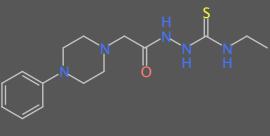
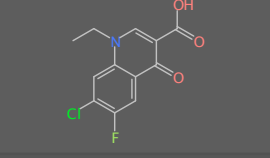
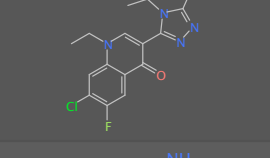
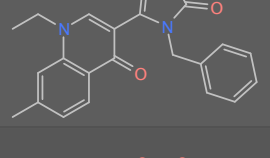
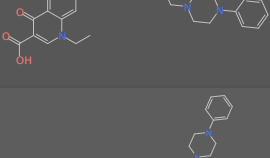
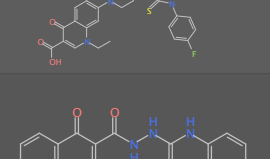
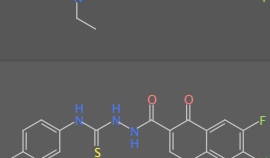
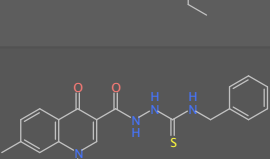

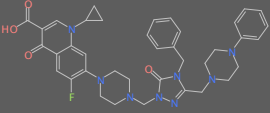
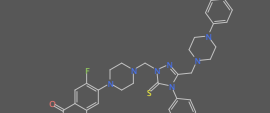
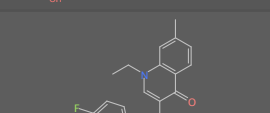
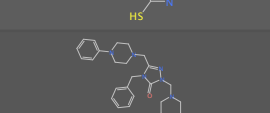
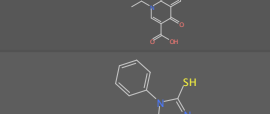
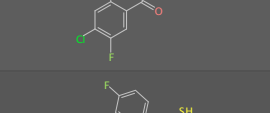
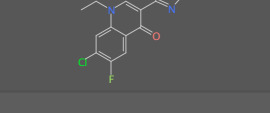
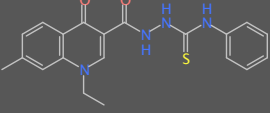
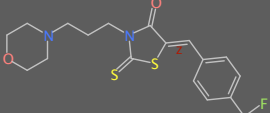
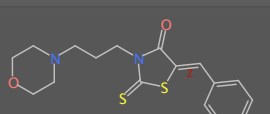
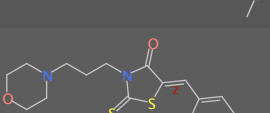


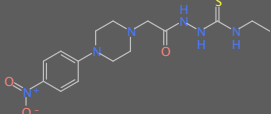
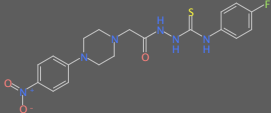
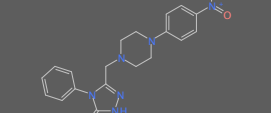
Structure	SMILES	Total Molwei...
	<chem>Cc3cc4N(CC)C=C(c2nnc(S)n2c1cccc1)C(=O)c4cc3</chem>	362.456
	<chem>CCNC(=S)NNC(=O)C2=CN(CC)c1cc(Cl)c(F)cc1C2=O</chem>	370.835
	<chem>S=C(NCc1cccc1)NNC(=O)C3=CN(CC)c2cc(Cl)c(F)cc2C3=O</chem>	432.906
	<chem>O=C(CN1CCN(CC1)c2cccc2)NNC(=S)Nc3cccc3</chem>	369.492
	<chem>Sc3nnc(CN1CCN(CC1)c2cccc2)n3CC</chem>	303.433
	<chem>O=C(CN1CCN(CC1)c2cccc2)NNC(=O)NCc3cccc3</chem>	367.451
	<chem>O=C(O)C2=CN(CC)c1cc(c(F)cc1C2=O)N7CCN(CN5N=C(CN3CCN(CC3)C)C)C5</chem>	682.823
	<chem>Sc4nnc(CN1CCN(CC1)c2cccc2)n4Cc3cccc3</chem>	365.504
	<chem>O=C(CN1CCN(CC1)c2cccc2)NNC(=S)Nc3ccc(F)cc3</chem>	387.482
	<chem>O=C3NN=C(CN1CCN(CC1)c2cccc2)N3c4cccc4</chem>	335.410
	<chem>S=C4OC(=NN4CN1CCN(CC1)c2cc3N(CC)C=C(C(=O)O)C(=O)c3cc2F)C1</chem>	607.709
	<chem>O=C(CN1CCN(CC1)c2cccc2)NNC(=S)NCc3cccc3</chem>	383.519

Structure	SMILES	Total Molwei...
	<chem>S=C3S\C(=C/c1ccccc1O)C(=O)N3CCCN2CCOCC2</chem>	364.489
	<chem>S=C3S\C(=C/c1c(F)cccc1Cl)C(=O)N3CCCN2CCOCC2</chem>	400.925
	<chem>Sc3nnc(C2=CN(CC)c1cc(C)ccc1C2=O)n3CC</chem>	314.412
	<chem>O=C4NN=C(CN1CCN(CC1)c2ccccc2)N4Cc3ccccc3</chem>	349.437
	<chem>CCNC(=S)NNC(=O)C2=CN(CC)c1cc(C)ccc1C2=O</chem>	332.427
	<chem>O=C(O)C3=CN(C1CC1)c2cc(c(F)cc2C3=O)N7CCN(CN6N=C(CN4CCN(C</chem>	646.790
	<chem>Sc4nnc(CN1CCN(CC1)c2ccccc2)n4c3ccccc3</chem>	351.477
	<chem>Cc3cc4N(CC)C=C(c2nnc(S)n2Cc1cccc1)C(=O)c4cc3</chem>	376.483
	<chem>O=C(O)C3=CN(C1CC1)c2cc(c(F)cc2C3=O)N8CCN(CN7N=C(CN4CCN(C</chem>	708.861
	<chem>S=C5OC(=NN5CN1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC</chem>	619.720
	<chem>Fc1ccc(cc1)n4c(CN2CCN(CC2)c3ccccc3)nnc4S</chem>	369.467
	<chem>Clc3cc4N(CC)C=C(c2nnc(S)n2Cc1cccc1)C(=O)c4cc3F</chem>	414.891

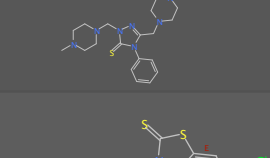
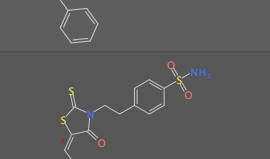

Structure	SMILES	Total Molwei...
	<chem>O=C(O)C3=CN(C1CC1)c2cc(c(F)cc2C3=O)N8CCN(CN6N=C(CN4CCN(C4)CC)CC6)CC8</chem>	694.834
	<chem>O=C(CN1CCN(CC1)c2ccccc2)NNC(=S)NCC</chem>	321.448
	<chem>O=C(O)C2=CN(CC)c1cc(Cl)c(F)cc1C2=O</chem>	269.658
	<chem>Sc3nnc(C2=CN(CC)c1cc(Cl)c(F)cc1C2=O)n3CC</chem>	352.820
	<chem>Cc1cc2c(cc1)C(=O)C(=CN2CC)C4=NNC(=O)N4Cc3ccccc3</chem>	360.416
	<chem>O=C(Nc1ccccc1)NNC(=O)C3=CN(CC)c2cc(Cl)c(F)cc2C3=O</chem>	402.812
	<chem>O=C(O)C2=CN(CC)c1cc(c(F)cc1C2=O)N7CCN(CN6N=C(CN3CCN(CC3)CC)CC6)CC7</chem>	696.850
	<chem>O=C(O)C2=CN(CC)c1cc(c(F)cc1C2=O)N6CCN(CN5N=C(CN3CCN(CC3)CC)CC5)CC6</chem>	634.779
	<chem>O=C(O)C2=CN(CC)c1cc(c(F)cc1C2=O)N7CCN(CN5N=C(CN3CCN(CC3)CC)CC5)CC7</chem>	700.813
	<chem>Fc1ccc(cc1)NC(=S)NNC(=O)C3=CN(CC)c2cc(C)ccc2C3=O</chem>	398.461
	<chem>Fc1ccc(cc1)NC(=S)NNC(=O)C3=CN(CC)c2cc(Cl)c(F)cc2C3=O</chem>	436.869
	<chem>S=C(NCc1ccccc1)NNC(=O)C3=CN(CC)c2cc(C)ccc2C3=O</chem>	394.498

Structure	SMILES	Total Molwei...
	<chem>O=C(O)C3=CN(C1CC1)c2cc(c(F)cc2C3=O)N8CCN(CN7N=C(CN4CCN(C</chem>	692.794
	<chem>O=C(O)C3=CN(C1CC1)c2cc(c(F)cc2C3=O)N8CCN(CN6N=C(CN4CCN(C</chem>	712.824
	<chem>Cc3cc4N(CC)C=C(c2nnc(S)n2c1ccc(F)cc1)C(=O)c4cc3</chem>	380.446
	<chem>O=C(O)C2=CN(CC)c1cc(c(F)cc1C2=O)N7CCN(CN6N=C(CN3CCN(CC3)</chem>	680.783
	<chem>Clc3cc4N(CC)C=C(c2nnc(S)n2c1cccc1)C(=O)c4cc3F</chem>	400.864
	<chem>Clc3cc4N(CC)C=C(c2nnc(S)n2c1ccc(F)cc1)C(=O)c4cc3F</chem>	418.854
	<chem>S=C3S\C=C/c1ccc(F)c(Br)c1)C(=O)N3CCCN2CCOCC2</chem>	445.376
	<chem>S=C(Nc1cccc1)NNC(=O)C3=CN(CC)c2cc(C)ccc2C3=O</chem>	380.471
	<chem>S=C3S\C=C/c1ccc(cc1)C(F)(F)F)C(=O)N3CCCN2CCOCC2</chem>	416.487
	<chem>S=C3S\C=C/c1ccc(OC)cc1)C(=O)N3CCCN2CCOCC2</chem>	378.516
	<chem>S=C3S\C=C/c1ccc(cc1)[N+][[O-])=O)C(=O)N3CCCN2CCOCC2</chem>	393.487
	<chem>S=C3S\C=C/c1ccc(Cl)cc1Cl)C(=O)N3CCCN2CCOCC2</chem>	417.380

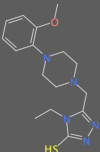
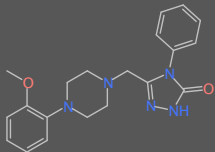
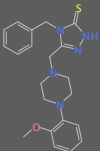
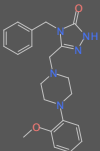
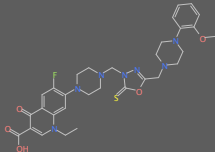
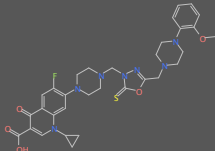
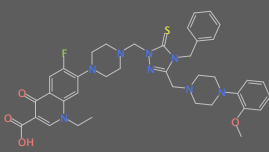
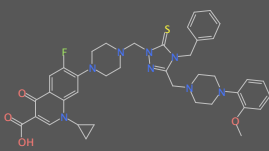
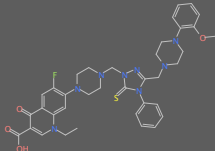
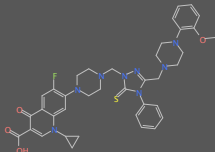
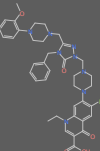
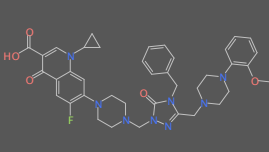
Structure	SMILES	Total Molwei...
	<chem>S=C3S\C(=C/c1cccnc1)C(=O)N3CCCN2CCOCC2</chem>	349.478
	<chem>S=C3S\C(=C/c1ccncc1)C(=O)N3CCCN2CCOCC2</chem>	349.478
	<chem>S=C3S\C(=C/c1ccccn1)C(=O)N3CCCN2CCOCC2</chem>	349.478
	<chem>S=C3S\C(=C/c1ccc(F)cc1)C(=O)N3CCCN2CCOCC2</chem>	366.480
	<chem>S=C3S\C(=C/c1ccc(OC)c(O)c1)C(=O)N3CCCN2CCOCC2</chem>	394.515
	<chem>S=C3S\C(=C/c1c(Cl)cccc1Cl)C(=O)N3CCCN2CCOCC2</chem>	417.380
	<chem>S=C3S\C(=C/c1ccccc1F)C(=O)N3CCCN2CCOCC2</chem>	366.480
	<chem>S=C3S\C(=C/c1cccc(F)c1)C(=O)N3CCCN2CCOCC2</chem>	366.480
	<chem>S=C1OC(=NN1CCC#N)CN2CCN(C)CC2</chem>	267.356
	<chem>S=C1OC(=NN1CCC#N)CN2CCN(CC2)c3ccccc3OC</chem>	359.453
	<chem>S=C3S\C(=C/c1cc(Br)ccc1F)C(=O)N3CCCN2CCOCC2</chem>	445.376
	<chem>O=C(Nc1cccc1)NNC(=O)C3=CN(CC)c2cc(C)ccc2C3=O</chem>	364.404

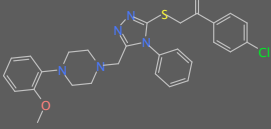
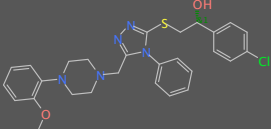
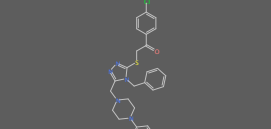
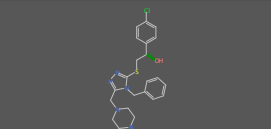
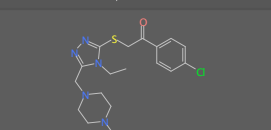
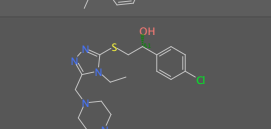
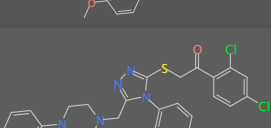
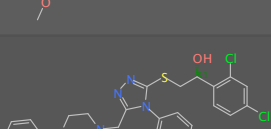
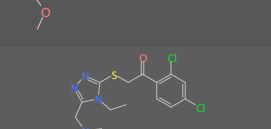
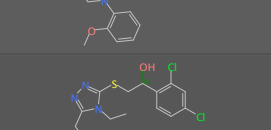
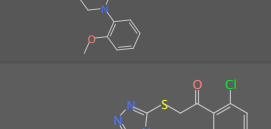
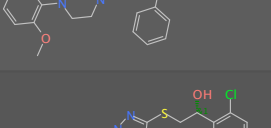
Structure	SMILES	Total Molwei...
	<chem>O=C(CN1CCN(CC1)c2ccccc2)NNC(=O)Nc3ccccc3</chem>	353.425
	<chem>S=C(Nc1ccccc1)NNC(=O)C3=CN(CC)c2cc(Cl)c(F)cc2C3=O</chem>	418.879
	<chem>O=C(CN1CCN(CC1)c2ccc(cc2)[N+](=[O-])=O)NN</chem>	279.299
	<chem>O=C(CN1CCN(CC1)c2ccc(cc2)[N+](=[O-])=O)NNC(=O)Nc3ccccc3</chem>	398.422
	<chem>O=C(CN1CCN(CC1)c2ccc(cc2)[N+](=[O-])=O)NNC(=S)NCC</chem>	366.445
	<chem>O=C(CN1CCN(CC1)c2ccc(cc2)[N+](=[O-])=O)NNC(=S)NCc3ccccc3</chem>	428.516
	<chem>O=C(CN1CCN(CC1)c2ccc(cc2)[N+](=[O-])=O)NNC(=O)NCc3ccccc3</chem>	412.449
	<chem>O=C(CN1CCN(CC1)c2ccc(cc2)[N+](=[O-])=O)NNC(=S)Nc3ccccc3</chem>	414.489
	<chem>O=C(CN1CCN(CC1)c2ccc(cc2)[N+](=[O-])=O)NNC(=S)Nc3ccc(F)cc3</chem>	432.479
	<chem>[O-][N+](=O)c1ccc(cc1)N4CCN(CC3=NNC(=O)N3Cc2ccccc2)CC4</chem>	394.434
	<chem>[O-][N+](=O)c1ccc(cc1)N4CCN(CC2=NNC(=O)N2c3ccccc3)CC4</chem>	380.407
	<chem>[O-][N+](=O)c1ccc(cc1)N4CCN(Cc3nnc(S)n3Cc2ccccc2)CC4</chem>	410.501

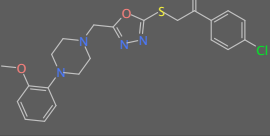
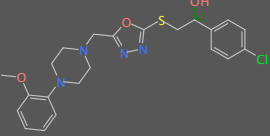
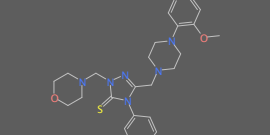
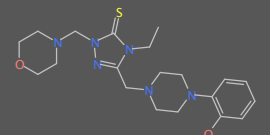
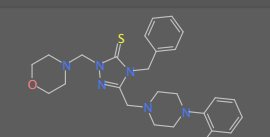
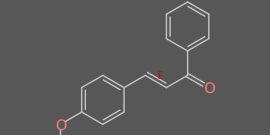
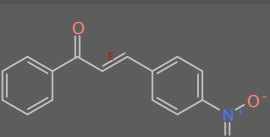
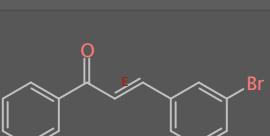
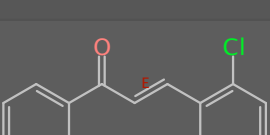
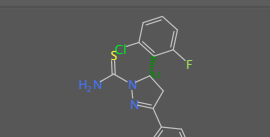
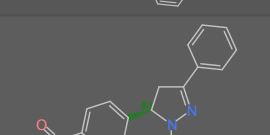
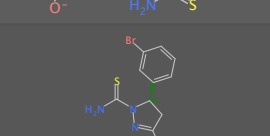
Structure	SMILES	Total Molwei...
	<chem>[O-][N+](=O)c1ccc(cc1)N4CCN(Cc2nnc(S)n2c3ccccc3)CC4</chem>	396.474
	<chem>[O-][N+](=O)c1ccc(cc1)N3CCN(Cc2nnc(S)n2CC)CC3</chem>	348.430
	<chem>[O-][N+](=O)c1ccc(cc1)N4CCN(Cc2nnc(S)n2c3ccc(F)cc3)CC4</chem>	414.464
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC6=NN(CN3CCN(CC3)c4cc5N(C</chem>	679.776
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC7=NN(CN3CCN(CC3)c4cc5N(C</chem>	691.787
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC7=NN(CN3CCN(CC3)c4cc5N(C</chem>	741.847
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC8=NN(CN3CCN(CC3)c4cc5N(C</chem>	753.858
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC6=NN(CN3CCN(CC3)c4cc5N(C</chem>	727.820
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC7=NN(CN3CCN(CC3)c4cc5N(C</chem>	739.831
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC6=NN(CN3CCN(CC3)c4cc5N(C</chem>	745.810
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC7=NN(CN3CCN(CC3)c4cc5N(C</chem>	757.821
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC7=NN(CN3CCN(CC3)c4cc5N(C</chem>	725.780

Structure	SMILES	Total Molwei...
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC8=NN(CN3CCN(CC3)c4cc5N(C</chem>	737.791
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC6=NN(CN3CCN(CC3)c4ccccc4)</chem>	584.747
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC5=NN(CN3CCN(CC3)c4ccccc4)</chem>	522.676
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC5=NN(CN3CCN(CC3)c4ccccc4)</chem>	570.720
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC4=NN(CN3CCN(C)CC3)C(=S)N</chem>	460.605
	<chem>[O-][N+](=O)c1ccc(cc1)N2CCN(CC2)CC4=NN(CN3CCN(C)CC3)C(=S)N</chem>	508.649
	<chem>S=C3S/C(=C/c1c(F)cccc1Cl)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	456.969
	<chem>S=C3S/C(=C/c1cccnc1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	405.522
	<chem>S=C3S/C(=C/c1cccc1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	404.534
	<chem>S=C3S/C(=C/c1ccc(OC)cc1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	434.560
	<chem>S=C3S/C(=C/c1ccc(Cl)cc1Cl)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	473.424
	<chem>S=C3S/C(=C/c1cccc1F)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	422.524

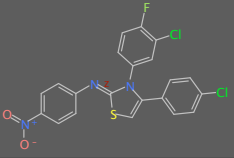
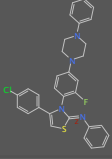
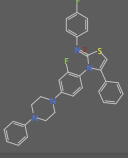
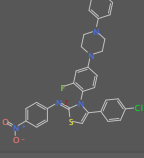
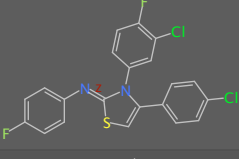
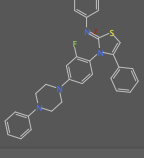
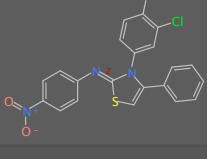
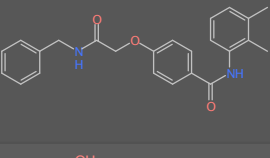
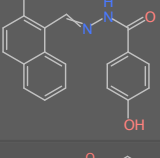
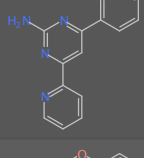
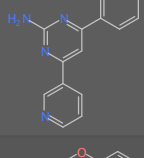
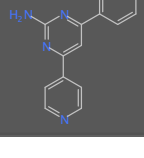
Structure	SMILES	Total Molwei...
	<chem>S=C3S/C(=C/c1ccc(cc1)C(F)(F)F)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	472.531
	<chem>S=C3S/C(=C/c1c(Cl)cccc1Cl)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	473.424
	<chem>S=C3S/C(=C/c1ccc(F)cc1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	422.524
	<chem>S=C3S/C(=C/c1cccc(F)c1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	422.524
	<chem>S=C3S/C(=C/c1ccc(OC)c(O)c1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	450.559
	<chem>S=C3S/C(=C/c1ccc(F)c(Br)c1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	501.420
	<chem>S=C3S/C(=C/c1ccccn1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	405.522
	<chem>S=C3S/C(=C/c1cccc(O)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	420.533
	<chem>S=C3S/C(=C/c1ccncc1)C(=O)N3CCc2ccc(cc2)S(N)(=O)=O</chem>	405.522
	<chem>O=C(CN1CCN(CC1)c2ccccc2OC)NNC(=O)NCc3ccccc3</chem>	397.477
	<chem>O=C(CN1CCN(CC1)c2ccccc2OC)NNC(=S)NCc3ccccc3</chem>	413.544
	<chem>COc4ccccc4N3CCN(Cc1nnc(S)n1c2ccccc2)CC3</chem>	381.503

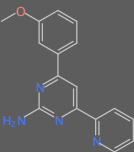
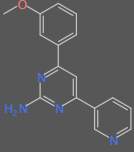
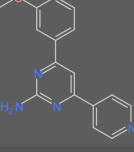
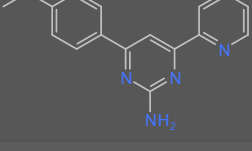
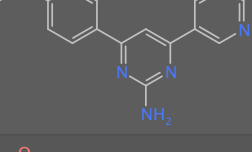
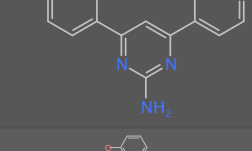
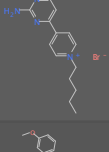

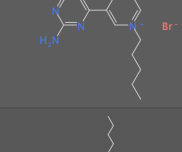
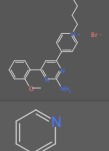
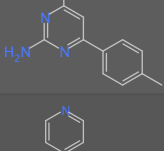
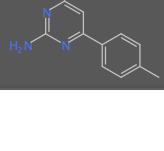
Structure	SMILES	Total Molwei...
	<chem>COc3ccccc3N2CCN(Cc1nnc(S)n1CC)CC2</chem>	333.459
	<chem>COc1ccccc1N4CCN(CC2 = NNC(=O)N2c3ccccc3)CC4</chem>	365.436
	<chem>COc1ccccc1N4CCN(CC3 = NNC(=S)N3Cc2ccccc2)CC4</chem>	395.530
	<chem>COc1ccccc1N4CCN(CC3 = NNC(=O)N3Cc2ccccc2)CC4</chem>	379.463
	<chem>S=C4OC(=NN4CN1CCN(CC1)c2cc3N(CC)C=C(C(=O)O)C(=O)c3cc2F)Cl</chem>	637.735
	<chem>S=C5OC(=NN5CN1CCN(CC1)c2cc3N(C=C(C(=O)O)C(=O)c3cc2F)C4CC</chem>	649.746
	<chem>O=C(O)C2 = CN(CC)c1cc(c(F)cc1C2=O)N7CCN(CN6N=C(CN3CCN(CC3)N</chem>	726.875
	<chem>O=C(O)C3 = CN(C1CC1)c2cc(c(F)cc2C3=O)N8CCN(CN7N=C(CN4CCN(CC4)N</chem>	738.886
	<chem>O=C(O)C2 = CN(CC)c1cc(c(F)cc1C2=O)N7CCN(CN5N=C(CN3CCN(CC3)N</chem>	712.849
	<chem>O=C(O)C3 = CN(C1CC1)c2cc(c(F)cc2C3=O)N8CCN(CN6N=C(CN4CCN(CC4)N</chem>	724.860
	<chem>O=C(O)C2 = CN(CC)c1cc(c(F)cc1C2=O)N7CCN(CN6N=C(CN3CCN(CC3)N</chem>	710.808
	<chem>O=C(O)C3 = CN(C1CC1)c2cc(c(F)cc2C3=O)N8CCN(CN7N=C(CN4CCN(CC4)N</chem>	722.819

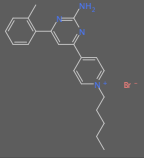
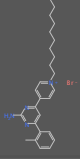
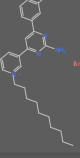
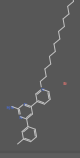
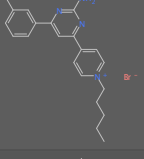
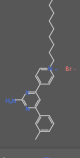

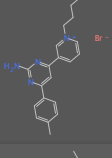
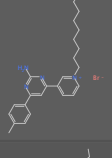
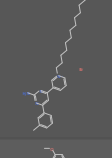

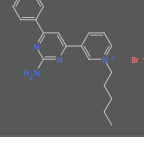
Structure	SMILES	Total Molwei...
	<chem>Clc1ccc(cc1)C(=O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5c4ccccc4</chem>	534.082
	<chem>Clc1ccc(cc1)C(O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5c4ccccc4</chem>	536.098
	<chem>Clc1ccc(cc1)C(=O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5Cc4ccccc4</chem>	548.109
	<chem>Clc1ccc(cc1)C(O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5Cc4ccccc4</chem>	550.125
	<chem>Clc1ccc(cc1)C(=O)CSc4nnc(CN2CCN(CC2)c3ccccc3OC)n4CC</chem>	486.038
	<chem>Clc1ccc(cc1)C(O)CSc4nnc(CN2CCN(CC2)c3ccccc3OC)n4CC</chem>	488.054
	<chem>Clc1ccc(c(Cl)c1)C(=O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5c4ccccc4</chem>	568.527
	<chem>Clc1ccc(c(Cl)c1)C(O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5c4ccccc4</chem>	570.543
	<chem>Clc1ccc(c(Cl)c1)C(=O)CSc4nnc(CN2CCN(CC2)c3ccccc3OC)n4CC</chem>	520.483
	<chem>Clc1ccc(c(Cl)c1)C(O)CSc4nnc(CN2CCN(CC2)c3ccccc3OC)n4CC</chem>	522.499
	<chem>Clc1ccc(c(Cl)c1)C(=O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5Cc4ccccc4</chem>	582.554
	<chem>Clc1ccc(c(Cl)c1)C(O)CSc5nnc(CN2CCN(CC2)c3ccccc3OC)n5Cc4ccccc4</chem>	584.570

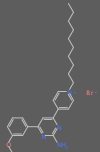
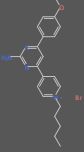
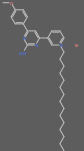
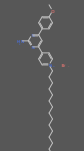
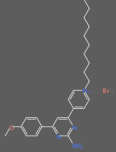
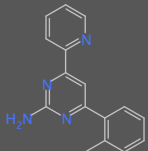
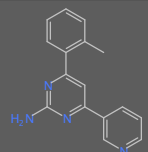
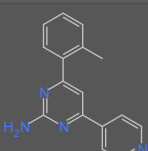

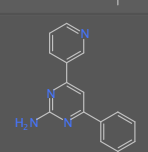
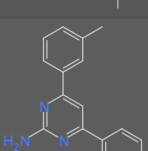

Structure	SMILES	Total Molwei...
	<chem>O=C(CSc3nnc(CN1CCN(CC1)c2ccccc2OC)o3)c4ccc(Cl)cc4</chem>	458.969
	<chem>OC(CSc3nnc(CN1CCN(CC1)c2ccccc2OC)o3)c4ccc(Cl)cc4</chem>	460.985
	<chem>COc1ccccc1N2CCN(CC2)CC5=NN(CN3CCOCC3)C(=S)N5c4ccccc4</chem>	480.635
	<chem>COc1ccccc1N2CCN(CC2)CC4=NN(CN3CCOCC3)C(=S)N4CC</chem>	432.591
	<chem>COc1ccccc1N2CCN(CC2)CC5=NN(CN3CCOCC3)C(=S)N5Cc4ccccc4</chem>	494.662
	<chem>COc2ccc(/C=C/C(=O)c1ccccc1)cc2</chem>	238.285
	<chem>O=[N+](([O-])c2ccc(/C=C/C(=O)c1ccccc1)cc2</chem>	253.256
	<chem>BrC2cc(/C=C/C(=O)c1ccccc1)ccc2</chem>	287.155
	<chem>Clc2ccccc2c2ccc(F)c2/C=C/C(=O)c1ccccc1</chem>	260.694
	<chem>S=C(N)N2N=C(CC2c1c(F)cccc1Cl)c3ccccc3</chem>	333.817
	<chem>S=C(N)N2N=C(CC2c1ccc(cc1)[N+](([O-])=O)c3ccccc3</chem>	326.379
	<chem>S=C(N)N2N=C(CC2c1cccc(Br)c1)c3ccccc3</chem>	360.278

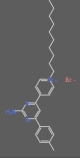


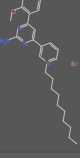
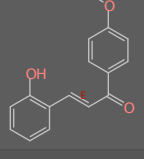
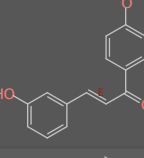
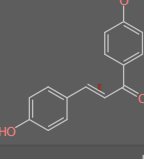
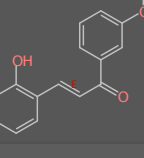
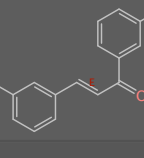
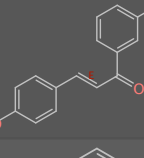
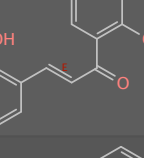
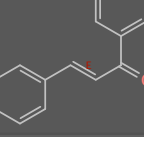
Structure	SMILES	Total Molwei...
	<chem>Fc2ccc(NC(=S)Nc1cccc1)cc2Cl</chem>	280.753
	<chem>BrC2cc(NC(=S)Nc1ccc(F)c(Cl)c1)ccc2</chem>	359.649
	<chem>BrC2ccc(NC(=S)Nc1ccc(F)c(Cl)c1)cc2</chem>	359.649
	<chem>Fc2ccc(NC(=S)Nc1cccc(F)c1)cc2Cl</chem>	298.743
	<chem>Clc1ccc(cc1)C3=CS/C(=N\c2ccc(F)cc2)N3c4ccc(C)cc4</chem>	394.900
	<chem>Clc1ccc(cc1)C3=CS/C(=N\c2cccc2)N3c4ccc(C)cc4</chem>	376.910
	<chem>[O-][N+](=O)c4ccc(\N=C1/SC=C(N1c2ccc(C)cc2)c3cccc3)cc4</chem>	387.462
	<chem>Cc1ccc(cc1)N3C(=CS/C3=N\c2cccc2)c4cccc4</chem>	342.465
	<chem>Clc4ccc(C2=CS/C(=N\c1cccc1)N2c3ccc(C)cc3)c(Cl)c4</chem>	411.355
	<chem>Cc1ccc(cc1)N3C(=CS/C3=N\c2ccc(F)cc2)c4cccc4</chem>	360.455
	<chem>Clc4ccc(C2=CS/C(=N\c1ccc(F)cc1)N2c3ccc(C)cc3)c(Cl)c4</chem>	429.345
	<chem>Clc1ccc(cc1)C3=CS/C(=N\c2cccc2)N3c4ccc(F)c(Cl)c4</chem>	415.318

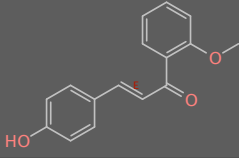
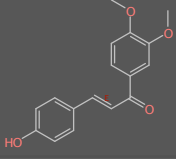
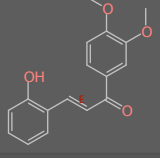
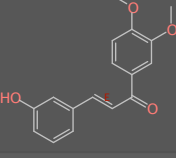
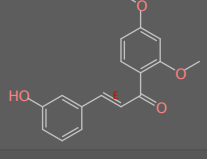
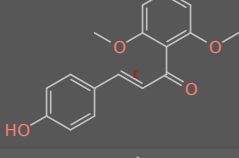
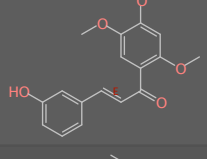
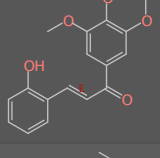
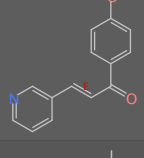
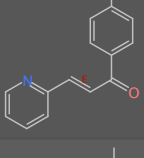
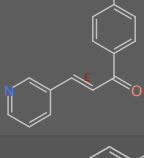
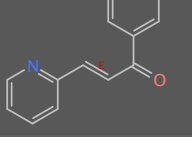
Structure	SMILES	Total Molwei...
	<chem>[O-][N+](=O)c4ccc(\N=C1/SC=C(N1c2ccc(F)c(Cl)c2)c3ccc(Cl)cc3)cc4</chem>	460.315
	<chem>Clc1ccc(cc1)C3=CS/C(=N\c2cccc2)N3c4ccc(cc4F)N5CCN(CC5)c6cccc</chem>	541.092
	<chem>Fc4cc(ccc4N2C(=CS/C2=N\c1ccc(F)cc1)c3cccc3)N5CCN(CC5)c6cccc</chem>	524.637
	<chem>[O-][N+](=O)c6ccc(\N=C1/SC=C(N1c2ccc(cc2F)N3CCN(CC3)c4cccc4</chem>	586.090
	<chem>Clc1ccc(cc1)C3=CS/C(=N\c2ccc(F)cc2)N3c4ccc(F)c(Cl)c4</chem>	433.308
	<chem>Fc4cc(ccc4N2C(=CS/C2=N\c1cccc1)c3cccc3)N5CCN(CC5)c6cccc6</chem>	506.647
	<chem>[O-][N+](=O)c4ccc(\N=C1/SC=C(N1c2ccc(F)c(Cl)c2)c3cccc3)cc4</chem>	425.870
	<chem>CC1=C(C(=CC=C1)NC(=O)C2=CC=C(C=C2)OCC(=O)NCC3=CC=CC=</chem>	388.466
	<chem>C1=CC=C2C(=C1)C=CC(=C2C=NNC(=O)C3=CC=C(C=C3)O)O</chem>	306.320
	<chem>NC1=NC(C2=CC=CC=C2OC)=CC(C3=CC=CC=N3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=CC=C2OC)=CC(C3=CC=CN=C3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=CC=C2OC)=CC(C3=CC=NC=C3)=N1</chem>	278.314

Structure	SMILES	Total Molwei...
	<chem>NC1=NC(C2=CC=CC(OC)=C2)=CC(C3=CC=CC=N3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=CC(OC)=C2)=CC(C3=CC=CN=C3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=CC(OC)=C2)=CC(C3=CC=NC=C3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=CC=N3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=CN=C3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=NC=C3)=N1</chem>	278.314
	<chem>NC1=NC(C2=CC=CC=C2OC)=CC(C3=CC=[N+](CCCCC)C=C3)=N1.[Br-]</chem>	429.361
	<chem>NC1=NC(C2=CC(OC)=CC=C2)=CC(C3=CC=C[N+](CCCCCCCCC)=C3)=N1.[Br-]</chem>	499.495
	<chem>NC1=NC(C2=CC(OC)=CC=C2)=CC(C3=CC=C[N+](CCCCC)=C3)=N1.[Br-]</chem>	429.361
	<chem>NC1=NC(C2=CC=CC=C2OC)=CC(C3=CC=[N+](CCCCCCCCC)C=C3)=N1.[Br-]</chem>	499.495
	<chem>NC1=NC(C2=CC=CN=C2)=CC(C3=CC=C(C)C=C3)=N1</chem>	262.315
	<chem>NC1=NC(C2=CC=NC=C2)=CC(C3=CC=C(C)C=C3)=N1</chem>	262.315

Structure	SMILES	Total Molwei...
	<chem>NC1=NC(C2=CC=[N+](CCCC)C=C2)=CC(C3=CC=CC=C3C)=N1.[Br-]</chem>	413.362
	<chem>NC1=NC(C2=CC=[N+](CCCCCCCCCO)C=C2)=CC(C3=CC=CC=C3C)=</chem>	483.496
	<chem>NC1=NC(C2=CC=C[N+](CCCCCCCCCO)=C2)=CC(C3=CC=CC(C)=C3)</chem>	483.496
	<chem>NC1=NC(C2=CC=C[N+](CCCCCCCCCCCCCO)=C2)=CC(C3=CC=CC(C)=C3)</chem>	553.630
	<chem>NC1=NC(C2=CC=[N+](CCCC)C=C2)=CC(C3=CC=CC(C)=C3)=N1.[Br-]</chem>	413.362
	<chem>NC1=NC(C2=CC=[N+](CCCCCCCCCO)C=C2)=CC(C3=CC=CC(C)=C3)</chem>	483.496
	<chem>NC1=NC(C2=CC=[N+](CCCCCCCCCCCCCO)C=C2)=CC(C3=CC=CC(C)=C3)</chem>	553.630
	<chem>NC1=NC(C2=CC=C[N+](CCCC)C=C2)=CC(C3=CC=C(C)C=C3)=N1.[Br-]</chem>	413.362
	<chem>NC1=NC(C2=CC=C[N+](CCCCCCCCCO)=C2)=CC(C3=CC=C(C)C=C3)</chem>	483.496
	<chem>NC1=NC(C2=CC=C[N+](CCCCCCCCCCCCCO)=C2)=CC(C3=CC=CC(C)=C3)</chem>	553.630
	<chem>NC1=NC(C2=CC(OC)=CC=C2)=CC(C3=CC=[N+](CCCCCCCCCCCCCO)C=C3)</chem>	569.629
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=C[N+](CCCC)C=C3)=N1.[Br-]</chem>	429.361

Structure	SMILES	Total Molwei...
	<chem>NC1=NC(C2=CC(OC)=CC=C2)=CC(C3=CC=[N+])(CCCCCCCCC)C=C3</chem>	499.495
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=[N+])(CCCC)C=C3)=N1</chem>	429.361
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=C[N+])(CCCCCCCCCCCCC)C=C3</chem>	569.629
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=[N+])(CCCCCCCCCCCCC)C=C3</chem>	569.629
	<chem>NC1=NC(C2=CC=C(OC)C=C2)=CC(C3=CC=[N+])(CCCCCCCCC)C=C3</chem>	499.495
	<chem>NC1=NC(C2=CC=CC=N2)=CC(C3=CC=CC=C3C)=N1</chem>	262.315
	<chem>NC1=NC(C2=CC=CN=C2)=CC(C3=CC=CC=C3C)=N1</chem>	262.315
	<chem>NC1=NC(C2=CC=NC=C2)=CC(C3=CC=CC=C3C)=N1</chem>	262.315
	<chem>NC1=NC(C2=CC=CC=N2)=CC(C3=CC=CC(C)=C3)=N1</chem>	262.315
	<chem>NC1=NC(C2=CC=CN=C2)=CC(C3=CC=CC(C)=C3)=N1</chem>	262.315
	<chem>NC1=NC(C2=CC=NC=C2)=CC(C3=CC=CC(C)=C3)=N1</chem>	262.315
	<chem>NC1=NC(C2=CC=C[N+])(CCCCCCCCCCCCC)=C2)=CC(C3=CC=C(C)C=C3</chem>	553.630

Structure	SMILES	Total Molwei...
	<chem>NC1=NC2=CC=[N+](CCCCCCCCC)C=C2)=CC(C3=CC=C(C)C=C3)</chem>	483.496
	<chem>NC1=NC2=CC=[N+](CCCCCCCCCCCC)C=C2)=CC(C3=CC=C(C)C=C3)</chem>	553.630
	<chem>NC1=NC2=CC=CC=C2OC)=CC(C3=CC=C[N+](CCCCCCCCCCCC)C=C3)</chem>	569.629
	<chem>NC1=NC2=CC=CC=C2OC)=CC(C3=CC=C[N+](CCCCCCCC)C=C3)</chem>	499.495
	<chem>O=C(/C=C/C1=CC=CC=C1OC)C2=CC=C(OC)C=C2</chem>	254.284
	<chem>O=C(/C=C/C1=CC=CC(O)=C1)C2=CC=C(OC)C=C2</chem>	254.284
	<chem>O=C(/C=C/C1=CC=C(O)C=C1)C2=CC=C(OC)C=C2</chem>	254.284
	<chem>O=C(/C=C/C1=CC=CC=C1OC)C2=CC(OC)=CC=C2</chem>	254.284
	<chem>O=C(/C=C/C1=CC=CC(O)=C1)C2=CC(OC)=CC=C2</chem>	254.284
	<chem>O=C(/C=C/C1=CC=C(O)C=C1)C2=CC(OC)=CC=C2</chem>	254.284
	<chem>O=C(/C=C/C1=CC=CC=C1OC)C2=CC=CC=C2OC</chem>	254.284
	<chem>O=C(/C=C/C1=CC=CC(O)=C1)C2=CC=CC=C2OC</chem>	254.284

Structure	SMILES	Total Molwei...
	<chem>O=C(/C=C/C1=CC=C(O)C=C1)C2=CC=CC=C2OC</chem>	254.284
	<chem>O=C(/C=C/C1=CC=C(O)C=C1)C2=CC=C(OC)C(OC)=C2</chem>	284.310
	<chem>O=C(/C=C/C1=CC=CC=C1O)C2=CC=C(OC)C(OC)=C2</chem>	284.310
	<chem>O=C(/C=C/C1=CC=CC(O)=C1)C2=CC=C(OC)C(OC)=C2</chem>	284.310
	<chem>O=C(/C=C/C1=CC=CC(O)=C1)C2=C(OC)C=C(OC)C=C2</chem>	284.310
	<chem>O=C(/C=C/C1=CC=C(O)C=C1)C2=C(OC)C=CC=C2OC</chem>	284.310
	<chem>O=C(/C=C/C1=CC=CC(O)=C1)C2=C(OC)C=C(OC)C(OC)=C2</chem>	314.336
	<chem>O=C(/C=C/C1=CC=CC=C1O)C2=CC(OC)=C(OC)C(OC)=C2</chem>	314.336
	<chem>O=C(/C=C/C1=CC=CN=C1)C2=CC=C(OC)C=C2</chem>	239.273
	<chem>O=C(/C=C/C1=CC=CC=N1)C2=CC=C(C)C=C2</chem>	223.274
	<chem>O=C(/C=C/C1=CC=CN=C1)C2=CC=C(C)C=C2</chem>	223.274
	<chem>O=C(/C=C/C1=CC=CC=N1)C2=CC=CC(C)=C2</chem>	223.274

Structure	SMILES	Total Molwei...
	<chem>O=C(/C=C/C1=CC=NC=C1)C2=CC=C(C)C=C2</chem>	223.274
	<chem>O=C(/C=C/C1=CC=NC=C1)C2=C(OC)C=CC=C2</chem>	239.273
	<chem>O=C(/C=C/C1=CC=C(O)C=C1)C2=C(OC)C=C(OC)C=C2OC</chem>	314.336
	<chem>O=C(/C=C/C1=CC=CC=N1)C2=CC(OC)=CC=C2</chem>	239.273
	<chem>O=C(/C=C/C1=CC=NC=C1)C2=CC(C)=CC=C2</chem>	223.274
	<chem>O=C(/C=C/C1=CC=CC=N1)C2=CC=C(OC)C=C2</chem>	239.273
	<chem>O=C(/C=C/C1=CC=CC=N1)C2=C(OC)C=CC=C2</chem>	239.273
	<chem>O=C(/C=C/C1=CC=NC=C1)C2=CC(OC)=CC=C2</chem>	239.273