

## **Supplementary Information**

### **Extracting SAR Information from a Large Collection of Anti-Malarial Screening**

#### **Hits by NSG-SPT Analysis**

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#### **Supplementary Figures S1-S5**

#### **Supplementary Table S1**

## Supplementary Figure Legends

### **Figure S1. Selected NSG regions after removal of known anti-malarial chemotypes.**

Three prominent local SAR regions that are highlighted in the NSG in Figure 3 of the manuscript are shown in detail.

**Figure S2. Corresponding SPTs.** For each of the local NSG regions displayed in Figure S1, the corresponding SPT is shown. Numbers correspond to Figure S1. Selected compounds are shown and informative SAR patterns are highlighted.

**Figure S3. Complete SPT.** The complete SPT for region 3 in Figure S2 is shown.

**Figure S4. Cluster and potency distribution.** Each cluster obtained by k-means clustering ( $k=60$ ) of the reduced GSK data set is represented by a boxplot that reports the distribution of potency values of the members. On the left axis, the cluster size, i.e. the number of compounds a cluster contains, is reported. The clusters are ordered by decreasing median potency from the top to the bottom, as indicated by the axis on the right (cluster rank). Potency values are reported on the horizontal axis as  $pXC_{50}$  values. Selected clusters mapped in Figure S5 are colored accordingly.

**Figure S5. NSG analysis and independent compound clustering.** The NSG corresponding to Figure 3 of the manuscript is displayed without potency-based coloring. Eight compound clusters obtained from standard k-means clustering ( $k=60$ ) are highlighted. Four clusters with highest median potency were selected together with four others that each contained one of the four most potent remaining compounds.

Figure S1

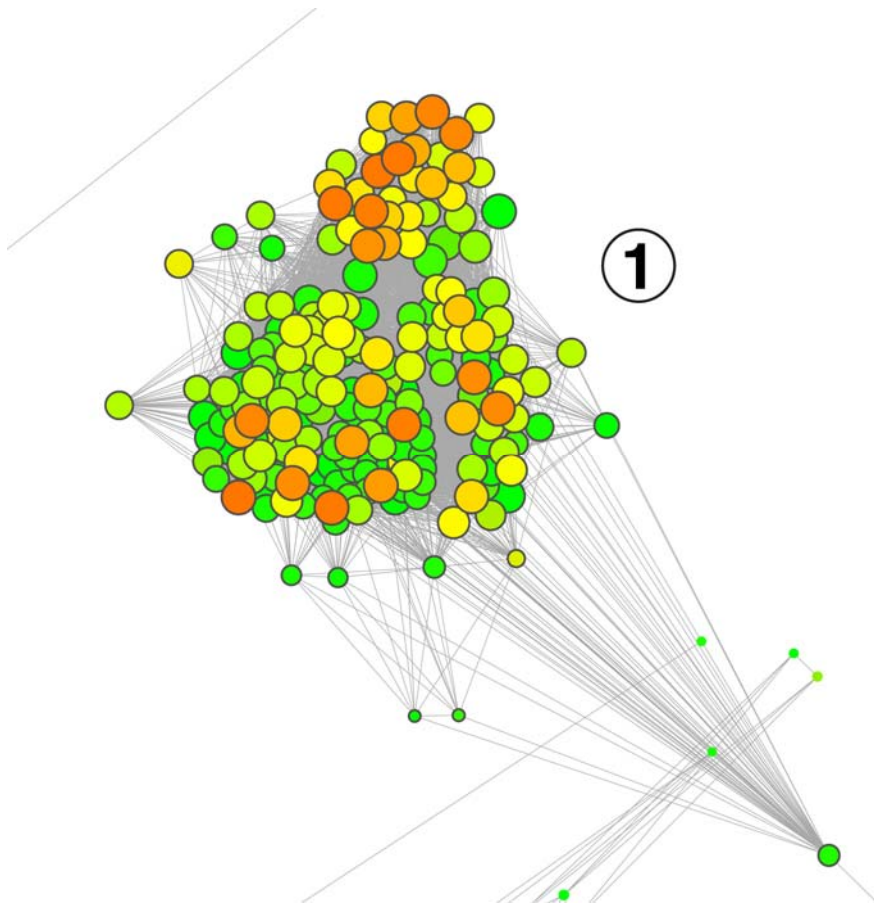


Figure S1 – continued

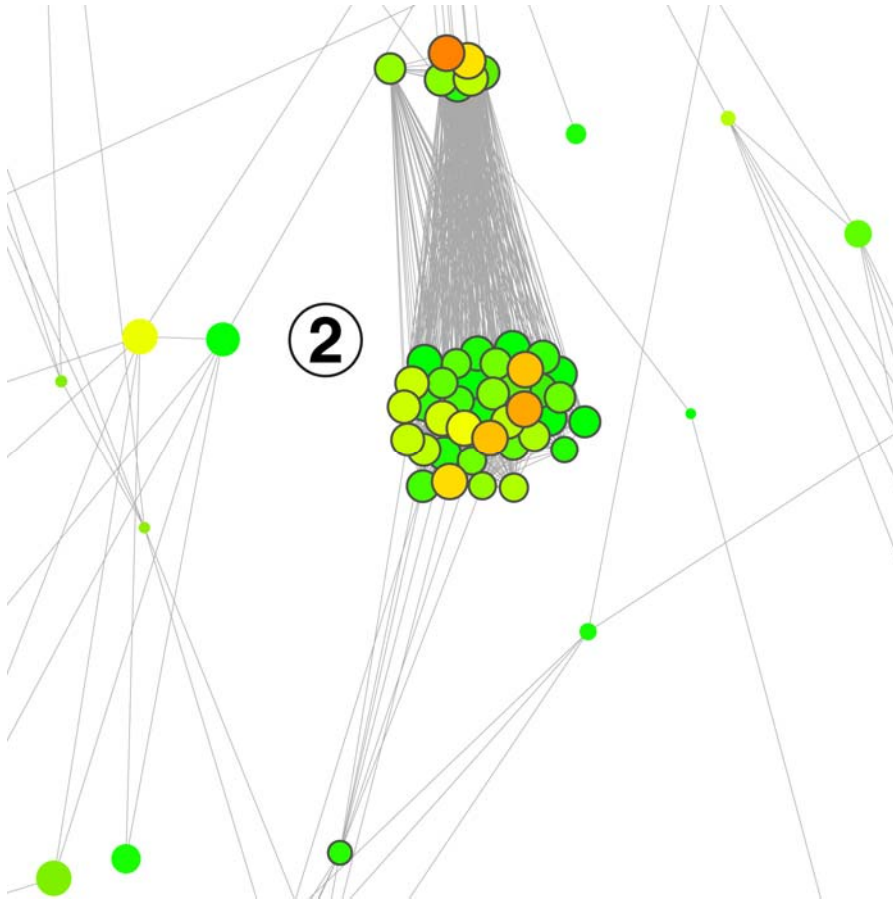


Figure S1 – continued

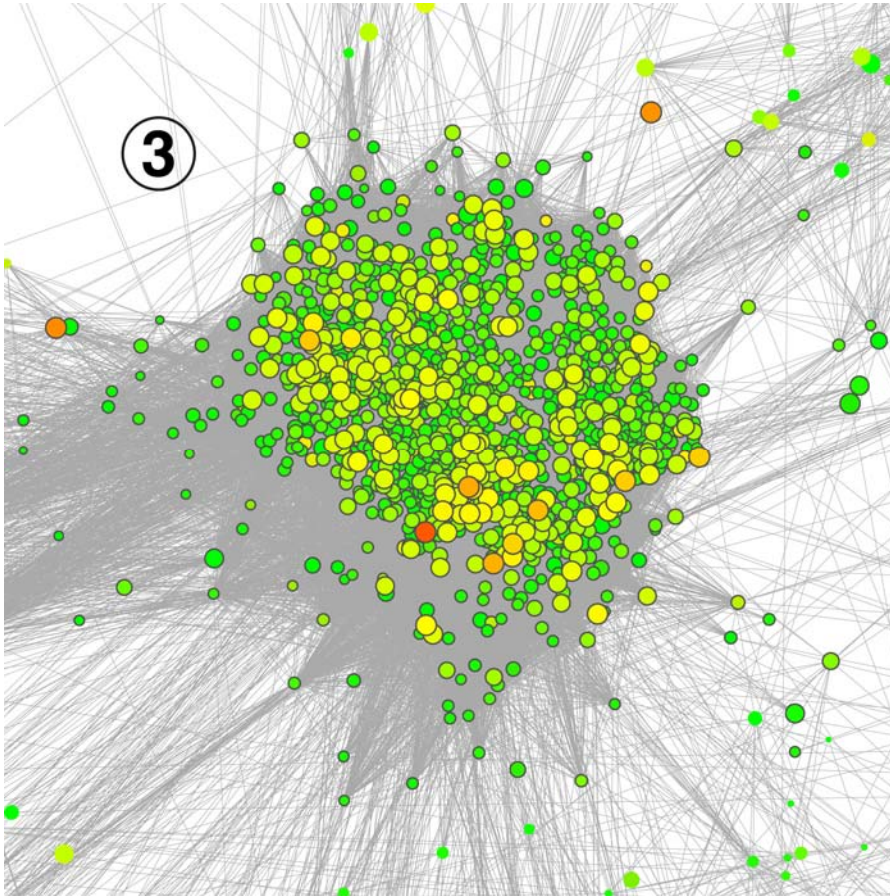


Figure S2

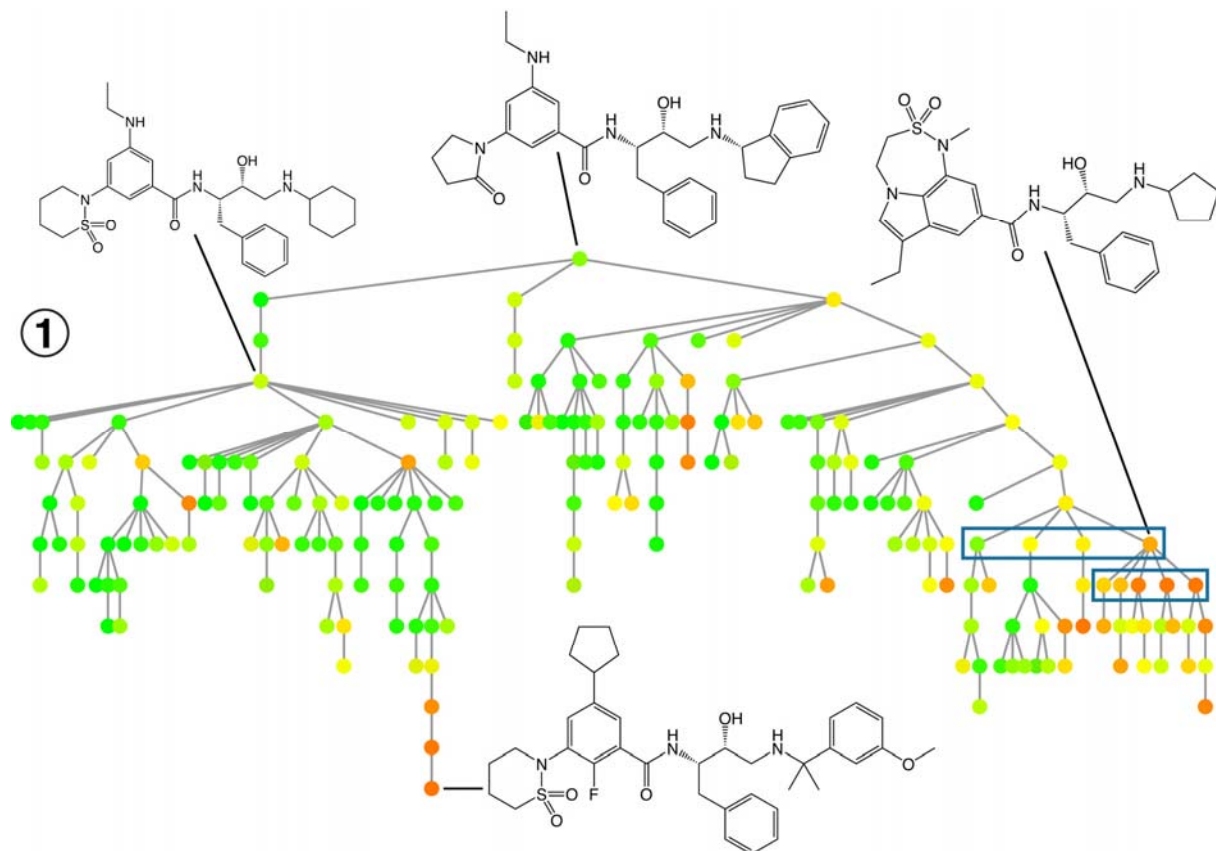


Figure S2 – continued

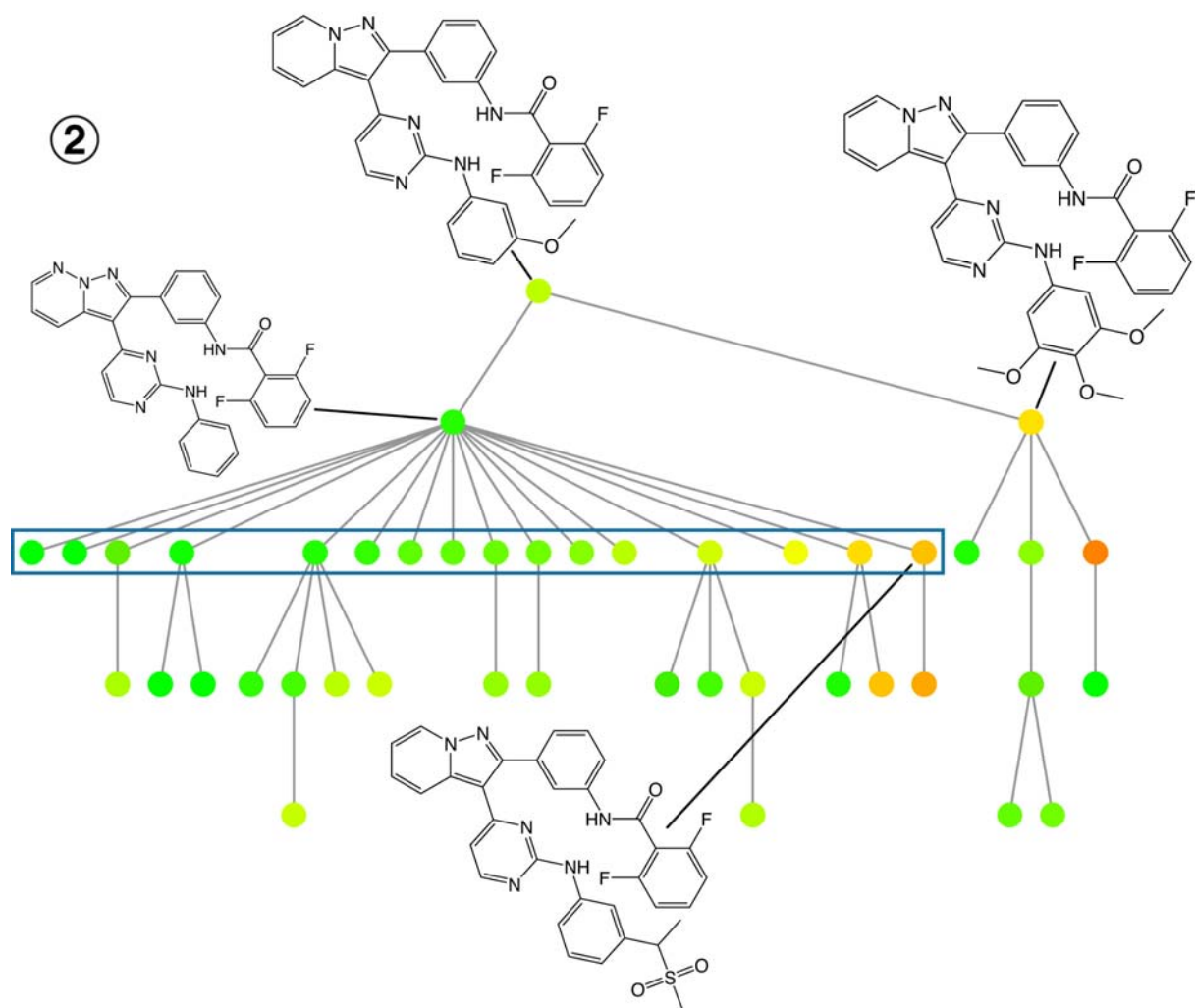


Figure S2– continued

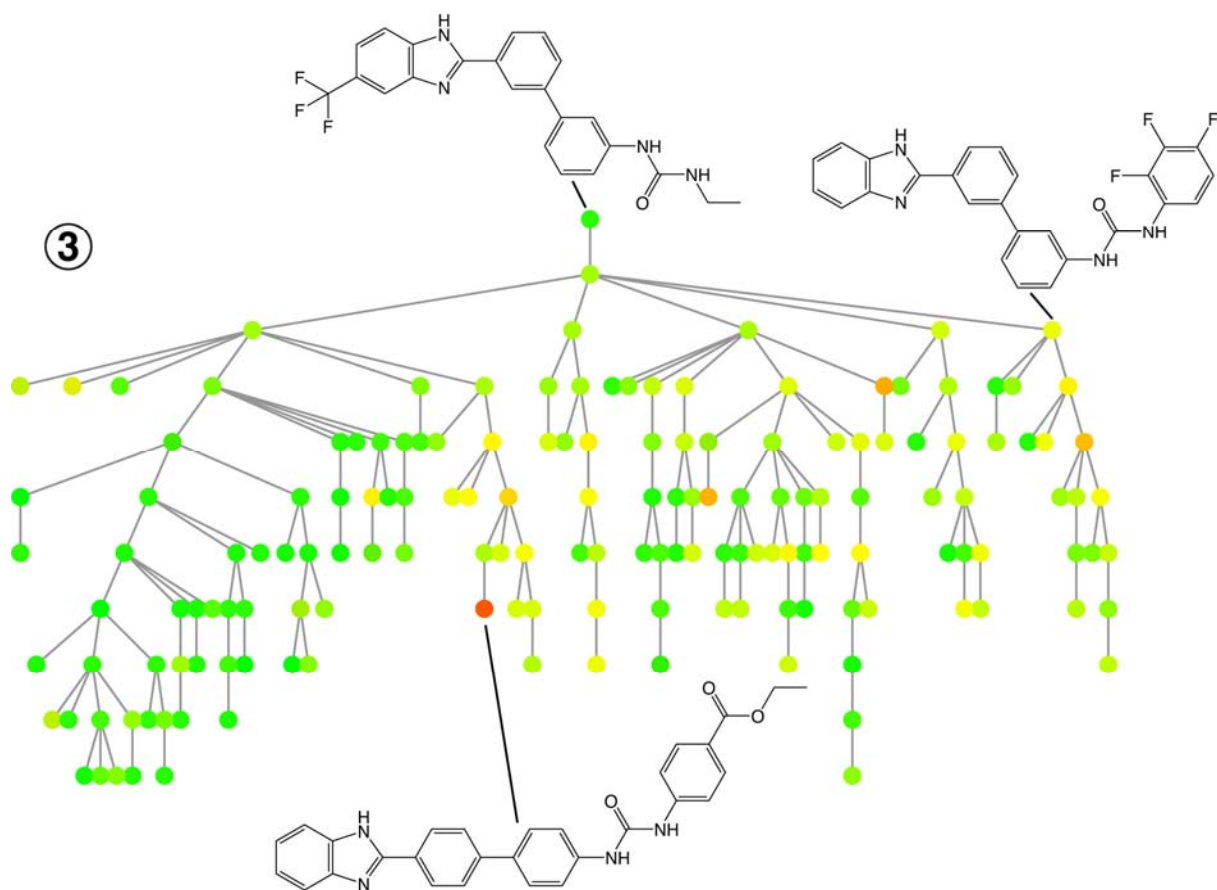




Figure S3

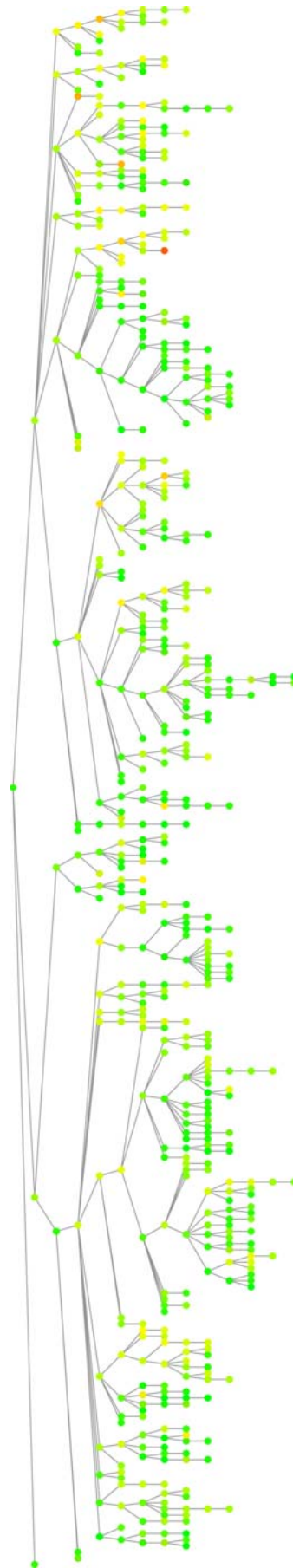


Figure S4

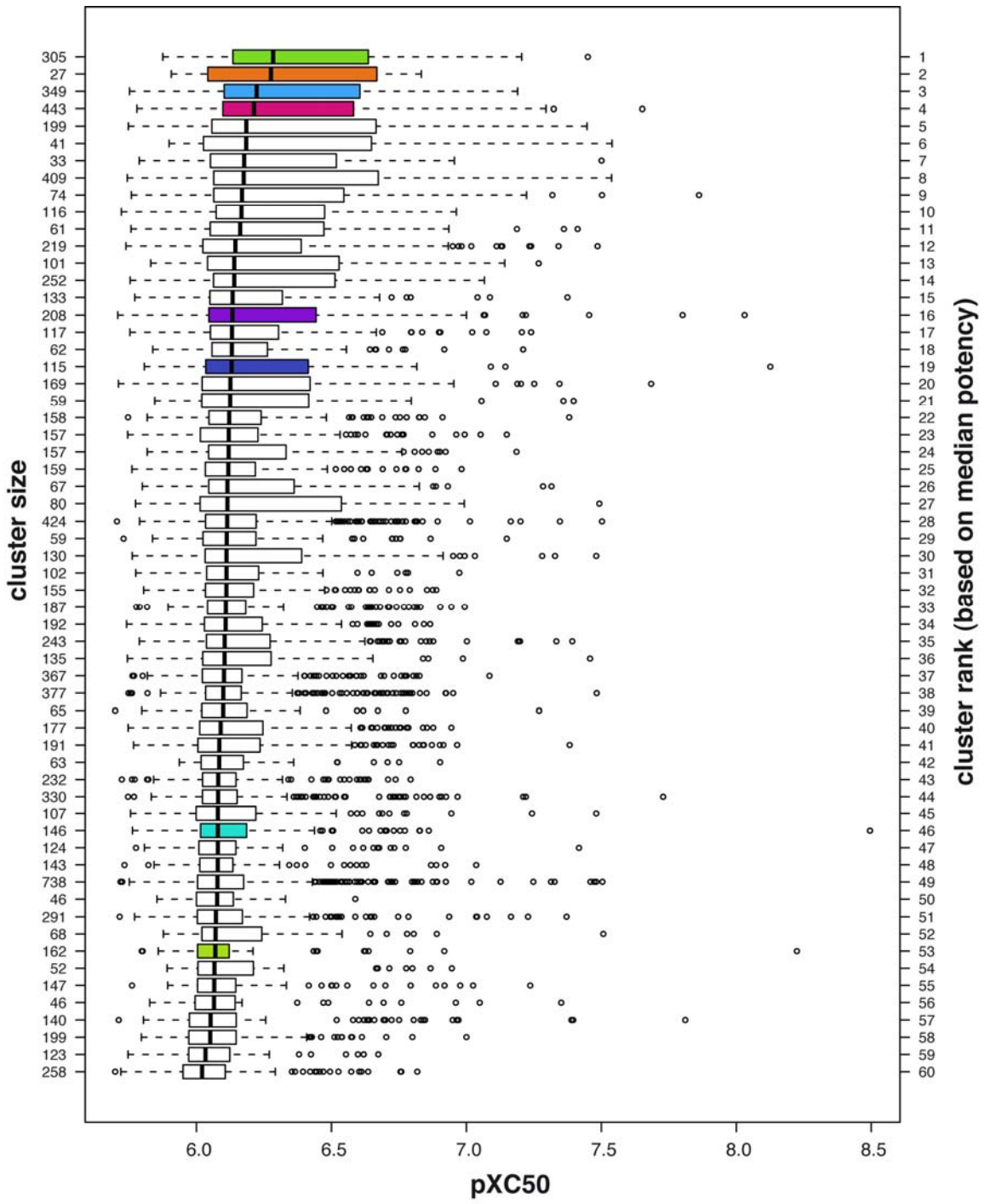
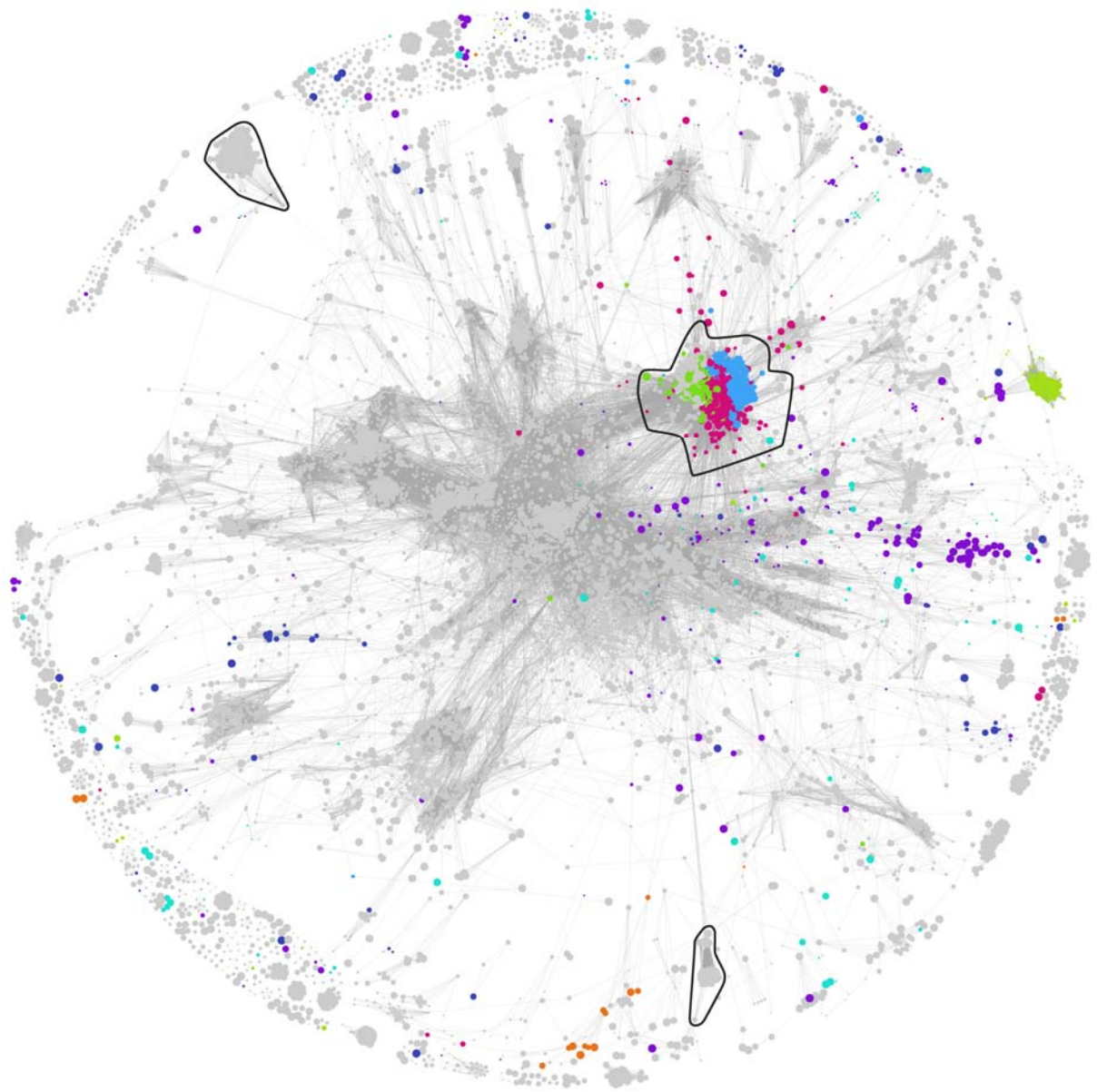


Figure S5



**Supplementary Table S1.** Compound IDs, SMILES strings, and potency values for cluster 1 (a) and 2 (b) from Figure 2a and cluster 1 (c), 2 (d) and 3 (e) from Figure 3a.

(a)

COMPOUND_ID	CANONICAL_SMILES	pXC50_3D7
286520	<chem>c1cc2c(c3c1[nH]cc3)c(nc(n2)N)N</chem>	5.9664
541129	<chem>CC(C)C(=O)n1c2ccc3c(c2cn1)c(nc(n3)N)N</chem>	5.98663
528514	<chem>COCn1ccc2c1ccc3c2c(nc(n3)N)N</chem>	6.00452
541638	<chem>CCCCCNc1c(nc2c(nc(nc2n1)N)N)c3ccccc3</chem>	6.02035
525503	<chem>c1ccc(cc1)COc2ccc(cc2)Cn3ccc4c3ccc5c4c(nc(n5)N)N</chem>	6.03033
42380	<chem>c1cc2c(c3c1CCC3)c(nc(n2)N)N</chem>	6.03259
287128	<chem>Cn1ccc2c1ccc3c2c(nc(n3)N)N</chem>	6.04485
538940	<chem>c1cc2c(ccn2CCCC3CCNC3)c4c1nc(nc4N)N</chem>	6.04695
525201	<chem>Cn1c2ccc3c(c2cc1c4cccc4)c(nc(n3)N)N</chem>	6.0518
542588	<chem>CC(C)(C)c1ccc(cc1)c2c(nc(nn2)N)N</chem>	6.06445
537098	<chem>CC(C)(C)c1ccc(cc1)Cc2ccc3c2c(nc(n3)N)N</chem>	6.07888
540873	<chem>c1ccc(cc1)Cc2ccc3c2c(nc(n3)N)N</chem>	6.08196
530471	<chem>CC(C)C(C(C)C)C(=O)n1cc2c(n1)ccc3c2c(nc(n3)N)N</chem>	6.10255
532155	<chem>c1cn(c2c1nc(nc2N)N)Cc3cc4c(cc3Cl)OCO4</chem>	6.11644
527111	<chem>c1ccc2c(c1)ccc3c2c(nc(n3)N)N</chem>	6.12529
532618	<chem>CC(C)CNc1c2c3ccn(c3ccc2nc(n1)N)CC(C)C</chem>	6.18791
529735	<chem>CC(C)C(C(C)C)C(=O)n1c2ccc3c(c2cn1)c(nc(n3)N)N</chem>	6.18829
528778	<chem>CN(C)c1ccc2c(c1Cl)c(nc(n2)N)N</chem>	6.32359
527483	<chem>c1cc(cnc1)Cn2cc3c(n2)ccc4c3c(nc(n4)N)N</chem>	6.44927
535016	<chem>CC(C)n1c2ccc3c(c2cn1)c(nc(n3)N)N</chem>	6.47789
534667	<chem>CCn1ccc2c1ccc3c2c(nc(n3)N)N</chem>	6.50506
540658	<chem>CC(C)Cn1cc2c(n1)ccc3c2c(nc(n3)N)N</chem>	6.519
541074	<chem>Cc1ccc(c(c1)Cn2ccc3c2c(nc(n3)N)N)C</chem>	6.52171
540581	<chem>c1cc2c(c3c1nn(c3)C4CCCC4)c(nc(n2)N)N</chem>	6.54287
532347	<chem>COCOCOCOCn1ccc2c1ccc3c2c(nc(n3)N)N</chem>	6.58057
528575	<chem>c1ccc(cc1)Cn2cc3c(n2)ccc4c3c(nc(n4)N)N</chem>	6.6676
528642	<chem>COCn1ccc2c1ccc3c2c(nc(n3)N)N</chem>	6.66983
537662	<chem>c1cc2c(ccn2CC3CC3)c4c1nc(nc4N)N</chem>	6.67607
528259	<chem>c1ccc(cc1)CN(Cc2cccc2)c3ccc4c(c3Cl)c(nc(n4)N)N</chem>	6.71604
539385	<chem>CCOCn1c2ccc3c(c2cc1c4cccc4)c(nc(n3)N)N</chem>	6.72947
533235	<chem>CN(C)S(=O)(=O)n1c2ccc3c(c2cn1)c(nc(n3)N)N</chem>	6.74942
542589	<chem>CCC(C)Oc1ccc2c(c1Cl)c(nc(n2)N)N</chem>	6.7525
528011	<chem>CCN(C)C(=O)n1c2ccc3c(c2cn1)c(nc(n3)N)N</chem>	6.75438
539206	<chem>CC(C)Cn1c2ccc3c(c2cn1)c(nc(n3)N)N</chem>	6.79777
530771	<chem>c1cc2c(ccn2CCCF)c3c1nc(nc3N)N</chem>	6.8259
529884	<chem>CCCCCn1ccc2c1ccc3c2c(nc(n3)N)N</chem>	6.82753
539074	<chem>c1cc2c(ccn2C3CCCC=C3)c4c1nc(nc4N)N</chem>	6.88094
528010	<chem>c1cc2c(ccn2C3CCCC3)c4c1nc(nc4N)N</chem>	6.90963
529425	<chem>c1cc2c(ccn2CCCCO)c3c1nc(nc3N)N</chem>	6.93012
526774	<chem>CC(C)(C)c1ccc(cc1)c2cc3c([nH]2)ccc4c3c(nc(n4)N)N</chem>	6.94675
538111	<chem>c1cc2c(ccn2CCCC(F)(F)F)c3c1nc(nc3N)N</chem>	7.0087
537331	<chem>c1cc2c(c3c1nn(c3)S(=O)(=O)N4CCCC4)c(nc(n2)N)N</chem>	7.0152
525834	<chem>c1ccc(cc1)Cn2cnc3c2ccc4c3c(nc(n4)N)N</chem>	7.02951
286974	<chem>Cc1cc2c(n1C)ccc3c2c(nc(n3)N)N</chem>	7.04525
528332	<chem>CC(C)c1cc2c(o1)ccc3c2c(nc(n3)N)N</chem>	7.06696
535950	<chem>CCC(CC)n1cc2c(n1)ccc3c2c(nc(n3)N)N</chem>	7.08923
536161	<chem>CCN1cc2c(n1)ccc3c2c(nc(n3)N)N</chem>	7.08965
532174	<chem>c1cc(c(c2c1nc(nc2N)N)Cl)N3CCOCC3</chem>	7.11408
524537	<chem>C=CCn1ccc2c1ccc3c2c(nc(n3)N)N</chem>	7.15499
541795	<chem>CC(C)Cn1ccc2c1ccc3c2c(nc(n3)NC(=O)C)N</chem>	7.15732
286288	<chem>CCc1cc2c(n1C(CC)CC)ccc3c2c(nc(n3)N)N</chem>	7.19591

537049	CCN(CC)S(=O)(=O)n1c2ccc3c(c2cn1)c(nc(n3)N)N	7.26076
529019	CC(CC=C)n1c2ccc3c(c2cn1)c(nc(n3)N)N	7.30066
526222	c1ccc(cc1)c2ccc(cc2)Cn3ccc4c3ccc5c4c(nc(n5)N)N	7.3159
524655	c1cc(cnc1)Cn2c3ccc4c(c3cn2)c(nc(n4)N)N	7.3174
287211	CCCc1cc2c(n1CC)ccc3c2c(nc(n3)N)N	7.32144
537510	CCCC(C)n1ccc2c1ccc3c2c(nc(n3)N)N	7.32219
539357	CN(C)S(=O)(=O)n1ccc2c1ccc3c2c(nc(n3)N)N	7.3377
286620	CC(C)c1cc2c([nH]1)ccc3c2c(nc(n3)N)N	7.40937
525411	CC(C)n1cc2c(n1)ccc3c2c(nc(n3)N)N	7.43237
528333	CC(C)Cn1ccc2c1ccc3c2c(nc(n3)N)N	7.46604
532592	CCN(CC)c1ccc2c(c1Cl)c(nc(n2)N)N	7.51005
524954	c1cc2c(cnn2S(=O)(=O)N3CCCC3)c4c1nc(nc4N)N	7.73087
288766	CCc1cc2c(n1C(C)(C)C)ccc3c2c(nc(n3)N)N	7.89615
287314	CCn1c2ccc3c(c2cc1C(C)C)c(nc(n3)N)N	7.90606
285858	CCc1cc2c(n1CC)ccc3c2c(nc(n3)N)N	7.98536
286070	COc1cc(cc(c1OC)OC)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.02946
533981	Cc1c(ccc2c1c(nc(n2)N)N)C(C)(C)C	8.059
285857	Cc1cc2c(n1C(C)C)ccc3c2c(nc(n3)N)N	8.06976
536359	c1ccnc(c1)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.08039
527334	Cc1cccc(c1)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.13378
529362	c1cc(ccc1Cn2ccc3c2ccc4c3c(nc(n4)N)N)F	8.1851
533945	CCC(C)(CC)C(=O)n1c2ccc3c(c2cn1)c(nc(n3)N)N	8.22209
541531	CCCC(CC)n1ccc2c1ccc3c2c(nc(n3)N)N	8.22792
531443	CCC(CC)n1c2ccc3c(c2cc1COC)c(nc(n3)N)N	8.25412
524705	CCC(C)(C)c1ccc2c(c1C)c(nc(n2)N)N	8.28276
524702	CCCC(CCC)n1ccc2c1ccc3c2c(nc(n3)N)N	8.30969
529823	c1cc(ccc1Cn2ccc3c2ccc4c3c(nc(n4)N)N)C#N	8.48242
524429	c1ccc2c(c1)cccc2Cn3ccc4c3ccc5c4c(nc(n5)N)N	8.49485
524869	CCC(C(C)C)n1ccc2c1ccc3c2c(nc(n3)N)N	8.49485
541564	Cc1cccc1Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.49485
524987	c1cc(ccc1Cn2ccc3c2ccc4c3c(nc(n4)N)N)Br	8.49485
528917	c1cc(ccc1Cn2ccc3c2ccc4c3c(nc(n4)N)N)Cl	8.49485
288654	CCC(C)(C)n1c(cc2c1ccc3c2c(nc(n3)N)N)C	8.49485
529873	c1cc(cc(c1F)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.49485
286710	Cc1ccc(cc1)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.49485
530049	COc1ccc(cc1)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.49485
540294	c1ccc(cc1)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.49485
530929	COc1cccc(c1)Cn2ccc3c2ccc4c3c(nc(n4)N)N	8.49485
531260	COc1ccc(cc1OC)Cn2c3ccc4c(c3cn2)c(nc(n4)N)N	8.49485
286631	CCC(CC)n1c(cc2c1ccc3c2c(nc(n3)N)N)C	8.49485
286526	CC(C)n1c2ccc3c(c2cc1C(C)C)c(nc(n3)N)N	8.49485
534641	c1cc2c(cc1Cn3ccc4c3ccc5c4c(nc(n5)N)N)OCO2	8.49485
535738	c1cc2c(ccn2Cc3cc4c(cc3Cl)OCO4)c5c1nc(nc5N)N	8.49485
286068	CCCc1cc2c(n1C(CC)CC)ccc3c2c(nc(n3)N)N	8.49485
285940	CCc1cc2c(n1C(C)CC)ccc3c2c(nc(n3)N)N	8.49485

(b)

COMPOUND_ID	CANONICAL_SMILES	pXC50_3D7
541505	<chem>Cc1ccc(cc1)S(=O)(=O)NC2=NC(=N)N(C(N2)(C)C)OCc3ccc(c(c3)Cl)Cl</chem>	5.94494
528127	<chem>c1ccc(cc1)Cc2ccc(cc2)OCCON3C(=N)N=C(NC34CCCCC4)N</chem>	5.94881
542722	<chem>COc1ccc(cc1OC)C2N=C(N=C(N2c3ccc(cc3)Cl)N)N</chem>	5.99961
524629	<chem>CN(C)c1ccc(cc1)N2C(=NC(=NC23CCCC3)N)N</chem>	6.02924
528799	<chem>CC1(N=C(N=C(N1OCCCOc2cc(c(cc2Cl)Cl)Cl)N)NC(=O)NC)C</chem>	6.02927
531153	<chem>CCCC1N=C(N=C(N1c2cccc2)N)N</chem>	6.08485
536935	<chem>CCC1(N=C(N=C(N1c2cccc2)N)N)C</chem>	6.10138
526121	<chem>CCCC1N=C(N=C(N1c2cccc(c2)N(=O)=O)N)N</chem>	6.11908
534155	<chem>Cc1cccc(c1C)N2C(=NC(=NC2(C)C)N)N</chem>	6.11982
531914	<chem>CC1(NC(=NC(=N)N1OCc2ccc3cccc3c2CON4C(=N)N=C(NC4(C)C)N)N)C</chem>	6.17833
528772	<chem>c1ccc(cc1)C=CC2N=C(N=C(N2OCCCCCON3C(N=C(N=C3N)N)C=Cc4cccc4)N)N</chem>	6.21124
532523	<chem>CC1(N=C(N=C(N1OCc2ccc(c(c2)Cl)Cl)NC(=O)NC)NC(=O)NC)C</chem>	6.22142
530768	<chem>CCCC1N=C(N=C(N1c2cccc(c2)C(F)(F)F)N)N</chem>	6.22594
536333	<chem>CCCCCCCOc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N</chem>	6.29911
536917	<chem>CCCOc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N</chem>	6.31205
532909	<chem>c1cc(ccc1N2C(=NC(=NC23CCCC3)N)N)Cl</chem>	6.38345
534963	<chem>CCCCCOc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N</chem>	6.46287
538554	<chem>CC1(N=C(N=C(N1c2ccc(cc2)Oc3cccc3)N)N)C</chem>	6.46778
534651	<chem>CC1(N=C(N=C(N1c2cccc2)N)N)C</chem>	6.4852
524411	<chem>CC1(N=C(N=C(N1c2ccc(c(c2)OC)OC)N)N)C</chem>	6.50728
542097	<chem>c1ccc(cc1)C2N=C(N=C(N2c3cccc3)N)N</chem>	6.53178
541825	<chem>CCOC(=O)NC1=NC(N(C(=N1)NC(=O)OCC)OCc2ccc(c(c2)Cl)Cl)(C)C</chem>	6.55556
529733	<chem>CC1(NC(=NC(=N)N1OCc2nc(nc(n2)Nc3cccc3)N)N)C</chem>	6.56294
524889	<chem>CCOc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N</chem>	6.58655
530434	<chem>CC1CCC2(CC1)N=C(N=C(N2OCc3cc4cccc4c5c3cccc5)N)N</chem>	6.61493
542654	<chem>CCCC1N=C(N=C(N1c2ccc(cc2)OC)N)N</chem>	6.63037
541538	<chem>CC1(N=C(N=C(N1c2ccc(cc2)N(=O)=O)N)N)C</chem>	6.63052
542586	<chem>CC1(NC(=NC(=N)N)NOCc2ccc(c(c2)Cl)Cl)C</chem>	6.64174
535665	<chem>CC1(NC(=NC(=N)N1OCCO)N)C</chem>	6.65584
529924	<chem>CC1CCC2(CC1)N=C(N=C(N2OCc3ccc(c4c3cccc4)Br)N)N</chem>	6.66602
524640	<chem>CCCCOc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N</chem>	6.66824
535018	<chem>CCCCCOc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N</chem>	6.68877
524477	<chem>c1cc(c(cc1CON2CNC(=NC2=N)N)Cl)Cl</chem>	6.71183
538465	<chem>CC1(N=C(N=C(N1O)N)N)C</chem>	6.71562
537305	<chem>C=CCc1cc(ccc1OCCCOc2c(nc(nc2N)N)N)Br</chem>	6.71614
526873	<chem>CC1(N=C(N=C(N1c2cc(c(cc2Cl)Cl)Cl)N)N)C</chem>	6.74172
537797	<chem>CCOC(=O)NC1=NC(N(C(=N1)NC(=O)OCC)OCc2cccc3c2ccc4c3cccc4)(C)C</chem>	6.76338
531957	<chem>CC1(NC(=NC(=N)N1OCCNCc2ccc(cc2)Cl)N)C</chem>	6.79588
539955	<chem>CCC1(N=C(N=C(N1c2ccc(cc2)Cl)N)N)C</chem>	6.79729
537628	<chem>C1CCC(CC1)CON2C(=N)N=C(NC23CCCC3)N</chem>	6.81061
528062	<chem>CC1CCC2(CC1)NC(=NC(=N)N2OCCCCCCCCO)N</chem>	6.83241
527586	<chem>c1ccc(cc1)CC2N=C(N=C(N2c3ccc(cc3)Cl)N)N</chem>	6.86299
530232	<chem>COc1ccc(cc1OC)C2N=C(N=C(N2OCc3cccc3)N)N</chem>	6.87679
528819	<chem>CCCCC1ccc(cc1)N2C(=NC(=NC2(C)C)N)N</chem>	6.88122
541363	<chem>CC1(N=C(N=C(N1OCc2cc3cccc3cc2CON4C(=NC(=NC4(C)C)N)N)N)C</chem>	6.89907
526273	<chem>CCOC(=O)NC1=NC(N(C(=N1)NC(=O)OCC)OCCCOc2ccc(cc2C)C)(C)C</chem>	6.901
536483	<chem>CC1(N=C(N=C(N1c2cccc(c2)I)N)N)C</chem>	6.90132
535386	<chem>CC1(N=C(N=C(N1c2ccc(cc2)OC)N)N)C</chem>	6.94634
526831	<chem>CCCC1N=C(N=C(N1c2ccc(cc2)C)N)N</chem>	7.02152
526798	<chem>CC1(N=C(N=C(N1c2ccc(c(c2)Cl)Oc3ccc(cc3)Cl)N)N)C</chem>	7.10294
531976	<chem>c1ccc(cc1)CCC2N=C(N=C(N2c3cccc3)N)N</chem>	7.1131
524860	<chem>CCCC1N=C(N=C(N1c2ccc(c(c2)C)C)N)N</chem>	7.13328
532784	<chem>CCCC1N=C(N=C(N1c2ccc(cc2)CC)N)N</chem>	7.17441
527826	<chem>CC1(N=C(N=C(N1OCCCON2C(=NC(=NC2(C)C)N)N)N)C</chem>	7.18073
529009	<chem>CC1(N=C(N=C(N1c2ccc(cc2)OCC#C)N)N)C</chem>	7.18204
526509	<chem>CC1(N=C(N=C(N1OCc2cccc3c2cccc3)N)NC(=O)Nc4ccc(cc4)N(=O)=O)C</chem>	7.22528
525681	<chem>CCC1(NC(=NC(=N)N1OCc2ccc(c(c2)Cl)Cl)N)CC</chem>	7.23255
535903	<chem>Cc1ccc(cc1)N2C(N=C(N=C2N)N)c3cccc3</chem>	7.24711

526851	CC1(N=C(N=C(N1c2ccc3ccccc3c2)N)N)C	7.26898
531021	CC1(NC(=NC(=N)N1OCCSCCON2C(=N)N=C(NC2(C)C)N)N)C	7.29597
525537	CC1(N=C(N=C(N1OCCc2cc(c(c2)OC)OC)OC)N)N)C	7.30749
526153	CC1(N=C(N=C(N1CCc2ccccc2)N)N)C	7.32462
524585	CCCC1N=C(N=C(N1c2ccc(cc2)Cl)N)N	7.33093
542656	CC1(NC(=NC(=N)N1OCc2c3ccccc3cc(c2OC)OC)N)C	7.33318
541420	CC1(N=C(N=C(N1c2ccc(cc2)I)N)N)C	7.35315
540626	CC1(NC(=NC(=N)N1OCCOc2ccc(cc2)C)C3ccccc3)N)C	7.35629
527643	c1ccc(cc1)CON2C(N=C(N=C2N)N)c3ccccc3	7.36532
531961	Cc1cc(cc(c1)N2C(=NC(=NC2(C)C)N)N)C	7.37715
538080	CCOC(=O)NC1=NC(=N)N(C(N1)(C)C)OCc2ccc(c(c2)Cl)Cl	7.39077
539298	CC1(N=C(N=C(N1OCCCOc2ccccc2)C(=O)O)N)N)C	7.3986
532043	CC1(NC(=NC(=N)N1OCCc2cc(c(c2)OC)OC)OC)N)C	7.40746
524865	c1ccc(cc1)CCC2N=C(N=C(N2c3ccc(cc3)Cl)N)N	7.42035
538575	CC1(N=C(N=C(N1c2ccccc2)Cl)N)N)C	7.42177
537162	CC1(N=C(N=C(N1OCc2cc(c(cc2Cl)CON3C(=NC(=NC3(C)C)N)N)Cl)N)N)C	7.42238
539784	Cc1ccc(cc1)N2C(=N)N=C(NC2(C)C)N	7.43668
529312	CCCc1cc(ccc1OCCCON2C(=NC(=NC2(C)C)NC(=O)OCC)NC(=O)OCC)C	7.4454
524688	CC1(N=C(N=C(N1OCC2COc3ccccc3O2)N)N)C	7.45613
542056	CC(=O)Nc1ccc(cc1)S(=O)(=O)NC2=NC(=N)N(C(N2)(C)C)OCc3ccc(c(c3)Cl)Cl	7.46963
541047	CCC(c1ccccc1)ON2C(=NC(=NC2(C)C)N)N	7.47493
537720	CC1N=C(N=C(N1OCc2ccccc2)N)N	7.48312
541502	CCOC(=O)NC1=NC(N(C(=N1)NC(=O)OCC)OCCCOc2cc(c(cc2Cl)Cl)Cl)(C)C	7.50627
535368	CC1(NC(=NC(=N)N1OCc2c3ccccc3ccc2OC)N)C	7.54037
530808	CCCc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N	7.54748
529494	CC=C CON1C(=N)N=C(NC1(C)C)N	7.55406
534193	CC1(N=C(N=C(N1c2ccc(cc2)C(C)(C)C)N)N)C	7.57352
527400	CC(C)C(=O)ONC1=NC(N(C(=N1)NOC(=O)C(C)C)OCCCOc2cc(c(cc2Cl)Cl)Cl)(C)C	7.57475
533818	CC1(NC(=NC(=N)N1OCCCN(C(=O)c2ccc(cc2)C(=O)NCCCON3C(=N)N=C(NC3(C)C)N)N)C	7.66548
537543	Cc1cc(ccc1Cl)N2C(=NC(=NC2(C)C)N)N	7.68008
537173	CCC(C)c1cccc(c1OCCCON2C(=NC(=NC2(C)C)N)N)C(C)CC	7.6991
532360	CC1(NC(=NC(=N)N1OCCN(C)c2ccccc2)N)C	7.71168
529801	c1ccc(cc1)C2N=C(N=C(N2c3ccc(c(c3)Cl)Cl)N)N	7.83565
541189	CC1(NC(=NC(=N)N1OCc2cc(c(cc2CON3C(=N)N=C(NC3(C)C)N)Cl)Cl)N)C	7.83689
536378	CCC(C)(C)c1ccc(cc1)N2C(=NC(=NC2(C)C)N)N	7.93
525631	CC1(N=C(N=C(N1c2cc(c(c2)Cl)Cl)Cl)N)N)C	7.94413
539767	CC(c1ccccc1)ON2C(=NC(=NC2(C)C)N)N	7.96282
538164	Cc1cc2ccccc2c(c1C)CON3C(=N)N=C(NC3(C)C)N	8.02247
541124	CC1(N=C(N=C(N1c2ccc(cc2)Br)N)N)C	8.03639
543059	CCc1ccc(cc1)N2C(=NC(=NC2(C)C)N)N	8.05434
530518	CC1(N=C(N=C(N1c2ccccc2)C(F)(F)F)N)N)C	8.06454
525486	CC(=O)NC1=NC(=NC(=O)C)N(C(N1)(C)C)OCCCOc2ccc(c(c2)Cl)Cl	8.07943
524645	CC1(N=C(N=C(N1OCc2ccccc2)C#N)N)N)C	8.1007
536182	CC1(N=C(N=C(N1OCc2ccc3ccccc3c2)N)NC(=O)c4ccc(cc4)N(=O)=O)C	8.12078
530224	CC1(NC(=NC(=N)N1OCCCOc2c(cccc2OC)OC)N)C	8.13806
530120	CC1(NC(=NC(=N)N1OCCCOc2ccc(cc2)N)N)C	8.15268
525105	CC1(N=C(N=C(N1OCc2ccccc3c2ccccc3)N)NC(=O)c4cc(cc(c4)N(=O)=O)N(=O)=O)C	8.16513
539291	Cc1ccc(cc1Cl)N2C(=NC(=NC2(C)C)N)N	8.1665
528184	CC1(N=C(N=C(N1c2ccc(c(c2)Cl)C(C)(C)C)N)N)C	8.1832
531569	CCCC(C)c1ccc(cc1)N2C(=NC(=NC2(C)C)N)N	8.20304
524583	CC1(NC(=NC(=N)N1OCc2ccc(c(c2)OC)OC)N)C	8.21773
538230	CC1(NC(=NC(=N)N1OCCc2ccc(c(c2)OC)OC)N)C	8.22819
524837	CC1(NC(=NC(=N)N1OCOc2ccc(cc2)Cl)N)C	8.3376
533539	CCCc1cc(ccc1OCCCON2C(=N)N=C(NC2(C)C)N)C(=O)C	8.33985
531304	CC1(N=C(N=C(N1OCC=Cc2ccccc2)N)N)C	8.37302
537904	CCOc1ccccc1CON2C(=NC(=NC2(C)C)N)N	8.43014
530222	CC1(N=C(N=C(N1OCc2ccc3c(c2)OCO3)N)N)C	8.43381
531500	Cc1cc(c(cc1C)CON2C(=N)N=C(NC2(C)C)N)C	8.43965
525815	CCC1N=C(N=C(N1OCc2ccc(c(c2)Cl)Cl)N)N	8.47502
538818	CC1(NC(=NC(=N)N1OCCCOc2cc(ccc2Cl)Cl)N)C	8.49485
538842	CC1(NC(=NC(=N)N1OCCc2ccc(cc2)N)N)C	8.49485

538977	CC1(NC(=NC(=N)N1OCCOc2cccc(c2)C(F)(F)N)N)C	8.49485
538794	CC1(NC(=NC(=N)N1OCCc2cccc3c2cccc3)N)C	8.49485
538720	CC1(NC(=NC(=N)N1OCCCOc2cc(cc(c2)Cl)Cl)N)C	8.49485
524927	CC(C)Oc1ccc(cc1)CCCON2C(=N)N=C(NC2(C)C)N	8.49485
538034	CCOC(=O)NC1=NC(=N)N(C(N1)(C)C)OCCCOc2cc(c(cc2Cl)Cl)Cl	8.49485
537851	CCCc1cccc(c1OCCCON2C(=N)N=C(NC2(C)C)N)C	8.49485
525208	CC(=O)NCC(=O)NC1=NC(=N)N(C(N1)(C)C)OCc2ccc3ccccc3c2	8.49485
537608	Cc1ccc(cc1C)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
525549	CC(CON1C(=NC(=NC1(C)C)N)N)c2ccc(cc2Cl)Cl	8.49485
531829	CC(CCON1C(=NC(=NC1(C)C)N)N)c2ccc(cc2)Cl	8.49485
524467	CC1(NC(=NC(=N)N1OCCCOc2cccc3c2cccc3)N)C	8.49485
542633	CCCOC(=O)c1ccc(cc1)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
542614	CC1(NC(=NC(=N)N1OCCCCCOc2ccc(c3c2cccc3)Cl)N)C	8.49485
542529	CC(COc1ccc(cc1)c2cccc2)CON3C(=NC(=NC3(C)C)N)N	8.49485
524695	CC1(N=C(N=C(N1OCCc2cccc2)N)N)C	8.49485
542036	CC1(NC(=NC(=N)N1OCCc2c(cccc2Cl)Cl)N)C	8.49485
524739	CC1(NC(=NC(=N)N1OCCc2ccc(cc2Cl)Cl)N)C	8.49485
541801	CC1(NC(=NC(=N)N1OCCCOc2ccc(cc2)OC)N)C	8.49485
541715	CCSc1cccc1CON2C(=N)N=C(NC2(C)C)N	8.49485
524772	CC1(NC(=NC(=N)N1OCCc2ccc(cc2)OC)N)C	8.49485
524800	CC1(NC(=NC(=N)N1OCCc2cccc2)N)C	8.49485
524801	CC1(NC(=NC(=N)N1OCC2CCCC2)N)C	8.49485
541413	CC1(NC(=NC(=N)N1OCCCCCOc2cc(c(c(c2)OC)OC)OC)N)C	8.49485
524822	CCc1ccc(cc1)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
541127	CC1(NC(=NC(=N)N1OCc2cccs2)N)C	8.49485
541061	CC(Cc1ccc(cc1Cl)Cl)CON2C(=NC(=NC2(C)C)N)N	8.49485
540842	c1c(c(cc(c1Cl)Cl)Cl)OCCCON2C(=N)N=C(NC23CCCC3)N	8.49485
540656	CC1(NC(=NC(=N)N1OCc2ccc(cc2)c3cccc3)N)C	8.49485
540612	CC(Cc1ccc(cc1)OC)CON2C(=NC(=NC2(C)C)N)N	8.49485
529779	CCCc1cc(ccc1OCCCON2C(=NC(=NC2(C)C)N)N)C	8.49485
539353	CC1(NC(=NC(=N)N1OCCSc2cc(sc2Cl)Cl)N)C	8.49485
539345	CC(CCON1C(=NC(=NC1(C)C)N)N)c2ccc(c(c2)Cl)Cl	8.49485
524856	CC1(NC(=NC(=N)N1OCCCOc2cccc2)N)C	8.49485
539136	CC1(NC(=NC(=N)N1OCCCOc2c(cccc2OC)CC=C)N)C	8.49485
539037	CCC1N=C(N=C(N1OCCCOc2c(cc(cc2Cl)Cl)Cl)N)N	8.49485
539033	CCOC(=O)c1cc(cc(c1OCCCON2C(=N)N=C(NC2(C)C)N)Cl)Cl	8.49485
539017	Cc1ccc2cccc2c1CCCON3C(=N)N=C(NC3(C)C)N	8.49485
532591	CC(C)c1ccc(cc1)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
527478	CCOc1ccc(cc1)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
532397	Cc1cc(c(c(c1C)OCCCON2C(=N)N=C(NC2(C)C)N)C)C	8.49485
532320	CCSc1ccc(cc1)CON2C(=NC(=NC2(C)C)N)N)C	8.49485
527707	CC1(NC(=NC(=N)N1OCOc2cc(c(cc2Cl)Cl)Cl)N)C	8.49485
527717	CC1(NC(=NC(=N)N1OCCCOc2cccc(c2)Cl)N)C	8.49485
527991	CC1(N=C(N=C(N1OCCCOc2ccc(cc2CC=C)Br)N)N)C	8.49485
528221	CC1(NC(=NC(=N)N1OCCOc2ccc3ccccc3c2)N)C	8.49485
531858	CC1(N=C(N=C(N1OCc2cccc3c2ccc4c3cccc4)N)N)C	8.49485
531837	CC1(N=C(N=C(N1OCc2ccc3ccccc3c2)N)N)C	8.49485
531799	Cc1cccc(c1C)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
531467	CC(C)C(=O)ONC1=NC(=N)N(C(N1)(C)C)OCCCOc2cc(c(cc2Cl)Cl)Cl	8.49485
531305	CCCc1cc(ccc1OCCCON2C(=N)N=C(NC2(C)C)N)OCCCOc3ccccc3	8.49485
531220	CCCc1cccc(c1OCCCON2C(=NC(=NC2(C)C)N)N)OC	8.49485
528250	CC1(N=C(N=C(N1OCCCOc2ccc(cc2)C(C)(C)C)N)N)C	8.49485
528252	Cc1cccc2c1cccc2CON3C(=NC(=NC3(C)C)N)N	8.49485
530893	Cc1ccc(cc1)CON2C(=N)N=C(NC2(C)C)N)C(C)C	8.49485
530819	CC1(NC(=NC(=N)N1OCCSc2cccc2)N)C	8.49485
528415	CC1(NC(=NC(=N)N1OCCCOc2ccc(cc2C(C)(C)C)C(C)(C)C)N)C	8.49485
528462	CC1N=C(N=C(N1OCc2cccc3c2cccc3)N)N	8.49485
530272	CC(C)Sc1ccc(cc1)CON2C(=N)N=C(NC2(C)C)N)Cl	8.49485
528526	CCOC(=O)c1cc(ccc1OCCCON2C(=N)N=C(NC2(C)C)N)Cl	8.49485
528590	CC1(NC(=NC(=N)N1OCc2cccc(c2Cl)Cl)N)C	8.49485
524852	Cc1cccc(c1OCCCON2C(=N)N=C(NC2(C)C)N)CC=C	8.49485



529742	CCCOc1ccc(cc1)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
528783	CC1(NC(=NC(=N)N1OCCc2cc(c(cc2Cl)Cl)Cl)N)C	8.49485
529477	CC1(N=C(N=C(N1c2ccc(c(c2)Cl)OCc3cccc(c3)C(=O)N(C)C)N)N)C	8.49485
529342	CC1(NC(=NC(=N)N1OCCCCCOc2ccccc2)N)C	8.49485
529307	CC1(NC(=NC(=N)N1OCCc2ccccc2OC)N)C	8.49485
529158	CCc1cccc1OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
537294	CC1(N=C(N=C(N1OCCCOc2cc(c(cc2Cl)Cl)N)N)C	8.49485
537164	c1ccc2c(c1)cccc2OCCCON3C(=N)N=C(NC34CCCC4)N	8.49485
537085	CC1(NC(=NC(=N)N1OCCCOc2ccc(cc2)N(=O)=O)N)C	8.49485
537078	CC1(NC(=NC(=N)N1OCc2cc(cc3c2OCOC3)Cl)N)C	8.49485
525601	Cc1ccc(cc1C)CON2C(=N)N=C(NC2(C)C)N	8.49485
536896	CCC1N=C(N=C(N1OCc2cccc3c2cccc3)N)N	8.49485
525634	CC1(NC(=NC(=N)N1OCCSc2ccccc2)N)C	8.49485
536381	Cc1ccc(c(c1)CC=C)OCCCON2C(=NC(=NC2(C)C)N)N	8.49485
525772	CC(=O)NC1=NC(N(C(=N1)NC(=O)C)OCc2ccc(c(c2)Cl)Cl)(C)C	8.49485
535970	CCC(c1ccc(cc1)Cl)ON2C(=NC(=NC2(C)C)N)N	8.49485
526115	CC1(NC(=NC(=N)N1OCCCCOc2ccccc2)N)C	8.49485
535647	CCC(CCON1C(=NC(=NC1(C)C)N)N)c2ccc(c(c2)Cl)Cl	8.49485
535464	CC1(NC(=NC(=N)N1OCCCOc2ccccc2Cl)N)C	8.49485
526119	CC1(NC(=NC(=N)N1OCCCCOc2ccc(cc2)OC)N)C	8.49485
535191	Cc1ccc(cc1C)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
526563	CC1(NC(=NC(=N)N1OCCCN(C(=O)c2ccc(cc2)N(=O)=O)N)C	8.49485
534978	CC1(N=C(N=C(N1c2ccc(c(c2)Cl)Cl)N)N)C	8.49485
526736	CC1(NC(=NC(=N)N1OCCCOc2ccccc2C(C)(C)C)N)C	8.49485
534838	Cc1cccc1OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
534669	CCC(C)Oc1ccc(cc1)CCCON2C(=NC(=NC2(C)C)N)N	8.49485
526941	CC1(N=C(N=C(N1OCCc2ccc3ccccc3c2)N)N)C	8.49485
534569	CCC(CCON1C(=NC(=NC1(C)C)N)N)c2ccc(cc2)Cl	8.49485
534373	CC1(NC(=NC(=N)N1OCCCCOc2ccc(cc2C3CCCC3)Cl)N)C	8.49485
534022	CC1(NC(=NC(=N)N1OCCc2ccccc2)C(F)(F)F)N)C	8.49485
533641	CCCOc1ccc(cc1)CCCON2C(=NC(=NC2(C)C)N)N	8.49485
533500	CCc1cccc(c1)OCCCON2C(=N)N=C(NC2(C)C)N	8.49485
533210	CCOc1ccc(cc1)CCCON2C(=N)N=C(NC2(C)C)N	8.49485
533001	CC1(NC(=NC(=N)N1OCCSc2ccc(c(c2)Cl)Cl)N)C	8.49485
527100	Cc1cc(c(c(c1)Br)OCCCON2C(=N)N=C(NC2(C)C)N)Br	8.49485
526948	Cc1ccc(c(c1)Cl)CON2C(=NC(=NC2(C)C)N)N	8.49485
533127	CC1(NC(=NC(=N)N1OCCCOc2c(cc(cc2Cl)Cl)Cl)N)C	8.53116

(c)

COMPOUND_ID	CANONICAL_SMILES	pXC50_3D7
533731	CCC1(CC1)NCC(C(Cc2ccccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)NCC)O	5.79437
524959	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCc4ccc5c(c4)OCCO5)O	5.86815
542708	CS(=O)(=O)N(c1ccc(cc1)F)c2cc(cc(c2)N3CCCC3=O)C(=O)NC(Cc4ccccc4)C(CNCc5cccc(c5)C(F)(F)F)O	5.87076
527834	COc1cc(cc(c1)OC)CNCC(C(Cc2ccccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)C5CCCC5)O	5.90494
527856	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNCc4cc(ccc4OC)C#N)O	5.91162
529378	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNC4(CCC4)Cc5cccc(c5)Cl)O	5.92907
535228	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCCc4cc(cc(c4)OC)OC)O	5.94299
541547	CCNc1cc(c(c(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3ccccc3)C(CNC(C)CC(C)C)O	5.95261
530426	CCCC1(CC1)NCC(C(Cc2ccccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)NCC)O	5.96587
535238	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNC4(CC4)CCC(C)C)O	5.96796
542640	CN(C)c1cc(cc2c1cc[nH]2)C(=O)NC(Cc3ccccc3)C(CNC4CCCC4)O	5.96927
422028	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNC4CCc5c4cccc5)O	5.98985
543109	c1ccc(cc1)CC(C(CNCCC(F)(F)F)O)NC(=O)c2ccccc2)CCC3CC3	5.98999
541528	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNC4(CC4)CC(C)C)O	5.99234
541358	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNC4CCCC4)O	5.9957
542559	CCNc1cc(c(c(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3ccccc3)C(CNC(C)(C)CC(C)(C)C)O	5.99647
534441	CCc1c[nH]c2c1cc(cc2N(c3ccccc3)S(=O)(=O)C)C(=O)NC(Cc4ccccc4)C(CNCc5cccc(c5)C(F)(F)F)O	6.00133
533669	CCCCCNCC(C(Cc1ccccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)NCC)O	6.00218
528671	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNCCc4cccc5c4cccc5)O	6.00805
526318	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4ccccc4)C(CNCCOC)O	6.02039
535050	CC(C)c1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNCc4cccc(c4)OC)O	6.02111
526187	CCCc1cc(c(c(c1)N2CCCC2=O)F)C(=O)NC(Cc3ccccc3)C(CNC(C)C)O	6.02566
529743	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCCc4cccc4)O	6.0285
534738	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3Cl)C(CNC(C)CCCC(C)C)O	6.03229
533461	CS(=O)(=O)N(c1cccc(c1)F)c2cc(cc(c2)N3CCCC3=O)C(=O)NC(Cc4ccccc4)C(CNCc5cccc(c5)C(F)(F)F)O	6.04096
527715	CCc1c[nH]c2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4ccccc4)C(CNCc5cccc(c5)OC)O	6.04122
527505	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNC(C)(C)Cc4cccc(c4)Cl)O	6.0523
542491	CCOCc1cccc(c1)C(=O)NC(Cc2ccccc2)C(CNCc3ccccc3OC)O	6.054
527135	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNCCc4cccc(c4)C(F)(F)F)O	6.05606
542314	CCc1cn(c2c1cc(cc2)C(=O)NC(Cc3ccccc3)C(CNC(C)(C)CCCC(C)C)O)CCS(=O)(=O)C	6.05709
530061	CCCN(CCC)C(=O)c1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCc4cccc(c4)C(F)(F)F)O	6.05769
539500	COc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNCc4cc(cc(c4)OC)OC)O	6.06933
539931	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNCCc4cccc4)O	6.07384
539002	CC(C)CCCC(C)(C)NCC(C(Cc1ccccc1)NC(=O)c2ccccc2)OCC3CC3)O	6.07394
532608	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNC(C)(C)CCCC(C)C)O	6.08275
536602	CCc1c[nH]c2c1cc(cc2N(c3ccccc3)S(=O)(=O)C)C(=O)NC(Cc4ccccc4)C(CNC(C)(C)CCCC(C)C)O	6.08464
537682	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNC(C)(C)(C)C)O	6.08612
542988	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4ccccc4)C(CNCC)O	6.09152
528485	c1cc(cc(c1)C(F)(F)F)CNCC(C(Cc2cc(cc(c2)F)F)NC(=O)c3cc(cc(c3)N4CCCC4=O)C5CCCC5)O	6.09535
539161	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3Cl)C(CNC4CCCC4)O	6.09553
534376	CC(C)Oc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCc4cc(cc(c4)OC)OC)O	6.09807
533866	CCNc1cc(c(c(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3ccccc3)C(CNCCC(C)(C)C)O	6.09833
532175	CC(C)CCCC(C)(C)NCC(C(Cc1ccccc1)NC(=O)c2ccccc2)CCC3CC3)O	6.09888
532537	CC(C)Nc1cc(cc(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3ccccc3)C(CNCc4cccc(c4)C(F)(F)F)O	6.09999
540719	CC(C)Nc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCc4cccc(c4)OC)O	6.10572
541569	CCc1cn(c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4ccccc4)C(CNCc5cccc(c5)OC)O)C	6.10587
537200	CCc1c[nH]c2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4ccccc4)C(CNC5CCCCC5)O	6.11138
535448	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNC(C)c4cccc(c4)OC)O	6.11385
536796	CCCNCC(C(Cc1ccccc1)NC(=O)c2cc(cc(c2)N3CCCC3=O)NCC)O	6.11931
534557	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccc(c(c3)F)F)C(CNCc4cccc(c4)OC)O	6.12559
528254	COc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCc4cc(cc(c4)OC)OC)O	6.12611
529692	CCOCc1cccc(c1)C(=O)NC(Cc2ccccc2)C(CNCc3cccc(c3)OC)O	6.13039
532671	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3ccccc3)C(CNCc4cc(cc(c4)OC)OC)O	6.13341
531691	CC(C)Oc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCc4cccc(c4)OC)O	6.13657
538957	COc1cccc(c1)C2(CCCCC2)NCC(C(Cc3ccccc3)NC(=O)c4cccc4)O	6.137
531121	COc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccccc3)C(CNCc4cccc(c4)OC)O	6.14188
532093	CCCC1(CCC1)NCC(C(Cc2ccccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)NCC)O	6.14256
527301	CCn1cnc2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4ccccc4)C(CNC5COCOC5)O	6.14764

538294	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)Cc4cccc(c4)OC)O	6.15064
537723	COc1cc(cc(c1)OC)CNCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)C5CCCC5)O	6.15242
527096	CCNc1cc(c(c1)N2CCCCS2(=O)=O)OC)C(=O)NC(Cc3cccc3)C(CNCc4cccc(c4)OC)O	6.16157
533574	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4(CCC4)C(C)C)O	6.16447
532322	CCCCC(C)(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCC3=O)NCC)O	6.17118
530511	CCc1c[nH]c2c1cc(cc2N3CCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)CCCC(C)C)O	6.17259
530137	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4C5CC6CC(C5)CC4C6)O	6.17497
527873	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc4cccc4)C(CNCc5cccc(c5)OC)O	6.17572
527239	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC(C)c4cccc4)O	6.17621
486417	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNCc5cccc5)O	6.17772
531048	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNCc4cccc(c4)c5cnnc5)O	6.17872
528703	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CCC(CC4)(C)C)O	6.18935
530056	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNCc4cccc(c4)n5cnc5)O	6.19733
533790	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccc3)C(CNC(C)CCCC(C)C)O	6.20834
528853	c1ccc(cc1)CC(C(CNCC(F)(F)F)O)NC(=O)c2cccc(c2)OCC3CC3	6.21041
531377	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cc(cc(c3)F)F)C(CNCc4cccc(c4)C(F)(F)F)O	6.2127
530807	COc1cccc(c1)CNCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)C5CCCC5)O	6.2225
526830	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc(c3)F)C(CNC(C)CCCC(C)C)O	6.22478
531871	CC(C)Oc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNCc4cc(cc(c4)OC)OC)O	6.22896
524925	CCn1ccc2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNCc5cccc(c5)OC)O	6.23069
535485	CCn1cnc2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	6.24138
539777	CCc1cn(c2c1cc(cc2)C(=O)NC(Cc3cccc3)C(CNC(C)(C)CCCC(C)C)O)CCOC	6.24469
530017	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNCCCc4ccc(cc4)OC)O	6.25501
534259	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CC5c4cccc5)O	6.25582
532724	CCCN(CCC)C(=O)c1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNCc4cccc(c4)OC)O	6.26026
528731	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNCc5ccc(cc5)C)O	6.26179
535339	CC(C)c1c[nH]c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNCc5cccc(c5)OC)O	6.27667
542062	COc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNCc4cc(cc(c4)OC)OC)O	6.28443
534800	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNCc4cccc(c4)OC)O	6.28578
526116	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNCCC(C)c4cccc4)O	6.29132
535811	CCc1c[nH]c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)CCCC(C)C)O	6.29138
526345	CCCC1(CCCC1)NCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)NCC)O	6.29696
536299	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC(C)Cc4cccc(c4)Cl)O	6.30451
539930	CCn1ccc2c1cc(cc2N3CCCC3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)CCCC(C)C)O	6.30879
536197	CCc1cn(c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)CCCC(C)C)O)C	6.31256
539142	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNCC(C)C)O	6.31407
532531	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)CCCC(C)C)O	6.35062
537511	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC4CCC(CC4)C(C)(C)C)O	6.35307
542597	CCn1ccc2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)CCCC(C)C)O	6.37868
530975	CCNc1cc(cc(c1)N2CC(CCS2(=O)=O)c3cccc3)C(=O)NC(Cc4cccc4)C(CNC(C)C)O	6.38505
536751	CCCCC(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)NCC)O	6.39968
536703	CCCCNCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)NCC)O	6.4002
540704	CCn1ccc2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)CCCC(C)C)O	6.45997
531124	CCc1cn2c3c1cc(cc3N(S(=O)(=O)C2)C)C(=O)NC(Cc4cccc4)C(CNC(C)C)O	6.49827
542158	CS(=O)(=O)N(c1cccc1)c2cc(cc(c2)N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC5CC5)O	6.51605
422026	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC4CCc5c4cccc5)O	6.53054
538376	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc(c3)Cl)C(CNC(C)CCCC(C)C)O	6.54514
533789	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNCc5cccc5C)O	6.56749
528471	CCC1(CCCC1)NCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)NCC)O	6.57607
536143	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)C4cccc4)O	6.58173
531861	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)CSCC(C)C)O	6.58527
537964	CCCC1(CCCC1)NCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)NCC)O	6.60745
543035	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNCc5cccc(c5)C)O	6.60923
537709	CCc1cn2c3c1cc(cc3N(S(=O)(=O)C2)C)C(=O)NC(Cc4cccc4)C(CNC(C)(C)CCCC(C)C)O	6.61979
529198	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CC5CCC4C5)O	6.62577
542041	CCc1c[nH]c2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)C(F)(F)F)O	6.64181
531004	CCn1cnc2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)C(F)(F)F)O	6.64374
535460	COc1cc(cc(c1)OC)CNCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCC4=O)C5CCCC5)O	6.64975
531366	COc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)c4cccc(c4)OC)O	6.65049
538916	CCCNCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)NCC)O	6.6507
541833	CC(C)CCCC(C)(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2F)N3CCCCS3(=O)=O)NC(C)C)O	6.65862

538657	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC45CC6CC(C4)CC(C6)C5)O	6.65963
529935	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC(C)CCCC(C)C)O	6.65965
530895	CCc1cn(c2c1cc(cc2)C(=O)NC(Cc3cccc3)C(CNC(C)(C)CCCC(C)C)O)CCc4cccc4	6.6601
533149	CCNc1cc(c(c(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3cccc3)C(CNC4CCC(CC4)(F)F)O	6.67376
534206	CCn1cc2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CCOCC5)O	6.68183
540034	CC(C)CCCC(C)(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)NC(C)C)O	6.68704
536573	CCNc1cc(c(c(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3cccc3)C(CNC(C)(C)CCCC(C)C)O	6.69494
525339	CCCCNCC(C(Cc1cccc1)NC(=O)c2cc3c(cn4c3c(c2)N(S(=O)(=O)CC4)C)CC)O	6.70445
527009	CCCC(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)NCC)O	6.70709
533757	CCc1c[nH]c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)OC)O	6.71597
539174	CCc1cn(c2c1cc(cc2)C(=O)NC(Cc3cccc3)C(CNCc4cccc(c4)C(F)(F)F)O)CCCO	6.73073
533531	CC(C)Nc1cc(c(c(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3cccc3)C(CNC4CCOCC4)O	6.73727
527994	CC(C)c1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC(C)C)O	6.74832
533586	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CCCC4)O	6.77031
541114	c1ccc(cc1)CC(C(CNC2CCCC2)O)NC(=O)c3cc(cc(c3)N4CCCC4=O)C5CCCC5	6.77161
540071	CCc1c[nH]c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNCc5cccc(c5)OC)O	6.77255
536023	CCc1cc(c(c(c1)N2CCCCS2(=O)=O)F)C(=O)NC(Cc3cccc3)C(CNC4CCOCC4)O	6.77893
541636	CCCC(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)NCC)O	6.78887
528026	c1ccc(cc1)CC(C(CNC2CCc3c2cccc3)O)NC(=O)c4cc(cc(c4)N5CCCC5=O)C6CCCC6	6.78927
527447	c1ccc(cc1)CC(C(CNC2CCc3cccc3C2)O)NC(=O)c4cc(cc(c4)N5CCCC5=O)C6CCCC6	6.79267
538326	CCCN(CCC)C(=O)c1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CC4)O	6.80553
528855	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4(CCCCC4)C)O	6.80687
538100	CC(C)c1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNCc5cccc(c5)OC)O	6.81125
534308	CC(C)(C)Nc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CCOCC4)O	6.82257
531412	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccc(cc3)Cl)C(CNC4CCCC4)O	6.82297
538000	CCn1c2cc(cc(c2n1)N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)C(F)(F)F)O	6.82698
542835	CCCC(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N3CCCCS3(=O)=O)C4CCCC4)O	6.83252
538502	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc(c4)Cl)C(CNC5CC5)O	6.83773
526920	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc(c4)F)C(CNC5CC5)O	6.84595
537334	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)c4cccc(c4)OC)O	6.84603
531966	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CCC(C4)(C)C)O	6.85918
534231	CCn1ccc2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	6.86176
530733	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC4CCSCC4)O	6.87505
537989	CCn1ccc2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)C(F)(F)F)O	6.8775
531686	CCn1ccc2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	6.91234
541375	CC(C)c1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC4CCCC4)O	6.91863
533327	CCn1ccc2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	6.92322
525517	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cc(cc(c4)F)F)C(CNC5CC5)O	6.92327
527407	CCc1cn(c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O)C	6.92723
531482	CCNc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3ccc(cc3)F)F)C(CNC4CCCC4)O	6.93143
532534	CCc1c[nH]c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)C(F)(F)F)O	6.93919
530456	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CC5)O	6.95001
532693	CCN1CCc2c1cc(cc2N3CCCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)C(F)(F)F)O	6.96285
526152	CCn1c2cc(cc(c2n1)N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)OC)O	6.96913
529474	CCc1cn(c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)C(F)(F)F)O)C	6.97479
538747	CC(C)Nc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC4CCCC4)O	6.98822
540084	CCc1c[nH]c2c1cc(cc2N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	6.9931
541922	CCCNCC(C(Cc1cccc1)NC(=O)c2cc3c(cn4c3c(c2)N(S(=O)(=O)CC4)C)CC)O	6.9936
536553	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CC5)O	7.00431
532978	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)CC)C(=O)NC(Cc4cccc4)C(CNC5CCOCC5)O	7.00525
530371	CCc1cc(c(c(c1)N2CCCC2=O)F)C(=O)NC(Cc3cccc3)C(CNC(C)(C)c4cccc(c4)OC)O	7.01907
534014	CCc1cn2c3c1cc(cc3N(S(=O)(=O)C2)C)C(=O)NC(Cc4cccc4)C(CNC5CCOCC5)O	7.05705
531093	CCc1cn2c3c1cc(cc3N(S(=O)(=O)C2)C)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	7.06005
538365	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C(C)C)C(=O)NC(Cc4cccc4)C(CNC5CCOCC5)O	7.07782
422010	CCNc1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC4CCCC4)O	7.07886
529614	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)CC)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	7.09387
537706	CC(C)Nc1cc(cc(c1)N2CCCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)c4cccc(c4)C(F)(F)F)O	7.10037
536260	CS(=O)(=O)N(c1cccc1)c2cc(cc(c2)N3CCCC3=O)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	7.10754
541845	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC(C)CC)O	7.12805
527848	CCN(C)c1cc(cc(c1)N2CCCC2=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)c4cccc(c4)OC)O	7.13677
541234	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc(c4)F)C(CNC5CCOCC5)O	7.16707

527286	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	7.1749
542262	CCNc1cc(cc(c1)N2CCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC45CCC(CC4)CC5)O	7.19892
538525	CCc1cn2c3c1cc(cc3N(S(=O)(=O)C2)C)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)OC)O	7.20944
539591	CC(C)CCCC(C)NCC(C(Cc1cccc1)NC(=O)c2cc(cc(c2)N(c3cccc3)S(=O)(=O)C)N4CCCC4=O)O	7.23386
535065	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc(c4)Cl)C(CNC5CCCC5)O	7.2434
540165	CC(C)c1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CCOCC5)O	7.26374
540708	CCNc1cc(cc(c1)N2CCCS2=O)C(=O)NC(Cc3cccc3)C(CNC(C)c4cccc4)O	7.26524
535845	CCC(c1cccc(c1)Cl)NCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)NCC)O	7.28651
531019	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CCOCC5)O	7.3213
531425	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	7.32892
529989	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc(c4)Cl)C(CNC5CCOCC5)O	7.35459
535438	CCNc1cc(cc(c1)N2CCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNCc4cc(cc(c4)OC)OC)O	7.36686
528183	CCn1ccc2c1cc(cc2N3CCCS3(=O)=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)OC)O	7.38093
539972	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNCC(C)C)O	7.42497
541055	CCCN(CCC)C(=O)c1cc(cc(c1)N2CCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)c4cccc(c4)C(F)(F)F)O	7.44141
532648	CCc1cn(c2c1cc(cc2N3CCCS3=O)C(=O)NC(Cc4cccc4)C(CNC(C)(C)c5cccc(c5)OC)O)C	7.44309
525238	CCC(c1cccc(c1)Cl)NCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCC4=O)C5CCCC5)O	7.45357
531046	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cc(cc(c4)F)F)C(CNC5CCCC5)O	7.4616
531951	CCNc1cc(cc(c1)N2CCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC45CCC(C4)CC5)O	7.46733
526988	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cc(cc(c4)F)F)C(CNC5CCOCC5)O	7.47334
538572	CCC(c1cccc(c1)Cl)NCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCC4=O)NCC)O	7.50026
537823	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)CC)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	7.5038
527527	CC(C)c1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc4)C(CNC5CCCC5)O	7.52328
530157	CCCN(CCC)C(=O)c1cc(cc(c1)N2CCCS2(=O)=O)C(=O)NC(Cc3cccc3)C(CNC(C)(C)c4cccc(c4)OC)O	7.52625
542347	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)C)C(=O)NC(Cc4cccc(c4)F)C(CNC5CCCC5)O	7.52679
529190	CCc1cn2c3c1cc(cc3N(S(=O)(=O)CC2)CC(F)(F)F)C(=O)NC(Cc4cccc4)C(CNC5CCOCC5)O	7.52836
542400	CC(C)(c1cccc(c1)OC)NCC(C(Cc2cccc2)NC(=O)c3cc(cc(c3)N4CCCCS4(=O)=O)C5CCCC5)O	7.53831

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COMPOUND_ID	CANONICAL_SMILES	pXC50_3D7
542494	<chem>Cn1cccc1C(=O)Nc2cccc(c2)c3c(c4ccccc4n3)c5ccnc(n5)Nc6ccc7c(c6)OCCO7</chem>	5.86943
541917	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(ccc(c4Cl)F)F)c5ccnc(n5)Nc6cccc(c6)F</chem>	5.94376
537852	<chem>CCN(CC)C(=O)Nc1ccc(cc1)c2c(c3ccccc3n2)c4ccnc(n4)Nc5cccc(c5)CCN(CC)CCO</chem>	5.95522
535475	<chem>Cc1c(nc2cc(ccc2n1)Nc3nccc(n3)c4c5ccccc5nc4c6cccc(c6)NC(=O)c7c(cccc7F)F)C</chem>	5.97177
540627	<chem>Cc1ccc(c(c1F)C(=O)Nc2cccc(c2)c3c(c4ccccc4n3)c5ccnc(n5)Nc6cccc(c6)F)F</chem>	5.97735
530976	<chem>CCS(=O)(=O)c1ccc(c(c1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F)OC</chem>	5.98621
537456	<chem>COc1cc(ccc1Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F)CS(=O)(=O)C</chem>	6.01483
528728	<chem>c1ccc(cc1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6cc(cccc6F)F</chem>	6.02089
536215	<chem>COCCOc1ccc(cc1F)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.02235
526244	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(ccc(c4F)F)F)c5ccnc(n5)Nc6cccc(c6)F</chem>	6.06776
529314	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6ccc(cc6)S(=O)(=O)N</chem>	6.11785
528162	<chem>COc1cccc(c1C(=O)Nc2cccc(c2)c3c(c4ccccc4n3)c5ccnc(n5)Nc6cccc(c6)F)OC</chem>	6.12543
539818	<chem>c1ccc(cc1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.13899
533988	<chem>c1ccc(cc1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.14546
538557	<chem>CCN(CCc1cccc(c1)Nc2nccc(n2)c3c4ccccc4nc3c5ccc(cc5)NC(=O)C(C)C)CCO</chem>	6.14652
536192	<chem>c1cc(cc(c1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.16015
531996	<chem>c1cc(cc(c1)NC(=O)c2c(cccc2F)F)c3c(c4ccccc4n3)c5ccnc(n5)Nc6cccc(c6)C(F)(F)F</chem>	6.18825
540895	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6cccc(c6)C(F)(F)F</chem>	6.20284
541540	<chem>CS(=O)(=O)Cc1ccc(cc1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)C(=O)Nc6c(cccc6F)F</chem>	6.27422
532692	<chem>c1cc(cc(c1)NC(=O)c2c(cccc2F)F)c3c(c4ccccc4n3)c5ccnc(n5)Nc6cccnc6</chem>	6.27732
527610	<chem>c1ccc(cc1)C(=O)Nc2cccc(c2)c3c(c4ccccc4n3)c5ccnc(n5)Nc6cccc(c6)NC(=O)CN</chem>	6.36502
537393	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6ccc(cc6)C(=O)NC7CC7</chem>	6.38632
531772	<chem>CCN(CC)CCCOc1ccc(cc1F)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.39017
537901	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6ccc(cc6)C(=O)N7CCOCC7</chem>	6.41678
530352	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)C(=O)Nc4c(cccc4F)F)c5ccnc(n5)Nc6cccc(c6)c7cnc7</chem>	6.44294
532490	<chem>COCCOc1ccc(cc1Cl)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.44845
529489	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6ccc(cc6)C7ccncc7</chem>	6.52886
535721	<chem>COc1ccc(cc1Cl)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.54657
533918	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)C4CCCC4)c5ccnc(n5)Nc6cccc(c6)c7cnc7</chem>	6.58361
525000	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6ccc(c(c6)F)NCCCN7CCOCC7</chem>	6.58634
537016	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4cc(ccc4F)F)c5ccnc(n5)Nc6cccc(c6)N7CCCC7=O</chem>	6.67305
539070	<chem>CS(=O)(=O)Cc1ccc(cc1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)C6CCCC6</chem>	6.69738
535316	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6ccc(cc6)c7cc[nH]n7</chem>	6.7232
527534	<chem>CC(=O)Nc1cccc(c1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.73558
541552	<chem>COc1cccc(c1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.74895
535061	<chem>c1cc(cc(c1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F)c7cnc7</chem>	6.77915
525581	<chem>CS(=O)(=O)Cc1ccc(cc1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.79041
529853	<chem>c1cc(cc(c1)NC(=O)c2c(cccc2F)F)c3c(c4ccccc4n3)c5ccnc(n5)Nc6ccc(cc6)N7CCOCC7</chem>	6.8018
535289	<chem>CS(=O)(=O)Cc1ccc(cc1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	6.82424
525025	<chem>CN1CCN(CC1)c2ccc(cc2)Nc3nccc(n3)c4c5ccccc5nc4c6cccc(c6)NC(=O)c7c(cccc7F)F</chem>	6.94981
530125	<chem>COc1cc(cc(c1OC)OC)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	7.11189
535545	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6cccc(c6)S(=O)(=O)N</chem>	7.1329
527930	<chem>c1ccn2c(c1)c(c(n2)c3cccc(c3)NC(=O)c4c(cccc4F)F)c5ccnc(n5)Nc6cccc(c6)CCS(=O)(=O)N</chem>	7.23367
525205	<chem>CC(c1cccc(c1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F)S(=O)(=O)C</chem>	7.24057
532918	<chem>CC(c1cccc(c1)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F)S(=O)(=O)C</chem>	7.34109
525842	<chem>COc1cc(cc(c1OC)OC)Nc2nccc(n2)c3c4ccccc4nc3c5cccc(c5)NC(=O)c6c(cccc6F)F</chem>	7.4867

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COMPOUND_ID	CANONICAL_SMILES	pXC50_3D7
541977	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCC(CC5)C(=O)N</chem>	5.75142
527260	<chem>c1ccc(cc1)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4</chem>	5.75415
537743	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)c5ccccc5)NC(=O)C</chem>	5.75873
542486	<chem>c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNC5CC5</chem>	5.77892
533656	<chem>CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3cc(s3)c4[nH]c5ccccc5n4</chem>	5.80679
533658	<chem>c1cc(cc(c1)C(=O)NCCN2CCCC2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F</chem>	5.8144
526983	<chem>Cc1cc(oc1C)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4</chem>	5.83815
532628	<chem>Cc1ccc(o1)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4cc5ccccc5[nH]4</chem>	5.8462
541152	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCN(CC5)c6ccc(cn6)C#N</chem>	5.84909
528876	<chem>c1ccc(cc1)n2ncc(n2)CNCc3ccc(cc3)c4ccc(s4)c5[nH]c6ccccc6n5</chem>	5.8526
532676	<chem>c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)C(=O)N5CCCCC5CN6CCC(C6)O</chem>	5.85295
537180	<chem>CN1CCN(CC1)Cc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4</chem>	5.85789
526614	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)C4CCCN(C4)C5CCC5</chem>	5.87007
529088	<chem>COC(=O)c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)C=CC(=O)Nc4ccc(c(c4)Cl)Cl</chem>	5.87282
529128	<chem>c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCCC(C5)O</chem>	5.87286
530587	<chem>c1ccc(cc1)n2ncc(n2)CNCc3ccc(cc3)c4cccc(c4)c5[nH]c6ccc(cc6n5)C(F)(F)F</chem>	5.87521
531298	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)NCc5ccc(cc5)F</chem>	5.87591
536119	<chem>Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)C(=O)NCc5nccn5C</chem>	5.87788
539124	<chem>CC(CN(C)C)C(=O)Nc1ccc(cc1)c2cc(sc2)c3[nH]c4cccc4n3</chem>	5.88092
538157	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)NCc5ccc(cc5)F</chem>	5.88475
527939	<chem>CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4</chem>	5.88986
525952	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCC(CC5)C(=O)N</chem>	5.89958
540901	<chem>CC(=O)Nc1ccc(cc1)c2cc(c(nc2)N)c3[nH]c4cc(ccc4n3)OC</chem>	5.90554
531213	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCN(CC5)c6ccc(cn6)C#N</chem>	5.90665
542156	<chem>c1ccc(cc1)n2ncc(n2)CNCc3ccc(cc3)c4cccc(c4)c5[nH]c6ccccc6n5</chem>	5.90974
542453	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCN5CCNCC5</chem>	5.91101
539359	<chem>Cn1cccc1CCNc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F</chem>	5.91208
536253	<chem>Cc1ccoc1C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4</chem>	5.91326
531417	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCNS(=O)(=O)C</chem>	5.91391
533917	<chem>Cn1cccc1CCNc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4</chem>	5.9169
530485	<chem>Cc1ccc(cc1S(=O)(=O)N2CCOCC2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4</chem>	5.91879
533326	<chem>Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)C(=O)NCCc5ccc(c(=O)[nH]5)O</chem>	5.92315
537470	<chem>Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)COC(C)C</chem>	5.92582
533339	<chem>Cc1cc2c(cc1C)nc([nH]2)c3ccc(cc3)C(=O)NCCC4CCCC4</chem>	5.92952
542339	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCC5CCCO5</chem>	5.93011
526441	<chem>Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCN(CC5)c6ccc(cn6)C#N</chem>	5.93523
534846	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCCN5CCNCC5</chem>	5.93856
541374	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)C(=O)NCCN5CCCC5</chem>	5.94396
536932	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)C=Cc4ccccc4</chem>	5.94428
542649	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)c6ccc(cn6)C#N</chem>	5.94581
536620	<chem>CNCCNc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F</chem>	5.94764
539822	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5ccccc5)C(=O)N</chem>	5.9482
526227	<chem>c1cc(ccc1)CNCCN2CCNCC2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F</chem>	5.94924
537636	<chem>c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)NCc5ccc(cc5)F</chem>	5.94951
528071	<chem>Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)c5c(nns5)C</chem>	5.95078
529941	<chem>c1ccc2c(c1)[nH]c(n2)c3cccc(n3)c4[nH]c5ccccc5n4</chem>	5.95268
535153	<chem>COCCN1CCN(CC1)Cc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4</chem>	5.95355
539648	<chem>c1cc(cc(c1)NC(=O)c2c[nH]cn2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F</chem>	5.95603
541907	<chem>Cn1cc(nc1)CCNC(=O)c2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4</chem>	5.95744
528285	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)C4CCN(CC4)Cc5ccccc5)F</chem>	5.95901
533877	<chem>CN1CCC(CC1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4</chem>	5.96088
527776	<chem>Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Cc5ccccc5</chem>	5.96337
531602	<chem>Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C(C(C)C)NC(=O)C</chem>	5.96374
529402	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)c6ccc(cn6)C#N</chem>	5.96492
524989	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCN5CCNCC5</chem>	5.96609
541399	<chem>CS(=O)(=O)NCCCNc1ccc(c1)c2ccc(s2)c3[nH]c4cccc4n3</chem>	5.96756
541971	<chem>c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5csnn5</chem>	5.96952
540752	<chem>c1ccc(cc1)C2CC2NC(=O)Nc3cccc(c3)c4cccc(c4)c5[nH]c6ccccc6n5</chem>	5.97077

530742	CN(CCN)Cc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)F	5.97209
539598	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)c5ccc(=O)[nH]n5	5.97234
534779	CCNC(=O)Nc1ccc(cc1)c2ccc(s2)c3[nH]c4c(cccc4n3)C	5.97239
528721	Cc1cc2c(cc1C)nc([nH]2)c3ccc(cc3)OCC(=O)NCc4ccc(cc4)C(C)(C)C	5.97465
529718	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CN5CCN(CC5)c6cnccn6	5.97489
535216	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5cnn6c5nccc6	5.97615
526807	CC(CN(C)C)C(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4cccc4n3	5.97619
538310	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Cc5c[nH]cn5	5.97648
536354	c1cc(cc(c1)F)CNC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	5.97708
530654	c1cc(ccc1c2[nH]c3ccc(c(cc3n2)F)F)C(=O)NCc4ccc(c(c4)Cl)Cl	5.97817
537149	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNC5CC5	5.97877
533123	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)C(=O)N5CCCC5CN6CCC(C6)O	5.97982
532787	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)CN5CCOCC5	5.98079
530002	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCCC5CN	5.98161
536297	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)CNC(=O)c5ccc(cc5)O	5.98171
530690	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCN5CCNCC5	5.98183
532677	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCC5CCCO5	5.98208
527641	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)c6ccc(cc6)C#N	5.98276
527965	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5cccnc5	5.98364
535280	CCNC(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4c(cccc4n3)C	5.98374
531659	Cc1c(sc(n1)C)CC(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	5.98694
527950	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CC5c6cccc6C(=O)N5	5.98717
538876	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCN5CCNCC5	5.9883
535364	c1cc(ccc1c2[nH]c3ccc(cc3n2)F)C(=O)NCc4ccc(c(c4)Cl)Cl	5.98831
531714	CC(C)C(C(=O)Nc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)NC(=O)C	5.98853
528739	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Cc5c[nH]cn5	5.98932
535014	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCN(CC5)CCC#N	5.98972
536271	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)CN5CCN(CC5)C	5.99079
532783	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCCNS(=O)(=O)C	5.99296
528863	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCN5CCCC5=O	5.99352
525038	CS(=O)(=O)NCCCNc1ccc(c1)c2cc(sc2)c3[nH]c4cccc4n3	5.99362
535853	CC(CN1CCN(CC1)C)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	5.99431
539570	CCOc1cccc(c1)C(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3	5.99695
526615	COCC1CCCN1Cc2ccc(cc2)c3ccc(s3)c4[nH]c5cccc5n4	5.99888
530128	CC(=O)N(C)c1cccc(c1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	5.99919
541948	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C(C)C(=O)NC(C)C	5.99995
535030	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)CS(=O)(=O)C	5.99995
542552	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCCNS(=O)(=O)C	6.00043
526128	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5cnccc5C(F)(F)F	6.00108
529270	CN(CCN)Cc1cccc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.0013
528190	CS(=O)(=O)NCCCNc1ccc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.0019
534254	c1cc(cc(c1)N)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.00349
524505	c1ccc(cc1)NC(=O)c2c[nH]cn2	6.00404
539952	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CNC(=O)c5ccc(cc5)O	6.00449
534991	Cc1cc2c(cc1C)nc([nH]2)c3ccc(cc3)OCC(=O)NCc4cccc(c4)C(F)(F)F	6.00516
525982	CC(=O)Nc1nc(cs1)C(=O)Nc2cccc(c2)c3ccc4c(c3)cn4COC	6.00554
536813	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CNc5ccc(cc5)C(=O)N	6.00568
539032	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5ccc(cc5)NC	6.00568
528451	CN1CCC(CC1)C(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.00568
531891	CC(C)(C)c1ccc2c(c1)nc([nH]2)c3ccc(cc3)C=CC(=O)NCc4cccc(c4)C(F)(F)F	6.00621
531474	c1cc(cc(c1)O)CC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.00726
525991	COc1cc(cc(c1OC)OC)C(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3	6.00789
532200	c1ccc2c(c1)C(CC(=O)N2)C(=O)Nc3cccc(c3)c4cccc(c4)c5[nH]c6cccc6n5	6.00856
542329	CNCc1ccc(c(c1)C(=O)OC)c2cccc(c2)CNCc3ccc(cc3)c4cccc4	6.00871
525179	Cn1ccnc1CNC(=O)c2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.00879
535395	c1ccc(c(c1)C(=O)N)OCC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.00966
540248	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)C(=O)c5cccn5C	6.01047
536596	CN1CCC(CC1)C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5cccc5n4	6.01055
527323	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCC5CCCO5	6.01214
527783	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCN(CC5)CCC#N	6.01245
535685	c1ccc(cc1)n2ncc(n2)CNCc3cccc(c3)c4cccc(c4)c5[nH]c6ccc(cc6n5)F	6.01287



529862	CC(=O)N(C)C1CCN(C1)Cc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.01289
527348	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCCN5CCNCC5	6.01331
536823	c1cc(cc(c1)NC(=O)c2c[nH]cn2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.01487
530377	CC(C1CCCN1C(=O)c2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4)O	6.01502
535295	c1cc(ccc1CN2CCN(CC2)c3ccc(cn3)C#N)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.01624
536862	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)c6ccc(cn6)C#N	6.01669
535206	c1cc(cc(c1)NC(=O)c2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.01676
533545	Cc1ccc2c(c1C)nc([nH]2)c3ccc(cc3)C(=O)NC4CCCC(C4)F	6.01676
542906	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)C(=O)NCCc5cn(cn5)C	6.01762
541295	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CN5CCN(CC5)c6ccc(cn6)C#N	6.01802
533897	c1cc(ccc1CN2CCCC2CN)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.01807
539234	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCCN5CCNCC5	6.01839
530085	c1ccc2c(c1)C(=O)CC(=O)Nc3ccc(cc3)c4cccc(c4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.01864
527332	CC(=O)N(C)C1CCN(C1)Cc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.01887
534856	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCN5CCCC5=O	6.01954
534568	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cccnc5C	6.01972
525644	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.02028
541207	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCCNC	6.02101
530750	c1cc(cc(c1)NC(=O)CCc2cccnc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.02104
525922	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)NCc5ccc(cc5)F	6.0241
536193	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)C4CCCN(C4)CC5CC5	6.02414
526545	CN(CCNCc1ccc(cc1)c2cccc(c2)c3[nH]c4cccc(c4n3)S(=O)(=O)C	6.02457
536524	CC(CN1CCN(CC1)C)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.02556
529630	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCCC(C5)O	6.02596
525134	Cn1cc(nc1)CCNC(=O)c2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.02659
540031	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)C(=O)NCCN5CCCC5	6.02781
536774	CS(=O)(=O)NCCCNCCc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F	6.02794
538324	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)Cc6cccnc6	6.02798
529910	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCN5CCNCC5	6.02842
531720	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCC(CC5)CO	6.02903
529192	CS(=O)(=O)NCCCNCCc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F	6.02937
529962	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCC5CN	6.02962
537577	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCC(CC5)C(=O)N	6.03068
541103	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	6.03246
530198	CCn1cc(cn1)CN2CCCC(C2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4	6.03311
534007	c1cc(ccc1CN2CCCC2CN)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.03335
540247	Cc1c(sc(n1)C)CC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.03386
533734	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)CCc5cccnc5	6.0351
526192	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5c5cnn(n5)c6ccccc6	6.03557
526309	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5csnn5	6.03592
540798	Cc1cccc(n1)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4	6.03646
540736	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)C(=O)NCCN5CCCC5	6.03685
538136	CC1CN(CC(O1)C)Cc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.03745
527028	c1ccc(cc1)n2ncc(n2)CNCc3ccc(cc3)c4cccc(c4)c5[nH]c6ccc(cc6n5)F	6.03761
538900	c1ccc(cc1)CNCc2c(ccc3c2nc([nH]3)c4cccc(c4)F)O	6.03814
526450	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCCC5CN	6.03886
538638	c1cc(ccc1CNCCN2CCNCC2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.04104
537166	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCC(CC5)CO	6.04108
540845	CC(=CCN1CCC(CC1)C(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3)C	6.04172
536259	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5cccc(c5)NC(=O)C	6.04204
536863	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCN(CC5)c6ccc(cn6)C#N	6.04207
538179	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCC(CC5)C(=O)N	6.04221
539036	Cc1cccc(c1)NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.04353
526419	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CNCCN5CCNCC5	6.04389
524504	COc1ccc(cc1)OCC(=O)Nc2cc(ccc2Cl)c3[nH]c4cccc4n3	6.04418
537055	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Cc5c[nH]cn5	6.04452
525265	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4cccc(c4)S(=O)(=O)N5CCOCC5	6.0447
532510	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C5CCCO5	6.04542
526151	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)C(=O)NCCN5CCCC5	6.04543
540106	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCC(CC5)CO	6.04654
543131	c1ccc(cc1)C2CC2NC(=O)Nc3cccc(c3)c4cccc(c4)c5[nH]c6ccccc6n5	6.04656

538412	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)Cc5cccn(=O)c5	6.04699
530422	c1cc(ccc1)CNCCCN2CCCC=O)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.04774
530937	CC(=O)Nc1cccc(c1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.0479
533561	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)NCc5cccc(c5)F	6.04866
542406	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCN(CC5)c6cnccn6	6.04901
528308	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCN5CCC(C5)N	6.04908
540996	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCC(C5)N	6.0497
533795	CC(C)C(C(=O)Nc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)NC(=O)C	6.05106
525507	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)COc5cccc5C(=O)N	6.0511
534644	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCCCC5	6.0511
534512	c1cc(ccc1)NC(=O)Nc2ccc(c(c2)Cl)Cl)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.0511
531178	Cc1c(snn1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.0513
534430	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)NCc5cccc(c5)F	6.05208
528052	Cc1c(snn1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccccc5n4	6.05316
538394	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)C(=O)N5CCCCC5CN6CCC(C6)O	6.05446
537570	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)Cc5cccn(=O)c5	6.05466
525214	CS(=O)(=O)NCCCNc1ccc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.05554
540598	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCC(CC5)C(=O)N	6.05624
540959	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)C(=O)NCCc5cn(cn5)C	6.05679
538267	CC1CN(CC(O1)C)Cc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.05737
529914	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)NC5CC5c6cccc6	6.05737
535355	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5cnn6c5nccc6	6.05934
530585	Cn1cncc1C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.0596
531875	Cc1c(snn1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.06073
531604	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCCCC5	6.06087
535610	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCC5CCCO5	6.06091
533280	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCCC(C5)O	6.06149
541939	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)CNc5ccc(cc5)C(=O)N	6.06189
533164	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCCCC5CN	6.06196
536200	c1cc(ccc1)NC(=O)CCc2cccn2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.06222
532539	Cn1cc(nc1)CCNC(=O)c2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.06258
529835	CS(=O)(=O)c1cccc1CNC(=O)c2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.06271
541990	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)c5cccc(c5)C(=O)N	6.06279
533710	CCCCOc1ccc(cc1)c2[nH]c3cccc3n2	6.06285
532296	CNCCNc1ccc(cc1)c2ccc(s2)c3[nH]c4cccc4n3	6.0632
530193	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)CCC#N	6.06336
533996	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)CNCCN5CCNCC5	6.06462
537177	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5cncn5C	6.06501
530582	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCCCN5CCC5=O	6.06585
527387	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)CNC(=O)c5ccc(cc5)O	6.06591
529694	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCCCO5	6.06592
530925	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCCC(C5)O	6.06599
527984	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)CCOC	6.06621
525383	Cn1cncc1C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.06663
540939	CC1CN(CC(O1)C)Cc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.0672
537238	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5ccc(=O)[nH]n5	6.06724
532782	c1cc(ccc1)CN2CCN(CC2)c3ccc(cc3)C#N)c4ccc(s4)c5[nH]c6ccc(cc6n5)F	6.06835
532910	c1cc(ccc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)NC(=O)c5ccoc5	6.06841
525315	CS(=O)(=O)NCCCNc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.06852
539376	Cn1cncc1C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.06856
537074	c1cc(ccc1)CN2CCCC(C2)O)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.06879
537745	c1cc(ccc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CN5CCC(CC5)C(=O)N	6.06892
541161	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCC(CC5)C(=O)N	6.06911
537229	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)NCc5cccc(c5)F	6.06912
539539	COc1ccc(o1)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4	6.06922
539781	COC(=O)c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)C(=O)NCc4ccc(c4)Cl)Cl	6.06964
537124	c1cc(ccc1)CN2CCCC(C2)O)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.07006
540113	c1cc(ccc1)CN2CCC(CC2)CO)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.07048
528100	c1cc(ccc1)CNCCN2CCNCC2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.07081
542384	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCC(C5)N	6.07118
535478	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCCCC5	6.07161

538012	CCOC(=O)c1ccc2c(c1)nc([nH]2)c3ccc(cc3)C(=O)NCc4ccc(cc4)C(C)(C)C	6.07207
538748	c1cc(ccc1CN2CCC(CC2)CO)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.07329
540292	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CNCCN5CCNCC5	6.07457
529777	CCN(CC(C)O)C(=O)c1ccc(cc1)c2ccc(cc2)c3[nH]c4c(cccc4n3)C	6.07555
525823	CC(C)(C)c1ccc(cc1)CNC(=O)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(C)(C)C	6.07578
526142	Cn1c(ccn1)C(=O)NCCNCc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.07584
531642	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCCN5CCCC5=O	6.07588
538223	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5ccncc5	6.07611
535298	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCCC(C5)O	6.07653
538560	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)C4CCN(CC4)Cc5ccc(cc5)F	6.07661
536585	Cc1c(snn1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.0767
540686	Cn1cccc1C(=O)C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.07687
541321	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)CCc5c[nH]cn5	6.07696
525422	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3cc(sc3)c4[nH]c5cccc5n4	6.07703
539568	COc1cccc(c1)c2cc([nH]n2)C(=O)Nc3ccc4c(c3)nc([nH]4)c5cccc5	6.07758
531595	COc1ccc2c(c1)cc([nH]2)C(=O)Nc3ccc4c(c3)nc([nH]4)c5cccc5	6.07875
538597	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)C(=O)NCCCN5CCCC5	6.07929
527515	Cc1cnc(cn1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.07951
536358	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)CN5CCCC5CN	6.07955
538925	CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.0798
536030	CNCCNCc1cccc(c1)c2ccc(s2)c3[nH]c4cccc4n3	6.0809
538673	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCCC(C5)O	6.08092
538543	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCC(C5)N	6.08104
531810	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)c5ccoc5	6.08121
527464	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C5CCN(CC5)C	6.0816
534070	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCCC5	6.08189
533998	Cc1c(sc(n1)C)CC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.0823
538788	CC(CN(C)C)C(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F	6.08318
531594	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.0832
537523	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)CN5CCN(CC5)C	6.08322
533542	Cc1c(snn1)C(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5cccc5n4	6.08373
541523	CNCCNCc1cccc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.08456
536384	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCN(CC5)CCO	6.0846
536285	c1ccc(cc1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.08509
525779	CCC(C)NC(=O)Nc1ccc(cc1)c2cccc(c2)c3[nH]c4cccc4n3	6.08565
541772	CN(C)CCCN1CCN(CC1)Cc2ccc(cc2)c3ccc(s3)c4[nH]c5cccc5n4	6.08598
542119	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)C(=O)c5cccn5C	6.08652
526416	CC(C)(C)c1ccc(cc1)CNC(=O)c2ccc(cc2)c3[nH]c4ccc(cc4n3)Cl	6.08687
539725	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCC#C	6.08704
530273	C1ccc(cc1)CNCc2cccc(c2)c3ccc(s3)c4[nH]c5cccc5n4	6.08723
537940	Cn1ncc1C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.08724
535960	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCOCC5	6.08734
537081	CN1CCC(CC1)C(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5cccc5n4	6.08808
529819	COc1ccc(cc1)CNCc2cccc(c2)c3ccc(s3)c4[nH]c5cccc5n4	6.08821
533299	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCCC5CN	6.08899
537103	CC(=O)Nc1ncc(s1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.08916
526272	c1cc(ccc1CN2CCN(CC2)c3ccc(cn3)C#N)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.08924
538470	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4cc(cnc4)Br	6.08962
535301	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCC(CC5)CO	6.08995
535593	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CN5CCCC5CN	6.09004
542664	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCC(CC5)CO	6.09025
543103	CS(=O)(=O)NCCCNc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)F	6.09077
540945	c1cc(ccc1CN2CCC(CC2)C(=O)N)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.09181
534623	CS(=O)(=O)c1cccc1CNC(=O)c2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.09182
529269	CCC(C)NC(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4c(cccc4n3)C	6.09199
524736	c1ccc(cc1)c2ccc(cc2)c3[nH]c4cccc4n3	6.09204
539311	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCCC5CO	6.09277
542242	CC(CN1CCN(CC1)C)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.09293
524977	Cc1cc2c(cc1)nc([nH]2)c3ccc(cc3)C(=O)NCc4cccc(c4)C(F)(F)F	6.09325
532453	c1cc(cc(c1)NC(=O)C)c2c[nH]cn2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.09348
530277	C#CCCC(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.09405

537239	CS(=O)(=O)NCCCNc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F	6.09451
527177	CCn1cc(c(n1)C)CN2CCCC(C2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4	6.09562
539071	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)c5csnn5	6.0958
541664	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(c(c4)N(=O)=O)Cl	6.0959
532061	COc1cccc(c1)C(=O)Nc2ccc(cc2)c3[nH]c4ccccc4n3	6.09593
539322	CC(C)(C)c1ccc2c(c1)nc([nH]2)c3ccc(cc3)C(=O)NCCCc4ccccc4	6.09622
538503	c1cc(ccc1NC(=O)Nc2[nH]c3ccc(cc3n2)N(=O)=O)Cl	6.09634
532629	CC(CN(C)C)C(=O)Nc1cccc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)F	6.09637
536202	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5ccsc5	6.09741
542877	CC(C)NCc1cccc(c1)c2cccc(c2)c3[nH]c4ccccc4n3	6.09749
536795	c1ccc2c(c1)[nH]c(n2)c3cc(ccs3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	6.09762
527875	CC(C1CCCN1C(=O)c2cccc(c2)c3ccc(s3)c4[nH]c5ccccc5n4)O	6.09797
530451	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCNC	6.09824
524774	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)Cc5c[nH]cn5	6.09851
542252	Cn1cncc1C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccccc5n4	6.09932
535285	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(c(c4)N(=O)=O)N5CCOCC5	6.09995
539845	c1cc(ccc1CN2CCCC2CN)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.10007
536208	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Cc5cccn5	6.10086
536825	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.10132
531580	CN1CCC(CC1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.10153
541032	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCC(C5)N	6.10246
536885	Cc1ccc2c(c1C)[nH]c(n2)c3ccc(cc3)C(=O)NCc4ccc(c(c4)Cl)Cl	6.10252
535840	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccc(=O)[nH]n5	6.10268
525490	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)c5ccncc5	6.10273
531085	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cccc(c5)NC(=O)C	6.10288
530246	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)c5csnn5	6.10364
529603	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NCc5cn6cccn6n5	6.10398
528558	c1cc(ccc1c2[nH]c3ccc(cc3n2)NC(=O)c4ccc(cc4)Br)NC(=O)c5ccc(cc5)Br	6.10444
542059	c1ccc(c(c1)C(=O)N)OCC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.10481
536696	CN(CCN)Cc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F	6.10493
541959	Cn1cccc1C(=O)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.10495
541060	c1ccc2c(c1)[nH]c(n2)c3cc(ccc3Cl)NC(=O)c4ccc(o4)c5ccc(cc5)Cl	6.10499
525683	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)CN5CCN(CC5)C	6.10506
534278	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)Cc5cccn(=O)c5	6.10581
529795	c1ccc(cc1)c2ccc(cc2)CNCCCNc3[nH]c4ccccc4n3	6.10602
534954	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCCC(C5)O	6.10807
539401	c1cc(ccc1CNCCN2CCNCC2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.10863
538301	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCCCC5CO	6.10867
539482	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)c5ccncc5	6.10887
529202	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCCC5CN	6.109
531237	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5ccccc5	6.10934
538426	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)Cc5c[nH]cn5	6.10948
537545	c1cc(cc(c1)C(F)(F)F)CNC(=O)c2ccc(cc2)c3[nH]c4cc(c(cc4n3)F)F	6.10989
538631	COc1ccc(cc1C(=O)Nc2ccc(cc2)c3[nH]c4ccccc4n3)Cl	6.11118
542078	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)C(=O)NCCN5CCCC5	6.11142
526194	CC(CN(C)C)C(=O)Nc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F	6.11167
540012	c1cc(cc(c1)NC(=O)Cc2c[nH]cn2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.11203
525699	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCC(C5)N	6.11205
535250	Cc1cc2c(cc1)nc([nH]2)c3ccc(cc3)C(=O)NCc4ccc(cc4)C(C)(C)C	6.11237
530869	CNCCNc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)F	6.11238
526757	c1cc(cc(c1)F)CNC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.11261
542429	Cc1cnc(cn1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.1131
525977	c1ccc(cc1)c2[nH]c3ccc(cc3n2)NC(=O)c4cc(n[nH]4)c5ccc6c(c5)OCCO6	6.1143
526320	c1cc(cc(c1)F)CNC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.11433
542279	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccccc5	6.11446
530323	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCOCC5	6.11464
529711	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCC(C5)CO	6.11485
533133	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCCC5CN	6.115
531012	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)c5cccc(c5)NC(=O)C	6.11516
542180	c1cc(cc(c1)F)CNC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.11551
537015	CCNC(=O)Nc1cccc(c1)c2ccc(s2)c3[nH]c4c(cccc4n3)C	6.11568

539014	Cc1c(snn1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.11569
525376	CN(C)CCNCc1cccc(c1)c2cccc(c2)c3[nH]c4cccc4n3	6.11589
534059	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCCNC	6.11591
527333	CC(=O)Nc1cccc(c1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.11685
540572	COc1ccc(cc1)NC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.11708
529221	c1ccc(cc1)CN2CCCN(CC2)c3ccc4c(c3)CCN(CC4)Cc5ccc(cc5)c6[nH]ccn6	6.11795
526749	CC(=O)Oc1ccc(cc1OC)C(=O)Nc2cccc(c2)c3[nH]c4cccc4n3	6.118
540834	CC(C)NCc1cccc(c1)c2ccc(cc2)c3[nH]c4cccc4n3	6.11846
535047	COCCN1CCN(CC1)Cc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.11859
525102	Cc1nc(n(n1)CC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F)C	6.11862
541020	Cc1ccc2c(c1)nc([nH]2)c3ccc(cc3)NC(=O)c4ccc(c(c4)OC)OC	6.11875
537500	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Cc5c[nH]cn5	6.11876
525757	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)C(C(C)C)NC(=O)C	6.11899
529187	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCCC5CN	6.11909
541201	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)NCc5cccc(c5)F	6.11938
528280	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCN(CC5)CCC#N	6.1197
539514	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)Cc5c[nH]cn5	6.11975
530493	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCC(C5)N	6.11982
532335	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CC(OC(C5)C)C	6.12077
536482	CCNC(=O)Nc1ccc(cc1)c2cccc(c2)c3[nH]c4c(ccc4n3)C	6.12143
527350	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Cc5c(nc(s5)C)C	6.12211
536979	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)NC(C)C	6.12265
526205	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)COc4cccc(c4)N(=O)=O	6.12273
535327	Cc1cccc1OCC(=O)Nc2ccc(cc2)c3[nH]c4cc5cccc5c4n3	6.1233
537844	c1cc(cc(c1)C(=O)NCCN2CCCC2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.12363
530412	c1cc(ccc1c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)C(=O)NCCN5CCCC5	6.12372
528700	CC(C)CN(C)Cc1ccc(cc1)c2ccc(s2)c3[nH]c4cccc4n3	6.1239
525971	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5ccc(cc5)S(=O)(=O)C	6.12391
539903	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCCC5CN	6.12409
533948	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCc5cccc(c5)N	6.12437
529573	CN(C)CCN(C)Cc1ccc(cc1)c2cccc(c2)c3[nH]c4cccc4n3	6.12449
533565	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)c6cncn6	6.12469
536794	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)C(=O)NCc5cccc5S(=O)(=O)C	6.12507
526324	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCCCC5	6.12513
542870	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCCCN5CCCC5=O	6.12527
526754	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(cc4)S(=O)(=O)N5CCCCC5	6.12572
524567	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCN(CC5)CCO	6.12579
537386	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)C(C)CN5CCN(CC5)C	6.12615
533963	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)C5CCN(CC5)C	6.12629
525473	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCCC5CN	6.12639
528065	CC(CN(C)C)C(=O)Nc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.12654
527219	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.12725
527714	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5ccc6c(c5)OCO6	6.1279
534124	C#CCNCc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.12821
537505	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)CCC#N	6.12837
531376	CC(CN(C)C)C(=O)Nc1cccc(c1)c2ccc(s2)c3[nH]c4cccc4n3	6.12882
530875	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCC(C5)N	6.12891
540830	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCCCN5CCCC5=O	6.12903
528638	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4cccc(c4)S(=O)(=O)N5CCCC5	6.12905
530413	CNCCNCc1cccc(c1)c2ccc(cc2)c3[nH]c4cccc4n3	6.1291
535116	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCCCC5	6.12951
535505	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)Cc5c[nH]cn5	6.1296
525600	CC(C1CCCN1C(=O)c2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F)O	6.12971
526354	Cc1cc(cc(c1)C)OCC(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3	6.12985
527231	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Cc5ccc5	6.13008
539110	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5cccc5	6.1301
534036	CN1CCN(CC1)CC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.13017
524972	c1ccc2c(c1)CCN2S(=O)(=O)c3ccc(cc3)C(=O)Nc4ccc(cc4)c5[nH]c6cccc6n5	6.13029
525203	CC(CN(C)C)C(=O)Nc1ccc(cc1)c2ccc(cc2)c3[nH]c4cccc4n3	6.13035
537586	CCOC(=O)NCC(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4c(cccc4n3)C	6.13087
529525	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)C(C)CN5CCN(CC5)C	6.13108

542478	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.13113
533381	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCC5CCCO5	6.13126
536808	COc(=O)C(c1ccc(cc1)O)NC(=O)c2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4	6.13215
533628	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CCC#C	6.13317
538105	CC(=O)Nc1nc(cs1)C(=O)Nc2cccc(c2)c3ccc4c(c3)cnn4CC5CC5	6.13346
528769	Cn1cncc1C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.13373
529723	c1ccc(cc1)NC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.13403
536635	CNc1ccc(cc1)CNCc2cccc(c2)c3ccc(s3)c4[nH]c5ccccc5n4	6.13414
526478	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CNCCN5CCC(C5)N	6.13417
537918	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)COc5ccccc5C(=O)N	6.13431
539772	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cccn5C	6.13462
530022	CC(C)(C)c1ccc2c(c1)nc([nH]2)c3ccc(cc3)C(=O)NCc4cccc(c4)C(F)(F)F	6.13489
532790	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCCc5cccn5C	6.13494
535042	Cc1cc(on1)CNC(=O)c2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.13557
532478	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCCNC	6.13572
531703	c1cc(ccc1c2ccc(cc2)NC(=O)Cc3c[nH]cn3)c4[nH]c5ccc(cc5n4)F	6.13583
527220	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)C(C)CN5CCN(CC5)C	6.13596
534306	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCN(CC5)CCO	6.13688
534769	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4cc(c(nc4)Cl)Cl	6.13763
535712	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)C(=O)N5CCCC5CN6CCC(C6)O	6.13808
526733	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCC(C5)N	6.13826
540647	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5c(cco5)C	6.13894
535709	Cn1cc(nc1)CCNC(=O)c2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.13914
530052	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)c5cccn5	6.13996
532587	CC(=O)N(C)c1cccc(c1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.14019
541019	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCC(CC5)CO	6.14041
537876	CN1CCC(CC1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.14047
526251	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)C(C)CN(C)C	6.1405
527684	Cn1ccnc1CNC(=O)c2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.14071
536771	COc1cc(ccc1OC)OC(=O)Nc2cccc(c2)c3[nH]c4cccc4n3	6.14109
532477	c1cc(ccc1)C(=O)NCCN2CCC2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.14129
532055	CC(CN(C)C)C(=O)Nc1ccc(cc1)c2cccc(c2)c3[nH]c4cccc4n3	6.14159
532342	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCCC(C5)N	6.14167
534751	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5c[nH]cn5	6.14167
532601	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5ccc(cc5)CN	6.1418
540973	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCCC(C5)N	6.14211
532973	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCC(CC5)CO	6.14255
529133	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)NC5CC5c6ccccc6	6.1433
533593	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)c5ccncc5	6.14337
536070	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCc5cnn(n5)c6ccccc6	6.14402
528800	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5ccc(cc5)CN	6.14419
530671	COCCN1CCN(CC1)Cc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.14422
540709	CN(C)CCNCc1ccc(cc1)c2cccc(c2)c3[nH]c4cccc4n3	6.14434
531070	CC(CN(C)C)C(=O)Nc1ccc(cc1)c2ccc(s2)c3[nH]c4cccc4n3	6.14449
529562	c1cc(ccc1)C(=O)N2CCCC2CN3CCC(C3)O)c4ccc(s4)c5[nH]c6ccc(cc6n5)F	6.14549
541395	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5ccccc5	6.14568
529450	Cn1cc(n(c1=O)C)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4	6.14586
533604	c1cc(ccc1)NC(=O)c2ccoc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.14607
529545	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)CCO	6.14767
538319	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5cccc(c5)N	6.14893
541686	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cccn5Cl	6.15035
542550	c1cc(ccc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CN5CCN(CC5)CCO	6.15101
532394	CS(=O)(=O)c1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.1512
525394	CN1CCC(CC1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.15136
542239	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.1514
531788	CC(CN(C)C)C(=O)Nc1cccc(c1)c2ccc(cc2)c3[nH]c4cccc4n3	6.15149
540938	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)C5c[nH]cn5	6.15155
532338	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)NC5CC5c6ccccc6	6.15162
536443	Cc1cnc(cn1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.15227
525456	c1ccc2c(c1)[nH]c(n2)c3cc(c3)c4cccc(c4)CNCCc5cccn5	6.1525
529927	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5ccoc5	6.15275

536343	c1cc(ccc1)NC(=O)c2ccncc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.15283
528909	CN1CCN(CC1)CC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.15305
531320	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)c6ccc(cc6)C#N	6.15372
537251	c1cc(ccc1)NC(=O)Cc2c[nH]cn2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.15486
528549	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCC5CCCO5	6.15512
527396	Cn1cc(nc1)CCNC(=O)c2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.15519
542190	Cn1ccnc1CNC(=O)c2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.15596
543091	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCC(C5)N	6.15626
526444	c1ccc(cc1)c2[nH]c3ccc(cc3n2)C#N	6.15628
530702	c1cc(ccc1)CN2CCC(CC2)CO)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.15701
526235	COc1ccc(cc1)c2cc([nH]n2)C(=O)Nc3ccc4c(c3)nc([nH]4)c5ccccc5	6.15734
526468	CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.15758
538281	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cnc5C(F)(F)F	6.15784
537413	CN1CCC(CC1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.15815
528568	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)Nc5ccsc5	6.15917
527353	COC(=O)c1cccc(c1)CNCc2cccc(c2)c3cc(sc3)c4[nH]c5ccccc5n4	6.15925
530243	c1cc(ccc1)c2ccc(cc2)NC(=O)CCc3c[nH]cn3)c4[nH]c5ccc(cc5n4)F	6.15946
528627	CNCCNCc1cccc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.15955
525072	c1cc(ccc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CNCc5ccccc5)N	6.15961
533987	CC(C1CCCN1C(=O)c2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F)O	6.16105
539608	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCCC5	6.16116
542061	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCCC(C5)O	6.16124
536725	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C(C)CN5CCOCC5	6.16199
529731	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Cc5c[nH]cn5	6.1626
531104	c1cc(ccc1)CN2CCN(CC2)c3cncnc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.16325
533802	c1cc(ccc1)NC(=O)c2csnn2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.16367
532875	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C(C)(C)c5ccccc5	6.16413
528016	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C5CC(=O)Nc6c5ccccc6	6.16429
530996	c1ccc2c(c1)[nH]c(n2)c3cc(c3)c4cccc(c4)CNCc5ccccc5)N	6.16437
532673	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCN(C)C	6.16623
525164	Cc1cn(c(=O)[nH]c1=O)CC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.16683
538542	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)C(C)CN(C)C	6.16701
540995	c1cc(ccc1)NC(=O)c2ccncc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.16713
538995	Cn1cc(nc1)CCNC(=O)c2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.16749
538756	c1cc(ccc1)CN2CCC(CC2)C(=O)N)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.16779
525547	CN1CCN(CC1)CC(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.16807
539688	CCNC(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.16847
533441	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(cc4)N(=O)N5CCCC5	6.16879
533330	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCC5CCCO5	6.16887
535439	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)Cc5ccccc5	6.1692
538053	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNC(C)C	6.17036
542247	CN1CCC(CC1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.1707
529017	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5c(cco5)C	6.17071
541434	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Cc5c[nH]cn5	6.17095
528825	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCCC(C5)N	6.1726
536664	c1ccc(cc1)CNC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.1731
533053	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)Nc5ccc(cc5)OC	6.17328
533876	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cnn6c5nccc6	6.17337
541341	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5ccc6c(c5)OCO6	6.17349
532655	Cc1cc(ccc1N(=O)=O)C(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3	6.1735
532522	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCCNC	6.17385
536799	CNCCNCc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F	6.17399
534523	c1cc(ccc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)NC(=O)c5c[nH]cn5	6.17404
532141	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)c5cncn5C	6.17405
541574	CC(=O)Nc1ncc(s1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.17466
535810	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)c5ccncc5	6.17766
528539	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCC5cnn(n5)c6ccccc6	6.17869
534139	c1ccc(cc1)CNC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.17908
533152	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCC(CC5)CO	6.1792
531645	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCc5ccc(cc5)NC	6.17963
526022	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5ccc(cc5)NC	6.18013

528842	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CCc5c[nH]cn5	6.18036
531406	c1cc(cc(c1)NC(=O)Cc2c[nH]cn2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.18038
540808	c1cc(ccc1CN2CCN(CC2)CCC#N)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.18118
529824	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cnccc5C(F)(F)F	6.18132
535898	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CNCCCN5CCCC5=O	6.18135
526743	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5cccnc5Cl	6.18266
533191	c1cc(ccc1c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)NC(=O)Cc5c[nH]cn5	6.18275
531917	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5ccc(=O)[nH]n5	6.1831
532080	CC(CN(C)C)C(=O)Nc1cccc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F	6.18479
525426	CC(=O)Nc1cccc(c1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.1855
541496	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)C(C)CN(C)C	6.18572
526659	c1ccc(cc1)n2ncc(n2)CNCc3cccc(c3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.18573
524855	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)C(=O)N5CCCCC5CN6CCC(C6)O	6.18583
540158	c1cc(ccc1CN2CCN(CC2)c3cnccn3)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.18608
537207	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cccc(c5)N(C)C(=O)C	6.18612
525862	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)CCc5c[nH]cn5	6.18668
530553	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.18885
535145	c1ccc(c(c1)C(=O)N)OCC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.1892
530970	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)c5cnn6c5nccc6	6.18921
526183	c1cc(ccc1CN2CCC(C2)N)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.18979
525493	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cccnc5	6.18995
532801	COc1ccc(cc1)CNCc2cccc(c2)c3cc(sc3)c4[nH]c5ccccc5n4	6.19034
539974	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)c5cncn5C	6.19074
528113	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5cnc(s5)NC(=O)C	6.19162
533644	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)CN5CCN(CC5)CCO	6.19271
525790	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCC(CC5)C(=O)N	6.19294
541555	COc1cccc1NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4	6.19314
539815	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCCC(C5)N	6.19365
526103	c1cc(cc(c1)F)CNC(=O)C=Cc2ccc(cc2)c3[nH]c4cc(ccc4n3)Cl	6.19384
531672	CCN(CC(C)O)C(=O)c1ccc(cc1)c2cccc(c2)c3[nH]c4c(cccc4n3)C	6.19457
538377	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4	6.19538
529183	Cc1cnc(cn1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.19598
542396	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCCC(C5)N	6.19612
526898	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)C(=O)N5CCCCC5C(C)O	6.1963
532027	Cn1cncc1C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4	6.19719
532920	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Cc5cccn(=O)c5	6.19725
528636	CC(=O)Nc1cccc(c1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.19829
532131	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)c5ccc(cc5)CC(=O)NC	6.19906
530509	CC(CN1CCN(CC1)C)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccccc5n4	6.19929
539583	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCCCN5CCCC5=O	6.19935
537903	c1ccc(cc1)C2CC2NC(=O)Nc3ccc(cc3)c4cccc(c4)c5[nH]c6cccccc6n5	6.20041
531387	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5c(nns5)C	6.20063
541898	CNCCNCc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.20172
525147	COc1cccc(c1)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4	6.2028
537143	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Cc5cccn(=O)c5	6.20302
526156	CCOC(=O)NCC(=O)Nc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.20328
538286	CC(C)CNCc1ccc(cc1)c2cccc(c2)c3[nH]c4cccc4n3	6.2036
540763	CCC(C)NC(=O)Nc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.20514
527798	CC(=O)Nc1ncc(s1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.20622
542077	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccc(cc5)N(C)C(=O)C	6.20738
536981	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCc5ccccc5	6.20857
539985	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cccc(c5)N(C)C(=O)C	6.20944
542779	c1cc(ccc1CN2CCN(CC2)c3cnccn3)c4ccc(s4)c5[nH]c6ccc(cc6n5)F	6.2098
533358	COc1ccc2c(c1)[nH]c(n2)c3ccc(cc3n2)c4ccc(cc4)NC(=O)CN5CCOCC5	6.21011
541998	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)CCO	6.21061
535452	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5ccccc5	6.21113
530539	Cc1ccoc1C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.21233
534429	c1cc2c(cc1c3[nH]c4ccc(cc4n3)NC(=O)C5CCCCC5)sc(n2)NC(=O)C6CCCCC6	6.2129
537719	c1cc(cc(c1)NC(=O)c2ccncc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.21325
535312	CCCN1CCN(CC1)Cc2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4	6.21376
537737	c1cncc(c1)CC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.21447



542459	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCC(CC5)C(=O)N	6.21464
525608	CCc1ccc(o1)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4[nH]c5ccccc5n4	6.21489
539293	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCN(CC5)CCO	6.2161
530872	c1cc(ccc1)NC(=O)c2cccnc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.21613
530042	CC(CN1CCN(CC1)C)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.21667
527890	CN(CCN)Cc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.21668
536758	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNc5ccc(cc5)CN	6.21735
528804	CNCCNCc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.21862
535756	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CNc5ccc(cc5)N	6.21913
531117	c1cc(ccc1)CNCCCN2CCCC2=O)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.21986
538476	c1cc(ccc1)CN2CCCC2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.22022
533607	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCC5CCCO5	6.22058
535046	Cc1c(cccn1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.22076
538736	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)CCO	6.22279
526079	Cn1cc(nc1)CCNC(=O)c2cccc(c2)c3ccc(s3)c4[nH]c5ccccc5n4	6.22289
532367	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCN(CC5)CCC#N	6.2229
526248	c1cc(ccc1)CNCC2CCCCO2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.22292
539149	c1cc(ccc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CNCCCN5CCCC5=O	6.22317
533523	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cnn6c5nccc6	6.22395
534870	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Cc5c(nc(s5)C)C	6.22462
536492	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCC(C5)N	6.22491
541597	CC(=O)N(C)C1CCN(C1)Cc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.22499
542806	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(s4)Cl	6.22561
535424	C1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cccnc5	6.22617
536500	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)Nc5ccc(cc5)Cl)Cl	6.22626
541370	CC(=O)Nc1cccc(c1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.22649
530703	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)c5c(nns5)C	6.22653
525745	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNc5cccc(c5)C(=O)N	6.22744
527945	c1ccc(cc1)CCN2CCN(CC2)C(=O)c3ccc(cc3)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.22798
527876	CC(=O)Nc1ccc(cc1)C(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4	6.22845
539586	CCOc1ccc(cc1N(=O)=O)C(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3	6.22872
536126	CS(=O)(=O)c1ccc(cc1)CNc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4	6.22916
534649	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCCCN5CCCC5=O	6.22939
528584	CC(=O)Nc1ncc(s1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.22947
539251	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCCCC5	6.22998
540182	c1cc(ccc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCC(CC5)CO	6.2305
531315	CN(CCC1CCCC1)Cc2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4	6.23081
535458	COC(=O)c1cccc(c1)CNc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.23084
533414	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)C(=O)NCCc5cn(cc5)C	6.23095
535880	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCCC(C5)N	6.23289
541396	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCCCC5	6.2331
536019	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C5CCC(CC5)OC	6.23316
532079	c1cc(ccc1)CNCCCN2CCCC2=O)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.23458
531163	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Cn5cc(c(=O)[nH]c5=O)C	6.23615
525906	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)Nc5ccccc5OC	6.237
535511	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cnc(cc5)C	6.23753
527589	CN1CCC(CC1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.23879
537722	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNc5ccccc5)N	6.24131
526491	c1cc(ccc1)NC(=O)c2cccnc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.24289
528866	c1ccc(cc1)CNc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4	6.24486
543080	CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.24491
526833	CN(C)CCNCc1ccc(cc1)c2ccc(s2)c3[nH]c4cccc4n3	6.24498
524973	Cc1c(c(on1)C)c2cccc(c2)CNc3ccc(cc3)c4cccc(c4)c5[nH]c6ccccc6n5	6.24499
525434	c1cc(ccc1)CN2CCN(CC2)CCO)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.24675
537512	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCCC(C5)N	6.2468
526084	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4	6.24693
527785	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl)Cl	6.2473
533317	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNc5cccc(c5)N	6.24761
536172	CC1CN(CC(O1)C)Cc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.24885
536566	CC(=O)N(C)C1CCN(C1)Cc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.24951
528158	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)CN5CCN(CC5)C	6.25016

533293	Cn1cncc1C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.25191
526042	c1cc(ccc1c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)C(=O)N5CCCC5CN6CCC(C6)O	6.25195
542299	Cn1c(ccn1)C(=O)NCCNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4	6.25222
533872	CC(=O)Nc1cccc(c1)NC(=O)CS2ccc(cc2)c3[nH]c4ccccc4n3	6.25259
534090	CS(=O)(=O)c1ccc(cc1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.25277
541218	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)CCO	6.25283
530543	CC(C)C(=O)Nc1ccc(cc1)c2cc(c(nc2)N)c3[nH]c4ccc(cc4n3)OC	6.25387
529857	c1cc(ccc1)NC(=O)CCc2c[nH]cn2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.25437
530720	Cc1c(c(on1)C)c2cccc(c2)CNCc3ccc(cc3)c4ccc(s4)c5[nH]c6ccccc6n5	6.25466
538658	Cc1c(c(on1)C)c2cccc(c2)CNCc3ccc(cc3)c4ccc(c4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.2551
540847	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CCc5c[nH]cn5	6.25753
538039	CC(=O)Nc1nc(cs1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4	6.25796
532870	c1ccc(cc1)n2ncc(n2)CNCc3cccc(c3)c4cccc(c4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.25817
528895	c1ccc2c(c1)[nH]c(n2)c3cc(cs3)c4ccc(cc4)NC(=O)Nc5ccsc5	6.25842
530644	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5cnn(n5)c6ccccc6	6.25888
540734	CCNCc1ccc(cc1)c2cccc(c2)c3[nH]c4ccccc4n3	6.25985
528356	CC(=O)Nc1cccc(c1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.26008
531912	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccc(cc5)C(=O)N	6.26147
539847	COC1CCC(CC1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.26167
525804	Cc1c(c(on1)C)c2cccc(c2)CNCc3ccc(cc3)c4ccc(c4)c5[nH]c6ccc(cc6n5)F	6.2636
530365	CC(C)(C)c1ccc(cc1)CNC(=O)C=Cc2ccc(cc2)c3[nH]c4ccc(cc4n3)C(C)(C)C	6.26378
536188	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5cccc(c5)C#N	6.2642
532470	COc1cccc1NC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.26449
530234	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5cccc(c5)N	6.26552
538107	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)Nc5ccsc5	6.26561
535792	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CNCc5CCCO5	6.26656
536826	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4cccc(c4)C#N	6.26708
542173	c1cc(ccc1CN2CCC(CC2)C(=O)N)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.26743
527673	CC(C1CCCN1C(=O)c2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F)O	6.26768
539529	c1ccc(cc1)n2ncc(n2)CNCc3ccc(cc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.26786
531855	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCCC(C5)N	6.2681
536022	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)C(C)CN5CCN(CC5)C	6.26981
525692	CC(C1CCCN1C(=O)c2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F)O	6.2709
525840	CC(C1CCCN1C(=O)c2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4)O	6.27284
531192	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CN5CCN(CC5)C	6.27328
536374	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccc(cc5)CC(=O)NC	6.27543
530347	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5ccncc5	6.27637
528361	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)C(=O)NCc5nccn5C	6.27747
539649	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CC(OC(C5)C)C	6.28181
528519	CC1CN(CC(O1)C)Cc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.28183
539155	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.28213
532057	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCCC5	6.28287
532970	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)NCc5ccccc5	6.28316
532429	c1cc(cc(c1)NC(=O)c2cccc(c2)C(=O)N)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.28389
529672	CN1CCN(CC1)CC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.28412
531322	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)C(=O)NCCN5CCCC5	6.28446
539139	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCCC(C5)N	6.28551
533363	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5cccc(c5)N	6.28652
525515	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)Nc5ccc(cc5)Cl	6.28673
528059	CS(=O)(=O)NCCNCNc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.2884
540069	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)c5ccncc5	6.28891
538248	c1cc(cc(c1)NC(=O)c2ccc(cc2)C(=O)N)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.28894
536010	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CNCc5CCCO5	6.2896
530689	CS(=O)(=O)c1ccc(cc1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.29007
535942	c1cc(ccc1c2[nH]c3ccc(cc3n2)Cc4ccc5c(c4)nc([nH]5)c6ccc(cc6)N)N	6.29078
537318	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCc5cccc(c5)N	6.29248
539827	Cn1cncc1C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.29301
534174	COc1ccc(cc1)NC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.29306
542684	CN(CCN)Cc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.29365
534613	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5ccccc5	6.29411
528363	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCC(CC5)CO	6.29581

541446	COc1cc(cc(c1)OC)C(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3	6.29595
526343	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cn(c(=O)n5C)C	6.29706
534690	COC(=O)c1cccc(c1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.29777
541330	CCNC(=O)Nc1ccc(cc1)c2cc(c(nc2)N)c3[nH]c4cc(ccc4n3)OC	6.30156
529891	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5ccncc5	6.3038
527259	Cn1cncc1C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.30749
525088	COC(=O)c1cccc(c1)CNCc2cccc(c2)c3ccc(s3)c4[nH]c5cccc5n4	6.30925
528372	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5ccc(cc5)CN	6.31086
533229	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)CN5CCC(CC5)CO	6.31606
526396	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCNC(=O)c5ccnn5C	6.31881
527508	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccncc5	6.31939
528012	c1cc(ccc1CN2CCC(CC2)CO)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.32184
536088	CN(C)CCNCc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F	6.324
531628	Cn1c(ccn1)C(=O)NCCNCc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.32527
533174	c1ccc2c(c1)C(=O)NC2=O)CC(=O)Nc3ccc(cc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.32802
535718	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCCCC5	6.32933
528424	CS(=O)(=O)NCCNCc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.33066
537816	c1cc(cc(c1)C(=O)N2CCCC2CN3CCC(C3)O)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.33216
527421	Cc1ccc(cc1NC(=O)C)C(=O)Nc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.33297
535417	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)C(=O)N5CCCCC5CN6CCC(C6)O	6.33471
541857	CC(=O)Nc1nc(cs1)C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.33714
535102	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(c4)NC(=O)c5c[nH]cn5	6.33779
536777	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.33813
533382	CS(=O)(=O)NCCNCc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.34042
536350	c1ccc(cc1)n2ncc(n2)CNCc3ccc(cc3)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.34078
536650	Cc1c(c(on1)C)c2cccc(c2)CNCc3cccc(c3)c4cccc(c4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.34104
534585	c1ccc(cc1)CNCc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.34116
542074	CC(=O)Nc1ncc(s1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.34294
540268	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)NCc5cccc(c5)F	6.34413
525131	c1ccc2c(c1)[nH]c(n2)c3cc(cs3)c4cccc(c4)CN5CCN(CC5)CCN6CCOCC6	6.34441
527864	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Cc5ccc(c(c5)O)OC	6.34452
529454	COc1ccc(cc1)NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.34503
529866	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCN5CCCC5=O	6.34868
527697	Cn1cncc1C(=O)Nc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.34928
538777	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCc5ccc(cc5)CN	6.35504
542836	c1cc(ccc1CNCC2CCCO2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.35608
542411	CNC(=O)Cc1ccc(cc1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.35669
536527	c1cc(cc(c1)N)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.35819
536383	Cc1c(snn1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.35926
532309	CC(C1CCCCN1C(=O)c2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F)O	6.36108
542955	c1ccc(cc1)n2ncc(n2)CNCc3ccc(cc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.36359
536578	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5cnn(n5)c6cccc6	6.3686
532213	Cc1c(c(on1)C)c2cccc(c2)CNCc3ccc(cc3)c4ccc(s4)c5[nH]c6ccc(cc6n5)F	6.37345
537583	c1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.3742
528373	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCC5CCCO5	6.37436
534008	CC(=O)Nc1nc(cs1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.37531
539687	CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.37627
527402	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5cccc(c5)N	6.38161
539928	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.38199
540200	CN1CCCC(C1)CN2CCN(CC2)Cc3cccc(c3)c4cc(sc4)c5[nH]c6cccc6n5	6.38334
525770	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)C(C)CN(C)C	6.38403
540987	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(cc4)S(=O)(=O)N5CCCCC5	6.38609
540011	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)CCc5c[nH]cn5	6.38676
525094	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cccc(c5)C(=O)N	6.3877
536685	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)C(C)CN(C)C	6.38853
529535	c1cc(ccc1CNCC2CCCO2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.39027
527157	CC(C)NCc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F	6.39208
532530	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCC(C)C	6.3924
536439	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5ccncc5	6.39365
534881	CC(CN1CCN(CC1)C)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.39432
542153	c1ccc2c(c1)[nH]c(n2)c3cc(cs3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.39581

535844	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCc5cccc(c5)C(=O)OC	6.39603
530985	Cn1cc(nc1)CCNC(=O)c2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.39621
529418	c1cc(ccc1CN)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.39629
526685	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc(cc5)OC	6.39845
527631	CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.39921
528902	CC(=O)Nc1ncc(s1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.40012
530714	CN(C)CCN1CCN(CC1)Cc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.40022
541389	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5ccc(s5)c6ccccn6	6.4019
528174	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCNC(=O)c5ccnn5C	6.40279
525543	Cc1ncc(s1)CN2CCC(CC2)C(=O)Nc3ccc(cc3)c4nc5cccc5o4	6.40509
531692	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5cccc5	6.40518
532816	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5cccc(c5)N	6.40873
530495	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)NCc5cccc(c5)F	6.4103
536987	Cn1cc(n(c1=O)C)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.41087
528142	CNCCNCc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F	6.41235
540232	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCCC(C5)N	6.41767
542506	c1cc(ccc1CNCCCN2CCCC=O)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.41993
537692	c1cc(ccc1CN2CCN(CC2)CCO)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.4213
537794	Cc1c(c(on1)C)c2cccc(c2)CNCc3cccc(c3)c4cccc(c4)c5[nH]c6cccc6n5	6.42333
538031	c1ccc(c(c1)C(=O)N)OCC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.42436
536676	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C(=O)c5cccn5C	6.42545
531870	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.42609
532949	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCC(C5)N	6.42776
543005	CN1CCN(CC1)CC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.43
525346	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)C(=O)N5CCCCC5(C)O	6.43032
527888	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5cccc(c5)c6c(noc6C)C	6.43225
534394	c1cc(ccc1c2ccc(cc2)C(=O)N3CCCCC3CN4CCC(C4)O)c5[nH]c6ccc(cc6n5)F	6.43371
525074	COc1ccc(cc1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.43381
534766	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCC5CCCO5	6.43498
538715	c1cc(cc(c1)NC(=O)c2cccnc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.44021
527145	c1ccc2cc3c(cc2c1)[nH]c(n3)c4ccc(cc4)NC(=O)c5cccc(c5)Br	6.44052
525835	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCc5cccc(c5)N	6.44325
537674	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)NC(=O)c4cccc(c4)NC(=O)c5ccc5	6.44344
537960	CC(C)(C)OC(=O)C1CCCN(C1)Cc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.44618
541470	COc(=O)c1cccc(c1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.4506
537208	CC(=O)Nc1ncc(s1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.45104
541149	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cnc(s5)NC(=O)C	6.45158
541145	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5ccc(cc5)C(=O)N	6.45475
538928	Cc1c(snn1)C(=O)Nc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.45509
539689	c1cc(cc(c1)NC(=O)Nc2ccsc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.45523
527180	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)c5cccc(c5)C(=O)N	6.45578
526059	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCCC(C5)N	6.45651
527169	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)c5cccc(c5)C(=O)N	6.45726
538425	c1cc(ccc1CN2CCCCC2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.45749
535760	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)CCc5c[nH]cn5	6.45856
540039	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5ccc(cc5)OC	6.4672
531119	C=CCOC(=O)N1CCC(C1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.46909
532657	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.47101
539429	c1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5cccc5n4	6.47145
542679	c1cc(cc(c1)NC(=O)c2ccncc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.47276
525436	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCCc5ccncc5	6.47388
533035	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNC(C)C	6.47429
529417	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5ccc(cc5)S(=O)(=O)C	6.47665
531965	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)c5ccc5	6.47785
536472	c1cc(cc(c1)F)CNC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.48087
541594	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.48168
529611	c1ccc(cc1)n2ncc(n2)CNCc3cccc(c3)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.48236
539372	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccc(c(c5)NC(=O)C)C	6.48339
541590	CS(=O)(=O)c1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.48672
528388	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccc(cc5)C(=O)N	6.49066
533662	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5cccc(c5)C(=O)OC	6.49261

539890	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5ccc(cc5)NC	6.49558
525795	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3O)NC(=O)c4ccc(cc4)N(=O)=O	6.49752
530951	CS(=O)(=O)c1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.50137
541492	CC(=O)N(C)c1ccc(cc1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.50307
533720	Cc1c(snn1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.50314
529716	CNCCNCc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.50374
542886	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C5CCN(CC5)C(=O)C	6.50473
539487	COc1ccc(cc1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.5074
537430	COc1ccc(cc1)NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.50989
531536	CN1CCN(CC1)CC(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.51007
532848	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CNCc5ccc(cc5)CN	6.51097
534480	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCCNC(=O)c5ccnn5C	6.51207
527146	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCN(CC5)CCN6CCOCC6	6.51248
538178	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5cccc(c5)C(=O)OC	6.51435
537409	COc1cccc1NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.51468
525951	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5csnn5	6.51646
529400	Cn1c(ccn1)C(=O)NCCNCc2cccc(c2)c3ccc(s3)c4[nH]c5cccc5n4	6.51909
538297	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)CCc5c[nH]cn5	6.52026
539879	c1cc(cnc1)c2cc(c3cc(ccc3n2)Cl)C(=O)Nc4ccc(cc4)S(=O)(=O)N5CCCC5	6.52286
534517	COc1ccc(cc1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.52305
530508	CNc1ccc(cc1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.52325
526600	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCN5CCCC5=O	6.52331
538930	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5ccc(cc5)S(=O)(=O)C	6.5239
535383	CN1CCN(CC1)CC(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5cccc5n4	6.52441
541287	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCN5CCCC5=O	6.52471
531456	COC(=O)c1cccc(c1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.52577
542042	Cn1c(ccn1)C(=O)NCCNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.52685
543037	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	6.53413
526666	CC(=O)Nc1nc(cs1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.53536
541463	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)CC5c6cccc6C(=O)N5	6.5391
538370	COC(=O)c1cccc(c1)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5cccc5n4	6.53917
532172	CC(=O)Nc1nc(cs1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.54097
542340	CC(C)NCc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F	6.54519
529167	c1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.54688
524998	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5cccc(c5)C(=O)OC	6.54839
527738	c1ccc(cc1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.54884
536301	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)CNC5ccc(cc5)C(=O)N	6.54923
528641	CC(C)(C)C(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3[nH]c4cccc4n3	6.55016
529642	CCOC(=O)c1ccc(cc1)c2cc(c(nc2)N)c3[nH]c4c(cccc4n3)C	6.55095
536449	CC(C1CCCN1C(=O)c2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F)O	6.55273
540058	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)CCN6CCOCC6	6.55284
540169	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)C(=O)N5CCCC5CN6CCC(C6)O	6.55422
542318	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccsc5	6.55495
532680	c1cc(cc(c1)NC(=O)c2ccncc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.55555
534929	c1cc(cc(c1)NC(=O)c2csnn2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.55573
532524	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)CNCC5CCCO5	6.55721
529907	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5ccoc5	6.55801
530868	Cc1cnc(cn1)C(=O)Nc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.56079
532300	c1cc(cc(c1)NC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F)C#N	6.56085
533448	CC(CN1CCN(CC1)C)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.56187
532947	CNC(=O)Cc1ccc(cc1)C(=O)Nc2cccc(c2)c3cc(sc3)c4[nH]c5cccc5n4	6.56312
533214	CCOC(=O)c1ccc(cc1)NC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.56418
534275	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)C(F)(F)F	6.56432
540004	C=CCOC(=O)N1CCC(C1)CNCc2cccc(c2)c3ccc(s3)c4[nH]c5cccc5n4	6.56497
534743	CC(C(=O)Nc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)NC(=O)C5CCCC5	6.56544
542521	CC(C)(C)OC(=O)C(CC(=O)N)NC(=O)c1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.56739
536005	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)CNC5ccc(cc5)C(=O)N	6.56863
530684	CS(=O)(=O)c1ccc(cc1)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.57172
532793	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCCC5	6.57296
537403	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(o4)c5cccc(c5)N(=O)=O	6.57407
538804	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5c(nns5)C	6.57417

526866	c1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.57558
537377	CC(C)NCc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.57586
543114	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5ccc(nc5)NC(=O)C	6.5773
532242	c1ccc(cc1)CNC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.57824
529214	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5ccc(cc5)OC	6.5804
534808	Cc1c(c(on1)C)c2cccc(c2)CNCc3cccc(c3)c4cc(sc4)c5[nH]c6cccc6n5	6.58062
537042	CC(C)NCc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.582
527262	Cn1c(ccn1)C(=O)NCCNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.58345
538104	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCc5ccc(cc5)CN	6.58348
525987	COC(=O)c1cccc(c1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.5838
542457	CC(=O)Nc1ncc(s1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.58478
538493	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5cccc(c5)N	6.5857
534329	c1cc(ccc1)NC(=O)Nc2ccc(c(c2F)F)F)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.58662
530833	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5c[nH]cn5	6.58773
535441	c1ccc2c(c1)[nH]c(n2)c3cc(cs3)c4cccc(c4)CNCCc5ccncc5	6.58868
538374	COC(=O)c1cccc(c1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.59083
530744	c1ccc2c(c1)[nH]c(n2)c3cc(cs3)c4cccc(c4)NC(=O)c5ccncc5	6.5923
530608	C=CCOC(=O)N1CCC(C1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.59419
529018	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc6c(c5)OCO6	6.59478
532253	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4ccc(s4)N(=O)=O	6.59884
539469	c1cc(ccc1)CN2CCN(CC2)c3ccncc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.60033
542991	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCC5CCN(C5)C(=O)OCC=C	6.60037
535094	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCC5CCCO5	6.60164
539753	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)c5cccc(c5)C(=O)N	6.60319
538579	COc1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.60376
535462	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCC5CCN(C5)C(=O)OCC=C	6.60528
541473	CC(CN(C)C)C(=O)Nc1cccc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.60533
532256	c1cc(ccc1)NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F)C#N	6.60716
537824	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5cccc5	6.60819
526285	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccsc5	6.60892
537145	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)CCN6CCOCC6	6.61151
525458	c1cc(ccc1)NC(=O)CCc2c[nH]cn2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.61289
541469	CC(=O)Nc1ccc(cc1)c2[nH]c3ccc(cc3n2)c4[nH]c5ccc(cc5n4)NC(=O)C	6.61624
529013	c1cc(ccc1)c2[nH]c3ccc(cc3n2)c4ccc5c(c4)[nH]c6ccc(cc6)Cl)Cl	6.61774
527411	COc1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5cccc5n4	6.61876
524474	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCc5cccc(c5)c6c(noc6)C	6.62113
540237	CC(=O)N1CCC(CC1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.62199
525673	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5csnn5	6.62334
542885	CC(=O)Nc1ccc(cc1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.62361
528131	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5ccc(c(c5F)F)F	6.62393
525899	COC(=O)c1cccc(c1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.62553
530584	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5ccc(cc5)OC	6.62586
527277	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)NCc5cccc(c5)F	6.62617
531894	CS(=O)(=O)c1cccc1)CNC(=O)c2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.62664
542414	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCN(CC5)CCN6CCOCC6	6.62668
529246	CC(=O)N(C)c1cccc(c1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.62682
538786	c1cc(cnc1)CCNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.62742
532491	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc(cc5)Cl	6.62769
527059	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccncc5	6.62769
539557	Cc1c(snn1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.62834
530404	CCOC1cc(ccc1OCC)OCC)C(=O)Nc2ccc(cc2)c3[nH]c4cccc4n3	6.63098
534407	Cn1cncc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.63157
525455	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.6331
541248	c1ccc2c(c1)c(=O)cc([nH]2)C(=O)Nc3cccc(c3)c4cc(sc4)c5[nH]c6cccc6n5	6.6336
541269	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5csc(n5)NC(=O)C	6.63425
530305	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5csc(n5)NC(=O)C	6.63435
529589	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)NCc5cccc5	6.63565
542346	c1ccc(cc1)NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.63589
533915	CC(=O)Nc1ccc(cc1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.63593
527291	CC(C)NCc1ccc(cc1)c2cccc(c2)c3[nH]c4cccc4n3	6.63614
528495	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.63656

533713	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)CCN6CCOCC6	6.63667
527878	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNC(C)C	6.6372
541550	c1ccc2c(c1)[nH]c(n2)c3cc(s3)c4cccc(c4)NC(=O)c5ccccc5	6.6383
539976	C=CCOC(=O)N1CCC(C1)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccccc5n4	6.64064
529541	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5ccc(cc5)C(=O)N	6.64108
534686	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccccc5	6.64125
537701	Cc1c(c(on1)C)c2cccc(c2)CNCc3cccc(c3)c4ccc(cc4)c5[nH]c6ccccc6n5	6.64134
539084	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)Nc5ccc(cc5)Cl	6.64457
531797	c1cc(cc(c1)NC(=O)NCc2ccc(cc2)F)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.64548
536772	c1cc(cc(c1)NC(=O)Nc2cccc(c2)c3ccc(c3)c4[nH]c5ccc(cc5n4)F)C#N	6.64702
525846	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)Cc5c[nH]cn5	6.64718
536972	c1cc(cc(c1)NC(=O)Nc2cccc(c2)c3ccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F)C#N	6.65021
527855	c1ccc(cc1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.65314
533570	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)NC(=O)c5csc(n5)NC(=O)C	6.65409
528110	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C(C)CN(C)C	6.65452
527325	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)Nc5ccc(cc5)Cl	6.65662
536890	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)NC(=O)c4cccc(c4)N(=O)=O	6.65685
535926	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccoc5	6.65913
527982	Cn1c(ccn1)C(=O)NCCNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.66232
536236	Cc1c(snn1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.66252
531832	c1cc(ccc1c2ccc(cc2)NC(=O)Nc3ccc(c(c3F)F)F)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.66439
529227	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCCNC(=O)c5ccnn5C	6.66646
528233	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5cccc(c5)c6c(noc6C)C	6.66678
535437	Cc1ccc(cc1NC(=O)C)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.66707
527740	COc1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4	6.67012
535141	CC(C)NCc1ccc(cc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F	6.67103
535705	c1cc(cc(c1)N)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.67182
534996	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCCc5ccccc5	6.6722
538909	Cc1c(c(on1)C)c2cccc(c2)CNCc3ccc(cc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.67285
525635	CCOC(=O)c1ccc(cc1)NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.6745
530294	CCOC(=O)c1ccc(cc1)NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.67454
531342	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)c5cnn6c5nccc6	6.6747
531062	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCN(CC5)c6ccncc6	6.67489
540999	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5cccc(c5)c6c(noc6C)C	6.67534
529085	c1ccc2c(c1)[nH]c(n2)c3cc(s3)c4cccc(c4)NC(=O)c5ccoc5	6.67621
526651	COC(=O)c1ccc2c(c1)[nH]c(n2)c3cc(cnc3N)c4cccc(c4)c5ccccc5	6.67633
541860	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5cccc(c5)C(=O)OC	6.67651
532866	CNc1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.67746
534132	CC(CN(C)C)C(=O)Nc1ccc(cc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.67816
525540	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CNCCc5ccccc5	6.68194
531214	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCc5ccccc5	6.68278
539563	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCCN5CCOCC5	6.68308
525730	C=CCOC(=O)N1CCC(C1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.68374
535691	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5c[nH]cn5	6.68657
537472	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.68701
527894	Cn1cncc1C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.68863
541497	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4	6.68951
539248	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5ccncc5	6.69079
529135	Cc1c(c(on1)C)c2cccc(c2)CNCc3cccc(c3)c4ccc(s4)c5[nH]c6cccccc6n5	6.69099
529365	CNCCNCc1cccc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F	6.69318
531024	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)c6ccncc6	6.69375
541342	COc1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.69514
534553	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCCc5ccccc5	6.69528
526722	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5ccncc5	6.69606
537963	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCN(CC5)c6ccncc6	6.69841
532001	CN(C)CCN1CCN(CC1)Cc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4	6.70032
525175	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	6.70078
531771	CCOC(=O)c1ccc(cc1)NC(=O)Nc2ccc(cc2)c3ccc(s3)c4[nH]c5c(cccc5n4)C	6.70115
542916	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)Nc5ccsc5	6.70185
540005	COc1ccc(cc1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.70785
529185	CN1CCC(CC1)N2CCN(CC2)Cc3cccc(c3)c4cccc(c4)c5[nH]c6cccccc6n5	6.71192

532302	CS(=O)(=O)c1ccc(cc1)CCNCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccc5n4	6.712
532971	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.71282
527967	CC(C)NCc1cccc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)F	6.71357
535255	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCCNC(=O)c5ccnn5C	6.71721
526489	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)F)c4ccc(cc4)CNCCCN5CCCC5=O	6.71809
532464	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCc5cccc(c5)c6c(noc6C)C	6.71871
527041	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)c5ccc(nc5)NC(=O)C	6.71992
542214	CCC(C)NC(=O)Nc1ccc(cc1)c2cccc(c2)c3[nH]c4c(ccc4n3)C	6.72379
535681	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5cccc(c5)C#N	6.72755
541572	Cn1c(ccn1)C(=O)NCCNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)F	6.72979
531255	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5cccc(c5)C(=O)OC	6.73021
526588	CC(=O)Nc1ncc(s1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)F	6.73337
527561	CC(=O)Nc1nc(cs1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)F	6.734
528589	CN1CCCC(C1)CN2CCN(CC2)Cc3ccc(cc3)c4cccc(c4)c5[nH]c6ccc(cc6n5)F	6.73529
537770	c1cc(ccc1)CN2CCC(C2)Nc3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.73561
535699	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5ccc(cc5)S(=O)(=O)C	6.73576
532354	c1cc(ccc1)CN2CCN(CC2)CCN3CCOCC3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.73805
534062	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.73966
539836	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNC5CCN(CC5)C	6.73974
536116	CS(=O)(=O)c1ccc(cc1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)F	6.73986
534301	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)c5csc(n5)NC(=O)C	6.74004
540807	Cc1c(c(on1)C)c2cccc(c2)CNCc3ccc(cc3)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)F	6.74115
534020	CC(C)NCc1ccc(cc1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)F	6.74128
542985	CC(=O)Nc1cccc(c1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5cccc5n4	6.74281
533744	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCc5ccc(cc5)OC	6.74495
526196	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5cccc5n4	6.74539
538025	c1cc(ccc1)CN2CCCC(C2)Nc3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.75114
538675	CNc1ccc(cc1)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)F	6.75119
531294	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.75325
543031	Cc1c(c(on1)C)c2cccc(c2)CNCc3cccc(c3)c4cccc(c4)c5[nH]c6ccc(cc6n5)F	6.75348
530189	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.75363
526688	c1ccc(cc1)NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.75417
530938	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)OC	6.75609
530438	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)C(C)CN5CCN(CC5)C	6.75657
527495	c1cc(cc(c1)F)c2cc(c(nc2)N)c3[nH]c4ccc(cc4n3)F	6.75692
542277	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.75981
532355	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5c[nH]c6c5cc(cc6)F	6.76019
530038	COc1ccc(cc1)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)F	6.76032
537032	CN1CCC(CC1)N2CCN(CC2)Cc3ccc(cc3)c4cccc(c4)c5[nH]c6ccc(cc6n5)F	6.76075
537009	Cc1c(c(on1)C)c2cccc(c2)CNCc3ccc(cc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)F	6.76325
534359	COC(=O)c1cccc(c1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)F	6.7642
538885	c1cc(cc(c1)N)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)F	6.76437
541148	CC(=O)Nc1nc(cs1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5cccc5n4	6.76477
542762	Cn1c(ccn1)C(=O)NCCNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)F	6.76507
526288	COc1ccc(cc1)NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.76619
528509	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccsc5	6.76673
540226	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccsc5	6.76997
528944	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)F)CNCc5ccncc5	6.7702
535188	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CNCc5ccncc5	6.77029
541776	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5F)F)F	6.77559
528159	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc6c(c5)OCO6	6.77716
531054	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5cnnc5C	6.77762
541402	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCNC(=O)c5ccnn5C	6.77784
541677	CNc1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)F	6.77844
538038	Cc1c(c(on1)C)c2cccc(c2)CNCc3cccc(c3)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)F	6.77936
539841	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)Nc5ccc(cc5)F	6.78215
535975	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.78297
529390	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5ccncc5	6.78388
529926	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)c6ccncc6	6.78556
534974	c1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)F	6.78695
528357	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)c6ccncc6	6.78755



531419	c1cc(ccc1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCCCC5	6.78803
538498	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)COc5ccccc5C(=O)N	6.79363
528512	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)CCN6CCOCC6	6.79626
540781	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CNCCc5ccncc5	6.80033
537645	c1cc(ccc1)CNCC2CCCO2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.80064
536078	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccccc5OC	6.80065
537132	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5ccc(cc5)c6csnn6	6.80111
534607	c1cc(ccc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)c6ccncc6	6.80148
540642	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)CCN6CCOCC6	6.80265
538126	c1cc(ccc1)CN)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.80332
525957	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	6.80365
529229	CN1CCCC(C1)CN2CCN(CC2)Cc3cccc(c3)c4ccc(cc4)c5[nH]c6cccc6n5	6.80367
542807	COC(=O)c1cccc(c1)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.80531
529967	CN1CCC(CC1)N2CCN(CC2)Cc3cccc(c3)c4ccc(cc4)c5[nH]c6cccc6n5	6.80654
536892	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5ccsc5	6.80717
527439	CS(=O)(=O)c1ccc(cc1)CNCc2ccc(cc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.80797
536017	COC(=O)c1cccc(c1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.80813
542328	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCN(CC5)CCN6CCOCC6	6.81395
527081	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCC(CC5)CCN6CCCCC6	6.81476
540042	c1cc(ccc1)CN2CCN(CC2)c3ccncc3)c4ccc(s4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.81491
532401	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCC(CC5)N6CCCCC6	6.8161
542514	c1ccc(cc1)CNCc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.81616
538231	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCN(CC5)c6ccncc6	6.81635
531998	CN1CCC(CC1)N2CCN(CC2)Cc3ccc(cc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.81655
533556	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	6.81831
534971	c1ccc2c(c1)[nH]c(n2)c3cc(c3)c4ccc(cc4)NC(=O)Nc5cccc(c5)C#N	6.81846
537672	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)NC(=O)c4ccc(o4)c5cccc(c5)N(=O)=O	6.8202
526200	Cn1c(ccn1)C(=O)NCCNCc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.82051
530057	COc1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.8222
528204	C=CCOC(=O)N1CCC(C1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.8226
538987	CC(=O)Nc1nc(cs1)C(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccccc5n4	6.82317
536002	c1cc(ccc1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)NC(=O)Nc5ccsc5	6.82514
542720	CN1CCCC(C1)CN2CCN(CC2)Cc3cccc(c3)c4ccc(s4)c5[nH]c6cccc6n5	6.82665
534056	c1ccc2c(c1)[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCN(CC5)c6ccncc6	6.82851
530009	CC(=O)Nc1cccc(c1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.82907
526939	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5ccccc5	6.83095
528154	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCC(C5)N	6.83191
525333	c1cc(ccc1)CN2CCN(CC2)CCN3CCOCC3)c4ccc(s4)c5[nH]c6ccc(cc6n5)F	6.834
530778	C=CCOC(=O)N1CCC(C1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.83473
537431	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)NC(=O)NCCc5ccc(cc5)F	6.83562
529752	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4cccc(c4)CNCCc5ccncc5	6.83577
542624	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCc5ccncc5	6.83605
539878	CN1CCCC(C1)CN2CCN(CC2)Cc3cccc(c3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.83766
526467	c1cc(ccc1)c2cccc(c2)c3[nH]c4ccc(cc4n3)F)CN5CCN(CC5)c6ccncc6	6.83768
529284	Cn1c(ccn1)C(=O)NCCNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.83794
528992	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc6c(c5)OCO6	6.83872
541741	CN1CCC(CC1)N2CCN(CC2)Cc3ccc(cc3)c4cccc(c4)c5[nH]c6cccc6n5	6.83896
539378	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCN(CC5)CCN6CCOCC6	6.83943
533143	CCOC(=O)c1ccc(cc1)NC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccccc5n4	6.83975
528949	CCOC(=O)c1ccc(cc1)NC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5c(cccc5n4)C	6.83982
539321	c1cc(ccc1)NC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F)C#N	6.83993
525820	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)C6CCN(CC6)C	6.84008
534339	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)CC6CCN(CC6)C	6.8412
532573	c1cc(ccc1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCCCC5	6.84159
534273	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCC(CC5)CCN6CCCCC6	6.84224
534538	CCOC(=O)c1ccc(cc1)NC(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5c(cccc5n4)C	6.84284
534276	c1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.84502
536574	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)OC	6.84631
536397	c1cc(ccc1)CNCc2ccncc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.84641
536852	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)CC6CCCN(CC6)C	6.84649
539924	c1cc(ccc1)CNCc2ccncc2)c3ccc(s3)c4[nH]c5ccc(cc5n4)F	6.84722

531982	c1cc(ccc1CN2CCC(CC2)CCN3CCCCC3)c4ccc(s4)c5[nH]c6ccc(cc6n5)F	6.8474
528434	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CN5CCC(CC5)CCN6CCCCC6	6.84766
525892	c1ccc2c(c1)[nH]c(n2)c3cc(cs3)c4cccc(c4)CN5CCC(CC5)CCN6CCCCC6	6.84773
526716	CN1CCC(CC1)NCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.84794
540815	c1cc(cc(c1)c2cccc(c2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCc5ccncc5	6.85015
532159	CN1CCCC(C1)CN2CCN(CC2)Cc3ccc(cc3)c4ccc(cc4)c5[nH]c6cccccc6n5	6.85221
535063	CN1CCC(CC1)N2CCN(CC2)Cc3ccc(cc3)c4ccc(s4)c5[nH]c6cccccc6n5	6.85249
527170	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCC(CC5)CCN6CCCCC6	6.85249
541519	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CN5CCN(CC5)c6ccncc6	6.8528
537772	C=CCOC(=O)N1CCC(C1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.85335
542148	CN1CCC(CC1)N2CCN(CC2)Cc3cccc(c3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	6.85392
538993	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCC(CC5)CCN6CCCCC6	6.85398
542561	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCc5ccncc5	6.85599
536348	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCc5ccncc5	6.85638
533056	CN1CCCC(C1)CN2CCN(CC2)Cc3cccc(c3)c4cccc(c4)c5[nH]c6cccccc6n5	6.85649
531097	c1cc(cc(c1)NC(=O)Nc2ccc(c(c2)Cl)Cl)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.85658
539092	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccccc5	6.85763
536694	CN1CCCC(C1)CN2CCN(CC2)Cc3cccc(c3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.85828
529833	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CNCc5ccncc5	6.85915
537934	CS(=O)(=O)c1ccc(cc1)CNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.85993
541380	Cn1c(ccn1)C(=O)NCCNCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccccc5n4	6.86253
540902	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)NC(=O)Nc5ccc6c(c5)OCO6	6.86464
537539	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCC(CC5)CCN6CCCCC6	6.86775
528569	COc1ccc(cc1)CNCc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.87089
529493	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCCc5ccc(cc5)OC	6.87174
537913	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.87333
525940	CN1CCCC(C1)CN2CCN(CC2)Cc3ccc(cc3)c4ccc(s4)c5[nH]c6cccccc6n5	6.87649
528312	c1ccc2c(c1)[nH]c(n2)c3cc(cs3)c4cccc(c4)NC(=O)c5cccc(c5)C(=O)N	6.87663
530320	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)CCc5c[nH]cn5	6.87866
542322	CN1CCCC(C1)CN2CCN(CC2)Cc3ccc(cc3)c4cccc(c4)c5[nH]c6cccccc6n5	6.88003
537689	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc(cc5)Cl	6.88136
526594	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)CCN6CCOCC6	6.88274
541892	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc(c(c5)Cl)Cl	6.88293
526125	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCc5ccc(cc5)OC	6.88645
525152	c1cc(ccc1CN2CCC(CC2)CCN3CCCCC3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.88821
542759	COC(=O)c1cccc(c1)CNCc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.88921
534434	c1cc(ccc1)CNCc2ccncc2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.89032
532616	CN1CCCC(C1)CN2CCN(CC2)Cc3ccc(cc3)c4ccc(s4)c5[nH]c6ccc(cc6n5)F	6.89768
532101	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCN(CC5)c6ccncc6	6.89849
535654	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CN5CCN(CC5)c6ccncc6	6.89911
526595	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)c5cccc(c5)C(=O)N	6.89915
531606	COc1ccc(cc1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.89942
537593	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3ccc(s3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.89965
527255	CN1CCC(CC1)NCc2ccc(cc2)c3cccc(c3)c4[nH]c5cccccc5n4	6.90091
534506	CCOC(=O)c1ccc(cc1)NC(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	6.91456
534591	Cn1c(ccn1)C(=O)NCCNCc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.9147
529501	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4cccc(c4)CN5CCN(CC5)CC6CCCN(C6)C	6.91617
539215	COc1cccc1NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.92165
526462	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4cccc(c4)NC(=O)Nc5ccc(c(c5F)F)F	6.92327
536488	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCc5ccncc5	6.9235
541881	CC(=O)Nc1ccc(cc1)C(=O)Nc2cccc(c2)c3cc(sc3)c4[nH]c5cccccc5n4	6.92502
525435	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)c6ccncc6	6.9267
542410	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCC5CCN(C5)C(=O)OCC=C	6.92716
542461	CN1CCCC(C1)CN2CCN(CC2)Cc3ccc(cc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.93017
526337	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4cccc(c4)CN5CCN(CC5)c6ccncc6	6.93149
528458	Cn1c(ccn1)C(=O)NCCNCc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.93173
532654	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5cccc(c5)C#N	6.9329
529747	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CNCCc5ccncc5	6.93296
530944	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccsc5	6.93312
537846	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4ccc(cc4)NC(=O)Nc5ccsc5	6.93379
536495	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4ccc(cc4)CNCCc5ccncc5	6.93961

526724	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5csc(n5)NC(=O)C	6.93988
525386	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5cccc(c5)C#N	6.94286
540838	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)CN5CCN(CC5)c6ccncc6	6.94371
537973	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4ccc(cc4)CNCCNc5ccnc5	6.9452
538050	Cc1cccc2c1[nH]c(n2)c3ccc(s3)c4ccc(cc4)NC(=O)Nc5ccsc5	6.94679
540555	c1cc(cc(c1)NC(=O)Nc2ccc(c(c2F)F)F)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	6.94708
541734	CNc1ccc(cc1)CNCc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.95194
534700	CC(=O)Nc1ccc(cn1)C(=O)Nc2ccc(cc2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	6.95484
529076	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)CNCC5CCN(C5)C(=O)OCC=C	6.96228
530540	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc(c(c5F)F)F	6.96778
533712	CN1CCC(CC1)N2CCN(CC2)Cc3cccc(c3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)F	6.97015
528167	CCOC(=O)c1ccc(cc1)NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5c(ccc5n4)C	6.97434
528663	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5cccc(c5)C#N	6.98147
528548	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	6.99897
536829	Cc1cccc2c1[nH]c(n2)c3ccc(cc3)c4ccc(cc4)CN5CCN(CC5)C6CCN(CC6)C	6.99909
538181	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)C(F)(F)F)c4ccc(cc4)CNCCc5ccncc5	7.00477
538738	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(c(c5)Cl)Cl	7.00504
539981	Cc1(c(snn1)C(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	7.01684
529997	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5cccc5OC	7.019
529949	CCOC(=O)c1ccc(cc1)NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	7.02357
536289	CCOC(=O)c1ccc(cc1)NC(=O)Nc2cccc(c2)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	7.0248
528151	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)NCc5ccc(cc5)F	7.04241
527679	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5cccc(c5)C#N	7.0446
524874	CC(=O)Nc1nc(cs1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)F	7.04962
539883	c1cc(cc(c1)c2[nH]c3ccc(cc3n2)F)c4cccc(c4)NC(=O)Nc5ccc(c(c5F)F)F	7.05033
536311	c1cc(cc(c1)c2ccc(s2)c3[nH]c4ccc(cc4n3)C(F)(F)F)CN5CCN(CC5)CCO	7.06226
525334	c1cc(cc(c1)c2ccc(cc2)c3[nH]c4ccc(cc4n3)F)CN5CCN(CC5)c6ccncc6	7.06679
537358	CC(=O)Nc1ccc(cn1)C(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccc(cc5n4)C(F)(F)F	7.13271
535592	CCOC(=O)c1ccc(cc1)NC(=O)Nc2cccc(c2)c3cccc(c3)c4[nH]c5ccccc5n4	7.16332
541018	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)c5ccc(nc5)NC(=O)C	7.18914
527638	Cc1cccc2c1[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)C5CC(=O)Nc6c5cccc6	7.18984
535121	c1cc(ccc1CN2CCN(CC2)c3ccncc3)c4ccc(cc4)c5[nH]c6ccc(cc6n5)C(F)(F)F	7.20511
528452	c1ccc2c(c1)[nH]c(n2)c3cccc(c3)c4cccc(c4)NC(=O)Nc5ccc(c(c5F)F)F	7.25863
525530	c1ccc2c(c1)[nH]c(n2)c3ccc(cc3)c4ccc(cc4)NC(=O)Nc5ccc(cc5)Cl	7.29503
541316	c1cc(cc(c1)NC(=O)Nc2ccc(cc2)Cl)c3ccc(cc3)c4[nH]c5ccc(cc5n4)F	7.32324
540625	c1cc(cnc1)c2[nH]c3cc(ccc3n2)Cl	7.41628
535843	CC(C)(C)c1ccc2c(c1)nc([nH]2)c3ccc(cc3)C=CC(=O)NCc4ccc(c(c4)Cl)Cl	7.4506
529304	CCOC(=O)c1ccc(cc1)NC(=O)Nc2ccc(cc2)c3ccc(cc3)c4[nH]c5ccccc5n4	7.65149