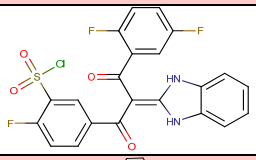
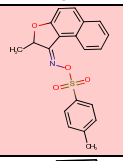
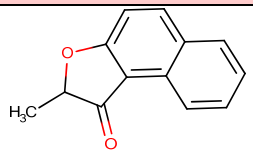
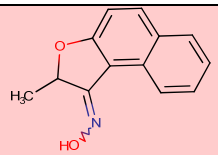
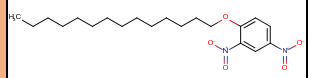
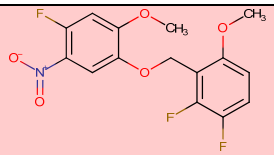
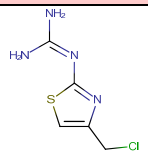
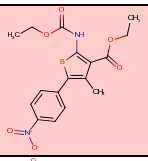
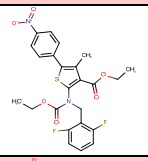
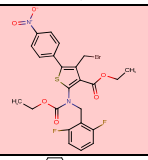
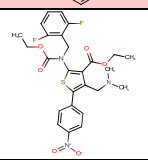
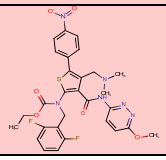
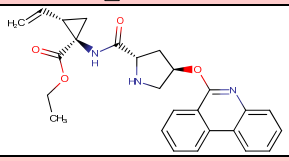
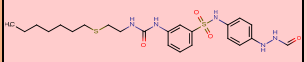
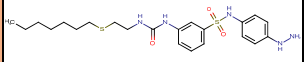
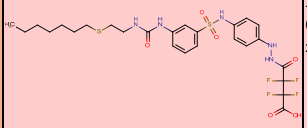
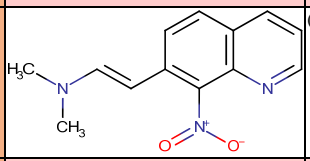
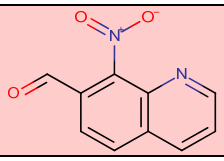
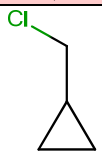
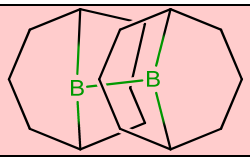
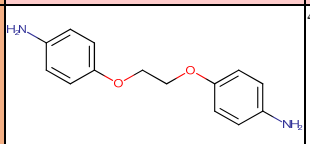
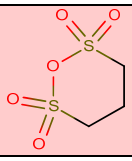
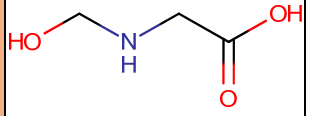
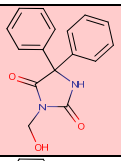
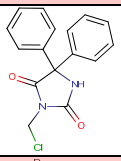
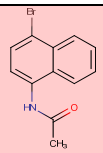
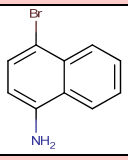
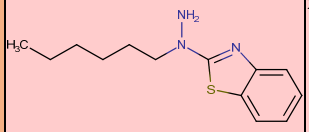
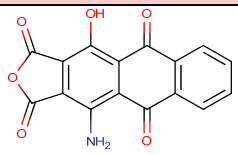
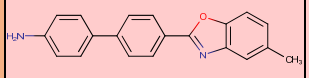
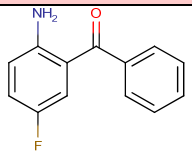
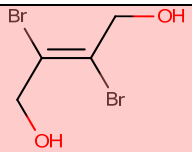
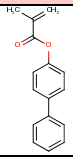
Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
21585	NO_CAS	A		5-[2-[1H-benzoimidazole-2(3H)-ylidene]-3-(2,5-difluorophenyl)-3-oxopropanoyl]-2-fluorobenzene-1-sulfonyl chloride	FC1=CC=C(F)C(=C1)C(=O)C(C(=O)C1=CC=C(F)C(=C1)S(Cl)(=O)=O)=C1NC2=CC=CC=C2N1
21339	NO_CAS	A		2-methylnaphtho[2,1-b]furan-1(2H)-one O-tosyl oxime	CC1OC2=CC=C3C=CC=CC3=C2\C1=N/OS(=O)(=O)C1=CC=C(C)C=C1
21337	NO_CAS	A		2-methylnaphtho[2,1-b]furan-1(2H)-one	CC1OC2=CC=C3C=CC=CC3=C2C1=O
21338	NO_CAS	A		2-methylnaphtho[2,1-b]furan-1(2H)-one oxime	CC1OC2=CC=C3C=CC=CC3=C2C1=NO
21194	NO_CAS	A		2,4-dinitro-1-tetradecyloxybenzene	CCCCCCCCCCCCCCOC1=CC=C(C=C1[N+]([O-])=O)[N+]([O-])=O
21468	NO_CAS	A		1,2-difluoro-3-[(4-fluoro-2-methoxy-5-nitrophenoxy)methyl]-4-methoxybenzene	COC1=CC=C(F)C(F)=C1COC1=CC(=C(F)C=C1OC)[N+]([O-])=O
21698	NO_CAS	A		2-(4-(chloromethyl)thiazol-2-YL)guanidine hydrochloride	C1=C(N=C(S1)N=C(N)N)CCl
23441	NO_CAS	A		ethyl 2-(ethoxycarbonylamino)-4-methyl-5-(4-nitrophenyl)thiophene-3-carboxylate	CCOC(=O)C1=C(SC(=C1C)C2=CC=C(C=C2)[N+](=O)[O-])NC(=O)OCC
23445	NO_CAS	A		ethyl 2-[(2,6-difluorophenyl)methyl-ethoxycarbonylamino]-4-methyl-5-(4-nitrophenyl)thiophene-3-carboxylate	CCOC(=O)C1=C(SC(=C1C)C2=CC=C(C=C2)[N+](=O)[O-])N(CC3=C(C=CC=C3F)F)C(=O)OCC
23453	NO_CAS	A		ethyl 4-(bromomethyl)-2-[(2,6-difluorophenyl)methyl-ethoxycarbonylamino]-5-(4-nitrophenyl)thiophene-3-carboxylate	CCOC(=O)C1=C(SC(=C1CBr)C2=CC=C(C=C2)[N+](=O)[O-])N(CC3=C(C=CC=C3F)F)C(=O)OCC
23444	NO_CAS	A		ethyl 2-[(2,6-difluorophenyl)methyl-ethoxycarbonylamino]-4-[(dimethylamino)methyl]-5-(4-nitrophenyl)thiophene-3-carboxylate	CCOC(=O)C1=C(SC(=C1CN(C)C)C2=CC=C(C=C2)[N+](=O)[O-])N(CC3=C(C=CC=C3F)F)C(=O)OCC

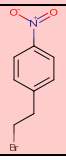
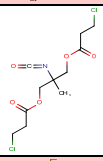
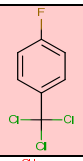
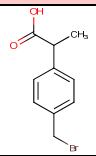
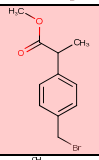
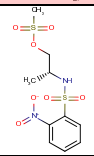
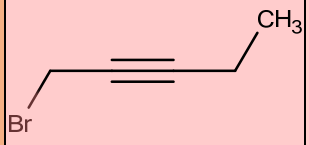
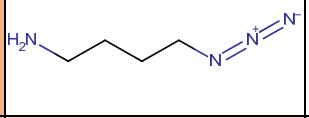
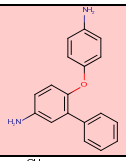
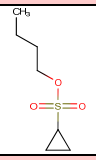
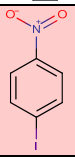
Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
23446	NO_CAS	A		ethyl N-[(2,6-difluorophenyl)methyl]-N-[4-[(dimethylamino)methyl]-3-[(6-methoxypyridazin-3-yl)carbamoyl]-5-(4-nitrophenyl)thiophen-2-yl]carbamate	CCOC(=O)N(CC1=C(C=CC=C1F)F)C2=C(C(=C(S2)C3=CC=C(C=C3)[N+](=O)[O-])CN(C)C)C(=O)NC4=NN=C(C=C4)OC
22111	NO_CAS	A		ethyl (1R,2S)-2-ethenyl-1-[[(2S,4R)-4-phenanthridin-6-yloxypyrrolidine-2-carbonyl]amino]cyclopropane-1-carboxylate	CCOC(=O)[C@]1(C[C@H]1C=C)NC(=O)[C@@H]2C[C@H](CN2)OC3=NC4=CC=CC=C4C5=CC=CC=C53
22162	NO_CAS	A		N-[4-(2-formylhydrazino)phenyl]-3-[3-[2-(heptylthio)ethyl]ureido]benzenesulfonamide ester	CCCCCCCSCCNC(=O)NC1=CC(=CC=C1)S(=O)(=O)NC2=CC=C(C=C2)NNC=O
22144	NO_CAS	A		3-[3-[2-(Heptylthio)ethyl]ureido]-N-(4-hydrazinophenyl)benzenesulfonamide hydrochloride	CCCCCCCSCCNC(=O)NC1=CC(=CC=C1)S(=O)(=O)NC2=CC=C(C=C2)NN
22070	NO_CAS	A		2,2,3,3-tetrafluoro-4-[2-[4-[3-[3-[2-(heptylthio)ethyl]ureido]phenylsulfonylamino]phenyl]hydrazino]-4-oxobutanoic acid potassium salt	CCCCCCCSCCNC(=O)NC1=CC(=CC=C1)S(=O)(=O)NC2=CC=C(C=C2)NNC(=O)C(C(C(=O)O)(F)F)(F)F
22059	176853-39-7	A		(E)-N,N-dimethyl-2-(8-nitroquinolin-7-yl)ethenamine	CN(C)/C=C/C1=C(C2=C(C=CC=N2)C=C1)[N+](=O)[O-]
22085	101327-87-1	A		8-nitro-7-quinolinecarboxaldehyde	C1=CC2=C(C(=C(C=C2)C=O)[N+](=O)[O-])N=C1
23683	5911-08-0	A		(chloromethyl)cyclopropane	C1CC1CCl
23764	21205-91-4	A		9,9'-bi-9-borabicyclo[3.3.1]nonane	B1(C2CCCC1CCC2)B3C4CCCC3CCC4
23657	6052-10-4	A		4,4'-(ethane-1,2-diylbis(oxy))dianiline	C1=CC(=CC=C1N)OCCOC2=CC=C(C=C2)N
23740	4720-58-5	A		1,2,6-oxadithiane 2,2,6,6-tetraoxide	C1CS(=O)(=O)OS(=O)(=O)C1

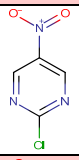
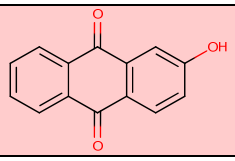
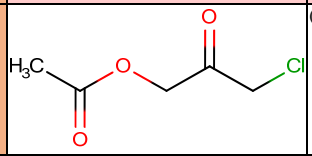
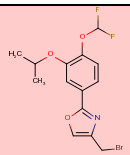
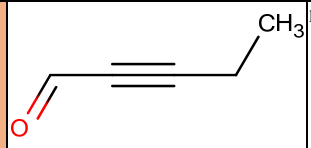
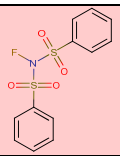
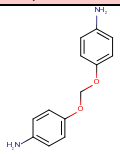
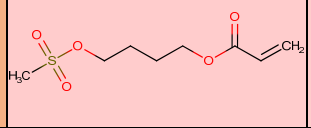
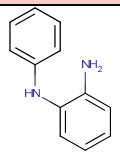
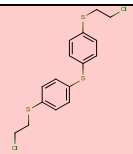
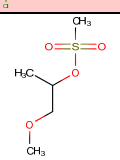
Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
23755	70161-44-3	A		sodium hydroxymethylglycinate	OCNCC(O)=O
23775	21616-46-6	A		3-(hydroxymethyl)-5,5-diphenylimidazolidine-2,4-dione	C1=CC=C(C=C1)C2(C(=O)N(C(=O)N2)CO)C3=CC=CC=C3
23684	93360-07-7	A		3-(chloromethyl)-5,5-diphenylhydantoin	C1=CC=C(C=C1)C2(C(=O)N(C(=O)N2)CCl)C3=CC=CC=C3
23799	91394-66-0	A		N-(4-bromonaphthalen-1-yl)acetamide	CC(=O)NC1=CC=C(C2=CC=CC=C21)Br
23798	2298-07-9	A		4-bromo-1-naphthylamine	C1=CC=C2C(=C1)C(=CC=C2Br)N
23812	1404197-89-2	A		2-(1-Hexylhydrazine-1-yl)benzothiazole	CCCCCCN(C1=NC2=CC=CC=C2S1)N
23845	82052-28-6	A		1-amino-4-hydroxy-9,10-dioxo-9,10-dihydroanthracene-2,3-dicarboxylic anhydride	NC1=C2C(=O)C3=C(C=CC=C3)C(=O)C2=C(O)C2=C1C(=O)OC2=O
24062	139036-50-3	A		4'-(5-methyl-2-benzoxazolyl)biphenyl-4-amine	CC1=CC2=C(C=C1)OC(=N2)C3=CC=C(C=C3)C4=CC=C(C=C4)N
23848	362-46-9	A		2-amino-5-fluorobenzophenone	C1=CC=C(C=C1)C(=O)C2=C(C=CC(=C2)F)N
23958	3234-02-4	A		(E)-2,3-dibromobut-2-ene-1,4-diol	C(/C(=C(/CO)\Br)/Br)O
24012	46904-74-9	A		(4-phenyl)phenyl methacrylate	CC(=C)C(=O)OC1=CC=C(C=C1)C2=CC=CC=C2

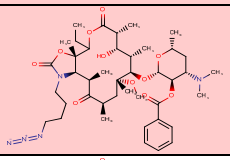
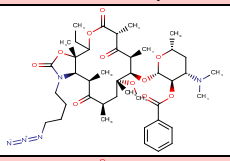
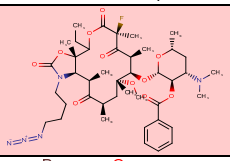
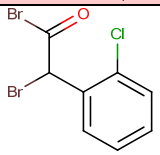
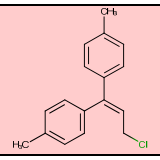
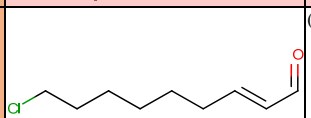
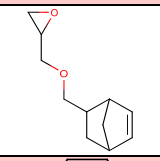
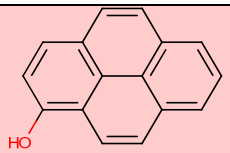
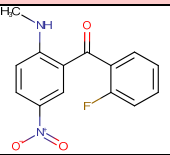
Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
24034	5339-26-4	A		4-nitrophenethyl bromide	C1=CC(=CC=C1CCBr)[N+](=O)[O-]
24098	886443-51-2	A		[3-(3-chloropropanoyloxy)-2-isocyanato-2-methylpropyl] 3-chloropropanoate	CC(COC(=O)CCCl)(COC(=O)CCCl)N=C=O
24504	402-42-6	A		1-fluoro-4-(trichloromethyl)benzene	C1=CC(=CC=C1C(Cl)(Cl)Cl)F
24511	111128-12-2	A		2-[4-(bromomethyl)phenyl]propanoic acid	CC(C1=CC=C(C=C1)CBr)C(=O)O
24537	99807-54-2	A		methyl 2-[4-(bromomethyl)phenyl]propanoate	CC(C1=CC=C(C=C1)CBr)C(=O)OC
24465	NO_CAS	A		(2R)-2-[[(2-nitrophenyl)sulfonyl]amino]propyl methanesulfonate	C[C@H](COS(C)(=O)=O)NS(=O)(=O)C1=CC=CC=C1[N+]([O-])=O
24510	16400-32-1	A		1-bromopent-2-yne	CCC#CCBr
24309	88192-20-5	A		4-azidobutan-1-amine	C(CCN=[N+]=[N-])CN
24321	1215223-23-6	A		6-(4-aminophenoxy)-[1,1'-biphenyl]-3-amine	C1=CC=C(C=C1)C2=C(C=CC(=C2)N)OC3=CC=C(C=C3)N
24732	83635-12-5	A		butyl cyclopropanesulfonate	CCCCOS(=O)(=O)C1CC1
24778	636-98-6	A		1-iodo-4-nitrobenzene	C1=CC(=CC=C1[N+](=O)[O-])I

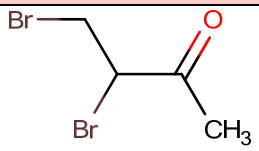
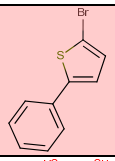
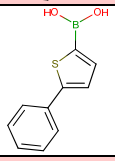
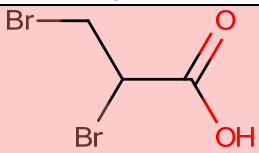
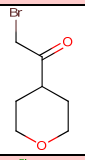
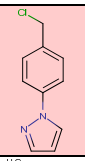
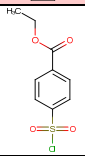
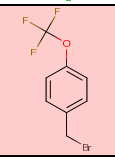
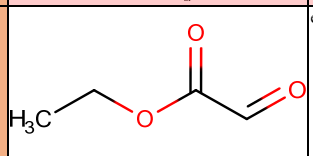
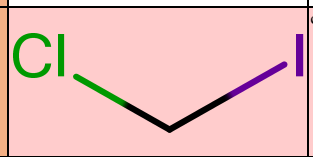
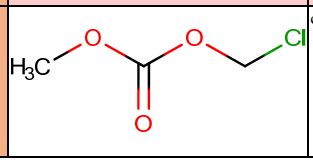
Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
24625	10320-42-0	A		2-chloro-5-nitropyrimidine	C1=C(C=NC(=N1)Cl)[N+](=O)[O-]
24720	605-32-3	A		2-hydroxyanthracene-9,10-dione	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C=C(C=C3)O
24616	40235-68-5	A		(3-chloro-2-oxopropyl) acetate	CC(=O)OCC(=O)CCl
24743	1574285-38-3	A		4-(bromomethyl)-2-[4-(difluoromethoxy)-3-isopropoxyphenyl]-oxazole	CC(C)OC1=C(C=CC(=C1)C2=NC(=CO2)CBr)OC(F)F
24756	55136-52-2	A		pent-2-ynal	CCC#CC=O
24718	133745-75-2	A		N-fluorobenzenesulfonimide	C1=CC=C(C=C1)S(=O)(=O)N(F)S(=O)(=O)C2=CC=CC=C2
25002	46843-47-4	A		4-[(4-aminophenoxy)methoxy]aniline	C1=CC(=CC=C1N)OCOC2=CC=C(C=C2)N
24989	561015-28-9	A		2-propenoic acid, 4-[(methylsulfonyl)oxy]butyl ester	CS(=O)(=O)OCCCCOC(=O)C=C
24952	534-85-0	A		2-aminodiphenylamine	C1=CC=C(C=C1)NC2=CC=CC=C2N
24854	152419-82-4	A		1-(2-chloroethylsulfanyl)-4-[4-(2-chloroethylsulfanyl)phenyl]sulfanylbenzene	C1=CC(=CC=C1SCCCl)SC2=CC=C(C=C2)SCCCl
25221	24590-51-0	A		1-methoxypropan-2-yl methanesulfonate	CC(COC)OS(=O)(=O)C

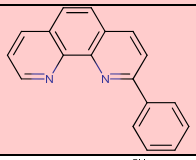
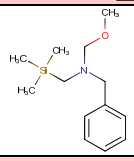
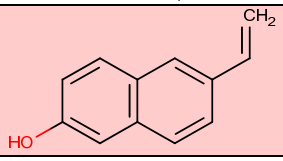
Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
25014	1145656-96-7	A		(2S,3R,4S,6R)-2-{[(3aS,4R,7R,8S,9S,10R,11R,13R,15R,15aR)-1-(4-azidobutyl)-4-ethyl-8-hydroxy-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-tetradecahydro-1H-oxacyclotetradeca[4,3-d][1,3]oxazol-10-yl]oxy}-4-(dimethylamino)-6-methyloxan-3-yl benzoate	CCC1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2OC(=O)C2=CC=CC=C2)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@H]2N(CCCCN=[N+]=[N-])C(=O)O[C@]12C)OC
25016	1145656-98-9	A		(2S,3R,4S,6R)-2-{[(3aS,4R,7R,9S,10R,11R,13R,15R,15aR)-1-(4-azidobutyl)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,8,14-tetraoxo-tetradecahydro-1H-oxacyclotetradeca[4,3-d][1,3]oxazol-10-yl]oxy}-4-(dimethylamino)-6-methyloxan-3-yl benzoate	CCC1OC(=O)[C@H](C)C(=O)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2OC(=O)C2=CC=CC=C2)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@H]2N(CCCCN=[N+]=[N-])C(=O)O[C@]12C)OC
25015	955377-54-5	A		(2S,3R,4S,6R)-2-{[(3aS,4R,7S,9S,10R,11R,13R,15R,15aR)-1-(4-azidobutyl)-4-ethyl-7-fluoro-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,8,14-tetraoxo-tetradecahydro-1H-oxacyclotetradeca[4,3-d][1,3]oxazol-10-yl]oxy}-4-(dimethylamino)-6-methyloxan-3-yl benzoate	CCC1OC(=O)[C@@](C)(F)C(=O)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2OC(=O)C2=CC=CC=C2)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@H]2N(CCCCN=[N+]=[N-])C(=O)O[C@]12C)OC
25185	NO_CAS	A		2-bromo-2-(2-chlorophenyl)acetyl bromide	ClC1=CC=CC=C1C(Br)C(Br)=O
25078	167859-39-4	A		3,3-di(p-tolyl)allyl chloride	CC1=CC=C(C=C1)C(=CCCl)C2=CC=C(C=C2)C
25301	115932-80-4	A		(E)-9-chlorononon-2-enal	C(CCCCl)CC/C=C/C=O
25306	17913-18-7	A		1-chloro-4-methoxybutane	COCCCCCl
25378	3188-75-8	A		2-(5-bicyclo[2.2.1]hept-2-enylmethoxymethyl)oxirane	C1C2CC(C1C=C2)COCC3CO3
25394	5315-79-7	A		1-hydroxypyrene	C1=CC2=C3C(=C1)C=CC4=C(C=CC(=C43)C=C2)O
25418	735-06-8	A		(2-fluorophenyl)-[2-(methylamino)-5-nitrophenyl]methanone	CNC1=C(C=C(C=C1)[N+](=O)[O-])C(=O)C2=CC=CC=C2F
25620	64818-36-6	A		hex-5-enyl methanesulfonate	CS(=O)(=O)OCCCCC=C

Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
25548	25109-57-3	A		3,4-dibromobutan-2-one	CC(=O)C(CBr)Br
25821	29488-24-2	A		2-bromo-5-phenylthiophene	C1=CC=C(C=C1)C2=CC=C(S2)Br
25736	306934-95-2	A		5-phenylthiophene-2-boronic acid	B(C1=CC=C(S1)C2=CC=CC=C2)(O)O
25748	600-05-5	A		2,3-dibromopropionic acid	C(C(C(=O)O)Br)Br
25818	141095-78-5	A		2-bromo-1-(oxan-4-yl)ethanone	C1COCCC1C(=O)CBr
25714	143426-52-2	A		1-[4-(chloromethyl)phenyl]pyrazole	C1=CN(N=C1)C2=CC=C(C=C2)CCl
25890	10486-51-8	A		ethyl 4-(chlorosulfonyl)benzoate	CCOC(=O)C1=CC=C(C=C1)S(=O)(=O)Cl
26049	50824-05-0	A		1-(bromomethyl)-4-(trifluoromethoxy)benzene	C1=CC(=CC=C1CBr)OC(F)(F)F
25889	924-44-7	A		ethyl glyoxylate	CCOC(=O)C=O
25940	593-71-5	A		chloroiodomethane	C(Cl)I
26201	40510-81-4	A		chloromethyl methyl carbonate	COC(=O)OCCl

Strong positive (Class A) in Ames assay in the Second AMES/QSAR International Challenge Project trial (80 chemicals)

Serial Id	CAS#	Ames result	Structure	Chemical name	SMILES
26299	109559-47-9	A		2-phenyl-1,10-phenanthroline	C1=CC=C(C=C1)C2=NC3=C(C=CC4=C3N=CC=C4)C=C2
26345	93102-05-7	A		N-benzyl-1-methoxy-N-((trimethylsilyl)methyl)methanamine	COCN(CC1=CC=CC=C1)C[Si](C)(C)C
26507	136896-92-9	A		6-ethenylnaphthalen-2-ol	C=CC1=CC2=C(C=C1)C=C(C=C2)O