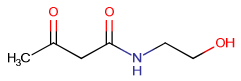
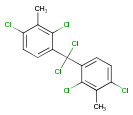
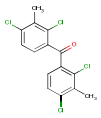
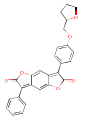
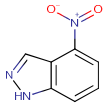
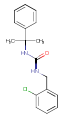
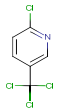
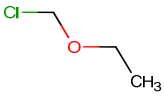
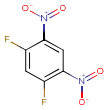
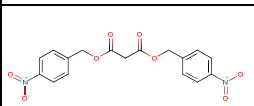
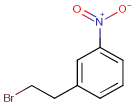
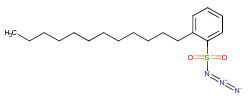
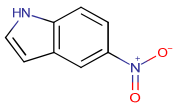
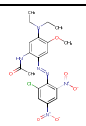
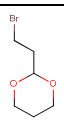
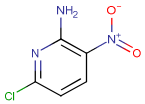
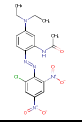
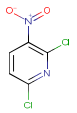
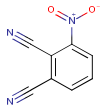
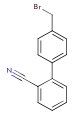
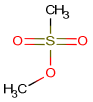
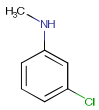
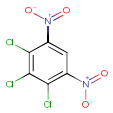
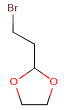
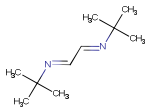
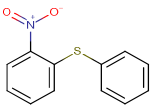
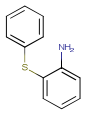
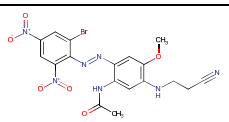
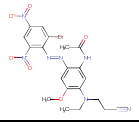
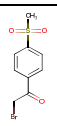
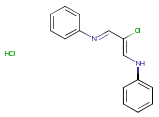
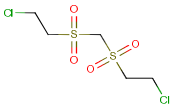
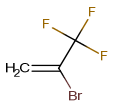
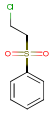
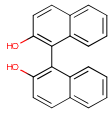
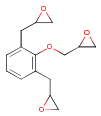
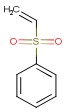
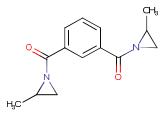
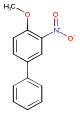
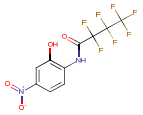
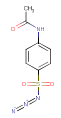
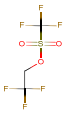
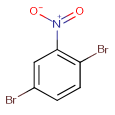
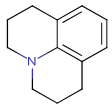
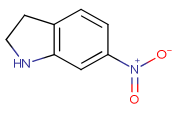
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

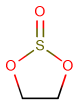
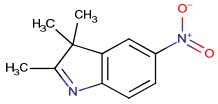
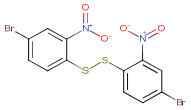
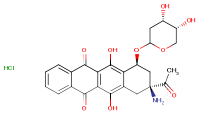
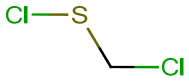
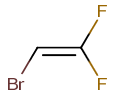
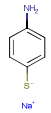
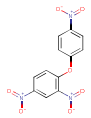
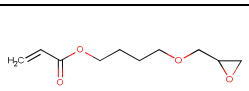
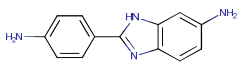
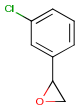
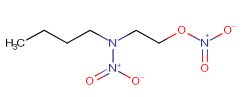
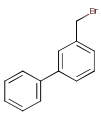
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

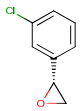
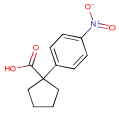
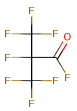
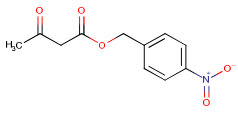
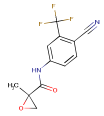
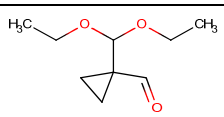
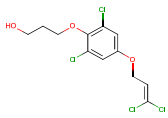
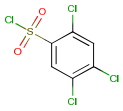
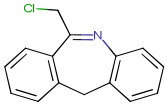
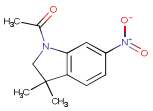
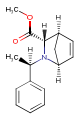
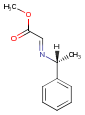
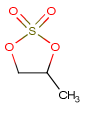
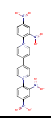
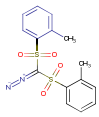
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

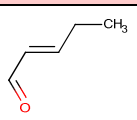
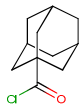
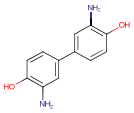
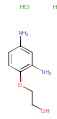
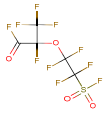
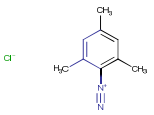
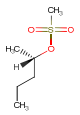
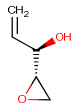
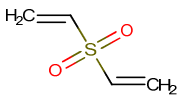
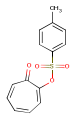
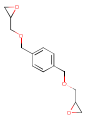
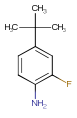
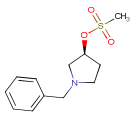
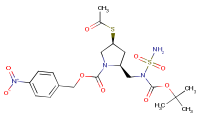
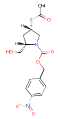
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

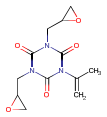
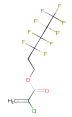
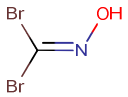
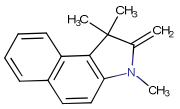
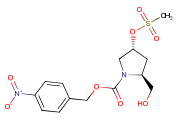
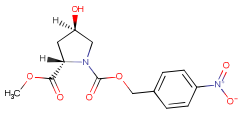
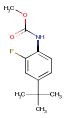
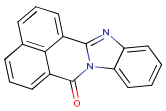
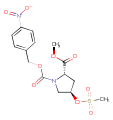
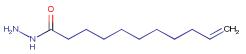
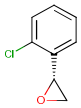
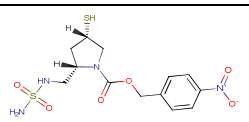
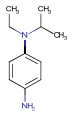
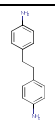
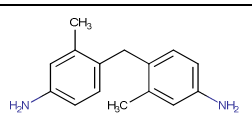
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

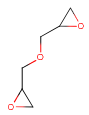
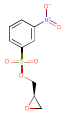
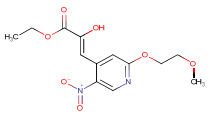
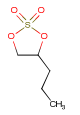
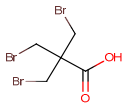
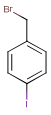
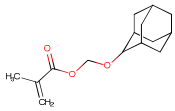
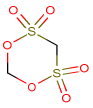
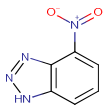
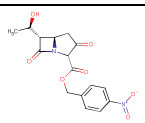
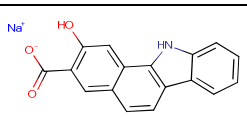
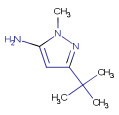
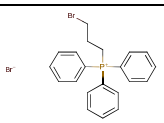
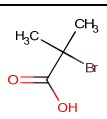
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

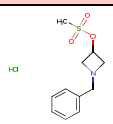
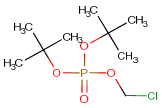
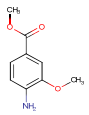
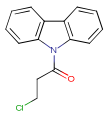
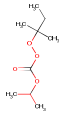
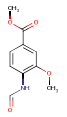
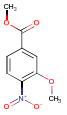
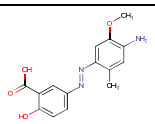
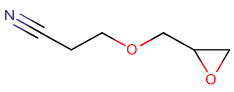
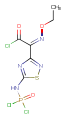
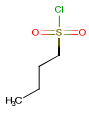
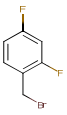
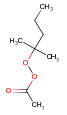
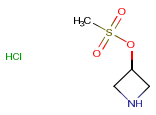
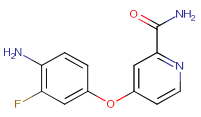
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

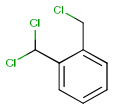
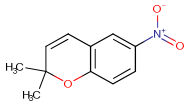
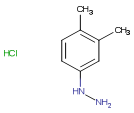
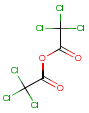
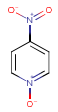
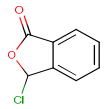
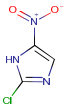
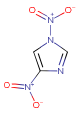
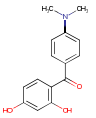
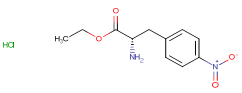
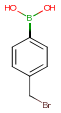
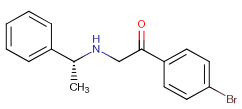
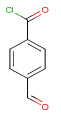
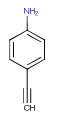
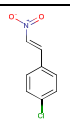
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

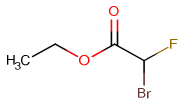
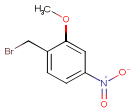
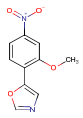
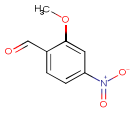
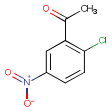
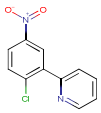
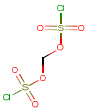
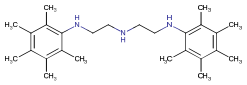
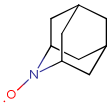
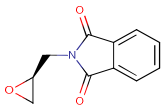
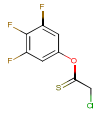
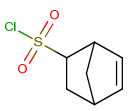
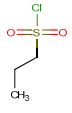
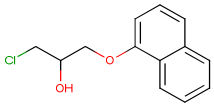
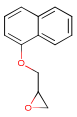
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

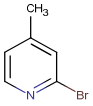
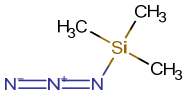
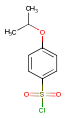
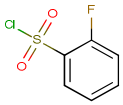
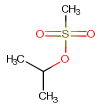
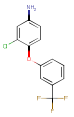
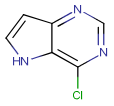
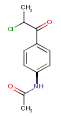
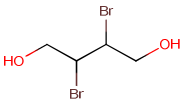
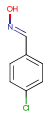
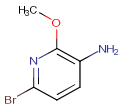
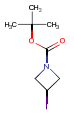
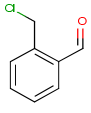
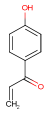
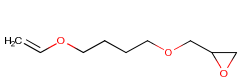
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

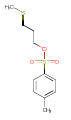
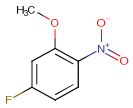
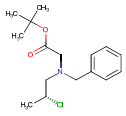
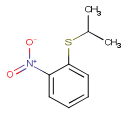
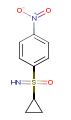
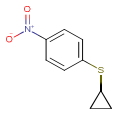
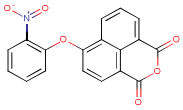
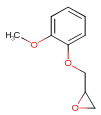
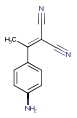
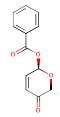
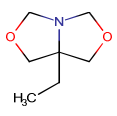
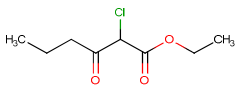
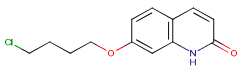
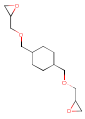
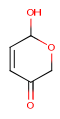
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

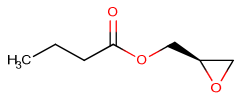
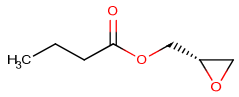
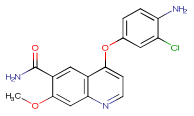
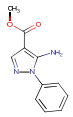
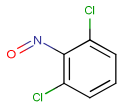
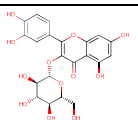
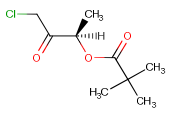
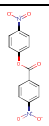
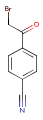
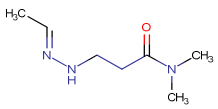
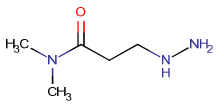
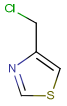
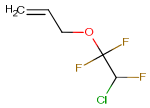
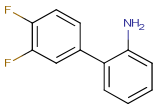
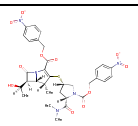
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

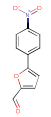
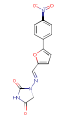
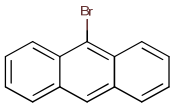
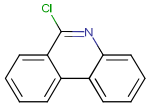
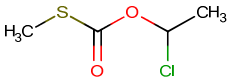
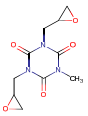
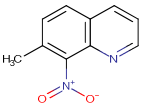
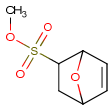
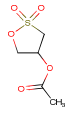
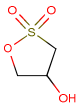
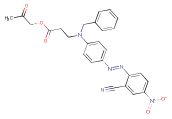
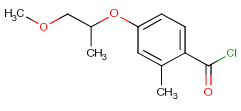
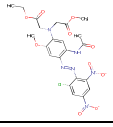
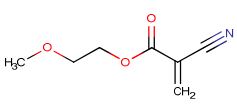
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

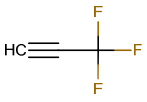
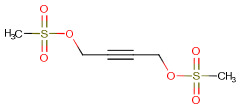
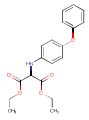
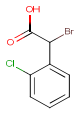
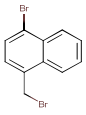
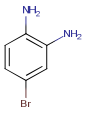
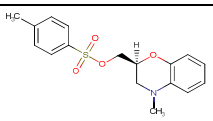
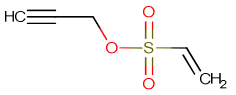
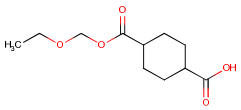
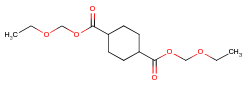
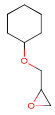
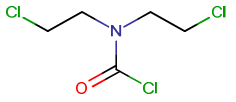
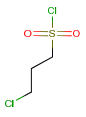
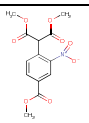
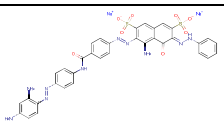
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

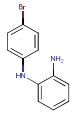
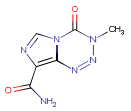
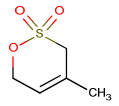
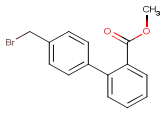
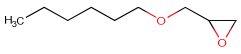
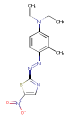
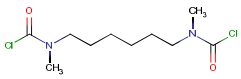
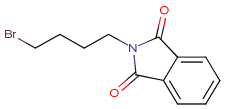
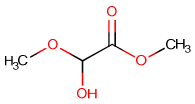
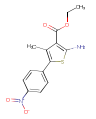
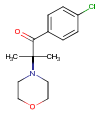
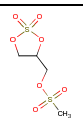
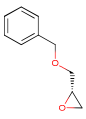
## Strong positive (Class A) in Ames assay in Phase II trial (253 chemicals)

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

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

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

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

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