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A new class of Indole-based HDAC8 inhibitors as potential anti-lung cancer agents: *In silico* design, synthesis, biological assessment and binding interaction analysis

Samima Khatun[1], Venkatesh Muthukumar[2], Ambati Himaja[2], Indrasis Dasgupta[1], Kalpataru Das[3], Balaram Ghosh[2,*], Shovanlal Gayen[1,*]

[1]*Laboratory of Drug Design and Discovery, Department of Pharmaceutical Technology, Jadavpur University, Kolkata, 700032, West Bengal, India.*

[2]*Epigenetic Research Laboratory, Department of Pharmacy, Birla Institute of Technology and Science-Pilani, Hyderabad Campus, Shamirpet, Hyderabad, 500078, India.*

[3]*Department of Chemistry, Dr. Harisingh Gour University (A Central University), Sagar, 470003, (MP) India*

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*Corresponding authors: Balaram Ghosh (balaram@hyderabad.bits-pilani.ac.in) and S. Gayen (shovanlal.gayen@gmail.com; sgayen.pharmacy@jadavpuruniversity.in)

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Table S1. Training set compounds in SMILES format

S. No.	Compounds	SMILES	Activity (nM)
1	1	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C=C(\F)CCS)OC1=O	0.41
2	3	O=C(CCCCCC(=O)N(Cc1ccc(Br)s1)c1ccc(OCCN2CCOCC2)cc1)NO	1.14
3	4	C[C@@H]1CN(C(=O)Nc2ccc(-c3nc(N4CCOCC4)c4cnn(CCCCCCC(=O)NO)c4n3)cc2)CCO1	1.28
4	5	O=C(CCCCCCCC(=O)c1ccc(-c2ccc(Br)cc2)cc1)NO	2
5	6	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3ccccc3F)ccc12)NO	2.4
6	8	COc1cc(OC)cc(-c2nnn([C@@H](Cc3ccccc3)C(=O)NO)c2C#CC2CC2)c1	3
7	9	COc1cccc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3c2)c1	3
8	10	CN1CC(C(=O)N[C@@H](CCCCCC(=O)c2ccon2)c2ncc(-c3ccccc3F)[nH]2)C1	3
9	11	COc1ccc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3c2)cc1OC	3.2
10	13	COc1cccc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3n2)c1	3.3
11	14	CCOc1cccc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3c2)c1	3.4
12	15	COc1ccc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3c2)cc1	3.6
13	16	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3cccc(Cl)c3)ccc12)NO	3.8
14	18	O=C(CCCCCCC/C(=N\O)c1ccc(-c2ccccc2)cc1)NO	4
15	19	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3ccccc3Cl)ccc12)NO	4
16	20	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3cccc(C(F)(F)F)c3)ccc12)NO	4.1
17	21	COc1ccccc1-c1ccc2c(NC(=O)CCCCCCC(=O)NO)n[nH]c2c1	4.2
18	23	COc1cc(OC)cc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3c2)c1	4.4
19	24	COc1cccc(-c2ccc3c(NC(=O)CCCCCC(=O)NO)n[nH]c3c2)c1	4.5
20	25	O=C(CCCCCCCC(=O)c1ccc(N2CCN(c3ccccc3)CC2)cc1)NO	4.5
21	26	COc1cc2ncnc(Nc3ccc(Br)cc3)c2cc1OCCCCCCC(=O)NO	4.6
22	28	O=C(CCCCCCCC(=O)c1ccc(-c2ccccc2)cc1)NO	5
23	29	COc1cc2ncnc(Nc3ccc(Cl)cc3Cl)c2cc1OCCCCCC(=O)NO	5.2
24	30	CCCCCCNNC(=O)c1cnc(N2CCN(Cc3c[nH]c4ccccc34)CC2)nc1	5.9
25	31	CC1(C)CC(=O)Nc2ccc(C(=O)NC[C@H]3CC[C@H](/C=C/C(=O)NO)CC3)cc21	6
26	33	O=C(NO)[C@H](Cc1c[nH]c2ccccc12)n1nnc(-c2ccccc2)c1C#CC1CC1	7
27	34	COc1ccc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3n2)cc1	7.2
28	35	O=C(NO)[C@H](Cc1ccccc1)n1nnc(-c2cccc(Cl)c2)c1C#CC1CC1	8
29	36	C=C(CCCCCCCC(=O)NO)c1ccc2ccccc2c1	8
30	38	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C(F)=C/CCS)OC1=O	8.5
31	39	O=C(CCCCCCC/C(=N\O)c1ccc2ccccc2c1)NO	8.5
32	40	O=C1CCC[C@@H](C(=O)N[C@@H](CCCCCS)C(=O)NCc2cccc(OCc3ccccc3)c2)N1	9
33	41	O=C(CCCCCCn1cc(Nc2ncc3ccn(Cc4ccccc4F)c3n2)cn1)NO	9.2
34	43	O=C(CCCCCCCC(=O)c1ccc(N2CCCCC2)cc1)NO	9.5
35	44	O=C(NO)[C@H](Cc1ccccc1)n1nnc(-c2ccccc2)c1C#Cc1ccccc1	10
36	45	C/C=C1\NC(=O)[C@H]2CSSCC/C=C/[C@@H](CC(=O)N[C@H](C(C)C)C(=O)N2)OC(=O)[C@H](C(C)C)NC1=O	10
37	46	N=C1Sc2ccccc2C2=NCCCN12	11
38	48	COc1ccc(-c2cc(OCCN(C)c3ncc(C(=O)NO)cn3)c3ncnc(C)c3c2)cn1	12

39	49	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3ccccc3)ccc12)NO	12.6
40	50	O=C(CCCCCCCOc1cccc(-c2nc3ccccc3[nH]2)c1)NO	12.88
41	51	COc1cc(OC)cc(N(CCNC(C)C)c2ccc3ncc(-c4cnn(CCCCCCC(=O)NO)c4)nc3c2)c1	13
42	53	CC(C)(C)c1ccc(S(=O)(=O)Nc2ccc(C(=O)NO)cc2)cc1	13.3
43	54	CCCCCCNNC(=O)c1cnc(N2CCN(Cc3cn(C)c4ccccc34)CC2)nc1	14
44	55	O=C(NO)c1ccc(NC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	14
45	56	COc1ccc(C(=O)CCCCCCCC(=O)NO)cc1	15
46	58	C[C@@H](c1ccccc1)n1c(-c2cccc(/C=C/C(=O)NO)c2)nc2ccccc21	16
47	59	CCCCCCNNC(=O)c1cnc(NCc2ccccc2)nc1	16
48	60	Cc1cc(C(=O)CCCCC[C@H](NC(=O)C2CN(C)C2)c2ncc(-c3ccccc3F)[nH]2)no1	16
49	61	Cc1c(Cc2ccccc2)nc(-c2cccc(/C=C/C(=O)NO)c2)n1CCc1ccccc1	16
50	63	Cc1cccc(CCNC(=O)[C@H](CCCCCS)NC(=O)[C@@H]2CCCC(=O)N2)c1	17
51	64	COc1ncc(-c2cc(OCCCCCCC(=O)NO)c3ncnc(C)c3c2)cc1F	18
52	65	COc1ccc(CC2C=Cc3cc(C(=O)NO)ccc32)cc1	18.3
53	66	CCCCCCNNC(=O)c1cnc(NCc2ccc(CNC(C)=O)cc2)nc1	19
54	68	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n(CCc2ccccc2)c1Cc1ccccc1	20
55	69	Cc1c(-c2ccccc2)nc(-c2cccc(/C=C/C(=O)NO)c2)n1CCc1ccccc1	20
56	70	O=C(/C=C/c1ccc(Cc2ccc(CO)cc2)cc1)NO	20
57	71	O=C(NO)c1ccc(NC(=O)c2ccc(C3CC3)cc2)cc1	20.4
58	73	CC(C)(C)OC(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	21
59	74	Cc1ccc(C(=O)Nc2ccc(C(=O)NO)cc2)cc1	21.6
60	75	CN(Cc1nc2c(N3CCOCC3)nc(-c3cnc(N)nc3)nc2n1C)c1ncc(C(=O)NO)cn1	22
61	76	O=C1CC/C=C/CCC(=O)N(Cc2cccc(/C=N/NC(=O)c3cccc(C(=O)NO)c3)c2)C[C@@H](c2ccccc2)O1	23
62	78	O=C1CCC[C@@H](C(=O)N[C@@H](CCCCCS)C(=O)NCc2ccc(C(F)(F)F)cc2)N1	23
63	79	CCCCCCNNC(=O)c1ccc(CNC(C)=O)cc1	23
64	80	CN(Cc1nc2c(N3CCOCC3)nc(-c3ccc(N)cc3)nc2n1C)c1ncc(C(=O)NO)cn1	24
65	81	CC1(C)CC(=O)Nc2ccc(C(=O)NC[C@H]3CC[C@@H](CCC(=O)NO)CC3)cc21	24
66	83	O=C(NO)c1cnc(N2CCN(S(=O)(=O)c3ccc4ccccc4c3)CC2)nc1	24.92
67	84	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n(CCc2ccccc2)c1-c1ccccc1	25
68	85	O=C(CCCCCCCCc1ccc2ccccc2c1)NO	25
69	86	O=C(/C=C/c1cccc(-c2nc3ccccc3n2CCc2ccccc2)c1)NO	25
70	88	COc1ccc(C(=O)NO)cc1OCc1ccccc1	25.40275576
71	89	C/C=C1\NC(=O)[C@@H](CS)NC(=O)[C@@H](C(C)C)NC(=O)C[C@@H](/C=C/CCS)OC(=O)[C@H](C(C)C)NC1=O	25.49509757
72	90	Cn1cc(CNCC2CCN(c3ncc(C(=O)NO)cn3)CC2)c2ccccc21	25.55597765
73	91	O=C(CC[C@@H](CCCC(=O)Nc1ccccc1)Cc1ccccc1)NO	27
74	93	COc1ccc(/C=C/C(=O)NO)c(-c2ccc(-c3ccccc3)cc2)c1	27.04986171
75	94	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C(F)=C/CCS)NC1=O	27.14
76	95	CC(C)(C)c1ccc(CN(C(=O)CNS(=O)(=O)c2ccc(F)cc2)c2ccc(C(=O)NO)cc2)cc1	28
77	96	CCCCCCNNC(=O)c1cnc(NCCc2ccccc2)nc1	28
78	2035	[N-]=[N+]=Nc1ccc(Cn2cc(NC(=O)CCCCCCC(=O)NO)cn2)cc1	28
79	98	C#CCOc1ccc(/C=N/NC(=O)c2cccc(C(=O)NO)c2)cc1	29
80	99	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	29

81	100	O=C(NO)c1cnc(N2CCN(C(/C=C/c3ccc(F)cc3)CO)CC2)nc1	30
82	2036	O=C(NO)c1ccc2c(c1)CN(Cc1ccc(-c3cccc([N+](=O)[O-])c3)o1)CC2	30
83	101	Cc1ccc(C(=O)NO)cc1NC(=O)c1ccc2ccccc2n1	30.3
84	103	CCN1CCC[C@@H](n2c(-c3cccc(/C=C/C(=O)NO)c3)nc(-c3ccccc3)c2C)C1	31
85	104	Cc1c(-c2ccccc2)nc(-c2cccc(/C=C/C(=O)NO)c2)n1[C@@H]1CCCN(C(C)C)C1	31
86	105	O=C(CCCCC[C@H](NC(=O)[C@H]1CCC(=O)N1)C(=O)NCCc1ccccc1)NO	31.6
87	106	CN1CC(C(=O)N[C@@H](CCCCCC(=O)c2ccon2)c2ncc(-c3ccccc3F)o2)C1	32
88	108	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3ccsc3)ccc12)NO	32.5
89	109	O=C(CCCCC[C@H](NC(=O)[C@H]1CCC(=O)N1)C(=O)Nc1cccc(C(F)(F)F)c1)NO	32.94996206
90	110	CC1(C)CC(=O)Nc2ccc(NC(=O)CCCCCCC(=O)NO)cc21	33
91	111	CC(C)(C)c1cccc(C(=O)Nc2ccc(C(=O)NO)cc2)c1	33.7
92	113	Cc1ccc(C(=O)NO)cc1NCc1ccc(Cl)cc1Cl	35
93	114	O=C(CCCCCCC(=O)c1ccc2ccccc2c1)NO	35
94	115	O=C(CCCCCCCC(O)c1ccc2ccccc2c1)NO	35
95	116	Nc1ccc(-c2nc(N3CCOCC3)c3cnn(CCCCCCC(=O)NO)c3n2)cc1	35.67
96	118	CCCCCCNNC(=O)c1ccc(-c2ccc(CNC(C)=O)cc2)cc1	36
97	119	O=C(/C=C/c1cccc(C(=O)NO)c1)Nc1ccccc1	37
98	120	CN(CC(=O)N(Cc1ccc(C(C)(C)C)cc1)c1ccc(C(=O)NO)cc1)S(=O)(=O)c1ccc(F)cc1	37.9
99	121	O=C(Cc1ccc(-c2csc(NC(=O)COc3ccccc3)n2)s1)NO	38
100	123	O=C(/C=C/c1ccc(CN(CCO)CCc2c[nH]c3ccccc23)cc1)NO	39.19183588
101	124	O=C1NC[C@@H](c2ccccc2)[C@@H]1C(=O)N[C@@H](CCCCCS)C(=O)Nc1ccccc1	40
102	125	O=C(/C=C/c1cccc(-c2nc3ccccc3n2Cc2ccccc2)c1)NO	40
103	126	CC(C)n1c(-c2cccc(/C=C/C(=O)NO)c2)nc2ccccc21	40
104	128	O=C(Cc1ccc(-c2csc(NC(=O)Cc3ccccc3)n2)s1)NO	41
105	129	O=C(NO)c1ccc(NC(=O)C2(c3c[nH]c(-c4ccccc4)n3)CCCC2)cc1	41
106	130	COc1cccc(-c2ccc3c(NC(=O)CCCCC(=O)NO)n[nH]c3c2)c1	41
107	131	COc1ccc(-c2cc(-c3ccn(Cc4ccc(C(=O)NO)cc4)n3)ccn2)cc1	41.6
108	133	CC(C)(C)c1ccc(NC(=O)c2ccc(C(=O)NO)cc2)cc1	43.9
109	134	O=C(NO)c1ccc(NC(=O)C2(c3ccc4ccccc4c3)CCOCC2)cc1	44
110	135	O=C(CCCCN1CCc2ccccc2C1c1ccccc1)NO	44
111	136	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C=C/C(F)(F)CS)OC1=O	44.09
112	138	O=C(CCCCCCCC(=O)c1ccc(C(F)(F)F)cc1)NO	45
113	139	CCCCCCNNC(=O)c1cccc(NCc2ccccc2)c1	46
114	140	COc1ccc(/C=C/C(=O)c2nnn(-c3ccc(Cl)cc3)c2C)cc1OC	47
115	141	O=C(/C=C/c1ccc(NC(=O)Cc2cccc3ccccc23)cn1)NO	47
116	143	O=C(CCCCCCC(=O)Nc1ccc2[nH]c(=O)ccc2c1)NO	48
117	144	CC1(C)CC(=O)Nc2ccc(C(=O)NCc3ccc(/C=C/C(=O)NO)cc3)cc21	49
118	145	O=C(/C=C/c1cccc(-c2nc3ccccc3n2-c2ccccc2)c1)NO	50
119	146	CCN1CCC[C@@H](n2c(-c3cccc(/C=C/C(=O)NO)c3)nc(Cc3ccccc3)c2C)C1	50
120	148	Cc1nc(-c2ccccc2)n(CCc2ccccc2)c1-c1cccc(/C=C/C(=O)NO)c1	50
121	149	Cc1c(Cc2ccccc2)nc(-c2cccc(/C=C/C(=O)NO)c2)n1CCN1CCOCC1	50
122	150	O=C(/C=C/c1cccc(-c2nc3ccccc3n2C2CCCCC2)c1)NO	50
123	151	Cc1c(-c2ccccc2)nc(-c2cccc(/C=C/C(=O)NO)c2)n1[C@@H]1CCCN(C)C1	50

124	153	C#CCN(C)CCCOc1cc(NC(=O)CCCCCCC(=O)NO)ccc1Cl	50
125	154	O=C(/C=C/c1cccc(-c2nc3ccccc3n2-c2ccc(Cl)cc2)c1)NO	50
126	155	CC(C)N(C(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1)c1ccc(C(=O)NO)cc1	51.42178527
127	156	COc1cc(NC(=O)NOCCCCCC(=O)NO)c2nc(OC)cc(C)c2c1	51.76485294
128	158	O=C(NO)c1cccc(C(=O)N/N=C/c2ccccc2)c1	52
129	159	O=C(NO)c1cccc(-c2nc(CSc3ccccc3)n[nH]2)c1	53
130	160	O=C(CCCCCCNC(=O)c1ccc2c(c1)CCC(=O)N2)NO	53
131	161	O=C(/C=C/c1ccccc1Cl)NO	54
132	163	C/C(=N\N(C)C(=O)c1ccc(N(C)C)cc1)c1ccc(C(=O)NO)cc1	54
133	164	CC1(C)CC(=O)Nc2ccc(C(=O)NCCCCCCC(=O)NO)cc21	55
134	165	O=C(CCN1CCc2ccccc2C1c1ccc(-c2ccccc2)cc1)NO	55
135	166	Cc1ccc2c(c1)C1=NCCCN1C(=S)S2	57
136	168	O=C1CC[C@@H](C(=O)N[C@@H](CCCCCS)C(=O)Nc2ccccc2)N1	59
137	169	CN1C(=O)CC(C)(C)c2cc(C(=O)NCCCCCCC(=O)NO)ccc21	59
138	170	O=C(NO)c1ccc(NC(=O)C2(c3ccc(Br)cc3)CCOCC2)cc1	59
139	171	C=C(c1cc(OC)c(OC)c(OC)c1)c1ccc(OC)cc1/C=C/C(=O)NO	60
140	173	COc1ccc(CS(=O)(=O)Nc2ccc(/C=C\C(=O)NO)cc2)cc1	60
141	174	O=C(CCCCCCC(=O)Nc1ccc2c(c1)/C(=C/c1ccc[nH]1)C(=O)N2)NO	60.2
142	175	COc1ccc(/C=N/NC(=O)CCCCCCCC(=O)NO)cc1	60.32
143	176	CC(C)N(C(=O)c1cccc(C(F)(F)F)c1F)c1ccc(C(=O)NO)cc1	60.82187107
144	178	O=C(NO)c1ccc(N(CC2CC2)C(=O)c2cccc(C(F)(F)F)c2)cc1	61.68306088
145	179	O=C1NCCC[C@H]1C(=O)N[C@@H](CCCCCS)C(=O)Nc1ccccc1	62
146	180	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C=C/CCS)OC1=O	62.06632659
147	181	CC(C)(C)c1cccc(C(=O)N(CC2CC2)c2ccc(C(=O)NO)cc2)c1	62.2430719
148	183	O=C(/C=C/c1cccc(-c2nc3ccccc3n2CCN2CCCC2)c1)NO	63
149	184	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n(CCN2CCOCC2)c1Cc1ccccc1	63
150	185	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NC(=O)Cc2ccccc2)cc1	63
151	186	Cc1nc(Cc2ccccc2)n(CCc2ccccc2)c1-c1cccc(/C=C/C(=O)NO)c1	63
152	188	COc1ccc(-n2c(-c3cccc(/C=C/C(=O)NO)c3)nc3ccccc32)cc1	63
153	189	CCCCCCNNC(=O)c1cnc(NCc2cccc3ccccc23)nc1	63
154	190	CC(C)N(C(=O)c1cccc(C(F)(F)F)c1)c1ccc(C(=O)NO)cc1	63.78675411
155	191	O=C(NO)c1ccc(Cn2sc3ccccc3c2=O)cc1	64
156	193	COc1ccc(C(=O)NO)cc1C(=O)Nc1ccc2c(c1)cc(C)c(=O)n2C	65
157	194	O=C(CCCCCCCC(=O)c1ccccc1)NO	65
158	195	COc1ccc(-c2nc(N3CCOCC3)c3sc(CN(C)c4ncc(C(=O)NO)cn4)cc3n2)cn1	65.16278326
159	196	O=C(/C=C/c1ccc(C(=O)NC(Cc2c[nH]c3ccccc23)C(=O)Nc2ccc3ccccc3c2)cc1)NO	65.7
160	198	O=C(NO)c1ccc(NC(=O)C2(c3ccc(-c4cn[nH]c4)cc3)CCCCC2)cc1	69
161	199	CC(C)N(C(=O)c1cccc(OC(F)(F)F)c1)c1ccc(C(=O)NO)cc1	69.05360237
162	200	COc1ccc(C(=O)NO)cc1NCc1ccccc1	69.49820142
163	201	Nc1nc2cc(-c3nn(CCCCCCC(=O)NO)c4ncnc(N)c34)ccc2o1	69.6491206
164	203	CCOc1ccc(C(C)=O)cc1NC(=O)c1cc(C(=O)NO)ccc1C	70
165	2037	O=C(/C=C/c1ccc(/C=N/OCc2ccc([N+](=O)[O-])cc2)cc1)NO	70
166	204	CN(C)c1cccc(C(=O)NO)c1	70.2
167	205	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(-c3ccc(C(=O)NO)cc3)c2c(=O)n1-c1ccccc1	71
168	206	O=C(NO)c1ccc(CN2C(=O)c3ccccc3S2(=O)=O)cc1-c1ccccc1	71
169	208	O=C(CCCCCCCN1C(=O)c2ccccc2C1=O)NO	71.4
170	209	Cn1c(=O)ccc2cc(C(=O)NCCCCCCC(=O)NO)ccc21	72

171	210	CC(C)C[C@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)c1cncn1)B(O)O	72
172	211	O=C(NO)c1ccc(F)c(NCc2ccccc2)c1	72
173	213	O=C(CCCCCCNC(=O)c1ccc2[nH]c(=O)ccc2c1)NO	73
174	214	CCCCC(CCCC(=O)Nc1ccccc1)CCC(=O)NO	74
175	215	CC(C)(C)c1ccc(CC(=O)Nc2ccc(C(=O)NO)cc2)cc1	74.3
176	216	COc1ccc(-c2cc(-c3ccccc3)[nH]c2C(=O)NCc2ccc(C(=O)Nc3ccccn3)cc2)cc1	74.8
177	218	O=C(/C=C/c1ccc(NS(=O)(=O)c2ccc(Cl)cc2)cc1)NO	75
178	219	CC1(Nc2ccc(C(=O)NO)cc2)CCN(c2ccc3ncccc3c2)C1=O	76
179	220	O=C(CCCCCCC(=O)Nc1cnn(Cc2ccccc2)c1)NO	76
180	221	S=C1Sc2cccc(I)c2C2=NCCCN12	76
181	223	Cc1c(-c2ccccc2)nc(-c2cccc(/C=C/C(=O)NO)c2)n1CCN1CCOCC1	79
182	224	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n(CCN2CCOCC2)c1-c1ccccc1	79
183	225	CCCCCCC(CCCC(=O)Nc1ccccc1)CCC(=O)NO	79
184	226	Cc1c(Cc2ccccc2)nc(-c2cccc(/C=C/C(=O)NO)c2)n1[C@@H]1CCCN(C)C1	79
185	228	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCCCCC(=O)NO)cc23)c1	79.8
186	229	O=C(NO)c1cccc(S(=O)(=O)NCc2ccccc2)c1	80
187	230	C#CCN(C)CCCOc1cc(NCc2ccc(/C=C/C(=O)NO)cc2)ccc1Cl	80
188	231	COc1ccc2cc(C(=O)NCCCCCCC(=O)NO)ccc2n1	80
189	233	CCN(c1ccc(C(=O)NO)cc1)S(=O)(=O)c1cccc(C(C)(C)C)c1	80.43693182
190	234	COc1ccc(C2c3ccccc3CCN2CCC(=O)NO)cc1	82
191	2038	O=C(CCCCCCC(=O)Nc1cnn(Cc2ccc([N+](=O)[O-])cc2)c1)NO	82
192	235	CC(C)N(Cc1ccc(CC(=O)NO)cc1)S(=O)(=O)c1cc(F)c(F)c(F)c1F	84.6
193	236	Cc1ccc2nc3c4ccccc4c(NCCCCCCC(=O)NO)nn3c(=O)c2c1	85.4
194	238	Cc1[nH]c2ccccc2c1C1=CCC(NCc2ccc(OCC(=O)NO)cc2F)CC1	86
195	239	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NC(=O)CCCc2ccccc2)cc1	86
196	240	CC(C)C(C(=O)Nc1ccc(C(=O)NO)cc1)c1ccccc1	87
197	241	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NC(=O)c2ccccc2)cc1	87
198	243	O=C(NO)c1ccc(CN2C(=O)c3cccc(F)c3C2=O)cc1-c1ccccc1	88
199	244	COc1ccc(C(=O)NO)cc1NC(=O)c1ccccc1	88.3
200	245	CN(C)c1ccc(C2(C(=O)Nc3ccc(C(=O)NO)cc3)CCCC2)cc1	89
201	246	COc1ccc(C(C)=O)cc1NC(=O)c1cc(C(=O)NO)ccc1C	90
202	248	O=C(COc1ccc(CNCCc2c[nH]c3ccccc23)c(F)c1)NO	90
203	249	COc1ccc(C(C)=O)cc1NC(=O)c1cc(C(=O)NO)ccc1Cl	90
204	250	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1[nH]c2nc1C(=O)NCCC/C=C\c1cccc-2c1	90
205	251	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NC(=O)CCc2ccccc2)cc1	90
206	253	COc1cc2cc(c1)COc1ccccc1NC(=O)[C@@H](CCCCCC(=O)NO)OCCC2	90.7
207	254	COc1ccc(Cn2ccc3cc(C(=O)NO)ccc32)cc1	92
208	255	CCN(C(=O)c1cc(C(C)(C)C)cc(C(C)(C)C)c1)c1ccc(C(=O)NO)cc1	92.8353381
209	256	COc1ccc(-c2nc(N3CCOCC3)c3nc(CN(C)c4ncc(C(=O)NO)cn4)n(C)c3n2)cc1	92.92
210	258	CCN(C(=O)c1cccc(C(F)(F)F)c1)c1ccc(C(=O)NO)cc1	94.71641885
211	259	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccc(F)cc32)cc1	95

212	260	COc1ccccc1C(=O)CCCCCCCC(=O)NO	95
213	261	Cc1ccc2nc3c4ccccc4c(NCCCCCCCC(=O)NO)nn3c(=O)c2c1	96.2
214	263	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccccc32)s1	97
215	264	C[C@@H](N)C(=O)NCc1nnc(-c2ccccc2)o1	98
216	265	CCc1nc2ccc(Cc3ccc(C(=O)NO)cc3)cc2c(=O)n1CCc1ccccc1	99
217	266	O=C(NO)c1ccc(CNC(=O)N2CCC(N3CC(c4ccccc4)(c4ccccc4)C3=O)CC2)cc1	99
218	268	CC(C)Oc1ccc(C(C)(C)O)cc1-c1cn(C)c(=O)c2[nH]c(C(=O)NCCCCCCCC(=O)NO)cc12	99.6
219	269	Cn1c(-c2cccc(/C=C/C(=O)NO)c2)nc2ccccc21	100
220	270	O=C(/C=C/c1ccc(NS(=O)(=O)c2cccc(C(F)(F)F)c2)cc1)NO	100
221	271	CC(C)(C)c1ccc(CS(=O)(=O)Nc2ccc(/C=C\C(=O)NO)cc2)cc1	100
222	273	O=C(/C=C/c1cccc(-c2nc3ccccc3n2CCN2CCCCC2)c1)NO	100
223	274	O=C(CCc1ccc(NS(=O)(=O)c2ccccc2)cc1)NO	100
224	275	Cc1nc(C)n(CCc2ccccc2)c1-c1cccc(/C=C/C(=O)NO)c1	100
225	276	CN1CC(C(=O)N[C@@H](CCCCCC(=O)c2ncco2)c2ncc(-c3ccc(F)cc3)[nH]2)C1	100
226	278	CCN1CCC[C@@H](n2c(Cc3ccccc3)nc(C)c2-c2cccc(/C=C/C(=O)NO)c2)C1	100
227	279	O=C(/C=C/c1ccc(NS(=O)(=O)c2ccc(Cl)c(Cl)c2)cc1)NO	100
228	280	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n([C@@H]2CCCN(C)C2)c1-c1ccccc1	100
229	281	O=C(NO)c1cccc(-c2cn(CCc3ccsc3)nn2)c1	100
230	283	Cc1ccc(CN(Cc2ccc(C(=O)NO)cc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	101
231	284	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2ccnc(c2)CNC(=O)C[C@@H](/C=C/CCS)OC1=O	101.8
232	285	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)cc1	103
233	286	O=C(CCCCCCN1C(=O)c2ccccc2C1=O)NO	103
234	288	CCC(C(=O)Nc1ccc(/C=C/C(=O)NO)nc1)c1ccccc1	104
235	289	Cc1ccc(C(=O)NO)cc1NC1CCCCC1	104.3
236	290	Cc1cccc(NC(=O)[C@H](CCCCCS)NC(=O)[C@@H]2CCC(=O)N2)c1	106
237	291	COc1ccc(-c2cc(C(=O)NCc3ccc(C(=O)NO)cc3)ccn2)cc1	107
238	293	Cn1c(CCCC(=O)O)nc2cc(N(CCCl)CCCl)ccc21	107
239	294	CCC(=O)CCCCC[C@@H]1NC(=O)[C@@H](C)n2nncc2[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	107.4709263
240	295	O=C(NO)c1cccc(CN(C2CC2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)c1	108
241	296	COc1ccc2c(c1)c(CC(=O)NCCCCCCC(=O)NO)c(C)n2C(=O)c1ccc(Cl)cc1	109
242	298	Cc1cc(C)c(CNC(=O)c2cc(-c3ccc(N4CCN(c5ncc(C(=O)NO)cn5)CC4)nc3)cc3c2cnn3C(C)C)c(=O)[nH]1	110
243	299	C/C(=N\NC(=O)c1ccc(N(C)C)cc1)c1ccc(C(=O)NO)cc1	110
244	300	O=C(NO)c1ccc(NC2CCN(c3ccc(C(F)(F)F)cc3)C2=O)cc1	110
245	301	Cc1cc(C)c(CNC(=O)c2cc(C)n(-c3cccc(NC(=O)CCCCCCC(=O)NO)c3)c2C)c(=O)[nH]1	110
246	303	O=C1CN(Cc2ccc(C(=O)NO)cc2)C(=O)[C@H](Cc2c[nH]c3ccccc23)N1	112
247	304	O=C(CCCCC[C@H](NC(=O)[C@@H]1CC(=O)N1)C(=O)Nc1ccccc1)NO	112.8760382
248	305	O=C(CCCCC[C@H](NC(=O)[C@@H]1CCC(=O)N1)C(=O)Nc1ccccc1)NO	112.8760382
249	306	O=C(CCCCCCC(=O)Nc1cccc(C(F)(F)F)c1)NO	113
250	308	Cc1cc2cc(NC(=O)c3cc(C(=O)NO)ccc3Cl)ccc2n(C)c1=O	113

251	309	COc1cc2c(cc1OC)C(=O)C(CC1CCN(Cc3ccc(/C=C/C(=O)NO)cc3)CC1)C2	113
252	310	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)CCCc2ccccc2)cc1	114
253	311	O=C(NO)c1cccc(C(=O)Nc2ccccc2)c1	114.8912529
254	313	COc1ccc2c(c1)c(CC(=O)O)c(C)n2Cc1ccc(-c2cn(CCCCCCC(=O)NO)nn2)cc1	116
255	314	O=C(O)c1cccc(-c2ccc(C3(C(=O)Nc4ccc(C(=O)NO)cc4)CCCC3)cc2)c1	118
256	315	O=C(CCCCC[C@H](NC(=O)C1CCNC1=O)C(=O)Nc1ccccc1)NO	118
257	316	COc1cc2cc(c1)COc1ccccc1NC(=O)C(CCCCCC(=O)NO)OC/C=C\2	119
258	318	CC(C)N(C(=O)c1ccc(F)c(C(F)(F)F)c1)c1ccc(C(=O)NO)cc1	119
259	319	Cc1ccc(C(=O)NO)cc1NCc1ccc2ccccc2c1	119
260	320	CC(Cc1nc2cc(/C=C/C(=O)NO)ccc2n1CCCO)c1ccccc1	119
261	321	O=C(NO)c1cccc(C(=O)NCCc2ccccc2)c1	120
262	323	O=C(NO)c1ccc(Cn2cc(Nc3ncc(Cl)c(Nc4ccc(F)cc4)n3)cn2)cc1	120
263	324	COc1ccc(C(=O)NO)cc1OCc1ccccc1Cl	120
264	325	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NC(=O)OCc2ccccc2)cc1	120
265	326	O=C(/C=C/c1cccc(-c2nc3ccccc3n2[C@@H]2CCCNC2)c1)NO	120
266	328	CS(=O)(=O)c1ccc(N2CCC(Nc3ccc(C(=O)NO)cc3)C2=O)cc1	120
267	329	CC(C)C[C@H]1CC(=O)N[C@@H](C)C(=O)N[C@@H](CCCCCC(=O)NO)C(=O)N[C@@H](Cc2cc3ccccc3[nH]2)C(=O)N1	120
268	330	O=C(NO)c1ccc(NC2CCN(c3ccc(Cl)cc3)C2=O)cc1	120
269	331	Cc1ccc(-c2nnc(CNC(=O)[C@@H](C)N)o2)cc1	121
270	333	COc1ccc(-c2cc(-c3ccccc3)[nH]c2C(=O)NCc2ccc(C(=O)Nc3ccccc3N)cc2)cc1	124.2
271	334	O=C(NO)c1ccc(N(Cc2ccccc2)C(=O)c2cccc(C(F)(F)F)c2)cc1	125.4368367
272	335	O=C(CCCCCCNC(=O)c1cnc(N(c2ccccc2)c2ccccc2)nc1)NO	129.5118259
273	336	CN(C)CCCNC(=O)c1cc(NC(=O)c2cc(NC(=O)c3cc(NC(=O)c4nc(NC(=O)CCCNC(=O)c5cc(NC(=O)c6cc(NC(=O)c7cc(NC(=O)c8nc(NC(=O)CCNC(=O)CCNC(=O)CCCCCCC(=O)NO)cn8C)cn7C)cn6C)cn5C)cn4C)cn3C)cn2C)cn1C	130
274	338	N#Cc1ccc2c(=O)n(CCc3ccccc3)c(=O)n(Cc3ccc(C(=O)NO)cc3)c2c1	130
275	339	Cc1cccc2c1C1=NCCCN1C(=S)S2	130
276	340	O=C(/C=C/c1cccc(S(=O)(=O)c2ccc3ccccc3n2)c1)NO	130
277	341	CN(/N=C/c1ccc(C(=O)NO)cc1)C(=O)c1ccc(N(C)C)cc1	130
278	343	O=C(NO)c1ccc(CN2CC(=O)N(Cc3ccc(Cl)cc3)[C@H](Cc3cccc3)C2=O)cc1	130
279	344	Cc1ccc(C(=O)NO)cc1NCCc1ccccc1	130
280	345	CCN(C(=O)c1cccc(C(C)(C)C)c1)c1ccc(C(=O)NO)cc1	130.1940859
281	346	CC(C)C[C@H]1CC(=O)N[C@@H](C)C(=O)N[C@@H](CCCCCC(=O)NO)C(=O)N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N1	130.9924048
282	348	O=C(CCCCCCNc1nn2c(=O)c3ccccc3nc2c2ccccc12)NO	131
283	349	O=C(/C=C/c1ccc(C(=O)NO)cc1)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)Nc1cccc(Cl)c1	132.3
284	350	CC(C)(C)c1ccc(-c2nnn([C@@H](Cc3ccccc3)C(=O)NO)c2C#CC2CC2)cc1	133
285	351	CC(C)(C)c1ccc(CN(C(=O)CN(Cc2c(F)c(F)c(F)c(F)c2F)S(C)(=O)=O)c2ccc(C(=O)NO)cc2)cc1	133
286	2040	NCC(=O)NCc1nnc(-c2ccc([N+](=O)[O-])cc2)o1	134
287	353	O=C(CCCCCCCCC(=O)c1ccccc1)NO	135
288	354	COC(=O)Cc1c(C)n(Cc2ccc(-c3cn(CCCCCCC(=O)NO)nn3)cc2)c2ccc(OC)cc12	135
289	355	NCC(=O)NCc1nnc(-c2ccc(F)cc2)o1	135

290	356	Cc1cccc(NC(=O)[C@H](CCCCCS)NC(=O)[C@@H]2CCCC(=O)N2)c1	135
291	358	O=C(NO)c1ccc(Cn2c(=O)[nH]c(=O)c3cccc(Cl)c32)cc1	137
292	359	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(CNC(=O)c3ccc(C(=O)NO)cc3)c2c(=O)n1-c1ccccc1	138
293	360	CC[C@H](C)[C@H](NC(=O)OC(C)(C)C)C(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(OC)cc1	139
294	361	Cc1ccc(-c2nnc(CNC(=O)CN)o2)cc1	139
295	363	O=C(/C=C/c1ccc(CN(CCO)CCc2cc3ccccc3[nH]2)cc1)NO	140
296	364	CCCOc1ccc(C(C)=O)cc1C(=O)Nc1cc(C(=O)NO)ccc1C	140
297	365	O=C(/C=C/c1ccc2c(c1)nc(-c1ccccn1)n2CCCO)NO	141
298	366	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)Cc2ccccc2)cc1	141
299	368	O=C(NO)c1cccc(NCc2ccccc2)c1	143.4
300	369	O=C(/C=C/c1ccc2c(c1)nc(COCc1ccccc1)n2CCCO)NO	145
301	370	O=C(NO)c1ccc(CN2CC(=O)N(Cc3ccccc3)[C@H](Cc3ccccc3)C2=O)cc1	145
302	371	CC[C@H](C)[C@H](NC(=O)CC(C)(C)C)C(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(OC)cc1	146
303	373	CC[C@H](C)[C@H](NC(=O)C1CCN(C(=O)OC(C)(C)C)CC1)C(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(OC)cc1	147
304	374	COc1ccc(C(=O)NO)cc1NCc1ccc(Cl)cc1	147
305	375	Nc1ccccc1NC(=O)c1ccc(CNC(=O)c2[nH]c(-c3ccsc3)cc2-c2ccc(O)cc2)cc1	148
306	376	Cn1c(CCc2ccccc2)nc2cc(/C=C/C(=O)NO)ccc21	148
307	378	CCC(=O)CCCCC[C@@H]1NC(=O)[C@H](CCCCNC(C)=O)NC(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	150
308	379	O=C(CCCCCNC(=O)Cn1cnc2c(N3CCOCC3)nc(Nc3ccccc3)nc21)NO	150
309	380	COc1ccc(N(C)c2cc(C#N)nc3ccccc23)cc1/C=C/C(=O)NO	150
310	381	COc1ccc(C(=O)NO)cc1NC(=O)c1cccc2c1/C(=N/O)c1ccccc1-2	150
311	383	CCC(=O)CCCCC[C@@H]1NC(=O)[C@H](CCCCCNC(C)=O)NC(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	150
312	384	O=C(NO)c1ccc(CN2CC(=O)N(Cc3cccc(Cl)c3)[C@H](Cc3ccccc3)C2=O)cc1	150
313	385	CN(CCc1ccccc1)S(=O)(=O)c1cccc(/C=C/C(=O)NO)c1	150
314	386	COc1ccc(-c2cc(-c3ccoc3)c(C(=O)NCc3ccc(C(=O)NO)cc3)[nH]2)cc1	150
315	388	O=C(NO)c1cccc(-c2csc(CSc3ccccc3)n2)c1	150
316	389	O=C(NO)c1ccc(CN(Cc2ccccc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	150
317	390	O=C(CCCCCCNC(=O)c1cnc(N(c2ccccc2)c2ccccc2Cl)nc1)NO	150.6542939
318	391	O=C(COc1ccc(C[C@H](NC(=O)CCc2ccccc2)C(=O)Nc2ccccc2)cc1)NO	151
319	393	O=C(CCc1ccc(Oc2cccs2)c(O)c1)Nc1ccc(C(=O)NO)cc1	152
320	394	O=C(CCCCCCCC(=O)c1cccnc1)NO	153
321	395	COc1ccc(-c2nnc(CNC(=O)[C@@H](C)N)o2)cc1	153
322	396	O=C(NO)c1ccc(Cn2c(=O)[nH]c(=O)c3ccc(F)cc32)cc1	154
323	398	O=C(NO)c1ccc(CN(Cc2ccccc2)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	155
324	399	O=C(NO)c1ccc(Cl)c(NC(=O)c2cccc3ccsc23)c1	155
325	400	Cc1ccc(NC(=O)[C@H](CCCCCC(=O)NO)NC(=O)[C@H]2CCC(=O)N2)cc1	156
326	401	COc1ccc(C(=O)NO)cc1CS(=O)(=O)Nc1ccc2c(c1)cc(C)c(=O)n2C	158

327	403	CCCCCc1c(-c2ccccc2)nnn1[C@@H](Cc1ccccc1)C(=O)NO	160
328	404	O=C(NO)c1ccc(NC2CCN(c3ccc(Cl)c(Cl)c3)C2=O)cc1	160
329	405	CN(C)CCn1c(-c2cccc(/C=C/C(=O)NO)c2)nc2ccccc21	160
330	406	CN1CCC[C@H](n2c(-c3cccc(/C=C/C(=O)NO)c3)nc3ccccc32)C1	160
331	408	Cc1cnc(Nc2ccc(OCCN3CCCC3)cc2)nc1Nc1ccc(C(=O)NO)cc1	160
332	409	COc1cc(C(=O)NO)ccc1Cn1ccc2cc(C(=O)NCC34C[C@H]5C[C@@H](C3)C[C@@H](C4)C5)ccc21	160
333	410	COc1ccc(-c2nc(NC(=O)NCCCC(=O)NO)cc3c2[nH]c2ccccc23)cc1	160
334	411	N#Cc1ccc(N2CCC(Nc3ccc(C(=O)NO)cc3)C2=O)cc1	160
335	413	O=C(/C=C/c1ccc2c(c1)nc(-c1ccncc1)n2CCCO)NO	161
336	414	CC(C)(C)c1ccc(C(=O)NCc2ccc(C(=O)NO)cc2)cc1	162
337	415	O=C(NO)c1ccc(CN2CC(=O)N(Cc3ccccc3Cl)[C@H](Cc3ccccc3)C2=O)cc1	162
338	416	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)[C@H](CC(C)C)NC(=O)OC(C)(C)C)cc1	163
339	418	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C(F)(F)[C@@H](/C=C/CCS)NC1=O	165.5
340	419	O=C(/C=C/c1cccc(S(=O)(=O)Nc2ccccc2)c1)NO	166.8977948
341	420	Cc1cc(-c2nc3sc4c(c3c(=O)[nH]2)CCN(C)C4)cc(C)c1OCCCCCC(=O)NO	167
342	421	COc1cccc(CNc2cc(C(=O)NO)ccc2OC)c1	167
343	423	CC(C)C(C(=O)Nc1ccc(/C=C/C(=O)NO)nc1)c1ccccc1	168
344	424	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccsc32)cc1	169
345	425	O=C(CCCCCCCNc1nn2c(=O)c3ccccc3nc2c2ccccc12)NO	170
346	426	N#Cc1ccc2c(c1)SC(=S)N1CCN=C21	170
347	428	CCOc1ccc(C(=O)NO)cc1NC(=O)c1ccccc1	171.5
348	429	CCc1nc2cc(Cc3ccc(C(=O)NO)cc3)ccc2c(=O)n1CCc1ccccc1	173
349	430	Nc1ccccc1NC(=O)c1ccc(CNC(=O)c2[nH]c(-c3ccc(O)cc3)cc2-c2ccoc2)cc1	174
350	431	CN1CCN(CCc2cn(CC3=CCC(C(=O)NO)C=C3)c3ccccc23)CC1	174
351	433	COc1ccc([C@H]2[C@H](COC(=O)c3ccc(C(=O)NO)cc3)C(=O)N2c2cc(OC)c(OC)c(OC)c2)cc1O	177
352	434	O=C(NO)c1ccc(Cl)c(C(=O)Nc2ccc(Cl)cc2)c1	177.4823935
353	435	O=C(/C=C/c1ccc(CNc2ccc3nc4n(c(=O)c3c2)CCCCC4)cc1)NO	178
354	436	O=C(NO)c1ccc(NC2CCN(c3cccc(Cl)c3)C2=O)cc1	180
355	438	O=C(CCCCCCNC(=O)c1csc(Br)n1)NO	180
356	439	COc1cccc2c(C(CCCCCC(=O)NO)c3c[nH]c4c(OC)cccc34)c[nH]c12	180
357	440	C[C@]1(Nc2ccc(C(=O)NO)cc2)CCN(c2ccc(Cl)cc2)C1=O	180
358	441	O=C(NO)c1cccc(-c2cn(CCc3ccccc3)nn2)c1	180
359	443	O=C(NO)c1ccc(CNC(=O)c2[nH]c(-c3ccc(O)cc3)cc2-c2ccoc2)cc1	180.6
360	444	COc1ccc(C(=O)NO)cc1OCc1ccc(Cl)cc1	181
361	445	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)[C@H](C)NC(=O)OC(C)(C)C)cc1	182
362	446	O=C(/C=C/c1ccc(NC(=O)Cc2ccccc2)cn1)NO	183
363	448	Nc1ccc(-c2nc(N3CCOCC3)c3ncn(CCCCCCC(=O)NO)c3n2)cn1	184
364	449	O=C(/C=C/c1cccn(CCCc2ccc3ccccc3c2)c1=O)NO	188
365	450	CC(=O)SCC(=O)CCCCCCCC(=O)Nc1ccccc1	190
366	451	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1ccc(Cl)cc1Cl)CC2	190
367	453	O=C(NO)c1ccc(Br)c(NC(=O)c2ccccc2)c1	191.4
368	454	CCn1c(C)nc2cc(/C=C/C(=O)NO)ccc21	192
369	455	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C(=O)OC(C)(	192

		C)C)C(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(OC)cc1	
370	456	Cc1[nH]c2ccccc2c1CCNCc1ccc(/C=C/C(=O)NO)cc1	193.4091649
371	458	Nc1nn(-c2ccccc2)nc1C(=O)NCc1ccc(C(=O)NO)cc1	195
372	459	O=C(COc1ccc(C[C@H](NC(=O)OCc2ccccc2)C(=O)Nc2ccccc2)cc1)NO	197
373	460	CC(C)N(CCn1c(-c2cccc(/C=C/C(=O)NO)c2)nc2ccccc21)C(C)C	200
374	461	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n(CCN2CCOCC2)c1C	200
375	463	Cc1nc2ccccc2n1Cc1ccc(C(=O)NO)cc1F	200
376	464	N[C@H](Cc1cccc(Cl)c1)C(=O)N1CCN(C(=O)c2cc(F)ccc2F)CC1	200
377	465	COc1ccc(-c2nc(NC(=O)NCCCCC(=O)NO)cc3c2[nH]c2ccccc23)cc1	200
378	466	O=C(CCCCCNC(=O)Cn1cnc2c(Nc3ccccc3)nc(Nc3ccccc3)nc21)NO	200
379	468	COc1ccc2[nH]c(C)c(CC(=O)N[C@@H](CCCCCC(=O)NO)C(=O)NCCc3c(-c4ccccc4)[nH]c4ccccc34)c2c1	200
380	469	O=C(NO)c1ccc(CNCc2nc(-c3ccccc3)no2)cc1	200
381	470	O=C(/C=C/c1cccc(S(=O)(=O)c2ccc3cccc(F)c3n2)c1)NO	200
382	471	Cn1cnc2cc(/C=C/C(=O)NO)ccc21	201
383	473	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2c(F)cc(F)c(Cl)c2F)cc1	201
384	474	COc1ccc(C(=O)NO)cc1NCc1cccc(Oc2ccccc2)c1	202
385	475	CCS/C(Nc1ccccc1)=C(\C#N)C(=O)N/N=C\c1ccc(Cl)cc1Cl	202
386	476	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2Cc1ccccn1)NO	202
387	478	O=C(/C=C/c1ccc2c(c1)nc(C1CCCCC1)n2CCCO)NO	203
388	479	Cc1ccc(C(=O)NO)cc1NC(=O)c1ccccc1	204
389	480	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(NCc3ccc(C(=O)NO)cn3)c2c(=O)n1-c1ccccc1	204
390	481	CC(C)CCN(CCCCCCC(=O)NO)c1ncc(C(=O)NCCCn2ccnc2)s1	204
391	483	O=C(NO)c1ccc(NC(=O)c2ccc(C3CCCCC3)cc2)cc1	208
392	484	CCN(c1ccc(C(=O)NO)cc1)S(=O)(=O)c1cccc(C(F)(F)F)c1	209.4277919
393	485	O=C(NO)c1ccc(NC2CCN(c3ccccc3)C2=O)cc1	210
394	486	O=C(NO)c1cccc(C(=O)NCc2ccccc2)c1	210
395	488	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1ccc(F)cc1F)CC2	210
396	489	CCOc1ccc(C2c3ccccc3CCN2CCC(=O)NO)cc1	210
397	490	C#CCN(C)Cc1cccc(NC(=O)CCCCCCC(=O)NO)c1	210
398	491	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	210
399	493	O=C(CCCCCCC(=O)Nc1ccccc1CN1CC[C@H](O)C1)NO	211
400	494	COc1ccc(C(=O)NO)cc1NC(=O)c1ccccc1Cl	211.16
401	495	N[C@@H](CCCCCC(=O)c1ccon1)c1ccn(-c2ccc(F)cc2)n1	212
402	496	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)[C@@H]2CCCN2C(=O)OC(C)(C)C)cc1	212
403	498	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2c(F)c(Cl)c(F)c(Cl)c2F)cc1	214
404	499	O=C(NO)c1ccc(Cl)c(NC(=O)c2cccc(OCc3ccccc3)c2)c1	214.4
405	500	CC(C)(C)c1[nH]c2ccccc2c1[C@H]1CCCN(Cc2ccc(/C=C/C(=O)NO)cc2F)C1	217
406	501	COc1ccc(-c2nc(N3CCOCC3)c3nc(CN(C)c4ncc(C(=O)NO)cn4)n(C)c3n2)cn1	217
407	503	O=C(c1ccc(-c2nc(COc3ccc(-c4nnco4)cc3)no2)s1)C(F)(F)F	220

408	504	CCOc1ccc(C(C)=O)cc1NC(=O)c1cc(C(=O)NO)ccc1Cl	220
409	505	O=C(NO)c1ccc(NC(=O)c2ccc(C(F)(F)F)cc2)cc1	220
410	506	CSc1ccc(C(=O)NO)cc1NC(=O)c1ccc(-c2ccccc2)cc1	220
411	508	O=C(CCCCCCNc1nn2c(=O)c3cc(Br)ccc3nc2c2ccccc12)NO	222
412	509	O=C(NO)c1ccc(Cn2c(=O)[nH]c(=O)c3cc(F)ccc32)cc1	222
413	510	CN(C(=O)CN(Cc1c(F)c(F)c(F)c(F)c1F)S(=O)(=O)c1ccc(F)cc1)c1ccc(C(=O)NO)cc1	224
414	511	CC(C)(C)c1cc(C(=O)N(CC2CC2)c2ccc(C(=O)NO)cc2)cc(C(C)(C)C)c1	225
415	513	Cc1ccc(C(=O)NO)cc1NCc1ccc(-c2ccccc2)cc1	227
416	514	COc1ccc(-c2cc(-c3ccccc3)[nH]c2C(=O)Nc2cccc(CC(=O)NO)c2)cc1	227
417	515	CC(C)(C)OC(=O)N[C@@H](Cc1ccc(OCC(=O)NO)cc1)C(=O)Nc1ccccc1	227
418	516	O=C(/C=C/c1ccc(C(=O)NC(Cc2c[nH]c3ccccc23)C(=O)Nc2ccc(I)cc2)cc1)NO	229.2
419	518	CC[C@H](C)[C@@H]1NC(=O)[C@@H](Cc2ccc(OC)cc2)NC(=O)[C@H](CCCCSCC(=O)C(F)(F)F)NC(=O)[C@H]2CCCN2C1=O	230
420	519	CN(C)c1ccc(C(=O)N/N=C/c2ccc(C(=O)NO)cc2)cc1	230
421	520	CCOc1ccc(C(=O)NO)cc1NC(=O)c1ccc(Cl)cc1Cl	230
422	521	COC(=O)[C@@H]1Cc2cccc(c2)C[C@H](NC(C)=O)C(=O)N[C@@H](CCCCCC(=O)NO)C(=O)N1	231
423	523	CC(C)Cc1nc2cc(/C=C/C(=O)NO)ccc2n1CCc1ccccn1	234
424	524	O=C(/C=C/c1ccc(/C=N/OCCN2CCOCC2)cc1)NO	235
425	525	COc1ccc(C(=O)Nc2cc(C(=O)NO)ccc2Cl)cc1	235.6
426	526	O=C(/C=C/c1ccc2c(c1)NCN2CCC1=CCCC=N1)NO	237
427	528	O=C(CCCCCCNc1nn2c(=O)c3cc(Cl)ccc3nc2c2ccccc12)NO	239
428	529	COc1ccc(C(=O)NO)cc1NC(=O)c1ccc(Cl)cc1	239.7
429	530	N=C(N)NCCC[C@@H]1NC(=O)C[C@H](Cc2ccc(O)cc2)NC(=O)[C@H](CC(=O)O)NC(=O)[C@H](CCCCCC(=O)NO)NC1=O	240
430	531	C=C(c1cc(OC)c(OC)c(OC)c1)c1ccc2c(c1)c(/C=C/C(=O)NO)cn2C	240
431	533	O=C(CCCCCC(c1c[nH]c2ccccc12)c1c[nH]c2ccccc12)NO	240
432	534	O=C(NO)c1ccc(CN(Cc2ccccc2F)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	241
433	535	O=C(/C=C/c1ccc(C(=O)NC(Cc2c[nH]c3ccccc23)C(=O)Nc2ccc(Cl)cc2)cc1)NO	243.1
434	536	CC(C)(C)c1ccc(C(=O)Nc2ccc(C(=O)NO)cc2)cc1	245
435	2041	Cc1c(NC(=O)NCCN2C(=O)S/C(=C\c3ccc([N+](=O)[O-])cc3)C2=O)c(=O)n(-c2ccccc2)n1C	245
436	538	Cc1ccc(C(=O)NO)cc1NCCCc1ccccc1	248
437	539	O=C(/C=C/C1CCN(CCc2c[nH]c3ccccc23)CC1)NO	250
438	540	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(NCc3ccc(C(=O)NO)cc3)c2c(=O)n1-c1ccccc1	250
439	541	CN1C(=O)C2CN(Cc3c2c2ccccc2n3Cc2ccc(C(=O)NO)cc2)C1=O	250
440	543	CC(C)(C)Oc1ccc(C[C@@H]2C(=O)Nc3ccccc3N2Cc2ccc(C(=O)NO)cc2)cc1	250
441	544	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CCCO)NO	251
442	545	O=C(CCCCC[C@H](NC(=O)C1CCCNC1=O)C(=O)Nc1ccccc1)NO	251
443	546	O=C(NO)c1ccc(CN2CC3(CCCCC3)c3ccccc32)cc1	253
444	548	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CCN1CCCCC1)NO	254
445	549	O=C(NO)c1ccc(Cl)c(NCc2ccccc2)c1	254
446	550	CCCCCCCC(=O)SCC/C=C(\F)[C@@H]1CC(=O)NCc2nc(cs2)C2=N[C@@](C)(CS2)C(=O)N[C@@H](C(C)C)C(=O)O1	255

447	551	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccccc32)c(F)c1	255
448	553	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C=C/CCS)NC1=O	255.3
449	554	COc1ccccc1-c1cnc(C(=O)NCCCCCCC(=O)NO)s1	255.89
450	555	Cc1ccc(C(=O)NO)cc1NCc1ccccc1	260
451	556	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(F)cc3)n1)CC2	260
452	558	Cc1ccc(CN2CCC(c3noc(CN(C)c4ncc(C(=O)NO)cn4)n3)CC2)cc1	260
453	559	S=C1Sc2ccc(Br)cc2C2=NCCN12	260
454	2042	CN(CCOc1no[n+]([O-])c1S(=O)(=O)c1ccccc1)C(=O)c1ccc(/C=C/C(=O)NO)cc1	260
455	2043	CNCCOc1no[n+]([O-])c1S(=O)(=O)c1ccccc1	260
456	560	COc1ccc(-c2nc3cc(/C=C/C(=O)NO)ccc3n2CC(O)CO)cc1	262
457	561	CC[C@H](C)[C@@H](CN1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(OC)cc1)NC(=O)OC(C)(C)C	263
458	563	CC(C)(C)c1ccc(C(=O)N(Cc2ccc(C(=O)NO)cc2)C2CC2)cc1	269
459	564	COc1ccc(NC(=O)c2cc(C(=O)NO)ccc2OC)cc1	270
460	565	Nc1ncc(-c2nc(N3CCOCC3)c3ccn(CCCCCCC(=O)NO)c3n2)cn1	270
461	566	O=C(CCCCCCNC(=O)NC(=O)c1ccccc1)NO	270
462	568	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2cc(F)c(F)c(F)c2)cc1	273
463	569	CC(C)CCc1c(OCCCCCCCCC(=O)NO)ccc(CCC(=O)NO)c1O	279.5
464	570	N[C@@H](CCCCCC(=O)c1ccon1)c1ncc(-c2ccccc2F)[nH]1	280
465	571	COc1ccc(N(C)c2nc(C)nc3ccccc23)cc1/C=C/C(=O)NO	280
466	573	COc1ccc(C(=O)NO)cc1C(=O)Nc1cccc(Cl)c1	280
467	574	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2ccc(F)cc2)cc1	281
468	575	O=C(NO)c1ccc(Cn2c(=O)[nH]c(=O)c3c(Cl)cccc32)cc1	281
469	576	CCN(C(=O)c1ccc(C(C)(C)C)cc1)c1ccc(C(=O)NO)cc1	281
470	578	O=C(CCCCCCNC(=O)c1ncc(-c2ccccc2)o1)NO	281.32
471	579	O=C(CCCCCCc1nc2ccc(Br)cc2[nH]1)NO	282
472	580	CCc1nc2c(Cc3ccc(C(=O)NO)cc3)cccc2c(=O)n1CCc1ccccc1	282
473	581	O=C(/C=C/c1ccc(CNC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1)NO	283
474	583	O=C(CCCCCC1OCCCCCCCCOc2ccccc2NC1=O)NO	286
475	584	Cc1ccc(C(=O)NO)cc1NCc1ccccc1Cl	286
476	585	COc1ccc([C@H]2[C@H](COC(=O)CCC(=O)NO)C(=O)N2c2cc(OC)c(OC)c(OC)c2)cc1O	288
477	586	COc1cc(OC)cc(N(CCNC(C)C)c2ccc3ncc(-c4cnn(CCOc5ccc(C(=O)NO)cc5)c4)nc3c2)c1	288
478	588	O=C(NO)c1ccc(CN2CCC(CN[C@@H]3C[C@H]3c3ccccc3)CC2)cc1	290
479	589	O=C(CCC(CCCC(=O)Nc1ccccc1)c1ccccc1)NO	290
480	590	CCOc1cc(C)nc(NC2CCc3ccc(C(=O)NO)cc3C2)n1	290
481	591	C#CCOc1ccc(/C=N/NC(=O)CCCCCCC(=O)NO)cc1	290
482	593	O=C(NO)c1ccc(Cl)c(NC(=O)c2ccc(Cl)cc2)c1	292
483	594	CCS/C(Nc1ccccc1)=C(\C#N)C(=O)Nc1ccc(OC)cc1	295
484	595	O=C(/C=C/c1ccc2c(c1)nc(COCc1ccccc1)n2CCc1cccnc1)NO	300
485	596	Cc1ccc(S(=O)(=O)Nc2ccc(/C=C/C(=O)NO)cc2)cc1	300
486	598	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccccc3Cl)n1)CC2	300
487	599	O=C(/C=C/c1ccc(NS(=O)(=O)c2ccc(Cl)cc2Cl)cc1)NO	300
488	600	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(C(F)(F)F)n1)CC2	300
489	601	O=C(NO)c1ccc(Cn2c(=O)[nH]c(=O)c3ccc(C(F)(F)F)cc32)cc1	302
490	603	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccccc32)cc1	309
491	604	O=C(/C=C/c1ccc(-c2ccc(O)cc2)cc1)NO	309.1601527
492	605	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3cccc(-c4cn(CCCCCCC(=O)NO)nn4)c3)[C@H]2O)[C@@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2	310

		C	
493	606	O=C(/C=C/c1cccc(-c2nc3ccccc3n2CC2CCNCC2)c1)NO	310
494	608	O=C(CCCCC(=O)Nc1ccc2c(c1)/C(=C/c1ccc[nH]1)C(=O)N2)NO	312
495	609	O=C(CCCCCCN(c1ccccn1)c1ccc2ccccc2n1)NO	312
496	610	COCCCn1c(CCc2ccccc2)nc2cc(/C=C/C(=O)NO)ccc21	313
497	611	CC[C@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@@H]2O)[C@@](C)(O)C[C@H](C)CN(C)[C@@H](C)[C@H](O)[C@@]1(C)O	314
498	613	O=C(NO)c1ccc(CN(Cc2cccnc2)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	316
499	614	O=C1CC[C@H](C(=O)N[C@@H](CCCCCS)C(=O)Nc2cccc(C(F)(F)F)c2)N1	316
500	615	O=C(NO)c1ccc(Cn2cc(CN3CCCC3)c3ccccc32)cc1	316.23
501	616	O=C(NO)c1ccc(F)c(NC(=O)c2ccccc2)c1	317.8
502	618	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(CNc3ncc(C(=O)NO)cn3)c2c(=O)n1-c1ccccc1	320
503	619	O=C(CCCCCCNCc1ccc2ccccc2c1)NO	320
504	620	O=C(CCCCCCn1cnc2c(N3CCOCC3)nc(-c3cccc(CO)c3)nc21)NO	320
505	621	O=C(/C=C/c1cccc(-c2ccc(O)cc2)c1)NO	320
506	623	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(N4CCOCC4)nc3)n1)CC2	320
507	624	O=C(NO)c1ccc(Cn2nnc(-c3ncccn3)n2)cc1	320
508	625	C#Cc1nc(C(=O)NCCCCCCC(=O)NO)cs1	320
509	626	O=C(NO)c1ccc(Cn2cc(Cc3ccccc3)c3ccccc32)cc1	324
510	628	O=C(CCCCCN(CCCc1ccccc1)C(=O)NC(=O)c1ccccc1)NO	328
511	629	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CCc1cccnc1)NO	329
512	630	C#CCN(C)CCCOc1ccc(NC(=O)CCCCCCC(=O)NO)cc1Cl	330
513	631	COc1ccc(COC(CCCCCC(=O)NO)C(=O)Nc2ccccc2)cc1	331
514	633	CC[C@H](C)[C@@H](CN1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(OC)cc1)NC(=O)CC(C)(C)C	333
515	634	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	334
516	635	CNC(=O)CCCCCCCn1nc(-c2ccc3oc(N)nc3c2)c2c(N)ncnc21	334
517	636	Cc1ccc(C(=O)NO)cc1NCc1c(Cl)cccc1Cl	335
518	638	COc1cc(-c2nc3cc(/C=C/C(=O)NO)ccc3n2CC(O)CO)ccc1OCc1ccccc1	336
519	639	O=C(CCN1CCc2ccccc2C1c1cccc(C(F)(F)F)c1)NO	340
520	640	C=C(c1ccc(OC)c(/C=C/C(=O)NO)c1)c1cc(OC)c(OC)c(OC)c1	340
521	641	O=C(NO)c1ccc(CNC(=O)c2[nH]c(-c3ccc(O)cc3)cc2-c2ccsc2)cc1	340.1
522	643	O=C(NO)c1ccc(C(F)(F)F)c(NC(=O)c2ccccc2)c1	342.2
523	644	COc1cc(/C=C2\SC(=O)N(CCNC(=O)Nc3c(C)n(C)n(-c4ccccc4)c3=O)C2=O)cc(OC)c1OC	344
524	645	O=C(/C=C/c1ccc2c(c1)nc(-c1ccccn1)n2CC(O)CO)NO	344
525	646	COc1ccc2c(c1)c(CC(=O)NCCCCCC(=O)NO)c(C)n2C(=O)c1ccc(Cl)cc1	345
526	648	O=C(CCCCCC(=O)NCCCN1c2ccccc2CCc2ccc(Cl)cc21)NO	345
527	649	O=C(/C=C/c1ccc2c(c1)NC(CCc1ccccc1)N2CCN1CCOCC1)NO	345
528	650	Cc1ccc(-c2nc(CNc3ccc(C(=O)NO)cc3)n(-c3ccccc3)n2)s1	349
529	651	CC(C)(C)OC(=O)NCCCC[C@H](NC(=O)OC(C)(C)C)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	350
530	653	CCCCCNNC(=O)c1ccc(-c2ccc(CNC(C)=O)cc2)cc1	350
531	654	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1cccc(F)c1)CC2	350
532	655	O=C(NO)c1cccc(-c2cn(Cc3ccccc3)nn2)c1	350

533	656	O=C(CCCCCCN(Cc1ccc(F)cc1)c1ncc(C(=O)NCCCn2ccnc2)s1)NO	351
534	658	CN(C)CC(C)(C)Cn1c(CCc2ccccc2)nc2cc(/C=C/C(=O)NO)ccc21	353
535	659	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc(CCCCCC(=O)NO)c2ccccc2n1	353
536	660	O=C(/C=C/c1ccc(C(=O)NO)cc1)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)Nc1ccc(Br)cc1	354.2
537	661	COc1cc(Cn2c(CCc3ccccc3)nc3cc(/C=C/C(=O)NO)ccc32)cc(OC)c1OC	355
538	663	CCCCCCCC(=O)SCC/C=C/[C@@H]1CC(=O)NCc2nc(cs2)C2=N[C@@](C)(CS2)C(=O)N[C@@H](C(C)C)C(=O)O1	357.9944134
539	664	CCCCNNC(=O)c1ccc(-c2ccc(CNC(C)=O)cc2)cc1	360
540	665	Cc1ccc(NC(=O)[C@H](CCCCCS)NC(=O)[C@@H]2CCCC(=O)N2)cc1	360
541	666	O=C(NO)[C@@H]1[C@H](c2ccccc2)[C@H]1c1ccc(-c2cnco2)cc1	360
542	668	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2Cc1ccccn1)NO	366
543	669	O=C(NO)c1ccc(CN(Cc2ccc(F)cc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	367
544	670	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1cccc(C(F)(F)F)c1)CC2	370
545	671	CC[C@H](C)[C@@H]1NC(=O)[C@@H](Cc2ccc(OC)cc2)NC(=O)[C@H](CCCCCC(=O)C(F)(F)F)NC(=O)[C@H]2CCCN2C1=O	370
546	673	N#Cc1ccc2c(c1)SC(=S)N1CCCN=C21	370
547	674	CN(C)Cc1c(C(=O)NCCOc2ccc(C(=O)NO)cc2)oc2ccccc12	370
548	675	O=C(NO)c1ccc(Cn2c(=O)[nH]c(=O)c3cc(Br)ccc32)cc1	371
549	676	O=C(CCCCCCS)NCc1ccc(C(F)(F)F)cc1	373
550	678	O=C(NO)c1ccc(CC(=O)N(CCO)C(=O)Cc2ccccc2)cc1	376
551	679	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2c(F)c(F)cc(F)c2F)cc1	378
552	680	COc1cc(OC)c2c(N3CCN(C)CC3)nc(-c3cc(C)c(OCCCCCC(=O)NO)c(C)c3)nc2c1	378.2
553	681	COc1cccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@](O)(C(C)=O)C[C@@H]3O[C@H]1C[C@H](NCc2ccc(-c3cn(CCCCCCCC(=O)NO)nn3)cc2)[C@H](O)[C@H](C)O1	379
554	683	COc1ccc2[nH]cc(Cn3cc(COc4ccc(/C=C/C(=O)NO)cc4OC)nn3)c2c1	380
555	684	CN1CCC(C(=O)N[C@@H](CCCCCC(=O)c2nccs2)c2ncc(-c3ccc(F)cc3)[nH]2)CC1	380
556	2045	O=C(NO)c1ccc(CNCc2nc(-c3ccc([N+](=O)[O-])cc3)no2)cc1	380
557	685	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(CCCCC(=O)NO)c2c(=O)n1-c1ccccc1	385
558	686	COc1ccc(S(=O)(=O)NC2CCc3ccc(C(=O)NO)cc3C2)cc1OC	390
559	688	COc1ccc2c(C(=O)c3cc(OC)c(OC)c(OC)c3)cn(Cc3ccc(C(=O)NO)cc3)c2c1	390
560	689	O=C(CCN1CCc2ccccc2C1c1cccc2ccccc12)NO	390
561	690	COC(=O)Cc1c(C)n(Cc2ccc(-c3cn(CCCCCCCC(=O)NO)nn3)cc2)c2ccc(OC)cc12	394
562	691	Cc1cc2ccccc2n1Cc1ccc(C(=O)NO)cc1	397
563	693	CN(C)Cc1cn(Cc2ccc(C(=O)NO)cc2)c2ccccc12	398.11
564	694	Cn1cncc1-c1cn(Cc2ccc(C(=O)NO)cc2)c2ccccc12	398.11
565	695	COc1cc2ccn(CCOc3ccc(NC(=O)CCCCCCC(=O)NO)cc3)c2cc1OC	398.3
566	696	O=C(Cc1ccc(CCCCc2cccc(C(F)(F)F)c2)cc1)NO	400
567	698	CCN1CCC[C@@H](n2c(-c3ccccc3)nc(C)c2-c2cccc(/C=C/C(=O)NO)c2)C1	400
568	699	O=C(CCCCCCCNC(=O)c1c(-c2ccc(O)cc2)sc2cc(O)ccc12)NO	400
569	700	O=C(/C=C/c1cccc(-c2nc3ccccc3n2CCN2CCOCC2)c1)NO	400

570	701	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3O)c(=O)c3ccccc32)cc1	400
571	703	COc1cc(OC)c2c(N3CCS(=O)(=O)CC3)nc(-c3cc(C)c(OCCCCCC(=O)NO)c(C)c3)nc2c1	403.5
572	704	O=C(CCCCCCCNC(=O)NC(=O)c1ccccc1)NO	405
573	705	O=C(CCCCCCC(=O)Nc1cccc(-c2cnnn2CC(O)c2cccc(Br)c2)c1)NO	406
574	706	O=C(NO)c1ccc(CNc2nccc(-c3cccnc3)n2)cc1	410
575	708	O=C(Cc1ccc(CCCCc2ccc3[nH]ccc3c2)cc1)NO	410
576	709	CCN(c1ccc(C(=O)NO)cc1)S(=O)(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1	410.4582805
577	710	O=C(NO)c1ccc(CN(Cc2cccc(F)c2)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	412
578	711	O=C(/C=C/c1ccc2c(c1)ncn2Cc1ccccc1)NO	412
579	713	O=C(NO)c1ccc(Cn2ccc3ccccc32)cc1	417
580	714	O=C(NO)c1ccc(CN2c3ccccc3NC(=O)[C@H]2Cc2ccc(F)c(F)c2)cc1	420
581	715	O=C(NO)c1cccc(C(=O)NCCc2cccnc2)c1	420
582	716	CCCCCCC(CCCC(=O)NO)CCC(=O)Nc1ccccc1	420
583	718	CC(C)c1cc(C(=O)N2Cc3ccc(NCc4ccc(C(=O)NO)cc4)cc3C2)c(O)cc1O	420
584	719	O=C(/C=C/C1CCN(Cc2cccc3ccccc23)CC1)NO	420
585	720	O=C(/C=C/c1ccc(CN(C(=O)c2c(F)c(F)c(F)c(F)c2F)C2CC2)cc1)NO	420
586	721	Cc1nc2c(/C=C/C(=O)NO)cccc2c(=O)n1-c1ccccc1	420
587	2046	CC(CNC(=O)c1ccc(/C=C/C(=O)NO)cc1)Oc1no[n+]([O-])c1S(=O)(=O)c1ccccc1	420
588	723	CN(C)CCc1cn(Cc2ccc(C(=O)NO)cc2)c2ccccc12	422
589	724	CC(C)c1cc(C(=O)N(C)c2ccc(NC(=O)CCCCCCC(=O)NO)cc2)c(O)cc1O	422
590	725	O=C(/C=C/c1ccc(C(=O)NC(Cc2c[nH]c3ccccc23)C(=O)Nc2ccc(Br)cc2)cc1)NO	423.1
591	726	O=C(NO)c1ccc(Cn2c(=O)n(CCc3cccc(F)c3)c(=O)c3ccccc32)cc1	429
592	728	COc1ccc(-c2nc(NC(=O)NCCC(=O)NO)cc3c2[nH]c2ccccc23)cc1	430
593	729	O=C(NO)C1=CCCCC1	431
594	730	O=C(CCCCCCC(=O)Nc1cccc(-c2cnnn2Cc2ccccc2)c1)NO	433
595	731	CCOc1ccc(C(=O)Nc2cc(C(=O)NO)ccc2OC)cc1	438.4
596	733	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(CC(O)c3cccc(Br)c3)nn2)c1)NO	440
597	734	O=C(NO)c1ccc2c(c1)nc(CCc1ccccc1)n2CCCO	441
598	735	O=C(/C=C/c1ccc(CNCc2ccc3ccccc3n2)cc1)NO	442
599	736	COc1ccc(C(=O)NO)cc1S(=O)(=O)Nc1ccc2c(c1)cc(C)c(=O)n2C	443
600	738	O=C(NO)c1ccc(Cl)c(NC(=O)c2cccc(Oc3ccccc3)c2)c1	448.6
601	739	O=C(NO)c1ccc(Cl)c(NC(=O)c2ccc(-c3ccccc3)cc2)c1	450
602	740	O=C1CCC[C@@H](C(=O)N[C@@H](CCCCCS)C(=O)NC2CCCC2)N1	450
603	741	COc1ccc(C(=O)CCCCCCC(=O)NO)cc1	450
604	743	O=C(CCn1c(=O)n(CCc2ccccc2)c(=O)c2ccccc21)NO	454
605	744	O=C(/C=C/c1ccc(Cc2ccc(O)c(Cl)c2)cc1)NO	460
606	2047	O=C(/C=C/c1ccc(C(=O)NCCCOc2no[n+]([O-])c2S(=O)(=O)c2ccccc2)cc1)NO	460
607	745	CCC/C=C/c1c(-c2ccccc2)nnn1[C@@H](Cc1ccccc1)C(=O)NO	464
608	746	Cc1cc2cc(NS(=O)(=O)Cc3cccc(C(=O)NO)c3)ccc2n(C)c1=O	465
609	748	O=C(CCCCCCn1cc(-c2ncnc3[nH]ccc23)cn1)NO	469
610	749	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1ccc(Cl)c(Cl)c1)CC2	470

611	750	O=C(/C=C/c1ccccc1Oc1c(Cl)cccc1Cl)NO	470
612	751	O=C(/C=C/C1CCN(Cc2cccc(Cl)c2)CC1)NO	470
613	753	COc1cc(C(=O)NO)ccc1CN(C(C)C)S(=O)(=O)c1cc(F)c(F)c(F)c1F	474
614	754	O=C(NO)c1ccc(CN(CCCCO)C(=O)Nc2ccccc2)cc1	478
615	755	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3cnc4ccccc4c3)n1)CC2	480
616	756	CC(C)(C)c1ccc(C2c3ccccc3CCN2CCC(=O)NO)cc1	480
617	758	COc1ccc(C(=O)NO)cc1NCc1ccc2ccccc2n1	481
618	2048	[N-]=[N+]=NCc1cc(N=[N+]=[N-])cc(C(=O)Nc2ccc(Cn3cc(NC(=O)CCCCCCC(=O)NO)cn3)cc2)c1	487
619	759	CCN(CC)Cc1ccc(Cn2c(=O)c(OCc3ccc(C(=O)NO)cc3)c(-c3cccnc3)c3ccccc32)cc1	490
620	760	NCc1ccc(NC(=O)N(CCCCO)Cc2ccc(C(=O)NO)cc2)cc1	498
621	761	O=C(CCCCCCC(=O)c1ccccc1)NO	500
622	763	S=c1[nH]cc(-c2ccncc2)[nH]1	500
623	764	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)CCc2ccccc2)cc1	502
624	765	O=C(NO)c1cc(F)c(Cn2nnc(-c3ncccn3)n2)c(F)c1	504
625	766	CCN(C(=O)c1ccc(C(=O)NO)cc1)c1cccc(C(C)(C)C)c1	508.7573095
626	768	O=C(NO)c1ccc(-c2cnnn2CC23CC4CC(CC(C4)C2)C3)s1	510
627	769	COc1ccc(C(=O)NO)cc1NC(=O)Cc1ccccc1	512.2
628	770	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)CNC(=O)OC(C)(C)C)cc1	514
629	771	COc1ccc(/C=C2\SC(=O)N(CCNC(=O)Nc3c(C)n(C)n(-c4ccccc4)c3=O)C2=O)cc1	517
630	773	COc1cncc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)c1	520
631	774	Cc1ccc(-c2cc(C(=O)NCCCCCCC(=O)NO)nn2-c2ccc(S(N)(=O)=O)cc2)cc1	520
632	775	S=C1Sc2cccc(Br)c2C2=NCCCN12	520
633	776	Cc1cncc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)c1	520
634	778	Cc1cccc(NC(=O)CCCCCCC(=O)NO)c1	523
635	779	COc1ccccc1CCn1c(=O)c2ccccc2n(Cc2ccc(C(=O)NO)cc2)c1=O	525
636	780	O=C(CCCCCCC(=O)Nc1cccc(-c2cnnn2Cc2ccc(F)cc2)c1)NO	529
637	781	C[C@H](NC(=O)[C@H](CC(=O)NCC(C)(C)C)NC(=O)c1ccc(C(=O)NO)cc1)C(=O)NCc1ccccc1	530
638	783	CC(C)C[C@H]1CC(=O)N[C@@H](Cc2ccccc2)C(=O)N[C@@H](CCCCCC(=O)O)C(=O)N[C@@H](Cc2cccc3ccccc23)C(=O)N1	530
639	784	O=C(/C=C/c1ccc(CNCCCN2c3ccccc3CCc3ccc(Cl)cc32)cc1)NO	533
640	785	O=C(CCCCCCNC(=O)c1c(-c2ccc(O)cc2)sc2cc(O)ccc12)NO	536.2835071
641	786	O=C(/C=C/c1ccc2c(c1)nc(-c1ccsc1)n2CCCO)NO	537
642	788	S=C1Sc2ccc(Cl)cc2C2=NCCCN12	540
643	789	CC(C)(C)OC(=O)n1cnc(C[C@@H]2NC(=O)[C@]3(C)CSC(=N3)c3csc(n3)CNC(=O)C[C@@H](/C=C/CCS)OC2=O)c1	540
644	790	Cc1ccc(-c2cc(C(=O)NCCCCCC(=O)NO)nn2-c2ccc(S(N)(=O)=O)cc2)cc1	544
645	791	CN1C(=O)CC[C@@H]1C(=O)N[C@@H](CCCCCS)C(=O)Nc1ccccc1	545
646	793	O=C(CCCCCCNCc1ccc(-c2ccccc2)s1)NO	550
647	794	CCN(CC)Cc1ccc(Cn2c(=O)c(OCc3ccc(C(=O)NO)cc3)c(-c3ccccc3)c3ccccc32)cc1	550
648	795	CCN(C(=O)c1ccccc1C(F)(F)F)c1ccc(C(=O)NO)cc1	550.3308096
649	796	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(Cc3ccc(F)cc3)nn2)c1)NO	552
650	798	COc1ccc(C(=O)NO)cc1CNc1ccc2c(c1)cc(C)c(=O)n2C	555
651	799	CCCNNC(=O)c1ccc(NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC(	557.3

		=O)c2ccc(OC)cc2)cc1	
652	800	COc1ccc(-c2cc(-c3ccccc3)[nH]c2C(=O)NCc2ccc(C(=O)Nc3ccccc3S)cc2)cc1	559
653	801	Cc1cc2cc(NS(=O)(=O)c3cc(C(=O)NO)ccc3Cl)ccc2n(C)c1=O	560
654	803	CC12CC3CC(C)(C1)CC(NS(=O)(=O)c1cccc(/C=C/C(=O)NO)c1)(C3)C2	562
655	804	Oc1cccn(CCCCCCCn2cc(-c3ccccc3)nn2)c1=S	565.2114649
656	805	O=C(NO)c1ccc(NC(=O)c2ccc(F)cc2)cc1	567
657	806	COc1ccc(-c2nc(NC(=O)NCCCC(=O)NO)cc3c4ccccc4n(C)c23)cc1	570
658	808	CN(C(=O)CN(C)S(=O)(=O)c1ccc(F)cc1)c1ccc(C(=O)NO)cc1	573
659	809	Cc1[nH]c2ccccc2c1/C=C/c1ccccc1-c1ccc(/C=C/C(=O)NO)cc1	580
660	810	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	580
661	811	O=C(COc1ccc2c(c1)CN(C(=O)OCc1ccccc1)[C@H](C(=O)NCCc1ccccc1)C2)NO	580
662	813	Nc1nc2ncc(CNc3ccc(C(=O)NO)cc3)nc2c(=O)[nH]1	581
663	814	O=C(NO)c1cccc(NC(=O)c2ccccc2)c1	582
664	815	O=C(NO)c1ccc2ccccc2n1	582.3
665	816	Cc1cc(F)cc(C)c1Oc1ccc(C(C)(C)O)cc1-c1cn(C)c(=O)c2[nH]c(C(=O)NCCCCCCC(=O)NO)cc12	583
666	818	CCOc1ccc(C(C)=O)cc1NC(=O)c1cccc(C(=O)NO)c1	590
667	819	C#Cc1cccc(Nc2ncnc3ccc(S(=O)(=O)n4ccc(/C=C/C(=O)NO)c4)cc23)c1	590
668	820	CCc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1CCc1ccc(OC)cc1	594
669	821	O=C(NO)c1ccc(CN2CCCc3cccnc32)c(F)c1	597
670	823	CC(C)C[C@H](NC(=O)OC(C)(C)C)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	600
671	824	CC(C)c1cc(C(C)C)c(C(C)C)cc1CS(=O)(=O)Nc1ccc(/C=C\C(=O)NO)cc1	600
672	825	CC(CCCCCC(=O)c1ccc2ccccc2c1)C(=O)NOCCCCC(=O)NO	600
673	826	O=C(/C=C/c1ccc(NS(=O)(=O)c2ccc(OC(F)(F)F)cc2)cc1)NO	600
674	828	S=C1Sc2cccc(Cl)c2C2=NCCN12	600
675	829	O=C(/C=C/c1ccc2c(=O)n(CCc3ccccc3)cnc2c1)NO	600
676	830	CC(C)Cc1nc2cc(/C=C/C(=O)NO)ccc2n1CCc1ccccc1	601
677	831	N[C@@H](CCCCCC(=O)c1ccon1)c1cc(-c2ccccc2F)on1	603
678	833	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3cccc(-c4cn(CCCCCC(=O)NO)nn4)c3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	604
679	834	CC(C)C[C@H]1CC(=O)N[C@@H](CCCNC(=N)N)C(=O)N[C@@H](CCCCCC(=O)O)C(=O)N[C@@H](Cc2cccc3ccccc23)C(=O)N1	607
680	835	O=C(CCCCCNC(=O)NC(=O)c1ccccc1)NO	608
681	836	Cc1nc2ccc(/C=C/C(=O)NO)cc2c(=O)n1-c1ccccc1	609
682	838	O=C(CCCCSc1nc(-c2ccc(-c3ccccc3)cc2)cc(=O)[nH]1)NO	610
683	839	O=C(Cc1ccc(CCCCc2ccccc2C(F)(F)F)cc1)NO	610
684	840	O=C(/C=C/c1ccc(NC(=O)C(Cc2ccccc2)c2ccccc2)cn1)NO	610.6659394
685	841	CCCCN(Cc1ccc(C(=O)NO)cc1)C(=O)Nc1ccc(CN)cc1	614
686	843	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	620
687	844	O=C(CCCCCCNCc1cc2ccccc2[nH]1)NO	620

688	845	O=C1CCSc2ccc(C(=O)NO)cc2N1	620
689	2050	O=C(CCCCCN1C(=O)c2cccc3c([N+](=O)[O-])ccc(c23)C1=O)NO	620
690	846	CC(C)(C)c1ccc(S(=O)(=O)NCc2ccc(C(=O)NO)cc2)cc1	622
691	848	O=C(NO)c1cccc(C(=O)NOCc2ccc(Cl)cc2Cl)c1	630
692	849	CCCCc1nc2cc(/C=C/C(=O)NO)ccc2n1CCN(CC)CC	630
693	850	CC(C)(C)OC(=O)N(Cc1ccc(C(C)(C)C)cc1)c1ccc(C(=O)NO)cc1	635
694	851	O=C(NO)c1ccc(CNc2cccc3ncccc23)cc1	636
695	853	O=C(NO)c1ccc(CN2c3ccccc3NC(=O)[C@H]2CCc2ccccc2)cc1	640
696	854	O=C(CCCCCC1OCCCCCOc2ccccc2NC1=O)NO	643
697	855	CC[C@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@@H]2O)[C@@](C)(O)C[C@H](C)CN(C)[C@@H](C)[C@H](O)[C@@]1(C)O	644
698	856	COc1ccc(C(=O)c2ccc3c(ccn3Cc3ccc(C(=O)NO)cc3)c2)cc1	646
699	858	NC(=O)c1ccc2c(c1)CCCN2Cc1ccc(C(=O)NO)cc1	651
700	2051	[N-]=[N+]=NCc1cc(N=[N+]=[N-])cc(C(=O)Nc2ccc(-c3cc(C(=O)NCCCCCCC(=O)NO)no3)cc2)c1	651
701	859	CC(C)N(Cc1ccc(C(=O)NO)cc1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	653
702	860	O=C(NO)c1cccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccccc32)c1	653
703	861	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NCCc2ccccc2)cc1	660
704	863	COC(=O)Cc1c(C)n(Cc2ccc(-c3cn(CCCCCC(=O)NO)nn3)cc2)c2ccc(OC)cc12	672
705	864	CC(C)c1cc(C(=O)N2Cc3ccc(/C=C/C(=O)NO)cc3C2)c(O)cc1O	675
706	865	O=C(NO)c1ccc2c(c1)CC(Nc1ccc(Br)cc1)CC2	680
707	866	O=C(NO)c1ccc(NC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1	682
708	868	O=C(NO)c1ccc(C(=O)Nc2ccccc2)cc1	689
709	869	O=CN(O)CCCCCC(C(=O)Nc1cnc2ccccc2c1)C(=O)Nc1cnc2ccccc2c1	690
710	870	CN1c2ccc(F)cc2C(=O)N2CCc3c([nH]c4ccc(OCc5ccc(/C=C/C(=O)Nc6ccccc6N)cc5)cc34)C21	690
711	871	O=C(NO)c1ccc(CN2c3ccccc3NC(=O)[C@H]2Cc2cccs2)cc1	690
712	873	O=C(CS)CCCCCCC(=O)Nc1ccccc1	690
713	874	O=C(COc1ccc2c(c1)CN(C(=O)CCc1ccccc1)[C@H](C(=O)NCCc1ccccc1)C2)NO	692
714	875	O=C(NO)c1ccc(CNC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	696.9935437
715	876	Cc1ccc(-c2cc(C(=O)NCCCCCCCC(=O)NO)nn2-c2ccc(S(N)(=O)=O)cc2)cc1	697
716	878	O=C(/C=C/c1cccc2ccccc12)NO	700
717	879	CC12CC3CC(C)(C1)CC(NCc1cccc(NC(=O)CCCCCCC(=O)NO)c1)(C3)C2	703
718	880	COc1ccc2c(c1)c(CC(=O)NCCCCCCCCC(=O)NO)c(C)n2C(=O)c1ccc(Cl)cc1	707
719	881	CC12CC3CC(C)(C1)CC(NC(=O)CCCCCCCCC(=O)NO)(C3)C2	707
720	2052	[N-]=[N+]=Nc1ccc(-c2cc(C(=O)NCCCCCCC(=O)NO)no2)cc1	707
721	883	CCCCCC[C@H](CCCCCC(=O)Nc1ccccc1)C(=O)NO	710
722	884	O=C(CCCCCCc1nc(-c2ccccc2Cl)no1)C(F)(F)F	710
723	885	COc1cccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@](O)(C(C)=O)C[C@@H]3O[C@H]1C[C@H](NCc2ccc(-c3cn(CCCCCCC(=O)NO)nn3)cc2)[C@H](O)[C@H](C)O1	710
724	886	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)	713

		C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	
725	888	CC(C)[C@H](NC(=O)OC(C)(C)C)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	720
726	889	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CCCN1CCCC1=O)NO	724
727	890	O=C(/C=C/c1ccc(C(c2c[nH]c3ccccc23)c2c[nH]c3ccccc23)cc1)NO	730
728	891	O=C(NO)c1ccc(CN2c3ccccc3NC(=O)[C@H]2Cc2ccc(O)cc2)cc1	730
729	893	COc1ccc2c(=O)n(CCc3ccccc3)c(=O)n(Cc3ccc(C(=O)NO)cc3)c2c1	731
730	894	Nc1ccc(F)cc1NC(=O)c1ccc(CNC(=O)/C=C/c2cccnc2)cc1	733
731	895	Nc1ncnc2c1c(-c1cnc3[nH]ccc3c1)nn2CCCCCCCCC(=O)NO	733
732	896	O=C(CCCCCCC(=O)Nc1ccc(-c2cnnn2CC(O)c2cccc(Br)c2)cc1)NO	737
733	898	O=C(NO)c1ccc(CN2C(=O)CCc3cc(Br)ccc32)cc1	743
734	899	CCCN1CC(=O)N2Cc3c(c4ccccc4n3Cc3ccc(C(=O)NO)cc3)CC2C1=O	747
735	900	CC[C@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)C)[C@H](C)O2)[C@H](C)[C@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@@H]2O)[C@@](C)(O)C[C@H](C)CN(C)[C@@H](C)[C@H](O)[C@@]1(C)O	749
736	901	CCC(=O)CCCCC[C@@H]1NC(=O)[C@H](CCCNC(=N)N)NC(=O)CCN(CC(C)C)C(=O)CN(CCc2c[nH]c3ccccc23)C1=O	750
737	903	COc1cc2ccn(CCCCOc3cccc(NC(=O)CCCCCCC(=O)NO)c3)c2c(OC)c1OC	752
738	904	COc1ccc(C(=O)c2ccc3c(ccn3Cc3ccc(C(=O)NO)cc3)c2)cc1OC	756
739	905	O=C(/C=C/c1ccccc1)NO	759
740	906	O=C(COc1ccc2c(c1)CN(C(=O)CCc1ccccc1)[C@H](C(=O)Nc1ccccc1)C2)NO	759
741	908	O=C(NO)c1ccc(NC2CCN(Cc3ccccc3)C2=O)cc1	760
742	909	CC(C)(C)OC(=O)N1CCC[C@H]1C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	760
743	910	CCCCCCCCc1nc2cc(/C=C/C(=O)NO)ccc2n1CCCO	763.4788799
744	911	CCc1nc2cc(F)c(/C=C/C(=O)NO)cc2c(=O)n1CCc1ccccc1	766
745	913	O=C(NO)c1ccc(Cl)c(NC(=O)c2ccc(-c3ccccc3)cc2Cl)c1	780
746	914	CCc1nc(N)nc(N)c1-c1ccc(-c2cn(CCCCCCC(=O)NO)nn2)cc1	780
747	915	CC[C@H](C)[C@@H]1NC(=O)[C@@H](Cc2ccc(OC)cc2)NC(=O)[C@H](CCCCCC(=O)C(F)(F)C(F)(F)F)NC(=O)[C@H]2CCCN2C1=O	780
748	916	O=CN(O)CCCCCCCC(=O)Nc1ccc2ccccc2c1	780
749	918	COc1cc2c(cc1-c1c(C)noc1C)[nH]c1ncnc(NCCCCCCC(=O)NO)c12	784
750	919	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@@](O)(CN(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	786
751	920	CCOC(=O)Nc1cccc(-c2csc(NC(=O)CCCCCC(=O)NO)n2)c1	787
752	921	COc1cc(-c2nc3cc(/C=C/C(=O)NO)ccc3n2CCCO)ccc1OCc1ccccc1	790
753	923	CC(C)(C)OC(=O)NCCC[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C=C/CCS)OC1=O	790
754	924	CC(/C=C/C(=O)NO)=C\[C@H](C)C(=O)c1ccc(N(C)C)cc1	790
755	925	O=C(NO)c1ccc(CN2CCCc3cc(-c4cc[nH]n4)ccc32)cc1	792
756	926	O=C(NO)c1ccc(Cn2c3c(c4ccccc42)COCC3)cc1	794.33
757	928	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C	796.2

		@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	
758	929	O=C(CCCCCCC(=O)Nc1ccc(-c2cn(Cc3ccc(F)cc3)nn2)cc1)NO	797
759	930	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)/C=C/C(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	800
760	931	Cc1ccc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)cc1	800
761	933	O=CN(O)CCCCCC(C(=O)Nc1ccc2ncccc2c1)C(=O)Nc1ccc2nccc2c1	800
762	934	CN(C)c1cccc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)c1	800
763	935	Nc1cc(F)ccc1NC(=O)c1ccc(CNC(=O)/C=C/c2cccnc2)cc1	801.6280283
764	936	CCC(=O)CCCCC[C@@H]1NC(=O)[C@H]2CC23CCN(CCCOCCCn2ccc4cc(ccc4c2=O)-c2cnc1[nH]2)CC3	808
765	938	O=C(NO)c1ccc(Cn2cnc(-c3ccccc3F)n2)c(F)c1	813
766	939	CC[C@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@H](C)O2)[C@H](C)[C@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)C)[C@@H]2O)[C@@](C)(O)C[C@H](C)CN(C)[C@@H](C)[C@H](O)[C@@]1(C)O	817
767	940	CN1CCc2c(c3ccccc3n2Cc2ccc(C(=O)NO)cc2)C1	817.2153476
768	941	CC(C)C[C@H](NC(=O)CNC(=O)c1cccc(/C=C/C(=O)NO)c1)B1O[C@@H]2[C@@H]3C[C@H](C[C@]2(C)O1)C3(C)C	819
769	943	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	825
770	944	O=C(NO)c1cccc(NC2CCCCC2)c1	830
771	945	O=C(NO)[C@@H]1[C@H](c2ccccc2)[C@H]1c1cc(Cl)c2c(c1)OCCO2	830
772	946	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3cccnc3)n1)CO2	830
773	2053	O=C(CCCCCCc1nc(-c2cccc([N+](=O)[O-])c2)no1)C(F)(F)F	830
774	948	CC12CC3CC(C)(C1)CC(NC(=O)CCCCCCC(=O)NO)(C3)C2	831
775	949	Cc1ccc(C(=O)NOCCCCCCC(=O)NO)cc1C	833
776	950	COc1ccc2c(c1)c(CCNC(C)=O)cn2Cc1ccc(C(=O)NO)cc1	834.8741702
777	951	CCN(CC)Cc1ccc2cc(COC(=O)Nc3ccc(C(=O)NO)cc3)ccc2c1	837
778	953	O=C(/C=C/c1ccc(NC(=O)Nc2ccc(Cl)cc2)cc1)NO	840
779	954	COc1ccc(C(=O)NO)cc1OCc1ccc(Cl)cc1Cl	840
780	955	COc1cc2c(cc1OC)C(=O)C(CC1CCN(Cc3ccc(NC(=O)CCCCCCC(=O)NO)cc3)CC1)C2	842
781	956	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccc(O)cc3)c(=O)c3ccccc32)cc1	845
782	958	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1ccc(Cl)cc1)CC2	850
783	959	COc1ccc(-c2noc(CNCc3ccc(C(=O)NO)cc3)n2)cc1	860
784	960	COc1ccc(C(=O)NO)cc1NCc1cccc2c1oc1ccccc12	860
785	961	O=C(NO)c1ccc(CN(Cc2ccc(F)cc2)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	860
786	963	O=C(CCCCCCCCC(=O)NCCCN1c2ccccc2CCc2ccc(Cl)cc21)NO	864
787	964	CC(C)C[C@H]1CC(=O)NC(C)(C)C(=O)N[C@@H](CCCCCC(=O)O)C(=O)N[C@@H](Cc2cccc3ccccc23)C(=O)N1	870
788	965	O=C(NO)[C@@H]1[C@H](c2ccccc2)[C@H]1c1ccc2nccnc2c1	870
789	966	CC(C)(C)OC(=O)N[C@@H](CO)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	870
790	968	COc1cc(-c2nc(NCc3ccc(C(=O)NO)cc3)cc3c2[nH]c2ccccc23)cc(OC)c1OC	875
791	969	CC(C)N(Cc1ccc(C(=O)NO)cc1)C(=O)c1c(F)c(F)c(F)c(F)c1F	876

792	970	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	877
793	971	CC(C)C(C(=O)Nc1ccc(C(=O)NO)nc1)c1ccccc1	882
794	973	Cn1cccc1C(=O)N1CCCc2cc(C(=O)NO)ccc2C1	890
795	974	CCc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1CCc1ccc(F)cc1	891
796	975	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(Cl)nc3)n1)CC2	900
797	976	O=C(NO)c1ccc(Cn2c3c(c4cc(F)ccc42)CS(=O)(=O)CC3)cc1	900
798	978	O=C(CCCCCCS)NCc1cccc(OCc2ccccc2)c1	904
799	979	Cc1cc2cc(NS(=O)(=O)c3ccc(C(=O)NO)cc3)ccc2n(C)c1=O	908
800	980	O=C(NO)c1cccc(S(=O)(=O)N[C@H](C(=O)Nc2ccccc2)c2ccccc2)c1	910
801	981	CCCCS(=O)(=O)NC1CCc2ccc(C(=O)NO)cc2C1	910
802	983	Cc1cn(Cc2ccc(C(=O)NO)cc2)c2ccccc12	911
803	984	Oc1cccn(CCCCCn2cc(-c3ccccc3)nn2)c1=S	917
804	985	C[C@@]12Nc3ccccc3[C@]1(O)CCN2Cc1ccc(/C=C/C(=O)NO)cc1	920
805	986	Cn1cc(CN2CCC(/C=C/C(=O)NO)CC2)c2ccccc21	920
806	988	O=C(NO)c1ccc(NC(=O)c2ccc(N3CCOCC3)cc2)cc1	921
807	989	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NCCCc2ccccc2)cc1	922
808	990	O=C(NO)c1cc2c(cc1F)CCC(NS(=O)(=O)c1cccc(Cl)c1)C2	930
809	2054	O=C(NO)c1ccc2c(c1)CC(Nc1ccc([N+](=O)[O-])cn1)CC2	930
810	991	Nc1cccc(-c2cc(C(=O)NCCCCCCCC(=O)NO)no2)c1	938
811	993	O=C(CCCCCCC(=O)Nc1cccc(-c2cnnn2-c2ccccc2)c1)NO	942
812	994	CCCCNc1nc(Cl)nc2c1ncn2Cc1ccc(C(=O)Nc2ccccc2N)cc1	948
813	995	O=C(CCCCCCc1nc(-c2cccs2)no1)C(F)(F)F	950
814	996	O=C(/C=C/C1CCN(Cc2ccc(Cl)cc2)CC1)NO	950
815	998	O=C(/C=C/c1ccc(C(F)(F)F)cc1)NO	954
816	999	COc1ccc(C(=O)NO)cc1NCc1ccc(OCCCCC(=O)Nc2ccc3c(c2)cc(C)c(=O)n3C)cc1	956
817	1000	CC(C)(C)OC(=O)NCCCC(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	960
818	1001	CCC(C(=O)Nc1ccc(C(=O)NO)nc1)c1ccccc1	964
819	1003	O=C(CCCCCNC(=O)c1ccc(NC(=O)NC(C(=O)Nc2cccc(C(F)(F)F)c2)c2ccccc2)cc1)NO	967
820	1004	CC1Sc2ccc(C(=O)NO)cc2NC1=O	970
821	1005	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1cccc(Cl)c1)CN2	970
822	1006	O=C(NO)c1ccc(CN(C(=O)c2c(F)c(F)c(F)c(F)c2F)C2CC2)cc1	971
823	1008	C[C@@H](NC(=O)c1cccc(=S)n1O)C(=O)O	980
824	1009	O=C(NO)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)s1	980
825	1010	O=C(NO)c1ccc(Cn2nnnc2-c2cccs2)cc1	984
826	1011	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@@](O)(CN(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)C)[C@@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@H](O)[C@]1(C)O	985
827	1013	Cc1ccc(-c2cc(C(F)(F)F)nn2-c2ccc(S(=O)(=O)NCCCCCCCCC(=O)NO)cc2)cc1	989
828	1014	O=C(/C=C/c1cccnc1)NC1CCc2ccc(C(=O)NO)cc2C1	990
829	1015	O=C(NO)c1ccc(CN2C(=O)CN(Cc3ccc(Cl)cc3)C2=O)cc1	994
830	1016	O=C(NO)c1cc(F)c(Cn2nnnc2-c2cccs2)c(F)c1	996
831	1017	C#Cc1ccc(C(=O)NO)s1	1000
832	1018	O=C(NO)c1ccc(CCCc2ccccc2)cc1	1000

833	1020	CC(=O)NCCCC[C@@H]1NC(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2cccc3ccccc23)NC(=O)[C@H](CCCCCC(=O)O)NC1=O	1000
834	1021	COc1ccc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)cn1	1000
835	1022	Cc1ccc2c(c1)SC(=S)N1CCCN=C21	1000
836	1023	S=C1Sc2ccc(I)cc2C2=NCCCN12	1000
837	1025	O=C(NO)c1cn(C2CCN(C(=O)Cc3ccc4ccccc4c3)CC2)nn1	1000
838	1026	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)OC(C)(C)C)cc1	1000
839	1027	S=C1Sc2cc(Br)ccc2C2=NCCN12	1000
840	1028	O=C(CCCc1ccc(NS(=O)(=O)c2ccccc2)cc1)NO	1000
841	1030	Cc1nc2c(c(N(C)c3ccc(OCCCCCC(=O)NO)cc3)n1)CCC2	1003
842	1031	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CCc1ccccc1)NO	1005
843	1032	O=C(/C=C/c1ccc(NC(=O)Cc2ccc3ccccc3c2)cn1)NO	1010
844	1033	Nc1ccccc1NC(=O)c1ccc(NC(=O)c2n[nH]cc2NC(=O)c2c(Cl)cccc2Cl)cc1	1010.16
845	1035	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	1020
846	1036	O=C(NO)c1ccc(Cl)c(OCc2ccc(Cl)cc2)c1	1020
847	1037	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2CCc2ccccc2)cc1	1020
848	1038	O=C(CCCCc1ccn(Cc2ccc(Nc3ccccc3)cc2)n1)NO	1024
849	1040	CC12CC3CC(C)(C1)CC(NCc1ccc(/C=C/C(=O)NO)cc1)(C3)C2	1030
850	1041	O=C(NO)c1ccc(C(=O)NCc2ccccc2)cc1	1030
851	1042	CC(C)(C)c1cccc(NC(=O)c2ccc(C(=O)NO)cc2)c1	1040
852	1043	Cc1cccc(C(=O)NOCCCCCC(=O)NO)c1	1043
853	1045	CC[C@@]1(O)C(=O)OCc2c1cc1n(c2=O)Cc2cc3cc(OCc4cn(CCCCCCC(=O)NO)nn4)ccc3nc2-1	1046
854	1046	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccc(F)cc3)c(=O)c3ccccc32)cc1	1049
855	1047	CN(C)c1ccc(CNC(=O)NCCC(=O)NO)cc1	1050
856	1048	CN(c1ccc(OCCCCCC(=O)NO)cc1)c1ncnc2ccccc12	1058
857	1050	O=C(NO)c1ccc(Cn2ccc3cc(C(=O)c4ccc(Cl)cc4)ccc32)cc1	1060
858	1051	Nc1nc2ncc(CNc3ccc(C(=O)NCCCCCCC(=O)NO)cc3)nc2c(=O)[nH]1	1060
859	1052	NC(=O)c1ccc2c(c1)CCCCN2Cc1ccc(C(=O)NO)cc1	1060
860	1053	CCCCN(Cc1ccc(C(=O)NO)cc1)C(=O)Nc1ccccc1	1064.697592
861	1055	O=C(CCCCCCCC(=O)NCCCN1c2ccccc2CCc2ccc(Cl)cc21)NO	1070
862	1056	CC12CC3CC(C)(C1)CC(NC(=O)CCCCCCCC(=O)NO)(C3)C2	1070
863	1057	O=C(CCCCCCS)Nc1ccccc1	1070
864	1058	CC(C)CCc1c(OCCCCCCCC(=O)NO)ccc2c1OC(=O)CC2	1075.12
865	1060	Nc1cc(F)ccc1NC(=O)c1ccc(CNC(=O)/C=C2\NC(=O)c3ccccc32)cc1	1080
866	1061	O=C(NO)c1ccc(Cl)c(NC(=O)c2ccc(Oc3ccccc3)cc2)c1	1080
867	1062	O=C(NO)c1ccc(CNC(=O)c2ccc(-c3csc(N4N=C(c5ccccc5)/C(=N/Nc5nccs5)C4=O)n3)cc2)cc1	1086.8
868	1063	COc1ccc(/C=C\c2cc(OC)c(OC)c(OC)c2)cc1/C=C/C(=O)Nc1ccccc1N	1090
869	1065	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CCCN1CCOCC1)NO	1090
870	1066	O=C(NO)c1ccc(NC(=O)C(Cc2ccccc2)c2ccccc2)cn1	1090
871	1067	O=C(NO)C1=CCCC1	1090
872	1068	O=C(Cc1ccccc1)Nc1ccc(C(=O)NO)nc1	1090
873	1070	O=C(CCCCCC1OCCCCCCOc2ccccc2NC1=O)NO	1100

874	1071	CN(C)S(=O)(=O)c1ccc(NCCCCCCC(=O)NO)c2nonc12	1100
875	1072	COc1ccc(C(=O)NO)cc1NC(=O)c1ccc(-c2ccccc2)cc1Cl	1100
876	1073	O=C(NO)c1ccc(CN2c3ccccc3CCC[C@@H]3CCCC[C@H]32)cc1	1100
877	1075	O=C(NO)c1ccc(CN2c3ccccc3S(=O)(=O)C[C@@H]3CCCC[C@@H]32)cc1	1100
878	1076	Cc1ccc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)c(F)c1	1100
879	1077	O=C(CCCCC/C=C/c1csc(Br)n1)NO	1100
880	1078	C[C@@]12CSC(=N1)c1csc(n1)CNC(=O)C[C@@H](/C=C/CCS)OC(=O)[C@H](CCCCNC(=O)O[C@@H]1CC/C=C/CCC1)NC2=O	1115
881	1080	COc1cccc(C(=O)c2ccc3c(ccn3Cc3ccc(C(=O)NO)cc3)c2)c1	1120
882	1081	O=C(CCCCCCCS)Nc1ccccc1	1120
883	1082	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1cccc(F)c1)CN2	1140
884	1083	COc1ccc(CCn2c(=O)c3ccccc3n(Cc3ccc(C(=O)NO)cc3)c2=O)cc1	1150
885	1085	O=C(NO)c1ccc(C(=O)NCCc2ccccc2)cc1	1150
886	1086	C[C@H](NC(=O)OC(C)(C)C)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	1150
887	1087	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3cc(F)ccc32)cc1	1155
888	1088	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1cccc(Cl)c1	1170
889	1090	O=C(NO)c1ccc(CN2C(=O)CCCc3cc(Cl)ccc32)cc1	1170
890	1091	COc1ccc(NC(=O)[C@H](Cc2ccc(OCC(=O)NO)cc2)NCc2ccccc2)cc1	1180
891	1092	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@@](O)(CN(C)Cc3ccc(-c4cn(CCCC(=O)NO)nn4)cc3)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	1180
892	1093	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@H](O)[C@]1(C)O	1180
893	1095	Cc1nc(N(C)c2ccc(OCC(=O)NO)cc2)c2ccccc2n1	1181
894	1096	O=C(NO)c1ccc(Cl)c(NC(=O)c2ccc(Cl)cc2Cl)c1	1184
895	1097	O=C(NO)c1ccc(CNc2cccc3cccnc23)cc1	1190
896	1098	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(C3CCCCC3)nn2)c1)NO	1190
897	1100	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccccc3-c3cn(CCCCCC(=O)NO)nn3)[C@H]2O)[C@@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	1190
898	1101	O=C(NO)c1cc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccccc32)cs1	1191
899	1102	O=C(NO)c1ccc(CN2CCCC2)cc1	1200
900	1103	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2coc(n2)CNC(=O)C[C@@H](/C=C/CCS)OC1=O	1200
901	1105	O=C(NO)c1ccc(C2CCCC2)cc1	1200
902	1106	Fc1ccc2c(c1)C1=NCCN1C(=S)S2	1200
903	1107	O=C(CCCCCC(Cc1ccccc1)C(=O)NO)Nc1ccccc1	1200
904	1108	Fc1cc(Br)cc2c1C1=NCCN1C(=S)S2	1200
905	1110	CC[C@H](C)[C@H]1NC(=O)[C@@H](CS)NC(=O)[C@@H](CCSC)NC(=O)C[C@@H](/C=C/CCS)OC(=O)C[C@@H]1O	1200
906	1111	O=C(/C=C/c1csc(Br)n1)NO	1200
907	1112	O=C(CCCCCCC(=O)Nc1ccc([C@H]2O[C@@H](CSc3nc(-c4ccccc4)c(-c4ccccc4)o3)C[C@@H](c3ccc(CO)cc3)O2)cc1)NO	1208.538499

908	1113	O=C(NO)c1ccc(CN2C(=O)CNC(=O)[C@H]2Cc2c[nH]c3ccccc23)cc1	1210
909	1115	COc1cc(NC(=O)NOCCCCCC(=O)NO)c2nccc(C)c2c1	1220
910	1116	COc1ccc(S(=O)(=O)NC2CNc3ccc(C(=O)NO)cc3C2)cc1OC	1220
911	1117	CCOc1cc(C(C)(C)C)ccc1C1=NC(c2ccc(Cl)cc2)C(c2ccc(Cl)cc2)N1C(=O)N1CCN(CCCCCCC(=O)NO)CC1	1224
912	1118	O=C(NCCc1cc(C(=O)NO)no1)c1ccc(Cl)c(Cl)c1	1230
913	1120	COc1cc2c(cc1OC)C(=O)C(CC1CCN(Cc3cccc(NC(=O)CCCCCCC(=O)NO)c3)CC1)C2	1240
914	1121	O=C(NO)c1ccc(Cn2ccc3cc(C(=O)c4ccc(F)cc4)ccc32)cc1	1240
915	1122	CC(C)[C@H](NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)CC(=O)[C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)CNC(=O)CNC(=O)CCCc1cn(-c2ccc(-c3cn(CCCCCCCC(=O)NO)nn3)cc2)nn1)C(=O)NCC(=O)NCC(N)=O	1243
916	1123	Cc1ccc(-c2noc(CNCc3ccc(C(=O)NO)cc3)n2)cc1	1250
917	1125	COc1cc(C(=O)c2ccc3c(ccn3S(=O)(=O)c3cccc(/C=C/C(=O)NO)c3)c2)cc(OC)c1OC	1260
918	1126	O=C(NC1CCc2ccc(C(=O)NO)cc2C1)OCc1cccnc1	1270
919	1127	Cc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1Cc1ccccc1	1270
920	1128	Oc1cccn(Cc2ccccc2)c1=S	1272
921	1130	O=C(NO)c1cc2c(cc1F)CCC(NS(=O)(=O)c1ccc(Cl)cc1)C2	1280
922	1131	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccccc3-c3cn(CCCCCCC(=O)NO)nn3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	1280
923	1132	O=C(/C=C/c1ccc(/C=N/OCc2c(F)c(F)c(F)c(F)c2F)cc1)NO	1290
924	1133	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccccc1	1290
925	1135	O=C(/C=C/C1CCN(Cc2csc3ccccc23)CC1)NO	1300
926	1136	O=C(Cc1ccc(CCCCc2ccc(C(F)(F)F)cc2)cc1)NO	1300
927	1137	Fc1ccc2c(c1)SC(=S)N1CCCN=C21	1300
928	1138	Cc1ccc2c(c1)C1=NCCN1C(=S)S2	1300
929	1140	CC(C)(C)C(=O)N1Cc2ccc(C(=O)NO)cc2C1	1300
930	1141	Cn1cccc1C(=O)N1Cc2ccc(C(=O)NO)cc2C1	1300
931	1142	CC[C@H](C)[C@H](NC(=O)OC(C)(C)C)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	1310
932	1143	CN1CCN(NC(=O)c2cccc(C(=O)NO)c2)CC1	1310
933	1145	CN(c1ccc(OCCCCC(=O)NO)cc1)c1ncnc2ccccc12	1326
934	1146	O=C(CCCCCN1C(=O)c2cccc3cccc(c23)C1=O)NO	1327.480006
935	1147	CCc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1CCCc1ccccc1	1330
936	1148	O=C(NO)c1ccc(C(=O)NCCc2ccncc2)cc1	1330
937	1150	CC(C)(C)OC(=O)N1CCC2(CC1)CN(Cc1ccc(C(=O)NO)s1)c1ccccc12	1344
938	1151	O=C(CCCCCS)Nc1ccccc1	1360
939	1152	O=C(NO)c1ccc(CNCc2nc(-c3ccc(C(F)(F)F)cc3)no2)cc1	1360
940	1153	O=C(NO)c1ccc(Cn2c3c(c4ccccc42)S(=O)(=O)CC3)cc1	1378.404875
941	1155	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O	1390
942	1156	O=C(/C=C/c1cccc(S(=O)(=O)n2ccc3cccnc32)c1)NO	1390
943	1157	O=C(NCC12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)c1ccc2c(ccn2Cc2ccc(C(=O)NO)c(F)c2)c1	1390
944	1158	CN(Cc1ccccc1)c1ccc2c3c(cccc13)C(=O)N(CCCCCC(=O)NO)C2=O	1400

945	1160	N=C(N)NCCC[C@@H]1NC(=O)C[C@H](Cc2ccc(O)cc2)NC(=O)[C@H](Cc2cccc3ccccc23)NC(=O)[C@H](CCCCCC(=O)O)NC1=O	1400
946	1161	CCc1nc2cc(/C=C/C(=O)NO)c(F)cc2c(=O)n1CCc1ccccc1	1400
947	1162	O=C(NO)[C@@H]1[C@H](c2ccccc2)[C@H]1c1ccc(-c2ncc(F)cn2)cc1	1400
948	1163	CCC(=O)CCCCC[C@@H]1NC(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC(=O)[C@H](CCCCCC(=O)CC)NC1=O	1400
949	1165	Nc1nc(-c2ccco2)c2cnn(Cc3cccc(OCCCCCCC(=O)NO)c3)c2n1	1408.9
950	1166	O=C(CCCCCCC(=O)NC1CCCC1)NO	1410
951	1167	COc1ccc(C(=O)c2ccc3c(ccn3S(=O)(=O)c3cccc(/C=C/C(=O)NO)c3)c2)cc1OC	1420
952	1168	CN(c1ccc(OCC(=O)NO)cc1)c1ncnc2ccccc12	1422
953	1170	O=C(CCCCCCC(=O)N/N=C/c1ccc(N(c2ccccc2)c2ccccc2)cc1)NO	1430
954	1171	CC(C)(C)OC(=O)N1CCC(C(=O)N2CC3(C[C@H]2C(=O)NCCCCCC(=O)NO)SCCS3)CC1	1440
955	1172	O=C(CCCCCNc1nc(Cl)nc2c1ncn2Cc1ccccc1)NO	1440
956	1173	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(Oc4ccccc4)cc3)n1)CC2	1440
957	1175	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccc(C(F)(F)F)cc32)cc1	1440.999653
958	1176	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2Cc1ccccc1)NO	1450
959	1177	O=C(CCCCCCNc1ncnc2ccc(F)cc12)NO	1460
960	1178	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1ccc(Cl)cc1)CN2	1460
961	1180	Cc1nc(N(C)c2ccc(OCCCC(=O)NO)cc2)c2ccccc2n1	1465
962	1181	C#CCN(C)CCCOc1cccc(NC(=O)CCCCCCC(=O)NO)c1Cl	1470
963	1182	O=C(NO)c1ccc(CN2c3ccccc3Sc3ccccc32)cc1	1480
964	1183	CN(C)c1ccc(-c2cn(CCCCCn3cccc(O)c3=S)nn2)cc1	1482
965	1185	Cc1ccc(C(=O)c2ccc3c(ccn3Cc3ccc(C(=O)NO)cc3)c2)cc1	1490
966	1186	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2ccnc(c2)CNC(=O)C[C@@H](/C=C/CCS)NC1=O	1491
967	1187	CCc1ccc(C#Cc2c(-c3ccccc3)nnn2[C@@H](Cc2ccccc2)C(=O)NO)cc1	1500
968	1188	O=C(CCCCCC(=O)c1ccccc1)NO	1500
969	1190	O=C(NO)[C@@H]1[C@H](c2ccccc2)[C@H]1c1ccc2c(c1)CN(CC(F)(F)F)C2=O	1500
970	1191	O=C(CCNC(=O)/C(Cc1ccc(O)c(Br)c1)=N/O)NO	1500
971	1192	O=C(NO)c1ccc(CN2C(=O)CCc3cc(C4CC4)ccc32)cc1	1500
972	1193	Cc1cc(Oc2ccccc2)nc(NC2CCc3ccc(C(=O)NO)cc3C2)n1	1500
973	1195	CC(C)c1cc(C(=O)N2Cc3ccc(NC(=O)CCCCCCC(=O)NO)cc3C2)c(O)cc1O	1510
974	1196	O=C(NO)c1cc2c(cc1F)CCC(Nc1nccc(-c3cccnc3)n1)C2	1510
975	1197	O=C(NO)c1ccc(CNCCCN2c3ccccc3CCc3ccc(Cl)cc32)cc1	1510
976	1198	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(Cl)cc3Cl)n1)CC2	1520
977	1200	O=C(CCCCCCOc1cccc(-c2nnc(-c3ccccc3Cl)s2)c1)NO	1521
978	1201	CC(C)[C@H](NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)CC(=O)[C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)CNC(=O)CNC(=O)CCCc1cn(-c2ccc(-c3cn(CCCCCCC(=O)NO)nn3)cc2)nn1)C(=O)NCC(=O)NCC(N)=O	1528
979	1202	COc1ccc(N(C)c2nc(C)nc3ccccc23)cc1OCCCCCCC(=O)NO	1531
980	1203	O=C(CCCc1csc(/C=C/c2ccccc2)n1)NO	1536
981	1205	CC(C)c1cc(C(=O)N2CCc3cc(NC(=O)CCCCCC(=O)NO)ccc32)c(O)cc1O	1550
982	1206	CC(C)c1cc(C(=O)N2CCc3cc(NCc4ccc(C(=O)NO)cc4)ccc32)c(	1550

		O)cc1O	
983	1207	COc1ccc(-c2ccc(/C=C/C=C/C(=O)NO)cc2)cc1	1560
984	1208	Nc1nc2ncc(CNc3ccc(C(=O)N[C@@H](CCC(=O)NCCCCCCCCC(=O)NO)C(=O)O)cc3)nc2c(=O)[nH]1	1560
985	1210	O=C(/C=C/c1cccn(CCc2ccc3ccccc3c2)c1=O)NO	1582.32
986	1211	Cc1c(C)n(Cc2ccc(C(=O)NO)cc2)c2ccccc12	1584.89
987	1212	Cc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1CCc1c[nH]c2ccccc12	1590
988	1213	O=C(CCCCCCC(=O)C(F)(F)F)Nc1ccccc1	1596.871942
989	1215	Cc1c(O)c(O)c2c(c1C=O)[C@@H]1O[C@H](O2)c2c(C)c(O)c(O)c(O)c2C1=O	1600
990	1216	COc1cc(C(=O)NN)ccc1COc1ccc(Cl)c(C)c1	1600
991	1217	COC(=O)c1ccc2ccccc2c1OCCCCCCCCC(=O)NO	1600
992	1218	S=C1Sc2cc(Cl)ccc2C2=NCCN12	1600
993	1220	S=C1Sc2ccc(Br)cc2C2=NCCCN12	1600
994	1221	CC(C)(C)OC(=O)N1CCC2(CC1)CN(Cc1ccc(C(=O)NO)cc1)c1ccccc12	1602
995	1222	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1cccc(OC(F)(F)F)c1)CN2	1610
996	1223	O=C(/C=C/c1ccc(Cl)cc1F)NCCCCCC(=O)NO	1619.7
997	1225	CC(=O)SCC/C=C/[C@@H]1CC(=O)N[C@H](C(C)C)C(=O)N[C@H](Cc2cn(C)cn2)C(=O)N[C@H](C(C)C)c2cn(nn2)CC(=O)O1	1620
998	1226	COc1cc2c(Oc3ccc(NC(=O)C4(C(=O)Nc5ccc(F)cc5)CC4)cc3F)ccnc2cc1OCCCCCC(=O)NO	1630
999	1227	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccc(Cl)cc32)cc1	1640
1000	1228	Cn1c(=O)c(OCc2ccc(C(=O)NO)cc2)c(C2CCCCC2)c2ccccc21	1640
1001	1230	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3cccc(Cl)c3)n1)CC2	1660
1002	1231	Cc1cccc(-c2cn(CCCCCn3cccc(O)c3=S)nn2)c1	1660
1003	1232	Cc1c2ccc(N(C)c3ccnc(Nc4ccc(C(=O)NCCCCCCCC(=O)NO)cc4)n3)cc2nn1C	1660
1004	1233	CC(C)c1cc(C(=O)N2CCc3cc(NC(=O)CCCCCCCCC(=O)NO)ccc32)c(O)cc1O	1670
1005	1235	Cc1nc(N(C)c2ccc(OCCCCC(=O)NO)cc2)c2ccccc2n1	1698
1006	1236	Cc1cccc2c1C1=NCCN1C(=S)S2	1700
1007	1237	O=C(CCCCCCCn1cc(Nc2ncc(Cl)c(Nc3ccc(F)cc3)n2)cn1)NO	1700
1008	1238	O=C(NO)c1ccc(Cn2c3c(c4ccccc42)CS(=O)(=O)CC3)cc1	1700
1009	1240	O=C(NO)c1cccc(CNc2ccccc2)c1	1700
1010	1241	COc1ccc(/C=C(\C)C(=O)c2cc(OC)c(OC)c(OC)c2)cc1OCCCC(=O)NO	1700
1011	1242	O=C(CCc1ccc(-c2ccc(O)cc2)cc1)NO	1700
1012	1243	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@@H](C)[C@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)C)[C@@H]2O)[C@](C)(O)C[C@H](C)CN(Cc2ccc(-c3cn(CCCCCCC(=O)NO)nn3)cc2)[C@H](C)[C@H](O)[C@@]1(C)O	1700
1013	1245	O=C(Nc1ccc2c(c1)N(Cc1ccc(C(=O)NO)cc1)CC2)Nc1ccc(Cl)c(C(F)(F)F)c1	1710
1014	1246	COc1cc(-c2nc3cc(/C=C/C(=O)NO)ccc3n2C)ccc1OCc1ccccc1	1710
1015	1247	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2CCCc2ccccc2)cc1	1720
1016	1248	N[C@@H](Cc1c[nH]c2ccccc12)C(=O)Nc1ccccc1-c1ccc(NC(=O)CCCCCCC(=O)NO)cc1	1720
1017	1250	CCc1c2c(nc3ccc(OCc4cn(CCCC(=O)NO)nn4)cc13)-c1cc3c(c(=O)n1C2)COC(=O)[C@]3(O)CC	1726
1018	1251	O=C(CCN1CCN(C(=O)Nc2ccnc3ccccc23)CC1)NO	1740
1019	1252	CN(C)c1ccc(NC(=O)NCCCCCCC(=O)NO)cc1	1740

1020	1253	Cc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1CCc1ccccc1	1750
1021	1255	CC(C)c1cc(C(=O)N2CCc3onc(C(=O)NCCCCCCC(=O)NO)c3C2)c(O)cc1O	1760
1022	1256	O=C(NO)c1ccc(Cn2c(=O)n(CCc3cccc(C(F)(F)F)c3)c(=O)c3ccccc32)cc1	1760
1023	1257	O=C(/C=C/c1ccc2c(c1)C(=O)CC1(CCN(Cc3ccccc3)CC1)O2)NO	1760
1024	1258	Cc1cccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)OC(C)(C)C)c1	1770
1025	1260	O=C(NO)c1ccc(C(=O)NCCCN2c3ccccc3CCc3ccc(Cl)cc32)cc1	1780
1026	1261	O=C(NO)c1ccc2c(c1)CC(Nc1ncc3cc(F)ccc3n1)CC2	1780
1027	1262	O=C(CCCCCCNCc1ccccc1)NO	1800
1028	1263	CCc1nc(N)nc(N)c1-c1ccc(/C=C/C(=O)NO)cc1	1800
1029	1265	CC(=O)SCC/C=C/[C@@H]1CC(=O)N[C@H](C(C)C)C(=O)N[C@H](Cc2ccccc2)C(=O)N[C@H](C(C)C)c2cn(nn2)CC(=O)O1	1800
1030	1266	COc1ccc(CNCCCCCCC(=O)NO)cc1OC	1800
1031	1267	Fc1ccc2c(c1)C1=NCCCN1C(=S)S2	1800
1032	1268	O=C(Cc1cccc2ccccc12)Nc1ccc(C(=O)NO)nc1	1810
1033	1270	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)Cc3ccc(-c4cn(CCCCC(=O)NO)nn4)cc3)[C@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	1820
1034	1271	COC[C@@H]1CCCN1Cc1ccc(C(=O)NO)cc1	1820
1035	1272	COC[C@@H]1CCCC1c1ccc(C(=O)NO)cc1	1820
1036	1273	O=C(CCCCCCc1nc(-c2cccnc2)no1)NO	1830
1037	1275	O=C(CCCC(=O)NCCCN1c2ccccc2CCc2ccc(Cl)cc21)NO	1850
1038	1276	CC(C)(C)OC(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	1860
1039	1277	COc1ccc(-c2noc(CCCCCCC(=O)C(F)(F)F)n2)cc1	1860
1040	1278	CN(C)c1ccc(-n2cc(Cn3cccc(O)c3=S)nn2)cc1	1868
1041	1280	CCCNc1nc(Cl)nc2c1ncn2Cc1ccc(C(=O)Nc2ccccc2N)cc1	1880
1042	1281	O=C(O)CCn1c(CCc2ccccc2)nc2cc(/C=C/C(=O)NO)ccc21	1890
1043	1282	O=C(CCCCN(Cc1ccccc1)Cc1ccccc1)NO	1900
1044	1283	O=C(NO)c1ccc(CNCc2ccsc2)cc1	1900
1045	1285	O=C(CCCCCCN1CCc2ccccc2C1)NO	1900
1046	1286	O=C(NO)c1ccc(CN2c3ccccc3C3C2CCS3(=O)=O)cc1	1900
1047	1287	N#Cc1cc(-c2ccccc2)ccc1Cn1cccc(O)c1=S	1907
1048	1288	CN1CC2(CCN(Cc3ccc(C(=O)NO)cc3)CC2)c2ccccc21	1910
1049	1290	CC(C)N(Cc1ccc(C(=O)NO)cc1)C(C)C	1920
1050	1291	O=C(NO)c1ccccc1	1920
1051	1292	O=C(CCCCCCc1nc(-c2cccs2)no1)NO	1920
1052	1293	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2Cc2ccccc2)cc1	1920
1053	1295	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc(CCCCC(=O)NO)c2ccccc2n1	1937
1054	1296	CCC(=O)CCCCC[C@H](NC(=O)C1CCC2(CC1)CN(C)C2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	1947
1055	1297	O=C(NO)c1ccc(Cn2ccc3cc(C(=O)NCC45C[C@H]6C[C@@H](C4)C[C@@H](C5)C6)ccc32)cc1	1950
1056	1298	Nc1cccc(-c2csc(NC(=O)CCCCCC(=O)NO)n2)c1	1950
1057	1300	CNC(=O)c1ccc(C(=O)NO)cc1	1950
1058	1301	CC(C)c1cc(C(=O)N2CCc3cc(NC(=O)CCCC(=O)NO)ccc32)c(O)cc1O	1960
1059	1302	O=C(CCCCCCNc1ncnc2ccc(Cl)cc12)NO	1970
1060	1303	O=C(CCCCCCC(=O)Nc1ccc(-c2cn(-c3ccccc3)nn2)cc1)NO	1970

1061	1305	Cc1nc2c(c(N(C)c3ccc(OCCCCC(=O)NO)cc3)n1)CCC2	1987
1062	1306	O=C(/C=C/c1ccc(NC(=O)Nc2ccc(Cl)c(C(F)(F)F)c2)cc1)NO	1990
1063	1307	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(Cc3ccccc3)nn2)c1)NO	1990
1064	1308	C[C@H](CN1CCC[C@@H]1C)NC(=O)c1ccc(-c2noc(C(F)(F)F)n2)cc1	2000
1065	1310	O=C(NO)c1ccc(CN2c3cc(C(F)(F)F)ccc3CCC[C@@H]3CCCC[C@H]32)cc1	2000
1066	1311	CN(/N=C/c1cccc(C(=O)NO)c1)C(=O)c1ccc(N(C)C)cc1	2000
1067	1312	C/C(=C\Cc1ccc(NS(=O)(=O)c2ccccc2)cc1)CC(=O)NO	2000
1068	1313	O=C(NO)c1ccc(CCCS(=O)(=O)c2ccccc2)cc1	2000
1069	1315	O=C(/C=C/c1ccc(OC[C@H](Cc2c[nH]c3ccccc23)NC(=O)c2ccc(Cl)cc2)cc1)NO	2000.8
1070	1316	CC(C)Cn1cnc2c(NCCCCCCC(=O)NO)nc(Cl)nc21	2010
1071	1317	O=C(CCCCCCC(=O)Nc1ccc(-c2cnnn2Cc2ccc(F)cc2)cc1)NO	2010
1072	1318	CC(C)c1cc(C(=O)N2Cc3ccc(NC(=O)CCCCCC(=O)NO)cc3C2)c(O)cc1O	2011
1073	1320	O=C(/C=C/c1ccc2cccnc2c1)NCCCCCC(=O)NO	2028.3
1074	1321	CCCN1CCC2(CC1)C[C@@H]2C(=O)N[C@@H](CCCCCC(=O)CC)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	2033
1075	1322	O=C(CCCCCCc1nc(-c2ccccc2)no1)NO	2050
1076	1323	Cc1cc(Cn2ccc3cc(C(=O)NCC45C[C@H]6C[C@@H](C4)C[C@@H](C5)C6)ccc32)ccc1C(=O)NO	2060
1077	1325	N#Cc1ccc(-c2ccc(Cn3cccc(O)c3=S)cc2)cc1	2075
1078	1326	O=C(CCCCCCc1nc(-c2ccc(Cl)cc2)no1)C(F)(F)F	2080
1079	1327	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)c4ccc(C(=O)Nc5ccccc5N)cc4)cc3)n2)cc(OC)c1OC	2080
1080	1328	Cc1cc(C)c(CNC(=O)c2cnn(-c3cccc(NC(=O)CCCCCCC(=O)NO)c3)c2C)c(=O)[nH]1	2080
1081	1330	CCC(=O)CCCCC[C@@H]1NC(=O)[C@H](C)N(C)C(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	2097.617696
1082	1331	CC(C)(C)C(=O)N1CCc2cc(C(=O)NO)ccc2C1	2100
1083	1332	O=C(NO)c1ccc(Cl)c(OCc2ccccc2Cl)c1	2100
1084	1333	CC(C)(CNC(=O)c1cccc(-c2noc(C(F)(F)F)n2)c1)c1coc(-c2ccccc2)n1	2100
1085	1335	Cc1c(O)c(O)c(O)c(C=O)c1-c1cc2c(C=O)c(C)c(O)c(O)c2o1	2100
1086	1336	Cn1cccc1C(=O)N1CCc2cc(C(=O)NO)ccc2C1	2100
1087	2056	O=C(CCCCCCNCc1ccc([N+](=O)[O-])cc1)NO	2100
1088	2057	O=C(NO)c1ccc(COc2no[n+]([O-])c2S(=O)(=O)c2ccccc2)cc1	2100
1089	1337	CC(/C=C/c1ccccc1)=C\C(=O)NCCCCCC(=O)NO	2116.3
1090	1338	COc1ccc(CNC(=O)c2cc(F)ccc2N2CCOCC2)cc1/C=C/C(=O)NO	2120
1091	1340	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccccc3)n1)CC2	2130
1092	1341	Cc1cc(Cl)ccc1-c1ccnc(NC2CCc3ccc(C(=O)NO)cc3C2)n1	2150
1093	1342	COc1cc2c(cc1OC)C(=O)C(CC1CCN(Cc3ccc(NCc4ccc(C(=O)NO)cc4)cc3)CC1)C2	2150
1094	1343	O=C(/C=C/c1cccc(S(=O)(=O)NCCCN2c3ccccc3CCc3ccc(Cl)cc32)c1)NO	2160
1095	1345	COc1cc(C(=O)c2ccc3c(ccn3Cc3ccc(/C=C/C(=O)NO)cc3)c2)cc(OC)c1OC	2170
1096	1346	COc1cc(OCc2cccc(-c3ccccc3)c2C)cc(OC)c1CNCCCCCCC(=O)NO	2175
1097	1347	O=C(NO)c1cccc(N(Cc2ccccc2)Cc2ccccc2)c1	2190
1098	1348	CN(C)c1ccc(C(=O)N/N=C/c2cccc(C(=O)NO)c2)cc1	2200
1099	1350	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(Cl)cc3)n1)CC2	2200
1100	1351	CCC(=O)CCCCC[C@@H]1NC(=O)[C@H](C)NC(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	2200
1101	1352	O=C(NO)c1cn(-c2cc(Cl)ccc2Oc2ccc(F)cc2)nn1	2200

1102	1353	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@@H]2C[C@](C)(OC)[C@@](O)(CN(C)C)[C@@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	2210
1103	1355	N#Cc1ccc2c(c1)CCCCN2Cc1ccc(C(=O)NO)cc1	2220
1104	1356	O=C1CCC[C@@H](C(=O)N[C@@H](CCCCCS)C(=O)N2CCc3ccccc3C2)N1	2230
1105	1357	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)Cc3ccc(-c4cn(CCC(=O)NO)nn4)cc3)[C@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	2230
1106	1358	Ic1ncccn1	2240
1107	1360	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	2240
1108	1361	COc1ccc(CNC(=O)c2cc(C(=O)Nc3ccccc3N)ccc2N2CCOCC2)cc1O	2244
1109	1362	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C(C)=O)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	2271
1110	1363	CC(C)[C@@H](C(=O)NO)n1nnc(-c2ccccc2)c1C#Cc1ccccc1	2300
1111	1365	Fc1cccc2c1C1=NCCCN1C(=S)S2	2300
1112	1366	CC(C)C[C@H]1CC(=O)N[C@@H](C)C(=O)N[C@@H](CCCCCC(=O)O)C(=O)N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N1	2300
1113	2058	O=C(COc1ccc2ccccc2c1/C=C1\SC(=O)NC1=O)Nc1ccc([N+](=O)[O-])cc1	2300
1114	1367	Nc1ncnc2c1c(-c1ccc(Cl)cc1)nn2-c1cccc(-c2cnnn2CCCCCC(=O)NO)c1	2311
1115	1368	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(NC(=O)CCCCCCC(=O)NO)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	2320
1116	2059	O=C(/C=C/c1ccc2cc(Oc3ccc([N+](=O)[O-])cc3)ccc2n1)NO	2320
1117	1370	O=C(CCCCCCC(=O)NCCCN1c2ccccc2CCc2ccc(Cl)cc21)NO	2330
1118	1371	O=C(CCCCCCS)NC1CCCC1	2330
1119	1372	O=C(NO)c1ccc(CN2C(=O)CNC(=O)[C@H]2Cc2ccccc2)cc1	2340
1120	1373	O=C(CCc1ccccc1)NO	2350
1121	1375	Nc1nc2ncc(CNc3ccc(C(=O)N[C@@H](CCC(=O)NCCCCCCCC(=O)NO)C(=O)O)cc3)nc2c(=O)[nH]1	2370
1122	1376	CCNc1nc(Cl)nc2c1ncn2Cc1ccc(C(=O)Nc2ccccc2N)cc1	2370
1123	1377	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@](C)(O)C[C@@H](C)CN(Cc2ccc(-c3cn(CCCCCC(=O)NO)nn3)cc2)[C@@H](C)[C@@H](O)[C@]1(C)O	2370
1124	1378	O=C(NO)c1ccc(CN(c2ccccc2)c2ccccc2)cc1	2380
1125	1380	Nc1nc2ncc(CNc3ccc(C(=O)N[C@@H](CCC(=O)NCCCCCCCC(=O)NO)C(=O)O)cc3)nc2c(=O)[nH]1	2390
1126	1381	O=C(CCCCCCOc1cccc(-c2nnc(-c3ccccc3)s2)c1)NO	2390
1127	1382	O=C(CCc1ccc(CC(=O)c2ccccc2)o1)NO	2400
1128	1383	O=C(/C=C/C1CCN(CCc2ccccc2)CC1)NO	2400
1129	2061	O=C(NO)c1ccc(Cn2c3c(c4cc(F)ccc42)C[S+]([O-])CC3)cc1	2400
1130	1385	Cc1ccccc1-c1cn(CCCCCn2cccc(O)c2=S)nn1	2402
1131	1386	O=C(NO)c1ccc2c(c1)CC(NC(=O)c1ccc(Cl)cc1)CN2	2410
1132	1387	CCCCNNC(=O)c1ccc(-c2ccccc2)cc1	2430
1133	1388	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@]	2450

		(C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	
1134	1390	Cc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1-c1ccccc1	2456.298028
1135	1391	CN(c1ccc(OCCCC(=O)NO)cc1)c1ncnc2ccccc12	2457
1136	1392	O=C(CCCCCN1C(=O)c2cccc3c(NCc4ccccc4)ccc(c23)C1=O)NO	2460
1137	1393	O=C(CCCCCn1cc(Nc2ncc(Cl)c(Nc3ccc(Cl)cc3)n2)cn1)NO	2470
1138	1395	O=C(NO)c1ccc(CNC(=O)N2CCC3(CC2)CN(Cc2ccccc2)c2ccccc23)cc1	2480
1139	1396	Cc1cccc(-c2ccc(Cn3cccc(O)c3=S)cc2)c1	2496
1140	1397	O=C(/C=C/C1CCN(Cc2ccccc2)CC1)NO	2500
1141	1398	O=C(CCCCc1ccn(-c2ccccc2)n1)NO	2515
1142	1400	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@@](O)(CN(C)Cc3ccc(-c4cn(CCCC(=O)NO)nn4)cc3)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)C)[C@@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@H](O)[C@]1(C)O	2530
1143	1401	Cc1ccc(-c2cn(CCCCCn3cccc(O)c3=S)nn2)cc1	2533
1144	1402	C/C=C1\NC(=O)c2csc(n2)[C@@H](C(C)C)NC(=O)C[C@@H](/C=C/CCS)OC(=O)[C@H](C(C)C)NC1=O	2550
1145	1403	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(F)cc1	2560
1146	2062	O=C(CCCCCCc1nc(-c2ccc([N+](=O)[O-])cc2)no1)NO	2560
1147	1405	CCC(=O)CCCCC[C@H](NC(=O)CC1CC2(C1)CN(C)C2)c1nc(-c2cc3ccccc3nc2OC)[nH]1	2573
1148	1406	CN(C)c1cccc2c(SNCCCCCC(=O)NO)cccc12	2580
1149	1407	CC(C)(C)OC(=O)Nc1cccc(-c2csc(NC(=O)CCCCCCCC(=O)NO)n2)c1	2580
1150	1408	CC(C)(C)OC(=O)Nc1cccc(-c2csc(NC(=O)CCCCCC(=O)NO)n2)c1	2580
1151	1410	O=C(NO)c1ccc2c(c1)CC(NC(=O)c1ccc(Cl)c(Cl)c1)CN2	2630
1152	1411	CCC(=O)CCCCC[C@H](NC(=O)C1CC2(C1)CN(C)C2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	2657
1153	1412	O=C(CCCCCCC(=O)Nc1ccc(-c2ccccc2NC(=O)[C@@H]2CCCN2)cc1)NO	2660
1154	1413	CC1(C)NC(=O)C[C@H](Cc2c[nH]c3ccccc23)NC(=O)[C@H](Cc2cccc3ccccc23)NC(=O)[C@H](CCCCCC(=O)O)NC1=O	2670
1155	1415	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)NCCc1ccccc1	2670
1156	1416	CCCc1ccc2c(c1)CCC(=O)N2Cc1ccc(C(=O)NO)cc1	2680
1157	1417	O=C(NO)c1ccc2c(c1)CC(Nc1ccc(F)cc1)CC2	2680
1158	1418	O=C(NO)c1coc(C(c2ccccc2)c2ccccc2)n1	2700
1159	1420	CN(C)c1ccc2c(c1)SC(=S)N1CCCN=C21	2700
1160	1421	O=C(COc1ccc2cc(/C=C3/SC(=O)NC3=O)ccc2c1)Nc1nc2ccccc2s1	2700
1161	1422	COc1cc(C(=O)c2csc(-c3ccc(/C=C/C(=O)NO)cc3)n2)cc(OC)c1OC	2710
1162	2063	[N-]=[N+]=Nc1ccc(-c2csc(NC(=O)CCCCCCC(=O)NO)n2)cc1	2710
1163	1423	CN(C)c1ccc(C(=O)N(CCCCCC(=O)NO)CC(=O)NCc2ccccc2)cc1	2750
1164	1425	O=C(/C=C/c1cccc(S(=O)(=O)n2ccc3cc(C(=O)c4ccc(F)cc4)ccc32)c1)NO	2750
1165	1426	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccc(O)cc32)cc1	2751
1166	1427	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@H](C)[C@@H](O[C@@	2770

		H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@](C)(O)C[C@@H](C)CN(Cc2ccc(-c3cn(CCCC(=O)NO)nn3)cc2)[C@@H](C)[C@@H](O)[C@]1(C)O	
1167	1428	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCCN(C)C2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	2778
1168	1430	Oc1cccn(Cc2ccc(-c3ccncc3)cc2)c1=S	2780
1169	1431	O=C(NCCN1CCCC1)c1ccc(-c2noc(C(F)(F)F)n2)cc1	2800
1170	1432	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2ccc3cnccc3c2)[nH]1	2800
1171	1433	O=C(NO)c1ccc(CC(=O)N(CCO)c2ccccc2)cc1	2800
1172	1435	Cc1cc(CNCCCCCCC(=O)NO)ccc1F	2800
1173	1436	O=CN(O)CCCCCCCC(=O)Nc1ccccc1	2800
1174	1437	CCc1nc(N)nc(N)c1-c1ccc(-c2cn(CCCCCC(=O)NO)nn2)cc1	2800
1175	1438	Cc1ccc(N)c(NC(=O)c2ccc(CNC(=O)OCc3cccnc3)cc2)c1	2800
1176	1440	COc1ccc(C(=O)c2ccc3c(ccn3Cc3ccc(/C=C/C(=O)NO)cc3)c2)cc1	2810
1177	1441	CCCCNNC(=O)c1ccc(Br)cc1	2817.800561
1178	1442	O=C(NO)c1ccc(CN2CCCCc3cc(-c4cc[nH]n4)ccc32)cc1	2820
1179	1443	COc1cc(Oc2ccc3nc(/C=C/C(=O)NO)ccc3c2)cc(OC)c1OC	2820
1180	1445	N#Cc1cccc(-c2cn(CCCCCn3cccc(O)c3=S)nn2)c1	2831
1181	1446	O=C(NO)c1ccc2c(c1)CC(NC(=O)c1ccc(-c3ccccc3)cc1)CN2	2850
1182	1447	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	2850
1183	1448	CN(C)c1ccc(-c2ccc(Cn3cccc(O)c3=S)cc2)cc1	2858
1184	1450	Cc1c2ccc(N(C)c3ccnc(Nc4ccc(/C=C/C(=O)NO)cc4)n3)cc2nn1C	2890
1185	1451	COc1ccc(CNC(=O)[C@H](CCC(=O)O)NC(=O)Cc2ccc(Br)cc2)cc1	2890
1186	2064	O=C(O)CC[C@@H](NC(=O)Cc1ccc(Br)cc1)C(=O)NCc1ccc([N+](=O)[O-])cc1	2890
1187	1452	O=C(NO)c1ccc2c(c1)CC(Nc1ccccn1)CC2	2900
1188	1453	CCCN(CCC)C[C@@H](C)NC(=O)c1ccc(-c2noc(C(F)(F)F)n2)cc1	2900
1189	1455	O=C(NO)c1ccc(CN2c3ccccc3CC[C@@H]3CCCC[C@H]32)cc1	2900
1190	1456	CC1(NCC(=O)NCc2ccc(/C=C/C(=O)NO)cc2)CCN(c2cnc(-c3cccc(Cl)c3Cl)c(N)n2)CC1	2900
1191	1457	N#CCc1ccc(-c2ccc(/C=C/C(=O)NO)cc2Cl)cc1C12CC3CC(CC(C3)C1)C2	2910
1192	1458	CCCCN(Cc1ccc(C(=O)NO)cc1)C(=O)CCCCn1cc(COc2cccc(Cc3cnc(NC(=O)CSc4nc(C)cc(C)n4)s3)c2)nn1	2940
1193	1460	O=C(CCCCCCNC(=O)c1cc(-c2ccc(F)cc2)[nH]n1)NO	2951
1194	1461	Cc1nc2c(c(N(C)c3ccc(OCC(=O)NO)cc3)n1)CCC2	2974
1195	1462	O=C(CCCCc1ccn(Cc2cccc(-c3ccccc3)c2)n1)NO	2984
1196	1463	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1nnc(-c2cc3ccccc3nc2OC)[nH]1	2988
1197	1465	C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@]2(O)c1cn(CCCCCCCC(=O)NO)nn1	3000
1198	1466	CC(=O)CCCCC[C@H](NC1CCCCN1C)C(=O)Nc1nc(-c2ccccc2)cs1	3000
1199	1467	CC(=O)CCCCC[C@H](NC(=O)C1CCCCN1C)C(=O)Nc1nc(-c2ccccc2)cs1	3000
1200	1468	O=C(NO)c1cccc(S(=O)(=O)N[C@@H](Cc2c[nH]c3ccccc23)C(=O)Nc2ccccc2)c1	3000
1201	1470	O=C(CCCCCOc1cccc(-c2nnc(-c3ccccc3)s2)c1)NO	3025
1202	1471	O=C(O)CC[C@H](NC(=O)Cc1ccc(Br)cc1)C(=O)NCc1ccccc1	3030

1203	1472	CC(C)(C)c1cc(CN(C(=O)c2cccc(C(F)(F)F)c2)c2ccc(C(=O)NO)cc2)cc(C(C)(C)C)c1	3030
1204	1473	CN(c1nccc(-c2cccnc2)n1)C1CCc2ccc(C(=O)NO)cc2C1	3040
1205	1475	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3ccc(C4CC4)cc32)cc1	3060
1206	1476	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCOCC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	3089
1207	1477	O=C(CCCCC(=O)NCCCN1c2ccccc2CCc2ccc(Cl)cc21)NO	3090
1208	1478	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2cc3cn(C)nc3cc2OC)[nH]1	3100
1209	1480	O=C(NO)c1sc2ccccc2c1Cl	3100
1210	1481	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(C2=CC3SC=NC3C=C2)[nH]1	3100
1211	1482	Cc1ccccc1-c1ccc(Cn2cccc(O)c2=S)cc1	3105
1212	1483	COc1cc(C(=O)c2csc(-c3ccc(/C=C/C(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	3110
1213	1485	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC1CC1)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	3129
1214	1486	O=C(CCCCCCC(=O)Nc1ccc(-c2cn(CC(O)c3cccc(Br)c3)nn2)cc1)NO	3130
1215	1487	CC(C)n1cnc2c(NCCCCCCC(=O)NO)nc(N)nc21	3130
1216	1488	Cc1cc(C)cc(C(=O)N(CC(=O)NCc2ccccc2)Cc2ccc(C(=O)Nc3cc(-c4ccccc4)ccc3N)cc2)c1	3130
1217	1490	O=C(NO)c1ccc(COC(=O)N2CCC3(CC2)CN(Cc2ccccc2)c2ccccc23)cc1	3190
1218	1491	Cc1cc2cc(NCc3cc(C(=O)NO)ccc3Cl)ccc2n(C)c1=O	3193
1219	1492	O=C(NO)c1ccc(CNCc2cccs2)cc1	3200
1220	1493	S=C1Sc2c(Cl)cccc2C2=NCCN12	3200
1221	1495	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	3210
1222	1496	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3cccc(-c4cn(CCCCCC(=O)NO)nn4)c3)[C@H]2O)[C@@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	3230
1223	1497	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(Cc1ccc(OC)cc1)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	3231
1224	1498	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCCCC(=O)NO)cc3)n2)cc(OC)c1OC	3280
1225	1500	O=C(O)c1cccc(=S)n1O	3300
1226	1501	Cc1cccc(C(=O)NO)c1	3300
1227	1502	Cn1cccc1C(=O)N1CCn2cc(C(=O)NO)cc2C1	3300
1228	1503	Oc1cccn(CCCCn2cc(-c3ccccc3)nn2)c1=S	3303
1229	1505	O=C(CCCCOCc1cc(-c2ccccc2)on1)NO	3320
1230	1506	COc1cccc(-c2ccc3c(NC(=O)C4CCC(C(=O)NO)CC4)n[nH]c3c2)c1	3340
1231	1507	CN(c1ccccc1Cl)S(=O)(=O)C1CC2OC1C(c1ccc(NC(=O)CCCCCCC(=O)O)cc1)=C2c1ccc(O)cc1	3350
1232	1508	O=C(NO)c1ccc2c(c1)CC(NC(=O)c1cccc(Cl)c1)CN2	3370
1233	1510	COc1ccc(N(C)c2nc(C)nc3ccccc23)cc1OCCCC(=O)NO	3398
1234	1511	O=C(N[C@@H](CCCCNC(=O)c1ncccc1O)c1ncc(-c2ccc3ccccc3c2)[nH]1)c1cncs1	3400
1235	1512	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cnc3ncccc3c2)[nH]1	3400
1236	1513	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)NCc1ccccc1	3410
1237	1515	Nc1cccc(-c2cc(C(=O)NCCCCC(=O)NO)no2)c1	3430
1238	1516	O=C(NO)c1ccc(CN2C(=O)C(Cc3ccccc3)N(Cc3cccnc3)C2=O)c	3441

		c1	
1239	1517	Nc1ccc(-c2cc(C(=O)NCCCCCCC(=O)NO)no2)cc1	3458
1240	1518	CN1CCC2(CC1)c1ccccc1N(Cc1ccc(C(=O)NO)cc1)C2c1ccccc1F	3490
1241	1520	O=C(CNS(=O)(=O)c1cccc(C(=O)NO)c1)Nc1ccccc1	3500
1242	1521	O=C(NO)c1ccc(CNCc2ccccc2)cc1	3500
1243	1522	CC(C)[C@H](NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCNC(=N)N)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)CC(=O)[C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)CNC(=O)CNC(=O)CCCc1cn(-c2ccc(-c3cn(CCCCCC(=O)NO)nn3)cc2)nn1)C(=O)NCC(=O)NCC(N)=O	3503
1244	1523	COc1cccc(C(=O)c2ccc3c(ccn3S(=O)(=O)c3cccc(/C=C/C(=O)NO)c3)c2)c1	3530
1245	1525	COc1ccc2[nH]cc(CCN(Cc3ccc(C(=O)NO)cc3)C(=O)/C=C/c3ccc(O)c(OC)c3)c2c1	3569.0036
1246	1526	O=C(CCCCNC(=O)c1cc(-c2ccccc2)on1)NO	3580
1247	1527	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3nccnc3c2)[nH]1	3600
1248	1528	O=C(CCC1C(=O)N(c2ccc(Cl)cc2)C(=O)N1Cc1ccccc1)Nc1ccc(C(=O)NO)cc1	3600
1249	1530	O=C(NCC1(c2nc(-c3ccccc3)cs2)CCOCC1)c1cccc(-c2noc(C(F)(F)F)n2)c1	3600
1250	1531	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccncc3nc2OC)[nH]1	3600
1251	1532	O=C(NO)c1ccc(CN2CCCc3cc(Cl)ccc32)cc1	3607.587092
1252	1533	CC(C)(C)OC(=O)Nc1ccc(-c2cc(C(=O)NCCCCC(=O)NO)no2)cc1	3650
1253	1535	Oc1ccc[nH]c1=S	3675
1254	1536	CCc1nc2ccc(/C=C/CC(=O)NO)cc2c(=O)n1-c1ccccc1	3690
1255	1537	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccccnc3cc2OC)[nH]1	3700
1256	1538	CC(C)[C@H]1NC(=O)[C@@H](C)[C@@H](C/C=C\CCC(=O)O)NC(=O)[C@@H](Cc2ccccc2)NC(=O)[C@@H](C)NC1=O	3700
1257	1540	O=C(NO)C1CCCCC1	3720
1258	1541	CC(C)c1cc(C(=O)N2Cc3ccc(NC(=O)CCCCCCCCC(=O)NO)cc3C2)c(O)cc1O	3720
1259	1542	N#Cc1ccc(NC2CCc3ccc(C(=O)NO)cc3C2)cc1Cl	3730
1260	1543	Cc1nc2ccc(/C=C/CC(=O)NO)cc2c(=O)n1-c1ccccc1	3730
1261	1545	COc1ccc(-c2ncc(/C=C/C(=O)NO)s2)cc1	3740
1262	2066	O=C(NO)c1ccc2c(c1)CC(Nc1ccc([N+](=O)[O-])cc1)CC2	3740
1263	1546	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc4ccccc4c3)n1)CC2	3780
1264	1547	Cc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)OC(C)(C)C)c(C)c1	3780
1265	1548	O=C(CCCCCONC(=O)c1ccc2ccccc2c1)NO	3790
1266	1550	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccc(C4CC4)nc3cc2OC)[nH]1	3800
1267	1551	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(CCc3ccc(C(=O)NO)cc3)c2c(=O)n1-c1ccccc1	3840
1268	1552	CC1=C(C)C(=O)C(CONC(=O)CCCCCCC(=O)Nc2ccccc2)=C(C)C1=O	3842
1269	1553	COc1ccc(/C=C/C(=O)c2cc(OC)c(OC)c(OC)c2)cc1OCCCCCCC(=O)NO	3880
1270	1555	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccc(C)nc3cc2OC)[nH]1	3900
1271	1556	CN(c1cccc2ccccc12)S(=O)(=O)C1CC2OC1C(c1ccc(NC(=O)CCCCCC(=O)O)cc1)=C2c1ccc(O)cc1	3940
1272	1557	C/C=C1\NC(=O)c2csc(n2)CNC(=O)C[C@@H](/C=C/CCSC(=O)CCCCCCC)OC(=O)[C@H](C(C)C)NC1=O	3960

1273	1558	O=C(CCCCCCC(=O)Nc1ccc(-c2cn(Cc3ccccc3)nn2)cc1)NO	3970
1274	1560	CN1CCc2c(n(Cc3ccc(C(=O)NO)cc3)c3ccccc23)C1	3981.07
1275	1561	O=C(NO)c1ccc(CN2C(=O)C(Cc3ccccc3)N(Cc3ccc(Cl)cc3)C2=O)cc1	3987.5
1276	1562	O=C(CCCc1ccccc1)NO	4000
1277	1563	Cc1ccccc1NC(=O)[C@@H]1Cc2ccc(OCC(=O)NO)cc2CN1C(=O)OC(C)(C)C	4000
1278	1565	O=CN(O)CCCCCCC(=O)Nc1ccccc1	4000
1279	1566	O=C(CCCCCCN(Cc1ccccc1)Cc1ccccc1)NO	4000
1280	1567	C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@]2(O)c1cn(CCCCCC(=O)NO)nn1	4000
1281	2067	O=C(COc1ccc2cc(/C=C3/SC(=O)NC3=O)ccc2c1)Nc1ccc([N+](=O)[O-])cc1	4000
1282	1568	O=C(CCCCCN1C(=O)c2cccc3c(Nc4cccc(F)c4)ccc(c23)C1=O)NO	4070
1283	1570	O=C(CCCCCN1C(=O)c2cccc3c(Nc4ccccc4)ccc(c23)C1=O)NO	4090
1284	2068	O=C(CCCCCCC(=O)Nc1nc(-c2cccc([N+](=O)[O-])c2)cs1)NO	4090
1285	1571	O=C(CCCCCCN(Cc1ccc(-c2ccccc2)s1)Cc1ccc(-c2ccccc2)s1)NO	4100
1286	1572	Nc1ccccc1NC(=O)c1ccc(CNc2nc(-c3ccccc3)cs2)cc1	4100
1287	1573	O=C(CCCCCCNC(=O)C(O)(O)C(F)(F)F)Nc1ccc(-c2ccccc2)cc1	4100
1288	1575	COc1cccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@](O)(C(C)=O)C[C@@H]3O[C@H]1C[C@H](NCc2ccc(-c3cn(CCCCCC(=O)NO)nn3)cc2)[C@H](O)[C@H](C)O1	4129
1289	1576	CC12CC3CC(C)(C1)CC(NC(=O)CCCCCC(=O)NO)(C3)C2	4140
1290	1577	O=C(NO)c1ccc(Cl)c(OCc2ccc(Cl)cc2Cl)c1	4150
1291	1578	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCCCCC(=O)NO)cc3)n2)cc(OC)c1OC	4170
1292	1580	CC(=O)SCCCCCCNC(=O)c1cc(-c2ccc(F)cc2)nn1C	4200
1293	1581	O=C(CS)NCCCCCC(=O)Nc1ccc(-c2ccccc2NC(=O)[C@@H]2CCCN2)cc1	4230
1294	1582	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1cccc2ccccc12	4250
1295	1583	Oc1cccn(Cc2ccc(-c3ccccc3)cc2)c1=S	4283
1296	1585	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccccc3-c3cn(CCCCCC(=O)NO)nn3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	4300
1297	1586	O=C(NO)c1ccc(CN2CCCCc3cc(Br)ccc32)cc1	4360
1298	1587	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3ncccc3c2)[nH]1	4400
1299	1588	CCCCCCNC(=O)[C@@H]1Cc2ccc(OCC(=O)NO)cc2CN1C(=O)OC(C)(C)C	4420
1300	2069	Nc1ccc(-c2cccs2)cc1NC(=O)c1ccc(-c2cn(C[S+]([O-])c3ccccc3)nn2)cc1	4454
1301	1590	Cc1ccc(C(=O)c2ccc3c(ccn3S(=O)(=O)c3cccc(/C=C/C(=O)NO)c3)c2)cc1	4480
1302	1591	O=C(COc1ccc2cc(/C=C3/SC(=O)NC3=O)ccc2c1)Nc1ccccc1	4500
1303	1592	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C(C)C)CC2)c1ncc(-c2cc3ccc(C)nc3cc2OC)[nH]1	4500
1304	1593	CC[C@H]1OC(=O)[C@@H](C)[C@H](O[C@@H]2C[C@](C)(OC)[C@@](O)(CN(C)Cc3ccc(-c4cn(CC(=O)NO)nn4)cc3)[C@@H](C)O2)[C@H](C)[C@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)C)[C@@H]2O)[C@@](C)(O)C[C@H](C)CN(C)[C@@H](C)[C@H](O)[C@@]1(C)O	4510
1305	1595	CC(C)(C)NC(=O)[C@@H]1Cc2ccc(OCC(=O)NO)cc2CN1C(=	4580

		O)OC(C)(C)C	
1306	1596	O=C(CCCCCCN(Cc1cc2ccccc2[nH]1)Cc1cc2ccccc2[nH]1)NO	4600
1307	1597	COc1ccc(N)c(NC(=O)c2ccc(CNC(=O)OCc3ccccnc3)cc2)c1	4600
1308	1598	Ic1ccncc1	4610
1309	1600	CC1(C)c2ccccc2N(Cc2ccc(C(=O)NO)cc2)C1c1ccncc1	4640
1310	1601	CCC(=O)CCCCCC(NC(=O)c1cncs1)c1[nH]c(-c2ccccc2)nc1C(N)=O	4701
1311	1602	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O	4750
1312	1603	COc1ccc(-c2ccc3nc(/C=C/C(=O)NO)ccc3c2)cc1	4770
1313	1605	O=C(CCCCCNC(=O)NC12CC3CC(CC(C3)C1)C2)NO	4815.391988
1314	1606	CC(=O)Nc1ccc(-c2cc(C(=O)NCCCCCCC(=O)NO)no2)cc1	4900
1315	1607	CCC(=O)CCCSC[C@@H]1NC(=O)[C@H](C)NC(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	4909.989817
1316	1608	COc1ccc(/C=C(\C)C(=O)c2cc(OC)c(OC)c(OC)c2)cc1OCCCCCCCC(=O)NO	4910
1317	1610	O=C(NO)c1ccc(OC2CCN(c3ccccc3)C2=O)cc1	4920
1318	1611	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(Cc1cccnc1)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	4924
1319	1612	Nc1ccccc1NC(=O)c1cnc(NCc2ccccc2)cn1	4936.789746
1320	1613	O=C(CCCC(=O)NCCc1ccccc1)NO	5000
1321	1615	Nc1ccccc1NC(=O)CCCCCC(=O)Nc1ccccc1	5000
1322	1616	CCOC(=O)NCCCC(=O)NCCc1ccccc1	5000
1323	1617	O=C(CCCCn1cc(Nc2ncc(Cl)c(Nc3ccc(F)cc3)n2)cn1)NO	5100
1324	1618	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCC(=O)NO)cc3)n2)cc(OC)c1OC	5140
1325	1620	COc1ccc(N(C)c2nc(C)nc3ccccc23)cc1OCCCCC(=O)NO	5189
1326	1621	N[C@@H](Cc1ccccc1)C(=O)Nc1ccccc1-c1ccc(NC(=O)CCCCCNC(=O)CS)cc1	5190
1327	1622	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(-c3ccc(C(F)(F)F)cc3)nn2)c1)NO	5220
1328	1623	CC(C)(C)OC(=O)Nc1ccc(-c2ncc(C(=O)NCCCCCCC(=O)NO)s2)cc1	5220
1329	1625	O=C(NO)[C@@H]1[C@H](c2ccccc2)[C@H]1c1cccc(-c2ncc(F)cn2)c1	5300
1330	1626	O=C(NO)c1ccc(CN2c3ccccc3C[C@@H]3CCCC[C@H]32)cc1	5300
1331	1627	O=C(CCCCCCNC(=O)C(O)(O)C(F)(F)F)Nc1nc2ccccc2s1	5300
1332	1628	Nc1ccccc1NC(=O)c1ccc(CSc2nnc(-c3ccncc3)n2-c2ccccc2)cc1	5320
1333	1630	COc1cc(C(=O)c2ccc3c(ccn3S(=O)(=O)c3ccc(/C=C/C(=O)NO)cc3)c2)cc(OC)c1OC	5340
1334	1631	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	5380
1335	1632	CCC(=O)CCCCC[C@H](NC(=O)C1CN(C)C1)c1[nH]c(-c2ccc(F)cc2)nc1C(N)=O	5383
1336	1633	Cc1ccc(-c2noc(CCCCCCC(=O)NO)n2)cc1	5390
1337	1635	S=C1Sc2cc(Cl)ccc2C2=NCCCN12	5400
1338	1636	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3nc(C4CC4)ccc3c2)[nH]1	5400
1339	1637	CCC(=O)CCCCC[C@H](NC(=O)C1CN(C)C1)c1[nH]c(-c2ccccc2)nc1C(N)=O	5422
1340	1638	Oc1cccn(Cc2ccc(Cn3cc(-c4ccccc4)nn3)cc2)c1=S	5470
1341	1640	Cc1ccc(NC(=O)C(Cc2c[nH]c3ccccc23)NC(=O)c2ccc(C(=O)NO)cc2)cc1	5500

1342	1641	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@@H](c3ccccc3)CN2)cc1	5500
1343	1642	CC1(C)c2cccc(C(=O)NO)c2CN1c1cnc(C(F)(F)F)cn1	5600
1344	1643	Brc1cncs1	5600
1345	1645	O=C(NO)c1ccc(CN2CCCCc3ccccc32)cc1	5610
1346	1646	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C(C)C)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	5664
1347	1647	Cc1cccc2sc(NC(=O)COc3ccc4cc(/C=C5/SC(=O)NC5=O)ccc4c3)nc12	5800
1348	1648	CC(=O)N[C@@H](Cc1ccc(OCc2ccccc2)cc1)C(=O)NO	5800
1349	1650	C=CCn1c(SCCCCCC(=O)Nc2ccccc2N)nnc1-c1ccncc1	5860
1350	1651	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O	5880
1351	1652	O=C(CCCCCCOc1cccc(-c2nc3ccccc3[nH]2)c1)NO	5980
1352	1653	CCCCCCCCCCCCCCCCCNNC(=O)c1cccs1	6000
1353	1655	Nc1ccc(F)cc1NC(=O)c1ccc(CNC(=O)OCc2cccnc2)cc1	6000
1354	1656	NCC(=O)Nc1ccccc1-c1ccc(NC(=O)CCCCCNC(=O)CS)cc1	6030
1355	1657	Oc1cccn(CCn2cc(-c3ccccc3)nn2)c1=S	6050
1356	1658	CC(C)C[C@H]1CC(=O)N[C@@H](C)C(=O)N[C@@H](CSCCC(=O)O)C(=O)N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N1	6050
1357	1660	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC(F)(F)F)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	6093
1358	1661	O=C(CS)NCCCCCC(=O)Nc1cccc2cccnc12	6120
1359	1662	Cc1nc2c(c(N(C)c3ccc(OCCCC(=O)NO)cc3)n1)CCC2	6190
1360	1663	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc(NCCCC(=O)NO)c2ccccc2n1	6194
1361	1665	O=C(NO)c1ccc(NC2CC(=O)N(c3ccccc3)C2)cc1	6250
1362	1666	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2ccc3c(=O)n(CC)ccc3c2)[nH]1	6261
1363	1667	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2cc3ccc(C)nc3cc2OC)[nH]1	6300
1364	1668	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCCC(=O)NO)cc3)n2)cc(OC)c1OC	6320
1365	1670	Oc1cccn(CCCn2cc(-c3ccccc3)nn2)c1=S	6400
1366	1671	CC(C)(C)OC(=O)Nc1ccc(-c2cc(C(=O)NCCCCCCC(=O)NO)no2)cc1	6522.630604
1367	1672	COc1cc(C(=O)c2csc(-c3ccc(C#CCCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	6550
1368	1673	O=C(NO)c1cccc(Oc2ccccc2)c1	6600
1369	1675	O=C(N[C@@H](CCCCCB(O)O)C(=O)Nc1cccc(-c2ccccc2)c1)c1cncs1	6600
1370	1676	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(NC(=O)CCCCCCC(=O)NO)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	6680
1371	1677	O=C(O)CCCCC[C@@H]1NC(=O)[C@H](Cc2c(F)c(F)c(F)c(F)c2F)NC(=O)C[C@H](Cc2ccc(O)cc2)NC(=O)[C@H](Cc2ccc3ccccc23)NC1=O	6700
1372	1678	Fc1cccc2c1SC(=S)N1CCN=C21	6700
1373	1680	Cc1ncc(-c2ccc(C(C(=O)NO)c3ccccc3F)cc2)cn1	6700
1374	1681	Cn1cc([C@H]2[C@H](C(=O)NO)[C@@H]2c2ccccc2)cn1	6700
1375	1682	O=C(CCN1CCc2ccccc2C1C1CCCCC1)NO	6700
1376	1683	O=C(CCC1C(=O)N(c2ccc(Cl)cc2)C(=O)N1Cc1ccc(Br)cc1)Nc1ccc(C(=O)NO)cc1	6700
1377	1685	Cc1ccc(NC(=O)CN(CCCCCC(=O)NO)C(=O)c2ccc(N(C)C)cc2	6760

		)cc1	
1378	1686	Oc1cccn(CCCCCCn2cc(-c3ccccc3)nn2)c1=S	6770.970462
1379	1687	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	6780
1380	1688	O=CN(O)CCCCCC(=O)Nc1ccccc1	6800
1381	1690	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccc(F)cc2)nc1C(N)=O	6802
1382	1691	Nc1nc(Nc2ccc(F)c(Cl)c2)c2ncn(Cc3ccc(C(=O)Nc4ccccc4N)cc3)c2n1	6810
1383	1692	CC(C)(C)OC(=O)Nc1ccc(-c2cc(NC(=O)CCCCCCC(=O)NO)no2)cc1	6851
1384	1693	CCC(=O)CCCCC[C@H](NC(=O)C12CCN(CC1)CC2)c1[nH]c(-c2ccc(F)cc2)nc1C#N	6929
1385	1695	O=CN(O)CCCCCNC(=O)c1ccc2ccccc2c1	7000
1386	1696	CN(C)c1ccc2c(c1)SC(=S)N1CCN=C21	7000
1387	1697	CC(=O)NCCCC[C@@H]1NC(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC(=O)[C@H](CSCCC(=O)O)NC1=O	7040
1388	1698	COc1cc(C(=O)c2csc(-c3ccc(O/C=C/c4ccc(CC(=O)NO)cc4)cc3)n2)cc(OC)c1OC	7100
1389	1700	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)Cc3ccc(-c4cn(CC(=O)NO)nn4)cc3)[C@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	7120
1390	1701	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	7130
1391	1702	N#Cc1ccc(-c2cn(CCCCCn3cccc(O)c3=S)nn2)cc1C(F)(F)F	7141.213482
1392	1703	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3nc(C)ccc3c2)[nH]1	7200
1393	1705	Cn1c(SCCCCCC(=O)Nc2ccccc2N)nnc1-c1ccncc1	7280
1394	1706	CC(C)c1cc(C(=O)N2Cc3ccc(NC(=O)CCC(=O)NO)cc3C2)c(O)cc1O	7319
1395	1707	Cc1cc(C)cc(C(=O)N(CCCCCC(=O)NO)CC(=O)NCc2ccccc2)c1	7330
1396	1708	CC12CC3CC(C)(C1)CC(NS(=O)(=O)c1ccc(/C=C/C(=O)NO)cc1)(C3)C2	7380
1397	1710	Cc1cc(Br)ccc1NC(=O)COc1ccc2cc(/C=C3/SC(=O)NC3=O)ccc2c1	7400
1398	1711	CC(C)c1cc(C(=O)N2Cc3ccc(NC(=O)CCCCC(=O)NO)cc3C2)c(O)cc1O	7415
1399	1712	C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@]2(O)c1cn(CCCCC(=O)NO)nn1	7416.198487
1400	1713	CCC(=O)CCCCCC(NC(=O)c1cncs1)c1[nH]c(-c2ccccc2)nc1C(=O)NC	7471
1401	1715	Cc1cccc(NC(=O)COc2ccc3cc(/C=C4/SC(=O)NC4=O)ccc3c2)n1	7500
1402	1716	CCC(=O)CCCCC[C@H](NC(=O)C1CCOCC1)c1[nH]c(-c2ccc(F)cc2)nc1C(N)=O	7566
1403	1717	Nc1nc2ncc(CNc3ccc(C(=O)NCCCCCCCCCC(=O)NO)cc3)nc2c(=O)[nH]1	7590
1404	1718	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2cc3cccnc3nc2OC)o1	7600
1405	1720	O=C(CCCCCCc1nc(-c2ccc(F)cc2)no1)C(F)(F)F	7650

1406	1721	CCCCCCC(=O)N(O)C1CC(=O)C(c2ccc(Cl)cc2)C1=O	7690
1407	1722	Nc1ccc(Cl)cc1NC(=O)c1ccc(CNC(=O)OCc2cccnc2)cc1	7700
1408	1723	O=C(NO)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	7700
1409	1725	Nc1ccccc1NC(=O)c1ccc(CNC(=O)OCc2cccnc2)cc1	7763.344198
1410	1726	COc1ccc2c(c1)C1=NCCN1C(=S)S2	7800
1411	1727	O=C(NO)c1ccc(CN2C(=O)C(Cc3ccccc3)N(Cc3ccccn3)C2=O)cc1	7826
1412	1728	Cn1c(SCc2ccc(C(=O)Nc3ccccc3N)cc2)nnc1-c1ccncc1	7850
1413	1730	COc1cc(C(=O)c2csc(-c3ccc(OCc4ccc(C(=O)NO)cc4)cc3)n2)cc(OC)c1OC	7980
1414	1731	Nc1ccccc1NC(=O)c1ccc(CNC2=NC(=O)C(c3ccccc3)N2)cc1	8000
1415	1732	Cc1coc(C(=O)CCCCC[C@H](NC(=O)C2CCN(C)CC2)c2ncc(-c3ccc(F)cc3)[nH]2)n1	8000
1416	1733	CCCCCCCCSSCC/C=C/[C@@H]1CC(=O)N[C@H](C(C)C)C(=O)N[C@H](C)C(=O)N[C@H](C(C)C)C(=O)NCC(=O)O1	8010
1417	1735	CC(C)(C)OC(=O)Nc1cccc(-c2cc(C(=O)NCCCCCCC(=O)NO)no2)c1	8104
1418	1736	O=C(CCCCN1C(=O)[C@@H](CS)N=C(c2ccccc2)c2ccccc21)NO	8110
1419	1737	O=C(NO)c1coc(-c2cccs2)n1	8130
1420	1738	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(Cc1ccccc1)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	8197
1421	1740	O=C(NO)c1ccc(CNCc2nc(-c3cccs3)no2)cc1	8260
1422	1741	COc1cc(C(=O)c2csc(-c3ccc(NCCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	8280
1423	1742	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3nc(OC)ccc3c2)[nH]1	8300
1424	1743	O=C(NCC12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)c1ccc2c(ccn2Cc2ccc(C(=O)NO)c(Br)c2)c1	8380
1425	1745	CC(C)(C)OC(=O)n1c(C[C@@H]2N=C(c3ccccc3)c3ccccc3N(CCCCC(=O)NO)C2=O)cc2ccccc21	8390
1426	1746	CCC(=O)CCCCC[C@@H]1NC(=O)C2CCN2CCCCCCOc2cccc2-c2cnc1[nH]2	8419
1427	1747	COc1cc(Cn2ccc3cc(C(=O)NCC45C[C@H]6C[C@@H](C4)C[C@@H](C5)C6)ccc32)ccc1C(=O)NO	8440
1428	1748	CN(Cc1ccc(C(=O)NO)cc1[18F])CC12CC3CC(CC(C3)C1)C2	8500
1429	1750	O=C(CCCCN1C(=O)[C@H](CCC(=O)NO)N=C(c2ccccc2)c2ccccc21)NO	8520
1430	1751	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cnc3ccccc3c2)[nH]1	8600
1431	1752	CC12CC3CC(C)(C1)CC(NCc1ccc(C(=O)NO)cc1)(C3)C2	8630
1432	1753	O=C(NO)c1ccc(CN2CCCCc3cc(Cl)ccc32)cc1	8640
1433	1755	O=C(CCCCCCc1nc(-c2ccc(F)cc2)no1)NO	8760
1434	1756	Cc1ccc(-c2cc(/C=C/c3ccc(C(=O)NO)cc3)ccn2)c(F)c1	8780
1435	1757	COc1cc(C(=O)c2csc(-c3ccc(OCCCC(=O)NO)cc3)n2)cc(OC)c1OC	8840
1436	1758	COc1ccc2sc(NC(=O)CCCCCCNC(=O)C(O)(O)C(F)(F)F)nc2c1	8900
1437	1760	COc1cc2c(Oc3ccc(NC(=O)C4(C(=O)Nc5ccc(F)cc5)CC4)cc3F)ccnc2cc1OCCCC(=O)NO	8940
1438	1761	Cc1ccc(NC(=O)COc2ccc3cc(/C=C4/SC(=O)NC4=O)ccc3c2)cc1	9000
1439	1762	Nc1ccccc1NC(=O)c1cnccn1	9012.649444
1440	1763	COc1ccc(-c2ncc(C(=O)NCCCCCCC(=O)NO)s2)c(OC)c1	9020
1441	1765	O=C(NO)C(c1ccc(-c2ncc(C(F)(F)F)cn2)cc1)c1ccccc1F	9100
1442	1766	COc1cc(C(=O)c2csc(-c3ccc(NCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	9110
1443	1767	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c	9200

		1ncc(-c2ccc(-c3cnccn3)cc2)[nH]1	
1444	1768	O=C(NO)c1cccc(S(=O)(=O)N[C@H](C(=O)NCc2ccccc2)c2cccc2)c1	9200
1445	1770	O=C(/C=C/c1ccc(/C=C(/CNC2CC2)c2ccc(F)cc2)cc1)NO	9300
1446	1771	O=C(N[C@@H](Cc1ccc(OCc2ccccc2)cc1)C(=O)NO)c1ccccc1	9300
1447	1772	O=C(CN1C(=O)S/C(=C/c2ccccn2)C1=O)Nc1nc2ccccc2s1	9300
1448	1773	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1[nH]c(-c2ccc(F)cc2)nc1C#N	9370
1449	1775	CCC(CC)c1ccc(C(=O)NO)cc1	9430
1450	1776	CCN(CC)Cc1ccc(C(=O)NO)cc1	9430
1451	1777	S=C1Oc2ccccc2C2=NCCCN12	9500
1452	1778	Nc1ccccc1NC(=O)c1ccc(CSC2=N[C@@H](c3ccccc3)CO2)cc1	9500
1453	1780	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C=C/CCSCCS)OC1=O	9600
1454	1781	COc1cc(Nc2nc(N)nc3c2ncn3Cc2ccc(C(=O)Nc3ccccc3N)cc2)cc(OC)c1	9610
1455	1782	Cn1cc(C(=O)Cl)cc1/C=C/C(=O)NO	9650
1456	1783	O=CN(O)CCCCCNC(=O)CCc1ccccc1	9700
1457	1785	CC(C)C[C@H]1CC(=O)N[C@@H](C)C(=O)N[C@@H](CSCC(=O)O)C(=O)N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N1	9700
1458	1786	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(C2=CC3OC=NC3C=C2)[nH]1	9700
1459	1787	O=C(CCCCCONC(=O)c1ccc2ccccc2n1)NO	9780
1460	1788	CN1c2ccc(F)cc2C(=O)N2CCc3c([nH]c4ccc(OCc5ccc(/C=C/C(=O)NO)cc5)cc34)C21	9800
1461	1790	O=C(CCCCCCNC(=O)C(O)(O)C(F)(F)F)Nc1ncc(-c2ccc(Br)cc2)s1	10000
1462	1791	Nc1nc2ncc(CNc3ccc(C(=O)N[C@@H](CCC(=O)NCCCCCCCC(=O)Nc4cc(-c5cccs5)ccc4N)C(=O)O)cc3)nc2c(=O)[nH]1	10000
1463	1792	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc(-c3ccncc3)cc2)[nH]1	10000
1464	1793	O=C(CCCCNCc1ccccc1)NO	10000
1465	1795	COc1ccc(C(=O)c2ccc3c(ccn3S(=O)(=O)c3ccc(/C=C/C(=O)NO)cc3)c2)cc1	10000
1466	1796	O=C(NO)c1coc(-c2cccc(-c3ccccc3)c2)n1	10080
1467	1797	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCCCCCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	10160
1468	1798	COc1ccccc1-c1ncc(C(=O)NCCCCCCC(=O)NO)s1	10190
1469	1800	CN(C)c1ccc(C(=O)NCCCCCNC(=O)CS)cc1	10200
1470	1801	O=C(CCCCCONC(=O)c1cc2ccccc2[nH]1)NO	10300
1471	1802	Cn1c(CCC(=O)NO)nc2ccccc2c1=O	10400
1472	1803	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O	10550
1473	1805	CCCNNC(=O)c1cnc(NCc2ccc(OC)cc2)cn1	10744
1474	2071	O=C(CCCCCOc1no[n+]([O-])c1S(=O)(=O)c1ccccc1)NO	10846.61237
1475	1806	O=C(/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1)NO	11000
1476	1807	C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@]2(O)c1cn(CCCC(=O)NO)nn1	11000
1477	1808	CC(C)(C)OC(=O)CC(O)/C=C/CCSSCC/C=C/C(O)CC(=O)OC(C)(C)C	11000
1478	1810	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(O)C	11050

		[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	
1479	1811	O=C(O)CCCCCSc1nnc(-c2ccncc2)n1-c1ccccc1	11050
1480	1812	C=CCn1c(SCCCCCC(=O)NO)nnc1-c1ccncc1	11060
1481	1813	O=C(CCCCCONC(=O)Nc1cnc2ccccc2c1)NO	11170
1482	1815	N[C@@H](Cc1c[nH]c2ccccc12)C(=O)Nc1ccccc1-c1ccc(NC(=O)CCCCCNC(=O)CS)cc1	11300
1483	1816	COc1ccc(-c2ncc(/C=C/C(=O)Nc3ccccc3N)s2)cc1OC	11550
1484	1817	O=C(Cc1ccccc1)NO	11620
1485	1818	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	11620
1486	1820	Cn1c(SCCCCCC(=O)O)nnc1-c1ccncc1	11950
1487	1821	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(-c3ccc(F)cc3)nn2)c1)NO	12000
1488	1822	COc1ccc2c(c1)SC(=S)N1CCN=C21	12000
1489	1823	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	12020
1490	1825	Cn1cc(C=O)cc1/C=C/C(=O)NO	12250
1491	1826	CCC(=O)CCCCC[C@H](NC(=O)c1cncs1)c1[nH]c(-c2ccc(F)cc2)nc1C#N	12260
1492	1827	CN(C)c1ccc(C(=O)NCCCNC(=O)CS)cc1	12300
1493	1828	O=C(CCCCCONC(=O)c1nccc2ccccc12)NO	12400
1494	1830	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@@H](c3ccccc3)[C@H](c3ccccc3)S2)cc1	12600
1495	1831	C#Cc1ccncc1	12600
1496	1832	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccc(-c3cccnc3)cc2)nc1C#N	12620
1497	1833	O=C(CCCCN1C(=O)[C@H](Cc2ccccc2)N=C(c2ccccc2)c2ccccc21)NO	12670
1498	1835	CN(C)S(=O)(=O)c1ccc(NCCCCCC(=O)NO)c2nonc12	12700
1499	1836	O=C(NO)c1ccc(CSc2nnc(-c3ccncc3)n2-c2ccccc2)cc1	12760
1500	1837	O=C(NO)c1csc(C(c2ccccc2)c2ccccc2)n1	12860
1501	1838	Fc1cccc2c1C1=NCCN1C(=S)S2	13000
1502	1840	COc1ccc(-c2cnc(NC(=O)CCCCCCNC(=O)C(O)(O)C(F)(F)F)s2)cc1	13000
1503	1841	Nc1ccccc1NC(=O)c1ccc(CNC2=NC(=O)C(Cc3ccccc3)N2)cc1	13000
1504	1842	N/N=C(\Cc1ccc(O)c(Br)c1)C(=O)NCCS	13000
1505	1843	Cc1ccc2c(c1)SC(=S)N1CCN=C21	13000
1506	1845	O=C(N[C@@H](CCCCNC(=O)c1ccccc1O)c1ncc(-c2ccc3ccccc3c2)[nH]1)c1cncs1	13000
1507	2072	O=C(CN1C(=O)S/C(=C/c2ccco2)C1=O)Nc1ccc([N+](=O)[O-])cc1	13000
1508	1846	COc1cccc(-c2ncc(/C=C/C(=O)Nc3ccccc3N)s2)c1	13370
1509	1847	O=C(CS)NCCCCCCNC(=O)Nc1ccccc1	13900
1510	1848	CNC(=O)c1cccc(C(=O)NO)c1	14000
1511	1850	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CCC(F)(F)F)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	14090
1512	1851	O=C(/C=C/c1ccc(Cn2cc(Nc3ncc(Cl)c(Nc4ccc(F)cc4)n3)cn2)cc1)NO	14100
1513	1852	COc1cc(-c2ncc(/C=C/C(=O)Nc3ccccc3N)s2)cc(OC)c1OC	14180
1514	1853	Nc1ccccc1NC(=O)c1ccc(CSC2=N[C@@H](c3ccccc3)CN2)cc1	14300
1515	1855	O=C(NO)c1coc(-c2ccc(Br)cc2)n1	14370
1516	1856	CC(=O)N[C@@H](Cc1ccc(OCCc2ccccc2)cc1)C(=O)NO	14400
1517	1857	COc1ccc(-c2ncc(C(=O)NCCCCCCCC(=O)NO)[nH]2)c(OC)c1	14560
1518	1858	O=C(NO)c1ccc(CN(Cc2nnnn2Cc2ccccc2)C(=O)c2ccccc2C(F)(F)F)cc1	14700
1519	1860	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@@H](c3ccc(O)cc3)CS2)cc1	15000
1520	1861	CCCC(=O)O	15000
1521	1862	COc1cccc(-c2ncc(C(=O)NCCCCCCCC(=O)NO)s2)c1	15230

1522	1863	O=C(NO)C1c2ccccc2-c2ccccc21	15247.95068
1523	1865	O=C1Nc2ccccc2/C1=N/NC(=S)Nc1ccc(C(=O)NO)cc1	15700
1524	1866	CCSC(=S)SCC(=O)c1ccc(OC)cc1	15848.93
1525	1867	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2cc3ccccc3nc2OC)o1	16000
1526	1868	O=C(COc1ccc2cc(/C=C3/SC(=O)NC3=O)ccc2c1)Nc1ccc(Br)cc1	16000
1527	1870	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccccc4)CC3c3ccc(C(F)(F)F)cc3)cc2)S1	16000
1528	1871	CCC(=O)CCCCC[C@H](NC(=O)c1ccon1)c1[nH]c(-c2ccc(F)cc2)nc1C#N	16190
1529	1872	COc1ccc2c(C(=O)c3cc(OC)c(OC)c(OC)c3)cn(S(=O)(=O)c3cccc(/C=C/C(=O)NO)c3)c2c1	16200
1530	1873	COc1ccc(CNC(=O)c2cc(F)ccc2N2CCOCC2)cc1OCC(=O)NO	16509
1531	1875	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccc(F)cc2)nc1C#N	16750
1532	1876	CCC(=O)CCCCCC(NC(=O)c1cncs1)c1[nH]c(-c2ccccc2)nc1C(=O)N1CCOCC1	16780
1533	1877	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3cccnc3cc2OC)o1	17000
1534	1878	CCOc1ccc2nc(NC(=O)COc3ccc4cc(/C=C5/SC(=O)NC5=O)ccc4c3)sc2c1	17000
1535	1880	O=C(/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)s1)NO	19000
1536	1881	O=C(CCN1CCc2ccccc2C1)NO	19000
1537	1882	O=C(CN1CCc2ccccc2C1c1ccccc1)NO	19000
1538	1883	O=C(NO)c1cccc(S(=O)(=O)N[C@@H](Cc2c[nH]c3ccccc23)C(=O)NCc2ccccc2)c1	19000
1539	1885	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccc(C(F)(F)F)cc2)nc1C#N	19190
1540	1886	CCC(=O)CCCCC[C@H](NC(=O)C1CN(C)C1)c1[nH]c(-c2ccc(F)cc2)nc1C#N	19650
1541	1887	O=C(NO)c1ccc(NC(=S)N/N=C/c2ccc(F)cc2)cc1	19700
1542	1888	COc1ccc(-c2ncc(C(=O)NCCCCCC(=O)NO)s2)c(OC)c1	19810
1543	1890	O=C(NO)c1cccc(-c2ccccc2)c1	20000
1544	1891	Nc1ccc(-c2cccs2)cc1NC(=O)c1ccc(N2CCC3(CC2)CNC(=O)O3)nc1	20000
1545	1892	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccc(C)nc3cc2OC)o1	20000
1546	1893	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccccc4)CC3c3ccccc3)cc2)S1	20000
1547	1895	O=C(NO)c1coc(-c2ccccc2Br)n1	20240
1548	1896	CSCC[C@@H]1N=C(c2ccccc2)c2ccccc2N(CCCCC(=O)NO)C1=O	20280
1549	1897	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccc(F)cc2F)nc1C#N	20730
1550	1898	CN1CCN(CCNC(=O)c2ccc(C(=O)NO)cc2)CC1	20910
1551	1900	S=C1Sc2ccccc2C2=NCCN12	21000
1552	1901	Fc1cccc2c1SC(=S)N1CCCN=C21	21000
1553	1902	CCC(=O)CCCCC[C@@H]1NC(=O)C2CCN2CCCCCOc2ccccc2-c2cnc1[nH]2	21460
1554	1903	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccccc3nc2OC)o1	21690
1555	1905	Cc1[nH]c2ccccc2c1CCNCc1ccc(/C=C/C(N)=O)cc1	22000
1556	1906	O=CN(O)CCCCCNC(=O)c1ccccc1	22000
1557	1907	CNC(=O)/C(CCCCCCC(=O)Nc1ccccc1)=N\O	22297.98197
1558	1908	CC(C)(C)OC(=O)C[C@@H]1N=C(c2ccccc2)c2ccccc2N(CCCCC(=O)NO)C1=O	22390

1559	1910	C=CCn1c(SCc2ccc(C(=O)Nc3ccccc3N)cc2)nnc1-c1ccncc1	22490
1560	1911	CC(=O)N1C(NCc2ccc(C(=O)Nc3ccccc3N)cc2)=NC(=O)C1Cc1ccccc1	22700
1561	1912	O=C(O)CC/C=C\C[C@@H]1NC(=O)[C@H]2CCCN2C(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	23000
1562	1913	O=C(N[C@@H](CCCCCB(O)O)C(=O)Nc1cccc(-c2ccccc2)c1)c1cccnc1	23000
1563	1915	O=C(CCCCN1C(=O)[C@H](CCC(=O)NC(c2ccccc2)(c2ccccc2)c2ccccc2)N=C(c2ccccc2)c2ccccc21)NO	23480
1564	1916	CC(=O)Nc1ccc(C(=O)CSc2nc(C)cc(O)n2)cc1	23900
1565	1917	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccc(C4CC4)nc3cc2F)o1	24000
1566	1918	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2cc3ccncc3nc2OC)o1	24000
1567	1920	CC(=O)N1C(NCc2ccc(C(=O)Nc3ccccc3N)cc2)=NC(=O)C1Cc1c[nH]c2ccccc12	24300
1568	1921	C[C@@H]1N=C(c2ccccc2)c2ccccc2N(CCCCC(=O)NO)C1=O	24750
1569	1922	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccc(F)cc4)CC3c3ccc(Cl)c(Cl)c3)cc2)S1	25000
1570	1923	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@H](c3ccccc3)[C@H](c3ccccc3)O2)cc1	25200
1571	1925	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccccc4)CC3c3ccc(F)cc3)cc2)S1	26000
1572	1926	CC(C)(C)OC(=O)CC[C@@H]1N=C(c2ccccc2)c2ccccc2N(CCCCC(=O)NO)C1=O	26070
1573	1927	O=C(NO)c1coc(-c2ccc3ccccc3c2)n1	26160
1574	1928	O=C(CCCCCn1cc(-c2ccc(C(=O)c3c(-c4ccc(O)cc4)sc4cc(O)ccc34)cc2)nn1)NO	26507.5461
1575	1930	C[Si](O)(O)CCCCCCC(=O)Nc1ccccc1	27000
1576	1931	CC(C)(C)OC(=O)N1C(NCc2ccc(C(=O)Nc3ccccc3N)cc2)=NC(=O)C1Cc1c[nH]c2ccccc12	27200
1577	1932	O=C(NO)c1coc(-c2ccc(-c3ccccc3)cc2)n1	27330
1578	1933	O=C(CCCCC[C@@H]1NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC(=O)[C@H]2CCCN2C(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O)NO	27600
1579	1935	O=C(N[C@@H](Cc1ccc(OCCc2ccccc2)cc1)C(=O)NO)c1ccccc1	27800
1580	1936	O=C(CS)NCCCCCC(=O)Nc1ccccc1	27892.65136
1581	1937	COc1ccc2cc(C(=O)/C=C/C=C/c3ccc(OC)c(OC)c3)c(=O)oc2c1	28000
1582	2073	COc1cc(COc2ccc(NC(=O)CCCCCCC(=O)OCc3ccc(CN=[N+]=[N-])cc3)cc2)cc(N=[N+]=[N-])c1	28000
1583	1938	C=CCn1c(SCc2ccc(C(=O)NO)cc2)nnc1-c1ccncc1	28370
1584	1940	COc1ccc2cc(-c3nc(C(=O)NO)co3)ccc2c1	29080
1585	1941	CNC(=O)/C(CCCCCCC(=O)Nc1cccc(-c2ccc(C(=O)O)cc2)c1)=N\O	29400
1586	1942	CCC(=O)CCCCC[C@H](NC(=O)CN(C)C)c1[nH]c(-c2ccc(F)cc2)nc1C#N	29490
1587	1943	C[C@@H](OCc1ccccc1)[C@@H]1N=C(c2ccccc2)c2ccccc2N(CCCCC(=O)NO)C1=O	29540
1588	1945	O=C(CCCCCCn1cc(-c2ccc(C(=O)c3c(-c4ccc(O)cc4)sc4cc(O)ccc34)cc2)nn1)NO	29900
1589	1946	CCCC[C@H]1NC(=O)C[C@H]2/C=C/CCSSC[C@@H](NC1=O)C(=O)N[C@H]([C@@H](C)CC)[C@@H](O)CC(=O)O2	30000
1590	1947	O=C(CCCCCCNC(=O)C(O)(O)C(F)(F)F)Nc1ncc(-c2ccc(O)cc2)s1	30000
1591	1948	S=C1Sc2c(Cl)cccc2C2=NCCCN12	30000
1592	1950	Cc1ccc(C(=O)N[C@@H](Cc2ccc(OCc3ccccc3)cc2)C(=O)NO)cc1	30700
1593	1951	O=C(NO)c1coc(-c2ccc(Cl)cc2)n1	30760

1594	1952	O=C(/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)cc1)NO	31000
1595	1953	Cc1cccc2c1SC(=S)N1CCN=C21	31000
1596	1955	Nc1ccccc1NC(=O)/C=C/c1ccc(NC(=O)Cc2ccccc2)cn1	31400
1597	1956	Nc1ccc(-c2cccs2)cc1NC(=O)c1ccc(CNC(=O)OCc2cccnc2)cc1	31738
1598	1957	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C(C)C)CC2)c1ncc(-c2cc3ccccc3nc2OC)o1	32920
1599	1958	O=C(NO)N1CCN(C(=S)N/N=C/c2ccccc2O)CC1	33670
1600	1960	Nc1ccccc1NC(=O)c1ccc(CNC2=NC(c3ccc(F)cc3)CO2)cc1	33900
1601	1961	CC(C)[C@H](NS(=O)(=O)c1cccc(C(=O)NO)c1)C(=O)Nc1ccccc1	33900
1602	1962	CC(C)Cc1nc2cc(CCC(=O)NO)ccc2n1CCCO	33960
1603	1963	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccccc4)CC3c3ccc(F)cc3F)cc2)S1	34000
1604	1965	Nc1ccccc1NC(=O)c1ccc(CNc2nccc(-c3cccnc3)n2)cc1	35000
1605	1966	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccccc4)CC3c3ccc(Br)cc3)cc2)S1	35000
1606	1967	CCC(C(=O)Nc1ccc(/C=C/C(=O)Nc2ccccc2N)nc1)c1ccccc1	35600
1607	2074	COC(=O)CCCCCCC(=O)Nc1cnn(Cc2cc(CN=[N+]=[N-])cc(N=[N+]=[N-])c2)c1	36000
1608	1968	O=C(NO)c1csc(-c2ccc(Br)cc2)n1	36360
1609	1970	CCOP(=O)(CNCc1ccc(C(=O)Nc2cc(-c3cccs3)ccc2N)cc1)OCC	37000
1610	1971	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2cccnc2OC)nc1C#N	38080
1611	1972	O=C(NO)c1noc(-c2ccccc2)n1	38500
1612	1973	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2cc3ccc(C)nc3cc2OC)o1	39000
1613	1975	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccccc2F)nc1C#N	39610
1614	1976	Nc1cc(Cl)ccc1NC(=O)c1ccc(CNC(=O)OCc2cccnc2)cc1	40000
1615	1977	O=C(NO)c1coc(-c2ccccc2)n1	41900
1616	1978	Ic1ccccn1	42000
1617	2076	CC(C)(C)OC(=O)CCCCCCC(=O)Nc1ccc(OCc2cc(CN=[N+]=[N-])cc(N=[N+]=[N-])c2)cc1	42600
1618	1980	CC(C)C(C(=O)Nc1ccc(/C=C/C(=O)Nc2ccccc2N)nc1)c1ccccc1	43100
1619	1981	O=C(NO)N1CCN(C(=S)N/N=C/c2ccc(Cl)cc2)CC1	43160
1620	1982	O=C(NO)c1coc(-c2ccc(F)cc2)n1	43350
1621	1983	CC(C)(C)OC(=O)N[C@@H](CCCCCS)C(=O)NC1CCCC1	44000
1622	1985	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1nnc(-c2cc3ccccc3nc2OC)o1	45000
1623	2077	COC(=O)CCCCCCNC(=O)c1cc(-c2ccc(NC(=O)c3cc(CN=[N+]=[N-])cc(N=[N+]=[N-])c3)cc2)on1	47100
1624	1986	CS(=O)(=O)N[C@@H](Cc1ccc(OCc2ccccc2)cc1)C(=O)O	47200
1625	1987	COC(=O)CCCCCCC(=O)Nc1ccc(OCc2cc(C)cc(C)c2)cc1	47800
1626	1988	COc1ccc(-c2nc(C(=O)NO)co2)cc1	50940
1627	1990	O=C(CCCCCCNC(=O)C(O)(O)C(F)(F)F)Nc1ccc(Cl)cc1	52000
1628	1991	Nc1ccccc1NC(=O)c1ccc(CNC2=NC(c3cccc(F)c3)CO2)cc1	52200
1629	1992	Cc1ccc(C(=O)N[C@@H](Cc2ccc(OCCc3ccccc3)cc2)C(=O)NO)cc1	52500
1630	1993	Cn1cc(C=O)cc1CCC(=O)NO	52560
1631	1995	Nc1ccccc1NC(=O)c1ccc(CNC2=NC(c3ccccc3)(c3ccccc3)CO2)cc1	53500
1632	1996	O=C(NO)C(c1ccccc1)c1ccccc1	53881.81422
1633	1997	CNC(=O)/C(CCCCCCC(=O)NC1c2ccccc2-c2ccccc21)=N\O	58400
1634	1998	O=C(NO)c1csc(-c2cnccn2)n1	61420
1635	2000	CNC(=O)/C(CCCCCCC(=O)Nc1ccc2ccccc2c1)=N\O	65000
1636	2001	CCC(C(=O)Nc1ccc(C(=O)Nc2ccccc2N)nc1)c1ccccc1	66200

1637	2078	COc1cc(COc2ccc(NC(=O)CCCCCCC(=O)OCCN=[N+]=[N-])cc2)cc(N=[N+]=[N-])c1	67500
1638	2002	Nc1ccccc1NC(=O)CCCCCC(c1c[nH]c2ccccc12)c1c[nH]c2ccccc12	74000
1639	2003	CC(C)C(C(=O)Nc1ccc(C(=O)Nc2ccccc2N)nc1)c1ccccc1	75200
1640	2005	CNC(=O)/C(CCCCCCC(=O)Nc1cccc(-c2cccnc2)c1)=N\O	76700
1641	2006	Nc1ccccc1NC(=O)/C=C/c1ccc(NC(=O)Cc2ccc3ccccc3c2)cn1	77100
1642	2007	Nc1ccccc1NC(=O)c1ccc(NC(=O)Cc2ccccc2)cn1	77100
1643	2008	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@H](c3ccccc3)CO2)cc1	80700
1644	2010	Cc1ccc(S(=O)(=O)N[C@@H](Cc2ccc(OCCc3ccccc3)cc2)C(=O)NO)cc1	82500
1645	2011	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@@H](c3ccc(O)cc3)CO2)cc1	83300
1646	2012	CNC(=O)/C(CCCCC[C@@H](C(=O)Nc1ccccc1)N(Cc1ccccc1)Cc1ccccc1)=N\O	87000
1647	2013	Nc1ccccc1NC(=O)c1ccc(CSC2=N[C@@H](Cc3ccccc3)CO2)cc1	88000
1648	2015	CNC(=O)/C(CCCCC[C@H](NCc1ccc(OC)cc1)C(=O)Nc1ccccc1)=N\O	94600
1649	2016	Nc1ccccc1NC(=O)c1ccc(NC(=O)Cc2cccc3ccccc23)cn1	98400
1650	2017	CS(=O)(=O)N[C@@H](Cc1ccc(OCCc2ccccc2)cc1)C(=O)O	102300
1651	2018	O=C(N[C@@H](Cc1ccc(OCc2ccccc2)cc1)C(=O)O)c1ccccc1	110500
1652	2020	Nc1ccccc1NC(=O)c1ccc(CSC2=N[C@@H](c3cccnc3)CO2)cc1	112000
1653	2021	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@H](Cc3c[nH]cn3)CO2)cc1	113000
1654	2022	O=C(CCC1=CCN(CCCc2ccc3ccccc3c2)C1=O)NO	119700
1655	2023	CC(=O)N[C@@H](Cc1ccc(OCCc2ccccc2)cc1)C(=O)O	120900
1656	2025	CCn1c(SCCCCCC(=O)Nc2ccccc2N)nnc1-c1ccncc1	198070
1657	2026	O=C(N[C@@H](Cc1ccc(OCCc2ccccc2)cc1)C(=O)O)c1ccccc1	253400
1658	2027	Cc1ccc(C(=O)N[C@@H](Cc2ccc(OCCc3ccccc3)cc2)C(=O)O)cc1	385600
1659	2028	N[C@H](Cc1ccc(Cl)cc1Cl)C(=O)O	410000
1660	2030	COC(=O)[C@H](Cc1ccc(OCc2ccccc2)cc1)NS(C)(=O)=O	753700
1661	2031	COC(=O)[C@H](Cc1ccc(OCCc2ccccc2)cc1)NC(C)=O	825100
1662	2032	COC(=O)[C@H](Cc1ccc(OCc2ccccc2)cc1)NC(C)=O	871500
1663	2033	COC(=O)[C@H](Cc1ccc(OCCc2ccccc2)cc1)NS(=O)(=O)c1ccc(C)cc1	961800

Table S2. Test set compounds in SMILES format

S.No	Compounds	SMILES	Activity (nM)
1	2	O=C(NO)[C@H](Cc1ccccc1)n1nnc(-c2ccccc2)c1C#CC1CC1	0.8
2	7	CN1c2ccc(NCc3ccc(-c4noc(CCCCCCC(=O)NO)n4)cc3)cc2C(=O)N2CCc3c([nH]c4ccc(O)cc34)C21	2.5
3	12	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3ccc(Cl)cc3)ccc12)NO	3.3
4	17	O=C(NO)[C@H](Cc1ccccc1)n1nnc(-c2ccsc2)c1C#CC1CC1	4
5	22	COc1cccc(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3c2)c1F	4.4
6	27	COc1ccc(F)c(-c2ccc3c(NC(=O)CCCCCCC(=O)NO)n[nH]c3c2)c1	4.9
7	32	O=C(CCCCCC/C=C/c1ccc2ccccc2c1)NO	6
8	37	CCCNNC(=O)c1cnc(N2CCN(Cc3c[nH]c4ccccc34)CC2)nc1	8.2
9	42	CC(C)(C)c1ccc(NS(=O)(=O)c2ccc(C(=O)NO)cc2)cc1	9.4
10	47	CN(Cc1nc2c(N3CCOCC3)nc(-c3ccncc3)nc2n1C)c1ncc(C(=O)NO)cn1	11
11	52	CCCCCCNNC(=O)c1cnc(N2CCN(CCc3c[nH]c4ccccc34)CC2)nc1	13
12	57	O=C1CN(Cc2ccc(C(=O)NO)cc2)C(=O)[C@H](Cc2ccccc2)N1	15.6
13	62	C[C@H](NC(=O)c1nc(-c2ncc(-c3ccccc3)s2)sc1C1CC1)c1ccc(C(=O)NO)cc1	16.84
14	2034	[N-]=[N+]=NCc1cc(Cn2cc(NC(=O)CCCCCCC(=O)NO)cn2)cc(N=[N+]=[N-])c1	17
15	67	COc1ccc(C(=O)NO)cc1S(=O)(=O)Nc1ccc(C)cc1	19.8
16	72	Cc1sc2c(c1C)C(c1ccc(Cl)cc1)=N[C@@H](CC(=O)Nc1ccc(C(=O)NO)cc1)c1nnc(C)n1-2	21
17	77	CCCCCCNNC(=O)c1cnc(N2CCN(CCc3cn(C)c4ccccc34)CC2)nc1	23
18	82	O=C(CCCCCCC(=O)Nc1n[nH]c2cc(-c3ccncc3)ccc12)NO	24.5
19	87	O=C(/C=C/c1cccc(-c2nc3ccccc3n2CCCc2ccccc2)c1)NO	25
20	92	Nc1nc2cc(-c3nn(CC4CCN(c5ncc(C(=O)NO)cn5)CC4)c4ncnc(N)c34)ccc2o1	27
21	97	CC(C)Oc1ccc(C(=O)NO)cc1NC(=O)c1ccccc1	29
22	102	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n(CCc2ccccc2)c1C	31
23	107	O=C(/C=C/c1cccc(C(=O)c2cc3ccccc3[nH]2)c1)NO	32
24	112	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	35
25	117	CC(C)N(C(=O)c1cc(C(C)(C)C)cc(C(C)(C)C)c1)c1ccc(C(=O)NO)cc1	35.68333
26	122	COc1ccc(C(=O)NO)cc1C(=O)Nc1ccc(Cl)cc1	38.98718
27	127	Cc1nc(-c2cccc(/C=C/C(=O)NO)c2)n([C@@H]2CCCN(C(C)C)C2)c1-c1ccccc1	40
28	132	O=C(NO)c1ccc(CNC(=O)N2CCC(N3C(=O)[C@H](c4ccccc4)[C@H]3c3ccccc3)CC2)cc1	42
29	137	O=C(CCCCCCCC(=O)c1ccc(Br)cc1)NO	45
30	142	O=C(/C=C/c1ccc(C(=O)NO)cc1)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)Nc1ccc(Cl)cc1	47.3
31	147	O=C(NO)c1cccc(S(=O)(=O)Nc2ccccc2)c1	50
32	152	CCN1CCC[C@@H](n2c(-c3cccc(/C=C/C(=O)NO)c3)nc(C)c2-c2ccccc2)C1	50
33	157	Cc1cccc(NC(=O)[C@H](CCCCCC(=O)NO)NC(=O)[C@H]2CCC(=O)N2)c1	52
34	162	COc1cccc(-c2ccc3c(NC(=O)CCCC(=O)NO)n[nH]c3c2)c1	54
35	167	COc1ccc(C(=O)NO)cc1NC(=O)c1ccc(-c2ccccc2)cc1	58.24946
36	172	O=C(NO)c1cccc(S(=O)(=O)NCCc2ccccc2)c1	60
37	177	O=C1C[C@@H](C(=O)N[C@@H](CCCCCS)C(=O)Nc2ccccc2)N1	61
38	182	CCN(CC)CCn1c(-c2cccc(/C=C/C(=O)NO)c2)nc2ccccc21	63
39	187	O=C(/C=C/c1cccc(-c2nc3ccccc3[nH]2)c1)NO	63

40	192	COc1ccc(-c2cc(-c3ccccc3)[nH]c2C(=O)NCc2ccc(C(=O)NCCS)cc2)cc1	64.1
41	197	CC(C)(C)c1ccc(CN(Cc2ccc(C(=O)NO)cc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	68
42	202	COc1ccc(-c2ccc(/C=C/C(=O)NO)cc2)cc1	69.8
43	207	O=C(NO)c1ccc(CCCN2CCC(CN[C@H]3C[C@@H]3c3ccccc3)CC2)cc1	71
44	212	O=C(NO)c1ccc(CN2C(=O)c3ccccc3C2=O)cc1-c1ccccc1	72
45	217	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCC(N(C)C)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	75
46	222	COc1ccc(C(=O)Nc2cc(C(=O)NO)ccc2OC)cc1	77.1
47	227	O=C(/C=C/c1cccc(C(=O)c2cc3ccccc3o2)c1)NO	79
48	232	O=C(NO)c1ccc2c(c1)C[C@H](Nc1nccc(-c3cccnc3)n1)CC2	80
49	237	CC(=O)N(Cc1ccc(C(C)(C)C)cc1)c1ccc(C(=O)NO)cc1	85.4
50	242	COc1ccccc1C(=O)N[C@H](COc1cccc(/C=C/C(=O)NO)c1)Cc1c[nH]c2ccccc12	87.4
51	247	COc1ccc(CS(=O)(=O)Nc2ccc(/C=C\C(=O)NO)cc2)cc1OC	90
52	252	O=C(NO)c1ccc(N(Cc2ccccc2)C(=O)CN(Cc2c(F)c(F)c(F)c(F)c2F)S(=O)(=O)c2ccc(F)cc2)cc1	90.6
53	257	O=C(CCCCCCC(=O)Nc1ccc2c(c1)CCC(=O)N2)NO	94
54	262	O=C(CCCCC[C@H](NC(=O)[C@@H]1CCCC(=O)N1)C(=O)Nc1ccccc1)NO	97
55	267	Cc1cccc(NC(=O)[C@H](CCCCCS)NC(=O)[C@H]2CCC(=O)N2C)c1	99
56	272	Cc1cccc(S(=O)(=O)Nc2ccc(/C=C/C(=O)NO)cc2)c1	100
57	277	CCN1CCC[C@@H](n2c(-c3cccc(/C=C/C(=O)NO)c3)nc(C)c2C)C1	100
58	282	COc1ccc(C(=O)NO)cc1C(=O)Nc1ccc2sccc2c1	100
59	287	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)[C@@H](NC(=O)OC(C)(C)C)C(C)C)cc1	104
60	292	O=C1CCC[C@H](C(=O)N[C@@H](CCCCCS)C(=O)Nc2ccccc2)N1	107
61	297	COc1cccc(C2c3ccccc3CCN2CCC(=O)NO)c1	110
62	302	Cc1ccc(C(=O)NO)cc1C(=O)Nc1ccc(Cl)cc1	111.9821
63	307	O=C(NO)c1ccc(CC(=O)N2CCC(N3CC(c4ccccc4)(c4ccccc4)C3=O)CC2)cc1	113
64	312	C[C@@H](N)C(=O)NCc1nnc(-c2ccc(F)cc2)o1	116
65	317	O=C(CCCCCCC(=O)Nc1cc(C(F)(F)F)ccc1Cl)NO	119
66	322	O=C(NO)c1ccc(Cl)c(NC(=O)c2ccccc2)c1	120
67	327	CCN1CCC[C@@H](n2c(-c3cccc(/C=C/C(=O)NO)c3)nc3ccccc32)C1	120
68	332	O=C(CCCCC[C@H](NC(=O)C1C(=O)NCC1c1ccccc1)C(=O)Nc1ccccc1)NO	123
69	2039	C[C@@H](N)C(=O)NCc1nnc(-c2ccc([N+](=O)[O-])cc2)o1	127
70	337	S=C1Sc2cccc(Cl)c2C2=NCCCN12	130
71	342	CCC(CCCC(=O)Nc1ccccc1)CCC(=O)NO	130
72	347	O=C(CCCCC[C@H](NC(=O)[C@@H]1CCCC(=O)N1)C(=O)NCCc1ccccc1)NO	131
73	352	CCC(=O)CCCCC[C@@H]1NC(=O)[C@H]2CCCCN2C(=O)[C@H]([C@H](C)CC)NC(=O)[C@H](Cc2cn(OC)c3ccccc23)NC1=O	134
74	357	CCc1ccc(C(=O)NO)cc1NCc1ccccc1	136
75	362	CC(C)(C)OC(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	140
76	367	COc1ccc(-c2nnc(CNC(=O)CN)o2)cc1	142
77	372	CC(C)(C)OC(=O)Nc1ccc(Cn2cc(NC(=O)CCCCCCC(=O)NO)cn2)cc1	147
78	377	CCOc1ccc(C(=O)NO)cc1NC(=O)c1ccc(-c2ccccc2)cc1	148.7
79	382	CCC(=O)CCCCC[C@@H]1NC(=O)[C@@H]2CCCN2C(=O)C[C@H](CC(C)C)NC(=O)[C@H](Cc2c[nH]c3ccccc23)NC1=O	150
80	387	O=C(NO)c1ccc(NC2CCN(c3ccccc3Cl)C2=O)cc1	150
81	392	COc1ccc(C(=O)NO)cc1NCCc1ccccc1	151
82	397	NCC(=O)NCc1nnc(-c2ccccc2)o1	155

83	402	Cc1ccc(-c2cc(C(F)(F)F)c(C#N)c(SCCC#N)n2)o1	159
84	407	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1cccc(Cl)c1)CC2	160
85	412	Cc1ccc(C(=O)NO)cc1NCc1ccc(Cl)cc1	161
86	417	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)c2ccccc2)cc1	164
87	422	CCCN1CC(=O)N2[C@H](Cc3c(n(Cc4ccc(C(=O)NO)cc4)c4ccccc34)[C@@H]2C)C1=O	168
88	427	COc1cccc(CN2C(=O)CN(Cc3ccc(C(=O)NO)cc3)C(=O)[C@H]2Cc2ccccc2)c1	171
89	432	COc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)[C@H](Cc2ccc(O)cc2)NC(=O)OC(C)(C)C)cc1	175
90	437	O=C(/C=C/c1ccccc1Sc1ccc(Cl)cc1)NO	180
91	442	COc1ccc(C(=O)NO)cc1NC(=O)c1cccc2cccnc12	180
92	447	CN(Cc1ccc(C(=O)NO)cc1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	184
93	452	O=C(CCN1CCc2ccccc2C1c1ccc(C(F)(F)F)cc1)NO	190
94	457	O=C(NO)c1cccc(-c2cn(CSc3ccccc3)nn2)c1	194.9002
95	462	CC1(C)CC(=O)Nc2ccc(C(=O)NCc3cccc(/C=C/C(=O)NO)c3)cc21	200
96	467	O=C(/C=C/c1ccc(NS(=O)(=O)c2ccccc2)cc1)NO	200
97	472	CC[C@H](C)[C@H](NC(=O)[C@@H](NC(=O)OC(C)(C)C)C(C)C)C(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(OC)cc1	201
98	477	CN1C(=O)CCC[C@H]1C(=O)N[C@@H](CCCCCS)C(=O)Nc1ccccc1	202
99	482	N[C@H](Cc1ccc(Cl)cc1Cl)C(=O)N1Cc2ccccc2C1	206.6826
100	487	O=C(NO)c1ccc(CN2c3ccccc3NC(=O)[C@@H]2Cc2ccccc2)cc1	210
101	492	O=C(Cc1ccc(CCCCc2ccc3c(c2)OCO3)cc1)NO	210
102	497	O=C(COc1ccc(C[C@H](NC(=O)OCc2ccccc2)C(=O)Nc2cccc(Cl)c2)cc1)NO	213
103	502	COc1cccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@](O)(C(C)=O)C[C@@H]3O[C@H]1C[C@H](N)[C@H](O)[C@H](C)O1	220
104	507	COc1cccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@](O)(C(C)=O)C[C@@H]3O[C@H]1C[C@H](NCc2ccc(NC(=O)CCCCCCC(=O)NO)cc2)[C@H](O)[C@H](C)O1	220
105	512	Cc1ccc(-c2cc(C(F)(F)F)nn2-c2ccc(S(=O)(=O)NCCCCCC(=O)NO)cc2)cc1	226
106	517	O=C(NO)c1ccc(CNCc2nc(-c3ccc(F)cc3)no2)cc1	230
107	522	COc1cc(C(=O)NO)ccc1CS(=O)(=O)Nc1ccc2c(c1)cc(C)c(=O)n2C	231
108	527	CC(C)Cc1nc2cc(/C=C/C(=O)NO)ccc2n1CCCO	238
109	532	COc1ccc(C(=O)NO)cc1NC(C)c1ccc(Cl)cc1	240
110	537	Cc1cccc(CCNC(=O)CCCCCCS)c1	246
111	542	CCCNNC(=O)c1cnc(N2CCN(C)CC2)nc1	250
112	547	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(CCCCCC(=O)NO)c2c(=O)n1-c1ccccc1	253
113	552	CCN(CC)CCn1c(CCc2ccccc2)nc2cc(/C=C/C(=O)NO)ccc21	255
114	557	O=C(NO)c1ccc(NC2CCN(CCc3ccccc3)C2=O)cc1	260
115	562	CC(C)CCc1c(OCCCCCCCC(=O)NO)ccc(CCC(=O)NO)c1O	267.85
116	567	C#Cc1nc(/C=C/CCCCCC(=O)NO)cs1	270
117	572	O=C(NO)[C@]1(F)[C@H](c2ccccc2)[C@H]1c1ccc(-c2ncc(F)cn2)cc1	280
118	577	O=C(/C=C/c1ccc(C(=O)NC(Cc2c[nH]c3ccccc23)C(=O)Nc2cccc(Br)c2)cc1)NO	281.1
119	582	CC(C)c1cc(C(=O)N2CCc3cc(NC(=O)CCCCCCC(=O)NO)ccc32)c(O)cc1O	284
120	587	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CCc1ccccn1)NO	290
121	2044	O=C(/C=C/c1ccc(C(=O)NCCOc2no[n+]([O-])c2S(=O)(=O)c2ccccc2)cc1)NO	290
122	592	CN1c2ccc(/C=C/C(=O)NO)cc2NC1CCc1ccccc1	291
123	597	O=C(NO)c1ccc(-c2cccc3ccccc23)cc1	300
124	602	O=C(CCCCCCNC(=O)c1ncc(-c2ccc(Br)cc2)o1)NO	302.73

125	607	CC(CCCCCC(=O)NO)n1cc(-c2ncnc3[nH]ccc23)cn1	310
126	612	O=C(NO)c1ccc(CN(C2CC2)S(=O)(=O)c2c(F)cc(F)cc2F)cc1	315
127	617	COc1ccc(C(=O)NO)cc1NC(=O)c1cccc2c1oc1ccccc12	320
128	622	O=C(CCCCCCNC(=O)Cn1cnc2c(Nc3ccccc3)nc(Nc3ccccc3)nc21)NO	320
129	627	O=C(NO)c1ccc(/C=C/c2nc3ccccc3c(=O)[nH]2)cc1	325
130	632	O=C(NO)c1ccc(CN(Cc2ccccn2)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	332
131	637	Cc1ccc(NC(=O)CCCCCCC(=O)NO)cc1	336
132	642	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2cccc(n2)CNC(=O)C[C@@H](/C=C/CCS)OC1=O	341.3
133	647	Cc1ccc(-c2cc(C(=O)NCCCCCCC(=O)NO)nn2-c2ccc(S(C)(=O)=O)cc2)cc1	345
134	652	O=C(NO)c1ccc(CNCc2nc(-c3ccc(Cl)cc3)no2)cc1	350
135	657	Nc1ccccc1NC(=O)c1ccc(Cn2cnc3c(Nc4ccc(C(=O)NO)cc4)nc(Cl)nc32)cc1	352
136	662	O=C(NO)c1ccc(NC(=O)c2cccc(C(F)(F)F)c2)cc1	356.5782
137	667	Cc1cc2cc(NS(=O)(=O)Cc3ccc(C(=O)NO)cc3)ccc2n(C)c1=O	360
138	672	O=C(NO)c1ccc2c(c1)CC(NS(=O)(=O)c1cccnc1)CC2	370
139	677	O=C(CCCCCCC(=O)NCCc1ccccc1)NO	376
140	682	O=C(CCCC(CCC(=O)Nc1ccccc1)Cc1ccccc1)NO	380
141	687	COc1ccc(-c2nc(C(=O)NCCCC(=O)NO)cc3c2[nH]c2ccccc23)cc1	390
142	692	CN1CCCC1c1cn(Cc2ccc(C(=O)NO)cc2)c2ccccc12	398.11
143	697	O=C(NO)c1ccc(CN(CCO)C(=O)Cc2ccccc2)cc1	400
144	702	COc1ccc(-c2nc3cc(/C=C/C(=O)NO)ccc3n2CCO)cc1	401
145	707	O=C(NCC12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)c1ccc2c(ccn2Cc2ccc(C(=O)NO)c(Cl)c2)c1	410
146	712	Cc1ccc(-c2cc(C(F)(F)F)nn2-c2ccc(S(=O)(=O)NCCCCCCC(=O)NO)cc2)cc1	412
147	717	S=C1Sc2cccc(Br)c2C2=NCCN12	420
148	722	COc1cc2ccn(CCOc3cccc(NC(=O)CCCCCCC(=O)NO)c3)c2c(OC)c1OC	420.9
149	727	CCCCC(CCCC(=O)NO)CCC(=O)Nc1ccccc1	430
150	732	O=C(NO)c1ccc(CN2C(=O)CNC(=O)[C@H]2Cc2cccs2)cc1	440
151	737	N[C@@H](CCCCCC(=O)c1ccon1)c1cnn(-c2ccc(F)cc2)n1	445
152	742	O=C(/C=C/c1ccc2c(c1)nc(CCc1ccccc1)n2CC(O)CO)NO	454
153	747	N[C@@H](CCCCCC(=O)c1ccon1)c1cnn(-c2ccc(F)cc2)c1	466
154	752	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3cccnc3)n1)CN2	470
155	757	Cc1ccc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)cn1	480
156	762	CCN1CCC[C@@H](n2c(C)nc(C)c2-c2cccc(/C=C/C(=O)NO)c2)C1	500
157	767	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3cccnc3Cl)n1)CC2	510
158	772	O=C(CCCCCCC(=O)Nc1ccc(-c2cnnn2-c2ccccc2)cc1)NO	518
159	777	O=C1CN(Cc2ccc(C(=O)NO)cc2)c2ccccc2N1	520
160	782	O=C(Cc1ccc(CCCCc2cc(F)c(F)cc2F)cc1)NO	530
161	787	O=C(NO)c1ccc(Cn2ccc3cc(C(=O)NCC45C[C@H]6C[C@@H](C4)C[C@@H](C5)C6)ccc32)c(F)c1	540
162	792	COc1ccc(C(=O)NO)cc1NC(=O)c1ccc(Cl)cc1Cl	548.3
163	797	CC(C)CCc1c(OCCCCCCC(=O)NO)ccc2ccc(=O)oc12	553.45
164	802	COc1ccc2c(ccn2CCOc2ccc(NC(=O)CCCCCCC(=O)NO)cc2)c1	560.9
165	807	CS(=O)(=O)Nc1ccc(-c2ccnc(Nc3ccc(N4CCC(C(=O)NCCCCCCCCC(=O)NO)CC4)cc3)n2)cc1	572
166	812	O=C(NO)c1ccc(CN(Cc2ccncc2)S(=O)(=O)c2cc(F)c(F)c(F)c2F)cc1	581
167	817	CC1(Nc2ccc(C(=O)NO)cc2)CCN(c2ccccc2)C1=O	590
168	822	O=C(NO)c1ccc2c(c1)C(=O)c1ccccc1C2=O	599
169	827	CN(c1ccc(/C=C/C(=O)NO)cc1)S(=O)(=O)c1ccccc1	600
170	2049	O=C(CCCCCC(c1c[nH]c2ccc([N+](=O)[O-])cc12)c1c[nH]c2ccc([N+](=O)[O-])cc12)NO	600
171	832	COC(=O)c1ccc(CO/N=C/c2ccc(/C=C/C(=O)NO)cc2)cc1	603

172	837	O=C(NO)c1ccc(-c2ccnc(Nc3ccc(N4CCOCC4)cc3)n2)cc1	609
173	842	COc1cccc(-c2nc(NCc3ccc(/C=C/C(=O)NO)cc3)cc3c2[nH]c2ccccc23)c1	617
174	847	O=C(/C=C/c1cccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)c1)NO	630
175	852	CC12CC3CC(C)(C1)CC(NCc1ccc(NC(=O)CCCCCCC(=O)NO)cc1)(C3)C2	638
176	857	O=CN(O)CCCCCCCC(=O)Nc1cccc2ccccc12	650
177	862	C#Cc1nc(/C=C/C=C/C(=O)NO)cs1	670
178	867	O=C(NO)c1ccc(N(Cc2cccc(C(F)(F)F)c2)C(=O)c2cccc(C(F)(F)F)c2)cc1	686.3643
179	872	Cn1cccc1C(=O)NCc1ccc(C(=O)NO)cc1	690
180	877	CCCNNC(=O)c1ccc(-c2ccc(CNC(C)=O)cc2)cc1	700
181	882	CC[C@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)Cc3ccc(-c4cn(CCCCC(=O)NO)nn4)cc3)[C@H](C)O2)[C@H](C)[C@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)C)[C@@H]2O)[C@@](C)(O)C[C@H](C)CN(C)[C@@H](C)[C@H](O)[C@@]1(C)O	709
182	887	CC(C)c1cc(-n2nnc(C(=O)NCCCCCCC(=O)NO)c2-c2ccc(CN3CCOCC3)cc2)c(O)cc1O	717
183	892	O=C(NO)c1ccc2c(c1)CC(Nc1ncccn1)CC2	730
184	897	O=C(CCCCCCOc1ccc2cc1COC/C=C/COCc1cccc(c1)-c1ccnc(n1)N2)NO	740
185	902	CN1CC(NS(=O)(=O)c2ccc(Cl)cc2)Cc2cc(C(=O)NO)ccc21	750
186	907	O=C(CCCCCCc1nc(-c2ccccc2)no1)C(F)(F)F	760
187	912	O=C(C=C1c2ccccc2-c2ccccc21)NCCCCCC(=O)NO	779
188	917	COc1cc2c(cc1-c1c(C)noc1C)[nH]c1nc(C)nc(NCCCCCCC(=O)NO)c12	782
189	922	O=C(CCCCCCC(=O)Nc1ccc(-c2cnnn2Cc2ccccc2)cc1)NO	790
190	927	CN(C)Cc1nn(Cc2ccc(C(=O)NO)cc2)c2ccccc12	794.33
191	932	Cc1ccc(-c2ccc(Cn3cccc(O)c3=S)cc2)cc1	800
192	937	COc1ccc(C(=O)c2ccc3c(ccn3S(=O)(=O)c3cccc(/C=C/C(=O)NO)c3)c2)cc1	812
193	942	CN(C)CCCNC(=O)c1cc(NC(=O)c2cc(NC(=O)c3cc(NC(=O)c4nc(NC(=O)CCCNC(=O)c5cc(NC(=O)c6cc(NC(=O)c7cc(NC(=O)c8nc(NC(=O)CCNC(=O)CCNC(=O)c9ccc(NC(=O)CCCCCCC(=O)NO)cc9)cn8C)cn7C)cn6C)cn5C)cn4C)cn3C)cn2C)cn1C	820
194	947	FC(F)(F)c1ccc2c(c1)C1=NCCCN1C(=S)S2	830
195	952	O=C(CCCCCCn1cc(Nc2ncc(Cl)c(Nc3cccc(Cl)c3)n2)cn1)NO	840
196	957	CC(C)Cc1nc2cc(/C=C/C(=O)NO)ccc2n1Cc1ccccc1	846
197	962	O=C(NO)c1ccc(NC2CCN(c3ccc(Cl)cc3)C2)cc1	860
198	967	O=C(/C=C/c1ccc(S(=O)(=O)NCCCN2c3ccccc3CCc3ccc(Cl)cc32)cc1)NO	874
199	972	O=C(/C=C/c1ccc2c(c1)nc(-c1ccncc1)n2CCO)NO	883
200	977	O=C(Cc1ccc(NS(=O)(=O)c2ccccc2)cc1)NO	900
201	982	O=C(/C=C/c1ccc(CNCc2ccc3cccc(Cl)c3n2)cc1)NO	911
202	987	O=C(NO)c1ccc(CNC(=O)c2ccc(Cl)c(Cl)c2)cc1	920
203	992	CNc1ccc(C(=O)NO)cc1	940
204	997	O=C(CCN1CCc2ccccc2C1c1ccccc1)NO	950
205	1002	O=C(NO)c1cccc(Cn2c(=O)[nH]c(=O)c3cccc(Cl)c32)c1	966
206	1007	O=C(Cc1ccc2ccccc2c1)Nc1ccc(C(=O)NO)nc1	976
207	1012	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@H]2O[C@@H](C)C[C@@H](N(C)Cc3ccc(-c4cn(CCCC(=O)NO)nn4)cc3)[C@@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@H](O)[C@]1(C)O	986
208	1019	CCCC[C@H]1NC(=O)C[C@@H](/C=C/CCS)OC(=O)C[C@H](O)[C@@H]([C@@H](C)CC)NC(=O)[C@@H](CS)NC1=O	1000

209	1024	S=C1Sc2ccc(I)cc2C2=NCCN12	1000
210	1029	CCCNNC(=O)c1cnc(NCc2ccccc2)nc1	1000
211	1034	CNc1nc(Cl)nc2c1ncn2Cc1ccc(C(=O)Nc2ccccc2N)cc1	1020
212	1039	O=C(CCCCCCc1nc(-c2ccc(C(F)(F)F)cc2)no1)C(F)(F)F	1030
213	1044	[11CH3]n1cc(CCNCc2ccc(/C=C/C(=O)NO)cc2)c2ccccc21	1044
214	1049	Cc1nc2cccc(/C=C/C(=O)NO)c2c(=O)n1-c1ccccc1	1060
215	1054	O=C(NO)c1ccc(Cn2c(=O)n(CCc3ccccc3)c(=O)c3cccnc32)cc1	1068
216	1059	COc1cc(NC(=O)NOCCCCCC(=O)NO)c2ncccc2c1	1080
217	1064	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)C)[C@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	1090
218	1069	Cc1c(NC(=O)CN2C(=O)S/C(=C\c3ccc(Br)cc3)C2=O)c(=O)n(-c2ccccc2)n1C	1093
219	1074	S=C1Sc2cc(Br)ccc2C2=NCCCN12	1100
220	1079	C#CCN(C)CCCOc1cc(NC(=O)CCCCCCCC(=O)NO)ccc1Cl	1120
221	1084	CC(C)(C)OC(=O)NCCCC[C@@H]1C(=O)Nc2ccccc2N1Cc1ccc(C(=O)NO)cc1	1150
222	1089	C#CCN(C)CCCOc1cc(NCc2ccc(C(=O)NO)cc2)ccc1Cl	1170
223	1094	CCc1nc2cc(/C=C/C(=O)NO)ccc2c(=O)n1CCc1ccccc1	1180
224	1099	CC(C)(C)OC(=O)NCC(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	1190
225	1104	O=C(N[C@@H](C(=O)O)c1ccccc1)c1cccc(=S)n1O	1200
226	1109	CC(C)(C)OC(=O)Nc1cccc(C(=O)/C=C/c2ccc(/C=C/C(=O)NO)cc2)c1	1200
227	1114	CC(C)c1cc(C(=O)N2CCc3cc(NC(=O)CCCCCCCC(=O)NO)ccc32)c(O)cc1O	1220
228	1119	COc1ccc(-c2ccnc(NC3CCc4ccc(C(=O)NO)cc4C3)n2)c(OC)c1	1230
229	1124	COc1ccc(CN2CCC(Nc3nc(Nc4ccc(NC(=O)CCCCCCC(=O)NO)cc4)nc4cc(OC)c(OC)cc34)CC2)cc1	1260
230	1129	Cc1cc(C)cc(C(=O)NOCCCCCC(=O)NO)c1	1278
231	1134	CCCCCC(CCCCCC(=O)Nc1ccccc1)C(=O)NO	1300
232	1139	O=C(NCCS)/C(Cc1ccc(O)c(Br)c1)=N/O	1300
233	1144	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(-c3cc(CO)cc(CO)c3)nn2)c1)NO	1320
234	1149	C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@@]2(O)c1cn(CCCCCCC(=O)NO)nn1	1341.641
235	1154	CC(=O)NCCCC[C@@H]1NC(=O)C[C@H](Cc2ccc(O)cc2)NC(=O)[C@H](Cc2cccc3ccccc23)NC(=O)[C@H](CCCCCC(=O)O)NC1=O	1380
236	1159	Nc1ccccc1NC(=O)c1ccc(CNC2=NC[C@@H](c3ccccc3)S2)cc1	1400
237	1164	O=C(CCN(Cc1ccccc1)Cc1ccccc1)NO	1400
238	1169	O=C(CCCCCCC(=O)N/N=C/c1cnc(N(c2ccccc2)c2ccccc2)nc1)NO	1430
239	1174	CC[C@@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2C[C@](C)(OC)[C@H](O)[C@@H](C)O2)[C@@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3cccc(-c4cn(CCCCCCC(=O)NO)nn4)c3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	1440
240	1179	N#Cc1ccc(-c2cn(CCCCCn3cccc(O)c3=S)nn2)cc1	1465
241	1184	N#Cc1ccc2c(c1)CCCN2Cc1ccc(C(=O)NO)cc1	1490
242	1189	S=C1Sc2ccccc2C2=NCCCN12	1500
243	1194	Cc1nc(N(C)c2ccc(OCCCCCC(=O)NO)cc2)c2ccccc2n1	1510
244	1199	CCCNc1ccc2c3c(cccc13)C(=O)N(CCCCCC(=O)NO)C2=O	1520
245	1204	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(F)c(Cl)c1	1550
246	1209	Oc1cccn(Cc2cn(-c3ccccc3)nn2)c1=S	1570
247	1214	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-	1600

		c2ccc3nc(CC)ccc3c2)[nH]1	
248	1219	N[C@@H](Cc1ccccc1)C(=O)Nc1ccccc1-c1ccc(NC(=O)CCCCCCC(=O)NO)cc1	1600
249	1224	O=C(NO)c1ccc(-c2nc3ccccc3c(=O)[nH]2)cc1	1620
250	1229	Cc1ccc(NC(=O)[C@@H]2Cc3ccc(OCC(=O)NO)cc3CN2C(=O)OC(C)(C)C)cc1	1650
251	1234	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(C(F)(F)F)cc3)n1)CC2	1690
252	1239	O=C(CCCCCCNCc1ccc(F)cc1)NO	1700
253	1244	N#Cc1cccc(-c2ccc(Cn3cccc(O)c3=S)cc2)c1	1701
254	1249	COc1cc2c(cc1OC)C(=O)C(CC1CCN(S(=O)(=O)c3cccc(/C=C/C(=O)NO)c3)CC1)C2	1720
255	1254	CC[C@H](Nc1ncnc2[nH]cnc12)c1nc2cccc(NCCCC(=O)NO)c2c(=O)n1-c1ccccc1	1758
256	1259	C#CCN(C)CCCOc1cc(NC(=O)CCCCCCC(=O)NO)c(Cl)cc1Cl	1780
257	1264	C#Cc1nc(/C=C/C(=O)NO)cs1	1800
258	1269	O=C(CCCCCN1C(=O)c2cccc3c(N4CCOCC4)ccc(c23)C1=O)NO	1810
259	1274	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)Cc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc3)[C@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	1840
260	1279	CCc1nc2cc(Cl)c(/C=C/C(=O)NO)cc2c(=O)n1CCc1ccccc1	1880
261	1284	CC(C)(C)OC(=O)NCCC(=O)N1CC2(C[C@H]1C(=O)NCCCCCC(=O)NO)SCCS2	1900
262	2055	[C-]#[N+]c1ccccc1-c1ccc(Cn2cccc(O)c2=S)cc1	1907
263	1289	CC(C)C(c1ccc(C(=O)NO)cc1)C(C)C	1920
264	1294	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1nnc(-c2cc3ccccc3nc2OC)[nH]1	1931
265	1299	COc1cc(CNc2nc(NCc3ccc(C(=O)Nc4ccccc4N)cc3)nc3[nH]ccc23)cc(OC)c1	1950
266	1304	CC(C)(C)OC(=O)N1Cc2cc(OCC(=O)NO)ccc2C[C@H]1C(=O)Nc1ccc(-c2ccccc2)cc1	1980
267	1309	O=C(NO)c1ccc(CN2c3ccncc3Sc3ncccc32)cc1	2000
268	1314	O=C1Sc2ccccc2C2=NCCCN12	2000
269	1319	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CN(C)C2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	2024
270	1324	N[C@@H](Cc1ccc(O)cc1)C(=O)Nc1ccccc1-c1ccc(NC(=O)CCCCCCC(=O)NO)cc1	2060
271	1329	O=C(NO)c1ccc(CN2C(=O)CCc3cc(Cl)ccc32)cc1	2080
272	1334	O=C(NO)c1ccc(NCc2csc3ccc(Br)cc23)cc1	2100
273	1339	O=C(CCCCC[C@H](NC(=O)[C@@H]1CCCC(=O)N1)C(=O)NC1CCCC1)NO	2130
274	1344	CC1(C)c2ccccc2N(Cc2ccc(C(=O)NO)cc2)C1c1cccnc1	2170
275	1349	O=C(NCc1ccc(C(=O)Nc2ccccc2O)cc1)OCc1cccnc1	2200
276	1354	COc1cc(-c2ncc(/C=C/C(=O)NO)s2)cc(OC)c1OC	2220
277	1359	O=C(NO)c1ccc2c(c1)CC(Nc1nccc(-c3ccc(F)c(Cl)c3)n1)CC2	2240
278	1364	S=C1Sc2cccc(I)c2C2=NCCN12	2300
279	1369	CCC(=O)CCCCC[C@H](NC(=O)[C@@H]1CCC12CCN(CC)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	2328
280	1374	CCCNNC(=O)c1ccc(Nc2ccccc2)cc1	2352
281	1379	O=C(NO)c1ccc(C(c2ccccc2)c2ccccc2)cc1	2380
282	2060	O=C(CCCCCCc1nc(-c2cccc([N+](=O)[O-])c2)no1)NO	2380
283	1384	O=C(/C=C/C=C/c1csc(Br)n1)NO	2400
284	1389	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccccc3-	2450

		c3cn(CCCCCCC(=O)NO)nn3)[C@H]2O)[C@@](C)(OC)C[C@@H](C)C2=NCCN3C(=O)O[C@@]1(C)[C@H]3[C@H]2C	
285	1394	C#CCN(C)CCCOc1cc(NC(=O)CCCCCCCCC(=O)NO)ccc1Cl	2480
286	1399	Cc1ccc2c(=O)n(CCc3ccccc3)c(=O)n(Cc3ccc(C(=O)NO)cc3)c2c1	2521
287	1404	COc1ccc(-c2ncc(/C=C/C(=O)NO)s2)c(OC)c1OC	2560
288	1409	CCc1c2c(nc3ccc(OCc4cn(CCCCCCCC(=O)NO)nn4)cc13)-c1cc3c(c(=O)n1C2)COC(=O)[C@]3(O)CC	2599
289	1414	O=C(NO)c1ccc2c(c1)CC(NC(=O)c1cccc(C(F)(F)F)c1)CN2	2670
290	1419	CC(C)C[C@H]1CC(=O)N[C@@H](C)C(=O)N[C@@H](CCCCCC(N)=O)C(=O)N[C@@H](Cc2c[nH]c3ccccc23)C(=O)N1	2700
291	1424	O=C(CCCCCCC(=O)Nc1cccc(-n2cc(C3CCCCC3)nn2)c1)NO	2750
292	1429	O=C(CCCCCCC(=O)Nc1cccc(-c2cn(-c3ccccc3)nn2)c1)NO	2780
293	1434	O=C(NO)c1ccc(Cn2c3c(c4cc(F)ccc42)CSCC3)cc1	2800
294	1439	COc1cccc(C(=O)NC2CNc3ccc(C(=O)NO)cc3C2)c1	2810
295	1444	Nc1ccc(-c2cc(C(=O)NCCCCC(=O)NO)no2)cc1	2830
296	1449	CCC(=O)CCCCC[C@H](NC(=O)C1=NOC2(CCN(C)CC2)C1)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	2885
297	1454	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2ccc3ccncc3c2)[nH]1	2900
298	1459	CC(C)c1cc(C(=O)N2CCc3cc(NC(=O)CCCCC(=O)NO)ccc32)c(O)cc1O	2940
299	1464	CCCNNC(=O)c1ccc(NC(=O)Cc2ccccc2)cc1	2991
300	1469	CCCCCNC(=O)[C@@H]1Cc2ccc(OCC(=O)NO)cc2CN1C(=O)OC(C)(C)C	3020
301	1474	O=C(NO)c1ccc(CCN2C(=O)c3cccc4c(N5CCOCC5)ccc(c34)C2=O)cc1	3050
302	1479	O=C(NO)c1ccc(CN2c3ccccc3Sc3cccnc32)cc1	3100
303	1484	O=C(CCCCOc1cccc(-c2nnc(-c3ccccc3)s2)c1)NO	3112
304	2065	O=C(CCCCCCc1nc(-c2ccc([N+](=O)[O-])cc2)no1)C(F)(F)F	3170
305	1489	Cc1ccc(-c2noc(CCCCCCC(=O)C(F)(F)F)n2)cc1	3190
306	1494	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@@H]2C[C@](C)(OC)[C@@](O)(CN(C)C)[C@@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	3200
307	1499	CC(C)(C)Oc1ccc(C[C@@H]2N=C(c3ccccc3)c3ccccc3N(CCCCC(=O)NO)C2=O)cc1	3300
308	1504	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1C[C@@]12CCN(C)C2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	3309
309	1509	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	3379
310	1514	CC(C)c1cc(C(=O)N(C)c2ccc(NC(=O)CCCCCCCC(=O)NO)cc2)c(O)cc1O	3410
311	1519	CC(C)[C@@H]1NC(=O)[C@]2(C)CSC(=N2)c2csc(n2)CNC(=O)C[C@@H](/C=C/CCC(=O)NO)OC1=O	3500
312	1524	C/C=C1\NC(=O)c2csc(n2)CNC(=O)C[C@@H](/C=C/CCS)OC(=O)[C@H](C(C)C)NC1=O	3550
313	1529	CS(=O)(=O)N[C@@H](Cc1ccc(OCc2ccccc2)cc1)C(=O)NO	3600
314	1534	O=C(CCCCCCc1nc(-c2ccccc2Cl)no1)NO	3650
315	1539	O=C(CCCCCNC(=O)c1cc(-c2ccc(F)cc2)[nH]n1)NO	3710
316	1544	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(O)C[C@@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O	3740
317	1549	COc1ccc(CC(=O)N[C@@H](CCC(=O)O)C(=O)NCc2ccccc2)cc1	3800
318	1554	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)/C=C/C(=O)NO)cc3)n2)cc(OC)c1OC	3900
319	1559	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-c2cc3ccccc3nc2OC)[nH]1	3978

320	1564	O=C(NO)c1ccc(-c2cn(CC34CC5CC(CC(C5)C3)C4)nn2)s1	4000
321	1569	CNc1nc(Nc2cnn(CCCCCCC(=O)NO)c2)ncc1Cl	4070
322	1574	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@@H](c3ccccc3)CS2)cc1	4100
323	1579	O=C(CCCCCCC(=O)Nc1cccc(-n2cc(-c3ccccc3)nn2)c1)NO	4180
324	1584	O=C(NO)C1[C@H](c2ccccc2)[C@H]1c1ccccc1	4300
325	1589	CC[C@H]1OC(=O)[C@H](C)[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)Cc3ccc(-c4cn(CCCCCCCC(=O)NO)nn4)cc3)[C@H]2O)[C@](C)(OC)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O	4420
326	1594	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3c(c2)C2CCC3C2)[nH]1	4527
327	1599	O=C(NO)c1ccc(/C=C/c2ccnc(-c3ccccc3O)c2)cc1	4620
328	1604	O=C(NO)[C@@H]1[C@H](c2ccccc2)[C@H]1c1ccnc(C2CC2)c1	4800
329	1609	O=C(CCCCc1ccn(Cc2ccc(-n3ccc4ccccc43)cc2)n1)NO	4918
330	1614	COc1nc2ccccc2cc1-c1cnc([C@@H](N)CCCCCC(=O)c2cnoc2C)[nH]1	5000
331	1619	Nc1ccccc1NC(=O)c1ccc(CSC2=N[C@@H](c3ccccc3)CS2)cc1	5160
332	1624	O=C(CCCCc1ccn(Cc2ccc(-c3ccccc3)cc2)n1)NO	5238
333	1629	CCC(=O)CCCCCC(NC(=O)c1cncs1)c1[nH]c(-c2ccccc2)nc1C(=O)NCCN(C)C	5335
334	1634	O=C(CCCCCCN(Cc1ccc2ccccc2c1)Cc1ccc2ccccc2c1)NO	5400
335	1639	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc(-c3cccnc3)cc2)[nH]1	5500
336	1644	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3c(=O)n(C)ccc3c2)[nH]1	5600
337	1649	CC(C)(C)OC(=O)Nc1cccc(-c2cc(C(=O)NCCCCC(=O)NO)no2)c1	5810
338	1654	O=C(CCCCCCC(=O)NC[C@H]1O[C@@H]2O[C@H]3[C@H](O)[C@@H](O)[C@@H](O[C@H]4[C@H](O)[C@@H](O)[C@@H](O[C@H]5[C@H](O)[C@@H](O)[C@@H](O[C@H]6[C@H](O)[C@@H](O)[C@@H](O[C@H]7[C@H](O)[C@@H](O)[C@@H](O[C@H]8[C@H](O)[C@@H](O)[C@@H](O[C@H]1[C@H](O)[C@H]2O)O[C@@H]8CO)O[C@@H]7CO)O[C@@H]6CO)O[C@@H]5CO)O[C@@H]4CO)O[C@@H]3CO)NO	6000
339	1659	CS(=O)(=O)Nc1ccc(-c2ccnc(Nc3ccc(N4CCC(C(=O)Nc5ccc(/C=C/C(=O)NO)cc5)CC4)cc3)n2)cc1	6065
340	1664	C=C(c1cc(OC)c(OC)c(OC)c1)c1ccc2c(c1)cc(/C=C/C(=O)NO)n2C	6200
341	1669	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1[nH]c(-c2ccc(F)cc2)nc1C(N)=O	6364
342	1674	O=C(COc1ccc2cc(/C=C3/SC(=O)NC3=O)ccc2c1)Nc1ccc(F)cc1	6600
343	1679	O=C(NO)c1ccc(CN2c3ccccc3C[C@@H]3CCCCC[C@H]32)cc1	6700
344	1684	O=C(CCCCN1C(=O)CN=C(c2ccccc2)c2ccccc21)NO	6720
345	1689	Cc1[nH]c2cc(O)ccc2c1CCNCc1ccc(/C=C/C(N)=O)cc1	6800
346	1694	O=C(/C=C/c1ccc(-c2ccc(O)c(C34CC5CC(CC(C5)C3)C4)c2)cc1)NO	6960
347	1699	Cn1c(SCCCCCC(=O)NO)nnc1-c1ccncc1	7100
348	1704	O=C(COc1ccc2cc(/C=C3/SC(=O)NC3=O)ccc2c1)Nc1cccc(F)n1	7200
349	2070	[N-]=[N+]=NCc1cc(COc2ccc(NC(=O)CCCCCCC(=O)NO)cc2)cc(N=[N+]=[N-])c1	7340
350	1709	Cc1cc(C)cc(C(=O)N(CCCCCC(=O)NO)CC(=O)NC2CCCCC2)c1	7400
351	1714	COc1cc(C(=O)c2csc(-c3ccc(OCCCCCCCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	7490
352	1719	COc1cccc(NC(=O)COc2ccc3cc(/C=C4/SC(=O)NC4=O)ccc3c2)c1	7600
353	1724	COc1ccc(Oc2ccc3nc(/C=C/C(=O)NO)ccc3c2)cc1	7750
354	1729	O=C(CCCCCONC(=O)c1cnc2ccccc2n1)NO	7950
355	1734	Nc1ccccc1NC(=O)c1ccc(CNC2=NC[C@H](c3ccccc3)O2)cc1	8100

356	1739	CN(c1ccc(C(=O)NO)cc1)C1CCN(c2ccccc2)C1=O	8200
357	1744	Cc1ccc(-c2noc(CCCCCCC(=O)Nc3ccccc3N)n2)cc1	8390
358	1749	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCCCCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	8500
359	1754	COc1cc(C(=O)c2csc(-c3ccc(NC(=O)CCCCC(=O)Nc4ccccc4N)cc3)n2)cc(OC)c1OC	8740
360	1759	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3nn(C)cc3c2)[nH]1	8900
361	1764	O=C(NO)[C@H](Cc1ccccc1)n1nnc(-c2ccccc2)c1C#Cc1ccc(-c2ccccc2)cc1	9100
362	1769	CN(C)c1ccc(C(=O)N(CC(=O)NCc2ccccc2)Cc2ccc(C(=O)Nc3ccccc3N)cc2)cc1	9210
363	1774	Nc1nc2ncc(CNc3ccc(C(=O)NCCCCCCCC(=O)NO)cc3)nc2c(=O)[nH]1	9380
364	1779	CS(=O)(=O)N[C@@H](Cc1ccc(OCCc2ccccc2)cc1)C(=O)NO	9500
365	1784	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc(-c3cccnc3)cc2)o1	9700
366	1789	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccc3nc(C)ccc3c2)nc1C#N	9835
367	1794	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccccc4)CC3c3ccc(Cl)c(Cl)c3)cc2)S1	10000
368	1799	CC[C@@H]1OC(=O)[C@@H](C)[C@H](O[C@H]2C[C@@](C)(OC)[C@](O)(CN(C)Cc3ccc(-c4cn(CCC(=O)NO)nn4)cc3)[C@H](C)O2)[C@H](C)[C@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@](C)(OC)C[C@H](C)C(=O)[C@@H](C)[C@@H](O)[C@@]1(C)O	10200
369	1804	Cc1ccc(C(=O)NCCCCCC(=O)Nc2ccccc2N)cc1	10700
370	1809	O=C(CCCCCCNC(=O)C(O)(O)C(F)(F)F)Nc1ccc(Br)cc1	11000
371	1814	CC(=O)c1cc(/C=C/C(=O)NO)n(C)c1	11250
372	1819	O=C(CS)NCCCCCn1ccc2cc(Cl)c(Cl)cc21	11849.05
373	1824	O=C(NO)c1csc(-c2ccccc2)n1	12120
374	1829	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1[nH]c(-c2ccc3nn(C)cc3c2)nc1C#N	12420
375	1834	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@H](Cc3ccccc3)CS2)cc1	12700
376	1839	S=C1Sc2ccc(Cl)cc2C2=NCCN12	13000
377	1844	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(C)CC2)c1ncc(-c2ccc3nnccc3c2)[nH]1	13000
378	1849	O=C(NO)c1cccc2ccccc12	14000
379	1854	CCCCCCCC(=O)SCC/C=C/[C@@H]1CC(=O)N[C@H](C(C)C)C(=O)N[C@H](C)C(=O)N[C@H](C(C)C)C(=O)NCC(=O)O1	14300
380	1859	CCC(=O)CCCCC[C@H](NC(=O)C1CN(C)C1)c1ncc(-c2ccccc2)[nH]1	14950
381	1864	CC12CC3CC(C)(C1)CC(NCc1ccc(NCc4ccc(C(=O)NO)cc4)cc1)(C3)C2	15300
382	1869	O=C(NO)c1cnc(NC2(c3ccccc3)CCC(F)(F)CC2)nc1	16000
383	1874	C[C@H]1CN(c2ccc(C(=O)Nc3ccccc3N)cn2)CCN1C(=O)OCc1ccccc1	16720
384	1879	CC(CCc1ccc(NS(=O)(=O)c2ccccc2)cc1)CC(=O)NO	17000
385	1884	CN(C)c1ccc(C(=O)NCCCCCCNC(=O)CS)cc1	19100
386	1889	CC(C)[C@@H]1N=C(c2ccccc2)c2ccccc2N(CCCCC(=O)NO)C1=O	19830
387	1894	O=C(NO)c1noc(-c2ccc(Br)cc2)n1	20040
388	1899	O=C(CCCCCCNC(=O)C(O)(O)C(F)(F)F)Nc1ncc(-c2ccccc2)s1	21000
389	1904	CC(C)(C)OC(=O)NCCCC[C@@H]1N=C(c2ccccc2)c2ccccc2N(CCCCC(=O)NO)C1=O	21790
390	1909	O=C(NO)c1ccc(NC2CCN(c3ccc(Cl)cc3)C2=O)c(Cl)c1	22400
391	1914	C[C@@]12Nc3ccccc3[C@]1(O)CCN2Cc1ccc(/C=C/C(N)=O)cc1	23000
392	1919	C[C@H](NS(=O)(=O)c1cccc(C(=O)NO)c1)C(=O)Nc1ccccc1	24200
393	1924	CCCC(=O)NO	26000
394	1929	CCC(=O)CCCCC[C@H](NC(=O)[C@H]1CC12CCN(CC)CC2)c1ncc(-	27000

		c2cc3cn(C)nc3cc2OC)o1	
395	1934	O=C(NO)c1ccc(NC(=S)N/N=C/c2ccccc2)cc1	27600
396	1939	O=C1NC(=O)/C(=C\c2ccc(OCC(=O)N3N=C(c4ccccc4)CC3c3ccccc3Cl)cc2)S1	29000
397	1944	Cn1c(SCc2ccc(C(=O)NO)cc2)nnc1-c1ccncc1	29760
398	1949	COc1ccc(-c2ccc(/C=C/C=C/C(=O)NO)cc2)cc1C12CC3CC(CC(C3)C1)C2	30600
399	1954	Cc1ccc(C2CC(c3ccccc3)=NN2C(=O)COc2ccc(/C=C3/SC(=O)NC3=O)cc2)cc1	31000
400	1959	Cc1ccc(-c2nc(C(=O)NO)co2)cc1	33890
401	1964	O=C(NO)c1csc(Cc2ccccc2)n1	35000
402	1969	CC(=O)N[C@@H](Cc1ccc(OCc2ccccc2)cc1)C(=O)O	36900
403	2075	COC(=O)CCCCCCC(=O)Nc1ccc(OCc2cc(CN=[N+]=[N-])cc(N=[N+]=[N-])c2)cc1	37400
404	1974	CCCC(CCC)C(=O)NO	39000
405	1979	Cc1ccc(S(=O)(=O)N[C@@H](Cc2ccc(OCc3ccccc3)cc2)C(=O)NO)cc1	42400
406	1984	COc1ccc(NC(=O)c2ccc(CNC(=O)OCc3cccnc3)cc2)c(N)c1	44000
407	1989	COc1ccc(NC(=O)CCCCCCNC(=O)C(O)(O)C(F)(F)F)cc1	51000
408	1994	Cc1cc(C)cc(COc2ccc(NC(=O)CCCCCCC(=O)OC(C)(C)C)cc2)c1	53200
409	1999	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@@H](Cc3ccccc3)CO2)cc1	63000
410	2004	Nc1ccccc1NC(=O)CCCc1ccc(N(CCCl)CCCl)cc1	75200
411	2009	Nc1ccccc1NC(=O)c1ccc(CNC2=NC(c3ccc(C(F)(F)F)cc3)CO2)cc1	82100
412	2014	O=C(O)CCCc1ccccc1	93000
413	2019	Nc1ccccc1NC(=O)c1ccc(CNC2=N[C@@H](c3cccnc3)CO2)cc1	111000
414	2024	CCCC(CCC)C(=O)O	137778.4
415	2029	Cc1ccc(S(=O)(=O)N[C@@H](Cc2ccc(OCc3ccccc3)cc2)C(=O)O)cc1	504700

Table S3. Results obtained from the training set of the HDAC8 inhibitors dataset in Recursive Partitioning

Model Information	Confusion Matrix			ROC Score	ROC_{Cv}
Tree 1: 69 leaves Error Rate (training data): 302.93 Min alpha: 0	Actual\Pred.	0	1	**0.90090**	0.77924
	0	663	170		
	1	133	697		
Tree 2: 52 leaves Error Rate (training data): 304.92 Min alpha: 0.8932	Actual\Pred.	0	1	0.88141	0.77198
	0	659	174		
	1	131	699		
Tree 3: 43 leaves Error Rate (training data): 316.98 Min alpha: 1.786	Actual\Pred.	0	1	0.86312	0.76575
	0	668	165		
	1	152	678		
Tree 4: 36 leaves Error Rate (training data): 330.89 Min alpha: 2.68	Actual\Pred.	0	1	0.84745	0.76449
	0	637	196		
	1	135	695		
Tree 5: 32 leaves Error Rate (training data): 343.9 Min alpha: 3.573	Actual\Pred.	0	1	0.84011	0.76600
	0	634	199		
	1	145	685		
Tree 6: 24 leaves Error Rate (training data): 375.87 Min alpha: 4.466	Actual\Pred.	0	1	0.81796	0.75234
	0	608	225		
	1	151	679		
Tree 7: 18 leaves Error Rate (training data): 406.83 Min alpha: 5.359	Actual\Pred.	0	1	0.79665	0. 75245
	0	583	250		
	1	157	673		
Tree 8: 14 leaves	Actual\Pred.	0	1		

Error Rate (training data): 429.83 Min alpha: 6.252	0	571	262	0.77584	0.74802
	1	168	662		
Tree 9: 13 leaves Error Rate (training data): 438.79 Min alpha: 10.72	Actual\Pred.	0	1	0.77302	0.71599
	0	556	277		
	1	162	668		
Tree 10: 6 leaves Error Rate (training data): 515.5 alpha: 11.61	Actual\Pred.	0	1	0.69954	0.67090
	0	435	398		
	1	118	712		
Tree 11: 5 leaves Error Rate (training data): 531.46 Min alpha: 17.86	Actual\Pred.	0	1	0.68915	0.66136
	0	418	415		
	1	117	713		
Tree 12: 4 leaves Error Rate (training data): 550.53 Min alpha: 21.44	Actual\Pred.	0	1	0.67382	0.66136
	0	428	405		
	1	146	684		
Tree 13: 3 leaves Error Rate (training data): 582.37 Min alpha: 32.16	Actual\Pred.	0	1	0.65173	0.63892
	0	365	468		
	1	115	715		
Tree 14: 2 leaves Error Rate (training data): 616.29 Min alpha: 35.73	Actual\Pred.	0	1	0.62941	0.63892
	0	326	507		
	1	110	720		

Table S4. Results obtained from the test set of the HDAC8 inhibitors dataset in Recursive Partitioning

Confusion Matrix			ROC Score	ROC Rating
Actual\Pred.	0	1	0.83877	Quality 0.839: Good
0	145	63		
1	39	168		

Actual\Pred.	0	1
0	149	59
1	37	170

0.81861 Quality 0.819: Good

Actual\Pred.	0	1
0	153	55
1	40	167

0.80451 Quality 0.805: Good

Actual\Pred.	0	1
0	146	62
1	36	171

0.80111 Quality 0.801: Good

Actual\Pred.	0	1
0	145	63
1	40	167

0.79872 Quality 0.799: Fair

Actual\Pred.	0	1
0	144	64
1	44	163

0.78472 Quality 0.785: Fair

Actual\Pred.	0	1
0	136	72
1	40	167

0.76813 Quality 0.768: Fair

Actual\Pred.	0	1
0	134	74
1	39	168

0.75116 Quality 0.751: Fair

Actual\Pred.	0	1
0	131	77
1	38	169

0.74925 Quality 0.749: Fair

Actual\Pred.	0	1
0	110	98
1	29	178

0.69714 Quality 0.697: Poor

Actual\Pred.	0	1
0	106	102
1	29	178

0.68645 Quality 0.686: Poor

Actual\Pred.	0	1
0	109	99
1	35	172

0.67823 Quality 0.678: Poor

Actual\Pred.	0	1
0	97	111
1	32	175

0.65771 Quality 0.658: Poor

Actual\Pred.	0	1
0	86	122
1	30	177

0.63427 Quality 0.634: Poor

Table S5. Statistical results for the RP model training set

Tree No: Depth:	ROC_{CV}	ROC	TP	FP	TN	FN	Acc	Pr	Se	Sp	F1	AUC_b	γ	$\rho+$	$\rho-$

Leaves		Score													
1:20:69	**0.779**	**0.901**	**697**	**170**	**663**	**133**	**0.818**	**0.804**	**0.840**	**0.796**	**0.821**	**0.818**	**0.636**	**4.115**	**0.201**
2:19:52	0. 772	0. 880	699	174	659	131	0.817	0.801	0.842	0.791	0.821	0.817	0.633	4.032	0.200
3:19:43	0. 766	0. 863	678	165	668	152	0.809	0.804	0.817	0.802	0.811	0.809	0.619	4.124	0.228
4:15:36	0. 764	0. 847	695	196	637	135	0.801	0.780	0.837	0.765	0.808	0.801	0.602	3.559	0.213
5:15:32	0. 766	0. 840	685	199	634	145	0.793	0.775	0.825	0.761	0.799	0.793	0.586	3.455	0.230
6:14:24	0. 752	0. 818	679	225	608	151	0.773	0.751	0.818	0.730	0.783	0.774	0.548	3.029	0.249
7:12:18	0. 752	0. 797	673	250	583	157	0.755	0.729	0.811	0700	0.768	0.755	0.511	2.702	0.270
8:12:14	0. 748	0. 776	662	262	571	168	0.741	0.717	0.798	0.685	0.755	0.742	0.483	2.536	0.295
9:11:13	0. 716	0. 773	668	277	556	162	0.736	0.707	0.805	0.668	0.753	0.736	0.472	2.420	0.292
10:4:6	0. 671	0. 699	712	398	435	118	0.690	0.641	0.858	0.522	0.734	0.690	0.380	1.795	0.272
11:3:5	0. 661	0. 689	713	415	418	117	0.680	0.632	0.859	0.502	0.729	0.680	0.361	1.724	0.281
12:3:4	0. 661	0. 674	684	405	428	146	0.669	0.628	0.824	0.514	0.713	0.669	0.338	1.695	0.342
13:2:3	0. 639	0. 652	715	468	365	115	0.649	0.604	0.862	0.438	0.710	0.650	0.300	1.533	0.316
14:1:2	0. 638	0. 629	720	507	326	110	0.629	0.587	0.868	0.391	0.700	0.629	0.259	1.425	0.337

Table S6. Statistical results for the RP model test set

Tree No: Depth: Leaves	***ROC* Score**	***TP***	***FP***	***TN***	***FN***	***Acc***	***Pr***	***Se***	***Sp***	***F1***	Auc_b	γ	$\rho+$	$\rho-$
1:20:69	**0.839**	**168**	**63**	**145**	**39**	**0.754**	**0.727**	**0.812**	**0.697**	**0.767**	**0.754**	**0.508**	**2.680**	**0.270**
2:19:52	0.819	170	59	149	37	0.769	0.742	0.821	0.716	0.780	0.769	0.538	2.896	0.250
3:19:43	0.804	167	55	153	40	0.771	0.752	0.807	0.736	0.779	0.771	0.542	3.051	0.263
4:15:36	0.801	171	62	146	36	0.764	0.734	0.826	0.702	0.777	0.764	0.528	2.771	0.2478
5:15:32	0.799	167	63	145	40	0.752	0.726	0.807	0.697	0.764	0.752	0.504	2.664	0.277
6:14:24	0.789	163	64	144	44	0.740	0.718	0.787	0.692	0.751	0.740	0.480	2.560	0.307
7:12:18	0.768	167	72	136	40	0.730	0.699	0.807	0.654	0.749	0.730	0.461	2.331	0.296
8:12:14	0.751	168	74	134	39	0.728	0.694	0.812	0.644	0.748	0.727	0.456	2.281	0.292
9:11:13	0.749	169	77	131	38	0.723	0.687	0.816	0.630	0.746	0.723	0.446	2.205	0.291
10:4:6	0.697	178	98	110	29	0.694	0.645	0.860	0.529	0.737	0.694	0.389	1.825	0.265
11:3:5	0.686	178	102	106	29	0.684	0.636	0.860	0.510	0.731	0.685	0.370	1.754	0.275
12:3:4	0.678	172	99	109	35	0.677	0.635	0.831	0.524	0.720	0.678	0.355	1.746	0.323
13:2:3	0.659	175	111	97	32	0.655	0.612	0.845	0.466	0.710	0.656	0.312	1.585	0.331
14:1:2	0.634	177	122	86	30	0.634	0.592	0.855	0.413	0.700	0.634	0.269	1.46	0.351

Table S7. Docking scores of the designed molecules (**M1**-**M12**)

COMPOUNDS	**FEATURES**	**DOCKING SCORES**
M1	Bayesian Fingerprints: G4,G6, G10, G11	-5.64
M2	Bayesian Fingerprint: G7	-6.30
M3	Bayesian Fingerprints: G8, G9	-2.04
M4	Bayesian Fingerprints: G12, G13	-5.85
M5	Bayesian Fingerprint: G14	-5.68
M6	Bayesian Fingerprint: G19	-7.41
M7	RP fingerprint: RP-2	-5.92
M8	RP fingerprint: RP-8	-6.10
M9	RP fingerprints: RP-19, RP-46	-6.19
M10	RP fingerprint: RP-29	**-7.97**
M11	RP fingerprint: RP-44	-4.54
M12	RP fingerprint: RP-29, Machine learning: SMR_VSA_3; CSN Analysis	**-8.56**

Table S8. Cytotoxicity profiles of reported selective HDAC8 inhibitors in different cancer cell lines

Reported selective HDAC8 inhibitors	Cytotoxicity		Journal	References
	Cell lines	IC_{50} (μM)		
16b	**A549**	7.1	*J. Med Chem. 2023*	Huang *et al*., 2023 [15]
16c		12.5		
16e (SZUH280)		9.6		
PCI-34051		15.8		
PCI-34051	**A549**	>33.3	*J. Med Chem. 2024*	Zhao *et al*., 2024 [16]
	HCT116	21.9±2.8		
NC-Z16	**A549**	32.9±0.4	*J. Med Chem. 2024*	Zhao *et al*., 2024 [16]
	HCT116	30.1±8.6		
Compound (**6c**)	**A549**	7.1	*Current study*	

Table S9. Docking scores of the synthesized molecules (**6a**-**6l**)

COMPOUNDS	DOCKING SCORES
6a	-7.97
6b	-8.56
6c	**-9.02**
6d	-7.49
6e	-7.40
6f	-6.48
6g	-8.14
6h	-7.79
6i	-8.85
6j	-8.66
6k	-8.59
6l	-8.58

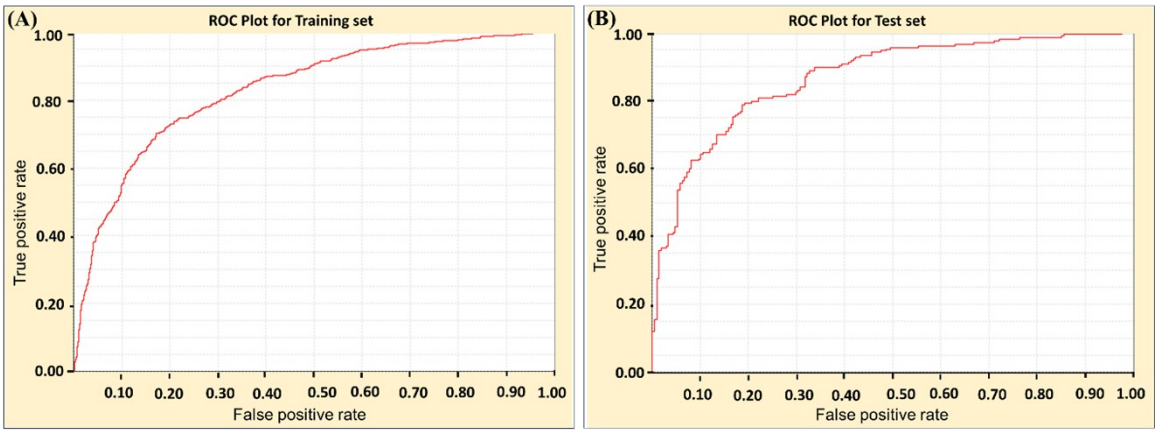


Fig. S1. (A) ROC plots illustrating the predictive performance of the Bayesian model for the A) Training set and (B) Test set, showing the relationship between sensitivity (true positive rate) and specificity (false positive rate) to evaluate the model's classification accuracy.

$$Accuracy\ (Acc) = \frac{TP + TN}{TP + TN + FP + FN} \quad (1)$$

$$Sensitivity\ (Se) = \frac{TP}{TP + FN};\ \begin{matrix} TP = Number\ of\ true\ positives \\ FN = Number\ of\ false\ negatives \end{matrix} \quad (2)$$

$$Specificity\ (Sp) = \frac{TN}{TN + FP};\ \begin{matrix} TN = Number\ of\ true\ negatives \\ FP = Number\ of\ false\ positives \end{matrix} \quad (4)$$

$$Precision\ (Pr) = \frac{TP}{TP + FP} \quad (4)$$

$$F1 = \frac{2TP}{2TP + FP + FN} \quad (5)$$

$$AUC_b = \frac{Se + Sp}{2} \quad (6)$$

$$\rho_+ = \frac{Se}{(1 - Sp)};\ \begin{matrix} where, \rho_+ > 1: Model\ is\ more\ likely\ to\ correctly\ identify\ positive\ instances \\ \rho_+ = 1: Model\ has\ no\ discriminatory\ power \\ \rho_+ < 1: Model\ is\ less\ likely\ to\ correctly\ identify\ positive\ instances \end{matrix} \quad (7)$$

$$\rho_- = \frac{(1 - Se)}{Sp};\ \begin{matrix} where, \rho_- < 1: Model\ is\ more\ likely\ to\ correctly\ identify\ negativce\ instances \\ \rho_- = 1: Model\ has\ no\ discriminatory\ power \\ \rho_- > 1: Model\ is\ less\ likely\ to\ correctly\ identify\ negative\ instances \end{matrix} \quad (8)$$

Fig. S2. Equations 1 to 8 used to calculate different statistical parameters for both training and test sets.

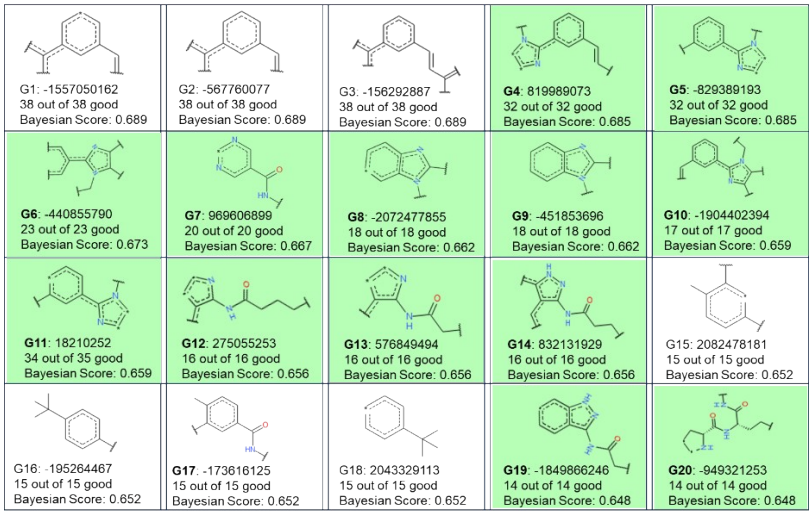


Figure S3. Favourable fingerprints associated with potent HDAC8 inhibition identified using Bayesian classification. The Bayesian score represents the frequency and significance of each structural feature within the dataset. Fingerprints shown in green correspond to fingerprints with nitrogen-containing ring system.

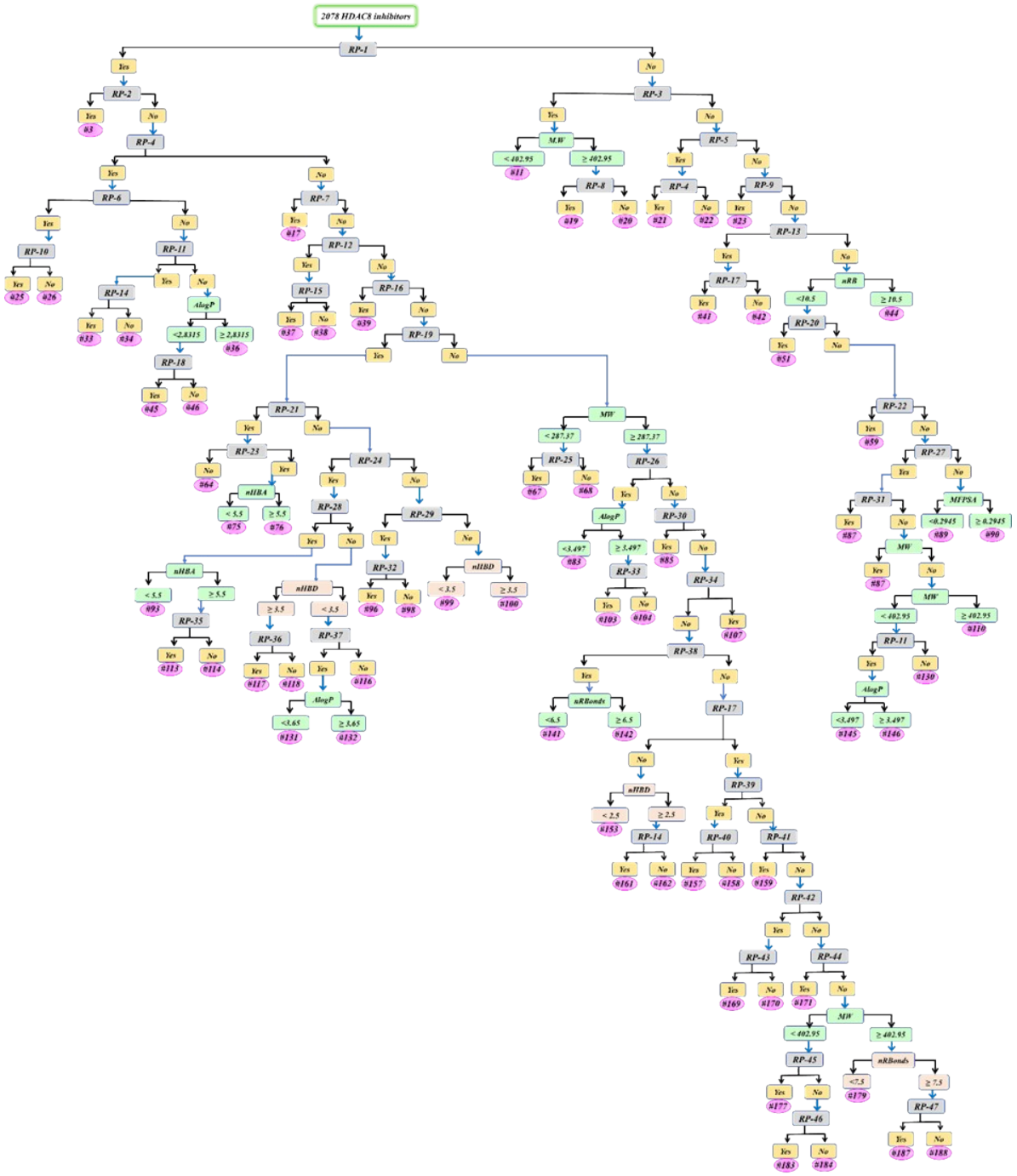


Fig. S4. Decision tree 1 depicting the hierarchical classification of HDAC8 inhibitors based on key molecular descriptors and sub-structural features. Each internal node represents a molecular descriptor used for splitting the dataset, while terminal nodes indicate the predicted activity class (active/inactive) along with the correctly classified compounds. The model highlights the relative importance of nitrogen-containing heterocyclic scaffolds in governing HDAC8 inhibitory activity.

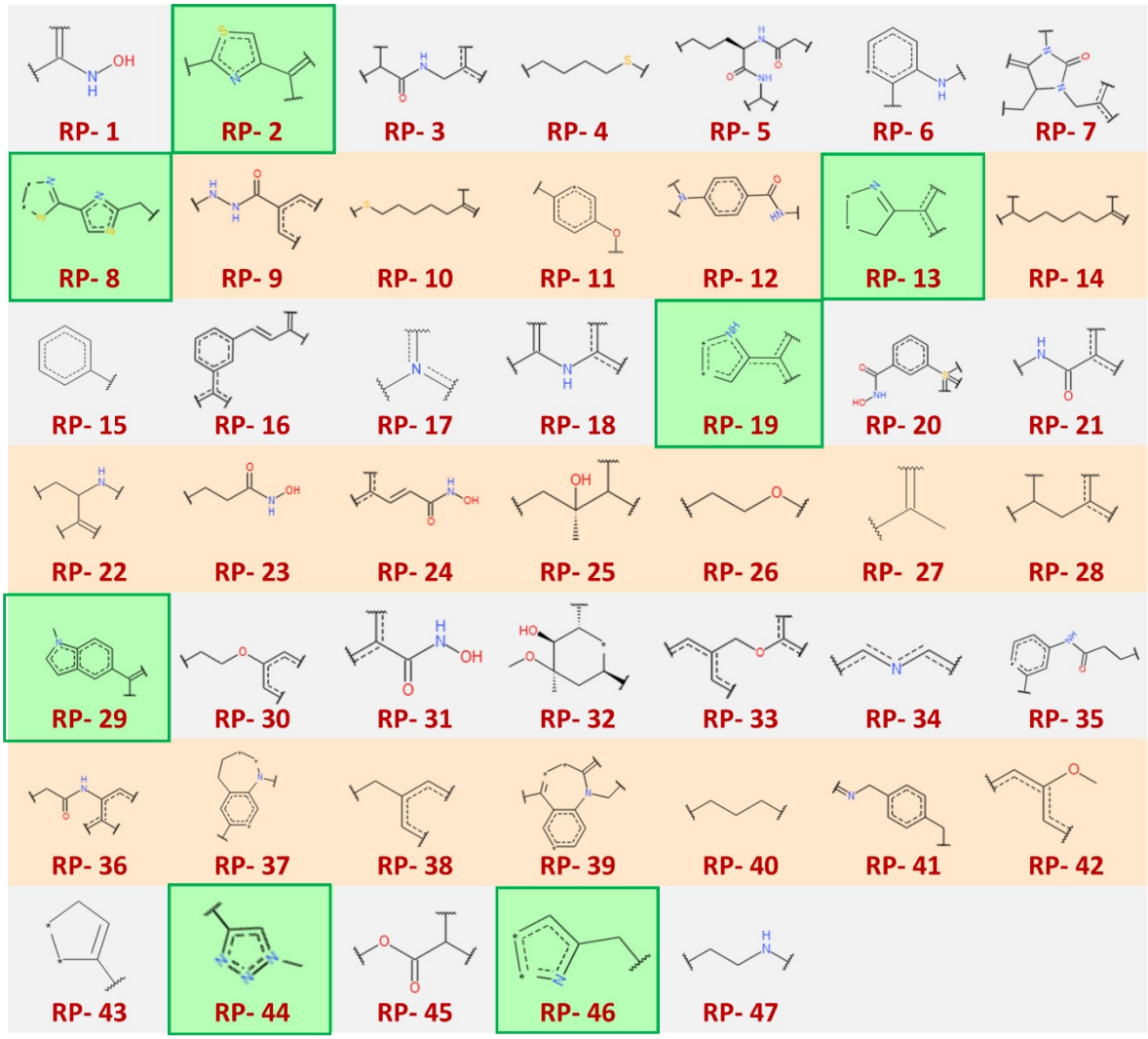


Fig. S5. List of 47 favourable fingerprints associated with potent HDAC8 inhibition identified generated by RP modelling study. The fingerprints containing nitrogen containing aromatic heterocycles are highlighted in green.

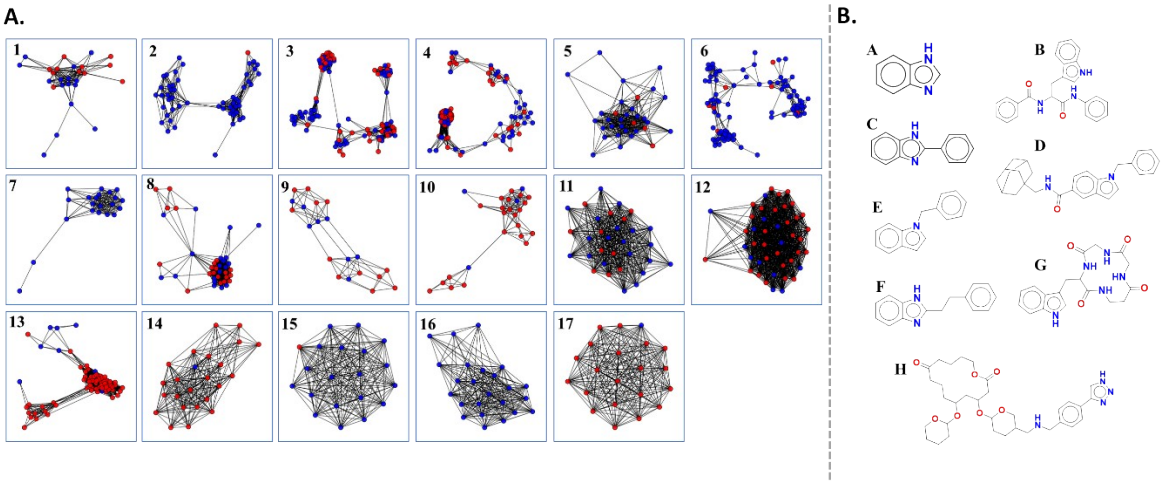


Fig. S6. A) A spring layout chemical space network (CSN) depicting 17 subgraphs/clusters of HDAC8 inhibitors, where node colors indicate activity classes and the line styles correspond to Tc-based similarity values. **B)** 2D representations of the common scaffolds identified in the study.

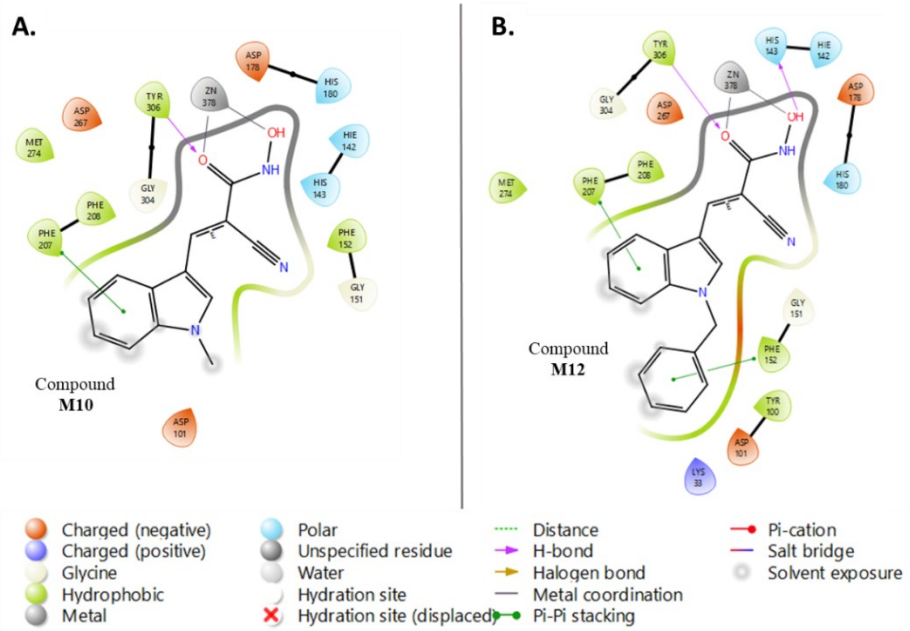


Fig. S7. 2D docking interactions of lead fingerprints **A) M10** and **B) M12** obtained from molecular docking studies (PDB: 1T69).

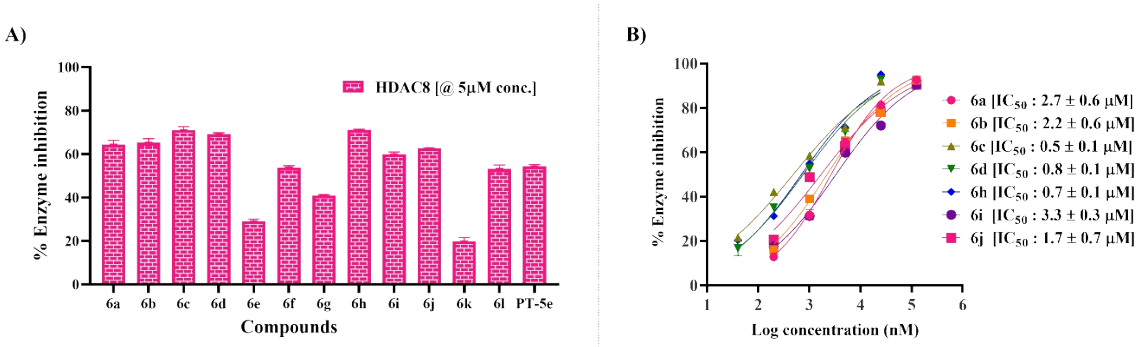


Fig. S8. A) Bargraph representing the % inhibition of the activity of HDAC8 by the synthesized compounds (**6a-6l**), along with the reference inhibitor **PT-5e** at 5µM concentration. Data are expressed as mean ± SD (n=2). **B)** Dose inhibition curve of lead molecules (**6a-6d**, **6h-6j**) against HDAC8 generated using a fluorophore-based enzymatic inhibition assay to determine their IC_{50} values. Data are presented as mean ± SD (n = 2).

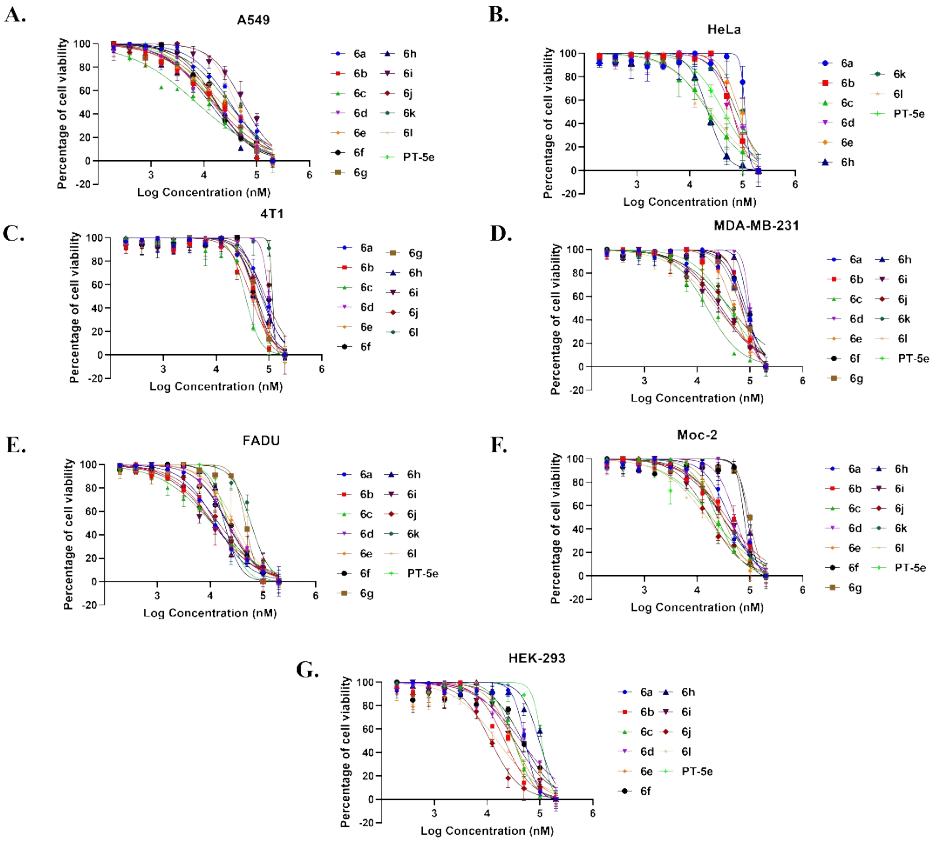


Fig. S9. Dose-response curves along with IC_{50} values of all synthesized compounds, including the reference compound **PT-5e**, were generated across six cancer cell lines: **(A)** A549 **(B)** HeLa **(C)** 4TI **(D)** MDA-MB-231 **(E)** FADU **(F)** Moc-2 and **(G)** HEK-293. The compounds were incubated with these cell lines for 72 hours, and cell viability was assessed using the MTT assay. Data are presented as mean ± SD (n=2) and plotted in a dose-response format. IC_{50} values were calculated through nonlinear regression analysis using GraphPad Prism 5.

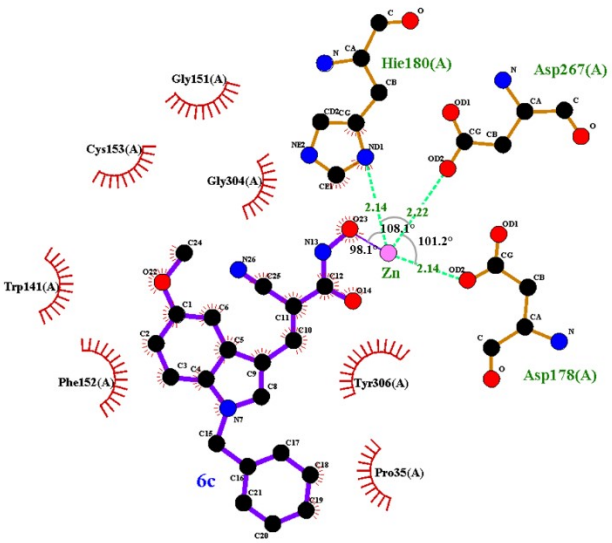


Fig. S10. 2D docking interactions of lead molecule **6c** in the active site of HDAC8 (PDB: 1VKG). Green dashed lines indicate polar interactions between the ligand and active site residues, including Asp178(A), Hie180(A), and Asp267(A), with bond distances (ranging from ~2.14 to 2.22 Å) and bond angles (ranging from 98.1° to 108°).

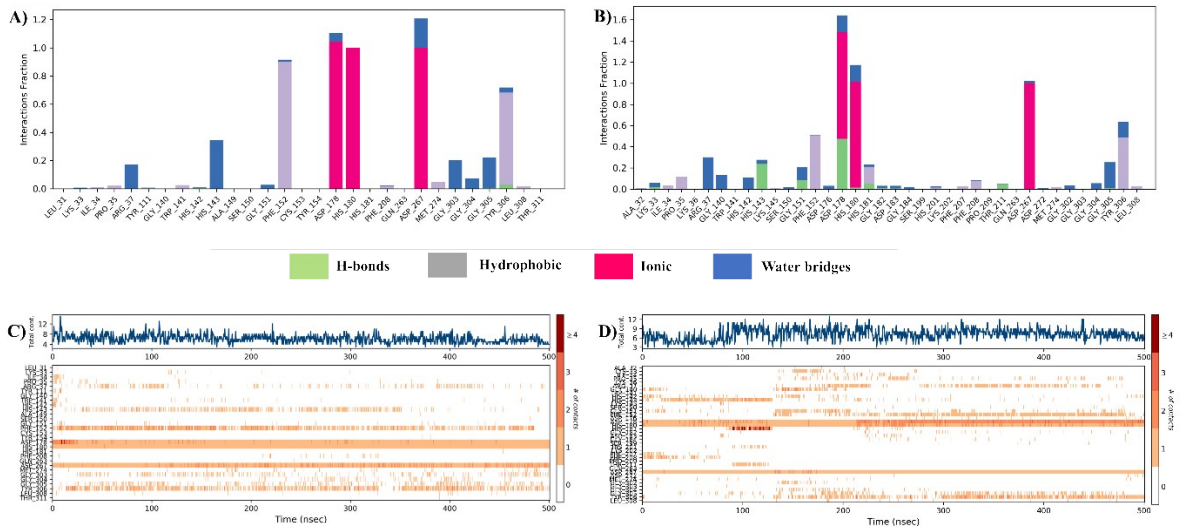


Fig. S11. (A) stacked bar chart illustrating the interaction fractions within the HDAC8-**6c** complex; **(B)** stacked bar chart showing the interaction fractions within the HDAC8-**PT-5e** complex; **(C)** timeline representation of ligand-protein contacts in the HDAC8-**6c** complex; **(D)** timeline representation of ligand-protein contacts in the HDAC8-**PT-5e** complex.

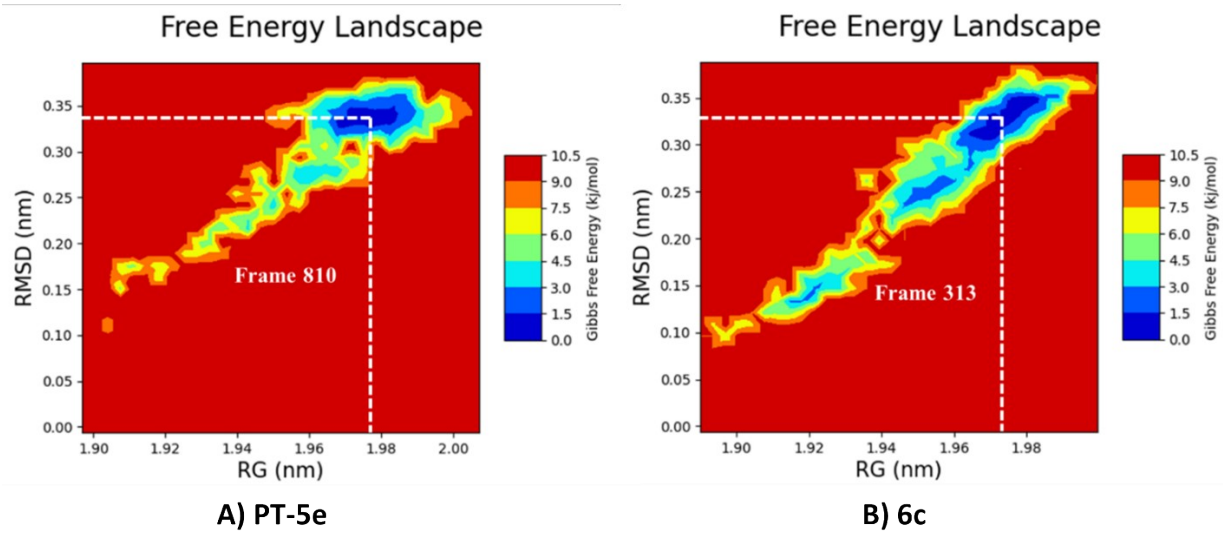
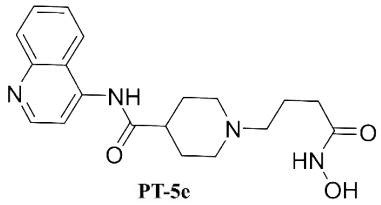


Fig. S12. 2D FEL plots of (A) HDAC8-**PT-5e** and (B) HDAC8-**6c** complexes



PT-5e

Fig. S13. Structure of reference molecule **PT-5e**

General methods for synthesis of intermediates

Synthesis of intermediates (2a-2d)

*Preparation of methyl (E)-2-cyano-3-(1H-indol-3-yl)acrylate (**2a**.* Methyl cyanoacetate (1.2 equiv, 2.31 mL, 24.79 mmol) was dissolved in MeOH (15 mL), followed by the addition of 0.03 equiv of KI (102.9 mg, 0.62 mmol) and 0.03 equiv of K_2CO_3 (85.69 mg, 0.62 mmol). After stirring for 20 min at room temperature, indole-3-carboxaldehyde (3g, 20.66 mmol) was added, and the reaction was allowed to proceed at RT for 4h. After completion (monitored by TLC), the solvent was removed under reduced pressure, and the residue was extracted with ethyl acetate, washed with water, dried over anhydrous Na_2SO_4, and concentrated to afford compound **2a** as a yellow solid in 95% (4.44 g) yield without further purification.

*Preparation of methyl (E)-2-cyano-3-(5-methoxy-1H-indol-3-yl)acrylate (**2b**.* Following the synthetic procedure of **2a** and adding 5-methoxyindole-3-carbaldehyde (2g, 11.4 mmol), compound **2b** was synthesized as yellow solid with a yield (2.80 g) of 96%.

*Preparation of methyl (E)-2-cyano-3-(2-methyl-1H-indol-3-yl)acrylate (**2c**.* Following the synthetic procedure of **2a** and adding 2-methylindole-3-carboxaldehyde (2g 12.56 mmol), compound **2c** was synthesized as pale-yellow solid (2.96 g) with a yield of 98%.

*Preparation of methyl (E)-2-cyano-3-(5-nitro-1H-indol-3-yl)acrylate (**2d**.* Following the synthetic procedure of **2a** and adding 5-nitroindole-3-carboxaldehyde (2g, 10.52 mmol), compound **2d** was synthesized (2.76 g) as brown coloured solid with 97% yield.

Synthesis of intermediates 3a-3l

Compounds **2a-2b** (1 equiv) was dissolved in ACN (15 ml), after which Cs_2CO_3 (2 equiv) and methyl/ethyl iodide (1.2 equiv.) were added. The reaction was allowed to proceed at RT for 4h and was monitored by TLC. The crude product was extracted with ethyl acetate and washed with water. The organic phase was separated, dried over anhydrous sodium sulfate, and concentrated under vacuum. The resulting solids (compounds **3a, 3b, 3d, 3f** and **3h***) were* obtained with more than 90% yield without further purification. Using the same procedure described above, compounds **2a-2d** were reacted with substituted benzyl bromides (1.2 equiv) in the presence of Cs_2CO_3 (2 equiv) in acetonitrile to afford compounds **3c**, **3e**, **3g**, and **3i-3l** in >85% yield without further purification.

Synthesis of intermediates 4a-4l.

Compound **3a-3l** (1 equiv) were dissolved in THF (5 ml) and treated with 0.5 N LiOH (3 equiv) at RT for 12 h. Upon completion of the reaction (monitored by TLC), THF was removed under reduced pressure and the resulting residue was dissolved in EtOAc and extracted with water. The aqueous layer was acidified with conc. HCl (pH 2-3) to precipitate the product, which was extracted with ethyl acetate, dried over anhydrous Na_2SO_4, and concentrated to afford crude compounds **4a-4l**.

Synthesis of intermediates 5a-5l

The acid derivatives **4a-4l** were dissolved in DMF (5 ml) in a clean, dry round-bottom flask under nitrogen atmosphere followed by the addition of HATU (1.2 equiv) and THP-protected hydroxylamine (1.2 equiv). The mixture was cooled to 0 °C in an ice bath, and DIPEA was added dropwise. After stirring at room temperature for 4-8 h (TLC monitored), the reaction was quenched with ice-cold water and extracted with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated. The crude product was purified by column chromatography (EtOAc:Hexane, 1.5:8.5) to afford THP-protected hydroxamic acids (**5a-5l**).

(S,E)-2-cyano-3-(1-methyl-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (5a). Yellow solid; yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.92 (s, 1H), 8.65 (s, 1H), 8.36 (s, 1H), 7.85 (dd, J = 6.8, 1.3 Hz, 1H), 7.41 – 7.28 (m, 3H), 5.09 (t, J = 2.8 Hz, 1H), 4.04 (td, J = 10.9, 3.0 Hz, 1H), 3.90 (s, 3H), 3.70 (ddd, J = 11.2, 5.3, 3.9 Hz, 1H), 1.95 – 1.81 (m, 3H), 1.71 – 1.61 (m, 3H).

(*S,E)-3-(1-benzyl-1H-indol-3-yl)-2-cyano-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5b**).* Yellow solid; yield: 67%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.59 (s, 1H), 8.61 (s, 1H), 8.40 (s, 1H), 7.96 – 7.90 (m, 1H), 7.65 – 7.59 (m, 1H), 7.38 – 7.18 (m, 8H), 5.64 (s, 2H), 4.98 (s, 1H), 4.12 – 4.01 (m, 1H), 3.59 – 3.49 (m, 1H), 1.72 (s, 3H), 1.55 (s, 3H).

*(S,E)-3-(1-benzyl-5-methoxy-1H-indol-3-yl)-2-cyano-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5c**).* Yellow solid; yield: 69%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.53 (s, 1H), 8.54 (s, 1H), 8.39 (s, 1H), 7.54 – 7.42 (m, 2H), 7.37 – 7.31 (m, 2H), 7.30 – 7.23 (m, 3H), 6.91 (dd, J = 8.9, 2.4 Hz, 1H), 5.59 (s, 2H), 4.98 (s, 1H), 4.12 – 4.04 (m, 1H), 3.82 (s, 3H), 3.57 – 3.48 (m, 1H), 1.72 (t, J = 3.0 Hz, 3H), 1.59 – 1.50 (m, 3H).

*(S,E)-2-cyano-3-(1-ethyl-5-methoxy-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5d**).* Maroon solid; yield: 62 %. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.50 (s, 1H), 8.43 (s, 1H), 8.38 (s, 1H), 7.56 (d, J = 8.9 Hz, 1H), 7.45 (d, J = 2.4 Hz, 1H), 6.96 (dd, J = 8.9, 2.4 Hz, 1H), 4.98 (t, J = 2.7 Hz, 1H), 4.34 (q, J = 7.1 Hz, 2H), 4.08 (ddd, J = 12.1, 8.5, 4.0 Hz, 1H), 4.02 (s, 2H), 3.85 (s, 3H), 3.71 (s, 3H), 3.59 – 3.50 (m, 1H), 1.72 (dt, J = 4.3, 2.2 Hz, 3H), 1.55 (d, J = 5.1 Hz, 3H), 1.41 (t, J = 7.2 Hz, 3H).

*(S,E)-2-cyano-3-(5-methoxy-1-(4-(trifluoromethyl)benzyl)-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5e**.* Yellow solid; yield: 59%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.63 (s, 1H), 8.53 (d, J = 3.2 Hz, 1H), 8.48 (s, 1H), 7.99 – 7.95 (m, 1H), 7.79 – 7.72 (m, 1H), 7.65 – 7.59 (m, 1H), 7.38 – 7.27 (m, 2H), 5.04 (s, 1H), 4.24 – 4.08 (m, 2H), 3.67 – 3.53 (m, 1H), 1.81 – 1.75 (m, 3H), 1.62 (s, 3H).

*(S,E)-2-cyano-3-(1-ethyl-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5f**.* Orange solid; yield: 70%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.57 (s, 1H), 8.49 (s, 1H), 8.39 (s, 1H), 7.93 (d, J = 7.7 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.42 – 7.23 (m, 2H), 4.99 (d, J = 2.8 Hz, 1H), 4.39 (q, J = 7.2 Hz, 2H), 1.72 (s, 3H), 1.55 (q, J = 7.2 Hz, 3H), 1.43 (t, J = 7.2 Hz, 3H).

*(S,E)-2-cyano-3-(5-methoxy-1-(4-(trifluoromethoxy)benzyl)-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5g**.* Yellow solid; yield: 68%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.55 (s, 1H), 8.56 (s, 1H), 8.40 (s, 1H), 7.50 (d, J = 8.9 Hz, 1H), 7.47 (d, J = 2.4 Hz,

1H), 7.38 – 7.33 (m, 4H), 6.92 (dd, J = 8.9, 2.4 Hz, 1H), 5.65 (s, 2H), 4.99 (d, J = 2.8 Hz, 1H), 4.08 (ddd, J = 12.3, 8.8, 3.8 Hz, 1H), 3.83 (s, 3H), 3.61 – 3.49 (m, 1H), 1.75 – 1.68 (m, 3H), 1.55 (d, J = 5.3 Hz, 3H).

*(S,E)-2-cyano-3-(5-methoxy-1-methyl-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5h**).* Brown solid; yield: 67%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.56 (s, 1H), 8.44 (s, 1H), 8.43 (s, 1H), 7.57 (d, J = 8.9 Hz, 1H), 7.50 (d, J = 2.3 Hz, 1H), 7.02 (dd, J = 8.9, 2.4 Hz, 1H), 5.03 (s, 1H), 4.13 (td, J = 10.2, 3.9 Hz, 1H), 3.98 (s, 3H), 3.90 (s, 3H), 3.62 – 3.57 (m, 1H), 1.80 – 1.74 (m, 3H), 1.60 (d, J = 5.5 Hz, 3H).

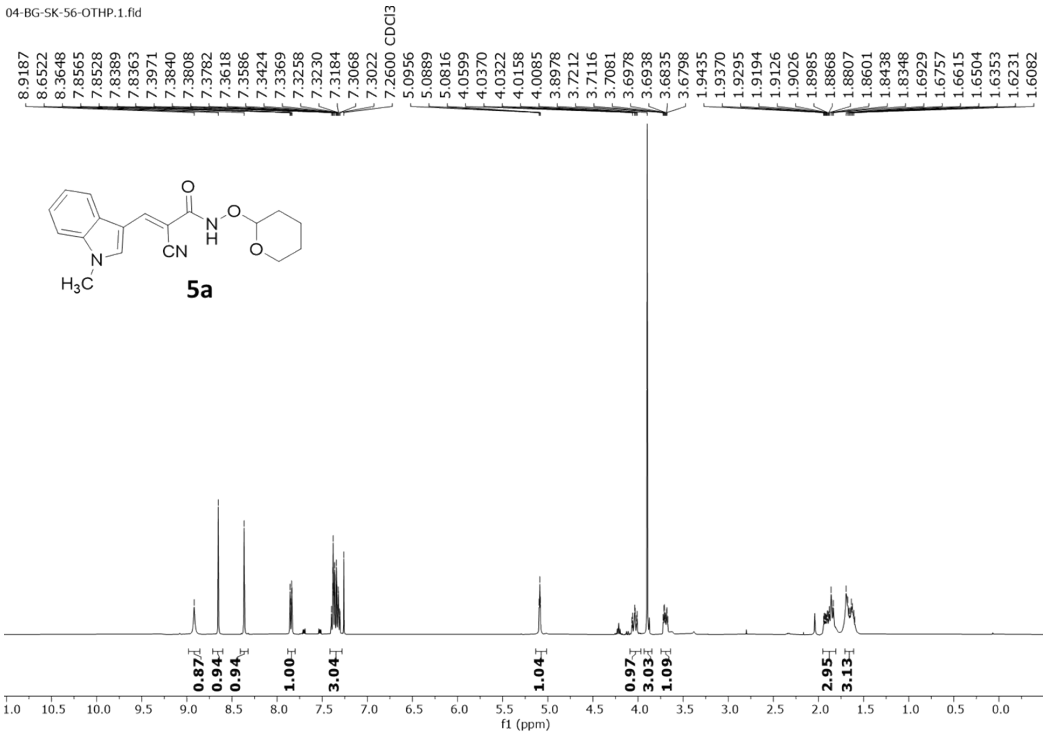
*(S,E)-2-cyano-3-(2-methyl-1-(4-(trifluoromethoxy)benzyl)-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5i**).* Green solid; Yield: 59%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.61 (s, 1H), 8.38 (s, 1H), 8.07 – 8.01 (m, 1H), 7.65 – 7.60 (m, 1H), 7.40 – 7.37 (m, 2H), 7.33 – 7.27 (m, 2H), 7.25 (s, 2H), 5.68 (s, 2H), 5.06 (d, J = 2.8 Hz, 1H), 4.21 – 4.08 (m, 1H), 3.60 (d, J = 11.3 Hz, 1H), 2.60 (s, 3H), 1.77 (s, 3H), 1.60 (s, 3H).

*(E)-2-cyano-3-(1-(4-methoxybenzyl)-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5j**).* Orange coloured solid; yield: 60%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.59 (s, 1H), 8.59 (s, 1H), 8.39 (s, 1H), 7.95 – 7.90 (m, 1H), 7.68 – 7.62 (m, 1H), 7.33 – 7.24 (m, 4H), 6.93 – 6.87 (m, 2H), 5.55 (s, 2H), 4.98 (s, 1H), 4.05 (d, J = 11.0 Hz, 1H), 3.71 (s, 3H), 3.59 – 3.51 (m, 1H), 1.72 (s, 2H), 1.55 (d, J = 5.1 Hz, 1H).

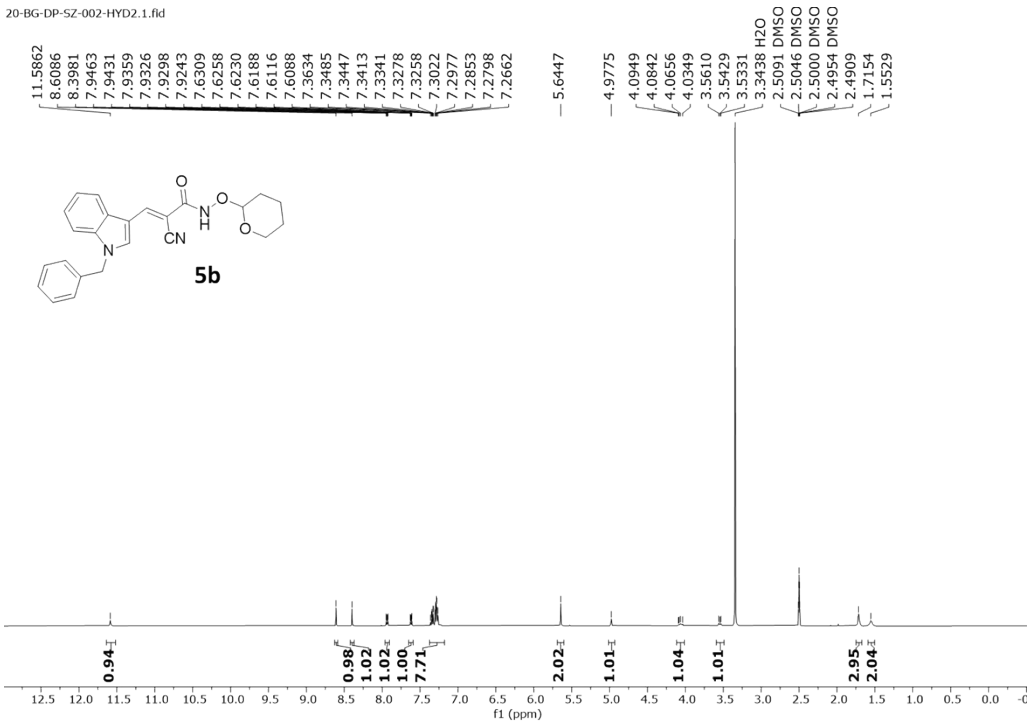
*(E)-2-cyano-3-(1-(4-fluorobenzyl)-2-methyl-1H-indol-3-yl)-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5k**.* Yellow solid; yield: 65%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 11.62 (s, 1H), 8.37 (s, 1H), 8.07 – 7.98 (m, 1H), 7.67 – 7.58 (m, 1H), 7.30 (tdd, J = 5.8, 4.1, 2.3 Hz, 2H), 7.19 (td, J = 6.7, 2.7 Hz, 4H), 5.62 (s, 2H), 5.05 (t, J = 2.6 Hz, 1H), 4.12 (s, 1H), 3.63 (d, J = 2.3 Hz, 1H), 2.61 (s, 3H), 1.77 (q, J = 2.0 Hz, 3H), 1.64 – 1.57 (m, 3H).

*(E)-3-(1-benzyl-5-nitro-1H-indol-3-yl)-2-cyano-N-((tetrahydro-2H-pyran-2-yl)oxy)acrylamide (**5l**).* Brown solid; yield: 66%. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 9.33 (s, 1H), 8.95 (s, 1H), 8.72 (s, 1H), 8.44 (s, 1H), 8.15 (s, 1H), 7.84 (s, 1H), 7.33 (dt, J = 23.5, 7.1 Hz, 4H), 5.99 – 5.38 (m, 2H), 4.96 (d, J = 26.5 Hz, 1H), 4.06 (s, 1H), 3.80 (s, 1H), 1.65 – 1.13 (m, 6H).

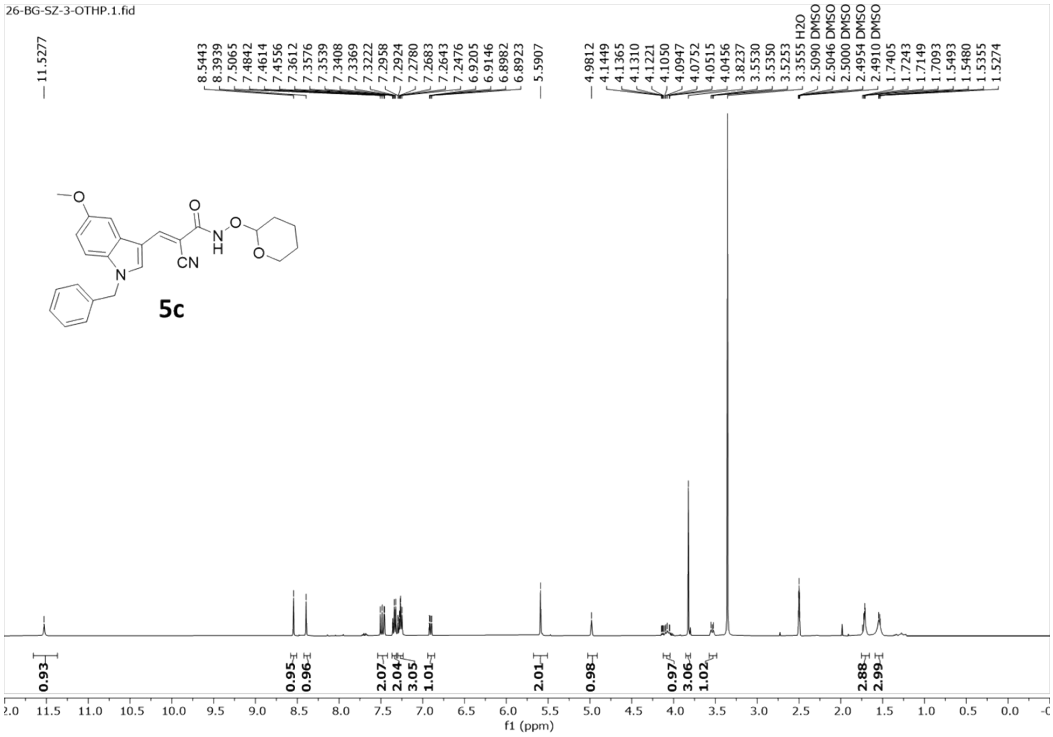
Supporting [1]HNMR spectra of intermediates (5a-5l)



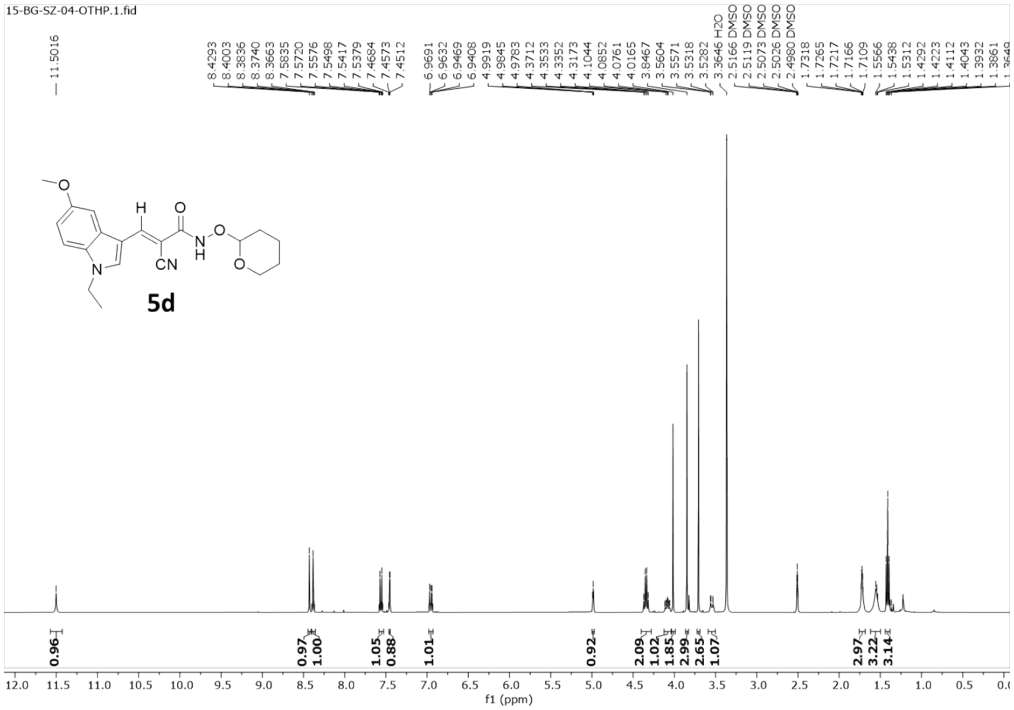
Supporting Spectra S1: [1]H NMR Spectra for the intermediate 5a.



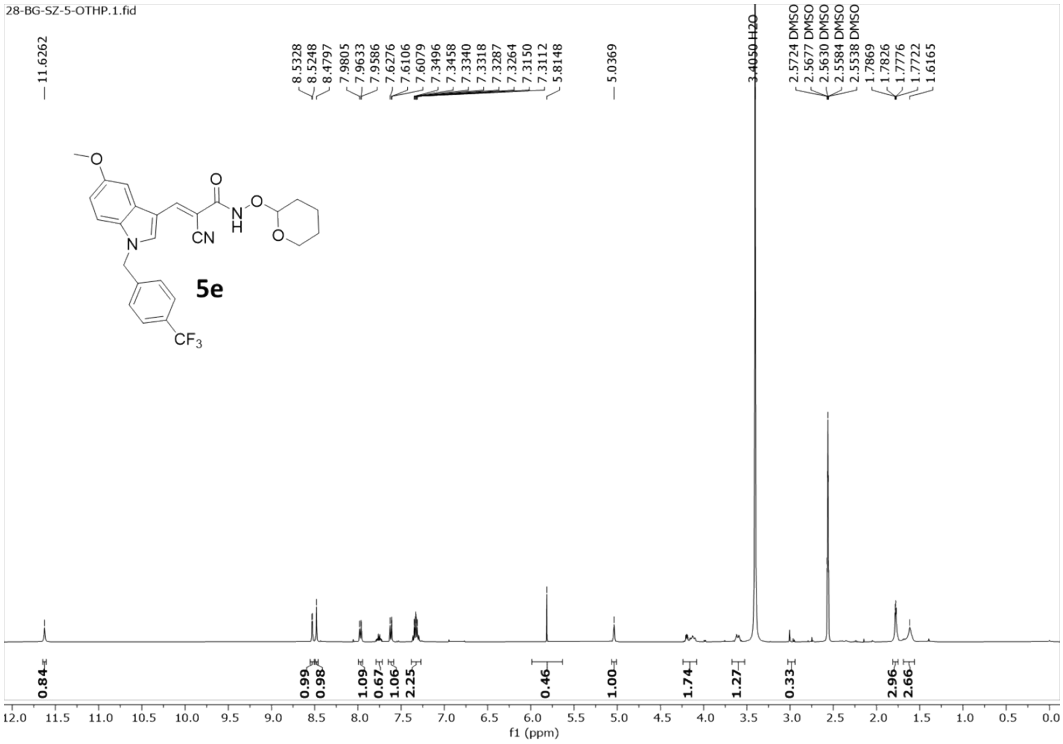
Supporting Spectra S2: [1]H NMR Spectra for the intermediate 5b.



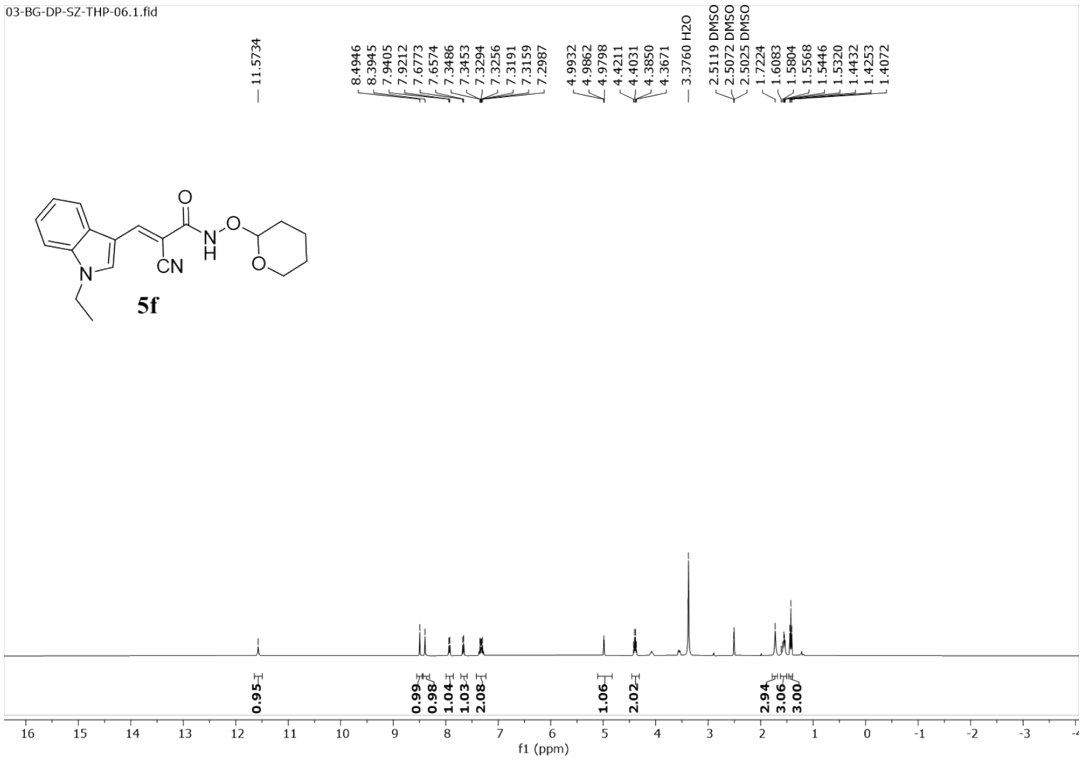
Supporting Spectra S3: ^{1}H NMR Spectra for the intermediate 5c.



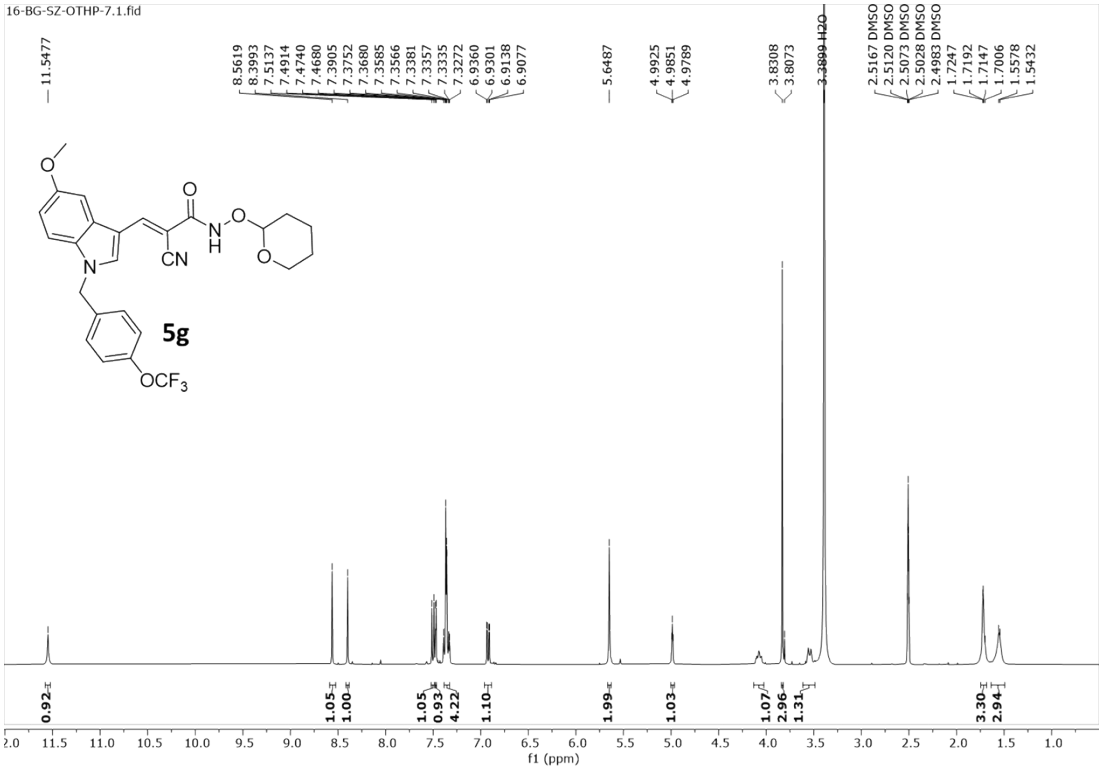
Supporting Spectra S4: ^{1}H NMR Spectra for the intermediate 5d.



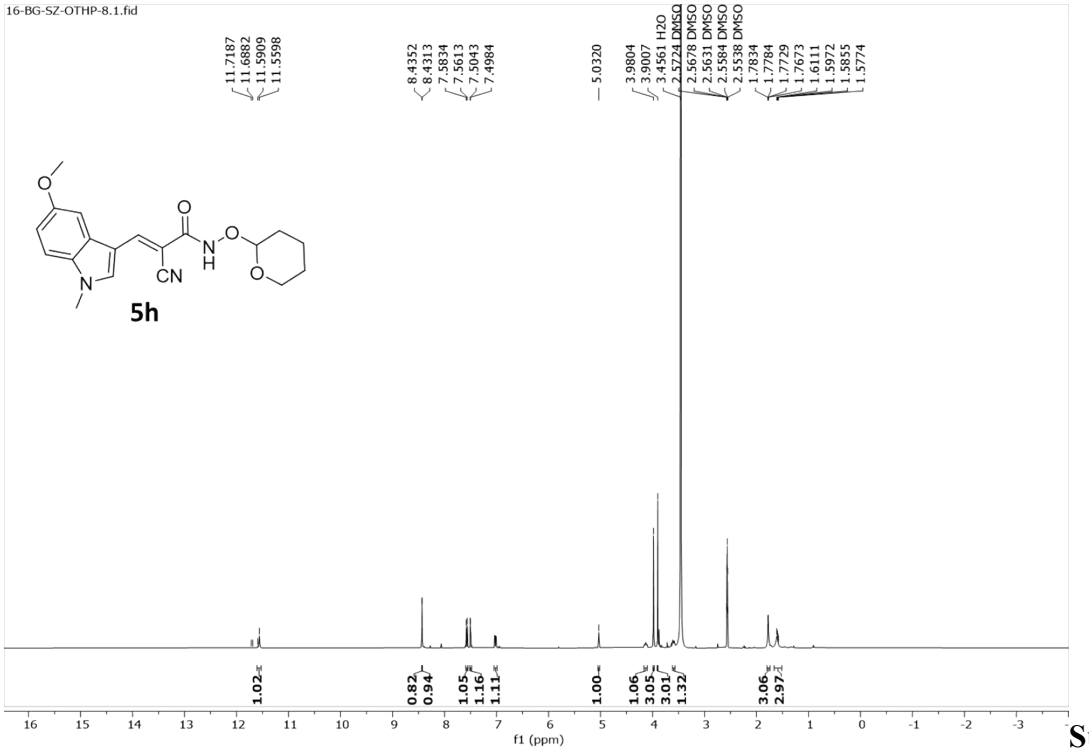
Supporting Spectra S5: ^{1}H NMR Spectra for the intermediate 5e.



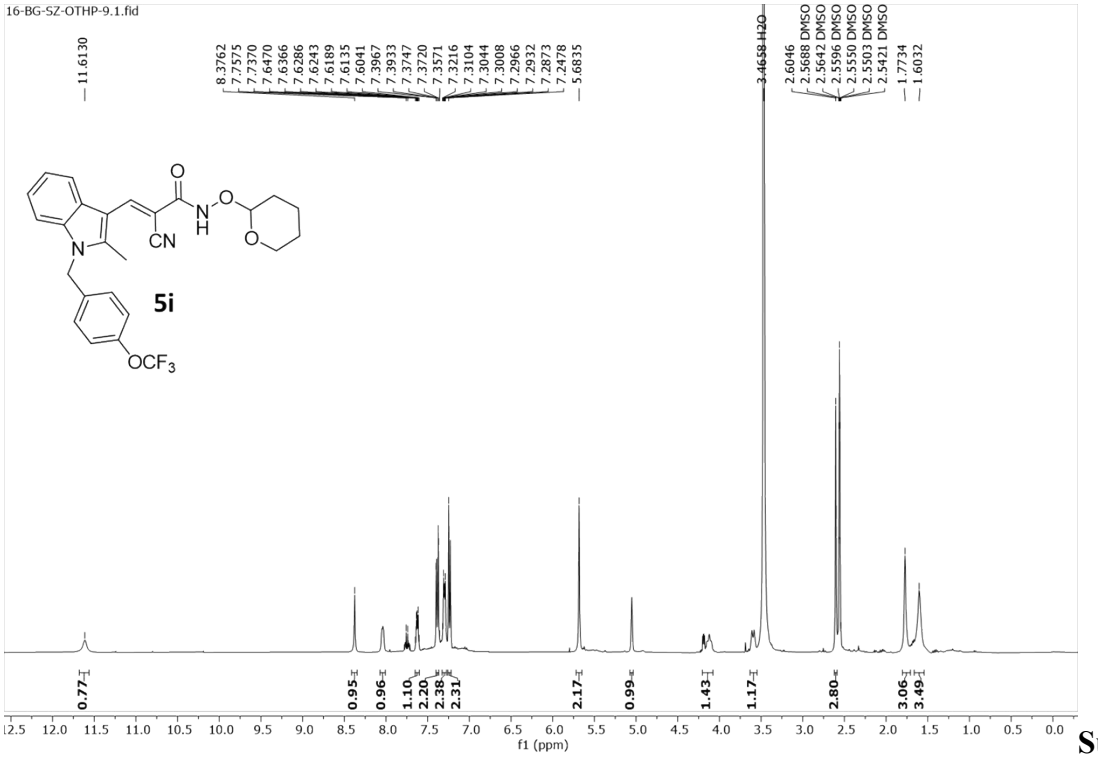
Supporting Spectra S6: ^{1}H NMR Spectra for the intermediate 5f.



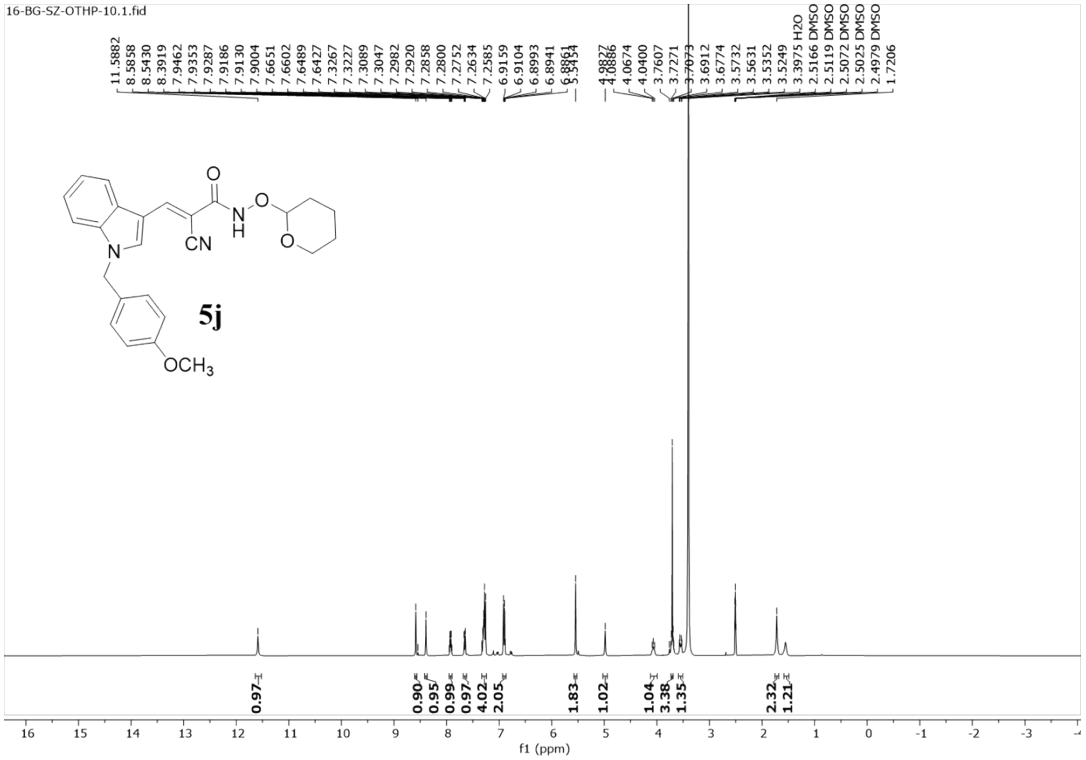
Supporting Spectra S7: ^{1}H NMR Spectra for the intermediate 5g.



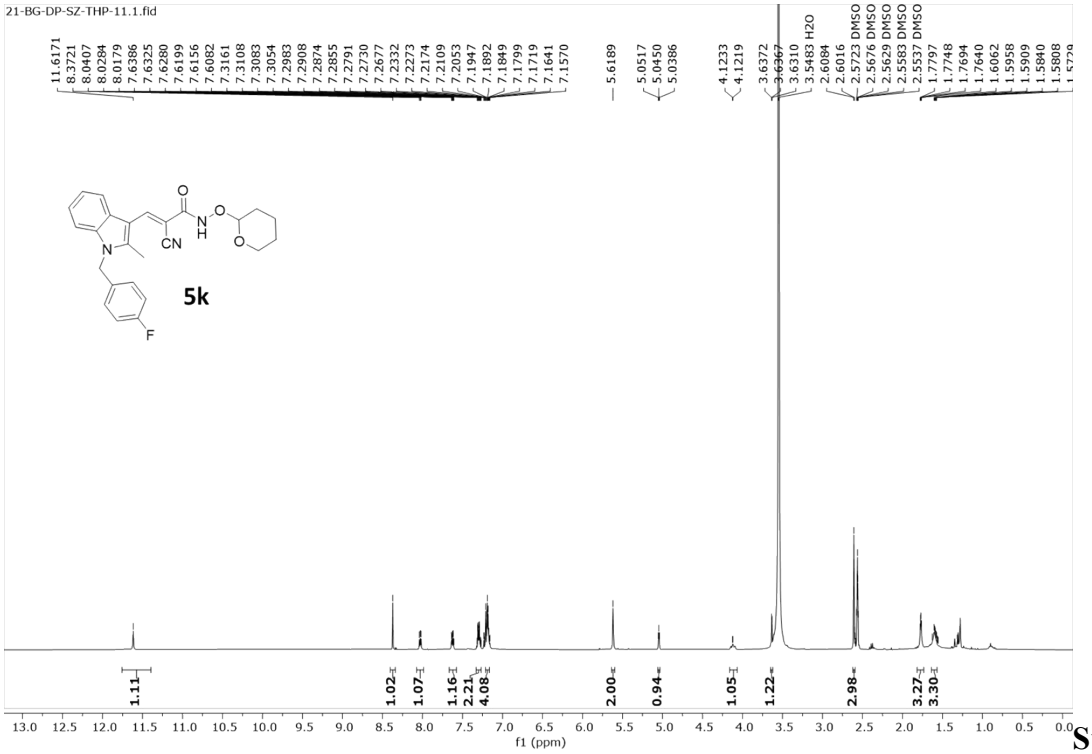
Supporting Spectra S8: ^{1}H NMR Spectra for the intermediate 5h.



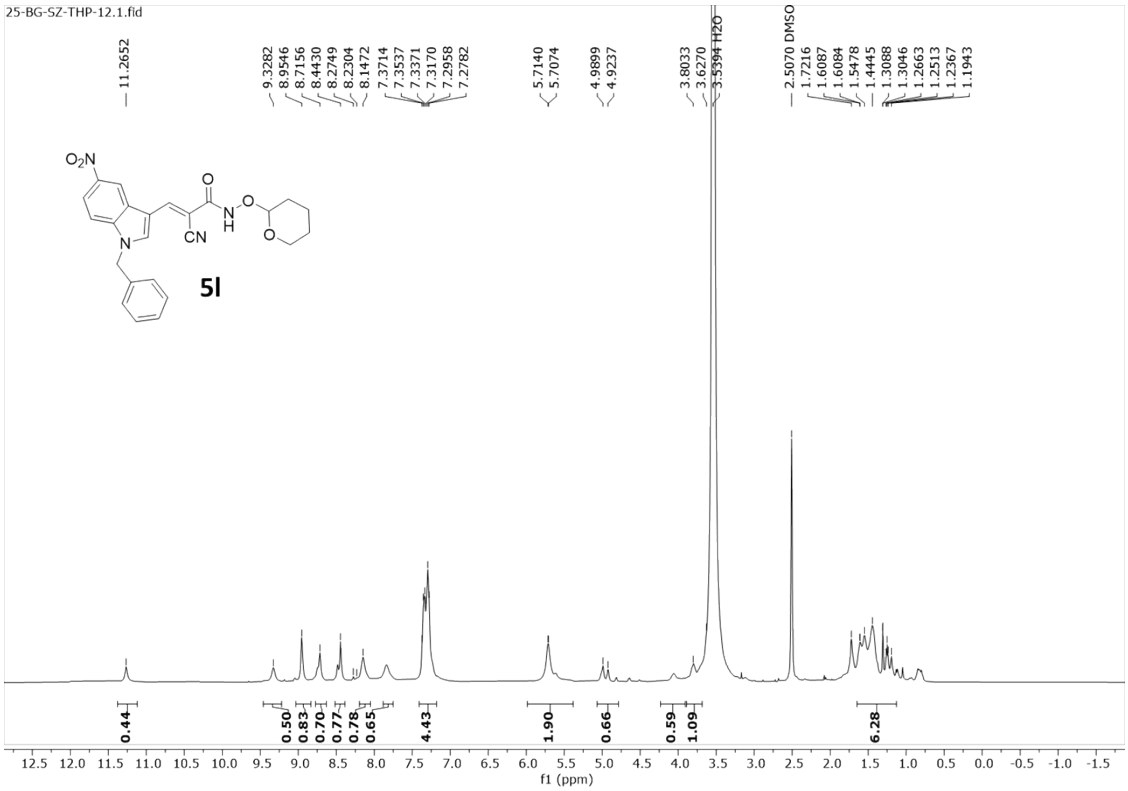
Supporting Spectra S9: ^{1}H NMR Spectra for the intermediate 5i.



Supporting Spectra S10: ^{1}H NMR Spectra for the intermediate 5j.

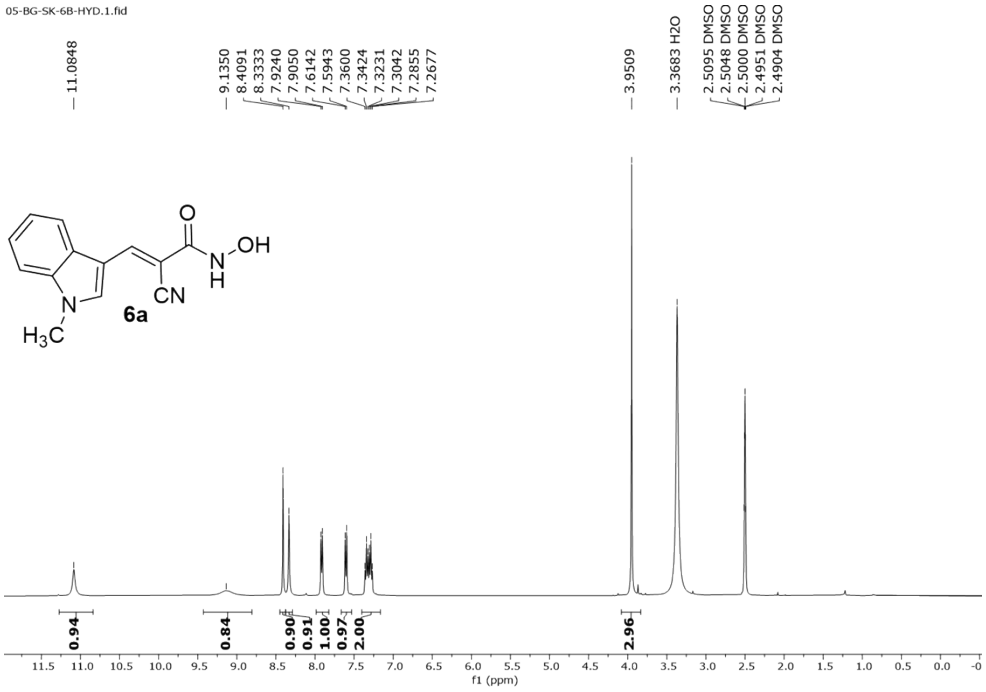


Supporting Spectra S11: ^{1}H NMR Spectra for the intermediate 5k.

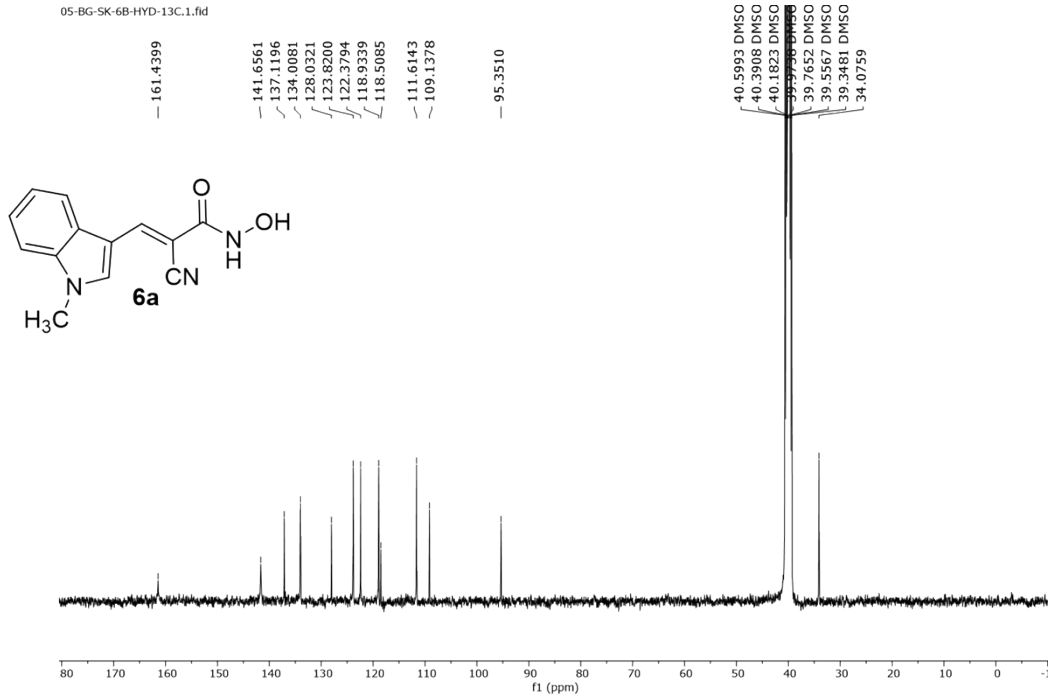


Supporting Spectra S12: ^{1}H NMR Spectra for the intermediate 5l.

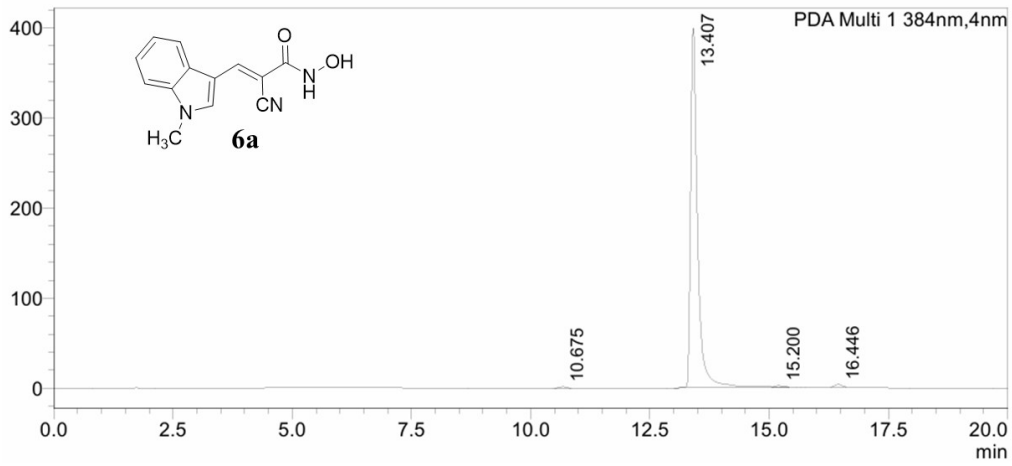
Supporting spectra (^{1}HNMR, ^{13}CNMR, ^{19}FNMR, HPLC, LCMS and HRMS) of final compounds (6a-6l)



Supporting Spectra S13: ^{1}H NMR Spectra for the compound 6a.



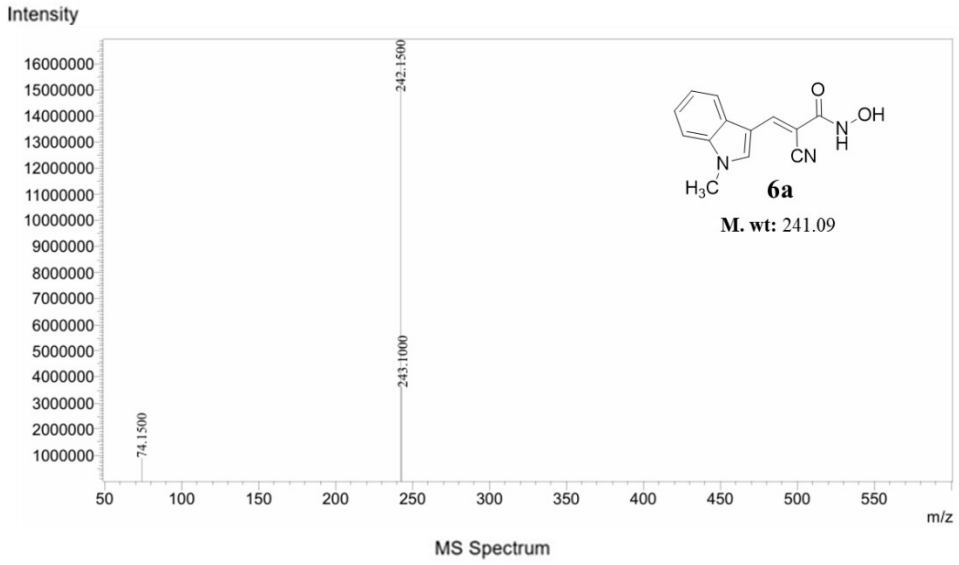
Supporting Spectra S14: ^{13}C NMR Spectra for the compound 6a.



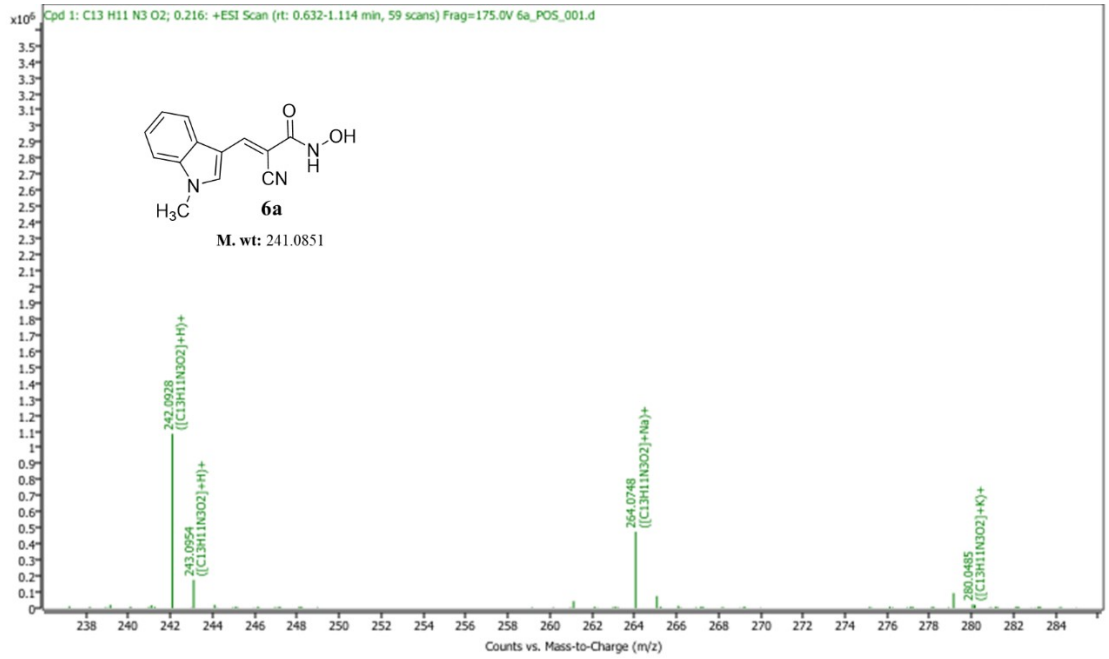
PDA Ch1 384nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.675	14620	1461	0.356	0.361
2	13.407	4057867	398895	98.716	98.607
3	15.200	11118	1388	0.270	0.343
4	16.446	27035	2785	0.658	0.688
Total		4110640	404529	100.000	100.000

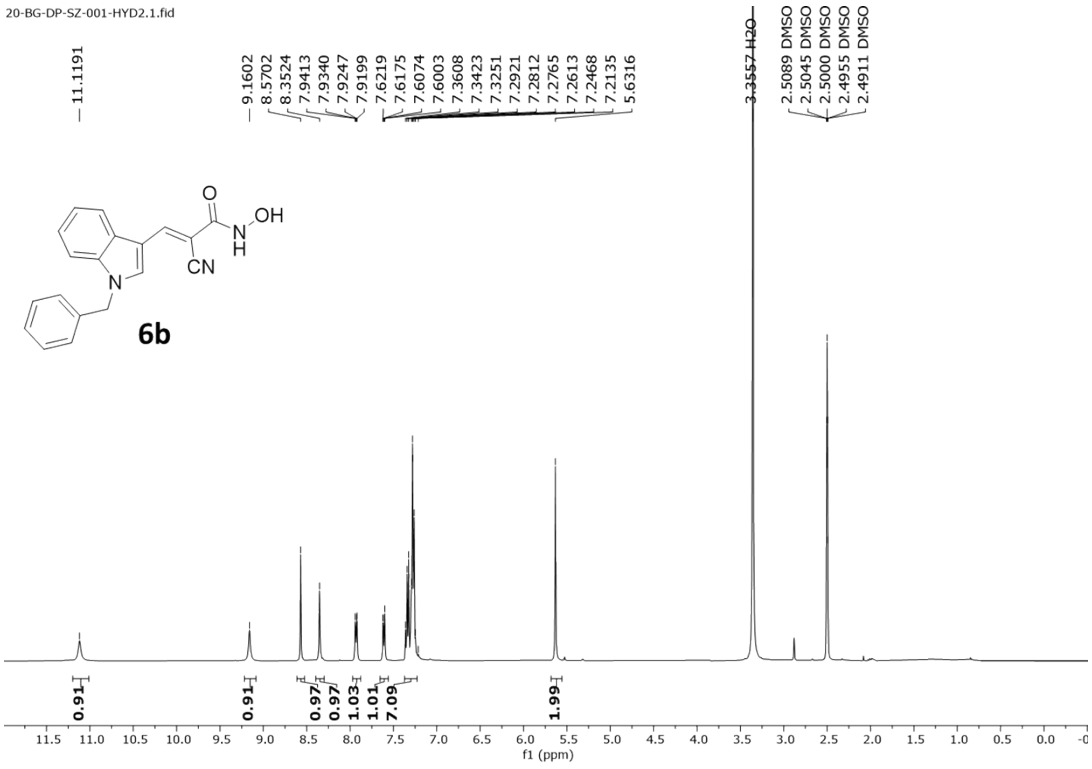
Supporting Spectra S15: HPLC traces of compound 6a.



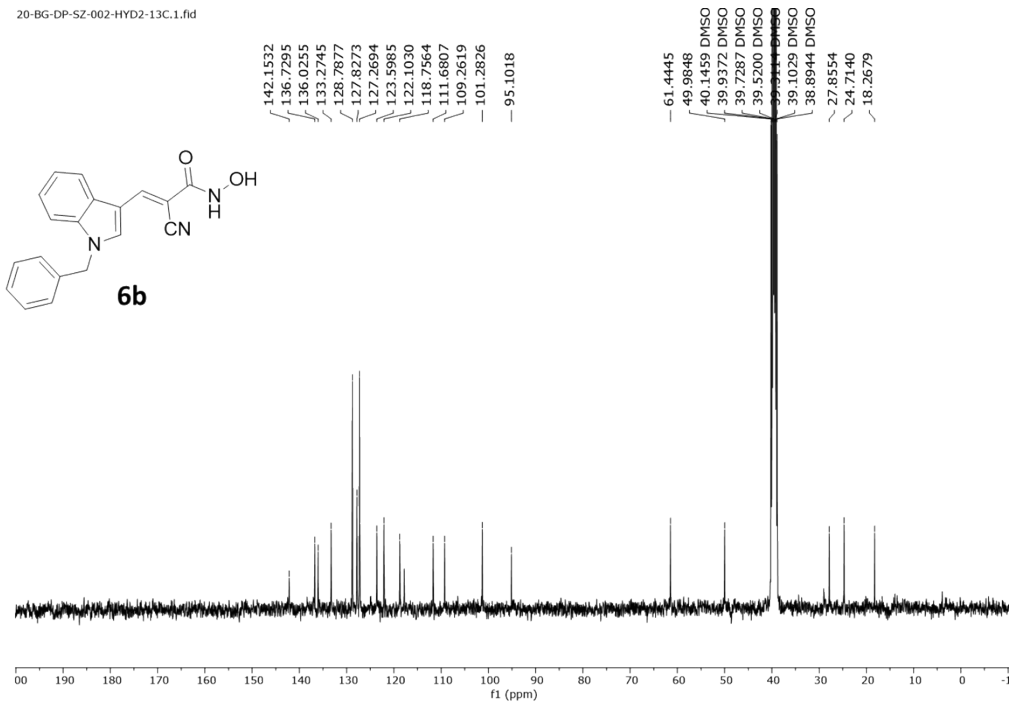
Supporting Spectra S16: LC-MS Spectra for the compound 6a.



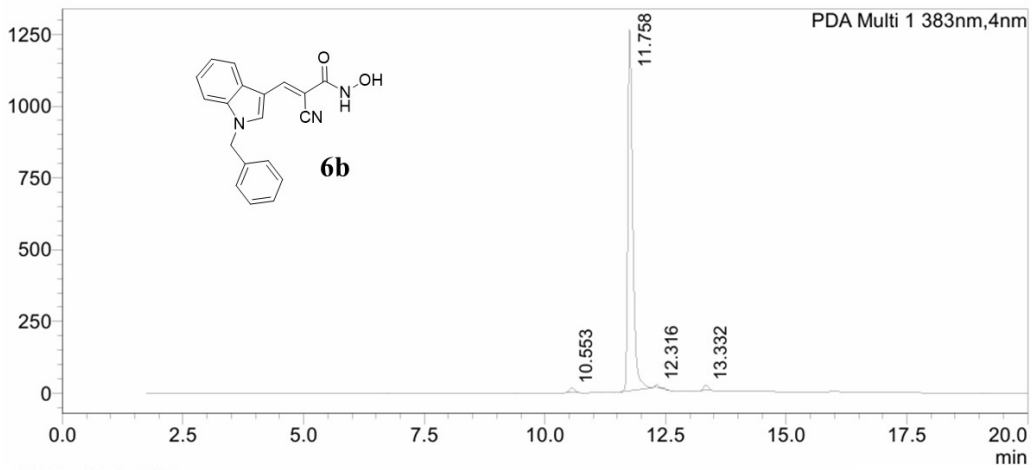
Supporting Spectra S17: HRMS Spectra for the compound 6a.



Supporting Spectra S18: ^{1}H NMR Spectra for the compound 6b.



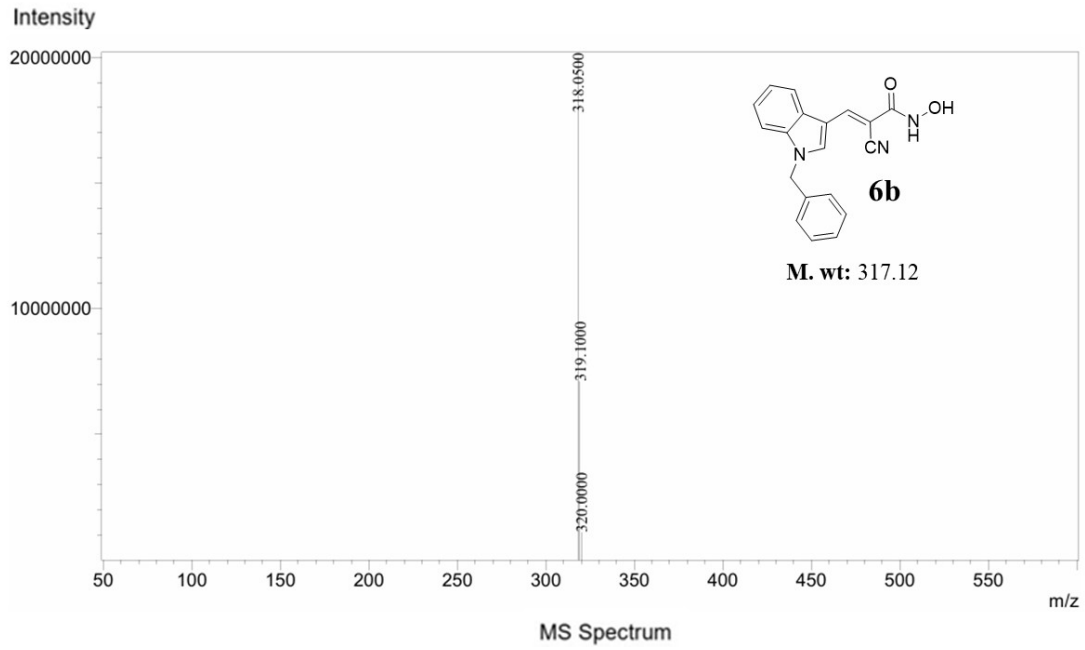
Supporting Spectra S19: ^{13}C NMR Spectra for the compound 6b.



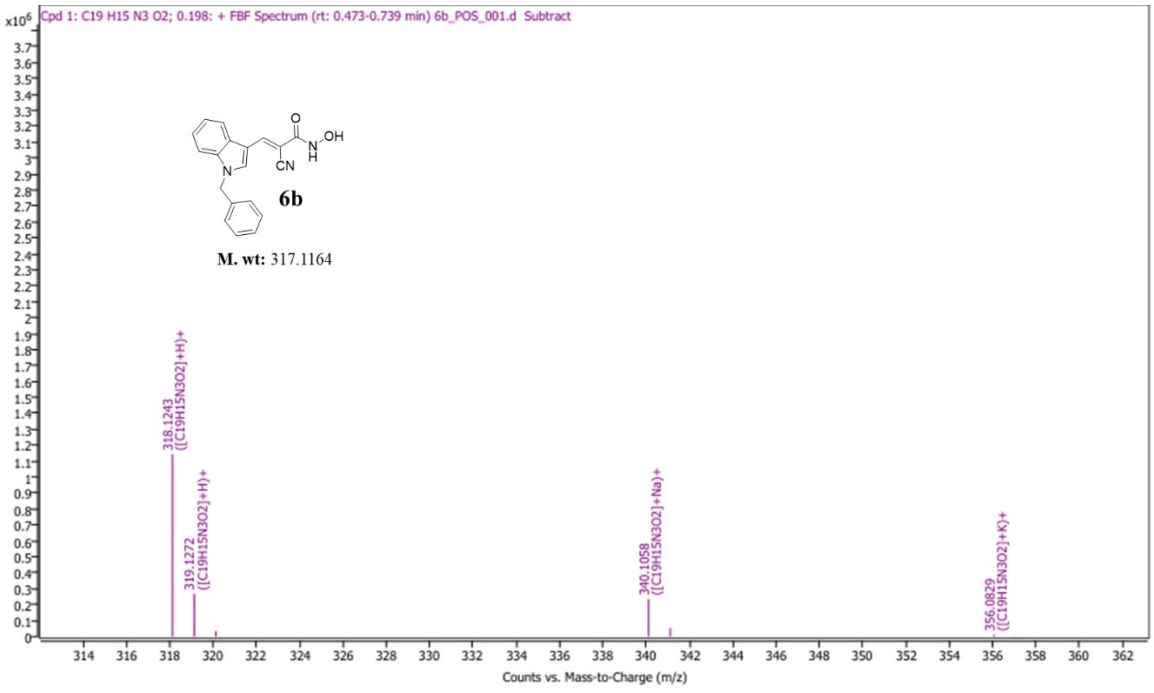
PDA Ch1 383nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	10.553	105869	14867	1.151	1.143
2	11.758	8919644	1259947	97.012	96.874
3	12.316	53485	7746	0.582	0.596
4	13.332	115357	18039	1.255	1.387
Total		9194354	1300599	100.000	100.000

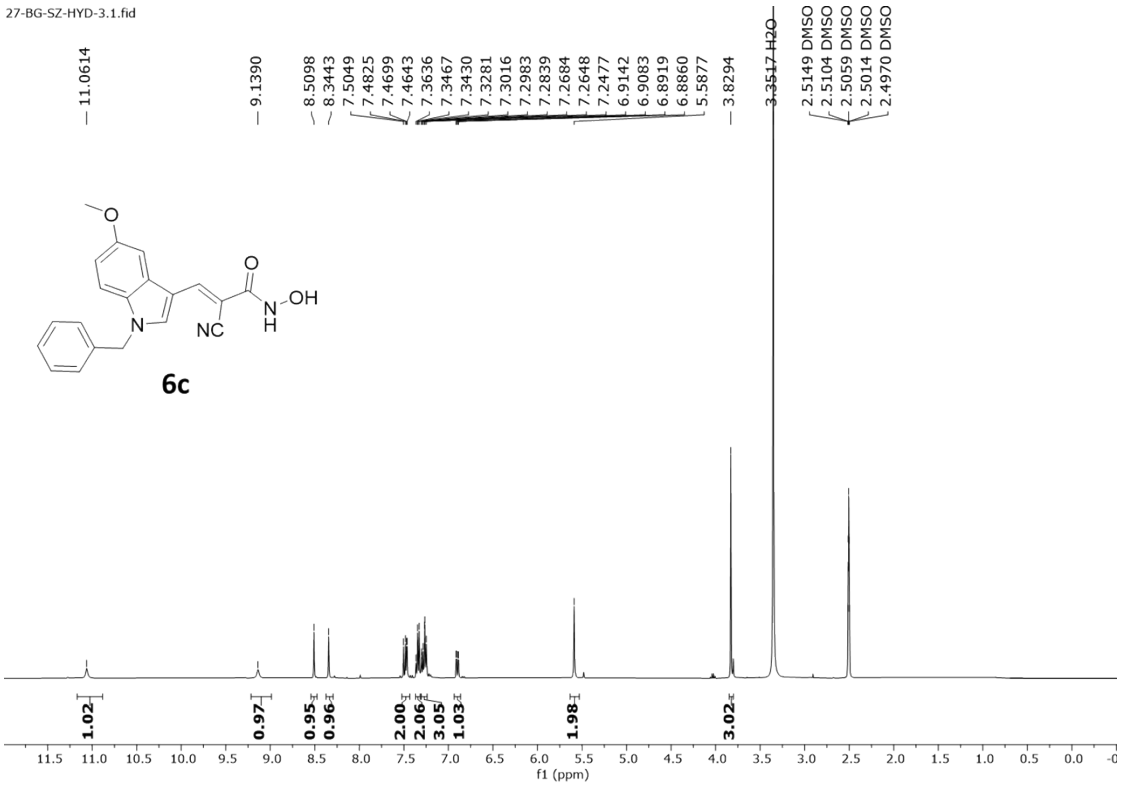
Supporting Spectra S20: HPLC traces of compound 6b.



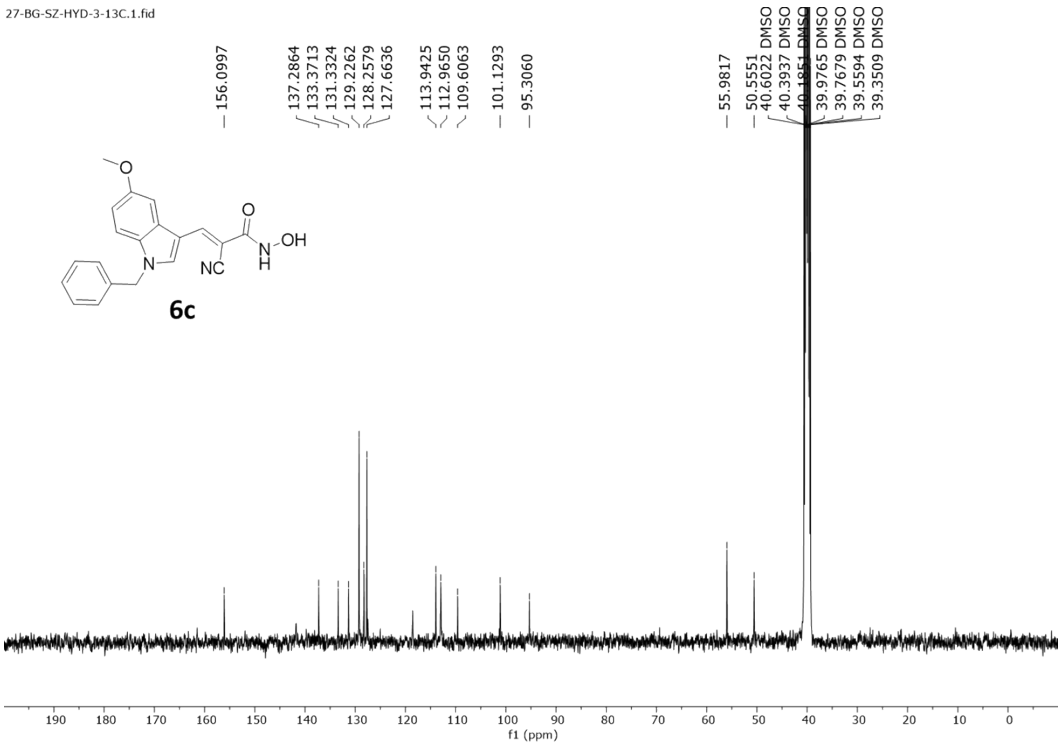
Supporting Spectra S21: LC-MS Spectra for the compound 6b.



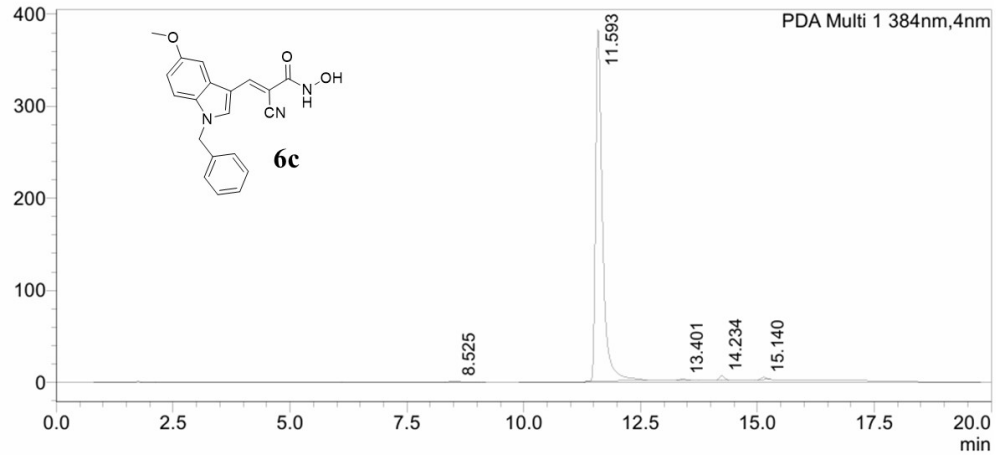
Supporting Spectra S22: HRMS Spectra for the compound 6b.



Supporting Spectra S23: ^{1}H NMR Spectra for the compound 6c.



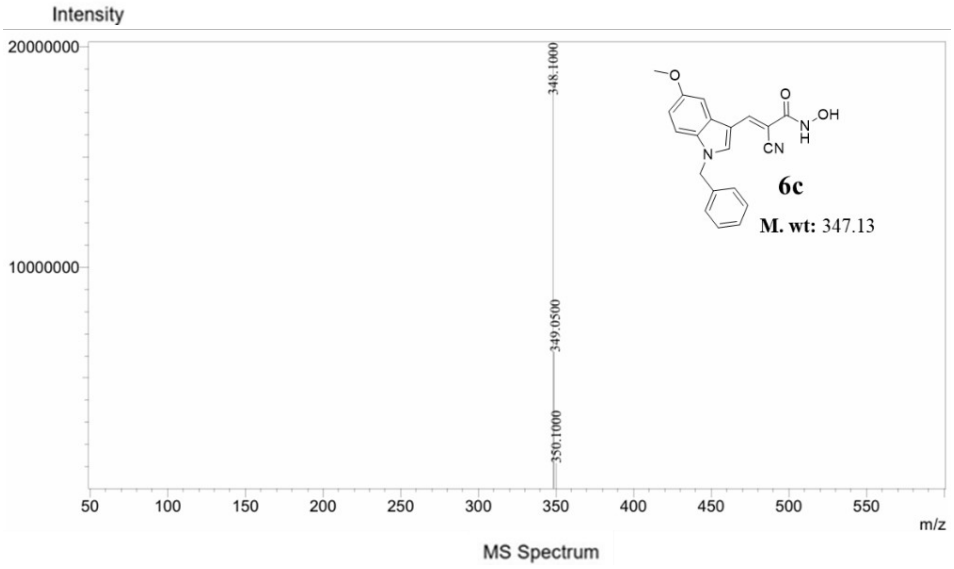
Supporting Spectra S24: ^{13}C NMR Spectra for the compound 6c.



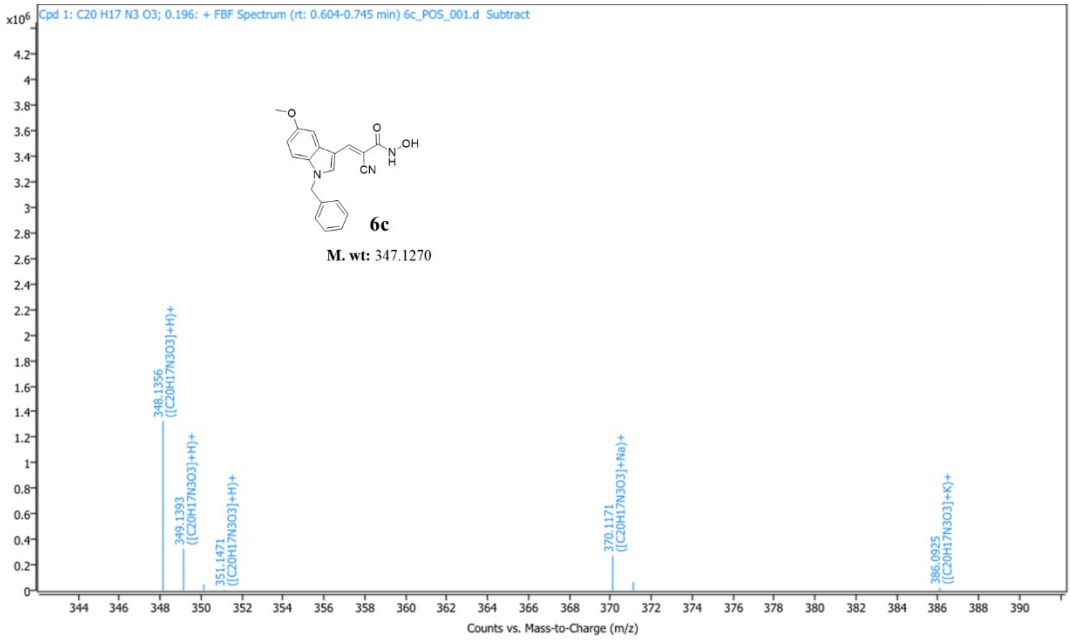
PDA Ch1 384nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	8.525	8820	1024	0.219	0.261
2	11.593	3957279	382542	98.250	97.578
3	13.401	11483	1553	0.285	0.396
4	14.234	30731	4428	0.763	1.129
5	15.140	19439	2491	0.483	0.635
Total		4027752	392038	100.000	100.000

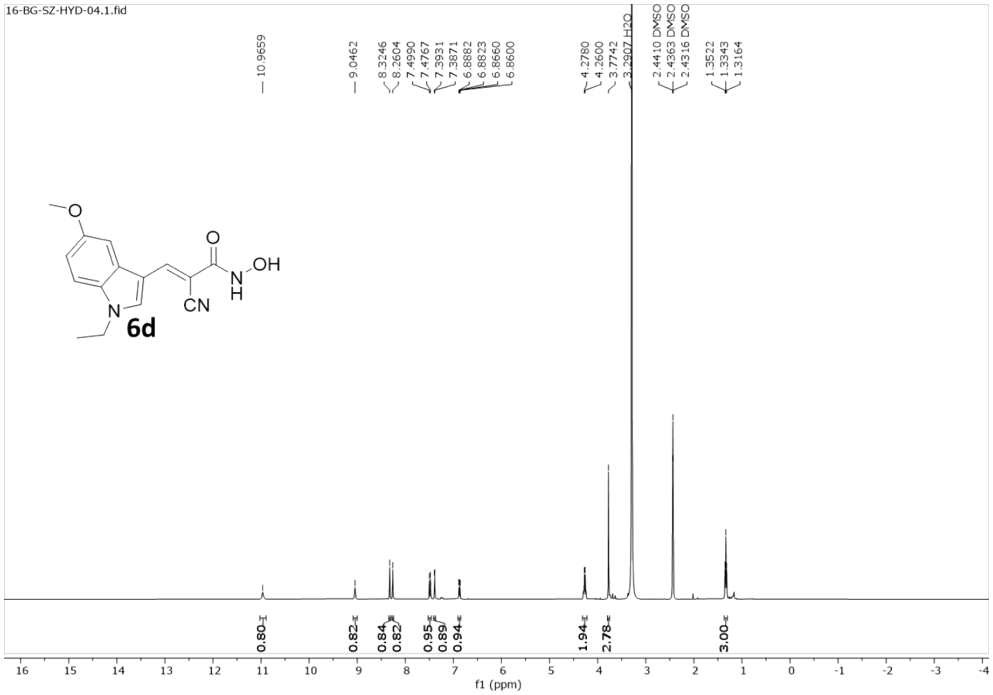
Supporting Spectra S25: HPLC traces of compound 6c.



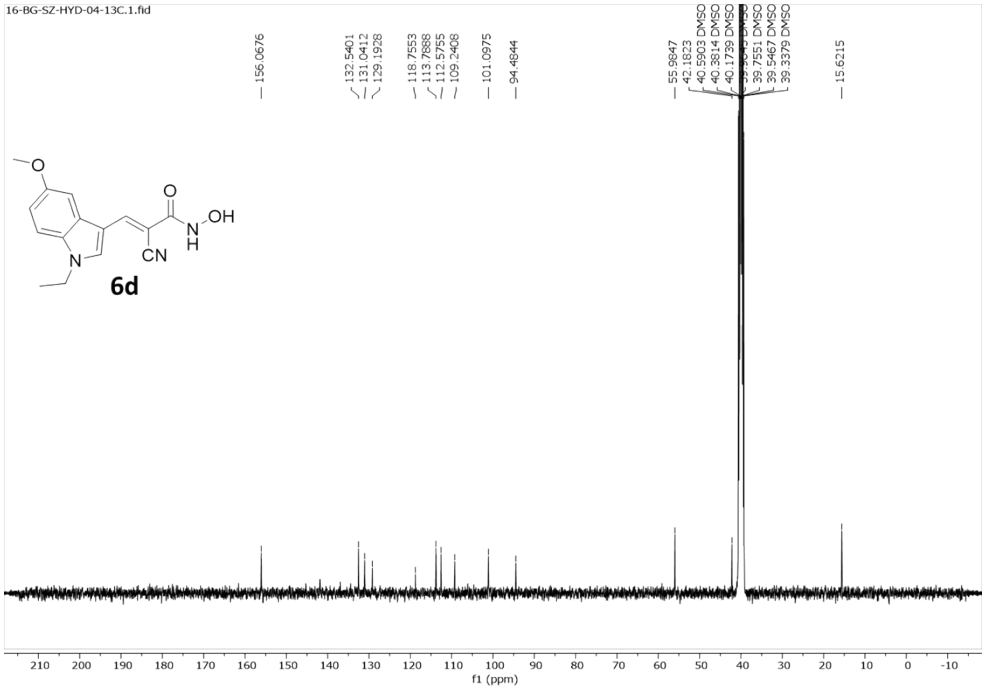
Supporting Spectra S26: LC-MS Spectra for the compound 6c.



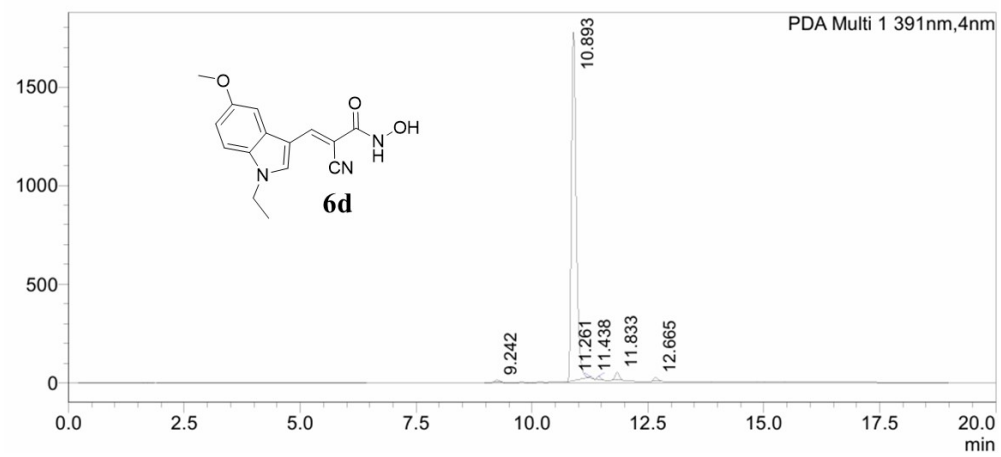
Supporting Spectra S27: HRMS Spectra for the compound 6c.



Supporting Spectra S28: ^{1}H NMR Spectra for the compound 6d.



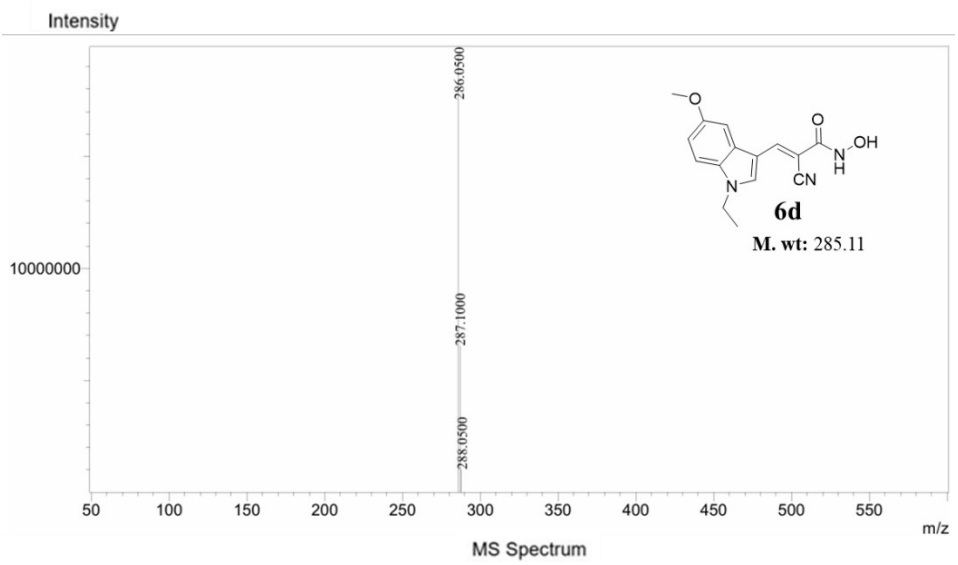
Supporting Spectra S29: ^{13}C NMR Spectra for the compound 6d.



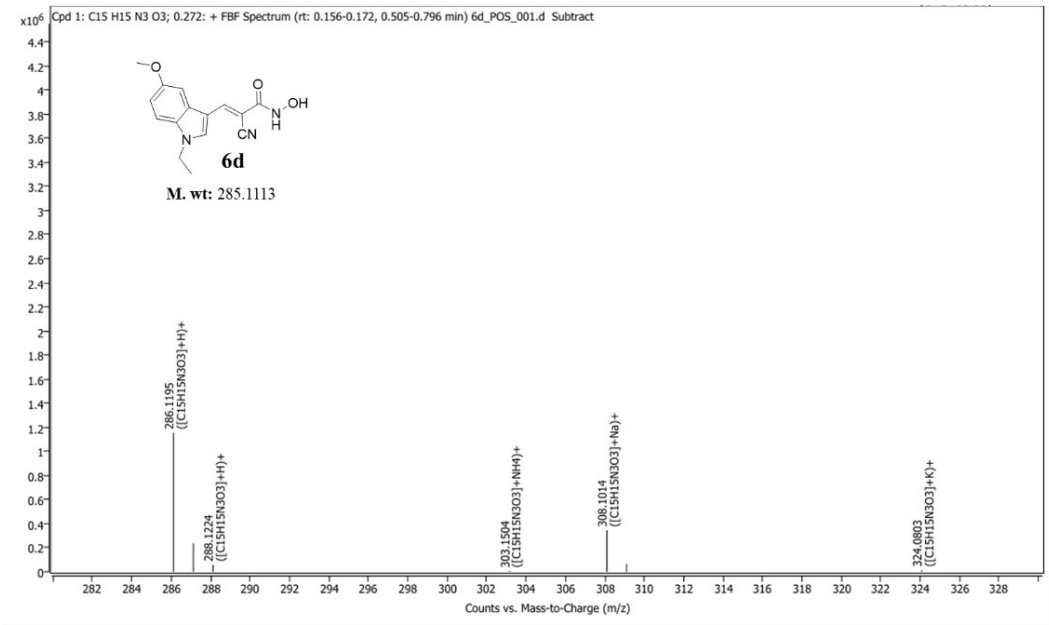
PDA Ch1 391nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	9.242	55968	8949	0.425	0.483
2	10.893	12681531	1766003	96.385	95.372
3	11.261	29746	7418	0.226	0.401
4	11.438	74014	15434	0.563	0.833
5	11.833	217936	36833	1.656	1.989
6	12.665	97902	17062	0.744	0.921
Total		13157096	1851699	100.000	100.000

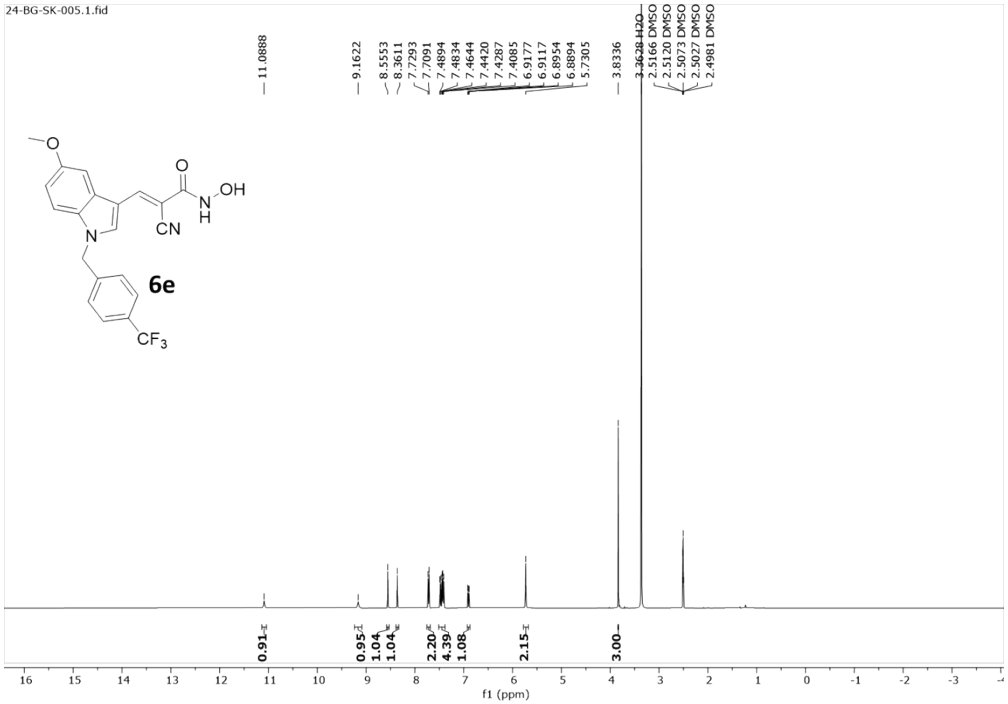
Supporting Spectra S30: HPLC traces of compound 6d.



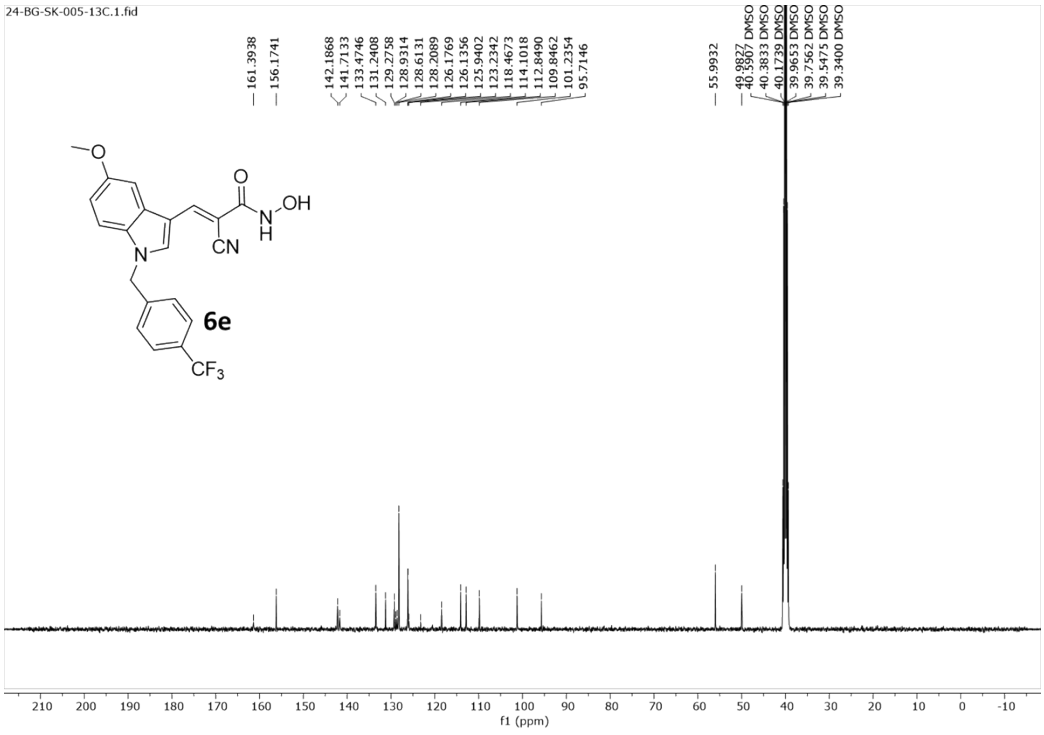
Supporting Spectra S31: LC-MS Spectra for the compound 6d.



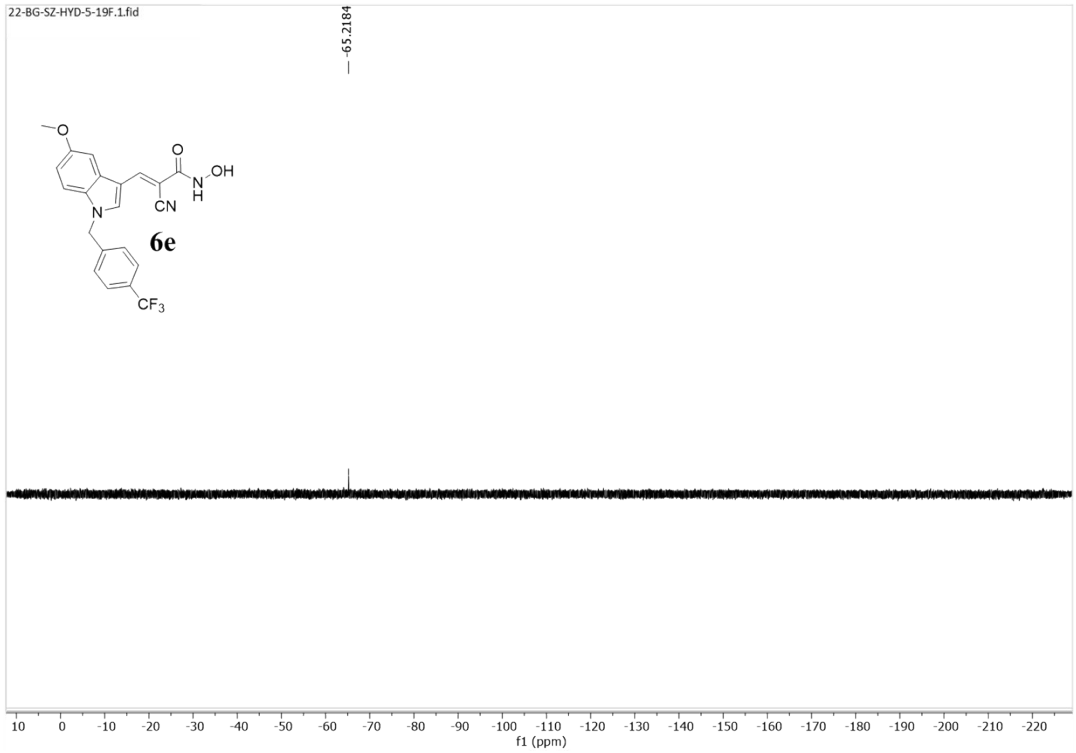
Supporting Spectra S32: HRMS Spectra for the compound 6d.



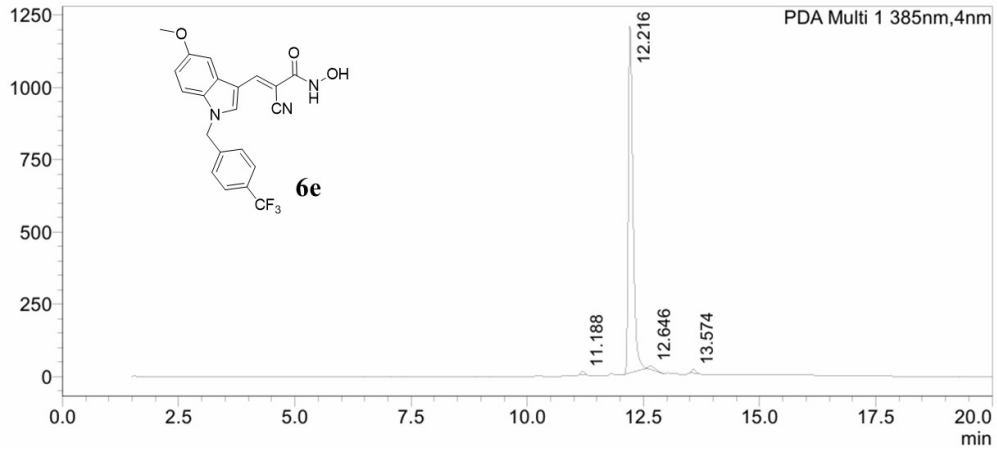
Supporting Spectra S33: ^{1}H NMR Spectra for the compound 6e.



Supporting Spectra S34: ^{13}C NMR Spectra for the compound 6e.



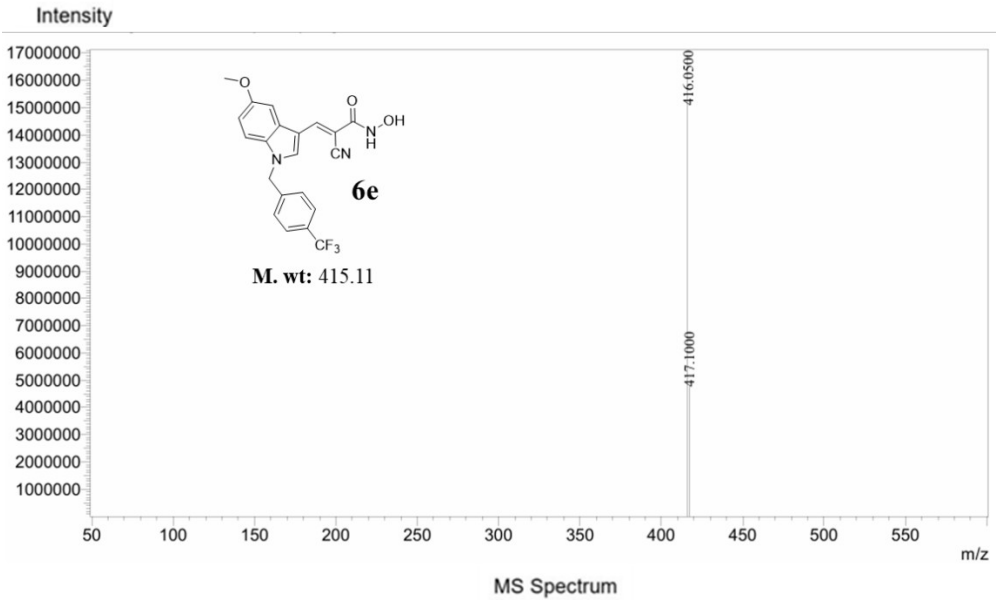
Supporting Spectra S35: ^{19}F NMR Spectra for the compound 6e.



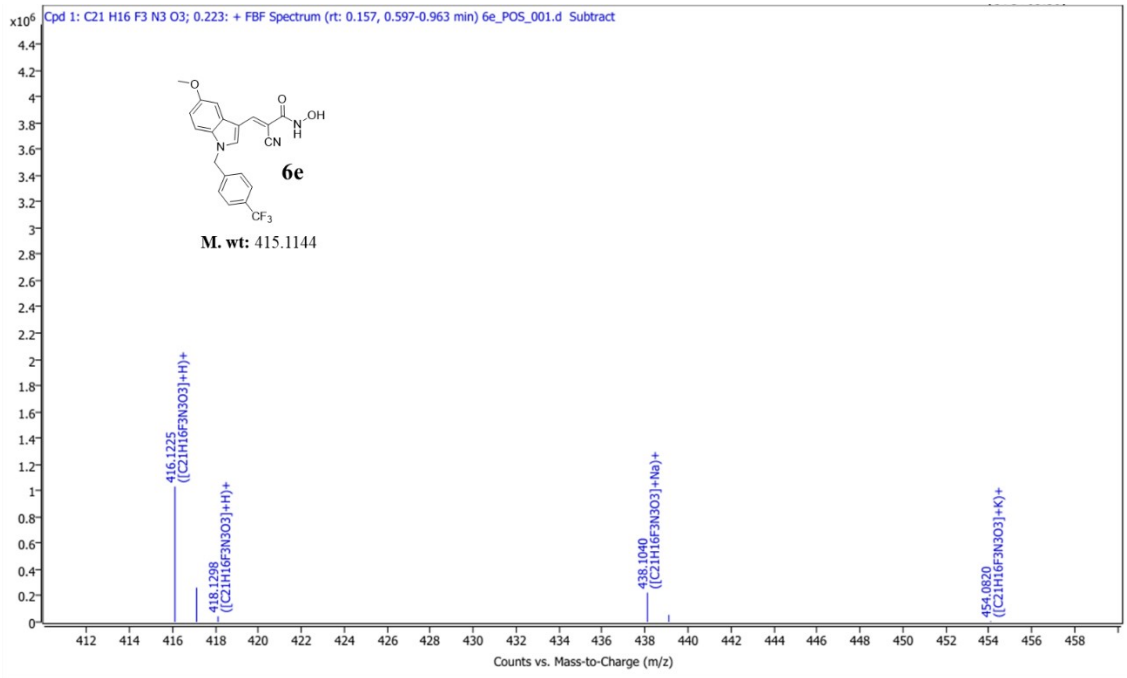
PDA Ch1 385nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.188	51279	9668	0.597	0.784
2	12.216	8354929	1198634	97.270	97.187
3	12.646	105064	11798	1.223	0.957
4	13.574	78140	13232	0.910	1.073
Total		8589412	1233332	100.000	100.000

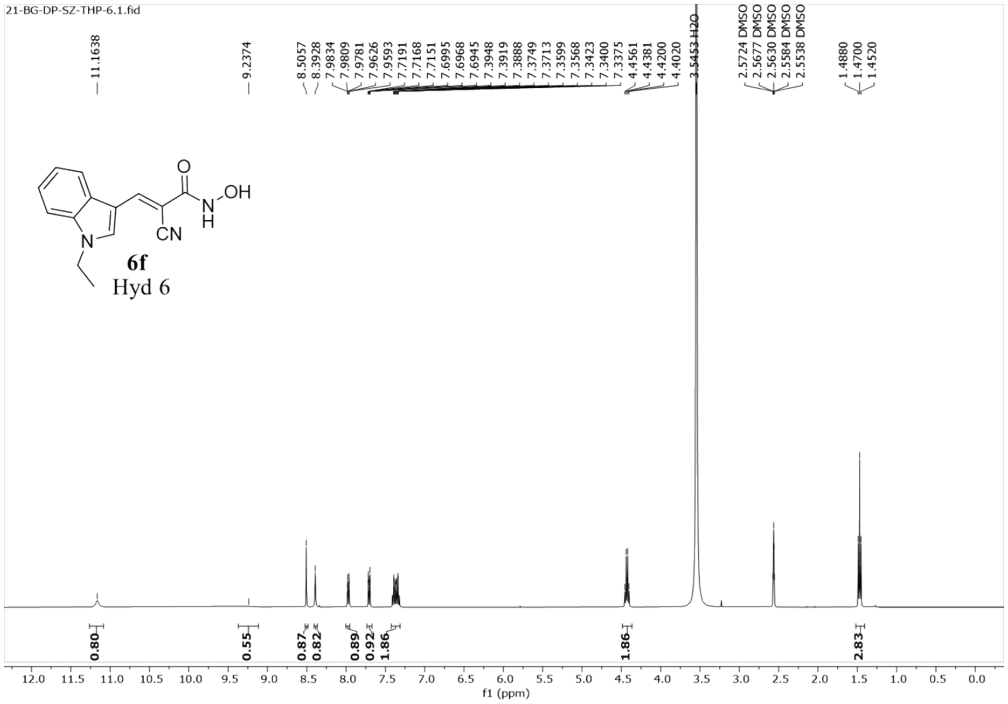
Supporting Spectra S36: HPLC traces of compound 6e.



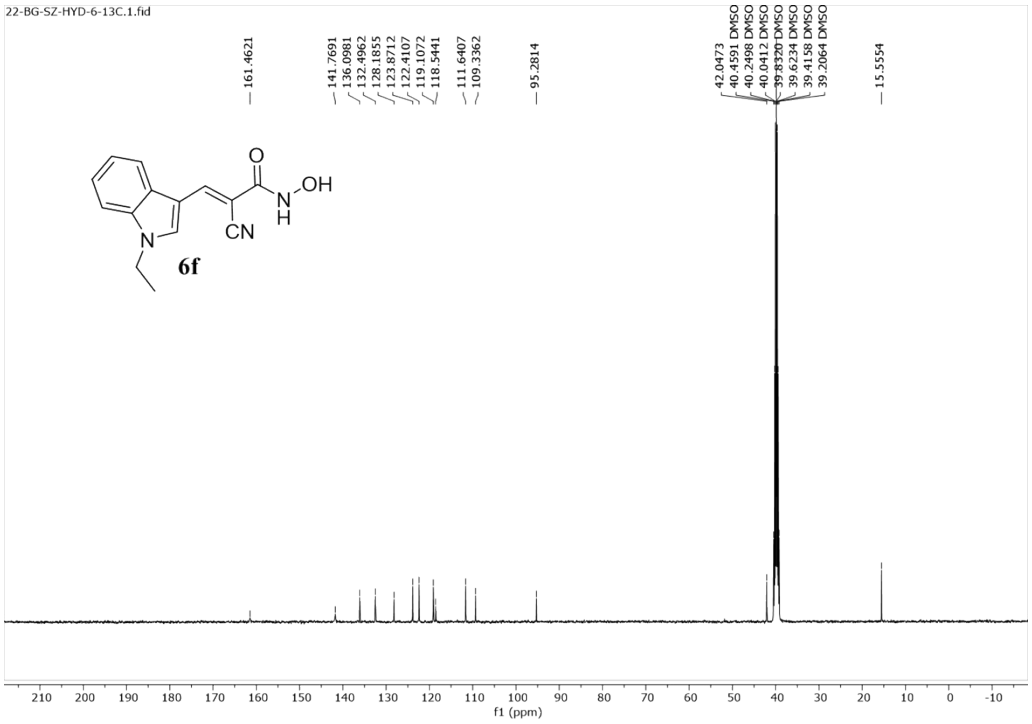
Supporting Spectra S37: LC-MS Spectra for the compound 6e.



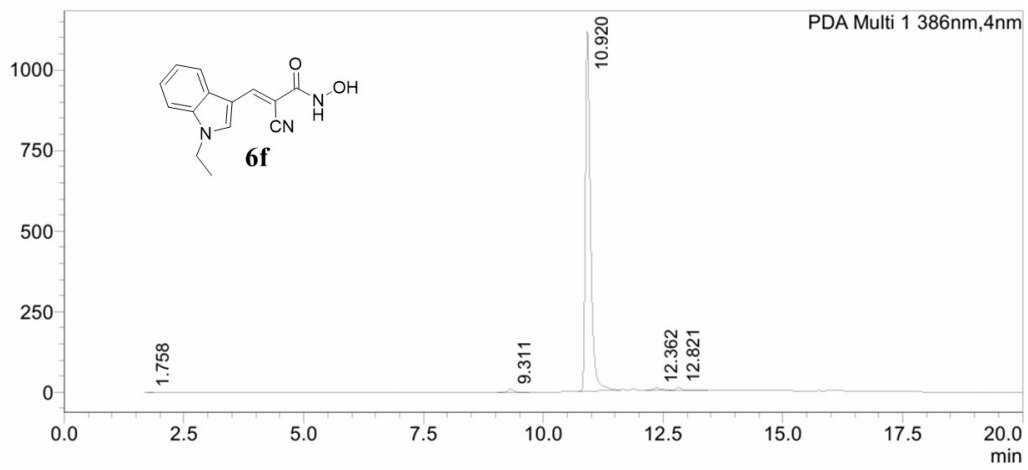
Supporting Spectra S38: HRMS Spectra for the compound 6e.



Supporting Spectra S39: ^{1}H NMR Spectra for the compound 6f.



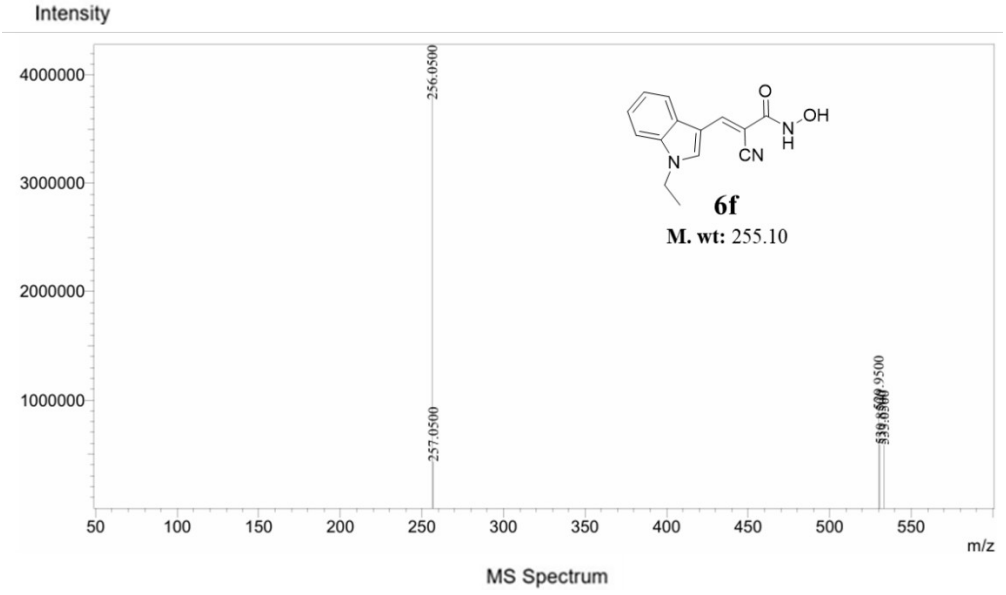
Supporting Spectra S40: ^{13}C NMR Spectra for the compound 6f.



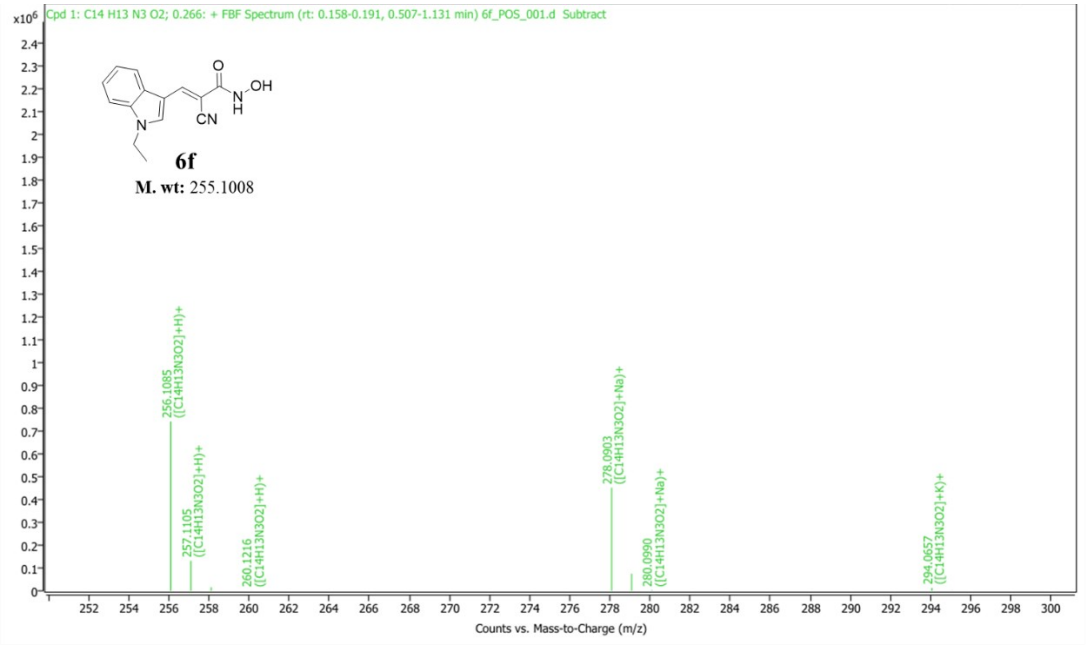
PDA Ch1 386nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	1.758	2996	820	0.035	0.072
2	9.311	84436	9655	0.974	0.844
3	10.920	8400757	1116924	96.920	97.593
4	12.362	93439	7016	1.078	0.613
5	12.821	86091	10050	0.993	0.878
Total		8667719	1144466	100.000	100.000

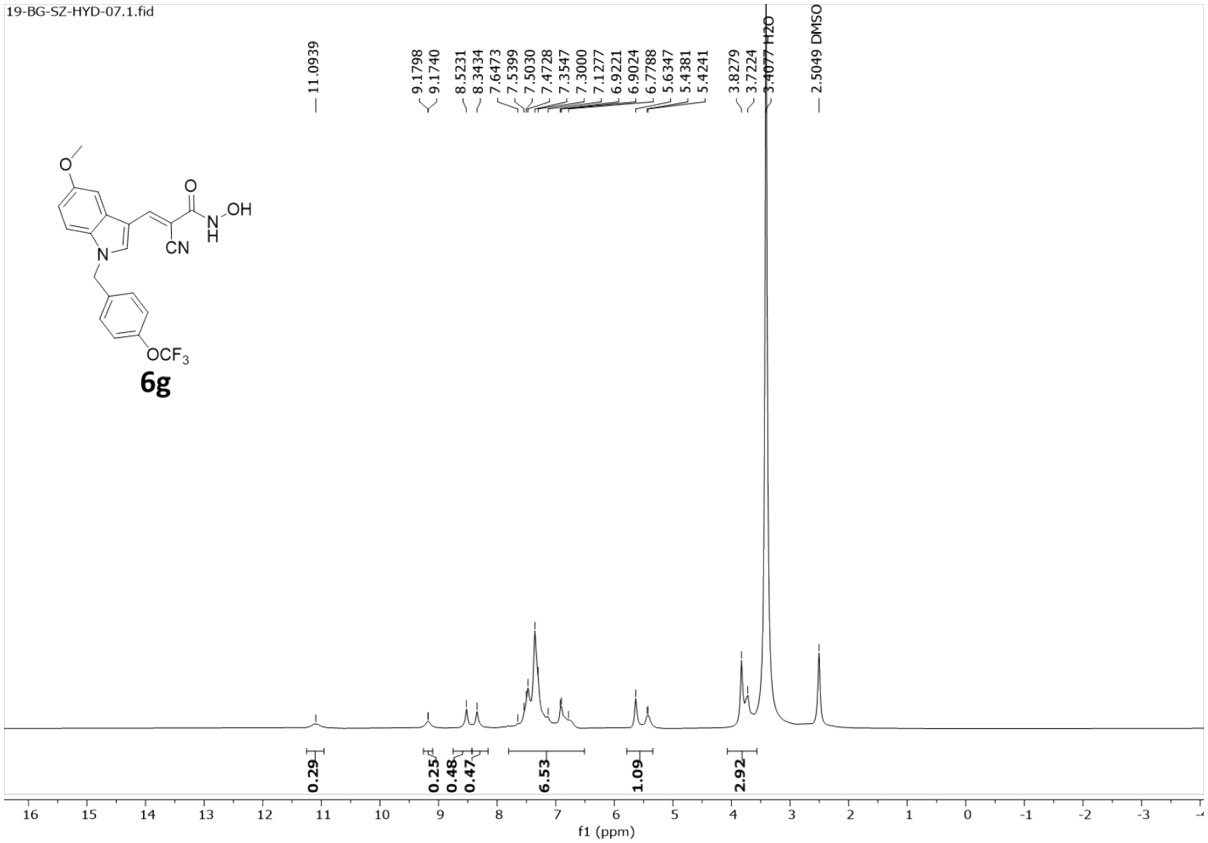
Supporting Spectra S41: HPLC traces of compound 6f.



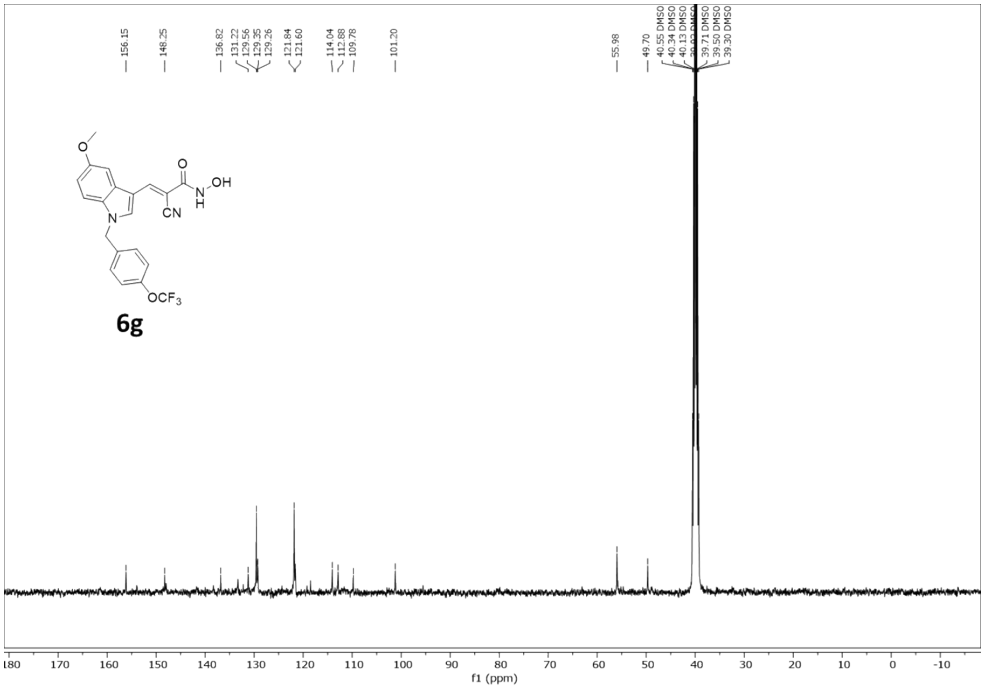
Supporting Spectra S42: LC-MS Spectra for the compound 6f.



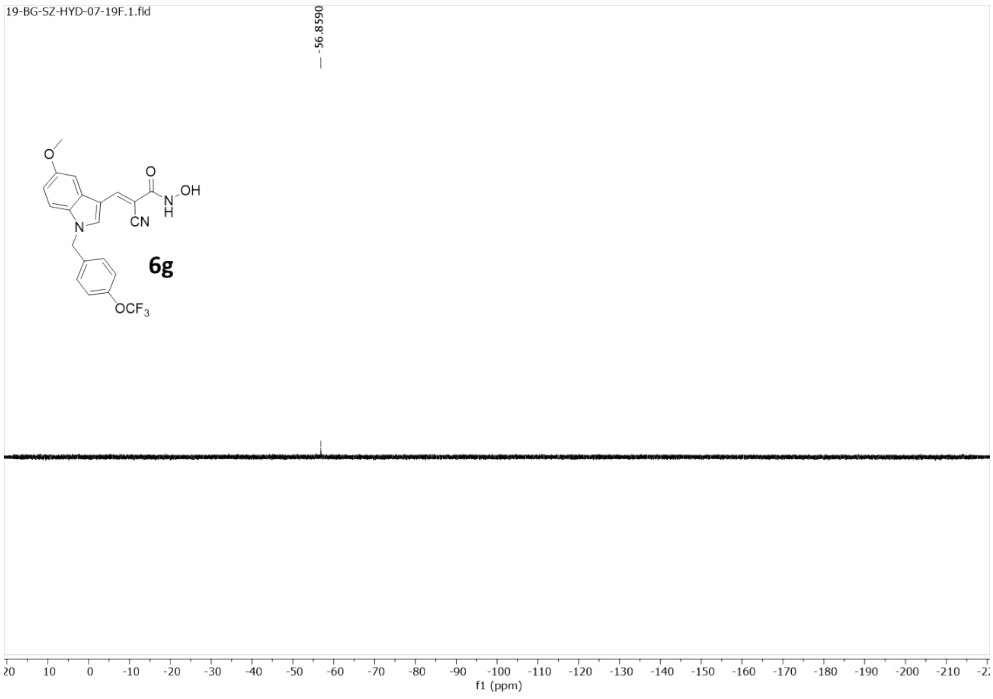
Supporting Spectra S43: HRMS Spectra for the compound 6f.



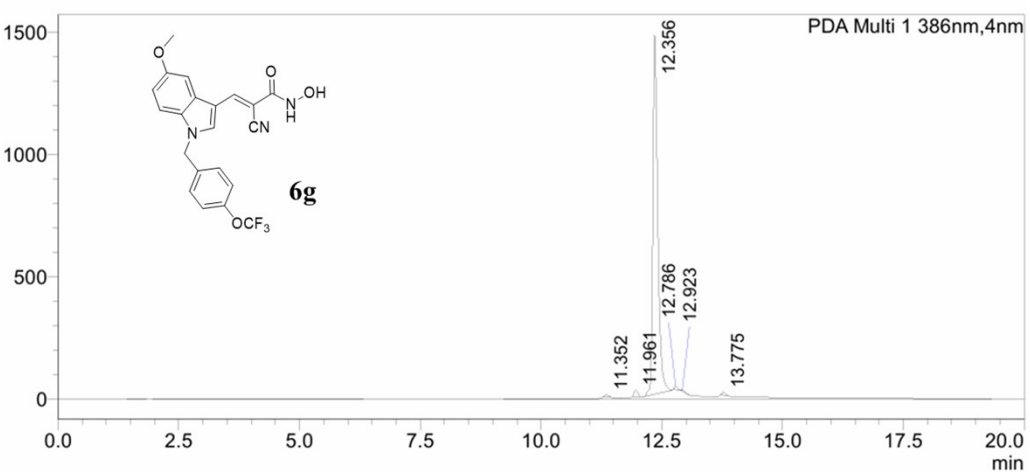
Supporting Spectra S44: ^{1}H NMR Spectra for the compound 6g.



Supporting Spectra S45: ^{13}C NMR Spectra for the compound 6g.



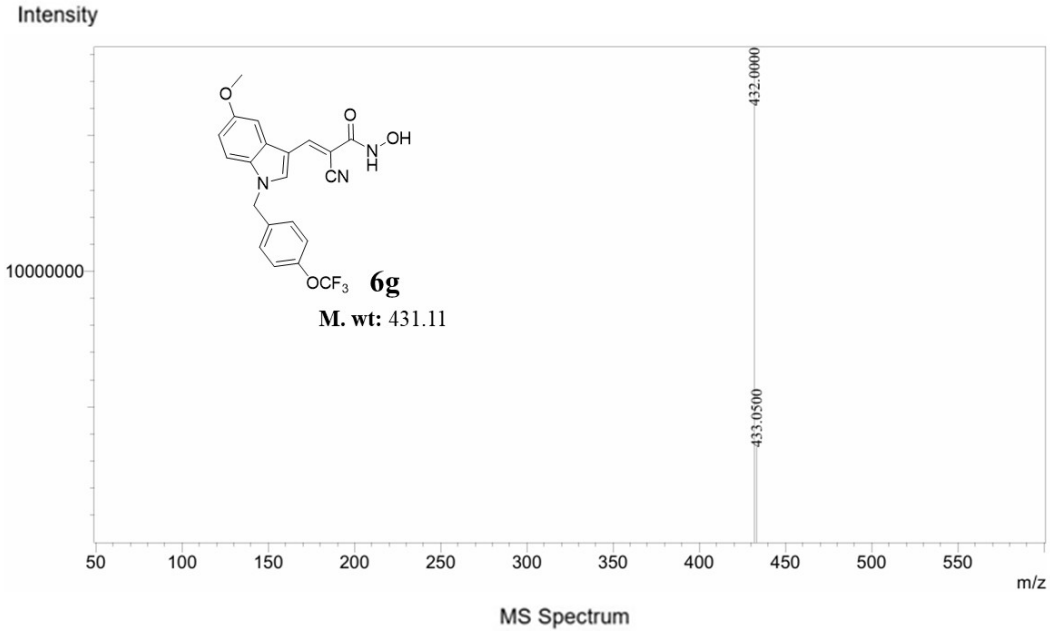
Supporting Spectra S46: ^{19}F NMR Spectra for the compound 6g.



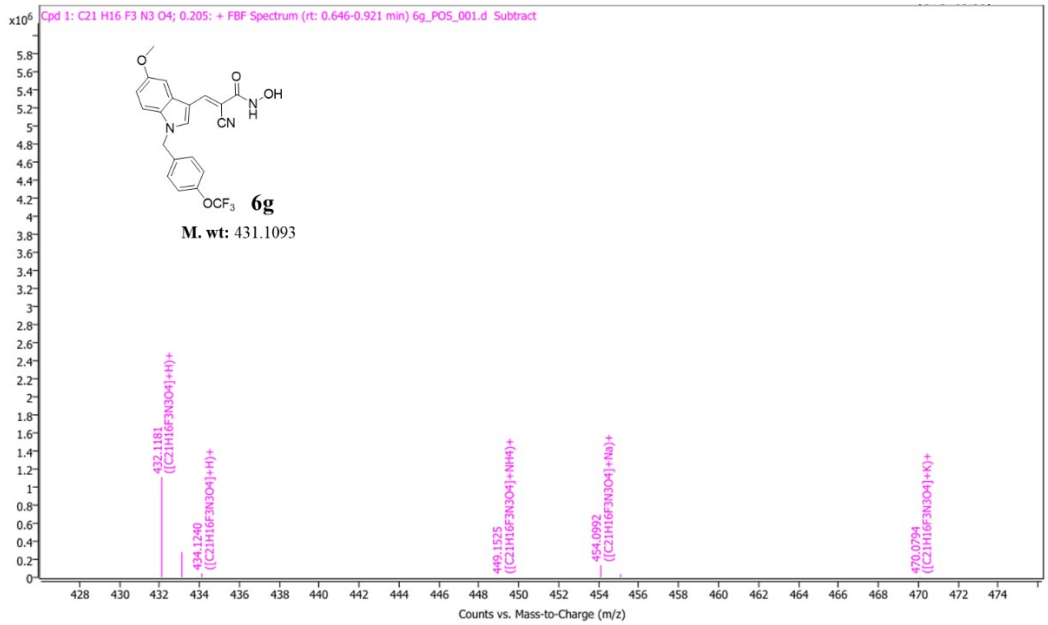
PDA Ch1 386nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.352	55378	9887	0.515	0.647
2	11.961	126335	24410	1.175	1.596
3	12.356	10442125	1469240	97.119	96.083
4	12.786	61499	13318	0.572	0.871
5	12.923	12457	1836	0.116	0.120
6	13.775	54106	10440	0.503	0.683
Total		10751901	1529132	100.000	100.000

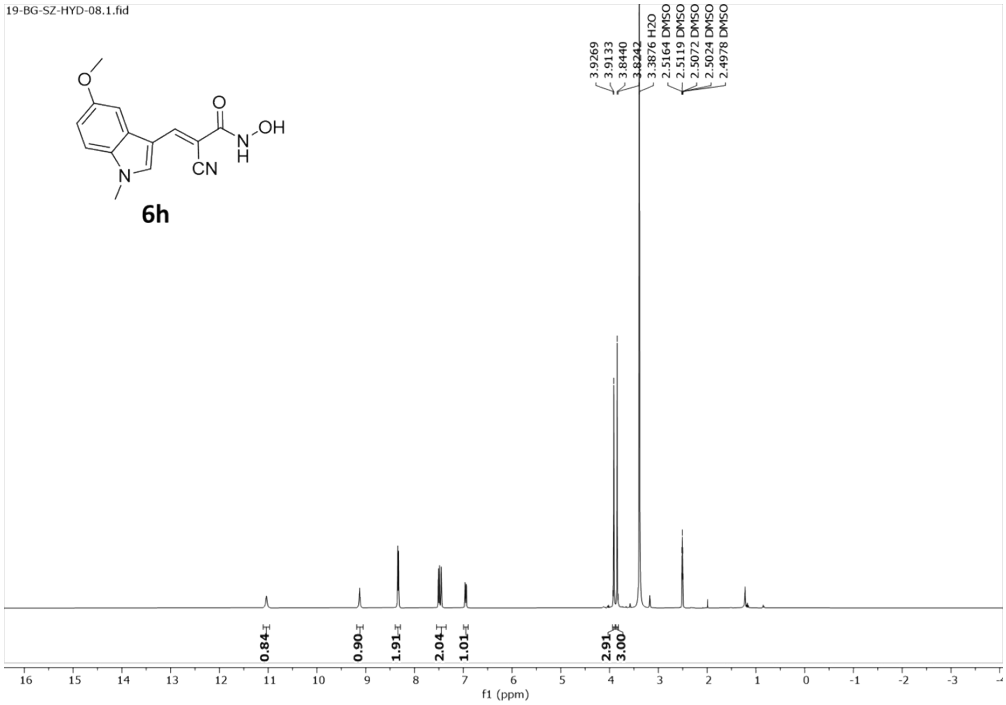
Supporting Spectra S47: HPLC traces of compound 6g.



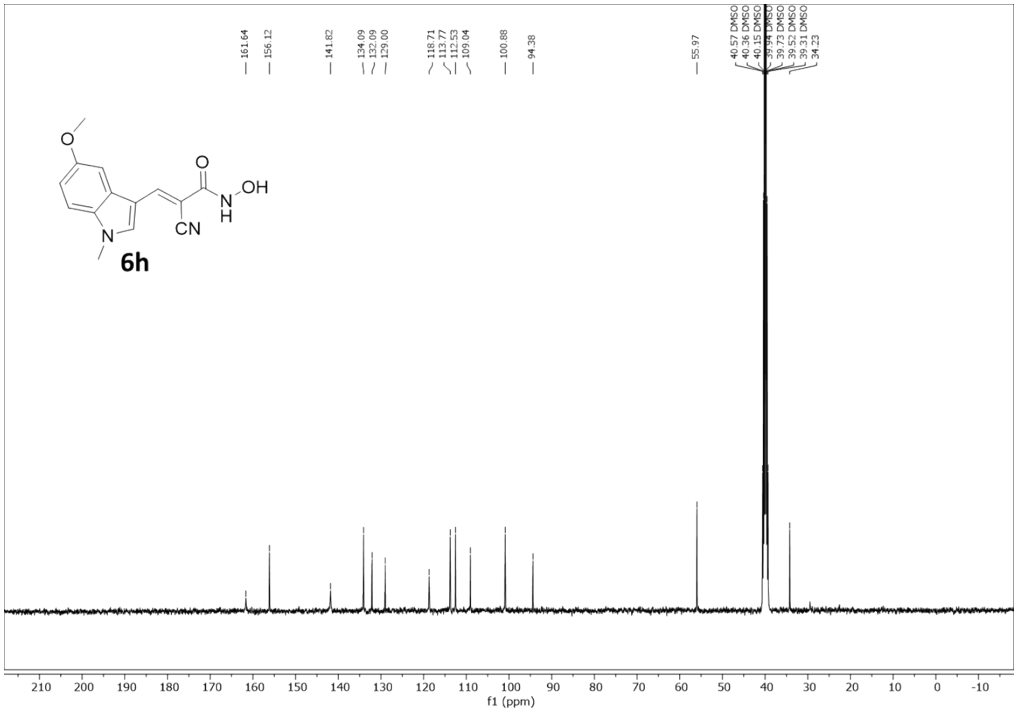
Supporting Spectra S48: LC-MS Spectra for the compound 6g.



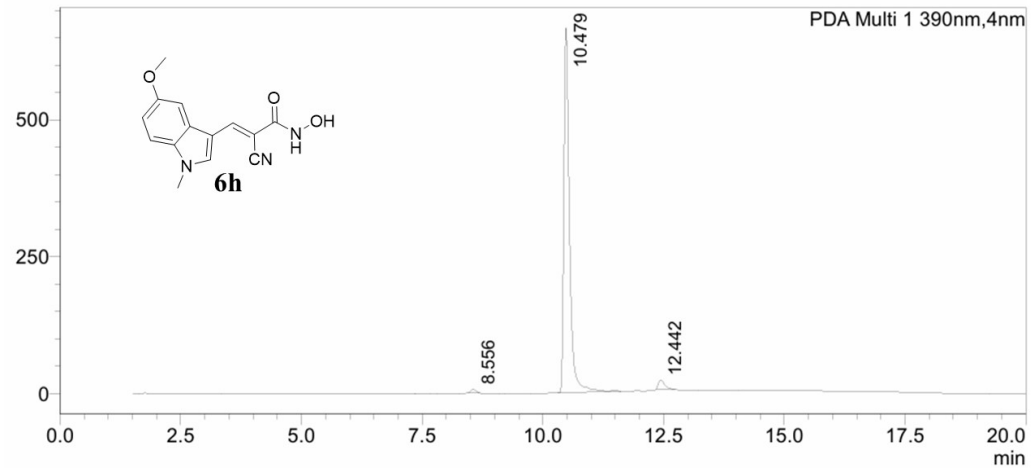
Supporting Spectra S49: HRMS Spectra for the compound 6g.



Supporting Spectra S50: ^{1}H NMR Spectra for the compound 6h.



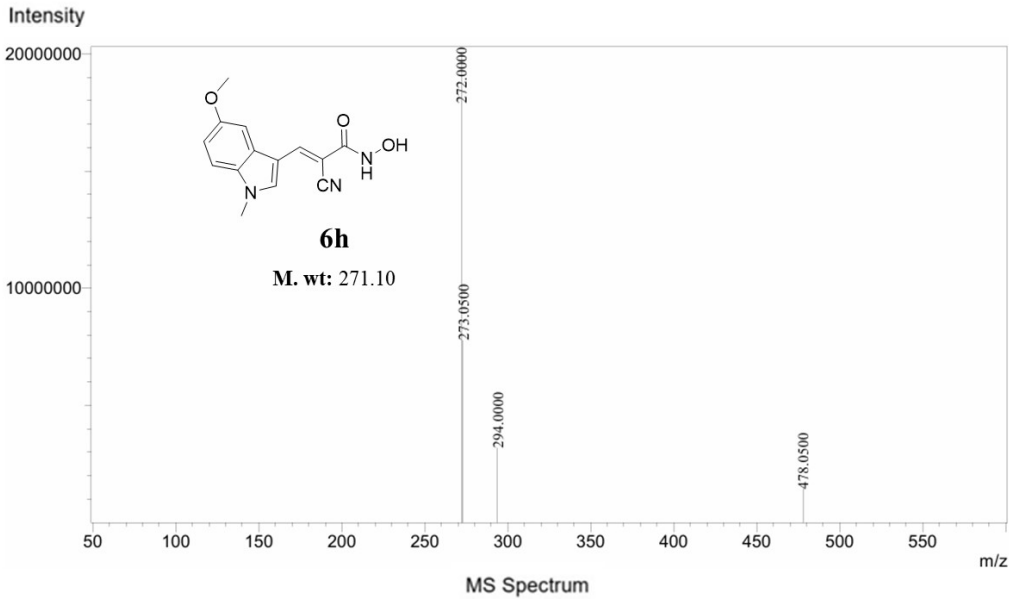
Supporting Spectra S51: ^{13}C NMR Spectra for compound 6h.



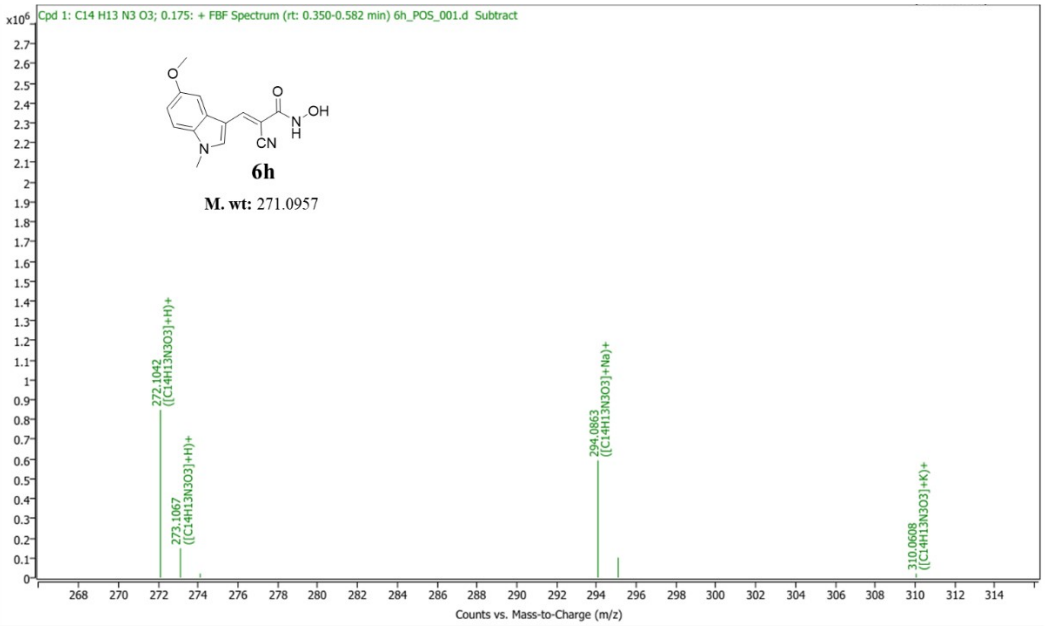
PDA Ch1 390nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	8.556	43165	5986	0.768	0.869
2	10.479	5419274	665982	96.420	96.683
3	12.442	158052	16863	2.812	2.448
Total		5620491	688832	100.000	100.000

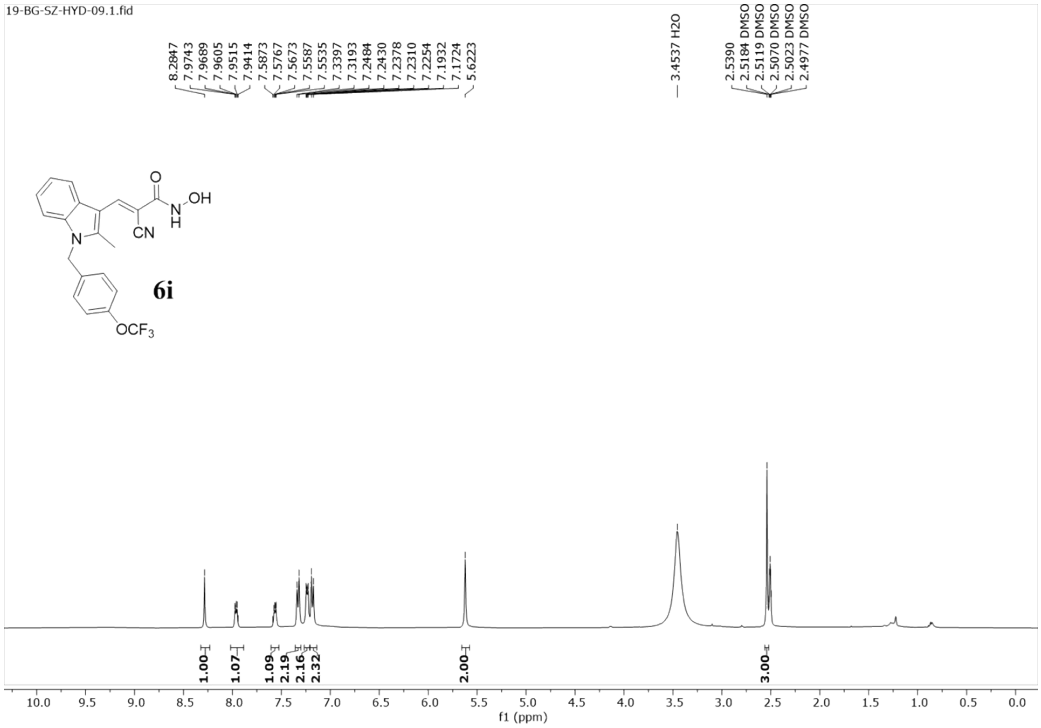
Supporting Spectra S52: HPLC traces of compound 6h.



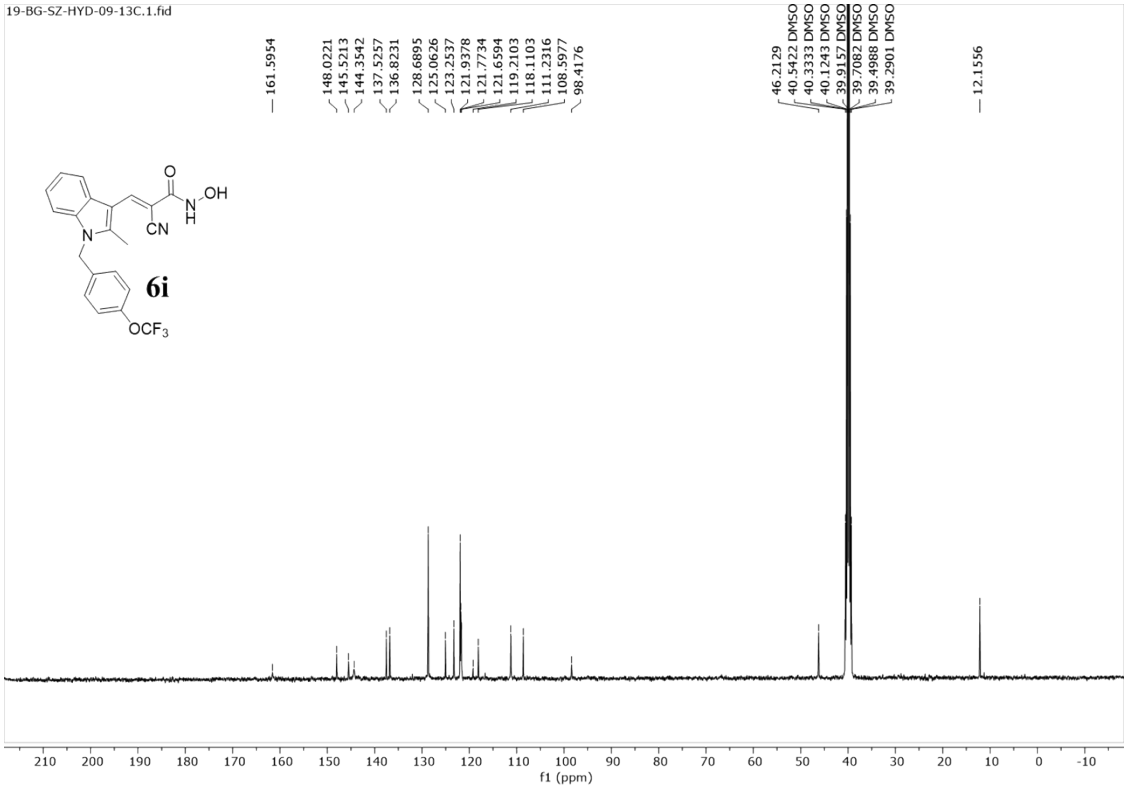
Supporting Spectra S53: LC-MS Spectra for the compound 6h.



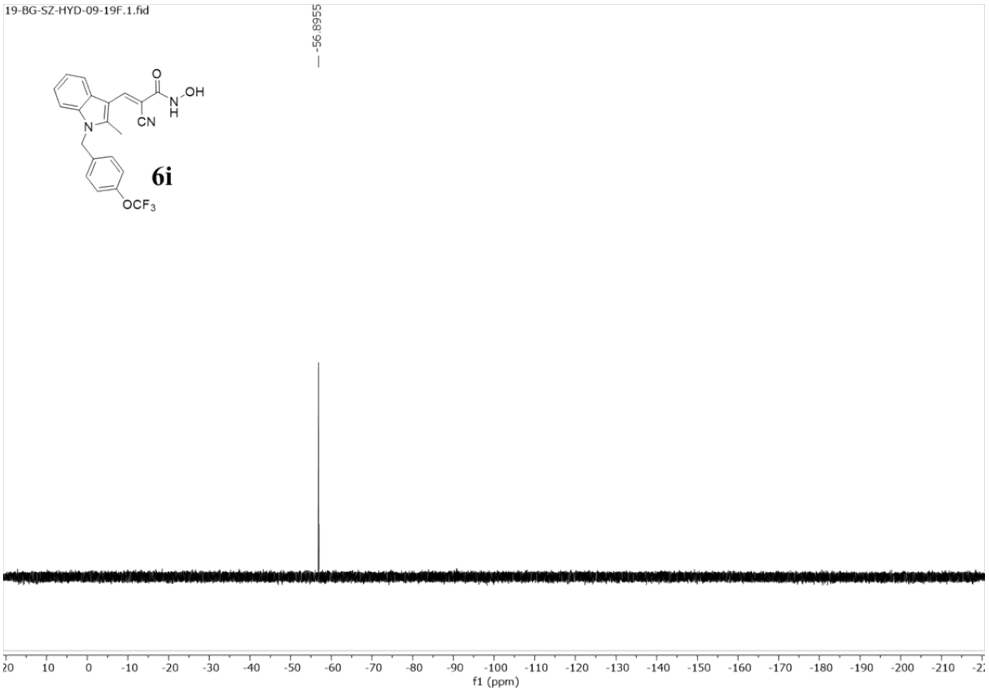
Supporting Spectra S54: HRMS Spectra for the compound 6h.



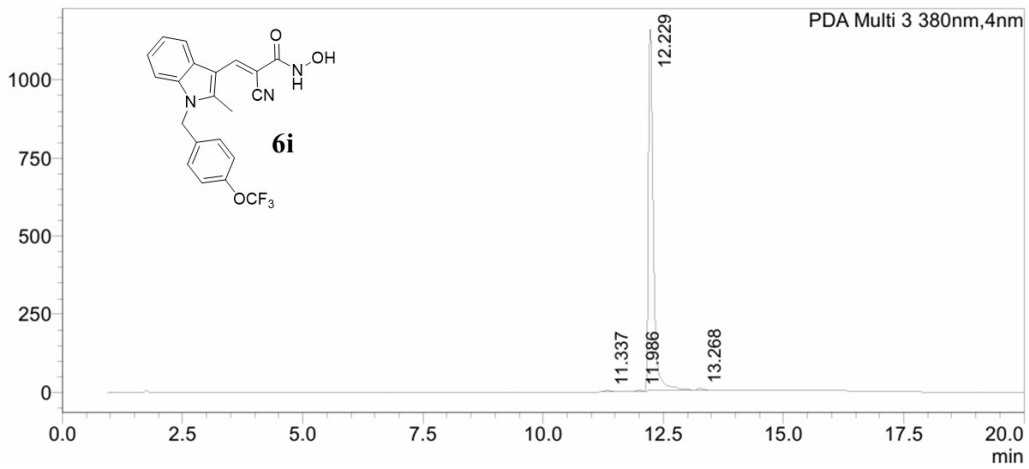
Supporting Spectra S55: ^{1}H NMR Spectra for compound 6i.



Supporting Spectra S56: ^{13}C NMR Spectra for compound 6i.



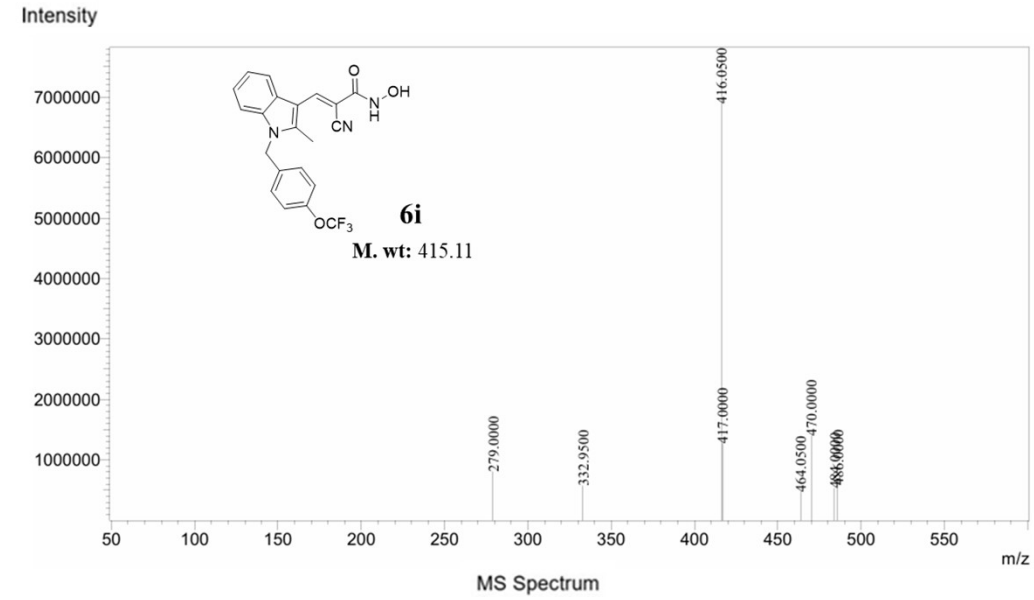
Supporting Spectra S57: ^{19}F NMR Spectra for compound 6i.



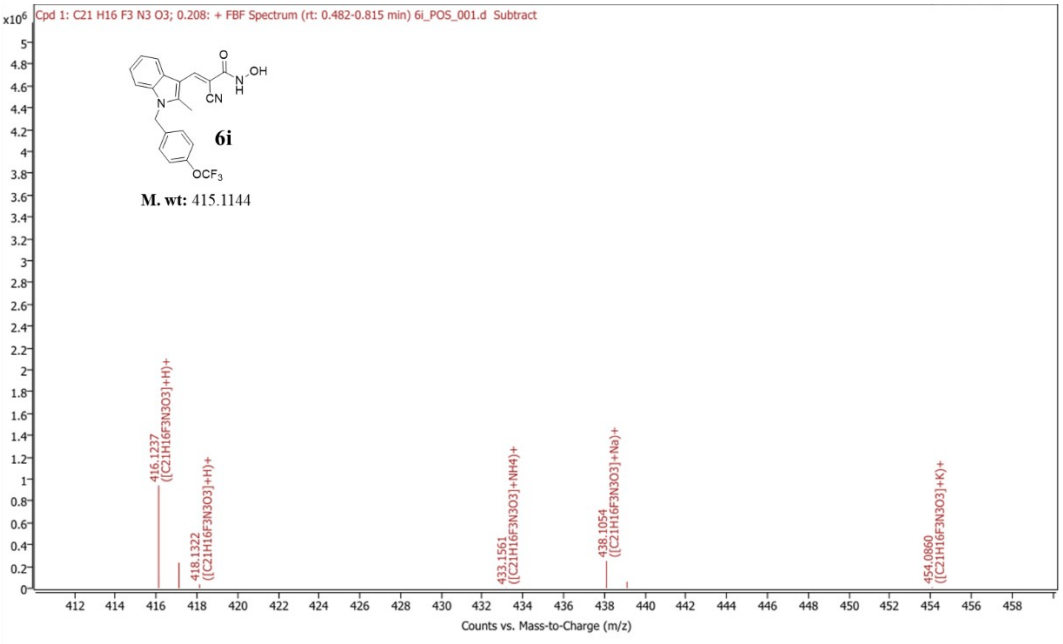
PDA Ch3 380nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.337	23484	4133	0.284	0.353
2	11.986	11037	1874	0.134	0.160
3	12.229	8181903	1156904	99.100	98.953
4	13.268	39745	6233	0.481	0.533
Total		8256169	1169143	100.000	100.000

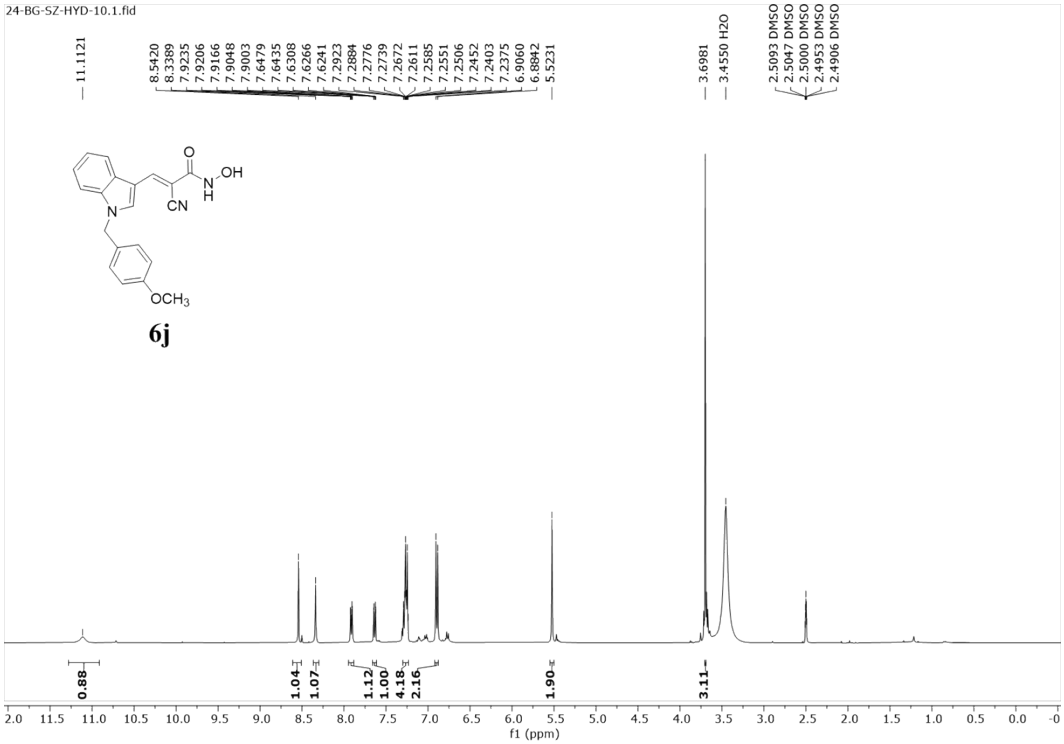
Supporting Spectra S58: HPLC traces of compound 6i.



Supporting Spectra S59: LC-MS Spectra for the compound 6i.

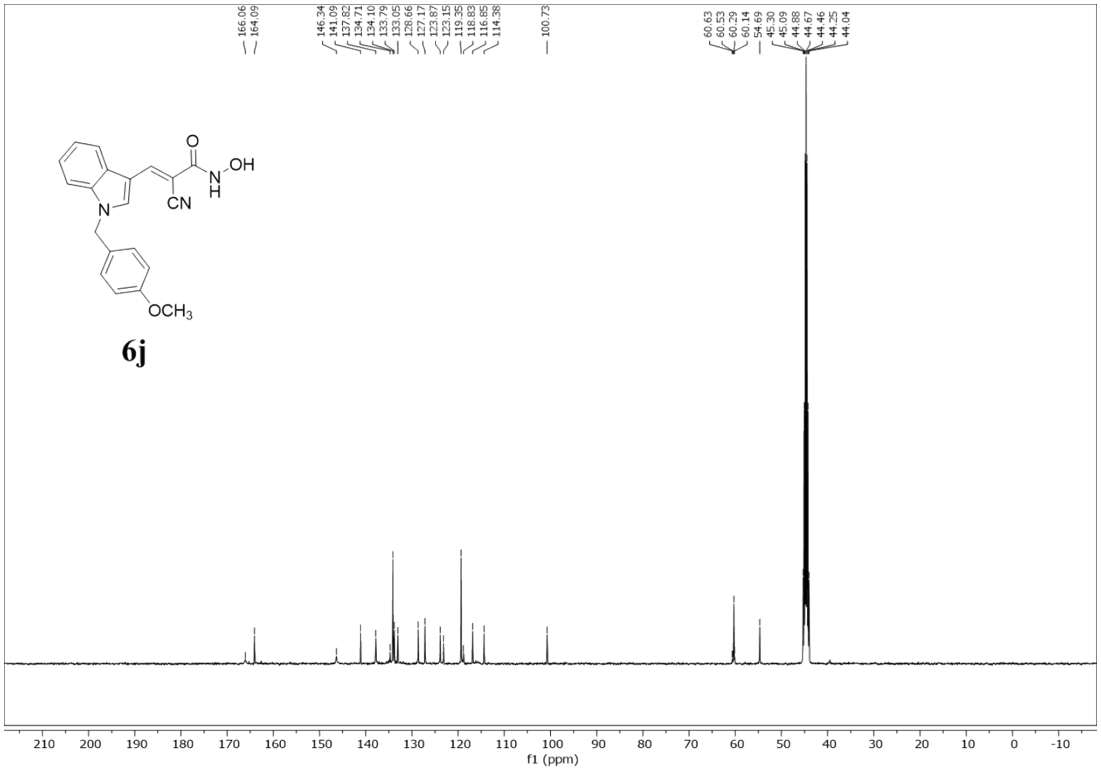


Supporting Spectra S60: HRMS Spectra for the compound 6i.



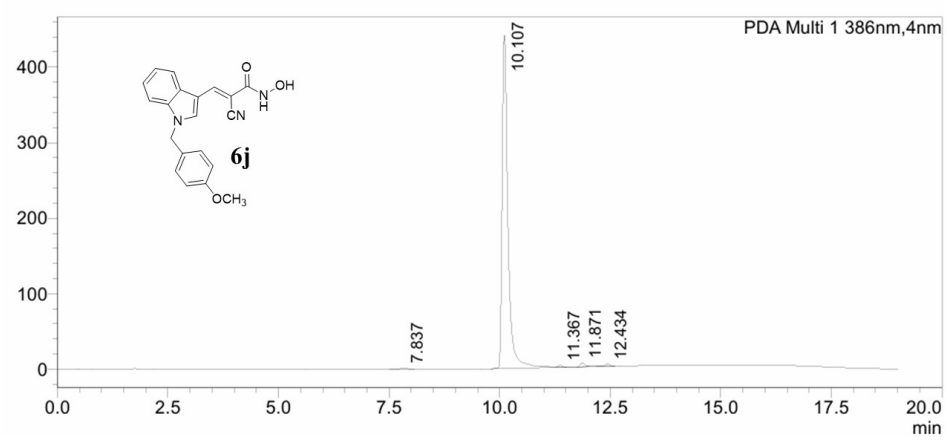
6j

Supporting Spectra S61: ^{1}H NMR Spectra for compound 6j.



6j

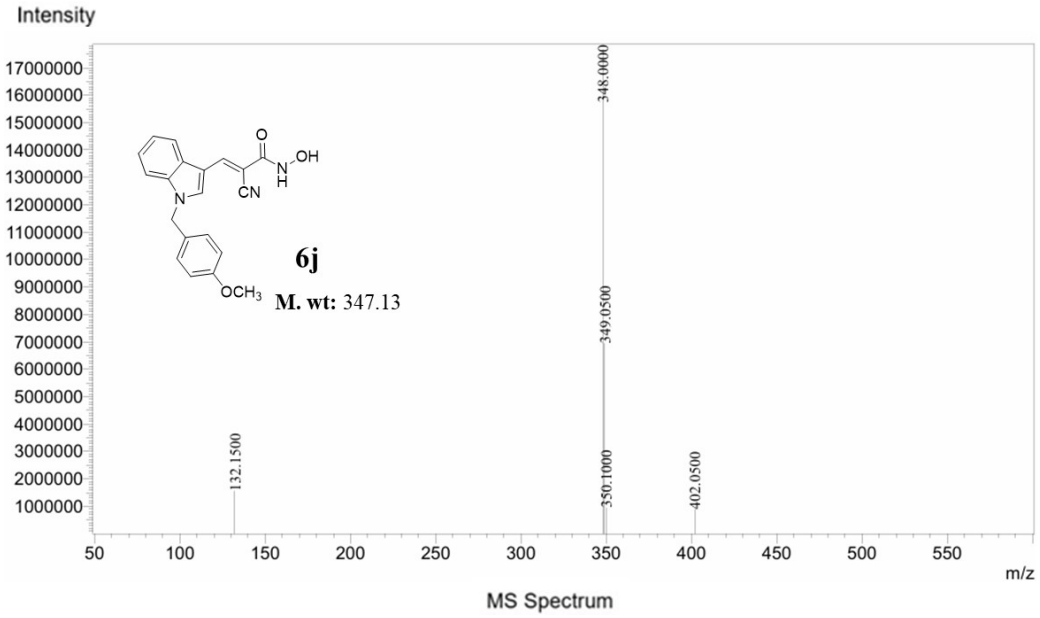
Supporting Spectra S62: ^{13}C NMR Spectra for compound 6j.



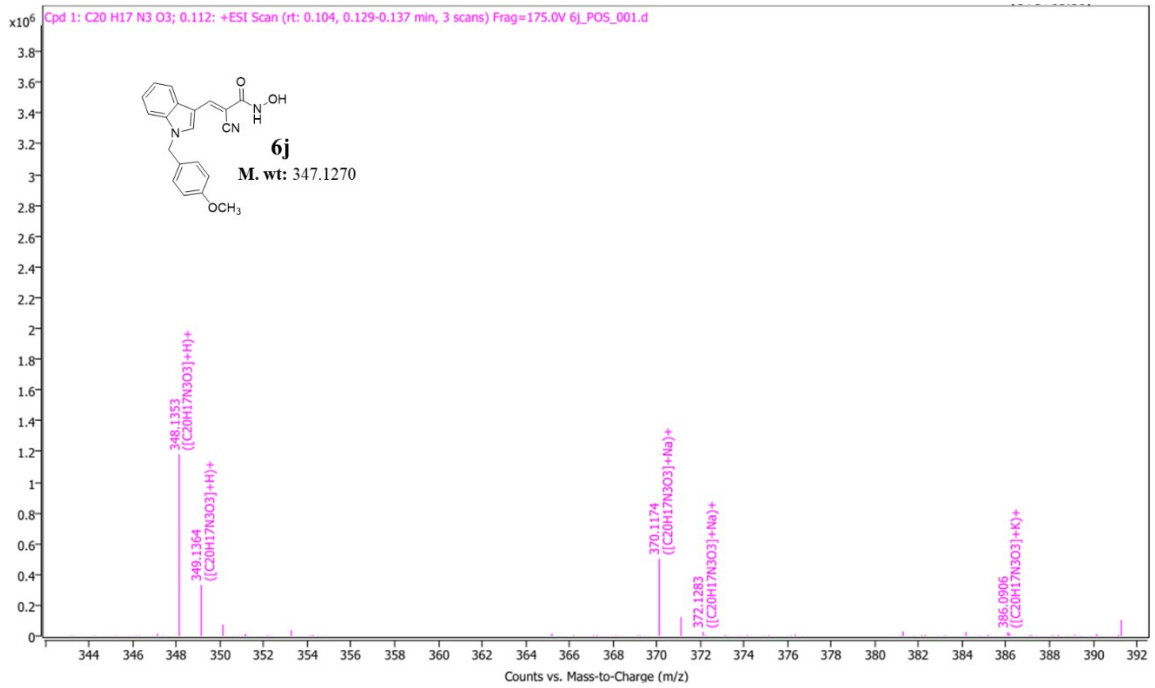
PDA Ch1 386nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	7.837	16273	1625	0.398	0.359
2	10.107	4001561	440828	97.959	97.302
3	11.367	11756	1956	0.288	0.432
4	11.871	33856	5487	0.829	1.211
5	12.434	21488	3153	0.526	0.696
Total		4084933	453049	100.000	100.000

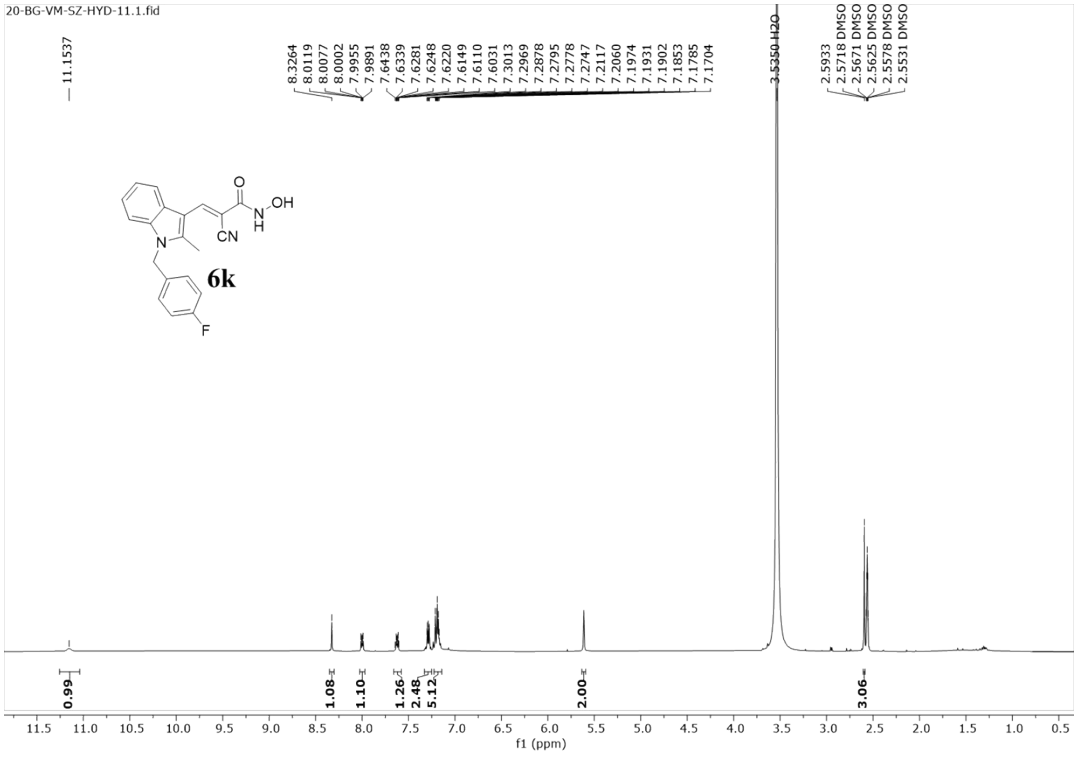
Supporting Spectra S63: HPLC traces of compound 6j.



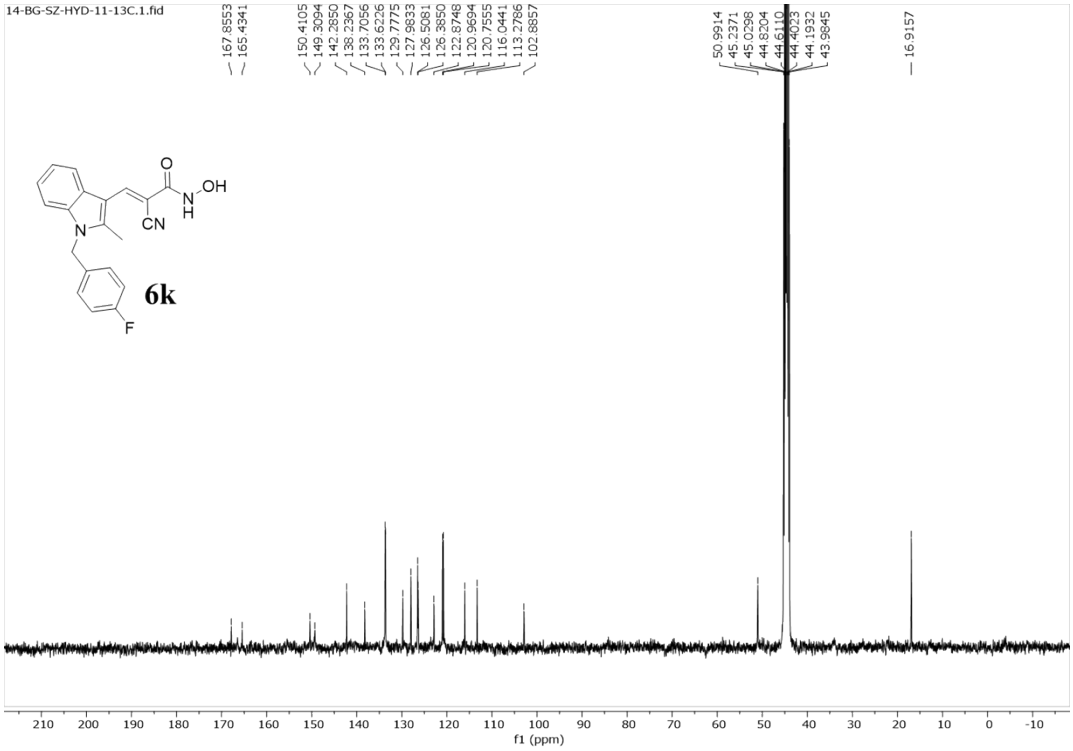
Supporting Spectra S64: LC-MS Spectra for the compound 6j.



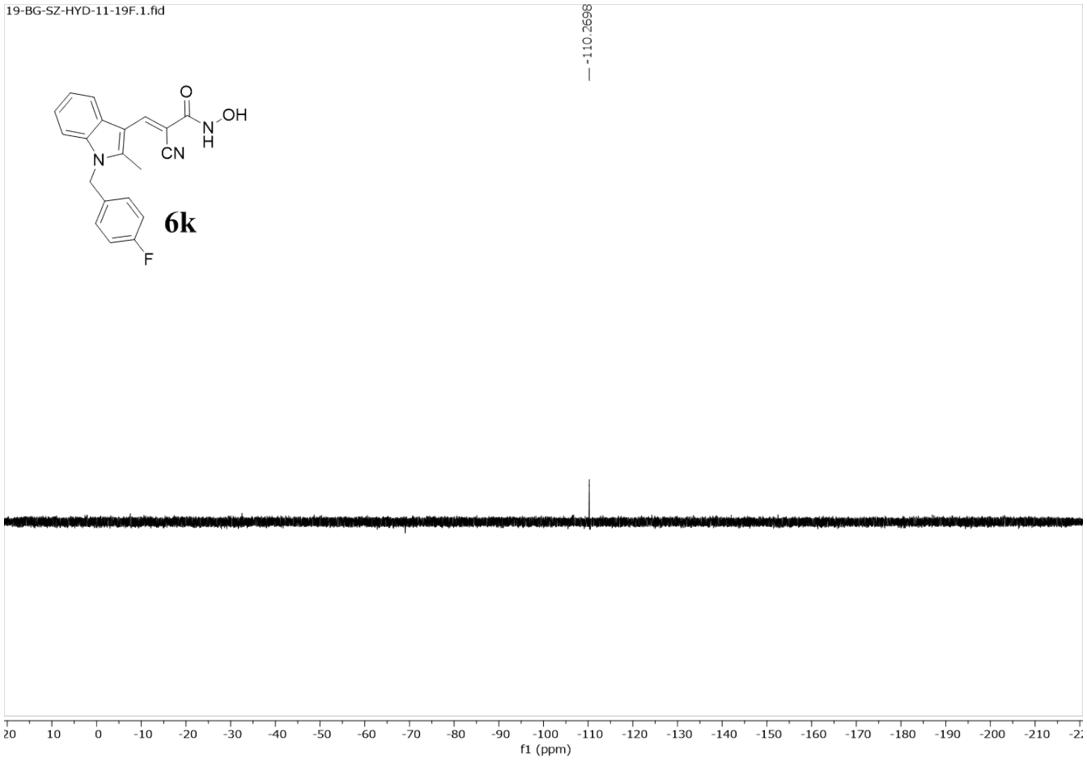
Supporting Spectra S65: HRMS Spectra for the compound 6j.



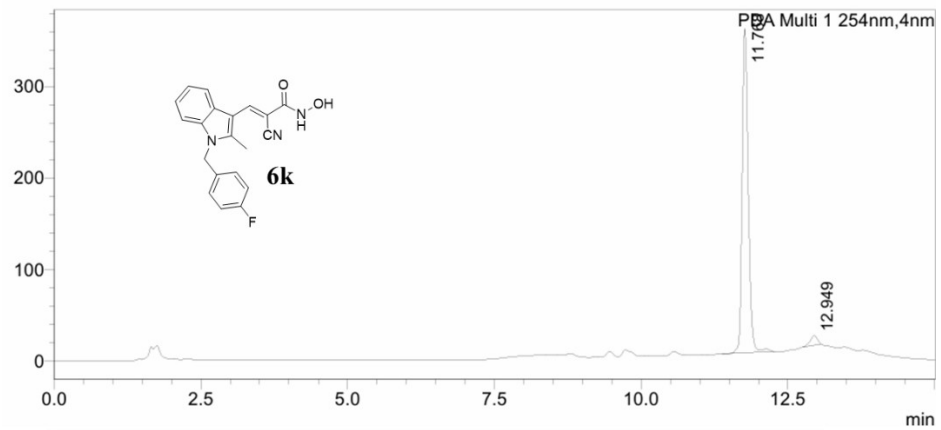
Supporting Spectra S66: ^{1}H NMR Spectra for compound 6k



Supporting Spectra S67: ^{13}C NMR Spectra for compound 6k



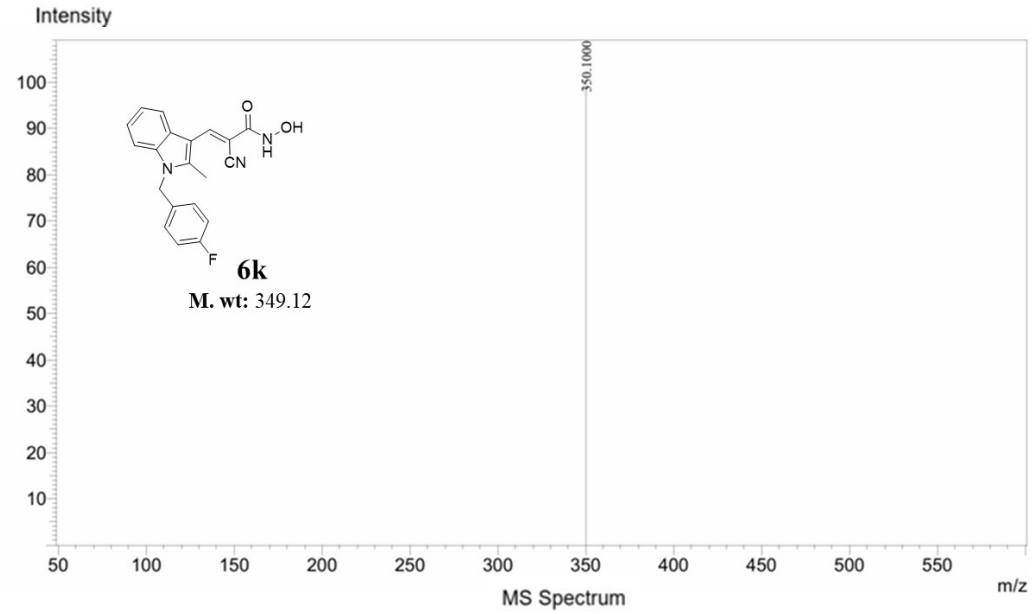
Supporting Spectra S68: ^{19}F NMR Spectra for compound 6k



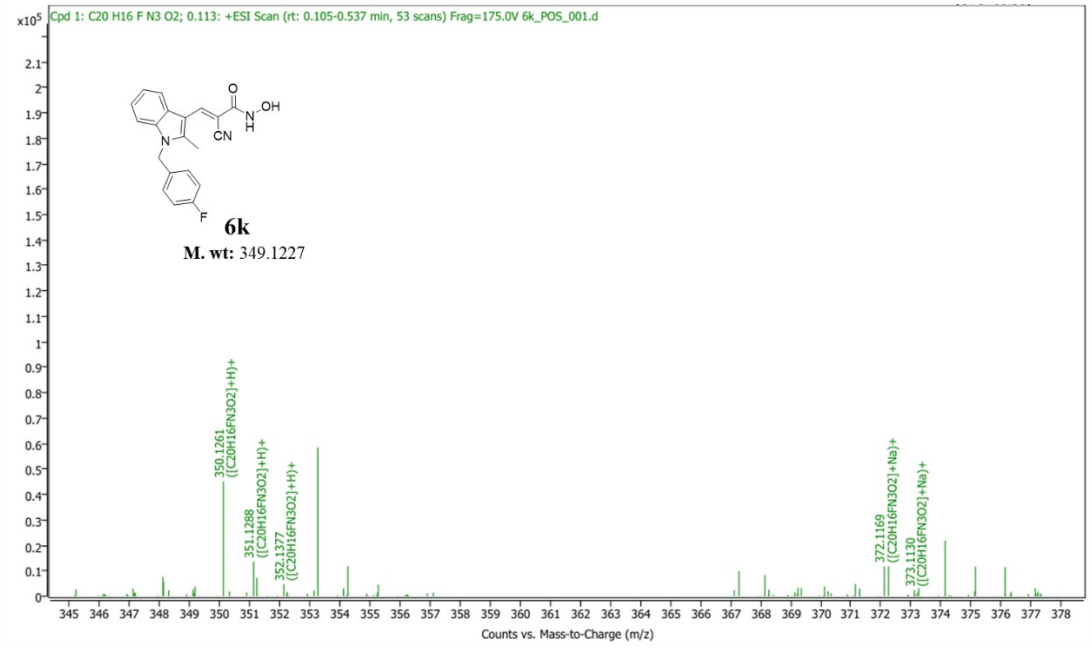
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Area%	Height%
1	11.768	2556600	354432	96.728	97.114
2	12.949	86485	10533	3.272	2.886
Total		2643085	364965	100.000	100.000

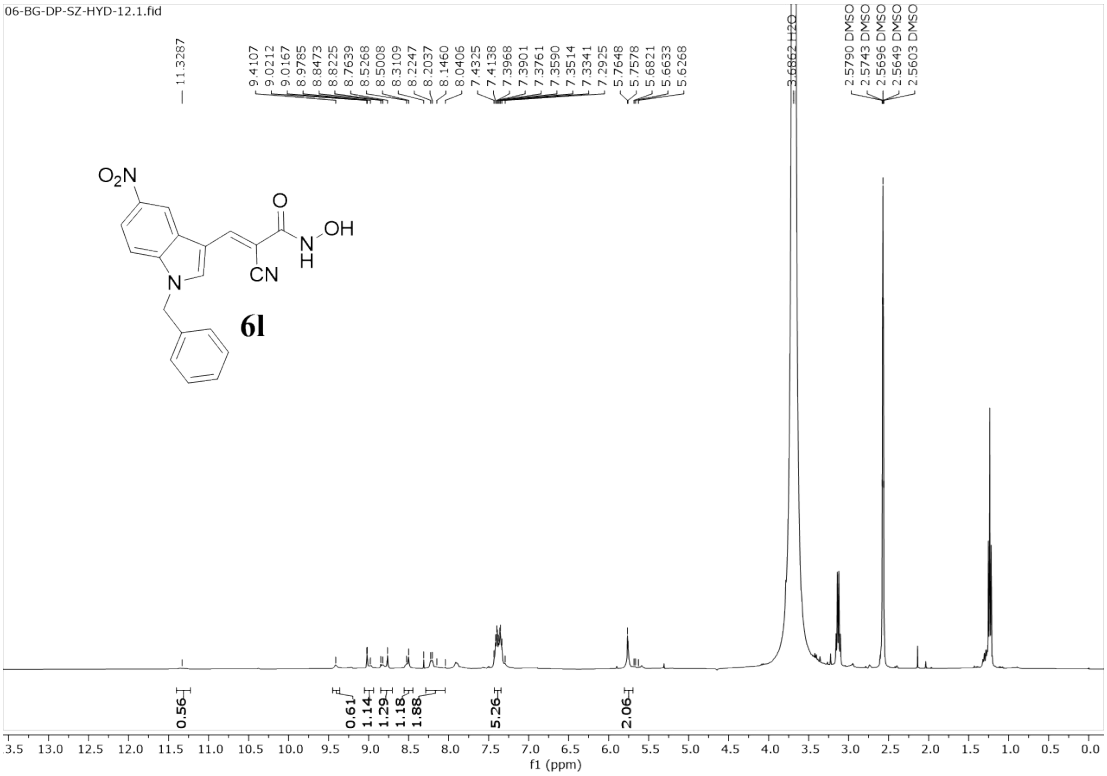
Supporting Spectra S69: HPLC traces of compound 6k.



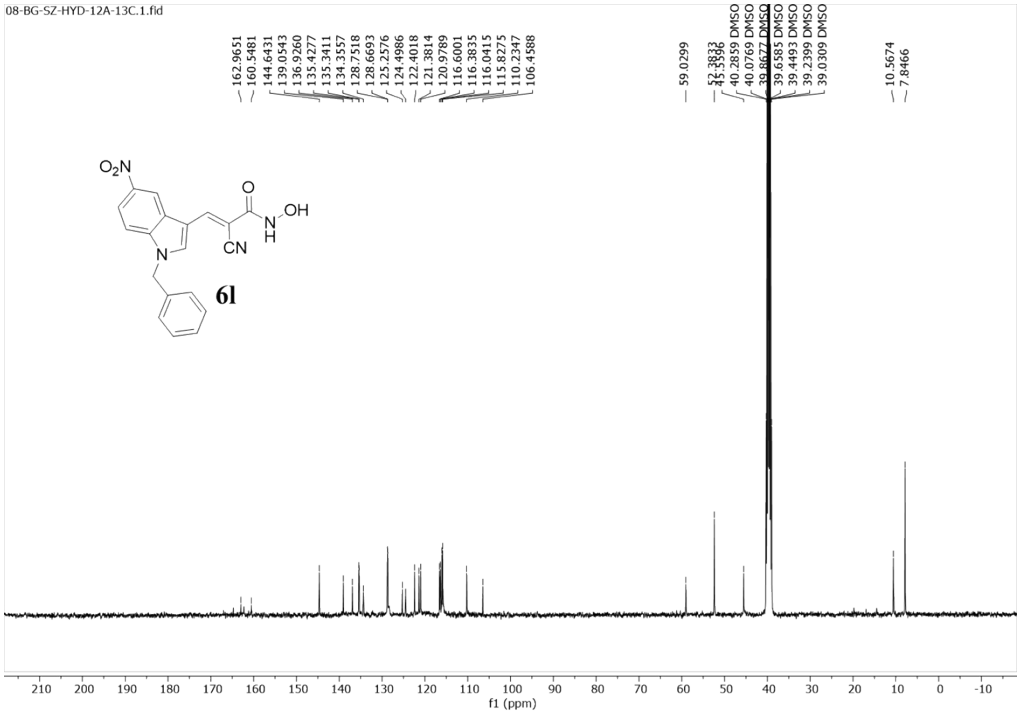
Supporting Spectra S70: LC-MS Spectra for the compound 6k.



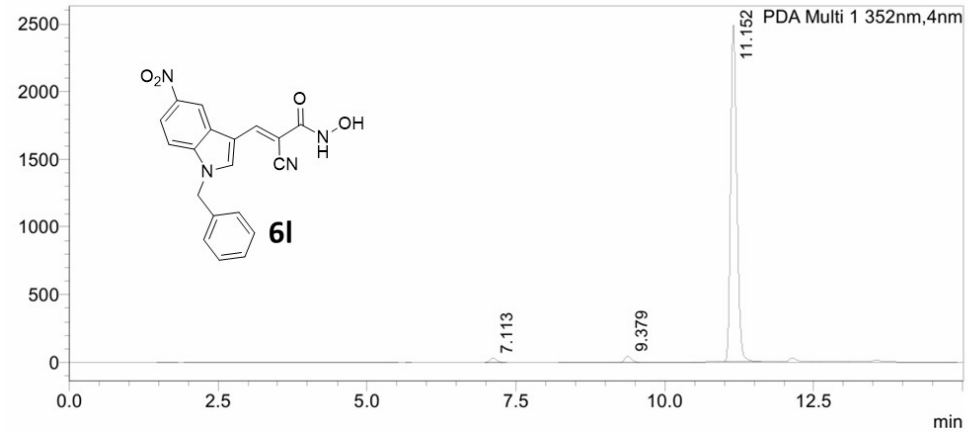
Supporting Spectra S71: HRMS Spectra for the compound 6k.



Supporting Spectra S72: ^{1}H NMR Spectra for compound 6l.



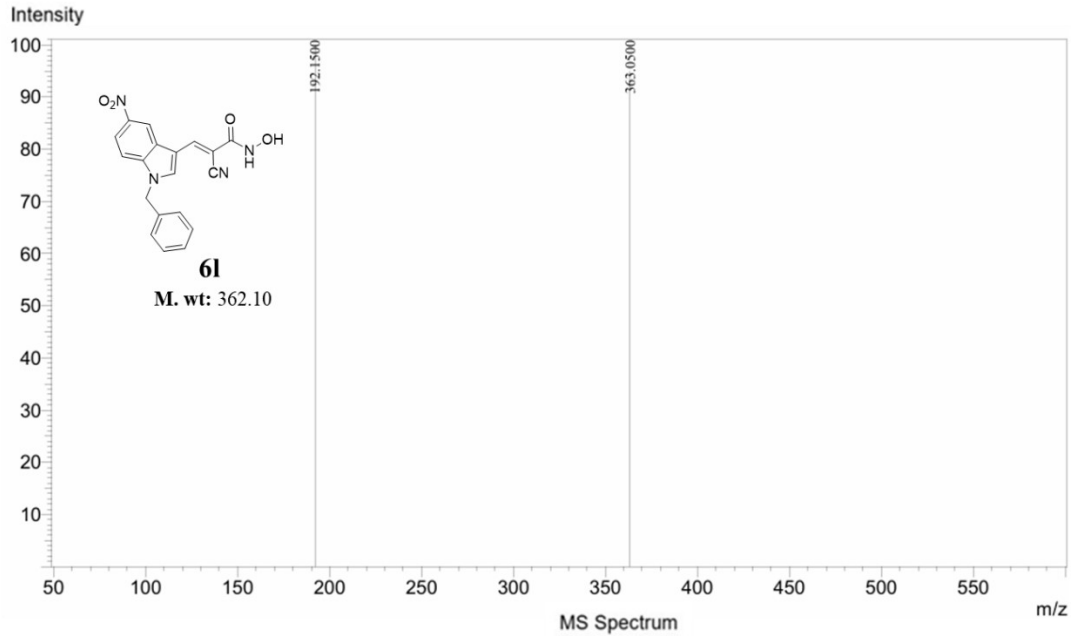
Supporting Spectra S73: ^{13}C NMR Spectra for compound 6l.



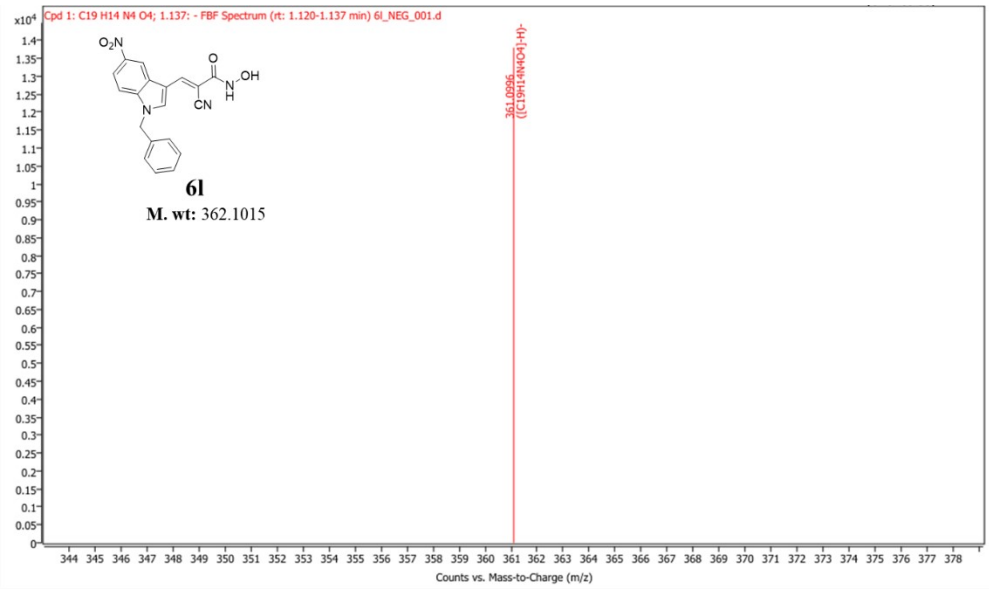
PDA Ch1 352nm

Peak#	Ret. Time	Area	Height	Area%	Height%	Tailing Factor
1	7.113	216705	30923	1.193	1.209	1.195
2	9.379	298783	43133	1.645	1.687	1.250
3	11.152	17649084	2483411	97.162	97.104	1.234
Total		18164572	2557467	100.000	100.000	

Supporting Spectra S74: HPLC traces of compound 6l.



Supporting Spectra S75: LC-MS Spectra for the compound 6l.



Supporting Spectra S76: HRMS Spectra for the compound 6l.