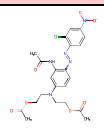
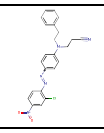
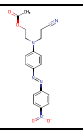
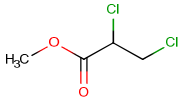
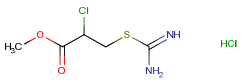
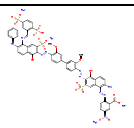
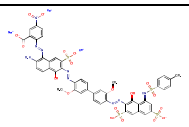
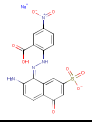
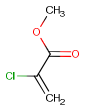
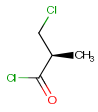
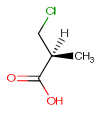
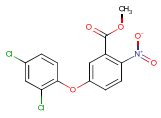
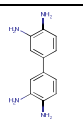
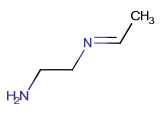
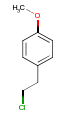
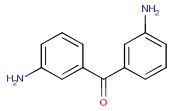
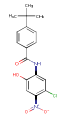
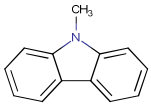
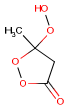
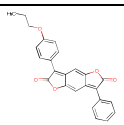
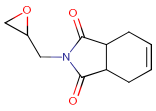
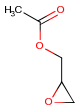
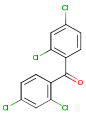
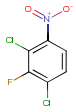
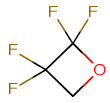
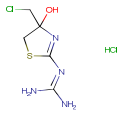
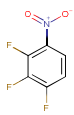
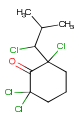
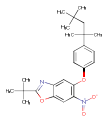
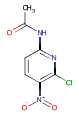
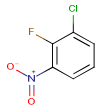
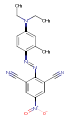
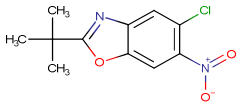
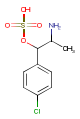
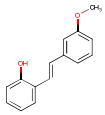
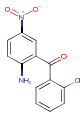
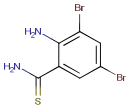
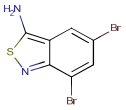
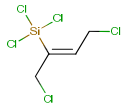
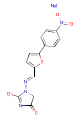
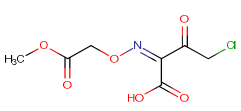
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
51	1533-78-4	A		5'-(bis(2-hydroxyethyl)amino)-2'-((2-chloro-4-nitrophenyl)azo)acetanilide,diacetate(ester)	CC(=O)NC1=C(C=CC(=C1)N(CCOC(=O)C)CCOC(=O)C)N=NC2=C(C=C(C=C2)[N+](=O)[O-])Cl
67	19649-68-4	A		3-[4-[(2-chloro-4-nitrophenyl)diazenyl]-N-phenethylanilino]propanenitrile	C1=CC=C(C=C1)CCN(CCC#N)C2=CC=C(C=C2)N=NC3=C(C=C(C=C3)[N+](=O)[O-])Cl
73	68391-42-4	A		2-[(2-cyanoethyl){4-[(E)-(4-nitrophenyl)diazenyl]phenyl}amino]ethylacetate	[O-][N+](=O)c2ccc(/N=N/c1ccc(N(CCOC(=O)C)CCC#N)cc1)cc2
175	3674-09-7	A		methyl2,3-dichloropropionate	COC(=O)C(CCl)Cl
320	54598-77-5	A		methyl3-carbamimidoylsulfanyl-2-chloropropanoate;hydrochloride	COC(=O)C(CSC(=N)N)Cl.Cl
322	75522-93-9	A		benzoicacid,2-((2-amino-6-((4'-((5-((2,5-disulfophenyl)azo)-1-hydroxy-6-(phenylamino)-3-sulfo-2-naphthalenyl)azo)-3,3'-dimethoxy(1,1'-biphenyl)-4-yl)azo)-5-hydroxy-7-sulfo-1-naphthalenyl)azo)-5-nitro-,tetrasodiumsalt	[Na+].[Na+].[Na+].[Na+].COC1=C(C=CC(=C1)C1=CC(OC)=C(C=C1)\N=N\C1=C(C=C2C(C=CC(NC3=CC=CC=C3)=C2\N=N\C2=C(C=CC(=C2)S([O-
323	75522-94-0	A		benzoicacid,2-((2-amino-5-hydroxy-6-((4'-((1-hydroxy-8-(((4-methylphenyl)sulfonyl)amino)-3,6-disulfo-2-naphthalenyl)azo)-3,3'-dimethoxy(1,1'-biphenyl)-4-yl)azo)-7-sulfo-1-naphthalenyl)azo)-5-nitro-,trisodiumsalt	[Na+].[Na+].[Na+].COC1=C(C=CC=C1)C1=CC(OC)=C(C=C1)\N=N\C1=C(C=C2C(C=CC(N)=C2\N=N\C2=C(C=C(C=C2)[N+]([O-])=O)C([O-])=O)=C1O)S([O-
324	67815-66-1	A		7-amino-4-hydroxy-8-((4-nitro-2-carboxyphenyl)azo)-2-naphthalenesulfonicacid,monosodiumsalt	C1=CC(=C(C=C1[N+](=O)[O-])C(=O)O)N/N=C\2/C(=CC=C3C2=CC(=CC3=O)S(=O)(=O)[O-])N.[Na+]
339	80-63-7	A		methyl2-chloroacrylate	COC(=O)C(=C)Cl
348	80141-51-1	A		(S)-3-chloro-2-methylpropionylchloride	C[C@H](CCl)C(=O)Cl
349	16674-04-7	A		(S)-3-chloro-2-methylpropionicacid	[H][C@@](C)(CCl)C(O)=O
541	42576-02-3	A		methyl5-(2,4-dichlorophenoxy)-2-nitrobenzoate	COC(=O)C1=C(C=CC(=C1)OC2=C(C=C(C=C2)Cl)Cl)[N+](=O)[O-]
662	91-95-2	A		3,3'-diaminobenzidine	C1=CC(=C(C=C1C2=CC(=C(C=C2)N)N)N)N
777	95465-58-0	A		N-ethylideneethylenediamine	C\C=N\CCN

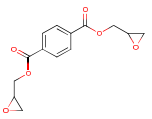
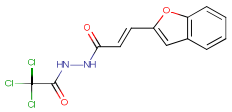
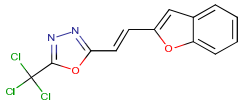
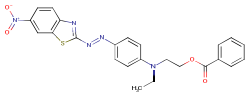
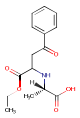
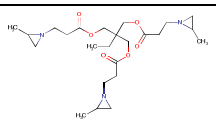
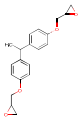
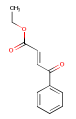
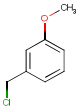
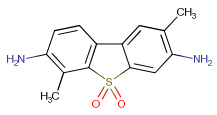
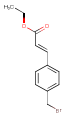
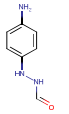
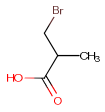
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
886	18217-00-0	A		p-(2-chloroethyl)anisole	COC1=CC=C(C=C1)CCCl
1003	611-79-0	A		4,4'-diaminobenzophenone	C1=CC(=CC(=C1)N)C(=O)C2=CC(=CC=C2)N
1037	94725-58-3	A		4-tert-butyl-5'-chloro-2'-hydroxy-4'-nitrobenzanilide	CC(C)(C)C1=CC=C(C=C1)C(=O)NC1=CC(Cl)=C(C=C1O)[N+]([O-])=O
1048	1484-12-4	A		9-methylcarbazole	CN1C2=CC=CC=C2C3=CC=CC=C31
1141	20748-96-3	A		5-hydroperoxy-5-methyl-1,2-dioxolan-3-one	CC1(CC(=O)OO1)OO
1145	79694-17-0	A		3-phenyl-7-(4-propoxyphenyl)-1,5-dioxa-s-indacene-2,6-dione	CCCOC1=CC=C(C=C1)C2=C3C=C4C(=C(C(=O)O4)C5=CC=CC=C5)C=C3OC2=O
1181	17620-38-1	A		N-oxiranylmethyl-4-cyclohexene-1,2-dicarbimide	C1C=CCC2C1C(=O)N(C2=O)CC3CO3
1190	6387-89-9	A		glycidyl acetate	CC(=O)OCC1CO1
1213	25187-08-0	A		2,2',4,4'-tetrachlorobenzophenone	C1=CC(=C(C=C1Cl)Cl)C(=O)C2=C(C=C(C=C2)Cl)Cl
1303	393-79-3	A		2,4-dichloro-3-fluoronitrobenzene	C1=CC(=C(C(=C1[N+](=O)[O-])Cl)F)Cl
1319	765-63-9	A		2,2,3,3-tetrafluorooxetane	C1C(C(O1)(F)F)(F)F
1417	95907-33-8	A		2-[4-(chloromethyl)-4-hydroxy-5H-1,3-thiazol-2-yl]guanidine hydrochloride	C1C(N=C(S1)N=C(N)N)(CCl)O.Cl
1446	771-69-7	A		2,3,4-trifluoronitrobenzene	C1=CC(=C(C(=C1[N+](=O)[O-])F)F)F
1548	89110-96-3	A		2,2,6-trichloro-6-(1-chloro-2-methylpropyl)cyclohexanone	CC(C)C(C1(CCCC(C1=O)(Cl)Cl)Cl)Cl

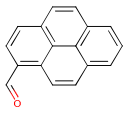
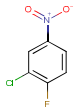
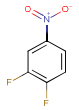
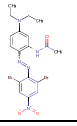
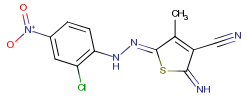
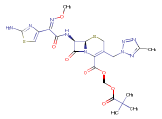
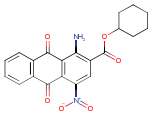
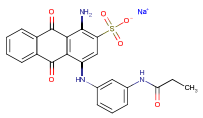
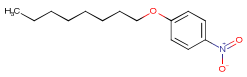
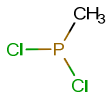
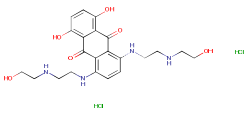
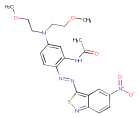
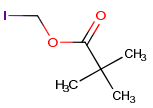
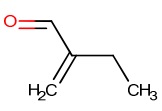
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
1583	102405-96-9	A		2-tert-butyl-6-nitro-5-[p-(1,1,3,3-tetramethylbutyl)phenoxy]benzoxazole	CC(C)(C)CC(C)(C)C1=CC=C(C=C1)OC2=C(C=C3C(=C2)N=C(O3)C(C)(C)C)[N+](=O)[O-]
1654	110882-70-7	A		N-(2-chloro-3-nitro-6-pyridyl)acetamide	CC(=O)NC1=NC(=C(C=C1)[N+](=O)[O-])Cl
1662	2106-49-2	A		3-chloro-2-fluoronitrobenzene	C1=CC(=C(C(=C1)Cl)F)[N+](=O)[O-]
1672	84870-65-5	A		4-(2,6-dicyano-4-nitrophenylazo)-3-methyl-N,N-diethylaniline	CCN(CC)C1=CC(C)=C(C=C1)\N=N\C1=C(C=C(C=C1C#N)[N+]([O-])=O)C#N
1718	102405-54-9	A		2-tert-butyl-5-chlolo-6-nitrobenzoxazole	CC(C)(C)C1=NC2=CC(=C(C=C2O1)[N+](=O)[O-])Cl
1745	86603-13-6	A		sulfuric acid hydrogen 2-amino-1-(p-chlorophenyl)propyl ester	CC(N)C(OS(O)(=O)=O)C1=CC=C(Cl)C=C1
1909	134964-55-9	A		2-(3-methoxystyryl)phenol	COC1=CC=CC(=C1)/C=C/C2=CC=CC=C2O
1924	2011-66-7	A		2-amino-2'-chloro-5-nitrobenzophenone	C1=CC=C(C(=C1)C(=O)C2=C(C=CC(=C2)[N+](=O)[O-])N)Cl
1925	14345-84-7	A		2-amino-3,5-dibromothiobenzamide	C1=C(C=C(C(=C1Br)N)C(=S)N)Br
1926	14346-17-9	A		3-amino-5,7-dibromo-2,1-benzisothiazole	C1=C(C=C(C2=NSC(=C21)N)Br)Br
1965	1586-88-5	A		trichloro[3-chloro-1-(chloromethyl)-1-propenyl]silane	ClC\C=C(\CCl)[Si](Cl)(Cl)Cl
1966	400-70-4	A		2,4-dichloro-5-trifluoromethyl-1-nitrobenzene	C1=C(C(=CC(=C1[N+](=O)[O-])Cl)Cl)C(F)(F)F
1996	14663-23-1	A		dantrolene sodium	C1C(=O)N=C(N1/N=C/C2=CC=C(O2)C3=CC=C(C=C3)[N+](=O)[O-])[O-].[Na+]
2080	84080-70-6	A		4-chloro-2-[(Z)-methoxycarbonylmethoxyimino]-3-oxobutyric acid	COC(=O)CO/N=C(/C(=O)CCl)\C(=O)O

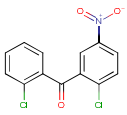
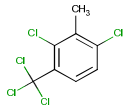
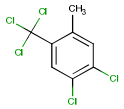
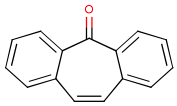
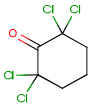
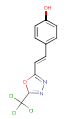
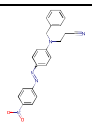
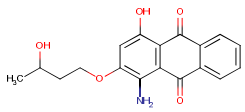
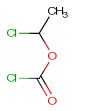
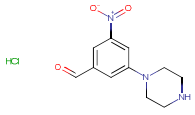
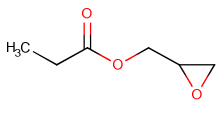
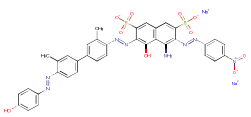
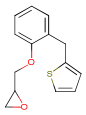
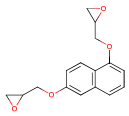
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
2082	7783-54-2	A		nitrogen trifluoride	N(F)(F)F
2104	7195-44-0	A		telephthalic acid diglycidyl	O=C(OCC1CO1)C1=CC=C(C=C1)C(=O)OCC1CO1
2131	93641-38-4	A		N'-[3-(benzofuran-2-yl)acryloyl]trichloroacetic acid hydrazide	ClC(Cl)(Cl)C(=O)NNC(=O)\C=C\C1=CC2=C(O1)C=CC=C2
2132	93641-24-8	A		2-[2-(benzofuran-2-yl)vinyl]-5-(trichloromethyl)-1,3,4-oxadiazole	ClC(Cl)(Cl)C1=NN=C(O1)\C=C\C1=CC2=CC=CC=C2O1
2153	68938-65-8	A		benzoic acid 2-[N-ethyl-p-(6-nitrobenzothiazol-2-ylazo)anilino]ethyl ester	CCN(CCOC(=O)C1=CC=CC=C1)C1=CC=C(C=C1)\N=N\C1=NC2=C(S1)C=C(C=C2)[N+]([O-])=O
2159	87269-99-6	A		N-(2-benzoyl-1-ethoxycarbonylethyl)alanine	[H][C@@](C)(NC(CC(=O)C1=CC=CC=C1)C(=O)OCC)C(O)=O
2196	64265-57-2	A		tris[3-(2-methylaziridin-1-yl)propionic acid]=propane-1,1,1-triyltrismethylene ester	CCC(COC(=O)CCN1CC1C)(COC(=O)CCN2CC2C)COC(=O)CCN3CC3C
2201	98460-24-3	A		2,2'-[ethylidenebis(4,1-phenyleneoxymethylene)]bisoxirane	CC(C1=CC=C(OCC2CO2)C=C1)C1=CC=C(OCC2CO2)C=C1
2228	15121-89-8	A		3-benzoylacrylic acid ethyl ester	CCOC(=O)\C=C\C(=O)C1=CC=CC=C1
2298	824-98-6	A		3-methoxybenzyl chloride	COC1=CC=CC(=C1)CCl
2303	55011-44-4	A		2,7-diamino-3,6-dimethyl-9-thia-9H-fluorene 9,9-dioxide	CC1=C(C=C2C(=C1)C3=C(S2(=O)=O)C(=C(C=C3)N)C)N
2362	78712-67-1	A		(E)-3-[p-bromomethylphenyl]acrylic acid ethyl ester	CCOC(=O)\C=C\C1=CC=C(CBr)C=C1
2367	63402-26-6	A		1-formyl-2-(4-aminophenyl)hydrazine	C1=CC(=CC=C1N)NNC=O
2472	56970-78-6	A		3-bromoisobutyric acid	CC(CBr)C(=O)O

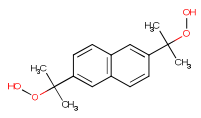
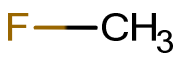
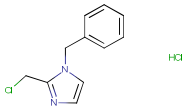
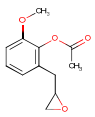
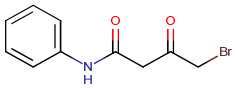
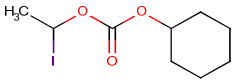
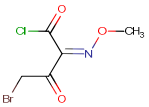
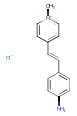
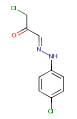
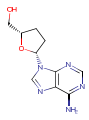
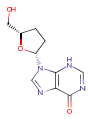
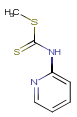
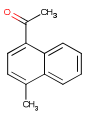
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
2577	3029-19-4	A		1-pyrenecarboxaldehyde	C1=CC2=C3C(=C1)C=CC4=C(C=CC(=C43)C=C2)C=O
2661	350-30-1	A		3-chloro-4-fluoronitrobenzene	C1=CC(=C(C=C1[N+](=O)[O-])Cl)F
2682	369-34-6	A		3,4-difluoronitrobenzene	C1=CC(=C(C=C1[N+](=O)[O-])F)F
2684	52583-53-6	A		2'-(2,6-dibromo-4-nitrophenylazo)-5'-diethylaminoacetanilide	CCN(CC)C1=CC(=C(C=C1)N=NC2=C(C=C(C=C2Br)[N+](=O)[O-])Br)NC(=O)C
2759	126389-08-0	A		2-amino-5-(2-chloro-4-nitrophenylazo)-4-methyl-3-thiophenecarbonitrile	CC1=C(C#N)C(=N)SC\1=N/NC1=C(Cl)C=C(C=C1)[N+]([O-])=O
2763	82547-81-7	A		cefteram pivoxil	CC1=NN(N=N1)CC2=C(N3[C@@H]([C@@H](C3=O)NC(=O)/C(=N\OC)/C4=CSC(=N4)N)SC2)C(=O)OCOC(=O)C(C)(C)C
2765	53814-79-2	A		1-amino-4-nitro-9,10-dihydro-9,10-dioxoanthracene-2-carboxylic acid cyclohexyl ester	NC1=C(C=C(C2=C1C(=O)C1=C(C=CC=C1)C2=O)[N+]([O-])=O)C(=O)OC1CCCCC1
2769	89923-62-6	A		1-amino-4-(3-propionylaminoanilino)-9,10-dihydro-9,10-dioxoanthracene-2-sulfonic acid sodium salt	CCC(=O)NC1=CC=CC(=C1)NC2=CC(=C(C3=C2C(=O)C4=CC=CC=C4C3=O)N)S(=O)(=O)[O-].[Na+]
2793	49562-76-7	A		p-octyloxynitrobenzene	CCCCCCCCOC1=CC=C(C=C1)[N+](=O)[O-]
2819	676-83-5	A		methyldichlorophosphine	CP(Cl)Cl
2858	70476-82-3	A		Mitoxantrone hydrochloride	C1=CC(=C2C(=C1NCCNCCO)C(=O)C3=C(C=CC(=C3C2=O)O)O)NCCNCCO.Cl.Cl
2864	105076-77-5	A		5'-[bis(2-methoxyethyl)amino]-2'-(5-nitro-2,1-benzisothiazol-3-ylazo)acetanilide	COCCN(CCOC)C1=CC(NC(C)=O)=C(C=C1)\N=N\C1=C2C=C(C=CC2=NS1)[N+]([O-])=O
2869	53064-79-2	A		iodomethyl pivalate	CC(C)(C)C(=O)OCI
2926	922-63-4	A		2-ethylacrolein	CCC(=C)C=O

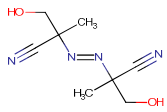
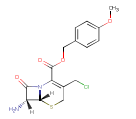
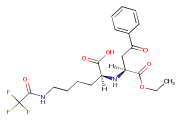
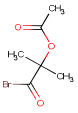
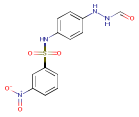
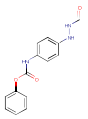
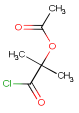
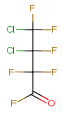
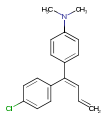
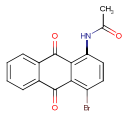
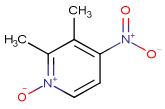
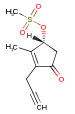
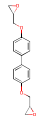
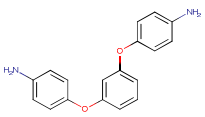
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
2968	54534-72-4	A		2,2'-dichloro-5-nitrobenzophenone	[O-][N+](=O)C1=CC=C(Cl)C(=C1)C(=O)C1=C(Cl)C=CC=C1
2970	99938-06-4	A		2,6-dichloro-3-(trichloromethyl)toluene	CC1=C(Cl)C=CC(=C1Cl)C(Cl)(Cl)Cl
2971	18964-69-7	A		4,5-dichloro-2-(trichloromethyl)toluene	CC1=CC(Cl)=C(Cl)C=C1C(Cl)(Cl)Cl
2983	2222-33-5	A		dibenzosuberenone	C1=CC=C2C(=C1)C=CC3=CC=CC=C3C2=O
2994	3776-30-5	A		2,2,6,6-tetrachlorocyclohexanone	C1CC(C(=O)C(C1)(Cl)Cl)(Cl)Cl
2997	96405-52-6	A		2-trichloromethyl-5-(4-hydroxystyryl)-1,3,4-oxadiazole	OC1=CC=C(C=C1)\C=C\C1=NN=C(O1)C(Cl)(Cl)Cl
3041	96662-24-7	A		3-[N-benzyl-4-(4-nitrophenylazo)anilino]propiononitrile	C1=CC=C(C=C1)CN(CCC#N)C2=CC=C(C=C2)N=NC3=CC=C(C=C3)[N+](=O)[O-]
3078	3224-15-5	A		1-amino-4-hydroxy-2-(3-hydroxybutoxy)anthraquinone	CC(CCOC1=C(C2=C(C(=C1)O)C(=O)C3=CC=CC=C3C2=O)N)O
3107	50893-53-3	A		1-chloroethyl chloroformate	CC(OC(=O)Cl)Cl
3159	86813-46-9	A		2-nitro-5-(1-piperazinyl)benzaldehyde	Cl.[O-][N+](=O)C1=CC(=CC(C=O)=C1)N1CCNCC1
3182	37111-25-4	A		propionic acid 2,3-epoxypropan-1-yl ester	CCC(=O)OCC1CO1
3223	68400-36-2	A		4-amino-5-hydroxy-6-[4'-(4-hydroxyphenylazo)-3,3'-dimethyl-4-biphenylylazo]-3-(4-nitrophenylazo)-2,7-naphthalenedisulfonic acid disodium salt	[Na+].[Na+].CC1=CC(=CC=C1\N=N\C1=CC=C(O)C=C1)C1=CC(C)=C(C=C1)\N=N\C1=C(O)C2=C(C=C(C(\N=N\C3=CC=C(C=C3)[N+]([O-])=O)=O)C2N)S([O-
3289	55506-46-2	A		2-[[2-(thiophen-2-ylmethyl)phenoxy]methyl]oxirane	C1C(O1)COC2=CC=CC=C2CC3=CC=CS3
3299	27610-48-6	A		1,6-bis(oxiran-2-ylmethoxy)naphthalene	C1C(O1)COC2=CC3=C(C=C2)C(=CC=C3)OCC4CO4

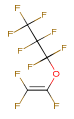
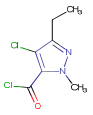
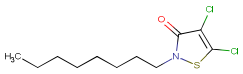
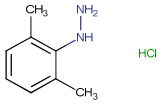
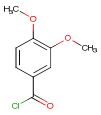
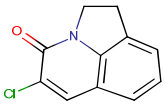
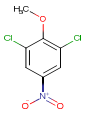
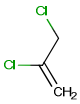
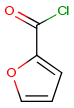
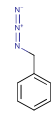
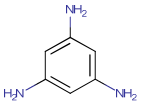
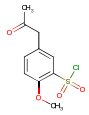
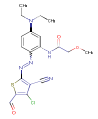
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
3304	96783-79-8	A		2,6-bis(1-hydroperoxy-1-methylethyl)naphthalene	CC(C)(OO)C1=CC2=C(C=C1)C=C(C=C2)C(C)(C)OO
3319	593-53-3	A		methyl fluoride	CF
3324	19276-03-0	A		1-benzyl-2-(chloromethyl)imidazole Hydrochloride	C1=CC=C(C=C1)CN2C=CN=C2CCl.Cl
3498	91520-02-4	A		[2-methoxy-6-(oxiran-2-ylmethyl)phenyl] acetate	CC(=O)OC1=C(C=CC=C1OC)CC2CO2
3564	1205-74-9	A		4-bromo-3-oxo-N-phenylbutanamide	C1=CC=C(C=C1)NC(=O)CC(=O)CBr
3643	102672-57-1	A		cyclohexyl 1-iodoethyl carbonate	CC(OC(=O)OC1CCCCC1)I
3669	115922-43-5	A		4-bromo-2-methoxyimino-3-oxobutanoyl chloride	CO\N=C(/C(Cl)=O)C(=O)CBr
3704	105757-36-6	A		pyridinium, 4-[2-(4-aminophenyl)ethenyl]-1-methyl-, chloride	[Cl-].C[N+]1=CC=C(\C=C\C2=CC=C(N)C=C2)C=C1
3733	77458-54-9	A		1-chloro-3-[2-(4-chlorophenyl)hydrazono]-2-propanone	ClCC(=O)\C=N\NC1=CC=C(Cl)C=C1
3763	4097-22-7	A		2',3'-dideoxyadenosine	C1C[C@@H](O[C@@H]1CO)N2C=NC3=C2N=CN=C3N
3764	69655-05-6	A		2',3'-dideoxyinosine	C1C[C@@H](O[C@@H]1CO)N2C=NC3=C2NC=NC3=O
3812	13037-46-2	A		methyl 2-pyridyldithiocarbamate	CSC(=S)NC1=CC=CC=N1
3844	28418-86-2	A		1-acetyl-4-methylnaphthalene	CC1=CC=C(C2=CC=CC=C12)C(=O)C
3934	354-64-3	A		pentafluoroiodoethane	C(C(F)(F)I)(F)(F)F

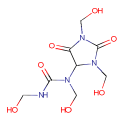
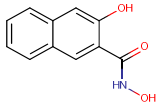
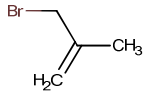
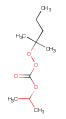
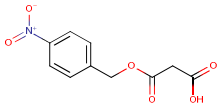
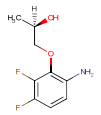
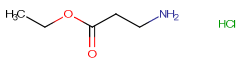
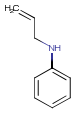
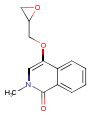
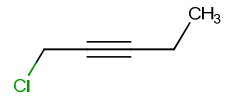
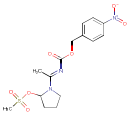
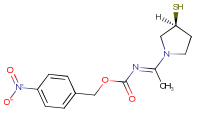
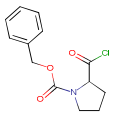
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
3956	19706-80-0	A		2,2'-azobis[2-(hydroxymethyl)propiononitrile]	CC(CO)(\N=N\C(C)(CO)C#N)C#N
3957	106773-36-8	A		(6R,7R)-7-amino-3-chloromethyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid 4-methoxybenzyl ester	[H][C@@]1(N)C(=O)N2C(C(=O)OCC3=CC=C(OC)C=C3)=C(CCl)CS[C@]12[H]
3974	116169-88-1	A		N2-[(S)-1-ethoxycarbonyl-3-oxo-3-phenylpropyl]-N6-trifluoroacetyl-L-lysine	[H][C@@](CCCCNC(=O)C(F)(F)F)(N[C@@]([H])(CC(=O)C1=CC=CC=C1)C(=O)OCC)C(O)=O
3999	40635-67-4	A		2-acetoxyisobutyryl bromide	CC(=O)OC(C)(C)C(=O)Br
4059	75753-05-8	A		N-[4-[(3-nitrophenyl)sulfonylamino]anilino]formamide	C1=CC(=CC(=C1)S(=O)(=O)NC2=CC=C(C=C2)NNC=O)[N+](=O)[O-]
4060	101907-41-9	A		phenyl N-[4-(2-formylhydrazinyl)phenyl]carbamate	C1=CC=C(C=C1)OC(=O)NC2=CC=C(C=C2)NNC=O
4099	40635-66-3	A		2-acetoxyisobutyryl chloride	CC(=O)OC(C)(C)C(=O)Cl
4113	678-06-8	A		3,4-dichloro-2,2,3,4,4-pentafluorobutyric acid fluoride	FC(=O)C(F)(F)C(F)(Cl)C(F)(F)Cl
4122	130288-19-6	A		N,N-dimethyl-4-[1-(4-chlorophenyl)-1,3-butadienyl]aniline	CN(C)C1=CC=C(C=C1)C(=C\C=C)\C1=CC=C(Cl)C=C1
4172	27563-14-0	A		1-(acetylamino)-4-bromoanthraquinone	CC(=O)NC1=C2C(=C(C=C1)Br)C(=O)C3=CC=CC=C3C2=O
4225	37699-43-7	A		2,3-dimethyl-4-nitropyridine 1-oxide	CC1=C(C=C[N+](=C1C)[O-])[N+](=O)[O-]
4293	95413-30-2	A		(R)-3-methyl-4-[(methylsulfonyl)oxy]-2-(2-propynyl)-2-cyclopenten-1-one	[H][C@]1(CC(=O)C(CC#C)=C1C)OS(C)(=O)=O
4365	2461-46-3	A		4,4'-bis(2,3-epoxypropoxy)biphenyl	C1C(O1)COC2=CC=C(C=C2)C3=CC=C(C=C3)OCC4CO4
4380	2479-46-1	A		4,4'-(1,3-phenylenedioxy)dianiline	C1=CC(=CC(=C1)OC2=CC=C(C=C2)N)OC3=CC=C(C=C3)N

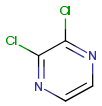
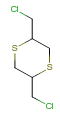
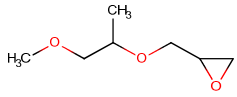
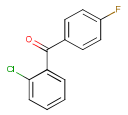
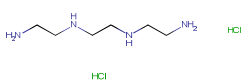
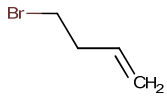
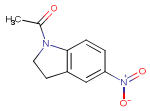
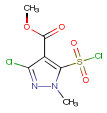
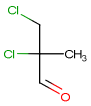
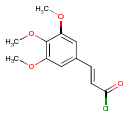
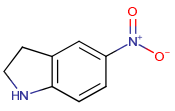
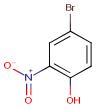
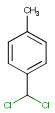
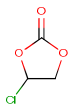
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
4391	1623-05-8	A		heptafluoropropyl trifluorovinyl ether	C(=C(F)F)(OC(C(C(F)(F)F)(F)F)(F)F)F
4445	129560-00-5	A		4-chloro-5-ethyl-2-methylpyrazole-3-carbonyl chloride	CCC1=NN(C(=C1Cl)C(=O)Cl)C
4466	64359-81-5	A		4,5-dichloro-2-n-octyl-4-isothiazolin-3-one	CCCCCCCCN1C(=O)C(=C(S1)Cl)Cl
4477	2538-61-6	A		2,6-dimethylphenylhydrazine hydrochloride	CC1=C(C(=CC=C1)C)NN.Cl
4481	3535-37-3	A		3,4-dimethoxybenzoyl chloride	COC1=C(C=C(C=C1)C(=O)Cl)OC
4565	88283-76-5	A		5-chloro-1,2-dihydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one	ClC1=CC2=C3N(CCC3=CC=C2)C1=O
4578	17742-69-7	A		2,6-deichloro-4-nitroanisole	COC1=C(C=C(C=C1Cl)[N+](=O)[O-])Cl
4670	3947-65-7	A		neamine	C1[C@H]([C@@H]([C@H]([C@@H]([C@H]1N)O[C@@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CN)O)O)N)O)O)N
4679	78-88-6	A		2,3-dichloropropene	C=C(CCl)Cl
4748	527-69-5	A		2-furoyl chloride	C1=COC(=C1)C(=O)Cl
4756	622-79-7	A		benzylazide	[N-]=[N+]=NCC1=CC=CC=C1
4759	108-72-5	A		1,3,5-benzenetriamine	C1=C(C=C(C=C1N)N)N
4777	80223-79-6	A		5-acetonyl-2-methoxybenzenesulfonyl chloride	CC(=O)CC1=CC(=C(C=C1)OC)S(=O)(=O)Cl
4808	122371-93-1	A		2'-(4-chloro-3-cyano-5-formyl-2-thienylazo)-5'-diethylamino-2-methoxyacetanilide	CCN(CC)C1=CC(=C(C=C1)N=NC2=C(C(=C(S2)C=O)Cl)C#N)NC(=O)COC

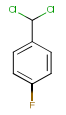
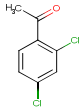
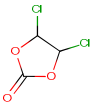
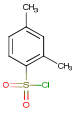
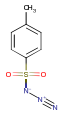
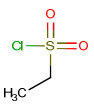
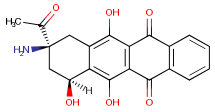
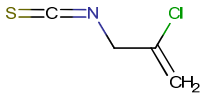
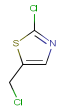
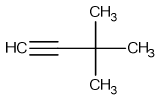
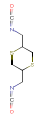
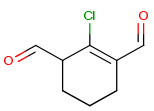
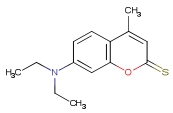
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
4857	78491-02-8	A		diazolidinylurea	C(NC(=O)N(CO)C1C(=O)N(C(=O)N1CO)CO)O
5004	22974-74-9	A		3-hydroxynaphthalene-2-carbohydroximic acid	C1=CC=C2C=C(C(=CC2=C1)C(=O)NO)O
5151	1458-98-6	A		3-bromo-2-methyl-1-propene	CC(=C)CBr
5152	132929-84-1	A		peroxycarbonic acid OO-(1,1-dimethylbutyl)O-isopropyl ester	CCCC(C)(C)OOC(=O)OC(C)C
5155	77359-11-6	A		4-nitrobenzyl hydrogen malonate	C1=CC(=CC=C1COC(=O)CC(=O)O)[N+](=O)[O-]
5171	124409-98-9	A		(R)-1-(2,3-difluoro-6-aminophenoxy)-2-propanol	[H][C@](C)(O)COC1=C(N)C=CC(F)=C1F
5176	4244-84-2	A		ethyl 3-aminopropanoate hydrochloride	CCOC(=O)CCN.Cl
5179	589-09-3	A		N-allylaniline	C=CCNC1=CC=CC=C1
5196	62775-08-0	A		2-methyl-4-(oxiran-2-ylmethoxy)isoquinolin-1-one	CN1C=C(C2=CC=CC=C2C1=O)OCC3CO3
5210	22592-15-0	A		1-chloro-2-pentyne	CCC#CCCl
5252	335-05-7	A		trifluoromethanesulfonyl fluoride	C(F)(F)(F)S(=O)(=O)F
5423	90505-34-3	A		[1-[(3R)-3-[(methylsulfonyl)oxy]pyrrolidine-1-yl]ethylidene]carbamic acid 4-nitrobenzyl ester	C\C(N1CCCC1OS(C)(=O)=O)=N/C(=O)OCC1=CC=C(C=C1)[N+]([O-])=O
5432	90505-36-5	A		[1-[(3S)-3-mercaptopyrrolidine-1-yl]ethylidene]carbamic acid 4-nitrobenzyl ester	[H][C@]1(S)CCN(C1)C(\C)=N\C(=O)OCC1=CC=C(C=C1)[N+]([O-])=O
5489	61350-60-5	A		2-chloroformyl-1-pyrrolidinecarboxylic acid benzyl ester	ClC(=O)C1CCCN1C(=O)OCC1=CC=CC=C1

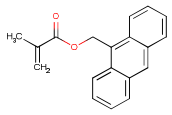
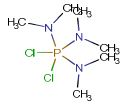
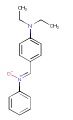
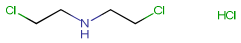
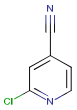
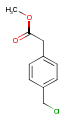
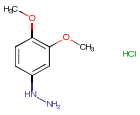
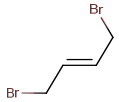
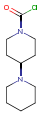
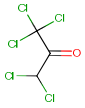
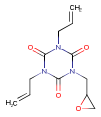
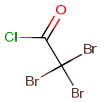
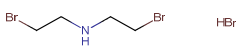
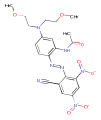
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
5609	4858-85-9	A		2,3-dichloropyrazine	C1=CN=C(C(=N1)Cl)Cl
5640	21273-22-3	A		2,5-bis(chloromethyl)-1,4-dithiane	ClCC1CSC(CCl)CS1
5873	132230-40-1	A		3-(2-methoxy-1-methylethoxy)-1,2-epoxypropane	COCC(C)OCC1CO1
6093	1806-23-1	A		2-chloro-4'-fluorobenzophenone	C1=CC=C(C(=C1)C(=O)C2=CC=C(C=C2)F)Cl
6296	38260-01-4	A		trientine hydrochloride	C(CNCCNCCN)N.Cl.Cl
6317	5162-44-7	A		4-bromobut-1-ene	C=CCCBr
6554	33632-27-8	A		1-acetyl-5-nitroindoline	CC(=O)N1CCC2=C1C=CC(=C2)[N+](=O)[O-]
6579	135397-28-3	A		3-chloro-5-(chlorosulfonyl)-1-methyl-1H-pyrazole-4-carboxylic acid methyl ester	COC(=O)C1=C(N(C)N=C1Cl)S(Cl)(=O)=O
6826	10141-22-7	A		2,3-dichloro-2-methylpropanal	CC(CCl)(C=O)Cl
6854	10263-19-1	A		3',4',5'-trimethoxycinnamoyl chloride	COC1=CC(=CC(=C1OC)OC)/C=C/C(=O)Cl
6856	32692-19-6	A		5-nitroindoline	C1CNC2=C1C=C(C=C2)[N+](=O)[O-]
6872	7693-52-9	A		4-bromo-2-nitrophenol	C1=CC(=C(C=C1Br)[N+](=O)[O-])O
8103	23063-36-7	A		1-(dichloromethyl)-4-methylbenzene	CC1=CC=C(C=C1)C(Cl)Cl
8508	3967-54-2	A		4-chloro-1,3-dioxolan-2-one	C1C(OC(=O)O1)Cl

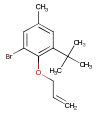
Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
8814	456-19-9	A		1-dichloromethyl-4-fluorobenzene	C1=CC(=CC=C1C(Cl)Cl)F
9280	2234-16-4	A		2',4'-dichloroacetophenone	CC(=O)C1=C(C=C(C=C1)Cl)Cl
9462	3967-55-3	A		4,5-dichloro-1,3-dioxolan-2-one	C1(C(OC(=O)O1)Cl)Cl
9484	609-60-9	A		2,4-dimethylbenzenesulfonyl chloride	CC1=CC(=C(C=C1)S(=O)(=O)Cl)C
9503	941-55-9	A		p-Toluenesulfonyl azide	CC1=CC=C(C=C1)S(=O)(=O)[N-][N+]#N
9760	594-44-5	A		ethanesulfonyl chloride	CCS(=O)(=O)Cl
10154	354-87-0	A		1,1,2,2,2-pentafluoroethanesulfonyl fluoride	C(C(F)(F)S(=O)(=O)F)(F)(F)F
10173	923-41-0	A		(7S,9S)-9-acetyl-9-amino-6,7,11-trihydroxy-5,7,8,9,10,12-hexahydro-5,12-naphthacenedione	[H][C@]1(O)C[C@@](N)(CC2=C(O)C3=C(C(=O)C4=C(C=CC=C4)C3=O)C(O)=C12)C(C)=O
10197	14214-31-4	A		2-chloro-3-isothiocyanato-1-propene	C=C(CN=C=S)Cl
10214	105827-91-6	A		2-chloro-5-chloromethylthiazole	C1=C(SC(=N1)Cl)CCl
10373	917-92-0	A		3,3-dimethyl-1-butyne	CC(C)(C)C#C
10392	144870-62-2	A		2,5-bis(isocyanatomethyl)-1,4-dithiane	O=C=NCC1CSC(CN=C=O)CS1
10479	83710-73-0	A		2-chloro-1-cyclohexene-1,3-dicarbaldehyde	ClC1=C(CCCC1C=O)C=O
10491	132220-02-1	A		7-(diethylamino)-4-methylchromene-2-thione	CCN(CC)C1=CC2=C(C=C1)C(=CC(=S)O2)C

Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
10556	31645-35-9	A		9-anthracenylmethyl methacrylate	CC(=C)C(=O)OCC1=C2C=CC=CC2=CC3=CC=CC=C31
10612	16490-49-6	A		chlorotris(dimethylamino)phosphonium chloride	CN(C)P(N(C)C)(N(C)C)(Cl)Cl
10623	93749-91-8	A		N-[4-(diethylamino)benzylidene]benzenamine N-oxide	CCN(CC)C1=CC=C(C=C1)\C=[N+](/[O-])C1=CC=CC=C1
10681	821-48-7	A		bis(2-chloroethyl)amine hydrochloride	C(CCl)NCCCl.Cl
10746	33252-30-1	A		2-chloro-4-cyanopyridine	C1=CN=C(C=C1C#N)Cl
10749	95360-33-1	A		methyl 2-[4-(chloromethyl)phenyl]acetate	COC(=O)CC1=CC=C(C=C1)CCl
10904	40119-17-3	A		(3,4-dimethoxyphenyl)hydrazine hydrochloride	COC1=C(C=C(C=C1)NN)OC.Cl
11051	821-06-7	A		1,4-dibromo-2-butene	C(/C=C/CBr)Br
11104	103816-19-9	A		4-piperidin-1-ylpiperidine-1-carbonyl chloride	C1CCN(CC1)C2CCN(CC2)C(=O)Cl
11116	1768-31-6	A		1,1,1,3,3-pentachloroacetone	C(C(=O)C(Cl)(Cl)Cl)(Cl)Cl
11178	20395-16-8	A		1,3-diallyl-5-(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	C=CCN1C(=O)N(CC=C)C(=O)N(CC2CO2)C1=O
11222	34718-47-3	A		tribromoacetyl chloride	C(=O)(C(Br)(Br)Br)Cl
11242	43204-63-3	A		bis(2-bromoethyl)amine hydrobromide	C(CBr)NCCBr.Br
11243	52583-35-4	A		5'-[bis(2-methoxyethyl)amino]-2'-[(2-cyano-4,6-dinitrophenyl)azo]acetoanilide	COCCN(CCOC)C1=CC(NC(C)=O)=C(C=C1)\N=N\C1=C(C=C(C=C1C#N)[N+]([O-])=O)[N+]([O-])=O

Strong positive (Class A) in Ames assay in Phase I trial (183 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
11256	188021-38-7	A		1-bromo-3-tert-butyl-5-methyl-2-prop-2-enoxybenzene	CC1=CC(=C(C(=C1)Br)OCC=C)C(C)(C)C