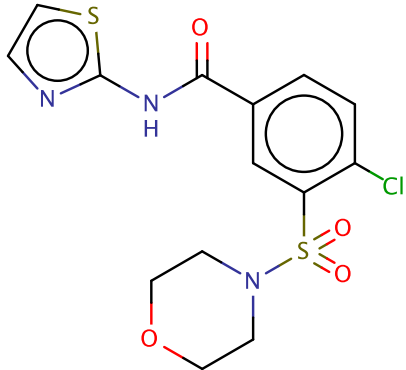
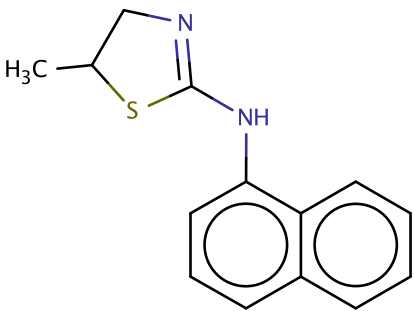
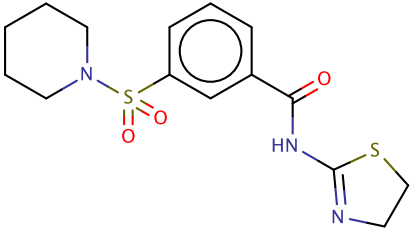
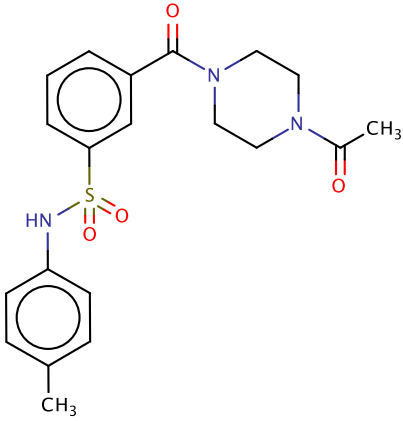
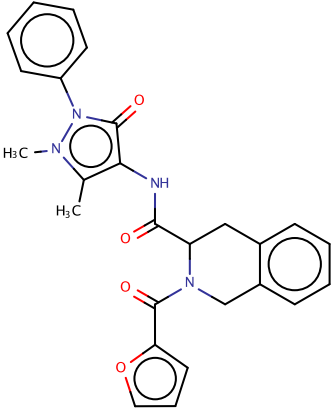


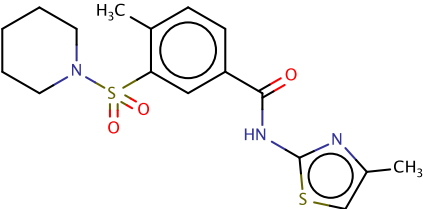
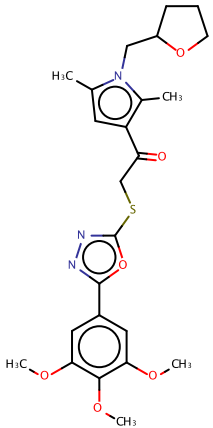
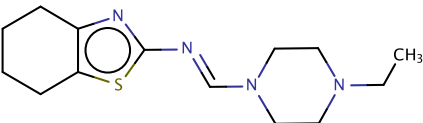
# Supplementary Materials: Pharmaceutical Machine Learning: Virtual High-Throughput Screens Identifying Promising and Economical Small Molecule Inhibitors of Complement Factor C1s.

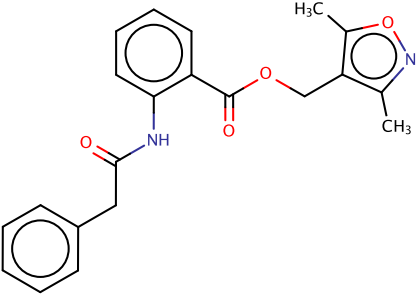
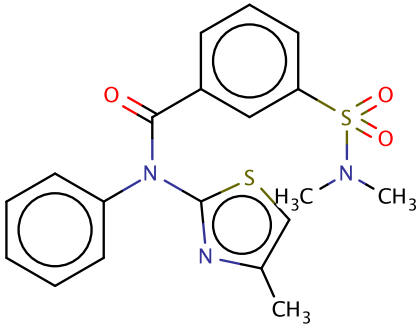
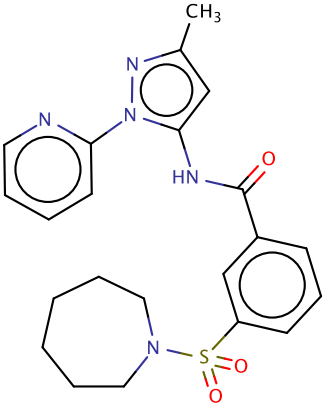
Jonathan Jun Feng Chen <sup>1,†</sup>, Lyndsey N. Schmucker <sup>2,†</sup> and Donald P. Visco Jr <sup>3,†\*</sup>

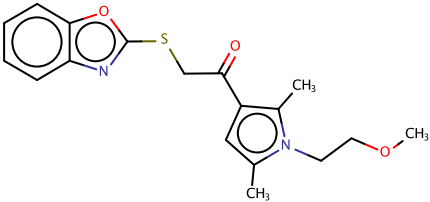
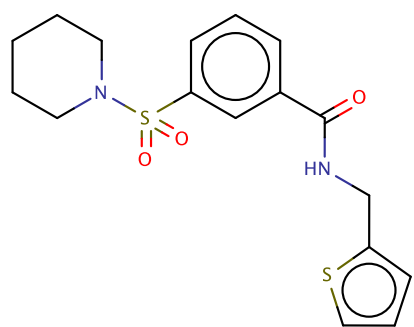
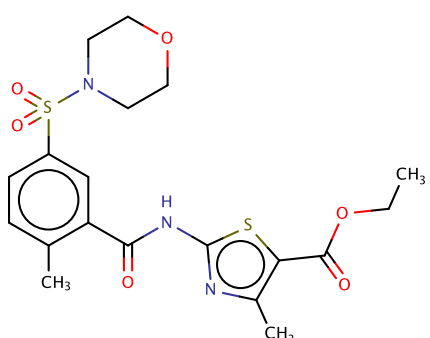
**Table S1.** Training Data. All data used to train the first-round classification and regression vHTS model. The same data is augmented with the *in vitro* experimental results and used to train the second-round classification and regression vHTS models. SID= PubChem Substance ID

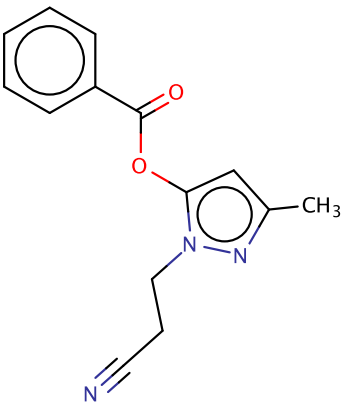
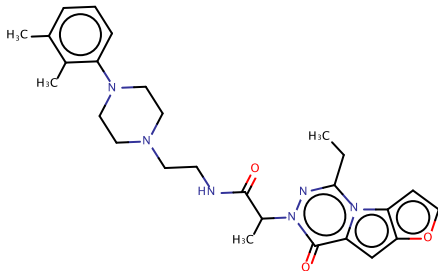
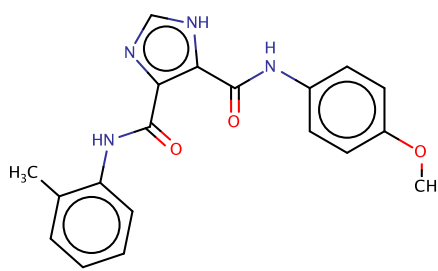
Structure	SID	Classification	Activity $IC_{50}[\mu M]$
	3711963	Inactive	N/A
	3712600	Inactive	N/A

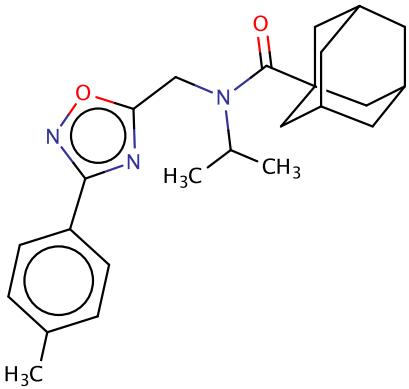
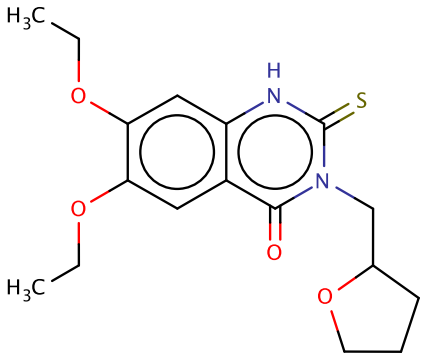
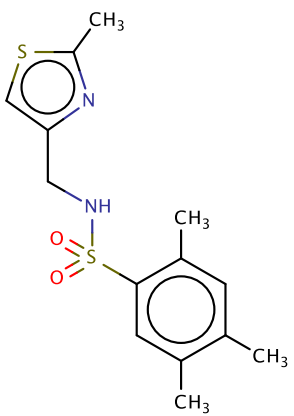
 <chem>C1CCN(C1)S(=O)(=O)Nc2ccc(cc2)C(=O)Nc3ccsc3</chem>	3712681	Inactive	N/A
 <chem>CC(=O)N1CCN(CC1)C(=O)c2ccc(cc2)NS(=O)(=O)Nc3ccc(C)cc3</chem>	3712850	Inactive	N/A
 <chem>Cc1nc2ccccc2n1C(C)Nc3ccccc3C(=O)N4CCN(CC4)C(=O)c5ccccc5C(=O)Nc6ccoc6</chem>	3713318	Inactive	N/A

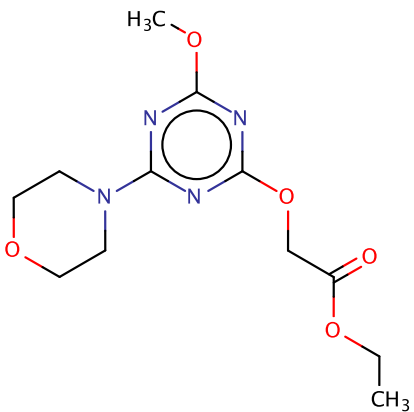
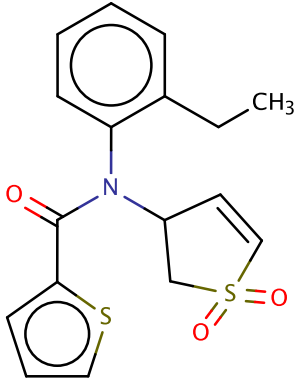
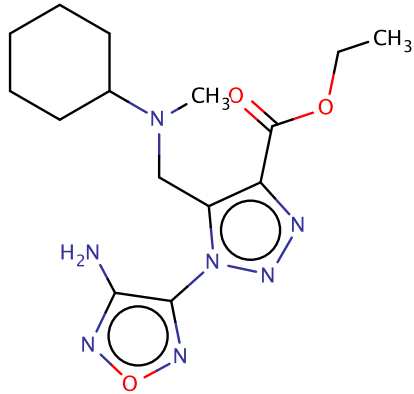
 <chem>Cc1nc(C)nc1NC(=O)c2ccc(C)cc2S(=O)(=O)N3CCCCC3</chem>	3713502	Inactive	N/A
 <chem>Cc1nc(C)nc1SCC(=O)Sc2ncnc2Oc3ccc(OC)c(OC)c3OC</chem>	3714494	Inactive	N/A
 <chem>Cc1nc2c(s1)CCCC2=Nc3ccncc3CC</chem>	3715220	Inactive	N/A

 <chem>CC1=CC=C(C=C1)NC(=O)c2ccccc2COC3=C(C)ON=C3</chem>	3715428	Inactive	N/A
 <chem>CC1=CN(C)C(S1)N(C)C(=O)c2ccccc2NS(=O)(=O)c3ccccc3</chem>	3715753	Inactive	N/A
 <chem>CC1=CC=C(C=C1)NC(=O)c2ccccc2NS(=O)(=O)N3CCCCC3</chem>	3715870	Inactive	N/A

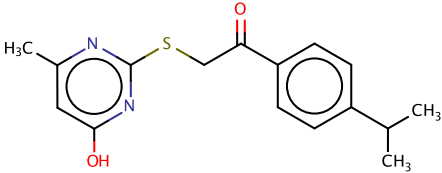
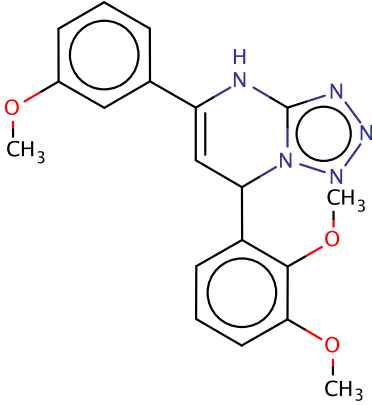
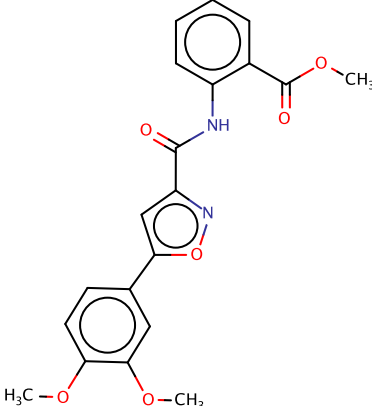
 <chem>Cc1c(C)nn(CCCS2c3ccccc3n2)C(=O)c1</chem>	3716178	Inactive	N/A
 <chem>CC1=CN=C(C1)NCC(=O)c2ccccc2S(=O)(=O)N3CCCCC3</chem>	3716847	Inactive	N/A
 <chem>CCOC(=O)c1c(C)nn(C1)c2c(C)ccc(S(=O)(=O)N3CCOCC3)c2</chem>	3717180	Inactive	N/A

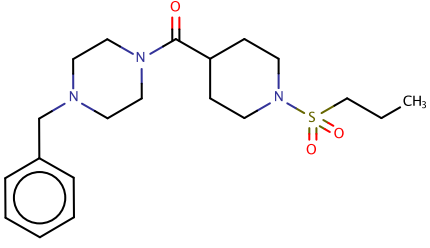
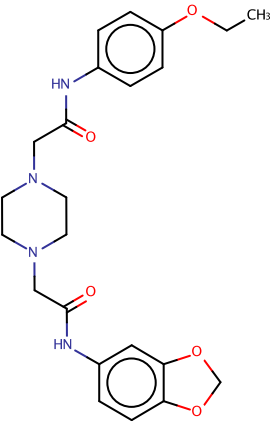
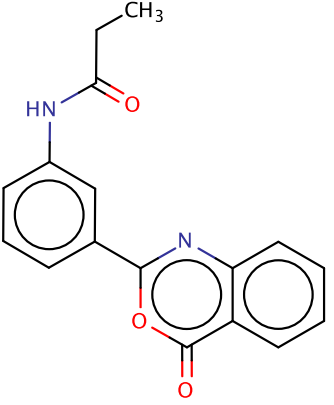
 <chem>CC1=CN(CCC#N)C1OC(=O)c2ccccc2</chem>	3717586	Active	2.14
 <chem>CC1=CN(C)C1C(=O)NCCC2CCN(Cc3ccccc3C)c23occc3</chem>	4240573	Inactive	N/A
 <chem>CC1=CN(C)C1C(=O)NC2=CC=C(OC)C=C2</chem>	4241692	Inactive	N/A

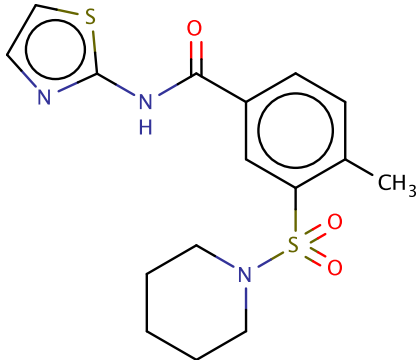
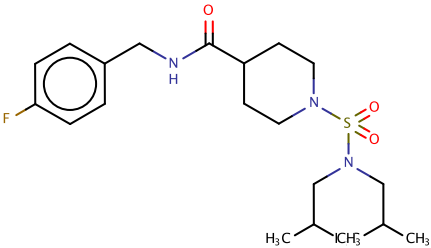
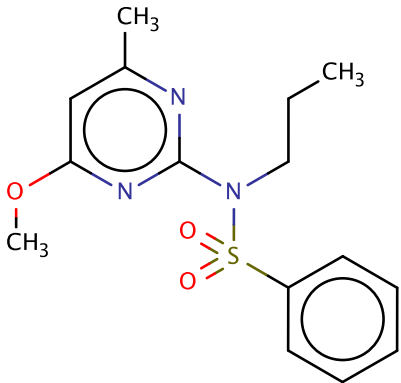
 <chem>Cc1ccc(cc1)c2nc3ocnc3n2N(C)C(=O)C45C6CC7C(C6)CC54</chem>	4242011	Inactive	N/A
 <chem>CCOC1=CC=C2C(=C1)N=C(S)N(C2=O)CC3OCC3</chem>	4242319	Inactive	N/A
 <chem>Cc1cc(C)c(C)c(C)c1S(=O)(=O)NCc2sc(C)n2</chem>	4243864	Inactive	N/A

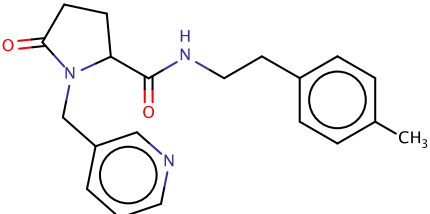
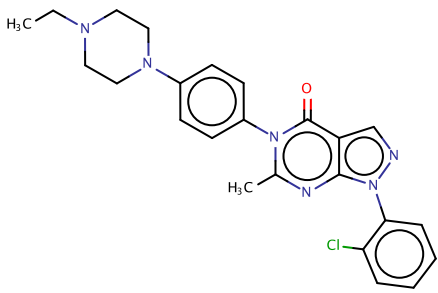
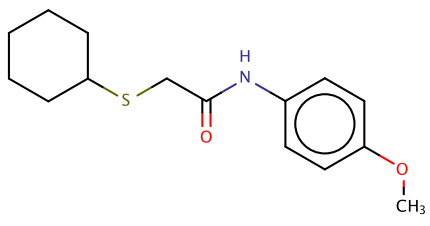
 <chem>CCOC(=O)COc1nc2nc(N3CCOCC3)c(O)c2n1</chem>	4244211	Inactive	N/A
 <chem>CC1=CC=C(C=C1)N(C2=CC=CS2)C3=CC=CS3=S</chem>	4245215	Inactive	N/A
 <chem>CCOC(=O)C1=CN2C(=N1)N=CN2C3=CC=CC=C3N4CCCCC4</chem>	4246549	Inactive	N/A

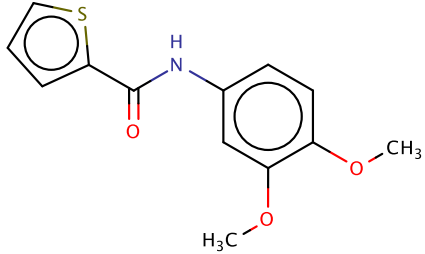
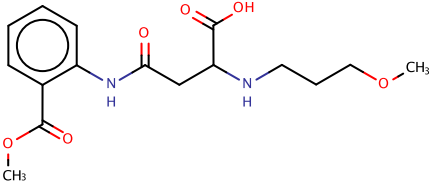
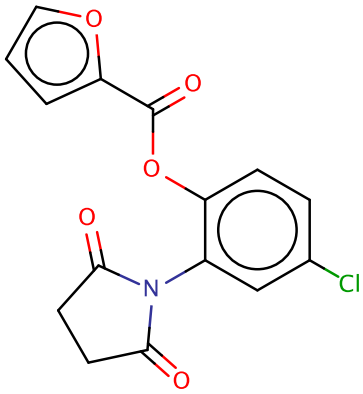


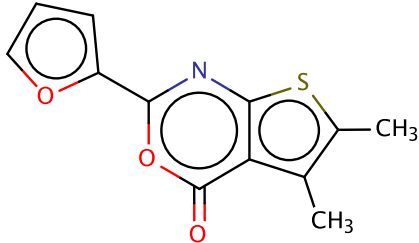
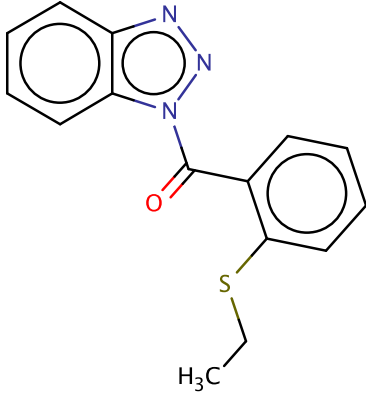
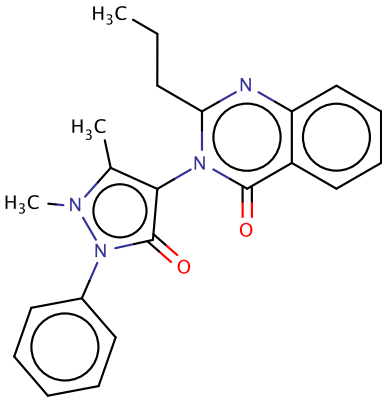
 <chem>CC1=CC=C(C=C1)C(=O)CS2=CC=C(O)N2C</chem>	4246823	Inactive	N/A
 <chem>CN1C=NC2=C1N=CN2C3=CC=C(OC)C=C3C4=CC=C(OC)C=C4</chem>	4246912	Inactive	N/A
 <chem>COC1=CC=C(C=C1)C2=NC3=CC=C(OC)C=C3N2C(=O)N4=CC=C(C=C4)C(=O)OC</chem>	4247384	Inactive	N/A

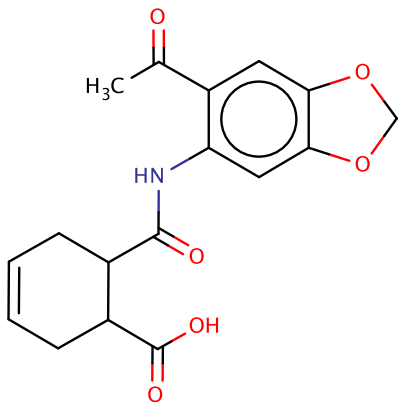
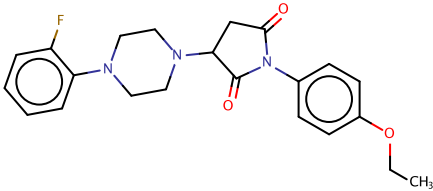
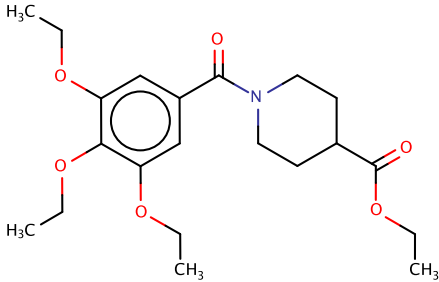
 <chem>CCCCS(=O)(=O)N1CCN(C1)C(=O)N2CCN(C2)Cc3ccccc3</chem>	4248033	Inactive	N/A
 <chem>CCOC1=CC=C(C=C1)NC(=O)CN2CCN(C2)CC(=O)Nc3cc4occc4c3</chem>	4248495	Inactive	N/A
 <chem>CCCC(=O)Nc1ccc(cc1)c2nc3ccccc3o2</chem>	4249007	Active	34.72

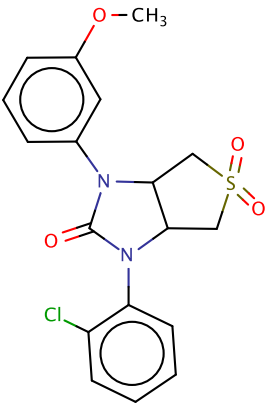
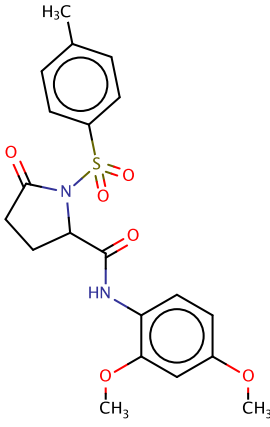
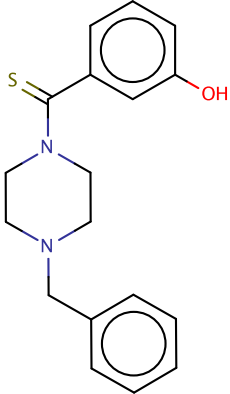
 <chem>Cc1ccc(cc1C(=O)Nc2cscn2)NS(=O)(=O)N3CCCCC3</chem>	4249302	Inactive	N/A
 <chem>CN1CC(C)CC1NS(=O)(=O)N2CCCC2C(=O)NCC3=CC=C(F)C=C3</chem>	4250394	Inactive	N/A
 <chem>CCN(CC)C1=NC(=C2C(=N1)OC)C=C2C3=CC=CC=C3S(=O)(=O)N3CCCC3</chem>	4251421	Inactive	N/A

 <chem>CC1=CC=C(C=C1)CCNC(=O)N2CCCC2C3=CC=NC=C3</chem>	4251548	Inactive	N/A
 <chem>CC1=CC=C(C=C1)N2CCN(C)CC2N3C(=O)N4C=CN(C)C4=N3C5=CC=C(C=C5)Cl</chem>	4251738	Inactive	N/A
 <chem>COc1ccc(NC(=O)CCSC2CCCCC2)cc1</chem>	4254582	Inactive	N/A

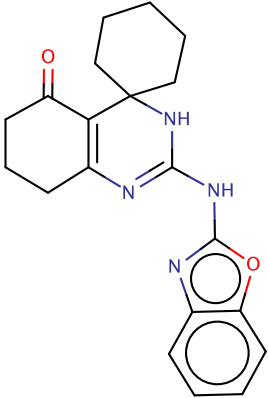
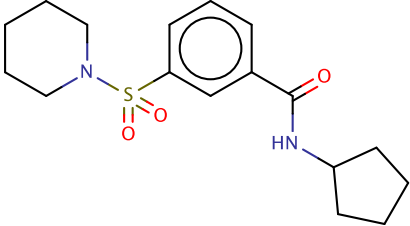
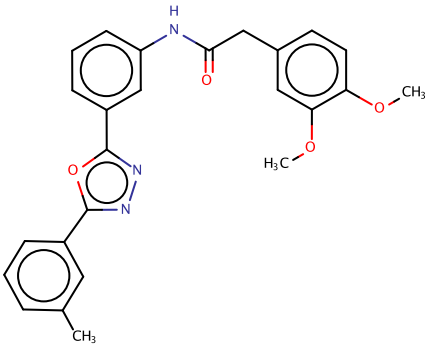
 <p>Chemical structure of 4-(3,4-dimethoxyphenyl)thiophene-2-carboxamide. It features a thiophene ring connected via a carbonyl group to an amide nitrogen, which is further attached to a benzene ring with methoxy groups at the 3 and 4 positions.</p>	4254762	Inactive	N/A
 <p>Chemical structure of N-(4-methoxybutyl)-2-(4-methoxyphenyl)acetamide. It consists of a benzamide core where the amide nitrogen is substituted with a 4-methoxybutyl group and the benzene ring has a methoxy group at the para position.</p>	4254843	Inactive	N/A
 <p>Chemical structure of N-(4-chlorophenyl)-2-(furan-2-yl)acetamide. It features a furan ring connected via a carbonyl group to an amide nitrogen, which is further attached to a benzene ring with a chlorine atom at the para position.</p>	4255208	Inactive	N/A

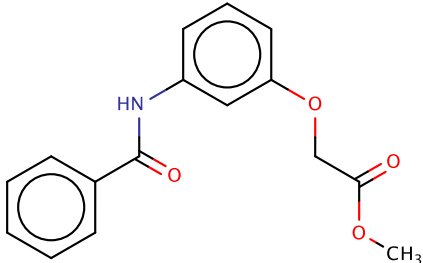
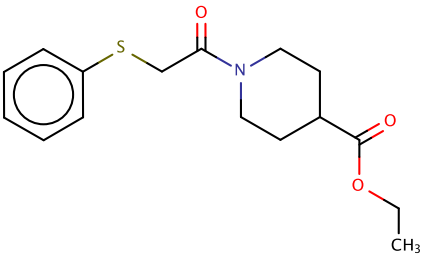
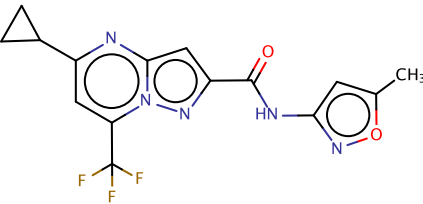
 <p>Chemical structure of a 5-methyl-2-(furan-2-yl)-1H-benzothiazol-4(1H)-one derivative. The structure features a benzothiazole core with a furan ring attached at the 2-position and two methyl groups at the 5-position.</p>	4255209	Inactive	N/A
 <p>Chemical structure of a 1H-benzotriazole-4-carbonyl derivative. The structure features a benzotriazole core with a carbonyl group at the 4-position and a propylsulfanyl group (-S-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>) at the 5-position.</p>	4255516	Active	30.99
 <p>Chemical structure of a complex benzothiazole derivative. The structure features a benzothiazole core with a carbonyl group at the 4-position, a propyl group at the 5-position, and a 1,3-dimethyl-5-phenyl-1H-imidazole-2-carbonyl group at the 2-position.</p>	4255537	Inactive	N/A

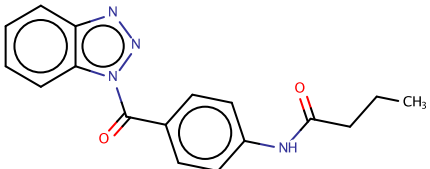
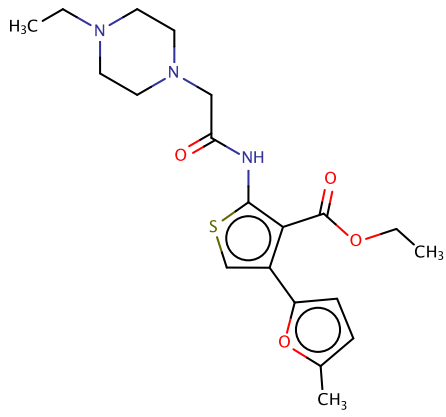
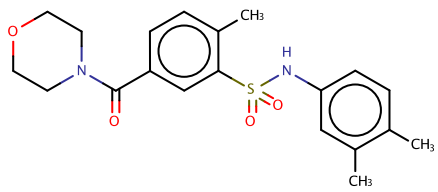
	4255573	Inactive	N/A
	4255800	Inactive	N/A
	4256088	Inactive	N/A

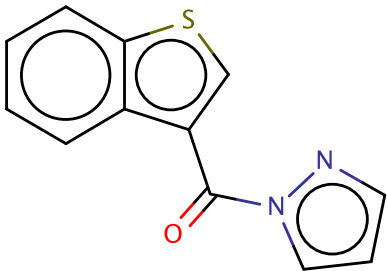
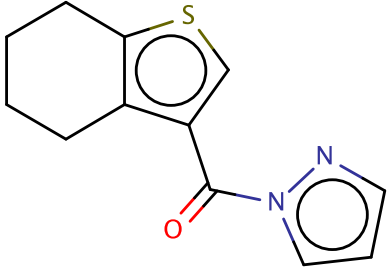
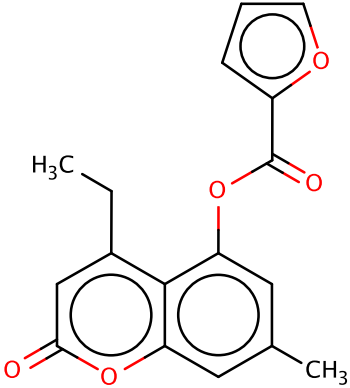
	4256347	Inactive	N/A
	4256651	Inactive	N/A
	4256969	Inactive	N/A

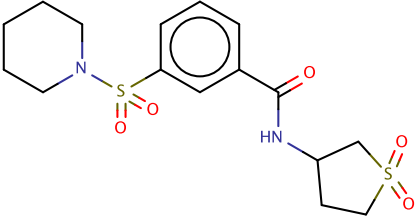
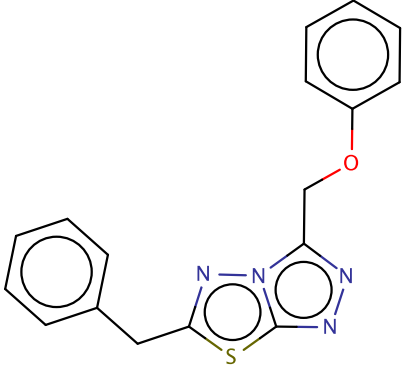
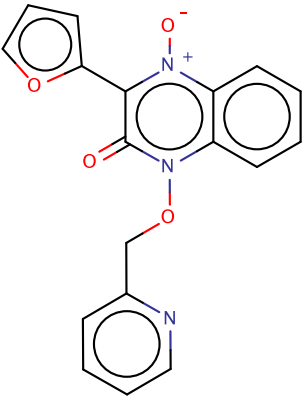


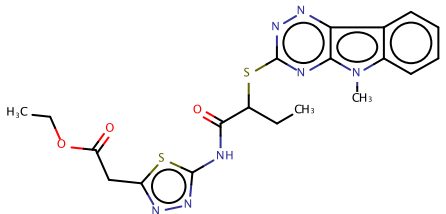
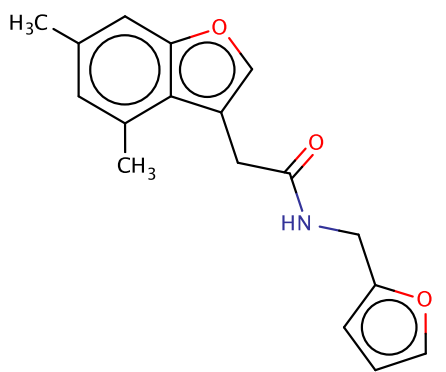
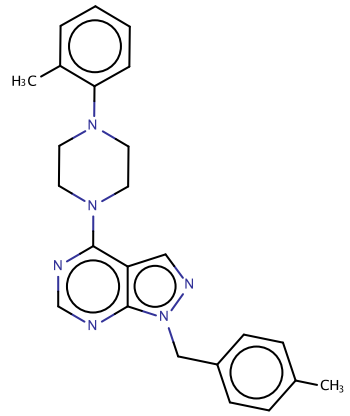
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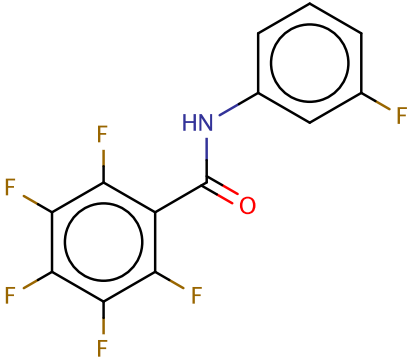
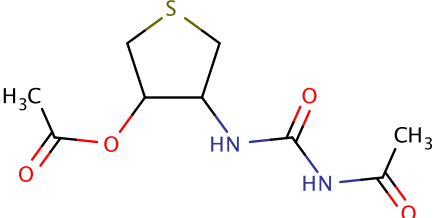
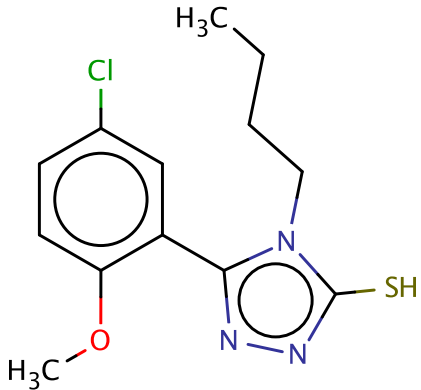
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 <chem>CCOC(=O)C1CCN(CC1)CCSc2ccccc2</chem>	4258729	Inactive	N/A
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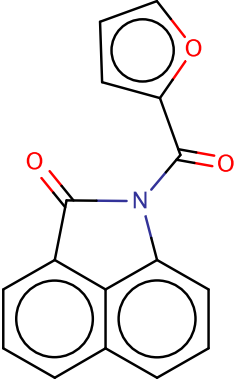
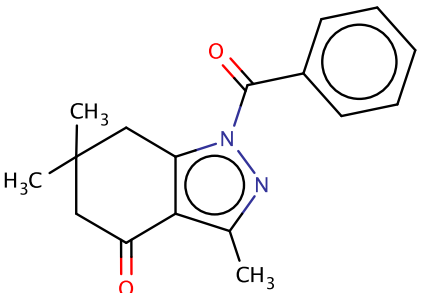
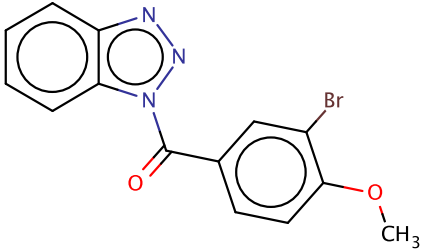
 <chem>CCCC(=O)Nc1ccc(cc1)C(=O)n2cnc3ccccc23</chem>	4258988	Active	0.38
 <chem>CCN1CCN(CC1)CC(=O)Nc2sc(C3C=CC(OC)C3)c2C(=O)OCC</chem>	4259517	Inactive	N/A
 <chem>CC1=CC=C(C=C1)S(=O)(=O)Nc2ccc(C)c(C)c2C(=O)N3CCCCO3</chem>	4259584	Inactive	N/A

 <p>Chemical structure of 2-(1H-indol-3-yl)propanoic acid imidazole salt. The structure shows an indole ring system with a propanoic acid chain attached to the 3-position, and an imidazole ring attached to the carboxylate group.</p>	4259744	Active	14.91
 <p>Chemical structure of 2-(1H-indolizino[1,2-b]pyridine-3-yl)propanoic acid imidazole salt. The structure shows an indolizino[1,2-b]pyridine ring system with a propanoic acid chain attached to the 3-position, and an imidazole ring attached to the carboxylate group.</p>	4260000	Active	3.83
 <p>Chemical structure of 2-(2-methyl-6-(methyl(methoxy)carbamoyl)phenyl)propanoic acid furfural salt. The structure shows a naphthalene ring system with a propanoic acid chain attached to the 2-position, a methyl group at the 6-position, and a methyl(methoxy)carbamoyl group at the 1-position. The propanoic acid chain is shown as a methyl group (H<sub>3</sub>C) and a carboxylate group (COO-). The furfural ring is shown as a furfural ring (furan-2-carbaldehyde).</p>	4260130	Active	10.1

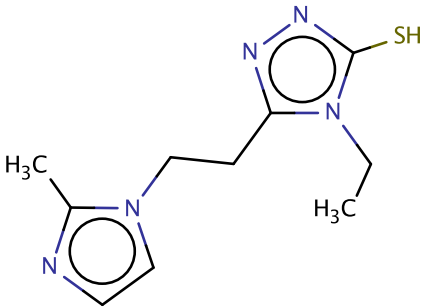
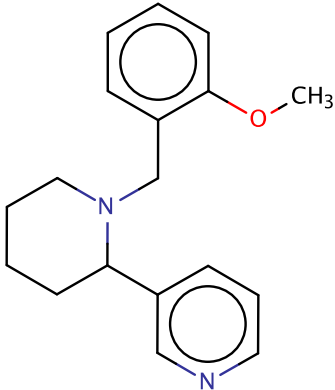
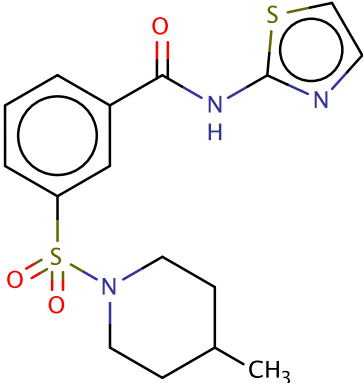
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	4261270	Inactive	N/A
	4261321	Active	37.87

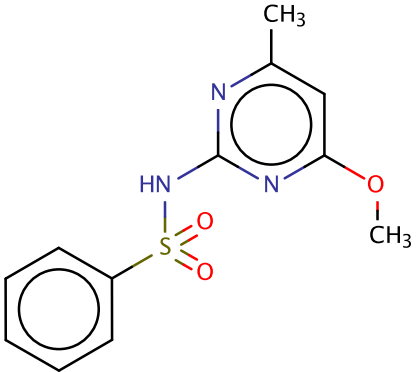
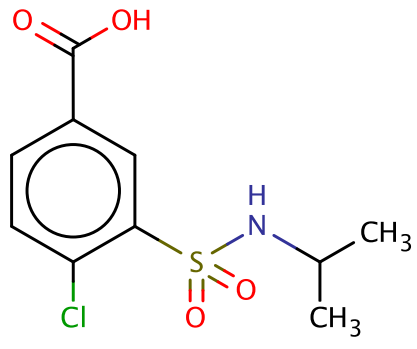
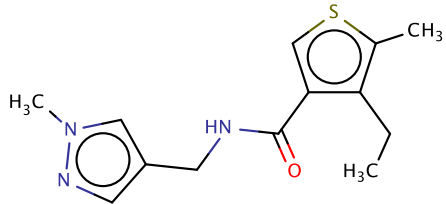
 <p>Chemical structure of compound 4261362: A complex molecule featuring a benzimidazole core. One nitrogen of the benzimidazole is substituted with a methyl group (CH<sub>3</sub>). The other nitrogen is linked via a sulfur atom to a propyl chain (CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>). The 2-position of the benzimidazole ring is substituted with a propyl chain (CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>) that is further linked to a thiazole ring. The thiazole ring is substituted at the 4-position with a propyl chain (CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>) that is linked to a carbonyl group (C=O), which is in turn linked to an ethoxy group (CH<sub>2</sub>-CH<sub>3</sub>).</p>	4261362	Inactive	N/A
 <p>Chemical structure of compound 4261432: A molecule consisting of a benzimidazole core. The benzimidazole ring is substituted at the 2-position with a propyl chain (CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>) that is linked to a carbonyl group (C=O). The carbonyl group is further linked to a methylene group (CH<sub>2</sub>), which is in turn linked to a nitrogen atom (NH). The nitrogen atom is further linked to a methylene group (CH<sub>2</sub>), which is in turn linked to a furan ring. The furan ring is substituted at the 2-position with a methyl group (CH<sub>3</sub>). The benzimidazole core is substituted at the 5-position with a methyl group (CH<sub>3</sub>) and at the 6-position with a methyl group (CH<sub>3</sub>).</p>	4261432	Inactive	N/A
 <p>Chemical structure of compound 4261564: A molecule consisting of a benzimidazole core. The benzimidazole ring is substituted at the 2-position with a methylene group (CH<sub>2</sub>), which is in turn linked to a methylene group (CH<sub>2</sub>), which is in turn linked to a benzene ring. The benzene ring is substituted at the 4-position with a methyl group (CH<sub>3</sub>). The benzimidazole core is substituted at the 5-position with a piperazine ring. The piperazine ring is further substituted at the 4-position with a benzene ring. The benzene ring is substituted at the 3-position with a methyl group (CH<sub>3</sub>).</p>	4261564	Inactive	N/A

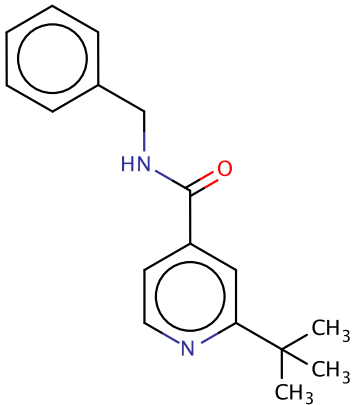
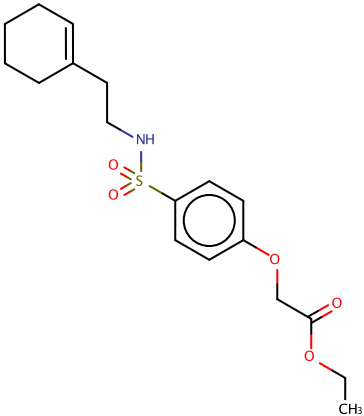
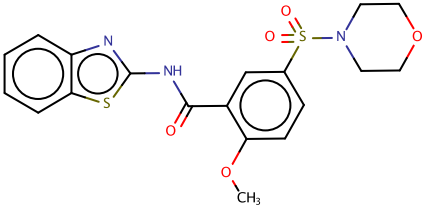
 <p>Chemical structure of 4-(2,3,4,5-tetrafluorophenyl)benzamide. It consists of a benzamide core where the para-substituted phenyl ring is replaced by a tetrafluorophenyl group.</p> <chem>NC(=O)c1ccc(cc1F)F</chem>	4261661	Inactive	N/A
 <p>Chemical structure of N-(2-(acetoxymethyl)thiolane)acetamide. It features a five-membered thiolane ring with a methyl acetate group at the 2-position and an acetamide group at the 3-position.</p> <chem>CC(=O)N[C@@H]1CCSC1OC(=O)C</chem>	4261818	Inactive	N/A
 <p>Chemical structure of 4-(4-chlorophenyl)-5-(3-methoxyphenyl)-1H-tetrazole. It consists of a 1H-tetrazole ring substituted at the 4-position with a 4-chlorophenyl group and at the 5-position with a 3-methoxyphenyl group.</p> <chem>COC1=CC=C(C=C1)c2nn[nH]c2C3=CC=C(C=C3)Cl</chem>	4261899	Inactive	N/A

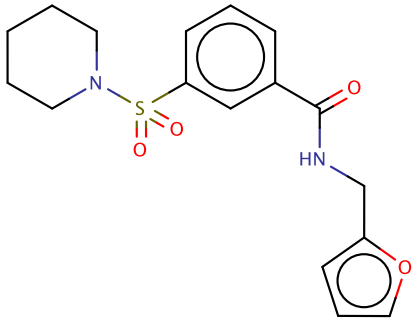
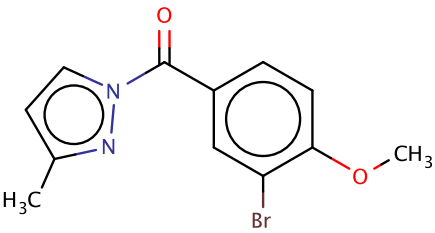
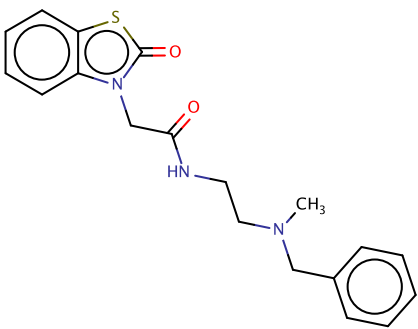
 <chem>O=C1C2=CC=CC=C2N1C(=O)C3=CC=CO3</chem>	4262775	Inactive	N/A
 <chem>CC1=C(C)N2C(=O)N1C(=O)C2C3=CC=CC=C3</chem>	4263151	Active	5.35
 <chem>COc1cc(Br)ccc1C(=O)N2C3=CC=CC=C3N2</chem>	4263449	Active	5.59

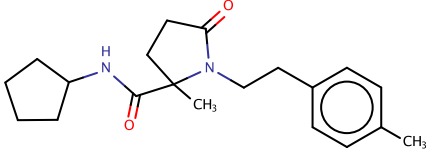
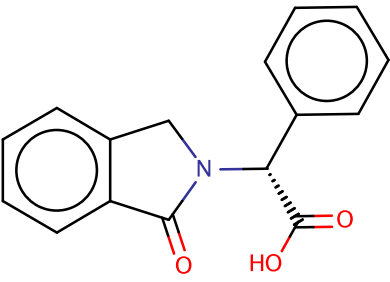
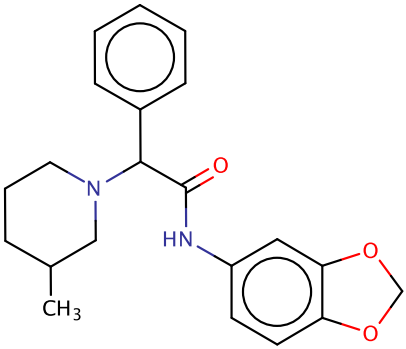


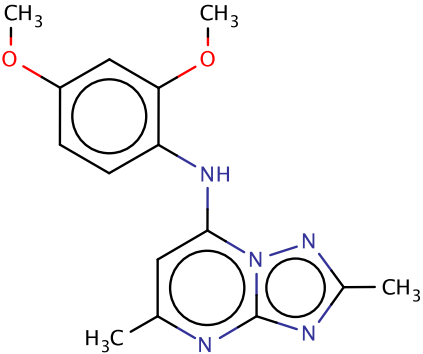
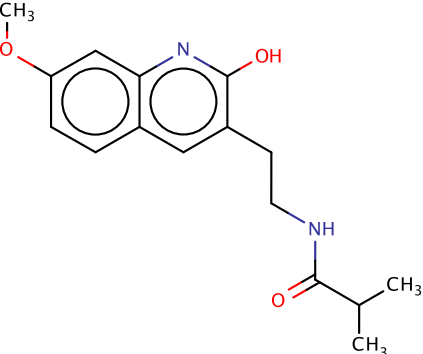
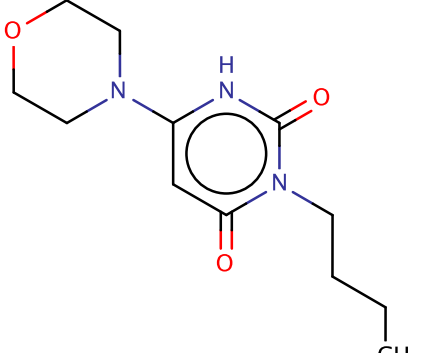
 <p>Chemical structure of 4-(2-methyl-1H-imidazol-3-yl)butan-1-yl-1H-thiazol-2-ylmethanethiol. It features a thiazole ring with a methyl group (H<sub>3</sub>C) and a thiol group (SH) at the 2-position, connected via a butyl chain to a 2-methyl-1H-imidazole ring.</p>	4263981	Inactive	N/A
 <p>Chemical structure of 1-(2-(4-methoxyphenyl)ethyl)piperidine. It consists of a piperidine ring substituted with a 2-(4-methoxyphenyl)ethyl group and a 2-pyridinyl group.</p>	4264329	Inactive	N/A
 <p>Chemical structure of 4-(4-(4-methylpiperidin-1-yl)sulfonylphenyl)thiazol-2-ylmethanethiol. It features a thiazole ring with a thiol group (SH) at the 2-position, connected via a methylene group to a carbonyl group, which is further connected to a 4-(4-methylpiperidin-1-yl)sulfonylphenyl group.</p>	4264469	Inactive	N/A

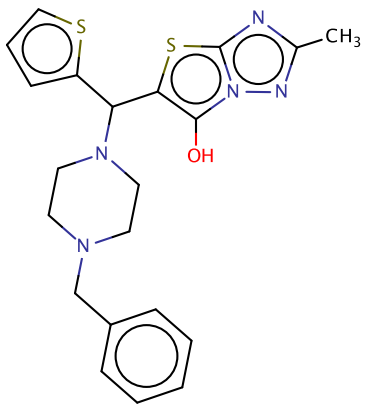
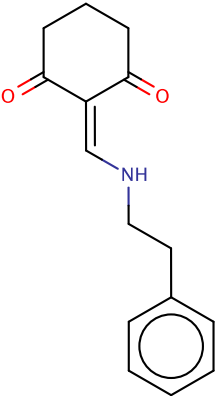
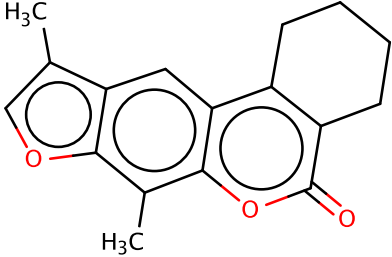
 <p>Chemical structure of 4-methyl-2-methoxy-N-(phenylsulfamoyl)pyridine. It features a pyridine ring with a methyl group (CH<sub>3</sub>) at the 4-position, a methoxy group (OCH<sub>3</sub>) at the 2-position, and a phenylsulfamoyl group (NH-SO<sub>2</sub>-C<sub>6</sub>H<sub>5</sub>) at the 1-position.</p>	4264491	Inactive	N/A
 <p>Chemical structure of 3-chloro-4-(propan-2-ylsulfamoyl)benzoic acid. It features a benzene ring with a carboxylic acid group (COOH) at the 1-position, a chlorine atom (Cl) at the 3-position, and a propan-2-ylsulfamoyl group (NH-SO<sub>2</sub>-CH(CH<sub>3</sub>)<sub>2</sub>) at the 4-position.</p>	4264513	Inactive	N/A
 <p>Chemical structure of N-(2-methyl-1,3,4-thiazol-5-yl)acetamide. It features a 1,3,4-thiazole ring with a methyl group (CH<sub>3</sub>) at the 2-position, and an acetamide group (NH-CO-CH<sub>3</sub>) at the 5-position.</p>	4265032	Inactive	N/A

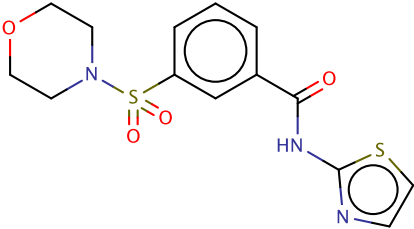
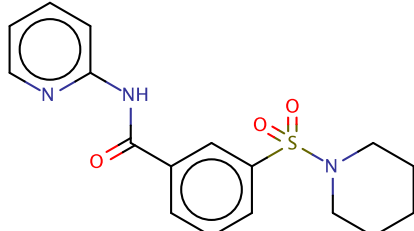
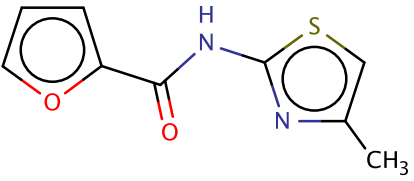
 <p>Chemical structure of 2-(2-(benzylamino)acetyl)pyridine-5-ylpropane-2,2-diol. It features a pyridine ring with a tert-butyl group at the 5-position and a 2-(benzylamino)acetyl group at the 2-position.</p>	4265342	Inactive	N/A
 <p>Chemical structure of 2-(2-(cyclohex-1-en-1-yl)ethyl)amino)ethyl 4-(ethoxycarbonyloxy)benzenesulfonate. It consists of a cyclohexene ring connected via a two-carbon chain to a secondary amine, which is further linked to a sulfonate group on a benzene ring. The benzene ring also has an ethyl ester group at the para position.</p>	4265617	Inactive	N/A
 <p>Chemical structure of 2-(2-(4-(methoxy)phenyl)pyridin-5-yl)propane-2,2-diol. It features a pyridine ring with a tert-butyl group at the 5-position and a 2-(4-methoxyphenyl)acetyl group at the 2-position.</p>	4265630	Inactive	N/A

	4265764	Inactive	N/A
	4265870	Inactive	N/A
	7965115	Inactive	N/A

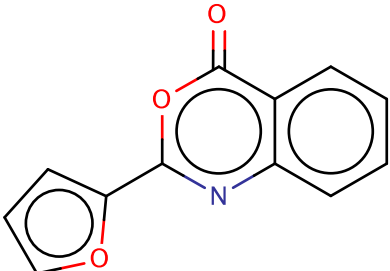
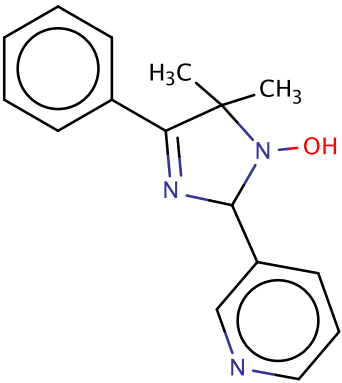
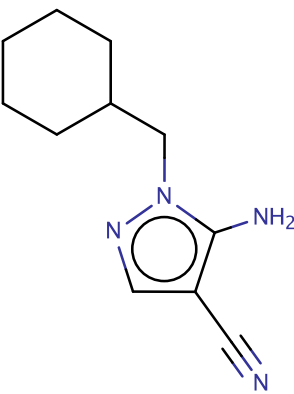
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 <chem>OC(=O)C[C@@H](c1ccccc1)c2c3ccccc3n2C(=O)c4ccccc4</chem>	7966122	Inactive	N/A
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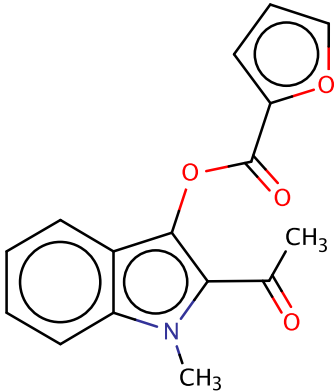
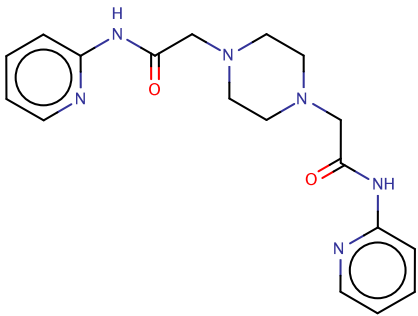
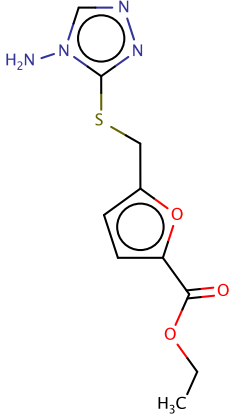
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 <chem>CC(C)C(=O)NCCCc1ccc2c(O)cnc2c1OC</chem>	7971047	Inactive	N/A
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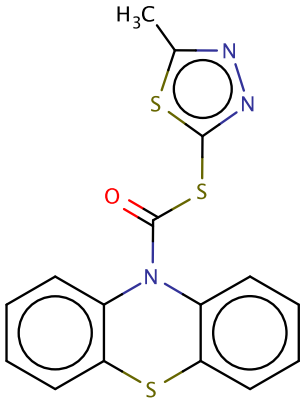
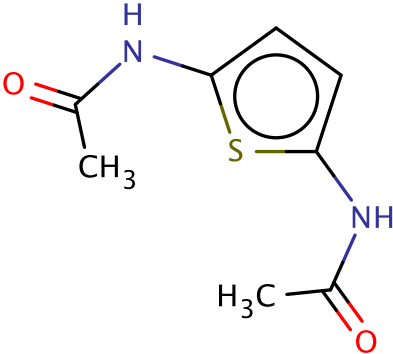
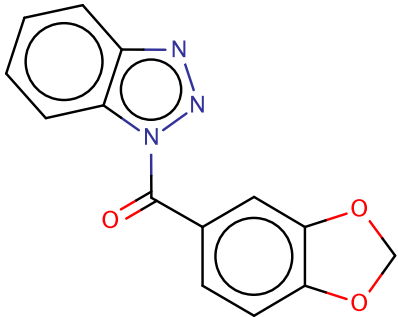
 <chem>Cc1nc2c(nc1O)CC3=CSC=C3N4CCN(CC4)Cc5ccccc5</chem>	7971311	Inactive	N/A
 <chem>O=C1CCCC(=O)N=C1NCCC2=CC=CC=C2</chem>	7972455	Inactive	N/A
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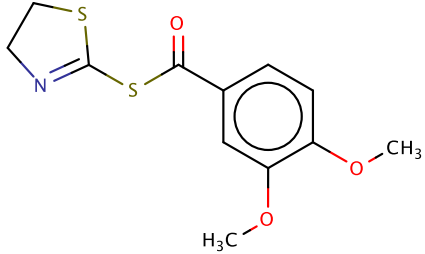
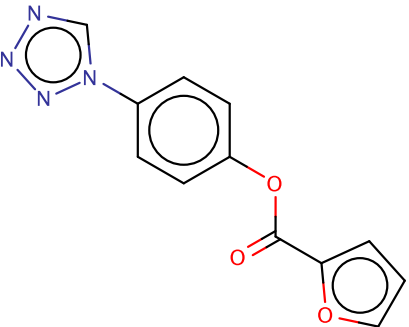
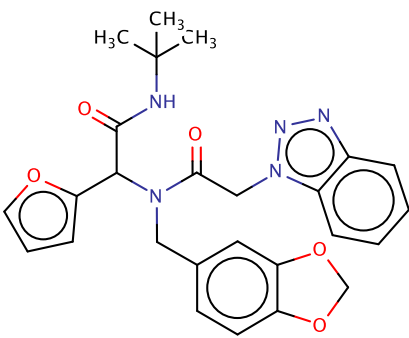
 <chem>C1CCN(C1)S(=O)(=O)NC(=O)c2ccc(cc2)NC3=CN=C(S3)</chem>	7972860	Inactive	N/A
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 <chem>CC1=CN=C(S1)NC(=O)c2ccoc2</chem>	7973018	Inactive	N/A

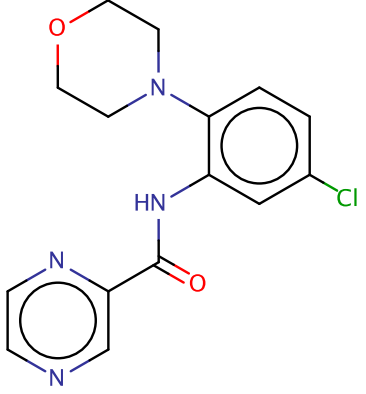
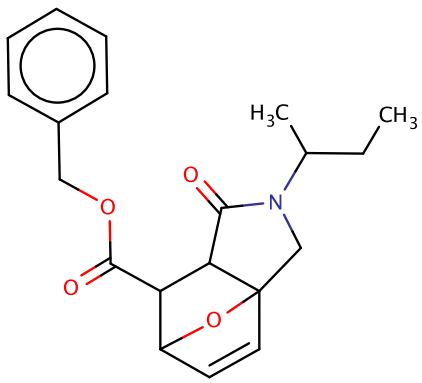
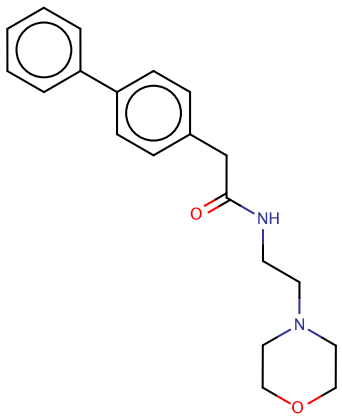


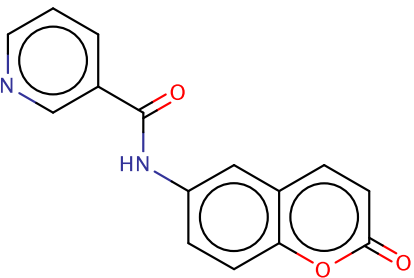
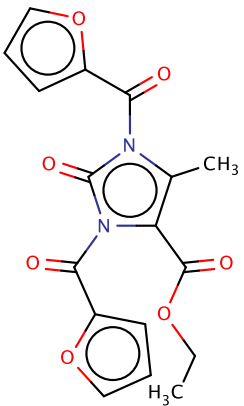
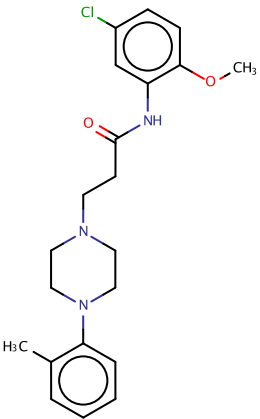
	7973318	Active	4.62
	7973389	Inactive	N/A
	7973713	Inactive	N/A

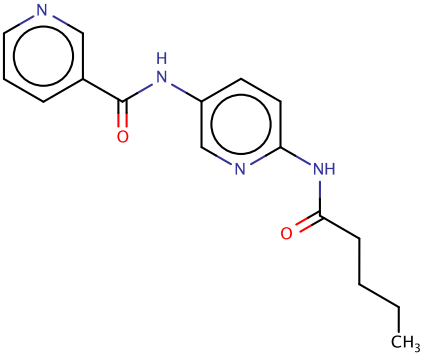
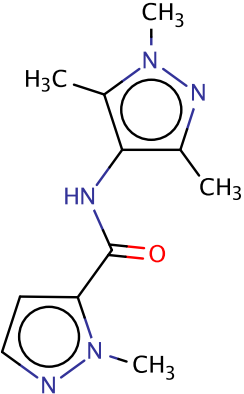
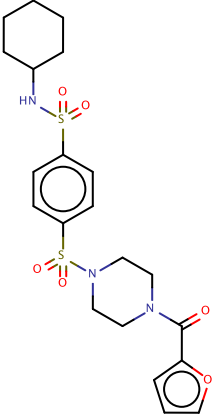
 <chem>CC(=O)c1c2c(c1)ccc3ccccc23OC(=O)C4=CC=CO4</chem>	7973891	Active	25.95
 <chem>C1=CN=C(C=C1)NC(=O)CN2CCN(CC2)C(=O)Nc3ccncc3</chem>	7973916	Inactive	N/A
 <chem>CCOC(=O)c1ccoc1CSc2nn[nH]2</chem>	7974410	Inactive	N/A

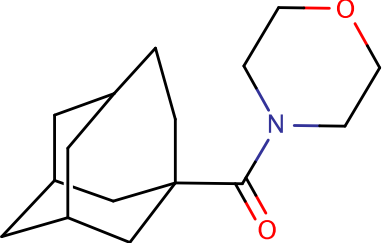
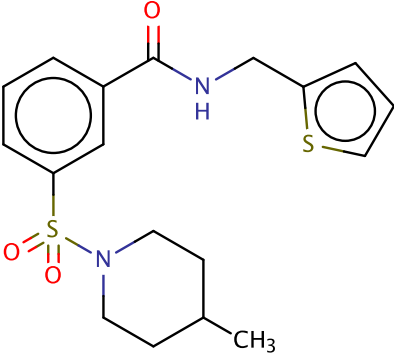
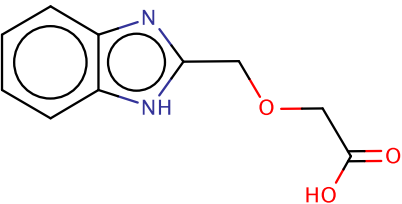
 <p>Chemical structure of 1-(2-methyl-1,3,4-thiazol-5-yl)sulfanylcarbonylpyrrolidine. It features a pyrrolidine ring connected via a carbonyl group to a sulfur atom, which is further connected to a 2-methyl-1,3,4-thiazole ring.</p>	7975174	Inactive	N/A
 <p>Chemical structure of N-(2-acetylphenyl)acetamide. It consists of a benzene ring with an acetamido group (-NHCOCH<sub>3</sub>) at the 1-position and an acetyl group (-COCH<sub>3</sub>) at the 2-position.</p>	7976940	Inactive	N/A
 <p>Chemical structure of 1-(1H-benzotriazol-5-yl)pyrrolidine-2-carbonyl-1,3-dioxolane. It features a benzotriazole ring system connected via a carbonyl group to a 1,3-dioxolane ring.</p>	7977382	Active	0.85

 <p>Chemical structure of 4-(3,4-dimethoxyphenyl)thiazolidine-2-thione. It features a thiazolidine-2-thione ring system connected to a benzene ring with methoxy groups at the 3 and 4 positions.</p>	7977978	Inactive	N/A
 <p>Chemical structure of 4-(1H-tetrazol-5-yl)phenyl 2-furancarboxylate. It consists of a tetrazole ring attached to a phenyl ring, which is further linked to a furan-2-carboxylate group.</p>	844155	Inactive	N/A
 <p>Chemical structure of a complex molecule. It features a central nitrogen atom bonded to a tert-butyl group, a furan-2-carboxylate group, a benzimidazole ring system, and a benzofuran ring system.</p>	844595	Inactive	N/A

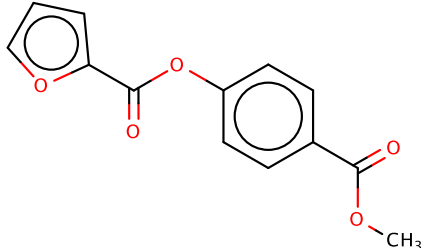
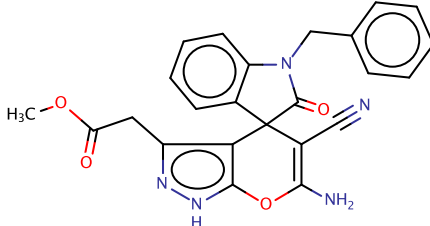
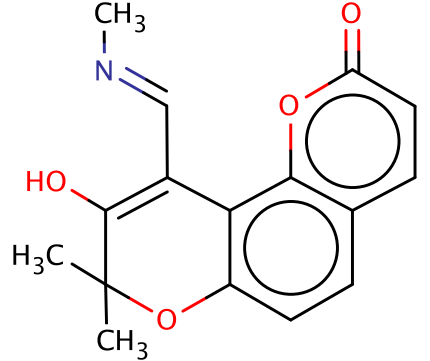
 <chem>C1=CN=C2C(=N1)C(=O)NC2c3ccc(Cl)cc3N4CCOCC4</chem>	845431	Inactive	N/A
 <chem>CC(C)C1CN(C1=O)C2=CC=CC=C2C(=O)OCC3=CC=CC=C3</chem>	846984	Inactive	N/A
 <chem>C1CCN(C1)CCNC(=O)CCc2ccc(cc2)-c3ccccc3</chem>	847433	Inactive	N/A

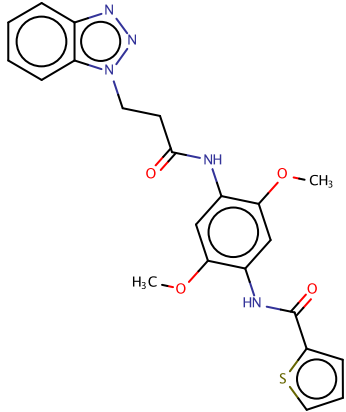
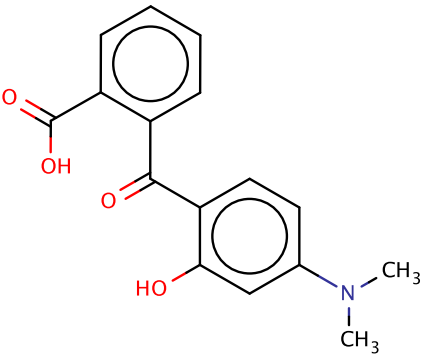
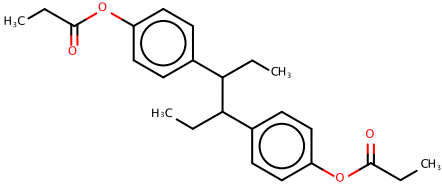
 <p>Chemical structure of a molecule featuring a pyridine ring connected via an amide bond to a naphthalene ring system. The naphthalene ring has a carbonyl group at the 1-position.</p>	847954	Inactive	N/A
 <p>Chemical structure of a complex bicyclic amide. It features a central five-membered ring with two nitrogen atoms, one of which is substituted with a methyl group (CH<sub>3</sub>). The structure includes a furan ring, a pyrrole ring, and a methylene group (H<sub>3</sub>C).</p>	848337	Active	8.54
 <p>Chemical structure of a piperazine derivative. The piperazine ring is substituted with a 4-chloro-3-methoxyphenyl group and a 4-methylphenyl group (H<sub>3</sub>C).</p>	848667	Inactive	N/A

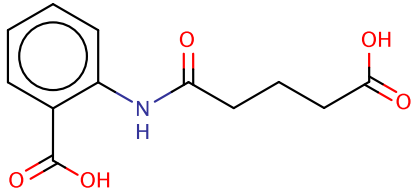
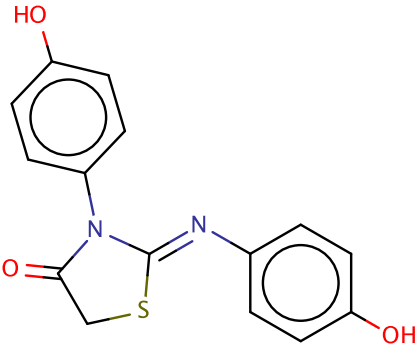
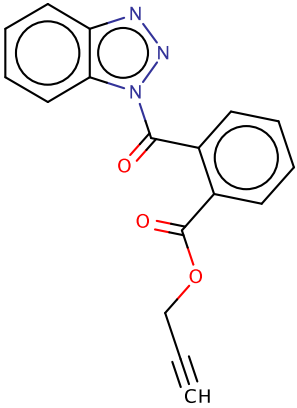
 <chem>CCCC(=O)Nc1cccnc1Nc2cccnc2C(=O)c3ccccn3</chem>	849229	Inactive	N/A
 <chem>Cc1c(C)nnc1NC(=O)c2c[nH]c2N</chem>	849832	Inactive	N/A
 <chem>O=C1C=CC=C1N2CCN(C2)S(=O)(=O)Nc3ccc(S(=O)(=O)Nc4ccccc4)cc3</chem>	850997	Inactive	N/A

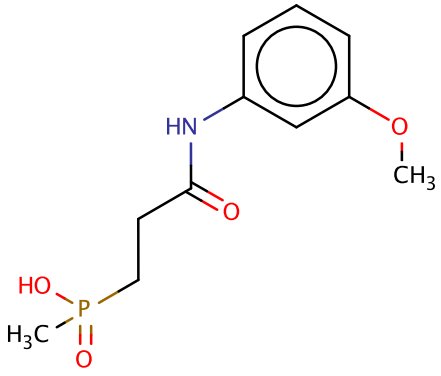
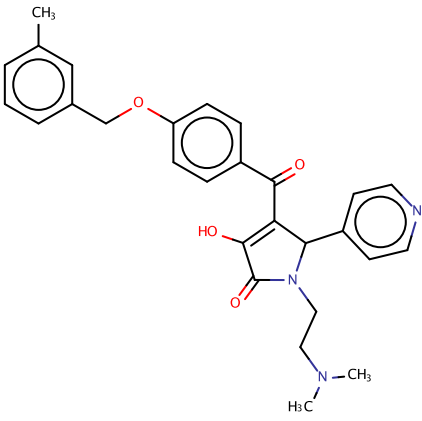
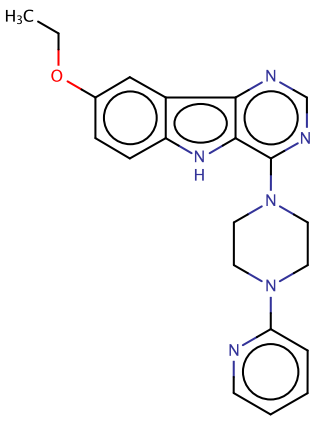
	851186	Inactive	N/A
	851359	Inactive	N/A
	851511	Inactive	N/A

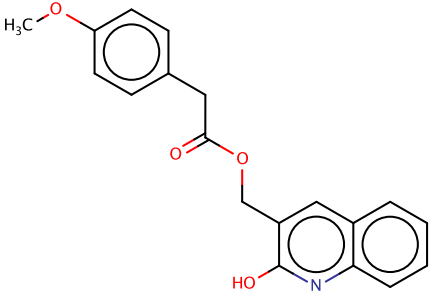
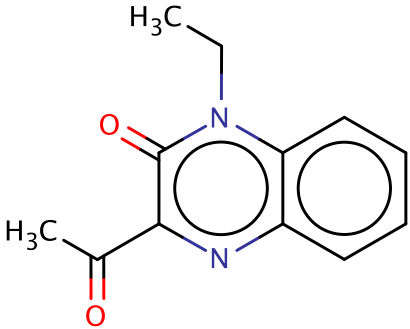
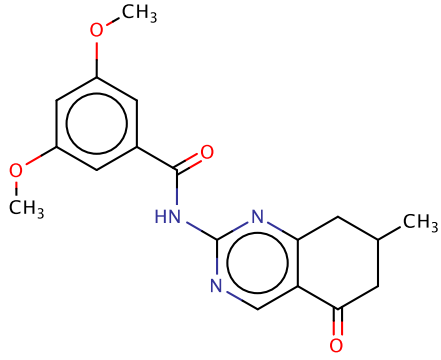


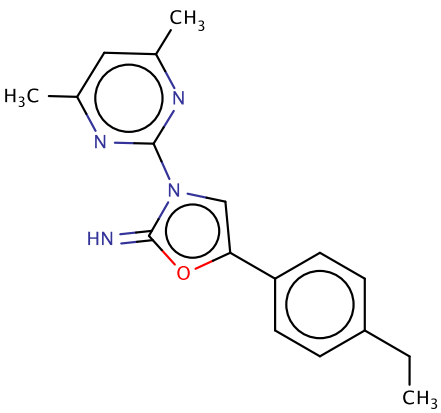
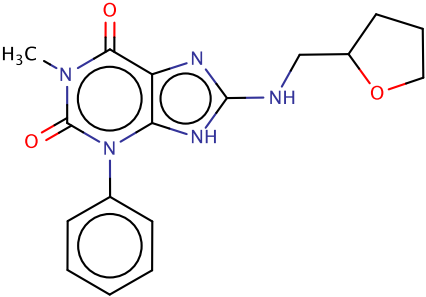
 <p>Chemical structure of methyl 4-(furan-2-ylmethoxy)benzoate. It consists of a furan ring connected via a methylene group to a methoxy group, which is further connected to a benzene ring. The benzene ring has a methyl ester group at the para position.</p>	851650	Active	17.07
 <p>Chemical structure of a complex heterocyclic molecule. It features a central benzimidazole-like core with a methyl ester group, a benzyl group, and a cyano group. The structure is highly substituted and contains multiple nitrogen and oxygen atoms.</p>	852054	Inactive	N/A
 <p>Chemical structure of a complex heterocyclic molecule. It features a central benzimidazole-like core with a methyl ester group, a methyl group, and a methyl group. The structure is highly substituted and contains multiple nitrogen and oxygen atoms.</p>	852663	Inactive	N/A

 <chem>COC1=CC(=C(C=C1)N(C)C)C(=O)NCCC2=CN3C=NC=C3N2</chem>	852804	Inactive	N/A
 <chem>CN(C)c1ccc(cc1C(=O)c2ccccc2C(=O)O)O</chem>	852974	Inactive	N/A
 <chem>CCCOC(=O)c1ccc(cc1C(CC)CC)c2ccc(cc2)C(=O)OCC</chem>	855949	Inactive	N/A

 <p>Chemical structure of 2-(2-(4-hydroxyphenyl)butanoyl)benzoic acid. It features a benzene ring with a carboxylic acid group (-COOH) at the 1-position and a butyrate ester group (-COOCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>-OH) at the 2-position.</p>	856413	Inactive	N/A
 <p>Chemical structure of 2-(4-hydroxyphenyl)-5-(4-hydroxyphenyl)thiazolidin-4(1H)-one. It consists of a thiazolidin-4(1H)-one ring system with a 4-hydroxyphenyl group attached to the nitrogen atom and a 5-(4-hydroxyphenyl) group attached to the 5-position of the ring.</p>	856534	Inactive	N/A
 <p>Chemical structure of 2-(2-(1H-benzotriazol-4-yl)phenyl)acetic acid ethyl ester. It features a benzotriazole ring system attached to a phenyl ring, which is further substituted with an ethyl ester group (-COOCH<sub>2</sub>CH<sub>3</sub>) and a terminal vinyl group (-CH=CH<sub>2</sub>).</p>	857178	Active	4.26

 <chem>COP(=O)(O)CCCNC(=O)c1cccc(OC)c1</chem>	859659	Inactive	N/A
 <chem>CN(C)CCN1C(=O)C(O)=C(C1=O)C(=O)c2ccc(OCC3=CC=C(C)C3)cc2</chem>	860659	Inactive	N/A
 <chem>CCOC1=CC=C2C(=C1)N=C3N=CN=C3N2N4CCN(CC4)N5=CC=CC=N5</chem>	862522	Inactive	N/A

 <p>Chemical structure of a molecule featuring a 4-methoxyphenyl group connected via a two-carbon chain to a carbonyl group, which is further linked to a methylene group attached to a quinoline ring system. The quinoline ring has a hydroxyl group at the 8-position.</p>	863457	Inactive	N/A
 <p>Chemical structure of a molecule consisting of a benzimidazole ring system substituted with a methyl group on the nitrogen at position 2 and an acetyl group at position 5.</p>	863929	Inactive	N/A
 <p>Chemical structure of a complex molecule featuring a quinoline ring system. It is substituted with a methyl group on the nitrogen at position 2, a methyl group at position 6, and a 3,5-dimethoxybenzoyl group at position 4.</p>	864485	Inactive	N/A

 <chem>Cc1cc(C)nc2n(c1)oc2c3ccc(C)cc3</chem>	865412	Inactive	N/A
 <chem>Cn1c(=O)c2nc(NC3CCOC3)c(=O)n2c1c4ccccc4</chem>	866130	Inactive	N/A