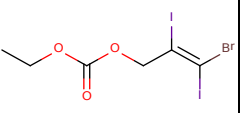
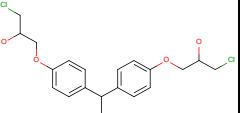
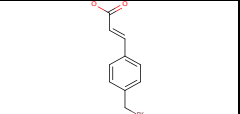
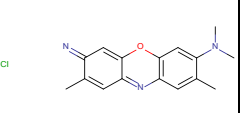
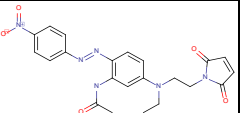
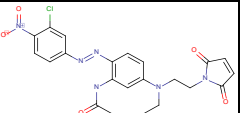
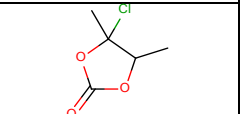
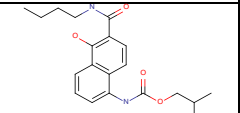
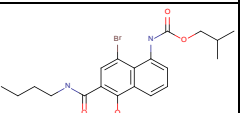
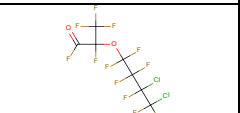
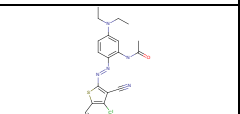
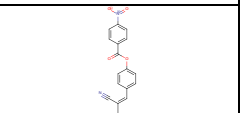
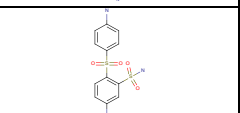
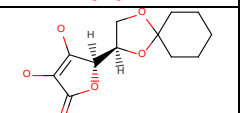
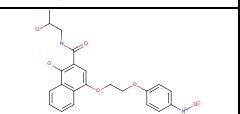
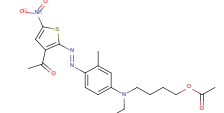
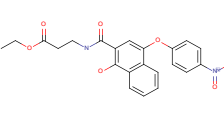
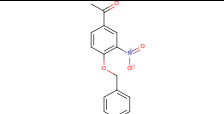
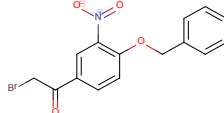
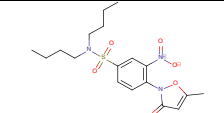
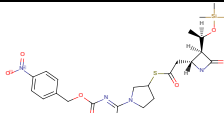
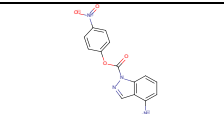
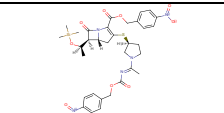
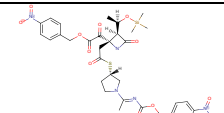
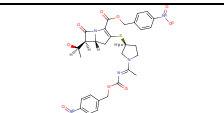
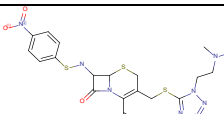
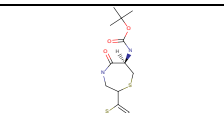
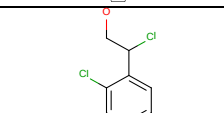
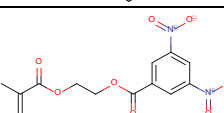
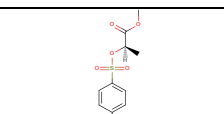


Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
811	NO_CAS	A		carbonic acid [(E)-3-bromo-2,3-diiodo-2-propenyl](ethyl) ester	CCOC(=O)OC/C=C(I)=C(I)Br
2202	NO_CAS	A		1,1-bis[p-(3-chloro-2-hydroxypropoxy)phenyl]ethane	CC(C1=CC=C(OCC(O)CCl)C=C1)C1=CC=C(OCC(O)CCl)C=C1
2361	927800-43-9	A		(E)-3-[p-(bromomethyl)phenyl]acrylic acid	OC(=O)/C=C/C1=CC=C(CBr)C=C1
2823	NO_CAS	A		N,N-dimethyl-N-(3-imino-2,8-dimethyl-3H-phenoxazin-7-yl)amine hydrochloride	Cl.CN(C)C1=CC2=C(C=C1)N=C1C=C(C)C(=N)C=C1O2
3237	NO_CAS	A		5'-[N-ethyl-N-[2-(2,5-dioxo-2,5-dihydro-1H-pyrrrol-1-yl)ethyl]amino]-2'-(4-nitrophenylazo)acetanilide	CCN(CC1C(=O)C=CC1=O)C1=CC(NC(C)=O)=C(C=C1)N=N\C1=CC=C(C=C1)[N+]([O-])=O
3245	NO_CAS	A		2'-(3-chloro-4-nitrophenylazo)-5'-[N-ethyl-N-[2-(2,5-dioxo-2,5-dihydro-1H-pyrrrol-1-yl)ethyl]amino]acetanilide	CCN(CC1C(=O)C=CC1=O)C1=CC(NC(C)=O)=C(C=C1)N=N\C1=CC=C(C(Cl)=C1)[N+]([O-])=O
3484	5368-01-4	A		4-chloro-4,5-dimethyl-1,3-dioxolan-2-one	CC1OC(=O)OC1(C)Cl
3561	NO_CAS	A		N-[6-(N-butylcarbamoyl)-5-hydroxy-1-naphthyl]carbamic acid isobutyl ester	CCCCNC(=O)C1=C(O)C2=C(C=C1)C(NC(=O)OCC(C)C)=CC=C2
3565	NO_CAS	A		N-[8-bromo-6-(N-butylcarbamoyl)-5-hydroxy-1-naphthyl]carbamic acid isobutyl ester	CCCCNC(=O)C1=C(O)C2=C(C(Cl)Br)=C1C(NC(=O)OCC(C)C)=CC=C2
4109	NO_CAS	A		2-(3,4-dichloro-1,1,2,2,3,4,4-heptafluorobutoxy)-2,3,3,3-tetrafluoropropionic acid fluoride	FC(=O)C(F)(OC(F)(F)C(F)(F)C(F)(F)Cl)C(F)Cl)C(F)(F)F
4807	104366-25-8	A		2'-[(4-chloro-3-cyano-5-formyl-2-thienyl)azo]-5'-(diethylamino)acetanilide	CCN(CC)C1=CC(NC(C)=O)=C(C=C1)N=N\C1=C(C#N)C(Cl)=C(S1)C=O
4848	67821-33-4	A		4-nitrobenzoic acid 4-(2,2-dicyanoethenyl)phenyl ester	[O-][N+](=O)C1=CC=C(C=C1)C(=O)OC1=CC=C(C=C(C#N)C#N)C=C1
5063	24573-61-3	A		2-(4-aminophenylsulfonyl)-5-nitrobenzenesulfonamide	NC1=CC=C(C=C1)S(=O)(=O)C1=C(C=C(C=C1)[N+]([O-])=O)S(N)(=O)=O
5223	NO_CAS	A		(5R)-5-[(2R)-1,4-dioxaspiro[4.5]decane-2-yl]-3,4-dihydroxyfuran-2(5H)-one	[H][C@@]1(COC2(CCCCC2)O1)[C@@]1([H])OC(=O)C(O)=C1O
5410	NO_CAS	A		1-hydroxy-N-(2-hydroxypropyl)-4-[2-(4-nitrophenoxy)ethoxy]naphthalene-2-carboxamide	CC(O)CNC(=O)C1=C(O)C2=C(C=CC=C2)C(OCCOC2=CC=C(C=C2)[N+]([O-])=O)=C1

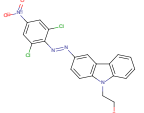
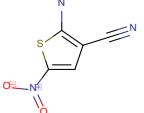
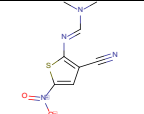
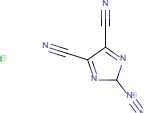
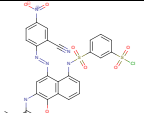
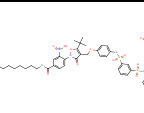
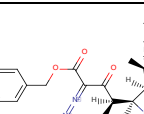
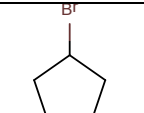
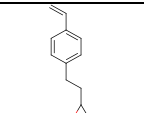
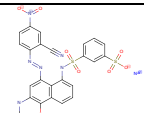
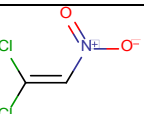
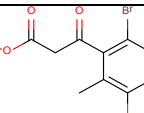
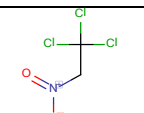
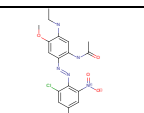
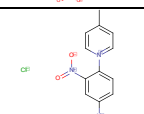
Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
5491	NO_CAS	A		acetic acid 4-[ethyl[4-(3-acetyl-5-nitro-2-thienylazo)-3-methylphenyl]amino]butyl ester	CCN(CCCOC(C)=O)C1=CC=C(\N=N\C=C=C(C=C(S2)N+([O-])=O)C(C)=O)C(C)=C1
5541	NO_CAS	A		3-[1-hydroxy-4-(4-nitrophenoxy)-2-naphthoylamino]propionic acid ethyl ester	CCOC(=O)CCNC(=O)C1=C(O)C2=C(C=CC=C2)C(OC2=CC=C(C=C2)N+([O-])=O)=O=C1
5560	NO_CAS	A		4'-benzyloxy-3'-nitroacetophenone	CC(=O)C1=CC(=C(OCC2=CC=CC=C2)C=C1)N+([O-])=O
5561	NO_CAS	A		4'-benzyloxy-3'-nitro-2-bromoacetophenone	[O-][N+](=O)C1=C(OCC2=CC=CC=C2)C=CC(=C1)C(=O)CBr
5620	NO_CAS	A		N,N-dibutyl-4-(2,3-dihydro-5-methyl-3-oxoisoxazole-2-yl)-3-nitrobenzenesulfonamide	CCCCN(CCCC)S(=O)(=O)C1=C(C=CC=C1)N1OC(C)=CC1=O[N+](O-)=O
5632	NO_CAS	A		N-[1-[3-[[[(2R,3S)-3-[(R)-1-(trimethylsilyloxy)ethyl]-4-oxo-2-azetidiny]]methylcarbonylthio]-1-pyrrolidinyl]ethylidene]carbamic acid p-nitrobenzyl ester	[H][C@](C)(O[Si](C)(C)C)[C@]1([H])C(=O)N[C@]1([H])CC(=O)SC1CCN(C1)C(C)=N(C(=O)OCC1=CC=C(C=C1)N+([O-])=O)=O
5635	NO_CAS	A		4-nitro-1H-indazole-1-carboxylic acid 4-nitrophenyl ester	[O-][N+](=O)C1=CC=C(OC(=O)N2N=CC3=C2C=CC=C3[N+](O-)=O)C=C1
5637	NO_CAS	A		(5R,6S)-3-[[[(3S)-1-[N-(p-nitrobenzyloxycarbonyl)acetimidoyl]-3-pyrrolidinyl]thio]-7-oxo-6-[(R)-1-(trimethylsilyloxy)ethyl]-1-azabicyclo[3.2.0]hepta-2-ene-2-carboxylic acid p-nitrobenzyl ester	[H][C@](C)(O[Si](C)(C)C)[C@]1([H])C(=O)N2C(C(=O)OCC3=CC=C(C=C3)N+([O-])=O)=O)C[C@]12[H]S[C@]11([H])CCN(C1)C(C)=N(C(=O)OCC1=CC=C(C=C1)N+([O-])=O)=O
5638	NO_CAS	A		2-[(2S,3S)-2-[[[(3S)-1-[N-(p-nitrobenzyloxycarbonyl)acetimidoyl]-3-pyrrolidinyl]thio]carbonylmethyl]-4-oxo-3-[(R)-1-(trimethylsilyloxy)ethyl]-2-azetidiny]-2-oxoacetic acid p-nitrobenzyl ester	[H][C@](C)(O[Si](C)(C)C)[C@]1([H])C(=O)N[C@]1(CC(=O)S[C@]1([H])CCN(C1)C(C)=N(C(=O)OCC1=CC=C(C=C1)N+([O-])=O)=O
5645	NO_CAS	A		(5R,6S)-6-[(R)-1-hydroxyethyl]-3-[[[(3S)-1-[N-(p-nitrobenzyloxycarbonyl)acetimidoyl]-3-pyrrolidinyl]thio]-7-oxo-1-azabicyclo[3.2.0]hepta-2-ene-2-carboxylic acid p-nitrobenzyl ester	[H][C@](C)(O)[C@]1([H])C(=O)N2C(C(=O)OCC3=CC=C(C=C3)N+([O-])=O)=O)C[C@]12[H]S[C@]11([H])CCN(C1)C(C)=N(C(=O)OCC1=CC=C(C=C1)N+([O-])=O)=O
5761	NO_CAS	A		3-[[[1-[2-(dimethylamino)ethyl]-1H-tetrazole-5-yl]thio]methyl]-7-[[[4-nitrophenyl]thio]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]octa-2-ene-2-carboxylic acid	CN(C)CCN1N=NN=C1SCC1=C(N2C(SC1)C(NSC1=CC=C(C=C1)N+([O-])=O)C2=O)C(O)=O
5926	NO_CAS	A		N-[(6R)-5-oxo-2-(2-thienyl)hexahydro-1,4-thiazepine-6-yl]carbamic acid tert-butyl ester	[H][C@]1(CSC(CNC1=O)C1=CC=CS1)NC(=O)OC(C)C
5942	NO_CAS	A		2-chloro-2-(2-chlorophenyl)ethanol	OCC(C)C1=CC=CC=C1Cl
5964	NO_CAS	A		3,5-dinitrobenzoic acid 2-(methacryloyloxy)ethyl ester	CC(=C)C(=O)OCCOC(=O)C1=C(C=CC=C1)N+([O-])=O[N+](O-)=O
5979	NO_CAS	A		(R)-2-(tosyloxy)propionic acid methyl ester	[H][C@](C)(OS(=O)(=O)C)C1=CC=C(C)C=C1C(=O)OC

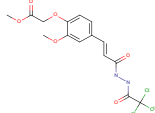
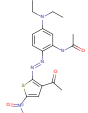
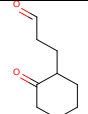
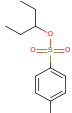
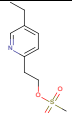
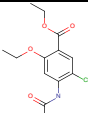
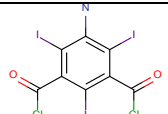
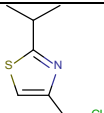
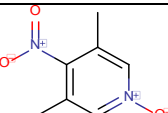
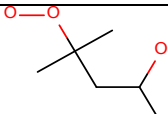
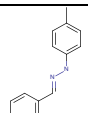
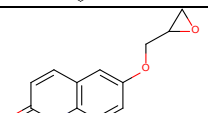
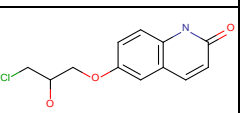
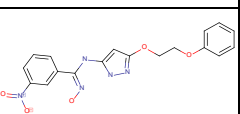
Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
6004	NO_CAS	A		N-(tert-butoxycarbonyl)-S-[2-nitro-1-(2-thienyl)ethyl]-L-cysteine	[H][C@@](CSC(C[N+](O-))=O)C1=CC=CS1)(NC(=O)OC(C)(C)C(O)=O
6149	NO_CAS	A		5-nitro-1H-indole-2-carboxylic acid ethyl ester	CCOC(=O)C1=CC2=C(N1)C=C(C=2)[N+](O-)=O
6223	NO_CAS	A		(2Z)-2-(5-amino-1,2,4-thiadiazole-3-yl)-2-(methoxyimino)acetic acid chloride	CO/N=C(/C(Cl)=O)C1=NSC(N)=N1
6224	NO_CAS	A		6-amino-7-fluoro-3,4-dihydro-2H-1,4-benzoxazine-3-one	NC1=CC2=C(OCC(=O)N2)C=C1F
6247	NO_CAS	A		1-(2-chloroethyl)-4-piperidinecarbonitrile hydrochloride	Cl.C1CCN1CCC(CC1)C#N
6274	NO_CAS	A		6-[(1,3-dimethylbutylidene)amino]-7-fluoro-3,4-dihydro-2H-1,4-benzoxazine-3-one	CC(C)C(C)C=N\C1=CC2=C(OCC(=O)N2)C=C1F
6275	NO_CAS	A		6-[(1,3-dimethylbutylidene)amino]-7-fluoro-4-(2-propynyl)-3,4-dihydro-2H-1,4-benzoxazine-3-one	CC(C)C(C)C=N\C1=CC2=C(OCC(=O)N2CC#C)C=C1F
6295	NO_CAS	A		1-(4-nitrophenoxy)-2-propanone	CC(=O)COC1=CC=C(C=C1)[N+](O-)=O
6307	NO_CAS	A		3-(hydroxymethyl)-1-(2-propynyl)-2,4-imidazolidinedione	OCN1C(=O)CN(CC#C)C1=O
6315	NO_CAS	A		2-(5-fluoro-2,4-dinitrophenoxy)acetic acid butyl ester	CCCCOC(=O)COC1=CC(F)=C(C=C1)[N+](O-)=O
6361	NO_CAS	A		N'-(4-aminophenyl)-2-(4-tert-pentylphenoxy)acetohydrazide	CCC(C)(C)C1=CC=C(OCC(=O)NNC2=CC=C(N)C=C2)C=C1
6395	NO_CAS	A		N,N-dimethyl-2-chloro-2-[4-chloro-2-(2-chlorobenzoyl)phenylazo]-3-oxobutanamide	CN(C)C(=O)C(Cl)(N=N\C1=CC=C(Cl)C=C1)C(=O)C1=CC=CC=C1Cl
6402	NO_CAS	A		4-chloro-2,3-dimethylpyridine 1-oxide	CC1=C(Cl)C=C[N+](O-)=C1C
6444	NO_CAS	A		1-(2,3-dibromopropyl)-1,2-diformylhydrazine	BrCC(Br)CN(C=O)C=O
6458	NO_CAS	A		carbonic acid ethyl 2-chloro-4-fluoro-5-nitrophenyl ester	CCOC(=O)OC1=CC=C(Cl)C(F)=C1[N+](O-)=O

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
6599	NO_CAS	A		2-[3-(2,6-dichloro-4-nitrophenylazo)-9H-carbazole-9-yl]ethanol	OCCN1C2=C(C=CC=C2)C2=C1C=CC(=C2)\N=N\ C1=C(Cl)C=C(C=C1Cl)[N+](O-)=O
6681	NO_CAS	A		2-amino-5-nitro-3-thiophenecarbonitrile	NC1=C(C=C(S1)[N+](O-)=O)C#N
6720	NO_CAS	A		N2-(3-cyano-5-nitro-2-thienyl)-N1,N1-dimethylformamidine	CN(C)C=N\ C1=C(C=C(S1)[N+](O-)=O)C#N
6727	NO_CAS	A		4,5-dicyano-2H-imidazole-2-diazonium chloride	[Cl-].[N#CC1=NC(N=C1C#N)[N+]#N
6812	NO_CAS	A		N-[5-(3-chlorosulfonylphenylsulfonfylamino)-4-(2-cyano-4-nitrophenylazo)-1-hydroxy-2-naphthyl]propionamide	CCC(=O)NC1=C(O)C2=C(C(NS(=O)(=O)C3=CC=CC(=C3)S(Cl)(=O)=O)=CC=C2)C(=C1)\N=N\ C1=CC=C(C=C1C#N)[N+](O-)=O
6867	NO_CAS	A		N-hexadecyl-4-[5-tert-butyl-4-[4-[3-[8-(2-cyano-4-nitrophenylazo)-6-(propionylamino)-5-hydroxy-1-naphthylaminosulfonyl]phenylsulfonfylamino]phenoxyethyl]-3-oxo-2,3-dihydroisoxazole-2-yl]-3-nitrobenzamide	CCCCCCCCCCCCCCCCNC(=O)C1=CC=C(N2OC(=C(COC3=C=C=C(NS(=O)(=O)C4=CC=CC(=C4)S(=O)(=O)N)C4=CC=CC5=C4C(=CC(NC(=O)CC)=C5O)\N=
6987	NO_CAS	A		(4R)-4-[(2R,3S)-3-[(1R)-1-(tert-butyl dimethylsilyloxy)ethyl]-4-oxo-2-azetidiny]-2-diazo-3-oxovaleric acid p-nitrobenzyl ester	[H][C@](C)(O[Si](C)(C)C(C)C)C(C)[C@@]1([H])C(=O)N[C@@]1([H])C@@([H])(C)C(=O)C(=[N+]=[N-])C(=O)OCC1=CC=C(C=C1)[N+](O-)=O
6991	NO_CAS	A		bromocyclopentane	BrC1CCCC1
7037	NO_CAS	A		1,2-epoxy-3-(4-vinylbenzyl)propane	C=CC1=CC=C(CCC2CO2)C=C1
7053	NO_CAS	A		3-[N-[8-(2-cyano-4-nitrophenylazo)-5-hydroxy-6-propionylamino-1-naphthyl]sulfamoyl]benzenesulfonic acid sodium salt	[Na+].CCC(=O)NC1=C(O)C2=C(C(NS(=O)(=O)C3=CC=CC(=C3)S(O-)))(=O)=O)CC=C2)C(=C1)\N=N\ C1=CC=C(C=C1C#N)[N+](O-)=O
7062	NO_CAS	A		1,1-dichloro-2-nitroethene	[O-][N+](=O)C=C(Cl)Cl
7070	NO_CAS	A		3-(4,6-dibromo-3-fluoro-2-methylphenyl)-3-oxopropionic acid ethyl ester	CCOC(=O)CC(=O)C1=C(Br)C=C(Br)C(F)=C1C
7089	NO_CAS	A		1,1,1-trichloro-2-nitroethane	[O-][N+](=O)CC(Cl)(Cl)Cl
7209	NO_CAS	A		2'-(2-chloro-4,6-dinitrophenylazo)-5'-ethylamino-4'-methoxyacetanilide	CCNC1=CC(NC(C)=O)=C(C=C1OC)\N=N\ C1=C(C=C(C=C1Cl)[N+](O-)=O)[N+](O-)=O
7296	NO_CAS	A		4-methyl-1-(2,4-dinitrophenyl)pyridinium · chloride	[Cl-].CC1=CC=[N+](C=C1)C1=CC=C(C=C1[N+](O-)=O)[N+](O-)=O

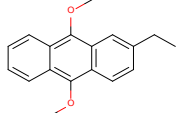
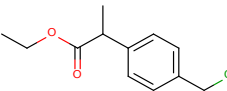
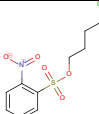
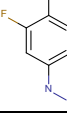
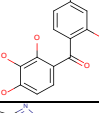
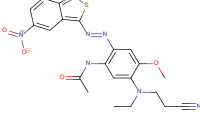
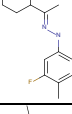
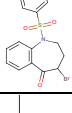
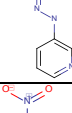
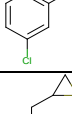

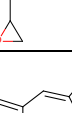
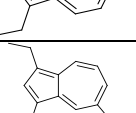
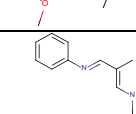
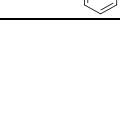
Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
7299	NO_CAS	A		2-[2-methoxy-4-[3-[2-(trichloroacetyl)hydrazino]-3-oxo-1-propenyl]phenoxy]acetic acid methyl ester	<chem>COC(=O)COC1=CC=C(C(=C(C(=O)=O)NNC(=O)C(Cl)(Cl)Cl)C=C1)OC</chem>
7323	NO_CAS	A		2'-(3-acetyl-5-nitro-2-thienylazo)-5'-diethylaminoacetanilide	<chem>CCN(CC)C1=CC(NC(C)=O)=C(C=C1)N=N\C1=C(C=C(S1)[N+](O-)=O)C(C)=O</chem>
7351	NO_CAS	A		3-(2-oxocyclohexyl)propanal	<chem>O=CCCC1CCCCC1=O</chem>
7404	NO_CAS	A		p-toluenesulfonic acid 1-ethylpropyl ester	<chem>CCC(CC)OS(=O)(=O)C1=CC=C(C)C=C1</chem>
7461	NO_CAS	A		methanesulfonic acid 2-(5-ethyl-2-pyridyl)ethyl ester	<chem>CCC1=CC=C(CCOS(C)(=O)=O)N=C1</chem>
7497	NO_CAS	A		4-(acetylamino)-5-chloro-2-ethoxybenzoic acid ethyl ester	<chem>CCOC(=O)C1=CC(Cl)=C(NC(C)=O)C=C1OCC</chem>
7512	NO_CAS	A		5-amino-2,4,6-triiodoisophthalic acid dichloride ester	<chem>NC1=C(I)C(C(Cl)=O)=C(I)C(Cl)=O=C1I</chem>
7549	NO_CAS	A		4-(chloromethyl)-2-isopropylthiazole	<chem>CC(C)C1=NC(CCl)=CS1</chem>
7554	NO_CAS	A		4,6-diamino-1,3-benzenediol dihydrochloride	<chem>Cl.Cl.NC1=CC(N)=C(O)C=C1O</chem>
7568	NO_CAS	A		3,5-dimethyl-4-nitropyridine 1-oxide	<chem>CC1=C[N+](O-)=CC(C)=C1[N+](O-)=O</chem>
7611	NO_CAS	A		3-hydroxy-1,1-dimethylbutyl hydroperoxide	<chem>CC(O)CC(C)(C)OO</chem>
7636	NO_CAS	A		benzaldehyde (4-methylphenyl)hydrazone	<chem>CC1=CC=C(C=C1)C=CC(=O)N=C(C=C1)C=C1</chem>
7681	NO_CAS	A		6-[(2,3-epoxypropane-1-yl)oxy]quinoline-2(1H)-one	<chem>O=C1NC2=C(C=C1)C=C(OCC1CO1)C=C2</chem>
7686	NO_CAS	A		6-(3-chloro-2-hydroxypropoxy)-1,2-dihydroquinoline-2-one	<chem>OC(CC)COC1=CC2=C(NC(=O)C=C2)C=C1</chem>
7739	NO_CAS	A		N2-hydroxy-N1-[3-(2-phenoxyethoxy)-1H-pyrazole-5-yl]-3-nitrobenzamide	<chem>O\N=C(NC1=CC(OCCOC2=CC=CC=C2)=NN1)C1=CC(=CC=C1)[N+](O-)=O</chem>

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
7743	NO_CAS	A		N1-[3-(2-phenoxyethoxy)-1H-pyrazole-5-yl]-3-nitrobenzamidine hydrochloride	Cl.[O-][N+](=O)C1=CC=CC(=C1)C(=N)NC1=CC(OCCOC2=CC=CC=C2)=NN1
7745	NO_CAS	A		3-[6-(2-phenoxyethoxy)-1H-pyrazolo[1,5-b][1,2,4]triazole-2-yl]aniline	NC1=CC=CC(=C1)C1=NN2N=C(OCCOC3=CC=CC=C3)C=C2N1
7748	NO_CAS	A		2-(2-fluoroacetylamino)-5-nitrobenzoic acid	OC(=O)C1=CC(=CC=C1NC(=O)CF)[N+](O-)=O
7762	NO_CAS	A		methacrylic acid 1,3-dioxo-2H-isoindole-2-ylmethyl ester	CC(=C)C(=O)OCN1C(=O)C2=C(C=CC=C2)C1=O
8013	NO_CAS	A		1-(ethenylsulfonylmethylsulfonyl)ethene	C=CS(=O)(=O)CS(=O)(=O)C=C
8072	NO_CAS	A		7-(1-imidazolyl)-6-nitro-2,3-dioxo-1,2,3,4-tetrahydro-1-quinoxalineacetic acid ethyl ester	CCOC(=O)CN1C(=O)C(=O)NC2=C1C=C(N1C=CN=C1)C(=C2)[N+](O-)=O
8073	NO_CAS	A		N-(indan-2-ylidene)aniline	C1C(CC2=C1C=CC=C2)=NC1=CC=CC=C1
8089	NO_CAS	A		2-(2-chloro-5-chloroacetyl-4-fluorophenoxy)-N-methylacetamide	CNC(=O)COC1=CC(C(=O)C(Cl)Cl)=C(F)C=C1
8106	NO_CAS	A		2-(4,α-dichlorobenzyl)pyridine	C1C(C1=CC=C(C1)C=C1)C1=NC=CC=C1
8116	NO_CAS	A		N,N-dimethyl-N'-(4-nitrosophenyl)-p-phenylenediamine	CN(C)C1=CC=C(NC2=CC=C(C=C2)N=O)C=C1
8134	NO_CAS	A		p-toluenethiosulfonic acid S-chloromethyl ester	CC1=CC=C(C=C1)S(=O)(=O)SCCl
8187	NO_CAS	A		3-amino-4'-bromobiphenyl-4-ol	NC1=C(O)C=CC(=C1)C1=CC=C(Br)C=C1
8218	NO_CAS	A		2-[2-chloro-4-fluoro-5-(5-hydroxy-1-methyl-1H-pyrazole-3-yl)phenoxy]-N-methylacetamide	CNC(=O)COC1=CC(C2=NN(C)C(O)=C2)=C(F)C=C1Cl
8275	NO_CAS	A		3-chloro-1-(1-bromovinyl)benzene	ClC1=CC=CC(=C1)C(Br)=C
8326	NO_CAS	A		4-acetoxy-2-(1-chloroethylthio)-6,7-difluoro-3-quinolinecarboxylic acid ethyl ester	CCOC(=O)C1=C(OC(C)=O)C2=C(C=C(F)C(F)=C2)N=C1SC(C)Cl

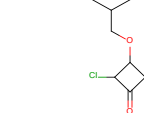
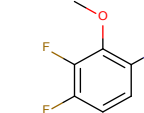
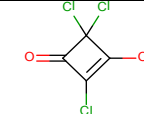
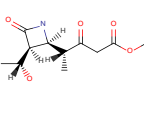
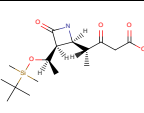
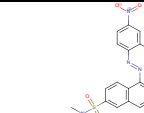
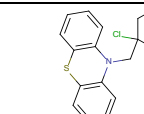
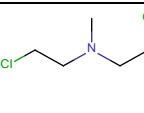
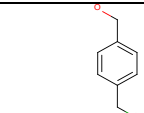
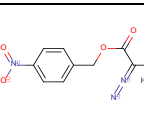
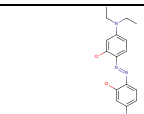
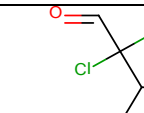
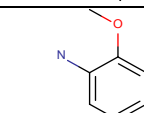
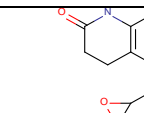
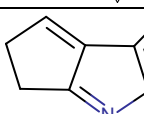
Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
8343	NO_CAS	A		2-ethyl-9,10-dimethoxyanthracene	<chem>CCC1=CC2=C(C=C1)C(OC)=CC=C2OC</chem>
8368	NO_CAS	A		2-(4-chloromethylphenyl)propionic acid ethyl ester	<chem>CCOC(=O)C(C)C1=CC=C(CCl)C=C1</chem>
8408	NO_CAS	A		2-nitrobenzenesulfonic acid 4-chlorobutyl ester	<chem>[O-][N+](=O)C1=C(C=CC=C1)S(=O)(=O)OCCCCl</chem>
8433	NO_CAS	A		3-fluoro-4-methylphenylhydrazine	<chem>CC1=CC=C(NN)C=C1F</chem>
8436	NO_CAS	A		2,2',3,4,4'-pentahydroxybenzophenone	<chem>OC1=CC(O)=C(C(=O)C1=CC(O)=C(O)C(=O)C1=CC(O)=C(O)C(=O)C1O</chem>
8524	NO_CAS	A		5'-[N-(2-cyanoethyl)-N-ethylamino]-4'-methoxy-2'-(5-nitro-2,1-benzisothiazole-3-ylazo)acetanilide	<chem>CCN(CCC#N)C1=CC(NC(C)=O)=C(C=C1OC)N=N1C1=C2C=C(C=CC2=NS1)[N+](O)=O</chem>
8533	NO_CAS	A		1-cyclohexylethanone 3-fluoro-p-tolylhydrazone	<chem>C/C(=N/NC1=CC=C(C(F)=C1)C)C(C)C1CCCC1</chem>
8602	NO_CAS	A		4-bromo-1-tosyl-2,3-dihydro-1H-1-benzazepine-5(4H)-one	<chem>CC1=CC=C(C=C1)S(=O)(=O)N1CCC(Br)C(=O)C2=C1C=CC=C2</chem>
8631	NO_CAS	A		3-methyl-2-butanone 3-pyridylhydrazone	<chem>CC(C)C(C)(C)=N\NC1=CN=CC=C1</chem>
8688	NO_CAS	A		5-chloro-2-nitrobenzenethiol	<chem>[O-][N+](=O)C1=C(S)C=C(Cl)C=C1</chem>
8726	NO_CAS	A		bis(thiirane-2-ylmethyl) sulfide	<chem>C(SCC1CS1)C1CS1</chem>
8727	NO_CAS	A		diglycidyl sulfide	<chem>C(SCC1CO1)C1CO1</chem>
8783	NO_CAS	A		1-ethyl-5-isopropylazulene	<chem>CCC1=CC=C2C=C(C=CC=C12)C(C)C</chem>
8784	NO_CAS	A		3-ethyl-7-isopropyl-1-azulenecarboxylic acid methyl ester	<chem>CCC1=C2C=CC=C(C=C2C(=C1)C(=O)OC)C(C)C</chem>
8884	NO_CAS	A		N-[2-methyl-3-(phenylimino)-1-propenyl]benzenamine hydrochloride	<chem>Cl.C/C(=C/NC1=CC=CC=C1)/C=N/C1=CC=CC=C1</chem>

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
8890	NO_CAS	A		4-methoxybiphenyl-3-amine hydrochloride	<chem>Cl.COC1=C(N)C=C(C=C1)C1=CC=CC=C1</chem>
8931	NO_CAS	A		3-ethyl-3-glycidylloxymethyloxetane	<chem>CCC1(COCC2CO2)COC1</chem>
9119	NO_CAS	A		1-chloromethylthio-4-nitrobenzene	<chem>[O-][N+](=O)C1=CC=C(SCC1)C=C1</chem>
9151	NO_CAS	A		1-dodecyloxy-2,4-dinitrobenzene	<chem>CCCCCCCCCCCCOC1=C(C=C(C=C1)[N+](=[O-])=O)[N+](=[O-])=O</chem>
9152	NO_CAS	A		4-dodecyloxy-1,3-phenylenediamine	<chem>CCCCCCCCCCCCOC1=C(N)C=C(N)C=C1</chem>
9180	NO_CAS	A		4-(2-biphenylcarbonylamino)benzoic acid chloride	<chem>ClC(=O)C1=CC=C(NC(=O)C2=C(C=CC=C2)C2=CC=CC=C2)C=C1</chem>
9181	NO_CAS	A		2-(4-biphenyl)-2-chloroacetic acid sodium salt	<chem>[Na+].[O-]C(=O)C(Cl)C1=CC=C(C=C1)C1=CC=CC=C1</chem>
9182	NO_CAS	A		2-biphenylcarboxylic acid chloride	<chem>ClC(=O)C1=C(C=CC=C1)C1=CC=CC=C1</chem>
9322	NO_CAS	A		6-nitroindole	<chem>[O-][N+](=O)C1=CC2=C(C=CN2)C=C1</chem>
9325	NO_CAS	A		diglycidyl persulfide	<chem>C(SSCC1CO1)C1CO1</chem>
9328	NO_CAS	A		N,N-bis(2-chloroethyl)-alpha-phenylbenzenemethanamine hydrochloride	<chem>Cl.C1CCCN(CCC1)C(C1=CC=CC=C1)C1=CC=CC=C1</chem>
9385	NO_CAS	A		4-methoxy-5-(3-morpholinopropoxy)-2-nitrobenzonitrile	<chem>COC1=CC(=C(C=C1)OCCCN1CCOCC1)C#N[N+](=[O-])=O</chem>
9538	NO_CAS	A		2'-fluoro-5'-nitroacetophenone	<chem>CC(=O)C1=C(F)C=CC(=C1)[N+](=[O-])=O</chem>
9543	NO_CAS	A		1-(2-fluoro-5-methylsulfonylamino-beta-oxophenethyl)-3,5,7-triaza-1-azoniatricyclo[3.3.1.1.3,7]decane bromide	<chem>[Br-].CS(=O)(=O)NC1=CC=C(F)C(=C1)C(=O)C[N+](C1N[C@]3C[N@](C1N)[C@]3)C1C2</chem>
9591	NO_CAS	A		4-(4-amino-2,5-dimethoxyphenylazo)benzoic acid hydrochloride	<chem>Cl.COC1=CC(N)=C(OC)C=C1\N=N/C1=CC=C(C=C1)C(O)=O</chem>

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
9612	NO_CAS	A		2-chloro-3-isobutoxy-1-cyclobutanone	CC(C)COC1CC(=O)C1Cl
9656	NO_CAS	A		1,2-difluoro-3-methoxy-4-nitrobenzene	COC1=C(C=CC(F)=C1F)[N+](=O)=O
9681	NO_CAS	A		2,4,4-trichloro-3-isobutoxy-2-cyclobutene-1-one	CC(C)COC1=C(Cl)C(=O)C1(Cl)Cl
9689	NO_CAS	A		(4R)-4-[(2R,3S)-3-[(1R)-1-hydroxyethyl]-4-oxoazetidine-2-yl]-3-oxovaleric acid 4-nitrobenzyl ester	[H][C@](C)(O)[C@@]1([H])C(=O)N[C@@]1([H])[C@@]([H])(C)C(=O)CC(=O)OCC1=CC=C(C=C1)[N+](=O)=O
9705	NO_CAS	A		(4R)-4-[(2R,3S)-3-[(1R)-1-(tert-butylidimethylsiloxy)ethyl]-4-oxoazetidine-2-yl]-3-oxovaleric acid 4-nitrobenzyl ester	[H][C@](C)(O)[Si](C)(C)C(C)(C)C[C@@]1([H])C(=O)N[C@@]1([H])[C@@]([H])(C)C(=O)CC(=O)OCC1=CC=C(C=C1)[N+](=O)=O
9753	NO_CAS	A		6-amino-5-[(2-hydroxy-4-nitrophenyl)azo]-N-methyl-2-naphthalenesulfonamide	CNS(=O)(=O)C1=CC=C(C=C1)C(N=NC1=CC=C(C=C1O)[N+](=O)=O)=C(N)C=C2
9767	NO_CAS	A		10-(3-chloro-1-azabicyclo[2.2.2]octane-3-ylmethyl)-10H-phenothiazine	C1C1(CN2C3=C(SC4=C2C=CC=C4)C=CC=C3)CN2CCC1CC2
9769	NO_CAS	A		N-(2-chloroethyl)-N-methyl-2-phenyl-2-chloroethanamine	CN(CCCl)CC(Cl)C1=CC=CC=C1
9781	NO_CAS	A		4-(chloromethyl)benzyl alcohol	OCC1=CC=C(CCl)C=C1
9783	NO_CAS	A		(4R)-2-diazo-3-oxo-4-[(2R,3S)-4-oxo-3-[(1R)-1-hydroxyethyl]azetidine-2-yl]valeric acid 4-nitrobenzyl ester	[H][C@](C)(O)[C@@]1([H])C(=O)N[C@@]1([H])[C@@]([H])(C)C(=O)C(=[N+]=[N-])C(=O)OCC1=CC=C(C=C1)[N+](=O)=O
9789	NO_CAS	A		5-(diethylamino)-5'-nitro-(2,2'-azobisphenol)	CCN(CC)C1=CC=C(N=C2C=C(C=C2O)[N+](=O)=O)C(O)=C1
9802	NO_CAS	A		2,2-dichloro-3-methylbutyraldehyde	CC(C)C(Cl)(Cl)C=O
9808	NO_CAS	A		3,4-difluoro-o-anisidine	COC1=C(F)C(F)=CC=C1N
9934	NO_CAS	A		5-glycidyl-3,4-dihydroquinoline-2(1H)-one	O=C1CCC2=C(N1)C=CC=C2C1CO1
9966	NO_CAS	A		2,3-dihydrocyclopenta[b]indole	C1CC2=NC3=C(C=CC=C3)C2=C1

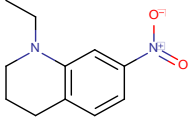
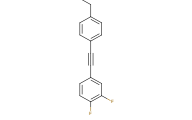
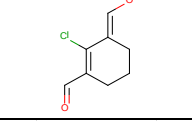
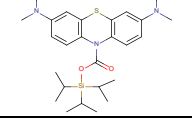
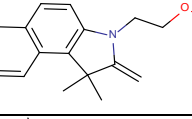
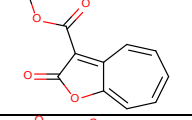
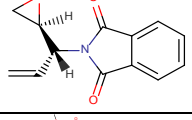
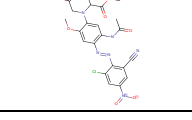
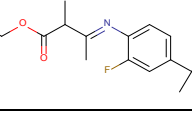
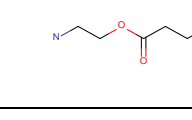
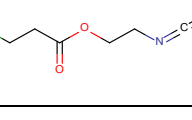
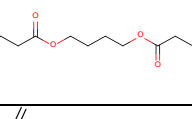
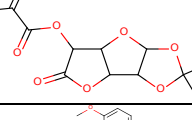
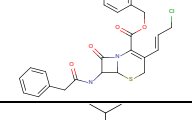
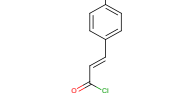
Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
10014	NO_CAS	A		3-pyridylhydrazine	<chem>NNC1=CN=CC=C1</chem>
10028	NO_CAS	A		4'-(bromomethyl)-2-biphenylcarboxylic acid tert-butyl ester	<chem>CC(C)(C)OC(=O)C1=C(C=CC=C1)C1=CC=C(CBr)C=C1</chem>
10047	NO_CAS	A		4-(4-methoxyphenylazo)aniline hydrochloride	<chem>Cl.COC1=CC=C(C=C1)N=N\C1=CC=C(N)C=C1</chem>
10049	NO_CAS	A		4-methoxybenzenediazonium chloride	<chem>[Cl-].COC1=CC=C(C=C1)[N+]#N</chem>
10063	NO_CAS	A		N-[2-[N2-[5-(hexahydro-1H-azepine-1-ylmethyl)-2-thienylcarbonyloxy]amidino]ethyl]phthalimide	<chem>N\C(CCN1C(=O)C2=CC=CC=C2C1=O)=N/OC(=O)C1=CC=C(CN2CCCCC2)S1</chem>
10148	NO_CAS	A		benzenethiosulfonic acid S-(chloromethyl) ester	<chem>ClCS(=O)(=O)C1=CC=CC=C1</chem>
10179	NO_CAS	A		(6R,7R)-7-amino-3-[(2S)-2-oxolanyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]octa-2-ene-2-carboxylic acid p-nitrobenzyl hydrochloride	<chem>Cl.[H][C@@]1(N)C(=O)N2C(C(=O)OCC3=CC=C(C=C3)[N+](=O)=O)=C(CS[C@]12[H])[C@]1([H])CCCO1</chem>
10183	NO_CAS	A		(7S,9S)-9-amino-6,7,11-trihydroxy-9-(2,5,5-trimethyl-1,3-dioxane-2-yl)-5,7,8,9,10,12-hexahydro-5,12-naphthacenedione hydrochloride	<chem>Cl.[H][C@@]1(O)C[C@@](N)(CC2=C(O)C3=C(C(O)=C12)C(=O)C1=C(C=CC=C1)C3=O)C1(C)OCC(C)CO1</chem>
10220	NO_CAS	A		4-[chloro(hydroxyimino)methyl]benzonitrile	<chem>O\N=C(/Cl)C1=CC=C(C=C1)C#N</chem>
10249	NO_CAS	A		2-chloro-2-propenyl thiocyanate	<chem>ClC(=C)CSC#N</chem>
10326	NO_CAS	A		(7S,9S)-9-acetyl-9-amino-7-(3-O,4-O-diacetyl-2-deoxy-beta-D-erythro-pentopyranosyloxy)-6,11-dihydroxy-5,7,8,9,10,12-hexahydro-5,12-naphthacenedione	<chem>[H][C@@]1([C@@]([H])(OC(C)=O)[C@@]([H])(CO1)OC(C)=O)O)[C@@]1([H])C[C@@](N)(C2=C(O)C3=C(C(O)=C12)C(=O)C1=C(C=CC=C1)C3=O)C(C)=</chem>
10387	NO_CAS	A		diacetic acid [5-acetylamino-4-(6-nitrobenzothiazole-2-ylazo)-2-methoxyphenyl]iminodiethylene ester	<chem>COCC1=CC(=N)N2C=NC3=C(S2)C=C(C=C3)[N+](=O)=O=C(NC(C)=O)C=C1N(CCO(C)=O)CCOC(C)=O</chem>
10401	NO_CAS	A		4,5-bis(2-methoxyethoxy)-2-nitrobenzonitrile	<chem>COCCOC1=C(OCCOC)C=C(C=C1)C#N[N+](=O)=O</chem>
10618	NO_CAS	A		5-(chloromethyl)-2-methoxybenzoic acid methyl ester	<chem>COC(=O)C1=CC(CCl)=CC=C1OC</chem>
10695	NO_CAS	A		2-(6-tert-butyl-7,7-dichloro-7H-pyrazolo[5,1-c][1,2,4]triazole-3-yl)-2-methylpropane-1-ol	<chem>CC(C)(C)C1=NN2C(=NN=C2C1(Cl)Cl)C(C)(C)CO</chem>

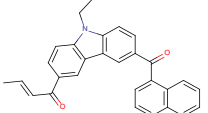
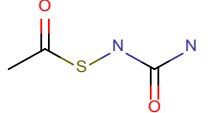
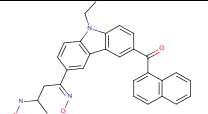
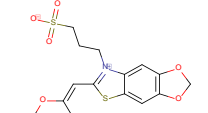
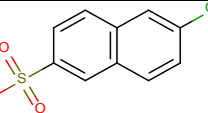
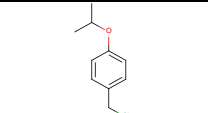
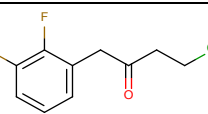
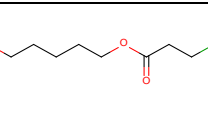
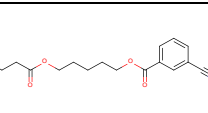
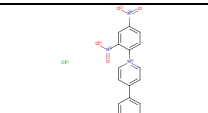
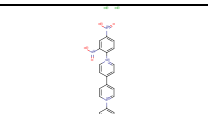
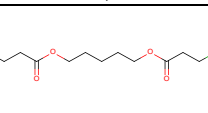
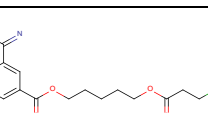
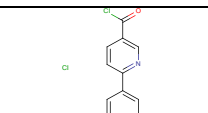
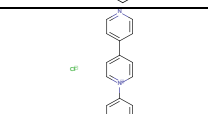
Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
10720	NO_CAS	A		2-(acetyloxyiminomethyl)-9H-thioxanthene-9-one	<chem>CC(=O)O\N=C\C1=CC2=C(SC3=C(C=CC=C3)C2=O)C=C1</chem>
11025	NO_CAS	A		6-chloro-4-hydroxy-1,1-dioxo-1-thia(VI)-2H-thieno[2,3-e]-1,2-thiazine-3-carboxylic acid methyl ester	<chem>COC(=O)C1=C(O)C2=C(C=C(Cl)S2)S(=O)(=O)N1</chem>
11264	NO_CAS	A		2-methyl-2-(2,2,2-tribromoacetyl-amino)propanoyl chloride	<chem>CC(C)(NC(=O)C(Br)(Br)Br)C(Cl)=O</chem>
11318	NO_CAS	A		2-chlorocarbonylpirazinium chloride	<chem>[Cl-].ClC(=O)C1=[NH+]C=CN=C1</chem>
11723	NO_CAS	A		4-isobutylbenzenesulfonyl chloride	<chem>CC(C)CC1=CC=C(C=C1)S(Cl)(=O)=O</chem>
11759	NO_CAS	A		acetic acid 3-[2,6-dichloro-4-(3,3-dichloroallyloxy)phenoxy]propyl ester	<chem>CC(=O)OCCOCOC1=C(Cl)C=C(COC(=O)C)C1Cl</chem>
11836	NO_CAS	A		bis[2,3,3,3-tetrafluoro-2-(trifluoromethyl)propanoic acid]octafluorobutane-1,4-diyl ester	<chem>FC(F)(F)C(F)(C(=O)OC(F)(F)C(F)(F)C(F)(F)OC(=O)C(F)(C(F)(F)C(F)(F)C(F)(F)OC(=O)C(F)(F)F</chem>
12113	NO_CAS	A		2-(fluoromethoxyimino)propane-1,3-dinitrile	<chem>FCON=C(C#N)C#N</chem>
12179	NO_CAS	A		(Z)-2-(5-amino-1,2,4-thiazole-3-yl)-2-fluoromethoxyiminoacetic acid methyl ester	<chem>COC(=O)C(=N/OCF)C1=NSC(N)=N1</chem>
12411	NO_CAS	A		4-chloromethyl-2-methylthiazole hydrochloride	<chem>Cl.CC1=NC(C)S1</chem>
12457	NO_CAS	A		2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoic acid 2-(trifluoromethyl)hexafluoropropyl ester	<chem>FC(F)(F)C(F)(F)C(F)(F)OC(F)(C(=O)OC(F)(F)C(F)(F)C(F)(F)OC(=O)C(F)(F)F</chem>
12639	NO_CAS	A		2-[(diphenylmethylene)amino]acetic acid methyl ester	<chem>COC(=O)CN=C(C1=CC=CC=C1)C1=CC=CC=C1</chem>
12655	NO_CAS	A		1,2,3-trimethyl-3H-benzo[e]indole	<chem>CN1C(C)=C(C)C2=C1C=CC1=C2C=CC=C1</chem>
12668	NO_CAS	A		1,1'-bis(2-hydroxy-5-biphenyl)-4,4'-bipyridinium dichloride	<chem>[Cl-].[Cl-].OC1=C(C=C(C=C1)[N+])1=CC=C(C=C1)C1=CC=[N+](C=C1)C1=CC(=O)C=C1)C1=CC=CC=C1)C1=CC=CC=C1</chem>
12711	NO_CAS	A		1-benzyl-1,2,3-trimethyl-1H-benzo[e]indole-3-ium • bromide	<chem>[Br-].CC1=[N+](C)C2=C(C3=C(C=C(C=C3)C=C2)C1)C)C1=CC=CC=C1</chem>

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
12795	NO_CAS	A		1-ethyl-7-nitro-1,2,3,4-tetrahydroquinoline	CCN1CCCC2=C1C=C(C=C2)[N+](O-)=O
12798	NO_CAS	A		4-[(4-ethylphenyl)ethynyl]-1,2-difluorobenzene	CCC1=CC=C(C=C1)C#CC1=CC(F)=C(F)C=C1
12825	NO_CAS	A		2-chloro-3-(hydroxymethylidene)-1-cyclohexene-1-ylcarbaldehyde	O(C=C1/CCCC(C=O)=C1Cl
12909	NO_CAS	A		3,7-bis(dimethylamino)-10H-phenothiazine-10-carboxylic acid triisopropylsilyl ester	CC(C)[Si](OC(=O)N1C2=C(SC3=C1C=CC(=C3)N(C)C)C=C(C=C2)N(C)C(C)C(C)C(C)C
12974	NO_CAS	A		3-(2-methoxyethyl)-1,1-dimethyl-2-methylene-1,2-dihydro-3H-benzo[e]indole	COCN1C(C=C(C)C(C)C)C2=C1C=CC1=C2C=CC=C1
13028	NO_CAS	A		2-oxo-2H-cyclohepta[b]furan-3-carboxylic acid methyl ester	COC(=O)C1=C2C=CC=CC=C2OC1=O
13126	NO_CAS	A		N-[(1R)-1-[(2S)-oxiranyl]-2-propenyl]phthalimide	[H][C@](C=C)(N1C(=O)C2=CC=CC=C2C1=O)[C@@]1([H])CO1
13204	NO_CAS	A		2-(N-{5-acetamido-4-[(2-chloro-6-cyano-4-nitrophenyl)diazenyl]-2-methoxyphenyl}-N-(methoxycarbonylmethyl)amino)propanoic acid methyl	COC(=O)CN(C(C)C(=O)OC)C1=CC(NC(C)=O)=C(C=C1OC)\N=N\N1=C(C=C(C=C1Cl)[N+](O-)=O)C#N
13405	NO_CAS	A		3-(4-tert-butyl-2-fluorophenylimino)-2-methylbutanoic acid ethyl ester	CCOC(=O)C(C)C(C)=N\C1=CC=C(C=C1F)C(C)C
13548	NO_CAS	A		3-chloropropanoic acid 2-aminoethy hydrochloride	Cl.NCCOC(=O)CCCl
13549	NO_CAS	A		3-chloropropanoic acid 2-isocyanatoethyl	ClCCC(=O)OCCN=C=O
13615	NO_CAS	A		bis(3-chloropropanoic acid)=butane-1,4-diyl	ClCCC(=O)OCCCCOC(=O)CCC1
13689	NO_CAS	A		methacrylic acid 4,4-dimethyl-10-oxo-3,5,7,11-tetraoxatricyclo[6.3.0.0.2,6]undecan-9-yl	CC(=C)C(=O)OC1C2OC3OC(C)C(C)OC32OC1=O
14786	NO_CAS	A		3-(3-chloro-1-propenyl)-8-oxo-7-(2-phenylacetyl-amino)-5-thia-1-azabicyclo[4.2.0]octa-2-ene-2-carboxylic acid 4-methoxybenzyl ester	COC1=CC=C(COC(=O)C2=C(CSC3C(NC(=O)CC4=CC=CC=C4)C(=O)N23)C=C(CCl)C=C1
15078	NO_CAS	A		3-(4-isopropylphenyl)acrylic acid chloride	CC(C)C1=CC=C(C=C(C(Cl)=O)C=C1



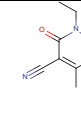
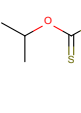




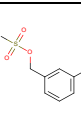

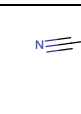
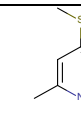
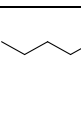
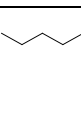

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
15086	NO_CAS	A		1-[9-ethyl-3-(1-naphthoyl)-9H-carbazole-6-yl]-2-butene-1-one	<chem>CCN1C2=C(C=C(C=C2)C(=O)\C=C\C)C2=C1C=CC(=C2)C(=O)C1=CC=CC2=C1C=CC=C2</chem>
15330	NO_CAS	A		S-(carbamoylamino) ethanethioate	<chem>CC(=O)SNC(N)=O</chem>
15375	NO_CAS	A		9-ethyl-6-(3-hydroxyamino-1-hydroxyiminobutyl)-9H-carbazole-3-yl(1-naphthyl) ketone	<chem>CCN1C2=C(C=C(C=C2)C(\CC(C)NO)=N(O)C2=C1C=CC(=C2)C(=O)C1=CC=CC2=C1C=CC=C2</chem>
15383	NO_CAS	A		3-[[6-(2-ethoxy-1-butenyl)-1,3-dioxolo[4,5-f]benzothiazole-7-ium]-7-yl]propane-1-sulfonate	<chem>CCO\C(CC)=C\C1=[N+](\CCCS([O-])(=O)=O)C2=CC3=C(OCCO3)C=C2S1</chem>
15410	NO_CAS	A		6-chloronaphthalene-2-sulfonic acid	<chem>OS(=O)(=O)C1=CC2=C(C=C1)C=C(Cl)C=C2</chem>
15414	NO_CAS	A		1-chloromethyl-4-isopropoxybenzene	<chem>CC(C)OC1=CC=C(CCl)C=C1</chem>
15724	NO_CAS	A		4-chloro-1-(2,3-difluorophenyl)butane-2-one	<chem>FC1=C(F)C(CC(=O)CCCl)=CC=C1</chem>
15729	NO_CAS	A		3-chloropropanoic acid 5-hydroxypentyl ester	<chem>OCCCCCOC(=O)CCCl</chem>
15742	NO_CAS	A		3-cyanobenzoic acid 5-(3-chloropropanoyloxy)pentyl ester	<chem>C1CCC(=O)OCCCCCOC(=O)C1=CC=C(C#N)</chem>
15779	NO_CAS	A		1-(2,4-dinitrophenyl)-4-(4-pyridyl)pyridinium chloride	<chem>[Cl-].[O-][N+](=O)C1=CC=C(C(=C1)[N+](O-)=O)[N+]1=CC=C(C=C1)C1=C=C=NC=C1</chem>
15780	NO_CAS	A		1-(2,4-dinitrophenyl)-1'-phenyl-4,4'-bipyridinium dichloride	<chem>[Cl-].[Cl-].[O-][N+](=O)C1=CC=C(C(=C1)[N+](O-)=O)[N+]1=CC=C(C=C1)C1=C=C[N+](C=C1)C1=CC=CC=C1</chem>
15838	NO_CAS	A		bis(3-chloropropanoic acid) entanep-1,5-diyl ester	<chem>C1CCC(=O)OCCCCCOC(=O)CCCl</chem>
15849	NO_CAS	A		3-(N-hydroxycarbamimidoyl)benzoic acid 5-(3-chloropropanoyloxy)pentyl ester	<chem>ONC(=N)C1=CC(=CC=C1)C(=O)OCCCCCOC(=O)CCCl</chem>
15871	NO_CAS	A		6-phenylnicotinoyl chloride hydrochloride	<chem>Cl.C1C(=O)C1=CN=C(C=C1)C1=CC=CC=C1</chem>
15872	NO_CAS	A		1-phenyl-4,4'-bipyridine-1-ium chloride	<chem>[Cl-].C1=CC=C(C(=C1)[N+]1=CC=C(C=C1)C1=CC=NC=C1</chem>

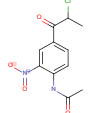
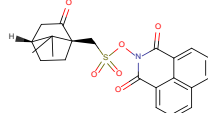
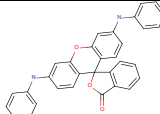
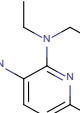
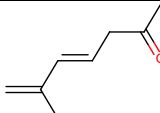
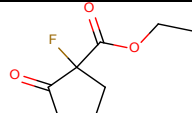
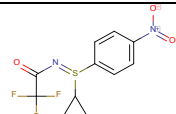
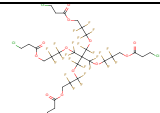
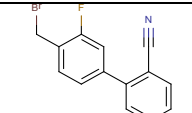
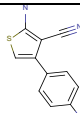
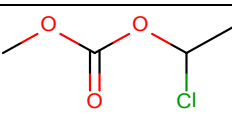
Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
15896	NO_CAS	A		1-(3-bromo-2-fluorophenyl)-2-chloroethane-1-one	<chem>FC1=C(Br)C=CC=C1C(=O)CCl</chem>
15995	NO_CAS	A		1-(1-amino-1H-pyrrole-2-yl)ethanone hydrochloride	<chem>Cl.CC(=O)C1=CC=CN1N</chem>
16058	NO_CAS	A		(2S)-4-(chloroformyl)-2-methyl-2,5-dihydro-1H-pyrrole-1-carboxylic acid allyl ester	<chem>[H][C@]1(C)C=C(CN1C(=O)OC C=C)C(Cl)=O</chem>
16430	NO_CAS	A		4-(N,N-diallylamino)benzene-1,3-diamine	<chem>NC1=CC(N)=C(C=C1)N(CC=C) CC=C</chem>
16431	NO_CAS	A		N,N-diallyl-2,4-dinitroaniline	<chem>[O-][N+](=O)C1=CC=C(N(CC=C)C C=C)C(=O)[N+](=O)C1=O</chem>
16832	NO_CAS	A		4-nitrobenzenesulfonic acid [(R)-2-methyloxiranyl]methyl ester	<chem>C[C@]1(COS(=O)(=O)C2=CC=C(C=C2)[N+](=O)C1=O)CO1</chem>
16936	NO_CAS	A		methacrylic acid 5-acetoxy-2-[4-(dimethylamino)benzoyl]phenyl ester	<chem>CN(C)C1=CC=C(C=C1)C(=O)C 1=CC=C(OC(C)=O)C=C1OC(=O)C(C)=C</chem>
17238	NO_CAS	A		3-bromo-1-oxo-1,3-dihydroisobenzofuran-5-carboxylic acid methyl ester	<chem>COC(=O)C1=CC2=C(C=C1)C(=O)OC2Br</chem>
17241	NO_CAS	A		3-(4-bromobutoxymethyl)-3-ethyloxetane	<chem>CCC1(COCCCCBr)COC1</chem>
17244	NO_CAS	A		4-bromomethyl-3-methylbenzoic acid methyl ester	<chem>COC(=O)C1=CC=C(CBr)C(C)=C1</chem>
17380	NO_CAS	A		4-chloro-2,2-dimethyl-4-pentenoic acid ethyl ester	<chem>CCOC(=O)C(C)(C)CC(Cl)=C</chem>
17403	NO_CAS	A		N-[4-(4,5-dihydrooxazole-2-yl)phenyl]hydroxylamine	<chem>ONC1=CC=C(C=C1)C1=NCCO1</chem>
17413	NO_CAS	A		(2S)-2-(3,4-difluorophenyl)oxirane	<chem>[H][C@]1(CO1)C1=CC=C(F)C(F)=C1</chem>
17433	NO_CAS	A		(4E)-dec-4-enohydrazide	<chem>CCCCC\C=C\CCC(=O)NN</chem>
17538	NO_CAS	A		5-bromo-2,2-dimethyl-4-oxopentanoic acid ethyl ester	<chem>CCOC(=O)C(C)(C)CC(=O)CBr</chem>

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
17570	NO_CAS	A		3-methyl-4-[(methylsulfonyloxy)methyl]benzoic acid methyl ester	<chem>COC(=O)C1=CC=C(COS(C)(=O)=O)C(C)=C1</chem>
18282	NO_CAS	A		2-[(4-vinyloxymethyl)cyclohexyl]methoxymethyl]oxirane	<chem>C=COCC1CCC(COCC2CO2)CC1</chem>
18417	NO_CAS	A		1-ethyl-3-cyano-4-methyl-5-(2-nitro-4-methoxyphenylazo)-6-hydroxy-1,2-dihydropyridine-2-one	<chem>CCN1C(O)=C([N=N]C2=CC=C(OC)C=C2[N+])([O-])=O)C(C)=C(C#N)C1=O</chem>
18565	NO_CAS	A		2,2-bis[isopropoxy(thiocarbonyl)thio]acetic acid methyl ester	<chem>COC(=O)C(SC(=S)OC(C)C)SC(=S)OC(C)C</chem>
18611	NO_CAS	A		1-(4-bromo-3-nitrophenyl)butane-1-one	<chem>CCCC(=O)C1=CC=C(Br)C(=C1)[N+](=O)[O-]</chem>
18625	NO_CAS	A		N-[chloro(6-phenyl-3-pyridyl)methylene]-2,1,3-benzoxadiazole-4-amine hydrochloride	<chem>Cl.C1/C(=N/C1=CC=CC2=NON=C12)C1=CN=C(C=C1)C1=CC=CC=C1</chem>
18643	NO_CAS	A		6-methyl-2,4-bis(methylthio)-3-nitropyridine	<chem>CSC1=C(C(SC)=NC(C)=C1)[N+](=O)[O-]</chem>
18681	NO_CAS	A		2-azido-1-(4-isopropoxy-2-methylphenyl)-2-methylpropane-1-one	<chem>CC(C)OC1=CC=C(C(=O)C(C)C)N=[N+]=[N-]C(C)=C1</chem>
18719	NO_CAS	A		benzoic acid 2-[[2-methyl-3'-[(methylsulfonyloxy)methyl]-4-biphenyl]oxy]ethyl ester	<chem>CC1=C(C=CC(OCCOC(=O)C2=CC=CC=C2)C1=CC=CC(COS(C)(=O)=O)=O)C1</chem>
18889	NO_CAS	A		4-butanoyl-2-nitrobenzonitrile	<chem>CCCC(=O)C1=CC=C(C#N)C(=C1)[N+](=O)[O-]</chem>
18898	NO_CAS	A		1-(4-fluorindol-3-yl)cyclopropane-1-carbonitrile	<chem>FC1=CC=CC2=C1C(=CN2)C1(C)C#N</chem>
18923	NO_CAS	A		2-bromo-N-[6-methyl-2,4-bis(methylsulfanyl)pyridin-3-yl]acetamide	<chem>CSC1=C(NC(=O)CBr)C(SC)=NC(C)=C1</chem>
18928	NO_CAS	A		4-(hexylsulfanyl)aniline	<chem>CCCCCCSC1=CC=C(N)C=C1</chem>
18929	NO_CAS	A		1-(hexylsulfanyl)-4-nitrobenzene	<chem>CCCCCCSC1=CC=C(C(=O)[N+](=O)[O-])C=C1</chem>
18966	NO_CAS	A		6-methyl-2,4-bis(methylsulfanyl)pyridin-3-amine	<chem>CSC1=C(N)C(SC)=NC(C)=C1</chem>

Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

Serial_Id	CAS#	AMES RESULT	Structure	Chemical_Name	SMILES
19083	NO_CAS	A		N-[4-(2-chloropropanoyl)-2-nitrophenyl]acetamide	CC(Cl)C(=O)C1=CC=C(NC(C)=O)C(=C1)[N+](=O)[O-]
19131	NO_CAS	A		[(1S,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptane-1-yl]methanesulfonic acid 1,3-dioxo-2,3-dihydro-1H-benzo[de]isoquinoline-2-yl ester	[H][C@@]12CC[C@@](C1)(CS(=O)(=O)ON3C(=O)C4=CC=CC5=C4C(=CC=C5)C3=O)(C(=O)C1)C2(C)C
19163	NO_CAS	A		3',6'-bis(phenylamino)spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one	O=C1OC2(C3=C1C=CC=C3)C1=CC=C(C=C1)C2(C(=O)C3=C(C=C3)NC(=O)C=C2)C=C1
19555	NO_CAS	A		3-amino-2-diethylamino-6-methylpyridine	CCN(CC)C1=NC(C)=CC=C1N
19801	NO_CAS	A		6-methylhepta-4,6-diene-2-one	CC(=O)C/C=C/C(C)=C
20043	NO_CAS	A		ethyl 1-fluoro-2-oxo-cyclopentane-1-carboxylate	CCOC(=O)C1(F)CCCC1=O
20233	NO_CAS	A		S-cyclopropyl-S-(4-nitrophenyl)-N-(2,2,2-trifluoroacetyl)sulfimin	[O-][N+](=O)C1=CC=C(C=C1)S(=N(C(=O)C(F)(F)F)C)C1CC1
20303	NO_CAS	A		bis(3-chloropropanoic acid)3,3'-[[[2,2-bis[[3-(3-chloropropanoyloxy)-1,1,2,2-tetrafluoropropoxy]difluoromethyl]-1,1,3,3-tetrafluoropropane-1,3-diyl]dioxy]bis(2,2,3,3-tetrafluoropropyl) ester	FC(F)(COC(=O)CCCl)C(F)(F)OC(F)(F)C(F)OC(F)(F)OC(F)(F)OC(F)(F)OC(F)(F)COC(=O)CCCl)C(F)(F)OC(F)(F)OC(F)(F)COC(=O)CCCl
20366	NO_CAS	A		4-(bromomethyl)-3'-fluorobiphenyl-2-carbonitrile	FC1=CC(=CC=C1CBr)C1=C(C=CC=C1)C#N
20474	NO_CAS	A		2-amino-4-(4-aminophenyl)thiophene-3-carbonitrile	NC1=C(C#N)C(=CS1)C1=CC=C(N)C=C1
20946	NO_CAS	A		1-chloroethyl methyl carbonate	COC(=O)OC(C)Cl