Supporting Information

LiCABEDS II. Modeling Ligand Selectivity for G-protein Coupled Cannabinoid Receptors

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PART 1

This part lists the compound structures, their binding affinities for both CB1 or CB2 receptors, and detailed assay protocol. Table S1 summarizes 12 novel compound structures and binding affinities. These compounds are derived from the scaffold shown in Figure S1. Table S2 shows the structures, binding affinities and predicted CB2 selectivity of another 26 compounds. These novel compounds serve as external testing set to assess the performance of selectivity prediction models.

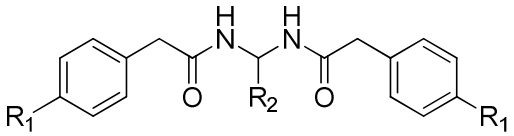


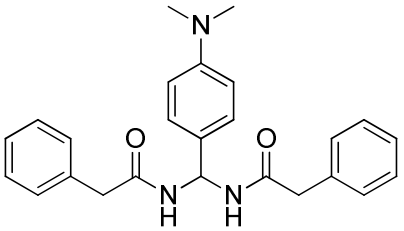
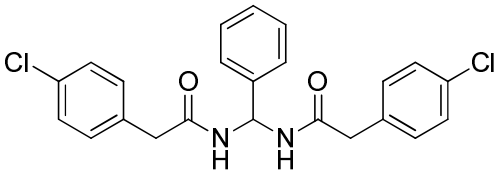
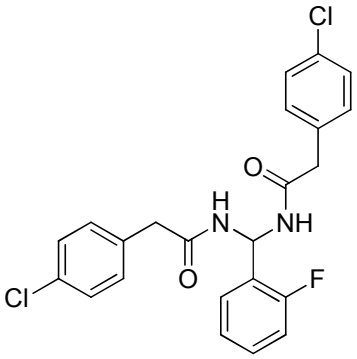
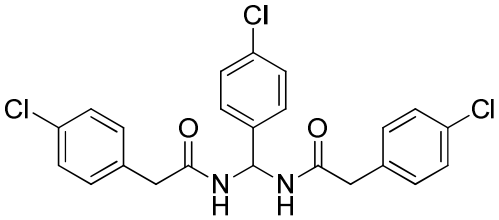
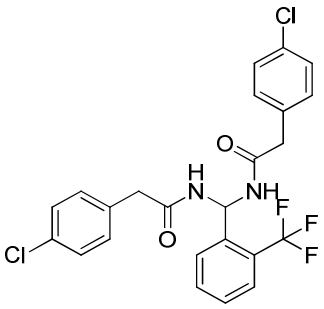
Figure S1: the scaffold of testing compounds summarized in Table S1

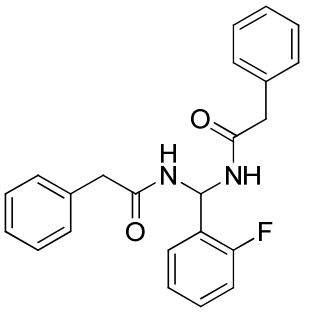
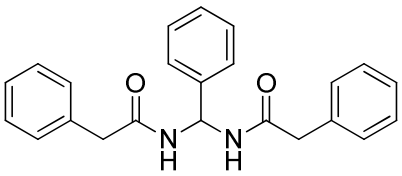
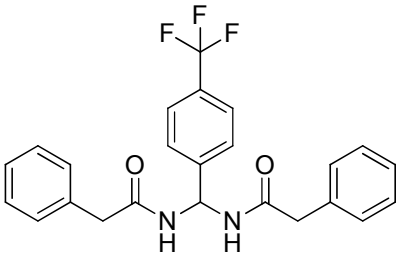
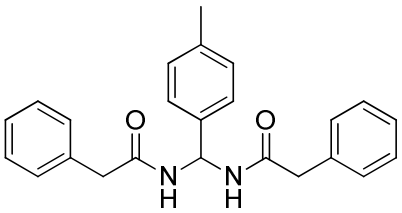
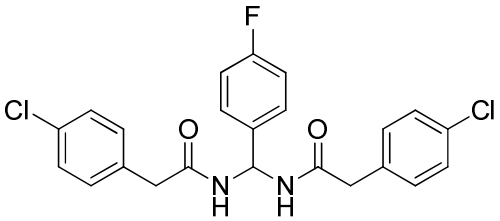
Table S1: the first compound collection for model validation

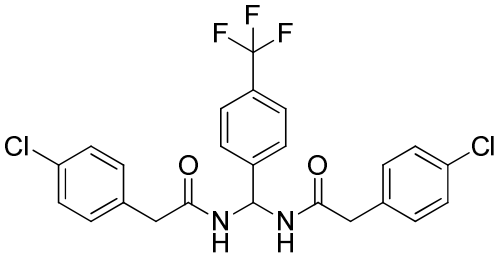
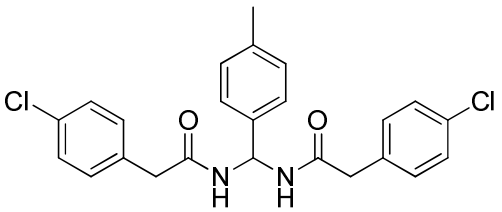
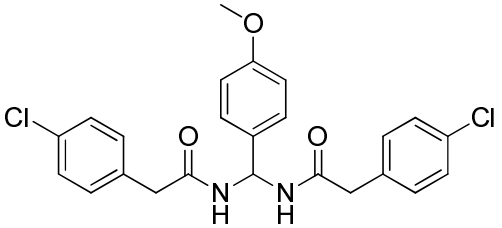
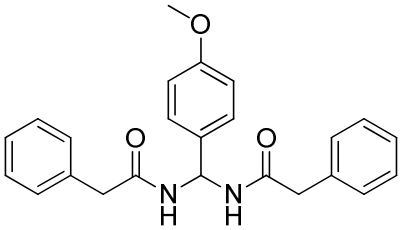
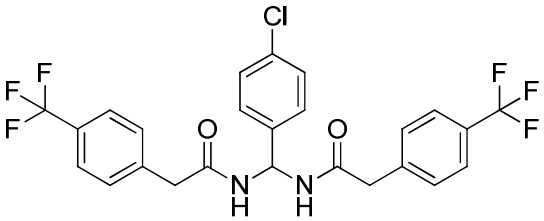
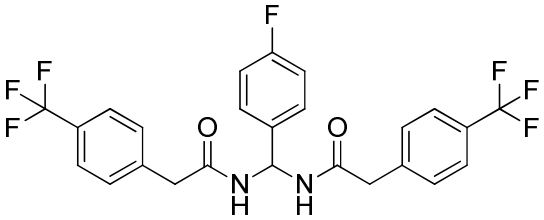
No.	Compd	R_1	R_2	MW	cLog P	K_i (CB_2), nM[b, c]	K_i (CB_1), nM[a, d]	SI[e]
1	PY1-37	H	$C_6H_5CH_2$	372.46	3.99	NB	NT	
2	PY1-38	H	$C_6H_5CH_2CH_2$	386.49	4.44	9,319	NT	
3	PY1-39	H	C_6H_5CH=CH	384.47	4.54	5,683	NT	
4	PY1-42	H	*p*-*i*-C_3H_7O-C_6H_4	416.51	4.55	313	> 20,000	> 64
5	PY1-45	H	*p*-Br-C_6H_4	437.33	4.70	2,226	NT	
6	PY1-48	H	*p*-C_2H_5O-C_6H_4	402.49	4.13	1,500	NT	
7	PY1-49	H	n-C_4H_9	338.44	3.75	35,970	NT	
8	PY1-50	H	n-C_5H_{11}	352.47	4.19	18,200	NT	
9	PY1-57	H	2-fluoro-4-methoxyphenyl	406.45	3.93	1071	NT	
10	PY1-58	H	*m*-F-C_6H_4	376.42	4.08	12,670	NT	
11	PY1-61	H	*p*-$(C_2H_5)_2$N-C_6H_4	429.55	4.76	64	> 20,000	> 313
12	PY1-63	H	*p*-*i*-C_3H_7-C_6H_4	400.51	5.18	85	> 20,000	> 235
SR1[f, g]					2.1	NT		
SR2[f, h]					NT	10.6		

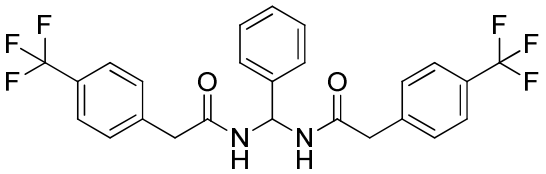
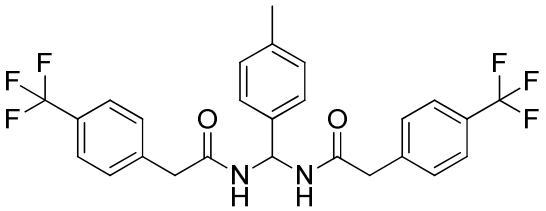
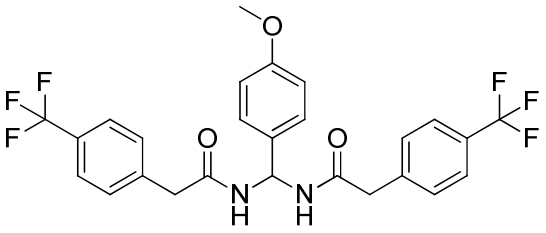
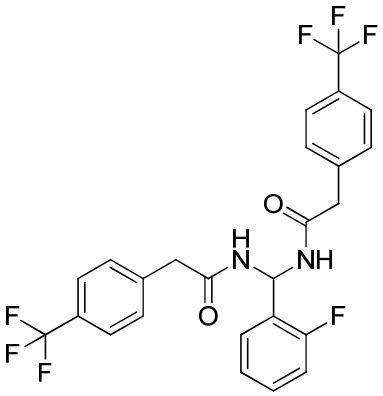
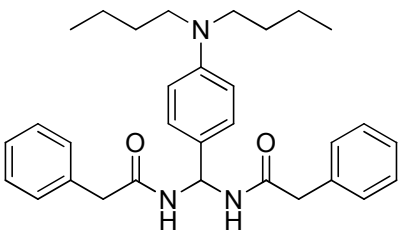
[a, b] Binding affinities of compounds for CB_1 and CB_2 receptor were evaluated using [^{3}H]-CP-55,940 radioligand competition binding assay. [c] NB no binding, K_i > 20,000 nM. [d] NT = not tested. [e] SI: selectivity index for CB_2, calculated as $K_i(CB_1)/K_i(CB_2)$ ratio. [f] The binding affinities of reference compounds were evaluated in parallel with compounds **1-12** under the same conditions. [g] CB_2 reference compound SR144528 (SR1). [h] CB_1 reference compound SR 141716 (SR2).

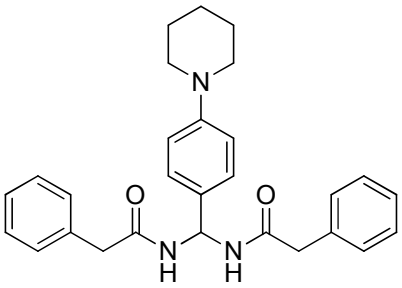
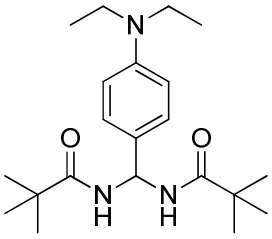
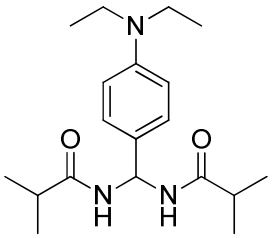
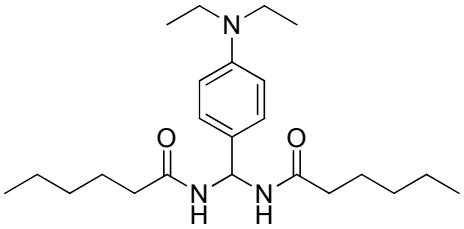
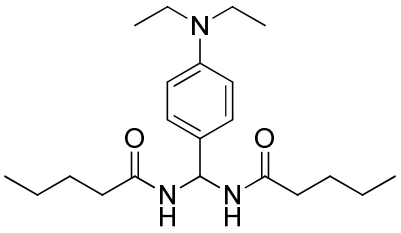
Table S2: the second compound collection for model validation

Compound Structure	Name	K_i nM (CB_2)	K_i nM (CB_1)	CB2 Selectivity	Prediction
	XIE95	709	NB	Selective	Non-selective
	HC1-9	1223	NB	Non-selective	Non-selective
	HC1-11	NB	NB	Non-selective	Non-selective
	HC1-13	188	9.1	Non-selective	Non-selective
	HC1-12	1225	95.84	Non-selective	Non-selective

	HC1-16	5237	2	Non-selective	Non-selective
	HC1-20	NB	18.47	Non-selective	Non-selective
	HC1-23	362	NB	Non-selective	Non-selective
	HC1-24	434	109	Non-selective	Non-selective
	HC1-25	NB	NB	Non-selective	Non-selective

	HC1-26	NB	7.7	Non-selective	Non-selective
	HC1-27	516	NB	Selective	Selective
	HC1-28	4872	NB	Non-selective	Non-selective
	HC1-29	5166	NB	Non-selective	Non-selective
	HC1-33	NB	NB	Non-selective	Non-selective
	HC1-35	1531	NB	Non-selective	Non-selective

	HC1-37	NB	NB	Non-selective	Non-selective
	HC1-38	NB	NB	Non-selective	Non-selective
	HC1-39	NB	NB	Non-selective	Non-selective
	HC1-40	1560	NB	Non-selective	Non-selective
	PY1-66	347	NB	Selective	Non-selective

	PY1-67	703	NB	Selective	Non-selective
	PY1-124	3553	NB	Non-selective	Selective
	PY1-143	587	NB	Selective	Selective
	PY1-144B	25.7	NB	Selective	Selective
	PY1-148	182	NB	Selective	Selective

Radioligand Competition Binding Assays. CB ligand competition binding assay was carried out as described previously[1]. Briefly, non-radioactive (or cold) ligands (PAM derivatives and reference ligands) were diluted in binding buffer (50 mM Tris-HCl (pH 7.4), 5 mM $MgCl_2$, 2.5 mM EGTA and 0.1% (w/v) fatty acid free BSA), supplemented with 10% dimethyl sulfoxide and 0.4% methyl cellulose. Each assay plate well contained a total of 200 µL of reaction mixture comprised of 5 µg of CB_1 (or CB_2) membrane protein, labeled [^{3}H]-CP-55,940 ligand at a final concentration of 3 nM and the unlabeled ligand at its varying dilutions as stated above. Plates were incubated at 30 ^{o}C for 1 h with gentle shaking. The reaction was terminated by rapid filtration through Unifilter GF/C filter plates using a Unifilter Cell Harvester (PerkinElmer). After the plate was allowed to dry overnight, 30 µL MicroScint-0 cocktail (PerkinElmer) was added to each well and the radioactivity was counted by using a PerkinElmer TopCounter. Data from these assays were analyzed using GraphPad Prism 5.0 Software. All assays were performed in duplicate and data points represented as mean±S.E.M. Bound radioactivity was analyzed for K_i values using non-linear regression analysis by GraphPad Prism 5.0 software.

The saturation binding of [^{3}H]-CP-55,940 to the membrane proteins was performed as described previously[2]. Briefly, the CB_1 (or CB_2) membrane fractions (5 µg) were incubated with increasing concentrations of [^{3}H]-CP-55,940 (0.05-4 nM) in 96-well plates at 30 °C with slow shaking for 1 h. The incubation buffer was composed of 50 mM Tris-HCl (pH 7.4), 5 mM $MgCl_2$, 2.5 mM EGTA and 0.1% (w/v) fatty acid free BSA. Ligand was diluted in incubation buffer supplemented with 10% dimethyl sulfoxide and 0.4% methyl cellulose. Non-specific binding was determined in the presence of 1:1000 unlabeled CP-55,940 (5,000 nM) in excess. The reaction was terminated and the radioactivity was counted as stated above. The difference between total and nonspecific binding equals the receptor specific binding. Non-linear regression analysis revealed the receptor density (B_{max}) and the equilibrium dissociation constant (K_d) values of [^{3}H]-CP-55,940 for the CB_2 receptor.

Supporting Information

1. Gertsch, J.; Leonti, M.; Raduner, S.; Racz, I.; Chen, J. Z.; Xie, X. Q.; Altmann, K. H.; Karsak, M.; Zimmer, A. Beta-caryophyllene is a dietary cannabinoid. *Proc Natl Acad Sci U S A* **2008,** 105, 9099-104.
2. Zhang, Y.; Xie, Z.; Wang, L.; Schreiter, B.; Lazo, J. S.; Gertsch, J.; Xie, X. Q. Mutagenesis and computer modeling studies of a GPCR conserved residue W5.43(194) in ligand recognition and signal transduction for CB2 receptor. *Int Immunopharmacol* **2011,** 11, 1303-10.

PART 2

The structures and bioactivity information of all annotated cannabinoid ligands involved in this study are listed in the following table. There are totally 703 cannabinoid ligands, including 147 CB2 selective compounds and 149 CB1 selective compounds. The remaining 407 compounds are neither CB1 selective nor CB2 selective. Note that CB1 non-selective compounds include 147 CB2 selective and 407 non-selective compounds. The same analogy applies to the CB2 non-selective. The table below lists the structures of these compounds in SMILES format, CAS index number, corresponding K_i values for CB1 and CB2 receptors, and reference information from which K_i values were extracted. The unit of K_i values is nM. CAS index number can be used to locate the structure information in Science Finder search engine (SciFinder®), while reference can be retrieved by reference index. These data have been deposited into our online compound repository, www.cbligand.org.

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Table S3: list of annotated CB ligands

SMILES Structure	CAS Number	Ki CB1	Ki CB2	Reference
CCCCCCC(C)(C)c1cccc(OCC/C=C/C/C=C/CCCC(=O)N[C@H](C)CO)c1	**1000174-11-7**	**8.55**	**21.48**	**2007:1195242**
O=C(N[C@H](C)CO)CCC/C=C\C/C=C\CCOc1ccc(C(C)(C)CCCCCC)cc1	**1000174-12-8**	**194.85**	**78.22**	**2007:1195242**
O=C(N[C@H](C)CO)CCC/C=C\C/C=C\C/C=C\c1ccccc1C(C)(C)CCCCCC	**1000174-13-9**	**86.33**	**257.33**	**2007:1195242**
O=C(N[C@H](C)CO)CCC/C=C\C/C=C\CCOc1cccc(C(C)(C)CCCCO)c1	**1000174-14-0**	**78.97**	**10.9**	**2007:1195242**
O=C(N[C@H](C)CO)CCC/C=C\C/C=C\CCOc1cccc(C(C)(C)CCCCBr)c1	**1000174-15-1**	**2.74**	**2.52**	**2007:1195242**
O=C(CCC/C=C\C/C=C\C/C=C\CCOc1cc(C(C)(CCCCCC)C)ccc1)N[C@@H](CO)C	**1000174-18-4**	**131.33**	**189**	**2007:1195242**
O=C(c1c(=O)c2c(n(c1)CCN1CCOCC1)nc(cc2)N(C)C)NC1CCCCC1	**1000376-74-8**	**5600**	**94**	**2007:1279246**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1)cc(cc2)OC)NC1CCCCC1	**1000376-77-1**	**170**	**79**	**2007:1279246**
O=C(c1c(=O)c2c(n(c1)CCN1CCOCC1)cc(cc2)OC)NC1CCCCC1	**1000376-78-2**	**2920**	**79**	**2007:1279246**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1)cccc2)NC1CCCCCC1	**1000376-79-3**	**17**	**6.4**	**2007:1279246**
O=C(c1c(=O)c2c(n(c1)CCN1CCOCC1)cccc2)NC1CCCCCC1	**1000376-80-6**	**290**	**28**	**2007:1279246**
O=C(c1n(Cc2ccccc2)c2c(ccc(N)n2)c(=O)c1)NC1CCCCC1	**1000376-84-0**	**5600**	**7900**	**2007:1279246**
O=c1n(C2CCCCC2)nc2c1cn(Cc1ccccc1)c1c2cccc1	**1000376-85-1**	**620**	**790**	**2007:1279246**
O=c1n(C2CCCCC2)nc2c1cn(Cc1ccccc1)c1c2ccc(Cl)c1	**1000376-86-2**	**560**	**1640**	**2007:1279246**
O=c1n(C2CCCCC2)nc2c1cn(CCN1CCOCC1)c1c2cccc1	**1000376-87-3**	**5600**	**7900**	**2007:1279246**
O=c1n(c2ccccc2)nc2c1cn(CCN1CCOCC1)c1c2cccc1	**1000376-88-4**	**2800**	**2280**	**2007:1279246**
Oc1c2c3cc(O)ccc3C(C)(C)Oc2cc(C(C)(C)CCCCCC)c1	**1002320-51-5**	**2.6**	**4.8**	**2007:1374805**
CC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1)C(C)(C)CCCCCC	**105823-04-9**	**23**	**2.9**	**1996:544126**
CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)NCCc1ccc(O)c(O)c1	**105955-13-3**	**3920**	**12900**	**2000:819929**
OCC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1O)C(C)(C)CCCCCC	**112830-95-2**	**0.73**	**0.52**	**1996:544126**
OCC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1O)C(C)(C)CCCCCC	**112924-45-5**	**1990**	**10000**	**1997:406316**
O=C(c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1)c1cccc2c1cccc2	**137642-54-7**	**0.75**	**1.91**	**2005:980153**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(CCCCCF)c1	**138886-82-5**	**57.5**	**8.71**	**2000:338367**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(CCCCC(F)(F)F)c1	**138886-83-6**	**19.95**	**30.2**	**2000:338367**
Oc1cc(CCCCC)cc(O)c1[C@@H]1C=C(C)CC[C@H]1C(=C)C	**13956-29-1**	**4365.2**	**2884**	**2000:338367**
OC[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(O)cc(C(C)(C)CCCCCC)c1)(C)C	**140835-14-9**	**2.3**	**2.3**	**1998:546552**
CCCCCCCCCCCCCC(=O)NCCO	**142-58-5**	**1000**	**1000**	**1999:584470**

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CCCCCCCCCCCC(=O)NCCO	**142-78-9**	**1000**	**1000**	**1999:584470**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N[C@H](C)CO	**150314-39-9**	**138**	**398.1**	**2000:338367**
O=C(c1c2ccccc2n(CCCC)c1C)c1cccc2c1cccc2	**155471-09-3**	**22**	**4.29**	**2000:554114**
O=C(c1c2ccccc2n(CCCCCC)c1C)c1cccc2c1cccc2	**155471-11-7**	**48**	**4.02**	**2000:554114**
O=C(c1c2ccccc2n(CCCCCCC)c1C)c1cccc2c1cccc2	**155471-12-8**	**311**	**141**	**2000:554114**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NC[C@H](O)C	**157182-47-3**	**12.5**	**20**	**1998:635184**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NC[C@H](O)C	**157182-48-4**	**5.6**	**12**	**1998:635184**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N[C@H](C)CO	**157182-50-8**	**195**	**83**	**1998:635184**
O=C(NN1CCCCC1)c1c(C)c(c2ccc(Cl)cc2)n(c2c(Cl)cc(Cl)cc2)n1	**158681-13-1**	**12.3**	**707.9**	**2000:338367**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCCOC	**158840-64-3**	**1819.7**	**446.7**	**2000:338367**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NC1CCCCC1	**158940-64-8**	**2.46**	**228**	**2002:372410**
CCCCC/C=C\C[C@@H](/C=C\C=C/C/C=C/CCCC(=O)NCCO)O	**161744-52-1**	**207**	**131**	**1998:486973**
N1(CCC2=C/C(=C\c3cccc4c3cccc4)/c3c2cccc3)CCOCC1	**161809-35-4**	**148**	**132**	**1998:762250**
CC1=C(c2c(/C/1=C/c1cccc3c1cccc3)cccc2)CCN1CCOCC1	**161809-36-5**	**1945**	**658**	**1998:762250**
CC1=C(c2c(/C/1=C/c1cccc3c1cccc3)cccc2)CCN1CCOCC1	**161809-41-2**	**2.89**	**2.05**	**1998:762250**
O=C(c1cccc2c1cccc2)c1ccn(CCCCC)c1	**162934-73-8**	**87.1**	**316.2**	**2000:338367**
O=C(c1c2ccc(I)cc2n(CCN2CCOCC2)c1C)c1ccc(OC)cc1	**164178-33-0**	**5152**	**31.2**	**1999:171151**
OC[C@]1(C)[C@H]2CC[C@H](CO)C[C@@H]2c2c(O)cc(C(C)(C)CCCCCC)cc2O1	**164228-44-8**	**1.9**	**1.4**	**1998:546552**
OCC[C@]1(C)[C@H]2CC[C@H](CO)C[C@@H]2c2c(O)cc(C(C)(C)CCCCCC)cc2O1	**164228-45-9**	**2.8**	**2.3**	**1998:546552**
OCCC[C@]1(C)[C@H]2CC[C@H](CO)C[C@@H]2c2c(O)cc(C(C)(C)CCCCCC)cc2O1	**164228-46-0**	**2.2**	**3.4**	**1998:546552**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)NCCO	**164228-50-6**	**45.8**	**3062**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCC(C)(C)C(=O)NCCO	**164228-51-7**	**72.2**	**10000**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C(C)C)C(=O)NCCO	**164228-53-9**	**3981.1**	**5128.6**	**2000:338367**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N1CCOCC1	**166100-34-1**	**1148.2**	**537**	**2000:338367**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)NCCF	**166100-39-6**	**5.75**	**131.8**	**2000:338367**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**168273-06-1**	**6.18**	**313**	**2002:372410**
CC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1OC)C(C)(C)CCCCCC	**174627-50-0**	**924**	**65**	**2006:156948**
C=C1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCCCCC)c1)(C)C	**174627-56-6**	**529**	**35**	**2006:156948**

Supporting Information

Oc1cc(C(C)(C)CCCCCC)cc(O)c1c1cc(C)cc(C)c1	**174627-58-8**	**79**	**2**	**2007:862454**
Oc1cc(C(C)(C)CCCCCC)ccc1c1cc(C)cc(C)c1	**174627-59-9**	**2.7**	**2.3**	**2007:652168**
N#Cc1ccc(C(=O)c2c3ccc(OC)cc3oc2c2ccc(OC)cc2)cc1	**176977-56-3**	**203**	**10000**	**1998:53483**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCC#C	**177037-50-2**	**10.8**	**290**	**1998:786633**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2(CCCCCC)SCCS2)c1	**179044-94-1**	**0.32**	**0.52**	**2003:473442**
CCCCCCC(=O)c1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(O)c1	**179044-95-2**	**21.7**	**83.7**	**1998:170464**
OC[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(O)cc(C#CCCCCC)c1)(C)C	**180989-25-7**	**5.8**	**61.6**	**1996:513738**
OC[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(O)cc(/C=C\CCCCC)c1)(C)C	**180989-26-8**	**0.8**	**9.5**	**1996:513738**
OC[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(O)cc(CCCCCCC)c1)(C)C	**180989-27-9**	**8.7**	**14.3**	**1996:513738**
OC[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(O)cc(/C=C\CCCCC)c1)(C)C	**181139-62-8**	**1.2**	**5.3**	**1996:513738**
OCC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1)C(C)(C)CCCCCC	**181764-31-8**	**1.2**	**0.032**	**1996:544126**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**183232-63-5**	**16.8**	**1430**	**1999:84973**
O=C(c1c(C)c(c2ccc(I)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**183232-66-8**	**7.49**	**2290**	**1999:84973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCC(C)(C(=O)N[C@@H](CO)C)C	**187224-15-3**	**220**	**10000**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCC(C)(C)C(=O)NC[C@H](O)C	**187224-16-4**	**1288**	**10000**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCC(C)(C)C(=O)NC[C@H](O)C	**187224-18-6**	**107**	**421**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCC(C)(C)C(=O)N[C@H](C)CO	**187224-20-0**	**876**	**10000**	**2001:466973**
CC1(Oc2cc(C(CCCCC#N)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**189148-90-1**	**1.75**	**1.1**	**2001:120397**
Cc1ccc(Cn2nc(C(=O)N[C@H]3C(C)(C)[C@@H]4CC[C@@]3(C)C4)cc2c2ccc(Cl)c(C)c2)cc1	**192703-06-3**	**50.3**	**1.99**	**2001:87292**
Oc1c2c3cc(C)ccc3C(C)(C)Oc2cc(C(C)(C)CCCCCC)c1	**194714-91-5**	**0.95**	**1.1**	**2007:1374805**
OCc1cc2c3c(O)cc(C(C)(C)CCCCCC)cc3OC(C)(C)c2cc1	**194714-92-6**	**1**	**2.24**	**2000:626409**
O=c1c2ccc(C)cc2c2c(O)cc(C(C)(C)CCCCCC)cc2o1	**194714-93-7**	**39**	**3.1**	**2007:1374805**
CCCCCc1c2CCCOc2c2[C@@H]3[C@H](CCC(=C)C3)C(C)(C)Oc2c1	**195866-29-6**	**884**	**200**	**1997:603435**
O=C1CC[C@H]2[C@@H](c3c4c(CCCO4)c(CCCCC)cc3OC2(C)C)C1	**195866-31-0**	**90**	**23**	**1997:603435**
O[C@H]1CC[C@H]2[C@@H](c3c4c(CCCO4)c(CCCCC)cc3OC2(C)C)C1	**195866-35-4**	**26**	**5.8**	**1997:603435**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C#CCCCCC)c1	**205746-46-9**	**0.65**	**3.1**	**2006:128508**
O[C@H](CCCCCC)c1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(O)c1	**205746-47-0**	**86.4**	**65.6**	**1998:170464**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C(=C)CCCCCC)c1	**205746-48-1**	**2.17**	**3.3**	**1998:170464**

Oc1cc(C2(CCCCCC)SCCS2)cc(O)c1[C@@H]1C=C(C)CC[C@H]1C(=C)C	**205746-54-9**	**136**	**50.4**	**1998:170464**
O=C(c1c(C)c(c2ccccc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**207805-44-5**	**123**	**217**	**1999:84973**
O=C(c1c2ccccc2n(CCCC)c1)c1cccc2c1cccc2	**208987-48-8**	**8.9**	**38**	**2000:554114**
O=C(c1c2ccccc2n(CC)c1C)c1cccc2c1cccc2	**209414-03-9**	**1180**	**964**	**2000:554114**
O=C(c1c2ccccc2n(C)c1)c1cccc2c1cccc2	**209414-04-0**	**10000**	**10000**	**2000:554114**
O=C(c1c2ccccc2n(CC)c1)c1cccc2c1cccc2	**209414-05-1**	**1340**	**2940**	**2000:554114**
O=C(c1cccc2c1cccc2)c1c2ccccc2n(CCC)c1	**209414-06-2**	**1050**	**170**	**2000:554114**
O=C(c1cccc2c1cccc2)c1c2ccccc2n(CCCCC)c1	**209414-07-3**	**9**	**2.94**	**2000:554114**
O=C(c1c2ccccc2n(CCCCCC)c1)c1cccc2c1cccc2	**209414-08-4**	**9.8**	**5.55**	**2000:554114**
O=C(c1c2ccccc2n(CCCCCCC)c1)c1cccc2c1cccc2	**209414-09-5**	**128**	**205**	**2000:554114**
O=C(c1ccc(OC)c2c1cccc2)c1c2ccccc2n(C)c1	**210179-35-4**	**10000**	**10000**	**2000:554114**
O=C(c1c2ccccc2n(CC)c1)c1ccc(OC)c2c1cccc2	**210179-37-6**	**817**	**633**	**2000:554114**
O=C(c1ccc(OC)c2c1cccc2)c1c2ccccc2n(CCC)c1	**210179-40-1**	**63**	**32**	**2000:554114**
O=C(c1c2ccccc2n(CCCC)c1)c1ccc(OC)c2c1cccc2	**210179-44-5**	**5.6**	**2.21**	**2000:554114**
O=C(c1ccc(OC)c2c1cccc2)c1c2ccccc2n(CCCCC)c1	**210179-46-7**	**1.2**	**12.4**	**2000:554114**
O=C(c1c2ccccc2n(CCCCCC)c1)c1ccc(OC)c2c1cccc2	**210179-48-9**	**5.3**	**6.4**	**2000:554114**
OCCNC(=O)CCC/C=C\C/C=C\C/C=C\C=C\[C@@H](CCCCC)O	**212144-00-8**	**738**	**1000**	**1998:486973**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc([C@]23C[C@@H]4C[C@H](C2)C[C@@H](C4)C3)c1	**212835-02-4**	**6.8**	**52**	**2006:128508**
OC[C@@H]1C[C@H]2[C@H](CC1)[C@](Oc1c2c(O)cc(C(C)(C)CCCCCC)c1)(CCl)C	**213915-67-4**	**40.7**	**9.7**	**1998:546552**
OC[C@@H]1C[C@H]2[C@H](CC1)[C@](Oc1c2c(O)cc(C(C)(C)CCCCCC)c1)(CCCl)C	**213915-68-5**	**2.2**	**4.3**	**1998:546552**
OC[C@@H]1C[C@H]2[C@H](CC1)[C@](Oc1c2c(O)cc(C(C)(C)CCCCCC)c1)(CC)C	**213915-69-6**	**11.1**	**21.5**	**1998:546552**
OC[C@@H]1C[C@H]2[C@H](CC1)[C@@](Oc1c2c(O)cc(C(C)(C)CCCCCC)c1)(C)CCC	**213915-70-9**	**14.4**	**38.9**	**1998:546552**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCNCCO	**215818-33-0**	**1300**	**4200**	**1998:635184**
C[C@@H](NCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)CO	**215818-34-1**	**980**	**2100**	**1998:635184**
CC(=O)NCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC	**215818-35-2**	**560**	**9600**	**1998:635184**
O=C(CCCN1CCOCC1)Oc1cc(C(C)(CCCCC#N)C)cc2c1[C@@H]1[C@@H](C(C)(O2)C)CC=C(C1)C	**216988-51-1**	**4.36**	**11.2**	**2000:309882**
N1(CCC2=C/C(=C\c3cccc4c3cccc4)/c3c2cccc3)CCOCC1	**220080-15-9**	**2.72**	**2.72**	**1998:762250**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(CC#CCCCN=[N+]=[N-])c1	**220543-77-1**	**5.24**	**7.4**	**1999:709954**

Supporting Information

CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCCCl	**220556-69-4**	**5.29**	**195**	**1998:786633**
O=C(c1c(C)c(c2ccc([N+](=O)[OH-])cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**221385-25-7**	**57.5**	**252**	**1999:84973**
O=C(c1c(C)c(c2ccccc2[N+](=O)[OH-])n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**221385-26-8**	**255**	**691**	**1999:84973**
O=C(c1c(C)c(c2ccc(N)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**221385-28-0**	**81.5**	**958**	**1999:84973**
O=C(c1c(C)c(c2ccccc2N)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**221385-29-1**	**346**	**931**	**1999:84973**
O=C(c1c(C)c(c2ccccc2I)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**221385-30-4**	**53.8**	**577**	**1999:84973**
O=C(c1c(C)c(CC)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**221385-33-7**	**183**	**744**	**1999:84973**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2)n1)NN1CCCCC1	**221385-35-9**	**60.4**	**836**	**1999:84973**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCC1	**221385-37-1**	**17.1**	**1310**	**1999:84973**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCCCCC1	**221385-38-2**	**7.85**	**215**	**1999:84973**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCOCC1	**221385-39-3**	**53.9**	**2450**	**1999:84973**
O=C(N1CCCCC1)c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1	**221385-40-6**	**125**	**4580**	**1999:84973**
CN1CCN(C(=O)c2c(C)c(c3ccc(Br)cc3)n(c3ccc(Cl)cc3Cl)n2)CC1	**221385-41-7**	**326**	**2340**	**1999:84973**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)NC1CCCCC1	**221385-42-8**	**11.7**	**1010**	**1999:84973**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)N(C1CCCCC1)C	**221385-43-9**	**76.7**	**1260**	**1999:84973**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCO	**221385-44-0**	**1120**	**19000**	**1999:84973**
O=C(c1c(C)c(c2ccc(Br)cc2)n(c2ccc(Cl)cc2Cl)n1)Nc1ccccc1	**221385-45-1**	**31.1**	**6750**	**1999:84973**
OCC(OCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)CO	**222723-55-9**	**21.2**	**3000**	**2001:266178**
CC1(Oc2cc(C(CCCCC(=O)N(C)C)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**228997-38-4**	**2.47**	**1.98**	**2001:120397**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NC1CC1	**229021-64-1**	**2.2**	**700**	**1999:335427**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(CC#CCCCCC)c1	**229030-02-8**	**4.26**	**9.33**	**1999:709954**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)Nc1ccc(OC)cc1	**231632-72-7**	**500**	**4000**	**2005:1241404**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C[C@]23C[C@@H]4C[C@H](C2)C[C@@H](C4)C3)c1	**249888-97-9**	**29.3**	**26.9**	**2005:529462**
CCCCCC#CCc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**252350-31-5**	**2.34**	**9.77**	**1999:709954**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCCCCC)c1)(C)C	**259869-52-8**	**7.9**	**5.2**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCCCCC)c1)(C)C	**259869-53-9**	**28**	**23**	**2006:156948**
CC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1)C(C)(C)CC	**259869-54-0**	**2290**	**14**	**2006:156948**
CC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1)C(C)(C)CCC	**259869-55-1**	**677**	**3.4**	**2006:156948**

Supporting Information

O=C(c1cc2c([nH]c1=O)c(OCCCCC)c(OC)cc2)NCc1ccc2OCOc2c1	**282089-49-0**	**2370**	**35.9**	**2001:87292**
Cc1c(CC(=O)N2CCOCC2)c2cc(OC)ccc2n1C(=O)c1ccc(Cl)cc1	**2854-32-2**	**2000**	**435**	**1999:714292**
O=C(c1cc2c3c(OC)cc(C(C)(C)CCCCCC)cc3OC(C)(C)c2cc1)OC	**305833-26-5**	**10000**	**529**	**2000:626409**
Cc1cc2c3ccc(C(C)(C)CCCCCC)cc3OC(C)(C)c2cc1	**305833-29-8**	**434**	**167**	**2000:626409**
O=C(c1cc2c3ccc(C(C)(C)CCCCCC)cc3OC(C)(C)c2cc1)OC	**305833-31-2**	**558**	**276**	**2000:626409**
OCc1cc2c3ccc(C(C)(C)CCCCCC)cc3OC(C)(C)c2cc1	**305833-32-3**	**2**	**1**	**2000:626409**
Oc1cc(C(C)(C)CCCCCC)ccc1c1cc(C)ccc1C(C)C	**305833-34-5**	**33**	**3**	**2002:336112**
Cc1cc2c3c(OC)cc(C(C)(C)CCCCCC)cc3OC(C)(C)c2cc1	**305833-35-6**	**681**	**286**	**2000:626409**
O=C(c1cc2c3c(O)cc(C(C)(C)CCCCCC)cc3OC(C)(C)c2cc1)OC	**305833-36-7**	**14**	**3.8**	**2000:626409**
O=C(c1cc2c3ccc(C(C)(C)CCC)cc3OC(C)(C)c2cc1)OC	**305833-37-8**	**10000**	**611**	**2000:626409**
OCc1cc2c3ccc(C(C)(C)CCC)cc3OC(C)(C)c2cc1	**305833-38-9**	**204**	**67**	**2000:626409**
Oc1c2c3cc(C)ccc3C(C)(C)Oc2cc(C(C)(C)CCC)c1	**305833-45-8**	**42**	**6**	**2000:626409**
Oc1cc(C(C)(C)CCC)ccc1c1cc(C)ccc1C(C)C	**305833-50-5**	**876**	**113**	**2002:336112**
O=C(c1c(C#N)c(c2ccc(OC)cc2)n(c2ccccc2Cl)n1)Nc1ccccc1	**312494-20-5**	**57**	**114**	**2000:677056**
O=C(c1cccc2c1cc(cc2)C)c1c2ccccc2n(CCC)c1C	**316189-64-7**	**343**	**16.3**	**2000:554114**
O=C(c1c2ccccc2n(CCCC)c1C)c1cccc2c1cc(cc2)C	**316189-65-8**	**58.7**	**3.47**	**2000:554114**
O=C(c1cccc2c1cc(cc2)C)c1c2ccccc2n(CCCCC)c1C	**316189-66-9**	**10.7**	**0.49**	**2000:554114**
O=C(c1c2ccccc2n(CCCCCC)c1C)c1cccc2c1cc(cc2)C	**316189-67-0**	**55.1**	**32.3**	**2000:554114**
O=C(c1c2cc(C)ccc2ccc1)c1cn(CCCCCCC)c2ccccc12	**316189-68-1**	**342**	**526**	**2000:554114**
O=C(c1c2ccccc2n(CCCCCCC)c1)c1cccc2c1cc(cc2)C	**316189-69-2**	**106**	**102**	**2000:554114**
O=C(c1c(C)n(CCC)c2ccccc12)c1c2ccccc2c(OC)cc1	**316189-70-5**	**476**	**97.3**	**2000:554114**
O=C(c1c2ccccc2c(OC)cc1)c1c(CCCC)n(CCC)c2ccccc12	**316189-71-6**	**40.7**	**59.1**	**2000:554114**
O=C(c1c2ccccc2c(OC)cc1)c1c(C)n(CCCC)c2ccccc12	**316189-72-7**	**33.7**	**13.3**	**2000:554114**
O=C(c1c2ccccc2c(OC)cc1)c1c(CCCCC)n(CCCC)c2ccccc12	**316189-73-8**	**140**	**312**	**2000:554114**
O=C(c1c(C)n(CCCCC)c2ccccc12)c1c2ccccc2c(OC)cc1	**316189-74-9**	**4.5**	**1.88**	**2000:554114**
O=C(c1c2ccccc2c(OC)cc1)c1c(CCCCCC)n(CCCCC)c2ccccc12	**316189-75-0**	**455**	**121**	**2000:554114**
O=C(c1c2ccccc2c(OC)cc1)c1c(C)n(CCCCCC)c2ccccc12	**316189-76-1**	**35.3**	**17.8**	**2000:554114**
O=C(c1c2ccccc2c(OC)cc1)c1c(C)n(CCCCCCC)c2ccccc12	**316189-77-2**	**381**	**155**	**2000:554114**

Supporting Information

CCCCC/C=C\C/C=C\CC/C=C\CCCC(=O)NCCc1ccc(O)c(O)c1	**320782-29-4**	**1000**	**11300**	**2000:819929**
CCCCCCC(C)(C)/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCc1ccc(O)c(OC)c1	**322399-51-9**	**261.8**	**10000**	**2001:122170**
O=C(NCc1ccc(O)c(OC)c1)CCC/C=C\C/C=C\C/C=C\C/C=C\C(C)(C)CCCCO	**322399-54-2**	**789.7**	**10000**	**2001:122170**
O=C(NCc1ccc(O)c(OC)c1)CCC/C=C\C/C=C\C/C=C\C/C=C\C(C)(C)CCCCBr	**322399-59-7**	**32.6**	**10000**	**2001:122170**
O=C(NCc1ccc(O)c(OC)c1)CCC/C=C\C/C=C\C/C=C\C/C=C\C(C)(C)CCCCC#N	**322399-60-0**	**67**	**5000**	**2001:122170**
O=C(N1/C(=N/c2ccccc2C(C)C)/SCC(C1)(C)C)OCC	**330479-67-9**	**5000**	**428**	**2007:684708**
O=c1c2ccc(O)cc2c2c(O)cc(C(C)(C)CCCCCC)cc2o1	**335371-37-4**	**400**	**0.82**	**2007:1374805**
Oc1c2c3cc(OC)ccc3C(C)(C)Oc2cc(C(C)(C)CCCCCC)c1	**335371-40-9**	**5.4**	**5.9**	**2007:1374805**
N#Cc1ccc(OCCCCC(c2cc3c([C@@H]4[C@H](CC=C(C)C4)C(C)(C)O3)c(O)c2)(C)C)cc1	**336104-65-5**	**1.5**	**1.14**	**2001:120397**
CC1(Oc2cc(C(CCCCC(=O)Nc3ccc(S(=O)(=O)N)cc3)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-66-6**	**41.5**	**10.3**	**2001:120397**
CC1(Oc2cc(C(CCCCC(=O)NN3CCCCC3)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-67-7**	**4.51**	**3.23**	**2001:120397**
CC1(Oc2cc(C(CCCCC(=O)Nc3c(Cl)cc(Cl)cc3)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-68-8**	**41.2**	**37.2**	**2001:120397**
CC1(Oc2cc(C(CCCCC(=O)N(CC)CC)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-69-9**	**23.9**	**2.47**	**2001:120397**
CC1(Oc2cc(C(CCCC[C@H](c3ccccc3)C#N)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-70-2**	**18.4**	**5.75**	**2001:120397**
CC1(Oc2cc(C(CCCCC(=O)NCc3ccc(S(=O)(=O)N)cc3)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-71-3**	**180**	**2.27**	**2001:120397**
CC1(Oc2cc(C(CCCCC(=O)O)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-73-5**	**222**	**4**	**2001:120397**
CC1(Oc2cc(C(CCCCCC#N)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-74-6**	**0.19**	**2.94**	**2001:120397**
CC1(Oc2cc(C(CCCCC(=O)Nc3ccc(Cl)cc3)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-76-8**	**395**	**11.3**	**2001:120397**
CC1(Oc2cc(C(CCCC[C@H](C#N)O)(C)C)cc(O)c2[C@H]2CC(=CC[C@H]12)C)C	**336104-77-9**	**21.3**	**3.22**	**2001:120397**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCCCC	**336615-64-6**	**11.4**	**1110**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCC	**336615-69-1**	**29.9**	**2960**	**2002:372410**
O=C(N[C@H](C)CO)CCC/C=C\C/C=C\C/C=C\C/C=C\C(C)(C)CCCCO	**342882-76-2**	**115.2**	**800.1**	**2001:122170**
O=C(N[C@H](C)CO)CCC/C=C\C/C=C\C/C=C\C/C=C\C(C)(C)CCCCC#N	**342882-77-3**	**3.4**	**3870**	**2001:122170**
O=C(N[C@H](C)CO)CCC/C=C\C/C=C\C/C=C\C/C=C\C(C)(C)CCCCBr	**342882-78-4**	**2.2**	**10000**	**2001:122170**
O=C(OC)[C@H](Cc1ccccc1)NC(=O)c1c2cccc(OC)c2n(CCN2CCOCC2)c1C	**354569-07-6**	**4000**	**8**	**2002:585100**
O=c1n(Cc2ccccc2OC)ccc2c1c1cccc(OC)c1n2CCN1CCOCC1	**354570-13-1**	**3700**	**67**	**2003:320274**
O=c1n([C@@H]2[C@@]3(C[C@@H](CC3)C2(C)C)C)ccc2c1c1cccc(OC)c1n2CCN1CCOCC1	**354570-35-7**	**16**	**1**	**2003:320274**
N=C(N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)NS(=O)(=O)c1ccc(F)cc1	**362519-28-6**	**52.6**	**1000**	**2003:1011327**

Supporting Information

N=C(N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)NS(=O)(=O)c1c(C)cc(C)cc1C	**362519-37-7**	**24.2**	**1000**	**2003:1011327**
CN(C)/C(=N\S(=O)(=O)c1ccc(Cl)cc1)/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1	**362519-41-3**	**280**	**1000**	**2003:1011327**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)c1ccc(Cl)cc1	**362519-49-1**	**25.2**	**1000**	**2003:1011327**
N=C(N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)NS(=O)(=O)c1ccc(Cl)cc1	**362519-50-4**	**16.1**	**1000**	**2003:1011327**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)c1cccc(Cl)c1	**362519-52-6**	**13.9**	**1000**	**2003:1011327**
O=S(=O)(N/C(=N\C)/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)c1ccc(C(F)(F)F)cc1	**362519-66-2**	**221**	**1000**	**2003:1011327**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)NCCO	**372504-52-4**	**54.1**	**4905**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)NCCO	**372504-55-7**	**35.3**	**4259**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)N[C@H](C)CO	**372504-60-4**	**7.42**	**1952**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)N[C@H](C)CO	**372504-63-7**	**185**	**4876**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)N[C@H](C)CO	**372504-66-0**	**389**	**2876**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CC[C@H](C)C(=O)N[C@H](C)CO	**372504-69-3**	**233**	**4695**	**2001:466973**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCc1cccn1C	**390824-18-7**	**124**	**70**	**2001:836853**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCc1ccoc1	**390824-20-1**	**1000**	**67**	**2001:836853**
CC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1F)CCCCCCC	**431041-31-5**	**1557**	**1508**	**2007:228762**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCC	**443141-78-4**	**46.3**	**3110**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NC(C)C	**443141-79-5**	**29.4**	**1740**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCCC	**443141-80-8**	**13.4**	**1600**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCC(C)C	**443141-81-9**	**11.5**	**704**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCCCCC	**443141-82-0**	**18.1**	**6870**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NN1CCOCC1	**443141-83-1**	**22.9**	**2400**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NO	**443141-84-2**	**1690**	**7820**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCO	**443141-85-3**	**385**	**4270**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCCO	**443141-86-4**	**160**	**1250**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NCCCCO	**443141-87-5**	**154**	**5720**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)N[C@H](C)CO	**443141-88-6**	**117**	**5900**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)N[C@H](C)CO	**443141-89-7**	**117**	**1770**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NN	**443141-90-0**	**374**	**12100**	**2002:372410**

Supporting Information

O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NNC	**443141-91-1**	**555**	**6660**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NNCC	**443141-92-2**	**143**	**6061**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NNCCC	**443141-93-3**	**74.8**	**2620**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NNCCCC	**443141-94-4**	**50.9**	**2850**	**2002:372410**
O=C(c1c(C)c(c2ccc(Cl)cc2)n(c2ccc(Cl)cc2Cl)n1)NNCC(C)C	**443141-95-5**	**41.8**	**2190**	**2002:372410**
O=C(c1ccccc1I)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1	**444912-55-4**	**1.8**	**2.2**	**2005:980153**
O=C(c1ccccc1I)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1	**444912-57-6**	**560**	**580**	**2005:980153**
O=C(c1ccccc1I)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1	**444912-75-8**	**2.8**	**2.9**	**2005:980153**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)c1ccc(Cl)cc1	**464213-10-3**	**7.8**	**7943**	**2003:1011327**
O=S(=O)(N/C(=N\C)/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)c1ccc(C(F)(F)F)cc1	**464213-13-6**	**35.9**	**3515**	**2003:1011327**
OCc1ccc(C(C)C)c(c2ccc(C(C)(C)CCCCCC)cc2O)c1	**468083-72-9**	**5**	**3**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1C1CCCC1	**468083-73-0**	**95**	**7**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1C1CCCCC1	**468083-74-1**	**11**	**1.5**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1C1CCCCCC1	**468083-75-2**	**18**	**2**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1[C@@H]1[C@@H]2C[C@H]3C[C@@H](C2)C[C@@H]1C3	**468083-76-3**	**7**	**3**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1C1CCSCC1	**468083-77-4**	**153**	**12**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1[C@@H]1CSCC1	**468083-78-5**	**138**	**28**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1C1CCN(C)CC1	**468083-79-6**	**10000**	**5424**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1C1=CCCCC1	**468083-80-9**	**97**	**28**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1[C@H]1[C@H](C)CCCC1	**468083-82-1**	**16**	**1**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1[C@H]1CC[C@H](C)CC1	**468083-83-2**	**45**	**5**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1[C@H]1CC[C@H](c2ccccc2)CC1	**468083-84-3**	**144**	**9**	**2002:336112**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1[C@@H]1C[C@H](C)CCC1	**468083-85-4**	**14**	**0.8**	**2002:336112**
Oc1cc(C(C)(C)CCC)cc(O)c1[C@@H]1C[C@H](C)CCC1	**468083-86-5**	**96**	**13**	**2002:336112**
C[C@@H]1C[C@H](c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CCC1	**468083-89-8**	**10000**	**466**	**2002:336112**
COc1c(C2CCOCC2)c(OC)cc(C(C)(C)CCCCCC)c1	**468083-90-1**	**10000**	**911**	**2002:336112**
OC1(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CCOCC1	**468083-92-3**	**10000**	**342**	**2002:336112**
OC1(CCC2(CC1)OCCO2)c1c(OC)cc(C(C)(C)CCCCCC)cc1OC	**468083-93-4**	**4581**	**126**	**2002:336112**

Supporting Information

O[C@H]1C[C@H]2O[C@@]2(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CC1	**468083-94-5**	**3758**	**1065**	**2002:336112**
O=C1CC=C(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CC1	**468083-95-6**	**8442**	**1773**	**2002:336112**
O=C1CCC(O)(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CC1	**468083-96-7**	**4572**	**346**	**2002:336112**
O=C1C[C@](O)(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)C[C@H](C)C1	**468083-97-8**	**1731**	**125**	**2002:336112**
OC1(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CCCCC1	**468083-98-9**	**5820**	**105**	**2002:336112**
O[C@]1(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)C[C@@H](O)C[C@@H](C)C1	**468084-00-6**	**1990**	**101**	**2002:336112**
O[C@]1(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CC[C@H](O)CC1	**468084-01-7**	**10000**	**1561**	**2002:336112**
O[C@@]1(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CC(C)(C)CCC1	**468084-02-8**	**7515**	**161**	**2002:336112**
O[C@]1(c2c(OCC)cc(C(C)(C)CCCCCC)cc2OCC)C[C@@H](C)CCC1	**468084-04-0**	**8810**	**858**	**2002:336112**
OC1(c2c(OC)cc(C(C)(C)CCCCCC)cc2OC)CCCCCC1	**468084-05-1**	**3201**	**64**	**2002:336112**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)NN1CCCCC1	**494844-07-4**	**0.00035**	**21**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1ccccc21)NN1CCCCC1	**494844-08-5**	**168**	**18.1**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)NN1CCCCCC1	**494844-12-1**	**0.001**	**2**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1ccc(Cl)cc21)NN1CCCCC1	**494844-13-2**	**31.2**	**26.8**	**2005:1118017**
Oc1ccc(C[C@@H](C(=O)OC)NC(=O)/C=C/c2ccc(OC)c(OCCCCC)c2)cc1	**501926-53-0**	**5700**	**120**	**2002:585100**
O=C(c1c2cccc(OC)c2n(CCN2CCOCC2)c1)N[C@@H]1[C@@]2(C[C@@H](CC2)C1(C)C)C	**501926-82-5**	**245**	**11**	**2003:320274**
O=C(c1c2cccc(OC)c2n(CCN2CCOCC2)c1C)N[C@@H]1[C@@]2(C[C@@H](CC2)C1(C)C)C	**501927-29-3**	**8**	**29**	**2003:320274**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)N(CC)C	**505030-92-2**	**117**	**1871**	**2005:1024928**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)N(CC)CC	**505031-03-8**	**30**	**3270**	**2005:1024928**
O=S(=O)(/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NC)N1CCCC1	**505031-04-9**	**231**	**1601**	**2005:1024928**
O=S(=O)(/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NC)N1CCCCC1	**505031-07-2**	**152**	**1321**	**2005:1024928**
O=S(=O)(/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NC)N(C)C(C)C	**505031-09-4**	**32**	**1126**	**2005:1024928**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)N1CCCCCCC1	**505031-10-7**	**125**	**2584**	**2005:1024928**
CN/C(=N\S(=O)(=O)N(C)C)/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1	**505031-11-8**	**223**	**3835**	**2005:1024928**
CCN/C(=N\S(=O)(=O)N(CC)CC)/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1	**505031-40-3**	**209**	**2864**	**2005:1024928**
CC(/N=C(\N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)/NS(=O)(=O)N(CC)CC)C	**505031-43-6**	**60**	**2755**	**2005:1024928**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2cccnc2)C1)\NS(=O)(=O)N(CC)CC	**505031-49-2**	**141**	**9077**	**2005:1024928**
O=S(=O)(/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NC)N1CCCCC1	**505031-78-7**	**58**	**3495**	**2005:1024928**

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O=C(c1c(C)n(c2ccc(Cl)cc2Cl)c(c2ccc(Cl)cc2)n1)NN1CCCCC1	**505073-38-1**	**403**	**208**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NOC(C)(C)C	**505073-41-6**	**333**	**242**	**2004:790826**
O=C(c1c(CC)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**505073-43-8**	**30**	**608**	**2004:790826**
O=C(c1c(C)n(c2ccc(Br)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**505073-44-9**	**60**	**489**	**2004:790826**
O=C(c1c(C)n(c2ccc(C(F)(F)F)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**505073-81-4**	**29**	**634**	**2004:790826**
O=C(c1c(C)n(c2ccc(F)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**505074-09-9**	**52**	**765**	**2004:790826**
O=C(c1c(C)n(c2ccc(OC)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**505074-10-2**	**106**	**326**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1C[C@H]2[C@H](CCC2)C1	**505074-28-2**	**40**	**1412**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)N[C@H]1CC[C@H](O)CC1	**505074-33-9**	**399**	**3469**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)N[C@@H]1[C@@H]2C[C@@H](CC2)C1	**505074-35-1**	**19**	**54**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCCC1	**505074-37-3**	**64**	**505**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCC1	**505074-38-4**	**27**	**774**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCOCC1	**505074-39-5**	**197**	**3297**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NCc1ccc(C(F)(F)F)cc1	**505074-51-1**	**171**	**1984**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NC1CCCC1	**505074-52-2**	**33**	**357**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NC1CCCCCC1	**505074-53-3**	**35**	**349**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)OC(C)(C)C	**505074-58-8**	**94**	**815**	**2004:790826**
O=C(c1c(C#N)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**505074-60-2**	**30**	**1590**	**2004:790826**
Oc1c2c3cc(C)ccc3C(C)(C)Oc2cc(CCCCC)c1	**521-35-7**	**309**	**95.5**	**2000:338367**
OCC1=CC[C@H]2[C@H](C1)c1c(OC2(C)C)cc(cc1)C(C)(C)CCCCCC	**525587-98-8**	**1.2**	**0.032**	**2006:156948**
O=C(c1c2cccc(OC)c2n(CCN2CCOCC2)n1)N[C@@H]1[C@@]2(C[C@@H](CC2)C1(C)C)C	**545424-33-7**	**24**	**2**	**2003:320274**
O=C(c1c2cccc(OC)c2n(CCN2CCOCC2)n1)N[C@@H](c1ccccc1)c1ncccc1	**545424-35-9**	**162**	**146**	**2003:320274**
O=C(c1ccc(C)c2c1cccc2)c1c2ccccc2n(CCCCC)c1C	**548461-82-1**	**5**	**0.73**	**2004:1043347**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NC1CCCCC1	**572889-89-5**	**35**	**160**	**2004:790826**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2(CCCCCC)CCCC2)c1	**579444-43-2**	**0.45**	**1.92**	**2003:473442**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2(CCCCCC)SCCCS2)c1	**579444-44-3**	**1.8**	**3.6**	**2003:473442**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2(CCCCCC)OCCO2)c1	**579444-45-4**	**0.52**	**0.22**	**2003:473442**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc([C@@]2(CCCCCC)Sc3ccccc3S2)c1	**579444-46-5**	**56.9**	**257**	**2003:473442**

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Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc([C@@]2(CCCCCC)S[C@H](C)[C@@H](C)S2)c1	**581068-72-6**	**32.3**	**19.7**	**2003:473442**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(CCCCC)c1	**5957-75-5**	**28.5**	**25**	**2003:462556**
O=C(c1nc(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)s1)NN1CCCCC1	**605670-36-8**	**1000**	**4668**	**2004:790826**
O=C(c1nc(c2ccc(Cl)cc2Cl)c(c2ccc(Cl)cc2)s1)NN1CCCCC1	**605670-37-9**	**227**	**5841**	**2004:790826**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C(C)(C)CCCCCC)c1	**61597-27-1**	**0.83**	**0.49**	**2003:473442**
O=C(c1ccc(C)c2c1cccc2)c1c2ccccc2n(CCCCC)c1	**619294-47-2**	**0.69**	**1.2**	**2004:1043347**
Oc1cc(C(C)(C)CCCCCC)cc(O)c1[C@@H]1CC(C)(C)CCC1	**620964-96-7**	**2**	**0.3**	**2002:336112**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2(C3CCCC3)SCCS2)c1	**623560-04-3**	**9.49**	**2.74**	**2003:462556**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2(C3CCCCC3)SCCS2)c1	**623560-05-4**	**1.86**	**1.05**	**2003:462556**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2(C3CCCCCC3)SCCS2)c1	**623560-08-7**	**1.76**	**6.62**	**2003:462556**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C(C)(C2CCCC2)C)c1	**623560-10-1**	**0.34**	**0.39**	**2003:462556**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C(C)(C2CCCCC2)C)c1	**623560-11-2**	**0.57**	**0.65**	**2003:462556**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C(C)(C2CCCCCC2)C)c1	**623560-12-3**	**0.94**	**0.22**	**2003:462556**
N=C(N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)NS(=O)(=O)c1ccc(C)cc1	**656827-41-7**	**197**	**1000**	**2003:1011327**
N=C(N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)NS(=O)(=O)c1ccc(OC)cc1	**656827-42-8**	**196**	**1000**	**2003:1011327**
O=S(=O)(/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\SC)c1ccc(C(F)(F)F)cc1	**656827-49-5**	**16.6**	**1000**	**2003:1011327**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)c1ccccc1Cl	**656827-52-0**	**75.4**	**1000**	**2003:1011327**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)c1ccc(F)cc1	**656827-72-4**	**338**	**1000**	**2003:1011327**
O=S(=O)(N/C(=N\C)/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)c1cccc(C(F)(F)F)c1	**656827-75-7**	**36.5**	**1000**	**2003:1011327**
O=S(=O)(N/C(=N\C)/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)c1ccc(C(F)(F)F)cc1	**656827-82-6**	**293**	**1000**	**2003:1011327**
CCCCCCCC/C=C\CCCCCCCC(=O)N[C@H](c1ccccc1)CO	**709671-89-6**	**2.7**	**2**	**2004:735312**
CCCCCCCC/C=C\CCCCCCCC(=O)N[C@H](CO)Cc1ccccc1	**709672-12-8**	**0.5**	**2.5**	**2004:735312**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C2SCCS2)c1	**71555-69-6**	**168**	**103**	**2003:473442**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1CC(F)(F)F	**784192-17-2**	**0.3**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1C1CCCCC1	**784192-19-4**	**20**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1CC	**784192-22-9**	**4**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1CC(F)F	**784192-23-0**	**0.6**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1CCF	**784192-24-1**	**3**	**10000**	**2005:1341997**

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O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1CCC	**784192-25-2**	**2**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1CCC(F)(F)F	**784192-27-4**	**1.8**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2nc(CC)n1CC(F)(F)F	**784192-59-2**	**1**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2nc(C(C)C)n1CC(F)(F)F	**784192-60-5**	**6**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2nc(C)n1CC(F)(F)F	**784192-63-8**	**0.6**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ccn1CC(F)(F)F	**784192-98-9**	**1**	**10000**	**2005:1341997**
O=C(c1nc(c2ccc(Cl)cc2Cl)n(c2ccc(Cl)cc2)n1)NN1CCCCC1	**793666-99-6**	**356**	**3562**	**2004:790826**
O=C(c1c(C)n(c2ncc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**796875-29-1**	**55**	**758**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)N1CC[C@H](O)CC1	**796875-33-7**	**172**	**3959**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)N1CCc2c(C1)cccc2	**796875-35-9**	**34**	**696**	**2004:790826**
O=C(c1c(C)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)N(CC)CC	**796875-36-0**	**828**	**2520**	**2004:790826**
O=C(c1c(Cl)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**796875-41-7**	**27**	**823**	**2004:790826**
O=C(c1c(Br)n(c2ccc(Cl)cc2)c(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**796875-42-8**	**23**	**746**	**2004:790826**
O=C(c1ccc(C)c2c1cccc2)c1c2ccccc2n(CCC)c1	**824955-98-8**	**1054**	**6.1**	**2004:1043347**
O=C(c1ccc(C)c2c1cccc2)c1c2ccccc2n(CCC)c1C	**824955-99-9**	**123**	**14**	**2004:1043347**
O=C(c1ccc(CC)c2c1cccc2)c1c2ccccc2n(CCC)c1	**824959-71-9**	**33**	**10**	**2004:1043347**
O=C(c1ccc(CC)c2c1cccc2)c1c2ccccc2n(CCC)c1C	**824959-72-0**	**70**	**12**	**2004:1043347**
O=C(c1ccc(CC)c2c1cccc2)c1c2ccccc2n(CCCCC)c1	**824959-81-1**	**0.46**	**0.69**	**2004:1043347**
O=C(c1ccc(CC)c2c1cccc2)c1c2ccccc2n(CCCCC)c1C	**824959-83-3**	**1.5**	**0.42**	**2004:1043347**
O=C(c1c2ccccc2n(CCC)c1)c1ccc(CCC)c2c1cccc2	**824959-87-7**	**26**	**9.6**	**2004:1043347**
O=C(c1c2ccccc2n(CCC)c1C)c1ccc(CCC)c2c1cccc2	**824960-01-2**	**52**	**12**	**2004:1043347**
O=C(c1c2ccccc2n(CCCCC)c1)c1ccc(CCC)c2c1cccc2	**824960-02-3**	**0.65**	**1.1**	**2004:1043347**
O=C(c1c2ccccc2n(CCCCC)c1C)c1ccc(CCC)c2c1cccc2	**824960-03-4**	**1.3**	**0.62**	**2004:1043347**
O=C(c1ccc(CCCC)c2c1cccc2)c1c2ccccc2n(CCC)c1	**824960-04-5**	**342**	**52**	**2004:1043347**
O=C(c1ccc(CCCC)c2c1cccc2)c1c2ccccc2n(CCC)c1C	**824960-05-6**	**147**	**49**	**2004:1043347**
O=C(c1ccc(CCCC)c2c1cccc2)c1c2ccccc2n(CCCCC)c1	**824960-06-7**	**14**	**7.2**	**2004:1043347**
O=C(c1ccc(CCCC)c2c1cccc2)c1c2ccccc2n(CCCCC)c1C	**824960-07-8**	**42**	**6.5**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)C)c1c2ccccc2n(CCC)c1	**824960-09-0**	**214**	**106**	**2004:1043347**

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O=C(c1cccc2c1cc(cc2)CC)c1c2ccccc2n(CCC)c1	**824960-57-8**	**338**	**123**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)CC)c1c2ccccc2n(CCC)c1C	**824960-63-6**	**1351**	**240**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)CC)c1c2ccccc2n(CCCCC)c1	**824960-64-7**	**8.4**	**3.8**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)CC)c1c2ccccc2n(CCCCC)c1C	**824960-71-6**	**28**	**5.6**	**2004:1043347**
O=C(c1c(OC)ccc2c1cccc2)c1c2ccccc2n(CCC)c1	**824960-73-8**	**3788**	**80**	**2004:1043347**
O=C(c1c(OC)ccc2c1cccc2)c1c2ccccc2n(CCC)c1C	**824960-74-9**	**10000**	**455**	**2004:1043347**
O=C(c1c(OC)ccc2c1cccc2)c1c2ccccc2n(CCCCC)c1	**824960-76-1**	**381**	**7.2**	**2004:1043347**
O=C(c1ccc(OCC)c2c1cccc2)c1c2ccccc2n(CCC)c1	**824960-95-4**	**220**	**74**	**2004:1043347**
O=C(c1ccc(OCC)c2c1cccc2)c1c2ccccc2n(CCC)c1C	**824960-96-5**	**767**	**221**	**2004:1043347**
O=C(c1ccc(OCC)c2c1cccc2)c1c2ccccc2n(CCCCC)c1	**824960-97-6**	**4.6**	**10.5**	**2004:1043347**
O=C(c1ccc(OCC)c2c1cccc2)c1c2ccccc2n(CCCCC)c1C	**824960-98-7**	**29**	**25**	**2004:1043347**
O=C(c1cccc2c1ccc(c2)OC)c1c2ccccc2n(CCC)c1	**824961-06-0**	**2358**	**138**	**2004:1043347**
O=C(c1cccc2c1ccc(c2)OC)c1c2ccccc2n(CCC)c1C	**824961-23-1**	**10000**	**30**	**2004:1043347**
O=C(c1cccc2c1ccc(c2)OC)c1c2ccccc2n(CCCCC)c1	**824961-41-3**	**44**	**1.9**	**2004:1043347**
O=C(c1cccc2c1ccc(c2)OC)c1c2ccccc2n(CCCCC)c1C	**824961-58-2**	**250**	**11**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)OC)c1c2ccccc2n(CCC)c1	**824961-59-3**	**204**	**71**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)OC)c1c2ccccc2n(CCC)c1C	**824961-60-6**	**1568**	**441**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)OC)c1c2ccccc2n(CCCCC)c1	**824961-61-7**	**6.6**	**6.9**	**2004:1043347**
O=C(c1cccc2c1cc(cc2)OC)c1c2ccccc2n(CCCCC)c1C	**824961-62-8**	**45**	**10.4**	**2004:1043347**
Oc1cc(C(C)(C)CCCCCC)ccc1[C@@H]1[C@@H](CCCO)CC[C@H](O)C1	**83002-05-5**	**61.66**	**23.4**	**2000:338367**
CC1=C[C@@H]2c3c(OC)cc(C(C)(C)CCCCC)cc3OC(C)(C)[C@H]2CC1	**832111-99-6**	**3134**	**18**	**2004:1043347**
O=C(c1c2CCc3cc(Cl)ccc3c2n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**852409-27-9**	**14.8**	**227**	**2005:288981**
O=C(c1c2CCc3cc(C)ccc3c2n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**852409-28-0**	**5.88**	**287**	**2005:288981**
O=C(c1c2CCc3cc(Br)ccc3c2n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**852409-29-1**	**4.87**	**367**	**2005:288981**
O=C(c1c2CCc3cc(I)ccc3c2n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**852409-30-4**	**4.11**	**1079**	**2005:288981**
O=C(c1c2CCc3ccccc3c2n(c2ccc(Cl)cc2Cl)n1)NN1CCCCC1	**852409-31-5**	**602**	**295**	**2005:288981**
O=C(c1c2CCc3cc(Cl)ccc3c2n(c2ccc(Cl)cc2)n1)NN1CCCCC1	**852409-32-6**	**142**	**550**	**2005:288981**
O=C(c1c2CCc3cc(Cl)ccc3c2n(c2ccccc2)n1)NN1CCCCC1	**852409-33-7**	**418**	**1375**	**2005:288981**

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O=C(c1c2CCc3cc(Cl)ccc3c2n(c2ccc(OC)cc2)n1)NN1CCCCC1	**852409-34-8**	**157**	**1875**	**2005:288981**
O=C(c1c2CCc3cc(Cl)ccc3c2n(c2ccc(Cl)cc2Cl)n1)NN1CCCC1	**852409-35-9**	**49**	**387**	**2005:288981**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2cnn1CC(F)(F)F	**857075-03-7**	**8**	**10000**	**2005:1341997**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc([C@@H]2[C@@H]3C[C@H]4C[C@@H](C3)C[C@@H]2C4)c1	**862075-65-8**	**34.9**	**14**	**2005:529462**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(/C=C\2/[C@@H]3C[C@H]4C[C@@H](C3)C[C@@H]2C4)c1	**862075-66-9**	**48.6**	**8.9**	**2005:529462**
Oc1c2[C@@H]3[C@H](CC=C(C)C3)C(C)(C)Oc2cc(C[C@@H]2[C@@H]3C[C@H]4C[C@@H](C3)C[C@@H]2C4)c1	**862075-67-0**	**79.7**	**76**	**2005:529462**
CCCCCn1c(C)c(C(=O)Cc2ccccc2F)c2c1cccc2	**864382-14-9**	**39**	**76**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccccc2)c2c1cccc2	**864445-37-4**	**90**	**159**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccccc2)c2c1cccc2	**864445-38-5**	**124**	**180**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccccc2C)c2c1cccc2	**864445-39-6**	**29**	**146**	**2005:760362**
Cc1ccccc1CC(=O)c1c2ccccc2n(CCCCC)c1C	**864445-40-9**	**23**	**19**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccc(C)cc2)c2c1cccc2	**864445-41-0**	**179**	**570**	**2005:760362**
Cc1ccc(CC(=O)c2c3ccccc3n(CCCCC)c2C)cc1	**864445-42-1**	**746**	**1353**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccccc2OC)c2c1cccc2	**864445-43-2**	**11**	**33**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccccc2OC)c2c1cccc2	**864445-44-3**	**25**	**82**	**2005:760362**
CCCCCn1cc(C(=O)Cc2cccc(OC)c2)c2c1cccc2	**864445-45-4**	**17**	**89**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2cccc(OC)c2)c2c1cccc2	**864445-46-5**	**62**	**84**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccc(OC)cc2)c2c1cccc2	**864445-47-6**	**1064**	**444**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccc(OC)cc2)c2c1cccc2	**864445-48-7**	**1678**	**645**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccccc2F)c2c1cccc2	**864445-49-8**	**23**	**39**	**2005:760362**
CCCCCn1cc(C(=O)Cc2cccc(F)c2)c2c1cccc2	**864445-50-1**	**72**	**91**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2cccc(F)c2)c2c1cccc2	**864445-51-2**	**430**	**182**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccc(F)cc2)c2c1cccc2	**864445-52-3**	**422**	**365**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccc(F)cc2)c2c1cccc2	**864445-53-4**	**2862**	**781**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccccc2Cl)c2c1cccc2	**864445-54-5**	**8**	**7**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccccc2Cl)c2c1cccc2	**864445-55-6**	**13**	**25**	**2005:760362**
CCCCCn1cc(C(=O)Cc2cccc(Cl)c2)c2c1cccc2	**864445-56-7**	**38**	**106**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2cccc(Cl)c2)c2c1cccc2	**864445-57-8**	**117**	**138**	**2005:760362**

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CCCCCn1cc(C(=O)Cc2ccc(Cl)cc2)c2c1cccc2	**864445-58-9**	**389**	**498**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccc(Cl)cc2)c2c1cccc2	**864445-59-0**	**1598**	**3723**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccccc2Br)c2c1cccc2	**864445-60-3**	**8.4**	**20**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccccc2Br)c2c1cccc2	**864445-61-4**	**15**	**29**	**2005:760362**
CCCCCn1cc(C(=O)Cc2ccc(Br)cc2)c2c1cccc2	**864445-62-5**	**1028**	**657**	**2005:760362**
CCCCCn1c(C)c(C(=O)Cc2ccc(Br)cc2)c2c1cccc2	**864445-63-6**	**3363**	**2679**	**2005:760362**
O=C(NC1CC1)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCCN=C=S	**867280-98-6**	**1.3**	**48.5**	**2005:990496**
O=C(NC1CC1)CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCCN=[N+]=[N-]	**867281-00-3**	**0.9**	**57.6**	**2005:990496**
O=C(c1c2ccc(I)cc2n(C[C@H]2N(C)CCCC2)c1)c1cccc2c1cccc2	**868542-00-1**	**18**	**9.8**	**2005:980153**
O=C(c1ccc(I)c2c1cccc2)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1	**868542-03-4**	**10**	**5.3**	**2005:980153**
O=C(c1ccccc1I)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1C	**868542-05-6**	**34**	**34**	**2005:980153**
O=C(c1cccc(I)c1)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1C	**868542-06-7**	**2900**	**9600**	**2005:980153**
O=C(c1ccc(I)cc1)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1C	**868542-07-8**	**1800**	**790**	**2005:980153**
O=C(c1ccccc1I)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1C	**868542-08-9**	**6.7**	**10**	**2005:980153**
O=C(c1ccccc1I)c1c2ccccc2n(C[C@H]2N(C)CCCC2)c1C	**868542-09-0**	**1200**	**83**	**2005:980153**
C/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NS(=O)(=O)N1CCCCCC1	**869278-54-6**	**155**	**1032**	**2005:1024928**
O=S(=O)(/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NC)N1CCSCC1	**869278-55-7**	**24**	**3526**	**2005:1024928**
O=S(=O)(/N=C(/N1N=C(c2ccc(Cl)cc2)[C@@H](c2ccccc2)C1)\NC)N1CCOCC1	**869278-56-8**	**75**	**5372**	**2005:1024928**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)NN1CCCC1	**870679-33-7**	**0.004**	**45**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)NC1CCCCC1	**870679-34-8**	**0.3**	**0.65**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)Nc1ccccc1	**870679-35-9**	**4.35**	**1.45**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)Nc1ccc(Cl)cc1	**870679-36-0**	**2.5**	**79**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)Nc1ccc(Cl)c(Cl)c1	**870679-37-1**	**25.83**	**500**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)Nc1ccc(C)cc1	**870679-38-2**	**5.74**	**65**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Cl)ccc21)Nc1ccc(OC)cc1	**870679-39-3**	**0.013**	**43.3**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1c(Cl)cccc21)NN1CCCCC1	**870679-40-6**	**9.84**	**31.6**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(Br)ccc21)NN1CCCCC1	**870679-41-7**	**0.008**	**37**	**2005:1118017**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(C)ccc21)NN1CCCCC1	**870679-42-8**	**0.0052**	**0.46**	**2005:1118017**

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O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1CCCc1cc(C)ccc21)NN1CCCC1	**870679-43-9**	**0.11**	**386**	**2005:1118017**
CC(C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873428-27-4**	**10000**	**111**	**2005:1233246**
CC(C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-28-5**	**10000**	**2317**	**2005:1233246**
CC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-30-9**	**10000**	**295**	**2005:1233246**
CC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873428-44-5**	**2449**	**160**	**2005:1233246**
CCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-46-7**	**4724**	**319**	**2005:1233246**
CCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873428-49-0**	**2162**	**108**	**2005:1233246**
CCCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873428-50-3**	**647**	**185**	**2005:1233246**
CCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873428-53-6**	**25**	**1**	**2005:1233246**
CCCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873428-56-9**	**332**	**146**	**2005:1233246**
CCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-58-1**	**1961**	**241**	**2005:1233246**
CCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-61-6**	**5837**	**108**	**2005:1233246**
CCCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-63-8**	**1243**	**52**	**2005:1233246**
CCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-65-0**	**4300**	**97**	**2005:1233246**
CCCCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873428-67-2**	**427**	**99**	**2005:1233246**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCc1cc(OC)ccc1OC	**873549-75-8**	**500**	**4100**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCc1ccc(OC)cc1OC	**873549-76-9**	**200**	**4000**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N1CCN(c2ccc(C)c(C)c2)CC1	**873549-77-0**	**400**	**4200**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N1CCN(c2ccc(Cl)cc2)CC1	**873549-78-1**	**600**	**10000**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N1CCN(c2ccc(F)cc2)CC1	**873549-79-2**	**300**	**5100**	**2005:1241404**
CCCCCCCC/C=C/C(=O)Nc1ccc(OC)cc1	**873549-80-5**	**4900**	**2500**	**2005:1241404**
CCCCCCCC/C=C/C(=O)NCCc1ccc(OC)cc1	**873549-82-7**	**2400**	**5100**	**2005:1241404**
CCCCCCCC/C=C/C(=O)NCCc1cc(OC)cc(OC)c1	**873549-83-8**	**2800**	**5200**	**2005:1241404**
CCCCCCCC/C=C\CCCCCCCCCCCC(=O)NCCc1c(OC)cc(OC)cc1	**873549-94-1**	**3700**	**10000**	**2005:1241404**
CCCCCCCC/C=C\CCCCCCCCCCCC(=O)Nc1ccc(N2CCOCC2)cc1	**873549-95-2**	**6400**	**10000**	**2005:1241404**
CCCCCCCC/C=C\CCCCCCCC(=O)Nc1ccc(OC)cc1	**873549-96-3**	**1600**	**10000**	**2005:1241404**
CCCCCCCC/C=C\CCCCCCCC(=O)NCc1ccc(OC)cc1	**873549-97-4**	**500**	**10000**	**2005:1241404**
CCCCCCCC/C=C\CCCCCCCC(=O)NCCc1ccc(OC)cc1	**873549-98-5**	**400**	**10000**	**2005:1241404**

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CCCCCCCC/C=C\CCCCCCCC(=O)NCCc1cc(OC)cc(OC)c1	**873549-99-6**	**1300**	**10000**	**2005:1241404**
CCCCCCCC/C=C\CCCCCCCC(=O)NCCc1ccc(OC)cc1OC	**873550-00-6**	**800**	**10000**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCc1ccc(OC)cc1	**873550-02-8**	**600**	**4500**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCCc1ccc(OC)cc1	**873550-03-9**	**2400**	**10000**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NCCc1ccc(OC)cc1OC	**873550-05-1**	**500**	**4000**	**2005:1241404**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)Nc1ccc(N2CCOCC2)cc1	**873550-06-2**	**150**	**4300**	**2005:1241404**
CC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873556-64-0**	**10000**	**47**	**2005:1233246**
CC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)c(OC)c1	**873556-69-5**	**2918**	**13**	**2005:1233246**
CCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873556-71-9**	**4307**	**24**	**2005:1233246**
CCC[C@H](C)Cc1cc2c([C@@H]3[C@H](CC=C(C)C3)C(C)(C)O2)cc1	**873556-72-0**	**1493**	**31**	**2005:1233246**
O=C(c1c(=O)c2c(n(c1)CCCCC)cccc2)Nc1cccc2c1cccc2	**875148-81-5**	**4083**	**371**	**2005:1298759**
O=C(c1c(=O)c2c(n(c1)CCCCC)cccc2)N[C@@H]1[C@@H]2C[C@H]3C[C@@H](C2)C[C@@H]1C3	**875148-95-1**	**1925**	**13.4**	**2005:1298759**
O=C(c1c(=O)c2c(n(c1)CCCCC)cccc2)N[C@H]1CCCc2c1cccc2	**875149-01-2**	**1045**	**60.2**	**2005:1298759**
O=c1c2nn(c3ccc(Cl)cc3)c(c3ccccc3Cl)c2ncn1N1CCCCC1	**876405-86-6**	**12**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1Cc1ccccc1	**876405-87-7**	**5**	**10000**	**2005:1341997**
O=c1c2nn(c3ccccc3Cl)c(c3ccc(Cl)cc3)c2ncn1CC(F)(F)C	**876405-88-8**	**0.2**	**10000**	**2005:1341997**
O=c1c2nn(c3ccc(Cl)cc3)c(c3ccccc3Cl)c2ncn1C1CCCCC1	**876405-89-9**	**38**	**10000**	**2005:1341997**
O=c1c2nn(c3ccc(Cl)cc3)c(c3ccccc3Cl)c2ncn1CC(F)(F)F	**876405-90-2**	**28**	**10000**	**2005:1341997**
Oc1c([C@@H]2C=C(C)CC[C@H]2C(=C)C)c(O)cc(c2ccc(C)cc2)c1	**881888-24-0**	**638.1**	**374.4**	**2006:128508**
Oc1cc(c2cccc3c2cccc3)cc(O)c1[C@@H]1C=C(C)CC[C@H]1C(=C)C	**881888-27-3**	**753.5**	**221.6**	**2006:128508**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(c2ccc(C)cc2)c1	**881888-28-4**	**95.49**	**71.81**	**2006:128508**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(c2ccc(CC)cc2)c1	**881888-29-5**	**119**	**51.7**	**2006:128508**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(c2ccc(CCC)cc2)c1	**881888-30-8**	**57.77**	**107.8**	**2006:128508**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(c2cccc3c2cccc3)c1	**881888-31-9**	**11.73**	**9.39**	**2006:128508**
N#CC1(c2cc(O)c([C@@H]3C=C(C)CC[C@H]3C(=C)C)c(O)c2)CCCC1	**881888-34-2**	**255.4**	**105**	**2006:128508**
N#CC1(c2cc(O)c([C@@H]3C=C(C)CC[C@H]3C(=C)C)c(O)c2)CCCCC1	**881888-35-3**	**319**	**110.7**	**2006:128508**
N#CC1(c2cc3c([C@@H]4[C@H](CCC(=C4)C)C(C)(C)O3)c(O)c2)CCCC1	**881888-36-4**	**27.9**	**25.2**	**2006:128508**
N#CC1(c2cc3c([C@@H]4[C@H](CCC(=C4)C)C(C)(C)O3)c(O)c2)CCCCC1	**881888-37-5**	**8.26**	**3.86**	**2006:128508**

Supporting Information

O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCC)c1)(C)C	**883111-53-3**	**812**	**198**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCCC)c1)(C)C	**883111-54-4**	**415**	**30**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCCCC)c1)(C)C	**883111-55-5**	**395**	**12**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCCCCC)c1)(C)C	**883111-56-6**	**100**	**10**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCC)c1)(C)C	**883111-57-7**	**1059**	**36**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCCC)c1)(C)C	**883111-58-8**	**118**	**5.3**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCCCC)c1)(C)C	**883111-59-9**	**63**	**2.7**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCC)c1)(C)C	**883111-60-2**	**3905**	**589**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCCC)c1)(C)C	**883111-61-3**	**906**	**69**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCCCC)c1)(C)C	**883111-62-4**	**376**	**38**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2c(OC)cc(C(C)(C)CCCCCC)c1)(C)C	**883111-63-5**	**135**	**30**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCC)c1)(C)C	**883111-64-6**	**4589**	**153**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCCC)c1)(C)C	**883111-65-7**	**295**	**48**	**2006:156948**
O[C@@H]1C[C@H]2[C@H](CC1)C(Oc1c2ccc(C(C)(C)CCCCC)c1)(C)C	**883111-67-9**	**127**	**34**	**2006:156948**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)NOCCO	**883296-70-6**	**470**	**81**	**2006:165889**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N(O)CCO	**883296-89-7**	**3900**	**1900**	**2006:165889**
CCCCCCCC/C=C\CCCCCCCC(=O)N(O)CCO	**883296-93-3**	**10000**	**5400**	**2006:165889**
CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)ONCCO	**883297-02-7**	**3500**	**2400**	**2006:165889**
CCCCCCCC/C=C\CCCCCCCC(=O)ONCCO	**883297-06-1**	**10000**	**8600**	**2006:165889**
Oc1cc(C(C)(C)CCCCCC)ccc1c1cccnc1	**895131-92-7**	**23**	**20**	**2007:652168**
O=C(OCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)N[C@H](C)CO)c1cc(I)ccc1N=[N+]=[N-]	**903514-40-9**	**570**	**220**	**2006:548780**
O=C(c1ccc2n(CCN(C)C)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-33-8**	**5000**	**876**	**2006:665189**
O=C(c1ccc2n(CCOC)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-34-9**	**5000**	**1259**	**2006:665189**
O=C(c1ccc2n(CC3CC3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-35-0**	**5000**	**84**	**2006:665189**
O=C(c1ccc2n(CC3CCCC3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-36-1**	**3220**	**6.8**	**2006:665189**
O=C(c1ccc2n(CC3CCCCC3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-37-2**	**844**	**8.1**	**2006:665189**
O=C(c1ccc2n(C[C@H]3NCCCC3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-39-4**	**5000**	**199**	**2006:665189**
O=C(c1ccc2n(CC3CCOCC3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-40-7**	**5000**	**8.5**	**2006:665189**

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O=C(c1ccc2n(Cc3ccccc3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-41-8**	**5000**	**11**	**2006:665189**
O=C(c1ccc2n(Cc3sccc3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-42-9**	**5000**	**14**	**2006:665189**
O=C(c1ccc2n(Cc3ccncc3)c(Cc3ccc4OCCc4c3)nc2c1)N(CC)CC	**909706-43-0**	**5000**	**154**	**2006:665189**
CC(C)CCn1c(Cc2ccc3OCCc3c2)nc2cc(NC)ccc12	**909706-46-3**	**5000**	**2267**	**2006:665189**
CC(C)(C)C(=O)N(c1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1)C	**909706-49-6**	**5000**	**52**	**2006:665189**
CC(C)(C)C(=O)Nc1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1	**909706-50-9**	**5000**	**4578**	**2006:665189**
O=C(N(c1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1)C)c1ccccc1	**909706-51-0**	**4511**	**85**	**2006:665189**
O=C(c1sccc1)N(c1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1)C	**909706-52-1**	**1030**	**49**	**2006:665189**
O=C(N(C)C)N(c1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1)C	**909706-54-3**	**5000**	**122**	**2006:665189**
O=C(Nc1ccccc1)N(c1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1)C	**909706-56-5**	**5000**	**1880**	**2006:665189**
S=C(Nc1ccccc1)N(c1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1)C	**909706-57-6**	**5000**	**521**	**2006:665189**
CC(C)CCn1c(Cc2ccc3OCCc3c2)nc2cc(N(C)Cc3ccccc3)ccc12	**909706-58-7**	**2884**	**103**	**2006:665189**
O=S(=O)(c1ccccc1)N(c1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1)C	**909706-59-8**	**822**	**4.2**	**2006:665189**
O=S(=O)(c1ccccc1)Nc1ccc2n(CCC(C)C)c(Cc3ccc4OCCc4c3)nc2c1	**909706-60-1**	**3531**	**30**	**2006:665189**
O=S(=O)(c1ccccc1)N(c1ccc2n(CC3CCCCC3)c(Cc3ccc4OCCc4c3)nc2c1)C	**909706-61-2**	**16**	**0.7**	**2006:665189**
O=C(c1c(=O)c2c(n(c1)Cc1ccc(F)cc1)nc(cc2)C)N[C@H]1CC[C@H](C)CC1	**913533-80-9**	**8.7**	**1.4**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1F)nc(cc2)C)N[C@H]1CC[C@H](C)CC1	**913533-81-0**	**37.5**	**8.4**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1)nc(cc2)C)NC1CCCCCC1	**913533-82-1**	**143.2**	**5.1**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccc(F)cc1)nc(cc2)C)NC1CCCCCC1	**913533-83-2**	**4.3**	**1**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1F)nc(cc2)C)NC1CCCCCC1	**913533-84-3**	**149.4**	**13.4**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1)nc(cc2)Cl)NC1CCCCC1	**913533-85-4**	**463.6**	**24.6**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccc(F)cc1)nc(cc2)Cl)NC1CCCCC1	**913533-86-5**	**495**	**21.4**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1F)nc(cc2)Cl)NC1CCCCC1	**913533-87-6**	**171.2**	**18.1**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)CCc1ccccc1)nc(cc2)C)NC1CCCCC1	**913533-89-8**	**1000**	**16.3**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccc(OC)cc1)nc(cc2)C)NC1CCCCC1	**913533-90-1**	**1000**	**35.8**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccc(F)cc1)nccc2)NC1CCCCC1	**913533-91-2**	**384.1**	**13**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1)nccc2)NC1CCCCC1	**913533-92-3**	**1000**	**48.6**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)CCN1CCOCC1)nccc2)NC1CCCCC1	**913533-93-4**	**1000**	**67.2**	**2006:908608**

Supporting Information

O=C(c1c(=O)c2c(n(c1)CCN1CCOCC1)nc(cc2)Cl)N[C@H]1CC[C@H](C)CC1	**913534-01-7**	**1000**	**40.5**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)Cc1ccccc1)cccc2)NC1CCCCC1	**913534-04-0**	**1000**	**4.8**	**2006:908608**
O=C(c1c(=O)c2c(n(c1)CCN1CCOCC1)cc(cc2)Cl)NC1CCCCC1	**913534-05-1**	**1000**	**3.3**	**2006:908608**
O=C(c1cccc2c1cccc2)c1cc(c2ccccc2)n(CCC)c1	**914458-17-6**	**404**	**104**	**2006:934979**
O=C(c1cc(c2ccccc2)n(CCCC)c1)c1cccc2c1cccc2	**914458-18-7**	**60**	**15**	**2006:934979**
O=C(c1cccc2c1cccc2)c1cc(c2ccccc2)n(CCCCC)c1	**914458-19-8**	**14**	**6.4**	**2006:934979**
O=C(c1cc(c2ccccc2)n(CCCCCC)c1)c1cccc2c1cccc2	**914458-20-1**	**11**	**7.1**	**2006:934979**
O=C(c1cc(c2ccccc2)n(CCCCCCC)c1)c1cccc2c1cccc2	**914458-21-2**	**21**	**62**	**2006:934979**
O=C(c1cc(c2ccccc2C)n(CCCCC)c1)c1cccc2c1cccc2	**914458-22-3**	**5.6**	**4**	**2006:934979**
O=C(c1cc(c2ccccc2CC)n(CCCCC)c1)c1cccc2c1cccc2	**914458-23-4**	**17**	**3.4**	**2006:934979**
O=C(c1cc(c2ccccc2CCCC)n(CCCCC)c1)c1cccc2c1cccc2	**914458-24-5**	**60**	**69**	**2006:934979**
O=C(c1cc(c2ccccc2OC)n(CCCCC)c1)c1cccc2c1cccc2	**914458-25-6**	**29**	**20**	**2006:934979**
O=C(c1cc(c2ccccc2F)n(CCCCC)c1)c1cccc2c1cccc2	**914458-26-7**	**7.7**	**3.3**	**2006:934979**
O=C(c1cc(c2ccccc2Cl)n(CCCCC)c1)c1cccc2c1cccc2	**914458-27-8**	**7.9**	**5.2**	**2006:934979**
O=C(c1cccc2c1cccc2)c1cc(c2ccccc2C(F)(F)F)n(CCCCC)c1	**914458-28-9**	**77**	**8.2**	**2006:934979**
O=C(c1cc(c2cccc(C)c2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-29-0**	**67**	**39**	**2006:934979**
O=C(c1cc(c2cccc(OC)c2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-30-3**	**53**	**23**	**2006:934979**
O=C(c1cc(c2cccc(F)c2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-31-4**	**16**	**9.1**	**2006:934979**
O=C(c1cc(c2cccc(Cl)c2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-32-5**	**70**	**16**	**2006:934979**
O=C(c1cccc2c1cccc2)c1cc(c2cccc(C(F)(F)F)c2)n(CCCCC)c1	**914458-33-6**	**245**	**71**	**2006:934979**
O=C(c1cccc2c1cccc2)c1cc(c2cccc([N+](=O)[OH-])c2)n(CCCCC)c1	**914458-34-7**	**100**	**41**	**2006:934979**
O=C(c1cc(c2ccc(C)cc2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-35-8**	**130**	**18**	**2006:934979**
O=C(c1cc(c2ccc(CC)cc2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-36-9**	**34**	**29**	**2006:934979**
O=C(c1cc(c2ccc(CCCC)cc2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-37-0**	**42**	**64**	**2006:934979**
O=C(c1cc(c2ccc(OC)cc2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-38-1**	**285**	**41**	**2006:934979**
O=C(c1cc(c2ccc(F)cc2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-39-2**	**41**	**33**	**2006:934979**
O=C(c1cc(c2ccc(Cl)cc2)n(CCCCC)c1)c1cccc2c1cccc2	**914458-40-5**	**276**	**25**	**2006:934979**
O=C(c1cccc2c1cccc2)c1cc(c2ccc(C(F)(F)F)cc2)n(CCCCC)c1	**914458-41-6**	**218**	**53**	**2006:934979**

Supporting Information

O=C(c1cccc2c1cccc2)c1cc(c2cccc3c2cccc3)n(CCCCC)c1	**914458-42-7**	**41**	**49**	**2006:934979**
O=C(c1cccc2c1cccc2)c1cc(c2ccc3ccccc3c2)n(CCCCC)c1	**914458-43-8**	**333**	**169**	**2006:934979**
O=C(c1cccc2c1cccc2)c1cc(c2cccnc2)n(CCCCC)c1	**914458-44-9**	**191**	**24**	**2006:934979**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)NC1CCCCC1	**919077-81-9**	**900**	**7.6**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)Nc1ccccc1	**919077-82-0**	**2409**	**32.8**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)Nc1ccc(Cl)cc1	**919077-83-1**	**10000**	**177**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)Nc1ccc(F)cc1	**919077-84-2**	**5000**	**61**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)Nc1ccc(C)cc1	**919077-85-3**	**5000**	**74**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)Nc1ccc(OC)cc1	**919077-87-5**	**10000**	**114**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)Nc1ccc(Cl)cc1Cl	**919077-89-7**	**2625**	**5000**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)NNc1ccccc1	**919077-90-0**	**2275**	**63**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)NNc1ccc([N+](=O)[OH-])cc1	**919077-92-2**	**4500**	**2116**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2ccc(C)c1)NNc1ccc(OC)cc1	**919077-93-3**	**5000**	**3000**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2cc(Cl)c(C)c1)NC1CCCCC1	**919077-94-4**	**833**	**25**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2cc(Cl)c(C)c1)NN1CCCCC1	**919077-95-5**	**916**	**200**	**2006:1212215**
O=C(c1nn(c2ccc(Cl)cc2Cl)c2c1Cc1c2cc(C)c(Cl)c1)NN1CCCCC1	**919077-96-6**	**1200**	**85**	**2006:1212215**
O=C1[C@@H]2[C@H](N(c3ccc(Cl)cc3Cl)C(=C2C)c2ccc(Cl)cc2)CCN1N1CCCCC1	**929199-32-6**	**2.2**	**1300**	**2007:81238**
O=C1[C@@H]2[C@H](N(c3ccc(Cl)cc3Cl)C(=C2C)c2ccc(Cl)cc2)CCN1C1CCCCC1	**929199-33-7**	**7.5**	**8300**	**2007:81238**
O=C1[C@@H]2[C@H](N(c3ccccc3Cl)C(=C2C)c2ccc(Cl)cc2)CCN1N1CCCCC1	**929199-75-7**	**3.5**	**1100**	**2007:81238**
O=C1[C@@H]2[C@H](N(c3ccccc3Cl)C(=C2C)c2ccc(OC)cc2)CCN1N1CCCCC1	**929199-76-8**	**20**	**850**	**2007:81238**
CCCCC/C=C/C/C=C/C/C=C/C/C=C/CCCC(=O)NCCO	**94421-68-8**	**13**	**65**	**1998:635184**
O=C(NCCO)CCCCCCCCOc1cc(CCCCC)cc(O)c1	**944395-58-8**	**130**	**390**	**2007:689135**
O=C(NC1CC1)CCCCCCCCOc1cc(CCCCC)cc(O)c1	**944395-59-9**	**16**	**39**	**2007:689135**
O=C(NCC1CC1)CCCCCCCCCCCOc1cc(CCCCC)cc(O)c1	**944395-60-2**	**510**	**80**	**2007:689135**
O=C(NCc1ccc(OC)c(O)c1)CCCCCCCCCCCOc1cc(CCCCC)cc(O)c1	**944395-62-4**	**2100**	**1650**	**2007:689135**
O=C(NCCO)CCCCCCCCCCCCOc1cc(CCCCC)cc(O)c1	**944395-63-5**	**60**	**39**	**2007:689135**
O=C(NC1CC1)CCCCCCCCCCCCOc1cc(CCCCC)cc(O)c1	**944395-64-6**	**750**	**310**	**2007:689135**
O=C(NCCO)CCCCCCCCOc1cc(O)ccc1CCCCCC	**944395-65-7**	**260**	**3940**	**2007:689135**

Supporting Information

O=C(NC1CC1)CCCCCCCOc1cc(O)ccc1CCCCCC	**944395-66-8**	**310**	**1800**	**2007:689135**
O=C(NCC1CC1)CCCCCCCCCCOc1cc(O)ccc1CCCCCC	**944395-67-9**	**750**	**470**	**2007:689135**
O=C(NCCc1ccc(O)c(O)c1)CCCCCCCCCCOc1cc(O)ccc1CCCCCC	**944395-68-0**	**2100**	**7900**	**2007:689135**
O=C(NCc1ccc(OC)c(O)c1)CCCCCCCCCCOc1cc(O)ccc1CCCCCC	**944395-69-1**	**2820**	**2100**	**2007:689135**
O=C(NCCO)CCCCCCCCCCOc1cc(O)ccc1CCCCCC	**944395-70-4**	**170**	**1420**	**2007:689135**
O=C(NC1CC1)CCCCCCCCCCOc1cc(O)ccc1CCCCCC	**944395-71-5**	**13**	**39**	**2007:689135**
O=C(NCCO)CCCCCCCOc1ccc(CCCCCC)c(O)c1	**944395-72-6**	**190**	**2400**	**2007:689135**
O=C(NC1CC1)CCCCCCCOc1ccc(CCCCCC)c(O)c1	**944395-73-7**	**56**	**280**	**2007:689135**
Nc1cc(C(C)(C)CCCCCC)ccc1c1cc(C)cc(C)c1	**946004-33-7**	**80**	**51**	**2007:652168**
O=C(c1cc(C(C)(C)CCCCCC)ccc1c1cc(C)cc(C)c1)OC	**946004-34-8**	**230**	**110**	**2007:652168**
O=C(c1cc(C(C)(C)CCCCCC)ccc1c1cc(C)cc(C)c1)N	**946004-35-9**	**370**	**320**	**2007:652168**
OCc1cc(C(C)(C)CCCCCC)ccc1c1cc(C)cc(C)c1	**946004-37-1**	**360**	**480**	**2007:652168**
NCc1cc(C(C)(C)CCCCCC)ccc1c1cc(C)cc(C)c1	**946004-38-2**	**1500**	**380**	**2007:652168**
O=C(OCc1cc(C(C)(C)CCCCCC)ccc1c1cc(C)cc(C)c1)CN1CCOCC1	**946004-40-6**	**370**	**0.81**	**2007:652168**
Cc1cc(c2ccc(C(C)(C)CCCCCC)cc2CN2CCOCC2)cc(C)c1	**946004-41-7**	**3900**	**660**	**2007:652168**
Oc1cc(C2(CCCCCC)CC2)ccc1c1cc(C)cc(C)c1	**946004-42-8**	**13**	**55**	**2007:652168**
Oc1cc(C2(CCCCCC)CCCC2)ccc1c1cc(C)cc(C)c1	**946004-43-9**	**2.9**	**5.5**	**2007:652168**
Oc1cc(C2(CCCCCC)CCCCC2)ccc1c1cc(C)cc(C)c1	**946004-44-0**	**1.8**	**1.7**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(C(=O)OC)C	**946004-46-2**	**160**	**16**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(CCC(=O)OC)C	**946004-47-3**	**120**	**5.6**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(CCCCC(=O)OC)C	**946004-48-4**	**24**	**14**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(CO)C	**946004-49-5**	**2200**	**600**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(CCCO)C	**946004-50-8**	**1100**	**56**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(CCCCCO)C	**946004-51-9**	**39**	**3.6**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(CCC(=O)NC)C	**946004-56-4**	**840**	**140**	**2007:652168**
CC(c1cc(O)c(c2cc(C)cc(C)c2)cc1)(CCCCC(=O)NC)C	**946004-57-5**	**96**	**39**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1c(C)cccc1C	**946004-58-6**	**1.7**	**18**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1cc(C)ccc1C	**946004-59-7**	**4.6**	**6.6**	**2007:652168**

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Oc1cc(C(C)(C)CCCCCC)ccc1c1cccc(C)c1C	**946004-60-0**	**49**	**20**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1ccc(C)c(C)c1	**946004-61-1**	**600**	**830**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1ccccc1OC	**946004-62-2**	**1.7**	**1**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1cccc(OC)c1OC	**946004-63-3**	**34**	**7.8**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1cccc(OC)c1	**946004-64-4**	**91**	**580**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1ccc(OC)c(OC)c1	**946004-65-5**	**1400**	**1700**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1ccccc1N	**946004-66-6**	**5.2**	**17**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1cccc(N)c1	**946004-67-7**	**15**	**44**	**2007:652168**
Oc1cc(C(C)(C)CCCCCC)ccc1c1ccc(N)cc1	**946004-68-8**	**320**	**1000**	**2007:652168**
N#Cc1cccc(c2ccc(C(C)(C)CCCCCC)cc2O)c1	**946004-69-9**	**27**	**45**	**2007:652168**
O=C(c1cc(O)c(c2cc(C)cc(C)c2)c(O)c1)OCCCCC	**949009-91-0**	**2000**	**1100**	**2007:862454**
O=C(c1cc(OC)c(c2cc(C)cc(C)c2)c(O)c1)OCCCCC	**949009-92-1**	**1400**	**270**	**2007:862454**
O=C(c1cc(O)c(c2ccccc2)c(O)c1)OCCCCC	**949009-94-3**	**10000**	**4000**	**2007:862454**
O=C(c1cc(O)c(c2cc(C)cc(C)c2)c(O)c1)OCCCC	**949009-95-4**	**2600**	**3200**	**2007:862454**
O=C(c1cc(O)c(c2cc(C)cc(C)c2)c(O)c1)OC	**949009-96-5**	**10000**	**4500**	**2007:862454**
O=C(c1cc(OC)c(c2cc(C)cc(C)c2)c(O)c1)OC	**949009-97-6**	**10000**	**6400**	**2007:862454**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCC)CCC2)c1	**951039-87-5**	**1.5**	**11.5**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCC)CCCCC2)c1	**951039-88-6**	**18.4**	**23.5**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCCC)CC2)c1	**951039-89-7**	**0.48**	**4.2**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCCC)CCC2)c1	**951039-90-0**	**2.7**	**52.3**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCCC)CCCC2)c1	**951039-91-1**	**9.9**	**45.5**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCCC)CCCCC2)c1	**951039-92-2**	**13.6**	**143.3**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(/C=C\CCCC)CC2)c1	**951039-99-9**	**1.5**	**1.7**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(/C=C\CCCC)CCC2)c1	**951040-00-9**	**0.93**	**1.2**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(/C=C\CCCC)CCCC2)c1	**951040-01-0**	**0.72**	**1.8**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(/C=C\CCCC)CCCCC2)c1	**951040-02-1**	**3.9**	**4.9**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(CCCCCCC)c1	**951040-04-3**	**8.8**	**20.8**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C(C)(C)CCCCCC)c1	**951040-05-4**	**0.9**	**1.4**	**2007:841173**

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Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCC)CC2)c1	**951040-06-5**	**0.44**	**0.86**	**2007:841173**
Oc1c2[C@@H]3[C@H](CCC(=C3)C)C(C)(C)Oc2cc(C2(CCCCCC)CCCC2)c1	**951040-07-6**	**0.45**	**1.92**	**2007:841173**
O=C(c1ccc2n(S(=O)(=O)c3ccccc3)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-26-2**	**259**	**17.9**	**2007:1170520**
O=C(c1ccc2[nH]c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-29-5**	**8000**	**4724**	**2007:1170520**
O=C(c1ccc2n(C)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-30-8**	**1811**	**84.7**	**2007:1170520**
O=C(c1ccc2n(CC=C)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-31-9**	**695**	**23.3**	**2007:1170520**
O=C(c1ccc2n(Cc3ccccc3)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-32-0**	**658**	**106**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)C)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-33-1**	**279**	**7.9**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-34-2**	**66.3**	**7**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)C(C)C)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-35-3**	**150**	**4.2**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)C3CC3)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-36-4**	**137**	**9.4**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CCC)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-37-5**	**195**	**22.3**	**2007:1170520**
CC(=O)n1c2c(CN(C3CCCC3)C2)c2c1ccc(c2)C(=O)N1CC[C@H](C)CC1	**959938-38-6**	**2331**	**88.1**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N1CCCCC1	**959938-39-7**	**818**	**17.5**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](F)CC1	**959938-40-0**	**2914**	**44.2**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N1CCOCC1	**959938-41-1**	**8000**	**308**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N1CC[C@H](OC)CC1	**959938-42-2**	**2131**	**27.6**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N(C)C(C)C	**959938-43-3**	**7222**	**107**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N(CCCC)C	**959938-44-4**	**779**	**22.3**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCCC4)C3)c2c1)N(C)CCC(C)C	**959938-45-5**	**1473**	**38.1**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN([C@@H]4COCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-46-6**	**973**	**27.8**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C4CCOCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-47-7**	**3021**	**216**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN([C@@H]4CCCCO4)C3)c2c1)N1CC[C@H](C)CC1	**959938-48-8**	**6183**	**17.6**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(CC=C)C3)c2c1)N1CC[C@H](C)CC1	**959938-49-9**	**263**	**6.4**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(C(C)C)C3)c2c1)N1CC[C@H](C)CC1	**959938-50-2**	**418**	**8.9**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(CCC)C3)c2c1)N1CC[C@H](C)CC1	**959938-51-3**	**604**	**11.1**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(CCCC)C3)c2c1)N1CC[C@H](C)CC1	**959938-52-4**	**341**	**16.8**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(CC4CC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-53-5**	**176**	**6.3**	**2007:1170520**

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O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(CC4CCCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-54-6**	**339**	**935**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(CCC4CCCCC4)C3)c2c1)N1CC[C@H](C)CC1	**959938-55-7**	**2742**	**1982**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3c(CN(Cc4ccccc4)C3)c2c1)N1CC[C@H](C)CC1	**959938-56-8**	**1273**	**37**	**2007:1170520**
O=C(c1ccc2n(S(=O)(=O)CC)c3cn(C4CCCC4)cc3c2c1)N1CC[C@H](C)CC1	**959938-57-9**	**66.3**	**7**	**2007:1170520**