

Supporting Information

Identification of Novel Aurora Kinase A (AURKA) Inhibitors *via* Hierarchical Ligand-Based Virtual Screening

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Table of Contents

Supplementary Tables (Tables S1- S5)

Supplementary Figures (Figures S1- S5)

Kinase assay method

Appendix

I Dataset 1

II Dataset 2

III Dataset 3

IV Filter Rules

Supplementary Tables

Table S1. Information for QSAR models based on dataset 2 and 3.

dataset	model type	model name	modeling method ^a	splitting method	N (all) ^b	N (training) ^c	N (test) ^d
dataset2	classification model	Model C1	SOM	random	1463	988 (561/427)	475 (271/204)
		Model C2	SVM	random			
dataset3	regression model	Model R1	MLR	random	356	259	97
		Model R2	MLR	SOM		263	93
		Model R3	SVM	random		259	97
		Model R4	SVM	SOM		263	93

a: modeling method. b: number of all compounds. c: number of compounds in a training set (highly active/weakly active). d: number of compounds in a test set (highly active/weakly active).

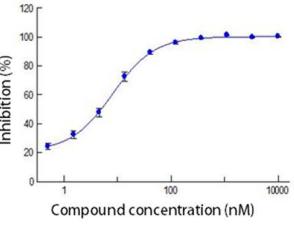
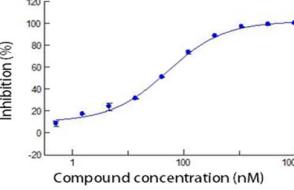
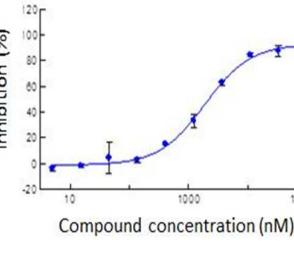
Table S2. The 29 selected molecular descriptors used in the classification models (Model C1 and Model C2) and the 21 selected molecular descriptors used in the quantitative predictive models (Model R1-R4).

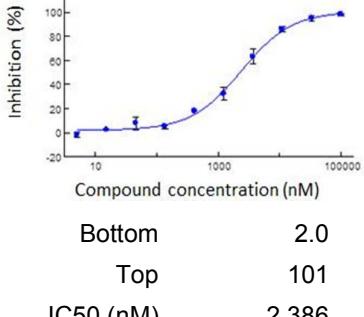
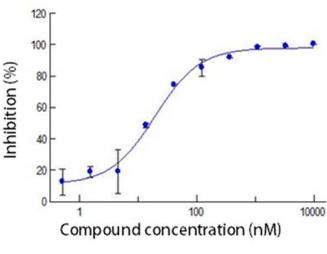
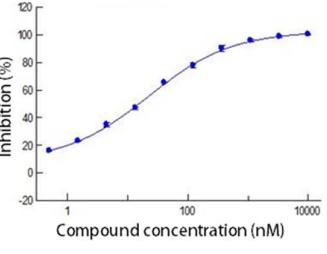
class	descriptor	
	classification model	regression model
I	HAcc_N	—
II	RDF_Polariz_27	RDF_Polariz_52
	2DACorr_LpEN_4	RDF_PiEN_16
	3DACorr_SigEN_6	RDF_PiEN_27
	RDF_SigEN_28	RDF_PiEN_68
	RDF_SigEN_29	RDF_PiEN_84
III	RDF_PiEN_18	RDF_LpEN_10
	RDF_PiEN_83	RDF_LpEN_54
	RDF_LpEN_26	RDF_LpEN_71
	RDF_LpEN_27	
	RDF_LpEN_46	
	RDF_LpEN_55	
IV	2DACorr_SigChg_1	2DACorr_SigChg_8
	2DACorr_SigChg_6	RDF_SigChg_16
	2DACorr_SigChg_8	RDF_SigChg_29
	RDF_TotChg_26	RDF_SigChg_113
	RDF_TotChg_32	RDF_PiChg_26
	RDF_TotChg_42	RDF_PiChg_39
	RDF_TotChg_44	RDF_PiChg_47
	RDF_TotChg_76	RDF_PiChg_52
	RDF_PiChg_29	RDF_PiChg_56
		RDF_TotChg_46
V		3DACorr_TotChg_2
	SurfACorr_HBP_2	
	SurfACorr_HBP_4	
	SurfACorr_HBP_6	
	SurfACorr_HBP_12	—
	SurfACorr_HPP_1	
VI	SurfACorr_HPP_6	
	InertiaX	NRotBond
	Rgyr	RDF_Ident_54
Total number	29	21

Table S3. Information of compound purity

compound	SMILES	Name	purity
#1	Clc1cnc(nc1Nc1cccc1S(=O)(=O)C(C)C)Nc1ccc(N2CCC([NH+]3CCN(CC3)C)CC2)cc1OC	-	100%
#2	Clc1c([C@H](Oc2cc(cnc2N)c2cn(nc2)C2CC[NH2+]CC2)C)c(Cl)ccc1F	Crizotinib	100%
#3	Clc1cc(Nc2nnc3c2cc(NC(=O)C=C)c(OCCC[NH+]2CCOCC2)c3)ccc1F	CI-1033	100%
#4	Clc1cccc(C)c1NC(=O)c1sc(ne1)Nc1nc(nc(N2CC[NH+](CC2)CCO)e1)C	Dasatinib	100%
#5	Clc1cc(Cl)c(OC)c1Ne1c2cc(OC)c(OCCC[NH+]3CCN(CC3)C)cc2ncc1C#N	Bosutinib	100%
#6	O(CCC[NH+]1CCCCC1)c1cc2nene(N3CCN(CC3)C(=O)Nc3ccc(OC(C)C)cc3)c2cc1OC	MLN-518	100%
#7	O1CCN(CC1)c1nc(nc(Oc2nnc(OCCOc3cccc3C)cc2)n1)Nc1ccc(cc1)C	-	100%
#8	s1c2c(nc1NC(=O)C1=CN(c3c(cc(F)e(N4CCN(CC4)C(=O)e4occc4)e3)C1=O)CC)cccc2	-	97%
#9	Clc1cc(Ne2nc(ne(n2)Ne2cc(Cl)ccc2C)N2CC[NH+]CC2)C)c(cc1)C	-	100%
#10	O=C(Nc1cc(Ne2nc(ccn2)-c2ccnc2)c(cc1)C)c1cc(cc1)C[NH+]1CCN(CC1)C	Imatinib	100%
#11	O1 C@ [(NC(=O) C@ @H)2C=C3 C@H ([N@H+](C2)C)Cc2c4c3cccc4[nH]c2](C)C(=O)N2[C@ @H (Cc3cccc3)C(=O)]	Ergotamine	97%
#12	FC(F)F)c1cc(NC(=O)e2cc(Ne3nc(ccn3)-c3ccnc3)c(cc2)C)cc(-n2cc(nc2)C)c1	Nilotinib	100%
#13	O(C(=O)CCN(C(=O)c1cc2ne(n(c2cc1)C)CNc1ccc(cc1)/C(=[NH+)/C(OCCCCCC)=O)/N)c1ncccc1)CC	Dabigatran	100%
#14	Clc1cc(Nc2nnc3c2cc(NC(=O)C=C/C[NH+](C)C)c(O[C@H]2CCOCC2)e3)ccc1F	Afatinib	100%
#15	S(CC(=O)Nc1ccc(OCC)cc1)c1nc(nc2Oc3c(cc(cc3)C)Cc12)-c1ccc(cc1)C	-	99%
#16	S(=O)(=O)(N1CCOCC1)c1cc(NC(=O)c2ccc(ne2)-n2ccnc2)ccc1OC	-	100%
#17	O1CC[NH+]1(CC1)C1(CCCCC1)CNC(=O)Nc1cc(OC)c(NC(=O)c2cccc2)cc1OC	-	100%
#18	S(CC(=O)NCC([NH+]1CCCOCC1)(C)C)c1n-2c(nn1)C=C(c1c-2cc(OC)cc1)C	-	95%
#19	O1CC[NH+]1(CC1)CCNc1nc(nc(n1)Nc1ccc(OC)cc1)Nc1ccc(OC)cc1	-	100%
#20	S(CC=1NC(=NC(=O)C=1)Nc1nc(c2c(n1)c(cc(c2)C)C)c1[nH]c2c(n1)cccc2	-	100%
#21	[NH+]1(CCN(CC1)c1nc(nc(n1)Nc1c2c(ccc1)cccc2)Nc1c2c(ccc1)cccc2)C	-	100%
#22	s1c2-c3n(C=Ne2c2c4c(CCC4)c(nc12)-c1cccc1)(SCC(=O)Nc1ccc(OC)cc1)nn3	-	98%
#23	Clc1cc(Nc2nc(ne(n2)N)C[NH+]2CCN(CC2)Cc2cc3OCOe3cc2)ccc1C	-	100%
#24	Fe1cc2e(N(C=C(C(=O)NCCc3ccc(O)cc3)C2=O)C2CC2)cc1N1CC[NH+]1(CC1)CC	-	100%
#25(ref)	FC(F)F)c1nc(ne1NC1CCCC1)Nc1cc2C3N(C(CC3)c2cc1)C(=O)CNC(=O)C	PF-03814735	100%
#26(ref)	O1CCN(CC1)Cc1cc2[nH]c(ne2cc1)-c1n[nH]cc1NC(=O)NC1CC1	AT-9283	100%
#27(ref)	S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)Cc(n1)Nc1n[nH]c(e1)C	VX-680	100%
#28(ref)	CO[C@ @H](C(=O)N1Cc2[nH]nc(NC(=O)c3ccc(cc3)N4CCN(C)CC4)c2C1)c5cccc5	PHA-739358	100%

Table S4. IC₅₀ curves for hit compounds experimented on Aurora Kinase A and B.

Compound	Compound concentration (nM)	Inhibition (%)	Inhibition (%)	Mean	SD	IC ₅₀ curve
Experimented on Aurora Kinase A						
#1	10000	99.8	100.4	100.1	0.44	 <p>Bottom: 20.98 Top: 100.22 IC50 (nM): 8.1 Hill: 1.12</p>
	3333	99.4	99.8	99.6	0.30	
	1111	101.1	101.3	101.2	0.15	
	370	99.0	99.1	99.0	0.07	
	123	95.4	96.2	95.8	0.59	
	41	89.8	88.6	89.2	0.89	
	14	74.9	70.2	72.5	3.33	
	5	49.8	45.5	47.7	3.04	
	2	34.2	30.3	32.3	2.74	
	1	25.6	22.7	24.2	2.07	
#2	10000	99.7	100.5	100.1	0.59	 <p>Bottom: 10.11 Top: 102.03 IC50 (nM): 50 Hill: 0.85</p>
	3333	98.7	99.5	99.1	0.52	
	1111	96.7	96.9	96.8	0.15	
	370	88.6	88.2	88.4	0.30	
	123	74.3	72.6	73.5	1.26	
	41	50.7	50.9	50.8	0.15	
	14	31.3	31.2	31.2	0.07	
	5	26.4	21.6	24.0	3.41	
	2	16.9	17.0	17.0	0.07	
	1	10.1	6.5	8.3	2.59	
#3	100000	92.7	90.8	91.8	1.35	 <p>Bottom: -1.4 Top: 93 IC50 (nM): 1,877 Hill: 1.12</p>
	33333	90.5	84.4	87.5	4.35	
	11111	85.1	83.1	84.1	1.45	
	3704	64.2	61.2	62.7	2.07	
	1235	36.8	29.4	33.1	5.18	
	412	15.4	14.5	14.9	0.62	
	137	4.0	0.9	2.4	2.18	
	46	12.6	-4.2	4.2	11.91	
	15	-1.2	-3.1	-2.1	1.35	
	5	-5.3	-2.8	-4.0	1.76	

Compound	Compound concentration (nM)	Inhibition (%)	Inhibition (%)	Mean	SD	IC ₅₀ curve
#4	100000	97.3	98.9	98.1	1.14	 <p>Bottom 2.0 Top 101 IC50 (nM) 2,386 Hill 1.06</p>
	33333	96.5	93.6	95.1	2.07	
	11111	87.5	84.2	85.8	2.28	
	3704	67.4	58.6	63.0	6.21	
	1235	36.2	28.4	32.3	5.49	
	412	18.0	17.9	17.9	0.10	
	137	3.7	6.6	5.1	2.07	
	46	11.7	4.2	8.0	5.28	
	15	2.6	2.1	2.3	0.41	
	5	-0.3	-3.5	-1.9	2.28	
Experimented on Aurora Kinase B						
#1	10000	100.4	100.3	100.3	0.08	 <p>Bottom 11.10 Top 97.97 IC50 (nM) 19 Hill 1.15</p>
	3333	99.2	98.8	99.0	0.30	
	1111	97.1	98.9	98.0	1.22	
	370	91.9	91.7	91.8	0.15	
	123	89.2	81.5	85.3	5.47	
	41	74.6	73.8	74.2	0.53	
	14	49.5	47.5	48.5	1.37	
	5	28.9	9.2	19.1	13.97	
	2	21.3	16.5	18.9	3.42	
	1	18.3	6.7	12.5	8.20	
#2	10000	100.0	100.5	100.3	0.30	 <p>Bottom 8.34 Top 103 IC50 (nM) 22 Hill 0.63</p>
	3333	98.2	99.1	98.6	0.61	
	1111	95.1	96.3	95.7	0.84	
	370	88.8	91.6	90.2	1.97	
	123	76.4	78.6	77.5	1.52	
	41	65.1	65.1	65.1	0.00	
	14	47.5	46.3	46.9	0.84	
	5	35.8	33.7	34.7	1.52	
	2	23.0	22.8	22.9	0.15	
	1	15.6	15.9	15.8	0.23	

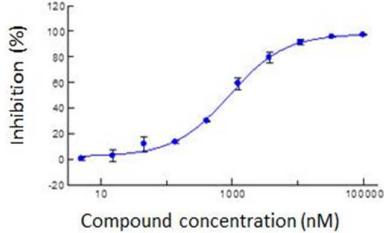
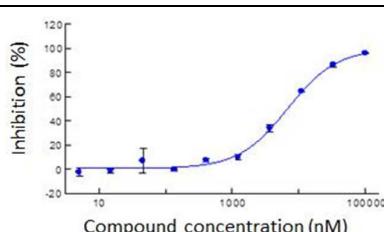
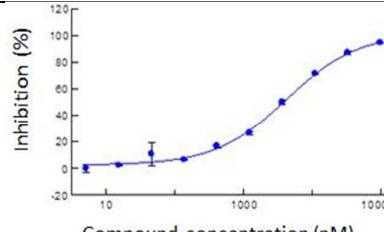
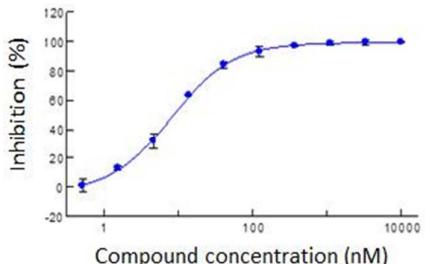
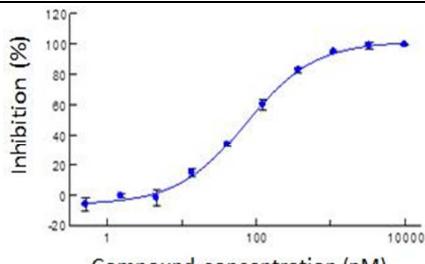
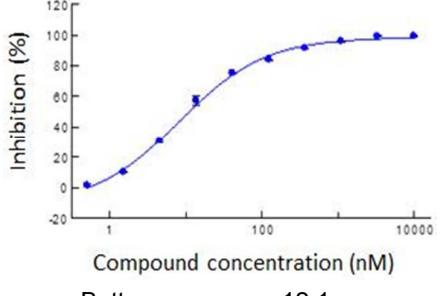
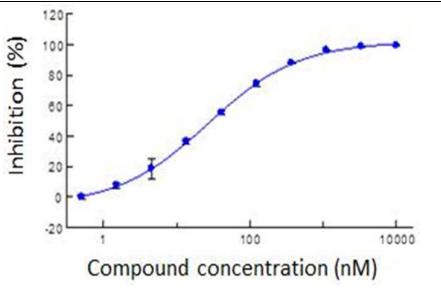
Compound	Compound concentration (nM)	Inhibition (%)	Inhibition (%)	Mean	SD	IC ₅₀ curve
#3	100000	96.8	97.3	97.1	0.41	 <p>Bottom 2.1 Top 98 IC50 (nM) 904 Hill 1.03</p>
	33333	95.7	95.1	95.4	0.41	
	11111	92.7	90.1	91.4	1.81	
	3704	82.4	76.2	79.3	4.45	
	1235	62.4	55.6	59.0	4.80	
	412	29.5	29.9	29.7	0.23	
	137	14.1	12.4	13.2	1.17	
	46	15.7	7.4	11.6	5.85	
	15	5.8	-0.8	2.5	4.68	
	5	-0.8	0.8	0.0	1.17	
#5	100000	95.7	96.1	95.9	0.29	 <p>Bottom 0.8 Top 100 IC50 (nM) 6,789 Hill 1.18</p>
	33333	87.6	85.0	86.3	1.81	
	11111	64.4	64.1	64.3	0.18	
	3704	35.9	32.0	33.9	2.81	
	1235	11.6	8.3	9.9	2.34	
	412	8.3	6.6	7.4	1.17	
	137	-0.8	0.0	-0.4	0.59	
	46	14.1	0.0	7.0	9.95	
	15	0.0	-2.5	-1.2	1.76	
	5	0.0	-5.0	-2.5	3.51	
#6	100000	94.8	94.3	94.5	0.35	 <p>Bottom 2.37 Top 102 IC50 (nM) 4,197 Hill 0.83</p>
	33333	88.1	85.8	87.0	1.58	
	11111	70.9	71.8	71.4	0.70	
	3704	50.9	49.1	50.0	1.29	
	1235	27.1	25.7	26.4	0.99	
	412	17.4	15.7	16.6	1.17	
	137	5.8	6.6	6.2	0.59	
	46	16.6	4.1	10.3	8.78	
	15	2.5	1.7	2.1	0.59	
	5	1.7	-2.5	-0.4	2.93	

Table S5. IC₅₀ curves for hit compounds #1 and #2 as control assay experiment.

Compound	Compound concentration (nM)	Inhibition (%)	Inhibition (%)	Mean	SD	IC ₅₀ curve								
Experimented on Aurora Kinase A														
#1	10000	99.8	99.1	99.4	0.54	 <table> <tr><td>Bottom</td><td>-4.1</td></tr> <tr><td>Top</td><td>99</td></tr> <tr><td>IC50 (nM)</td><td>7.9</td></tr> <tr><td>Hill</td><td>1.05</td></tr> </table>	Bottom	-4.1	Top	99	IC50 (nM)	7.9	Hill	1.05
Bottom	-4.1													
Top	99													
IC50 (nM)	7.9													
Hill	1.05													
3333	100.8	98.1	99.4	1.98										
1111	99.8	97.8	98.8	1.44										
370	97.3	96.5	96.9	0.54										
123	95.6	90.3	93.0	3.77										
41	85.7	82.6	84.1	2.25										
14	63.4	63.1	63.3	0.18										
5	35.2	28.2	31.7	4.94										
2	12.1	14.0	13.0	1.35										
1	3.8	-2.3	0.8	4.31										
#2	10000	99.6	99.4	99.5	0.09	 <table> <tr><td>Bottom</td><td>-6.3</td></tr> <tr><td>Top</td><td>102</td></tr> <tr><td>IC50 (nM)</td><td>72</td></tr> <tr><td>Hill</td><td>0.94</td></tr> </table>	Bottom	-6.3	Top	102	IC50 (nM)	72	Hill	0.94
Bottom	-6.3													
Top	102													
IC50 (nM)	72													
Hill	0.94													
3333	100.7	97.7	99.2	2.16										
1111	95.3	94.4	94.8	0.63										
370	84.2	81.4	82.8	1.98										
123	62.7	57.5	60.1	3.68										
41	34.5	32.6	33.6	1.35										
14	13.0	16.4	14.7	2.42										
5	2.0	-5.7	-1.8	5.48										
2	0.1	-1.8	-0.8	1.35										
1	-3.3	-9.3	-6.3	4.22										

Compound	Compound concentration (nM)	Inhibition (%)	Inhibition (%)	Mean	SD	IC ₅₀ curve
Experimented on Aurora Kinase B						
#1	10000	99.6	98.6	99.1	0.70	 <p>Bottom -12.1 Top 98 IC50 (nM) 8.0 Hill 0.77</p>
	3333	98.7	99.2	98.9	0.32	
	1111	95.6	95.8	95.7	0.19	
	370	91.1	91.2	91.2	0.13	
	123	83.7	84.0	83.9	0.25	
	41	75.4	74.6	75.0	0.57	
	14	54.9	59.2	57.0	3.06	
	5	31.1	30.0	30.5	0.76	
	2	9.9	9.9	9.9	0.00	
	1	1.8	0.9	1.4	0.64	
#2	10000	99.4	98.8	99.1	0.45	 <p>Bottom -5.6 Top 102 IC50 (nM) 27 Hill 0.70</p>
	3333	98.7	98.5	98.6	0.19	
	1111	96.4	95.8	96.1	0.38	
	370	87.6	87.8	87.7	0.13	
	123	75.8	72.9	74.3	2.04	
	41	56.2	54.3	55.3	1.34	
	14	35.2	37.6	36.4	1.66	
	5	23.1	14.0	18.6	6.50	
	2	9.0	6.3	7.7	1.91	
	1	0.9	-0.9	0.0	1.27	

Supplementary Figures

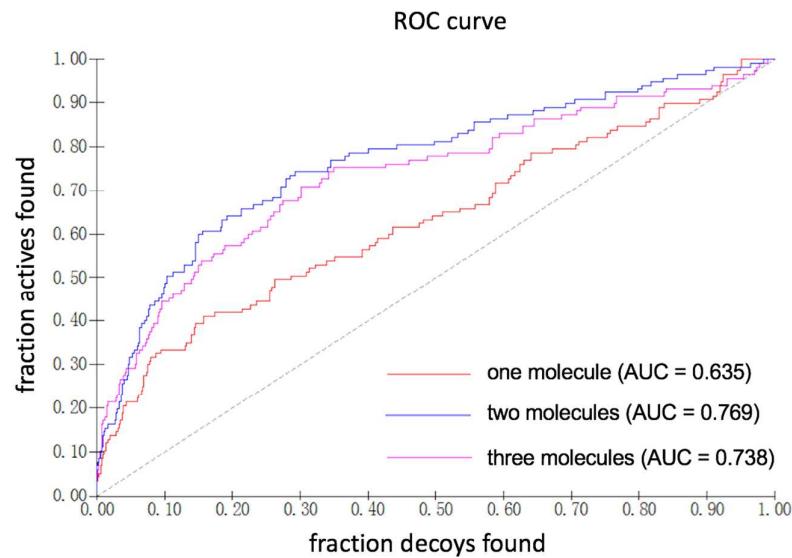


Figure S1. The ROC curves for queries overlaid by one molecule, two molecules and three molecules together the AUC (area under the curve).

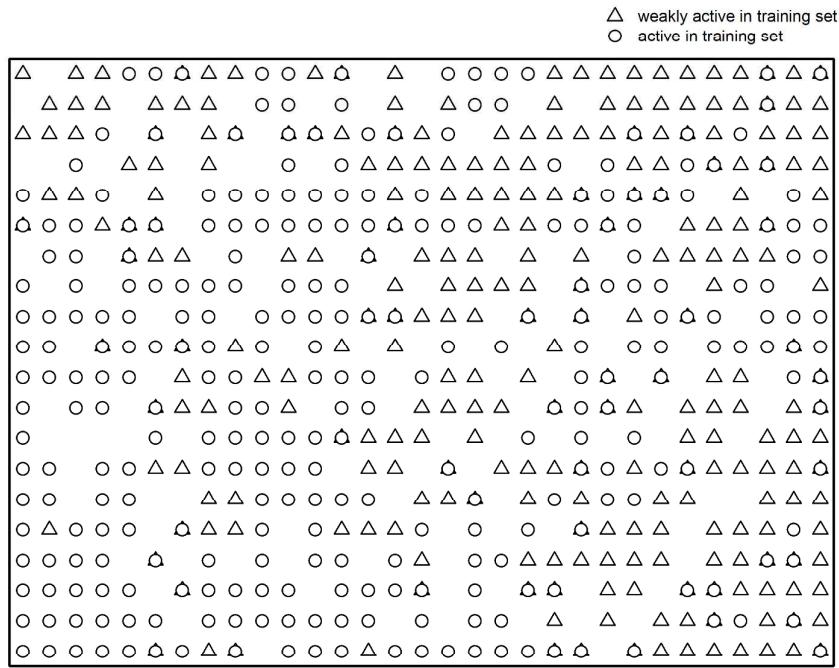


Figure S2. Rectangular Kohonen's self-organizing map (size 31×20) on the basis of most frequent occupation for the training set split from dataset 2. Circles represent highly active AURKA inhibitors and triangles represent weakly active AURKA inhibitors.

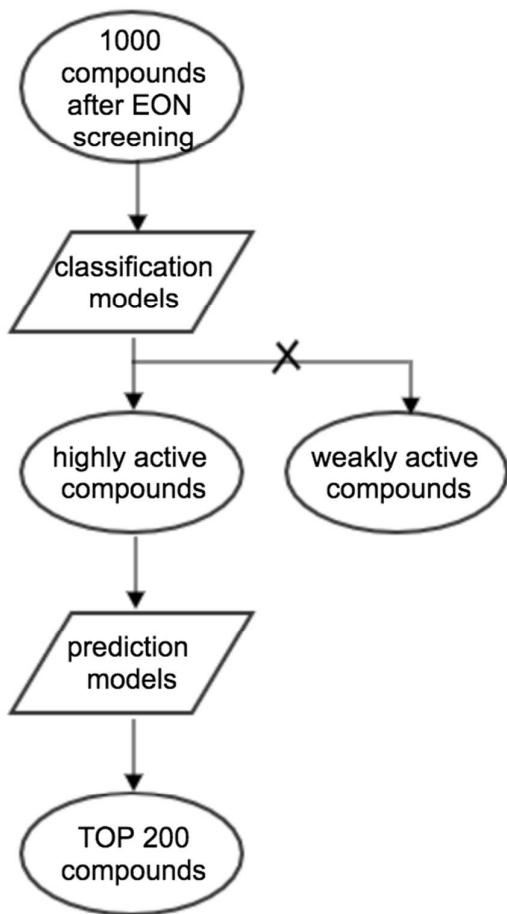
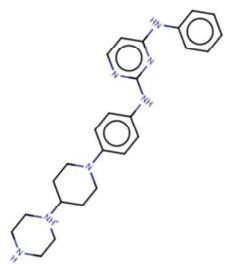
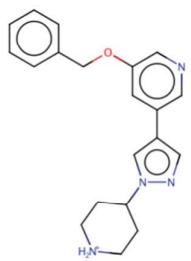


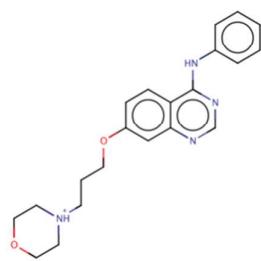
Figure S3. QSAR protocol for the compounds from J&K database.



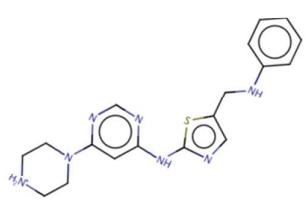
scaffold of Hit1



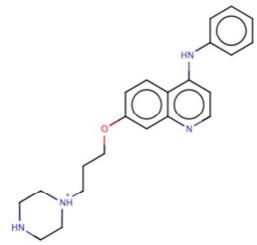
scaffold of Hit2



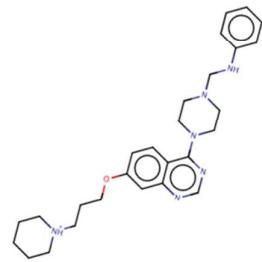
scaffold of Hit3



scaffold of Hit4

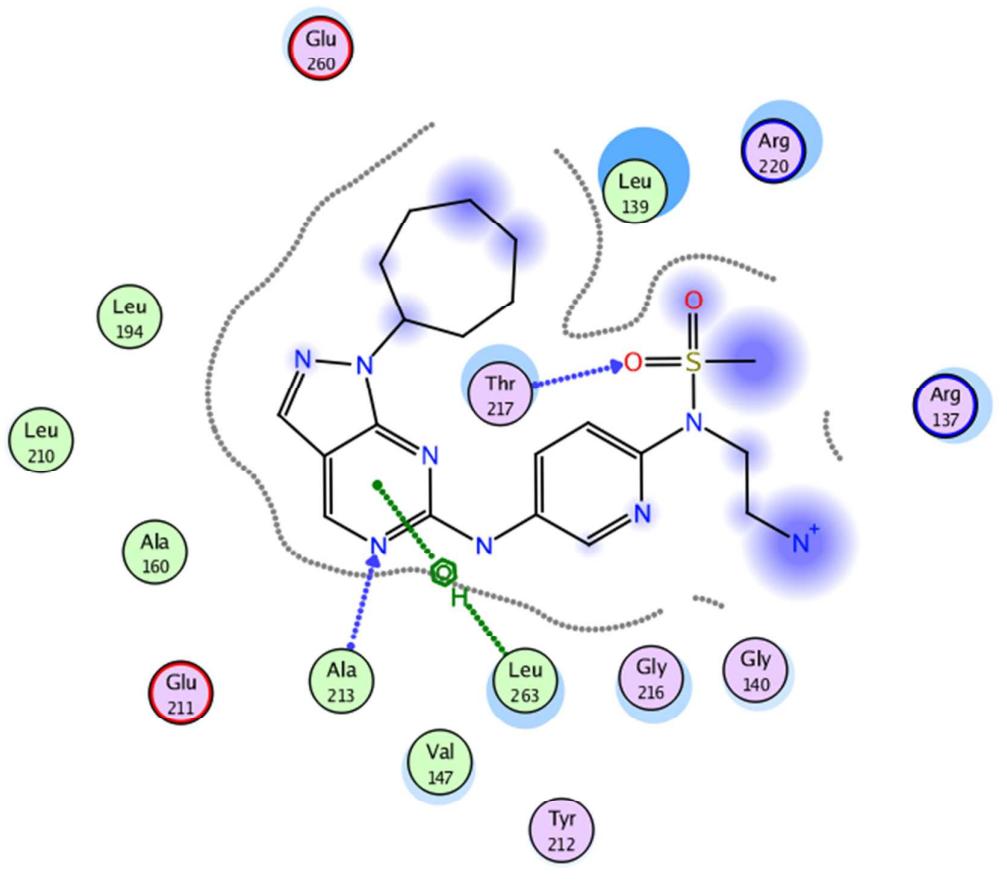


scaffold of Hit5



scaffold of Hit6

Figure S4. Bemis-Murcko scaffolds for hits1-6.



- | | | | |
|---------------------|----------------------|-----------------------|------------------|
| ○ polar | → sidechain acceptor | ○ solvent residue | ○○ arene-arene |
| ● acidic | ← sidechain donor | ○ metal complex | ○○H arene-H |
| ○ basic | → backbone acceptor | solvent contact | ○+○ arene-cation |
| ○ greasy | ← backbone donor | metal contact | |
| ○ proximity contour | ● ligand exposure | ○ receptor contact | |

Figure S5. Receptor-ligand interactions between hit1 and AURKA (PDB code: 3r21) at the ATP-binding site. Image produced by MOE (version 2011).

Kinase assay method

By using Mobility Shift Assay, we screened 28 compounds against Aurora A and B kinase in vitro. The compounds were tested twice from 10 μ M or 100 μ M for 10 concentrations (see the Table S4 and Table S5 for the details of compound concentration). The details of the experimental process are as following:

1. Prepare 1x kinase base buffer and stop buffer for testing kinases

1) 1x Kinase base buffer. 50 mM HEPES, pH 7.5; 0.0015% Brij-35 (use 0.015% Brij-35 in the control assay); 10 mM MgCl₂; 2 mM DTT. 2) 2x Stop buffer. 100 mM HEPES, pH 7.5; 0.015% Brij-35; 0.2% Coating Reagent #3; 50 mM EDTA

2. Prepare compound

1) Dilute the compound to 50X of the final desired highest inhibitor concentration in reaction by 100% DMSO (500 μ M solution). 2) Serially dilute the compound for a total of 10 concentrations. 3) Add 100 μ l of 100% DMSO to two empty wells for no compound control and no enzyme control in the same 96-well plate. Mark the plate as source plate. 4) Prepare intermediate plate. Transfer 10 μ l of compound from source plate to a new 96-well plate as the intermediate plate. Add 90 μ l of 1x kinase buffer to each well of the intermediate plate. Mix the compounds in intermediate plate for 10 min on shaker.

3. Prepare assay plate

Transfer 5 μ l of each well from the 96-well intermediate plate to a 384-well plate in duplicates.

4. Kinase reaction

1) Prepare 2.5x enzyme solution. Add kinase in 1x kinase base buffer. 2) Prepare 2.5x peptide solution Add FAM-labeled peptide and ATP in the 1x kinase base buffer. 3) Assay plate already contains 5 μ l of compound in 10% DMSO. 4) Transfer 2.5x enzyme solution to the assay plate Add 10 μ l of 2.5x enzyme solution to each well of the 384-well assay plate. 5) Incubate at room temperature for 10 min. 6) Transfer 2.5x peptide solution to the assay plate Add 10 μ l of 2.5x peptide solution to each well of the 384-well assay plate. 7) Kinase reaction and stop Incubate at 28 $^{\circ}$ C for 1hr. Add 25 μ l of stop buffer to stop reaction.

5. Caliper reading Collect data on Caliper.
6. Do control assay to avoid aggregation for compounds with high bioactivity (IC50 < 500nM). The steps are the same as the former five steps except using 0.015% Brij-351 when preparing 1x kinase base buffer and stop buffer for testing kinases (step 1) for the control assay.

Appendix

I. Dataset 1

The PDB codes for the compounds in dataset 1 (72 compounds in total) are as followed: 0BX, 0BY, 0BZ, 0C0, 0C3, 0C4, 0C5, 0C6, 0C7, 0C8, 0C9, 0FY, 0K6, 2JZ, 2VU, 45B, 48B, 83H, 97B, 400, 626, A0H, ANP, AND, ADP, AK8, AKI, ANP, ASH, ATP, CC3, CJ5_nh, D36, D37, E9Z, EML, FH3, FH5, HPM, JVE, L0C, L0D, L0E, L0F, L0G, LJE, LJF, MMH, MPY, N13, N15, NHI, NHJ, NHU, NRM, OFI, P9J, PEG, PFQ, PG4, QMN, RO9, VEK, VX6, WPH, X6D, XU1, XU2, Y3M, YM4, YPH, ZZL.

II. Dataset 2

smiles IC₅₀(nM) label index

Clc1cc(ccc1F)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCCN2CCOCC2)c3)cn1
 0.15000001 1 1
 o1c2ncnc(NCCc3nc[nH]c3)c2c(c1-c1cccc1)-c1cccc1 0.296 1 2
 S1[C@H](NC=C1CC(=O)Nc1cc(F)ccc1)Nc1ncnc2c1cc(OC)c(OCCCN1CCC(CC1)C
 OP(O)(O)=O)c2 0.30000001 1 3
 o1c2ncnc(NCCO)c2c(c1-c1cccc1)-c1cccc1 0.30899999 1 4
 Clc1c(cccc1Cl)C(=O)N1CCN(CC1)Cc1cc(Nc2scen2)ccc1 0.5 1 5
 OC(=O)c1cc(Nc2nc3n(ccc3cn2)C2CCCCC2)ccc1 0.60000002 1 6
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)C)cc(n1)Nc1n[nH]c(c1)C
 0.69999999 1 7
 Clc1cc(ccc1)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCN2CCCCC2)c3)cn1
 0.80000001 1 8
 O(C[C@@H](O)CN1CCCCC1)c1cc2ncnc(Nc3cnc(nc3)NC(=O)c3cccc3)c2cc1OC
 0.80000001 1 9
 o1c2ncnc(N3CCC(O)CC3)c2c(c1-c1cccc1)-c1cccc1 0.80699998 1 10
 Fc1c(cccc1C(F)(F)F)C(=O)N1CCN(CC1)Cc1nc(Nc2n[nH]cc2)ccc1 0.89999998 1
 11
 Clc1cc2c(-c3nc(ncc3CN=C2c2c(OC)cccc2F)Nc2cc(OC)c(cc2)C(O)=O)cc1 1 1
 12
 Fc1cccc1C(NC(=O)c1oc2c([nH]nc2NC(=O)c2ccc(cc2)CN2CCOCC2)c1)(C)C 1
 1 13
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)C(=O)Nc1ccc(F)cc1 1 1
 14
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCOC)c2)CC(=O)Nc1cc(F)ccc1 1 15
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCN(CC2)C(C)(C)C)cc(n1)Nc1n[nH]c(c1)C 1.3
 1 16
 Fc1cccc(F)c1NC(=O)Nc1c[nH]nc1-c1[nH]c2c(n1)cc(cc2)CN1CCOCC1 1.5 1 17
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCCCC2)cc(n1)Nc1n[nH]c(c1)C 1.6 1 18
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCN(CC2)C)cc(n1)Nc1n[nH]c(c1)C 1.6 1 19
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCOCC2)cc(n1)Nc1n[nH]c(c1)C 1.7 1 20
 o1c2ncnc(NCCN3CCOCC3)c2c(c1-c1cccc1)-c1cccc1 1.766 1 21
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CCO)c
 2)cccc1F 1.89 1 22
 P(OCCN1CCN(CC1)C(=O)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(F)c
 cc3)c2cc1)(O)(O)=O 1.91 1 23
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CCO)
 c2)ccc1 1.9299999 1 24
 Br1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)CN1CCOCC1 2 1
 25
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)C3CC3)ccc2N\1 2 1 26

FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)CCn1ccnc1 2 1 27
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CN1CCOCC1 2 1 28
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC[C@H]1CO)c2)CC(=O)Nc1cccc(F)c1F
 2 1 29
 O=C1Nc2c(cc3[nH]c-4c(CCCc5c-4n[nH]c5C)c3c2)C1(C)C 2 1 30
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)[C@@@H]3N(CCCC3)C)ccc2N
 \1 2 1 31
 O(C)c1ccc(NC(=O)Nc2cc3NC(=O)/C(/c3cc2)=C\c2[nH]cc(C(O)=O)c2C)cc1
 2.0899999 1 32
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CCO)
 c2)cc(F)c1 2.29 1 33
 Fc1cccc1NC(=O)Nc1c[nH]nc1-c1[nH]c2c(n1)cc(cc2)CN1CCOCC12.8 1 34
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CCF)c
 2)ccc1 2.8599999 1 35
 Brclcnc(nc1Nc1cc2[nH]ncc2cc1)Nc1cc2c(CS(=O)(=O)C2)cc1 3 1 36
 Brclcnc(nc1Nc1cc2nc([nH]c2cc1)C(F)(F)F)Nc1cc2c(CS(=O)(=O)C2)cc1 3 1 37
 Brclcnc(nc1Nc1cc2nc[nH]c2cc1)Nc1cc2c(CS(=O)(=O)C2)cc1 3 1 38
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)Cn1nccc1 3 1 39
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)N1CCN(CC1)Cn1nccc1 3 1
 40
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1scen1)-c1ccc(cc1)CN1CCOCC1 3
 1 41
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)NCCN1CCOCC1 3
 1 42
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3ncnc(nc3)NC(=O)c3cccc3)c2cc1OC 3 1 43
 O1CCN(CC1)Cc1cc2[nH]c(nc2cc1)-c1n[nH]cc1NC(=O)NC1CC1 3 1 44
 S1(=O)(=O)Cc2cc(Nc3nc(NC=4C=C[C@H]5NC(=N[C@@H]5C=4)C(F)(F)F)c([N+]
](=O)[O-])cn3)ccc2C1 3 1 45
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)-c1[nH+]ccn1C 3 1 46
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)N(CCCn1ccnc1)CC 3
 1 47
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCN1CCOCC1 3
 1 48
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O) 3 1 49
 s1cccc1C(=O)N[n+]1[nH]c2cc(oc2c1)C(=O)NC(C)(C)c1cccc1 3 1 50
 o1c2ncnc(NCCN3ccnc3)c2c(c1-c1cccc1)-c1cccc1 3.3110001 1 51
 Clc1cccc1NC(=O)c1ccc(Nc2nc(ncc2F)Nc2ccc(cc2)CC(=O)N2CCN(CC2)CC)cc1
 3.4000001 1 52
 Clc1cccc1NC(=O)c1ccc(Nc2nc(ncc2F)Nc2ccc(cc2)CNCCN2CCNCC2)cc1
 3.4000001 1 53
 O1CCN(CC1)Cc1cc2nc([nH]c2cc1)-c1n[nH]cc1NC(=O)c1cccc1 3.5 1 54
 S(c1ccc(NC(=O)CC)c1)c1nc(N2CCNCC2)cc(n1)Nc1n[nH]c(c1)C 3.7 1 55
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCNCC3)c2)ccc

1 3.77 1 56
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1ncsc1)-c1ccc(OC)cc1 4 1 57
 Clc1cc2c(-c3nc(ncc3CN=C2c2c(F)cccc2F)Nc2ccc(cc2)C(O)=O)cc1 4 1 58
 Clc1cnc(nc1Nc1cc2[nH]c(nc2cc1)C(F)(F)F)NC=1C=C[C@@@H]2[C@@@H](C=1)CS(=O)(=O)C2 4 1 59
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(N(C(=O)C3CCN(CC3)C)CC)ccc2N\1
 4 1 60
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)Cn3ccnc3)ccc2N\1 4 1 61
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)CCN1CCOCC1 4 1 62
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)Cn1ccnc14 1 63
 FC(F)(F)c1nc(ncc1C(OC)=O)/C(/C(=O)N)=C\1\Nc2c(N/1)cccc24 1 64
 O=C1N(c2c(cc3[nH]c-4c(CCCc5c-4n[nH]c5C)c3c2)C1(C)C)CC4 1 65
 S1(=O)(=O)Cc2cc(Nc3nc(Nc4cc5NC(=O)Nc5cc4)c([N+](=O)[O-])cn3)ccc2C1 4
 1 66
 S1(=O)(=O)Cc2cc(Nc3nc(Nc4cc5nc([nH]c5cc4)C(F)(F)F)c(cn3)C)ccc2C1 4 1
 67
 S\1c2cc(NC(=O)Cn3ccnc3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 4 1 68
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)N(CCO)CC 4 1 69
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCn1ccnc1 4 1
 70
 o1c2c([nH]nc2NC(=O)c2ccc(N3CCCN(C3)C)cc2)cc1C(=O)NC1(CC1)c1cccc1 4
 1 71
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)C(=O)Nc1cccc1 4 1 72
 s1cc(nc1NC(=O)Nc1cc(cc(c1)C(F)(F)F)CN1CCCC1)CCNc1ncnc2c1scc2 4 1
 73
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)C 4 1 74
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN(C(CO)(C)C)CC 4 1 75
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN(C(CO)(C)C)CC(F)(F)F 4 1
 76
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN(C(CO)(C)C)CC(F)F 4 1 77
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CC(F)(F)C(F)(F)C1 4 1 78
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CC(F)(F)C1 4 1 79
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CC(F)(F)CC1 4 1 80
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CC(F)(F)CCC1 4 1 81
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CC(F)C1 4 1 82
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CCC(CC1)C(F)(F)F 4 1 83
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CCC(F)(F)CC1 4 1 84
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CCC(F)CC1 4 1 85
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1CCCC1 4 1 86
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1C[C@@@H](F)CC1 4 1 87
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CN1C[C@@@H](F)CCC1 4 1 88
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CNCC(F)(F)C(F)(F)F 4 1 89
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)CNCCCC(F)(F)F 4 1 90

s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)CC)C 4 1 91
 s1nc(cc1NC1=NC(SC)=Cn2c1ncc2-c1cn[nH]c1)C 4 1 92
 s1nc(cc1NC1=NC=Cn2c1ncc2-c1cn[nH]c1)C 4 1 93
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)[C@H]3N(CCCC3)C)ccc2N\1
 4 1 94
 Clc1cccc1NC(=O)c1ccc(Nc2nc(ncc2F)Nc2ccc(cc2)CC(=O)N2CCN(CC2)C(=O)C)c
 c1 4.3000002 1 95
 Clc1cccc1NC(=O)c1ccc(Nc2nc(ncc2F)Nc2ccc(cc2)CNC(=O)CN2CCNCC2)cc1
 4.3000002 1 96
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)C3CC
 3)c2)ccc1 4.6199999 1 97
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccnc1)-c1ccc(cc1)CN1CCOCC1 5 1
 98
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccnc1)-c1ccc(cc1)CN1CCOCC1 5 1
 99
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)C3(N)CC3)ccc2N\1 5 1
 100
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)CCN3CCOCC3)ccc2N\1 5
 1 101
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(O)=O 5 1 102
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)CCO 5 1 103
 S1(=O)(=O)Cc2cc(Nc3nc(Nc4cc5nc[nH]c5cc4)c(F)cn3)ccc2C1 5 1 104
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CCN1CCS(=O)(=O)CC1 5
 1 105
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)Cn1ccnc1 5 1 106
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCNC)CO)c2)CC(=O)Nc1cc(F)ccc1 5 1
 107
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCOCC3)cc2)cc1C(=O)N[C@H](C)c1cccc1 5
 1 108
 s1cccc1CC(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(cc2)C(C)(C)C)C1 5 1 109
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)C)c2)cc1
 5.0700002 1 110
 O1CCN(CC1)Cc1cc2nc([nH]c2cc1)-c1n[nH]cc1NC(=O)NC1CCCCC1 5.6999998
 1 111
 O=C(Nc1c[nH]nc1-c1[nH]c2c(n1)cccc2)c1cccc1 5.9000001 1 112
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccnc1)-c1ccc(cc1)CN1CCOCC1 6 1
 113
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccnc1)-c1ccc(cc1)CN1CCOCC1 6 1
 114
 Clc1cccc1C(=O)Nc1ccc(Nc2nc(ncc2F)Nc2ccc(O)cc2)cc1 6 1 115
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)C(N)(C)C)ccc2N\1 6 1
 116
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)C3CCN(CC3)C)ccc2N\1 6

1 117
FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)CCN3CCN(CC3)C)ccc2N\1
 6 1 118
FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N(CC)c1cccnc1 6 1
 119
FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N(CCCN1CCOCC1)C
 C 6 1 120
O(C[C@@H](O)CN1CCCCC1)c1cc2ncnc(Nc3cnc(nc3)NC(=O)c3cccc3)c2cc1OC
 6 1 121
O=C(Nc1n[nH]c2c1CN(C2)C(=O)[C@H](O)c1cccc1)c1ccc(N2CCN(CC2)C)cc1 6
 1 122
S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)C)cc(n1)Nc1[nH]nc(c1)C 6 1
 123
S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCN1CCOCC1 6
 1 124
S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCN1CCOCC1 6
 1 125
S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CCc1n(cnc1)C 6 1
 126
s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)e2)CCCC 6 1 127
s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@@H](C)c1cccc1
 6 1 128
s1nc(cc1NC1=NC=Cn2c1ncc2-c1cn[nH]c1)C1CCN(S(=O)(=O)C)CC1 6 1
 129
S(=O)(=O)(N1CCCC1)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(F)ccc3)c
 2cc1 6.04 1 130
S(=O)(=O)(N1C[C@@H](F)CC1)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3
cc(F)ccc3)c2cc1 6.29 1 131
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3C[C@H](N[C@
@H](C3)C)C)c2)ccc1 6.4200001 1 132
FC(F)(F)c1nc(nc(N)c1)/C(/C(=O)N)=C\1\Nc2c(N/1)cccc2 7 1 133
FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)CCN3CCOCC3)ccc2N\1 7
 1 134
FC1(F)CCN(CC1)CCNC(=O)c1cc2N\C(\Nc2cc1)=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F
 7 1 135
S(=O)(=O)(N1CCCC1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC
 3)cc1 7 1 136
S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C(F)(F)F)C(C)(C)C)cccc2 7 1 137
S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CCN1CCOCC1 7 1
 138
S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CN1CCNCC1 7 1 139
o1c2ncnc(N[C@H](CO)c3cccc3)c2c(c1-c1cccc1)-c1cc(NC(=O)C=C)ccc1 7 1
 140

BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1ncnc1)-c1ccc(OC)cc1 8 1 141
 Clc1cnc(nc1Nc1ccc(O)cc1)Nc1ccc(O)cc1 8 1 142
 FC(F)(F)c1nc(nc(c1)C)/C(/C(=O)N)=C\1\Nc2c(N/1)cccc2 8 1 143
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)CCn3ccnc3)ccc2N\1 8 1
 144
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)-c1cccnc18 1 145
 S(=O)(=O)(N)c1cc(Nc2nc(ccn2)C=2[C@H]3[C@@H](N=CC=C3)N(C=2)CCC)ccc1
 8 1 146
 S(=O)(=O)(N1CCc2c1cccc2)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)
)CCC3)cc1 8 1 147
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)C(=O)N1CCN(CC1)C 8 1
 148
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)c1cccnc1)C 8 1 149
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)[C@H]3CCN(C3)C)ccc2N\1
 8 1 150
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1cccnc1)-c1ccc(OC)cc1 9 1 151
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccnc1)-c1ccc(OC)cc1 9 1 152
 Clc1cc(NC(=O)Nc2sc(cn2)CCNc2ncnc3c2scc3)ccc1 9 1 153
 Clc1cc(NC(=O)Nc2scc(n2)CCNc2ncnc3c2scc3)ccc1 9 1 154
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(N3CCN(CC3)C)ccc2N\1 9 1
 155
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N1CCN(CC1)C 9 1
 156
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)CO 9 1 157
 F[C@@H](C(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)C1)c1cccc1
 9 1 158
 Fc1cccc1NC(=O)c1ccc(Nc2nc(ncc2F)Nc2ccc(O)cc2)cc1 9 1 159
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](CC)c1cccc1
 9 1 160
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1F)cccc2 9 1
 161
 s1cc(nc1NC(=O)Nc1cc(ccc1)C)CCNc1ncnc2c1scc2 9 1 162
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CC3C
 C3)c2)ccc1 9.5100002 1 163
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(N2CCNCC2)cc1 10 1
 164
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)CN 10 1 165
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)CN1CCNCC1 10 1
 166
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)N1CCNCC1 10 1 167
 Clc1cccc1NC(=O)c1ccc(Nc2nc(ncc2F)Nc2ccc(O)cc2)cc1 10 1 168
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(N2CCN(CC2)C)cc1 10 1
 169

Clc1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)Cn1nccc1 10 1
 170
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)N1CCN(CC1)C 10 1 171
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)N1CCN(CC1)Cn1nccc1 10 1
 172
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)CN(C)C)ccc2N\1 10 1
 173
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N(CCCn1ccnc1)CC 10
 1 174
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N(CCO)CCO 10 1
 175
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N1CCNCC1 10 1
 176
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N1C[C@H](N)CC1 10
 1 177
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)NCCN1CCOCC1 10
 1 178
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)Nc1ccncc1 10 1
 179
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C\1/Nc2c(N/1)cccc2 10 1 180
 Fc1ccc(cc1)C(=O)Nc1c[nH]nc1-c1[nH]c2c(n1)cc(cc2)CN1CCOCC1 10 1 181
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C(F)(F)F)-c1ccncl)cccc2 10 1 182
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C(F)(F)F)C(F)(F)F)cccc2 10 1 183
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C)C(F)(F)F)cccc2 10 1 184
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)N)C(F)(F)F)cccc2 10 1 185
 S\1c2cc(N)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 10 1 186
 S\1c2cc(OCCn3ccnc3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 10 1 187
 S\1c2cc(S(=O)(=O)NCCN3CCOCC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F
 10 1 188
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)-c1ccncc1 10 1 189
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)N(CCCN1CCOCC1)CC
 10 1 190
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)N1CCC(N)CC1 10 1
 191
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)[C@H]3CCNC3)ccc2N\1 10
 1 192
 Clc1cc(NC(=O)Nc2scc(n2)CCNc2ncnc3c2scc3)ccc1F 11 1 193
 Clc1cc(Nc2ncnc3c2cc(NC(=O)\C=C\CN(C)C)c(O[C@H]2CCOC2)c3)ccc1F 11 1
 194
 s1c(ccc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)C(=O)Nc1cccc1 11 1
 195
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCOCC3)cc2)cc1C(=O)NCc1cccc1 11 1
 196

BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccc(Cl)cc1)-c1ccc(cc1)CN1CCOCC1 12 1
 197
 O1CCN(CC1)Cc1cc2nc([nH]c2cc1)-c1n[nH]cc1NC(=O)Nc1cccc1 12 1 198
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1)c1c
 ccccc1 12 1 199
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC(CC1)CO)c2)CNS(=O)(=O)c1cc(F)ccc1
 12 1 200
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1ccc(O)cc1)Nc1ccc(O)cc1 13 1 201
 O([C@@@H](C(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)C1)c1cccc1
)C 13 1 202
 O1CCN(CC1)Cc1cc2nc([nH]c2cc1)-c1n[nH]cc1NC(=O)Nc1ccnc1 13 1 203
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](C)c1cccc1 13
 1 204
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\c=C=c2cc(NC(=O)N3CCN(CC3)C)cc2)cc1C 13
 1 205
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\c=C=c2cc(NC(=O)N3CCN(CC3)C)cc2)cc1C 13
 1 206
 S(=O)(N1CCN(CC1)C)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(F)ccc3)
 c2cc1 13.94 1 207
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)-c1cc(ccc1)C(=O)C 14
 1 208
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)CN(C)C 14 1
 209
 FC(F)(F)c1cnc(nc1Nc1ccc(O)cc1)Nc1ccc(O)cc1 14 1 210
 Fc1ccc(cc1)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 14 1 211
 Fc1cccc1C(=O)Nc1ccc(Nc2nc(ncc2F)Nc2ccc(O)cc2)cc1 14 1 212
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1ccc(OC)cc1)Nc1ccc(O)cc1 14 1 213
 S(=O)(=O)(N1CCCCC1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CC
 C3)cc1 14 1 214
 [nH]1nc(Nc2nc(nc(N3CCN(CC3)C)c2)\c=C\c2cccc2)cc1C14 1 215
 s1c2c(nc1-c1ccc(Nc3ncne4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2 14 1
 216
 s1nc(cc1NC1=NC(NN2CCCC2=O)=Cn2c1ncc2-c1cn[nH]c1)C 14 1 217
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(N2CCN(CC2)C)cc1 15 1
 218
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)N1CCN(CC1)C 15 1 219
 BrC1cnc2nc([nH]c2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(N2CCN(CC2)C)cc1 15 1
 220
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1scen1)-c1ccc(cc1)CN(C)C 16 1
 221
 O(c1ncnc1-c1nc(nc1)NC)c1ccc(NC(=O)c2cccc2Nc2cccc2)cc1 16 1 222
 OC(=O)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 16 1 223
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(OC)cc1 17 1 224

O1CCN(CC1)CCCOc1cc2ncnc(Nc3cnc(nc3)NC(=O)CCCC)c2cc1OC 17 1
 225
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)Cc1ccnc1 17 1 226
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)Cc1cnnc1 17 1 227
 S1[C@@H]2[C@@H](N=CN=C2NCCC(C=C/C(Nc2[nH]c(N)c(n2)\C=C(\C(F)(F)F)\C)=C)C=C1 17 1 228
 s1c2c(ncnc2NCCc2ccc(Nc3[nH]c4ncc(cc4n3)C(F)(F)F)cc2)cc1 17 1 229
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\C=C\c2cccc2)cc1C 17 1 230
 s1nc(cc1NC1=NC(=C[NH+]2C1=NC=C2c1cn[nH]c1)C1CC1)C 17 1 231
 Fc1cnc(nc1Nc1ccc(NC(=O)c2cccc2)cc1)Nc1ccc(O)cc1 18 1 232
 O1C2n3c4c(c5c(CNC5=O)c5c6c(n(c45)[C@]1(C)[C@H](OC)[C@H](NC)C2)cccc6)
 c1c3cccc1 18 1 233
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](CN1CCOCC1)
 c1cccc1 18 1 234
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCOCC3)cc2)cc1C(=O)N[C@H](CN1CCCC1)c1cc
 ccc1 18 1 235
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN(CC(C)C)CCO)c4)c2)cccc1F
 18 1 236
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1cc(O)ccc1)Nc1ccc(O)cc1 19 1 237
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1cccc1)Nc1ccc(O)cc1 19 1 238
 O(c1cccc1-c1nc(nc1)NC)c1c2c(cccc2)c(Nc2[nH]c3e(n2)cccc3)cc1 19 1 239
 O=C(Nc1cc2c([nH]nc2\C=C\c2cccc2)cc1C)Cc1cccc1 19 1 240
 Cl\C(=C\c1nc([nH]c1N)NC(=C=C/C(CCNC1ncnc2c1scc2)=C)=C)\C 20 1 241
 Clc1cc(Nc2ncnc3c2cc(OCCCN2CCOCC2)c(OC)c3)ccc1F 20 1 242
 Clc1cc2nc([nH]c2nc1)Nc1ccc(cc1)CCNc1ncnc2c1scc2 20 1 243
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(OCCO)cc1 20 1 244
 FC(F)(F)c1nc(nc1)/C(/C(=O)N)=C/1\Nc2cc(N(C(=O)CN(CC)CC)CC)ccc2N\1 20
 1 245
 FC(F)(F)c1nc(nc1)/C(/C(=O)N)=C/1\Nc2cc(N(CC)C(=O)N3CCCCC3)ccc2N\1 20
 1 246
 FC(F)(F)c1nc(nc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)-c1ncnc120 1 247
 FC(F)(F)c1nc(nc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)N1CCC(N)CC1 20 1
 248
 FC(F)(F)c1nc(nc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)NCCCN1CCN(CC1)C
 C 20 1 249
 FC(F)(F)c1nc(nc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)NCCN1ccnc1 20 1
 250
 FC(F)(F)c1nc(nc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)Nc1ccc(cc1)CN1CCOC
 C1 20 1 251
 FC(F)(F)c1nc(nc1C(=O)NCCN1CCOCC1)/C(/C(=O)N)=C/1\Nc2cc(C)c(cc2N/1)C
 20 1 252
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1cccc1C)Nc1ccc(O)cc1 20 1 253
 Fc1cnc(nc1Nc1cccc1OC)Nc1ccc(O)cc1 20 1 254

S1(=O)(=O)Cc2cc(Nc3nc(Nc4cc5nc([nH]c5cc4)C(F)(F)F)ccn3)ccc2C1 20 1
 255
 S\1[C@@@H]2[C@@@H](N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C=CC(=C2)CCc1c
 ccnc1 20 1 256
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(C(F)(F)F)c(cn1)C(O)=O)cccc2 20 1 257
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(C(F)(F)F)c(cn1)C(OC)=O)cccc2 20 1 258
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(OC)n1)C(F)(F)F)cccc2 20 1 259
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)cc(OCCN1CCOCC1)cc2 20 1
 260
 S\1c2cc(C(=O)NCCN3CCOCC3)c(F)cc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F
 20 1 261
 S\1c2cc(N3CCC(N4CCOCC4)CC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 20
 1 262
 S\1c2cc(NC(=O)CN(C)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 20 1
 263
 S\1c2cc(OCCN3CCOCC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 20 1
 264
 S\1c2cc(S(=O)(=O)N3CCN(CC3)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 20
 1 265
 S\1c2cc(S(=O)(=O)NCCN3CCOCC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F
 20 1 266
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)N1CCNCC120 1
 267
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)N1C[C@H](N)CC1 20
 1 268
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NC1CCNCC1 20 1
 269
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCN1CCN(CC1)CC
 20 1 270
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCN1CCN(CC1)C 20
 1 271
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CCN1CCS1 20 1
 272
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CCc1[nH+]ccn1C 20 1
 273
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CCn1ccnc1 20 1 274
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CN1CCN(CC1)C 20 1
 275
 FC(F)(F)c1nc([nH+]cc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)[C@@@H]3CCNC3)ccc2N\
 1 20 1 276
 FC(F)(F)c1nc(ccn1)/C(/C(=O)N)=C/1\Nc2cc(N(C(=O)[C@@@H]3N(CCC3)C)CC)ccc
 2N1 20 1 277
 S(=O)(=O)(N(C)C)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)c

c1 21 1 278
 O=C(Nc1cc2c([nH]nc2\c=C\c2cccc2)cc1)Cc1cccc1 22 1 279
 O=C(Ne1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1)CN1CCCC1)CC)Nc1ccc
 cc1 22 1 280
 O=C(Ne1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1ccc(cc1)CN1CCCC1)CC)Nc1ccc
 cc1 22 1 281
 O=C(Ne1ccc(cc1)-c1nn(cc1C=1[C@H]2[C@@H](NC(=C2)c2cc(ccc2)CN2CCCC2)
 N=CC=1)CC)Nc1cccc1 22 1 282
 s1c(cnc1NC(=O)Nc1cc(ccc1)C(F)(F)F)CCNc1ncnc2c1scc2 22 1 283
 s1cc(nc1NC(=O)Nc1cc(ccc1)C(F)(F)F)CCNc1ncnc2c1scc2 22 1 284
 s1nc(cc1NC1=NC(SCC)=Cn2c1ncc2-c1cn[nH]c1)C 22 1 285
 O1CCN(CC1)Cc1ccc(cc1)-c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)NCC)cc1)C
 C 23 1 286
 O1CCN(CC1)Cc1ccc(cc1)C=1N[C@H]2N=CC=C([C@@H]2C=1)c1cn(nc1-c1ccc(
 NC(=O)NCC)cc1)CC 23 1 287
 Oc1ccc(Nc2nc(ncc2C#N)Nc2ccc(O)cc2)cc1 23 1 288
 s1cc(nc1NC(=O)Nc1cc(F)ccc1)CCNc1ncnc2c1scc2 23 1 289
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)c1ccc(cc1)C 23 1 290
 Clc1cc2nc(sc2cc1)-c1ccc(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)cc1 24 1
 291
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)[C@H](C)c1cccc1)c1ccc(N2CCN(CC2)C)cc1 24
 1 292
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)c1cc(ccc1)C 24 1 293
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1ccc(F)cc1)Nc1ccc(O)cc1 25 1 294
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCOCC3)cc2)cc1C(=O)N[C@H](CN1CCOCC1)c1c
 cccc1 25 1 295
 Fc1ccc(F)cc1CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 25 1 296
 O1CCC(NC(=O)Nc2c[nH]nc2-c2[nH]c3c(n2)cc(cc3)CN2CCOCC2)CC1 26 1
 297
 s1c2c(nc1-c1cc(F)c(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2 26
 1 298
 s1c2cc(F)ccc2nc1-c1ccc(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)cc1 26 1
 299
 Clc1cc(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)ccc1-c1sc2c(n1)cccc2 27
 1 300
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)Nc1c(cccc1CC)CC)c1ccc(N2CCN(CC2)C)cc1 27
 1 301
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](CN1CCCC1)c
 1cccc1 27 1 302
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C(F)(F)F)C 27 1 303
 Cl\c(=C\c1nc([nH]c1)NC(\c=C/C/CCNc1ncnc2c1scc2)=C)=C\c 28 1 304
 Clc1cc2nc([nH]c2cc1)Nc1ccc(cc1)CCNc1ncnc2c1scc2 28 1 305
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1cccc1O)Nc1ccc(O)cc1 28 1 306

s1c2c(ncnc2NCCC(\C=C/C/C(Nc2[nH]c(C)c(n2)\C=C/C)=C)cc1 28 1 307
 s1c2c(ncnc2NCCc2ccc(Nc3[nH]c4c(n3)cccc4)cc2)cc1 28 1 308
 O(c1c2c(cccc2)c(Nc2[nH]c3c(n2)cccc3)cc1C)c1ncnc1-c1nc(nc1)NC 29 1
 309
 S(=O)(=O)(N1CCOCC1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)C
 CC3)cc1 29 1 310
 O(C)c1ccc(N2N=C(Nc3n[nH]c(c3)C)c3c(cccc3)C2=O)cc1 29 1 311
 Br\c1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1ncn1C)-c1ccc(cc1)CN1CCOCC1 30 1
 312
 Br\c1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(OCCO)cc1 30 1 313
 Clc1cc2N/C(/Nc2cc1F)=C(/C(=O)N)\c1nc(ccn1)C(F)(F)F 30 1 314
 FC(F)(F)c1nc(nc1)C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(OC)=O 30 1 315
 FC(F)(F)c1nc(nc1C(=O)NCCN1CCOCC1)/C(/C(=O)N)=C\1/Nc2c(N/1)cccc2 30
 1 316
 Fc1cc(F)cc2N/C(/Nc12)=C(/C(=O)N)\c1nc(ccn1)C(F)(F)F 30 1 317
 Fc1cnc(nc1Nc1ccc(O)cc1)Nc1ccc(O)cc1 30 1 318
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cc(N2CCN(CC2)C)ccc1)C 30 1 319
 S(=O)(=O)(N)c1cc(Nc2nc(ccn2)C=2[C@H]3[C@@@H](N=CC=C3)N(C=2)CC)ccc1
 30 1 320
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)cccc2 30 1 321
 S\1c2cc(N(CCN3CCCCC3)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 30 1
 322
 S\1c2cc(N3CCC(N4CCCCC4)CC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 30
 1 323
 S\1c2cc(N3CCN(CC3)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 30 1
 324
 S\1c2cc(NCCN3CCOCC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 30 1
 325
 S\1c2cc(OCCCN3CCOCC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 30 1
 326
 S\1c2cc(S(=O)(=O)N3CCNCC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 30
 1 327
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCN 30 1
 328
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)C(=O)NCCN 30 1 329
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CCN1CCC(F)(F)CC1 30 1
 330
 s1cc(nc1NC(=O)Nc1c2[nH]ccc2ccc1)CCNc1ncnc2c1scc2 30 1 331
 s1nc(cc1NC1=NC(S(=O)C)=Cn2c1nc2-c1cn[nH]c1)C 30 1 332
 S(=O)(=O)(NC)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 31 1 333
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@@@H](CC)c1cccc
 1 31 1 334

O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)c1ccccc1 31 1 335
 Brclnc2[nH]c(nc2c1N1CCN(CC1)Cc1ncn1C)-c1ccc(OC)cc1 32 1 336
 O(C)c1ccc(cc1)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O32 1 337
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NCc1ccccc1 32 1
 338
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)Nc1cc(NC(=O)C)ccc1 33 1 339
 Oclccc(Nc2nc(nc2C)Nc2ccc(O)cc2)cc1 34 1 340
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1)CC
 34 1 341
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)C(C)C 35 1 342
 S(=O)(=O)(Nc1cc2c([nH]nc2\C=C\c2cccc2)cc1)Cc1ccccc1 35 1 343
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\C=C\c2ccc(cc2)CN2CCN(CC2)C)cc1 35 1
 344
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\C=C\c2cc(ccc2)CN2CCN(CC2)C)cc1 35 1
 345
 Fc1nc(nc1Nc1ccc(cc1)C(=O)Nc1cc(OC)ccc1)Nc1ccc(O)cc1 36 1 346
 O(C)c1cc(ccc1)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O36 1 347
 Fc1ccc(N2N=C(Nc3n[nH]c(c3)C)c3c(cccc3)C2=O)cc1 37 1 348
 S1(=O)(=O)Cc2cc(Nc3nc(Nc4cc5nc[nH]c5cc4)ccn3)ccc2C1 38 1 349
 Clc1ccc(NC(=O)Nc2scc(n2)CCNc2ncn3c2scc3)cc1 39 1 350
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1ccc(cc1)CN(C)C)CC)NCC 39
 1 351
 S(=O)(=O)(CC=C)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc
 1 39 1 352
 Brclnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccc(Cl)cc1)-c1ccc(OC)cc1 40 1 353
 FC(F)(F)c1nc(nc1C(=O)N)NCCN1CCOCC1/C(/C(=O)N)=C\1/Nc2cc(C)c(cc2N/1)
 C 40 1 354
 Fc1cc2N\C(\Nc2cc1F)=C(/C(=O)N)\c1nc(ccn1)C(F)(F)F 40 1 355
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C(F)(F)F)-c1nc(ccc1)cccc2 40 1 356
 S\1c2cc(OCCN3CCN(CC3)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 40 1
 357
 S\1c2cc(OCCN(C)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 40 1 358
 S\1c2cc(OCCN3CCN(CC3)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 40 1
 359
 S\1c2cc(Oc3ccncc3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 40 1 360
 s1c2c(ncnc2NCCC(\C=C/C(Nc2[nH]c(C)c(n2)\C=C(\C(F)(F)F)/C)=C)=C)cc1 40
 1 361
 s1c2c(ncnc2NCCc2ccc(Nc3[nH]c4c(n3)cc(cc4)C(F)(F)F)cc2)cc1 40 1 362
 Fc1ccc(cc1)-c1nn(Nc2ccc(Oc3nc(ccc3-c3nc(ncc3)NC)cc2)c2c1cccc2 41 1
 363
 o1cccc1C(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(cc2)C(C)(C)C)C1 41 1 364
 s1cc(nc1NC(=O)Nc1cc(ccc1)C#C)CCNc1ncn2c1scc2 41 1 365
 Clc1nc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1scen1)-c1ccc(N(C)C)cc1 42 1

FC(F)(F)Cn1nc(c2CCc3c(nc(nc3)Nc3cccc3)-c12)C(=O)N 42 1 367
 FC(F)(F)c1cc(Nc2nc(ncc2)Nc2cc(NC(=O)C3CC3)ccc2)ccc1 42 1 368
 O(C)c1ccc(OC)cc1CC(=O)Nc1cc2c([nH]nc2\c=C\c2cccc2)cc1C 42 1 369
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1ccc(cc1)CN1CCCC1)CC)NCC
 42 1 370
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1ccc(cc1C)CN(C)C)CC)Nc1cccc
 1 42 1 371
 [nH]1nc-2c(CCCc3c-2[nH]c2c3cccc2)c1C 42 1 372
 o1c2ncnc(NCCc3ccc(NC(=O)Nc4cccc4)cc3)c2c(c1-c1cccc1)-c1cccc1 43 1
 373
 s1c(cnc1Nc1nenc2c1cc(OC)c(OCCN1CCOCC1)c2)C 43 1 374
 O(CCCN1CCN(CC1)CC)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 44 1 375
 s1c(-c2nc(ncc2)Nc2ccc(N3CCOCC3)cc2)c(nc1N)C 44 1 376
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC(C)(C)c1cccc1 44
 1 377
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1ccc(cc1)CN(C)C)CC)Nc1cccc1
 45 1 378
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC1CCCC2c1cccc2 45
 1 379
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C)C1(N2C[C@H](O[C@H](C2)C)C)C
 C1 45 1 380
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C#N)C 46 1 381
 O=C(N1CCNCC1)c1ccc(cc1)\C=C\C1=NN[C@H]2[C@H]1C=CC=C2 48 1
 382
 O=C(N1CCNCC1)c1ccc(cc1)\C=C\c1n[nH]c2c1cccc2 48 1 383
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC(c1cccc1)c1cccc1
 48 1 384
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NCC 48 1 385
 Fc1nc(nc1Nc1ccc(cc1)C(=O)NCCC)Nc1ccc(O)cc1 49 1 386
 Fc1cc(cc(F)c1)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 49 1 387
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)NCCN 50 1
 388
 Fc1nc(nc1Nc1ccc(cc1)C(=O)Nc1cc(ccc1)C)Nc1ccc(O)cc1 50 1 389
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 50 1 390
 S(=O)(=O)(N)c1cc(Nc2nc(ccn2)-c2c3c(n(c2)CCC)cncc3)ccc1 50 1 391
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(C(F)(F)c(cn1)C(=O)NCCN1CCOCC1)cccc2 50
 1 392
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(OCCN3CCOCC3)n1)C(F)(F)F)cccc2 50 1
 393
 S\1c2cc(NC(=O)CN)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 50 1 394
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)CC(=O)NCCN1CCOCC1 50
 1 395

s1cc(nc1NC(=O)Nc1cc(OC)ccc1)CCNc1ncnc2c1scc2 50 1 396
 s1ccnc1NC(=O)CN1CCN(CC1)c1c2nc([nH]c2ncc1C#N)-c1ccc(N(C)C)cc1 50 1
 397
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)CN1CCOCC1)C 50 1 398
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)NC(C)C)Nc1ccc(O)cc1 51 1 399
 O1CCN(CC1)c1ccc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)cc1 51 1 400
 [nH]1nc-2c(CCc3c-2[nH]c2c3cccc2)c1C 51 1 401
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1scen1)-c1ccc(OC)cc1 52 1
 402
 Fc1cc(Nc2ncnc3c2cc(cc3)C#CO)ccc1 52 1 403
 s1c(cnc1NC(=O)Nc1cccc1)CCNc1ncnc2c1scc2 52 1 404
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC1CCc2c1cccc2 52
 1 405
 s1cc(nc1NC(=O)Nc1cccc1)CCNc1ncnc2c1scc2 52 1 406
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1ccc(N2CCN(CC2)C)cc1)C 53 1 407
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1)CN(C)C)CC)Nc1cccc1
 53 1 408
 s1cc(nc1NC(=O)Nc1cc(cc(c1)C(F)(F)F)CCN1CCC1)CCNc1ncnc2c1scc2 53 1
 409
 s1ccnc1NC(=O)CN1CCN(CC1)c1c2nc([nH]c2ncc1C1CC1)-c1ccc(OC)cc1 53 1
 410
 Clc1cc2sc(nc2cc1)-c1ccc(Nc2ncnc3c2cc(OC)c(OCCCN2CCN(CC2)C)c3)cc1 54 1
 411
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)NC1CC1)Nc1ccc(O)cc1 54 1 412
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1scen1)-c1ccc(N(C)C)cc1 55 1
 413
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1ccncc1)-c1ccc(N(C)C)cc1 55 1 414
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)Cc1noc(c1)C)-c1ccc(cc1)CN 55 1 415
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCOCC1)e2)CC(=O)N(CC)c1cccc1 55 1
 416
 S(=O)(=O)(C)c1ccc(cc1)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 56 1
 417
 S(=O)(=O)(CC)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 57 1 418
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1)CN1CCCC1)CC)NCC
 58 1 419
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1cc(F)ccc1)Nc1ccc(O)cc1 59 1 420
 O1CCN(CC1)Cc1ccc(cc1)C=1N[C@H]2N=CC=C([C@@@H]2C=1)c1cn(nc1-c1ccc(
 NC(=O)Nc2cccc2)cc1)CC 59 1 421
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC(C)C 59 1 422
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(NC(=O)CN(CC)CC)ccc2N\1 60 1
 423
 FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)NC1CCNCC1 60 1

424

FC(F)(F)c1nc(ncc1C(=O)NCCCN1CCOCC1)/C(/C(=O)N)=C\1/Nc2c(N/1)cccc2 60
1 425
O(c1ncccc1-c1c[nH]nc1N)c1ccc(Nc2nnn(c3c2cccc3)-c2ccc(cc2)C)cc1 60 1
426
S\1c2c(N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F)cccc2C(=O)NCCN1CCOCC1 60
1 427
s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cc(cc2)C(F)(F)
F 60 1 428
S\1c2cc(NC(=O)[C@H]3CCN(C3)C)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F
60 1 429
O(CCCN1CCC(O)CC1)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 61 1 430
S(=O)(=O)(N)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 61
1 431
O(c1ccc(NC(=O)c2cccc2Nc2cccc2)cc1C)c1ncccc1-c1nc(ncc1)NC 62 1 432
O=C(Nc1ccc(cc1)-c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)cc1)CC)
C 62 1 433
s1c2cc(OC)ccc2nc1-c1ccc(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)cc1 62
1 434
S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1)Cc
1cccc1 63 1 435
Clc1ccc(NC(=O)c2ccc(Nc3nc(ncc3F)Nc3ccc(O)cc3)cc2)cc1 64 1 436
s1c2c(ncnc2NCCC(\C=C(\F)/C(Nc2[nH]c(C)c(n2)\C=C(\C(F)(F)F)/C)=C)cc1 64
1 437
s1c2c(ncnc2NCCc2cc(F)c(Nc3[nH]c4c(n3)cc(cc4)C(F)(F)F)cc2)cc1 64 1 438
O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)Cc1cccc1 65 1 439
S1C=Cn2c1nc(c2-c1nc(ncc1)Nc1cc(N2CCOCC2)ccc1)-c1cc(NC(=O)Cc2cccc2)ccc
1 65 1 440
s1c2c(nc1-c1cc(OC)c(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2 65
1 441
s1cccc1CC(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)C1 65 1
442
FC(F)(F)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 66 1 443
s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](C)c1cccc1 66
1 444
Fc1nc(nc1Nc1cccc1C)Nc1ccc(O)cc1 67 1 445
O(C)c1ccc(cc1)C(=O)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 67 1 446
O=C1N(c2c(cc3[nH]c(nc3c2)-c2n[nH]c(c2)C)C1(C)C)CC 69 1 447
Brc1cc(ccc1Cc1cccc1)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCN2CCOCC2)c3)c
n1 70 1 448
FC(F)(F)c1nc(ncc1)/C(/C(=O)N)=C/1\Nc2cc(ccc2N\1)C(=O)NCCN(C)C 70 1
449
O1CCN(CC1)Cc1cc(ccc1)-c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)NCC)cc1)C

C 70 1 450
 O=C(Nc1c[nH]nc1-c1[nH]c2c(n1)cccc2)C 70 1 451
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C)C(OC)=O)cccc2 70 1 452
 S\1c2cc(ccc2N/C/1=C(\C(=O)N)/c1nc(OC)ccn1)CN1CCOCC1 70 1 453
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)CC(=O)c1cccc1 71 1 454
 O=C1Nc2c(cc3c4CCCC5c(n[nH]c5C)-c4[nH]c3c2)C1(C)C 72 1 455
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1cc(Cl)ccc1)-c1ccc(N(C)C)cc1 75
 1 456
 Fc1cnc(nc1Nc1ccc(cc1)C)Nc1ccc(O)cc1 75 1 457
 S1(=O)(=O)Cc2cc(Nc3nc(Nc4cc5nc([nH]c5cc4)C(F)(F)F)c(cn3)CCC)ccc2C1
 75.099998 1 458
 Fc1cnc(nc1Nc1ccc(OC)cc1)Nc1ccc(O)cc1 78 1 459
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1cccc1OC)Nc1ccc(O)cc1 78 1 460
 Brclsc(nc1)Nc1ccc(cc1)C(O)=O 79 1 461
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)[C@H](C)c1cccc1)-c1ccc(N(C)C)cc1 79 1
 462
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\c=C/c2ccc(cc2)CN2CCN(CC2)C)cc1C 79 1
 463
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\c=C\c2cc(ccc2)CN2CCN(CC2)C)cc1C 79 1
 464
 Fc1cnc(nc1Nc1cccc1)Nc1cccc1 80 1 465
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C)C)cccc2 80 1 466
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)NCCN1CCOCC1)C(F)(F)F)cccc2 80 1
 467
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1scen1)-c1cccc1 81 1 468
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1nc(oc1)C(C)C)-c1ccc(OC)cc1 81 1
 469
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)Cc1nc(oc1)C(C)C)-c1ccc(cc1)CN1CCOCC1 81
 1 470
 S(=O)(=O)(N1CCOCC1)c1ccc(NC2=NC=Cn3c2ncc3-c2cn[nH]c2)cc1 81 1
 471
 S(=O)(=O)(N)c1ccc(Nc2nc(ccn2)-c2c3c(n(c2)CCC)cncc3)cc1 82 1 472
 o1c2ncnc(N[C@H](CO)c3cccc3)c2c(c1-c1cccc1)-c1ccc(NC(=O)C=C)cc1 82 1
 473
 s1c2c(nc1-c1ccc(Oc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2 82 1
 474
 s1nc(cc1NC1=NC(SCCN(C)C)=Cn2c1ncc2-c1cn[nH]c1)C 82 1 475
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)CCN)C 83 1 476
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(OCC)=O)C(=O)CCC3)cc1)
 c1cccc1 84 1 477
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)[C@H](C)c1ccen1)-c1ccc(N(C)C)cc1 85 1
 478
 Clc1cc2sc(nc2cc1)-c1cc(F)c(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)cc1 85

1 479
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3nc(nc3)NC(=O)c3ccc(cc3)CC)c2cc1OC 85 1
 480
 s1nc(cc1NC1=NC(Sc2ccc(F)cc2)=Cn2c1ncc2-c1cn[nH]c1)C 85 1 481
 S1(=O)(=O)Cc2cc(Nc3nc(Nc4cc5[nH]nc(NC(=O)c6ccc(cc6)C(C)(C)C)c5cc4)c(cn3)
 C(F)(F)F)ccc2C186 1 482
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN(CCC)CCO)c4)c2)cccc1F 87
 1 483
 Oc1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 90 1 484
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(C(F)(F)F)c(cn1)C(=O)NCCCN1CCOCC1)cccc2 90
 1 485
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1O)cccc2 91 1
 486
 s1cccc1CC(=O)Nc1cc2c([nH]nc2\c=C\c2cccc2)cc1N1CCCC1 91 1 487
 O=C(N)c1n[nH]c-2c1CCc1c-2nc(nc1)Nc1cccc1 92 1 488
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)Cc1ccc(NC(=O)C)cc1 93 1 489
 Clc1ccc(N2N=C(Nc3n[nH]c(c3)C)c3c(cccc3)C2=O)cc1 93 1 490
 S(=O)(=O)(Nc1nccen1)c1ccc(NC(=S)N2CCN(CC2)c2ncnc3[nH]c4cc(OC)c(OC)cc4
 c23)cc1 94 1 491
 Clc1cc(NC(=O)Nc2scc(n2)CCNc2ncnc3c2scc3)ccc1Cl 96 1 492
 Brclsc(nc1)Nc1ccc(cc1)C(=O)NCCOC 97 1 493
 ClC1=N[C@@@H]2[C@H](NC=C2c2nc(nc2)Nc2cc(S(=O)(=O)N)ccc2)C(=C1)C 98
 1 494
 O(C)c1cc(ccc1)C(=O)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 100 1 495
 O(CCCO)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 100 1 496
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)Nc1c(cccc1CC)CC)c1ccc(cc1)C(C)(C)C 100 1
 497
 O=C1NCc2c1c(ccc2)-c1[nH]c2c(c1)cccc2 100 1 498
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)CCCC(=O)NO)cc(n1)Nc1[nH]nc(c
 1)C 100 1 499
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)CCCCCC(=O)NO)cc(n1)Nc1[nH]nc(c
 1)C 100 1 500
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)CCCCCCC(=O)NO)cc(n1)Nc1[nH]n
 c(c1)C 100 1 501
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)CCCCCCCC(=O)NO)cc(n1)Nc1[nH]
 nc(c1)C 100 1 502
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)c2ncc(cn2)C(=O)NO)cc(n1)Nc1[nH]
]nc(c1)C 100 1 503
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(Nc2[nH]nc(c2)C)cc(n1)NCCCCCCC(=O)NO
 100 1 504
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(Nc2[nH]nc(c2)C)cc(n1)NCCCCCCC(=O)NO
 100 1 505
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(Nc2[nH]nc(c2)C)cc(n1)NCCNCCCCCCC(=O)N

O 100 1 506
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(C(F)(F)F)c(cn1)C(=O)N1CCN(CC1)C)cccc2
 100 1 507
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(OC)ccn1)cccc2 100 1 508
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(ccn1)-c1cccc1)cccc2 100 1 509
 S\1c2cc(N3C[C@@@H](N)CC3)ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 100 1
 510
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)Nc1cccc1 105 1
 511
 s1nc(cc1NC1=NC(SC(C)(C)C)=Cn2c1ncc2-c1cn[nH]c1)C 105 1 512
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC[C@H]1CO)c2)CC(=O)Nc1cc(OC)ccc1
 106 1 513
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)Cc1ccc([N+](=O)[O-])cc1 109 1
 514
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3ccc(NC(=O)c4cccc4)cc3)c2cc1OC 110 1
 515
 [nH]1nc-2c(CCc3c-2[nH]c2c3cccc2)c1C1CC1 110 1 516
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2 110 1
 517
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC(CC1)CO)c2)CNC(=O)c1cc(F)ccc1
 111 1 518
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1C)CN(C)C)CC)Nc1cccc
 1 113 1 519
 Clc1cnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1cccc1)-c1ccc(N(C)C)cc1 115 1
 520
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)CC(C)C 115 1 521
 O=C(C)c1ccc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)cc1 116 1 522
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(=O)NC)C(=O)CCC3)cc1)c
 1cccc1 117 1 523
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1ccnc1)-c1ccc(N(C)C)cc1 118 1
 524
 FC(F)(F)c1nc([nH]c1)-c1n[nH]cc1\C=C\c1ccnc1 120 1 525
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1OC)cccc2
 120 1 526
 s1cc(nc1C)CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 120 1 527
 s1cnc(C)c1CN1N=C(Nc2n[nH]c(c2)C)c2c(cccc2)C1=O 120 1 528
 O=C(Nc1cc(ccc1)-c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)cc1)CC)
 C 126 1 529
 O(C)c1ccc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)cc1 128 1 530
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1)CN(C)C)CC)NCC
 128 1 531
 Fc1cnc(nc1Nc1ccc(OC)cc1)Nc1ccc(OC)cc1 130 1 532
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)Cc1cccc1)c1ccc(cc1)C(C)(C)C 130 1 533

O1CCN(CC1)CCOc1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 135 1 534
 Brc1sc(nc1)Nc1ccc(cc1)C(=O)NC 140 1 535
 Clc1cc(NC(=O)c2ccc(Nc3nc(ncc3F)Nc3ccc(O)cc3)cc2)ccc1 140 1 536
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)Cc1cccc1)c1ccc(N2CCN(CC2)C)cc1 140 1
 537
 S(=O)(=O)(Nc1cc2c([nH]nc2)C=C/c2ccc(NC(=O)N3CCN(CC3)C)cc2)cc1N1CCCC
 1)C 140 1 538
 S(=O)(=O)(Nc1cc2c([nH]nc2)C=C\c2cc(NC(=O)N3CCN(CC3)C)ccc2)cc1N1CCCC
 1)C 140 1 539
 O(c1ncccc1-c1nc(ncc1)NC)c1ccc(Nc2nnnc(c3c2cccc3)-c2cccc2)cc1 149 1 540
 Oc1ccc(Nc2nc(ccn2)C=2[C@H]3[C@H](NC=2)C=CC=C3)cc1 150 1 541
 Oc1ccc(Nc2nc(ncc2CC)Nc2ccc(O)cc2)cc1 150 1 542
 BrC=1N2[C@H](NC=1)C(=NC(=C2)c1cccn1)Nc1ccc(N2CCOCC2)cc1 152 1
 543
 BrC1n2c(nc1)C(=NC(=C2)c1cccn1)Nc1ccc(N2CCOCC2)cc1 152 1 544
 O(C)c1cc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)ccc1 158 1 545
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)CC(=O)NCCC(C)C 158 1
 546
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)N)Nc1ccc(O)cc1 160 1 547
 O1c2cc(ccc2OC1)C(=O)Nc1n[nH]c2c1CN(C2)C(=O)C(C)C 160 1 548
 [nH]1nc(c2cc(-c3ccncc3)c(N3CCCC3)cc12)\C=C\c1cccc1 160 1 549
 o1cccc1C(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)C1 160 1
 550
 o1cccc1C(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(N3CC[NH+](CC3)C)cc2)C1 160 1
 551
 s1c2c(nc1-c1cc(Nc3nc(Nc4n[nH]c(e4)C)ccn3)ccc1)cccc2 160 1 552
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C1CCCCC1 169 1 553
 s1c2c(nc1-c1ccc(Oc3ncnc4c3cc(OC)c(OCCN3CCCC3)c4)cc1)cccc2 170 1
 554
 s1nc(cc1NC1=NC=Cn2c1nc2-c1cn(nc1)C)C1CCN(S(=O)(=O)C)CC1 170 1
 555
 O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)Nc1ccc(N2CCN(CC2)C)cc1)C 175 1 556
 O=C(C)c1cc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)ccc1 176 1 557
 Brc1cnc2[nH]c(nc2c1N1CCN(S(=O)(=O)c2cccc2)CC1)-c1ccc(N(C)C)cc1 178 1
 558
 Fc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 178 1 559
 O(CCCN1CCCCC1)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 179 1 560
 Fc1cnc(nc1Nc1cc(cc1)C)Nc1ccc(O)cc1 180 1 561
 Fc1cnc(nc1Nc1ccc(cc1)C(=O)Nc1ccc(cc1)C)Nc1ccc(O)cc1 180 1 562
 O=C1Nc2c(cc3[nH]c(nc3c2)-c2n[nH]c(c2)C)C1(C)C 180 1 563
 s1cc(nc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)C(=O)Nc1cccc1 182 1
 564
 ClC=1N2[C@H](NC=1)C(=NC(=C2)c1cccn1)Nc1ccc(N2CCOCC2)cc1 190 1

565

Clc1n2c(nc1)C(=NC(=C2)c1ccnc1)Nc1ccc(N2CCOCC2)cc1 190 1 566
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN(CCO)CC)c4)c2)ccc1
190 1 567
O(C)c1cc2[nH]c(cc2cc1)-c1n[nH]c2c1nccc2 190 1 568
O1CCN(CC1)CCNC(=O)c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)cc
1)CC 197 1 569
Fc1cnc(nc1Nc1ccc(F)cc1)Nc1ccc(F)cc1 200 1 570
Ic1cc2S\C(Nc2cc1)=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 200 1 571
O(CCN1CCCC1)e1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 200 1 572
S\1c2c(N/C/1=C(\C(=O)N)/c1nc(ccn1)C)cccc2 200 1 573
S\1c2c(N/C/1=C(\C(=O)N)/c1ncc(cn1)CC)cccc2 200 1 574
S\1c2cc([N+](=O)[O-])ccc2N/C/1=C(\C(=O)N)/c1nc(ccn1)C(F)(F)F 200 1 575
[nH]1nc(c2cc(N)c(N3CCCC3)cc12)\C=C\c1cccc1 200 1 576
s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1F)cccc2 200 1
577
O=C(NCCN1CCN(CC1)C)c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)
cc1)CC 203 1 578
O(C)c1cc2nc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 205 1 579
O1CCN(CC1)c1ccc(NC2=NC(=CN3[C@@H]2NC=C3C)c2ccnc2)cc1 208 1
580
O1CCN(CC1)c1ccc(NC2=NC(=Cn3c2ncc3C)c2ccnc2)cc1 208 1 581
O=C/1Nc2c(cccc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2 208 1 582
Br\c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 210 1
583
Br\c1cnc2[nH]c(nc2c1N1CCN(CC1)CC(C)C)-c1ccc(N(C)C)cc1 210 1 584
Clc1cc2[nH]c(nc2cc1)-c1n[nH]c2c1cc(OCc1cccc1)cc2 210 1 585
Oc1ccc(Nc2nc(ccn2)C=2[C@H]3[C@@H](N=CC=C3)N(C=2)CCC)cc1 210 1
586
O=C(NC1CC1)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 213 1 587
S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(=O)N2CCCC2)C(=O)CCC
3)cc1)c1cccc1 218 1 588
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN(CCC)CCO)c4)c2)ccc1
220 1 589
s1c2c(nc1-c1cc(F)c(Oc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2
220 1 590
o1c2ncnc(N[C@H](CO)c3cccc3)c2c(c1-c1cccc1)-c1cccc1 223 1 591
O=C(NCCN1CCN(CC1)C)c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc
2)cc1)CC 228 1 592
s1c2c(nc1-c1cc(O)c(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2
230 1 593
s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1C)cccc2 230 1
594

O=[N+](O-)c1cc2c([nH]nc2\c=C\c2cccc2)cc1N1CCCC1 240 1 595
 s1cccc1CC(=O)Nc1cc2c([nH]nc2C#Cc2cccc2)cc1C 240 1 596
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)c1ccc(cc1)C(C)(C)C 240 1 597
 Clc1c2nc([nH]c2ncc1Cl)-c1ccc(N(C)C)cc1 250 1 598
 O1CCN(CC1)Cc1ccc(cc1)-c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)N(C)C)cc1)
 CC 250 1 599
 O1CCN(CC1)Cc1ccc(cc1)C=1N[C@H]2N=CC=C([C@@H]2C=1)c1cn(nc1-c1ccc(
 NC(=O)N(C)C)cc1)CC 250 1 600
 s1c2c(ncnc2NCCn2nnc(NC(=O)Nc3cc(ccc3)C(F)(F)F)c2)cc1 250 1 601
 O=C/1Nc2c(cc(NC(=O)C)cc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2 252 1
 602
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)c1cccc1)-c1ccc(N(C)C)cc1 258 1 603
 Fc1cnc(nc1Nc1cc(OC)ccc1)Nc1ccc(O)cc1 260 1 604
 s1nc(O)c(/C(=N/C(CO)C)/N)c1Nc1ccc(Oc2cccc2)cc1 260 1 605
 s1nc(O)c(C(NC(CO)C)=N)c1Nc1ccc(Nc2cccc2)cc1 265 1 606
 FC(F)(F)c1ccc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)cc1 270 1 607
 O(C)c1cc(Nc2nc(nc(n2)NC(Cc2c3ccnec3[nH]c2)C(=O)N)Nc2cc3c(nc3)cc2)ccc1O
 C 270 1 608
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)C 270 1 609
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)Cc1ccncc1 270 1 610
 O=C1N(N=C(Nc2n[nH]c(c2)C)c2c1cccc2)Cc1ncncc1 270 1 611
 Oclccc(Nc2nc(ccn2)C=2[C@H]3[C@@H](N=CC=C3)N(C=2)CC)cc1 270 1
 612
 s1cc(nc1NC(=O)NC1CCCC1)CCNc1ncnc2c1scc2 270 1 613
 S(=O)(=O)(Cc1cccc1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC
 3)cc1 271 1 614
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)C(=O)Nc1cccc1)-c1ccc(N(C)C)cc1 277 1
 615
 Brclcnc2[nH]c(nc2c1N1CCN(CC1)CC(=O)Nc1cccc1)-c1ccc(N(C)C)cc1 277 1
 616
 Clc1cccc1NC(=O)Nc1scc(n1)CCNc1ncnc2c1scc2 280 1 617
 Oclcc(Nc2nc(ccn2)C=2[C@H]3[C@H](NC=2)C=CC=C3)ccc1 280 1 618
 [nH]1nc(c2c1ccc(C#N)c2C)\C=C\c1ccc(cc1)CN1CCN(CC1)C 280 1 619
 [nH]1nc(c2c1ccc(C#N)c2C)\C=C\c1cc(ccc1)CN1CCN(CC1)C 280 1 620
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(=O)N2CCOCC2)C(=O)CC
 C3)cc1)c1cccc1 281 1 621
 O(N)C(=O)c1cc(Nc2nc(ccn2)C=2[C@H]3[C@@H](N=CC=C3)N(C=2)CC)ccc1
 290 1 622
 s1c2c(nc1-c1cc(OC(F)(F)F)c(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)ccc
 c2 290 1 623
 FC(F)(F)c1nc([nH]c1)-c1n[nH]cc1\c=C\c1c2c(cccc2)cnc1 300 1 624
 O(C)c1nc(nc1)/C(=O)N=C\1/Nc2c(N/1)cccc2 300 1 625
 [nH]1c-2c(CCc3c-2n[nH]c3)c2c1cccc2 300 1 626

s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1O)cccc2 300 1
 627
 o1c2ncnc(NCCc3ccc(NC(=O)c4cccc4)cc3)c2c(c1-c1cccc1)-c1cccc1 304 1
 628
 O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 312 1 629
 Fc1cc(ccc1)C(=O)Nc1ncc(Nc2ncnc3Oc4cc(OC)ccc4CNc23)cn1 320 1 630
 s1c2c(nc1-c1ccc(Nc3nc(Nc4n[nH]c(c4)C)ccn3)cc1OC)cccc2 320 1 631
 Brc1sc(nc1)Nc1ccc(cc1)C(=O)NC(COC)C 330 1 632
 Fc1ccc(cc1)C(=O)Nc1ncc(Nc2ncnc3Oc4cc(OC)ccc4CNc23)cn1 330 1 633
 o1c2ncnc(N3CC(NC(C3)C)C)c2c(c1-c1cccc1)-c1cccc1 334 1 634
 O(C)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 338 1 635
 O=C1NCc2c1c(ccc2)-c1[nH]cccc1 338 1 636
 OCc1[nH]nc-2c1CCc1c-2[nH]c2c1cccc2 340 1 637
 s1c2c(nc1-c1cc(C)c(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2
 340 1 638
 [nH]1nc(c2c1ccc(-c1cc(N)ccc1)c2C)\C=C/c1ccc(cc1)CN1CCN(CC1)C 350 1
 639
 [nH]1nc(c2c1ccc(-c1cc(cc(N)c1)C)c2C)\C=C\c1cc(ccc1)CN1CCN(CC1)C 350 1
 640
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OC)c(OC)c4)cc1)cccc2 350 1 641
 O(C)c1cc(ccc1O)-c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc
 1 357 1 642
 Brc1sc(nc1)Nc1ccc(NC(=O)C)cc1 360 1 643
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN(CCO)CC)c4)c2)cccc1F
 360 1 644
 Fc1cc\2c(NC(=O)/C/2=C\c2[nH]c(C)c(C(=O)C)c2CCC(O)=O)cc1 362 1 645
 OCCNC(=O)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 364 1 646
 Brc1cnc2[nH]c(nc2c1N1CCNCC1)-c1ccc(N(C)C)cc1 365 1 647
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1)CN1CCCC1)CC)N(C)C
 366 1 648
 s1c2c(nc1-c1ccc(Nc3nc(Nc4n[nH]c(c4)C)ccn3)cc1)cccc2 370 1 649
 O=C(NCc1cccc1)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 374 1 650
 OC(Cn1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1)CO 377 1
 651
 s1cccc1-c1nnc(nc1Nc1cc2nc([nH]c2cc1)C(F)(F)F)Nc1cc2c(CS(=O)(=O)C2)cc1
 383 1 652
 O1c2cc(ccc2OC1)C(=O)Nc1n[nH]c2c1CN(C2)C(=O)NC(C)C 390 1 653
 [nH]1nc(N)c2c1cc(cc2)-c1nc(ncc1)N 390 1 654
 s1c2c(nc1-c1cc(F)c(Nc3ncnc4c3cc(OCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2
 390 1 655
 O(C)c1cc2c(ncnc2Nc2ccc(NC(=O)c3cccc3)cc2)cc1OC393 1 656
 s1nc(cc1NC1=NC(S(=O)(=O)C)=Cn2c1ncc2-c1cn[nH]c1)C 603 0 657
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 605 0 658

O(C)c1ccccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 607 0 659
 ClC1=N[C@@@H]2[C@H](NC=C2c2nc(ncc2)Nc2ccc(S(=O)(=O)N)cc2)C(=C1)C
 620 0 660
 [nH]1nc(c2cc(NCc3ncccc3)c(N3CCCC3)cc12)\C=C\c1ccccc1 620 0 661
 O1CCN(CC1)c1cc(Nc2nc-3c(CC(c4c-3n(nc4C(=O)NC)C)(C)C)cn2)ccc1 625 0
 662
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3nc(NC(=O)c4cccc4)cn3)c2cc1OC 629 0
 663
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc[nH]c2ncc1)CC)Nc1ccccc1 631 0 664
 O1CCN(CC1)Cc1cc(Nc2nc-3c(CC(c4c-3n(nc4C(=O)NC)C)(C)C)cn2)ccc1 638 0
 665
 Fc1nc(nc1Nc1ccc(cc1)C(=O)N(C)C)Nc1ccc(O)cc1 640 0 666
 O=C(Nc1cc2c([nH]nc2C2CC2c2cccc2)cc1)Cc1ccccc1 640 0 667
 o1c2ncnc(NCCc3ccc(N)cc3)c2c(c1-c1ccccc1)-c1ccccc1 640 0 668
 o1c2ncnc(NCCc3ccc(O)cc3)c2c(c1-c1ccccc1)-c1ccccc1 640 0 669
 s1nc(cc1NC1=NC=Cn2c1ncc2-c1cn(nc1)C)C(C)C 640 0 670
 O1CCN(CC1)c1ccc(Nc2nc-3c(CC(c4c-3n(nc4C(=O)NC)C)(C)C)cn2)cc1 649 0
 671
 BrC1cnc2[nH]c(nc2c1N1CCN(CC1)CC1CC1)-c1ccc(OC)cc1 650 0 672
 O=C1NN=C(Nc2n[nH]c(c2)C)c2c1cccc2 650 0 673
 O(C)c1ccc(cc1)C(=O)Nc1n[nH]c2c1CN(C2)C(=O)C 660 0 674
 O=C(N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)CC1)c1ccccc1 670 0
 675
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCc1ccc(NC(=O)C)cc1)C 672 0 676
 Fc1nc(nc1Nc1cc(ccc1)C)Nc1cc(ccc1)C 680 0 677
 Clc1cc(Nc2nenc3c2cc(OCCCN2CCN(CC2)C)c(OC)c3)ccc1-c1sc2c(n1)cccc2 690 0
 678
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3nc(nc3)NC(=O)c3ccncc3)c2cc1OC 690 0
 679
 Oc1cc(Nc2nc(ccn2)C=2[C@H]3[C@@@H](N=CC=C3)N(C=2)CC)ccc1 710 0
 680
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)Nc1ccc(NC(=O)C)cc1 719 0 681
 O=C1Nc2c(cc(NC(=O)c3cccc3)cc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2
 720 0 682
 FC(F)(F)c1ccc(cc1)C(=O)CN1N=C(Nc2n[nH]c(c2)C)c2c(ccc2)C1=O 720 0
 683
 O=C1Nc2c(cc([N+](=O)[O-])cc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2
 724 0 684
 BrC1sc(nc1)Nc1cc(ccc1)C(=O)NC 740 0 685
 FC(F)(F)c1cc2nc([nH]c2nc1)-c1ccc(N(C)C)cc1 740 0 686
 o1c2ncnc(NCCOCCO)c2c(c1-c1ccccc1)-c1ccccc1 760 0 687
 FC(F)(F)c1cc(ccc1)C(=O)Nc1nn(c2c1ccc(Oc1c3cc(OC)c(OC)cc3ncc1)c2)C 764 0
 688

OCCn1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1 792 0 689
 o1c2ncnc(N[C@H](CO)C)c2c(c1-c1cccc1)-c1cccc1 792 0 690
 o1c2ncnc(NCCC(OCC)=O)c2c(c1-c1cccc1)-c1cccc1 796 0 691
 Clc1nccc2c1n(cc2-c1nc(ncc1)Nc1cc(O)ccc1)CC 800 0 692
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCN(CCO)CC)c4)c2)cccc1F 800 0
 693
 s1c2c(nc1-c1cc(O)c(Nc3ncnc4c3cc(OCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2
 800 0 694
 Clc1nccc2c1n(cc2-c1nc(ncc1)Nc1cc(S(=O)(=O)N)ccc1)CCC 800 0 695
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)Nc1cccc1 804 0 696
 O1C(OC)(C=CC1OC)CNc1ncnc2oc(c(c12)-c1cccc1)-c1cccc1 827 0 697
 O(C)c1cc(ccc1)CNC(=O)c1c(n[nH]c1NN=C\c1ccc(OC)cc1)C 838 0 698
 s1c2c(nc1-c1ccc(Nc3nc(N4CCN(CC4)C)ccn3)cc1)cccc2 840 0 699
 O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1ccc(N(C)C)cc1)(C)C)C 855 0 700
 [nH]1nc-2c(Cc3c-2[nH]c2c3cccc2)c1C 870 0 701
 s1ccnc1NC(=O)CN1CCN(CC1)c1c2nc([nH]c2ncc1)-c1ccc(N(C)C)cc1 870 0
 702
 s1c(cnc1Nc1ncc(cc1)CN1CCN(CC1)C(=O)NC)C#N 880 0 703
 S(=O)(=O)(C)c1ccc(cc1)CNc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 890 0 704
 BrC1sc(nc1)Nc1cc(OC)ccc1 900 0 705
 BrC1sc(nc1)Nc1ccc(Oc2ccncc2)cc1 900 0 706
 S\1c2c(N/C/1=C(\C(=O)N)/c1nc(cc(n1)C)C(O)=O)cccc2 900 0 707
 [nH]1c2c(nc1-c1n[nH]cc1)cccc2 910 0 708
 FC(F)(F)c1cc(Nc2nc(Nc3cc(NC(=O)C4CC4)ccc3)ccn2)ccc1 931 0 709
 o1c2ncnc(NCc3ccc(N)cc3)c2c(c1-c1cccc1)-c1cccc1 945 0 710
 O(C)c1cc(NC(=O)c2c(n[nH]c2N\N=C\c2ccc(OC)cc2)C)ccc1OC 960 0 711
 O(c1ccc(NC(=O)c2cc(Oc3cccc3)ccc2)cc1C)c1ncccc1-c1nc(ncc1)NC 964 0
 712
 OCCCn1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1 969 0 713
 O1c2c(cc(OC)cc2)CNc2c1ncnc2Nc1nc(nc1)NC(=O)c1cccc1 970 0 714
 o1c2ncnc(NC[C@H](O)C)c2c(c1-c1cccc1)-c1cccc1 973 0 715
 BrC1sc(nc1)Nc1ccc(cc1)C(=O)N(CCOC)C 980 0 716
 Ic1cc(F)c(Nc2c(F)c(F)c(cc2C(O)=O)CN)Cc2ccc(S(=O)(=O)C)cc2)cc1 1000 0
 717
 O(c1ncccc1-c1nc(ncc1)NC)c1cc(C)c(NC(=O)c2cccc2Nc2cccc2)cc1 1000 0
 718
 O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1cc(N2CCN(CC2)C)ccc1)(C)C)C 1000
 0 719
 O=C1N(N=C(Nc2n[nH]cc2)c2c1cccc2)c1ccc(cc1)C 1000 0 720
 O\c1cc\2c(N/C(=C\3/c4cc([N+](=O)[O-])ccc4NC/3=O)/C/2=N\O)cc1 1000 0
 721
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 1004 0 722
 Fc1cc(Oc2ncnc3c2n(cc3)C)ccc1NC(=O)Nc1cc(ccc1)C(F)(F)F 1050 0 723

Oc1ccc(Nc2nc(ccn2)C=2[C@H]3[C@H](N(C=2)C)C=CC=C3)cc1 1050 0
 724

O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1ccc(N2CCN(CC2)C)cc1)(C)C)C 1051
 0 725

O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)NCCc1c2c([nH]c1)cccc2 1071 0
 726

O(C)c1cccc1NC(=O)c1c(n[nH]c1N\N=C\c1ccc(OC)cc1)C 1087 0 727

Brc1sc(nc1)Nc1cc(ccc1)C 1100 0 728

Brc1sc(nc1)Nc1cccc1 1100 0 729

Clc1sc(nc1)Nc1ccc(F)cc11100 0 730

Fc1cc(ccc1)C(=O)Nc1ncc(Nc2ncnc3Oc4c(cc(OC)cc4)CNc23)cn1 1100 0
 731

[nH]1c2c(cc1-c1n[nH]c(c1)C)cccc2 1100 0 732

[nH]1nc-2c(-c3c-2[nH]c2c3cccc2)c1C 1100 0 733

s1c2c(cc1-c1cc(cc3c1[nH]nc3)-c1c3nc(nc3n(c1)CCN)N)cccc2 1100 0 734

O(C)c1cc(ccc1)CNc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 1144 0 735

O=[N+]([O-])c1cc(Nc2nc(ccn2)C=2[C@H]3[C@@H](N=CC=C3)N(C=2)CCC)ccc1
 1160 0 736

Fc1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 1181 0 737

O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1cc(ccc1)CN1CCN(CC1)C)(C)C)C 1184
 0 738

O(C)c1cccc1CCNc1nc(nc(n1)NCCc1c2ccnc2[nH]c1)N(CCCC)C 1200 0
 739

O1c2cc(OC)c(OC)cc2CNc2c1ncnc2Nc1nc(nc1)NC(=O)c1ccc(cc1)C 1200 0
 740

s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cc(cc2)C(F)(F)
 F 1200 0 741

s1c2c(ncnc2NCCc2ccc(NC(=O)Nc3cc(ccc3)C(F)(F)F)cc2)cc1 1200 0 742

s1c2c(ncnc2NCCn2cc(nc2)NC(=O)Nc2cc(ccc2)C(F)(F)F)cc1 1200 0 743

Brc1sc(nc1)Nc1cc(ccc1)C(=O)NCCOC 1220 0 744

S(=O)(=O)(N1CCC(CC1)C(=O)N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)CC
 1)C 1237 0 745

O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1)CN(C)C)CC)N(C)C
 1259 0 746

Fc1cc\2c(NC(=O)/C/2=C/2\Nc3c(cccc3)\C\2=N/O)cc1 1270 0 747

Clc1ncccc2c1n(cc2-c1nc(nc1)Nc1cc(S(=O)(=O)N)ccc1)CC 1280 0 748

O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCCc1ccc(N2CCN(CC2)C)cc1)C 1287 0
 749

S(=O)(=O)(N1CCC(CC1)C(=O)N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)CC
 1)c1cccc1 1288 0 750

s1c2c(nc1-c1cc(OC)c(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2
 1300 0 751

s1c2c(nc1-c1ccc(Nc3cc(ncc3)Nc3n[nH]c(c3)C)cc1)cccc2 1300 0 752

O(CC)C(=O)N1CCC(CC1)C(=O)N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)C
 C1 1308 0 753
 FC(F)(F)c1ccc(NC(=O)C=2C(n3c4c(nc3NC=2C)cccc4)c2occc2)cc1 1320 0
 754
 O=[N+](O-)c1cc(Nc2nc(ccn2)C=2[C@H]3[C@@H](N=CC=C3)N(C=2)CC)ccc1
 1340 0 755
 O(C1CCN(CC1)C)c1ccc(Nc2nc-3c(CC(c4c-3n(nc4C(=O)NC)C)(C)C)cn2)cc1
 1343 0 756
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)NCCc1cccc1 1350 0 757
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C(C)C 1392 0 758
 Brclsc(nc1)Nc1ccc(Oc2cccc2)cc1 1400 0 759
 P(OCCN(CCCOc1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(F)ccc3)c2cc1)C)(O)(O)=O
 1400 0 760
 s1c(cnc1NC=1NC=2[C@H](N=1)C=CCC=2)CCNC1=NC=N[C@H]2[C@H]1SC=C
 2 1400 0 761
 s1c(cnc1Nc1[nH]c2c(n1)cccc2)CCNc1nenc2c1sec2 1400 0 762
 s1c(cnc1Nc1ncc(cc1)CN1CCOCC1)C#N 1400 0 763
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCN(CCO)CC)c4)c2)ccc1 1400 0
 764
 O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1cc(N(C)C)ccc1)(C)C)C 1437 0
 765
 Fc1ccc(NC(=O)c2c(n[nH]c2N\N=C\c2ccc(OC)cc2)C)cc1 1447 0 766
 O(C)c1ccc(cc1)CNc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 1447 0 767
 Brclsc(nc1)Nc1ccc(cc1)C(=O)NCCO 1480 0 768
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)NCCc1cccnc1 1484 0 769
 Brclsc(nc1)Nc1cc(ccc1)C#N 1500 0 770
 s1c2c(nc1-c1ccc(Nc3nc(NC)ccn3)cc1)cccc2 1500 0 771
 O(c1ccc(NC(=O)c2cccc2Oc2cccc2)cc1C)c1ncccc1-c1nc(ncc1)NC 1544 0
 772
 Clc1cc(ccc1)C(=O)Nc1cc(C)c(Oc2ncccc2-c2nc(ncc2)NC)cc1 1546 0 773
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)Nc1ccc(N(C)C)cc1 1568 0 774
 O(C)c1ccc(cc1)CCNC(=O)c1c(n[nH]c1N\N=C\c1ccc(OC)cc1)C 1580 0 775
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)NCc1cccc1 1580 0 776
 O(C1CCN(CC1)C)c1cc(Nc2nc-3c(CC(c4c-3n(nc4C(=O)NC)C)(C)C)cn2)ccc1
 1584 0 777
 S(=O)(=O)(N1CCN(CC1)C1CCN(CC1)c1cc(OC)c(Nc2nc(ccn2)-c2n3c(nc2-c2cc(cc
 2)C(=O)Nc2c(F)cccc2F)C=CC=C3)cc1)C 1600 0 778
 s1nc(cc1NC1=NC=Cn2c1ncc2-c1cn(nc1)C)C1CCNCC1 1600 0 779
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OCCN3CCN(CC3)C)e(OC)c4)cc1OC)cccc2
 1600 0 780
 O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1ccc(cc1)CN1CCN(CC1)C)(C)C)C 1615
 0 781
 O(C)c1ccc(cc1)CNC(=O)c1c(n[nH]c1N\N=C\c1ccc(OC)cc1)C 1623 0 782

S(=O)(=O)(N1CCOCC1)c1cc(Nc2nc(ccn2)-c2c3c(n(c2)CCC)cncc3)ccc1C 1650
 0 783
 BrC1ccc(cc1)CNc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 1688 0 784
 BrC1sc(nc1)Nc1ccc(OC)cc1 1700 0 785
 BrC1sc(nc1)Nc1ccc(cc1)C(=O)C 1700 0 786
 O=C(Nc1cc2c([nH]nc2CCc2cccc2)cc1)Cc1cccc1 1700 0 787
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)CN(C)C)CC)Nc1cccc1 1701 0
 788
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)NCc1cc(NC(=O)C)ccc1 1746 0
 789
 O=C/1Nc2c(cccc2)\C\1=C\c1[nH]c2c(c1CCC(OCC)=O)C(=O)CCC2 1780 0
 790
 O1c2c(CNc3c1ncnc3Nc1cnc(nc1)NC(=O)c1cccc1)cccc2 1900 0 791
 o1cccc1-c1nc(NC(C)C)c2cc(ccc2n1)\C=C\C(O)(C)C 1900 0 792
 s1cccc1CC(=O)Nc1ccc2[nH]nc(c2c1C)\C=C/c1ccc(cc1)CN1CCN(CC1)C 1900
 0 793
 s1cccc1CC(=O)Nc1ccc2[nH]nc(c2c1C)\C=C\c1cc(ccc1)CN1CCN(CC1)C 1900
 0 794
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCc1ccncc1)C 1923 0 795
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)NCc1nc[nH]c1 1937 0 796
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(=O)NCc1cccc1 1942 0 797
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C1CCN(CC1)C(=O)C 1970 0
 798
 Fc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(OCC)=O)C(=O)CCC3)cc1 1980 0
 799
 BrC1sc(nc1)Nc1cccc1 2000 0 800
 Fc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\O 2000 0 801
 Ic1cc(F)c(Nc2c(F)c(F)c(cc2C(O)=O)CNC(=O)[C@@@H](N)CC(=O)N)cc1 2000
 0 802
 BrC1sc(nc1)Nc1ccc(cc1)C#N 2100 0 803
 Fc1cccc1CCNc1nc(nc(n1)Nc1cc2c(nccc2)cc1)Nc1cc(OC)c(cc1)C 2100 0
 804
 O1CCN(CC1)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2ccncc2)cc1 2120 0 805
 O1CCN(CC1)c1ccc(NC2=NC(=Cn3c2ncc3)c2ccncc2)cc1 2120 0 806
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCc1cc(N2CCN(CC2)C)ccc1)C 2136 0
 807
 O1c2c3c4c(cc2OC1)C(=O)Nc4cc1c3cccc1O 2140 0 808
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)C)c1ccc(cc1)C 2140 0 809
 FC(F)(F)Cn1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1 2150 0
 810
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCCN2CCCC2)C(=O)CCC3)cc1
)c1cccc1 2170 0 811

S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCN(C)C)C(=O)CCC3)cc1)c1cccc1 2190 0 812
 O1c2c(CNc3c1ncnc3Nc1nc(nc1)NC(=O)c1cccc1)c(OC)ccc2 2200 0 813
 Br1sc(nc1)Nc1cc(ccc1)C(OCC)=O 2250 0 814
 S(=O)(=O)(N1CCc2c1cccc2)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCN(C)C)C(=O)CCC3)cc1 2270 0 815
 Br1sc(nc1)Nc1ccc(cc1)C(=O)NCCN1CCOCC1 2300 0 816
 O=C/1Nc2c(cccc2)\C\1=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C 2300 0 817
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCc1ccnc1)C 2306 0 818
 O=C(N1Cc2c([nH]nc2NC(=O)Cc2cccc2)C1)C 2310 0 819
 O(C)c1ccc(-n2nc(c3CCc4c(nc(nc4)NC4CCCC4)-c23)C(=O)N)cc1 2312 0 820
 S(=O)(=O)(N1CCc2c1cccc2)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCN(CC)CC)C(=O)CCC3)cc1 2340 0 821
 Clc1ccc(cc1)C(=O)Nc1cc(C)c(Oc2ncccc2-c2nc(ncc2)NC)cc1 2342 0 822
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)-c1cccc1 2360 0 823
 Br1sc(nc1)Nc1ccc(cc1)C(F)(F)F 2400 0 824
 Clc1c2nc([nH]c2ncc1)-c1ccc(N(C)C)cc1 2400 0 825
 O1CCN(CC1)CCNCc1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)cc1)C 2445 0 826
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCN(CC)CC)C(=O)CCC3)cc1)c1cccc1 2450 0 827
 Clc1ncccc1n(cc2-c1nc(ncc1)Nc1ccc(O)cc1)CC 2460 0 828
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cccc4)c2)ccc1 2478.6001 0 829
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 2497 0 830
 O=C(Nc1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2ccnc2)cc1)C 2500 0 831
 O=C(Nc1ccc(NC2=NC(=Cn3c2ncc3)c2ccnc2)cc1)C 2500 0 832
 s1c(cnc1Nc1cccc1)C#N 2500 0 833
 s1cc(cc1NC1=NC=Cn2c1ncc2-c1cn(nc1)C)C 2500 0 834
 s1cc(nc1NC(=O)c1cc(ccc1)C(F)(F)CCNc1ncnc2c1scc2 2500 0 835
 Br1sc(nc1)Nc1cccc1OC 2700 0 836
 o1cccc1-c1nc(NC(C)C)c2cc(ccc2n1)C#CCO 2700 0 837
 Clc1cc2nncnc(Nc3ccc(cc3)-c3sc4c(n3)cccc4)c2cc1C 2700 0 838
 s1c2c(nc1-c1ccc(Nc3ncnc4c3scc4)cc1)cccc2 2800 0 839
 OCCNc1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)cc1)CC 2819 0 840
 Br1sc(nc1)Nc1ccc(cc1)C 2840 0 841
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)CCN1CCCCC1 2848 0 842
 O(C)c1cc(ccc1)CCNC(=O)c1c(n[nH]c1N\N=C\c1ccc(OC)cc1)C 2895 0 843
 Br1ccc(Nc2sc(Br)cn2)cc1 2900 0 844
 O(C)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2ccnc2)cc1 2900 0 845
 O(C)c1ccc(NC2=NC(=Cn3c2ncc3)c2ccnc2)cc1 2900 0 846

O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1NC)C 2900 0 847
 O=C(NCCCC)c1cc(NC(=O)CCCCCNc2ncnc3[nH]cnc23)ccc1 2900 0 848
 O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1cc(ccc1)CN(C)C)(C)C)C 2940 0
 849
 Brclsc(nc1)Nc1ccc(Cl)cc1 3000 0 850
 Brclsc(nc1)Nc1cccc1C 3000 0 851
 Clc1ncnc2[nH]c3cc(OC)c(OC)cc3c12 3000 0 852
 Ic1cc(F)c(Nc2c(F)c(F)c(cc2C(O)=O)\C=N\NC(=O)c2oc(cc2)CO)cc13000 0
 853
 o1cccc1C1n2c3c(nc2NC(C)=C1C(=O)Nc1ccc([N+](=O)[O-])cc1)cccc3 3000 0
 854
 O=C(N(O)C)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 3057 0 855
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)C)c1cccc1 3110 0 856
 S(=O)(=O)(N1CCC(CC1)C(=O)N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)NC)C)cn2)C
 C1)c1cccc13112 0 857
 O(C)c1c(OC)cc(cc1OC)C=1CNC(=O)C=1c1c2c([nH]c1)cccc2 3200 0 858
 O(C)c1c(OC)cc(cc1OC)C=1CNC(=O)C=1c1c2c(n(c1)C)cccc2 3200 0 859
 s1c2c(ncnc2NCCc2ccc(NC(=O)c3cc(ccc3)C(F)(F)F)cc2)cc13200 0 860
 s1c2c(nc1-c1ccc(N(C)c3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1OC)cccc2
 3300 0 861
 O=C(NCC)Cn1nc(c(c1)-c1c2cc[nH]c2nc1)-c1ccc(NC(=O)Nc2cccc2)cc1 3392
 0 862
 Clc1cc2c([nH]cc2C(=O)c2c(F)c(NS(=O)(=O)CCC)ccc2F)nc1 3400 0 863
 O(C)c1c2c([nH]nc2C)nc2c1cc(OC)cc2 3500 0 864
 O1c2c(cc(OC)cc2)CNc2c1ncnc2Nc1nc(nc1)NC(=O)c1ccc(cc1)C 3500 0
 865
 S(=O)(=O)(N1CCC(CC1)C(=O)N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)NC)C)cn2)C
 C1)C 3500 0 866
 Brclsc(nc1)Nc1ccnc1 3600 0 867
 O(C)c1cccc1CCNc1nc(nc(n1)NC(Cc1c2ccnc2[nH]c1)C(=O)N)Nc1cc2c(nc2)cc1
 3700 0 868
 O1c2c(CNc3c1ncnc3Nc1nc(nc1)NC(=O)c1ccc(cc1)C)cccc2 3700 0 869
 S(=O)(=O)(N(C)C)c1ccc(NC2=NC=Cn3c2nc3-c2cn(nc2)C)cc1 3700 0 870
 O=C(Nc1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2ccnc2)cc1)c1cccc1 3750 0
 871
 O=C(Nc1ccc(NC2=NC(=Cn3c2nc3)c2ccnc2)cc1)c1cccc1 3750 0 872
 O(C)c1cccc1CCNc1nc(nc(n1)NC(Cc1c2ccnc2[nH]c1)C(=O)N)N(CCCC)C 3800
 0 873
 s1c(cnc1Nc1nc(cc1)CN1CCN(CC1)C)C#N 3800 0 874
 O=C(N(O)C1CCCCC1)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 3839 0
 875
 O=C(Nc1ccc(cc1)-c1[nH]nc1-c1c2cc[nH]c2nc1)Nc1cccc1 3848 0 876
 O=C(Nc1ccc(cc1)-c1n[nH]cc1-c1c2cc[nH]c2nc1)Nc1cccc1 3848 0 877

S(=O)(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCCN2C
 COCC2)c3)cn1 3900 0 878
 S(=O)(=O)(N(CCC)CCC)c1ncc(cn1)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCCN2C
 COCC2)c3)cn1 3900 0 879
 Ic1cc(F)c(Nc2c(F)c(F)c(cc2C(O)=O)\C=N\NC(=O)CS(=O)(=O)c2ccc(Cl)cc2)cc1
 4000 0 880
 O=C/1Nc2c(cccc2)\C\1=C/1\Nc2c(cccc2)\C\1=N\O 4000 0 881
 s1c2c(nc1-c1cc(F)c(Nc3ncnc4c3scc4)cc1)cccc2 4000 0 882
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)-c1cccc1 4050 0 883
 O(C)c1cc2[nH]c(nc2cc1)-c1n[nH]cc1\C=C\c1cc(cnc1)C#N 4200 0 884
 O1CCN(CC1)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3c2ccnc2)c2ccnc2)cc1
 4200 0 885
 O1CCN(CC1)c1ccc(NC2=NC(=Cn3c2ncc3-c2ccnc2)c2ccnc2)cc1 4200 0
 886
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)NCCCC)Cc1ccc(N2CCCC2)cc1 4200 0
 887
 Oc1ccc(Nc2nc(ccn2)C=2[C@H]3[C@H](N(C=2)c2ccccc2)C=CC=C3)cc1 4200
 0 888
 O=C/1Nc2c(cccc2)\C\1=C/1\Nc2c(cccc2)\C\1=N\OC 4300 0 889
 [nH]1c2ncccc2nc1-c1ccc(N(C)C)cc1 4300 0 890
 [nH]1c2ncccc2nc1-c1ccc(cc1)-c1ncccc1 4400 0 891
 [nH]1c2ncccc2nc1-c1ccc(cc1)C1NCCCC1 4400 0 892
 s1c(cnc1Nc1ncc(cc1)CN1CCN(CC1)CC)C#N 4400 0 893
 s1c2c(nc1-c1cc(C)c(Nc3ncnc4c3cc(OC)c(OC)c4)cc1)cccc2 4400 0 894
 S(=O)(=O)(Nc1cc(ccc1)C=1N=C(Nc2ccc(OC)cc2)[C@@@H]2N(C=1)C=CN2)c1cccn
 c1 4500 0 895
 S(=O)(=O)(Nc1cc(ccc1)C=1N=C(Nc2ccc(OC)cc2)c2n(C=1)ccn2)c1ccnc1 4500
 0 896
 Brclsc(nc1)Nc1ccc(cc1)C(=O)NCCN(CC)CC 4520 0 897
 O=C(N(O)Cc1cccc1)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C4564 0 898
 OCCNc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 4597 0 899
 [nH]1c2ncccc2nc1-c1ccc(N2CCCC2)cc1 4600 0 900
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCc1ncccc1)C 4643 0 901
 Oc1cc(Nc2nc(ccn2)C=2[C@H]3[C@H](N(C=2)c2ccccc2)C=CC=C3)ccc1 4670
 0 902
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C(=O)N1CCN(CC1)C)C 4708
 0 903
 Fc1cc(ccc1)C(=O)Nc1n[nH]c2c1CN(C2)C(=O)C 4850 0 904
 s1cc(nc1CC(=O)Nc1cc(ccc1)C(F)(F)F)CCNc1ncc2c1scc2 4900 0 905
 Clc1cc2nc([nH]c2nc1)-c1ccc(N(C)C)cc1 4970 0 906
 Brclsc(nc1)Nc1c2c(ccc1)cccc2 5000 0 907
 O(C)c1c2c3cc(O)ccc3cc3NC(=O)c(cc1O)c23 5000 0 908
 O1c2cc(N(CC)CC)ccc2CNc2c1ncc2Nc1ncc(nc1)NC(=O)c1cccc1 5000 0

909

O(C)c1ccc(cc1)C(=O)Nc1cccc1C(=O)NC(Cc1ccc(O)cc1)C(=O)Nc1ccc(cc1C)C
 5090 0 910

O(C)c1cccc1CCNc1nc(nc(n1)NC)Nc1cc2c(nccc2)cc1 5100 0 911

O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)CNCCN1CCN(CC1)C)CC)Nc1cc
 ccc1 5111 0 912

O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)CNCCN1CCN(CC1)C)CC)Nc1cccc
 c1 5111 0 913

Brc1sc(nc1)Nc1ccc(cc1)C(=O)NCCN(C)C 5250 0 914

O(C)c1ccc(cc1)C=N\Nc1[nH]nc(C)c1C(OCc1cccc1)=O 5250 0 915

O(C)c1cc2c(ncnc2Ne2ccc(N3Cc4c(C3)cccc4)cc2)cc1OC 5300 0 916

Brc1sc(nc1)Nc1ccc(cc1)C(=O)NCCN1CCCC1 5320 0 917

s1c(cnc1Nc1ncc(cc1)CN1CCN(CC1)CCO)C#N 5400 0 918

O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)CNCCN(C)C)CC)Nc1cccc1
 5477 0 919

O(C)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2cc(N)ccc2)cc1 5480 0 920

O(C)c1ccc(NC2=NC(=Cn3c2ncc3)c2cc(N)ccc2)cc1 5480 0 921

Brc1sc(nc1)NC(=O)c1cccc1 5500 0 922

Brc1sc(nc1)Nc1cccc1F 5500 0 923

Clc1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2ccnc2)cc1 5500 0 924

Clc1ccc(NC2=NC(=Cn3c2ncc3)c2ccnc2)cc1 5500 0 925

s1c2c(nc1-c1cc(Nc3nc(nc4c3cc(OC)c(OC)c4)Nc3n[nH]c(c3)C)ccc1)cccc2 5500
 0 926

O=C(Nc1ccc(cc1)-c1n(ncc1-c1c2cc[nH]c2ncc1)CC)Nc1cccc1 5600 0 927

o1cccc1-c1nn2c(NC3=C(CN(Cc4cccc4OC)C3=O)C2=O)c1 5600 0 928

O=C(N)Cn1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1 5676 0
 929

Brc1sc(nc1)Nc1ccc(cc1)C(OCC)=O 5700 0 930

Clc1cc2nccc(Nc3ccc(cc3)-c3sc4c(n3)cccc4)c2cc1 5700 0 931

O(C(=O)c1[nH]nc-2c1CCc1c-2[nH]c2c1cccc2)CC 5700 0 932

Clc1cc(NC(=O)C=2C(n3c4c(nc3NC=2C)cccc4)c2occc2)ccc1F 5730 0 933

O=C(Nc1ccc(cc1)-c1n(ncc1-c1c2cc[nH]c2ncc1)C(C)(C)C)Nc1cccc1 5770 0
 934

s1c2c(nc1-c1ccc(Nc3ncnc4[nH]cnc34)cc1OC)cccc2 5800 0 935

S(=O)(=O)(Nc1ccc(cc1)CCNc1ncnc2oc(c(c12)-c1cccc1)-c1cccc1)1cccc1 5831
 0 936

Oc1cc(Nc2nc(ccn2)C=2[C@H]3[C@H](N(C=2)C)C=CC=C3)ccc1 5840 0
 937

s1ccnc1NC(=O)CN1CCN(CC1)c1ncnc2c1cc(OC)c(OC)c2 5900 0 938

s1c2c(nc1-c1ccc(Nc3nc(nc4c3cc(OC)c(OC)c4)Nc3n[nH]c(c3)C)cc1)cccc2 6000
 0 939

OCCn1nc(c2CCc3c(nc(nc3)NC3CCCC3)-c12)C(=O)N 6040 0 940

Fc1ccc(NC(=O)C=2C(n3c4c(nc3NC=2C)cccc4)c2occc2)cc16150 0 941

O1CCCC1n1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1 6195 0
942

O1CCC[C@@@H]1Cn1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1
6195 0 943

O(C)c1cccc1CCNc1nc(nc(n1)NC(Cc1c2ccnc2[nH]c1)C(=O)N)N([C@@@H](C)c1c
cccc1)C 6300 0 944

Clc1c([C@H](Oc2cc3cc(cnc3cc2)\C=C\C(=O)N)C)c(Cl)ccc1F 6400 0 945

Clc1cc(Nc2nenc3c2cc(OC)c(OC)c3)ccc1F 6500 0 946

O(C)c1c(OC)cc(cc1OC)C1=C(CNC1=O)c1c2c(n(c1)COc1cccc1)cccc2 6500 0
947

O(C)c1ccc(cc1)-c1[nH]c2ncccc2n1 6600 0 948

S(=O)(=O)(Nc1cc(ccc1)C=1N=C(Nc2ccc(OC)cc2)[C@@@H]2N(C=1)C=CN2)c1ccc(
OC)cc1 6700 0 949

S(=O)(=O)(Nc1cc(ccc1)C=1N=C(Nc2ccc(OC)cc2)c2n(C=1)ccn2)c1ccc(OC)cc1
6700 0 950

n12c(ncc1)C(=NC(=C2)c1ccnc1)Nc1cccc1 6700 0 951

n1cc(ccc1)C=1N=C(Nc2cccc2)[C@@@H]2N(C=1)C=CN2 6700 0 952

Clc1cc(cc(-n2nc(c3c2cc(nc3)N[C@@@H](C)c2cccc2)C)c1)-c1cccc1NC(=O)C
6800 0 953

O1CCN(CC1)C(=O)Cn1nc(c(c1)-c1c2cc[nH]c2ncc1)-c1ccc(NC(=O)Nc2cccc2)cc1
6810 0 954

[nH]1c2ncc(cc2nc1-c1ccc(N(C)C)cc1)C 6900 0 955

n1c(ccnc1Nc1cc(ccc1)C#N)C=1[C@H]2[C@@H](N=CC=C2)N(C=1)CC 6990
0 956

[nH]1c2nccc(c2nc1-c1ccc(N(C)C)cc1)C 7000 0 957

O(C)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2cc(NC(=O)Nc3cccc3)ccc2)cc1
7200 0 958

O(C)c1ccc(NC2=NC(=Cn3c2ncc3)c2cc(NC(=O)Nc3cccc3)ccc2)cc1 7200 0
959

s1cc(nc1NC(=O)N(C)c1cccc1)CCNc1ncnc2c1scc2 7200 0 960

O(C)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2cc(NC(=O)COc)ccc2)cc1 7310
0 961

O(C)c1ccc(NC2=NC(=Cn3c2ncc3)c2cc(NC(=O)COc)ccc2)cc1 7310 0 962

o1cccc1C1n2c3c(nc2NC(C)=C1C(=O)Nc1ccc(OC)cc1)cccc3 7580 0 963

Brc1sc(nc1)Nc1ccncc1 7800 0 964

O(C)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2cc(NC(=O)Nc3ccc(OC)cc3)ccc2)cc
1 7900 0 965

O(C)c1ccc(NC2=NC(=Cn3c2ncc3)c2cc(NC(=O)Nc3ccc(OC)cc3)ccc2)cc1 7900
0 966

o1cccc1-c1nn2c(NC3=C(CN(Cc4ccc(OC)cc4)C3=O)C2=O)c1 8000 0 967

s1c2c(nc1-c1ccc(Nc3ncnc4[nH]ccc34)cc1)cccc2 8000 0 968

OC1CCC(NC(=O)c2cc3Cc4c([nH]nc4-c4ccc(cc4)-c4ccc(OC)cc4)-c3cc2)CC1 8090
0 969

Fc1ccc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2occc2)cc1 8100 0 970
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc[nH]c2ncc1)C(C)(C)C)Nc1cccc1 8155 0
 971
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)C)c1ccc(cc1)C#N 8500 0 972
 O=C(C)c1cc(ccc1)-c1cc2nc([nH]c2nc1)-c1ccc(N(C)C)cc1 9000 0 973
 Brclsc(nc1)Nc1ccc(NC(=O)c2cccc2)cc1 9200 0 974
 o1cccc1C1c2c(n[nH]c2)NC(C)=C1C(=O)Nc1ccc(OC)cc1 9250 0 975
 Brclsc(nc1)Nc1cc(F)ccc19300 0 976
 s1c2c(nc1-c1cc(C)c(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2
 9400 0 977
 O(C)c1cc2c(ncnc2N2CCN(CC2)Cc2c3c(ccc2)cccc3)cc1OC 9600 0 978
 O(C)c1ccc(NC2=NC(=CN3[C@@@H]2NC=C3)c2nn(cc2)C)cc1 9700 0 979
 O(C)c1ccc(NC2=NC(=Cn3c2ncc3)c2nn(cc2)C)cc1 9700 0 980
 O(C)c1c(OC)cc(cc1OC)C1=C(c2c3c([nH]c2)cccc3)C(=O)NC1=O 9900 0
 981
 Brclsc(nc1)NC(=O)Nc1cccc1 10000 0 982
 Brclsc(nc1)Nc1cc(ccc1)C(F)(F)F 10000 0 983
 FC(F)(F)c1nc([nH]c1)-c1n[nH]cc1\C=C\c1cc(cnc1)CNCC 10000 0 984
 [nH]1c2ncccc2nc1-c1cc(N(C)C)ccc1 10000 0 985
 n12c(nc1-c1cn(nc1)C)C(=NC=C2)Nc1cc(N(C)C)ccc1 10000 0 986
 s1cc(nc1NC(=O)Cc1cc(ccc1)C(F)(F)F)CCNc1ncne2c1sec2 10000 0 987
 s1cc(nc1NC1=NC=Cn2c1ncc2-c1cn(nc1)C)C 10000 0 988
 s1nc(nc1NC1=NC=Cn2c1ncc2-c1cn(nc1)C)C 10000 0 989
 Oc1cc(O)ccc1-c1ccc(cc1)-c1[nH]nc(Nc2ccc(cc2)CNC(C)C)c1 10050 0 990
 O(C(=O)c1c(n[nH]c1N\N=C\c1cc2c([nH]cc2)cc1)C)CC11505 0 991
 Oc1ccc(cc1)CC(NC(=O)c1cccc1N)C(=O)Nc1ccc(cc1)C 11940 0 992
 [nH]1c2c(nc1-c1ccc(N(C)C)cc1)ccnc2 12500 0 993
 Brclsc(nc1)Nc1ccc([N+](=O)[O-])cc1 13000 0 994
 O(C(=O)c1c(n[nH]c1N\N=C\c1c2c([nH]cc2)ccc1)C)CC13740 0 995
 O=C1N(N=C(Nc2n[nH]c3c2cccc3)c2c1cccc2)c1cccc1 14000 0 996
 O=C1NCc2c1c(ccc2)C(=O)N 14340 0 997
 Clc1cc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2occc2)ccc1F 15000 0 998
 o1cccc1-c1nn2c(NC3=C(CN(Cc4cccc4)C3=O)C2=O)c1 15100 0 999
 O(C)c1ccc(cc1)\C=N\Nc1[nH]nc(C)c1C(OCC)=O 15140 0 1000
 o1cccc1-c1nn2c(NC3=C(CN(Cc4cc(OC)ccc4)C3=O)C2=O)c1 15200 0 1001
 O(C)c1c(OC)cc(cc1OC)C1=C(CNC1=O)c1c2c([nH]c1)cccc2 16000 0 1002
 O(C)c1cc(ccc1)-c1[nH]c2ncccc2n1 16000 0 1003
 O(C)c1ccc(cc1)C=1CNC(=O)C=1c1c2c([nH]c1)cccc2 16000 0 1004
 O(C)c1cc2c(ncnc2N2CCN(CC2)CC(=O)N(C)c2cccc2)cc1OC 16500 0 1005
 O(CC)c1cc2c(nc(nc2C)Nc2nc(O)c3c(n2)cccc3)cc1 16720 0 1006
 O=C(NCCCC)c1cc(NC(=O)CCCCCCNc2ncnc(N)c2)ccc1 17000 0 1007
 Brclsc(nc1)Nc1ccc(OC(F)(F)F)cc1 17200 0 1008
 Oc1cc(ccc1)-c1cc2nc([nH]c2nc1)-c1ccc(N(C)C)cc1 18000 0 1009

o1cccc1-c1nn2c(NC3=C(CN(Cc4cc(NC(=O)C)ccc4)C3=O)C2=O)c1 18300 0
 1010
 O(CC(O)Cn1c2c(nc1N\N=C\c1cccc1O)N(C)C(=O)NC2=O)c1ccc(OC)cc1 18400
 0 1011
 Fc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C 20000 0 1012
 O(C)c1ccc(cc1)-c1cc2nc([nH]c2nc1)-c1ccc(N(C)C)cc1 20000 0 1013
 s1c2c(ncnc2NCCe2cc(NC(=O)Ne3cc(ccc3)C(F)(F)F)ccc2)cc1 20000 0 1014
 S(=O)(=O)(Nc1nccn1)c1ccc(N)cc1 21000 0 1015
 O(Cc1cccc1)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 21230 0 1016
 Clc1c([C@H](Oc2cc3cc(cnc3cc2)C2CC2C(=O)N)C)c(Cl)ccc1F 22000 0 1017
 O(C)c1cc2c(ncnc2N2CCN(CC2)C(C)c2cccc2)cc1OC 25000 0 1018
 s1cnc(-c2nesc2)c1NC(=O)Cc1c2c(ccc1)cncc2 27000 0 1019
 O(C)c1c(OC)cc(cc1OC)C1=C(CNC1=O)c1c2c(n(c1)COCC)cccc2 29000 0
 1020
 O(C)c1cccc1-c1[nH]c2ncccc2n1 29000 0 1021
 O(C)c1c(OC)cc(cc1OC)C1=C(CNC1=O)c1c2c(n(c1)COCC(C)(C)C)cccc2 30000 0
 1022
 O(C)c1c(OC)cc(cc1OC)C1=C(CNC1=O)c1c2c(n(c1)COCC(C)C)cccc2 33000 0
 1023
 O(C)c1cc2c(ncnc2N2CCN(CC2)CCOc2cccc2)cc1OC 35000 0 1024
 Fc1ccc(cc1)CN1CCN(CC1)c1nene2c1cc(OC)c(OC)c2 40000 0 1025
 Clc1ccc(NC(=O)C=2C(C3=C(NC=2C)CC(CC3=O)(C)C)c2cccc2)cc1 40340 0
 1026
 O(C)c1c(OC)cc(cc1OC)C1=C(CNC1=O)c1c2c(n(c1)CC(O)CO)cccc2 47000 0
 1027
 Clc1cc([N+](=O)[O-])ccc1NC(=O)c1cc(Cl)ccc1O 54100 0 1028
 O(C)c1cc2c(ncnc2N2CCN(CC2)CCc2cccc2)cc1OC 76000 0 1029
 O(C)c1cc2[nH]c(cc2cc1)C(=O)C1CCC(CC1)C(C(=O)NCCCC=1CCCCC=1)C 86150
 0 1030
 O(C)c1cc2c(ncnc2N2CCN(CC2)CC(=O)N2CCCC2)cc1OC 98000 0 1031
 O(CC)c1ccc(Nc2nc3N(C)C(=O)NC(=O)c3n2CC(=O)Nc2ccc(OCC)cc2)cc1 98700
 0 1032
 BrC1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\O 100000 0 1033
 Clc1cc(Nc2nenc(N)e2C(=O)NCCN2CCCCC2)ccc1OCc1cccc1 100000 0 1034
 s1c(-c2nc(ncc2)Nc2cc(OC)c(OC)c(OC)c2)c(nc1C)C 0.40000001 1 1035
 S(c1ccc(NC(=O)CC)cc1)c1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 1 1 1036
 OC(CCCC(Nc1nc(Nc2n[nH]c(c2)C)cc(C)c1C#N)C)(C)C 1200 0 1037
 Clc1cc(Sc2nc(Nc3n[nH]c(c3)C)c3c(n2)cccc3)ccc1Cl 2 1 1038
 S(c1ccc(NS(=O)(=O)C)cc1)c1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 2 1 1039
 Clc1cc(Cl)ccc1Sc1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 2 1 1040
 S(c1ccc(NC(=O)C)cc1)c1nc(cc(n1)Nc1n[nH]c(c1)C)-c1cccc1 2.4000001 1
 1041
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCC2)cc(n1)Nc1n[nH]c(c1)C 2.4000001 1

1042
 Clc1c(Sc2nc(Nc3n[nH]c(c3)C)c3c(n2)cccc3)cccc1Cl 3 1 1043
 S(c1ccc(NC(=O)CC)cc1)c1nc(cc(n1)Nc1n[nH]c(c1)C)-c1cccn1 3.9000001 1
 1044
 Clc1cc(Sc2nc(Nc3n[nH]c(c3)C)c3c(n2)cccc3)ccc1 4 1 1045
 S(c1ccc(NC(=O)C)cc1)c1nc(Nc2[nH]nc(c2)C)c2c(n1)cccc2 4 1 1046
 Clc1cccc1Sc1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 5 1 1047
 Clc1cccc(Cl)c1Sc1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 5 1 1048
 S(c1ccc(NC(=O)CC)cc1)c1nc(cc(n1)Nc1n[nH]c(c1)C)C 5.0999999 1 1049
 Clc1ccc(Sc2nc(Nc3n[nH]c(c3)C)c3c(n2)cccc3)cc1 6 1 1050
 S(CCCCCCO)c1nc(Nc2n[nH]c(c2)C)cc(C)c1C#N 8.5 1 1051
 S(c1ccc(NC(OC(C)(C)C)=O)cc1)c1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 9 1
 1052
 O(c1ncccc1-c1nc(ncc1)NC)c1c2c(cccc2)c(NC(=O)Nc2cccc2)cc1 52 1 1053
 s1c(cnc1NC(=O)Nc1cc(ccc1)CCN1CCC1)CCNc1ncnc2c1sc2 53 1 1054
 O1CCN(CC1)Cc1ccc(cc1)-c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)
 cc1)CC 59 1 1055
 Brc1cc(ccc1C)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCN2CCOCC2)c3)cn1 70
 1 1056
 O1CCN(CC1)Cc1cc(ccc1)-c1[nH]c2nccc(c2c1)-c1cn(nc1-c1ccc(NC(=O)Nc2cccc2)
 cc1)CC 94 1 1057
 S(=O)(=O)(N(Cc1ccncc1)c1ncc(Nc2nc3n(ncc3cn2)C2CCCCCC2)cc1)C 95 1
 1058
 Clc1cc(NC(=O)Nc2sc(cn2)CCNc2ncnc3c2sc3)ccc1Cl 96 1 1059
 S(=O)(=O)(C=1C=Nc2n(nc(c2)C)C=1c1cccc1)c1cccc1 101 1 1060
 S(=O)(=O)(C=1C=Nc2n(ncn2)C=1c1cccc1)c1cccc1 104 1 1061
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3ccc(NC(=O)c4cccc4)cc3)c2cc1OC 110 1
 1062
 S(=O)(=O)(N(CCO)c1ncc(Nc2nc3n(ncc3cn2)C2CCCCCC2)cc1)C 110 1 1063
 Clc1ccc(cc1)-c1nn2c(N=CC(S(=O)(=O)c3cccc3)=C2c2cccc2)c1 120 1 1064
 Fc1ccc(cc1)C1N(CCC1Nc1nc(cnc1)C(=O)c1c2c(ncnc2N)n(c1)C(C)C)C=O 140 1
 1065
 o1c2c(nc1Nc1c3c(cccc3)c(Oc3ncccc3-c3nc(ncc3)NC)cc1)cccc2 141 1 1066
 S(=O)(=O)(N(CCN1CCOCC1)c1ncc(Nc2nc3n(ncc3cn2)C2CCCCCC2)cc1)C 150 1
 1067
 O=C(Nc1c(cccc1CC)CC)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 152 1 1068
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(Nc2nc(nc(N3CCN(CC3)CCO)c2)C)c1)c1cccc1
 170 1 1069
 S(=O)(=O)(N(CCN)c1ncc(Nc2nc3n(ncc3cn2)C2CCCCCC2)cc1)C 180 1 1070
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN(CCO)CC)c4)c2)ccc1
 190 1 1071
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(cc2)CN2CCOCC2)c1)c1cccc1
 220 1 1072

O(c1ncccc1-c1nc(ncc1)NC)c1c2c(cccc2)c(NC(=O)NC(C)(C)C)cc1 225 1 1073
 S(=O)(=O)(N(CCN(C)C)c1ncc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 260 1
 1074
 s1c(cnc1NC(=O)NC1CCCC1)CCNc1ncnc2c1scc2 270 1 1075
 Clc1cccc1NC(=O)Nc1sc(cn1)CCNc1ncnc2c1scc2 280 1 1076
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(Nc2nc(nc(N3CCN(CC3)C)c2)C)c1)c1cccc1
 290 1 1077
 S(=O)(=O)(Nc1cc2c(C=Cc3ncc(cc3C2=O)-c2cn(nc2)C)cc1)N(CC1OCCOC1)C
 290 1 1078
 O(c1ncccc1-c1nc(ncc1)NCCC1N(CCC1)C)c1c2c(cccc2)c(Nc2[nH]c3c(n2)cccc3)cc1
 327 1 1079
 O(c1ncccc1-c1nc(ncc1)NCC1CCN(CC1)CC)c1c2c(cccc2)c(Nc2[nH]c3c(n2)cccc3)cc
 1 332 1 1080
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(N3CCN(CC3)C)cc2)c1)c1cccc1
 340 1 1081
 S(=O)(=O)(N(CCN1CCCC1)c1ncc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 350 1
 1082
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN(CCO)CC)c4)c2)cccc1F
 360 1 1083
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(ccc2CC)CC)C)cn1)C(=O)N1C
 CCN(CC1)C372 1 1084
 s1c2c(nc1Nc1c3c(cccc3)c(Oc3nc3c-3nc(ncc3)NC)cc1)cccc2 380 1 1085
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(N3CCOCC3)cc2)c1)c1cccc1
 390 1 1086
 O=C(NCCc1cccc1)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 677 0 1087
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(Nc2nc(nc(NCCN3CCOCC3)c2)C)c1)c1cccc1
 680 0 1088
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(ccc2CC)CC)C)cn1)C(=O)NCC
 N(C)C 750 0 1089
 Fc1ccc(cc1NC(=O)Nc1ccc(cc1)-c1c2c([nH]nc2N)ccc1)C 760 0 1090
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(ccc2CC)CC)C)cn1)C(=O)N
 768 0 1091
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCN(CCO)CC)c4)c2)cccc1F 1400
 0 1092
 O=C(c1c2c(ncnc2N)n(c1)C(C)C)c1nc(NC2CCN(C(=O)C)C2c2cccc2)cnc1 820 0
 1093
 O=C(NC1CCCC1)c1cc(-n2c3nc(ncc3cc2)Nc2cc(N3CCN(CC3)C)ccc2)ccc1 820 0
 1094
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2cc(N3CCN(CC3)C)ccc2)c1)c1cccc1
 850 0 1095
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(N3CCN(CC3)C)cc2)c1)c1ccc(OC)
 cc1 1000 0 1096
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(N3CCN(CC3)C)cc2)c1)CC 1640

0 1097
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(N3CCN(CC3)C)cc2)c1)C(C)C
 1000 0 1098
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2cc(N3CCOCC3)ccc2)c1)c1cccc1
 1000 0 1099
 s1c2c(nc(nc2N2CCOCC2)-c2cnc(nc2C)N)cc1C(O)(C)C10000 0 1100
 O1C2CC(N(C2)CCn2nc3c(ccc3-c3nc4c(nc3O)cccc14)c2O)C 1000 0 1101
 O(c1nc1-c1nc(ncc1)NC)c1c2c(ccc2)c(Nc2[nH]c3c(n2)ccnc3)cc11067 0
 1102
 Fc1cc(ccc1)C(=O)Nc1ncc(Nc2ncnc3Oc4cc(OC)c(OC)cc4CNc23)cn1 1100 0
 1103
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(OCCN3CCCC3)cc2)c1)c1cccc1
 1170 0 1104
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc([nH]c2ncc1)-c1cc(ccc1)CN(C)C)CC)N(C)C
 1259 0 1105
 FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(ccc2CC)CC)C)cn1)C(=O)
 NCCN(C)C 1376 0 1106
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(ccc2CC)CC)C)cn1)C(=O)NC1
 CCN(CC1)C1450 0 1107
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(NC(=O)c2ccc(N3CCN(CC3)C)cc2)c1)CCC
 1640 0 1108
 O(c1nc1-c1nc(ncc1)NCC(CN(C)C)(C)C)c1c2c(ccc2)c(Nc2[nH]c3c(n2)cccc3)cc
 1 1658 0 1109
 Clc1cc(S(=O)(=O)Nc2cc(ccc2)-c2n[nH]c(NC(=O)c3ccc(N4CCN(CC4)C)cc3)c2)ccc
 1 1710 0 1110
 O1c2c-3c(cc(O)c2O)C(Oc2c-3c(cc(O)c2O)C1=O)=O 2480 0 1111
 s1c(cnc1NC(=O)c1cc(ccc1)C(F)(F)F)CCNc1ncnc2c1scc2 2500 0 1112
 Fc1cc(NC(=O)Nc2ccc(Nc3ncnc4c3ccc(OCC3CCN(CC3)C)c4)cc2)ccc1 2680 0
 1113
 S(c1ccc(NC(=O)CC)cc1)c1nc(cc(n1)Nc1n[nH]c(c1)C)C(C)(C)C 10 1 1114
 Clc1cc(ccc1)[C@H](NC(=O)c1[nH]cc(c1)-c1nc(ncc1C)Nc1c2OCCOc2ccc1)CO 11
 1 1115
 s1c(-c2nc(ncc2)Nc2ccc(N3CCN(CC3)C(=O)C)cc2)c(nc1NC)C 12 1 1116
 s1c(-c2nc(ncc2)Nc2ccc(N3CCOCC3)cc2)c(nc1NCC)C 14 1 1117
 OCC(NC(=O)c1[nH]cc(c1)-c1nc(ncc1C)Nc1cccc1)c1cccc1 15 1 1118
 Clc1cc(ccc1)C(NC(=O)c1[nH]cc(c1)-c1nc(ncc1C)Nc1c2OCOc2ccc1)CO 15 1
 1119
 S(c1cc(OC)c(OC)cc1)c1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 17 1 1120
 [nH]1nc(Nc2nc(nc3c2cccc3)N(C)c2cccc2)cc1C 17 1 1121
 S(c1ccc(NC(=O)C)cc1)c1nc(cc(n1)Nc1n[nH]c(c1)C)C 18 1 1122
 s1c(-c2nc(ncc2)Nc2ccc(N3CCOCC3)cc2)c(nc1NC)C 19 1 1123
 S(c1cccc1)c1nc(Nc2n[nH]c(c2)C)c2c(n1)cccc2 20 1 1124
 [nH]1nc(Nc2nc(nc3c2cccc3)Nc2cccc2)cc1C 24 1 1125

S(c1ccc(NC(=O)C)cc1)c1nc(Nc2n[nH]cc2)c2c(n1)cccc2 24 1 1126
 s1c(-c2nc(ncc2)Nc2ccc(N)cc2)c(nc1C)C 31 1 1127
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC[C@H]3CO)c4)c2)cccc
 1F 950 0 1128
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)CCO)c4)c2)cccc
 1F 55 1 1129
 [nH]1nc(cc1Nc1nc(nc2c1cccc2)-c1cccc1)C 58 1 1130
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN(CCO)C)c4)c2)ccc1 65 1
 1131
 s1c(-c2nc(ncc2)Nc2cc([N+](=O)[O-])ccc2)c(nc1N)C 73 1 1132
 [nH]1nc(Nc2nc(nc3c2cccc3)-c2ccncc2)cc1C 81 1 1133
 S(c1ccc(NC(=O)C)cc1)c1nc(Nc2n[nH]c(c2)C)ccn1 86 1 1134
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC[C@H]3CO)c4)c2)ccc
 1 1400 0 1135
 Clc1cc(ccc1)[C@H](NC(=O)c1[nH]cc(c1)-c1nc(ncc1C)Nc1cccc(OC)c1OC)CO
 200 1 1136
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC(O)CC3)c4)c2)cccc1F
 220 1 1137
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC(CC3)CO)c4)c2)cc(F)
 c1 230 1 1138
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC(CC3)CCO)c4)c2)cccc
 1F 280 1 1139
 Fc1c(NC(=O)Cn2ncc(Nc3ncnc4c3cc(OC)c(OCCCN3CCCC3CO)c4)c2)cccc1F
 340 1 1140
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCCN(CCC)CCO)c4)c2)cccc1F 87 1
 1141
 FC(F)(F)c1cc(NC(=O)c2cc(C#Cc3n(C)c(nc3)C(=O)NC)c(cc2)C)ccc1CN1CCN(CC1
)CCO 3000 0 1142
 O(C)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1 3168 0
 1143
 Clc1ccc(NC(=O)Nc2ccc(Oc3cc(ncc3)C(=O)NC)cc2)cc1C(F)(F)F 3800 0
 1144
 Oc1c(ccc(O)c1O)C1=CC(=O)c2c(C1=O)c([N+](=O)[O-])ccc2 4800 0 1145
 s1c(cnc1CC(=O)Nc1cc(ccc1)C(F)(F)CCNc1ncnc2c1sc2 4900 0 1146
 Clc1ccc(S(=O)(=O)Nc2cc(ccc2)-c2n[nH]c(NC(=O)c3ccc(N4CCN(CC4)C)cc3)c2)cc
 1 4990 0 1147
 O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1ccc(cc1)CN(C)C)(C)C)C 855 0 1148
 FC(F)(F)c1cc(NC(=O)c2cc(-c3cc4c(nc(nc4)NC)cc3)c(cc2)C)c(OC2CCN(CC2)C)cc1
 25000 0 1149
 FC(F)(F)c1cc(NC(=O)c2cc(-c3cc4c(nc(nc4)NCCN4CCOCC4)cc3)c(cc2)C)ccc1
 25000 0 1150
 O(C)c1c(OC)cc(Nc2nc(Nc3cc4c(nc3)cccc4)ccn2)cc1OC 5000 0 1151
 O(CCCN1CCCCC1)c1ccc(Nc2nc(Nc3cc4c(nc3)cccc4)ccn2)cc1 5000 0 1152

O(C)c1c(OC)cc(cc1OC)C1=C(c2c3c([nH]c2)cccc3)C(=O)NC1=O 5400 0
 1153
 S1SCC(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(C
 CC2)C(=O)C(N)C1)CCCNC(N)=N)Cc1cccc1)CC(C)C)Cc1c2c([nH]c1)cccc2)C(=O)
)NCC(=O)N 6000 0 1154
 Oc1c(ccc(O)c1O)C1=CC(=O)c2c(C1=O)c(O)ccc2O 6200 0 1155
 S1SCC(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(NC(=O)
 C(N)C1)C(O)C)CCCNC(N)=N)Cc1c2c([nH]c1)cccc2)Cc1c2c([nH]c1)cccc2)CC(C)
 C)C(=O)NCC(=O)N 7000 0 1156
 s1c(cnc1NC(=O)N(C)c1cccc1)CCNc1ncnc2c1sc2 7200 0 1157
 Clc1ccc(cc1)C=1n2ncnc2N=CC=1S(=O)(=O)c1cccc1 9238 0 1158
 S(=O)(=O)(N1CCN(CC1)C1CCN(CC1)c1cc(OC)c(Nc2nc(ccn2)-c2n3c(nc2-c2cc(cc
 2)C(=O)Nc2c(F)cccc2F)C=CC=C3)cc1CC)C 9500 0 1159
 O(C)c1c(OC)cc(cc1OC)C1=C(c2c3c([nH]c2)cccc3)C(=O)NC1=O 9900 0
 1160
 Ic1ccc(Nc2sc(Br)cn2)cc1 10000 0 1161
 BrC1sc(nc1)Nc1cccc1C(F)(F)F 10000 0 1162
 BrC1sc(nc1)Nc1ccc(F)cc1F 10000 0 1163
 BrC1sc(nc1)Nc1cc(F)ccc1F 10000 0 1164
 BrC1sc(nc1)Nc1cc(Cl)c(Cl)cc1 10000 0 1165
 BrC1sc(nc1)Nc1cc(Cl)cc(Cl)c1 10000 0 1166
 BrC1sc(nc1)Nc1cc(cc(c1)C)C 10000 0 1167
 s1c2c(nc1-c1cc(Nc3ncnc4[nH]cnc34)ccc1)cccc2 10000 0 1168
 s1c2c(nc1-c1cc(Nc3ncnc4[nH]cnc34)ccc1)cccc2 8000 0 1169
 s1c2c(nc1-c1ccc(Nc3nc(nc4c3cc(OC)c(OC)c4)NC)cc1)cccc2 10000 0 1170
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OC)c4)cc1OC)cccc2 10000 0 1171
 O1c2c(CNc3c1ncnc3Nc1cnc(nc1)NC(=O)c1cccc1)cccc2OC 10000 0 1172
 [nH]1c2cc(N3CCN(CC3)C)ccc2nc1-c1n[nH]cc1\C=C\c1ccnc1 10000 0 1173
 FC(F)(F)c1cc(Nc2ncnc(Nc3cc(NC(=O)C4CC4)ccc3)c2)ccc1 10000 0 1174
 [nH]1cc(nc1-c1n[nH]cc1\C=C\c1ccnc1)C#N 10000 0 1175
 BrC1sc(nc1)Nc1cc(cc(c1)C(F)(F)C(F)(F)F 10000 0 1176
 BrC1sc(nc1)N 10000 0 1177
 BrC1sc(nc1)NC(=O)C 10000 0 1178
 s1ccnc1Nc1ccc(F)cc1 10000 0 1179
 O=C(NC1CCCC1)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 10000 0 1180
 O=C(Nc1cccc1)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 10000 0 1181
 s1c(cnc1NC(=O)Cc1cc(ccc1)C(F)(F)F)CCNc1ncnc2c1sc2 10000 0 1182
 O=C(N)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1cccc1)(C)C)C 10000 0 1183
 O1c2cc(ccc2OC1)C(=O)Nc1n[nH]c2c1CN(C2)C(=O)C 10000 0 1184
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)Nc1cccc1)C 10000 0 1185
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)N)Cc1cccc1 10000 0 1186
 Fc1cccc1CC(=O)Nc1n[nH]c2c1CN(C2)C(=O)NCCCC10000 0 1187
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)NCCCC)Cc1cc2c(cc1)cccc2 10000 0 1188

O=C1N(CCC1)c1ccc(cc1)CC(=O)Nc1n[nH]c2c1CN(C2)C(=O)NCCCC 10000 0
 1189
 O=C(Nc1n[nH]c2c1CN(C2)C(=O)NCCCC)C(C)c1cc2c(cc1)cccc2 10000 0
 1190
 Fc1ccc(cc1)C(=O)Nc1n[nH]c2c1CN(C2)C(=O)C 10000 0 1191
 Clc1cccc(Cl)c1C(=O)Nc1c[nH]nc1C(=O)NC1CCNCC1 10000 0 1192
 Brc1nc(sc1)Nc1ccc(F)cc1 10000 0 1193
 Brc1sc(nc1)N(C)c1ccc(F)cc1 10000 0 1194
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)cc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)CCO)cn1
 10000 0 1195
 O=C(Nc1ccc(cc1)-c1nn(cc1-c1c2cc[nH]c2ncc1)CC)N(C)C 10000 0 1196
 O(C)c1ccc(N2CCN(CC2)C)cc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0
 1197
 O(C(=O)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C)CC 10000 0 1198
 S(C)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0 1199
 O=C(C)c1c(N2CCN(CC2)C)cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000
 0 1200
 O=C(C)c1cc(N2CCN(CC2)C)ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000
 0 1201
 O=C(C)c1ccc(N2CCN(CC2)C)cc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000
 0 1202
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OC)c4)cc1O)cccc2 10000 0 1203
 Clc1cc(Nc2ncnc3c2ccc(Cl)c3)ccc1-c1sc2c(n1)cccc2 10000 0 1204
 Clc1cc2ncnc(Nc3ccc(cc3F)-c3sc4c(n3)cccc4)c2cc1 10000 0 1205
 Clc1cc2nccc(Nc3cc(OC)c(cc3)-c3sc4c(n3)cccc4)c2cc1 10000 0 1206
 Clc1cc(Nc2nenc3c2sc3)ccc1-c1sc2c(n1)cccc2 10000 0 1207
 s1c2c(nc1-c1ccc(Nc3ncnc4c3scc4)cc1OC)cccc2 10000 0 1208
 s1c2c(nc1-c1ccc(Nc3ncnc4[nH]cnc34)cc1)cccc2 10000 0 1209
 s1c2c(nc1-c1ccc(Nc3nc(OC)nc4[nH]ccc34)cc1OC)cccc2 10000 0 1210
 s1c2c(nc1-c1ccc(Nc3nc(OC)nc4[nH]ccc34)cc1)cccc2 10000 0 1211
 s1c2c(nc1-c1ccc(Nc3ncnc4[nH]ccc34)cc1OC)cccc210000 0 1212
 s1c2c(nc1-c1ccc(Nc3nc(N(C)C)ccn3)cc1)cccc210000 0 1213
 s1c2c(nc1-c1ccc(Nc3nc(ncc3)NC)cc1)cccc2 10000 0 1214
 s1c2c(nc1-c1ccc(Nc3cc(ncc3)C(=O)NC)cc1)cccc2 10000 0 1215
 s1c2c(nc1-c1ccc(Nc3cc(ncc3)NC)cc1)cccc2 10000 0 1216
 O=C(N)c1cc([nH]c1-c1cccc1)-c1nc(ncc1)N 10000 0 1217
 Fc1cc(cc(F)c1)C(=O)Nc1n[nH]c2c1CN(C(=O)C(C)(C)C)C2(C)C 10000 0
 1218
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)N)C 10000 0 1219
 O1CCN(CC1)CCNc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0 1220
 s1c2c(nc(nc2N2CCOCC2)-c2cnc(nc2)N)cc1C(O)(C)C 10000 0 1221
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C1CCN(CC1)C 10000 0 1222
 FC(F)(F)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0 1223

FC(F)(F)c1cc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)ccc1 10000 0 1224
 O=C(C)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0 1225
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1[N+](=O)[O-])C 10000 0 1226
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cc([N+])(=O)[O-])ccc1)C 10000 0 1227
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1ccc([N+])(=O)[O-])cc1)C 10000 0 1228
 [nH]1nc(c2cc(NCc3nc3)N3CCN(CC3)C)cc12)\C=C\c1cccc1 10000 0
 1229
 O(C)c1cc(N2CCN(CC2)C)ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0
 1230
 O(C(=O)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)C 10000 0 1231
 O=C(N)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0 1232
 S(=O)(=O)(N)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0 1233
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1-c1cccc1)C 10000 0 1234
 O(c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)c1cccc1 10000 0 1235
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1Cc1cccc1)C 10000 0 1236
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1Nc1cccc1)C 10000 0 1237
 O=C(c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)c1cccc1 10000 0 1238
 S(c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)c1cccc1 10000 0 1239
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1NC(=O)C)C 10000 0 1240
 s1c2c(ne1-c1cc(O)c(Ne3nc4e3cc(OC)c(OC)c4)cc1)cccc2 350 1 1241
 O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C)C 10000 0 1242
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C(=O)C)C 10000 0 1243
 O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C(=O)C)C 10000 0 1244
 O=C(N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)NC)C)cn2)CC1)c1cccc1 10000 0
 1245
 O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C(=O)N1CCN(CC1)C)C
 10000 0 1246
 O(CC)C(=O)N1CCC(CC1)C(=O)N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)NC)C)cn2)
 CC1 10000 0 1247
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCCN1CCCC1)C 10000 0 1248
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 10000 0 1249
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)CC)C 10000 0 1250
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 10000 0 1251
 O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 10000 0 1252
 O=C(NC(CN(C)C)C)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 10000 0 1253
 O=C(N(CCN(C)C)C)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 10000 0 1254
 O=C(N1CCN(CC1)C)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 10000 0 1255
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C 10000 0 1256
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)-c1ncccc1 10000 0 1257
 FC(F)(F)Oc1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 10000 0 1258
 FC(F)(F)Oc1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1 10000
 0 1259
 FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)

N 10000 0 1260
 FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)
 N1CCN(CC1)C 10000 0 1261
 FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)
 N1CCCC1CN1CCCC1 10000 0 1262
 FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)
 N1CCC(N(C)C)CC1 10000 0 1263
 FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)
 N1CCN(CC1)C 10000 0 1264
 Clc1c(NC(=O)N(C)c2ncnc(Nc3ccc(N4CCN(CC4)CC)cc3)c2)c(Cl)c(OC)cc1OC
 10000 0 1265
 Clc1c2n(c3c(c2ccc1Cl)C(C#N)C1(NC3=O)CCNCC1)C 10000 0 1266
 o1nc(C(=O)NCc2ccncc2)c1-c1ccc(OC)cc1 10000 0 1267
 O=C1NC=Cc2c1cccc2Cc1n2N=C(C=Cc2nn1)c1cn(nc1)C 10000 0 1268
 O=C1NC=Cc2c1cccc2Cc1n2N=C(C=Cc2nn1)c1cccc1 10000 0 1269
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)cc1Nc1nc(ccn1)-c1n(cc(c1)C(=O)N)C 10000 0
 1270
 FC(F)(F)Cn1cc(cc1-c1nc(ncc1)Nc1cc(N2CCN(CC2)C)ccc1OC(F)(F)F)C(=O)N
 10000 0 1271
 FC(F)(F)Oc1ccc(N2CCNCC2)cc1Nc1nc(ccn1)-c1n(cc(c1)C(=O)N)C 10000 0
 1272
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)cc1Nc1nc(ccn1)-c1n(cc(c1)C(=O)N)CCO 10000
 0 1273
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)(OC(C)(C)C)=O)cc1Nc1nc(ccn1)-c1n(cc(c1)C(=O)
 N)C 10000 0 1274
 O=C1NCCc2[nH]c(cc12)-c1nc(ncc1)N 10000 0 1275
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)cc1Nc1nc(ccn1)-c1n(c2c(c1)C(=O)N)NCC2)C
 10000 0 1276
 FC(F)(F)Cn1c2c(cc1-c1nc(ncc1)Nc1cc(N3CCN(CC3)C)ccc1OC(F)(F)F)C(=O)NCC
 2 10000 0 1277
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)cc1Nc1nc(ccn1)-c1n(c2c(c1)C(=O)N)NCC2)CCO
 10000 0 1278
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)cc1Nc1nc(ccn1)-c1n(c2c(c1)C(=O)N(CC2)C(OC
 C)(C)C)=O)C 10000 0 1279
 ClC=1C(=O)N(C=NC=1OCc1ccc(F)cc1F)c1cc(ccc1C)C(=O)NCCO 10000 0
 1280
 o1c2ncnc(NCCC(=O)Nc3cccc3)c2c(c1-c1cccc1)-c1cccc1 5831 0 1281
 Oc1cc(O)ccc1C1=CC(=O)c2c(cccc2O)C1=O 12000 0 1282
 s1c2c(ncnc2NCCc2ccc(cc2)C(=O)Nc2cc(ccc2)C(F)(F)F)cc120000 0 1283
 s1cc(nc1NC(=O)Nc1cc(ccc1)C(F)(F)F)CCNc1ncnc2c1sec2 20000 0 1284
 Fc1cc2[nH]c(cc2cc1)C(=O)N1C[C@]2(CCN(C2)C2CC[C@H](NC2)C)c2c1cccc2
 1890 0 1285
 O=C1NC(=Cc2n(nc(N)c12)C)c1ccc(N2CCN(CC2)C)cc1 52000 0 1286

O=C1CCCC2n(c-3c(c12)C(=O)c1c-3cccc1)C(C)C 110 1 1287
 O=C(NC1CCCCC1)C1CCC(N(C1)c1nc(nc(c1)-c1cc2[nH]nc(N)c2cc1)NC)C 39810
 0 1288
 O1CCN(CC1)CCCN1cc(c2c1cccc2)C1=C(c2c3ncccc3n(c2)C)C(=O)NC1=O 1790
 0 1289
 O=C1NC(=O)C(n2c3c(nc3)cc2)=C1c1c2c(n(c1)CCn1ccnc1)cccc2 260 1 1290
 Clc1c([C@@@H](Oc2cc3c(nc3)cc2)C)c(Cl)ccc1F 50000 0 1291
 O(C)c1ccc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2cccc2)cc1 50000 0 1292
 O=C(Nc1ccc([N+]=(O)[O-])cc1)C=1C(c2c(n[nH]c2)NC=1C)c1ccccc1 50000 0
 1293
 FC(F)(F)c1ccc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2cccc2)cc1 50000 0
 1294
 Clc1cc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2cccc2)ccc1F 50000 0 1295
 Fc1ccc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2cccc2)cc1 50000 0 1296
 s1cccc1C1c2c(n[nH]c2)NC(C)=C1C(=O)Nc1ccc(OC)cc1 50000 0 1297
 s1cccc1C1c2c(n[nH]c2)NC(C)=C1C(=O)Nc1ccc([N+]=(O)[O-])cc1 50000 0
 1298
 s1cccc1C1c2c(n[nH]c2)NC(C)=C1C(=O)Nc1ccc(cc1)C(F)(F)F 50000 0 1299
 Clc1cc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2sc2ccc2)ccc1F 50000 0 1300
 o1cccc1C1c2c(n[nH]c2)NC(C)=C1C(=O)Nc1ccc([N+]=(O)[O-])cc1 50000 0
 1301
 FC(F)(F)c1ccc(NC(=O)C=2C(c3c(n[nH]c3)NC=2C)c2occc2)cc1 50000 0 1302
 O1CC(N2CCN(CC2)c2cc3c(cc2CC)C(=O)c2c([nH]c4cc(ccc24)C#N)C3(C)C)C1
 50000 0 1303
 O1CC(N2CCC(CC2)c2cc3c(cc2)C(=O)c2c([nH]c4cc(ccc24)C#N)C3(C)C)C1 50000
 0 1304
 S1SCC(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)CNC(=O)C(NC(=O)C(NC(=O)C(NC1)CC(O)=O)C(O)C)CCCNC(N)=N)CCCNC(N)=N)C(=O)NCC(=O)N
 91000 0 1305
 Clc1cc(Nc2nenc(N)c2C(=O)Nc2cccc2)ccc1OCc1ccccc1 100000 0 1306
 Clc1cc(Nc2nenc(N)c2-c2oc(nn2)CCN2CCOCC2)ccc1OCc1ccccc1 100000 0
 1307
 O(C)c1cc2[nH]c(nc2cc1)-c1n[nH]cc1\C=C\c1cc(cnc1)C(=O)NCC 100000 0
 1308
 O(C)c1cc2[nH]c(nc2cc1)-c1n[nH]cc1\C=C\c1cc(cnc1)C(OC)=O 100000 0 1309
 O=C1NCc2c1c(ccc2)C(O)=O 100000 0 1310
 O=C1NCc2c1c(ccc2)C(OC)=O 100000 0 1311
 O=C1N(Cc2c1c(ccc2)-c1n(ccc1)C(OC(C)(C)C)=O)C 100000 0 1312
 Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)C\1=O 100000 0 1313
 Fc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC 100000 0 1314
 Fc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)C\1=O 100000 0 1315
 Br1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)C\1=O 100000 0 1316
 Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC 100000 0 1317

BrC1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C 100000 0 1318
 BrC1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC 100000 0 1319
 Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C 100000 0 1320
 Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=O 100000 0 1321
 Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\O 100000 0 1322
 Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC 100000 0 1323
 Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\O 100000 0 1324
 Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C 100000 0 1325
 Clc1cc(Nc2ncnc(N)c2C(=O)NNC(=O)CCN2CCOCC2)ccc1OCc1cccc1 100000 0
 1326
 Clc1cc(Nc2ncnc(N)c2C(OCc2cc(F)ccc2)=O)ccc1OCc1cccc1 100000 0 1327
 Clc1cc(Nc2nenc(N)c2C(=O)N(CC)CC)ccc1OCc1cccc1 100000 0 1328
 Clc1cc(Nc2ncnc(N)c2C(=O)NCCOC)ccc1OCc1cccc1 100000 0 1329
 Clc1cc(Nc2ncnc(N)c2C(=O)NCCc2ccc(OC)cc2)ccc1OCc1cccc1 100000 0
 1330
 Clc1cc(Nc2ncnc(N)c2C(=O)NCCN2CCOCC2)ccc1OCc1cccc1 100000 0 1331
 Clc1ccc(cc1)Cn1cc(c2c1cccc2)CCC(=O)Nc1ccncc1 100000 0 1332
 Clc1cc(Nc2ncnc(C)c2C#Cc2cc(F)c(cc2)CN2CCCC2)ccc1OCc1cc(F)ccc1 100000
 0 1333
 Clc1ccc(cc1)-c1sc(CCNC(=O)C(=O)Nc2cc(NC(=O)C)ccc2)c(n1)C 100000 0
 1334
 BrC1sc(nc1)NC(=O)CSc1sc2c(n1)cc(OC)cc2 100000 0 1335
 Clc1ccc(cc1)Cn1cc(c2c1cccc2)CCC(=O)Nc1ccc([N+](=O)[O-])cc1 100000 0
 1336
 S1SCC(NC(=O)C(NC(=O)C(NC(=O)CNC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(N)C1)Cc1nc[nH]c1)CCC(=O)N)CC(O)=O)C(O)C)C(=O)NCC(=O)N 137000
 0 1337
 S1SCC(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)CNC(=O)C(N)C1)Cc1nc[nH]c1)CCC(=O)N)C(C)C)C(=O)NCC(=O)N234000 0
 1338
 S1SCC(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)CNC(=O)C(NC(=O)C(N)C1)CC(O)=O)C(C)C)Cc1c2c([nH]c1)cccc2)Cc1nc[nH]c1)C(=O)NCC(=O)N 242000 0 1339
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(Nc2nc(nc(N3CCN(CC3)C)c2)C)c1)CCCC 1000000 0 1340
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(Nc2nc(nc(N3CCN(CC3)C)c2)C)c1)c1cc(ccc1)C 1000000 0 1341
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(Nc2nc(nc(NCCN3CCOCC3)c2)C)c1)c1cccc1 1000000 0 1342
 S(=O)(=O)(Nc1cc(ccc1)-c1n[nH]c(Nc2nc(nc(NCCN(C)C)c2)C)c1)c1cccc1 1000000 0 1343
 s1c2cc(ccc2nc1NC(=O)NCc1ccc(OC)cc1)-c1[nH]nnn1 4800000 0 1344
 O(C)c1ccc(cc1)CNC(=O)Nc1nccc(c1)-c1[nH]nnn1 1e+008 0 1345

O(C)c1ccc(cc1)CNC(=O)Nc1nccc(c1)C#N 1e+008 0 1346
 S(c1ccc(NC(=O)C2CC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)cc(NC(=O)CCN1
 CCCCC1)c2 38 1 1347
 S(c1ccc(NC(=O)C2CC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)cc(NC(=O)CN1C
 COCC1)c2 7 1 1348
 S(c1ccc(NC(=O)C2CC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)cc(NC(=O)CN1C
 CCC1)c2 23 1 1349
 S(c1ccc(NC(=O)C2CC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)cc(NC(=O)CN1C
 CCC1CO)c2 10 1 1350
 S(c1ccc(NC(=O)C2CC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)cc(NC(=O)C(=O)
 N1CCN(CC1)C)c2 7 1 1351
 S(c1ccc(NC(=O)CN2C[C@H](OC(C)(C)C)C[C@@H]2CO)cc1)C=1N=C(Nc2n[nH]
 c(c2)C)c2n(N=1)ccc2 301 1 1352
 S(c1ccc(NC(=O)CN2C[C@H](Oc3ccc(F)cc3)C[C@H]2CO)cc1)C=1N=C(Nc2n[nH]
 c(c2)C)c2n(N=1)ccc2 53 1 1353
 S(c1ccc(NC(=O)CN2C[C@@H](F)C[C@@H]2CO)cc1)C=1N=C(Nc2n[nH]c(c2)C)c
 2n(N=1)ccc2 15 1 1354
 S(c1ccc(NC(=O)CN2CC(F)(F)C[C@H]2CO)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)
 1ccc2 8 1 1355
 S(c1ccc(NC(=O)CN2CCC[C@H]2CO)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2
 14 1 1356
 S(c1ccc(NC(=O)CN(C)C)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2 31 1
 1357
 S(c1ccc(NC(=O)CN2CCOCC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2 85
 1 1358
 S(c1ccc(NC(=O)CNC2CCCC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2 143 1
 1359
 S(c1ccc(NC(=O)CNC2CC2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2 32 1
 1360
 S(c1ccc(NC(=O)CN2C[C@H](Oc3ccc(F)cc3)[C@H](O)C2)cc1)C=1N=C(Nc2n[nH]
 c(c2)C)c2n(N=1)ccc2 7 1 1361
 S(c1ccc(NC(=O)CN2C[C@H](Oc3cc(F)cc(F)c3)[C@@H](O)C2)cc1)C=1N=C(Nc2n
 [nH]c(c2)C)c2n(N=1)ccc2 26 1 1362
 S(c1ccc(NC(=O)CN2C[C@H](Oc3ccc(F)cc3F)[C@@H](O)C2)cc1)C=1N=C(Nc2n[nH]
 c(c2)C)c2n(N=1)ccc2 13 1 1363
 S(c1ccc(NC(=O)CN2C[C@H](Oc3cc(F)ccc3)[C@@H](O)C2)cc1)C=1N=C(Nc2n[nH]
 c(c2)C)c2n(N=1)ccc2 17 1 1364
 S(c1ccc(NC(=O)CN2C[C@H](Oc3cccc3F)[C@@H](O)C2)cc1)C=1N=C(Nc2n[nH]
 c(c2)C)c2n(N=1)ccc2 10 1 1365
 S(c1ccc(NC(=O)CN2C\C(=N/O)[C@H](OC(C)(C)C)C2)cc1)C=1N=C(Nc2n[nH]c(c
 2)C)c2n(N=1)ccc2 9 1 1366
 S(c1ccc(NC(=O)CN2C[C@@H](OC3CCCC3)[C@@H](O)C2)cc1)C=1N=C(Nc2n[nH]
 c(c2)C)c2n(N=1)ccc2 11 1 1367

$S(c1ccc(NC(=O)CN2C[C@H](OCC3CC3)[C@@@H](O)C2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 7 1 1368
 $S(c1ccc(NC(=O)CN2C[C@H](OC(C)C)[C@@@H](O)C2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 8 1 1369
 $S(c1ccc(NC(=O)CN2C[C@H](OCCOC)[C@@@H](O)C2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 5 1 1370
 $S(c1ccc(NC(=O)CN2C[C@H](OC(CC)(C)C)[C@H](O)C2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 5 1 1371
 $S(c1ccc(NC(=O)CN2C[C@@@H](OC(C(F)(F)F)(C)C)[C@H](O)C2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 6 1 1372
 $S(c1ccc(NC(=O)CN2C[C@H](O)[C@@@H](F)C2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 5 1 1373
 $S(c1ccc(NC(=O)CN2C[C@H](OC(C)(C)C)[C@@@H](O)C2)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 12 1 1374
 $S(c1ccc(NC(=O)CN2CC(N)CC2CO)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 381 1 1375
 $S(c1ccc(NC(=O)CN2CC(O)CC2CO)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 58 1 1376
 $S(c1ccc(NC(=O)CN2CC(SC(C)(C)C)CC2CO)cc1)C=1N=C(Nc2n[nH]c(c2)C)c2n(N=1)ccc2$ 111 1 1377
 $Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCNC CO)c4)c2)ccc1$ 690 0 1378
 $Clc1cc(ccc1)[C@H](NC(=O)c1[nH]cc(c1)-c1nc(ncc1C)Nc1cccc1CC)CO$ 720 0 1379
 $FC(F)(F)c1cc(ccc1)-c1n2N=C(NC3CCNCC3)C=Cc2nn1$ 800 0 1380
 $O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc([N+](=O)[O-])cc c3)c2cc1OC$ 890 0 1381
 $Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCC N3CCC[C@H]3CO)c4)c2)cccc1F$ 39 1 1382
 $Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCC N(CCC)CCO)c4)c2)ccc1$ 220 1 1383
 $O=C1NC=C(C=C1NC(=O)c1ccc(N2CCCC2CN2CCCC2)cc1)c1nc(NC)cnc1$ 1000 0 1384
 $Fc1cc(NC(=O)Cn2ncc(Nc3ncnc4c3cc(OC)c(OCCC N(CCO)CC)c4)c2)ccc1$ 1100 0 1385
 $Fc1cc(NC(=O)Cn2ncc(Nc3ncnc4c3cc(OC)c(OCCC N3CCC[C@H]3CO)c4)c2)ccc1$ 1300 0 1386
 $Fc1cccc1NC(=O)Cc1[nH]nc(Nc2ncnc3c2cc(OC)c(OCCC N2CCC(CC2)CO)c3)c1$ 140 1 1387
 $Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCC N3CCC[C@H]3CO)c4)c2)ccc1$ 110 1 1388
 $O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cccc3)c2cc1OC$ 1600 0 1389

O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(OC)ccc3)c2cc1O
 C 1900 0 1390
 Clc1cccc1Nc1nc(n(n1)-c1ncnc1)N 2000 0 1391
 Fc1ccc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCC(CC3)CO)c4)c2)cc1
 2000 0 1392
 O(C)c1cccc1Nc1nc(n(n1)-c1ncnc(NCCN(C)C)c1)N 2100 0 1393
 Clc1cccc1Nc1nc(n(n1)-c1ncc(cc1)C#N)N 2500 0 1394
 O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(ccc3)C#N)c2cc1
 OC 2600 0 1395
 O1CCN(CC1)c1cc(OC)c(Nc2nc(n(n2)-c2ncc(cc2)C#N)N)cc1 2600 0 1396
 Fc1cc(NC(=O)Cn2ncc(Nc3ncnc4c3ccc(OCCN3CCCC3CO)c4)c2)ccc1 3000 0
 1397
 Fc1ccc(N2CCOCC2)cc1Nc1nc(n(n1)-c1ncnc1)N 3000 0 1398
 O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(O)ccc3)c2cc1OC
 4000 0 1399
 O1CCN(CC1)c1cc(Ne2nc(n(n2)-c2ncc2)N)c(OC)cc1 4000 0 1400
 O(C)c1cccc1Nc1nc(n(n1)-c1ncnc1)N 7000 0 1401
 o1c2c(c3c1ncnc3NCc1ccc(OC)c1)cccc2 1000000 0 1402
 Clc1cc(ccc1)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCN2CCOCC2)c3)cn1 0.1 1
 1403
 O1CCN(CC1)Cc1cc2nc([nH]c2cc1)-c1n[nH]cc1NC(=O)NC1CC1 3 1 1404
 OC(=O)c1cc(Nc2nc3n(ccc3cn2)-c2ncc2)ccc1 0.60000002 1 1405
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)C)cc(n1)Nc1[nH]nc(c1)C
 0.60000002 1 1406
 S1(=O)(=O)CCN(CC1)c1ccc(Nc2nc3n(ccc3cn2)-c2ncc2)cc1 0.80000001 1
 1407
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)CC(=O)Nc1cccc1 1 1
 1408
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC(CC1)CO)c2)CC(=O)Nc1cc(F)ccc1 1
 1409
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCN(CC2)C2CC2)cc(n1)Nc1n[nH]c(c1)C 1 1
 1410
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCN(CC2)CC)cc(n1)Nc1n[nH]c(c1)C 1 1
 1411
 Clc1cc2c(-c3nc(ncc3CN=C2c2c(F)cccc2F)Nc2ccc(cc2)C(O)=O)cc1 1 1 1412
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)CC(=O)Nc1cc(F)ccc1 1 1
 1413
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN(CCO)CC)c2)CC(=O)Nc1cc(F)ccc1 1 1
 1414
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN(CC#C)CC)c2)CC(=O)Nc1cc(F)ccc11 1
 1415
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC(CC1)CC)c2)CC(=O)Nc1cc(F)ccc1 1
 1 1416

s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCN(CC1)C)c2)CC(=O)Nc1cc(F)ccc1 1
 1 1417
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCCC1CO)c2)CC(=O)Nc1cc(F)ccc1 1 1
 1418
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)C)cc(n1)Nc1[nH]nc(c1)C 1.4 1
 1419
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCCCC2)cc(n1)Nc1n[nH]c(c1)C 1.6 1 1420
 n1c2n(ccc2cnc1Nc1cc(N2CCN(CC2)C)ccc1)-c1cccc1 3 1 1421
 s1c(cnc1NC(=O)Nc1cc(cc(c1)C(F)(F)F)CN1CCCC1)CCNc1ncnc2c1scc2 4 1
 1422
 n1cccc1-n1c2nc(ncc2cc1)Nc1cc(N2CCN(CC2)C)ccc1 5 1 1423
 S(=O)(=O)(N(CCCN1CCOCC1)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 5
 1 1424
 S(=O)(=O)(N(C(C)C)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 5 1 1425
 O(C)c1cc(-n2c3nc(ncc3cc2)Nc2cc(N3CCN(CC3)C)ccc2)ccc1 6 1 1426
 O(CCN1CCN(Nc2nc3n(ccc3cn2)C2CCCCC2)CC1)C 6 1 1427
 S(=O)(=O)(N(CCO)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 6 1 1428
 S(=O)(=O)(C)c1cc(-n2c3nc(ncc3cc2)Nc2ccc(N3CCN(CC3)C)cc2)ccc1 9 1
 1429
 s1c(cnc1NC(=O)Nc1cc(ccc1)C)CCNc1ncnc2c1scc2 9 1 1430
 S(=O)(=O)(N(CCCN1CCCCC1)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 9
 1 1431
 S(=O)(=O)(C)c1cc(-n2c3nc(ncc3cc2)Nc2cc(N3CCN(CC3)C)ccc2)ccc1 10 1
 1432
 O=C(N)c1cc(-n2c3nc(ncc3cc2)Nc2cc(N3CCN(CC3)C)ccc2)ccc1 11 1 1433
 Clc1cc(NC(=O)Nc2sc(cn2)CCNc2ncnc3c2scc3)ccc1F 11 1 1434
 n1c2n(ccc2cnc1Nc1cc(N2CCN(CC2)C)ccc1)-c1ccnc1 12 1 1435
 S1(=O)(=O)CCN(CC1)c1ccc(Nc2nc3n(ccc3cn2)C2CCCCC2)cc1 12 1 1436
 n1c2n(ccc2cnc1Nc1cc(N2CCN(CC2)C)ccc1)-c1cc(ccc1)C#N 13 1 1437
 n1c2n(ccc2cnc1Nc1ccc(N2CCN(CC2)C)cc1)-c1ccnc1 13 1 1438
 S(=O)(=O)(N(CCO)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 13 1 1439
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C(=O)N1CCCC1)C14 1 1440
 S(=O)(=O)(N(CCN1CCOCC1)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 14 1
 1441
 FC(F)(F)c1cc2[nH]c(nc2cc1)Nc1c2c(cccc2)c(Oc2ncccc2-c2nc(ncc2)NC)cc1 16 1
 1442
 s1nc(cc1NC1=NC(=Cn2c1ncc2-c1cn[nH]c1)C1CC1)C 17 1 1443
 S(=O)(=O)(Nc1ncc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 17 1 1444
 O(C)c1cc(-n2c3nc(ncc3cc2)Nc2ccc(N3CCN(CC3)C)cc2)ccc1 18 1 1445
 n1c2n(ccc2cnc1Nc1ccc(N2CCN(CC2)C)cc1)C1Cc2c(C1)cccc2 18 1 1446
 S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)C)cc(n1)Nc1[nH]nc(c1)C 20 1
 1447
 S(=O)(=O)(N(CCN)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 20 1 1448

s1c(cnc1NC(=O)Nc1cc(F)ccc1)CCNc1nenc2c1scc223 1 1449
 S(=O)(=O)(C=1C=Nc2n(nc(c2)-c2ccc(OC)cc2)C=1c1cccc1)c1cccc1 25 1
 1450
 n1c2n(ccc2cnc1Nc1cc(N2CCN(CC2)C)ccc1)-c1cc(ccc1)C(C)C 29 1 1451
 s1c(cnc1NC(=O)Nc1c2[nH]ccc2ccc1)CCNc1nenc2c1scc2 30 1 1452
 S(=O)(=O)(N(Cc1ccncc1)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1)C 30 1
 1453
 Clc1cc2c(-c3nc(ncc3CN=C2c2c(F)cccc2F)Nc2ccc(cc2)C(O)=O)cc1 34 1 1454
 Clc1ccc(NC(=O)Nc2sc(cn2)CCNc2nenc3c2scc3)cc1 39 1 1455
 n1c2n(ccc2cnc1Nc1ccc(N2CCN(CC2)C)cc1)C1C2CC(C1)CC2 39 1 1456
 Brclc2n(nc1-c1cccc1)C(c1cccc1)=C(S(=O)(=O)c1cccc1)C=N2 39 1 1457
 O1C(C)C(O)C(N)CC1OC1CC(O)(Cc2c1c(O)c1c(C(=O)c3c(C1=O)c(OC)ccc3)c2O)
 C(=O)CO 40 1 1458
 s1c(cnc1NC(=O)Nc1cc(ccc1)C#C)CCNc1nenc2c1scc2 41 1 1459
 n1c2n(ccc2cnc1Nc1ccc(N2CCN(CC2)C)cc1)C1CCCCC1 47 1 1460
 O1CCN(CC1)c1ccc(Nc2nc3n(ncc3cn2)C2CCCCC2)cc1 49 1 1461
 s1c(cnc1NC(=O)Nc1cc(OC)ccc1)CCNc1nenc2c1scc2 50 1 1462
 S(=O)(=O)(C=1C=Nc2n(nc(c2)-c2cccc2)C=1c1cccc1)c1cccc1 51 1 1463

III. Dataset 3

smiles pIC₅₀(nM) index

Clc1cc(ccc1F)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCCN2CCOCC2)c3)cn1	9.8239088	1
OC(=O)c1cc(Nc2nc3n(ccc3cn2)C2CCCCC2)ccc1	9.2218485	2
S(c1ccc(NC(=O)C2CC2)cc1)c1nc(N2CCN(CC2)Cc(n1)Nc1n[nH]c(c1)C	9.1549015	3
Clc1cc(ccc1)C(=O)Nc1ncc(Nc2ncnc3c2cc(OC)c(OCCN2CCCCC2)c3)cn1	9.0969105	4
O(C[C@@H](O)CN1CCCCC1)c1cc2ncnc(Nc3nc(nc3)NC(=O)c3cccc3)c2cc1OC	9.0969105	
	5	
Fc1c(cccc1C(F)(F)F)C(=O)N1CCN(CC1)Cc1nc(Nc2n[nH]cc2)ccc1	9.0457573	6
Fc1cccc1C(NC(=O)c1oc2c([nH]nc2NC(=O)c2ccc(cc2)CN2CCOCC2)c1)(C)C	9	7
s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)C(=O)Nc1ccc(F)cc1	9	8
s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCOC)c2)CC(=O)Nc1cc(F)ccc19	9	
Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CCO)c2)cccc1F		
	8.7235384	10
P(OCCN1CCN(CC1)C(=O)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(F)ccc3)c2cc1)(O)		
(O)=O	8.7189665	11
s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC[C@H]1CO)c2)CC(=O)Nc1cccc(F)c1F	8.6989698	
	12	
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CCO)c2)cc(F)c1		
	8.6401644	13
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CCF)c2)ccc1		
	8.5436344	14
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCNCC3)c2)ccc1	8.4236584	
	15	
o1c2c([nH]nc2NC(=O)c2ccc(N3CCN(C3)Cc2)cc1C(=O)NC1(CC1)c1cccc1	8.3979397	16
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)C3CC3)c2)ccc1		
	8.3353577	17
s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCNCCO)c2)CC(=O)Nc1cc(F)ccc1	8.3010302	18
s1cccc1CC(=O)N1Cc2c([nH]nc2NC(=O)c2ccc(cc2)C(C)(C)C)C1	8.3010302	19
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)C)c2)ccc1		
	8.2949924	20
O(C[C@@H](O)CN1CCCCC1)c1cc2ncnc(Nc3nc(nc3)NC(=O)c3cccc3)c2cc1OC	8.2218485	
	21	
s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)CCCC	8.2218485	22
s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)Cc2)cc1C(=O)N[C@@H](C)c1cccc1	8.2218485	
	23	
S(=O)(=O)(N1CCCC1)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(F)ccc3)c2cc1		
	8.2189627	24
S(=O)(=O)(N1C[C@@H](F)CC1)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(F)ccc3)c2c		
c1	8.2013493	25
Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3C[C@H](N[C@@H](C3)C)c2)ccc1	8.1924648	26

S(=O)(=O)(N1CCc2c1cccc2)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 8.0969105 27
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](CC)c1cccc1 8.0457573
 28
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1F)cccc2 8.0457573 29
 Fc1cc(NC(=O)Cc2[nH]nc(Ne3ncnc4c3ccc(c4)-c3ccc(cc3)C(=O)N3CCN(CC3)CC3CC3)c2)ccc1
 8.0218191 30
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCOCC3)cc2)cc1C(=O)NCc1cccc1 7.9586072 31
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1)c1cccc1
 7.9208188 32
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC(CC1)CO)c2)CNS(=O)(=O)c1cc(F)ccc1 7.9208188
 33
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](C)c1cccc1 7.8860564 34
 S(=O)(N1CCN(CC1)C)c1ccc(cc1)-c1cc2ncnc(Nc3n[nH]c(e3)CC(=O)Nc3cc(F)ccc3)c2cc1
 7.8557372 35
 S(=O)(=O)(N1CCCCC1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 7.8538718 36
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3cnc(nc3)NC(=O)CCCC)c2cc1OC 7.7695513 37
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](CN1CCOCC1)c1cccc1
 7.7447276 38
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCOCC3)cc2)cc1C(=O)N[C@H](CN1CCCC1)c1cccc1
 7.7447276 39
 S(=O)(=O)(N(C)C)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 7.6777806 40
 Clc1cc2nc(sc2cc1)-c1ccc(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)cc1 7.6197886 41
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCOCC3)cc2)cc1C(=O)N[C@H](CN1CCOCC1)c1cccc1
 7.6020598 42
 s1c2c(nc1-c1cc(F)c(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)C)c4)cc1)cccc2 7.5850267 43
 s1c2cc(F)ccc2nc1-c1ccc(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)cc1 7.5850267 44
 Clc1cc(Nc2ncnc3c2cc(OC)c(OCCN2CCN(CC2)C)c3)ccc1-c1sc2c(n1)cccc2 7.5686364 45
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](CN1CCCC1)c1cccc1
 7.5686364 46
 S(=O)(=O)(N1CCOCC1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 7.5376019 47
 S(=O)(=O)(NC)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 7.5086384
 48
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@@H](CC)c1cccc1 7.5086384
 49
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NCc1cccc1 7.4948502 50
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1)CC 7.4685211
 51
 S(=O)(=O)(CC=C)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 7.4089355
 52

FC(F)(F)Cn1nc(c2CCc3c(nc(nc3)Nc3cccc3)-c12)C(=O)N 7.3767509 53
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCOCC1)c2)C 7.3665314 54
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC(C)(C)c1cccc1 7.3565474 55
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC1CCCc2c1cccc2 7.3467875 56
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC(c1cccc1)c1cccc1 7.318759
 57
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NCC 7.318759 58
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 7.3010302 59
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC1CCc2c1cccc2 7.2839966 60
 Clc1cc2sc(nc2c1)-c1ccc(Nc2ncnc3c2cc(OC)c(OCCCN2CCN(CC2)C)c3)cc1 7.2676063 61
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCOCC1)c2)CC(=O)N(CC)c1cccc1 7.2596374 62
 S(=O)(=O)(CC)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 7.2441254
 63
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)NC(C)C 7.2291479 64
 O(c1cccc1-c1c[nH]nc1N)c1ccc(Ne2nnc(c3c2cccc3)-c2ccc(cc2)C)cc1 7.221849 65
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)cc(cc2)C(F)(F)F 7.221849
 66
 O(CCCN1CCC(O)CC1)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 7.2146702 67
 S(=O)(=O)(N)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 7.2146702 68
 s1c2cc(OC)ccc2nc1-c1ccc(Nc2ncnc3c2cc(OC)c(OCCCN2CCN(CC2)C)c3)cc1 7.2076082 69
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1)Cc1cccc1
 7.2006593 70
 s1c2c(nc1-c1cc(OC)c(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)cccc2 7.1870866 71
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)N[C@H](C)c1cccc1 7.1804562 72
 Brclcc(ccc1Cc1cccc1)C(=O)Nc1nc(Nc2ncnc3c2cc(OC)c(OCCCN2CCOCC2)c3)cn1
 7.154902 73
 s1c2c(nc1-c1ccc(Oc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)cccc2 7.0861859 74
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(OCC)=O)C(=O)CCC3)cc1)c1cccc1
 7.0757208 75
 Clc1cc2sc(nc2c1)-c1cc(F)c(Nc2ncnc3c2cc(OC)c(OCCCN2CCN(CC2)C)c3)cc1 7.070581 76
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3cnc(nc3)NC(=O)c3ccc(cc3)CC)c2cc1OC 7.070581 77
 Oc1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 7.0457573 78
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)O)cccc2 7.0409584 79
 O=C(N)c1n[nH]c-2c1CCc1c-2nc(nc1)Nc1cccc1 7.036212 80
 O(CCCO)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 7 81
 O=C1NCc2c1c(ccc2)-c1[nH]c2c(c1)cccc2 7 82
 s1c2c([nH]nc2NC(=O)c2ccc(N3CCN(CC3)C)cc2)cc1C(=O)Nc1cccc1 6.9788108 83
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCC[C@H]1CO)c2)CC(=O)Nc1cc(OC)ccc1 6.9746943
 84
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3ccc(NC(=O)c4cccc4)cc3)c2cc1OC 6.9586072 85
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2 6.9586072 86
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCC(CC1)CO)c2)CNC(=O)c1cc(F)ccc1 6.9546771 87
 O=C(C)c1ccc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)cc1 6.9355421 88

S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(=O)NC)C(=O)CCC3)cc1)c1cccc1
 6.9318142 89
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1OC)cccc2 6.9208188 90
 O(C)c1ccc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)cc1 6.8927898 91
 O1CCN(CC1)CCOc1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 6.8696661 92
 O(C)c1cc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)ccc1 6.801343 93
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCOCC1)c2)CC(=O)NCCC(C)C6.801343 94
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C1CCCCC1 6.7721133 95
 s1c2c(nc1-c1ccc(Oc3ncnc4c3cc(OC)c(OCCN3CCCC3)c4)cc1)cccc2 6.7695513 96
 O=C(C)c1cc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)ccc1 6.7544875 97
 Fc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 6.7495799 98
 O(CCCN1CCCCC1)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 6.7471471 99
 O(CCN1CCCCC1)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 6.6989698 100
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1F)cccc2 6.6989698 101
 O(C)c1cc2nc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 6.6882463 102
 O=C/1Nc2c(cccc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2 6.6819367 103
 Brc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 6.6777806 104
 O=C(NC1CC1)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 6.6716204 105
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(=O)N2CCCC2)C(=O)CCC3)cc1)c1cccc1
 1 6.6615434 106
 s1c2c(nc1-c1cc(F)c(Oc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)cccc2 6.6575775 107
 s1c2c(nc1-c1cc(O)c(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)cccc2 6.6382723 108
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1C)cccc2 6.6382723 109
 O=C/1Nc2c(cc(NC(=O)C)cc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2 6.5985994 110
 s1nc(O)c(C(NC(CO)C)=N)c1Nc1ccc(Nc2cccc2)cc1 6.5767541 111
 FC(F)(F)c1ccc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)cc1 6.5686364 112
 S(=O)(=O)(Cc1cccc1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 6.5670309 113
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(=O)N2CCOCC2)C(=O)CCC3)cc1)c1ccc
 cc1 6.5512938 114
 s1c2c(nc1-c1cc(OC(F)(F)F)c(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)cccc2
 6.5376019 115
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1O)cccc2 6.5228786 116
 O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C 6.5058455 117
 s1c2c(nc1-c1ccc(Ne3nc(Nc4n[nH]c(c4)C)ccn3)cc1OC)cccc2 6.4948502 118
 O(C)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 6.4710832 119
 O=C1NCc2c1c(ccc2)-c1[nH]ccc1 6.4710832 120
 s1c2c(nc1-c1cc(C)c(Nc3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1)cccc2 6.4685211 121
 s1c2c(nc1-c1ccc(Ne3ncnc4c3cc(OC)c(OC)c4)cc1)cccc2 6.4559321 122
 O(C)c1cc(ccc1O)-c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1 6.4473319
 123
 Fc1cc\2c(NC(=O)/C/2=C\c2[nH]c(C)c(C(=O)C)c2CCC(O)=O)cc1 6.4412913 124
 s1c2c(nc1-c1ccc(Nc3nc(Nc4n[nH]c(c4)C)ccn3)cc1)cccc2 6.4317985 125

s1c2c(nc1-c1cc(F)c(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2 6.4089355 126
 O(C)c1cc2c(ncnc2Nc2ccc(NC(=O)c3cccc3)cc2)cc1OC6.4056072 127
 Clc1cc2nc(sc2cc1)-c1ccc(Nc2ncnc3c2cc(OCCCN2CCN(CC2)C)c(OC)c3)cc16.3979402 128
 O=C/1Nc2c(cccc2)\C\1=C\c1[nH]c(C)c(CCC(O)=O)c1C 6.3580303 129
 S(=O)(=O)(Cc1ccc(F)cc1)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 6.3535962 130
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCC[C@H]1CO)c2)CC(=O)Nc1cccc1C(=O)N
 6.3448615 131
 Fc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CC(C3)(C)C)cc1 6.3410354 132
 Fc1cc(NC(=O)Cc2oc(nc2)Nc2ncnc3c2cc(OC)c(OCCCN2CCOCC2)c3)ccc1 6.3260579 133
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCCN1CCC[C@H]1CO)c2)CC(=O)Nc1cc(N(C)C)ccc1
 6.3160529 134
 O(C)c1cc(ccc1OC)-c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(O)=O)C(=O)CCC3)cc1
 6.251812 135
 S(=O)(=O)(N1CCc2c1cccc2)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(=O)N2CCOCC2)C(=O)C
 CC3)cc1 6.2494917 136
 s1cc(nc1Nc1ncnc2c1cc(OC)c(OCCCN1CCOCC1)c2)CC(=O)Nc1cc(F)ccc1 6.2380724 137
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1C)C 6.2182446 138
 O(C)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 6.2168112 139
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3nc(NC(=O)c4cccc4)cn3)c2cc1OC 6.2013493 140
 Clc1cc(Nc2ncnc3c2cc(OCCCN2CCN(CC2)C)c(OC)c3)ccc1-c1sc2c(n1)cccc26.1611509 141
 O1CCN(CC1)CCCOc1cc2ncnc(Nc3nc(nc3)NC(=O)c3ccncc3)c2cc1OC 6.1611509 142
 O=C/1Nc2c(cc(NC(=O)c3cccc3)cc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2 6.1426673
 143
 O=C/1Nc2c(cc([N+](=O)[O-])cc2)\C\1=C\c1[nH]c2c(c1CCC(O)=O)C(=O)CCC2 6.1402617 144
 s1c2c(nc1-c1cc(O)c(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2 6.09691 145
 s1c2c(nc1-c1ccc(Nc3nc(N4CCN(CC4)C)ccn3)cc1)cccc2 6.0757208 146
 Fc1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5.9277501 147
 O(C)c1cccc1CCNc1nc(nc(n1)NCCc1c2ccnc2[nH]c1)N(CCCC)C 5.9208188 148
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cc(cc2)C(F)(F)F 5.9208188
 149
 s1c2c(ncnc2NCCc2ccc(NC(=O)Nc3cc(ccc3)C(F)(F)F)cc2)cc1 5.9208188 150
 s1c2c(nc1-c1cc(OC)c(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2 5.8860564 151
 s1c2c(nc1-c1ccc(Nc3cc(nc3)Nc3n[nH]c(c3)C)cc1)cccc2 5.8860564 152
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C(C)C 5.8563609 153
 s1c2c(nc1-c1ccc(Nc3nc(NC)ccn3)cc1)cccc2 5.8239088 154
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1OC)cccc2 5.7958798 155
 O=C/1Nc2c(cccc2)\C\1=C\c1[nH]c2c(c1CCC(OCC)=O)C(=O)CCC25.7495799 156
 Fc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCC(OCC)=O)C(=O)CCC3)cc1 5.7033348 157
 Fc1cccc1CCNc1nc(nc(n1)Nc1cc2c(nccc2)cc1)Nc1cc(OC)c(cc1)C 5.6777806 158
 S(=O)(=O)(N1CCc2c1cccc2)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCCN(C)C)c(=O)CCC3)cc1
 5.6439743 159
 S(=O)(=O)(N1CCc2c1cccc2)c1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCCN(CC)CC)c(=O)CCC3)cc

1 5.630784 160
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)-c1ccccc1 5.6270881 161
 S(=O)(=O)(Nc1cc\2c(NC(=O)/C/2=C\c2[nH]c3c(c2CCCN(CC)CC)C(=O)CCC3)cc1)c1cccc1
 5.6108341 162
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cccc4)c2)ccc1 5.6057935 163
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1N)C 5.6025815 164
 Clc1cc2ncnc(Nc3ccc(cc3)-c3sc4c(n3)cccc4)c2cc1C 5.5686364 165
 s1c2c(nc1-c1ccc(Nc3ncnc4c3sc4)cc1)cccc2 5.5528421 166
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)CCN1CCCCC1 5.5454602 167
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1NC)C 5.5376019 168
 s1c2c(nc1-c1ccc(N(C)c3ncnc4c3cc(OC)c(OCCCN3CCN(CC3)C)c4)cc1OC)cccc25.4814858 169
 O(C)c1cccc1CCNc1nc(nc(n1)NC(Cc1c2ccnc2[nH]c1)C(=O)N)Nc1cc2c(nccc2)cc1 5.4317985
 170
 O(C)c1cccc1CCNc1nc(nc(n1)NC(Cc1c2ccnc2[nH]c1)C(=O)N)N(CCCC)C 5.4202166 171
 S(=O)(=O)(N(CCC)CCC)c1ccc(cc1)C(=O)Nc1ncc(Nc2nenc3c2cc(OC)c(OCCN2CCOCC2)c3)cn
 1 5.4089355 172
 S(=O)(=O)(N(CCC)CCC)c1ncc(cn1)C(=O)Nc1ncc(Nc2nenc3c2cc(OC)c(OCCN2CCOCC2)c3)cn
 1 5.4089355 173
 s1c2c(nc1-c1cc(F)c(Nc3ncnc4c3sc4)cc1)cccc2 5.3979402 174
 s1c2c(nc1-c1cc(C)c(Nc3ncnc4c3cc(OC)c(OC)c4)cc1)cccc2 5.3565474 175
 O(C)c1ccc(cc1)C(=O)Nc1cccc1C(=O)NC(Cc1ccc(O)cc1)C(=O)Nc1ccc(cc1C)C 5.293282 176
 O(C)c1cccc1CCNc1nc(nc(n1)NC)Nc1cc2c(nccc2)cc1 5.2924299 177
 O(C)c1cc2c(ncnc2Nc2ccc(N3Cc4c(C3)cccc4)cc2)cc1OC 5.2757239 178
 s1c2c(nc1-c1cc(Nc3nc(nc4c3cc(OC)c(OC)c4)Ne3n[nH]c(c3)C)cccc1)cccc2 5.2596374 179
 Clc1cc2ncnc(Nc3ccc(cc3)-c3sc4c(n3)cccc4)c2cc1 5.2441254 180
 s1c2c(nc1-c1ccc(Nc3ncnc4[nH]cnc34)cc1OC)cccc2 5.2365718 181
 s1c2c(nc1-c1ccc(Nc3nc(nc4c3cc(OC)c(OC)c4)Nc3n[nH]c(c3)C)cccc1)cccc2 5.221849 182
 O(C)c1cccc1CCNc1nc(nc(n1)NC(Cc1c2ccnc2[nH]c1)C(=O)N)N([C@@@H](C)c1cccc1)C
 5.2006593 183
 Clc1cc(Nc2nenc3c2cc(OC)c(OC)c3)cccc1F 5.1870866 184
 s1c2c(nc1-c1ccc(Nc3ncnc4[nH]ccc34)cc1)cccc2 5.09691 185
 s1c2c(nc1-c1cc(C)c(Nc3ncnc4c3cc(OCCCN3CCN(CC3)C)c(OC)c4)cc1)cccc2 5.0268722 186
 Oe1ccc(cc1)CC(NC(=O)c1cccc1N)C(=O)Nc1ccc(cc1)C 4.9229956 187
 O=C1NCc2c1c(ccc2)C(=O)N 4.843451 188
 O(CC)c1cc2c(nc(nc2C)Nc2nc(O)c3c(n2)cccc3)cc1 4.7767639 189
 O(CC(O)Cn1c2c(nc1N\N=C\c1cccc1O)N(C)C(=O)NC2=O)c1ccc(OC)cc1 4.7351823 190
 O(Cc1cccc1)c1cc2cc([nH]c2cc1)-c1c2c(CNC2=O)ccc1 4.6730499 191
 O(C)c1cc2[nH]c(cc2cc1)C(=O)C1CCC(CC1)C(C(=O)NCCC=1CCCCC=1)C 4.0647449 192
 O(CC)c1ccc(Nc2n3N(C)C(=O)NC(=O)c3n2CC(=O)Nc2ccc(OCC)cc2)cc1 4.0056829 193
 s1c(-c2nc(ncc2)Nc2cc(OC)c(OC)c(OC)c2)c(nc1C)C 9.3979397 194
 OC(CCCC(Nc1nc(Nc2n[nH]c(c2)C)cc(C)c1C#N)C)(C)C 5.9208188 195
 S(CCCCCCO)c1nc(Nc2n[nH]c(c2)C)cc(C)c1C#N 8.0705814 196
 S(=O)(=O)(C=1C=Nc2n(nc(c2)C)C=1c1cccc1)c1cccc1 6.9956784 197

S(=O)(=O)(C=1C=Nc2n(ncn2)C=1c1cccc1)c1ccccc1 6.9829664 198
 Clc1ccc(cc1)-c1nn2c(N=CC(S(=O)(=O)c3cccc3)=C2c2ccccc2)c1 6.9208188 199
 O=C(Nc1c(cccc1CC)CC)c1nn(c-2c1CCc1c-2nc(nc1)Nc1ccccc1)C 6.8181562 200
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)N1CCC(N(C)C)CC
 1 6.3151546 201
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)N1CCCC1CN1CC
 CC1 6.3089185 202
 O=C(NCc1ccccc1)c1nn(c-2c1CCc1c-2nc(nc1)Nc1ccccc1)C 6.1694112 203
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)NCCN(C)C
 6.124939 204
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)N 6.1146388 205
 FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)NCCN(C)C
 5.8613815 206
 O(C)c1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)NC1CCN(CC1)C
 5.8386321 207
 s1c(-c2nc(ncc2)Nc2ccc(N3CCN(CC3)C(=O)C)cc2)c(nc1NC)C 7.9208188 208
 s1c(-c2nc(ncc2)Nc2ccc(N3CCOCC3)cc2)c(nc1NCC)C 7.8538718 209
 s1c(-c2nc(ncc2)Nc2ccc(N3CCOCC3)cc2)c(nc1NC)C 7.7212462 210
 s1c(-c2nc(ncc2)Nc2ccc(N)cc2)c(nc1C)C 7.5086384 211
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCC[C@H]3CO)c4)c2)cccc1F
 6.0222764 212
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)CCO)c4)c2)cccc1F
 7.2596374 213
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCN(CC3)CCO)c4)c2)cccc1F 7.1870866 214
 s1c(-c2nc(ncc2)Nc2cc([N+](=O)[O-])cc2)c(nc1N)C 7.1366773 215
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCC[C@H]3CO)c4)c2)cccc1F
 5.8538718 216
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCC(O)CC3)c4)c2)cccc1F 6.6575775
 217
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCC(CC3)CO)c4)c2)cc(F)c1
 6.6382723 218
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCN3CCC(CC3)CCO)c4)c2)cccc1F
 6.5528421 219
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCCN(CCC)CCO)c4)c2)cccc1F 7.0604806 220
 O(C)c1ccccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1 5.4992146 221
 O=C(NC)c1nn(c-2c1C(Cc1c-2nc(nc1)Nc1ccc(cc1)CN(C)C)(C)C)C 6.0680337 222
 S1SCC(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C
 (N)C1)CCCNC(N)=N)Cc1ccccc1)CC(C)C)Cc1c2c([nH]c1)cccc2)C(=O)NCC(=O)N 5.221849
 223
 S1SCC(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(NC(=O)C(N)C1)
 C(O)C)CCCNC(N)=N)Cc1c2c([nH]c1)cccc2)Cc1c2c([nH]c1)cccc2)CC(C)C)C(=O)NCC(=O)N
 5.154902 224
 Clc1ccc(cc1)C=1n2ncnc2N=CC=1S(=O)(=O)c1ccccc1 5.0344219 225

s1c2c(nc1-c1cc(Nc3ncnc4[nH]cnc34)ccc1)cccc2 5 226
 s1c2c(nc1-c1cc(Nc3ncnc4[nH]ccc34)ccc1)cccc2 5.09691 227
 s1c2c(nc1-c1ccc(Nc3nc(nc4c3cc(OC)c(OC)c4)NC)cc1)cccc2 5 228
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OC)c4)cc1OC)cccc2 5 229
 Clc1cccc(Cl)c1C(=O)Nc1c[nH]nc1C(=O)NC1CCNCC15 230
 FC(F)(F)Oc1ccc(N2CCN(CC2)C)cc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)CCO)cn1 5 231
 O(C)c1ccc(N2CCN(CC2)C)cc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 232
 O(C(=O)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C)CC 5 233
 S(C)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 234
 O=C(C)c1c(N2CCN(CC2)C)cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 235
 O=C(C)c1cc(N2CCN(CC2)C)ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 236
 O=C(C)c1ccc(N2CCN(CC2)C)cc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 237
 s1c2c(nc1-c1ccc(Nc3ncnc4c3cc(OC)c(OC)c4)cc1O)cccc2 5 238
 Clc1cc(Nc2ncnc3c2ccc(Cl)e3)ccc1-c1sc2c(n1)cccc2 5 239
 Clc1cc2ncnc(Ne3ccc(cc3F)-c3sc4c(n3)cccc4)c2cc1 5 240
 Clc1cc2nccc(Nc3cc(OC)c(cc3)-c3sc4c(n3)cccc4)c2cc1 5 241
 Clc1cc(Nc2ncnc3c2scc3)ccc1-c1sc2c(n1)cccc2 5 242
 s1c2c(nc1-c1ccc(Ne3ncnc4c3scc4)cc1OC)cccc2 5 243
 s1c2c(nc1-c1ccc(Ne3ncnc4[nH]cnc34)cc1)cccc2 5 244
 s1c2c(nc1-c1ccc(Ne3nc(OC)nc4[nH]ccc34)cc1OC)cccc2 5 245
 s1c2c(nc1-c1ccc(Ne3nc(OC)nc4[nH]ccc34)cc1)cccc2 5 246
 s1c2c(nc1-c1ccc(Nc3ncnc4[nH]ccc34)cc1OC)cccc25 247
 s1c2c(nc1-c1ccc(Ne3nc(N(C)C)ccn3)cc1)cccc25 248
 s1c2c(nc1-c1ccc(Ne3nc(ncc3)NC)cc1)cccc2 5 249
 s1c2c(nc1-c1ccc(Ne3cc(ncc3)C(=O)NC)cc1)cccc2 5 250
 s1c2c(nc1-c1ccc(Ne3cc(ncc3)NC)cc1)cccc2 5 251
 O=C(N)c1cc([nH]c1-c1cccc1)-c1nc(ncc1)N 5 252
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)N)C 5 253
 O1CCN(CC1)CCNc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 254
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1)C1CCN(CC1)C 5 255
 FC(F)(F)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 256
 FC(F)(F)c1cc(Nc2nc-3c(CCc4c-3n(nc4C(=O)N)C)cn2)ccc1 5 257
 O=C(C)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 258
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1[N+](=O)[O-])C 5 259
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cc([N+](=O)[O-])ccc1)C 5 260
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1ccc([N+](=O)[O-])cc1)C 5 261
 O(C)c1cc(N2CCN(CC2)C)ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 262
 O(C(=O)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)C 5 263
 O=C(N)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 264
 S(=O)(=O)(N)c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1 5 265
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1-c1cccc1)C 5 266
 O(c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)c1cccc1 5 267
 O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1Cc1cccc1)C 5 268

$O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1Nc1cccc1)C$ 5 269
 $O=C(c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)c1cccc1$ 5 270
 $S(c1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1)c1cccc1$ 5 271
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)Nc1cccc1NC(=O)C)C$ 5 272
 $O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C)C$ 5 273
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C(=O)C)C$ 5 274
 $O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C(=O)C)C$ 5 275
 $O=C(N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)NC)C)cn2)CC1)c1cccc1$ 5 276
 $O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)C(=O)N1CCN(CC1)C)C$ 5 277
 $O(CC)C(=O)N1CCC(CC1)C(=O)N1CCC(Nc2nc-3c(CCc4c-3n(nc4C(=O)NC)C)cn2)CC1$ 5 278
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NCCN1CCCCC1)C$ 5 279
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCCC1)C$ 5 280
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCN(CC1)CC)C$ 5 281
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C$ 5 282
 $O=C(NC)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C$ 5 283
 $O=C(NC(CN(C)C)C)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C$ 5 284
 $O=C(N(CCN(C)C)C)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C$ 5 285
 $O=C(N1CCN(CC1)C)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)C$ 5 286
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)Cc1cccc1$ 5 287
 $O=C(N)c1nn(c-2c1CCc1c-2nc(nc1)NC1CCCC1)-c1ncccc1$ 5 288
 $FC(F)(F)Oc1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)N)C)cn1$ 5 289
 $FC(F)(F)Oc1cccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1$ 5 290
 $FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)N$ 5 291
 $FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)NC1CCN(CC1)C$ 5 292
 $FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)N1CCCC1C$
 $N1CCCC1$ 5 293
 $FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)N1CCC(N(C)C)CC1$ 5 294
 $FC(F)(F)Oc1cc(ccc1Nc1nc-2c(CCc3c-2n(nc3C(=O)Nc2c(cccc2CC)CC)C)cn1)C(=O)N1CCN(CC1)C$ 5 295
 $ClC=1C(=O)N(C=NC=1OCc1ccc(F)cc1F)c1cc(ccc1C)C(=O)NCCO$ 5 296
 $s1cc(nc1NC(=O)Nc1cc(ccc1)C(F)(F)F)CCNc1nenc2c1scc2$ 4.6989698 297
 $S1SCC(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)CNC(=O)C(NC(=O)C(N)C1)C$
 $C(O)=O)C(O)C)CCCNC(N)=N)CCCNC(N)=N)C(=O)NCC(=O)N$ 4.0409584 298
 $Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)C\1=O$ 4 299
 $Fc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC$ 4 300
 $Fc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)C\1=O$ 4 301
 $Brc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)C\1=O4$ 302
 $Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC$ 4 303
 $Brc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C$ 4 304
 $Brc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC$ 4 305
 $Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C$ 4 306

Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)C\1=O4 307
 Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\O 4 308
 Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC 4 309
 Ic1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\O 4 310
 Clc1c2NC(=O)/C(/c2ccc1)=C/1\Nc2c(cccc2)\C\1=N\OC(=O)C 4 311
 Clc1ccc(cc1)-c1sc(CCNC(=O)C(=O)Nc2cc(NC(=O)C)ccc2)c(n1)C 4 312
 Brc1sc(nc1)NC(=O)CSc1sc2c(n1)cc(OC)cc2 4 313
 S1SCC(NC(=O)C(NC(=O)C(NC(=O)CNC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(N)C1)C
 c1nc[nH]c1)CCC(=O)N)CC(O)=O)C(O)C)C(=O)NCC(=O)N 3.8632793 314
 S1SCC(NC(=O)C2N(CCC2)C(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)CNC(=O)C(N)C1)C
 N)C1)Cc1nc[nH]c1)CCC(=O)N)C(C)C)C(=O)NCC(=O)N 3.630784 315
 S1SCC(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C(=O)C(NC(=O)CNC(=O)C(NC(=O)C(N)C1)C
 C(O)=O)C(C)C)Cc1c2c([nH]c1)cccc2)Cc1nc[nH]c1)C(=O)NCC(=O)N 3.6161847 316
 s1c2cc(ccc2nc1NC(=O)NCc1ccc(OC)cc1)-c1[nH]nnn1 2.3187587 317
 O(C)c1ccc(cc1)CNC(=O)Nc1nccc(c1)-c1[nH]nnn1 1 318
 O(C)c1ccc(cc1)CNC(=O)Nc1nccc(c1)C#N1 319
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC(CC3)CO)c4)c2)cccc1F 6.3872161
 320
 Clc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4e3cc(OC)c(OCCCN3CCC(CC3)CO)c4)c2)ccc1 6.3467875
 321
 FC(F)(F)c1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC(CC3)CO)c4)c2)ccc1
 6.2924299 322
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCNCCO)c4)c2)ccc1 6.1611509 323
 O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc([N+](=O)[O-])ccc3)c2cc1OC
 6.0506101 324
 Fc1c(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCCN3CCC[C@H]3CO)c4)c2)cccc1F 7.4089355
 325
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCCN(CCC)CCO)c4)c2)ccc1 6.6575775 326
 Fc1cccc1NC(=O)Cc1[nH]nc(Nc2ncnc3c2cc(OC)c(OCCCN2CCC(CC2)CO)c3)c1 6.8538718
 327
 Fc1cc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3ccc(OCCCN3CCC[C@@H]3CO)c4)c2)ccc1 6.9586072
 328
 O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cccc3)c2cc1OC 5.7958798 329
 O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(OC)ccc3)c2cc1OC 5.7212462
 330
 Clc1cccc1Nc1nc(n(n1)-c1ncccc1)N 5.6989698 331
 Fc1ccc(NC(=O)Cc2[nH]nc(Nc3ncnc4c3cc(OC)c(OCCCN3CCC(CC3)CO)c4)c2)cc1 5.6989698
 332
 O(C)c1cccc1Nc1nc(n(n1)-c1ncnc(NCCN(C)C)c1)N 5.6777806 333
 Clc1cccc1Nc1nc(n(n1)-c1ncc(cc1)C#N)N 5.6020598 334
 O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(ccc3)C#N)c2cc1OC
 5.5850267 335
 O1CCN(CC1)c1cc(OC)c(Nc2nc(n(n2)-c2ncc(cc2)C#N)N)cc1 5.5850267 336

Fc1ccc(N2CCOCC2)cc1Nc1nc(n(n1)-c1ncccc1)N 5.5228786 337
 O(CCCN1CCC(CC1)CO)c1cc2ncnc(Nc3n[nH]c(c3)CC(=O)Nc3cc(O)ccc3)c2cc1OC 5.3979402
 338
 O1CCN(CC1)c1cc(Nc2nc(n(n2)-c2ncccc2)N)c(OC)cc1 5.3979402 339
 O(C)c1cccc1Nc1nc(n(n1)-c1ncccc1)N 5.154902 340
 o1c2c(c3c1ncce3NCc1ccc(OC)cc1)cccc2 3 341
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)CC(=O)Nc1cccc1 9 342
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC(CC1)CO)c2)CC(=O)Nc1cc(F)ccc1 9 343
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCN(CC2)C2CC2)cc(n1)Nc1n[nH]c(c1)C 9 344
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCN(CC2)CC)cc(n1)Nc1n[nH]c(c1)C 9 345
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCOCC1)c2)CC(=O)Nc1cc(F)ccc1 9 346
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN(OC)CC)c2)CC(=O)Nc1cc(F)ccc1 9 347
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN(CC#C)CC)c2)CC(=O)Nc1cc(F)ccc19 348
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCC(CC1)CC)c2)CC(=O)Nc1cc(F)ccc1 9 349
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCN(CC1)C)c2)CC(=O)Nc1cc(F)ccc1 9 350
 s1c(cnc1Nc1ncnc2c1cc(OC)c(OCCN1CCCC1CO)c2)CC(=O)Nc1cc(F)ccc1 9 351
 S(c1ccc(NC(=O)CC)cc1)c1nc(N2CCCCCC2)cc(n1)Nc1n[nH]c(c1)C 8.7958803 352
 S(=O)(=O)(C=1C=Nc2n(nc(c2)-c2ccc(OC)cc2)C=1c1cccc1)c1cccc1 7.6020598 353
 Brc1c2n(nc1-c1cccc1)C(c1cccc1)=C(S(=O)(=O)c1cccc1)C=N2 7.4089355 354
 O1C(C)C(O)C(N)CC1OC1CC(O)(Cc2c1c(O)c1c(C(=O)c3c(C1=O)c(OC)ccc3)c2O)C(=O)CO
 7.3979402 355
 S(=O)(=O)(C=1C=Nc2n(nc(c2)-c2cccc2)C=1c1cccc1)c1cccc1 7.2924299 35

IV Filter Rules

```
#Copyright (C) 2000–2005, 2010 by OpenEye Scientific Software, Inc.  
#This file defines the rules for filtering multi-structure files based on  
#properties and substructure patterns.  
  
MIN_MOLWT      130          "Minimum molecular weight"  
MAX_MOLWT      781          "Maximum molecular weight"  
  
MIN_NUM_HVY    9            "Minimum number of heavy atoms"  
MAX_NUM_HVY    55           "Maximum number of heavy atoms"  
  
MIN_RING_SYS   0            "Minumum number of ring systems"  
MAX_RING_SYS   5            "Maximum number of ring systems"  
  
MIN_RING_SIZE   0            "Minimum atoms in any ring system"  
MAX_RING_SIZE   20           "Maximum atoms in any ring system"  
  
MIN_CON_NON_RING 0            "Minimum number of connected non-ring atoms"  
MAX_CON_NON_RING 19           "Maximum number of connected non-ring atoms"  
  
MIN_FCNGRP     0            "Minimum number of functional groups"  
MAX_FCNGRP     7            "Maximum number of functional groups"  
  
MIN_UNBRANCHED 1            "Minimum number of connected unbranched non-ring atoms"  
MAX_UNBRANCHED 13           "Maximum number of connected unbranched non-ring atoms"  
  
MIN_CARBONS    3            "Minimum number of carbons"  
MAX_CARBONS    41           "Maximum number of carbons"  
  
MIN_HETEROATOMS 1            "Minimum number of heteroatoms"  
MAX_HETEROATOMS 14           "Maximum number of heteroatoms"  
  
MIN_Het_C_Ratio 0.04        "Minimum heteroatom to carbon ratio"  
MAX_Het_C_Ratio 4.0          "Maximum heteroatom to carbon ratio"  
  
MIN_HALIDE_FRACTION 0.0       "Minimum Halide Fraction"  
MAX_HALIDE_FRACTION 0.66      "Maximum Halide Fraction"  
  
#count ring degrees of freedom = (#BondsInRing) - 4 - (RigidBondsInRing) -  
(BondsSharedWithOtherRings)  
#must be >= 0, from JCAMP 14:251–265, 2000.  
ADJUST_ROT_FOR_RING true        "BOOLEAN for whether to estimate degrees of freedom in
```

rings"

MIN_ROT_BONDS	0	"Minimum number of rotatable bonds"
MAX_ROT_BONDS	16	"Maximum number of rotatable bonds"
MIN_RIGID_BONDS	4	"Minimum number of rigid bonds"
MAX_RIGID_BONDS	55	"Maximum number of rigid bonds"
MIN_HBOND_DONORS	0	"Minimum number of hydrogen-bond donors"
MAX_HBOND_DONORS	9	"Maximum number of hydrogen-bond donors"
MIN_HBOND_ACCEPTORS	0	"Minimum number of hydrogen-bond acceptors"
MAX_HBOND_ACCEPTORS	13	"Maximum number of hydrogen-bond acceptors"
MIN_LIPINSKI_DONORS	0	"Minimum number of hydrogens on O & N atoms"
MAX_LIPINSKI_DONORS	6	"Maximum number of hydrogens on O & N atoms"
MIN_LIPINSKI_ACCEPTORS	1	"Minimum number of oxygen & nitrogen atoms"
MAX_LIPINSKI_ACCEPTORS	14	"Maximum number of oxygen & nitrogen atoms"
MIN_COUNT_FORMAL_CRG	0	"Minimum number formal charges"
MAX_COUNT_FORMAL_CRG	4	"Maximum number of formal charges"
MIN_SUM_FORMAL_CRG	-2	"Minimum sum of formal charges"
MAX_SUM_FORMAL_CRG	2	"Maximum sum of formal charges"
MIN_CHIRAL_CENTERS	0	"Minimum chiral centers"
MAX_CHIRAL_CENTERS	21	"Maximum chiral centers"
MIN_XLOGP	-3.0	"Minimum XLogP"
MAX_XLOGP	6.85	"Maximum XLogP"

#choices are insoluble<poorly<moderately<soluble<very<highly

MIN_SOLUBILITY	insoluble	"Minimum solubility"
----------------	-----------	----------------------

PSA_USE_SandP false "Count S and P as polar atoms"

MIN_2D_PSA 0.0 "Minimum 2-Dimensional (SMILES) Polar Surface Area"

MAX_2D_PSA 205.0 "Maximum 2-Dimensional (SMILES) Polar Surface Area"

AGGREGATORS true "Eliminate known aggregators"

PRED_AGG false "Eliminate predicted aggregators"

#secondary filters (based on multiple primary filters)

```
GSK_VEBER      false    "PSA>140 or >10 rot bonds"  
MAX_LIPINSKI   3        "Maximum number of Lipinski violations"  
MIN_ABS        0.11     "Minimum probability F>10% in rats"  
PHARMACOPIA    false    "LogP > 5.88 or PSA > 131.6"
```

ALLOWED_ELEMENTS H, C, N, O, F, P, S, Cl, Br, I

ELIMINATE_METALS Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd

#acceptable molecules must have <= instances of each of the patterns below

#specific, undesirable functional groups

```
RULE 0 quinone  
RULE 0 pentafluorophenyl_esters  
RULE 0 paranitrophenyl_esters  
RULE 0 HOBT_esters  
RULE 0 triflates  
RULE 0 lawesson_s_reagent  
RULE 0 phosphoramides  
RULE 1 beta_carbonyl_quat_nitrogen  
RULE 0 acylhydrazide  
RULE 0 cation_C_Cl_I_P_or_S  
RULE 0 phosphoryl  
RULE 0 alkyl_phosphate  
RULE 1 phosphinic_acid  
RULE 0 phosphanes  
RULE 0 phosphoranes  
RULE 0 imidoyl_chlorides  
RULE 0 nitroso  
RULE 0 N_P_S_Halides  
RULE 0 carbodiimide  
RULE 0 isonitrile  
RULE 0 triacyloxime  
RULE 0 cyanohydrins  
RULE 0 acyl_cyanides  
RULE 0 sulfonylnitrile  
RULE 0 phosphonylnitrile  
RULE 0 azocyanamides  
RULE 0 beta_azo_carbonyl  
RULE 2 polyenes  
RULE 0 saponin_derivatives  
RULE 1 cytochalasin_derivatives  
RULE 4 cycloheximide_derivatives
```

```
RULE 1 monensin_derivatives
RULE 1 squalestatin_derivatives

#functional groups which often eliminate compounds from consideration

RULE 0 acid_halide
RULE 0 aldehyde
RULE 3 alkyl_halide
RULE 0 anhydride
RULE 0 azide
RULE 0 azo
RULE 2 di_peptide
RULE 1 michael_acceptor
RULE 0 beta_halo_carbonyl
RULE 3 nitro
RULE 0 oxygen_cation
RULE 0 peroxide
RULE 0 phosphonic_acid
RULE 0 phosphonic_estер
RULE 0 phosphoric_acid
RULE 0 phosphoric_estер
RULE 1 sulfonic_acid
RULE 0 sulfonic_estер
RULE 0 tricarbo_phosphene
RULE 0 epoxide
RULE 0 sulfonyl_halide
RULE 0 halopyrimidine
RULE 0 perhalo_ketone
RULE 0 aziridine
RULE 1 oxaryl
RULE 0 alphahalo_amine
RULE 0 halo_amine
RULE 1 halo_alkene
RULE 0 acyclic_NCN
RULE 0 acyclic_NS
RULE 0 SCN2
RULE 0 terminal_vinyl
RULE 0 hetero_hetero
RULE 0 hydrazine
RULE 0 N_methoyl
RULE 2 NS_beta_halothyl
RULE 0 propiolactones
RULE 0 iodoso
```

```
RULE 0 iodoxy
RULE 0 noxide
```

```
#groups of molecules
```

```
RULE 2 dye
```

```
#functional groups which are allowed, but may not be wanted in high quantities
#common functional groups
```

```
RULE 6 alcohol
RULE 5 alkene
RULE 4 amide
RULE 4 amino_acid
RULE 3 amine
RULE 3 primary_amine
RULE 3 secondary_amine
RULE 3 tertiary_amine
RULE 2 carboxylic_acid
RULE 6 halide
RULE 4 iodine
RULE 3 ketone
RULE 4 phenol
RULE 2 imine
RULE 1 methyl_ketone
RULE 1 alkylaniline
RULE 2 sulfonamide
RULE 1 sulfonylurea
RULE 0 phosphonamide
RULE 1 alphahalo_ketone
RULE 0 oxaziridine
RULE 1 cyclopropyl
RULE 2 guanidine
RULE 0 sulfonimine
RULE 0 sulfinimine
RULE 1 hydroxamic_acid
RULE 0 sulfinylthio
RULE 0 disulfide
RULE 0 enol_ether
RULE 2 enamine
RULE 0 organometallic
RULE 0 dithioacetal
```

```
RULE 1 oxime
RULE 0 isothiocyanate
RULE 0 isocyanate
RULE 2 lactone
RULE 2 lactam
RULE 1 thioester
RULE 1 carbonate
RULE 0 carbamic_acid
RULE 1 thiocarbamate
RULE 0 triazine
RULE 1 malonic
```

```
#other functional groups
```

```
RULE 2 alkyne
RULE 4 aniline
RULE 4 aryl_halide
RULE 2 carbamate
RULE 3 ester
RULE 6 ether
RULE 1 hydrazone
RULE 0 nonacylhydrazone
RULE 1 hydroxylamine
RULE 2 nitrile
RULE 2 sulfide
RULE 2 sulfone
RULE 2 sulfoxide
RULE 1 thiourea
RULE 1 thioamide
RULE 1 thiol
RULE 2 urea
```

```
RULE 0 hemiketal
RULE 0 hemiacetal
RULE 0 ketal
RULE 3 acetal
RULE 0 aminal
RULE 0 hemiaminal
```

```
#protecting groups
```

```
RULE 0 benzyloxycarbonyl_CBZ
RULE 0 t_butoxycarbonyl_tBOC
```

```
RULE 0 fluorenylmethoxycarbonyl_Fmoc
RULE 1 dioxolane_5MR
RULE 1 dioxane_6MR
RULE 1 tetrahydropyran_THP
RULE 1 methoxyethoxymethyl_MEM
RULE 2 benzyl_ether
RULE 2 t_butyl_ether
RULE 0 trimethylsilyl_TMS
RULE 0 t_butyldimethylsilyl_TBDMS
RULE 0 triisopropylsilyl_TIPS
RULE 0 t_butyldiphenylsilyl_TBDPS
RULE 1 phthalimides_PHT
```