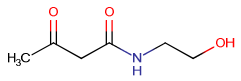
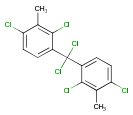
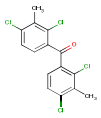
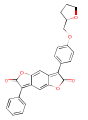
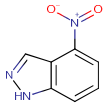
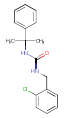
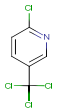
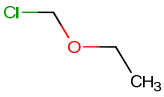
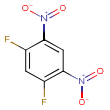
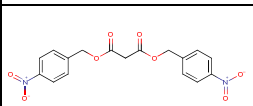
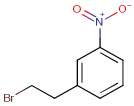
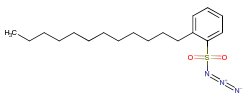
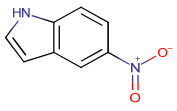
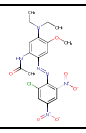
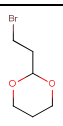
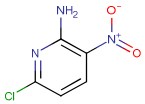
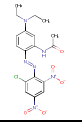
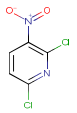
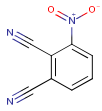
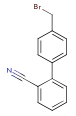
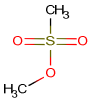
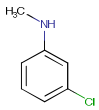
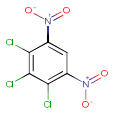
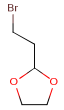
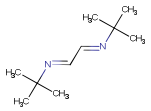
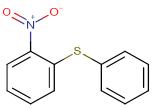
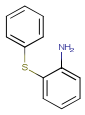
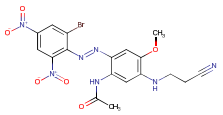
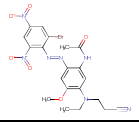
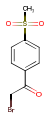
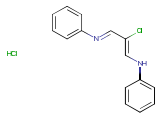
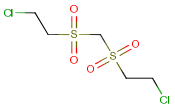
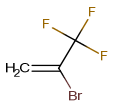
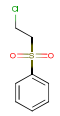
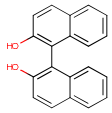
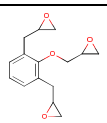
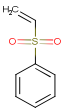
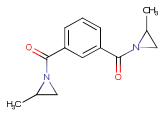
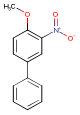
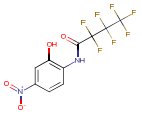
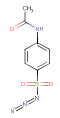
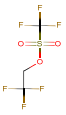
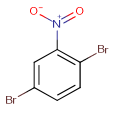
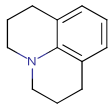
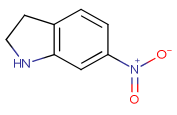
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
570	24309-97-5	A		N-(2-hydroxyethyl)acetoacetamide	CC(=O)CC(=O)NCCO
2969	115571-65-8	A		dichlorobis(2,4-dichloro-3-methylphenyl)methane	CC1=C(Cl)C(=CC=C1Cl)C(Cl)(Cl)C1=CC=C(Cl)C(C)=C1Cl
2995	29598-81-0	A		2,2',4,4'-tetrachloro-3,3'-dimethylbenzophenone	CC1=C(Cl)C=CC(C(=O)C2=CC=C(Cl)C(C)=C2Cl)=C1Cl
5548	134724-55-3	A		3-[4-(oxolan-2-ylmethoxy)phenyl]-7-phenylfuro[2,3-f][1]benzofuran-2,6-dione	C1CC(OC1)COC2=CC=C(C=C2)C3=C4C=C5C(=C(C(=O)O5)C6=CC=CC=C6)C=C4OC3=O
5633	2942-40-7	A		4-nitro-1H-indazole	C1=CC2=C(C=NN2)C(=C1)[N+](=O)[O-]
5736	99485-76-4	A		1-[(2-chlorophenyl)methyl]-3-(2-phenylpropan-2-yl)urea	CC(C)(C1=CC=CC=C1)NC(=O)NCC2=CC=CC=C2Cl
5944	69045-78-9	A		2-chloro-5-(trichloromethyl)pyridine	C1=CC(=NC=C1C(Cl)(Cl)Cl)Cl
6097	3188-13-4	A		chloromethoxyethane	CCOCCl
6267	327-92-4	A		1,5-difluoro-2,4-dinitrobenzene	C1=C(C(=CC(=C1[N+](=O)[O-])F)F)[N+](=O)[O-]
6326	67245-85-6	A		bis[(4-nitrophenyl)methyl] propanedioate	C1=CC(=CC=C1COC(=O)CC(=O)OCC2=CC=C(C=C2)[N+](=O)[O-])[N+](=O)[O-]
6513	16799-04-5	A		1-(2-bromoethyl)-3-nitrobenzene	C1=CC(=CC(=C1)[N+](=O)[O-])CCBr
6748	79791-38-1	A		N-diazo-2-dodecylbenzenesulfonamide	CCCCCCCCCCCCC1=CC=CC=C1S(=O)(=O)N=[N+]=[N-]
6752	6146-52-7	A		5-nitroindole	C1=CC2=C(C=CN2)C=C1[N+](=O)[O-]
6811	79295-99-1	A		N-[2-[(2-chloro-4,6-dinitrophenyl)diazenyl]-5-(diethylamino)-4-methoxyphenyl]acetamide	CCN(CC)C1=C(OC)C=C(\N=N\C2=C(C=C(C=C2Cl)[N+]([O-])=O)[N+]([O-])=O)C(NC(C)=O)=C1
7114	33884-43-4	A		2-(2-bromoethyl)-1,3-dioxane	C1COC(OC1)CCBr

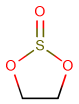
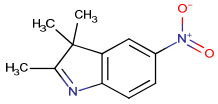
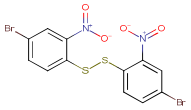
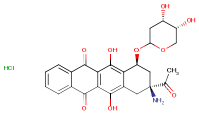
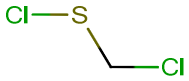
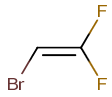
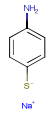
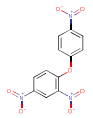
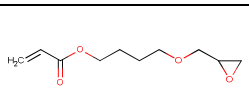
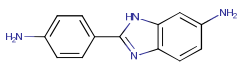
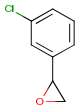
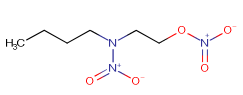
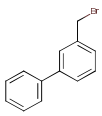
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
7164	27048-04-0	A		2-amino-6-chloro-3-nitropyridine	C1=CC(=NC(=C1[N+](=O)[O-])N)Cl
7210	66557-45-7	A		N-[2-[(2-chloro-4,6-dinitrophenyl)diazenyl]-5-(diethylamino)phenyl]acetamide	CCN(CC)C1=CC(NC(C)=O)=C(C=C1)\N=N\C1=C(C=C(C=C1Cl)[N+]([O-])=O)[N+]([O-])=O
7223	16013-85-7	A		2,6-dichloro-3-nitropyridine	C1=CC(=NC(=C1[N+](=O)[O-])Cl)Cl
7248	51762-67-5	A		3-nitrophthalonitrile	C1=CC(=C(C(=C1)[N+](=O)[O-])C#N)C#N
7446	114772-54-2	A		4'-bromomethyl-2-cyanobiphenyl	C1=CC=C(C(=C1)C#N)C2=CC=C(C=C2)CBr
7463	66-27-3	A		methyl methanesulfonate	COS(=O)(=O)C
7548	7006-52-2	A		3-chloro-N-methylaniline	CNC1=CC(=CC=C1)Cl
7588	6379-46-0	A		2,3,4-trichloro-1,5-dinitrobenzene	C1=C(C(=C(C(=C1[N+](=O)[O-])Cl)Cl)Cl)[N+](=O)[O-]
7619	18742-02-4	A		2-(2-bromoethyl)-1,3-dioxolane	C1COC(O1)CCBr
7699	30834-74-3	A		N,N'-ditert-butylethane-1,2-diimine	CC(C)(C)\N=C\C=N\C(C)(C)C
7851	4171-83-9	A		2-nitrophenyl phenyl sulfide	C1=CC=C(C=C1)SC2=CC=CC=C2[N+](=O)[O-]
7879	1134-94-7	A		2-phenylsulfanylaniline	C1=CC=C(C=C1)SC2=CC=CC=C2N
7895	53950-33-7	A		N-[2-[(2-bromo-4,6-dinitrophenyl)diazenyl]-5-(2-cyanoethylamino)-4-methoxyphenyl]acetamide	COC1=C(NCCC#N)C=C(NC(C)=O)C(=C1)\N=N\C1=C(C=C(C=C1Br)[N+]([O-])=O)[N+]([O-])=O
7896	22578-86-5	A		2'-(2-bromo-4,6-dinitrophenylazo)-5'-[N-(2-cyanoethyl)-N-ethylamino]-4'-methoxyacetanilide	CCN(CCC#N)C1=C(OC)C=C(\N=N\C2=C(C=C(C=C2Br)[N+]([O-])=O)[N+]([O-])=O)C(NC(C)=O)=C1
7898	50413-24-6	A		2-bromo-1-(4-methylsulfonylphenyl)ethanone	CS(=O)(=O)C1=CC=C(C=C1)C(=O)CBr

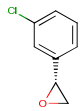
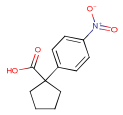
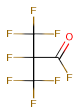
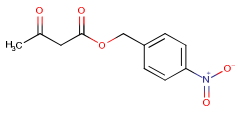
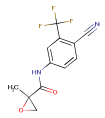
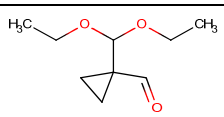
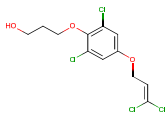
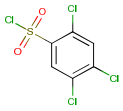
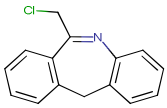
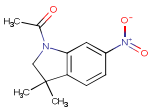
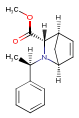
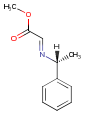
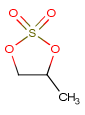
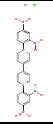
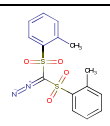
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
7936	6684-16-8	A		N-(2-chloro-3-phenyliminoprop-1-enyl)aniline hydrochloride	Cl.ClC(=C/NC1=CC=CC=C1)\C=N\C1=CC=CC=C1
8009	41123-59-5	A		bis[(2-chloroethyl)sulfonyl]methane	ClCCS(=O)(=O)CS(=O)(=O)CCCl
8161	1514-82-5	A		2-bromo-3,3,3-trifluoroprop-1-ene	C=C(C(F)(F)F)Br
8354	938-09-0	A		2-chloroethylsulfonylbenzene	C1=CC=C(C=C1)S(=O)(=O)CCCl
8537	602-09-5	A		1-(2-hydroxynaphthalen-1-yl)naphthalen-2-ol	C1=CC=C2C(=C1)C=CC(=C2C3=C(C=CC4=CC=CC=C43)O)O
8569	13561-08-5	A		2-[[2,6-bis(oxiran-2-ylmethyl)phenoxy]methyl]oxirane	C1C(O1)CC2=C(C(=CC=C2)CC3CO3)OCC4CO4
8586	5535-48-8	A		phenyl vinyl sulfone	C=CS(=O)(=O)C1=CC=CC=C1
8734	7652-64-4	A		1,1'-(1,3-phenylenedicarbonyl)bis(2-methylaziridine)	CC1CN1C(=O)C2=CC(=CC=C2)C(=O)N3CC3C
8889	15854-73-6	A		4-methoxy-3-nitrobiphenyl	COC1=C(C=C(C=C1)C2=CC=CC=C2)[N+](=O)[O-]
9015	2712-83-6	A		2,2,3,3,4,4,4-heptafluoro-N-(2-hydroxy-4-nitrophenyl)butanamide	C1=CC(=C(C=C1[N+](=O)[O-])O)NC(=O)C(C(C(F)(F)F)(F)F)(F)F
9072	2158-14-7	A		N-(4-azidosulfonylphenyl)acetamide	CC(=O)NC1=CC=C(C=C1)S(=O)(=O)N=[N+]=[N-]
9156	6226-25-1	A		2,2,2-trifluoroethyl trifluoromethanesulfonate	C(C(F)(F)F)OS(=O)(=O)C(F)(F)F
9293	3460-18-2	A		2,5-dibromonitrobenzene	C1=CC(=C(C=C1Br)[N+](=O)[O-])Br
9307	479-59-4	A		julolidine	C1CC2=C3C(=CC=C2)CCCN3C1
9321	19727-83-4	A		6-nitroindoline	C1CNC2=C1C=CC(=C2)[N+](=O)[O-]

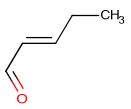
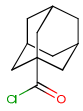
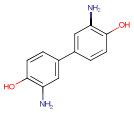
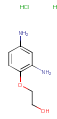
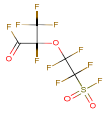
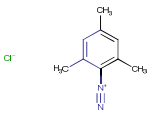
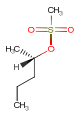
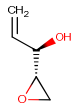
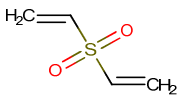
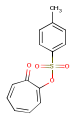
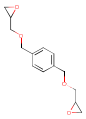
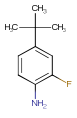
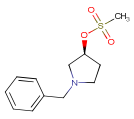
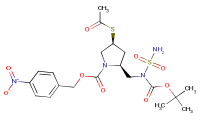
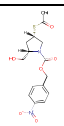
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
9796	3741-38-6	A		ethylene sulfite	C1COS(=O)O1
9837	2314-97-8	A		trifluoroiodomethane	C(F)(F)I
9838	3484-22-8	A		2,3,3-trimethyl-5-nitro-3H-indole	CC1=NC2=C(C1(C)C)C=C(C=C2)[N+](=O)[O-]
10005	76209-05-7	A		bis(4-bromo-2-nitrophenyl) disulfide	[O-][N+](=O)C1=CC(Br)=CC=C1SSC1=CC=C(Br)C=C1[N+]([O-])=O
10172	110311-30-3	A		amrubicin hydrochloride	CC(=O)[C@]1(C[C@@H](C2=C(C3=C(C(=C2C1)O)C(=O)C4=CC=CC=C4C3=O)O)OC5C[C@@H]([C@@H](CO5)O)O)N.Cl
10484	26826-80-2	A		chloro(chlorosulfanyl)methane	ClCSCl
10951	359-08-0	A		2-bromo-1,1-difluoroethylene	C(=C(F)F)Br
11001	6976-04-1	A		4-(sodiothio)aniline	[Na+].NC1=CC=C([S-])C=C1
11342	2363-36-2	A		2,4-dinitro-1-(4-nitrophenoxy)benzene	C1=CC(=CC=C1[N+](=O)[O-])OC2=C(C=C(C=C2)[N+](=O)[O-])[N+](=O)[O-]
11455	119692-59-9	A		acrylic acid 4-(glycidyloxy)butyl ester	C=CC(=O)OCCCCOCC1CO1
11478	7621-86-5	A		2-(4-aminophenyl)-1H-benzo[d]imidazol-5-amine	C1=CC(=CC=C1C2=NC3=C(N2)C=C(C=C3)N)N
11518	20697-04-5	A		(3-chlorophenyl)oxirane	C1C(O1)C2=CC(=CC=C2)Cl
11565	82486-82-6	A		nitric acid 2-(butyl-nitro-amino)-ethyl ester	CCCCN(CCO[N+]([O-])=O)[N+]([O-])=O
11650	14704-31-5	A		3-(bromomethyl)biphenyl	C1=CC=C(C=C1)C2=CC(=CC=C2)CBr
11682	33574-02-6	A		iodomethylcyclopropane	C1CC1CI

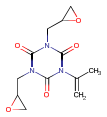
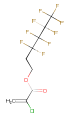
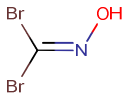
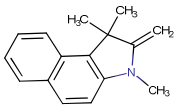
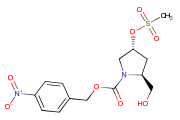
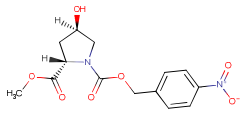
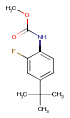
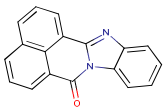
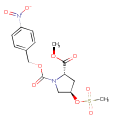
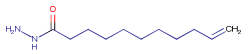
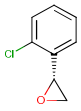
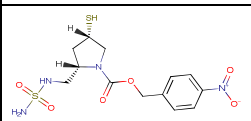
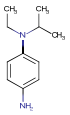
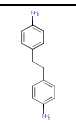
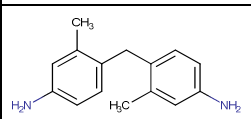
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
11754	62600-71-9	A		(2R)-2-(3-chlorophenyl)oxirane	C1[C@H](O1)C2=CC(=CC=C2)Cl
11829	52648-77-8	A		1-(4-nitrophenyl)cyclopentane-1-carboxylic acid	C1CCC(C1)(C2=CC=C(C=C2)[N+](=O)[O-])C(=O)O
11884	677-84-9	A		2-(trifluoromethyl)-2,3,3,3-tetrafluoropropionic acid fluoride	FC(=O)C(F)(C(F)(F)F)C(F)(F)F
11965	61312-84-3	A		4-nitrobenzyl acetoacetate	CC(=O)CC(=O)OCC1=CC=C(C=C1)[N+](=O)[O-]
12021	90357-51-0	A		N-(4-cyano-3-(trifluoromethyl)phenyl)-2-methyloxirane-2-carboxamide	CC1(CO1)C(=O)NC2=CC(=C(C=C2)C#N)C(F)(F)F
12026	400709-86-6	A		1-(diethoxymethyl)cyclopropane-1-carbaldehyde	CCOC(C1(CC1)C=O)OCC
12031	178043-48-6	A		3-[2,6-dichloro-4-(3,3-dichloroprop-2-enoxy)phenoxy]propan-1-ol	C1=C(C=C(C(=C1Cl)OCCCO)Cl)OCC=C(Cl)Cl
12057	15945-07-0	A		2,4,5-trichlorobenzenesulfonyl chloride	C1=C(C(=CC(=C1Cl)Cl)Cl)S(=O)(=O)Cl
12210	215353-44-4	A		6-(chloromethyl)-11H-dibenzo[b,e]azepine	ClCC1=NC2=C(CC3=C1C=CC=C3)C=CC=C2
12443	453562-68-0	A		1-(3,3-dimethyl-6-nitroindolin-1-yl)ethanone	CC(=O)N1CC(C2=C1C=C(C=C2)[N+](=O)[O-])(C)C
12505	130194-96-6	A		(1S,3S,4R)-2-[(1R)-1-phenylethyl]-2-azabicyclo[2.2.1]hepta-5-ene-3-carboxylic acid methyl ester	[H][C@](C)(N1[C@@]2([H])C[C@]([H])(C=C2)[C@@]1([H])C(=O)OC)C1=CC=CC=C1
12506	153831-92-6	A		N-[(1R)-1-phenylethyl]iminoacetic acid methyl ester	[H][C@](C)(\N=C\C(=O)OC)C1=CC=CC=C1
12528	5689-83-8	A		4-methyl-1,3,2-dioxathiolane 2,2-dioxide	CC1COS(=O)(=O)O1
12664	41168-79-0	A		1,1'-bis(2,4-dinitrophenyl)-4,4'-bipyridinium dichloride	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])[N+]2=CC=C(C=C2)C3=CC=[N+](C=C3)C4=C(C=C(C=C4)[N+](=O)[O-])[N+](=O)[O-].[Cl-
12670	14159-45-6	A		1-[diazo-(2-methylphenyl)sulfonylmethyl]sulfonyl-2-methylbenzene	CC1=CC=CC=C1S(=O)(=O)C(=[N+]=[N-])S(=O)(=O)C2=CC=CC=C2C

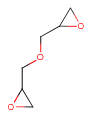
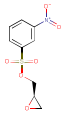
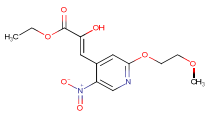
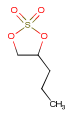
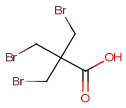
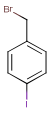
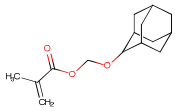
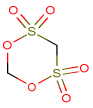
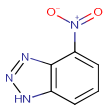
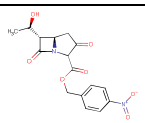
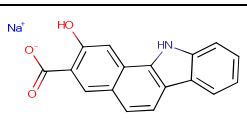
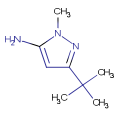
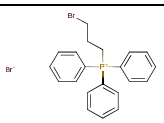
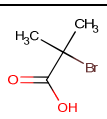
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
12718	1576-87-0	A		2-pentenal	CC/C=C/C=O
12771	2094-72-6	A		adamantane-1-carbonyl chloride	C1C2CC3CC1CC(C2)(C3)C(=O)Cl
12839	4194-40-5	A		3,3'-diaminobiphenyl-4,4'-diol	C1=CC(=C(C=C1C2=CC(=C(C=C2)O)N)N)O
12840	66422-95-5	A		2-(2,4-diaminophenoxy)ethanol dihydrochloride	C1=CC(=C(C=C1N)N)OCCO.Cl.Cl
12882	4089-57-0	A		2,3,3,3-tetrafluoro-2-[1,1,2,2-tetrafluoro-2-(fluorosulfonyl)ethoxy]propionic acid fluoride	FC(=O)C(F)(OC(F)(F)C(F)(F)S(F)(=O)=O)C(F)(F)F
12897	158091-65-7	A		2,4,6-trimethylbenzenediazonium chloride	[Cl-].CC1=CC(C)=C([N+]#N)C(C)=C1
12968	119992-81-3	A		(S)-1-methylbutyl methanesulfonate	[H][C@](C)(CCC)OS(C)(=O)=O
13027	102490-00-6	A		(1R)-1-[(2S)-oxiran-2-yl]prop-2-en-1-ol	C=C[C@H]([C@@H]1CO1)O
13063	77-77-0	A		divinyl sulfone	C=CS(=O)(=O)C=C
13108	38768-08-0	A		tropolone tosylate	CC1=CC=C(C=C1)S(=O)(=O)OC2=CC=CC=CC2=O
13112	29513-13-1	A		2-[[4-(oxiran-2-ylmethoxymethyl)phenyl]methoxymethyl]oxirane	C1C(O1)COCC2=CC=C(C=C2)COCC3CO3
13137	129373-04-2	A		4-tert-butyl-2-fluoroaniline	CC(C)(C)C1=CC(=C(C=C1)N)F
13165	118354-71-5	A		[(3S)-1-benzylpyrrolidin-3-yl] methanesulfonate	CS(=O)(=O)O[C@H]1CCN(C1)CC2=CC=CC=C2
13202	491878-06-9	A		(4-nitrophenyl)methyl (2S,4S)-4-acetylsulfanyl-2-[[(2-methylpropan-2-yl)oxycarbonyl-sulfamoylamino]methyl]pyrrolidine-1-carboxylate	CC(=O)S[C@H]1C[C@H](N(C1)C(=O)OCC2=CC=C(C=C2)[N+](=O)[O-])CN(C(=O)OC(C)(C)C)S(=O)(=O)N
13203	104773-40-2	A		(2S,4S)-4-(acetylthio)-2-(hydroxymethyl)pyrrolidine-1-carboxylic acid 4-nitrobenzyl ester	[H][C@]1(CN(C(=O)OCC2=CC=C(C=C2)[N+]([O-])=O)[C@]([H])(CO)C1)SC(C)=O

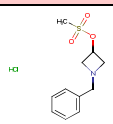
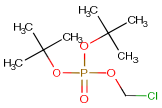
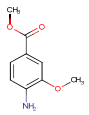
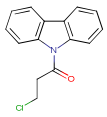
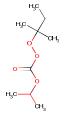
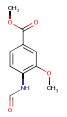
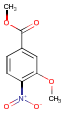
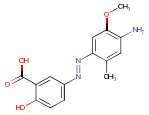
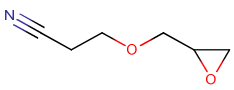
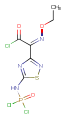
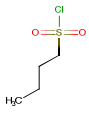
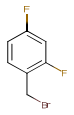
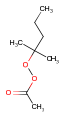
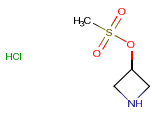
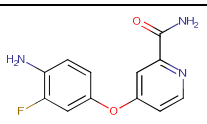
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
13218	69731-45-9	A		1-allyl-3,5-diglycidyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	CC(=C)N1C(=O)N(C(=O)N(C1=O)CC2CO2)CC3CO3
13242	701909-41-3	A		2-chloroacrylic acid 3,3,4,4,5,5,6,6,6-nonafluorohexyl ester	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)CCOC(=O)C(Cl)=C
13302	74213-24-4	A		dibromoformaldoxime	ON=C(Br)Br
13354	344928-74-1	A		1,1,3-trimethyl-2-methylene-2,3-dihydro-1H-benzo[e]indole	CN1C(=C)C(C)(C)C2=C1C=CC1=C2C=CC=C1
13384	127626-37-3	A		(4-nitrophenyl)methyl (2S,4R)-2-(hydroxymethyl)-4-methylsulfonyloxypyrrolidine-1-carboxylate	CS(=O)(=O)O[C@@H]1C[C@H](N(C1)C(=O)OCC2=CC=C(C=C2)[N+](=O)[O-])CO
13386	101803-29-6	A		(2S,4R)-4-hydroxy-2-(methoxycarbonyl)pyrrolidine-1-carboxylic acid 4-nitrobenzyl ester	[H][C@]1(O)CN(C(=O)OCC2=CC=C(C=C2)[N+]([O-])=O)[C@@]([H])(C1)C(=O)OC
13406	623548-14-1	A		4-tert-butyl-2-fluorophenylcarbamic acid methyl	COC(=O)NC1=CC=C(C=C1F)C(C)(C)C
13427	23749-58-8	A		7H-benzimidazo[2,1-a]benz[de]isoquinolin-7-one	C1=CC=C2C(=C1)N=C3N2C(=O)C4=CC=CC5=C4C3=CC=C5
13455	138324-82-8	A		(2S,4R)-2-methyl 1-(4-nitrobenzyl) 4-((methylsulfonyl)oxy)pyrrolidine-1,2-dicarboxylate	COC(=O)[C@@H]1C[C@H](CN1C(=O)OCC2=CC=C(C=C2)[N+](=O)[O-])OS(=O)(=O)C
13521	5458-77-5	A		undec-10-enehydrazide	C=CCCCCCCCCC(=O)NN
13546	62566-66-9	A		(2R)-2-(2-chlorophenyl)oxirane	C1[C@H](O1)C2=CC=CC=C2Cl
13597	148017-03-2	A		(2S,4S)-2-sulfamoylaminomethyl-4-mercaptopyrrolidine-1-carboxylic acid 4-nitrobenzyl ester	[H][C@@]1(S)CN(C(=O)OCC2=CC=C(C=C2)[N+]([O-])=O)[C@]([H])(CNS(N)(=O)=O)C1
13767	91215-79-1	A		4-N-ethyl-4-N-propan-2-ylbenzene-1,4-diamine	CCN(C1=CC=C(C=C1)N)C(C)C
13772	621-95-4	A		4,4'-diaminodibenzyl	C1=CC(=CC=C1CCC2=CC=C(C=C2)N)N
14011	97-28-9	A		4,4'-methylenebis(3-methylaniline)	CC1=CC(N)=CC=C1CC1=CC=C(N)C=C1C

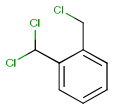
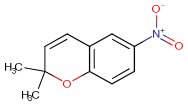
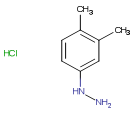
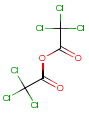
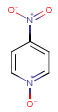
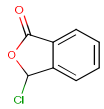
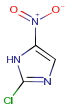
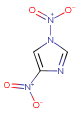
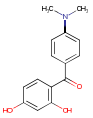
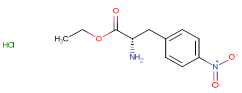
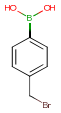
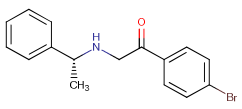
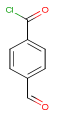
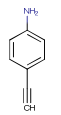
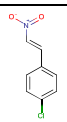
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
14383	2238-07-5	A		2-(oxiran-2-ylmethoxymethyl)oxirane	C1C(O1)COCC2CO2
14875	115314-17-5	A		(R)-glycidyl 3-nitrobenzenesulfonate	C1[C@@H](O1)COS(=O)(=O)C2=CC=CC(=C2)[N+](=O)[O-]
15545	794470-22-7	A		2-hydroxy-3-[2-(2-methoxyethoxy)-5-nitropyridine-4-yl]propenoic acid ethyl ester	CCOC(=O)C(\O)=C\C1=CC(OCCOC)=NC=C1[N+]([O-])=O
15565	165108-64-5	A		4-propyl-1,3,2-dioxathiolane 2,2-dioxide	CCCC1COS(=O)(=O)O1
15568	52813-48-6	A		3-bromo-2,2-bis(bromomethyl)propanoic acid	C(C(CBr)(CBr)C(=O)O)Br
15571	16004-15-2	A		1-(bromomethyl)-4-iodobenzene	C1=CC(=CC=C1CBr)I
15583	791611-93-3	A		methacrylic acid 2-adamantyloxymethyl ester	CC(=C)C(=O)OCOC1C2CC3CC(C2)CC1C3
15720	426253-76-1	A		(2S)-4-(chloroacetyl)-2-methyl-2,5-dihydro-1H-pyrrole-1-carboxylic acid allyl ester	[H][C@]1(C)C=C(CN1C(=O)OCC=C)C(=O)CCl
15759	99591-74-9	A		1,5,2,4-dioxadithiane, 2,2,4,4-tetraoxide	O=S1(=O)CS(=O)(=O)OCO1
15833	6299-39-4	A		4-nitro-1H-benzotriazole	[O-][N+](=O)C1=CC=CC2=C1N=NN2
15847	74288-40-7	A		(4-nitrophenyl)methyl (5R,6S)-6-[(1R)-1-hydroxyethyl]-3,7-dioxo-1-azabicyclo[3.2.0]heptane-2-carboxylate	C[C@H]([C@@H]1[C@H]2CC(=O)C(N2C1=O)C(=O)OCC3=CC=C(C=C3)[N+](=O)[O-])O
15855	116353-24-3	A		sodium 2-hydroxy-11H-benzo[a]carbazole-3-carboxylate	C1=CC=C2C(=C1)C3=C(N2)C4=CC(=C(C=C4C=C3)C(=O)[O-])O.[Na+]
15886	118430-73-2	A		5-tert-butyl-2-methylpyrazol-3-amine	CC(C)(C)C1=NN(C(=C1)N)C
15897	3607-17-8	A		3-bromopropyltriphenylphosphonium bromide	C1=CC=C(C=C1)[P+](CCCBr)(C2=CC=CC=C2)C3=CC=CC=C3.[Br-]
15899	2052-01-9	A		2-bromo-2-methylpropionic acid	CC(C)(C(=O)O)Br

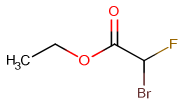
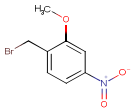
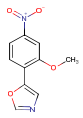
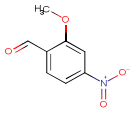
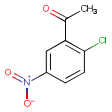
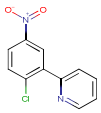
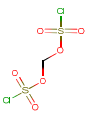
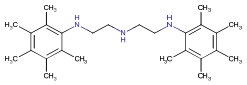
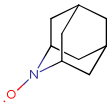
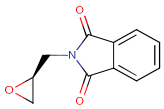
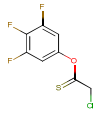
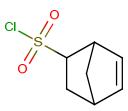
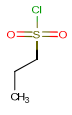
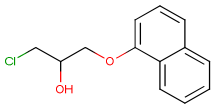
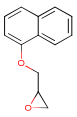
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
15938	292163-60-1	A		methanesulfonic acid 1-benzylazetidine-3-yl hydrochloride	Cl.CS(=O)(=O)OC1CN(CC2=CC=CC=C2)C1
15946	229625-50-7	A		ditert-butyl chloromethyl phosphate	CC(C)(C)OP(=O)(OCCl)OC(C)(C)C
16003	41608-64-4	A		methyl 4-amino-3-methoxybenzoate	COC1=C(C=CC(=C1)C(=O)OC)N
16048	2499-66-3	A		1-(9H-Carbazole-9-yl)-3-chloropropane-1-one	ClCCC(=O)N1C2=C(C=CC=C2)C2=C1C=CC=C2
16235	2372-22-7	A		isopropoxyperformic acid 1,1-dimethylpropyl ester	CCC(C)(C)OOC(=O)OC(C)C
16252	700834-18-0	A		methyl 4-formylamino-3-methoxybenzoate	COC1=C(C=CC(=C1)C(=O)OC)NC=O
16290	5081-37-8	A		methyl 3-methoxy-4-nitrobenzoate	COC1=C(C=CC(=C1)C(=O)OC)[N+](=O)[O-]
16348	85720-86-1	A		5-[(4-amino-5-methoxy-2-methylphenyl)diazenyl]-2-hydroxybenzoic acid	COC1=C(N)C=C(C)C(=C1)\N=N\C1=CC=C(O)C(=C1)C(O)=O
16390	10433-39-3	A		3-(oxiranylmethoxy)-propanenitrile	N#CCCOCC1CO1
16451	90211-01-1	A		[(Z)-2-[5-(dichlorophosphinylamino)-1,2,4-thiadiazole-3-yl]-2-(ethoxyimino)acetyl] chloride	CCO\N=C(C(Cl)=O)\C1=NSC(NP(Cl)(Cl)=O)=N1
16570	2386-60-9	A		butane-1-sulfonyl chloride	CCCCS(=O)(=O)Cl
16588	23915-07-3	A		1-(bromomethyl)-2,4-difluorobenzene	C1=CC(=C(C=C1F)F)CBr
16589	18260-97-4	A		peroxyacetic acid 1,1-dimethylbutyl ester	CCCC(C)(C)OOC(C)=O
16624	36476-89-8	A		3-methanesulfonatoazetidine hydrochloride	CS(=O)(=O)OC1CNC1.Cl
16677	757251-54-0	A		4-(4-amino-3-fluorophenoxy)-pyridine-2-carboxylic acid amide	C1=CC(=C(C=C1OC2=CC(=NC=C2)C(=O)N)F)N

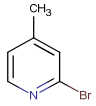
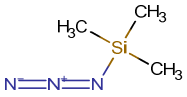
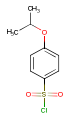
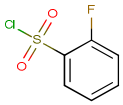
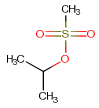
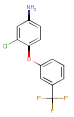
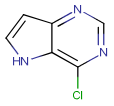
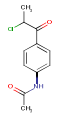
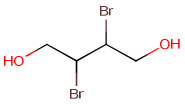
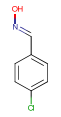
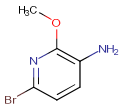
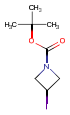
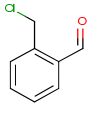
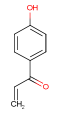
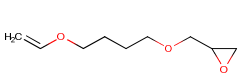
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
16751	30293-58-4	A		1-(chloromethyl)-2-(dichloromethyl)benzene	C1=CC=C(C(=C1)CCl)C(Cl)Cl
16798	33143-28-1	A		2,2-dimethyl-6-nitro-2H-chromene	CC1(C=CC2=C(O1)C=CC(=C2)[N+](=O)[O-])C
16800	60481-51-8	A		3,4-dimethylphenylhydrazine hydrochloride	CC1=C(C=C(C=C1)NN)C.Cl
16822	4124-31-6	A		(2,2,2-trichloroacetyl) 2,2,2-trichloroacetate	C(=O)(C(Cl)(Cl)Cl)OC(=O)C(Cl)(Cl)Cl
16831	1124-33-0	A		4-nitropyridine 1-oxide	C1=C[N+](=CC=C1[N+](=O)[O-])[O-]
17070	6295-21-2	A		3-chlorophthalide	C1=CC=C2C(=C1)C(OC2=O)Cl
17080	57531-37-0	A		2-chloro-4-nitroimidazole	C1=C(NC(=N1)Cl)[N+](=O)[O-]
17123	19182-81-1	A		1,4-dinitroimidazole	C1=C(N=CN1[N+](=O)[O-])[N+](=O)[O-]
17125	160818-07-5	A		(2,4-dihydroxyphenyl)-(4-dimethylaminophenyl)methanone	CN(C)C1=CC=C(C=C1)C(=O)C2=C(C=C(C=C2)O)O
17178	58816-66-3	A		3-(4-nitrophenyl)-L-alanine ethyl ester hydrochloride	CCOC(=O)[C@H](CC1=CC=C(C=C1)[N+](=O)[O-])N.Cl
17243	68162-47-0	A		[4-(bromomethyl)phenyl]boronic acid	B(C1=CC=C(C=C1)CBr)(O)O
17513	920804-14-4	A		1-(4-bromophenyl)-2-[[(1R)-1-phenylethyl]amino]ethanone	C[C@H](C1=CC=CC=C1)NCC(=O)C2=CC=C(C=C2)Br
17551	16173-52-7	A		4-formylbenzoyl chloride	C1=CC(=CC=C1C=O)C(=O)Cl
17634	14235-81-5	A		4-ethynylaniline	C#CC1=CC=C(C=C1)N
17676	5153-70-8	A		1-chloro-4-(2-nitroethenyl)benzene	[O-][N+](=O)\C=C\C1=CC=C(Cl)C=C1

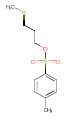
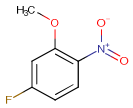
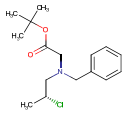
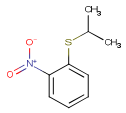
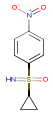
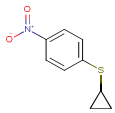
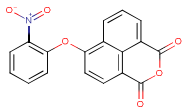
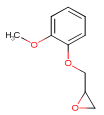
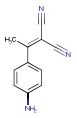
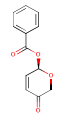
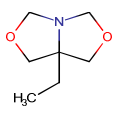
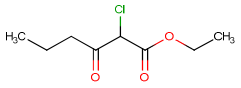
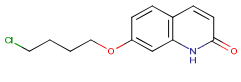
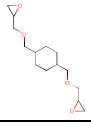
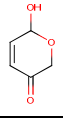
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
17784	401-55-8	A		ethyl 2-bromo-2-fluoroacetate	CCOC(=O)C(F)Br
17786	90434-16-5	A		1-(bromomethyl)-2-methoxy-4-nitrobenzene	COC1=CC(=CC=C1CBr)[N+]([O-])=O
17817	198821-78-2	A		5-(2-methoxy-4-nitrophenyl)-1,3-oxazole	COC1=C(C=CC(=C1)[N+](=O)[O-])C2=CN=CO2
17818	136507-15-8	A		2-methoxy-4-nitrobenzaldehyde	COC1=CC(=CC=C1C=O)[N+]([O-])=O
17910	23082-50-0	A		2'-chloro-5'-nitroacetophenone	CC(=O)C1=C(C=CC(=C1)[N+](=O)[O-])Cl
17911	879088-40-1	A		2-(2-chloro-5-nitrophenyl)pyridine	C1=CC=NC(=C1)C2=C(C=CC(=C2)[N+](=O)[O-])Cl
17987	92975-18-3	A		bis(chlorosulfonyloxy)methane	C(OS(=O)(=O)Cl)OS(=O)(=O)Cl
17996	862464-60-6	A		bis[2-(pentamethylphenylamino)ethyl]amine	CC1=C(C)C(C)=C(NCCNCCNC2=C(C)C(C)=C(C)C(C)=C2C)C(C)=C1C
18094	57625-08-8	A		2-azatricyclo[3.3.1.13,7]decan-2-oxyl	C1C2CC3CC1CC(C2)N3[O]
18137	161596-47-0	A		2-[[(2S)-oxiran-2-yl]methyl]isoindole-1,3-dione	C1[C@@H](O1)CN2C(=O)C3=CC=CC=C3C2=O
18170	95986-39-1	A		chlorothioacetic acid O-(3,4,5-trifluorophenyl) ester	FC1=CC(OC(=S)CCl)=CC(F)=C1F
18249	498563-29-4	A		bicyclo[2.2.1]hepta-5-ene-2-sulfonyl chloride	ClS(=O)(=O)C1CC2CC1C=C2
18310	10147-36-1	A		1-propanesulfonyl chloride	CCCS(=O)(=O)Cl
18446	20133-93-1	A		1-chloro-3-(1-naphthoxy)-2-propanol	C1=CC=C2C(=C1)C=CC=C2OCC(CCl)O
18557	2461-42-9	A		glycidyl 1-naphthyl ether	C1C(O1)COC2=CC=CC3=CC=CC=C32

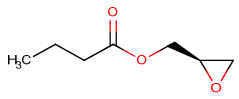
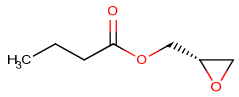
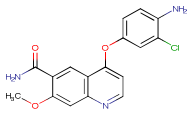
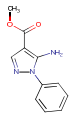
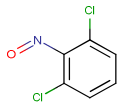
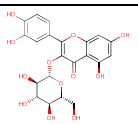
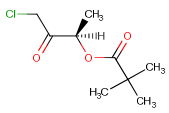
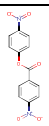
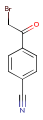
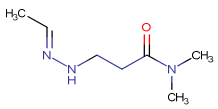
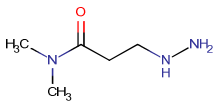
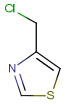
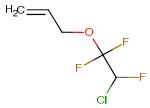
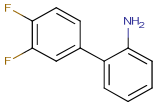
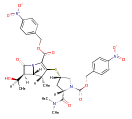
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
18616	4926-28-7	A		2-bromo-4-methylpyridine	CC1=CC(=NC=C1)Br
18682	4648-54-8	A		azidotrimethylsilane	C[Si](C)(C)N=[N+]=[N-]
18725	98995-40-5	A		4-isopropoxybenzenesulfonyl chloride	CC(C)OC1=CC=C(C=C1)S(Cl)(=O)=O
18905	2905-21-7	A		2-fluorobenzenesulfonyl chloride	C1=CC=C(C(=C1)F)S(=O)(=O)Cl
18956	926-06-7	A		isopropylmethanesulfonate	CC(C)OS(=O)(=O)C
19073	40718-14-7	A		3-chloro-4-[3-(trifluoromethyl)phenoxy]aniline	NC1=CC=C(OC2=CC=CC(=C2)C(F)(F)F)C(Cl)=C1
19081	84905-80-6	A		4-chloro-5H-pyrrolo[3,2-d]pyrimidine	ClC1=C2NC=CC2=NC=N1
19084	81112-08-5	A		N-[4-(2-chloropropanoyl)phenyl]acetamide	CC(C(=O)C1=CC=C(C=C1)NC(=O)C)Cl
19122	20163-90-0	A		2,3-dibromo-1,4-butanediol	C(C(C(CO)Br)Br)O
19360	3848-36-0	A		4-chlorobenzaldehyde oxime	C1=CC(=CC=C1/C=N/O)Cl
19477	89466-18-2	A		6-bromo-2-methoxypyridin-3-amine	COC1=C(N)C=CC(Br)=N1
19510	254454-54-1	A		3-iodo-azetidine-1-carboxylic acid tert-butyl ester	CC(C)(C)OC(=O)N1CC(I)C1
19636	108683-62-1	A		2-(chloromethyl)benzaldehyde	ClCC1=C(C=O)C=CC=C1
19729	95605-38-2	A		1-(4-hydroxyphenyl)prop-2-en-1-one	OC1=CC=C(C=C1)C(=O)C=C
19737	16801-21-1	A		2-(4-ethenoxybutoxymethyl)oxirane	C=COCCCCOCC1CO1

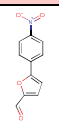
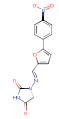
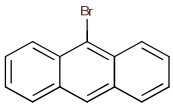
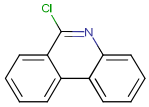
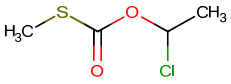
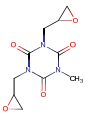
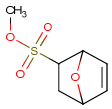
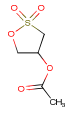
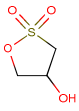
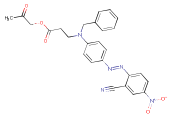
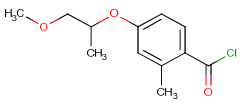
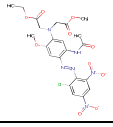
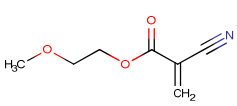
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
19802	187722-18-5	A		3-methylsulfanylpropyl 4-methylbenzenesulfonate	CSCCCOS(=O)(=O)C1=CC=C(C)C=C1
20046	448-19-1	A		4-fluoro-2-methoxy-1-nitrobenzene	COC1=C(C=CC(=C1)F)[N+](=O)[O-]
20065	888494-24-4	A		glycine, N-[(2R)-2-chloropropyl]-N-(phenylmethyl)-,1,1-dimethylethyl ester	C[C@@H](Cl)CN(CC(=O)OC(C)(C)C)CC1=CC=CC=C1
20172	70415-85-9	A		1-nitro-2-propan-2-ylsulfanylbenzene	CC(C)SC1=CC=CC=C1[N+]([O-])=O
20226	942410-33-5	A		1-(S-cyclopropylsulfonimidoyl)-4-nitrobenzene	[O-][N+](=O)C1=CC=C(C=C1)S(=N)(=O)C1CC1
20228	851008-48-5	A		1-(cyclopropylthio)-4-nitrobenzene	C1CC1SC2=CC=C(C=C2)[N+](=O)[O-]
20296	111669-59-1	A		6-(2-nitrophenoxy)-1H,3H-naphtho[1,8-cd]pyran-1,3-dione	[O-][N+](=O)C1=C(OC2=C3C=CC=C4C(=O)OC(=O)C(C=C2)=C34)C=CC=C1
20413	2210-74-4	A		2-[(2-methoxyphenoxy)methyl]oxirane	COC1=CC=CC=C1OCC2CO2
20488	122520-80-3	A		2-[1-(4-aminophenyl)ethylidene]propanedinitrile	CC(=C(C#N)C#N)C1=CC=C(C=C1)N
20503	582302-79-2	A		benzoic acid (2R)-5-oxo-5,6-dihydro-2H-pyran-2-yl ester	O=C(O[C@H]1OCC(=O)C=C1)C1=CC=CC=C1
20512	7747-35-5	A		5-ethyl-3,7-dioxa-1-azabicyclo[3.3.0]octane	CCC12COCN1COC2
20551	67271-32-3	A		ethyl 2-chloro-3-oxohexanoate	CCCC(=O)C(C(=O)OCC)Cl
20557	913613-82-8	A		7-(4-chlorobutoxy)-1H-quinolin-2-one	C1=CC(=CC2=C1C=CC(=O)N2)OCCCCCl
20635	14228-73-0	A		2-[[4-(oxiran-2-ylmethoxymethyl)cyclohexyl]methoxymethyl]oxirane	C1CC(CCC1COCC2CO2)COCC3CO3
20648	35436-57-8	A		2-hydroxy-2H-pyran-5-one	C1C(=O)C=CC(O1)O

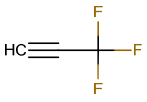
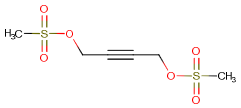
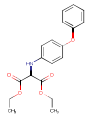
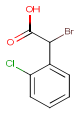
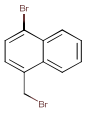
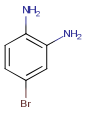
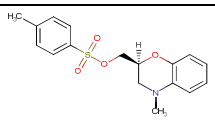
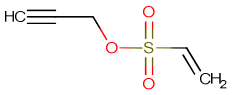
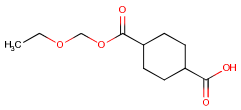
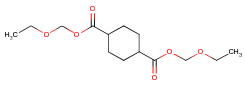
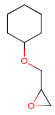
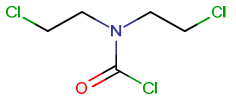
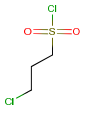
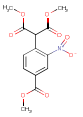
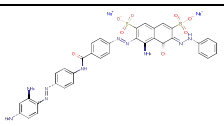
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
20661	60456-26-0	A		(R)-glycidyl butyrate	CCCC(=O)OC[C@H]1CO1
20662	65031-96-1	A		(S)-(+)-glycidyl butyrate	CCCC(=O)OC[C@@H]1CO1
20769	417722-93-1	A		4-(4-amino-3-chlorophenoxy)-7-methoxyquinoline-6-carboxamide	COC1=CC2=C(C=C1C(N)=O)C(OC1=CC=C(N)C(Cl)=C1)=CC=N2
20779	29097-01-6	A		5-amino-1-phenyl-1H-pyrazole-4-carboxylic acid methyl ester	COC(=O)C1=C(N)N(N=C1)C1=CC=CC=C1
20903	1194-66-7	A		1,3-dichloro-2-nitrosobenzene	ClC1=CC=CC(Cl)=C1N=O
20912	482-35-9	A		isoquercitrin	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O)O
20932	832151-99-2	A		2,2-dimethylpropanoic acid (1R)-3-chloro-1-methyl-2-oxopropyl ester	[H][C@](C)(OC(=O)C(C)(C)C)C(=O)CCl
20975	1037-31-6	A		4-nitrophenyl 4-nitrobenzoate	C1=CC(=CC=C1C(=O)OC2=CC=C(C=C2)[N+](=O)[O-])[N+](=O)[O-]
21031	20099-89-2	A		4-(2-bromoacetyl)benzonitrile	C1=CC(=CC=C1C#N)C(=O)CBr
21134	112858-31-8	A		3-(2-ethylidenehydrazinyl)-N,N-dimethylpropanamide	C\C=N\NCCC(=O)N(C)C
21275	107746-30-5	A		3-hydrazino-N,N-dimethylpropanamide	CN(C)C(=O)CCNN
21699	3364-76-9	A		4-(chloromethyl)-1,3-thiazole	C1=C(N=CS1)CCl
21719	380-44-9	A		3-(2-chloro-1,1,2-trifluoroethoxy)prop-1-ene	C=CCOC(C(F)Cl)(F)F
21729	873056-62-3	A		2-(3,4-difluorophenyl)aniline	C1=CC=C(C(=C1)C2=CC(=C(C=C2)F)F)N
21738	96036-02-1	A		(4R,5S)-3-[[(3S)-1-(4-nitrobenzyloxycarbonyl)-5β-(dimethylaminocarbonyl)pyrrolidine-3β-yl]thio]-4α-methyl-6β-[(1R)-1-hydroxyethyl]-7-oxo-1-azabicyclo[3.2.0]hepta-2-ene-2-carboxylic acid 4-nitrobenzyl ester	[H][C@](C)(O)[C@@]1([H])C(=O)N2C(C(=O)OCC3=CC=C(C=C3)[N+]([O-])=O)=C(S[C@]3([H])CN(C(=O)OCC4=CC=C(C=C4)[N+]([O-

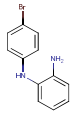
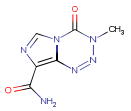
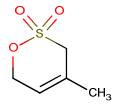
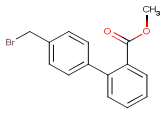
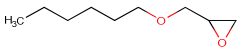
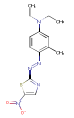
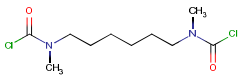
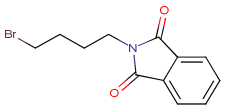
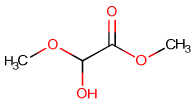
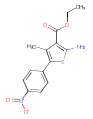
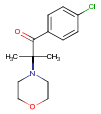
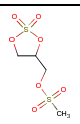
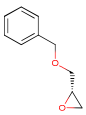
Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
21782	7147-77-5	A		5-(4-nitrophenyl)furan-2-carbaldehyde	C1=CC(=CC=C1C2=CC=C(O2)C=O)[N+](=O)[O-]
21783	7261-97-4	A		dantrolene	C1C(=O)NC(=O)N1/N=C/C2=CC=C(O2)C3=CC=C(C=C3)[N+](=O)[O-]
21841	1564-64-3	A		9-bromoanthracene	C1=CC=C2C(=C1)C=C3C=CC=CC3=C2Br
22012	15679-03-5	A		6-chlorophenanthridine	C1=CC=C2C(=C1)C3=CC=CC=C3N=C2Cl
22066	91507-67-4	A		thiocarbonic acid O-(1-chloroethyl) S-methyl ester	CSC(=O)OC(C)Cl
22089	69804-58-6	A		1-methyl-3,5-bis(oxiran-2-ylmethyl)-1,3,5-triazinane-2,4,6-trione	CN1C(=O)N(C(=O)N(C1=O)CC2CO2)CC3CO3
22189	7471-63-8	A		7-methyl-8-nitroquinoline	CC1=C(C2=C(C=CC=N2)C=C1)[N+](=O)[O-]
22290	625392-85-0	A		methyl 7-oxabicyclo[2.2.1]hept-2-ene-5-sulfonate	COS(=O)(=O)C1CC2C=CC1O2
22328	1263199-75-2	A		2-acetoxy-1,3-propanesultone	CC(=O)OC1COS(=O)(=O)C1
22336	373-91-1	A		trifluoromethyl hypofluorite	C(OF)(F)(F)F
22342	10200-48-3	A		2,2-dioxooxathiolan-4-ol	C1C(CS(=O)(=O)O1)O
22444	1021394-33-1	A		3-[N-benzyl-4-[(2-cyano-4-nitrophenyl)azo]anilino]propanoic acid 2-oxopropyl ester	CC(=O)COC(=O)CCN(CC1=CC=CC=C1)C1=CC=C(C=C1)\N=N\C1=CC=C(C=C1C#N)[N+]([O-])=O
22470	1253521-36-6	A		4-(2-methoxy-1-methylethoxy)-2-methylbenzoyl chloride	COCC(C)OC1=CC=C(C(Cl)=O)C(C)=C1
22510	213831-09-5	A		N-[5-(acetylamino)-4-[(2-chloro-4,6-dinitrophenyl)azo]-2-methoxyphenyl]-N-(2-ethoxy-2-oxoethyl)glycine methyl ester	CCOC(=O)CN(CC(=O)OC)C1=CC(NC(C)=O)=C(C=C1OC)\N=N\C1=C(C=C(C=C1Cl)[N+]([O-])=O)[N+]([O-])=O
22583	27816-23-5	A		2-methoxyethyl 2-cyanoprop-2-enoate	COCCOC(=O)C(=C)C#N

Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
22628	661-54-1	A		3,3,3-trifluoropropyne	C#CC(F)(F)F
22645	2917-96-6	A		4-methylsulfonyloxybut-2-ynyl methanesulfonate	CS(=O)(=O)OCC#CCOS(=O)(=O)C
22659	861640-76-8	A		diethyl 2-(4-phenoxyanilino)propanedioate	CCOC(=O)C(C(=O)OCC)NC1=CC=C(C=C1)OC2=CC=CC=C2
22677	29270-30-2	A		2-bromo-2-(2-chlorophenyl)acetic acid	C1=CC=C(C(=C1)C(C(=O)O)Br)Cl
22682	79996-99-9	A		1-bromo-4-(bromomethyl)naphthalene	C1=CC=C2C(=C1)C(=CC=C2Br)CBr
22683	1575-37-7	A		4-bromobenzene-1,2-diamine	C1=CC(=C(C=C1Br)N)N
22725	502434-59-5	A		4-methylbenzenesulfonic acid [(2S)-4-methyl-3,4-dihydro-2H-1,4-benzooxazine-2-yl]methyl ester	[H][C@@]1(COS(=O)(=O)C2=CC=C(C)C=C2)CN(C)C2=C(O1)C=CC=C2
22785	1326236-05-8	A		2-propynyl vinylsulfonate	C=CS(=O)(=O)OCC#C
22823	1173478-74-4	A		4-(ethoxymethoxycarbonyl)cyclohexane-1-carboxylic acid	CCOCOC(=O)C1CCC(CC1)C(O)=O
22824	1187579-75-4	A		bis(ethoxymethyl) cyclohexane-1,4-dicarboxylate	CCOCOC(=O)C1CCC(CC1)C(=O)OCOCC
22826	3681-02-5	A		2-(cyclohexyloxymethyl)oxirane	C1CCC(CC1)OCC2CO2
22889	2998-56-3	A		N,N-bis(2-chloroethyl)carbamoyl chloride	C(CCl)N(CCCl)C(=O)Cl
23031	1633-82-5	A		3-chloropropane-1-sulfonyl chloride	C(CS(=O)(=O)Cl)CCl
23062	1160293-27-5	A		dimethyl 2-(4-methoxycarbonyl-2-nitrophenyl)propanedioate	COC(=O)C1=CC(=C(C=C1)C(C(=O)OC)C(=O)OC)[N+](=O)[O-]
23080	57131-19-8	A		2,7-naphthalenedisulfonic acid, 4-amino-3-((4'-((2,4-diaminophenyl)azo)(4,4'-benzanilide)-4-yl)azo)-5-hydroxy-6-(phenylazo)-disodium salt	[Na+].[Na+].NC1=CC(N)=C(C=C1)N=NC1=CC=C(NC(=O)C2=CC=C(C=C2)\N=N\C2=C(C=C3C=C(\C(=N/NC4=CC=CC=C4)C(=O)C3=C2N)S([O-

Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
23109	100953-52-4	A		N-(4-bromo-phenyl)-benzene-1,2-diamine	C1=CC=C(C(=C1)N)NC2=CC=C(C=C2)Br
23126	85622-93-1	A		3-methyl-4-oxoimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide	CN1C(=O)N2C=NC(=C2N=N1)C(=O)N
23129	64931-17-5	A		4-methyl-3,6-dihydrooxathiine 2,2-dioxide	CC1=CCOS(=O)(=O)C1
23138	114772-38-2	A		methyl 2-[4-(bromomethyl)phenyl]benzoate	COC(=O)C1=CC=CC=C1C2=CC=C(C=C2)CBr
23203	5926-90-9	A		2-(hexoxymethyl)oxirane	CCCCCCOCC1CO1
23237	70693-64-0	A		N,N-diethyl-3-methyl-4-[(5-nitro-1,3-thiazol-2-yl)diazenyl]aniline	CCN(CC)C1=CC(C)=C(C=C1)\N=N\C1=NC=C(S1)[N+]([O-])=O
23258	99191-71-6	A		N,N'-dimethyl-N,N'-hexanediyl-bis-carbamoyl chloride	CN(CCCCCCN(C)C(=O)Cl)C(=O)Cl
23359	5394-18-3	A		N-(4-bromobutyl)phthalimide	C1=CC=C2C(=C1)C(=O)N(C2=O)CCCCBr
23379	19757-97-2	A		methyl 2-hydroxy-2-methoxyacetate	COC(C(=O)OC)O
23440	174072-89-0	A		ethyl 2-amino-4-methyl-5-(4-nitrophenyl)thiophene-3-carboxylate	CCOC(=O)C1=C(SC(=C1C)C2=CC=C(C=C2)[N+](=O)[O-])N
23476	88324-57-6	A		1-(4-chlorophenyl)-2-methyl-2-morpholin-4-ylpropan-1-one	CC(C)(C(=O)C1=CC=C(C=C1)Cl)N2CCOCC2
23491	1373610-00-4	A		(2,2-dioxo-1,3,2-dioxathiolan-4-yl)methyl methanesulfonate	CS(=O)(=O)OCC1COS(=O)(=O)O1
23605	16495-13-9	A		(2S)-2-(phenylmethoxymethyl)oxirane	C1[C@H](O1)COCC2=CC=CC=C2