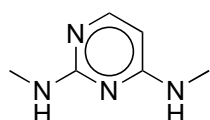
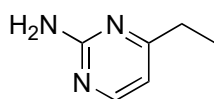


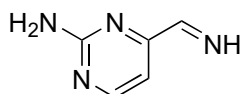
CNc1nc(OC)ccn1



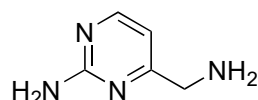
CNc1nc(NC)ncc1



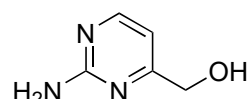
NC1=NC=CC(CC)=N1



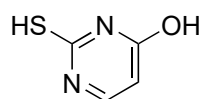
NC1=NC=CC(C=N)=N1



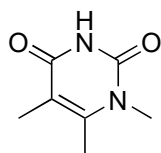
NC1=NC=CC(CN)=N1



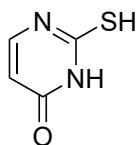
NC1=NC=CC(CO)=N1



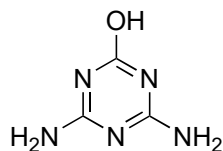
OC1=CC=NC(S)=N1



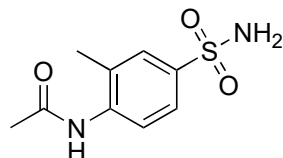
O=C1N(C(C)=C(C(N1)=O)C)C



O=C1C=CN=C(N1)S

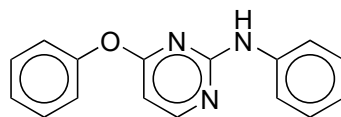
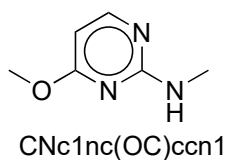


NC1=NC(N)=NC(O)=N1



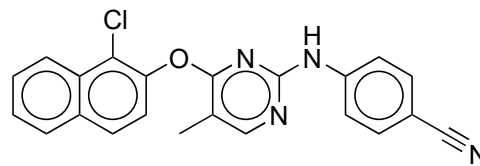
CC(NC1=C(C=C(C=C1)S(N)(=O)=O)C)=O

	AllAve
AveStepTime	29.09998
StepNum	27.125
TotalTime	805.2031



FXQ-2009-220-10S

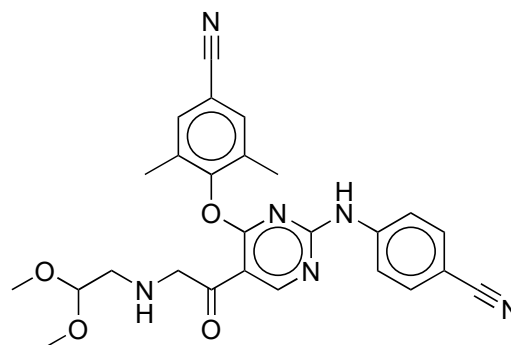
FXQ-2009-220-10S.log
26.94117647
17
458



CC1CNC(NC2CCC(C#N)CC2)NC1OC3CCCCC2C1Cl

GSX-2019-EJMC277-5-15a5

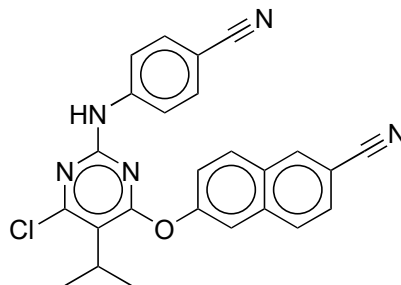
GSX-2019-EJMC277-5-15a5.log
33.03846154
52
1718



COC(CNCC(=O)O)C1CNC(NC2CCC(C#N)CC2)NC1OC3C(C)CC(C#N)CC3OC

LHY-2009-1539-1P

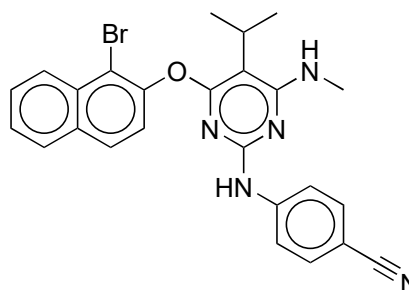
LHY-2009-1539-1P.log
31.02941176
34
1055



CC(C)c1c(Cl)nc(NC2CCC(C#N)CC2)nc1Oc3ccc2cc(C#N)ccc2c3

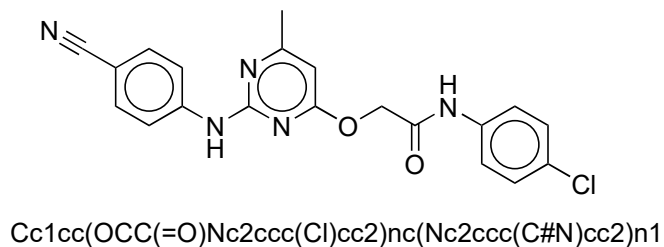
WHQ-2014-SQER-761-66

WHQ-2014-SQER-761-66.log
36.03571429
28
1009

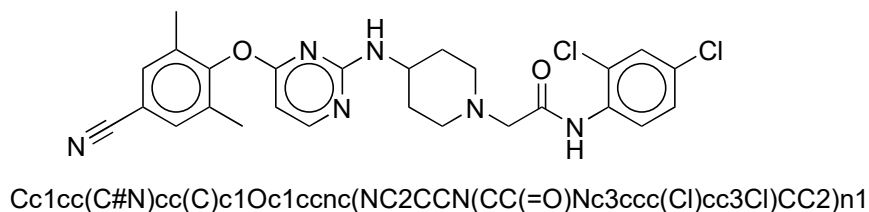


CNc1nc(NC2CCC(C#N)CC2)nc1Oc3ccc3c(Br)c1C(C)C

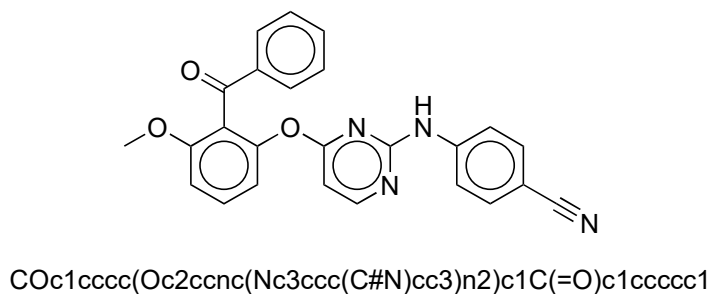
WHQ-2015-BMC-624-3-3i	
WHQ-2015-BMC-624-3-3i.log	
21.95833333	
23	
505.0416667	



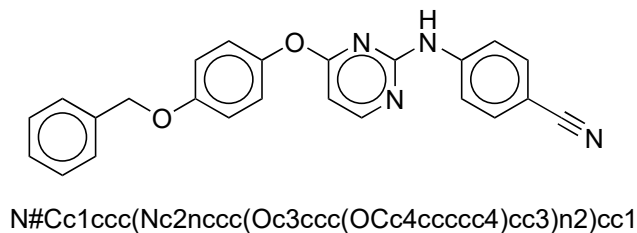
WZY-2015-EJMC-1-4-7n	
WZY-2015-EJMC-1-4-7n.log	
31.51724138	
29	
914	

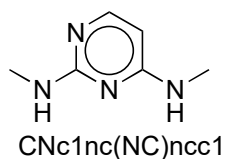


YSQ-2013-EJMC-134-1d	
YSQ-2013-EJMC-134-1d.log	
30.77777778	
18	
554	

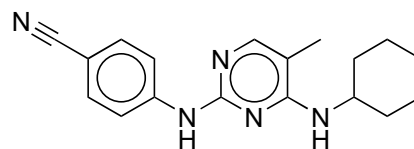


YSQ-2013-EJMC-134-1f	
YSQ-2013-EJMC-134-1f.log	
25.5952381	
42	
1075	





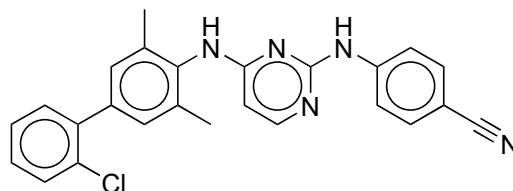
GSX-2011-BMC-7093-1j	
GSX-2011-BMC-7093-1j.log	
	18.70588235
	17
	318



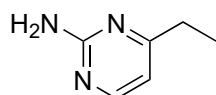
Cc1cnc(Nc2ccc(C#N)cc2)nc1NC1CCCCC1

JKJ-2018-EJMC-726-3-4f

JKJ-2018-EJMC-726-3-4f.log	
	28.29032258
	31
	877



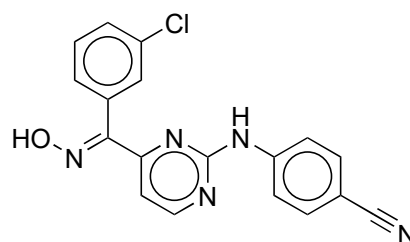
Cc1cc(-c2ccccc2Cl)cc(C)c1Nc1ccnc(Nc2ccc(C#N)cc2)n1



NC1=NC=CC(CC)=N1

FXQ-2010-2371-12F

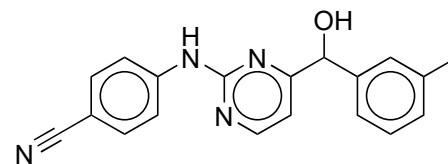
FXQ-2010-2371-12F.log	
	20.05263158
	19
	381



N#Cc1ccc(Nc2nccc(/C(=N/O)c3ccccc(Cl)c3)n2)cc1

GSX-2011-BMC-5117-10e

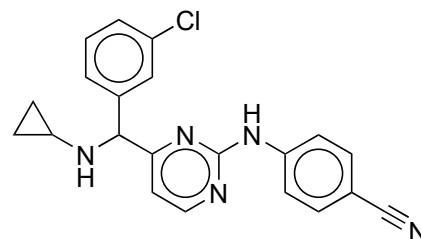
GSX-2011-BMC-5117-10e.log	
	17.63636364
	33
	582



Cc1cccc(C(O)c2ccnc(Nc3ccc(C#N)cc3)n2)c1

LY-2014-EJPS-334-2-1g

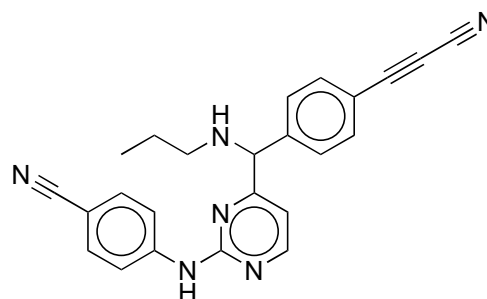
LY-2014-EJPS-334-2-1g.log	
	25.7037037
	27
	694



N#Cc1ccc(Nc2nccc(C(NC3CC3)c3ccccc(Cl)c3)n2)cc1

MG-2014-EJMC-600-4-1l

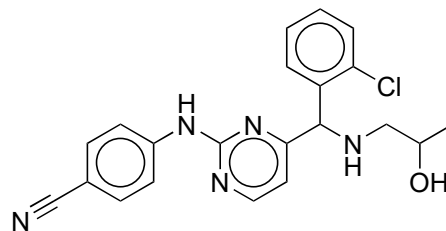
MG-2014-EJMC-600-4-1l.log	
	28.60869565
	23
	658



CCCNC(c1ccc(C#CC#N)cc1)c1ccnc(Nc2ccc(C#N)cc2)n1

MG-2014-EJMC-600-4-1r

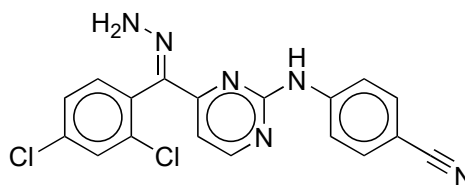
MG-2014-EJMC-600-4-1r.log
27.82142857
28
779



CC(O)CNC(c1ccnc(Nc2ccc(C#N)cc2)n1)c1ccccc1Cl

MXD-2011-CMC-2225-9o

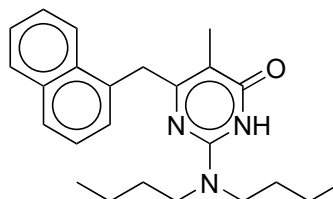
MXD-2011-CMC-2225-9o.log
21.20833333
24
509



N#Cc1ccc(Nc2nccc(/C(=N/N)c3ccc(Cl)cc3Cl)n2)cc1

WYP-2008-171-6Q

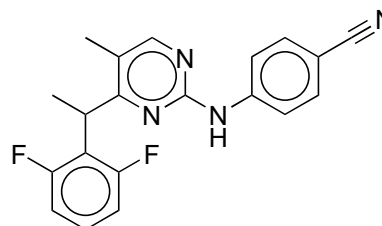
WYP-2008-171-6Q.log
31.68292683
41
1299



CCCCN(CCCC)c1nc(Cc2cccc3ccccc23)c(C)c(=O)[nH]1

YSQ-2012-CMC-152-17R

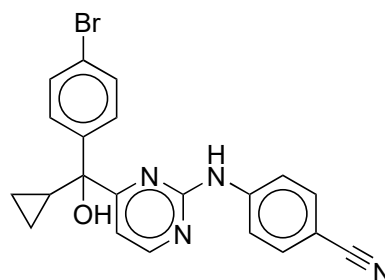
YSQ-2012-CMC-152-17R.log
22.66666667
24
544



Cc1cnc(Nc2ccc(C#N)cc2)nc1C(C)c1c(F)cccc1F

YZH-2014-BMC-2535-2-3p

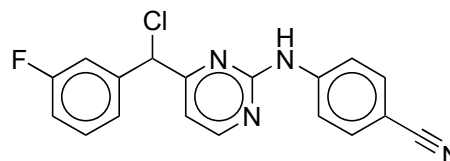
YZH-2014-BMC-2535-2-3p.log
28.25925926
27
763



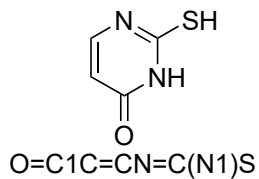
N#Cc1ccc(Nc2nccc(C(O)(c3ccc(Br)cc3)C3CC3)n2)cc1

YZH-2014-BMC-3220-2-7e

YZH-2014-BMC-3220-2-7e.log
18.625
24
447

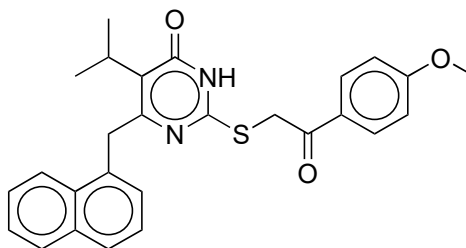


N#Cc1ccc(Nc2nccc(C(Cl)c3cccc(F)c3)n2)cc1



HYP2004-3175-4O

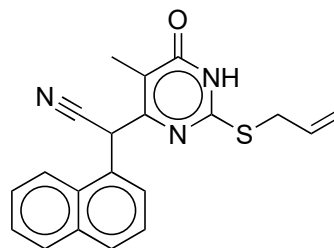
HYP2004-3175-4O.log	
	38.8
	40
	1552



COc1ccc(C(=O)CSc2nc(Cc3cccc4ccccc34)c(C(C)C)c(=O)[nH]2)cc1

LJ-2007-1780-3D

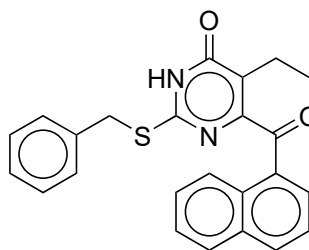
LJ-2007-1780-3D.log	
	24.84210526
	19
	472



C=CCSc1nc(C(C#N)c2cccc3ccccc23)c(C)c(=O)[nH]1

LJ-2007-1780-4J

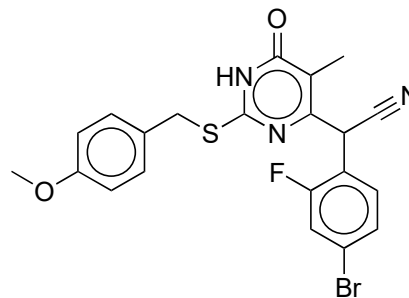
LJ-2007-1780-4J.log	
	30.72727273
	22
	676



CCc1c(C(=O)c2cccc3ccccc23)nc(SCc2ccccc2)[nH]c1=O

WHQ-2014-MCC-5468-3-1r

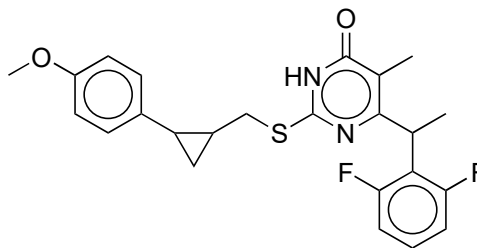
WHQ-2014-MCC-5468-3-1r.log	
	30.33333333
	27
	819



COc1ccc(CSc2nc(C(C#N)c3ccc(Br)cc3F)c(C)c(=O)[nH]2)cc1

YSQ-2012-CMC-152-12

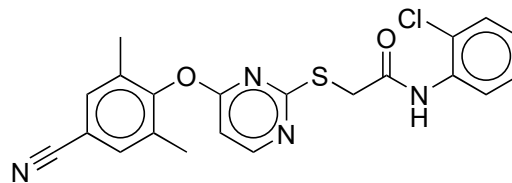
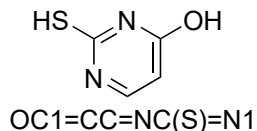
YSQ-2012-CMC-152-12.log	
	29.54166667
	23
	679.4583333



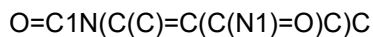
COc1ccc(C2CC2CSc2nc(C(C)c3c(F)cccc3F)c(C)c(=O)[nH]2)cc1

WZY-2015-BMC-4248-3-3d

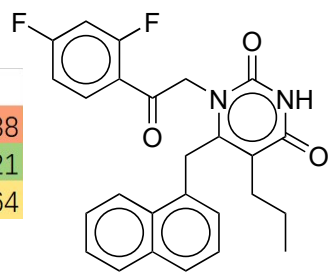
WZY-2015-BMC-4248-3-3d.log	
	28.65217391
	23
	659



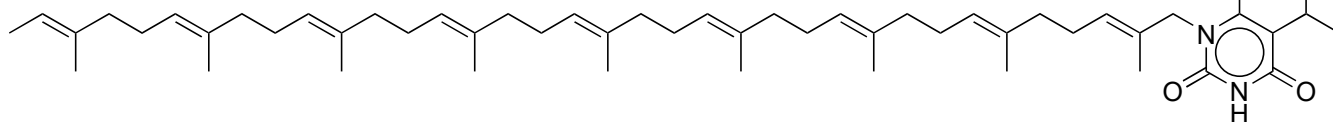
Cc1cc(C#N)cc(C)c1Oc1ccnc(SCC(=O)Nc2ccccc2Cl)n1



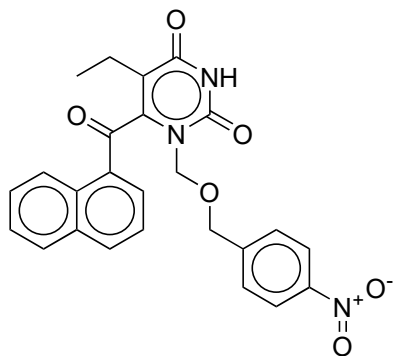
HYP2005-1237-4-33.log	
	36.38095238
	21
	764

CCCc1c(Cc2cccc3ccccc23)n(CC(=O)c2ccc(F)cc2F)c(=O)[nH]c1=O

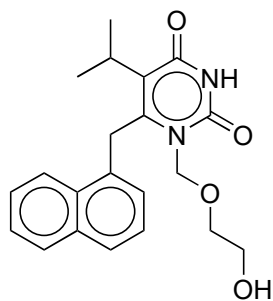
LJ-2006-1250-24

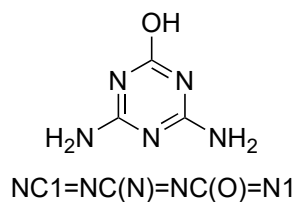
[illegible]

LJ-2007-200-22.log	
	41.07407407
	27
	1109

CCc1c(C(=O)c2cccc3ccccc23)n(COCc2ccc([N+](=O)[O-])cc2)c(=O)[nH]c1=O

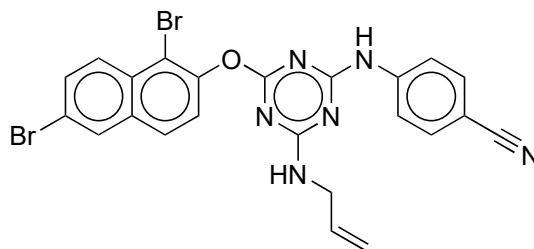
MG2003-255-4.log	
	31.18181818
	22
	686

CC(C)c1c(Cc2cccc3ccccc23)n(COCCO)c(=O)[nH]c1=O

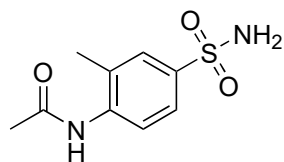


CFE-2008-ZL-12

CFE-2008-ZL-12.log	
33.16666667	
30	
995	

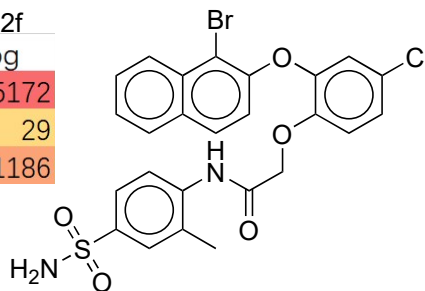


C=CCNc1nc(Nc2ccc(C#N)cc2)nc(Oc2ccc3cc(Br)ccc3c2Br)n1



GSX-2011-BMC-4220-12f

GSX-2011-BMC-4220-12f.log	
40.89655172	
29	
1186	

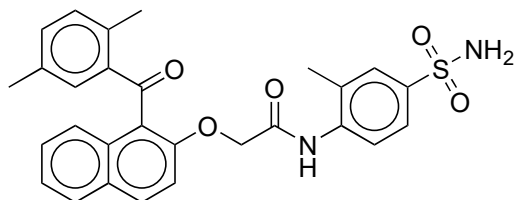


CC(NC1=C(C=C(C=C1)S(N)(=O)=O)C)=O

Cc1cc(S(N)(=O)=O)ccc1NC(=O)COc1ccc(Cl)cc1Oc1ccc2ccccc2c1Br

MXD-2011-BMC-4601-10e

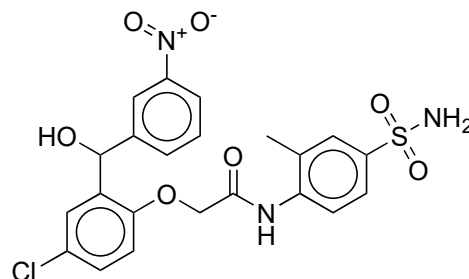
MXD-2011-BMC-4601-10e.log	
39.48648649	
37	
1461	



Cc1ccc(C)c(C(=O)c2c(OCC(=O)Nc3ccc(S(N)(=O)=O)cc3C)ccc3ccccc23)c1

MXD-2011-BMC-4704-7h

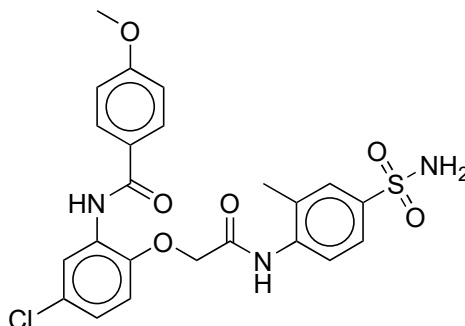
MXD-2011-BMC-4704-7h.log	
37.77777778	
72	
2720	



Cc1cc(S(N)(=O)=O)ccc1NC(=O)COc1ccc(Cl)cc1C(O)c1cccc([N+](=O)[O-])c1

MXD-2012-EJMC-504-3-13j

MXD-2012-EJMC-504-3-13j.log	
33	
39	
1287	



COc1ccc(C(=O)Nc2cc(Cl)ccc2OCC(=O)Nc2ccc(S(N)(=O)=O)cc2C)cc1