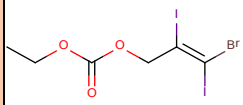
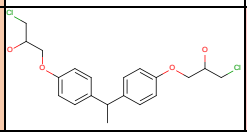
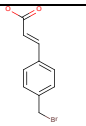
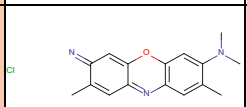
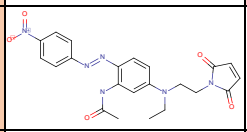
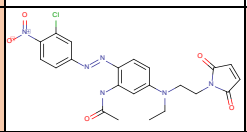
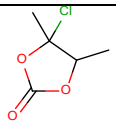
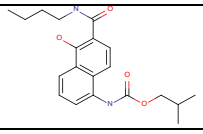
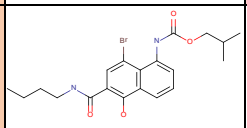
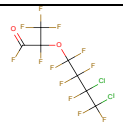
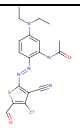
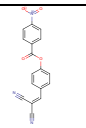
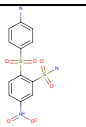
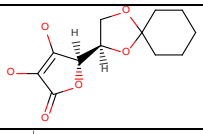
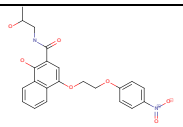
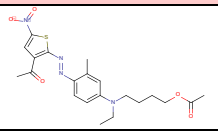
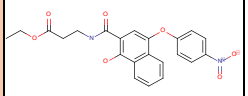
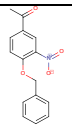
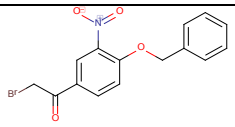
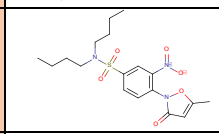
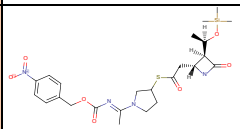
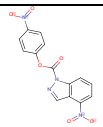
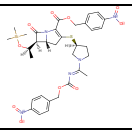
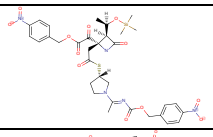
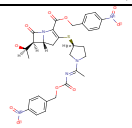
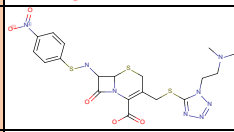
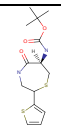
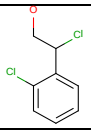
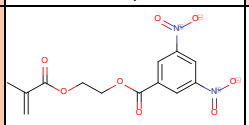
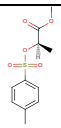
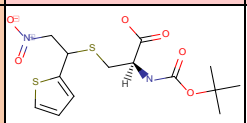
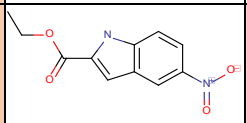
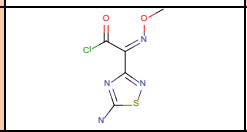
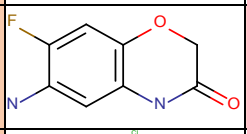
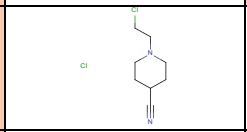
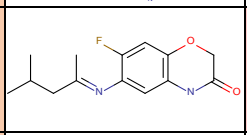
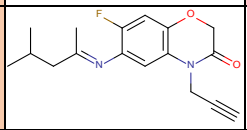
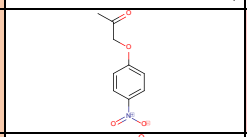
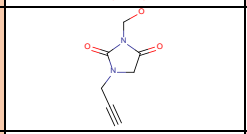
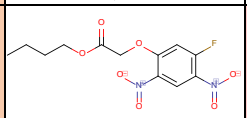
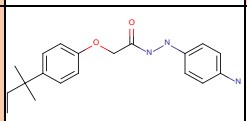
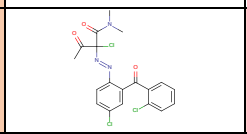
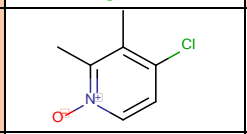
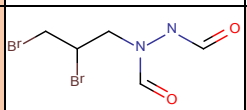
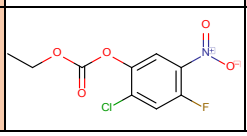
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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(I)=C(\Br)I |
| 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=C1C)N=C1C=C(C)C(=N)C=C1O2 |
| 3237 | NO_CAS | A |  | 5'-[N-ethyl-N-[2-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)ethyl]amino]-2'-(4-nitrophenylazo)acetanilide | CCN(CCN1C(=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-pyrrol-1-yl)ethyl]amino]acetanilide | CCN(CCN1C(=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(Br)=C1)C(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)(Cl)C(F)(F)Cl)C(F)(F)F |
| 4807 | 104366-25-8 | A |  | 2'-[(4-chloro-3-cyano-5-formyl-2-thienyl)azo]-5'-(diethylamino)acetoanilide | 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 |

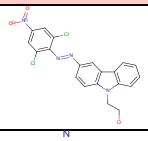
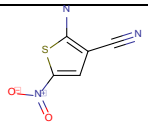
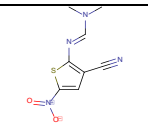
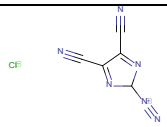
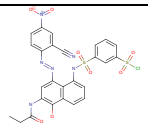
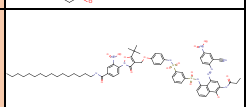
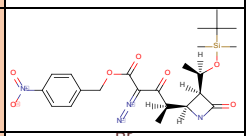
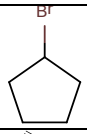
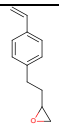
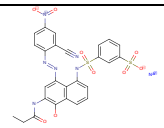
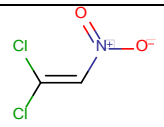
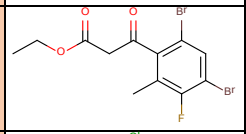
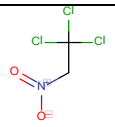
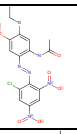
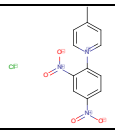
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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(CCCCOC(C)=O)C1=CC=C(\N=N\C2=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)=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=CC(=C(C=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-azetidinyl]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 |
| 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)=C(C[C@]12[H])S[C@@]1([H])CCN(C1)C(\C)=N\C(=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-(trimethylsiloxy)ethyl]-2-azetidinyl]-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- |
| 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)=C(C[C@]12[H])S[C@@]1([H])CCN(C1)C(\C)=N\C(=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)C |
| 5942 | NO_CAS | A |  | 2-chloro-2-(2-chlorophenyl)ethanol | OCC(Cl)C1=CC=CC=C1Cl |
| 5964 | NO_CAS | A |  | 3,5-dinitrobenzoic acid 2-(methacryloyloxy)ethyl ester | CC(=C)C(=O)OCCOC(=O)C1=CC(=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)C1=CC=C(C)C=C1)C(=O)OC |

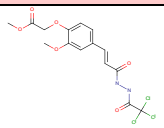
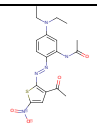
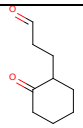
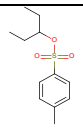
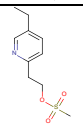
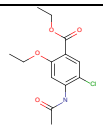
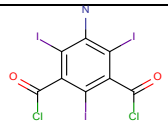
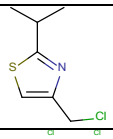
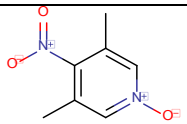
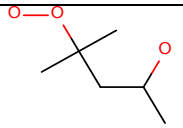
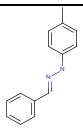
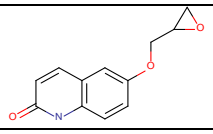
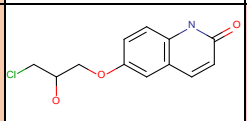
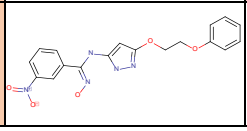
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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)C(O)=O |
| 6149 | NO_CAS | A |  | 5-nitro-1H-indole-2-carboxylic acid ethyl ester | CCOC(=O)C1=CC2=C(N1)C=CC(=C2)[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.ClCCN1CCC(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)[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=C1C(=O)C1=CC=CC=C1Cl)C(C)=O |
| 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(NC=O)C=O |
| 6458 | NO_CAS | A |  | carbonic acid ethyl 2-chloro-4-fluoro-5-nitrophenyl ester | CCOC(=O)OC1=CC(=C(F)C=C1Cl)[N+]([O-])=O |

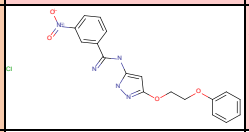
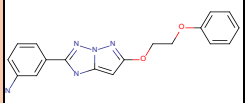
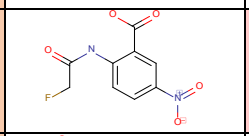
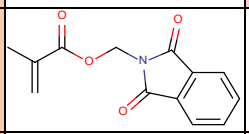
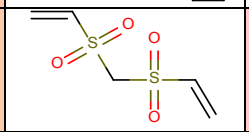
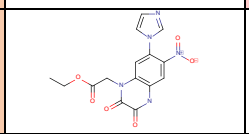
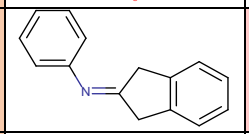
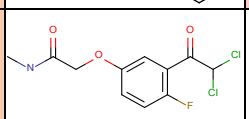
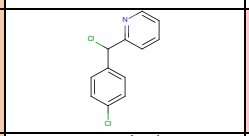
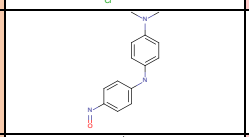
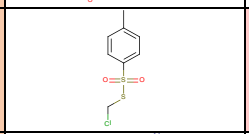
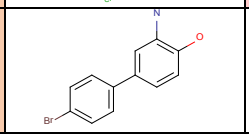
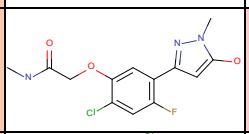
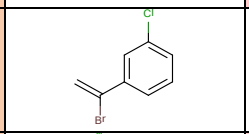
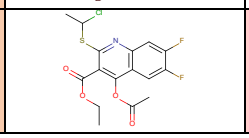
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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-chlorosulfonylphenylsulfonylamino)-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]phenylsulfonylamino]phenoxymethyl]-3-oxo-2,3-dihydroisoxazole-2-yl]-3-nitrobenzamide | CCCCCCCCCCCCCCCCCNC(=O)C1=CC=C(N2OC(=C(COC3=CC=C(NS(=O)(=O)C4=CC=CC(=C4)S(=O)(=O)NC4=CC=CC5=C4C(=CC(NC(=O)CC)=C5O)\N= |
| 6987 | NO_CAS | A |  | (4R)-4-[(2R,3S)-3-[(1R)-1-(tert-butyldimethylsilyloxy)ethyl]-4-oxo-2-azetidinyl]-2-diazo-3-oxovaleric acid p-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)C(=[N+]=[N-])C(=O)OCC1=CC=C(C=C1)[N+ |
| 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- |
| 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 |

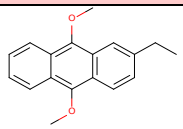
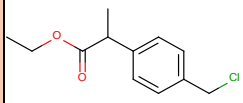
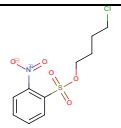
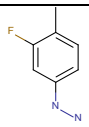
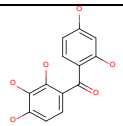
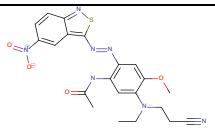
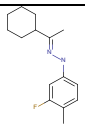
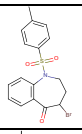
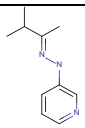
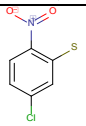
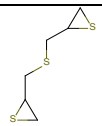
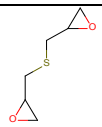
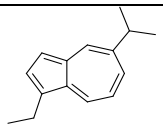
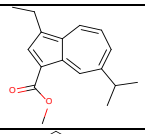
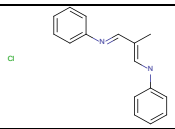
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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 | COC(=O)COC1=CC=C(\C=C\C(=O)NNC(=O)C(Cl)(Cl)Cl)C=C1OC |
| 7323 | NO_CAS | A |  | 2'-(3-acetyl-5-nitro-2-thienylazo)-5'-diethylaminoacetoanilide | CCN(CC)C1=CC(NC(C)=O)=C(C=C1)\N=N\C1=C(C=C(S1)[N+]([O-])=O)C(C)=O |
| 7351 | NO_CAS | A |  | 3-(2-oxocyclohexyl)propanal | O=CCCC1CCCCC1=O |
| 7404 | NO_CAS | A |  | p-toluenesulfonic acid 1-ethylpropyl ester | CCC(CC)OS(=O)(=O)C1=CC=C(C)C=C1 |
| 7461 | NO_CAS | A |  | methanesulfonic acid 2-(5-ethyl-2-pyridyl)ethyl ester | CCC1=CC=C(CCOS(C)(=O)=O)N=C1 |
| 7497 | NO_CAS | A |  | 4-(acetylamino)-5-chloro-2-ethoxybenzoic acid ethyl ester | CCOC(=O)C1=CC(Cl)=C(NC(C)=O)C=C1OCC |
| 7512 | NO_CAS | A |  | 5-amino-2,4,6-triiodoisophthalic acid dichloride ester | NC1=C(I)C(C(Cl)=O)=C(I)C(C(Cl)=O)=C1I |
| 7549 | NO_CAS | A |  | 4-(chloromethyl)-2-isopropylthiazole | CC(C)C1=NC(CCl)=CS1 |
| 7554 | NO_CAS | A | | 4,6-diamino-1,3-benzenediol dihydrochloride | Cl.Cl.NC1=CC(N)=C(O)C=C1O |
| 7568 | NO_CAS | A |  | 3,5-dimethyl-4-nitropyridine 1-oxide | CC1=C[N+]([O-])=CC(C)=C1[N+]([O-])=O |
| 7611 | NO_CAS | A |  | 3-hydroxy-1,1-dimethylbutyl hydroperoxide | CC(O)CC(C)(C)OO |
| 7636 | NO_CAS | A |  | benzaldehyde (4-methylphenyl)hydrazone | CC1=CC=C(N\N=C\C2=CC=CC=C2)C=C1 |
| 7681 | NO_CAS | A |  | 6-[(2,3-epoxypropane-1-yl)oxy]quinoline-2(1H)-one | O=C1NC2=C(C=C1)C=C(OCC1CO1)C=C2 |
| 7686 | NO_CAS | A |  | 6-(3-chloro-2-hydroxypropoxy)-1,2-dihydroquinoline-2-one | OC(CCl)COC1=CC2=C(NC(=O)C=C2)C=C1 |
| 7739 | NO_CAS | A |  | N2-hydroxy-N1-[3-(2-phenoxyethoxy)-1H-pyrazole-5-yl]-3-nitrobenzamidine | O\N=C(\NC1=CC(OCCOC2=CC=CC=C2)=NN1)C1=CC(=CC=C1)[N+]([O-])=O |

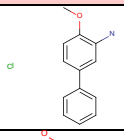
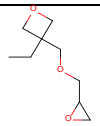
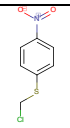
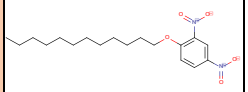
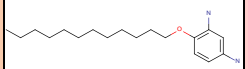
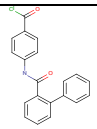
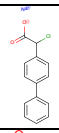
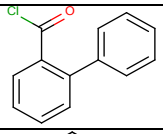
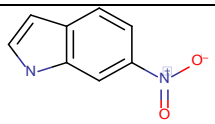
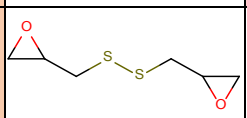
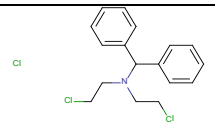
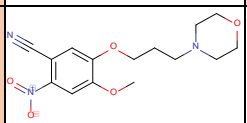
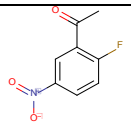
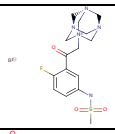
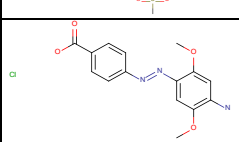
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| Serial_Id | CAS# | AMES RESULT | Structure | Chemical_Name | SMILES |
|---|---|---|---|---|---|
| 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 | ClC(C1=CC=C(Cl)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 |

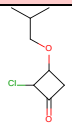
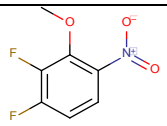
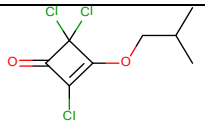
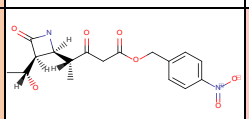
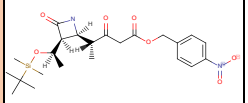
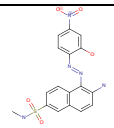
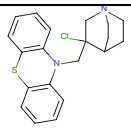
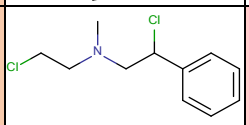
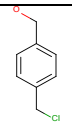
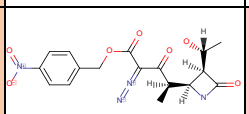
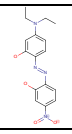
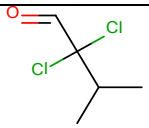
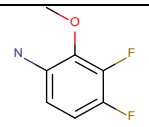
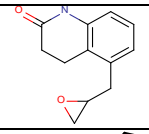
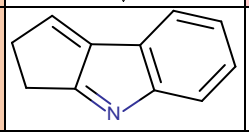
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| Serial_Id | CAS# | AMES RESULT | Structure | Chemical_Name | SMILES |
|---|---|---|---|---|---|
| 8343 | NO_CAS | A |  | 2-ethyl-9,10-dimethoxyanthracene | CCC1=CC2=C(C=C1)C(OC)=C1C=CC=CC1=C2OC |
| 8368 | NO_CAS | A |  | 2-(4-chloromethylphenyl)propionic acid ethyl ester | CCOC(=O)C(C)C1=CC=C(CCl)C=C1 |
| 8408 | NO_CAS | A |  | 2-nitrobenzenesulfonic acid 4-chlorobutyl ester | [O-][N+](=O)C1=C(C=CC=C1)S(=O)(=O)OCCCCCl |
| 8433 | NO_CAS | A |  | 3-fluoro-4-methylphenylhydrazine | CC1=CC=C(NN)C=C1F |
| 8436 | NO_CAS | A |  | 2,2',3,4,4'-pentahydroxybenzophenone | OC1=CC(O)=C(C=C1)C(=O)C1=CC=C(O)C(O)=C1O |
| 8524 | NO_CAS | A |  | 5'-[N-(2-cyanoethyl)-N-ethylamino]-4'-methoxy-2'-(5-nitro-2,1-benzisothiazole-3-ylazo)acetoanilide | CCN(CCC#N)C1=CC(NC(C)=O)=C(C=C1OC)\N=N\C1=C2C=C(C=CC2=NS1)[N+]([O-])=O |
| 8533 | NO_CAS | A |  | 1-cyclohexylethanone 3-fluoro-p-tolylhydrazone | C\C(=N/NC1=CC=C(C)C(F)=C1)C1CCCCC1 |
| 8602 | NO_CAS | A |  | 4-bromo-1-tosyl-2,3-dihydro-1H-1-benzazepine-5(4H)-one | CC1=CC=C(C=C1)S(=O)(=O)N1CCC(Br)C(=O)C2=C1C=CC=C2 |
| 8631 | NO_CAS | A |  | 3-methyl-2-butanone 3-pyridylhydrazone | CC(C)C(\C)=N\NC1=CN=CC=C1 |
| 8688 | NO_CAS | A |  | 5-chloro-2-nitrobenzenethiol | [O-][N+](=O)C1=C(S)C=C(Cl)C=C1 |
| 8726 | NO_CAS | A |  | bis(thiirane-2-ylmethyl) sulfide | C(SCC1CS1)C1CS1 |
| 8727 | NO_CAS | A |  | diglycidyl sulfide | C(SCC1CO1)C1CO1 |
| 8783 | NO_CAS | A |  | 1-ethyl-5-isopropylazulene | CCC1=CC=C2C=C(C=CC=C12)C(C)C |
| 8784 | NO_CAS | A |  | 3-ethyl-7-isopropyl-1-azulenecarboxylic acid methyl ester | CCC1=C2C=CC=C(C=C2C(=C1)C(=O)OC)C(C)C |
| 8884 | NO_CAS | A |  | N-[2-methyl-3-(phenylimino)-1-propenyl]benzenamine hydrochloride | Cl.C\C(=C/NC1=CC=CC=C1)\C=N\C1=CC=CC=C1 |

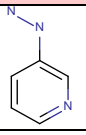
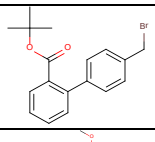
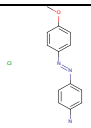
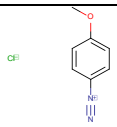
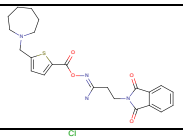
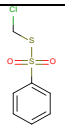
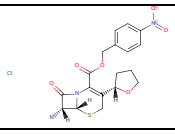
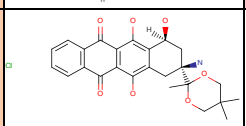
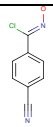
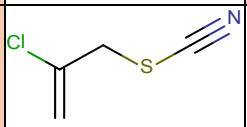
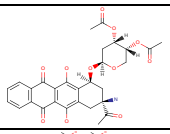
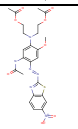
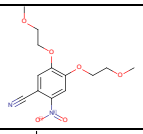
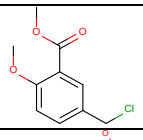
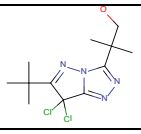
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| Serial_Id | CAS# | AMES RESULT | Structure | Chemical_Name | SMILES |
|---|---|---|---|---|---|
| 8890 | NO_CAS | A |  | 4-methoxybiphenyl-3-amine hydrochloride | Cl.COC1=C(N)C=C(C=C1)C1=CC=CC=C1 |
| 8931 | NO_CAS | A |  | 3-ethyl-3-glycidyloxymethyloxetane | CCC1(COCC2CO2)COC1 |
| 9119 | NO_CAS | A |  | 1-chloromethylthio-4-nitrobenzene | [O-][N+](=O)C1=CC=C(SCCl)C=C1 |
| 9151 | NO_CAS | A |  | 1-dodecyloxy-2,4-dinitrobenzene | CCCCCCCCCCCCOC1=C(C=C(C=C1)[N+]([O-])=O)[N+]([O-])=O |
| 9152 | NO_CAS | A |  | 4-dodecyloxy-1,3-phenylenediamine | CCCCCCCCCCCCOC1=C(N)C=C(N)C=C1 |
| 9180 | NO_CAS | A |  | 4-(2-biphenylylcarbonylamino)benzoic acid chloride | ClC(=O)C1=CC=C(NC(=O)C2=C(C=CC=C2)C2=CC=CC=C2)C=C1 |
| 9181 | NO_CAS | A |  | 2-(4-biphenylyl)-2-chloroacetic acid sodium salt | [Na+].[O-]C(=O)C(Cl)C1=CC=C(C=C1)C1=CC=CC=C1 |
| 9182 | NO_CAS | A |  | 2-biphenylcarboxylic acid chloride | ClC(=O)C1=C(C=CC=C1)C1=CC=CC=C1 |
| 9322 | NO_CAS | A |  | 6-nitroindole | [O-][N+](=O)C1=CC2=C(C=CN2)C=C1 |
| 9325 | NO_CAS | A |  | diglycidyl persulfide | C(SSCC1CO1)C1CO1 |
| 9328 | NO_CAS | A |  | N,N-bis(2-chloroethyl)-α-phenylbenzenemethanamine hydrochloride | Cl.ClCCN(CCCl)C(C1=CC=CC=C1)C1=CC=CC=C1 |
| 9385 | NO_CAS | A |  | 4-methoxy-5-(3-morpholinopropoxy)-2-nitrobenzonitrile | COC1=CC(=C(C=C1OCCCN1CCOCC1)C#N)[N+]([O-])=O |
| 9538 | NO_CAS | A |  | 2'-fluoro-5'-nitroacetophenone | CC(=O)C1=C(F)C=CC(=C1)[N+]([O-])=O |
| 9543 | NO_CAS | A |  | 1-(2-fluoro-5-methylsulfonylamino-β-oxophenethyl)-3,5,7-triaza-1-azoniatricyclo[3.3.1.13,7]decane bromide | [Br-].CS(=O)(=O)NC1=CC=C(F)C(=C1)C(=O)C[N+]12C[N@]3C[N@](C[N@](C3)C1)C2 |
| 9591 | NO_CAS | A |  | 4-(4-amino-2,5-dimethoxyphenylazo)benzoic acid hydrochloride | Cl.COC1=CC(N)=C(OC)C=C1\N=N\C1=CC=C(C=C1)C(O)=O |

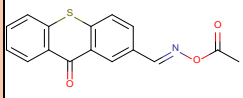
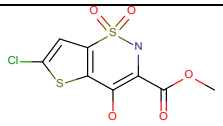
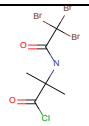
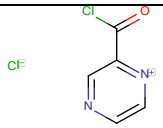
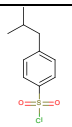
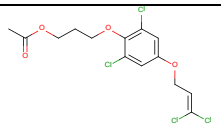
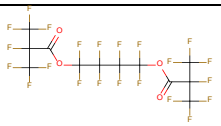
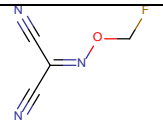
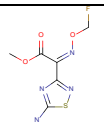
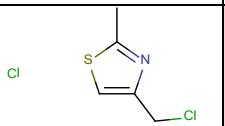
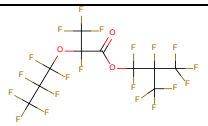
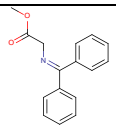
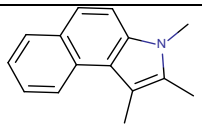
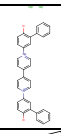
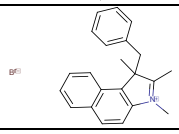
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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-butyldimethylsiloxy)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=CC2=C(C=C1)C(\N=N\C1=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 | ClC1(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=N\C2=CC=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=C2CC1CO1 |
| 9966 | NO_CAS | A |  | 2,3-dihydrocyclopenta[b]indole | C1CC2=NC3=C(C=CC=C3)C2=C1 |

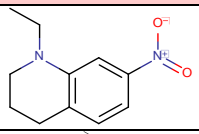
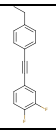
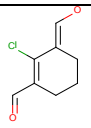
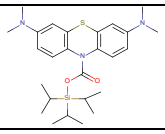
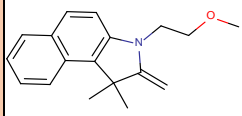
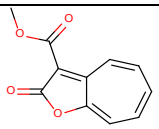
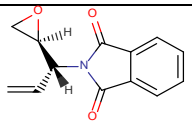
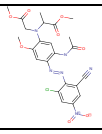
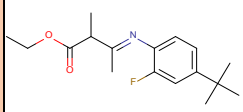
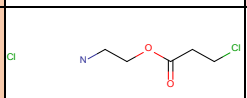
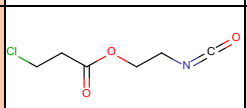
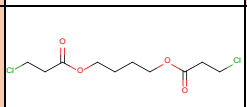
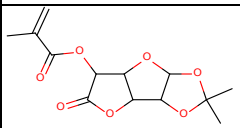
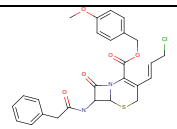
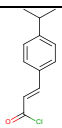
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| Serial_Id | CAS# | AMES RESULT | Structure | Chemical_Name | SMILES |
|---|---|---|---|---|---|
| 10014 | NO_CAS | A |  | 3-pyridylhydrazine | NNC1=CN=CC=C1 |
| 10028 | NO_CAS | A |  | 4'-(bromomethyl)-2-biphenylcarboxylic acid tert-butyl ester | CC(C)(C)OC(=O)C1=C(C=CC=C1)C1=CC=C(CBr)C=C1 |
| 10047 | NO_CAS | A |  | 4-(4-methoxyphenylazo)aniline hydrochloride | Cl.COC1=CC=C(C=C1)\N=N\C1=CC=C(N)C=C1 |
| 10049 | NO_CAS | A |  | 4-methoxybenzenediazonium chloride | [Cl-].COC1=CC=C(C=C1)[N+]#N |
| 10063 | NO_CAS | A |  | N-[2-[N2-[5-(hexahydro-1H-azepine-1-ylmethyl)-2-thienylcarbonyloxy]amidino]ethyl]phthalimide | N\C(CCN1C(=O)C2=CC=CC=C2C1=O)=N/OC(=O)C1=CC=C(CN2CCCCCC2)S1 |
| 10148 | NO_CAS | A |  | benzenethiosulfonic acid S-(chloromethyl) ester | ClCSS(=O)(=O)C1=CC=CC=C1 |
| 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 | 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 |
| 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 | 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)(C)CO1 |
| 10220 | NO_CAS | A |  | 4-[chloro(hydroxyimino)methyl]benzonitrile | O\N=C(/Cl)C1=CC=C(C=C1)C#N |
| 10249 | NO_CAS | A |  | 2-chloro-2-propenyl thiocyanate | ClC(=C)CSC#N |
| 10326 | NO_CAS | A |  | (7S,9S)-9-acetyl-9-amino-7-(3-O,4-O-diacetyl-2-deoxy-β-D-erythro-pentopyranosyloxy)-6,11-dihydroxy-5,7,8,9,10,12-hexahydro-5,12-naphthacenedione | [H][C@@]1(C[C@]([H])(OC(C)=O)[C@@]([H])(CO1)OC(C)=O)O[C@@]1([H])C[C@@](N)(CC2=C(O)C3=C(C(O)=C12)C(=O)C1=C(C=CC=C1)C3=O)C(C)= |
| 10387 | NO_CAS | A |  | diacetic acid [5-acetylamino-4-(6-nitrobenzothiazole-2-ylazo)-2-methoxyphenyl]iminodiethylene ester | COC1=CC(\N=N\C2=NC3=C(S2)C=C(C=C3)[N+]([O-])=O)=C(NC(C)=O)C=C1N(CCOC(C)=O)CCOC(C)=O |
| 10401 | NO_CAS | A |  | 4,5-bis(2-methoxyethoxy)-2-nitrobenzonitrile | COCCOC1=C(OCCOC)C=C(C(=C1)C#N)[N+]([O-])=O |
| 10618 | NO_CAS | A |  | 5-(chloromethyl)-2-methoxybenzoic acid methyl ester | COC(=O)C1=CC(CCl)=CC=C1OC |
| 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 | CC(C)(C)C1=NN2C(=NN=C2C1(Cl)Cl)C(C)(C)CO |

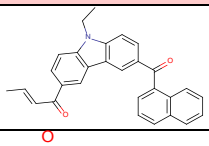
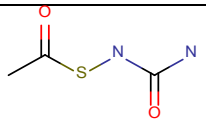
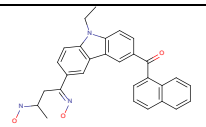
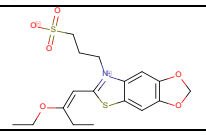
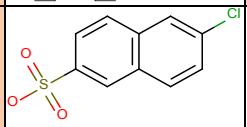
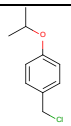
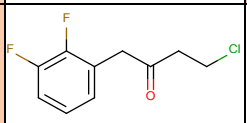
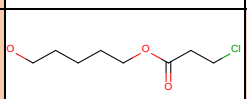
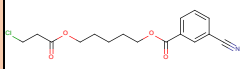
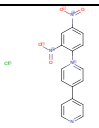
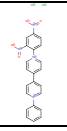
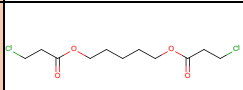
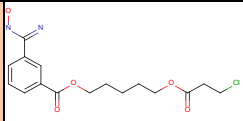
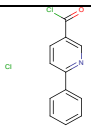
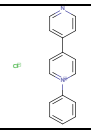
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| Serial_Id | CAS# | AMES RESULT | Structure | Chemical_Name | SMILES |
|---|---|---|---|---|---|
| 10720 | NO_CAS | A |  | 2-(acetyloxyiminomethyl)-9H-thioxanthene-9-one | CC(=O)O\N=C\C1=CC2=C(SC3=C(C=CC=C3)C2=O)C=C1 |
| 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 | COC(=O)C1=C(O)C2=C(C=C(Cl)S2)S(=O)(=O)N1 |
| 11264 | NO_CAS | A |  | 2-methyl-2-(2,2,2-tribromoacetylamino)propanoyl chloride | CC(C)(NC(=O)C(Br)(Br)Br)C(Cl)=O |
| 11318 | NO_CAS | A |  | 2-chlorocarbonylpirazinium chloride | [Cl-].ClC(=O)C1=[NH+]C=CN=C1 |
| 11723 | NO_CAS | A |  | 4-isobutylbenzenesulfonyl chloride | CC(C)CC1=CC=C(C=C1)S(Cl)(=O)=O |
| 11759 | NO_CAS | A |  | acetic acid 3-[2,6-dichloro-4-(3,3-dichloroallyloxy)phenoxy]propyl ester | CC(=O)OCCCOC1=C(Cl)C=C(OCC=C(Cl)Cl)C=C1Cl |
| 11836 | NO_CAS | A |  | bis[2,3,3,3-tetrafluoro-2-(trifluoromethyl)propanoic acid]octafluorobutane-1,4-diyl ester | FC(F)(F)C(F)(C(=O)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)OC(=O)C(F)(C(F)(F)F)C(F)(F)F)C(F)(F)F |
| 12113 | NO_CAS | A |  | 2-(fluoromethoxyimino)propane-1,3-dinitrile | FCON=C(C#N)C#N |
| 12179 | NO_CAS | A |  | (Z)-2-(5-amino-1,2,4-thiadiazole-3-yl)-2-fluoromethoxyiminoacetic acid methyl ester | COC(=O)C(=N/OCF)\C1=NSC(N)=N1 |
| 12411 | NO_CAS | A |  | 4-chloromethyl-2-methylthiazole hydrochloride | Cl.CC1=NC(CCl)=CS1 |
| 12457 | NO_CAS | A |  | 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoic acid 2-(trifluoromethyl)hexafluoropropyl ester | FC(F)(F)C(F)(F)C(F)(F)OC(F)(C(=O)OC(F)(F)C(F)(C(F)(F)F)C(F)(F)F)C(F)(F)F |
| 12639 | NO_CAS | A |  | 2-[(diphenylmethylene)amino]acetic acid methyl ester | COC(=O)CN=C(C1=CC=CC=C1)C1=CC=CC=C1 |
| 12655 | NO_CAS | A |  | 1,2,3-trimethyl-3H-benzo[e]indole | CN1C(C)=C(C)C2=C1C=CC1=C2C=CC=C1 |
| 12668 | NO_CAS | A |  | 1,1'-bis(2-hydroxy-5-biphenylyl)-4,4'-bipyridinium dichloride | [Cl-].[Cl-].OC1=C(C=C(C=C1)[N+]1=CC=C(C=C1)C1=CC=[N+](C=C1)C1=CC(=C(O)C=C1)C1=CC=CC=C1)C1=CC=CC=C1 |
| 12711 | NO_CAS | A |  | 1-benzyl-1,2,3-trimethyl-1H-benzo[e]indole-3-ium・bromide | [Br-].CC1=[N+](C)C2=C(C3=C(C=CC=C3)C=C2)C1(C)CC1=CC=CC=C1 |

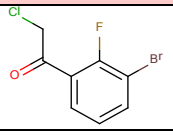
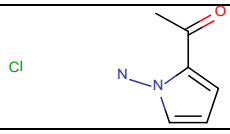
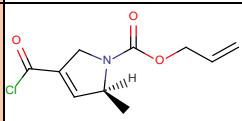
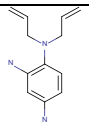
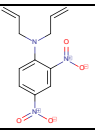
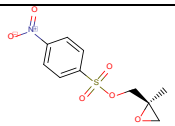
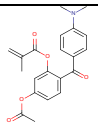
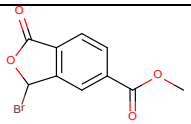
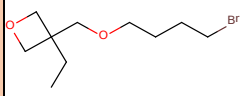
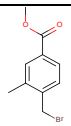
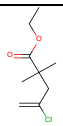
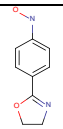
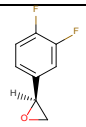
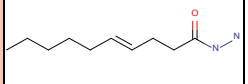
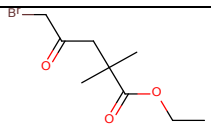
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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 | COCCN1C(=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\C1=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)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)CCCl |
| 13689 | NO_CAS | A |  | methacrylic acid 4,4-dimethyl-10-oxo-3,5,7,11-tetraoxatricyclo[6.3.0.02,6]undecan-9-yl | CC(=C)C(=O)OC1C2OC3OC(C)(C)OC3C2OC1=O |
| 14786 | NO_CAS | A |  | 3-(3-chloro-1-propenyl)-8-oxo-7-(2-phenylacetylamino)-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 |

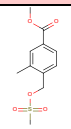
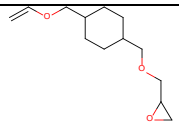
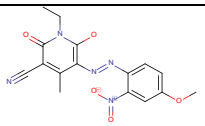
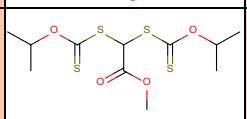
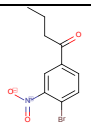
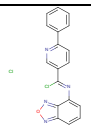
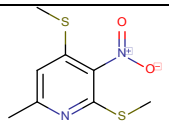
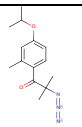
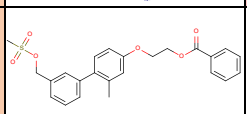
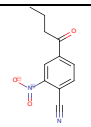
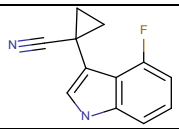
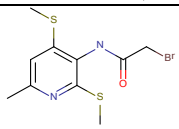
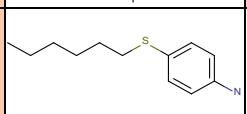
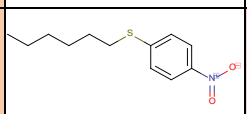
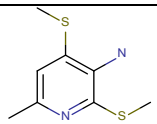
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

| 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 | CCN1C2=C(C=C(C=C2)C(=O)\C=C\C)C2=C1C=CC(=C2)C(=O)C1=CC=CC2=C1C=CC=C2 |
| 15330 | NO_CAS | A |  | S-(carbamoylamino) ethanethioate | CC(=O)SNC(N)=O |
| 15375 | NO_CAS | A |  | 9-ethyl-6-(3-hydroxyamino-1-hydroxyiminobutyl)-9H-carbazole-3-yl(1-naphthyl) ketone | CCN1C2=C(C=C(C=C2)C(\CC(C)NO)=N\O)C2=C1C=CC(=C2)C(=O)C1=CC=CC2=C1C=CC=C2 |
| 15383 | NO_CAS | A |  | 3-[[6-(2-ethoxy-1-butenyl)-1,3-dioxolo[4,5-f]benzothiazole-7-ium]-7-yl]propane-1-sulfonate | CCO\C(CC)=C\C1=[N+](CCCS([O-])(=O)=O)C2=CC3=C(OCO3)C=C2S1 |
| 15410 | NO_CAS | A |  | 6-chloronaphthalene-2-sulfonic acid | OS(=O)(=O)C1=CC2=C(C=C1)C=C(Cl)C=C2 |
| 15414 | NO_CAS | A |  | 1-chloromethyl-4-isopropoxybenzene | CC(C)OC1=CC=C(CCl)C=C1 |
| 15724 | NO_CAS | A |  | 4-chloro-1-(2,3-difluorophenyl)butane-2-one | FC1=C(F)C(CC(=O)CCCl)=CC=C1 |
| 15729 | NO_CAS | A |  | 3-chloropropanoic acid 5-hydroxypentyl ester | OCCCCCOC(=O)CCCl |
| 15742 | NO_CAS | A |  | 3-cyanobenzoic acid 5-(3-chloropropanoyloxy)pentyl ester | ClCCC(=O)OCCCCCOC(=O)C1=CC=CC(=C1)C#N |
| 15779 | NO_CAS | A |  | 1-(2,4-dinitrophenyl)-4-(4-pyridyl)pyridinium chloride | [Cl-].[O-][N+](=O)C1=CC=C(C(=C1)[N+]([O-])=O)[N+]1=CC=C(C=C1)C1=CC=NC=C1 |
| 15780 | NO_CAS | A |  | 1-(2,4-dinitrophenyl)-1'-phenyl-4,4'-bipyridinium dichloride | [Cl-].[Cl-].[O-][N+](=O)C1=CC=C(C(=C1)[N+]([O-])=O)[N+]1=CC=C(C=C1)C1=CC=[N+](C=C1)C1=CC=CC=C1 |
| 15838 | NO_CAS | A |  | bis(3-chloropropanoic acid) entanep-1,5-diyl ester | ClCCC(=O)OCCCCCOC(=O)CCCl |
| 15849 | NO_CAS | A |  | 3-(N-hydroxycarbamimidoyl)benzoic acid 5-(3-chloropropanoyloxy)pentyl ester | ONC(=N)C1=CC(=CC=C1)C(=O)OCCCCCOC(=O)CCCl |
| 15871 | NO_CAS | A |  | 6-phenylnicotinoyl chloride hydrochloride | Cl.ClC(=O)C1=CN=C(C=C1)C1=CC=CC=C1 |
| 15872 | NO_CAS | A |  | 1-phenyl-4,4'-bipyridine-1-ium chloride | [Cl-].C1=CC=C(C=C1)[N+]1=CC=C(C=C1)C1=CC=NC=C1 |

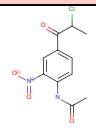
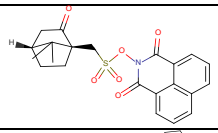
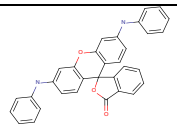
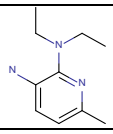
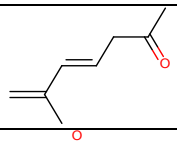
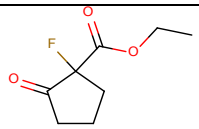
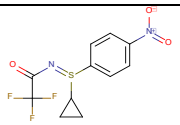
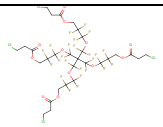
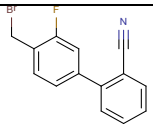
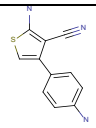
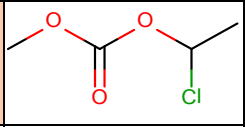
# Strong positive (Class A) in Ames assay in Phase III trial (236 chemicals)

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

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

# 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@@](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=C(OC3=C2C=CC(NC2=CC=CC=C2)=C3)C=C(NC2=CC=CC=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)\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(C(F)(F)OC(F)(F)C(F)(F)COC(=O)CCCl)(C(F)(F)OC(F)(F)C(F)(F)COC(=O)CCCl)C(F)(F)OC(F)(F)C(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 |