hsa4780 KO5638 NFE2L2; NFE2 like bZIP transcription factor 2	**urinary bladder** kidney large intestine **liver** spleen	**liver** **urinary bladder** kidney ear Zymbals gland	**stomach** **liver** **lung** **urinary bladder** vascular system thyroid gland	**liver** **stomach** **lung** vascular system hematopoietic system	**Liver Neoplasms** **Liver Neoplasms, Experimental** Urinary Bladder Neoplasms **Lung Neoplasms** Stomach Neoplasms Adenoma
Dibromoacetonitrilquinone	81-49-2					Mouse	Male	B6C3F1	Diet	103	104	Positive	Forestomach	Carcinoma - squamous cell									
Dibromoacetonitrilquinone	81-49-2					Rat	Female	Fischer 344	Diet	66	66	Not specified		Caecum : Adenoma - polypoid Colon : Adenoma - polypoid Rectum : Adenoma - polypoid									
Dibromoacetonitrilquinone	81-49-2					Rat	Female	Fischer 344	Diet	40	66	Not specified		Caecum : Adenoma - polypoid Colon : Adenoma - polypoid Rectum : Adenoma - colloid									
Dibutyl phthalate	84-74-2	C(C)=,C(C)(C(CCC)=O)C=C(C=C1)(O(CCCC)=O	급성 독성(흡입: 증기) - 구분4 생식독성 - 구분1B 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 14, 25, **29**, **30**, 52, 53, 58, 60, 61, 64, 66, 67, 71, 107, 112, 122, 123, 131, 153, **165**, **167**, **200**, 214, 218	Carcinogenicity data available: EPA OPP-Group D Not Classifiable as to Human Carcinogenicity Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6C3F1	Diet	30 d	Not specified	Not specified			STAR CYP11A1 **AR** CGA CYP17A1 **EGR1**	LAMP3 PAPSS1 ABIC12 SMARCC1 MTTH	AKR1B10 FECH FTL PTGR1 SPAG6	hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (3) hsa:1081 K08622 CGA; glycoprotein hormones, alpha polypeptide hsa:1583 K00486 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa:1586 K00512 CYP17A1; cytochrome P450 family 17 subfamily A member 1 hsa04934 Cushing syndrome - Homo sapiens (human) (2) hsa:1583 K00486 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa:1586 K00512 CYP17A1; cytochrome P450 family 17 subfamily A member 1 hsa04917 Prolactin signaling pathway - Homo sapiens (human) (2) hsa:1081 K08622 CGA; glycoprotein hormones, alpha polypeptide hsa:1586 K00512 CYP17A1; cytochrome P450 family 17 subfamily A member 1	hematopoietic system kidney liver urinary bladder	hematopoietic system liver urinary bladder	liver vascular system	liver stomach pituitary gland	Mammary Neoplasm, Animal Neoplasm Metastasis
Dichlone	117-80-6	C1=,C(=C(C2(C)=C1)(C(C)=O)C(2=O)(O)(C)C)=O	급성 독성(경구) - 구분3 급성 독성(경피) - 구분3 피부 부식성/피부 자극성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 14, 19, 21, 23, 25, 27, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 150, 153, 163, **165**, **167**, 187, **200**, 214, 307, 310, 318	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (pretreaning) then diet	76	76	Negative	Liver	Hepatoma	AR DIO1 DIO2 DIO3 HD	CTSD NGK4 SNAG4 IFIH1 AIBN7	ERCC3 LRP6 POB FAM171A1 HGFA12A	hsa04919 Thyroid hormone signaling pathway - Homo sapiens (human) (3) hsa:1733 K01562 DIO1; iodothyronine deiodinase 1 hsa:1734 K17904 DIO2; iodothyronine deiodinase 2 hsa:1735 K07734 DIO3; iodothyronine deiodinase 3	kidney thyroid gland oral cavity nasal cavity	liver kidney urinary bladder ear Zymbals gland **uterus**	vascular system liver stomach urinary bladder small intestine lung	thyroid gland vascular system urinary bladder liver hematopoietic system stomach pituitary gland **ovary** small intestine peritoneal cavity	-
Dichlone	117-80-6					Mouse	Male	B6AKF1	Gavage (pretreaning) then diet	76	76	Negative	Liver	Hepatoma									
Dichlone	117-80-6					Mouse	Female	B6C3F1	Gavage (pretreaning) then diet	76	76	Negative	Liver	Hepatoma									
Dichlone	117-80-6					Mouse	Male	B6C3F1	Gavage (pretreaning) then diet	76	76	Negative	Liver	Hepatoma									
Dichlorodiphenyldichloroethane	72-54-8	C1=,C(=CC(=C(C1)Cl)C2=C(C=C(C=C2)Cl)C(Cl)Cl)	급성 독성(경구) - 구분3 급성 독성(경피) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(유) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 14, 19, 23, 25, 27, **29**, **30**, 34, 40, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 107, 112, 117, 122, 123, 148, 153, **165**, **167**, 187, **200**, 214, 307, 318	Cancer slope factor: 6.9e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6AKF1	Gavage (pretreaning) then diet	76	76	Not specified	Liver	Hepatoma	**AR** ~~EGR1~~ NRF2 ~~TP53~~ ~~Tumor~~ ~~Neoplasms~~ ~~MYMD~~ TYMB	CYP11A1 MANSC1 TGFB2 MAPK13 METTL21D	CYP2B6 CYP2A4 CYP11B1 ADAMTS9 ERCC3	hsa05200 Pathways in cancer - Homo sapiens (human) (9) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:238 K05109 ALK; ALK receptor tyrosine kinase hsa:3815 K05091 KIT; KIT proto-oncogene, receptor tyrosine kinase hsa:5155 K05089 PDGFRB; platelet derived growth factor receptor beta hsa:5468 K08539 PPARG; peroxisome proliferator activated receptor gamma hsa04151 PI3K-Akt signaling pathway - Homo sapiens (human) (2) hsa:3815 K05091 KIT; KIT proto-oncogene, receptor tyrosine kinase hsa:5155 K05089 PDGFRB; platelet derived growth factor receptor beta hsa04072 Phospholipase D signaling pathway - Homo sapiens (human) (2) hsa:3815 K05091 KIT; KIT proto-oncogene, receptor tyrosine kinase hsa:5155 K05089 PDGFRB; platelet derived growth factor receptor beta	liver thyroid gland kidney	liver kidney	liver lung vascular system small intestine stomach	lung hematopoietic system vascular system liver small intestine thyroid gland urinary bladder	-
Dichlorodiphenyldichloroethane	72-54-8					Mouse	Male	B6AKF1	Gavage (pretreaning) then diet	76	76	Not specified	Liver	Hepatoma									
Dichlorodiphenyldichloroethane	72-54-8					Mouse	Female	B6C3F1	Gavage (pretreaning) then diet	76	76	Not specified	Liver	Hepatoma									
Dichlorodiphenyldichloroethane	72-54-8					Mouse	Female	B6C3F1	Diet	79	90	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dichlorodiphenyldichloroethane	72-54-8					Mouse	Male	B6C3F1	Gavage (pretreaning) then diet	76	76	Not specified	Liver	Hepatoma									
Dicofol	115-32-2	C(C(Cl)(c=1C=,C(C)=CC=1)C(=1C(C(Cl)=CC=C)C=CC=1)Cl)(Cl)(Cl)	급성 독성(경구) - 구분4 급성 독성(경피) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(유) 생식세포 변이원성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분1	7, 8, 11, 14, 19, 23, 25, 27, **29**, 30, 34, 36, 43, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 148, 153, 163, **165**, **167**, 187, **200**, 214, 307, 318	Carcinogenicity data available EPA OPP-Group C Possible Human Carcinogen	Mouse	Female	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic	**EGR1** **AR** ~~Tumor~~ ~~TTR~~ ~~CYP1A1~~ NRF2 AUB	MANSC1 TGFB2 GAA30 BMOH1 MRGZB	ADAMTS9 ERCC3 NEX2 ANO1 MLPH	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (3) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:367 K08557 AR; androgen receptor hsa:5579 K19662 PRKCB; protein kinase C beta hsa04918 Thyroid hormone synthesis - Homo sapiens (human) (2) hsa:5579 K19662 PRKCB; protein kinase C beta hsa:7276 K20731 TTR; transthyretin hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:367 K08557 AR; androgen receptor hsa:5579 K19662 PRKCB; protein kinase C beta	thyroid gland	-	liver vascular system	hematopoietic system liver lung thyroid gland	Prostatic Neoplasm
Dicofol	115-32-2					Mouse	Male	B6C3F1	Diet	78	91	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dicofol	115-32-2					Rat	Female	Osborne-Mendel	Diet	78	111	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dicofol	115-32-2					Rat	Male	Osborne-Mendel	Diet	78	110	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Diethenylbenzene	1321-74-0	C=1(C)=CC=CC=1)C=C(C=C,C=,C=C(C)=CC=,C=C(C=C,C=,C)=CC=CC=,C=C(C=,C=C)=C	인화성 액체 - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(유) 생식세포 변이원성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분2	8, 11, **29**, **30**, 52, 53, 60, 61, 67, 112, **165**, **167**, **200**	-	Mouse	Female	B6C3F1/N	Inhalation	95 d	91 d	Not specified			-			oral cavity spleen hematopoietic system stomach kidney Mattoni head cancers	mammary gland **uterus** nasal cavity hematopoietic system stomach thyroid gland oral cavity	lung stomach vascular system small intestine urinary bladder	**ovary** lung stomach thyroid gland urinary bladder pituitary gland peritoneal cavity small intestine	-
Diethyl phthalate	84-66-2	O(C(C)(C1=C(C(O(C)=O)(C=CC=C1)=O	급성 독성(흡입: 증기) - 구분3 심한 눈 손상성/눈 자극성 - 구분2A(유) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	57, 131	Carcinogenicity data available EPA OPP-Group D Not Classifiable as to Human Carcinogenicity Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1/N	Dermal	736 d	730 d	Not specified	Abdomen-skin	Tumour - mast cell - benign	CGA CYP11A1 STAR CYP19A1	LAMP3 ABIC12 PAPSS1 DSG SERPINB1	AKR1B10 CASP2 CYP4A11 FTL SPAG6	hsa04925 Aldosterone synthesis and secretion - Homo sapiens (human) (2) hsa:1583 K00486 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa:6770 K16831 STAR; steroidogenic acute regulatory protein hsa04927 Cortisol synthesis and secretion - Homo sapiens (human) (2) hsa:1583 K00486 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa:6770 K16831 STAR; steroidogenic acute regulatory protein hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (2) hsa:1583 K00486 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa:6770 K16831 STAR; steroidogenic acute regulatory protein	kidney hematopoietic system liver Mattoni head cancers stomach	hematopoietic system liver small intestine stomach oral cavity	liver stomach kidney thyroid gland	liver stomach urinary bladder peritoneal cavity pituitary gland	Breast Neoplasm Mammary Neoplasm, Animal Adenoma, Liver Cell
Diethyl phthalate	84-66-2					Mouse	Male	B6C3F1	Dermal	2 yrs	2 yrs	Not specified	Adrenal gland-capsule	Adenoma									
Diethyl phthalate	84-66-2					Rat	Female	Fischer 344	Dermal	104 d	730 d	Not specified	Adrenal gland-cortex	Adenoma									
Diethyl phthalate	84-66-2					Rat	Male	Fischer 344	Dermal	456 d	730 d	Not specified	Adrenal gland-cortex	Adenoma									
Diflatone	21626-89-1	C1N(N)(C(C2=C1C=,C(=,C(=O)(C(C4=,C(C3=O)(C=,C(=,C4	-	-	-	Mouse	Female	BALB/cLac/ME	Diet	80	119	Positive	Liver	Adenoma - hepatocellular	GUSB	IL1R1 BAGAL75 NGK4 WDR4 PPP1CA	SAT CYP2E1 TMN71 KIF34 MT1B	hsa00053 Ascorbate and aldarate metabolism - Homo sapiens (human) (1) hsa:2990 K01195 GUSB; glucuronidase beta hsa00983 Drug metabolism - other enzymes - Homo sapiens (human) (1) hsa:2990 K01195 GUSB; glucuronidase beta hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa:2990 K01195 GUSB; glucuronidase beta	oral cavity	all tumor bearing animals	vascular system stomach urinary bladder small intestine thyroid gland	liver vascular system **ovary** thyroid gland urinary bladder small intestine	-

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Diflubenzuron	21424-69-1					Mouse	Male	BALB/c(c.w/ref)	Diet	80	119	Positive	Liver	Adenoma - hepatocellular									
Diglycidyl resorcinol ether	101-90-6	C1[c+]CC+CC[c+]C1[O]CC2CO2OCC3OC3	경성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(사)(B) 피부 과민성 : 구분1(사/1B) 생식세포 변이원성 : 구분2 **발암성 : 구분2** 만성 수생환경 유해성 : 구분3	7, 14, 19, 23, 25, 27, **29**, **30**, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, **165**, **167**, **187**, **200**, 204, 207, 318	Cancer slope factor: 0.00049 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	103	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic	-				stomach nasal cavity hematopoietic system thyroid gland	stomach nasal cavity	stomach kidney	stomach pituitary gland	Stomach Neoplasm
Diglycidyl resorcinol ether	101-90-6					Mouse	Male	B6C3F1	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Diglycidyl resorcinol ether	101-90-6					Rat	Female	Fischer 344	Gavage	103	104	Positive	Forestomach	Carcinoma - squamous cell									
Diglycidyl resorcinol ether	101-90-6					Rat	Female	Fischer 344	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Diglycidyl resorcinol ether	101-90-6					Rat	Male	Fischer 344	Gavage	103	104	Positive	Forestomach	Carcinoma - squamous cell									
Diglycidyl resorcinol ether	101-90-6					Rat	Male	Fischer 344	Gavage	98	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dimethyl terephthalate	120-61-6	C1[c+]CC+CC+C1C(=O)OC(C)(=O)OC	특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분1	57, 131	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic	AR	SERPINB1 CAD8F4B AKR1B1 IGJ7 TRAF5	AKR1B10 FBCN PTGR1 FTL PGD	hsa05275 Prostate cancer - Homo sapiens (human) (1) hsa:367 408557 AR; androgen receptor hsa05200 Pathways in cancer - Homo sapiens (human) (1) hsa:367 408557 AR; androgen receptor hsa04114 Oocyte meiosis - Homo sapiens (human) (1) hsa:367 408557 AR; androgen receptor	hematopoietic system kidney vascular system ear Zymbals gland Maltoni head cancers	hematopoietic system clitoral gland urinary bladder	urinary bladder vascular system	urinary bladder pituitary gland peritoneal cavity liver **ovary**	-
Dimethyl terephthalate	120-61-6					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dimethyl terephthalate	120-61-6					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dimethyl terephthalate	120-61-6					Rat	Male	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Dinitrotoluene	25321-14-6	[N+](C1=CC[N+](=O)[O-])=CC=C1C[c+]=O[O-]	경성 독성(경구) : 구분3 경성 독성(경피) : 구분4 경성 독성(흡입) :분진/미스트 : 구분3 생식세포 변이원성 : 구분2 **발암성 : 구분1B** 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	-	Carcinogenicity data available: PPRTV (ORNL)-Likely to be carcinogenic to humans Genotoxicity Data: genotoxic	Rat	Male	Fischer 344	Diet	52	52	Positive	Liver	Carcinoma- hepatocellular- trabecular	-				-	-	-	-
Dinoseb	88-85-7	C+1[N+](=O)[O-])=CC(O)C=C(N+](=O)[O-])C=C+1[C](C)C)O	경성 독성(경구) : 구분2 경성 독성(경피) : 구분1 경성 독성(흡입) :분진/미스트 : 구분2 피부 과민성 : 구분1(사/1A) 생식독성 : 구분1A 경성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	6, 7, 8, 11, 18, 19, 23, 25, 27, **29**, **30**, 34, 36, 37, 43, 46, 51, 52, 53, 57, 58, 60, 61, 62, 67, 72, 107, 111, 112, 117, 122, 123, 131, 148, 150, 153, 163, **165**, 166, **167**, **187**, **200**, 220, 307, 318	Carcinogenicity data available: EPA, OPP Group C Possible Human Carcinogen Genotoxicity Data: clastogenic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	GCLC GCLM HMOX1 NQO1 SOK17	NQO1 CYP1A1	GCLM SERPINB8 TANK02 EHHADH CORO1C	hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa:1728 430015 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:2730 411205 GCLM; glutamate-cysteine ligase modifier subunit hsa:3162 420510 HMOX1; heme oxygenase 1 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa:1728 430015 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:3162 420510 HMOX1; heme oxygenase 1 hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (2) hsa:1728 430015 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:3162 420510 HMOX1; heme oxygenase 1	-	-	thyroid gland kidney	**ovary**	-
Dinoseb	88-85-7					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Dinoseb	88-85-7					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Dinoseb	88-85-7					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Dioxin	1746-01-6	[O]C3c1cC(OC2c1Cl)c(Cl)c(c(Cl)c2Cl)[O]C1c(Cl)c(c(Cl)c(Cl)c1Cl)Cl	경성 독성(경구) : 구분1 경성 독성(경피) : 구분1 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(사)(B) 생식독성 : 구분1A 특정표적장기 독성(1회 노출) : 구분1 특정표적장기 독성(반복 노출) : 구분1 경성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	21, **29**, **30**, 49, 53, 54, 57, 61, 67, 112, 131, 150, 160, **167**, **200**, 310	Cancer slope factor: 38 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: NTP RCC-Known Human Carcinogen	Mouse	Female	B6C3F1	Gavage	104	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular	AHR CYP1A1 TIPARP AHRR CYP1A2 ARNT NQO1	ARNT CADPS2 CCDC40 TNFI2 GCA	RAM171A1 HSPA12A LBX2 MAFGKT3P3 MAANX	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (4) hsa:1543 437408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:1544 437409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1545 437410 CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa:405 409087 ARNT; aryl hydrocarbon receptor nuclear translocator hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (4) hsa:1543 437408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:1544 437409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1545 437410 CYP1B1; cytochrome P450 family 1 subfamily B member 1 hsa:405 409087 ARNT; aryl hydrocarbon receptor nuclear translocator hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa:1543 437408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:1544 437409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1545 437410 CYP1B1; cytochrome P450 family 1 subfamily B member 1	thyroid gland oral cavity	liver **lung** kidney thyroid gland urinary bladder hematopoietic system	liver vascular system urinary bladder	thyroid gland liver urinary bladder vascular system peritoneal cavity stomach pituitary gland **ovary**	Carcinoma, Hepatocellular Breast Neoplasm Carcinoma Lung Neoplasm Ovarian Neoplasm lymphatic Metastasis
Dioxin	1746-01-6					Mouse	Male	B6C3F1	Gavage	104	104	Positive	Liver	Adenoma - hepatocellular									
Dioxin	1746-01-6					Mouse	Male	Swiss/NrRlcp	Gavage	52	104	Positive	Liver	Multiple tumour types									
Dioxin	1746-01-6					Rat	Female	Osborne-Mendel	Gavage	104	105	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Diphenhydramine hydrochloride	147-24-0	C1=CC=C(C=C1)C(C2=CC=CC=C2)OCCN(C)C.Cl	경성 독성(경구) : 구분4 심한 눈 손상성/눈 자극성 : 구분2A(사)(B) 만성 수생환경 유해성 : 구분2	33, 34, 46, 52, 58, 61, 62, 91, 93, 94, 96, 97, 98, 126, 131, 195, 197, 203, 204	-	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic	HRH1 BCHE CXCL8 SLC22A2	TAGLN IGJ4 BHGALTS	SLC24A4 FNDC4 RN4BB IFIT1 WBP11	hsa04062 Chemokine signaling pathway - Homo sapiens (human) (1) hsa:3576 410830 CXCL8; C-X-C motif chemokine ligand 8 hsa05142 Chagas disease - Homo sapiens (human) (1) hsa:3576 410830 CXCL8; C-X-C motif chemokine ligand 8 hsa05323 Rheumatoid arthritis - Homo sapiens (human) (1) hsa:3576 410830 CXCL8; C-X-C motif chemokine ligand 8	all tumor bearing animals	thyroid gland nasal cavity lung	kidney lung vascular system thyroid gland	peritoneal cavity stomach lung hematopoietic system	Endometrial Neoplasm Melanoma
Diphenhydramine hydrochloride	147-24-0					Mouse	Male	B6C3F1	Diet	105	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Diphenhydramine hydrochloride	147-24-0					Rat	Female	Fischer 344	Diet	106	128	Negative	Liver	Nodule - neoplastic									
Diphenhydramine hydrochloride	147-24-0					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									
Diphenyl carbonate	102-09-0	O(C)(OC1=CC=CC=C1)=O)C2=CC=CC=C2	경성 독성(경구) : 구분4 생식독성 : 구분2 경성 수생환경 유해성 : 구분1	-	Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				nasal cavity stomach thyroid gland ear Zymbals gland urinary bladder Maltoni head cancers oral cavity	urinary bladder nasal cavity thyroid gland hematopoietic system	urinary bladder stomach kidney vascular system	**ovary** urinary bladder thyroid gland pituitary gland stomach peritoneal cavity	-
Diphenyl carbonate	102-09-0					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Diphenyl carbonate	102-09-0					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Haemangioma									
Diphenyl carbonate	102-09-0					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Diphenylacetonitrile	86-29-3	NMC(C1=CC=CC=C1)C=3C=CC=CC=2	-	7, 8, 11, 25, **29**, **30**, 34, 36, 52, 53, 58, 60, 61, 67, 72, 107, 112, 122, 123, 153, 163, **165**, **167**, **200**	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				spleen Maltoni head cancers	kidney	lung	hematopoietic system lung **ovary** pituitary gland peritoneal cavity	-
Diphenylacetonitrile	86-29-3					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Diphenylacetonitrile	86-29-3					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Diphenylacetonitrile	86-29-3					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Dipropyl-4,7-methylenediisoy-3-methyl-1,2,3,4-tetrahydronaphthalene-1,2-dicarboxylate	83-59-0	C1=C3C(=CC2=C1OCO2)C(O)CCC(=O)C(C)CC(=O)C)C3C	-	-	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				-	-	-	-	-
Dipropyl-4,7-methylenediisoy-3-methyl-1,2,3,4-tetrahydronaphthalene-1,2-dicarboxylate	83-59-0					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Dipropyl-4,7-methylenediisoy-3-methyl-1,2,3,4-tetrahydronaphthalene-1,2-dicarboxylate	83-59-0					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Dipropyl-4,7-methylenediisoy-3-methyl-1,2,3,4-tetrahydronaphthalene-1,2-dicarboxylate	83-59-0					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Direct Black 38	1937-37-7	S(C=4C)Na.NC1=CC=C(C=c1S(C)=O)C=C=C(N=NC3=C(C=C(C=C3)N(Na)=O)C=S(C(=4)=O)C5)[O-][c+](=O)=O.c1[C=S(O)Na.NC6=CC=CC=C6]N[O]=[c+](=O)=O.[Na+].[Na+]	심한 눈 손상성/눈 자극성 : 구분2A(사)(B) **발암성 : 구분1B** 생식독성 : 구분2	7, 21, 25, **29**, **30**, 41, 52, 53, 57, 67, 112, 120, 123, 131, 150, 152, 163, **167**, **200**, 310	Cancer slope factor: 0.0001 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Mixed	ICR	Drinking water	57	57	Positive	Liver	Hepatoma	-				-	-	-	-	-
Direct Black 38	1937-37-7					Rat	Female	Fischer 344	Diet	13	13	Positive	Liver	Adenoma - hepatocellular | Carcinoma\hepatocellular | Nodule - neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Direct Black 38	1937-37-7					Rat	Male	Fischer 344	Diet	13	13	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Direct Blue 15, tetrasodium	2429-74-5	[Na+].[Na+].[Na+].[Na+].O=S(=O)(S[C-]=C[N-]NC4=CC=C(C=1C=C(S=O)(=O)O[Na])C=1C=C(C=1[OC]N=NC=2C(S(=O)=O)=CQ(O)[C-]=C(C=2)C(=O)O)C=1C=C(C=1C(=O)=O)O)=O)C=1[N-]NC=C=NCC(=O)[N-]C=1[N-]NC=C=NCC(=O)[N-]C=1[N-]NC=C=NCC(=O)[N-]C=1[N-]NC=C=NCC(=O)[N-]C=1[N-]NC(=O)[N-]	생식세포 변이원성 - 구분2 발암성 - 구분2	-	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Female	Fischer 344	Drinking water	96	97	Positive	Clitoral gland	Adenoma | Adenoma - bilateral	-				-	-	-	-	Cell Transformation, Neoplastic
Direct Blue 15, tetrasodium	2429-74-5					Rat	Male	Fischer 344	Drinking water	97	97	Positive	Adrenal gland medulla	Pheochromocytoma|benign | Pheochromocytoma - benign - bilateral									
Direct Blue 218	28407-37-6	[Na+].[Na+].[Na+].[Na+].O=S(=O)[C-]=C=2Na(NC=1C=C(C=C=1O)[C@CC=2C=4[C=]=O)C=C(C=4)C=3C=C(S=O)(=O)O)=O)[C-]=C(C=4C(=C(S(=O)=O)O)[C-]=C7C=4C(=C(S(=O)=O)O)=[C-]=C7[N-]Na)=N[C-]=C(C=3)C=1[N-]Na)=N[C-]=C(C=1C=C(C=1C=C(C=1C

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Efavirapine.HCl enhancdate	119011-76-8	[C+]1[C]COP(OC1)[C]2=[C]NC(=O)C2[C]3=[C]C=[C]C=C2[N+](O)=[C]NO[C]3NO[C]NC(=O)C=[C]C=[C]BC(N)=[C]C=[C]SC(N)=[C]CC[C]	-	-	-	Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular	-				-	-	-	-	-
Efavirapine.HCl enhancdate	119011-76-8					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Efavirapine.HCl enhancdate	119011-76-8					Rat	Female	Fischer 344/DuCrl	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Efavirapine.HCl enhancdate	119011-76-8					Rat	Male	Fischer 344/DuCrl	Diet	104	104	Negative	Liver	Multiple tumour types									
Ellagic acid	476-66-4	C=12C3=C4OC(C=1C=1C(C=C2OC(C3=C(C=C4C(O)=C3O)O)=O)=O)=O	-	-	-	Rat	Female	Fischer 344/DuCrj	Diet	52	52	Not specified	Liver	Multiple tumour types	TNFSF11 NFE2L2 TNF IL1B CASP3 RELA MMP2 TP53	NCPS6 GPD1 TFAM UGP2 IL1R1	TCF12 IGFBP2 EP300 BLM CBP72	hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (5) hsa3553 KEGG:19:IL1B; interleukin 1 beta hsa4780 KEGG:8:NFE2L2; NFE2 like b2P transcription factor 2 hsa5370 KEGG:5:RELA; RELA proto-oncogene, NF-kB subunit hsa7124 KEGG:6:TNF; tumor necrosis factor hsa836 KEGG:2:CASP3; caspase 3 hsa05418 Fluid shear stress and atherosclerosis - Homo sapiens (human) (5) hsa3553 KEGG:19:IL1B; interleukin 1 beta hsa4313 KEGG:8:MMP2; matrix metallopeptidase 2 hsa4780 KEGG:8:NFE2L2; NFE2 like b2P transcription factor 2 hsa5370 KEGG:5:RELA; RELA proto-oncogene, NF-kB subunit hsa7124 KEGG:6:TNF; tumor necrosis factor hsa04933 AGE-RAGE signaling pathway in diabetic complications - Homo sapiens (human) (5) hsa3553 KEGG:19:IL1B; interleukin 1 beta hsa4313 KEGG:8:MMP2; matrix metallopeptidase 2 hsa5370 KEGG:5:RELA; RELA proto-oncogene, NF-kB subunit hsa7124 KEGG:6:TNF; tumor necrosis factor hsa836 KEGG:2:CASP3; caspase 3	kidney urinary bladder	small intestine urinary bladder	kidney	**ovary** pituitary gland hematopoietic system	Cell Transformation, Neoplastic Urinary Bladder Neoplasm Skin Neoplasm
Emodin	518-82-1	C1(C=3C)(C)(C)=C1(C)=CC)=C2O(C)C(O)=O)=CC)=C(O)=C3O)=O	원한 눈 손상성/눈 자극성 - 구분2A(GB) 만성 수생환경 유해성 - 구분2	6, 7, 8, 11, 14, 18, 19, 21, 23, 25, 27, 29, 30, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 102, 111, 112, 117, 122, 123, 131, 148, 150, 152, 163, 165, 166, 167, 187, 200, 214, 217, 310, 318	-	Mouse	Female	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma,hepatocellular | Hepatoblastoma	TGFB1 CASP3 ABCB11 CYP1A2 CYP3A4	CTSD TACR3 BDCK1 BDCK2 DVER	FOXO1 BACSAP1 TBP12 UBE2C RBCC3	urinary bladder kidney stomach large intestine liver vascular system	urinary bladder small intestine	stomach kidney thyroid gland liver	pituitary gland liver vascular system	Leukemia-Lymphoma, Adult T-Cell
Emodin	518-82-1					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Kidney	Adenoma - tubular | Carcinoma - tubular									
Emodin	518-82-1					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Hepatoblastoma									
Emodin	518-82-1					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Hepatoblastoma									
Erythrosin B	16423-68-0	[C-4]=[C]OC=[C]C(I)=[C]O[C=,2C]=[C]C=[C]C=[C]C3=[C]C(I)=[C]O[C=,2][O-][C=3][N+](=O)[O-] [C-4]=[C]OC=[C]C(I)=[C]O[C=,2C]=[C]C=[C]C3=[C]C(I)=[C]O[C=,2][O-][C=3][N+](=O)[O-]	경성 독성(경구) - 구분4	7, 8, 11, 14, 19, 21, 23, 25, 27, 29, 30, 36, 41, 43, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 97, 98, 107, 111, 112, 117, 122, 123, 131, 148, 150, 153, 165, 167, 187, 199, 200, 203, 204, 214, 220, 307, 310, 318	Genotoxicity Data: clastogenic	Mouse	Female	CD1	Diet	104	104	Negative	Multiple sites	Multiple tumour types	CDK2 UGT1A6 UGT2B7 ABCB1	-	-	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa54278 KEGG:6:UGT1A6; UDP glucuronosyltransferase family 1 member A6 hsa7364 KEGG:6:UGT2B7; UDP glucuronosyltransferase family 2 member B7 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (2) hsa54278 KEGG:6:UGT1A6; UDP glucuronosyltransferase family 1 member A6 hsa7364 KEGG:6:UGT2B7; UDP glucuronosyltransferase family 2 member B7 hsa01240 Biosynthesis of cofactors - Homo sapiens (human) (2) hsa54278 KEGG:6:UGT1A6; UDP glucuronosyltransferase family 1 member A6 hsa7364 KEGG:6:UGT2B7; UDP glucuronosyltransferase family 2 member B7	-	-	-	-	Thyroid Neoplasm Skin Neoplasm
Erythrosin B	16423-68-0					Mouse	Male	CD1	Diet	104	104	Not specified	Multiple sites	Lymphoma - lymphocytic									
Erythrosin B	16423-68-0					Rat	Female	Osborne-Mendel	Diet	104	104	Not specified	Liver	Multiple tumour types									
Erythrosin B	16423-68-0					Rat	Male	Osborne-Mendel	Diet	104	104	Not specified	Liver	Multiple tumour types									
Estazolam	29975-16-4	C=1N2C(=NN=1)CN=C(C3=CC=CC=C3Cl)C4=CC=CC=C4	자료없음	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Angioma	AKR1C1 AKR1C2 AKR1C3 CYP3A4 TBN TBNR	VTN TGFBR3 TNC MYBL1	REL SCGN HPN INHBE	hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (3) hsa1576 KEGG:6:CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa1646 KEGG:6:AKR1C2; aldo-keto reductase family 1 member C2 hsa8644 KEGG:6:AKR1C3; aldo-keto reductase family 1 member C3 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (2) hsa1576 KEGG:6:CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa1646 KEGG:6:AKR1C2; aldo-keto reductase family 1 member C2 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1646 KEGG:6:AKR1C2; aldo-keto reductase family 1 member C2 hsa8644 KEGG:6:AKR1C3; aldo-keto reductase family 1 member C3	-	-	-	-	-
Estazolam	29975-16-4					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Angioma									
Estazolam	29975-16-4					Rat	Female	SD	Diet	104	104	Negative	Liver	Carcinoma - hepatocellular									
Estazolam	29975-16-4					Rat	Male	SD	Diet	104	104	Negative	Liver	Carcinoma - hepatocellular									
Ethamoxytriphetol	67-48-1	C1=CC=CC=C1C(C2=CC=CC=C2)(CC3=CCC(C=C3)OCCN(C)C)CC	-	-	-	Rat	Female	Not specified	Gavage	52	52	Negative	Mammary tissue	Multiple tumour types	-				stomach vascular system kidney nasal cavity	stomach	kidney	-	-
Ethosuximide	938-73-8	C1(=CC=CC=C1C)(C2=CC)ONOCC	원한 눈 손상성/눈 자극성 - 구분2A(GB) 급성 수생환경 유해성 - 구분3	36, 46	-	Mouse	Female	B6C3F1	Diet	96	100	Not specified	Liver	Multiple tumour types	-				urinary bladder stomach kidney nasal cavity	ear Zymbals gland urinary bladder mammary gland small intestine stomach hematopoietic system	kidney thyroid gland liver urinary bladder vascular system	urinary bladder hematopoietic system	**Liver Neoplasm, Experimental**
Ethosuximide	938-73-8					Mouse	Male	B6C3F1	Diet	96	100	Positive	Liver	Multiple tumour types									
Ethinylestradiol	57-63-6	O[C@]4CC#C)[C@@]3CCC)[C@@]2C1=CC=C(C=C1)CC)[C@@]1CC[C@@]([C@@]3(C4)H)([H])[H]	경성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 원한 눈 손상성/눈 자극성 - 구분2A(GB) **발암성 - 구분1A** 생식독성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	8, 11, 14, 19, 23, 27, 29, 30, 34, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 97, 98, 107, 111, 112, 117, 122, 123, 148, 150, 165, 167, 187, 195, 200, 203, 204, 214, 220, 307, 318	Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: predicted to be non-genotoxic	Rat	Female	Sic-Wistar	Gavage	52	52	Positive	Liver	Carcinoma - hepatocellular	ESR1 IL1B ESR2 ABCB11 NR1H4 C3 ABCC2	TPM1 CDLSA2 PRBAF1 ERP27 KIF23	CILRL3 DSPTOR AGER CIGH IERS1	hsa04976 Bile secretion - Homo sapiens (human) (2) hsa8647 KEGG:6:ABCB11; ATP binding cassette subfamily B member 11 hsa9971 KEGG:7:NR1H4; nuclear receptor subfamily 1 group H member 4 hsa05131 Shigellosis - Homo sapiens (human) (2) hsa3553 KEGG:19:IL1B; interleukin 1 beta hsa718 KEGG:9:C3; complement C3	-	liver ear Zymbals gland	stomach	pituitary gland hematopoietic system	Carcinoma, Hepatocellular Urinary Bladder Neoplasm Endometrial Neoplasm Adenocarcinoma Pancreatic Neoplasm Mesothelioma
Ethoxyquin	91-53-2	C(C)(C)NC=1C=1C=1C(=CC=1C)=C2(C)OCC	경성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 원한 눈 손상성/눈 자극성 - 구분2A(GB) 특정표적장기 독성(반복 노출) - 구분2 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 14, 27, 29, 30, 34, 36, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 112, 122, 123, 131, 148, 150, 165, 167, 200, 214, 220, 318	Genotoxicity Data: non-genotoxic	Rat	Female	Fischer 344	Diet	58	58	Negative	Kidney	Multiple tumour types	NFE2L2 NQO1 NFKBIA CYP3A4 GSTM4 GSTM1	MYBL1	AKR1B10	hsa01100 Metabolic pathways - Homo sapiens (human) (4) hsa1728 KEGG:5:NQO1; NAD(P)H quinone dehydrogenase 1 hsa2297 KEGG:7:GSTA5; glutathione S-transferase alpha 5 hsa231 KEGG:1:AKR1B1; aldo-keto reductase family 1 member B hsa2941 KEGG:7:GSTA4; glutathione S-transferase alpha 4 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (2) hsa2297 KEGG:7:GSTA5; glutathione S-transferase alpha 5 hsa23077 KEGG:8:AKR7A3; aldo-keto reductase family 7 member A3 hsa2941 KEGG:7:GSTA4; glutathione S-transferase alpha 4 hsa05225 Hepatocellular carcinoma - Homo sapiens (human) (3) hsa1728 KEGG:5:NQO1; NAD(P)H quinone dehydrogenase 1 hsa2297 KEGG:7:GSTA5; glutathione S-transferase alpha 5 hsa2941 KEGG:7:GSTA4; glutathione S-transferase alpha 4	-	ear Zymbals gland	**kidney** thyroid gland	urinary bladder	Carcinoma, Renal Cell Precancerous Conditions Urinary Bladder Neoplasm Kidney Neoplasm Stomach Neoplasm Carcinoma, Hepatocellular **Liver Neoplasm**
Ethoxyquin	91-53-2					Rat	Female	Fischer 344	Diet	78	78	Negative	Kidney	Multiple tumour types									
Ethoxyquin	91-53-2					Rat	Male	Fischer 344	Diet	60	60	Not specified	Liver	Multiple tumour types									
Ethoxyquin	91-53-2					Rat	Male	Fischer 344	Diet	58	58	Negative	Kidney	Multiple tumour types									
Ethyl methylphenylglycidate	77-83-8	O1(C)C1(C)OC(=O)C2=CC=CC=C2)C	원한 눈 손상성/눈 자극성 - 구분2A(GB) 만성 수생환경 유해성 - 구분2	7, 8, 11, 25, 29, 30, 34, 36, 52, 53, 58, 60, 67, 72, 112, 122, 123, 152, 163, 165, 167, 200	Genotoxicity Data: clastogenic	Rat	Female	Wistar	Diet	104	104	Negative	Liver	Haemangioendothelioma	-				-	-	-	-	-
Ethyl methylphenylglycidate	77-83-8					Rat	Male	Wistar	Diet	104	104	Negative	Liver	Multiple tumour types									
Ethylbenzene	100-41-4	C1=CC=CC(=C1)C	인화성 액체 - 구분2 급성 독성(흡입 증기) - 구분4 **발암성 - 구분2** 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2 흡인 유해성 - 구분1 만성 수생환경 유해성 - 구분3	-	Cancer slope factor: 2.5e-06 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: Health Canada - Group D: IRIS (not classifiable as to human carcinogenicity) (IRIS, 1991)/Group 2B: IARC (possibly carcinogenic to humans)/ GCDWQ: HC, 1986 Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Inhalation	103	104	Positive	Harderian gland	Adenoma	BAX BCL2 CASP3 CYCS CASP9 **CYP2E1**	NGF BAC1 ALDH1BA1 IRF2 TIAM	2CCHC2 DENND5A BCL2A1 MAP3K8 NFATS	hsa05014 Amyotrophic lateral sclerosis - Homo sapiens (human) (4) hsa54205 KEGG:8:CYCS; cytochrome c, somatic hsa596 KEGG:7:BCL2; BCL2 apoptosis regulator hsa836 KEGG:7:BCL2; caspase 2 hsa842 KEGG:9:CASP9; caspase 9 hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (4) hsa54205 KEGG:8:CYCS; cytochrome c, somatic hsa596 KEGG:7:BCL2; BCL2 apoptosis regulator hsa836 KEGG:7:BCL2; caspase 2 hsa842 KEGG:9:CASP9; caspase 9 hsa01524 Platinum drug resistance - Homo sapiens (human) (4) hsa54205 KEGG:8:CYCS; cytochrome c, somatic hsa596 KEGG:7:BCL2; BCL2 apoptosis regulator hsa836 KEGG:7:BCL2; caspase 2 hsa842 KEGG:9:CASP9; caspase 9	kidney Malignant neoplasms nasal cavity oral cavity spleen hematopoietic system thyroid gland	kidney thyroid gland ear Zymbals gland **uterus** nasal cavity hematopoietic system	lung thyroid gland stomach liver vascular system urinary bladder small intestine	thyroid gland liver **ovary** pituitary gland urinary bladder lung stomach peritoneal cavity vascular system	Neoplasm Neuroectodermal Tumor, Primitive
Ethylbenzene	100-41-4					Mouse	Male	B6C3F1	Inhalation	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Hepatoblastoma									
Ethylbenzene	100-41-4					Rat	Female	Fischer 344	Inhalation	104	105	Positive	Kidney	Adenoma - tubular									
Ethylbenzene	100-41-4					Rat	Male	Fischer 344	Inhalation	104	105	Positive	Adrenal gland medulla	Pheochromocytoma|malign | Pheochromocytoma: benign: bilateral									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Ethylphenacemide	90-49-2	C1=CC=C(C=C1)C(CC)(NCN)=O|=O	-	-	-	Rat	Male	Fischer 344	Diet	71	71	Not specified	Liver	Hepatoma	-				large intestine	**uterus** small intestine hematopoietic system	urinary bladder	**ovary**	-
Ethynodiol diacetate, Mestranol mixture	8056-92-6	C1[C@@H]4[C@C]1=C[C@@]3[C@]2[C@@]([C@]1(C)CC[C@@H]4)[C-]=C1[C@]2[C@@](O)(CC[C@@]1(C(=O)[O])[C@]1(C)CC[C-]=C[C-]=C)C[C-]=C[C-]=C[C@]2[C@@]3[C@@H](C)[C@]1(C)[C@@H](O)C[C-]=C[C@@H](N)[C-]=C[C-]=C[C-]=C

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Fenvalerate	51630-58-1					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Fenvalerate	51630-58-1					Mouse	Female	C57BL/6	Gavage	104	114	Negative	Liver	Tumour - liver cell									
Fenvalerate	51630-58-1					Mouse	Male	C57BL/6	Gavage	104	114	Negative	Liver	Tumour - liver cell									
Fluoroxazole	84386-73-9	N=1C=NNC=1[C](C=2C(=O)=2C)=CC=2F(F)(F)ON(N=ON=C)O		27, 122, 123, 150, 220	-	Mouse	Female	CD1	Diet	104	104	Negative	Liver	Carcinoma - hepatocellular	CYP2C9 CYP2C19 CYP19A1 CYP3A4 CYP11A1 NR1I3	KIR11 ERBB3 NAPTL1	SQLE TMEM40	hsa01100 Metabolic pathways - Homo sapiens (human) (4) hsa1557 K17721 CYP2C19; cytochrome P450 family 2 subfamily C member 19 hsa1576 K17686 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa1588 K07434 CYP19A1; cytochrome P450 family 19 subfamily A member 1 hsa1595 K08812 CYP11A1; cytochrome P450 family 11 subfamily A member 1 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (2) hsa1576 K17686 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa1588 K07434 CYP19A1; cytochrome P450 family 19 subfamily A member 1 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (2) hsa1557 K17721 CYP2C19; cytochrome P450 family 2 subfamily C member 19 hsa1576 K17686 CYP3A4; cytochrome P450 family 3 subfamily A member 4	liver esophagus	-	-	hematopoietic system	Liver Neoplasm, Experimental Liver Neoplasms Glioblastoma
Fluoroxazole	84386-73-9					Mouse	Male	CD1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Fluoroxazole	84386-73-9					Rat	Female	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Fluoroxazole	84386-73-9					Rat	Male	SD	Diet	104	104	Positive	Adrenal gland medulla	Pheochromocytoma									
Fluometuron	2164-17-2	C1=C(C=C(C=C1N(C)N(C)C)=C)C(F)(F)F	급성 독성(경구) : 구분4 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 57, 58, 61, 107, 121	Carcinogenicity data available: EPA OPP Group C Possible Human Carcinogen Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic					all tumor bearing animals	ear Zymbals gland	urinary bladder stomach thyroid gland kidney	lung liver stomach	-
Fluometuron	2164-17-2					Mouse	Male	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Fluometuron	2164-17-2					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Fluometuron	2164-17-2					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Food Blue 2	860-22-0	[Na+].[Na+].O=S(=O)(C1=CC2=C(C=C1)N(C)C2=O)=C4NC=3C=CC(S(=O)(=O)[O-])=CC=3C4=O)[O-]	급성 독성(경구) : 구분4 만한 눈 손상 또는 자극성 : 구분2A/2B	21, 41, 46, 57, 131, 150, 210	Genotoxicity Data: clastogenic	Mouse	Female	CD1	Diet	84	84	Negative	Liver	Nodular hyperplasia	CYP1A1 AxaB GRIN2A CHRNA4 CHRNB2	-	-	hsa05033 Nicotine addiction - Homo sapiens (human) (2) hsa1137 K04806 CHRNA4; cholinergic receptor nicotinic alpha 4 subunit hsa2903 K05209 GRIN2A; glutamate ionotropic receptor NMDA type subunit 2A hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa1137 K04806 CHRNA4; cholinergic receptor nicotinic alpha 4 subunit hsa196 K09363 AHR; aryl hydrocarbon receptor hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (2) hsa1137 K04806 CHRNA4; cholinergic receptor nicotinic alpha 4 subunit hsa2903 K05209 GRIN2A; glutamate ionotropic receptor NMDA type subunit 2A	-	-	-	-	Skin Neoplasm
Food Blue 2	860-22-0					Mouse	Male	CD1	Diet	84	84	Negative	Liver	Nodular hyperplasia									
Food Blue 2	860-22-0					Mouse	Female	SD	Diet	100	100	Negative	Multiple sites	Multiple tumour types									
Food Blue 2	860-22-0					Mouse	Male	SD	Diet	95	95	Negative	Multiple sites	Multiple tumour types									
Food Blue 2	3844-45-9	O=S(=O)(C5=C(C)=C2C=CC(=[N+](CC=1C=CS(=O)=O)=O)=C(C=1S(CC[C-](C2)=O)=O)=C4C(C=CS(=O)=O)=O)[O-]=CC=C4[C]C(=CC=CS[O-])[Na+].[Na+]	피부접촉	7, 14, 19, 23, 25, 29, 30, 52, 53, 57, 64, 66, 67, 71, 111, 112, 117, 122, 123, 148, 152, 165, 167, 187, 200, 214, 307, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Female	CD1	Diet	104	104	Negative	Liver	Haemangioma	GRIN2A CHRNA4 CHRNB2 IYD	-	-	hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (1) hsa1141 K04813 CHRNB2; cholinergic receptor nicotinic beta 2 subunit hsa04725 Cholinergic synapse - Homo sapiens (human) (1) hsa1141 K04813 CHRNB2; cholinergic receptor nicotinic beta 2 subunit hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa1141 K04813 CHRNB2; cholinergic receptor nicotinic beta 2 subunit	-	-	-	-	-
Food Blue 2	3844-45-9					Mouse	Male	CD1	Diet	104	104	Negative	Liver	Carcinoma - hepatocellular									
Food Blue 2	3844-45-9					Rat	Mixed	Osborne-Mendel	Diet	104	104	Not specified	Liver	Hepatoma									
Food Green 3	2353-45-9	[Na+].[Na+].O=S(=O)[C-](C=C(C=C(C=C1)[N+](C2C=CC(S(=O)=O)=CC=2)=C1)S(=O)=O)=C(C=C2C(C(S=O)=O)=C(C=C2)C(C6=C(C=CC(S(=O)=O)[O-])=CC=C6)=C3C=CC(=C(C=C3)S(O)[O-])=C(C=C4)[C-]=S(O)[O-]	피부접촉	7, 8, 11, 14, 19, 20, 23, 25, 27, 29, 30, 34, 36, 41, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 150, 153, 163, 165, 167, 187, 200, 214, 307, 310, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Female	C.Delta(Fos)	Diet	104	104	Negative	Liver	Adenoma - hepatocellular	IYD	-	-	hsa04918 Thyroid hormone synthesis - Homo sapiens (human) (1) hsa:38434 K17721 IYD; iodotyrosine deiodinase	-	-	-	-	-
Food Green 3	2353-45-9					Mouse	Male	C.Delta(Fos)	Diet	104	104	Not specified	Liver	Multiple tumour types									
Food Green 3	2353-45-9					Rat	Female	Osborne-Mendel	Diet	104	104	Negative	Liver	Multiple tumour types									
Food Green 3	2353-45-9					Rat	Male	Osborne-Mendel	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Food Orange 4	1936-15-8	[Na+].[Na+].O=S(=O)[C-]2C1=C(C=C1C=C(S(=O)=O)=O)[O-]C(=2)O[N]=NC3=CC=CC=C3[O-]	피부접촉	27, 41	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic	-	-	-	-	-	-	-
Food Orange 4	1936-15-8					Mouse	Male	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Food Orange 4	1936-15-8					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Food Orange 4	1936-15-8					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Food Violet 2	1694-08-3	[Na+].[O-]S(=O)(=S(C=1C(C[N+])=C4C=CC(=C(C=1C=CC(=C(C=1C=CC(=C(C=1[N](C)C)C2=CC=C)C=C2)N(CC)C3=CC(S(=O)=O)[C-]=O)=C(C=3)[O-])=C(C=C4)[O-])	발암성 - 구분2 만한 수생환경 유해성 : 구분3	-	Cancer slope factor: 5.7e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	ASH-CS1	Diet	80	80	Negative	Liver	Multiple tumour types	-	-	-	-	-	-	-
Food Violet 2	1694-08-3					Mouse	Male	ASH-CS1	Diet	80	80	Negative	Liver	Multiple tumour types									
Food Violet 2	1694-08-3					Rat	Female	SD	Diet	52	52	Positive	Ear canal	Carcinoma									
Food Violet 2	1694-08-3					Rat	Female	SD	Diet	51	52	Positive	Mammary gland	Carcinoma									
Fullerene	99685-96-8	C12=C3C4=C5C1=C6C7=C8C2=C9C10=C3C11=C12C4=C1[C]1[C]2[C]3[C]4=C5[C]5[C]6[C]7=C8C[N]4=C7C1[C]5=C1[C]6[C]8=C9C[N]3=C10C[N]2=C11[C]1[C]4[C]2[C]1[C]3[C]2[C]4[C]5[C]6[C]7[C]8[C]9[C]1[C]2[C]3

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
gamma-Oryzanol	11042-64-1					Rat	Male	Fischer 344/DuCrl	Diet	104	105	Negative	Liver	Nodule- neoplastic									
Gemfibrozil	25812-30-0	CC(C)(C)CCOC(=O)C(C)Oc1ccc(CCc1ccc(Cl)cc1)cc1O	경성 독성(경구) : 구분4 만성 수생환경 유해성 : 구분4	6, 7, 8, 11, 18, 25, 29, 30, 34, 36, 37, 51, 52, 53, 58, 60, 61, 67, 72, 110, 122, 123, 153, 162, 165, 166, 167, 200, 318	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	CD1	Diet	78	78	Negative	Liver	Adenoma - hepatocellular	PPARA CYP2C8 IL1B SOC3 NR1H3 SERPINE1	AKR1C3 CCL5 STAT1B CCDC50 STX1A	NR1H2 PPARD PPARA ABCA1 PCDH17	hsa05417:Lipid and atherosclerosis - Homo sapiens (human) (2) hsa1558:K17718:CYP2C8; cytochrome P450 family 2 subfamily C member 8 hsa3553:K04519:IL1R; interleukin 1 beta hsa04932:Non-alcoholic fatty liver disease - Homo sapiens (human) (2) hsa10062:K08536:NR1H2; nuclear receptor subfamily 1 group H member 3 hsa3553:K04519:IL1R; interleukin 1 beta hsa05152:Tuberculosis - Homo sapiens (human) (1) hsa3553:K04519:IL1R; interleukin 1 beta	liver stomach	-	kidney liver	liver	**Liver Neoplasms** Adenoma, Liver Cell Carcinoma, Hepatocellular
Gemfibrozil	25812-30-0					Mouse	Male	CD1	Diet	78	78	Negative	Liver	Multiple tumour types									
Gemfibrozil	25812-30-0					Rat	Female	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Gemfibrozil	25812-30-0					Rat	Male	SD	Diet	104	104	Positive	Adrenal gland	Pheochromocytoma									
Genistein	446-72-0	C1=c(C=c(C2=c(=O)c(C(=c(=O)c(C(=c(=O)c(C(

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Ibuprofen	15687-27-1	C1(=CC=C(C=C1)C(C)C(O)=O)CC(C)C	특정성 표적 - 최고급 1 급성 독성(경구) - 구분4 만성 수생환경 유해성 - 구분2	6, 18, **29**, **30**, 34, 36, 37, 51, 52, 53, 58, 61, 67, 72, 112, 162, 166, 168, **167**, **200**, 318	Genotoxicity Data: predicted to be genotoxic	Rat	Male	Fischer 344	Diet	54	54	Not specified	Colon	Multiple tumour types	TNF PTGS2 NGFR IL18 IFNG PTGS1	BACE1 FABP4 NGF ALDH1B1 TCR1	GCLC TFF1 HPGD GCLM FAM49A	hsa05140 Leishmaniasis - Homo sapiens (human) (3) hsa:3458 K04687 IFNG; interferon gamma hsa:3553 K04519 IL1B; interleukin 1 beta hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa04060 Cytokine-cytokine receptor interaction - Homo sapiens (human) (3) hsa:3458 K04687 IFNG; interferon gamma hsa:3553 K04519 IL1B; interleukin 1 beta hsa:4804 K05263 NGFR; nerve growth factor receptor hsa04657 IL-17 signaling pathway - Homo sapiens (human) (3) hsa:3458 K04687 IFNG; interferon gamma hsa:3553 K04519 IL1B; interleukin 1 beta hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2	-	-	lung	lung	Prostatic Neoplasm Mammary Neoplasm, Experimental Adenocarcinoma Colorectal Neoplasm Pancreatic Neoplasm
Indole	120-72-9	C1=CC=C2C(=C1)C(=CN2)	급성 독성(경구) - 구분4 급성 독성(경피) - 구분2 피부 부식성/피부 자극성 - 구분2 **발암성 - 구분1A** 급성 수생환경 유해성 - 구분1	8, 11, 21, 41, 57, 60, 131, 158, 310	Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	Swiss	Diet	70	70	Negative	Urinary bladder	Carcinoma	NRG2 ABCB1 **CYP1A2** CYP1A CYP1A1 EPO	CROB141 HEATR3 FTSD1 G10F1 IL1R1	SAT AHRR H61 EPSB12 GIPC	hsa00976 Bile secretion - Homo sapiens (human) (2) hsa:1576 K17688 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:5243 K05658 ABCB1; ATP binding cassette subfamily B member 1 hsa05206 Gastric cancer - Homo sapiens (human) (1) hsa:5243 K05658 ABCB1; ATP binding cassette subfamily B member 1	thyroid gland ear Zymbals gland spleen all tumor bearing animals oral cavity urinary bladder	all tumor bearing animals	urinary bladder vascular system liver stomach thyroid gland	thyroid gland urinary bladder vascular system liver stomach **ovary** hematopoietic system	-
Indole-3-carbinol	700-06-1	C1=C(C=C2C(=C1)C(=CN2)CO)	-	7, 8, 11, 14, 19, 21, 23, 25, 28, 29, **30**, 34, 36, 41, 43, 46, 52, 53, 57, 58, 60, 61, 63, 64, 66, 67, 71, 72, 100, 109, 162, 163, 167, 191, 112, 117, 122, 123, 131, 150, 152, 162, 165, **167**, 177, 187, **200**, 214, 260, 307, 310, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1/N	Gavage	94 d	90 d	Not specified	Forestomach	Multiple tumour types	TNF CYP1A1 IL1 NFKB1 NFKBIA **AHR** CYP1A2	CYMPK DMXL1 FSD2R1 FABP4 TAG2N	SAT SP1 CDPT3 LST1 C10ORF118	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (4) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:1728 K00355 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:196 K09083 AHR; aryl hydrocarbon receptor hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (3) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:196 K09083 AHR; aryl hydrocarbon receptor hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa04659 Th17 cell differentiation - Homo sapiens (human) (2) hsa:196 K09083 AHR; aryl hydrocarbon receptor hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit	thyroid gland	all tumor bearing animals	vascular system thyroid gland urinary bladder stomach lung	thyroid gland vascular system hematopoietic system lung pituitary gland	**Liver Neoplasm** Liver Neoplasm, Experimental **Breast Neoplasm** Ovarian Cyst Uterine Cervical Neoplasm
Indole-3-carbinol	700-06-1					Mouse	Female	B6C3F1/N	Gavage	2 yrs	2 yrs	Not specified	Adrenal gland cortex	Adenoma									
Indoleban	100643-96-7	C(C)(C)C=1C=C(C=C(C=1)CC(NH)=O)=CC=C(N(C)=O)				Rat	Female	Fischer 344	Diet	104	104	Positive	Adrenal gland medulla	Multiple tumour types						all tumor bearing animals			
Indoleban	100643-96-7					Rat	Male	Fischer 344	Diet	95	95	Positive	Adrenal gland medulla	Multiple tumour types									
Indomethacin	53-86-1	C1=CC(=CCC2=C1N(C(=C2CC(=O)O)C)C(=O)C(Cl)=CC=C)C(=O)O	급성 독성(경구) - 구분2 피부 과민성 - 구분1(A/1A) 생식세포 변이원성 - 구분2 만성 수생환경 유해성 - 구분3	6, 18, 28, 34, 36, 37, 51, 58, 61, 62, 63, 72, 100, 101, 102, 103, 162, 166, 177, 218	Genotoxicity Data: clastogenic	Rat	Male	Fischer 344/DuCr	Diet	52	52	Not specified	Forestomach	Multiple tumour types	INS PTGS2 MIF2 TNF NOS2	TCR1 MAP4K4 ROCK1 TUBGCP3 NPM1	HPGD PPARD TMEM4K PPARA GCLC	hsa04657 IL-17 signaling pathway - Homo sapiens (human) (2) hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa05165 Human papillomavirus infection - Homo sapiens (human) (2) hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa04064 NF-kappa B signaling pathway - Homo sapiens (human) (2) hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor	-	mammary gland stomach	-	-	Mammary Neoplasm, Animal **Liver Neoplasm** Urolithiasis Neoplasm Kidney Neoplasm Leydig Cell Tumor
Indomethacin	53-86-1					Rat	Female	SD	Drinking water	92	92	Positive	Liver	Multiple tumour types									
Ipazilide fumarate	115436-74-7	O(C(C(N(C(C(C)C)C)C)N)=O)C(C)=C(C=C(C=C(C=C(C=C(C)=O)C(C)=C(C)=O)O)=O)=O				Rat	Female	SD	Gavage	52	52	Negative	Liver	Multiple tumour types									
Ipazilide fumarate	115436-74-5					Rat	Male	SD	Gavage	52	52	Negative	Liver	Multiple tumour types									
Isoguajazole maleate	64504-69-8	C1=CC(=CC(=C1)C(N)C(N)C2=NC1=NC(NH)N(C)=C(O)O)=O)=O)=O				Rat	Male	Wistar	Diet	50	50	Negative	Liver	Multiple tumour types									
Isoniazid	89667-48-3	C1=CC=C(C=N1)C(=O)NNC(=O)C=2C=NC=CC=2				Mouse	Female	CD1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Isoniazid	89667-48-3					Mouse	Male	CD1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Isoniazid	89667-48-3					Rat	Male	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Isobutyl 4-hydroxybenzoate	4247-02-3	C1=C(C=CC(=C1)C(OCC)(C)C)=O)O	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(/2B)	19, 23, **29**, **30**, 52, 53, 61, 67, 111, 112, 117, **165**, **167**, 187, **200**, 307	-	Mouse	Female	ICR/Ivl	Diet	102	106	Negative	Liver	Multiple tumour types	**AR** **ESR1** SPC1 **NR1I2** STMN1	LAMP3 PAPSS1 ZFAND5 SEC16A AIMC2	AKR1B10 OS9 IL10RB PTGR1 PCK	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2 hsa:9970 K08641 NR1I2; nuclear receptor subfamily 1 group I member 2 hsa04915 Estrogen signaling pathway - Homo sapiens (human) (2) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2 hsa01522 Endocrine resistance - Homo sapiens (human) (2) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2	kidney hematopoietic system vascular system	hematopoietic system small intestine	kidney liver thyroid gland	liver pituitary gland lung hematopoietic system	-
Isobutyl 4-hydroxybenzoate	4247-02-3					Mouse	Male	ICR/Ivl	Diet	102	104	Negative	Liver	Multiple tumour types									
Isoeugenol	97-54-1	C1=C(C=C(C=C1)C=C)OC	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(/2B) 피부 과민성 - 구분1(A/1A) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분3	8, 11, **29**, **30**, 34, 36, 46, 52, 53, 57, 58, 60, 61, 67, 72, 112, 131, 163, **165**, **167**, **200**	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1/N	Gavage	93 d	91 d	Not specified			CXCL8 NCOA1 AHR GCLM **HMOX1** **SF** SOCS3 ZFP36	HYIX CXCL2 EJPS ITGB8 CROBP4B	P7GR1 AKR1B10 FTL MGST1 GCLC	hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa:2730 K11205 GCLM; glutamate-cysteine ligase modifier subunit hsa:3162 K00510 HMOX1; heme oxygenase 1 hsa:4843 K12241 NOS2; nitric oxide synthase 2 hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa:3162 K00510 HMOX1; heme oxygenase 1 hsa:3558 K05409 IL2; interleukin 2 hsa:4843 K12241 NOS2; nitric oxide synthase 2 hsa05142 Chagas disease - Homo sapiens (human) (2) hsa:3558 K05409 IL2; interleukin 2 hsa:4843 K12241 NOS2; nitric oxide synthase 2	kidney stomach vascular system skin nasal cavity	stomach hematopoietic system	stomach urinary bladder	stomach	-
Isoeugenol	97-54-1					Mouse	Female	B6C3F1/N	Gavage	327 d	730 d	Not specified	Adrenal gland capsule	Adenoma									
Isopropyl (2,4-dichlorophenoxy)acetate	94-11-1	C1=C(C=C(Cl)=C1)OCC(O)(C)(C)=O)Cl	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 MPF in 과분화/암 독작용 - 구분2(A/2B)	8, 11, 60	-	Mouse	Female	B6A/F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Carcinoma - hepatocellular	-				-	-	kidney liver	-	-
Isopropyl (2,4-dichlorophenoxy)acetate	94-11-1					Mouse	Male	B6A/F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Isopropyl (2,4-dichlorophenoxy)acetate	94-11-1					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Isopropyl (2,4-dichlorophenoxy)acetate	94-11-1					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Isosafrole	120-58-1	C1=C(C=C2C=C1OCO2)C=CC	급성 독성(경구) - 구분4	8, 11, 60	Carcinogenicity data available: IARC Group 2 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6A/F1	Gavage (preweaning) then diet	81	81	Not specified	Liver	Hepatoma	CYP1A2 **CYP1A1** CYP1A ABCB1	IRF7 MYBL1 CTPS1 SNHG8 CXCL2	MGST1 SOD2 CASP2 AKR1B10 TNNI3K2	hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (1) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa00830 Retinol metabolism - Homo sapiens (human) (1) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa00380 Tryptophan metabolism - Homo sapiens (human) (1) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1	stomach liver	stomach	stomach vascular system liver	stomach lung liver	-
Isosafrole	120-58-1					Mouse	Male	B6A/F1	Gavage (preweaning) then diet	81	81	Not specified	Liver	Hepatoma									
Isosafrole	120-58-1					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	81	81	Not specified	Liver	Hepatoma									
Isosafrole	120-58-1					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	81	81	Not specified	Liver	Hepatoma									
Isoxaflutole	141379-73-8	C1(=NC(C=4N(C2=C1C(=C(S2)CCC3=CC=CC=C3)CCC3=CC=CC=C3)CCC3=CC=CC=C3)C(C)=CC=CC=C5)C5)	-	7, 14, 19, 23, 25, 27, **29**, **30**, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, **165**, 167, 187, **200**, 204, 307, 318	-	Rat	Female	SD(CrlCD)	Gavage	52	52	Negative	Liver	Multiple tumour types	-				-	-	-	-	-
Isoxaflutole	141379-73-8					Rat	Male	SD(CrlCD)	Gavage	52	52	Negative	Liver	Multiple tumour types									
Kanechlor 400	12737-87-0	C1(=CC(=CC(=C1)C(Cl)=CC(=CC=C)=C)Cl)C(Cl)C(Cl)	-	-	-	Rat	Female	Donryu	Diet	26	84	Negative	Liver	Multiple tumour types	**KRAS**	FABP4 ABNT CASP12 CCDC49 FNIP2	IEL FAM171A1 HSPA12A LIM2 MAP3K7IP2	**hsa04540 Gap junction - Homo sapiens (human) (1)** **hsa:3845 K07827 KRAS; KRAS proto-oncogene, GTPase** **hsa04213 Longevity regulating pathway - multiple species - Homo sapiens (human) (1)** **hsa:3845 K07827 KRAS; KRAS proto-oncogene, GTPase** **hsa05170 Human immunodeficiency virus 1 infection - Homo sapiens (human) (1)** **hsa:3845 K07827 KRAS; KRAS proto-oncogene, GTPase**	thyroid gland hematopoietic system ear Zymbals gland oral cavity kidney nasal cavity liver Maltoni head cancers	liver thyroid gland hematopoietic system kidney **uterus** urinary bladder nasal cavity lung clitoral gland	liver vascular system lung small intestine	thyroid gland urinary bladder vascular system liver pituitary gland peritoneal cavity stomach small intestine **ovary**	Adenoma
Kava kava extract	9000-38-8	COC1=CC(=O)OC(C)C)C=CC2=CC=CC=C2COC3=CC=CC=C3COC4=CC(=CC(=O)O4)OC.COC(=O)C(=C)C(=O)OC(C)C(=O)C=CC=C(C)C=CC=CC=CC

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Leucomalachite green	129-73-7	N(C=1C=CC(=CC=1)C(=1C=2C=CC(=CC=2)C=1C=CC(N)C(=)C=CC=1)=1C=CC=1)(C)C	-	8, 11, 14, 19, 23, 34, 36, 43, 58, 60, 61, 64, 66, 71, 72, 111, 117, 122, 133, 150, 163, 187, 214, 220, 307, 318	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	C57BL/6N x C3H/HeN MTV-	Diet	2 yrs	2 yrs	Not specified	Axillary lymph node	Lymphoma - malignant	CDKN1A MDM2 MKRT TP0	CTPS1 RPRM INCENP BCC2 E9HC2	SAT ENC1 SRBP1 ITGAM P2RY14	hsa05165: Human papillomavirus infection - Homo sapiens (human) (1) hsa:4193 #36643 MDM2; MDM2 proto-oncogene hsa04144: Endocytosis - Homo sapiens (human) (1) hsa:4193 #36643 MDM2; MDM2 proto-oncogene hsa01524: Platinum drug resistance - Homo sapiens (human) (1) hsa:4193 #36643 MDM2; MDM2 proto-oncogene	thyroid gland liver spleen all tumor bearing animals	thyroid gland liver **uterus** ear Zymbals gland **lung** clitoral gland urinary bladder	vascular system thyroid gland **lung** urinary bladder	liver **lung** vascular system peritoneal cavity thyroid gland hematopoietic system **ovary** urinary bladder stomach	**Lung Neoplasms** Adenoma
Leucomalachite green	129-73-7					Rat	Female	Fischer 344	Diet	726 d	730 d	Not specified	Abdomen	Lipoma									
Leucomalachite green	129-73-7					Rat	Male	Fischer 344	Diet	726 d	730 d	Not specified	Adrenal gland cortex	Adenoma									
Leucturacol hydrochloride	27912-14-7	C1=CC=C(C2=C(C(=CC(=C2)O)O)O)C(=O)OC(=O)[N]C(C)(C)C(=O)O.Cl				Mouse	Female	CF-1	Diet	78	78	Not specified	Liver	Hepatoma					large intestine				
Leucturacol hydrochloride	27912-14-7					Mouse	Male	CF-1	Diet	78	78	Not specified	Liver	Hepatoma - benign									
Leucturacol hydrochloride	27912-14-7					Rat	Female	Wistar	Diet	78	78	Not specified	Liver	Tumour - hepatocellular									
Leucturacol hydrochloride	27912-14-7					Rat	Female	Wistar	Diet	104	104	Not specified	Liver	Hepatoma - benign Hepatoma - benign									
Leucturacol hydrochloride	27912-14-7					Rat	Female	Wistar	Diet	52	52	Not specified	Liver										
Leucturacol hydrochloride	27912-14-7					Rat	Female	Wistar	Diet	78	78	Not specified	Liver	Multiple tumour types									
Leuprorelin acetate hydrochloride	43003-72-3	C(=O)(C=1C=CC=CC=1)C(N)[N]C(C=1C=CC=CC=1)C(=O)N(C)C(C(=O)N(C)C(C(=O)N(C)C(

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Meyoramine maleate	59-23-6					Rat	Female	Fischer 344	Drinking water	110	122	Positive	Liver	Carcinoma : hepatocellular									
Mesidine hydrochloride	6334-11-8	C=1(C(=CC(=CC=1)C)C)N)C	-	-	-	Mouse	Female	CD-1 Hsd(ICR)	Diet	77	94	Positive	Liver	Hepatoma	-				spleen liver urinary bladder oral cavity ear Zymbals gland Malloni head cancers skin	urinary bladder lung liver clitoral gland thyroid gland uterus ear Zymbals gland oral cavity	urinary bladder thyroid gland vascular systems liver	urinary bladder thyroid gland vascular system liver	-
Mesidine hydrochloride	6334-11-8					Mouse	Male	CD-1 Hsd(ICR)	Diet	77	94	Positive	Liver	Hepatoma									
Mesidine hydrochloride	6334-11-8					Rat	Male	SD	Diet	73	77	Positive	Liver	Hepatoma									
Mestranol	72-33-3	O[C@]4(CC[C@@]3(C)[C@@]2(C)[C]=CC=C(C=c1C(C)C)[C@]3(C)[C@@](A)(C)[H])[C@]2[H])[C@]4[H]	피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) 발암성 - 구분1A 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 19, 22, 27, 28, 30, 52, 53, 60, 61, 67, 97, 98, 111, 112, 117, 122, 167, 187, 195, 200, 202, 204, 207	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	ICR x B6SF1 (MTV+)	Diet	104	104	Not specified	Mammary tissue	Multiple tumour types	ESR1 AR SGK1 AIP ESR2 GRB10 NR1I2	TPM1 CGGBP2 PBRM1 EIF2S1 KIF22	OLFML2 DEFB108 CIB1 SDR16 HES2	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2100 KEGG11 ESR2; estrogen receptor 2 hsa367 KEGG17 AR; androgen receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa2100 KEGG11 ESR2; estrogen receptor 2 hsa367 KEGG17 AR; androgen receptor hsa01522 Endocrine resistance - Homo sapiens (human) (1) hsa2100 KEGG11 ESR2; estrogen receptor 2	-	liver ear Zymbals gland	stomach	pituitary gland	Carcinoma, Hepatocellular Liver Neoplasms Adenoma
Mestranol	72-33-3					Mouse	Female	CBGF	Diet	78	78	Negative	Liver	Tumour : hepatocellular									
Mestranol	72-33-3					Mouse	Male	CBGF	Diet	78	78	Negative	Liver	Tumour : hepatocellular									
Mestranol	72-33-3					Mouse	Female	B10 (MTV+)	Diet	104	104	Not specified	Mammary tissue	Multiple tumour types									
Mestranol-norethynodrel mix	8015-30-3	O[C@]4(CC[C@@]3(C)[C@@]2(C)[C]=CC=C(C=c1C(C)C)[C@]3(C)[C@@](A)(C)[H])[C@]2[H])[C@]4[H]			-	Mouse	Female	A/He	Diet	104	104	Negative	Liver	Hepatoma	-				-	-	-	-	-
Mestranol-norethynodrel mix	8015-30-3	CCC(=O)[C@]1(O)CC[C@H]2[C@H]3[C@H](C[C@]4(C)C=CC(=O)C=C[C@H]34)C[C@]12C				Mouse	Female	A/He	Diet	104	104	Negative	Liver	Hepatoma									
Mestranol-norethynodrel mix	8015-30-3					Mouse	Female	A/He	Diet	104	104	Negative	Liver	Multiple tumour types									
Mestranol-norethynodrel mix	8015-30-3					Mouse	Female	BALB/c	Diet	96	96	Not specified	Multiple sites	Carcinoma : squamous cell									
Mestranol-norethynodrel mix	8015-30-3					Mouse	Female	BALB/c	Diet	104	104	Negative	lung	Multiple tumour types									
Mestranol-norethynodrel mix	8015-30-3					Mouse	Female	BALB/c	Diet	104	104	Negative	lung	Multiple tumour types									
Mestranol-norethynodrel mix	8015-30-3					Mouse	Female	C3H/He (MTV+)	Diet	104	104	Negative	Liver	Hepatoma									
Mestranol-norethynodrel mix	8015-30-3					Mouse	Female	C3H/B	Diet	104	104	Negative	Liver	Hepatoma									
Mestranol-norethynodrel mix	8015-30-3					Mouse	Female	C3H/B	Diet	104	104	Negative	Liver	Hepatoma									
Methaphenilene	450-78-7	C2C(NC(CN(C)CC1=CC=C(C=C1)=C)=C=C2	-	-	-	Rat	Female	Fischer 344	Drinking water	82	130	Negative	Liver	Multiple tumour types					all tumor bearing animals				-
Methaphenilene	450-78-7					Rat	Male	Fischer 344	Drinking water	82	130	Negative	Liver	Multiple tumour types									
Methoxyphenylacetic acid	1701-77-5	C1=CC=CC(=C1C(C)O)=O)OC	-	-	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				stomach kidney vascular system skin	-	vascular system kidney	-	-
Methoxyphenylacetic acid	1701-77-5					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Methoxyphenylacetic acid	1701-77-5					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Methoxyphenylacetic acid	1701-77-5					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Methoxychlor	72-43-5	C1=C(C=CC(=C1)C(C2=C(C=C(C=C2)Cl)Cl)(Cl)Cl)OC	경口 독성(분진) - 구분4 특정표적장기 독성(반복 노출) - 구분2(위장계열) 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 14, 19, 20, 27, 29, 30, 34, 36, 43, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 111, 112, 117, 122, 123, 150, 165, 167, 187, 192, 200, 214, 220, 307, 318	Carcinogenicity data available: NIOSH potential occupational carcinogen	Mouse	Female	B6C3F1	Diet	78	92	Not specified	Liver	Adenoma : hepatocellular | Carcinoma:hepatocellular | Nodule : neoplastic	ESR1 AR SOD2 CYP2B6 Fos6 CYP11A1	TGFB2 CSORF4B HSD17B1 MANSC1 HOXA10	ADAMTS9 HES2 MLPH ERCC2 ANO1	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (3) hsa1555 K17709 CYP2B6; cytochrome P450 family 2 subfamily B member 6 hsa2100 KEGG11 ESR2; estrogen receptor 2 hsa367 KEGG17 AR; androgen receptor hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2100 KEGG11 ESR2; estrogen receptor 2 hsa367 KEGG17 AR; androgen receptor hsa04024 cAMP signaling pathway - Homo sapiens (human) (1) hsa5888 K05250 ESR2; Activin receptor-like kinase 2 subunit beta	liver stomach ear Zymbals gland	liver stomach	liver lung urinary bladder stomach	hematopoietic system lung liver urinary bladder	Ovarian Neoplasm Testicular Neoplasm Breast Neoplasm
Methoxychlor	72-43-5					Mouse	Male	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma : hepatocellular | Carcinoma:hepatocellular | Nodule : neoplastic									
Methoxychlor	72-43-5					Rat	Female	Osborne-Mendel	Diet	117	117	Not specified	Liver	Multiple tumour types									
Methoxychlor	72-43-5					Rat	Female	Osborne-Mendel	Diet	104	104	Negative	Liver	Multiple tumour types									
Methyl clofenapate	21340-68-1	CCC(C)OC1=CC=C(C=C1)C(=O)C=C(C=C2)C(C)OC)=O			-	Mouse	Female	Elderly Park	Diet	16	78	Not specified	Liver	Multiple tumour types	ACOX1 CLU CYP3A23-3A1 CYP4A1 EHHADH FTH1 GSTA2	APOA1 TUBGCP3 SOD1 MANSC1 MYOSC	CPT1A CYP4A11 NR1H2 ABCA1 PPARD	hsa00280 Valine, leucine and isoleucine degradation - Homo sapiens (human) (1) hsa1962 K07514 EHHADH; enoyl-CoA hydratase and 3-hydroxyacyl CoA dehydrogenase hsa04978 Mineral absorption - Homo sapiens (human) (1) hsa2495 K00522 FTH1; ferritin heavy chain 1 hsa00650 Butanoate metabolism - Homo sapiens (human) (1) hsa1962 K07514 EHHADH; enoyl-CoA hydratase and 3-hydroxyacyl CoA dehydrogenase	liver vascular system stomach skin	liver stomach	liver	liver urinary bladder	-
Methyl clofenapate	21340-68-1					Mouse	Female	Elderly Park	Diet	52	78	Not specified	Liver	Multiple tumour types									
Methyl clofenapate	21340-68-1					Mouse	Female	Elderly Park	Diet	78	78	Positive	Liver	Adenoma : hepatocellular									
Methyl clofenapate	21340-68-1					Mouse	Female	Elderly Park	Multiple routes	78	78	Positive	Liver	Adenoma : hepatocellular									
Methyl clofenapate	21340-68-1					Mouse	Male	Elderly Park	Diet	26	78	Positive	Liver	Multiple tumour types									
Methyl clofenapate	21340-68-1					Mouse	Male	Elderly Park	Diet	52	78	Positive	Liver	Multiple tumour types									
Methyl clofenapate	21340-68-1					Mouse	Male	Elderly Park	Diet	78	78	Positive	Liver	Adenoma : hepatocellular									
Methyl parathion	298-00-0	O(P)(SC)(OC1=CC=C(C=C1)[N+](=O)[O-])=O)=S)C	경口 독성(분진) - 구분2 경口 독성(분말) - 구분3 경口 독성(용액) - 구분4 특정표적장기 독성(반복 노출) - 구분2 경口 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 14, 19, 21, 23, 25, 29, 30, 45, 52, 53, 57, 61, 64, 66, 67, 71, 97, 98, 111, 112, 117, 122, 123, 131, 150, 152, 165, 167, 187, 195, 200, 203, 204, 214, 307, 310, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Diet	102	102	Not specified	Liver	Adenoma : hepatocellular | Carcinoma:hepatocellular | Nodule : neoplastic	ACHE BCHE AR CAT	FOSFRL CCR6 DSG	CYP1A2 CYP2B6 CYP3A4 NR1I3 EHHADH	hsa05200 Pathways in cancer - Homo sapiens (human) (1) hsa367 K08557 AR; androgen receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa367 K08557 AR; androgen receptor hsa05215 Prostate cancer - Homo sapiens (human) (1) hsa367 K08557 AR; androgen receptor	skin ear Zymbals gland	hematopoietic system	thyroid gland urinary bladder	-	-
Methyl parathion	298-00-0					Mouse	Male	B6C3F1	Diet	102	102	Not specified	Liver	Adenoma : hepatocellular | Carcinoma:hepatocellular | Nodule : neoplastic									
Methyl parathion	298-00-0					Rat	Female	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma : hepatocellular | Carcinoma:hepatocellular | Nodule : neoplastic									
Methyl parathion	298-00-0					Rat	Male	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma : hepatocellular | Carcinoma:hepatocellular | Nodule : neoplastic									
Methylnitrosophenylnitrosamine	937-25-7	C1=C(C=CC(=C1N)N=O)=O	-	-	-	Rat	Male	Fischer 344	Drinking water	50	114	Positive	Liver	Nodule : hyperplastic	-				esophagus thyroid gland	esophagus uterus	lung	lung	Carcinoma Esophageal Neoplasm
Methylheperidin	1103-07-1	C1=c(C(=c(C(=c1)C)C)=O)C(C)N)(C)C2=c(C(C=c(C(C=c2)C=c2)OC)OC)OC)C)N)(C)C)N)(C)C)N)(C

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Mitotane	53-19-0					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Mitotane	53-19-0					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Mitotane	53-19-0					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Mixture of Aspirin, Phenacetin and Caffeine	8003-03-0	C=1(C(O)=O)C(OC(=O)C)=CC=CC=1N3C(NC(C3)=C2N=CN(C)=C(O)C=2)NC=4C=CC(=C(C)=4)OCC)=O)C	-	-	-	Mouse	Female	B6C3F1	Diet	78	94	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic	-				-	-	-	-	-
Mixture of Aspirin, Phenacetin and Caffeine	8003-03-0					Mouse	Male	B6C3F1	Diet	78	94	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Mixture of Aspirin, Phenacetin and Caffeine	8003-03-0					Mouse	Female	CS7BL/6	Diet	77	77	Negative	Liver	Carcinoma - hepatocellular									
Mixture of Aspirin, Phenacetin and Caffeine	8003-03-0					Mouse	Male	CS7BL/6	Diet	77	77	Negative	Liver	Carcinoma - hepatocellular									
Mofebutene	125533-88-0	CC(=O)C(=O)C=C(C=C(C)OCCNBCCOCC2)N3C=3C=CC4=C(C=3)C(C)(C)CCC4C)C			-	Mouse	Female	MMTV/NULI (Taconic)	Diet	178.d	182.d	Not specified			-				kidney stomach	vascular system	thyroid gland	hematopoietic system	-
Monobenzyl ether of Hydroquinone	103-16-2	O(C=1C=CC(=CC=1)O)CC2=CC=CC=C2	피부 과민성 - 구분1(1A/1B) 안전 수생환경 유해성 - 구분2	10, 25, 23, **29, 30**, 34, 36, 41, 46, 52, 53, 57, 58, 61, 67, 72, 111, 152, 117, 131, 150, 162, 165, 167, 187, **200**, 307, 310	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				stomach nasal cavity urinary bladder kidney vascular system	stomach urinary bladder hematopoietic system nasal cavity	stomach kidney thyroid gland vascular system	stomach **ovary** thyroid gland pituitary gland peritoneal cavity vascular system hematopoietic system urinary bladder	-
Monobenzyl ether of Hydroquinone	103-16-2					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Monobenzyl ether of Hydroquinone	103-16-2					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Monobenzyl ether of Hydroquinone	103-16-2					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Monuron	150-68-5	C1(=CC=C(C=1Cl)N(C)C)=O)Cl	급성 독성(경구) - 구분4 심한 눈 손상/눈 자극성 - 구분2A(2B) 생식세포 변이원성 - 구분2 **발암성 - 구분2** 안전 수생환경 유해성 - 구분3	**29, 30**, 52, 53, 57, 61, 67, 112, 130, **165, 167, 200**	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma	ALDH1A3 C6 MIR182 MIR183A ~~MIR345~~ ~~MIR96~~ TNN-49	ALDH1B1 RPM6 CCNC ARH1 C17ORF75	CYP2B6 CYP1A2 CYP3A4 INS LDT1	hsa05206 MicroRNAs in cancer - Homo sapiens (human) (2) hsa-miR7040 K16882 MIR144; microRNA 144 hsa-miR7053 K17114 MIR96; microRNA 96 hsa04810 Regulation of actin cytoskeleton - Homo sapiens (human) (1) hsa7230 K03985 C6; complement C6 hsa05020 Prion disease - Homo sapiens (human) (1) hsa-miR-49 MIR381 K8; mitochondrial K8	**kidney** all tumor bearing animals	thyroid gland **uterus** lung ear Zymbals gland	**kidney** urinary bladder vascular system	urinary bladder	Liver Neoplasm, Experimental Kidney Neoplasm
Monuron	150-68-5					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Monuron	150-68-5					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Monuron	150-68-5					Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
m-Phenylenediamine	108-45-2	C1=C(N)C=CC=C1N	급성 독성(경구) - 구분4 급성 독성(흡입) - 구분4 급성 독성(흡입: 분진/미스트) - 구분4 심한 눈 손상/눈 자극성 - 구분2A(2B) 피부 과민성 - 구분1(1A/1B) 생식세포 변이원성 - 구분2 특정표적장기 독성(반복 노출) - 구분2 특정표적장기 독성(반복 노출) - 구분1 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	10, 21, 41, 57, 131, 150, 310	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Drinking water	78	84	Negative	Liver	Haemangioma	-				spleen ear Zymbals gland thyroid gland urinary bladder	urinary bladder **uterus** ear Zymbals gland thyroid gland hematopoietic system clitoral gland lung liver kidney mammary gland nasal cavity	thyroid gland urinary bladder liver vascular system lung	thyroid gland liver urinary bladder vascular system **ovary** hematopoietic system stomach peritoneal cavity	-
m-Phenylenediamine	108-45-2					Mouse	Male	B6C3F1	Drinking water	78	84	Negative	Liver	Haemangioma									
Myristicin	607-91-0	C1=C(C=C(C2=C1OCO2)OCC)=C	-	-	-	Mouse	Female	B6C3F1/N	Gavage	92.d	91.d	Not specified			CYP1A2 ~~CYP2A3~~ ~~ABCC3~~ ~~ABL1~~	G2E5 CAB39	SOD3 ITGA6 TNNI3K2 CASP2 MGST1	hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (1) hsa-1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (5) hsa-1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa-1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1	stomach liver kidney	stomach	stomach liver vascular system	liver lung stomach	-
N-(4-Aminophenyl)aniline	101-54-2	C1=C(C=CC(=C1)N)C2=CC=CC=C2N	급성 독성(경구) - 구분4 피부 과민성 - 구분1(1A/1B) 급성 수생환경 유해성 - 구분1	6, 7, 14, 18, 19, 23, 25, 27, **29, 30**, 36, 37, 46, 51, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 91, 93, 94, 95, 96, 106, 111, 112, 117, 122, 123, 126, 131, 150, 153, **165**, 166, 167, 187, 197, **200**, 214, 220, 307, 318	Genotoxicity Data: predicted to be genotoxic	Rat	Female	Fischer 344	Diet	2 yrs	2 yrs	Not specified	Adrenal gland	Pheochromocytoma	CYP1A1	CCR6 DNAJC12 AMH R2 TEP1 MYO5C	HTATIP2 CYTIP SOD3 CCR5 TNNI3K2	hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (1) hsa-1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (1) hsa-1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa-1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1	spleen liver thyroid gland ear Zymbals gland all tumor bearing animals	**uterus** thyroid gland urinary bladder ear Zymbals gland hematopoietic system clitoral gland lung kidney	thyroid gland urinary bladder vascular system	thyroid gland urinary bladder vascular system liver hematopoietic system **ovary**	-
N-(4-Aminophenyl)aniline	101-54-2					Rat	Male	Fischer 344	Diet	2 yrs	2 yrs	Not specified	Adrenal gland	Pheochromocytoma									
N-(Trichloromethylthio)phthalimide	133-07-3	C1=CC=CC2=C(N(SC(Cl)(Cl)Cl)C)=O	급성 독성(흡입: 분진/미스트) - 구분4 심한 눈 손상/눈 자극성 - 구분2A(2B) 피부 과민성 - 구분1(1A/1B) **발암성 - 구분2** 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 14, 19, 22, 23, 27, **29, 30**, 32, 34, 36, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, **165, 167**, 187, **200**, 214, 307, 318	Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	HPRT1 ABCB1A ABCC3 ABCC5 ABCF1 ABHD6	CCNC NGK4 TIMM TEP1 MYO5C	SAT POR VASN UBP6 GNAI1	hsa01523 Antifolate resistance - Homo sapiens (human) (2) hsa-10057 K05648 ABCC5; ATP binding cassette subfamily C member 5 hsa-8714 K05667 ABCC3; ATP binding cassette subfamily C member 3 hsa02010 ABC transporters - Homo sapiens (human) (2) hsa-10057 K05648 ABCC5; ATP binding cassette subfamily C member 5 hsa-8714 K05667 ABCC3; ATP binding cassette subfamily C member 3 hsa04976 Bile secretion - Homo sapiens (human) (1) hsa-8714 K05667 ABCC3; ATP binding cassette subfamily C member 3	kidney	**uterus** kidney	**stomach** small intestine vascular system urinary bladder	small intestine hematopoietic system vascular system **stomach** urinary bladder	Stomach Neoplasm Adenocarcinoma Carcinoma, Squamous Cell Neoplasm, Experimental Papilloma
N-(Trichloromethylthio)phthalimide	133-07-3					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N-(Trichloromethylthio)phthalimide	133-07-3					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N-(Trichloromethylthio)phthalimide	133-07-3					Mouse	Female	B6C3F1	Diet	104	104	Positive	Duodenum	Adenocarcinoma									
N-(Trichloromethylthio)phthalimide	133-07-3					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N-(Trichloromethylthio)phthalimide	133-07-3					Mouse	Male	B6C3F1	Diet	104	104	Positive	Duodenum	Adenocarcinoma									
N,4-Dinitroso-N-methylaniline	99-80-9	N(N(C=1C=CC(N=O)=CC=1)C)=O	안전 수생환경 유해성 - 구분2	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Rat	Male	CII	Intraperitoneal	26	86	Positive	Liver	Hepatoma	-				spleen liver esophagus urinary bladder	esophagus **uterus** urinary bladder liver	-	-	-
N,N,N'-Tetramethyl-4,4'-methylenedianiline	101-61-1	C2N(C)C=1C=C(C(C1=CC=C(N(C)C)C=C1)C)=C2	**발암성 - 구분1B**	8, 11, 19, 20, 23, **29, 30**, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 62, 67, 72, 107, 111, 112, 117, 121, 148, 150, 162, 165, 167, 187, **200**, 307, 310	Cancer slope factor: 1.3e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	78	91	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular					**thyroid gland** liver vascular system ear Zymbals gland	**thyroid gland** liver lung mammary gland ear Zymbals gland	kidney vascular system **thyroid gland**	liver peritoneal cavity	Thyroid Neoplasm
N,N,N'-Tetramethyl-4,4'-methylenedianiline	101-61-1					Mouse	Male	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
N,N,N'-Tetramethyl-4,4'-methylenedianiline	101-61-1					Rat	Female	Fischer 344	Diet	59	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
N,N,N'-Tetramethyl-4,4'-methylenedianiline	101-61-1					Rat	Male	Fischer 344	Diet	59	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
N,N,N-Trimethylbenzenemethanaminium chloride	56-93-9	C1=CC=CC(=C1C(N=)C)C)C(C)=)	피부 부식성/피부 자극성 - 구분2 심한 눈 손상/눈 자극성 - 구분2A(2B)	**29, 30**, 52, 53, 57, 112, **165, 167, 200**	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Gavage	92.d	91.d	Not specified			-								-
N,N,N'-bis(2-Hydroxyethyl)-2-nitro-p-phenylenediamine	23229-34-4	[N+](C)(C)[O-])=CC(=1C)=CC=CC(=1)N(CCO)CCO)NCCO	피부염증	7, 19, 23, 29, **29, 30**, 43, 52, 53, 67, 111, 112, 117, 122, 123, 153, **165, 166, 167**, 187, **200**, 307	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Diet	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic	-				skin vascular system large intestine hematopoietic system	lung	thyroid gland kidney	hematopoietic system liver lung	-
N,N'-bis(2-Hydroxyethyl)-2-nitro-p-phenylenediamine	23229-34-4					Mouse	Male	B6C3F1	Diet	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
N,N'-bis(2-Hydroxyethyl)-2-nitro-p-phenylenediamine	23229-34-4					Rat	Female	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
N,N'-bis(2-Hydroxyethyl)-2-nitro-p-phenylenediamine	23229-34-4					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
N,N'-Bis-fructose-2,2'-diylbiscetamide	304-28-9	C1=C(C)=CC=C1N(C)C(=O)C=2C=CC(=CC=2C(=O)N(C)C)=O		**29, 30**, 52, 53, 67, 112, **165, 167, 200**	-	Cynomolgus monkey	Mixed	Not specified	Diet	258	1513	Not specified	Lung	Carcinoma - alveolar/bronchiolar	-								-
N,N'-Bis-fructose-2,2'-diylbiscetamide	304-28-9					Rhesus monkey	Mixed	Not specified	Diet	258	1664	Not specified	Multiple sites	Tumour - malignant									
N,N'-Di-2-naphthyl-p-phenylenediamine	93-46-9	C1(=CC=C(C=C1)N(C2=CC=3(C(=C2)=CC=CC=3)N(C4=CC=5(C(=C4)=CC=CC=5	급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	19, 23, 23, 27, 36, 41, 46, 57, 61, 111, 117, 131, 150, 187, 307, 310	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				liver spleen ear Zymbals gland thyroid gland	ear Zymbals gland urinary bladder **uterus** hematopoietic system thyroid gland clitoral gland	urinary bladder liver thyroid gland vascular system	urinary bladder thyroid gland **ovary** liver vascular system stomach pituitary gland hematopoietic system	-
N,N'-Di-2-naphthyl-p-phenylenediamine	93-46-9					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N,N'-Di-2-naphthyl-p-phenylenediamine	93-46-9					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
N,N'-Di-2-naphthyl-p-phenylenediamine	93-46-9			-	-	Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N,N-Diethyl-3-methylbenzamide	134-62-3	C(C)(=O)c1cc(C)ccc1)(C)N(CC)CC)=O	경련 독성(흡연) - 구분4 경련 독성(흡입) 위험 - 구분3 심한 눈 손상성/눈 자극성 - 구분2A(2B) 특정표적장기 독성(반복 노출) - 구분2 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분3	8, 11, 57, 60	Carcinogenicity data available: EPA OPP Group D Not Classifiable as to Human Carcinogenicity Genotoxicity Data: predicted to be genotoxic	Mouse	Female	CD1	Diet	78	78	Negative	Liver	Adenoma - hepatocellular	AGXE CORT C19Q86 IL10 IL6 CYP1A2	TMEM194A TBX15 CCDC93 CTX1A CAPRIN1	TNNT1 MT1B LST1 VASP IRT1	hsa05152 Tuberculosis - Homo sapiens (human) (2) hsa:3569 IL5RA; IL6; interleukin 6 hsa:3586 IL10RA; IL10; interleukin 10 hsa05321 Inflammatory bowel disease - Homo sapiens (human) (2) hsa:3569 IL5RA; IL6; interleukin 6 hsa:3586 IL10RA; IL10; interleukin 10 hsa05133 Pertussis - Homo sapiens (human) (2) hsa:3569 IL5RA; IL6; interleukin 6 hsa:3586 IL10RA; IL10; interleukin 10	all tumor bearing animals	all tumor bearing animals	lung urinary bladder	-	-
N,N-Diethyl-3-methylbenzamide	134-62-3					Mouse	Male	CD1	Diet	78	78	Negative	Liver	Adenoma - hepatocellular									
N,N-Diethyl-3-methylbenzamide	134-62-3					Rat	Female	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
N,N-Diethyl-3-methylbenzamide	134-62-3					Rat	Male	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
N,N-Diethyl-4-((1-oxido-4-pyridinyl)azo)benzenamine	7347-48-1	[N+]([O-])c1cc(/N=N/c1ccc(N(CC)CC)cc1)ccc1	-	-	-	Rat	Male	SD	Diet	52	52	Positive	Liver	Multiple tumour types	-				liver spleen vascular system nasal cavity esophagus	nasal cavity ear Zymbals gland thyroid gland esophagus	thyroid gland	-	-
N,N-Dimethyl-4-(m-tolyiazo)aniline	55-80-1					Rhesus monkey	Mixed	Not specified	Diet	208	1456	Not specified	Liver	Carcinoma - hepatocellular									
N,N-Dimethyl-4-(m-tolyiazo)aniline	55-80-1	N(c)Nc1ccc(/C=C/c1ccc(/C=C/c1)C)c2ccc(N(C)C)cc2	-	8, 11, 16, 20, 22, 29, 30, 34, 36, 41, 52, 53, 57, 58, 60, 61, 67, 72, 111, 152, 117, 131, 150, 163, 166, 167, 187, 200, 207, 310	-	Rat	Male	AfpkcAPESD	Gavage	52	52	Positive	Liver	Carcinoma - hepatocellular	TAT	CTPS1 INCENP RPRM CCNC DHFR	ENC1 ITGAM SRRP1 PXRP14 SAT	hsa00130 Ubiquinone and other terpenoid-quinone biosynthesis - Homo sapiens (human) (1) hsa:6888 KDOB15; TAT; tyrosine aminotransferase hsa00400 Phenylalanine, tyrosine and tryptophan biosynthesis - Homo sapiens (human) (1) hsa:6888 KDOB15; TAT; tyrosine aminotransferase hsa00350 Tyrosine metabolism - Homo sapiens (human) (1) hsa:6888 KDOB15; TAT; tyrosine aminotransferase	spleen liver vascular system **thyroid gland** all tumor bearing animals	liver **thyroid gland** urinary bladder clitoral gland	**thyroid gland** vascular system urinary bladder kidney	liver urinary bladder vascular system	Carcinoma, Hepatocellular **Liver Neoplasm, Experimental** Neoplasm Metastasis Precancerous Conditions Thyroid Neoplasm
N,N-Dimethyl-4-(m-tolyiazo)aniline	55-80-1					Rat	Male	Fischer 344/DuCrl	Diet	104	104	Positive	Liver	Carcinoma - hepatocellular									
N,N-Dimethylaniline	121-69-7	C1=CC=CC(=C1)N(C)C	경련 독성(흡연) - 구분4 경련 독성(흡입) - 구분4 경련 독성(흡입) 위험 - 구분3 심한 눈 손상성/눈 자극성 - 구분2A(2B) **발암성 - 구분2** 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분3	29, 30, 52, 53, 57, 67, 112, 131, 165, 167, 200	Carcinogenicity data available: PPRTV (ORNL) - Suggestive evidence of carcinogenic potential for oral exposure. Inadequate information for inhalation. Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Forestomach	Papilloma - squamous cell	CYP2A13 TCF7L2 AXIN2 FMO1 FMO2	CTPS1 INCENP RPRM CCNC RCC2	SRRP1 ENC1 SAT ITGAM PXRP14	hsa04934 Cushing syndrome - Homo sapiens (human) (2) hsa:6934 KDM4B; TCF7L2; transcription factor 7 like 2 hsa:8313 KDM5B; AXIN2; axin 2 hsa05217 Basal cell carcinoma - Homo sapiens (human) (2) hsa:6934 KDM4B; TCF7L2; transcription factor 7 like 2 hsa:8313 KDM5B; AXIN2; axin 2 hsa05210 Colorectal cancer - Homo sapiens (human) (2) hsa:6934 KDM4B; TCF7L2; transcription factor 7 like 2 hsa:8313 KDM5B; AXIN2; axin 2	thyroid gland spleen liver all tumor bearing animals	thyroid gland liver **uterus** ear Zymbals gland lung urinary bladder hematopoietic system clitoral gland nasal cavity kidney	vascular system thyroid gland lung urinary bladder	liver thyroid gland urinary bladder peritoneal cavity vascular system lung stomach **ovary** hematopoietic system	-
N,N-Dimethylaniline	121-69-7					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma(hepatocellular | Nodule - neoplastic									
N,N-Dimethylaniline	121-69-7					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma(hepatocellular | Nodule - neoplastic									
N,N-Dimethylaniline	121-69-7					Rat	Male	Fischer 344	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma(hepatocellular | Nodule - neoplastic	-								
N,N'-Dimethyl-N,N'-dinitrosophthalamide	3851-16-9	C(C1=C(C(N(N=O)C)=O)C=CC=C1)(N(N=O)C)=O	-	-	-	Rat	Male	Wistar	Gavage	67	67	Not specified	Liver	Multiple tumour types	-				stomach oral cavity nasal cavity	all tumor bearing animals	lung kidney vascular system	lung vascular system hematopoietic system	-
N,N-Dimethyl-p-toluidine	99-97-8	C=1(N(C)C)C=CC(=CC=1)C	인화성 액체 - 구분4 경련 독성(흡입) - 구분1 경련 독성(흡입) 위험 - 구분3 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(2B) **발암성 - 구분2** 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분3	8, 11, 21, 29, 30, 34, 41, 52, 53, 57, 58, 60, 67, 112, 131, 150, 165, 167, 200, 310	Carcinogenicity data available: CalEPA Likely Human Carcinogen Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1/N	Gavage	93 d	91 d	Not specified			ID4 ABHD3 ABHD11A ABHD5	CTPS1 RPRM INCENP CXCR7 DHFR	ENC1 SRRP1 ITGAM PXRP14 SAT		**liver** spleen thyroid gland oral cavity all tumor bearing animals	thyroid gland **liver** clitoral gland ear Zymbals gland lung urinary bladder nasal cavity oral cavity	vascular system thyroid gland urinary bladder kidney lung	**liver** vascular system urinary bladder peritoneal cavity thyroid gland	**Liver Neoplasm** Nose Neoplasm
N,N'-Diphenylguanidine	102-06-7	C(NC1=CC=CC=C1)(NC2=CC=CC=C2)=N	경련 독성(흡연) - 구분4 심한 눈 손상성/눈 자극성 - 구분2A(2B) 생식독성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 만성 수생환경 유해성 - 구분3	7, 10, 19, 21, 23, 25, 29, 30, 41, 46, 52, 53, 57, 60, 61, 67, 111, 152, 117, 122, 126, 128, 131, 150, 153, 165, 167, 187, 200, 207, 310	Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Diet	94 d	91 d	Not specified			KCNH2 SLC26A2	DHFR ALDH18A1 HIPO MYO5C TEP1	SLC2A4 INS PPARGC1A VASN LST1		spleen thyroid gland liver ear Zymbals gland all tumor bearing animals	ear Zymbals gland **uterus** mammary gland hematopoietic system stomach urinary bladder small intestine kidney clitoral gland thyroid gland lung liver	thyroid gland urinary bladder liver vascular system	thyroid gland urinary bladder vascular system liver **ovary** hematopoietic system stomach	-
N,N-Diphenyl-p-phenylenediamine	74-31-7	N(C1=CC=CC=C1)(C2=CC=CC=C2)C3=CC=CC=C3	피부 과민성 - 구분1(1A/1B)	19, 21, 23, 29, 30, 41, 52, 53, 57, 61, 67, 111, 112, 117, 131, 150, 160, 167, 187, 200, 207, 310	Carcinogenicity data available: PPRTV (ORNL) - Inadequate for an assessment of carcinogenic potential Genotoxicity Data: genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	MAPK1 MAPK2 AIP CAT EGR1	MYOSC TEP1 PIGER1 COG5 DNAAF2	SAT VASN HTATIP2 HPGD HSPA1L	hsa04068 FoxO signaling pathway - Homo sapiens (human) (2) hsa:5595 KEGG: MAPK2; mitogen-activated protein kinase 2 hsa:847 KEGG: CAT; catalase hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa:5595 KEGG: MAPK2; mitogen-activated protein kinase 2 hsa:847 KEGG: CAT; catalase hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa:5595 KEGG: MAPK2; mitogen-activated protein kinase 2 hsa:847 KEGG: CAT; catalase	spleen thyroid gland liver ear Zymbals gland all tumor bearing animals	**uterus** thyroid gland hematopoietic system urinary bladder kidney ear Zymbals gland clitoral gland lung all tumors bearing animals	thyroid gland urinary bladder liver vascular system small intestine	thyroid gland **ovary** urinary bladder vascular system pituitary gland stomach peritoneal cavity small intestine	-
N,N-Diphenyl-p-phenylenediamine	74-31-7					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N,N-Diphenyl-p-phenylenediamine	74-31-7					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N,N-Diphenyl-p-phenylenediamine	74-31-7					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N,N-Diphenyl-p-phenylenediamine	74-31-7					Rat	Female	Fischer 344/DuCrl	Diet	104	112	Negative	Liver	Cholangiocarcinoma									
N,N-Diphenyl-p-phenylenediamine	74-31-7					Rat	Male	Fischer 344/DuCrl	Diet	104	112	Negative	Liver	Nodule - hyperplastic									
N,N-Dipropyl-4-(4'-pyridyl)-1'-oxidoaniline	-	N(C1=CC=C(C=C1)N(=NC=2C=C(N+]=CC=2)[O-])(CC)CC)CC				Rat	Male	SD	Diet	52	52	Not specified	Liver	Multiple tumour types									
N-1-Oxoremidifluorene	63019-65-8	C1=C(C)c2C=c1ccc4c3c(c(=O)c2)c2c(N(C)C)=O)c(C)c=O	-	-	-	Rat	Female	Buffalo	Diet	53	93	Positive	Ear canal	Carcinoma - squamous cell	-				kidney skin spleen	ear Zymbals gland mammary gland liver	urinary bladder thyroid gland vascular system	urinary bladder stomach **ovary** vascular system	-
N-1-Naphthyl-1,2-ethylenediamine dihydrochloride	1465-25-4	C1=CC=C2C(=C1N(CC)NC=c4C=C2Cl.Cl	-	6, 7, 18, 19, 21, 23, 25, 27, 34, 36, 37, 41, 51, 57, 58, 61, 62, 72, 115, 117, 122, 123, 131, 150, 153, 163, 166, 187, 220, 227, 310, 318	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	104	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma(hepatocellular | Nodule - neoplastic	-				ear Zymbals gland spleen all tumors bearing animals	**uterus** hematopoietic system ear Zymbals gland urinary bladder lung mammary gland clitoral gland small intestine	thyroid gland urinary bladder kidney	thyroid gland urinary bladder **ovary** lung	-
N-1-Naphthyl-1,2-ethylenediamine dihydrochloride	1465-25-4					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma(hepatocellular | Nodule - neoplastic									
N-1-Naphthyl-1,2-ethylenediamine dihydrochloride	1465-25-4					Rat	Female	Fischer 344	Diet	104	107	Not specified	Liver	Adenoma - hepatocellular | Carcinoma(hepatocellular | Nodule - neoplastic									
N-1-Naphthyl-1,2-ethylenediamine dihydrochloride	1465-25-4					Rat	Male	Fischer 344	Diet	104	107	Not specified	Liver	Adenoma - hepatocellular | Carcinoma(hepatocellular | Nodule - neoplastic									
N2-gamma-Glutamyl-p-hydroxybenzoic acid	-	C1=C(C=CC(=C1O)C(=O)NNC(CC(@H)(N)C)=O)C(=O)O				Mouse	Female	Swiss	Gavage	52	123	Not specified	Liver	Multiple tumour types	-				-	-	-	-	-
N2-gamma-Glutamyl-p-hydroxybenzoic acid	-					Mouse	Male	Swiss	Gavage	52	123	Positive	Liver	Multiple tumour types	-				-	-	-	-	-
N-4'-(4'-Fluorobiphenyl)acetamide	398-32-3	N(C=2C=CC(C1=CC=C(C=C1)F)=CC=2)C(=O)C	-	-	-	Rat	Male	Fischer 344	Diet	52	52	Positive	Kidney	Adenocarcinoma	-				kidney thyroid gland urinary bladder nasal cavity esophagus liver skin	ear Zymbals gland urinary bladder mammary gland	urinary bladder thyroid gland kidney liver	urinary bladder liver lung	-
N-9H-Fluoren-2-yl-2,2,2-trifluoroacetamide	363-17-7	C=1C=C(C=C2C=1C3=C(C2)C=CC=C3)N(C)C(F)(F)F)=O	-	8, 11, 21, 29, 30, 34, 36, 41, 52, 53, 57, 58, 60, 61, 67, 72, 107, 152, 122, 123, 131, 150, 163, 166, 167, 200, 220, 310	-	Rat	Female	Buffalo	Diet	53	54	Positive	Ear canal	Carcinoma - squamous cell	-				kidney liver skin stomach	ear Zymbals gland liver mammary gland	urinary bladder thyroid gland kidney	urinary bladder stomach liver	-
N'-Acetyl-4-(hydroxymethyl)phenylhydrazine	65704-38-5	N(C1=CC=C(C=C1)CO)N(C)=O	-	-	-	Mouse	Female	Swiss	Drinking water	115	115	Positive	Blood vessel	Multiple tumour types	-				-	ear Zymbals gland mammary gland	vascular system lung kidney thyroid gland urinary bladder	vascular system lung hematopoietic system	-
N'-Acetyl-4-(hydroxymethyl)phenylhydrazine	65704-38-5					Mouse	Male	Swiss	Drinking water	115	115	Positive	Blood vessel	Multiple tumour types									
Nafenopin	3771-19-5	C(C)(C)(=O)C(O)(C3=CC=C(C1C1CCCC2=C1C=CC=C2)C=C3	경련 독성(흡연) - 구분4 **발암성 - 구분2** 만성 수생환경 유해성 - 구분4	29, 30, 34, 36, 52, 53, 58, 67, 72, 112, 163, 166, 167, 200	Carcinogenicity data available: CalEPA Likely Human Carcinogen	Rat	Male	Fischer 344	Diet	108	108	Positive	Liver	Carcinoma - hepatocellular	PPARA CYP4A1 ACAA1 ACOX1	ABCA1 TNFD2 NCPD8 NAPTL1 IBP10	PPARA PXRP14 PPARD FDXD1 CPT1A	hsa00280 Valine, leucine and isoleucine degradation - Homo sapiens (human) (1) hsa:20 KEGG: ACAA1; acetyl-CoA acyltransferase 1 hsa04146 Peroxisome - Homo sapiens (human) (1) hsa:20 KEGG: ACAA1; acetyl-CoA acyltransferase 1 hsa00592 alpha-Linolenic acid metabolism - Homo sapiens (human) (1) hsa:20 KEGG: ACAA1; acetyl-CoA acyltransferase 1	liver stomach	liver stomach ear Zymbals gland	liver stomach	pituitary gland liver	-

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Naftenopin	2771-18-0					Rat	Male	SD	Diet	60	60	Positive	Liver	Multiple tumour types									
Naftenopin	2771-18-5					Rat	Female	Wistar	Diet	55	55	Not specified	Liver	Adenoma- hepatocellular									
Naftenopin	2771-18-3					Rat	Female	Wistar	Diet	70	70	Positive	Liver	Adenoma- hepatocellular									
Naphthalene	91-20-3	C1=12C(=CC=CC=1)C=CC=C2	인화성 고체 - 구분2 급성 독성(경구) - 구분4< **발암성 - 구분2** 생식세포 변이원성 - 구분2 만성 수생환경 유해성 - 구분1	8, 11, **29**, **30**, 34, 52, 53, 57, 58, 60, 61, 62, 67, 112, **165**, **167**, **200**	Cancer slope factor: 1.4e-05 ug/m3-1 (carcinogenicity, oral) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Inhalation	103	104	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic	CYP1B CYP2E2 AHR GCLC SCGB1A1 EPHB1	AIRN7 CADPS2 CCDC49 FMR2 GCA	FAM171A1 HSPA12A LIM2 MAFIK7BP3 NMNAT	hsa04904 Cushing syndrome - Homo sapiens (human) (1) hsa:196 409363 AHR; aryl hydrocarbon receptor hsa00480 Glutathione metabolism - Homo sapiens (human) (1) hsa:2729 411204 GCLC; glutamate-cysteine ligase catalytic subunit hsa00270 Cysteine and methionine metabolism - Homo sapiens (human) (1) hsa:2729 411204 GCLC; glutamate-cysteine ligase catalytic subunit	thyroid gland spleen ear Zymbals gland kidney oral cavity hematopoietic system nasal cavity urinary bladder Multiple head cancers	hematopoietic system **uterus** urinary bladder kidney nasal cavity thyroid gland clitoral gland ear Zymbals gland	urinary bladder thyroid gland **lung** stomach vascular system liver kidney small intestine preputial gland	**ovary** thyroid gland urinary bladder stomach pituitary gland vascular system **lung** liver peritoneal cavity	**Lung Neoplasms** **Liver Neoplasms, Experimental** Nose Neoplasm Neoplasm Metastasis
Naphthalene	91-20-3					Mouse	Male	B6C3F1	Inhalation	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Naphthalene	91-20-3					Rat	Female	Fischer 344	Inhalation	105	105	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
Naphthalene	91-20-3					Rat	Male	Fischer 344	Inhalation	104	104	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
N-Cyclohexyl-2-benzothiazolylsulphenamide	95-33-0	C1=CC=CC2=C(N)=C(SC2(NC)(C)CCCC)1	피부 과민성 - 구분1(1A/1B) 생식독성 - 구분2 특정표적장기 독성(반복 노출) - 구분2 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 19, 20, 21, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 62, 67, 72, 111, 112, 117, 122, 123, 131, 150, 163, **165**, 167, 187, **200**, 220, 307, 310	Genotoxicity Data: inconclusive	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	AHR	-	CCR5 FHYH INS SCSDL FNDC4	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa:196 409363 AHR; aryl hydrocarbon receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa:196 409363 AHR; aryl hydrocarbon receptor hsa04659 Th17 cell differentiation - Homo sapiens (human) (1) hsa:196 409363 AHR; aryl hydrocarbon receptor	-	all tumor bearing animals	thyroid gland	-	-
N-Cyclohexyl-2-benzothiazolylsulphenamide	95-33-0					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N-Cyclohexyl-2-benzothiazolylsulphenamide	95-33-0					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
N-Cyclohexyl-2-benzothiazolylsulphenamide	95-33-0					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Nefiracetam	77191-36-7	C1CCC(N1CC(N(C=2C(=CC=CC=2)C)C)=O)=O	-	8, 11, 60	-	Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Adenoma- hepatocellular	PTGS2	ALDH1B1 DHRS NPR1 HSPD NADK	TMEM41B CNTN1 SLC16A1 TCN1B MT1B	hsa04064 NF-kappa B signaling pathway - Homo sapiens (human) (1) hsa:5743 411987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa:5743 411987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa00590 Arachidonic acid metabolism - Homo sapiens (human) (1) hsa:5743 411987 PTGS2; prostaglandin-endoperoxide synthase 2	oral cavity spleen liver nasal cavity	liver ear Zymbals gland nasal cavity vascular system	urinary bladder thyroid gland kidney	-	-
Nefiracetam	77191-36-7					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Adenoma- hepatocellular									
Nefiracetam	77191-36-7					Rat	Female	Fischer 344/DuCrl	Diet	104	104	Negative	Liver	Tumour- hepatocellular									
Nefiracetam	77191-36-7					Rat	Male	Fischer 344/DuCrl	Diet	104	104	Negative	Liver	Adenoma- hepatocellular									
N-Hydroxy-4-acetylaminobiphenyl	4463-22-0	N(C(=O)C)C=1C=CC=CC=1)C2=CC=CC=C2)O	-	-	-	Rat	Female	Not specified	Diet	43	65	Negative	Liver	Multiple tumour types	-				liver spleen	liver urinary bladder ear Zymbals gland	urinary bladder thyroid gland	liver urinary bladder stomach vascular system	-
N-Hydroxy-N-nitrosobenzenamine, ammonium salt	135-20-6	C1=CC=CC2=C(N(N=O)[O-])NH4+]	급성 독성(경구) - 구분3 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A(1B) **발암성 - 구분1A**	8, 11, 21, 29, 30, 34, 36, 41, 52, 53, 57, 58, 60, 61, 67, 72, 112, 131, 150, 163, **165**, **167**, **200**, 310	Cancer slope factor: 6.3e-05 ug/m3-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: mutagenic	Mouse	Female	B6C3F1	Diet	78	95	Positive	Harderian gland	Adenoma	-					-	-	-	-
N-Hydroxy-N-nitrosobenzenamine, ammonium salt	135-20-6					Mouse	Male	B6C3F1	Diet	78	95	Positive	Harderian gland	Adenoma									
N-Hydroxy-N-nitrosobenzenamine, ammonium salt	135-20-6					Rat	Female	Fischer 344	Diet	78	106	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
N-Hydroxy-N-nitrosobenzenamine, ammonium salt	135-20-6					Rat	Male	Fischer 344	Diet	78	105	Positive	Body cavity	Mesothelioma									
Nitazoxanide	55981-09-4	N1=c(SC)=C1[N]N=]([O-])=O)NC(C=2C=CC=CC=2OC(=O)C)=O	-	7, 11, 21, 22, 25, 27, **29**, **30**, 34, 36, 41, 46, 52, 53, 57, 58, 61, 62, 72, 111, 112, 117, 122, 123, 131, 150, 152, 163, **165**, **167**, 187, **200**, 307, 310	-	Mouse	Female	B6C3F1/N	Gavage	92 d	91 d	Not specified	Thyroid gland	Adenoma- follicular cell	EIF2A EIF2AK2 ATF4 IFNA2 ABCC1	MYBL1 TGFI STAT1B STEAP1 DHRS	PCDH17 CKS1B AURKA ABCA1 TMEM4X	hsa05010 Alzheimer disease - Homo sapiens (human) (2) hsa:468 404374 ATF4; activating transcription factor 4 hsa:5610 416195 EIF2AK2; eukaryotic translation initiation factor 2 alpha kinase 2 hsa04141 Protein processing in endoplasmic reticulum - Homo sapiens (human) (2) hsa:468 404374 ATF4; activating transcription factor 4 hsa:5610 416195 EIF2AK2; eukaryotic translation initiation factor 2 alpha kinase 2 hsa05160 Hepatitis C - Homo sapiens (human) (2) hsa:3440 415414 IFNA2; interferon alpha 2 hsa:5610 416195 EIF2AK2; eukaryotic translation initiation factor 2 alpha kinase 2	-	mammary gland kidney all tumor bearing animals	urinary bladder liver	hematopoietic system	-
Nitrobenzene	98-95-3	C1=CC=CC(=C1)[N+](]O-])=O	인화성 액체 - 구분4 급성 독성(경구) - 구분4 급성 독성(경피) - 구분3 급성 독성(흡입: 증기) - 구분3 **발암성 - 구분2** 생식독성 - 구분2 특정표적장기 독성(반복 노출) - 구분1 만성 수생환경 유해성 - 구분3	**29**, **30**, 52, 53, 57, 67, 112, 131, **165**, **167**, **200**	Cancer slope factor: 4e-05 ug/m3-1 (carcinogenicity, oral) Carcinogenicity data available: IRIS-Likely to be carcinogenic to humans (Combined route) Genotoxicity Data: non-genotoxic	Mouse	Female	B6C3F1	Inhalation	107	107	Positive	Liver	Adenoma- hepatocellular	FAS FASL	CCR6 PDGFRL DSE OAS1 CCR7	CCR5 KRT34 EHHADH MGST1 SERPINB8		kidney thyroid gland spleen ear Zymbals gland skin hematopoietic system liver urinary bladder	**uterus** hematopoietic system clitoral gland kidney urinary bladder **lung** mammary gland ear Zymbals gland	thyroid gland vascular system kidney urinary bladder **lung** liver stomach small intestine	**ovary** vascular system hematopoietic system stomach urinary bladder liver thyroid gland peritoneal cavity small intestine	**Lung Neoplasms** **Adenoma** Bone Marrow Neoplasm Breast Neoplasm Carcinoma Carcinoma, Hepatocellular
Nitrobenzene	98-95-3					Mouse	Male	B6C3F1	Inhalation	107	107	Positive	Liver	Adenoma- hepatocellular									
Nitrobenzene	98-95-3					Rat	Female	Fischer 344	Inhalation	60	60	Not specified	Kidney	Multiple tumour types									
Nitrobenzene	98-95-3					Rat	Female	Fischer 344	Inhalation	107	107	Positive	Kidney	Multiple tumour types									
Nitrofen	1836-75-5	C1=CC=C(C)=C1)OC2=CC=C(C=C2[N+](]O-])=O)Cl)Cl	급성 독성(경구) - 구분4 **발암성 - 구분1A** 생식독성 - 구분1B 만성 수생환경 유해성 - 구분2	6, 8, 11, 14, 16, 18, 19, 21, 27, **29**, **30**, 34, 36, 37, 51, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 131, 150, 163, 165, 166, **167**, 187, **200**, 214, 220, 281, 307, 312, 318	Cancer slope factor: 2.3e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	78	91	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular	NKX2-1 SFTPB SFTPC FOXA2 SFTPA1	FABP4 CYP1A1 DSE OAS1 PDGFRL	SOD3 TINM22 CYTIP ITL EHHADH	hsa04950 Maturity onset diabetes of the young - Homo sapiens (human) (1) hsa:3170 408835 FOXA2; forkhead box A2 hsa04213 Longevity regulating pathway - multiple species - Homo sapiens (human) (1) hsa:3170 408835 FOXA2; forkhead box A2	thyroid gland liver kidney hematopoietic system	liver	vascular system liver stomach thyroid gland kidney	liver vascular system urinary bladder thyroid gland stomach	-
Nitrofen	1836-75-5					Mouse	Female	B6C3F1	Diet	78	92	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Nitrofen	1836-75-5					Mouse	Male	B6C3F1	Diet	78	91	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular									
Nitrofen	1836-75-5					Mouse	Male	B6C3F1	Diet	78	92	Positive	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Nitrosobenzthiazuron	51542-32-7	C1=CC2=C(C=C1[N]=C(S2)NC(=O)N(C)N=O)	-	-	-	Rat	Mixed	Wistar	Gavage	51	58	Positive	Forestomach	Carcinoma - squamous cell	-				large intestine skin stomach esophagus	all tumor bearing animals	urinary bladder kidney	hematopoietic system lung	-
Nitrosodiphenylamine	86-30-6	C2(N(N=O)C1=CC=CC=C1)=CC=CC=C2	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 특정표적장기 독성(1회 노출) - 구분2 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분2	8, 11, **29**, **30**, 34, 46, 52, 53, 57, 58, 60, 61, 67, 112, 131, **165**, **167**, **200**	Cancer slope factor: 2.6e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: inconclusive	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma	-				urinary bladder spleen thyroid gland oral cavity hematopoietic system vascular system nasal cavity ear Zymbals gland	urinary bladder **uterus** hematopoietic system nasal cavity	vascular system urinary bladder lung thyroid gland	**ovary** thyroid gland urinary bladder vascular system stomach	Cell Transformation, Neoplastic
Nitrosodiphenylamine	86-30-6					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Nitrosodiphenylamine	86-30-6					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
Nitrosodiphenylamine	86-30-6					Mouse	Female	B6C3F1	Diet	98	101	Not specified	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
N-Methyl-N'-bis(2-hydroxyethyl)-2-nitro-p-phenylenediamine	2784-94-3	[N+](]O-])=O)C=1C)=CC=C(C=1)N(CCO)CCO)NC	생식세포 변이원성 - 구분2 **발암성 - 구분2**	-	Cancer slope factor: 1.5e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	91	91	Positive	Liver	Adenoma- hepatocellular	-				skin	lung	thyroid gland kidney liver	liver hematopoietic system lung	-
N-Methyl-N'-bis(2-hydroxyethyl)-2-nitro-p-phenylenediamine	2784-94-3					Mouse	Female	B6C3F1	Diet	100	100	Positive	Liver	Adenoma- hepatocellular									
N-Methyl-N'-bis(2-hydroxyethyl)-2-nitro-p-phenylenediamine	2784-94-3					Mouse	Female	B6C3F1	Diet	38	100	Positive	Liver	Adenoma- hepatocellular									
N-Methyl-N'-bis(2-hydroxyethyl)-2-nitro-p-phenylenediamine	2784-94-3					Mouse	Female	B6C3F1	Diet	64	100	Positive	Liver	Adenoma- hepatocellular									
N-Methyl-N'-bis(2-hydroxyethyl)-2-nitro-p-phenylenediamine	2784-94-3					Mouse	Female	B6C3F1	Diet	91	91	Positive	Liver	Adenoma- hepatocellular									
N-Methyl-N'-bis(2-hydroxyethyl)-2-nitro-p-phenylenediamine	2784-94-3					Mouse	Female	B6C3F1	Diet	100	100	Positive	Liver	Adenoma- hepatocellular									
N-Methyl-N-nitrosobenzamide	6341-2-06-8	C(N(N=O)C)=O)C=1=C=C=C=C=1	-	-	-	Rat	Female	MRC-Wistar	Drinking water	52	130	Positive	Liver	Multiple tumour types	-				stomach oral cavity nasal cavity	all tumor bearing animals	lung kidney vascular system	lung hematopoietic system vascular system	-
N-Methyl-N-nitrosobenzamide	6341-2-06-8					Rat	Male	MRC-Wistar	Drinking water	52	130	Positive	Forestomach	Carcinoma - squamous cell									
N-Methyl-N-nitrosobenzenethanamine	13256-11-6	N(=O)N(CCC1=CC=CC=C1)C	-	-	-	Rat	Male	Fischer 344	Drinking water	32	127	Positive	Forestomach	Carcinoma- basal cell	-				stomach oral cavity esophagus nasal cavity liver vascular system	nasal cavity liver **uterus** lung vascular system	lung kidney stomach	lung	-
N-Methyl-N-nitrosobenzenethanamine	13256-11-6					Rat	Male	Fischer 344	Drinking water	104	127	Positive	Forestomach	Carcinoma- basal cell									
N-Methyl-p-nitro-N-nitrosoaniline	940-41-9	C1=CC=CC(=C1N(N=O)C)N=]=O)[O-]	-	8, 11, 21, **29**, **30**, 34, 36, 41, 52, 53, 57, 58, 60, 61, 67, 72, 112, 131, 150, 163, **165**, **167**, **200**, 310	-	Rat	Male	Fischer 344	Drinking water	50	114	Negative	Liver	Nodule- hyperplastic	-				esophagus thyroid gland liver	**uterus** liver hematopoietic system lung all tumor bearing animals	thyroid gland vascular system lung kidney	vascular system	-
N-Nitroso-2-phenylethylurea	777-79-7	C1=CC=CC=C1)CCN(N=O)C(=O)N				Syrian hamster	Female	Not specified	Gavage	20	75	Positive	Forestomach	Carcinoma									
N-Nitroso-2-phenylethylurea	777-79-7					Syrian hamster	Male	Not specified	Gavage	20	75	Positive	Forestomach	Carcinoma									
N-Nitrosochlordazepoxide	5175-17-4	C1(N(C(N=O)=N)C2=C(C1=[N+](]C1[O-])C2)=CC=CC=C2)C=CC=C2)Cl				Mouse	Female	ICR/Ha x BALB/cF1	Drinking water	73	106	Negative	Liver	Multiple tumour types					esophagus	all tumor bearing animals		-	-
N-Nitrosochlordazepoxide	5175-17-4					Mouse	Male	ICR/Ha x BALB/cF1	Drinking water	73	106	Negative	lung	Multiple tumour types									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
N-Nitrosoephedrine	17608-59-2	C1=CC=CC=C1[C]([N]=O)C(O)	-	-	-	Rat	Male	SD	Gavage	104	104	Positive	Forestomach	Carcinoma - squamous cell	-				stomach liver lung	uterus nasal cavity vascular system	kidney	-	-
N-Nitrosomethylphenidate	55017-03-4	C(C)(C)C1=O)C1NCCCC1(N=O)C2=CC=CC=C2	-	-	-	Mouse	Female	(C57BL/6 x B6AF1/J1)	Drinking water	73	106	Negative	Liver	Multiple tumour types	-				all tumor bearing animals	vascular system	stomach	-	-
N-Nitrosomethylphenidate	55017-03-4					Mouse	Male	(C57BL/6 x B6AF1/J1)	Drinking water	73	106	Negative	Liver	Multiple tumour types									
N-Nitroso-N-methyl-(2-tosyloxy)ethylamine	66398-63-8	O=S(=O)(C=1C=CC(=CC=1)C)OCCN([N]=O)C	-	-	-	Rat	Female	Fischer 344	Gavage	121	121	Positive	Liver	Carcinoma - hepatocellular	-				vascular system liver spleen oral cavity nasal cavity esophagus stomach lung large intestine	vascular system liver small intestine nasal cavity	-	-	-
N-Nitroso-N-methyl-(2-tosyloxy)ethylamine	66398-63-8					Rat	Male	Fischer 344	Gavage	121	121	Positive	Liver	Carcinoma - hepatocellular									
N-Nitroso-N-methylaniline	614-00-6	N([N]=O)c1=CC=CC=1)(C)=O	-	-	-	Rat	Female	Chester Beatty	Drinking water	67	67	Positive	Liver	Multiple tumour types	CYP2A13 **CYP2E1**	CCK1 CTSD1 B4GALT5 SRPK2 SPA17	TNNT1 CNTN1 SAT ITGA4 KIT14		esophagus all tumor bearing animals	uterus liver esophagus hematopoietic system all tumor bearing animals	lung vascular system	-	Carcinoma Esophageal Neoplasm
N-Nitroso-N-methylaniline	614-00-6					Rat	Male	Chester Beatty	Drinking water	60	60	Positive	Liver	Multiple tumour types									
N-Nitroso-N-methylaniline	614-00-6					Rat	Female	Fischer 344	Drinking water	50	114	Positive	Liver	Carcinoma									
N-Nitroso-N-methylaniline	614-00-6					Rat	Male	Fischer 344	Drinking water	50	114	Positive	Liver	Carcinoma									
N-Nitroso-N-methylaniline	614-00-6					Rat	Mixed	SD	Drinking water	104	104	Positive	Oesophagus	Multiple tumour types									
N-Nitrosopropoxur	38777-13-8	C1=CC=C(C(=C1)OC(N)N=O)C(=O)OC(C)C	-	-	-	Rat	Male	SD	Gavage	31	90	Positive	Forestomach	Carcinoma	-				stomach nasal cavity vascular system esophagus	nasal cavity vascular system stomach oral cavity small intestine	-	-	-
Nonabromodiphenyl	27753-52-2	C1=C(C(=C(C(=C1Br)Br)Br)Br)C=2C(=C(C=C(C=2Br)Br)Br)Br	-	-	-	Mouse	Female	B6C3F1	Diet	78	78	Positive	Liver	Carcinoma - hepatocellular	-				liver large intestine kidney urinary bladder Mahoni head cancers	liver kidney urinary bladder	liver stomach lung	liver stomach lung	-
Nonabromodiphenyl	27753-52-2					Mouse	Male	B6C3F1	Diet	78	78	Positive	Liver	Carcinoma - hepatocellular									
Nonoxynol	26027-38-3	C1=C(C=CC(=C1)OCCOCCOCCO)C(CCCCCCCCC	만성 수생환경 유해성 - 구분3	7, 8, 11, 19, 23, 25, **29, 30**, 34, 44, 46, 52, 53, 58, 60, 61, 62, 67, 111, 112, 117, 122, 123, 148, 150, 153, **160, 167, 187**, 200, 207	-	Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Carcinoma - hepatocellular	CXCL8 IL1A IL1B TLR4	-	-	hsa04010 MAPK signaling pathway - Homo sapiens (human) (2) hsa:3552 K04283 IL1A; interleukin 1 alpha hsa:3553 K04519 IL1B; interleukin 1 beta hsa04940 Type I diabetes mellitus - Homo sapiens (human) (2) hsa:3552 K04283 IL1A; interleukin 1 alpha hsa:3553 K04519 IL1B; interleukin 1 beta hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa:3552 K04283 IL1A; interleukin 1 alpha hsa:3553 K04519 IL1B; interleukin 1 beta	hematopoietic system urinary bladder nasal cavity stomach	ear Zymbals gland stomach	kidney lung thyroid gland liver	lung
Nonoxynol	26027-38-3					Rat	Female	Fischer 344/DuCrl	Diet	52	52	Negative	Liver	Multiple tumour types									
Nonoxynol	26027-38-3					Rat	Female	Fischer 344/DuCrl	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Noramincophenazone methanesulphonate sodium salt	68-89-3	[Na+].[O-]S(=O)(=O)N(C)C2=C(N(N(C1=CC=CC=C1)C2=O)C)C(=O)[O-]	자료없음	**29, 30**, 52, 53, 67, 112, **165, 167, 200**	-	Mouse	Female	B6C3F1	Drinking water	75	86	Positive	Liver	Carcinoma - hepatocellular						-		-	-
Noramincophenazone methanesulphonate sodium salt	68-89-3					Mouse	Male	B6C3F1	Drinking water	77	86	Positive	Liver	Multiple tumour types									
Noramincophenazone methanesulphonate sodium salt	68-89-3					Rat	Male	Fischer 344/DuCrl	Drinking water	72	83	Not specified	Kidney	Multiple tumour types									
Noramincophenazone methanesulphonate sodium salt	68-89-3					Rat	Female	Wistar	Diet	104	130	Negative	Liver	Adenoma									
Noramincophenazone methanesulphonate sodium salt	68-89-3					Rat	Male	Wistar	Diet	104	130	Negative	Liver	Adenoma									
Norphenazone	89-25-8	N1(N(=C)CC1=O)C(C)=2=CC=CC=C2	만성 수생환경 유해성 - 구분3	8, 11, 14, 21, 28, 34, 34, 41, 43, 57, 58, 60, 63, 64, 66, 71, 72, 100, 101, 102, 103, 131, 150, 163, 177, 214, 310, 318	Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6C3F1	Diet	102	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	IL1B TNF NOS2 IL6 NGF	HRPD	TMEM40 UCT2B15	hsa05010 Alzheimer disease - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa05133 Pertussis - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor	spleen	all tumor bearing animals	urinary bladder	-	-
Norphenazone	89-25-8					Mouse	Male	B6C3F1	Diet	102	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Norphenazone	89-25-8					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Norphenazone	89-25-8					Rat	Male	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
N-Phenyl-1,4-benzenediamine monohydrochloride	2198-59-6	N(C=1C=CC(N)=CC=1)(C=2C=CC=CC=2)Cl	자료없음	19, 23, 46, 61, 111, 117, 187, 207	-	Mouse	Female	B6C3F1	Diet	48	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				spleen liver thyroid gland ovary Zymbals gland all tumor bearing animals	uterus thyroid gland urinary bladder ear Zymbals gland hematopoietic system clitoral gland lung kidney	thyroid gland urinary bladder liver vascular system	thyroid gland urinary bladder vascular system liver hematopoietic system **ovary**	-
N-Phenyl-1,4-benzenediamine monohydrochloride	2198-59-6					Mouse	Male	B6C3F1	Diet	48	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
N-Phenyl-1,4-benzenediamine monohydrochloride	2198-59-6					Rat	Female	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
N-Phenyl-1,4-benzenediamine monohydrochloride	2198-59-6					Rat	Male	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
N-Phenyl-2-naphthalenamine	135-88-6	N(C=1C=C(C)C=CC=1)C=2C=CC=C(C)C=2	생식세포변이성 발암성 - 구분2 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2A/2B 피부 과민성 - 구분1(A/B) **발암성 - 구분2** 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 19, 21, 23, 25, 28, **29**, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 63, 67, 72, 100, 101, 102, 103, 111, 112, 117, 122, 123, 131, 150, 153, 163, **165, 167**, 177, 187, **200**, 207, 310	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma	-				liver spleen ear Zymbals gland thyroid gland	ear Zymbals gland urinary bladder **uterus** hematopoietic system thyroid gland clitoral gland	urinary bladder liver thyroid gland vascular system	urinary bladder thyroid gland **ovary** liver vascular system stomach pituitary gland hematopoietic system	-
N-Phenyl-2-naphthalenamine	135-88-6					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
N-Phenyl-2-naphthalenamine	135-88-6					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
N-Phenyl-2-naphthalenamine	135-88-6					Mouse	Female	B6C3F1	Diet	102	104	Not specified	Kidney	Adenocarcinoma - tubular | Adenomatous									
N-Phenyl-2-naphthalenamine	135-88-6					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Not specified	Liver	Hepatoma									
N-Phenyl-2-naphthalenamine	135-88-6					Mouse	Male	B6C3F1	Diet	102	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Ochratoxin A	303-47-9	[C@H]1(OC(=O)c2=C(O)c=CC=c(Cl)c2)C(=O)N[C@H](C(=O)O)CC(=CC=C(C)C=1)C	급성 독성(경구) - 구분2 **발암성 - 구분1B** 생식독성 - 구분1B 특정표적장기 독성(반복 노출) - 구분2 특정표적장기 독성(반복 노출) - 구분2 만성 수생환경 유해성 - 구분4	-	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	104	104	Positive	Kidney	Multiple tumour types	CASP3 NFKB2 BCL2 CASP9 BAX	SHC1 AKRC13 TIRAP RHOB HSPA5	SOD3 CGREF NDUFB2 NQO1 CYP286	hsa05170 Human immunodeficiency virus 1 infection - Homo sapiens (human) (3) hsa:596 K02161 BCL2; BCL2 apoptosis regulator hsa:842 K04399 CASP9; caspase 9 hsa:983 K02087 CDK1; cyclin dependent kinase 1 hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa:4780 K05638 NFE2L2; NFE2 like bZIP transcription factor 2 hsa:596 K02161 BCL2; BCL2 apoptosis regulator hsa:842 K04399 CASP9; caspase 9 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (3) hsa:4780 K05638 NFE2L2; NFE2 like bZIP transcription factor 2 hsa:596 K02161 BCL2; BCL2 apoptosis regulator hsa:842 K04399 CASP9; caspase 9	kidney urinary bladder	kidney **mammary gland**	kidney	**liver**	Breast Neoplasms Carcinoma Cell Transformation, Neoplastic Mammary Neoplasm, Experimental Precancerous Conditions Liver Neoplasms Adenoma
Ochratoxin A	303-47-9					Mouse	Male	B6C3F1	Diet	104	104	Positive	Kidney	Adenoma									
Ochratoxin A	303-47-9					Rat	Female	DA	Gavage	110	110	Negative	Liver	Multiple tumour types									
Ochratoxin A	303-47-9					Rat	Male	DA	Gavage	110	110	Positive	Kidney	Adenocarcinoma									
Oestradiol	50-28-2	C1=C(C=C2C(=C1)[C@]3([C@]([C@H](C2)[C@@H](C[C@](C[C@H](C[C@H](C[C@H](C[C@H])O)O)O)O)O)O)O	**발암성 - 구분1A** 생식독성 - 구분1B 특정표적장기 독성(1회 노출) - 구분1 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 14, 19, 23, 27, **28, 30**, 34, 34, 46, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 111, 112, 117, 122, 163, **165, 167, 187, 200**, 204, 302, 318	Cancer slope factor: 0.011 (ug/m3)-1 (Genotoxicity, Inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	C3H (MTV+)	Diet	104	104	Not specified	Mammary gland	Adenocarcinoma	ESR1 ESR2 PGR EGF	BPRM PRRM1 PLEC LYCAM SRP27	KIT5A GRIA1 TFF3 OSPM1 PDS5B	hsa05224 Breast cancer - Homo sapiens (human) (8) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2 hsa:5241 K08556 PGR; progesterone receptor hsa04915 Estrogen signaling pathway - Homo sapiens (human) (3) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2 hsa:5241 K08556 PGR; progesterone receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (3) hsa:2099 K08550 ESR1; estrogen receptor 1 hsa:2100 K08551 ESR2; estrogen receptor 2 hsa:5241 K08556 PGR; progesterone receptor	-	liver ear Zymbals gland	stomach lung	pituitary gland hematopoietic system stomach lung	Mammary Neoplasm, Animal Polycystic Ovary Syndrome Cell Transformation, Neoplastic Ovarian Neoplasm Breast Neoplasm
Oestradiol	50-28-2					Mouse	Female	C3H/He1 (MTV-)	Diet	78	78	Not specified	**Ovary**	Adenoma - tubular									
Oestradiol	50-28-2					Mouse	Female	C3H/He1 (MTV-)	Diet	104	104	Not specified	Mammary gland	Adenocarcinoma									

Chemical Name	CAS No.	SMILES	GHS Classific	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Oestradiol	50-28-2					Mouse	Female	C3H/He/ MTV(+)	Diet	52	52	Not specified	Mammary gland	Adenocarcinoma									
Oestradiol mustard	22966-79-6	C1[n+](C(=O)C=C1)C(C)(BCl)CC(=O)CC(=O)C=C(C)C(=O)[N][C@](C)([C@H]([C@H]([C@H]

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Parathion	56-38-2					Rat	Male	Osborne-Mendel	Diet	80	112	Not specified	Adrenal gland	Adenoma - cortical									
p-Carboxaphenylhydroxine hydrochloride	24589-77-3	C1=C(C=CC(=C1)C(C(=O)NNC))	-	-	-	Mouse	Female	Swiss	Drinking water	121	121	Positive	Large arteries	leiomyoma	-				spleen	kidney hematopoietic system mammary gland clitoral gland	lung vascular system	hematopoietic system lung stomach liver	-
p-Carboxaphenylhydroxine hydrochloride	24589-77-3					Mouse	Male	Swiss	Drinking water	120	120	Positive	Large arteries	leiomyoma									
p-Chloroaniline hydrochloride	20265-96-7	C[N]c1CC=C(C)C(C=C1.Cl	-	7, 21, 26, **28, 30**, 34, 36, 41, 52, 53, 57, 58, 61, 67, 72, 112, 122, 123, 131, 150, 163, **165, 166, 167, 200**, 310	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Gavage	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				thyroid gland spleen ear Zymbals gland liver kidney urinary bladder	urinary bladder thyroid gland **uterus** liver ear Zymbals gland lung hematopoietic system kidney clitoral gland	liver vascular system urinary bladder thyroid gland lung	thyroid gland liver urinary bladder vascular system hematopoietic system lung	-
p-Chloroaniline hydrochloride	20265-96-7					Mouse	Male	B6C3F1	Gavage	102	105	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
p-Chloroaniline hydrochloride	20265-96-7					Rat	Female	Fischer 344	Gavage	103	105	Not specified	Adrenal gland medulla	Pheochromocytomabenign									
p-Chloroaniline hydrochloride	20265-96-7					Rat	Male	Fischer 344	Gavage	103	105	Positive	Adrenal gland medulla	Pheochromocytomabenign | Pheochromocytoma- benign- bilateral									
Pemoline magnesium hydroxide	18968-99-5	C1=CC=CC2=C1(C2C(N(=O)Mg)(O)O	-	-	-	Rat	Female	SD	Diet	46	66	Not specified	Liver	Multiple tumour types	-				stomach thyroid gland spleen oral cavity ear Zymbals gland urinary bladder	stomach kidney **uterus** hematopoietic system ear Zymbals gland lung urinary bladder mammary gland	stomach urinary bladder vascular system thyroid gland lung	stomach hematopoietic system urinary bladder thyroid gland **ovary** vascular system lung liver	-
Pemoline magnesium hydroxide	18968-99-5					Rat	Female	SD	Diet	46	66	Not specified	Liver	Multiple tumour types									
Penicillin V potassium	132-98-9	C)C(=O)[H]1C(C)(C)S[C@@]2[C@@H](C(=O)N1)N(C)C(=O)C(=C2)c1ccc(Br)cc1	자료없음	46, 61	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Gavage	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-								
Penicillin V potassium	132-98-9					Mouse	Male	B6C3F1	Gavage	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Penicillin V potassium	132-98-9					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Clitoral gland	Adenoma									
Penicillin V potassium	132-98-9					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Pentabromodiphenyl ether	32534-81-9	C1(=C(C(=C(C)=C(Br)c)c)c)Oc2c(Br)cc(Br)cc2Br	생식독성 : 수컷독성 특정표적장기 독성(반복 노출) : 구분2 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	21, 27, **29, 30**, 41, 52, 53, 57, 61, 67, 112, 131, 150, **165, 167, 200**, 310	Carcinogenicity data available: IRIS-D (Not classifiable as to human carcinogenicity)	Mouse	Female	B6C3F1/N	Gavage	93 d	91 d	Not specified			CYP1A1 CYP3A22-3A1 TTR CXCL8 CYP2B1	ERNA3 CDKN2B BAGAL75 RBM12 SRGAP1	CYP1A2 CYP3A4 C1QBG6 DIO1 STGALA1		liver large intestine urinary bladder kidney thyroid gland	liver kidney urinary bladder thyroid gland	liver stomach lung	liver stomach thyroid gland urinary bladder lung pituitary gland **ovary**	-
Pentachlorobenzene	608-93-5	C=1(C(=C(C(=C(C=1)Cl)Cl)Cl)Cl)Cl	인화성 고체 : 구분2 급성 독성(경구) : 구분4 생식독성 : 구분2 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, **29, 30**, 52, 53, 58, 60, 67, 107, 112, **165, 167, 200**	Carcinogenicity data available: IRIS-D (Not classifiable as to human carcinogenicity) Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1/N	Diet	92 d	91 d	Not specified			**CYP2E1** CYP11A1 GSTP1 AHR COMT	FABP4 AIRN7 CADPS2 CCDC49 FNIP2	BGL FAM171A1 HSPA12A UM2 MAPK7IP3		thyroid gland oral cavity hematopoietic system kidney nasal cavity ear Zymbals gland liver Maltoni head-cancers lung	liver kidney thyroid gland lung hematopoietic system **uterus** nasal cavity urinary bladder	liver vascular system small intestine	thyroid gland liver urinary bladder vascular system peritoneal cavity pituitary gland **ovary** small intestine stomach	-
Pentachloroanisole	1825-21-4	C(c(c(C(=C(C)=C)c)c)Cl)Cl)C(C)Cl)Cl	급성 독성(경구) : 구분2	8, 11, **29, 30**, 52, 53, 60, 61, 67, 112, **165, 167, 200**	-	Mouse	Female	B6C3F1/N	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	DIO2 DIO3 DNH THRAA THRB	NIR4 FABP4 VTN ACSL3 IRS7	ERCC3 MGST1 GATA1 SOD3 PC8		kidney hematopoietic system nasal cavity ear Zymbals gland thyroid gland stomach urinary bladder oral cavity	kidney hematopoietic system urinary bladder liver **uterus** nasal cavity stomach	vascular system liver urinary bladder	urinary bladder liver vascular system thyroid gland peritoneal cavity	-
Pentachloroanisole	1825-21-4					Mouse	Male	B6C3F1/N	Gavage	103	104	Positive	Adrenal gland medulla	Pheochromocytomabenign									
Pentachloroanisole	1825-21-4					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Adrenal gland medulla	Pheochromocytomabenign									
Pentachloroanisole	1825-21-4					Rat	Male	Fischer 344	Gavage	103	104	Positive	Adrenal gland medulla	Pheochromocytomabenign									
Pentachloronitrobenzene	82-68-8	C(c(c(C(=C(C)=C)c)Cl)C)C)C)Cl)(N+](O-])=O	급성 독성(경구) : 구분4 피부 과민성 : 구분1A(사람) 특정표적장기 독성(반복 노출) : 구분2 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 14, 16, **29, 30**, 34, 36, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 107, 112, 122, 123, 131, 150, 163, **165, 167, 200**, 214, 220, 281, 312, 318	Carcinogenicity data available: EPA: OPP-Group C Possible Human Carcinogen Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6AKF1	Gavage (pmewaring) then diet	77	77	Not specified	Liver	Hepatoma	NFE2L2 ACSM1 CES1 EPHX1	PDGFRL CAS1 CYP11A1 DSE CCS7	MGST1 EHHADH GSDB1 SOD3 CYP3F		thyroid gland kidney ear Zymbals gland liver lung nasal cavity oral cavity	kidney hematopoietic system **uterus** lung liver clitoral gland urinary bladder thyroid gland	liver vascular system thyroid gland kidney	vascular system **ovary** liver urinary bladder thyroid gland stomach	-
Pentachloronitrobenzene	82-68-8					Mouse	Male	B6AKF1	Gavage (pmewaring) then diet	77	77	Positive	Liver	Hepatoma									
Pentachloronitrobenzene	82-68-8					Mouse	Female	B6C3F1	Gavage (pmewaring) then diet	77	77	Not specified	Liver	Hepatoma									
Pentachloronitrobenzene	82-68-8					Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Pentachloronitrobenzene	82-68-8					Mouse	Female	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma- hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Pentachlorophenol	87-86-5	C1(=C(C(=C(C)=C)Cl)Cl)C(Cl)Cl)Cl	급성 독성(경구) : 구분2 급성 독성(경피) : 구분3 급성 독성(흡입: 분진/미스트) : 구분2 피부 부식성/자극성 자극성 : 구분2 심한 눈 손상/눈 자극성 : 구분2A(사람) **발암성 : 구분2** 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	6, 7, 8, 11, 14, 18, 19, 21, 26, 27, 28, **29, 30**, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 131, 140, 150, 153, 163, **165, 166, 167, 187, 200**, 214, 220, 307, 310, 318	Cancer slope factor: 4.6e-06 ug/m3-1 (carcinogenicity, oral) Carcinogenicity data available: IRIS-Likely to be carcinogenic to humans Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (pmewaring) then diet	76	76	Negative	Liver	Hepatoma	IL1B CASP3 HMGB1 HSPA1A IL6 JUNP	CYP11A1 MMP4 PLSCR4 PCDLCE2 XIRBAP	ERCC3 PC8 VANIN ABHD2 CDY15		hsa05134 Legionellosis - Homo sapiens (human) (3) hsa:3303 K03283 HSPA1A; heat shock protein family A (Hsp70) member 1A hsa:3569 K05405 IL6; interleukin 6 hsa:836 K02187 CASP3; caspase 3 hsa05020 Prion disease - Homo sapiens (human) (3) hsa:3303 K03283 HSPA1A; heat shock protein family A (Hsp70) member 1A hsa:3569 K05405 IL6; interleukin 6 hsa:836 K02187 CASP3; caspase 3 hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (3) hsa:3303 K03283 HSPA1A; heat shock protein family A (Hsp70) member 1A hsa:3569 K05405 IL6; interleukin 6 hsa:836 K02187 CASP3; caspase 3	nasal cavity hematopoietic system thyroid gland kidney oral cavity urinary bladder	liver kidney hematopoietic system thyroid gland	liver vascular system	liver vascular system thyroid gland **ovary** pituitary gland urinary bladder	**Carcinoma, Hepatocellular** **Liver Neoplasm** Leukemia, Myeloid, Acute Adrenal Gland Neoplasm Adenoma, Liver Cell
Pentachlorophenol	87-86-5					Mouse	Male	B6AKF1	Gavage (pmewaring) then diet	76	76	Negative	Liver	Multiple tumour types									
Pentachlorophenol	87-86-5					Mouse	Female	B6C3F1	Gavage (pmewaring) then diet	76	76	Negative	Liver	Hepatoma									
Pentachlorophenol	87-86-5					Mouse	Female	B6C3F1	Diet	103	105	Positive	Adrenal gland medulla	Pheochromocytomabenign | Pheochromocytoma- benign- bilateral									
Pentachlorophenol	87-86-5					Mouse	Female	B6C3F1	Diet	102	105	Positive	Liver	Adenoma- hepatocellular | Carcinomahepatocellular									
Pentachlorophenol	87-86-5					Mouse	Male	B6C3F1	Gavage (pmewaring) then diet	76	76	Negative	Liver	Hepatoma									
Pentachlorophenol	87-86-5					Mouse	Male	B6C3F1	Diet	103	105	Positive	Adrenal gland medulla	Pheochromocytomabenign | Pheochromocytoma- benign- bilateral									
Pentachlorophenol	87-86-5					Mouse	Male	B6C3F1	Diet	103	105	Positive	Adrenal gland medulla	Pheochromocytomabenign | Pheochromocytoma- benign- bilateral									
Phenacetin	62-44-2	C1=C(C=CC(=C1N(C)C(=O)CC	급성 독성(경구) : 구분4 생식세포 변이원성 : 구분2 **발암성 : 구분1A** 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2	-	Cancer slope factor: 6.3e-07 (ug/m3)-1 (carcinogenicity) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	96	104	Positive	Liver	Carcinoma- hepatocellular	CYP1A2 CYP3A1 PTGS1 AADAC CYP7A	ALDH1BA1 CSQBG40 HMPD GUP1 AIM1	CEP72 CDY15 EUOV13 GAL3ST3 GCOM1		hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:5742 K00509 PTGS1; prostaglandin-endoperoxide synthase 1 hsa04726 Serotonergic synapse - Homo sapiens (human) (1) hsa:5742 K00509 PTGS1; prostaglandin-endoperoxide synthase 1 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (1) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1	urinary bladder kidney nasal cavity stomach skin	urinary bladder ear Zymbals gland nasal cavity mammary gland stomach small intestine	thyroid gland kidney urinary bladder liver	urinary bladder liver	Carcinoma, Renal Cell Urinary Bladder Neoplasm Kidney Neoplasm Carcinoma, Transitional Cell Ureteral Neoplasm Urologic Neoplasm
Phenacetin	62-44-2					Mouse	Male	B6C3F1	Diet	96	104	Positive	Kidney	Adenoma- renal cell									
Phenacetin	62-44-2					Mouse	Female	C57BL/6	Diet	77	77	Negative	Liver	Multiple tumour types									
Phenacetin	62-44-2					Mouse	Male	C57BL/6	Diet	77	77	Negative	Liver	Nodule- hyperplastic									
Phenacetin	62-44-2					Rat	Female	SD	Diet	110	110	Positive	Eye canal	Carcinoma- squamous cell									
Phenazone	60-80-0	C=1(N(N(C(C=1)=O)C)=CC=CC=C2)C)C	급성 독성(경구) : 구분4 특정표적장기 독성(반복 노출) : 구분2	8, 11, 60	Genotoxicity Data: non-genotoxic	Rat	Male	SD	Diet	114	114	Positive	Liver	Cholangioma - cystic	IL1B TNF NOS2 IL6 NGF	SLC15A1 ALDH1BA1 HMPD TOB1 NGF	TMS4B4X DIAPH3 LST1 C10ORF118 SAT		hsa05133 Pertussis - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa05142 Chagas disease - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor hsa05146 Amoebiasis - Homo sapiens (human) (3) hsa:3569 K05405 IL6; interleukin 6 hsa:4843 K13241 NOS2; nitric oxide synthase 2 hsa:7124 K03156 TNF; tumor necrosis factor	urinary bladder kidney oral cavity	small intestine all tumor bearing animals	-	-	Carcinoma Urinary Bladder Neoplasm Kidney Neoplasm
Phenazone	60-80-0					Rat	Male	SD	Diet	88	88	Not specified	Liver	Multiple tumour types									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Phenazopyridine hydrochloride	136-40-3	N1=C(C=CC(=C1N)N(C=N)C=N)C=CC=C(C=C2)NC1	경성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(사) **발암성 : 구분1B**	6, 8, 14, 18, 19, 21, 23, 27, **29**, **30**, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 107, 111, 112, 117, 122, 123, 131, 148, 150, 163, 165, 166, **167**, 187, **200**, 214, 220, 307, 310, 318	Cancer slope factor: 4.3e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	80	105	Positive	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic	-				spleen ear Zymbals gland large intestine liver vascular system urinary bladder	ear Zymbals gland small intestine liver urinary bladder kidney clitoral gland **uterus** hematopoietic system lung	liver vascular system thyroid gland urinary bladder	liver vascular system thyroid gland urinary bladder	-
Phenazopyridine hydrochloride	136-40-3					Mouse	Male	B6C3F1	Diet	80	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic									
Phenazopyridine hydrochloride	136-40-3					Rat	Female	Fischer 344	Diet	78	105	Positive	Colon	Adenocarcinoma									
Phenazopyridine hydrochloride	136-40-3					Rat	Male	Fischer 344	Diet	78	104	Positive		Colon : Adenocarcinoma | Adenoma Rectum : Adenocarcinoma									
Phenelzine hydrogen sulphate	156-51-4	C(CC1=CC=CC=C1)NN.OS(O)(=O)=O	경성 독성(경구) : 구분3 생식세포 변이원성 : 구분2	21, 29, **30**, 41, 52, 53, 57, 61, 67, 112, 117, 150, **166**, **167**, **200**, 310	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	Swiss	Drinking water	93	93	Positive	Blood vessel	Angiosarcoma	-			-					-
Phenelzine hydrogen sulphate	156-51-4					Mouse	Male	Swiss	Drinking water	99	99	Negative	Liver	Multiple tumour types									
Phenesterine	3546-10-9	[C@H](C[C@]4[H])([C@]([C@]([C@]5[C@]([C@]([C@H]([C]1=[C]([C@]([C@]([C]2[H])[C@]([C]3[H])([C]([C]([C]

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Phenothiazine	92-84-2	N(1)C(c2)C(=z)C(=y)C=xC=wC=vC=uC=tC=s1	경구 독성(분말) : 구분4 피부 과민성 : 구분1(A/1B) 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분3	8, 11, 27, 29, 30, 34, 36, 52, 53, 57, 58, 60, 61, 67, 72, 107, 112, 131, 148, 163, 165, 167, 200	Carcinogenicity data available: PPRTV (ORNL) - Inadequate for an assessment of carcinogenic potential Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma	AR ESR1 NR1I2 Estrogen ARL1	CRH TMEM74A CCNC TIMP TAGLN	FNDC4 SCSDL WFF1 HMGCS1 HPN	hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2099 KO05132 ESR1: estrogen receptor 1 hsa5468 KO06130 PPARG: peroxisome proliferator activated receptor gamma hsa05205 Proteoglycans in cancer - Homo sapiens (human) (1) hsa2099 KO05132 ESR1: estrogen receptor 1 hsa05216 Thyroid cancer - Homo sapiens (human) (1) hsa5468 KO06130 PPARG: peroxisome proliferator activated receptor gamma	spleen thyroid gland hematopoietic system ear Zymbals gland all tumor bearing animals	all tumor bearing animals	thyroid gland **urinary bladder**	thyroid gland **urinary bladder** stomach	Urinary Bladder Neoplasm
Phenothiazine	92-84-2					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenothiazine	92-84-2					Mouse	Female	B6C3F1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenothiazine	92-84-2					Mouse	Male	B6C3F1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenoxybenzamine hydrochloride	63-92-3	N(CC(c1c(CC(c2C(=O)C(=z)C=vCC(=tC(=s2)C)C)C)C)C)	경구 독성(분말) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 발암성 : 구분1B 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2 만성 수생환경 유해성 : 구분1	7, 14, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 112, 122, 123, 152, 163, 165, 167, 200, 214, 318	Cancer slope factor: 030077 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Intraperitoneal	52	84	Positive	Abdominal cavity	Sarcoma	NR1I3 SLC22A2 CALCA ADRA1A GAL	FOS1 B4GALT5	TNNT1	hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (2) hsa148 KO4125 ADRA1A: adrenoceptor alpha 1A hsa796 K12332 CALCA: calcitonin related polypeptide alpha hsa04270 Vascular smooth muscle contraction - Homo sapiens (human) (2) hsa148 KO4125 ADRA1A: adrenoceptor alpha 1A hsa796 K12332 CALCA: calcitonin related polypeptide alpha hsa04970 Salivary secretion - Homo sapiens (human) (1) hsa148 KO4125 ADRA1A: adrenoceptor alpha 1A	all tumor bearing animals	kidney ear Zymbals gland nasal cavity stomach all tumor bearing animals	kidney stomach	hematopoietic system lung **urinary bladder**	Urinary Bladder Neoplasm Carcinoma, Small Cell Leukemia, Lymphocytic, Chronic, B-Cell Neoplasm, Squamouse Cell Sarcoma, Experimental
Phenoxybenzamine hydrochloride	63-92-3					Mouse	Male	B6C3F1	Intraperitoneal	51	83	Positive	Abdominal cavity	Sarcoma									
Phenoxybenzamine hydrochloride	63-92-3					Rat	Female	SD	Intraperitoneal	52	83	Positive	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic									
Phenoxybenzamine hydrochloride	63-92-3					Rat	Male	SD	Intraperitoneal	52	83	Positive	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic									
Phenyl glycidyl ether	122-60-1	C1(c2C(c3C(c4C(O)CC)CO))	경구 독성(증기) : 구분2 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 피부 과민성 : 구분1(A/1B) 발암성 : 구분1B 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 만성 수생환경 유해성 : 구분3	-	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Rat	Female	SD	Inhalation	104	104	Positive	Nasal cavity	Carcinoma - epidermoid	NFE2L2 AKR1C2	TBX15 IL1R1 FGMS11 AKC4.13 ABCC13	FNDC4 WBFI1 SERPINA2 GDF03 HPN		stomach nasal cavity hematopoietic system thyroid gland	stomach nasal cavity	stomach kidney	stomach pituitary gland peritoneal cavity	-
Phenyl glycidyl ether	122-60-1					Rat	Male	SD	Inhalation	104	104	Positive	Nasal cavity	Multiple tumour types									
Phenyl isothiocyanate	103-72-0	C1(=CC=CC=c1)N(=c=S	분말 : 구분3 경구 독성(분말) : 구분4 만성 수생환경 유해성 : 구분1	61	Carcinogenicity data available: PPRTV (ORNL) - Inadequate for an assessment of carcinogenic potential Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Haemangioma	-				spleen thyroid gland ear Zymbals gland Mathoni head cancers	thyroid gland **uterus** clitoral gland urinary bladder	thyroid gland urinary bladder vascular system	thyroid gland urinary bladder vascular system	-
Phenyl isothiocyanate	103-72-0					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenyl isothiocyanate	103-72-0					Mouse	Female	B6C3F1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenyl isothiocyanate	103-72-0					Mouse	Male	B6C3F1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenylbutazone	50-33-9	C1(=CC=c2C(=c1)N(N(C2=o)C(=o)C(C)C)c3c(O)CCCC)=O	경구 독성(분말) : 구분3 경구 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 29, 30, 34, 36, 52, 53, 58, 60, 61, 67, 72, 112, 163, 165, 167, 200	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic	TNF CYP1A4 ABCC1 CSTP1 SOD1 UGT1A8	SRBB2 ABCC5 NADK SMARCC1 NS2	CYP2A4 TNNT1 PPP1CB LZIA FAM49A	hsa00983 Drug metabolism - other enzymes - Homo sapiens (human) (2) hsa1576 K17689 CYP1A4: cytochrome P450 family 1 subfamily A member 4 hsa2950 K23790 GSTP1: glutathione S-transferase pi 1 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (2) hsa1576 K17689 CYP1A4: cytochrome P450 family 1 subfamily A member 4 hsa2950 K23790 GSTP1: glutathione S-transferase pi 1 hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1576 K17689 CYP1A4: cytochrome P450 family 1 subfamily A member 4 hsa2950 K23790 GSTP1: glutathione S-transferase pi 1	-	kidney ear Zymbals gland **uterus**	liver	lung	Urinary Bladder Neoplasm Carcinoma Papilloma Kidney Neoplasm **Liver Neoplasm** Leukemia, Myeloid, Acute
Phenylbutazone	50-33-9					Mouse	Male	B6C3F1	Gavage	103	104	Positive	Liver	Adenoma- hepatocellular									
Phenylbutazone	50-33-9					Rat	Female	Donryu	Diet	104	110	Negative	Adrenal gland	Pheochromocytoma									
Phenylbutazone	50-33-9					Rat	Male	Donryu	Diet	104	110	Negative	Kidney	Multiple tumour types									
Phenylbutazone	50-33-9					Rat	Female	Fischer 344	Gavage	103	105	Positive	Kidney	Carcinoma, transitional cell									
Phenylbutazone	50-33-9					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Kidney	Adenoma- renal tubule- bilateral | Adenoma, tubular									
Phenylethyl-3-methylsiloxane	71835-85-9	C1(=C(c2C=c3C(C(O)C(C=c2)=c3)=C(c4C(C(O)C(O)=c4)=O				Rat	Male	Fischer 344	Diet	55	55	Negative	Colon	Multiple tumour types									
Phenylhydrazine	100-63-0	N(N(C=1C=CC=CC=1	인화성 액체 : 구분4 경구 독성(분말) : 구분3 경구 독성(캡슐) : 구분2 경구 독성(캡슐 증가) : 구분1 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 피부 과민성 : 구분1(A/1B) 생식세포 변이원성 : 구분2 발암성 : 구분1B 생식독성 : 구분2 특정표적장기 독성(반복 노출) : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 14, 19, 25, 27, 29, 30, 34, 36, 41, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 117, 131, 150, 152, 163, 167, 187, 192, 200, 214, 217, 218, 318	Carcinogenicity data available: NIOSH-potential occupational carcinogen Genotoxicity Data: genotoxic	Mouse	Female	Swiss	Gavage	39	55	Negative	lung	Multiple tumour types	CCND1 GPT SOD1 Estrogen HMOX1	CCNC MTTH MMOSC DNAH10 TEP1	SAT HTATIP2 CTORF63 ARF1A1 VASN	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa2875 K00814 GPT: glutamic-pyruvic transaminase hsa5743 K11987 PTGS2: prostaglandin-endoperoxide synthase 2 hsa05222 Small cell lung cancer - Homo sapiens (human) (2) hsa4609 K04077 MYC: MYC proto-oncogene, bHLH transcription factor hsa5743 K11987 PTGS2: prostaglandin-endoperoxide synthase 2 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa4609 K04077 MYC: MYC proto-oncogene, bHLH transcription factor hsa5743 K11987 PTGS2: prostaglandin-endoperoxide synthase 2	ear Zymbals gland spleen all tumors bearing animals	mammary gland hematopoietic system kidney **uterus** thyroid gland	lung vascular system urinary bladder stomach	hematopoietic system lung stomach vascular system thyroid gland urinary bladder **ovary** liver	-
Phenylhydrazine hydrochloride	59-88-1	N(N(C=1C=CC=CC=1.Cl	피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 피부 과민성 : 구분1(A/1B) 생식세포 변이원성 : 구분2 발암성 : 구분1B 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극)	14, 25, 29, 30, 41, 52, 53, 57, 64, 66, 67, 71, 112, 131, 150, 165, 167, 200, 214, 310, 318	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	Swiss	Drinking water	112	112	Positive	Blood vessel	Angioma	-				ear Zymbals gland spleen all tumors bearing animals	mammary gland hematopoietic system kidney **uterus** thyroid gland	lung vascular system urinary bladder stomach	hematopoietic system lung stomach vascular system thyroid gland urinary bladder **ovary** liver	-
Phenylhydrazine hydrochloride	59-88-1					Mouse	Male	Swiss	Drinking water	112	112	Positive	Blood vessel	Multiple tumour types									
Phenylmercury acetate	62-38-4	CC(O)(c(C1=cC=cC=c(C1)=O	경구 독성(분말) : 구분3 생식독성 : 구분1B 특정표적장기 독성(반복 노출) : 구분1 경구 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	7, 8, 11, 14, 16, 19, 23, 25, 27, 29, 30, 33, 34, 36, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 126, 131, 148, 150, 152, 163, 164, 165, 167, 187, 200, 214, 220, 281, 307, 312, 318	-	Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma	NOG	TOB1 SERPINB1 IRF2 CTSD9L STAT5B	FCDH17 POU6A SPAG4 AURKA PLAG4	hsa04350 TGF-beta signaling pathway - Homo sapiens (human) (1) hsa9241 K04658 NOG: noggin	-	-	-	pituitary gland	-
Phenylmercury acetate	62-38-4					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenylmercury acetate	62-38-4					Mouse	Female	B6C3F1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenylmercury acetate	62-38-4					Mouse	Male	B6C3F1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Phenylthiourea	103-85-5	N(C(=S)N(C1=cC=cC=c1)	-	29, 30, 52, 53, 67, 91, 93, 94, 96, 112, 165, 167, 197, 200	Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic	TAS2R38 CYP1A BBP4 THRSP CYP2B10 CYP4A14 PPARA	TEP1 PHF14 ALDH1BA1 TBX15 MYO5C	CYORF63 POR CYP4F2 VASN RNF72		CYP2D1 SCSDL CYP2B6 CYORF11B KRT2				
Phenylthiourea	103-85-5					Mouse	Male	B6C3F1	Diet	78	91	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic									
Phenylthiourea	103-85-5					Rat	Female	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic									
Phenylthiourea	103-85-5					Rat	Male	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Nodule- neoplastic									
Phenytoin	57-41-0	C1(=CC=C(C=c1)C(2(C(N(C(N(C2=o)=O)C)=O)C)c3=CC=CC=C3	경구 독성(분말) : 구분4 생식세포 변이원성 : 구분1B 발암성 : 구분1A 생식독성 : 구분1A 특정표적장기 독성(1회 노출) : 구분1 특정표적장기 독성(반복 노출) : 구분1	16, 23, 27, 29, 30, 34, 52, 53, 57, 58, 61, 67, 91, 93, 94, 96, 111, 152, 117, 122, 123, 131, 150, 163, 165, 167, 187, 197, 200, 220, 307	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	78	86	Negative	Liver	Adenoma- hepatocellular	PRKDC CYP2C9 CYP3A4 CYP2B6 NR1I2 CYP2C19	SLC15A1 CCNC SLC16A1 CTPS1 NQO1	CYP2D1 SCSDL CYP2B6 CYORF11B KRT2	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1555 K17709 CYP2B6: cytochrome P450 family 2 subfamily B member 6 hsa1553 K17716 CYP2C9: cytochrome P450 family 2 subfamily C member 9 hsa1576 K17689 CYP1A4: cytochrome P450 family 1 subfamily A member 4 hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa1555 K17709 CYP2B6: cytochrome P450 family 2 subfamily B member 6 hsa1553 K17716 CYP2C9: cytochrome P450 family 2 subfamily C member 9 hsa1576 K17689 CYP1A4: cytochrome P450 family 1 subfamily A member 4 hsa00982 Drug metabolism - cytochrome P450 - Homo sapiens (human) (3) hsa1555 K17709 CYP2B6: cytochrome P450 family 2 subfamily B member 6 hsa1553 K17716 CYP2C9: cytochrome P450 family 2 subfamily C member 9 hsa1576 K17689 CYP1A4: cytochrome P450 family 1 subfamily A member 4	oral cavity	all tumor bearing animals	urinary bladder thyroid gland	**liver** **ovary** urinary bladder hematopoietic system	Carcinoma, Hepatocellular Liver Neoplasm, Experimental **Liver Neoplasm** Neuroblastoma Head and Neck Neoplasm Multiple Myeloma
Phenytoin	57-41-0					Mouse	Female	B6C3F1	Diet	106	106	Positive	Liver	Adenoma- hepatocellular									
Phenytoin	57-41-0					Mouse	Male	B6C3F1	Diet	78	86	Negative	Liver	Adenoma- hepatocellular									
Phenytoin	57-41-0					Mouse	Male	B6C3F1	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Hepatoblastoma									
Phenytoin	57-41-0					Mouse	Male	CD(SD)F1	Diet	52	52	Not specified	Liver	Adenoma- hepatocellular									
Phenytoin	57-41-0					Rat	Female	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma(hepatocellular | Hepatoblastoma									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADRs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Phthalaldehyde	643-79-8	O=CC1=CC=CC=C1C=O	피부 부식성/피부 자극성 - 구분1(A/1B/1C) 경성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 131, 152, 162, 166, 167, 187, 200, 214, 217, 218	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1/N	Inhalation	96 d	90 d	Not specified			Il4 Il1 Acta2 Aktc1 Ccl16	Il12 Snx22 Wdr84 Dse Tram1	Hta1b2 Slc14a1 Gcgm Atf3h Gclc	hsa04672 Intestinal immune network for IgA production - Homo sapiens (human) (2) hsa:3567 ILS3438 IL5; interleukin 5 hsa:3579 K10589 ACDA; activation induced cytidine deaminase hsa05200 Pathways in cancer - Homo sapiens (human) (1) hsa:3567 ILS3438 IL5; interleukin 5 hsa04660 T cell receptor signaling pathway - Homo sapiens (human) (1) hsa:3567 ILS3438 IL5; interleukin 5	spleen oral cavity Maltoni head cancers ear Zymbals gland hematopoietic system thyroid gland kidney nasal cavity	kidney lung **uterus** thyroid gland clitoral gland hematopoietic system liver nasal cavity	stomach thyroid gland vascular system urinary bladder lung small intestine	stomach thyroid gland **ovary** urinary bladder pituitary gland vascular system peritoneal cavity small intestine	-
Phthalamide	88-96-0	C1(=C(C(=O)NH2)=CC=CT)C(=O)N	-	46	-	Mouse	Female	B6C3F1	Diet	103	103	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	-				spleen all tumor bearing animals	**uterus** hematopoietic system	vascular system lung urinary bladder thyroid gland liver small intestine	**ovary** hematopoietic system vascular system thyroid gland lung urinary bladder stomach small intestine	-
Phthalamide	88-96-0					Mouse	Male	B6C3F1	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Phthalamide	88-96-0					Rat	Female	Fischer 344	Diet	106	106	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Phthalamide	88-96-0					Rat	Male	Fischer 344	Diet	106	106	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Phthalic anhydride	85-44-9	C1=CC=CC2=C(C(=O)OC2=O)=O	급성 독성(경구) - 구분4 심한 눈 손상/눈 자극성 - 구분2A/2B 호흡기 과민성 - 구분1(A/1B) 피부 과민성 - 구분1(1A/1B) 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극)	-	Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	Il4 Il13 Ifng Il10 Il1 Nfkbia Map3k5 Tnf	GFLD1 NCPS6 TIAM1 IL1R1 WWP2	TCF12 IGFBP2 EF2D2 PPP1R14C KIAA0247	hsa04660 T cell receptor signaling pathway - Homo sapiens (human) (3) hsa:3458 K04687 IFNG; interferon gamma hsa:3567 K05428 IL5; interleukin 5 hsa:3586 K05443 IL10; interleukin 10 hsa:5599 K04440 MAPK8; mitogen-activated protein kinase 8 hsa:5601 K04440 MAPK9; mitogen-activated protein kinase 9 hsa04658 Th1 and Th2 cell differentiation - Homo sapiens (human) (5) hsa:3458 K04687 IFNG; interferon gamma hsa:3567 K05428 IL5; interleukin 5 hsa:3596 K05455 IL13; interleukin 13 hsa:5599 K04440 MAPK8; mitogen-activated protein kinase 8 hsa:5601 K04440 MAPK9; mitogen-activated protein kinase 9 hsa05200 Pathways in cancer - Homo sapiens (human) (5) hsa:3458 K04687 IFNG; interferon gamma hsa:3567 K05428 IL5; interleukin 5 hsa:3596 K05455 IL13; interleukin 13 hsa:5599 K04440 MAPK8; mitogen-activated protein kinase 8 hsa:5601 K04440 MAPK9; mitogen-activated protein kinase 9	kidney thyroid gland hematopoietic system ear Zymbals gland urinary bladder Maltoni head cancers spleen large intestine oral cavity liver	kidney hematopoietic system thyroid gland **uterus** clitoral gland urinary bladder	urinary bladder vascular system kidney small intestine lung	**ovary** hematopoietic system pituitary gland urinary bladder thyroid gland stomach peritoneal cavity small intestine vascular system	-
Phthalic anhydride	85-44-9					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Phthalic anhydride	85-44-9					Rat	Female	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Phthalic anhydride	85-44-9					Rat	Male	Fischer 344	Diet	105	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Piperonyl butoxide	51-03-6	C=1C=2c(C(=O)C=1CCC(OCCOCCOCCC)OCC)2	급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 14, 21, 29, 33, 34, 36, 41, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 107, 112, 131, 150, 163, 165, 167, 208, 214, 216, 218	Carcinogenicity data available EPA: OPP-Group C Possible Human Carcinogen Genotoxicity Data: non-genotoxic	Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma	CYP1A1 CYP1A2 Ahr CYP2B10 Ccna1 Gpx2 Pcbd Sod3	LAMP2	CYP1A2 PPP1CB CASP2	hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1728 K00355 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:2877 K00432 GPX2; glutathione peroxidase 2 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa:1728 K00355 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:2735 K16767 GLI1; GLI family zinc finger 1 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1728 K00355 NQO1; NAD(P)H quinone dehydrogenase 1	liver stomach	liver	liver vascular system stomach	liver stomach lung	Cell Transformation, Neoplastic **Liver Neoplasm** Precancerous Conditions **Liver Neoplasm, Experimental** Neoplasm, Experimental **Adenoma, Liver Cell**
Piperonyl butoxide	51-03-6					Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma									
Piperonyl butoxide	51-03-6					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Piperonyl butoxide	51-03-6					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma									
Piperonyl butoxide	51-03-6					Mouse	Female	B6C3F1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma									
Piperonyl butoxide	51-03-6					Mouse	Female	B6C3F1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma									
Piperonyl butoxide	51-03-6					Mouse	Female	B6C3F1	Diet	112	112	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Piperonyl butoxide	51-03-6					Mouse	Male	B6C3F1	Gavage (preweaning) than diet	76	76	Negative	Liver	Hepatoma									
Piperonyl butoxide	51-03-6					Mouse	Male	B6C3F1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma									
Piperonyl butoxide	51-03-6					Mouse	Male	B6C3F1	Diet	112	112	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Piperonyl sulphoxide	120-62-7	C1=CC(=CC2=C1OCO2)C([S+]([C]CCCCCCCC)O-)[C	-	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 166, 167, 187, 200, 204, 207, 218	-	Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma	-				stomach	stomach	liver	-	-
Piperonyl sulphoxide	120-62-7					Mouse	Male	B6AKF1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma									
Piperonyl sulphoxide	120-62-7					Mouse	Female	B6AKF1	Gavage (preweaning) than diet	76	76	Not specified	Liver	Hepatoma									
Piperonyl sulphoxide	120-62-7					Mouse	Female	B6AKF1	Diet	104	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Piricisic acid	50892-23-4	N=1C(=NC(=CC=1FNC=2C(=CC=CC=2)C(O)SCC)O)=O	-	6, 8, 11, 18, 34, 36, 37, 51, 57, 58, 60, 61, 72, 162, 166, 218	-	Mouse	Male	C3b	Diet	53	63	Positive	Liver	Carcinoma - hepatocellular	PPARA NCF1 ACOX1 LICP2	APOA1 MYBL1	PPARD PPARA HPGD	hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (1) hsa:653361 K08801 NCF1; neutrophil cytosolic factor 1 hsa04024 cAMP signaling pathway - Homo sapiens (human) (1) hsa:51 K00232 ACOX1; acyl-CoA oxidase 1 hsa01212 fatty acid metabolism - Homo sapiens (human) (1) hsa:51 K00232 ACOX1; acyl-CoA oxidase 1	liver	-	liver	liver	**Carcinoma, Hepatocellular** **Liver Neoplasm** Precancerous Conditions **Liver Neoplasm, Experimental** **Adenoma, Liver Cell** Neoplasm
Piricisic acid	50892-23-4					Rat	Male	Fischer 344	Diet	60	60	Positive	Liver	Carcinoma - hepatocellular									
Piricisic acid	50892-23-4					Rat	Male	Fischer 344	Diet	69	69	Positive	Liver	Carcinoma - hepatocellular - trabecular									
Piricisic acid	50892-23-4					Rat	Male	Fischer 344	Diet	37	52	Not specified	Liver	Adenoma - hepatocellular									
Piricisic acid	50892-23-4					Rat	Male	Fischer 344	Diet	37	104	Not specified	Liver	Adenoma - hepatocellular									
Piricisic acid	50892-23-4					Rat	Male	Fischer 344	Diet	52	52	Positive	Liver	Adenoma - hepatocellular									
Piriniuil	65089-17-0	N=1C(=NC(=CC=1FNC=2C(=CC=CC=2)C(C)(O)SCC)=O)NCCO	-	-	-	Mouse	Female	C3b	Diet	82	82	Positive	Liver	Carcinoma - hepatocellular	CAT HMGCR LDLR	APOA1 MYBL1 DHFR	PPARD PPARA	hsa04976 Bile secretion - Homo sapiens (human) (1) hsa:3156 K00021 HMGCR; 3-hydroxy-3-methylglutaryl-CoA reductase hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa:3156 K00021 HMGCR; 3-hydroxy-3-methylglutaryl-CoA reductase hsa00900 Terpenoid backbone biosynthesis - Homo sapiens (human) (1) hsa:3156 K00021 HMGCR; 3-hydroxy-3-methylglutaryl-CoA reductase	liver	-	liver	liver	Carcinoma, Hepatocellular
Piriniuil	65089-17-0					Rat	Male	Fischer 344	Diet	75	82	Positive	Liver	Carcinoma - hepatocellular									
Pirimerol hydrochloride	61477-94-9	C1=CC=CNc(C1C(CCCN2)C(=O)c)CCC(=O)c(NCl=CC=CC=3)O.Cl			-	Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular	-				stomach	stomach ear Zymbals gland	stomach	-	-
Pirimerol hydrochloride	61477-94-9					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Pirimerol hydrochloride	61477-94-9					Rat	Female	Wistar	Diet	104	104	Negative	Liver	Multiple tumour types									
Pirimerol hydrochloride	61477-94-9					Rat	Male	Wistar	Diet	104	104	Negative	Adrenal gland	Adenoma - cortical									
Piroxicam	36322-90-4	O1N(C(=)C(C=)C1=)C1=CC=CC=2O(S)(NC3=NC=CC=C3)=O(C)(=O)=O	급성 독성(경구) - 구분3 호흡기 과민성 - 구분1(A/1B) 피부 과민성 - 구분1(A/1B) 생식세포 변이원성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	21, 41, 57, 131, 150, 202	-	Rat	Male	Fischer 344	Diet	54	54	Not specified	Colon	Multiple tumour types	PTGS2 CDKN1A CYP2C9 MPO PTGS1	SNX1 CCNC BAD1 DHFR TGFI	BACGAP1 FANCI EAM115A NBT2 ADIPOQ	hsa05202 Transcriptional misregulation in cancer - Homo sapiens (human) (2) hsa:1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa:4353 K10789 MPO; myeloperoxidase hsa04921 Oxytocin signaling pathway - Homo sapiens (human) (1) hsa:1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A hsa05218 Melanoma - Homo sapiens (human) (1) hsa:1026 K06625 CDKN1A; cyclin dependent kinase inhibitor 1A	-	small intestine all tumor bearing animals	-	-	**Lung Neoplasm** Colonic Neoplasm Esophageal Neoplasm Mesothelioma Urinary Bladder Neoplasm Neoplasm

Chemical Name	CAS No.	SMILES	GHS Classific.	ADRs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Polybrominated biphenyl	59536-65-1	C1(Br)=C(Br)C(C)=C(C=1)Br)Br)Br)=C(C=C(C)=C2Br)Br)Br	발암성 : 구분1B 특정표적장기 독성(반복 노출) : 구분2	21, 27, **29**, **30**, 41, 52, 53, 57, 67, 112, 135, 150, **165**, **167**, **200**, 310	Carcinogenicity data available: IARC Group 2A - Probably carcinogenic to humans	Rat	Female	Spartan	Diet	57	57	Negative	Liver	Multiple tumour types	**AHR**	CDKN2B BAGAT1S STRA3 RBM13 SRGAP1	CYP1A2 CYP3A4 CTDRED STGALA1 CTSD2	hsa04659 Th17 cell differentiation - Homo sapiens (human) (1) hsa-196 409083 AHR; aryl hydrocarbon receptor hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (5) hsa-196 409083 AHR; aryl hydrocarbon receptor hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa-196 409083 AHR; aryl hydrocarbon receptor	liver large intestine	liver urinary bladder	liver	liver stomach	-
p-Phenylacetanilide	4075-79-0	CC(NC(=O)C=C(C=C)C=C)C(=O)C=CC=CC=C2)=O		-	-	Rat	Female	Not specified	Diet	43	65	Positive	Liver	Multiple tumour types	-				urinary bladder kidney nasal cavity skin spleen liver	urinary bladder ear Zymbals gland mammary gland hematopoietic system **uterus** nasal cavity liver small intestine lung kidney	urinary bladder thyroid gland kidney liver vascular system	urinary bladder vascular system stomach **ovary** liver thyroid gland lung	-
p-Phenylenediamine	106-50-3	C=1)NC=CC(N)=CC=1	급성 독성(경구) : 구분3 급성 독성(흡입) 분진/미스트 : 구분2 심한 눈 손상/눈 자극성 : 구분2A(AOR) 피부 과민성 : 구분1(1A/1B) 특정표적장기 독성(반복 노출) : 구분1 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	8, 11, 19, 21, 23, 27, **29**, **30**, 41, 46, 52, 53, 57, 60, 61, 67, 111, 152, 157, 522, 123, 130, 150, **160**, **162**, **167**, 187, **200**, 220, 307, 310	Carcinogenicity data available: PPRTV (ORNL)- Inadequate for an assessment of carcinogenic potential Genotoxicity Data: genotoxic	Rat	Female	Fischer 344	Diet	80	80	Not specified	Adrenal gland	Pheochromocytoma	CXCL8 **MMP14** CD86 PRDM1 MRGPRX2 Tnf	CCR6 DNAJC2 AMH R2 TEF1 MYOSC	HTATIP2 MGST1 BCL2A1 CYP3F SOD3	hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (1) hsa-2162 830510 HMOX1; heme oxygenase 1 hsa05206 MicroRNAs in cancer - Homo sapiens (human) (1) hsa-2162 830510 HMOX1; heme oxygenase 1 hsa05320 Autoimmune thyroid disease - Homo sapiens (human) (1) hsa-942 405413 CD86; CD86 molecule	spleen ear Zymbals gland thyroid gland urinary bladder	urinary bladder ear Zymbals gland **uterus** thyroid gland hematopoietic system kidney lung clitoral gland liver mammary gland nasal cavity small intestine stomach	thyroid gland urinary bladder vascular system liver vascular system lung small intestine	thyroid gland liver urinary bladder vascular system hematopoietic system **ovary** stomach pituitary gland peritoneal cavity lung small intestine	-
p-Phenylenediamine	106-50-3					Rat	Male	Fischer 344	Diet	80	80	Not specified	Adrenal gland	Pheochromocytoma									
p-Phenylenediamine dihydrochloride	624-18-0	C=1)NC=CC(N)=CC=1.Cl.Cl	급성 독성(경구) : 구분3 급성 독성(흡입) : 구분4 급성 독성(흡입) 분진/미스트 : 구분2 심한 눈 손상/눈 자극성 : 구분2A(AOR) 피부 과민성 : 구분1(1A/1B) 특정표적장기 독성(반복 노출) : 구분1 급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	61	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic	-				spleen ear Zymbals gland thyroid gland urinary bladder	urinary bladder ear Zymbals gland **uterus** thyroid gland hematopoietic system kidney lung clitoral gland liver mammary gland nasal cavity small intestine stomach	thyroid gland urinary bladder liver vascular system lung small intestine	thyroid gland liver urinary bladder vascular system hematopoietic system **ovary** stomach pituitary gland peritoneal cavity lung small intestine	-
p-Phenylenediamine dihydrochloride	624-18-0					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
p-Phenylenediamine dihydrochloride	624-18-0					Rat	Female	Fischer 344	Diet	103	116	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
p-Phenylenediamine dihydrochloride	624-18-0					Rat	Male	Fischer 344	Diet	103	116	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Practolol	6673-35-4	C1=C(C)=CC=C1OCC(O)CNC(C)C(NC)C(=O		46	-	Mouse	Female	Alderly Park	Multiple routes	78	78	Negative	Liver	Multiple tumour types	ADRB2 MAPK1 **MAPK14** RDX	ALDH1BA1 NADK CARKMI HMPO ITGAV	CBP22 CDYS1 ELOVL1 GAUS71 GCOM1	hsa04380 Osteoclast differentiation - Homo sapiens (human) (2) hsa-5594 404371 MAPK1; mitogen-activated protein kinase 1 hsa-5595 404371 MAPK2; mitogen-activated protein kinase 3 hsa05211 Renal cell carcinoma - Homo sapiens (human) (2) hsa-5594 404371 MAPK1; mitogen-activated protein kinase 1 hsa-5595 404371 MAPK2; mitogen-activated protein kinase 3 hsa04664 Fc epsilon RI signaling pathway - Homo sapiens (human) (2) hsa-5594 404371 MAPK1; mitogen-activated protein kinase 1 hsa-5595 404371 MAPK2; mitogen-activated protein kinase 3	all tumor bearing animals	nasal cavity ear Zymbals gland stomach mammary gland	kidney thyroid gland urinary bladder	-	-
Practolol	6673-35-4					Mouse	Male	Alderly Park	Multiple routes	78	78	Negative	Liver	Multiple tumour types									
Practolol	6673-35-4					Rat	Female	Alpk:APfSD	Diet	104	104	Negative	Liver	Multiple tumour types									
Practolol	6673-35-4					Rat	Male	Alpk:APfSD	Diet	104	104	Negative	Liver	Multiple tumour types									
Procarbazine hemihydrate	150821-03-7	C1=NN(=NN1)C(=2)OC3=C(C(C=2)=O)C=CC=C3NC(=O)C(4=CC(=C(C=C4)OCCCCS5=CC=CC=C5.O.Cl)C(=NN(=NN6)C=7OC8=C(C(C=7)=O)C(=CC=C8NC(=O)C9=CC=CC=C9NC(=O)C10=CC=CC=C10)OCCCCC5%10=CC=CC=C%10						Rat	Female	JcrSD	Gavage	52	52	Negative	Liver	Multiple tumour types									
Procarbazine hemihydrate	150821-03-7					Rat	Female	JcrSD	Gavage	52	52	Negative	Liver	Multiple tumour types									
Procarbazine hemihydrate	150821-03-7					Rat	Male	JcrSD	Gavage	52	52	Negative	Liver	Multiple tumour types									
Procarbazine hemihydrate	150821-03-7					Rat	Male	JcrSD	Gavage	52	56	Negative	Liver	Nodule- neoplastic									
Procarpam	2955-38-6	C(C)CC1(N)C=4C=CC(=CC=4)C=2C=C=CC=2)=NCC3=O)O	급성 수생환경 유해성 : 구분1 만성 수생환경 유해성 : 구분1	14, 15, 23, 27, **29**, **30**, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 113, 160, **165**, 167, 187, **200**, 214, 307, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	CF-1	Diet	80	80	Negative	Bone	Osteoma	-			-	-	liver	liver	-
Procarpam	2955-38-6					Mouse	Male	CF-1	Diet	80	80	Negative	Liver	Adenoma - hepatocellular									
Procarpam	2955-38-6					Rat	Female	Wistar	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Procarpam	2955-38-6					Rat	Male	Wistar	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Prednimustine	29069-24-7	C(C)[C@H](O)C[C@H](C)C[C@H](C[C@](C)(Cl)C=C)C=C1CC(C=C1)C(C)[C@](C)(C[C@](C)(C[C@H](C)C)[C@](C)(C)C)C(C)C)C(C)C=C=C=C=C(N)C(C)C(C)=O=O	급성 독성(경구) : 구분4 특정표적장기 독성(반복 노출) : 구분2 특정표적장기 독성(반복 노출) : 구분2 위험 수생환경 유해성 : 구분4	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Rat	Female	SD	Gavage	78	104	Positive	Ear canal- external	Carcinoma - squamous cell	-				liver all tumor bearing animals	ear Zymbals gland	stomach	hematopoietic system lung	Hodgkin Disease
Pirenidone hydrochloride	40179-40-3	C1=CC(=O)C=4C1OCC(NCCNC(=O)C(NC2=O)=O)C(O)C.Cl			-	Mouse	Female	CD1	Diet	78	78	Not specified	Liver	Carcinoma - hepatocellular	-				skin	all tumor bearing animals	urinary bladder kidney	hematopoietic system	-
Pirenidone hydrochloride	40179-40-3					Mouse	Male	CD1	Diet	78	78	Not specified	Liver	Adenoma									
Primidone	125-33-7	C(C)(C)C(NCNC1=O)=O)=CC=CC=C2	급성 독성(경구) : 구분4 발암성 : 구분2	**29**, 30, 34, 52, 53, 58, 67, 112, **165**, **167**, **200**	Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	101	104	Positive	Liver	Adenoma - hepatocellular	ABCB11 C3 IL1A IL24 PON1 S100A8 S100A9 SLPI	SLC16A1 ZBED2 CCR7 ALDH1BA1 NEF	TRIM23 SGK2 PPARA PCB FABP4	hsa04060 Cytokine-cytokine receptor interaction - Homo sapiens (human) (2) hsa-11009 420668 IL24; interleukin 24 hsa-3552 404383 IL1A; interleukin 1 alpha hsa04657 IL-17 signaling pathway - Homo sapiens (human) (2) hsa-6279 421127 S100A8; S100 calcium binding protein A8 hsa-6280 421128 S100A9; S100 calcium binding protein A9 hsa04933 AGE-RAGE signaling pathway in diabetic complications - Homo sapiens (human) (2) hsa-2152 403801 F2; coagulation factor II; tissue factor hsa-3552 404383 IL1A; interleukin 1 alpha	-	all tumor bearing animals	thyroid gland liver urinary bladder	liver thyroid gland	-
Primidone	125-33-7					Mouse	Male	B6C3F1	Diet	101	103	Positive	Liver	Adenoma - hepatocellular									
Primidone	125-33-7					Rat	Female	Fischer 344	Diet	101	103	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Hepatoblastoma									
Primidone	125-33-7					Rat	Male	Fischer 344	Diet	99	103	Not specified	Adrenal gland medulla	Pheochromocytoma benign Pheochromocytoma- benign- bilateral									
Probenecid	57-66-9	O=S(=O)(C1=CC=C(C=C1)C(O)=O)NCCCCCCC	-	8, 11, 60	Genotoxicity Data: predicted to be non-genotoxic	Mouse	Female	B6C3F1	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular	SLC22A8 SLC22A6 ABCC1 ABCC2	TGFI NAPEL1 GEMIN4 PRMC8 CCDC93	INS PCDH17 CBG1 TMEM52 ZCCHC24	hsa01523 Antifolate resistance - Homo sapiens (human) (1) hsa-4363 405665 ABCC1; ATP binding cassette subfamily C member 1 hsa04977 Vitamin digestion and absorption - Homo sapiens (human) (1) hsa-4363 405665 ABCC1; ATP binding cassette subfamily C member 1 hsa02010 ABC transporters - Homo sapiens (human) (1) hsa-4363 405665 ABCC1; ATP binding cassette subfamily C member 1	spleen	-	thyroid gland	liver thyroid gland	-
Probenecid	57-66-9					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Probenecid	57-66-9					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Probenecid	57-66-9					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									
Procarbazine	671-16-9	C1=C(C=CC(=C1C(C(NC)C)=O)C(NNC	-	-	Cancer slope factor: 0.004 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Rat	Male	BR-46	Intravenous	52	104	Positive	Multiple sites	Multiple tumour types	FGF4B LHB MGMT AMH AOC2	ALDH1BA1 TRIM4P SHC1 FKBP5 HMPO	C10ORF11B TFI1 OS9 TMEM49B IGKC	hsa04024 cAMP signaling pathway - Homo sapiens (human) (2) hsa-268 404665 AMH; anti-Mullerian hormone hsa-3972 408521 LHB; luteinizing hormone subunit beta hsa04060 Cytokine-cytokine receptor interaction - Homo sapiens (human) (1) hsa-268 404665 AMH; anti-Mullerian hormone hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa-3972 408521 LHB; luteinizing hormone subunit beta	all tumor bearing animals	**uterus** all tumor bearing animals	kidney	lung	Breast Neoplasm Adenocarcinoma
Procarbazine hydrochloride	366-70-1	C1=C(C=CC(=C1C(C(NC)C)=O)C(NNC)C)	급성 독성(경구) : 구분4 발암성 : 구분1B 생식독성 : 구분2	8, 11, 28, 40, 61, 63, 100, 101, 102, 103, 177	Cancer slope factor: 0.0004 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Cynomolgus monkey	Mixed	Not specified	Multiple routes	825	980	Positive	Bone	Osteosarcoma	-								-
Procarbazine hydrochloride	366-70-1					Mouse	Female	B6C3F1	Intraperitoneal	52	85	Positive	Brain	Neuroblastoma - olfactory									
Procarbazine hydrochloride	366-70-1					Mouse	Male	B6C3F1	Intraperitoneal	52	85	Positive	Brain	Neuroblastoma - olfactory									
Procarbazine hydrochloride	366-70-1					Mouse	Female	Swiss	Intraperitoneal	26	76	Positive	Liver	Lymphosarcoma									
Proflavine hydrochloride	952-23-8	N1=C(C)=CC=2C1=CC(N)=CC=2)C==CC1=C(N)C=1	만성 수생환경 유해성 : 구분2	-	-	Mouse	Female	B6C3F1	Diet	103	103	Inadequate test	Liver	Adenoma - hepatocellular | Carcinomahepatocellular	-				ear Zymbals gland spleen all tumors bearing animals	ear Zymbals gland **uterus** urinary bladder clitoral gland thyroid gland mammary gland hematopoietic system small intestine	liver urinary bladder thyroid gland vascular system lung	liver thyroid gland urinary bladder hematopoietic system vascular system stomach	-
Proflavine hydrochloride	952-23-8					Mouse	Male	B6C3F1	Diet	103	103	Inadequate test	Liver	Adenoma - hepatocellular | Carcinomahepatocellular | Nodule- neoplastic									

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Proflavine hydrochloride	952-23-8					Rat	Female	Fischer 344	Diet	109	109	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Proflavine hydrochloride	952-23-8					Rat	Male	Fischer 344	Diet	109	109	Inadequate test		Large intestine - Sarcoma Small intestine - Adenocarcinoma | Leiomyosarcoma									
Promethazine hydrochloride	58-33-3	N1(C3=CSC=2C7=CC=CC=2)C=CC=C3C(CN(C)C)C1	급성 독성(경구) : 구분3 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(사) 피부 과민성 : 구분1(1A/1B) 특정표적장기 독성(1회 노출) : 구분3(호흡기 자극)	7, 8, 11, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 60, 61, 67, 72, 111, 112, 117, 122, 123, 150, 153, 163, 165, 167, 187, 200, 220, 307	-	Mouse	Female	B6C3F1	Gavage	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma	-				skin all tumor bearing animals	ear Zymbaki gland uterus all tumor bearing animals	-	-	-
Promethazine hydrochloride	58-33-3					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma									
Promethazine hydrochloride	58-33-3					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma									
Promethazine hydrochloride	58-33-3					Rat	Male	Fischer 344	Gavage	102	102	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Hepatoblastoma									
Pronamide	23950-58-5	CC(C)NC(C)=1C=2C(C=C(C=1)Cl)=O)CHC	급성 독성(흡입: 분진/미스트) : 구분4 발암성 : 구분2 만성 수생환경 유해성 : 구분2	8, 11, 19, 23, 34, 36, 57, 58, 60, 61, 62, 72, 107, 111, 121, 122, 123, 150, 167, 187, 207	Carcinogenicity data available: CalEPA-Cidety Human Carcinogen	Mouse	Male	B6C3F1	Diet	52	52	Not specified	Liver	Carcinoma - hepatocellular	NR1I2 AR ESR1 CYP2B10 TP53 ABL CYP2B1 CYP1A2 CYP4A1 CYP4A10	AKR1C3 SHC1 TRIAP TBX15 MIRNL2	CISH INS IERS1 EDC32 ADAMTS9	hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa2099 KEGG:SS ESR1; estrogen receptor 1 hsa367 KEGG:T AR; androgen receptor hsa5468 KEGG:SS PPARG; peroxisome proliferator-activated receptor gamma hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa1576 KI:7689 CYP1A4; cytochrome P450 family 3 subfamily A member 4 hsa2099 KEGG:SS ESR1; estrogen receptor 1 hsa367 KEGG:T AR; androgen receptor hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (1) hsa5468 PPARG; peroxisome proliferator-activated receptor gamma	all tumor bearing animals	-	liver kidney	-	Liver Neoplasm, Experimental Leydig Cell Tumor
Pronamide	23950-58-5					Mouse	Male	B6C3F1	Diet	78	78	Not specified	Liver	Carcinoma - hepatocellular									
Pronamide	23950-58-5					Mouse	Male	B6C3F1	Diet	104	104	Positive	Liver	Carcinoma - hepatocellular									
Propham	122-42-9	C1=CC=1C(C=C(N)OC(C)C)=O	급성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 만성 수생환경 유해성 : 구분3	8, 11, 29, 30, 52, 53, 60, 67, 152, 165, 167, 200	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	ESR1 NR1 VTG1 VTG2	TPM1 IKBKAP CSL4B ALDH18A1 CAPRIN1	PCR FGF21 VASN RNF12 CACNG4	hsa04021 Apelin signaling pathway - Homo sapiens (human) (1) hsa4886 KI:1821 NR1; nuclear respiratory factor 1 hsa05016 Huntington disease - Homo sapiens (human) (1) hsa4886 KI:1821 NR1; nuclear respiratory factor 1	spleen	-	urinary bladder thyroid gland kidney	urinary bladder	-
Propham	122-42-9					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Propham	122-42-9					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Propham	122-42-9					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Propranolol hydrochloride	318-98-9	C=12C(OCC(ONC)C)C)O=CC=CC=1C=2C=CC=C2Cl	급성 독성(경구) : 구분4 심한 눈 손상성/눈 자극성 : 구분2A(사용) 생식세포 변이원성 : 구분2	18, 23, 29, 30, 34, 36, 52, 53, 58, 67, 72, 111, 112, 117, 163, 165, 167, 187, 200, 307	-	Mouse	Female	CD1	Diet	78	92	Negative	Liver	Multiple tumour types	-				all tumor bearing animals	nasal cavity	kidney	-	-
Propranolol hydrochloride	318-98-9					Mouse	Male	CD1	Diet	78	92	Negative	Liver	Adenoma -									
Propranolol hydrochloride	318-98-9					Rat	Female	Fischer 344	Gavage	88	91	Negative	Liver	Multiple tumour types									
Propranolol hydrochloride	318-98-9					Rat	Male	Fischer 344	Gavage	88	91	Negative	Liver	Multiple tumour types									
Propyl gallate	121-79-9	C1(=C(C(=CC(=C1O)O)OC)=O)O(O)O	피부 과민성 : 구분1(1A/1B)	6, 8, 21, 27, 28, 29, 30, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 62, 63, 67, 72, 100, 101, 103, 105, 110, 112, 122, 123, 128, 150, 163, 165, 166, 167, 177, 200, 220, 310, 318	Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular	ESR1 HGNC HIF1A MDC1 ACLY AKR1C2	LAMP3 ITGAV GSS TSFM ABIN12	PTGR1 FTL AKR1B10 FECH HMOX1	hsa04919 Thyroid hormone signaling pathway - Homo sapiens (human) (1) hsa2091 KI:8268 HIF1A; hypoxia inducible factor 1 subunit alpha hsa04659 Th17 cell differentiation - Homo sapiens (human) (1) hsa2091 KI:8268 HIF1A; hypoxia inducible factor 1 subunit alpha hsa04140 Autophagy - animal - Homo sapiens (human) (1) hsa2091 KI:8268 HIF1A; hypoxia inducible factor 1 subunit alpha	kidney hematopoietic system stomach	hematopoietic system stomach	stomach kidney	pituitary gland	Cell Transformation, Neoplastic Liver Neoplasm
Propyl gallate	121-79-9					Mouse	Male	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Propyl gallate	121-79-9					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Propyl gallate	121-79-9					Rat	Male	Fischer 344	Diet	103	105	Not specified	Adrenal gland	Pheochromocytoma									
Propyzamide	23950-58-5	C1=C(=CC(=C(N(C(=O)C(C)(C)C)C)C)Cl)C(=C(C=C)C)=O				Mouse	Female	CD1	Diet	86	86	Negative	Liver	Carcinoma - hepatocellular	-				spleen		urinary bladder	hematopoietic system	
Propyzamide	23950-58-5					Mouse	Male	CD1	Diet	86	86	Negative	Liver	Carcinoma - hepatocellular									
Protocatechuic acid	99-50-3					Syrian hamster	Female	Not specified	Diet	49	52	Negative	Liver	Multiple tumour types									
Protocatechuic acid	99-50-3	C1(=CC=C(C(=C1O)O)C(=O)O)	-	-	Genotoxicity Data: predicted to be genotoxic	Rat	Male	Fischer 344/DuCr	Diet	51	52	Not specified	Forestomach	Multiple tumour types	TNF HRAS CASP3 CASP1 CAT EPO	SERPINB1 CCDC83 STX1A SEC16A CBFPQ	PTGR1 AKR1B10 FTL FECH PLA2G6	hsa05205 Proteoglycans in cancer - Homo sapiens (human) (3) hsa2091 KI:8268 HIF1A; hypoxia inducible factor 1 subunit alpha hsa7422 KI:5448 VEGFA; vascular endothelial growth factor A hsa836 KI:2187 CASP3; caspase 3 hsa05167 Kaposi sarcoma-associated herpesvirus infection - Homo sapiens (human) (3) hsa2091 KI:8268 HIF1A; hypoxia inducible factor 1 subunit alpha hsa7422 KI:5448 VEGFA; vascular endothelial growth factor A hsa836 KI:2187 CASP3; caspase 3 hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa2091 KI:8268 HIF1A; hypoxia inducible factor 1 subunit alpha hsa7422 KI:5448 VEGFA; vascular endothelial growth factor A hsa836 KI:2187 CASP3; caspase 3	kidney urinary bladder stomach	urinary bladder stomach cloaca gland	stomach kidney thyroid gland	ovary pituitary gland stomach thyroid gland	-
Purpurin	81-54-9	C1(C(=C(C(=C1O)=O)C=CC)=C2O)(O)O=C(=C2O)(O)O)=O(=CC=CC=3)=O	-	8, 11, 19, 23, 23, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 67, 72, 111, 112, 117, 121, 150, 163, 165, 167, 187, 200, 307, 310	-	Rat	Male	Fischer 344	Diet	74	74	Positive	Urinary bladder	Carcinoma - squamous cell	-				urinary bladder kidney stomach large intestine liver vascular system	urinary bladder small intestine	stomach liver thyroid gland	pituitary gland stomach vascular system thyroid gland ovary liver hematopoietic system	-
Pyrimethamine	58-14-0	N=1C(=C(C(=NC=1N)C)C=2C=CC(=CC=2)Cl)N	급성 독성(경구) : 구분4 만성 수생환경 유해성 : 구분2	7, 8, 10, 19, 23, 25, 27, 29, 30, 33, 34, 46, 52, 53, 58, 60, 61, 67, 91, 93, 94, 96, 97, 98, 107, 111, 112, 117, 122, 123, 126, 135, 153, 165, 167, 187, 198, 197, 200, 203, 204, 307	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	B6C3F1	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic	SLC47A1 SLC47A2 CASP3 BCL6 CASP7 CAT	SLC15A1 HAPD	LST1 GRIP1 AHRR SP1 CYTH1	hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (3) hsa836 KI:2187 CASP3; caspase 3 hsa840 KI:4287 CASP7; caspase 7 hsa05010 Alzheimer disease - Homo sapiens (human) (2) hsa836 KI:2187 CASP3; caspase 3 hsa840 KI:4287 CASP7; caspase 7 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa836 KI:2187 CASP3; caspase 3 hsa840 KI:4287 CASP7; caspase 7	-	ear Zymbaki gland small intestine	thyroid gland liver	thyroid gland liver	Adenocarcinoma Melanoma, Experimental Mycosis Fungoides
Pyrimethamine	58-14-0					Mouse	Male	B6C3F1	Diet	78	104	Inadequate test	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Pyrimethamine	58-14-0					Rat	Female	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Pyrimethamine	58-14-0					Rat	Male	Fischer 344	Diet	78	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Pyrogallol	87-66-1	C1=C(C(=C(C=C1)O)O)O	급성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(사용) 생식세포 변이원성 : 구분2 특정표적장기 독성(반복 노출) : 구분2(간 장기 손상) 만성 수생환경 유해성 : 구분2	7, 19, 23, 25, 29, 30, 46, 52, 53, 67, 111, 112, 117, 122, 123, 165, 167, 187, 200, 307	Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1/N	Dermal	93 d	91 d	Not specified		Multiple tumour types	CASP3 CYCPA2 CAT CYP2E1 SOD1 SOD2	HEATR3 CYORF41 IFIH1 COG3 DNAAF2	HES1 HIVEP1 GNAI1 LIPH PITPNM1	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1571 KI:2743 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa847 KI:3781 CAT; catalase hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1571 KI:2743 CYP2E1; cytochrome P450 family 2 subfamily E member 1 hsa847 KI:3781 CAT; catalase hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (1) hsa847 KI:3781 CAT; catalase	stomach kidney urinary bladder hematopoietic system nasal cavity thyroid gland oral cavity	stomach urinary bladder hematopoietic system kidney thyroid gland small intestine nasal cavity uterus	stomach kidney thyroid gland lung vascular system	ovary thyroid gland stomach pituitary gland urinary bladder vascular system peritoneal cavity	-
Quercetin	117-39-5	C1(=C(C(=CC2=C1C(=C(C(O)C2=O)C=1C(=CC(=C(C=1)O)O)O)O)	급성 독성(경구) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(사용) 생식세포 변이원성 : 구분2 특정표적장기 독성(반복 노출) : 구분2(간 장기 손상) 만성 수생환경 유해성 : 구분2	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 41, 46, 52, 53, 57, 58, 60, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 126, 150, 153, 162, 165, 167, 187, 200, 214, 220, 307, 310, 318	Carcinogenicity data available: IARC-Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: genotoxic	Mouse	Female	D2L	Diet	120	120	Negative	Liver	Multiple tumour types	TNF HMOX1 IL1B NOS2 BCL2 NFE2L2	IFIH1 COG3 DNAAF2 FABP1 FCHSD2	GNAI1 LIPH PITPNM1 AHRR GCKR	hsa05132 Tuberculosis - Homo sapiens (human) (4) hsa3553 KI:6459 IL1B; interleukin 1 beta hsa4843 KI:5241 NOS2; nitric oxide synthase 2 hsa596 KI:2161 BCL2; BCL2 apoptosis regulator hsa836 KI:2187 CASP3; caspase 3 hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa3162 KI:8530 HMOX1; heme oxygenase 1 hsa4843 KI:5241 NOS2; nitric oxide synthase 2 hsa596 KI:2161 BCL2; BCL2 apoptosis regulator hsa836 KI:2187 CASP3; caspase 3	urinary bladder kidney vascular system stomach all tumor bearing animals	urinary bladder small intestine	stomach urinary bladder	pituitary gland stomach	Mammary Neoplasm, Animal Pancreatic Neoplasm Leukemia Neoplasm Invasiveness Neoplasm
Quercetin	117-39-5					Mouse	Male	D2L	Diet	115	115	Negative	Heart	Sarcoma - spindle cell									
Quercetin	117-39-5					Rat	Female	Fischer 344	Diet	64	64	Negative	Skin/soft tissue	Multiple tumour types									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Quercetin	117-39-5					Rat	Female	Fischer 344	Diet	103	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Quercetin	117-39-5					Rat	Male	Fischer 344	Diet	64	64	Negative	Multiple sites	Multiple tumour types									
Quercetin dihydrate	6151-25-3	C1(=CC(=C2C(=C(C(O)C(=C(C2)-O)O)C3=CC(=C(C=C3)O)O)O)O)O.O	-	19, 21, 22, 29, 30, 41, 46, 52, 53, 57, 61, 67, 111, 112, 117, 131, 150, 165, 167, 187, 200, 207, 310	-	Rat	Female	ACI	Diet	77	77	Negative	Adrenal gland	Adenoma - cortical	TNF CASP3 HMOX1 IL1B NOS2 BCL2 NFKB1A	IFIH1 COG5 DNAAF2 FABP1 FCHSD2	GNAI1 LIPH PITPNM1 KHNYN GCK6	hsa05152 Tuberculosis - Homo sapiens (human) (4) hsa:3553 IL1B, interleukin 1 beta hsa:4843 NOS2, nitric oxide synthase 2 hsa:596 BCL2, BCL2 apoptosis regulator hsa:836 CASP3, caspase 3 hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (4) hsa:3553 IL1B, interleukin 1 beta hsa:4843 NOS2, nitric oxide synthase 2 hsa:596 BCL2, BCL2 apoptosis regulator hsa:836 CASP3, caspase 3 hsa05200 Pathways in cancer - Homo sapiens (human) (4) hsa:3162 HMOX1, heme oxygenase 1 hsa:4843 NOS2, nitric oxide synthase 2 hsa:596 BCL2, BCL2 apoptosis regulator hsa:836 CASP3, caspase 3	urinary bladder kidney vascular system stomach all tumor bearing animals	urinary bladder small intestine	stomach urinary bladder	pituitary gland stomach	Mammary Neoplasm, Animal Pancreatic Neoplasm Leukemia Neoplasm Invasiveness Neoplasm
Quercetin dihydrate	6151-25-3					Rat	Female	ACI	Diet	121	121	Negative	Adrenal gland	Adenoma - cortical									
Quercetin dihydrate	6151-25-3					Rat	Male	ACI	Diet	77	77	Negative	Adrenal gland	Pheochromocytoma									
Quercetin dihydrate	6151-25-3					Rat	Male	ACI	Diet	121	121	Negative	Cecum	Adenocarcinoma									
Quercetin dihydrate	6151-25-3					Rat	Female	Fischer 344	Diet	77	77	Negative	Adrenal gland	Adenoma - cortical									
Quercetin dihydrate	6151-25-3					Rat	Male	Fischer 344	Diet	77	77	Negative	Multiple sites	Multiple tumour types									
Quinapril hydrochloride	82586-55-8	C1[C@H](N[C@@H](CCC2=CC=CC=C2)C)[C@@H](O)N2[C@H](CCC2)CC=C1C=C3C(OCC=3)=O)C(O)=O.Cl	-	19, 23, 111, 117, 187, 307	-	Mouse	Female	B6C3F1	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular	AGT NPPA ACE EDN1 IL6 RTN4rl1 RBN	-	CASP2	hsa04924 Renin secretion - Homo sapiens (human) (2) hsa:1636 KIT,SCF, ACE, angiotensin I converting enzyme hsa:1906 KIT,SCF, EDNRB, endothelin 1 hsa:4878 KIT,SCF, NPPA, natriuretic peptide A hsa05410 Hypertrophic cardiomyopathy - Homo sapiens (human) (3) hsa:1636 KIT,SCF, ACE, angiotensin I converting enzyme hsa:1906 KIT,SCF, EDNRB, endothelin 1 hsa:3569 KIT,SCF, IL6, interleukin 6 hsa04066 HIF-1 signaling pathway - Homo sapiens (human) (3) hsa:1906 KIT,SCF, EDNRB, endothelin 1 hsa:3569 KIT,SCF, IL6, interleukin 6 hsa:4878 KIT,SCF, NPPA, natriuretic peptide A	all tumor bearing animals skin	ear Zymbals gland	kidney	liver	-
Quinapril hydrochloride	82586-55-8					Mouse	Male	B6C3F1	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular									
Quinapril hydrochloride	82586-55-8					Rat	Female	Wistar	Gavage	104	104	Negative	Liver	Multiple tumour types									
Quinapril hydrochloride	82586-55-8					Rat	Male	Wistar	Gavage	104	104	Negative	Liver	Multiple tumour types									
Ramoxirtron.HCl	132607-72-3	C[C@@H](CCC2=C(C1(N=C(N2)[C]=C)N[C-4=C]C=C(C=C4[C]=C)O.Cl	-	46	-	Mouse	Female	B6C3F1	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular	HTR3A	SLC15A1 ALDH1BA1 EXD3 CTPS1 SNA1	LST1 SF1 TMEM41B C10ORF118 WIPF1	hsa04726 Serotonergic synapse - Homo sapiens (human) (1) hsa:3359 HTR3A, 5-hydroxytryptamine receptor 3A hsa04742 Taste transduction - Homo sapiens (human) (1) hsa:3359 HTR3A, 5-hydroxytryptamine receptor 3A	-	ear Zymbals gland	urinary bladder	hematopoietic system lung vascular system liver	-
Ramoxirtron.HCl	132607-72-3					Mouse	Male	B6C3F1	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular									
Ramoxirtron.HCl	132607-72-3					Rat	Female	Fischer 344	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular									
Ramoxirtron.HCl	132607-72-3					Rat	Male	Fischer 344	Gavage	104	104	Negative	Liver	Adenoma - hepatocellular									
Resorcinol	108-46-3	C1=C(O)C=CC=C1O	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상/눈 자극성 - 구분2 피부 과민성 - 구분1(A/1B) 특정표적장기 독성(1회 노출) - 구분1 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분3	28, 29, 30, 34, 52, 53, 57, 58, 63, 67, 100, 101, 102, 103, 107, 111, 112, 117, 131, 150, 167, 177, 187, 200	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Gavage	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	TNR AKR1B10 AOC [illegible] MFO PTGS2 TPO	HEATR3 CYORF4 WNIP2 TBC1D9 IFIH1	ERCC2 RACGAP1 ADAMTS9 TRIP13 ECT2	hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa:324 KEGG:BRS: APC, APC regulator of WNT signaling pathway hsa:4286 KEGG:BRS: MITF, melanocyte inducing transcription factor hsa:5743 KEGG:BRS: PTGS2, prostaglandin-endoperoxide synthase 2 hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa:57016 KEGG:BRS: AKR1B10, aldo-keto reductase family 1 member B10 hsa:5743 KEGG:BRS: PTGS2, prostaglandin-endoperoxide synthase 2 hsa05010 Alzheimer disease - Homo sapiens (human) (2) hsa:324 KEGG:BRS: APC, APC regulator of WNT signaling pathway hsa:5743 KEGG:BRS: PTGS2, prostaglandin-endoperoxide synthase 2	kidney urinary bladder stomach hematopoietic system nasal cavity thyroid gland oral cavity Maltoni head cancers ear Zymbals gland vascular system large intestine spleen	urinary bladder stomach hematopoietic system small intestine kidney thyroid gland nasal cavity liver **uterus**	thyroid gland stomach kidney vascular system lung	**ovary** thyroid gland stomach pituitary gland urinary bladder vascular system hematopoietic system liver peritoneal cavity	-
Resorcinol	108-46-3					Mouse	Male	B6C3F1	Gavage	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Resorcinol	108-46-3					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Resorcinol	108-46-3					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Resveratrol	501-36-0	C1(=C(C(=C(C(=C1)O)C=C)C=C)C=C)C=C2O)O	-	8, 14, 19, 21, 22, 27, 28, 29, 30, 34, 36, 41, 43, 46, 52, 53, 57, 58, 61, 62, 63, 64, 66, 67, 71, 72, 100, 101, 102, 103, 107, 111, 112, 117, 131, 150, 163, 165, 167, 177, 187, 200, 214, 307, 310, 318	-	Mouse	Female	B6C3F1/N	Gavage	17 d	17 d	Not specified			SIRT1 TNF IL1B CASP3 IL6 PTGS2 TPS3	CYORF40 WNIP2 RNF72 MANSC1 RNF144A	TCF12 PLA2G6 EP300 ERCC2 OGG1	hsa04657 IL-17 signaling pathway - Homo sapiens (human) (3) hsa:3553 IL1B, interleukin 1 beta hsa:3569 IL6, interleukin 6 hsa:5743 PTGS2, prostaglandin-endoperoxide synthase 2 hsa:7124 TNF, tumor necrosis factor hsa:836 CASP3, caspase 3 hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (5) hsa:3553 IL1B, interleukin 1 beta hsa:3569 IL6, interleukin 6 hsa:5743 PTGS2, prostaglandin-endoperoxide synthase 2 hsa:7124 TNF, tumor necrosis factor hsa:836 CASP3, caspase 3 hsa05010 Alzheimer disease - Homo sapiens (human) (5) hsa:3553 IL1B, interleukin 1 beta hsa:3569 IL6, interleukin 6 hsa:5743 PTGS2, prostaglandin-endoperoxide synthase 2 hsa:7124 TNF, tumor necrosis factor hsa:836 CASP3, caspase 3	**stomach** kidney urinary bladder ear Zymbals gland skin nasal cavity	**stomach** urinary bladder hematopoietic system small intestine	**stomach** kidney lung thyroid gland liver	**ovary** **stomach** pituitary gland thyroid gland	Prostatic Neoplasm Breast Neoplasm Neoplasm Metastasis Carcinoma, Hepatocellular Colorectal Neoplasm Stomach Neoplasm
Rifampicin	13292-46-1	C1=C(C@@H](C[C@@H](C[C@H](C[C@H](C[C@@H](C[C@@H](C[C@@H](C(OC=CO)C[C@]4(OC=3)C[C]=C(O)C2=C(O)C(NC[C]=C1)C=O)=O)C[C=4C=O)O)C=NNSCNC(C)C)C)C)O)C)O)C)O)C	급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 14, 19, 21, 23, 25, 28, 29, 30, 34, 44, 46, 52, 53, 57, 58, 60, 61, 62, 63, 64, 66, 67, 71, 100, 101, 102, 103, 111, 112, 117, 122, 123, 131, 152, 165, 167, 177, 187, 200, 214, 307, 318	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	BALB/c	Drinking water	60	112	Negative	Liver	Hepatoma	NR1I2 CYP3A4 ABCB1 CYP2B6 PXRDC CYP2C9 BCOA1	-	CYP2C19 CYP3A4 CYP2B1 ABCA1 CYP2B6	hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa:1555 KIT,TOR CYP2B6, cytochrome P450 family 2 subfamily B member 6 hsa:1559 KIT,TOR CYP2C9, cytochrome P450 family 2 subfamily C, member 9 hsa:1576 KIT,TOR CYP3A4, cytochrome P450 family 3 subfamily A member 4 hsa00982 Drug metabolism - cytochrome P450 - Homo sapiens (human) (3) hsa:1555 KIT,TOR CYP2B6, cytochrome P450 family 2 subfamily B member 6 hsa:1559 KIT,TOR CYP2C9, cytochrome P450 family 2 subfamily C, member 9 hsa:1576 KIT,TOR CYP3A4, cytochrome P450 family 3 subfamily A member 4 hsa00830 Retinol metabolism - Homo sapiens (human) (3) hsa:1555 KIT,TOR CYP2B6, cytochrome P450 family 2 subfamily B member 6 hsa:1559 KIT,TOR CYP2C9, cytochrome P450 family 2 subfamily C, member 9 hsa:1576 KIT,TOR CYP3A4, cytochrome P450 family 3 subfamily A member 4	-	-	-	**liver**	**Liver Neoplasm**
Rifampicin	13292-46-1					Mouse	Male	BALB/c	Drinking water	60	112	Negative	Liver	Hepatoma									
Rifampicin	13292-46-1					Mouse	Female	CD1(ICr)	Drinking water	60	106	Positive	Liver	Hepatoma									
Rifampicin	13292-46-1					Mouse	Male	CD1(ICr)	Drinking water	60	106	Positive	Liver	Hepatoma									
Rifampicin	13292-46-1					Rat	Female	Wistar	Drinking water	104	138	Negative	Liver	Hepatoma									
Rifampicin	13292-46-1					Rat	Male	Wistar	Drinking water	104	138	Negative	Liver	Hepatoma									
Ripazepam	26308-28-1	N2C(CN=C(C=1C=CC=CC=1)Cl)=C(C=1)[C]=C2C(=NNS(CC)C)=O	피부감염	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans	Mouse	Female	CD1	Diet	78	78	Positive	Liver	Adenoma - hepatocellular	-				skin	all tumor bearing animals	liver thyroid gland urinary bladder	liver hematopoietic system	-
Ripazepam	26308-28-1					Mouse	Male	CD1	Diet	78	78	Positive	Liver	Adenoma - hepatocellular									
Ripazepam	26308-28-1					Rat	Female	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Ripazepam	26308-28-1					Rat	Male	SD	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Rosamone	121-19-7	O=[As](O)(C=1C=CC(=CC(=1)[C]=1)[N+]))[O-]=O(O)O	급성 독성(경구) - 구분3	-	-	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	CEP192 MMP9 PECAM1 ACD1 ACTB	PDGFRL	-	hsa05418 Fluid shear stress and atherosclerosis - Homo sapiens (human) (2) hsa:4318 KEGG:MMP9, matrix metallopeptidase 9 hsa:5175 KEGG:PECAM1, platelet and endothelial cell adhesion molecule 1 hsa04670 Leukocyte transendothelial migration - Homo sapiens (human) (2) hsa:4318 KEGG:MMP9, matrix metallopeptidase 9 hsa:5175 KEGG:PECAM1, platelet and endothelial cell adhesion molecule 1 hsa04668 TNF signaling pathway - Homo sapiens (human) (1) hsa:4318 KEGG:MMP9, matrix metallopeptidase 9	-	-	thyroid gland kidney	-	Neoplasm Invasiveness
Rosamone	121-19-7					Mouse	Male	B6C3F1	Diet	103	105	Not specified	Adrenal gland	Adenoma - cortical | Adenomacortical adenocarcinoma									
Rosamone	121-19-7					Mouse	Male	Swiss-Webster	Diet	104	104	Negative	Multiple sites	Multiple tumour types									
Rosamone	121-19-7					Mouse	Male	Swiss-Webster	Diet	104	104	Negative	Liver	Hepatoma									
Rutin sodium sulfate	12768-44-6	C(@H](C@@H](C[C@H](C[C@@H](O[C@@H](O[C@@H](C[C@@H](O[C@@H](C[C@@H](C[C@@H](O)O)C=4C=3C=C=C)C=C)C=C)C=C)C=C)C=C)C=C)C=C)C=C)O)O				Rat	Female	SD	Gavage	104	138	Negative	Liver	Carcinoma - hepatocellular									
Rutin sodium sulfate	12768-44-6					Rat	Male	SD	Gavage	104	138	Negative	Liver	Carcinoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Rutoside	153-18-4	C1[C@@H]([C@H]([C@@H](O)[C@H]([C@H](O)CO)O)O)O[C@H]([C@H](O)[C@H](O)[C@H](O)[C@H]([C@@H](O)[C@H](O)CO)O)O)O[C@H]1OC[C@H]1[C@H]([C@H]([C@@H](O)[C@H](O)CO)O)O)O[C@]1(OC=C2C(=C(O)C=C(O)C=C2O)C=C1=O)C=2C=C(O)C=C(O)C=2	자료없음	29, 30, 52, 53, 67, 112, 165, 167, 200	Genotoxicity Data: clastogenic	Rat	Female	ACI	Diet	77	77	Negative	Pituitary gland	Adenoma	TNF CASP3 IL6 BCL2 IL1B PTGS2 BAX	DMBL1 CILINA1 CXCL10 ADAMTS9 TUBGCP3	TCF12 KDELC1 FOAD CSF72 DSTN	hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (5) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:3569 K05405 IL6; interleukin 6 hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:596 K02161 BCL2; BCL2 apoptosis regulator hsa:836 K02187 CASP3; caspase 3 hsa05162 Human cytomegalovirus infection - Homo sapiens (human) (4) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:3569 K05405 IL6; interleukin 6 hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:836 K02187 CASP3; caspase 3 hsa04668 TNF signaling pathway - Homo sapiens (human) (4) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:3569 K05405 IL6; interleukin 6 hsa:5743 K11987 PTGS2; prostaglandin-endoperoxide synthase 2 hsa:836 K02187 CASP3; caspase 3	kidney vascular system	small intestine	kidney	-	Melanoma Multiple Myeloma Leukemia
Rutoside	153-18-4					Rat	Female	ACI	Diet	121	121	Negative	Adrenal gland	Pheochromocytoma									
Rutoside	153-18-4					Rat	Male	ACI	Diet	77	77	Negative	Adrenal gland	Adenoma - cortical									
Rutoside	153-18-4					Rat	Male	ACI	Diet	121	121	Negative	Colon	Adenoma									
Saccharin	81-07-2	O1N(NC(=O)C1C=CC=C2)=O2)=O1=O	자료없음	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Female	Swiss	Diet	76	76	Negative	Liver	Hepatoma	PPARA TBPV1 TADIB2 ARSFA ARP CA2	SNA1 CCNC BARD1 TGFI1 DnlB	BACSAP1 FANO EAMT11A SAT NIT2	hsa05323 Rheumatoid arthritis - Homo sapiens (human) (1) hsa:7422 K05468 VEGFA; vascular endothelial growth factor A hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa:7422 K05468 VEGFA; vascular endothelial growth factor A hsa04010 MAPK signaling pathway - Homo sapiens (human) (1) hsa:7422 K05468 VEGFA; vascular endothelial growth factor A	spleen	all tumor bearing animals	thyroid gland urinary bladder	thyroid gland urinary bladder	Carcinoma Adenocarcinoma Urinary Bladder Neoplasm Stomach Neoplasm Neoplasm, Experimental
Saccharin	81-07-2					Mouse	Female	Swiss	Diet	91	91	Negative	Urinary bladder	Carcinoma - urothelial									
Saccharin	81-07-2					Mouse	Male	Swiss	Diet	91	91	Negative	Urinary bladder	Carcinoma - transitional cell									
Saccharin	81-07-2					Rat	Male	Fischer 344	Diet	72	73	Negative	Forestomach	Papilloma									
Safrole	94-59-7	C1=C(C=CC2=C1OCO2)CC=C	인체 독성(흡연) : 구분4 피부 부식성/피부 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A(2B) 생식세포 변이원성 : 구분2 발암성 : 구분1B 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분2	6, 18, 19, 23, 36, 37, 51, 57, 58, 61, 111, 117, 131, 166, 187, 301, 318	Cancer slope factor: 4.3e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: inconclusive	Mouse	Female	B6AKF1	Gavage (pmearning) then diet	81	81	Positive	Liver	Hepatoma	CYP1A2 CYP2D6 CYP1A1 CASP2 CASP9 CYP1A CYP3A4	E2F3 TIMM HSPA6 AIRN1 CASPS2	ITGA6 SOD3 MGST1 TNNB2I CASP2	hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (3) hsa:1543 K07408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa:836 K02187 CASP3; caspase 3 hsa:842 K04389 CASP9; caspase 9 hsa05169 Epstein-Barr virus infection - Homo sapiens (human) (2) hsa:836 K02187 CASP3; caspase 3 hsa:842 K04389 CASP9; caspase 9 hsa05130 Pathogenic Escherichia coli infection - Homo sapiens (human) (2) hsa:836 K02187 CASP3; caspase 3 hsa:842 K04389 CASP9; caspase 9	stomach liver	stomach liver	stomach liver vascular system	liver stomach lung	Liver Neoplasm, Experimental Liver Neoplasm
Safrole	94-59-7					Mouse	Male	B6AKF1	Gavage (pmearning) then diet	81	81	Not specified	Liver	Hepatoma									
Safrole	94-59-7					Mouse	Female	B6C3F1	Gavage	90	90	Positive	Liver	Carcinoma - hepatocellular									
Safrole	94-59-7					Mouse	Female	B6C3F1	Gavage (pmearning) then diet	81	81	Positive	Liver	Hepatoma									
Safrole	94-59-7					Mouse	Male	B6C3F1	Gavage	90	90	Not specified	Liver	Carcinoma - hepatocellular									
Safrole	94-59-7					Mouse	Male	B6C3F1	Gavage (pmearning) then diet	81	81	Positive	Liver	Hepatoma									
Safrole	94-59-7					Mouse	Male	BALB/c	Diet	52	52	Positive	Liver	Adenoma - hepatocellular									
Safrole	94-59-7					Mouse	Male	BALB/c	Diet	52	75	Positive	Liver	Adenoma - hepatocellular									
Safrole	94-59-7					Mouse	Female	CD1	Diet	51	71	Positive	Liver	Carcinoma - hepatocellular									
Safrole	94-59-7					Mouse	Female	CD1	Diet	52	88	Positive	Liver	Hepatoma									
Salazosulfapyridine	599-79-1	O=S(=O)(C=1C=CC(=CC=1)N=NC2=CC(=CC=C2)C(=O)NC3=NC=CC=C3)	-	-	-	Mouse	Female	B6C3F1	Gavage	104	105	Positive	Liver	Adenoma - hepatocellular	TNF IL1B BILA IL6 ABCG2 CXCL8 MPO	TGFI CCNC SNA1 PRKAC8 KSAP1	ADIPOQ BACSAP1 INS FANO TMEM4K	hsa04152 Acetylcholine resistance - Homo sapiens (human) (4) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:3569 K05405 IL6; interleukin 6 hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa:9429 K05687 ABCG2; ATP binding cassette subfamily G member 2 (Junior blood group) hsa05132 Salmonella infection - Homo sapiens (human) (4) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:3569 K05405 IL6; interleukin 6 hsa:3576 K10830 CXCL8; C-X-C motif chemokine ligand 8 hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit hsa04933 AGE-RAGE signaling pathway in diabetic complications - Homo sapiens (human) (4) hsa:3553 K04519 IL1B; interleukin 1 beta hsa:3569 K05405 IL6; interleukin 6 hsa:3576 K10830 CXCL8; C-X-C motif chemokine ligand 8 hsa:5970 K04735 RELA; RELA proto-oncogene, NF-kB subunit	urinary bladder spleen	urinary bladder kidney	thyroid gland liver	liver thyroid gland	Colonic Neoplasm Carcinoma, Hepatocellular Stomach Neoplasm Thyroid Neoplasm Carcinoma, Transitional Cell Urologic Neoplasm
Salazosulfapyridine	599-79-1					Mouse	Male	B6C3F1	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular									
Salazosulfapyridine	599-79-1					Rat	Female	Fischer 344	Gavage	104	105	Positive	Kidney	Papilloma - transitional cell									
Salazosulfapyridine	599-79-1					Rat	Male	Fischer 344	Gavage	26	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
Salazosulfapyridine	599-79-1					Rat	Male	Fischer 344	Gavage	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Hepatoblastoma									
Salbutamol	18559-94-9	N(CC(C=1C=CC(=C(C=1)CO)O)O)(C)(C)C	-	46	-	Rat	Female	SD	Diet	80	80	Positive	Mesovarium	Leiomyoma	ADRB2 TNF NR3C1 IL6 ADRB1 ADRB3 LPO	CRH SDC4	SYPR SYBAM CA2	hsa04080 Neuroactive ligand-receptor interaction - Homo sapiens (human) (3) hsa:152 K04141 ADRB1; adrenoceptor beta 1 hsa:155 K04143 ADRB3; adrenoceptor beta 3 hsa:2908 K05771 NR3C1; nuclear receptor subfamily 3 group C member 1 hsa04020 Calcium signaling pathway - Homo sapiens (human) (2) hsa:152 K04141 ADRB1; adrenoceptor beta 1 hsa:155 K04143 ADRB3; adrenoceptor beta 3 hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa:3569 K05405 IL6; interleukin 6 hsa:7124 K03156 TNF; tumor necrosis factor	stomach	-	kidney	-	Smooth Muscle Tumor Uterine Neoplasm
Salbutamol	18559-94-9					Rat	Female	SD	Diet	104	104	Positive	Mesovarium	Leiomyoma									
Sevoflurane	28523-86-6	S(C(C(=N)C(=O)[H])([H])C(C(F)(F)F)(F)F)(C(F)(F)F)(F)F				Mouse	Female	C57BL/6	Diet	26 or 52	26 or 52	Not specified	Kidney								kidney		
Sevoflurane	28523-86-6			36, 81		Rat	Female	Fischer 344/N	Diet	52	52	Negative	Liver	Multiple tumour types							kidney	lung	
Sevoflurane	28523-86-6					Rat	Male	Fischer 344/N	Diet	52	52	Negative	Liver	Multiple tumour types									
Sertraline hydrochloride	79559-97-0	C1=CC(=C2C(=C1)[C@H]([C@H](C2)[C@H]2C=3C=CC(Cl)=CC=3C=C2)=C1)C=3[N].Cl	-	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 200, 204, 301, 318	-	Mouse	Female	CD1	Diet	104	104	Negative	lung	Adenoma - alveolar/bronchiolar	-				-	-	-	-	-
Sertraline hydrochloride	79559-97-0					Mouse	Male	CD1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular									
Sertraline hydrochloride	79559-97-0					Rat	Female	Long-Evans	Diet	104	104	Negative	Thyroid gland	Adenoma - follicular cell									
Sodium 2,4-dinitrophenol	1011-73-0	C1[N]=[c]=[c](O-[])=[c]([N+]=[c]=O)=[c]=[c]=C1[O-].[Na+]	폭발성 물질 - 등급1.3 미세 유해성 표현요소 - 구분3	-	-	Mouse	Female	DBA	Diet	90	90	Negative	Mammary gland	Carcinoma	-				-	-	-	-	-
Sodium 2-biphenylolate	132-27-4	C1[=c]([O-])C=1C=C=C(C)C2=C1C=C=C2[Na+]	인체 독성(흡연) : 구분4 피부 부식성/피부 자극성 : 구분1(1A/1B/1C) 심한 눈 손상성/눈 자극성 : 구분1 발암성 : 구분2 특정표적장기 독성(1회 노출) : 구분2(마취작용)	-	Cancer slope factor: 8.6e-07 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: predicted to be clastogenic	Mouse	Female	B6C3F1	Diet	96	104	Negative	Liver	Carcinoma - hepatocellular	-				-	-	-	-	-
Sodium 2-biphenylolate	132-27-4					Mouse	Male	B6C3F1	Diet	96	104	Negative	Liver	Carcinoma - hepatocellular									
Sodium 2-biphenylolate	132-27-4					Rat	Female	Fischer 344/DuCrl	Diet	65	65	Positive	Urinary bladder	Carcinoma - transitional cell									
Sodium 2-biphenylolate	132-27-4					Rat	Female	Fischer 344/DuCrl	Diet	104	106	Positive	Urinary bladder	Carcinoma - transitional cell									
Sodium 2-biphenylolate	132-27-4					Rat	Female	Fischer 344/DuCrl	Diet	104	123	Positive	Urinary bladder	Carcinoma - transitional cell									
Sodium aristocholate	10190-99-5	C=2(C=1C(C=CC=1C(C)=C)C=3C=2C(=CC4=C3OCO4)C)[O-]=O)[N+](O-[=O].[Na+].C=4(C=C5(C(C=CC=C5)=C7C=4C)=CC8=C7OCO8)C)[O-]=O)[N+](O-[=O].[Na+]	-	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 165, 167, 187, 200, 204, 301, 318	-	Rat	Female	Wistar	Gavage	52	69	Positive	Forestomach	Carcinoma - squamous cell	CYP1A1 SOD1 CYP1A2 CASP3 LDHA SLIT2 GRIM1	-	-	hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa:1728 K00355 NQO1; NAD(P)H quinone dehydrogenase 1 hsa:836 K02187 CASP3; caspase 3 hsa:999 K05689 CDH1; cadherin 1 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1728 K00355 NQO1; NAD(P)H quinone dehydrogenase 1 hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa:1544 K07409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa:1728 K00355 NQO1; NAD(P)H quinone dehydrogenase 1	-	-	-	-	Carcinoma Neoplasm Invasiveness Urinary Bladder Neoplasm Carcinoma, Transitional Cell Urologic Neoplasm Kidney Neoplasm
Sodium aristocholate	10190-99-5					Rat	Male	Wistar	Gavage	52	69	Positive	Forestomach	Carcinoma - squamous cell									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Sodium benzoate	532-32-1	C1=CC=CC=C1(C)(O-)[=O].[Na+]	자료없음	-	Genotoxicity Data: clastogenic	Mouse	Female	Swiss	Drinking water	134	134	Negative	Liver	Multiple tumour types	TNF CASP3 DAO OTC CAT Il6	-	-	hsa01100 Metabolic pathways - Homo sapiens (human) (3) hsa1410 K00273 D-AO; D-amino acid oxidase hsa5009 K00611 OTC; ornithine transcarbamylase hsa847 K03781 CAT; catalase hsa05014 Amyotrophic lateral sclerosis - Homo sapiens (human) (2) hsa836 K02187 CASP3; caspase 3 hsa847 K03781 CAT; catalase hsa05022 Pathways of neurodegeneration - multiple diseases - Homo sapiens (human) (2) hsa836 K02187 CASP3; caspase 3 hsa847 K03781 CAT; catalase	-	-	-	-	-
Sodium benzoate	532-32-1					Mouse	Male	Swiss	Drinking water	113	113	Negative	Liver	Hepatoma									
Sodium benzoate	532-32-1					Rat	Female	Fischer 344	Diet	104	108	Negative	Multiple sites	Multiple tumour types									
Sodium benzoate	532-32-1					Rat	Male	Fischer 344	Diet	104	108	Negative	Multiple sites	Multiple tumour types									
Sodium bilthionolate	6385-58-6	C1=C(C)=CC=C1(C)(S)[O-].[SC(=CC(=CC=C2)[O-])C2(S)[O-]].[Na+].[Na+]	-	7, 14, 19, 23, 25, 27, 29, 30, 34, 36, 46, 52, 53, 58, 61, 64, 66, 67, 71, 72, 111, 112, 117, 122, 123, 153, 163, 166, 167, 187, 200, 204, 207, 218	-	Mouse	Female	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma	-				-	-	-	-
Sodium bilthionolate	6385-58-6					Mouse	Male	B6AKF1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Sodium bilthionolate	6385-58-6					Mouse	Female	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Hepatoma									
Sodium bilthionolate	6385-58-6					Mouse	Male	B6C3F1	Gavage (preweaning) then diet	76	76	Negative	Liver	Multiple tumour types									
Sodium saccharin	128-44-9	[Na+].[O-]c2c.c(S(=O)(=O)N1C(=C(C=C(C=C1)C(=N2)[O-])	자료없음	29, 30, 52, 53, 67, 112, 165, 167, 200	Genotoxicity Data: clastogenic	Cynomolgus monkey	Mixed	Not specified	Diet	1221	1221	Not specified	Multiple sites	Tumour - malignant									
Sodium saccharin	128-44-9					Mouse	Female	CD-1 HsMICR	Diet	104	104	Negative	Liver	Multiple tumour types									
Sodium saccharin	128-44-9					Mouse	Male	CD-1 HsMICR	Diet	104	104	Negative	Liver	Hepatoma									
Sodium saccharin	128-44-9					Rat	Male	ACI	Diet	52	52	Positive	Urinary bladder	Carcinoma: transitional cell									
Sodium saccharin	128-44-9					Rat	Male	Anaibuminsemic Sprague-Dawley	Diet	80	80	Negative	Urinary bladder	Carcinoma									
Sodium saccharin	128-44-9					Rat	Male	Fischer 344	Diet	100	104	Negative	Urinary bladder	Multiple tumour types									
Sodium saccharin	128-44-9					Rat	Male	Fischer 344	Diet	102	104	Negative	Urinary bladder	Multiple tumour types									
Sodium saccharin	128-44-9					Rat	Male	Fischer 344	Diet	104	104	Negative	Urinary bladder	Multiple tumour types									
Sodium saccharin	128-44-9					Rat	Male	Fischer 344	Diet	52	52	Negative	Urinary bladder	Multiple tumour types									
Sodium saccharin	128-44-9					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Multiple tumour types									
Sodium sphenisuphonate	1300-72-7	O=S(=O)(C=1C=C2C=CC=C(C=C2C=C1)C)C)[O-].[Na+]	자료없음	57, 131		Mouse	Female	B6C3F1	Dermal	90 d	90 d	Not specified											
Solvent Blue 18	2475-45-8	C1(=C)C(C(=2C(C1=O)=C)C=CC=2N(N)=O)C)=CC=CN	흡흡기 과민성 : 구분1(1A/1B) 피부 과민성 : 구분1(1A/1B) 발암성 : 구분1B 급성 수생환경 유해성 : 구분1	-	Cancer slope factor: 1.3e-06 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Diet	103	106	Not specified	Liver	Adenoma - hepatocellular	H2AX KRT14	AMH R2 CCR6 DNASE2 TBP1 IL1R1	HTATSF2 CASP2 CYTIP SAT RNFT2		urinary bladder kidney spleen liver large intestine all tumor bearing animals	urinary bladder uterus ear Zymbals gland kidney liver thyroid gland clitoral gland lung hematopoietic system	thyroid gland vascular system urinary bladder liver stomach lung	thyroid gland liver vascular system urinary bladder lung hematopoietic system stomach ovary pituitary gland	-
Solvent Blue 18	2475-45-8					Mouse	Male	B6C3F1	Diet	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular									
Solvent Blue 18	2475-45-8					Rat	Female	Fischer 344	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Solvent Blue 18	2475-45-8					Rat	Male	Fischer 344	Diet	103	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Sotalol hydrochloride	959-24-0	CS(NC1=CC=C(C=C1)C(=O)C(=CC=C2)C(=O)C=3C(O)=[O]=[O]=C)C		46		Mouse	Female	CD1	Diet	78	92	Negative	Liver	Multiple tumour types					all tumor bearing animals		thyroid gland		
Sotalol hydrochloride	959-24-0					Mouse	Male	CD1	Diet	78	92	Negative	Liver	Adenoma									
Sotalol hydrochloride	959-24-0					Rat	Female	Long-Evans	Diet	78	104	Negative	Liver	Cholangioma									
Sotalol hydrochloride	959-24-0					Rat	Male	Long-Evans	Diet	78	104	Negative	Liver	Adenoma - hepatocellular									
Steviglmatocytin	10048-13-2	C3=.C)C1=C(OC2=.C)C1=O)C(=C-C(2O)C4=C3O)C@@[S]C@[4C=C(O)]=O)[=O]=O)OC	급성 독성(경구) : 구분4 피부 부식성/자극 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A/2B) 변이원성 : 구분2 발암성 : 구분2 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1 특정표적장기 독성(반복 노출) : 구분2	-	Cancer slope factor: 0.01 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen	Cynomolgus monkey	Mixed	Not specified	Gavage	663	663	Positive	Adrenal gland	Adenoma - cortical	MSH1 CDK1 CDC25C CCNB1 CYP3A4 CHEK1	PLCG2 ACOT2 CCL16 GFLD1 SLC41A2	KIAA0247 PPP1R14C CARKN PLK4 BLM							
Steviglmatocytin	10048-13-2					Mouse	Female	B6F1	Diet	55	68	Positive	Brown fat - dorsal	Angiosarcoma									
Steviglmatocytin	10048-13-2					Mouse	Female	B6F1	Diet	55	73	Positive	Brown fat - dorsal	Angiosarcoma									
Steviglmatocytin	10048-13-2					Rat	Male	ACI/N	Diet	120	122	Positive	Liver	Carcinoma - hepatocellular									
Styrene	100-42-5	C1=CC=CC(=C1)C=C	인화성 액체 : 구분2 급성 독성(흡입) 유가스 : 구분4 피부 부식성/자극 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A/2B) 변이원성 : 구분2 발암성 : 구분2 생식독성 : 구분2 특정표적장기 독성(1회 노출) : 구분1(호흡기 자극) 특정표적장기 독성(반복 노출) : 구분1 흡인 유해성 : 구분1	-	Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	78	91	Not specified	Liver	Adenoma - hepatocellular	CYP2E1 TNF CXCL8 Il6	SEEM1 IRF2 TRAM2 RNF72 CYLNR40	FGFR1 WT1 SOD3 TNNC2 HTATSF2		oral cavity stomach kidney spleen Malloni head cancers ear Zymbals gland	mammary gland uterus nasal cavity stomach oral cavity	lung stomach vascular system small intestine	ovary lung stomach thyroid gland urinary bladder peritoneal cavity pituitary gland small intestine	Breast Neoplasm Lung Neoplasm Urinary Bladder Neoplasm Lymphoma, Non-Hodgkin Mammary Neoplasm, Animal Mastocytosis, Systemic
Styrene	100-42-5					Mouse	Male	B6C3F1	Gavage	78	91	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Styrene	100-42-5					Mouse	Female	CD1	Inhalation	52	52	Not specified	Lung	Adenoma - alveolar/bronchiolar									
Styrene	100-42-5					Mouse	Female	CD1	Inhalation	78	78	Not specified	Lung	Adenoma - alveolar/bronchiolar									
Styrene	100-42-5					Mouse	Female	CD1	Inhalation	98	98	Positive	Lung	Multiple tumour types									
Styrene	100-42-5					Mouse	Male	CD1	Inhalation	52	52	Not specified	Lung	Adenoma - alveolar/bronchiolar									
Styrene	100-42-5					Mouse	Male	CD1	Inhalation	78	78	Not specified	Lung	Adenoma - alveolar/bronchiolar									
Styrene	100-42-5					Mouse	Male	CD1	Inhalation	104	105	Positive	Liver	Adenoma - hepatocellular									
Styrene	100-42-5					Rat	Female	Fischer 344	Gavage	90	97	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Styrene oxide	96-09-3	O1(C)C1(C2)=CC=CC=C2	인화성 액체 : 구분4 급성 독성(경구) : 구분4 피부 부식성/자극 자극성 : 구분2 심한 눈 손상성/눈 자극성 : 구분2A/2B) 피부 과민성 : 구분1(1A/1B) 변이원성 : 구분2 발암성 : 구분1B	8, 11, 19, 22, 29, 30, 52, 53, 57, 60, 67, 111, 112, 165, 167, 187, 200, 207	Cancer slope factor: 4.6e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: genotoxic	Mouse	Female	B6C3F1	Gavage	104	107	Positive	Forestomach	Carcinoma - squamous cell	EPHB1 GSTM1 CASP3 Il2 Il10	TRAF5 CAPRIN1 GSS PGM2L1 DSE	AURKA CDK6B MDUF82 KRT34 CASP2	Fugal1524 Platinum drug resistance - Homo sapiens (human) (2) hsa2944 K00799 GSTM1; glutathione S-transferase mu 1 hsa836 K02187 CASP3; caspase 3 hsa05200 Pathways in cancer - Homo sapiens (human) (2) hsa2944 K00799 GSTM1; glutathione S-transferase mu 1 hsa836 K02187 CASP3; caspase 3 hsa05130 Pathogenic Escherichia coli infection - Homo sapiens (human) (1) hsa836 K02187 CASP3; caspase 3	stomach hematopoietic system thyroid gland vascular system nasal cavity all tumor bearing animals	stomach hematopoietic system nasal cavity all tumor bearing animals	stomach vascular system	stomach pituitary gland peritoneal cavity urinary bladder thyroid gland	Stomach Neoplasm Liver Neoplasm, Experimental
Styrene oxide	96-09-3					Mouse	Male	B6C3F1	Gavage	104	107	Positive	Forestomach	Carcinoma - squamous cell									
Styrene oxide	96-09-3					Rat	Female	Fischer 344	Gavage	104	107	Positive	Forestomach	Carcinoma - squamous cell									
Styrene oxide	96-09-3					Rat	Male	Fischer 344	Gavage	104	107	Positive	Forestomach	Carcinoma - squamous cell									
Styrene/beta-nitrostyrene	-	C1=CC=CC(=C1)C=C(C2)=CC=CC(=C2)C=C2N=[]([O-])=O	-	-	-	Mouse	Female	B6C3F1	Gavage	78	92	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic	-					-	-	-	-
Styrene/beta-nitrostyrene	-					Mouse	Male	B6C3F1	Gavage	79	92	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Styrene/beta-nitrostyrene	-					Rat	Female	Fischer 344	Gavage	79	108	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Styrene/beta-nitrostyrene	-					Rat	Male	Fischer 344	Gavage	79	108	Not specified	Liver	Adenoma - hepatocellular | Carcinoma/hepatocellular | Nodule - neoplastic									
Sulindac sulfone	59973-80-7	O=S(=O)(C=3C=C(C(=C2C1=C(C=C(C=C1)C)=C2)C)C)=O)=O)=CC=3C		29, 30, 52, 53, 61, 67, 112, 165, 167, 200		Rat	Male	Fischer 344	Diet	53	53	Negative	Colon	Multiple tumour types					spleen				
Sulphadimidine	57-68-1	O=S(=O)(C=1C=CC(=CC=1)NNC2=NC(=CC(=N2)C)C	심한 눈 손상성/눈 자극성 : 구분2A/2B)	8, 11, 60	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	52	52	Not specified	Liver	Adenoma - hepatocellular	NAT2 NAT1 CYP2A6 NR1I2	KEAP1 CTPS1 INCENP HBP1 CCR6	SAT TACC1 INS PIR HYI0	Fugal0983 Drug metabolism - other enzymes - Homo sapiens (human) (2) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa10 K00622 NAT1; N-acetyltransferase 1 hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa10 K00622 NAT1; N-acetyltransferase 1 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (2) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa10 K00622 NAT1; N-acetyltransferase 1	spleen urinary bladder	kidney small intestine urinary bladder vascular system ear Zymbals gland	thyroid gland urinary bladder	thyroid gland urinary bladder liver	Adenoma Thyroid cancer, follicular Thyroid Neoplasm
Sulphadimidine	57-68-1					Mouse	Female	B6C3F1	Diet	78	78	Not specified	Liver	Adenoma - hepatocellular									
Sulphadimidine	57-68-1					Mouse	Female	B6C3F1	Diet	104	104	Positive	Liver	Adenoma - hepatocellular									
Sulphadimidine	57-68-1					Mouse	Male	B6C3F1	Diet	52	52	Not specified	Liver	Adenoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADIs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Sulphafurazole	127-69-5	C=1(C(C)=NOC=1NS(=O)(=O)C=2C=1(C(=2C=1(C(=C2)N))NC)	표준기 과민성 : 구분1(A/1B)	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: predicted to be genotoxic	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic	AIB CYP3A4 PON1 SRXN1	KEAP1 CTPS1 BNC5MP RCC2 BGLAP	SAT PIR TACC3 HTR3 INS	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (1) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa00830 Retinol metabolism - Homo sapiens (human) (1) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4 hsa00591 Linoleic acid metabolism - Homo sapiens (human) (1) hsa1576 K17689 CYP3A4; cytochrome P450 family 3 subfamily A member 4	spleen urinary bladder	urinary bladder	thyroid gland urinary bladder	thyroid gland urinary bladder	-
Sulphafurazole	127-69-5					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Sulphafurazole	127-69-5					Rat	Female	Fischer 344	Diet	103	106	Not specified	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Sulphafurazole	127-69-5					Rat	Male	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma- hepatocellular | Carcinoma|hepatocellular | Nodule- neoplastic									
Suaibazone	27470-51-0	C(O)C(CCC(O)=O)=O)=C(C1(C)N)NC(=1)=C(=2)=CC=CC=C2)C(=2=CC=C=C(C=C(C=2)=O)CCCC	-	8, 11, 60	-	Rat	Female	Fischer 344/DuCr)	Diet	104	104	Negative	Liver	Multiple tumour types	PKLR	ZBED2 TRAJA NDE1 WDR4 SMARCC1	IL23A KATS TMEM71 PCDH17 TMEM4A	hsa00620 Pyruvate metabolism - Homo sapiens (human) (1) hsa5213 K12406 PKLR; pyruvate kinase L/R hsa01100 Metabolic pathways - Homo sapiens (human) (1) hsa5213 K12406 PKLR; pyruvate kinase L/R hsa01200 Carbon metabolism - Homo sapiens (human) (1) hsa5213 K12406 PKLR; pyruvate kinase L/R	-	easy Zymbals gland	kidney	lung	**Liver Neoplasm, Experimental**
Suaibazone	27470-51-0					Rat	Male	Fischer 344/DuCr)	Diet	104	104	Negative	Adrenal gland	Pheochromocytoma									
Tamoxifen citrate	54965-24-1	C(1=CC=CC=C1(C)(C=2CC=2C=CC=C2)OCCN(C)C)=1C(=2C=CC=C2)OCCN(C)C)=1C(=2C=CC=C2)OCCN(C)C)=O)=C(=O)O.O	-	6, 7, 8, 11, 14, 16, 18, 19, 20, 25, 27, 29, 30, 34, 36, 37, 43, 46, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 107, 111, 112, 117, 120, 123, 131, 153, 163, 165, 166, 167, 187, 200, 214, 281, 302, 312, 318	-	Mouse	Female	Elderly Park	Multiple routes	65	65	Positive	Liver	Multiple tumour types	ESR1 LDL GPER1 ESRRG CYP19A1 PGR CYP22A CYP19A4	-	-	hsa04152 Endocrine resistance - Homo sapiens (human) (4) hsa1565 K17712 CYP20A; cytochrome P450 family 2 subfamily D member 6 hsa2100 K08551 ESR2; estrogen receptor 2 hsa2852 K04246 GPER1; G protein-coupled estrogen receptor 1 hsa595 K04503 CCND1; cyclin D1 hsa05224 Breast cancer - Homo sapiens (human) (3) hsa2100 K08551 ESR2; estrogen receptor 2 hsa5241 K08556 PGR; progesterone receptor hsa595 K04503 CCND1; cyclin D1 hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (3) hsa2100 K08551 ESR2; estrogen receptor 2 hsa5241 K08556 PGR; progesterone receptor hsa595 K04503 CCND1; cyclin D1	-	-	-	-	Carcinoma, Renal Cell **Liver Neoplasm, Experimental** Precancerous Conditions
Tamoxifen citrate	54965-24-1					Mouse	Male	Elderly Park	Multiple routes	65	65	Positive	Liver	Hepatoblastoma									
Tamoxifen citrate	54965-24-1					Mouse	Male	Elderly Park	Multiple routes	56	56	Not specified	Not applicable	Mortality									
Tamoxifen citrate	54965-24-1					Mouse	Male	Elderly Park	Multiple routes	56	56	Not specified	Not applicable	Mortality									
Tamoxifen citrate	54965-24-1					Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Adenoma- hepatocellular									
Tamoxifen citrate	54965-24-1					Mouse	Female	C57BL/6	Diet	52	52	Negative	Liver	Carcinoma- hepatocellular									
Tamoxifen citrate	54965-24-1					Mouse	Female	DBA/2	Diet	52	52	Negative	Liver	Carcinoma- hepatocellular									
Tamoxifen citrate	54965-24-1					Rat	Female	Alpk:APFD	Gavage	88	107	Positive	Liver	Adenoma- hepatocellular									
Tamoxifen citrate	54965-24-1					Rat	Male	Alpk:APFD	Gavage	88	107	Positive	Liver	Adenoma- hepatocellular									
Tamoxifen citrate	54965-24-1					Rat	Female	Fischer 344/Tox	Diet	86	86	Positive	Liver	Carcinoma- hepatocellular									
Tannins	1401-55-4	C(C1=(C(=2)C(=C(OC(C=2=C(=C)=2)=C2)O)O)O)=O)O)O)=O)O)C(@H)O)C(C1=(C(=2)=C(O)=C2)O)C(=O)=C(=C(=C(=C(=O)O)=O)O)O)=O)O)C@@H)O)C(C1=(C(=2)=C(O)=C2)O)C(=O)=C(=C(=C(=C(=O)O)=O)O)O)=O)O)C@@H)OR)C(C(N)=O=C(=2)=C(=C(N)=O)C(C(N)=O=C(=2)=C(=C(N)=O)C(=2)=C(=C(N)=O)C(=2)=C(=C(N)=O)

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Tetradifon	116-29-0	O=S(=O)(C1=CC=CC(=CC=1)Cl)C1=CC=1Cl)C2=CC(=O)C=1C2C)Cl)	경성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	7, 8, 11, 19, 21, 25, 27, 29, 30, 34, 36, 43, 46, 52, 53, 58, 60, 61, 62, 67, 72, 111, 112, 117, 122, 123, 152, 163, 166, 167, 187, 200, 207	-	Mouse	Female	B6AKR1	Gavage (pretreating) than diet	76	76	Negative	Liver	Hepatoma	EGR1 EDN2	FABP4 AIRN7 CADPS2 CCDC49 FNIP2	BEL S100A SAT CYP11B2 DAAH1TA1	-	spleen thyroid gland	-	-	thyroid gland urinary bladder	-
Tetradifon	116-29-0					Mouse	Male	B6AKR1	Gavage (pretreating) than diet	76	76	Negative	Liver	Hepatoma									
Tetradifon	116-29-0					Mouse	Female	B6C3F1	Gavage (pretreating) than diet	76	76	Negative	Liver	Hepatoma									
Tetradifon	116-29-0					Mouse	Male	B6C3F1	Gavage (pretreating) than diet	76	76	Negative	Liver	Hepatoma									
Tetraul	2227-13-6	C1=C(C)=CC(=C1OC)B(C2=CC=C(C=C2)Cl)Cl	-	8, 11, 29, 30, 52, 53, 60, 67, 112, 165, 167, 200	-	Rat	Female	Wistar	Diet	116	116	Negative	Liver	Multiple tumour types	-				thyroid gland large intestine spleen ear Zymbals gland	ear Zymbals gland thyroid gland uterus	thyroid gland liver	thyroid gland liver urinary bladder	-
Tetraul	2227-13-6					Rat	Female	Wistar	Diet	104	104	Negative	Liver	Multiple tumour types									
Tetraul	2227-13-6					Rat	Male	Wistar	Diet	116	116	Negative	Liver	Hepatoma									
Tetraul	2227-13-6					Rat	Male	Wistar	Diet	104	104	Negative	Liver	Multiple tumour types									
Thiabendazole	148-79-8	C1[n]=NC2=C(N)[C]=CC=C2[C]=3N=CSC==3	경성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 10, 11, 21, 29, 30, 34, 41, 46, 52, 53, 57, 58, 60, 61, 67, 112, 122, 123, 131, 150, 166, 167, 200, 220, 310	Carcinogenicity data available EPA OPP Likely to be Carcinogenic to Humans (High Doses), Not Likely to be Carcinogenic to Humans (Low Doses) Genotoxicity Data: genotoxic	Mouse	Male	B6C3F1	Diet	52	52	Negative	Liver	Adenoma- hepatocellular	CYP1A1 CYP1A2 CYP2B1 CYP2B2 GCLC RND3 ACOT12	SLC15A1	CYP1A2 CYP2A4 CYP2B6 SCSDL	hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1544 607409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa2729 611204 GCLC; glutamate-cysteine ligase catalytic subunit hsa00830 Retinol metabolism - Homo sapiens (human) (1) hsa1544 607409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa00232 Caffeine metabolism - Homo sapiens (human) (1) hsa1544 607409 CYP1A2; cytochrome P450 family 1 subfamily A member 2	-	stomach mammary gland ear Zymbals gland small intestine all tumor bearing animals	urinary bladder	hematopoietic system	Urinary Bladder Neoplasm
Thiabendazole	148-79-8					Mouse	Female	C57 CD-1 (ICR)	Diet	78	78	Negative	Liver	Multiple tumour types									
Thiabendazole	148-79-8					Mouse	Male	C57 CD-1 (ICR)	Diet	78	78	Negative	Liver	Adenoma- hepatocellular									
Thiabendazole	148-79-8					Rat	Female	Fischer 344/DuCrl	Diet	65	65	Not specified	Urinary bladder	Multiple tumour types									
Thiamphenicol	15318-45-3	O=S(=O)(C1=CC=C(C=C1)[C@H]([C@@H](CO)NC(=O)C(Cl)Cl)=O)C(C	만성 수생환경 유해성 - 구분2	-	-	Rat	Female	Fischer 344/DuCrl	Drinking water	104	108	Negative	Liver	Multiple tumour types	ABCG2 SLC1A2	FABP4	-		spleen	-	-	-	-
Thiamphenicol	15318-45-3					Rat	Male	Fischer 344/DuCrl	Drinking water	104	108	Negative	Liver	Adenoma- hepatocellular									
Tiliric acid	37087-04-8	O=[S](O)N1[C@H]([C@H]([C@H]1[C]N[C]C(=O)[C]=C(C=C(C)=C)[C]N)O)=O				Rat	Male	Fischer 344	Diet	70	71	Positive	Liver	Carcinoma- hepatocellular	-				liver				
Tilmicosol hydrochloride	62774-06-3	C1=CC=C(C)=C1C(N(C=C2)CC(C)=C)C(=C2)CC(C)=C)C(=O)=O			-	Mouse	Female	CD1	Gavage	80	80	Negative	Liver	Multiple tumour types	-				skin	nasal cavity ear Zymbals gland	stomach	hematopoietic system	-
Tilmicosol hydrochloride	62774-06-3					Mouse	Male	CD1	Gavage	80	80	Negative	Liver	Adenoma- hepatocellular									
Tilmicosol hydrochloride	62774-06-3					Rat	Female	SD	Gavage	104	104	Negative	Liver	Adenoma- hepatocellular									
Tilmicosol hydrochloride	62774-06-3					Rat	Male	SD	Gavage	104	104	Negative	Liver	Adenoma- hepatocellular									
Tocopherols	1406-66-2	C1(=C(C)=C(C)=C1[R]([C]CC[C]([C]CCC[C]([C]CCC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)CCC)[R])[R])[R])O)=C(C)=C4[C]=C3[R]([C]CC[C]4[C]CCC[C]3[C]CCC[C]([C]CCC[C]([C]CCC[C]([

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Tolazamide	1156-19-0	N1(CCCCCC1)NC(NS(=O)(=O)C2=CC=C(C)C=C2)C=O	경구 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	57, 61	-	Mouse	Female	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	DDIT3 INS1	CTSF1 INC5NP	ING		spleen	vascular system	thyroid gland	-	-
Tolazamide	1156-19-0					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Tolazamide	1156-19-0					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Tolazamide	1156-19-0					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Tolbutamide	64-77-7	O=S(=O)(C1=CC=C(C)C=C1)NC(NCCCC)=O	생식독성 - 구분1A	-	Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Diet	78	103	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	CYP2C9 CYP2C19 INS INS1 SLC2A1 ABCC8 ALB	CTSF1	ING	hsa04911 Insulin secretion - Homo sapiens (human) (3) hsa:2630 KH5426 INS; insulin hsa:6513 KE7299 SLC2A1; solute carrier family 2 member 1 hsa:6833 KE9032 ABCC8; ATP binding cassette subfamily C member 8 hsa04066 HIF-1 signaling pathway - Homo sapiens (human) (2) hsa:2630 KH5426 INS; insulin hsa:6513 KE7299 SLC2A1; solute carrier family 2 member 1 hsa04931 Insulin resistance - Homo sapiens (human) (2) hsa:2630 KH5426 INS; insulin hsa:6513 KE7299 SLC2A1; solute carrier family 2 member 1	spleen large intestine skin	-	thyroid gland	-	-
Tolbutamide	64-77-7					Mouse	Male	B6C3F1	Diet	78	102	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Tolbutamide	64-77-7					Rat	Female	Fischer 344	Diet	78	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Tolbutamide	64-77-7					Rat	Male	Fischer 344	Diet	78	106	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Toluene	108-88-3	C1=CC=CC(=C1)C	인화성 액체 - 구분2 피부 부식성/피부 자극성 - 구분2 생식독성 - 구분2 특정표적장기 독성(1회 노출) - 구분3(마취졸림) 특정표적장기 독성(반복 노출) - 구분2 흡인 유해성 - 구분1	-	Carcinogenicity data available: EPA OPP-Group D Not Classifiable as to Human Carcinogenicity Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Inhalation	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	AR TP53 IL4 TNF IL1B KDR3 CASP3	CTSD IRF2 TADA2 RNF12 DHFR	BCL2A1 MAP3K8 ZC3HC1 DENND5A NFATS	hsa05140 Leishmaniasis - Homo sapiens (human) (3) hsa:3553 KH4519 IL1B; interleukin 1 beta hsa:3565 KE5430 IL4; interleukin 4 hsa:7124 KE0156 TNF; tumor necrosis factor hsa04657 IL-17 signaling pathway - Homo sapiens (human) (3) hsa:3553 KH4519 IL1B; interleukin 1 beta hsa:3565 KE5430 IL4; interleukin 4 hsa:7124 KE0156 TNF; tumor necrosis factor hsa04640 Hematopoietic cell lineage - Homo sapiens (human) (3) hsa:3553 KH4519 IL1B; interleukin 1 beta hsa:3565 KE5430 IL4; interleukin 4 hsa:7124 KE0156 TNF; tumor necrosis factor	oral cavity spleen Malignant head cancers liver kidney nasal cavity urinary bladder vascular system ear Zymbals gland	urinary bladder clitoral gland nasal cavity liver oral cavity thyroid gland **uterus** kidney stomach lung	urinary bladder thyroid gland vascular system kidney lung stomach small intestine liver	urinary bladder **ovary** thyroid gland vascular system pituitary gland stomach liver peritoneal cavity small intestine	Neoplasm
Toluene	108-88-3					Mouse	Male	B6C3F1	Inhalation	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Toluene	108-88-3					Rat	Female	Fischer 344	Inhalation	105	105	Negative	Liver	Multiple tumour types									
Toluene	108-88-3					Rat	Female	Fischer 344	Inhalation	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Toluene	108-88-3					Rat	Male	Fischer 344	Inhalation	106	106	Negative	Liver	Multiple tumour types									
Toluene diisocyanates	26471-62-5	C1=C(C=C(C)=C1)[N]=C=O)N=C=O)N=C=O)C=2[C]=CC=CC=2N=C=O)N=C=O)C	경구 독성(흡입): 유기 - 구분1 피부 부식성/피부 자극성 - 구분2 심한 눈 손상/눈 자극성 - 구분2A(2B) 호흡기 과민성 - 구분1(1A/1B) 피부 과민성 - 구분1(1A/1B) 발암성 - 구분2 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극) 위험성 수생환경 유해성 - 구분3	14, 19, 21, 23, 41, 57, 64, 66, 71, 111, 117, 131, 150, 187, 204, 207, 210, 318	Cancer slope factor: 1.1e-05 (ug/m3)-1 (carcinogenicity, inhalation) Carcinogenicity data available: CalEPA-Likely Human Carcinogen Genotoxicity Data: inconclusive	Mouse	Female	B6C3F1	Gavage	105	107	Positive	-	Abdominal cavity : Haemangiosarcoma Liver : Haemangiosarcoma | Adenomahepatocellular **Ovary** : Haemangiosarcoma Skin - subcutaneous tissue : Haemangioma Spleen : Haemangioma	skin spleen hematopoietic system Malignant head cancers	liver mammary gland **uterus** hematopoietic system clitoral gland	vascular system urinary bladder thyroid gland	liver vascular system urinary bladder	-
Toluene diisocyanates	26471-62-5					Mouse	Male	B6C3F1	Gavage	105	107	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Toluene diisocyanates	26471-62-5					Mouse	Female	CD1	Inhalation	104	104	Negative	Liver	Adenoma - hepatocellular									
Toluene diisocyanates	26471-62-5					Mouse	Male	CD1	Inhalation	104	104	Negative	Liver	Adenoma - hepatocellular									
Toluene-2,6-diamine dihydrochloride	15481-70-6	C1=CC(=C(C)=C1)N(C)N(C)C1	-	-	-	Mouse	Female	B6C3F1	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic	-				spleen liver urinary bladder ear Zymbals gland thyroid gland kidney	urinary bladder **uterus** ear Zymbals gland clitoral gland lung liver thyroid gland mammary gland hematopoietic system small intestine	thyroid gland urinary bladder vascular system liver	liver thyroid gland vascular system urinary bladder hematopoietic system **ovary**	-
Toluene-2,6-diamine dihydrochloride	15481-70-6					Mouse	Male	B6C3F1	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Toluene-2,6-diamine dihydrochloride	15481-70-6					Rat	Female	Fischer 344	Diet	103	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Toluene-2,6-diamine dihydrochloride	15481-70-6					Rat	Male	Fischer 344	Diet	103	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma|hepatocellular | Nodule - neoplastic									
Toluene-2-sulphonamide	88-19-7	NS(C1=CC=CC=C1C)=O)=O	경구 독성(경구) - 구분4 호흡결막자극 독성(반복 노출) - 구분2	43	Genotoxicity Data: inconclusive	Rat	Female	SD	Diet	142	142	Not specified	Liver	Nodule - neoplastic					spleen Malignant head cancers	-	thyroid gland	urinary bladder thyroid gland	-
Toluene-2-sulphonamide	88-19-7					Rat	Male	SD	Diet	142	142	Not specified	Liver	Angiosarcoma									
Toluene-2-sulphonamide	88-19-7					Rat	Mixed	SD	Diet	133	142	Positive	Liver	Carcinoma									
Toluene-2-sulphonamide	88-19-7					Rat	Female	Wistar	Drinking water	102	102	Negative	Liver	Carcinoma - hepatocellular									
Tomelukast	88107-10-2	C(CC1=NN=NN1)CCOC2=CC=C(C)C=C2[C]C(O)C(C)=O	-	6, 8, 11, 14, 18, 19, 23, 29, 30, 34, 36, 37, 46, 51, 52, 53, 58, 60, 61, 62, 64, 66, 67, 71, 72, 111, 152, 157, 163, 165, 166, 167, 187, 200, 214, 307, 318	-	Mouse	Female	B6C3F1	Diet	104	104	Positive	Liver	Adenoma - hepatocellular	CYP27B1 PAX PPP PPARA PPARG RORA	NOP56	NR1H2 OSS	hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa:5468 KO8530 PPARG; peroxisome proliferator-activated receptor gamma hsa:572 KO2158 BAX; BCL2 associated agonist of cell death hsa:581 KO2159 BAK; BCL2 associated X, apoptosis regulator hsa05160 Hepatitis C - Homo sapiens (human) (3) hsa:5465 KO7294 PPARA; peroxisome proliferator-activated receptor alpha hsa:572 KO2158 BAX; BCL2 associated agonist of cell death hsa:581 KO2159 BAK; BCL2 associated X, apoptosis regulator hsa04932 Non-alcoholic fatty liver disease - Homo sapiens (human) (3) hsa:5465 KO7294 PPARA; peroxisome proliferator-activated receptor alpha hsa:5468 KO8530 PPARG; peroxisome proliferator-activated receptor gamma hsa:581 KO2159 BAK; BCL2 associated X, apoptosis regulator	-	-	liver	liver	-
Tomelukast	88107-10-2					Mouse	Male	B6C3F1	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular									
Toremifene citrate	89778-27-8	C(C)=C(C1=CC=C(C=C1)OCCN(C)C)C2=CC=CC=C2[C]=C=CC=C2[C]=C=CC=C2[C](C)C)O[C](C)C)O)=O)C(C)=O)C(C)=O)O	-	7, 8, 11, 14, 19, 23, 23, 27, 29, 30, 34, 36, 46, 52, 53, 58, 60, 61, 62, 64, 66, 67, 71, 72, 111, 152, 157, 163, 123, 150, 165, 166, 167, 187, 200, 214, 307, 318	-	Rat	Female	SD	Gavage	52	52	Negative	Liver	Multiple tumour types	-				-	-	-	-	-
Toremifene citrate	89778-27-8					Rat	Female	SD	Gavage	52	65	Negative	Liver	Multiple tumour types									
Toremifene citrate	89778-27-8					Rat	Female	SD	Gavage	52	65	Negative	Liver	Adenoma - hepatocellular									
Toremifene citrate	89778-27-8					Rat	Female	SD	Gavage	52	65	Negative	Liver	Adenoma - hepatocellular									
Toremifene citrate	89778-27-8					Rat	Female	SD	Gavage	52	52	Negative	Liver	Multiple tumour types									
trans-(±)-[2-(Thiocyanatoethyl)-2-phenylcyclohex-5-enyl]dimethylammonium hydrogen fumarate	55567-81-2	C(=O)(OCC)[C@]1[C@H]2=CCC1(NC)C)C2=CC=CC=C2)C3=CC=CC=C3)C(C)C)O)[C(C)O]=O)C(C)=O)C(C)=O)O	-	-	-	Mouse	Female	CF-1	Diet	80	80	Negative	Liver	Adenoma - hepatocellular	-				-	-	-	-	-
trans-(±)-[2-(Thiocyanatoethyl)-2-phenylcyclohex-5-enyl]dimethylammonium hydrogen fumarate	55567-81-2					Mouse	Male	CF-1	Diet	80	80	Negative	Liver	Adenoma - hepatocellular									
trans-(±)-[2-(Thiocyanatoethyl)-2-phenylcyclohex-5-enyl]dimethylammonium hydrogen fumarate	55567-81-2					Rat	Female	Wistar	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
trans-(±)-[2-(Thiocyanatoethyl)-2-phenylcyclohex-5-enyl]dimethylammonium hydrogen fumarate	55567-81-2					Rat	Male	Wistar	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									

Chemical Name	CAS No.	SMILES	GHS Classific.	ADPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Triamterene	396-01-0	N1=c(N)=c(N[C]c=C1N)N=c(C)=N2(N)C(=c(C=c(C=c(N	급성 독성(경구) - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상/눈 자극성 - 구분2A(사)(B) 발암성 - 구분2 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극)	14, 15, 21, 22, 27, 28, 30, 34, 36, 41, 46, 52, 53, 57, 58, 61, 64, 66, 67, 71, 72, 111, 112, 118, 120, 150, 163, 166, 167, 187, 200, 214, 307, 310, 318	Carcinogenicity data available CalEPA Likely Human Carcinogen	Mouse	Female	B6C3F1	Diet	104	104	Positive	Liver	Adenoma - hepatocellular	ABCB1A ABCG2 ACE BCAT1 CYP2A5 EGFR HMOX1	SLC15A1 BCAS3 VPRBP RNF186 FHIT	GRIP1 LGT1 SP1 DNMT3A CYYR1	hsa05171 Coronavirus disease - COVID-19 - Homo sapiens (human) (2) hsa1636 KEGG: ACE; angiotensin I converting enzyme hsa1956 KEGG: EGFR; epidermal growth factor receptor hsa01100 Metabolic pathways - Homo sapiens (human) (2) hsa1544 KEGG: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa586 KEGG: BCAT1; branched chain amino acid transaminase 1 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (2) hsa1544 KEGG: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1956 KEGG: EGFR; epidermal growth factor receptor	ear Zymbals gland large intestine spleen	ears Zymbals gland small intestine clitoral gland	liver urinary bladder	liver hematopoietic system vascular system	liver Neoplasm
Triamterene	396-01-0					Mouse	Female	B6C3F1	Diet	104	104	Positive	Liver	Adenoma - hepatocellular									
Triamterene	396-01-0					Mouse	Male	B6C3F1	Diet	104	104	Positive	Harderian gland	Adenoma									
Triamterene	396-01-0					Mouse	Male	B6C3F1	Diet	104	104	Positive	Liver	Adenoma - hepatocellular | Carcinoma-hepatocellular									
Trichloroethylpentachlorobenzene	29082-74-4	C1(c(c(C(c(c(Cl)c(Cl)Cl)Cl)Cl)Cl)Cl)Cl	-	-	-	Mouse	Male	C57BL/10SnSn	Diet	78	78	Not specified	Liver	Nodule - hyperplastic	AHR NRF2 ARNTM1 UGT1A6A CYP1A1 CYP1A2 CYP2B10	IR27 GJA1 SNAI1B CTSD MYO5C	NQO1 URP6 GAUN5 MCCC1 NPTX1	hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (3) hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KEGG: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa4616 KEGG: NRF2; nuclear respiration factor 2 subfamily 1 group I member 2 hsa05204 Chemical carcinogenesis - DNA adducts - Homo sapiens (human) (3) hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KEGG: CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa6817 KEGG: SULT1A1; sulfotransferase family 1A member 1 hsa00140 Steroid hormone biosynthesis - Homo sapiens (human) (2) hsa1543 KEGG: CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KEGG: CYP1A2; cytochrome P450 family 1 subfamily A member 2	kidney hematopoietic system thyroid gland	kidney	-	thyroid gland	-
Trichloroethylpentachlorobenzene	29082-74-4					Rat	Female	SD	Diet	52	52	Not specified	Liver	Multiple tumour types									
Trichloroethylpentachlorobenzene	29082-74-4					Rat	Male	SD	Diet	52	52	Not specified	Liver	Multiple tumour types									
Triceryl phosphate	1330-78-5	O=P(OC1c(c(C(c(c(c(C)c)OC2)=CC=c(C=c(C)c)OC3=CC=c(C=c(C)c)C)OC3=CC=c(C=c(C)c)C)OC	생식독성 - 구분2 만성 수생환경 유해성 - 구분2	8, 11, 19, 20, 22, 28, 30, 34, 36, 41, 52, 53, 57, 58, 60, 67, 72, 111, 112, 117, 120, 150, 163, 166, 167, 187, 200, 307, 310	-	Mouse	Female	B6C3F1	Diet	104	105	Not specified	Liver	Adenoma - hepatocellular | Carcinoma-hepatocellular | Hepatoblastoma	CASP3 CYP1A4 IGF1 TNFSF ACHE ACSL1	CTSD TNFSF10A TPM1 IKBKAP RNFT2	CYP2D CACNG4 CHRNE STGALI1 PLAGG6	hsa05224 Breast cancer - Homo sapiens (human) (1) hsa3479 KEGG: IGF1; insulin like growth factor 1 hsa04935 Growth hormone synthesis, secretion and action - Homo sapiens (human) (1) hsa3479 KEGG: IGF1; insulin like growth factor 1 hsa04913 Ovarian steroidogenesis - Homo sapiens (human) (1) hsa3479 KEGG: IGF1; insulin like growth factor 1	kidney urinary bladder Multiple head cancers spleen hematopoietic system large intestine	urinary bladder kidney	kidney stomach urinary bladder	hematopoietic system stomach urinary bladder pituitary gland	-
Triceryl phosphate	1330-78-5					Mouse	Male	B6C3F1	Diet	104	105	Not specified	Liver	Adenoma									
Triceryl phosphate	1330-78-5					Rat	Female	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma-hepatocellular | Hepatoblastoma									
Triceryl phosphate	1330-78-5					Rat	Male	Fischer 344	Diet	104	104	Not specified	Liver	Adenoma - hepatocellular | Carcinoma-hepatocellular | Hepatoblastoma									
Triflusalin	1582-09-8	[N+](O)([c-]c(C(c(c(C)c)c(N+](O)[c-])c(C)c)c(C)c)C(F)(F)F)N(CCC)CCC	급성 독성(경구) - 구분4 피부 부식성 - 구분1(A/1B) 발암성 - 구분2 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	8, 11, 14, 28, 29, 30, 52, 53, 57, 58, 60, 61, 63, 64, 66, 67, 71, 100, 105, 106, 150, 107, 112, 120, 165, 167, 177, 200, 214, 318	Carcinogenicity data available EPA OPP Group D Possible Human Carcinogen	Mouse	Female	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular	NRF2 AR ESR1 PPARG ARA ESR1L	CYP1A1	TNNT1 TNNI3K TMEM46 EIF4G1	hsa05200 Pathways in cancer - Homo sapiens (human) (3) hsa2099 KEGG: ESR1; estrogen receptor 1 hsa367 KEGG: AR; androgen receptor hsa5468 KEGG: PPARG; peroxisome proliferator activated receptor gamma hsa05207 Chemical carcinogenesis - receptor activation - Homo sapiens (human) (2) hsa2099 KEGG: ESR1; estrogen receptor 1 hsa367 KEGG: AR; androgen receptor hsa05205 Proteoglycans in cancer - Homo sapiens (human) (1) hsa2099 KEGG: ESR1; estrogen receptor 1	-	lung ear Zymbals gland	**thyroid gland** stomach	stomach liver lung	Thyroid Neoplasm Colonic Neoplasm Neoplasm
Triflusalin	1582-09-8					Mouse	Female	B6C3F1	Diet	78	90	Positive	Liver	Adenoma - hepatocellular | Carcinoma-hepatocellular									
Triflusalin	1582-09-8					Mouse	Male	B6C3F1	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Triflusalin	1582-09-8					Mouse	Male	B6C3F1	Diet	78	90	Not specified	Liver	Adenoma - hepatocellular | Carcinoma-hepatocellular | Hepatoblastoma									
Triflusalin	1582-09-8					Mouse	Female	NMRI	Diet	104	104	Negative	Liver	Adenoma - hepatocellular									
Triprolidine hydrochloride monohydrate	6138-79-0	C1(C(CN(CC=c(C(2)=CC=c(C=c(2)(C)C)=NC=c(C=c(3)C)C)	급성 독성(경구) - 구분4	-	-	Mouse	Female	B6C3F1	Diet	65	65	Not specified	Liver	Multiple tumour types	HRH1 CXCL8 BMP6 CD14 CD40	SNA1 SLC26A1 MYBL1 DMB DNAG2	SLC2A4 CNTN1 TMEM41B IFIT1 ASAH1	hsa04064 NF-kappa B signaling pathway - Homo sapiens (human) (2) hsa3576 KEGG: CXCL8; C-X-C motif chemokine ligand 8 hsa929 KEGG: CD14; CD14 molecule hsa04060 Cytokine-cytokine receptor interaction - Homo sapiens (human) (2) hsa3576 KEGG: CXCL8; C-X-C motif chemokine ligand 8 hsa654 KEGG: BMP6; bone morphogenetic protein 6 hsa04620 Toll-like receptor signaling pathway - Homo sapiens (human) (2) hsa3576 KEGG: CXCL8; C-X-C motif chemokine ligand 8 hsa929 KEGG: CD14; CD14 molecule	oral cavity stomach nasal cavity spleen esophagus vascular system	ear Zymbals gland clitoral gland stomach vascular system oral cavity nasal cavity small intestine	stomach urinary bladder	hematopoietic system lung	Melanoma
Triprolidine hydrochloride monohydrate	6138-79-0					Mouse	Female	B6C3F1	Diet	104	105	Negative	Liver	Adenoma - hepatocellular									
Triprolidine hydrochloride monohydrate	6138-79-0					Mouse	Male	B6C3F1	Diet	65	65	Not specified	Liver	Carcinoma - hepatocellular									
Triprolidine hydrochloride monohydrate	6138-79-0					Mouse	Male	B6C3F1	Diet	104	105	Negative	Liver	Adenoma - hepatocellular									
Trp-P-2 acetate	72254-58-1	C1=CC=C2C(=C1NC3=C2C(=NC(=C3)N)CC(C)(C)=O				Mouse	Female	CDF1	Diet	88	88	Positive	Liver	Carcinoma - hepatocellular									
Trp-P-2 acetate	72254-58-1					Mouse	Male	CDF1	Diet	88	88	Positive	Liver	Carcinoma - hepatocellular									
Trp-P-2 acetate	72254-58-1					Rat	Female	ACI	Diet	124	124	Positive	Brain	Adenoma									
Trp-P-2 acetate	72254-58-1					Rat	Male	ACI	Diet	124	124	Not specified	Liver	Multiple tumour types									
Turmeric yellow	458-37-7	C2(c(C(c=c(C)C=c(C)C)C=c(C)C)C=CC1=c(C=c(C)c)c(1)OC)O)=O)=c(C2)O)OC	피부감염	7, 14, 19, 23, 25, 27, 28, 29, 34, 36, 46, 52, 53, 58, 61, 62, 64, 66, 67, 71, 72, 111, 112, 117, 132, 133, 148, 153, 163, 165, 167, 187, 200, 214, 307, 318	Genotoxicity Data: predicted to be genotoxic	Rat	Male	Fischer 344	Diet	55	55	Negative	Colon	Multiple tumour types	TNF HMOX1 BRAF BCL2 CASP3 RELA IL1B	HTRX CXCL2 EJPS TNFRSF10B KBKS	VASP NQO1 SREF2 GCLM GASS	hsa05200 Pathways in cancer - Homo sapiens (human) (5) hsa3162 KEGG: HMOX1; heme oxygenase 1 hsa4780 KEGG: NFE2L2; NFE2 like bZIP transcription factor 2 hsa596 KEGG: BCL2; BCL2 apoptosis regulator hsa5970 KEGG: RELA; proto-oncogene, NF-kB subunit hsa836 KEGG: CASP3; caspase 3 hsa05418 Fluid shear stress and atherosclerosis - Homo sapiens (human) (4) hsa3162 KEGG: HMOX1; heme oxygenase 1 hsa4780 KEGG: NFE2L2; NFE2 like bZIP transcription factor 2 hsa596 KEGG: BCL2; BCL2 apoptosis regulator hsa5970 KEGG: RELA; proto-oncogene, NF-kB subunit hsa05417 Lipid and atherosclerosis - Homo sapiens (human) (4) hsa4780 KEGG: NFE2L2; NFE2 like bZIP transcription factor 2 hsa596 KEGG: BCL2; BCL2 apoptosis regulator hsa5970 KEGG: RELA; proto-oncogene, NF-kB subunit hsa836 KEGG: CASP3; caspase 3	**stomach** kidney	**stomach**	**stomach**	-	**Lung Neoplasms** Breast Neoplasm Prostatic Neoplasm Carcinoma, Hepatocellular Stomach Neoplasm Colonic Neoplasm

Chemical Name	CAS No.	SMILES	GHS Classific.	AOPs	Cancer Information	Species	Sex	Strain	Route	Exposure time (weeks)	Experiment time (weeks)	Result	Tumor site	Tumor types	Top Interacting Genes	Down regulation	Up regulation	KEGG pathways	Rats_Male	Rats_Female	Mice_Male	Mice_Female	Cancer curated human
Urapidil	34661-75-1	N1(C)N(CCC1)C2=CC=CC=C2OC(CC)NC3=CC(NC)=NC=C3=O			-	Rat	Female	Sc:Wistar	Gavage	52	52	Negative	Liver	Multiple tumour types	-				all tumor bearing animals	all tumor bearing animals	urinary bladder	-	-
Urapidil	34661-75-1				-	Rat	Male	Sc:Wistar	Gavage	52	52	Negative	Liver	Multiple tumour types									
Vanicid	146-17-7	C1=NC=CC(=C1)C(NN=CC2=CC(=CC=C2)[OC]=O			-	Mouse	Mixed	Not specified	Gavage	52	52	Positive	lung	Adenocarcinoma	-				stomach	stomach mammary gland	lung	lung	-
Vinyltoluenes	25013-15-4	C1=CC=CC(=C1)C=CC2=CC=CC=C2)C=C	인화성 액체 - 구분3 급성 독성(경구) - 구분5 급성 독성(흡입) 증기 - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2(A/2B) 특정표적장기 독성(1회 노출) - 구분3(호흡기 자극성)	-	Carcinogenicity data available: IARC Group 3 - Not classifiable as to its carcinogenicity to humans Genotoxicity Data: clastogenic	Mouse	Female	B6C3F1	Inhalation	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	-				oral cavity Malignt head cancers spleen stomach nasal cavity	mammary gland oral cavity stomach nasal cavity liver	lung stomach vascular system urinary bladder	**ovary** lung urinary bladder stomach	-
Vinyltoluenes	25013-15-4					Mouse	Male	B6C3F1	Inhalation	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Vinyltoluenes	25013-15-4					Rat	Female	Fischer 344	Inhalation	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Vinyltoluenes	25013-15-4					Rat	Male	Fischer 344	Inhalation	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Watanidipine.2HCl	132743-71-2	C1=C(C(C)=C(NH)C(C)=O)OCCC=aC=CC)=CC=2NNCCN(CC)C(C=4C=CC=CC=4)C=3C=CC=CC=3)C=4C=CC=CC=4)C=1C=CC=CC=1			-	Mouse	Female	B6C3F1	Diet	78	78	Negative	Liver	Adenoma- hepatocellular					all tumor bearing animals	-	-	-	-
Watanidipine.2HCl	132743-71-2					Mouse	Male	B6C3F1	Diet	78	78	Negative	Liver	Adenoma- hepatocellular									
Watanidipine.2HCl	132743-71-2					Rat	Female	Fischer 344/DuCr	Diet	104	104	Negative	Liver	Adenoma- hepatocellular									
Watanidipine.2HCl	132743-71-2					Rat	Male	Fischer 344/DuCr	Diet	104	104	Negative	Liver	Adenoma- hepatocellular									
Xibenolol.HCl	15263-30-8	C1=CC=CC(=C1)C1C(O)CC(CNC(C)C)C(O)=C1	-			Mouse	Female	B6C3F1	Diet	82	92	Negative	Liver	Multiple tumour types	-				skin		kidney		-
Xibenolol.HCl	15263-30-8					Mouse	Male	B6C3F1	Diet	82	92	Negative	Liver	Multiple tumour types									
Xylazine.HCl	23076-35-9	C1=CC=C(C)=C1C(NC=2SCCCN=2)C.Cl	-	-	-	Rat	Male	Fischer 344/DuCr	Diet	52	52	Not specified	Thyroid gland	Adenoma- follicular cell	-				spleen liver	small intestine hematopoietic system mammary gland ear Zymbals gland	thyroid gland urinary bladder vascular system liver	thyroid gland urinary bladder hematopoietic system vascular system pituitary gland liver	-
Xylene	1330-20-7	C1=CC=C(C=C1)C=CC=2C=CC=CC=2)C=C=3C=CC=CC=3)C=CC=3)C	인화성 액체 - 구분3 급성 독성(경구) - 구분4 급성 독성(흡입) 증기 - 구분4 피부 부식성/피부 자극성 - 구분2 심한 눈 손상성/눈 자극성 - 구분2(A/2B) 특정표적장기 독성(1회 노출) - 구분1(호흡기 자극성) 특정표적장기 독성(1회 노출) - 구분3(마취작용) 특정표적장기 독성(반복 노출) - 구분1 흡인 유해성 - 구분1		Carcinogenicity data available: IRIS-Data are inadequate for an assessment of human carcinogenic potential Genotoxicity Data: inconclusive	Mouse	Female	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic	**CYP2E1** CYP2B1 **CAT** **Cyp2e1** CYP1A1 CYP2A6 HGF06	-	-	hsa01100 Metabolic pathways - Homo sapiens (human) (4) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1548 K17683 CYP2A6; cytochrome P450 family 2 subfamily A member 6 hsa847 K03781 CAT; catalase hsa00980 Metabolism of xenobiotics by cytochrome P450 - Homo sapiens (human) (3) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa1548 K17683 CYP2A6; cytochrome P450 family 2 subfamily A member 6 hsa05208 Chemical carcinogenesis - reactive oxygen species - Homo sapiens (human) (3) hsa1543 KO7408 CYP1A1; cytochrome P450 family 1 subfamily A member 1 hsa1544 KO7409 CYP1A2; cytochrome P450 family 1 subfamily A member 2 hsa847 K03781 CAT; catalase	oral cavity spleen Malignt head cancers **liver** nasal cavity vascular system urinary bladder ear Zymbals gland kidney thyroid gland hematopoietic system lung stomach	**liver** clitoral gland oral cavity urinary bladder nasal cavity lung thyroid gland **uterus** kidney stomach hematopoietic system	urinary bladder thyroid gland lung vascular system kidney small intestine	urinary bladder thyroid gland **ovary** vascular system pituitary gland **liver** stomach peritoneal cavity small intestine	**Liver Neoplasm** Neuroectodermal Tumors, Primitive
Xylene	1330-20-7					Mouse	Male	B6C3F1	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Xylene	1330-20-7					Rat	Female	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Xylene	1330-20-7					Rat	Male	Fischer 344	Gavage	103	104	Not specified	Liver	Adenoma- hepatocellular | Carcinoma/hepatocellular | Nodule- neoplastic									
Zinc 2-mercaptobenzothiazole	155-04-4	C1=CC=CC2=C1SC(=N2)[Zn]SC4=NC=3C=CC=CC=3S4	피부 과민성 - 구분1(1A/1B) 급성 수생환경 유해성 - 구분1 만성 수생환경 유해성 - 구분1	-	-	Mouse	Female	B6AF1	Gavage (preweaning) thas diet	76	76	Negative	Liver	Hepatoma	-				-	-	-	-	-
Zinc 2-mercaptobenzothiazole	155-04-4					Mouse	Male	B6AF1	Gavage (preweaning) thas diet	76	76	Negative	Liver	Hepatoma									
Zinc 2-mercaptobenzothiazole	155-04-4					Mouse	Female	B6C3F1	Gavage (preweaning) thas diet	76	76	Negative	Liver	Hepatoma									
Zinc 2-mercaptobenzothiazole	155-04-4					Mouse	Male	B6C3F1	Gavage (preweaning) thas diet	76	76	Negative	Liver	Hepatoma									

연구진

연 구 기 관 : **산업안전보건연구원**

연구책임자 : 임경택(선임연구위원, 흡입독성연구센터)

연구기간

2023. 01. 01. ~ 2023. 11. 30.

본 연구보고서의 내용은 연구책임자의 개인적 견해이며,
우리 연구원의 공식견해와 다를 수도 있음을 알려드립니다.

산업안전보건연구원장

페닐화합물류 노출에 의한 랫드와 마우스의
성별·장기별 발암성 고찰
(2023-산업안전보건연구원-981)

발 행 일 : 2023년 12월 31일
발 행 인 : 산업안전보건연구원 원장 김은아
연구책임자 : 산업화학연구실 선임연구위원 임경택
발 행 처 : 안전보건공단 산업안전보건연구원
주 소 : (44429) 울산광역시 중구 종가로 400
전 화 : 042-869-8533
팩 스 : 042-869-8691
Homepage : http://oshri.kosha.or.kr
I S B N : 979-11-93642-44-3
공공안심글꼴 : 무료글꼴, 한국출판인회의, Kopub바탕체/돋움체

OPEN 공공누리
출처표시 상업용금지 변경금지
공공저작물 자유이용허락

페닐화합물류 노출에 의한 랫드와 마우스의 성별·장기별 발암성 고찰

표지
랑데뷰 226g(인쇄용지)

내지
네오스타 미색 80g(인쇄용지)
저탄소제품 708kg CO_2 eq./ton

환경보호를 위해
저탄소용지(친환경용지)를
사용하였습니다.

친환경 환경부
CO_2 탄소발자국 708kg 환경부 저탄소

산업재해예방
안전보건공단
산업안전보건연구원