LAMPIRAN

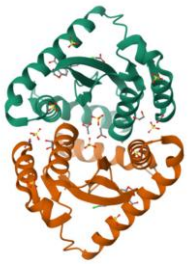
Lampiran 1.

PREPARASI PROTEIN TARGET INHIBITOR HIV INTEGRASE

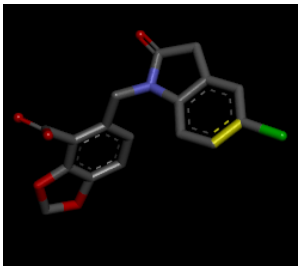
Target kerja yang digunakan yaitu enzim HIV integrase yang diunduh dari situs *Protein Data Bank* (PDB) Kode PDB ID 3NF7.

- PDB DOI: https://doi.org/10.2210/pdb3NF7/pdb
- Classification: HYDROLASE/HYDROLASE INHIBITOR
- Organism(s): Human immunodeficiency virus 1
- Mutation(s): Yes
- Method: X-RAY DIFFRACTION
- Resolution: 1.80 Å

Berikut visualisasi dari target kerja dan ligan alami yang digunakan bisa dilihat pada gambar.



(a)



(b)

(a) Struktur Kristal Enzim HIV Integrase

(b) Ligan Alami CIW 5-[(5-chloro-2-oxo-2,3-dihydro-1H-indol-1-yl)methyl]-1,3-benzodioxole-4-carboxylic acid

(Sumber: RSCB *Protein Data Bank*)

Lampiran 2. Preparasi senyawa aktif berdasarkan IC50

No	IDPubchem	Ic50	No	IDPubchem	Ic50	No	IDPubchem	Ic50
1	CHEMBL366356	0.6	48	CHEMBL212000	0.036	95	CHEMBL198160	0.0087
2	CHEMBL357646	0.97	49	CHEMBL212000	0.036	96	CHEMBL198160	0.0087
3	CHEMBL357646	0.97	50	CHEMBL212000	0.036	97	CHEMBL212921	0.08
4	CHEMBL357646	0.97	51	CHEMBL212000	0.036	98	CHEMBL212921	0.08
5	CHEMBL32865	0.01	52	CHEMBL1159988	0.36	99	CHEMBL371007	0.01
6	CHEMBL193759	0.01	53	CHEMBL1159988	0.36	100	CHEMBL371007	0.01
7	CHEMBL212412	0.07	54	CHEMBL1159988	0.36	101	CHEMBL370620	0.2
8	CHEMBL212412	0.07	55	CHEMBL1159988	0.36	102	CHEMBL202166	0.6
9	CHEMBL196391	2.71	56	CHEMBL339815	0.79	103	CHEMBL217285	0.06
10	CHEMBL1159989	0.32	57	CHEMBL108760	0.08	104	CHEMBL217285	0.06
11	CHEMBL1159989	0.32	58	CHEMBL129964	0.70	105	CHEMBL204656	0.00021
12	CHEMBL1159989	0.32	59	CHEMBL175266	0.21	106	CHEMBL204656	0.00021
13	CHEMBL1159989	0.32	60	CHEMBL199874	0.5	107	CHEMBL320261	0.059
14	CHEMBL1159990	0.23	61	CHEMBL199874	0.5	108	CHEMBL321391	0.5
15	CHEMBL1159990	0.23	62	CHEMBL35842	0.05	109	CHEMBL212213	0.0072
16	CHEMBL1159990	0.23	63	CHEMBL35842	0.05	110	CHEMBL212213	0.0072
17	CHEMBL142072	0.05	64	CHEMBL431948	0.68	111	CHEMBL421353	0.126
18	CHEMBL142072	0.05	65	CHEMBL431948	0.68	112	CHEMBL437708	0.08
19	CHEMBL553067	0.5	66	CHEMBL431948	0.68	113	CHEMBL437708	0.08
20	CHEMBL553067	0.5	67	CHEMBL431948	0.68	114	CHEMBL437708	0.08
21	CHEMBL553067	0.5	68	CHEMBL431948	0.68	115	CHEMBL407451	0.2
22	CHEMBL553067	0.5	69	CHEMBL431948	0.68	116	CHEMBL407451	0.2
23	CHEMBL553067	0.5	70	CHEMBL431948	0.68	117	CHEMBL217776	0.2
24	CHEMBL553067	0.5	71	CHEMBL431948	0.68	118	CHEMBL217776	0.2
25	CHEMBL553067	0.5	72	CHEMBL431948	0.68	119	CHEMBL217776	0.2
26	CHEMBL553067	0.5	73	CHEMBL431948	0.68	120	CHEMBL217776	0.2
27	CHEMBL111182	0.6	74	CHEMBL431948	0.68	121	CHEMBL217776	0.2
28	CHEMBL130911	0.19	75	CHEMBL431948	0.68	122	CHEMBL217776	0.2
29	CHEMBL213852	0.15	76	CHEMBL431948	0.68	123	CHEMBL35109	2.3
30	CHEMBL209488	0.21	77	CHEMBL431948	0.68	124	CHEMBL35109	2.3
31	CHEMBL209488	0.21	78	CHEMBL431948	0.68	125	CHEMBL35109	2.3
32	CHEMBL149674	0.6	79	CHEMBL431948	0.68	126	CHEMBL415678	0.43
33	CHEMBL149674	0.6	80	CHEMBL380034	0.85	127	CHEMBL415678	0.43
34	CHEMBL217020	0.05	81	CHEMBL164		128	CHEMBL415678	0.43
35	CHEMBL217020	0.05	82	CHEMBL210233	0.02	129	CHEMBL441683	0.04
36	CHEMBL217020	0.05	83	CHEMBL206604	8.2	130	CHEMBL441683	0.04
37	CHEMBL217020	0.05	84	CHEMBL206604	8.2	131	CHEMBL212982	0.033
38	CHEMBL217020	0.05	85	CHEMBL378373	0.43	132	CHEMBL212982	0.033
39	CHEMBL216874	0.01	86	CHEMBL86133		133	CHEMBL190009	
40	CHEMBL216874	0.01	87	CHEMBL385825	0.059	134	CHEMBL143614	0.1
41	CHEMBL288097	0.6	88	CHEMBL385825	0.059	135	CHEMBL377501	0.012
42	CHEMBL216389	0.44	89	CHEMBL385825	0.059	136	CHEMBL204751	0.25
43	CHEMBL216389	0.44	90	CHEMBL385825	0.059	137	CHEMBL204751	0.25
44	CHEMBL216389	0.44	91	CHEMBL385825	0.059	138	CHEMBL378395	0.35

45	CHEMBL216389	0.44	92	CHEMBL385825	0.059	139	CHEMBL378395	0.35
46	CHEMBL378029	0.015	93	CHEMBL419981	0.19	140	CHEMBL144613	0.47
47	CHEMBL211028	0.01	94	CHEMBL129148	0.89	141	CHEMBL18635	0.11

No	IDPubchem	Ic50	No	IDPubchem	Ic50
142	CHEMBL148364	0.88	189	CHEMBL210234	0.007
143	CHEMBL148364	0.88	190	CHEMBL379658	0.01
144	CHEMBL148364	0.88	191	CHEMBL209958	0.08
145	CHEMBL209307	0.04	192	CHEMBL209958	0.08
146	CHEMBL386515	0.05	193	CHEMBL441250	0.66
147	CHEMBL386515	0.05	194	CHEMBL441250	0.66
148	CHEMBL209854	0.036	195	CHEMBL441250	0.66
149	CHEMBL209854	0.036	196	CHEMBL386710	0.02
150	CHEMBL179		197	CHEMBL386710	0.02
151	CHEMBL312608	0.9	198	CHEMBL267578	0.81
152	CHEMBL368084	0.02	199	CHEMBL414850	0.0005
153	CHEMBL368084	0.02	200	CHEMBL385951	0.07
154	CHEMBL211110	0.19	201	CHEMBL385951	0.07
155	CHEMBL211110	0.19	202	CHEMBL385951	0.07
156	CHEMBL379382	0.33	203	CHEMBL472863	0.37
157	CHEMBL379382	0.33	204	CHEMBL472863	0.37
158	CHEMBL379974	0.35	205	CHEMBL87764	
159	CHEMBL379974	0.35	206	CHEMBL86448	
160	CHEMBL377621	0.42	207	CHEMBL36070	0.04
161	CHEMBL377621	0.42	208	CHEMBL209614	0.6
162	CHEMBL129073	0.60	209	CHEMBL209614	0.6
163	CHEMBL209872	0.025	210	CHEMBL232801	0.17
164	CHEMBL36303	0.1	211	CHEMBL340775	0.2
165	CHEMBL611459				
166	CHEMBL68013				
167	CHEMBL68013				
168	CHEMBL68013				
169	CHEMBL68013				
170	CHEMBL68013				
171	CHEMBL68013				
172	CHEMBL68013				
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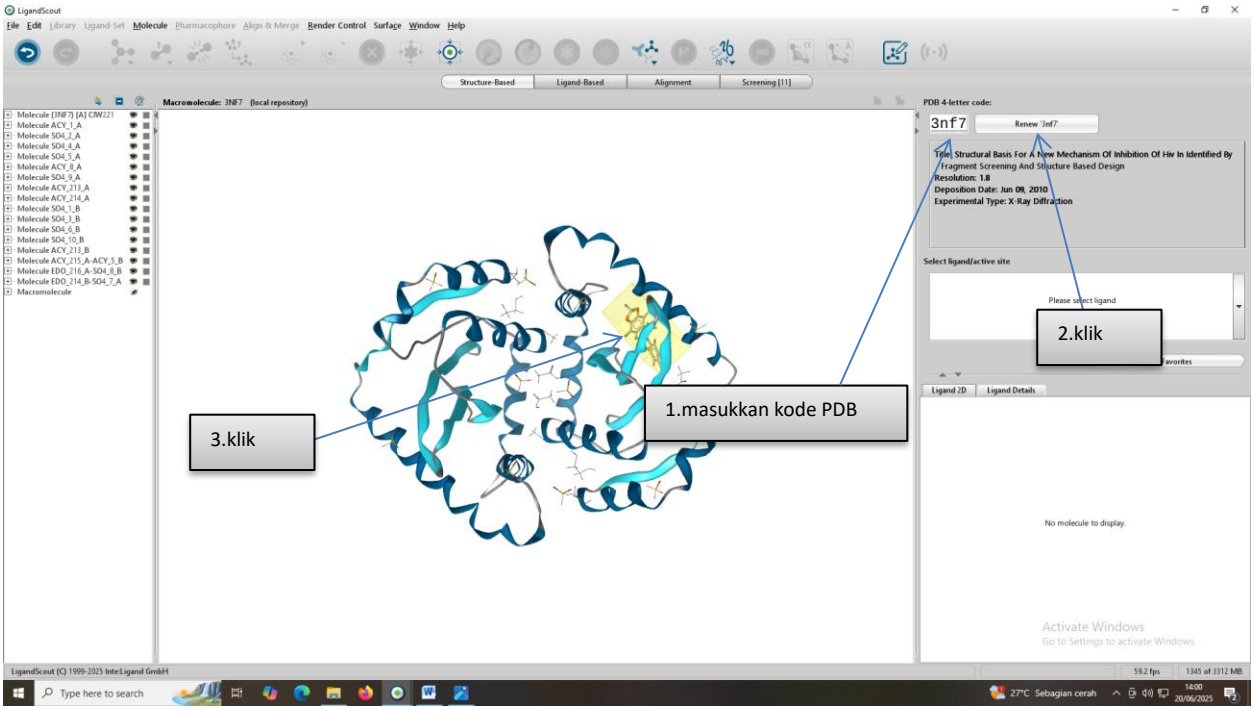
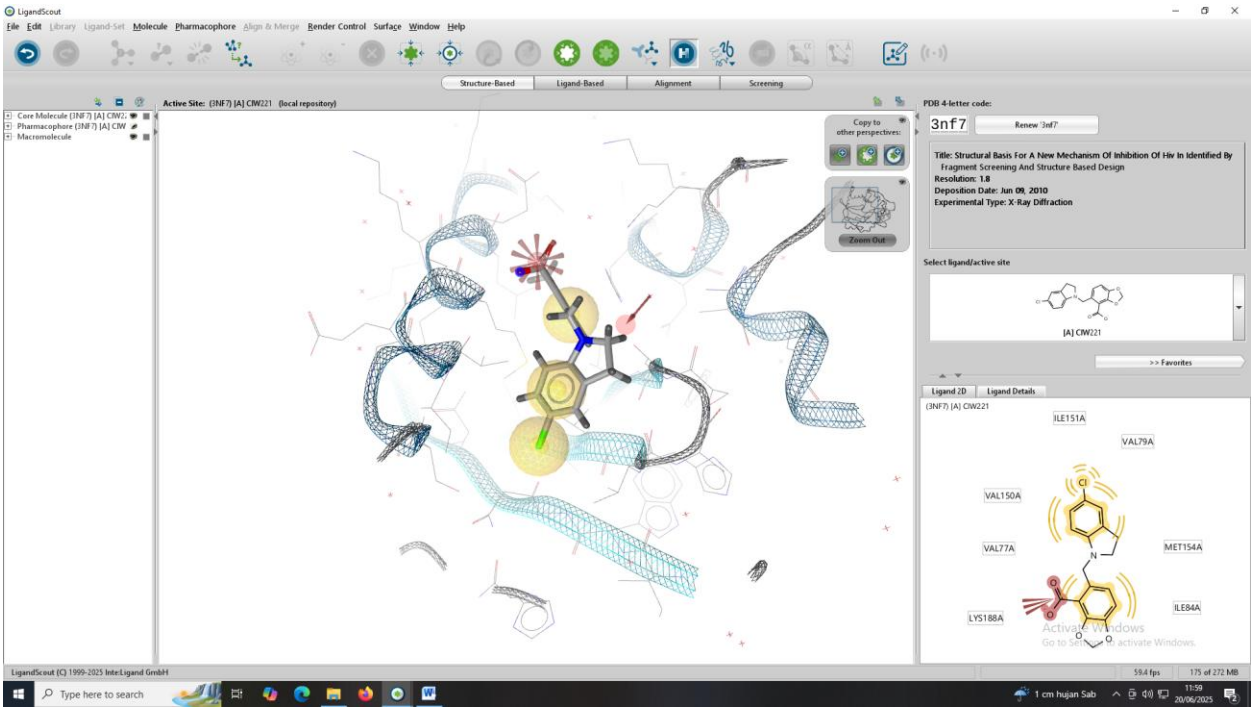
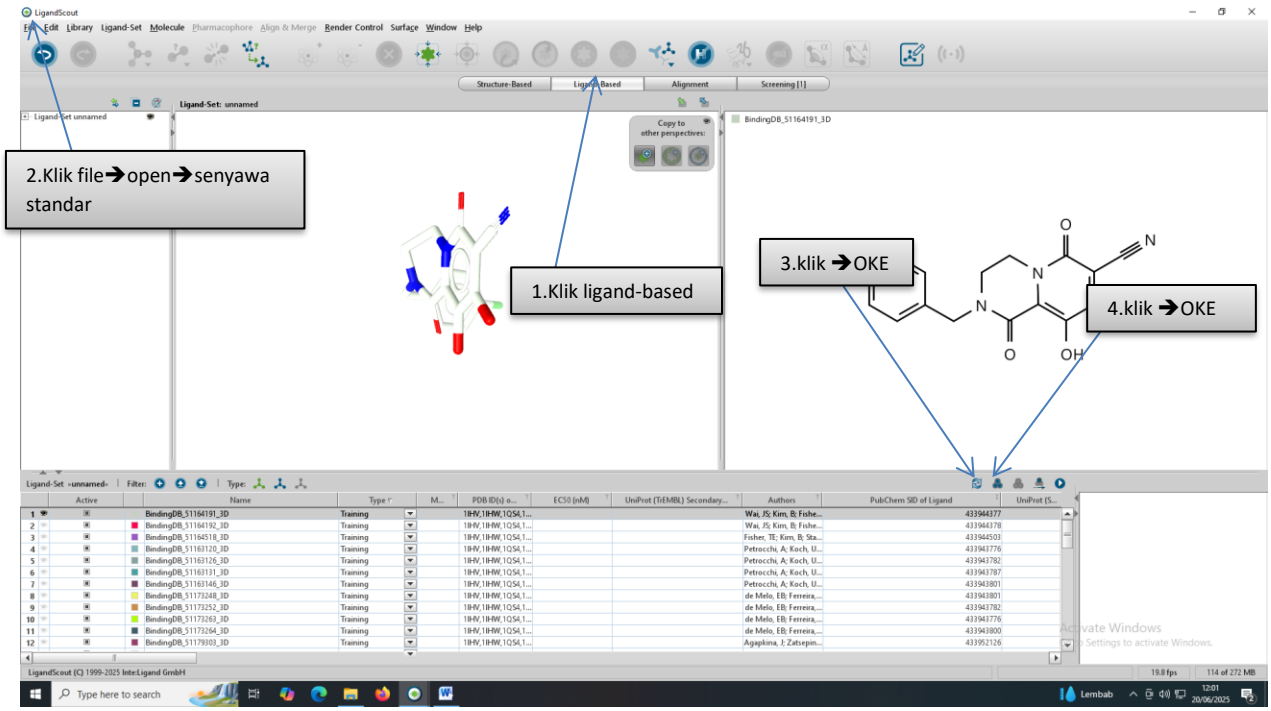
176	CHEMBL68013				
177	CHEMBL68013				
178	CHEMBL68013				
179	CHEMBL68013				
180	CHEMBL68013				
181	CHEMBL68013				
182	CHEMBL413552	0.1			

183	CHEMBL63592	0.08
184	CHEMBL63592	0.08
185	CHEMBL63592	0.08
186	CHEMBL59548	0.6
187	CHEMBL59548	0.6
188	CHEMBL198001	5.3

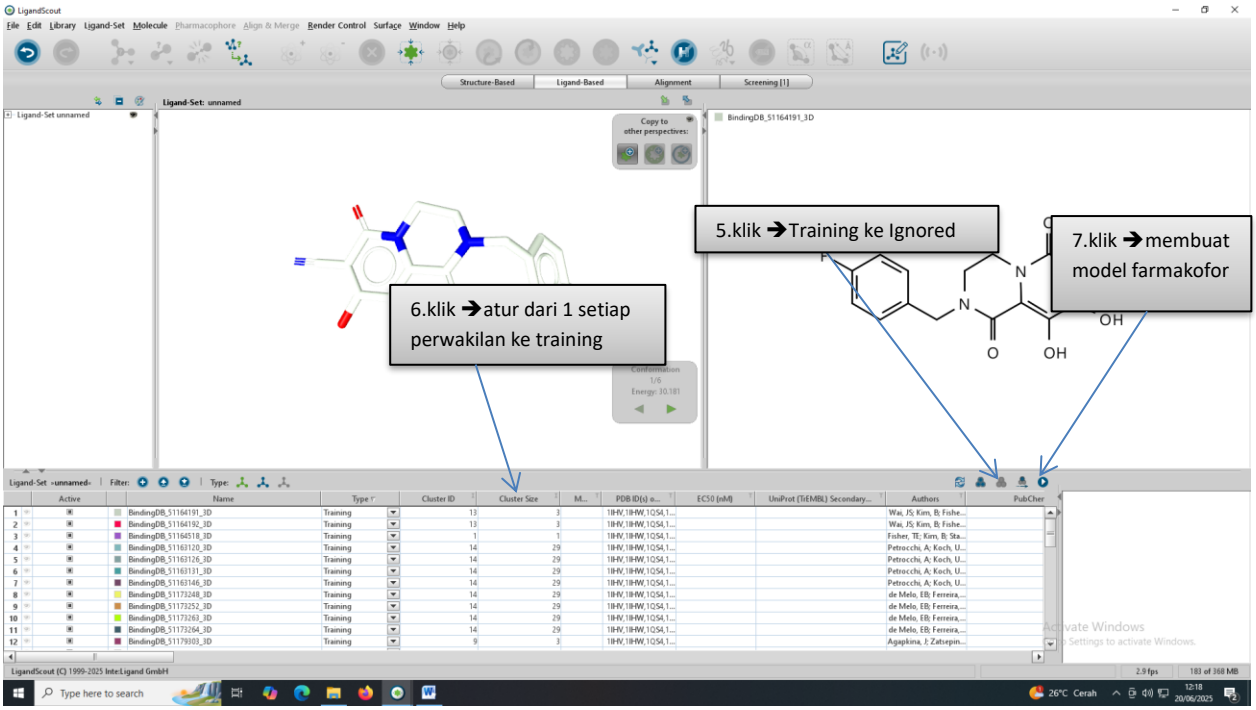
Lampiran 3. Validasi metode farmakofor



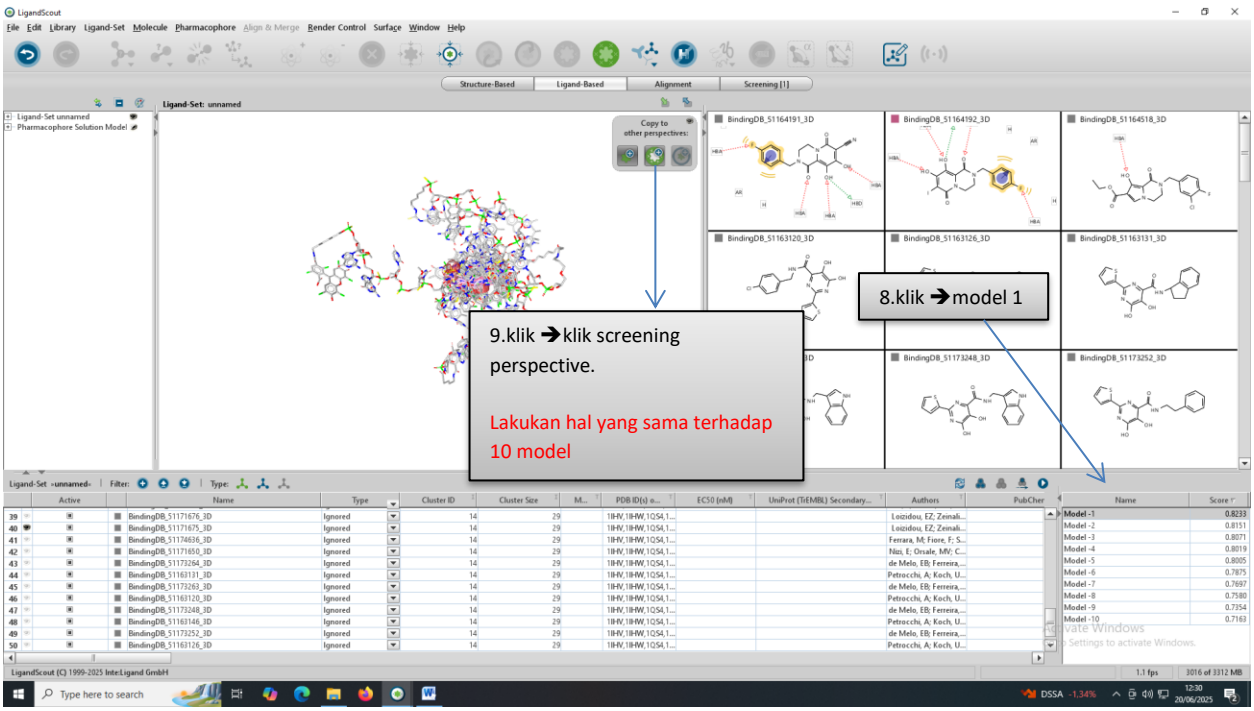




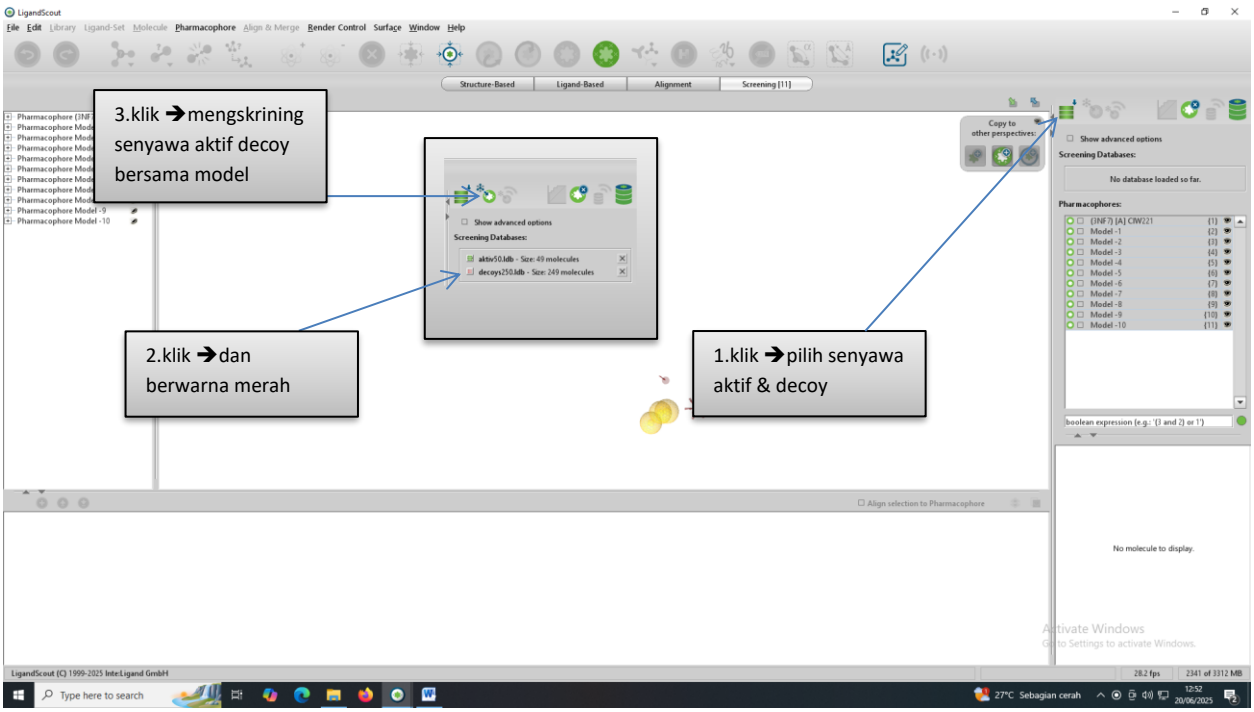
Menentukan cluster id dan cluster zise dari senyawa standar yang di download dari bindingDB



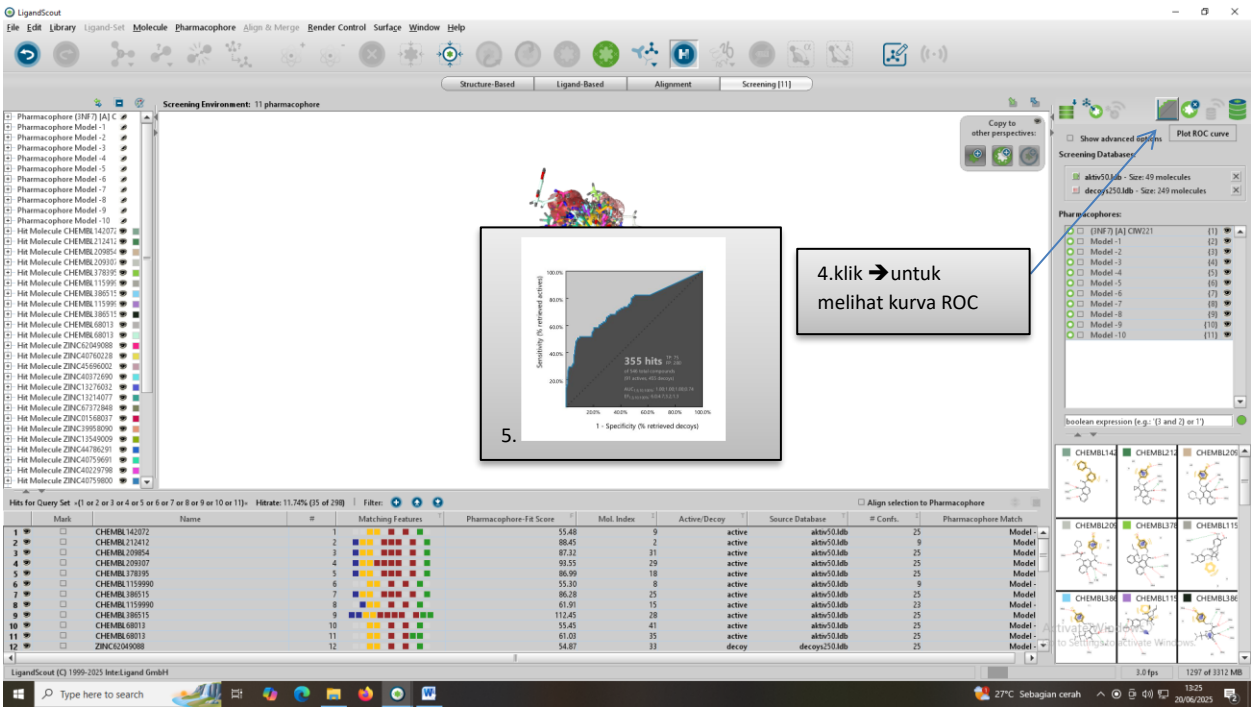
Membuat model farmakofor dari senyawa standar



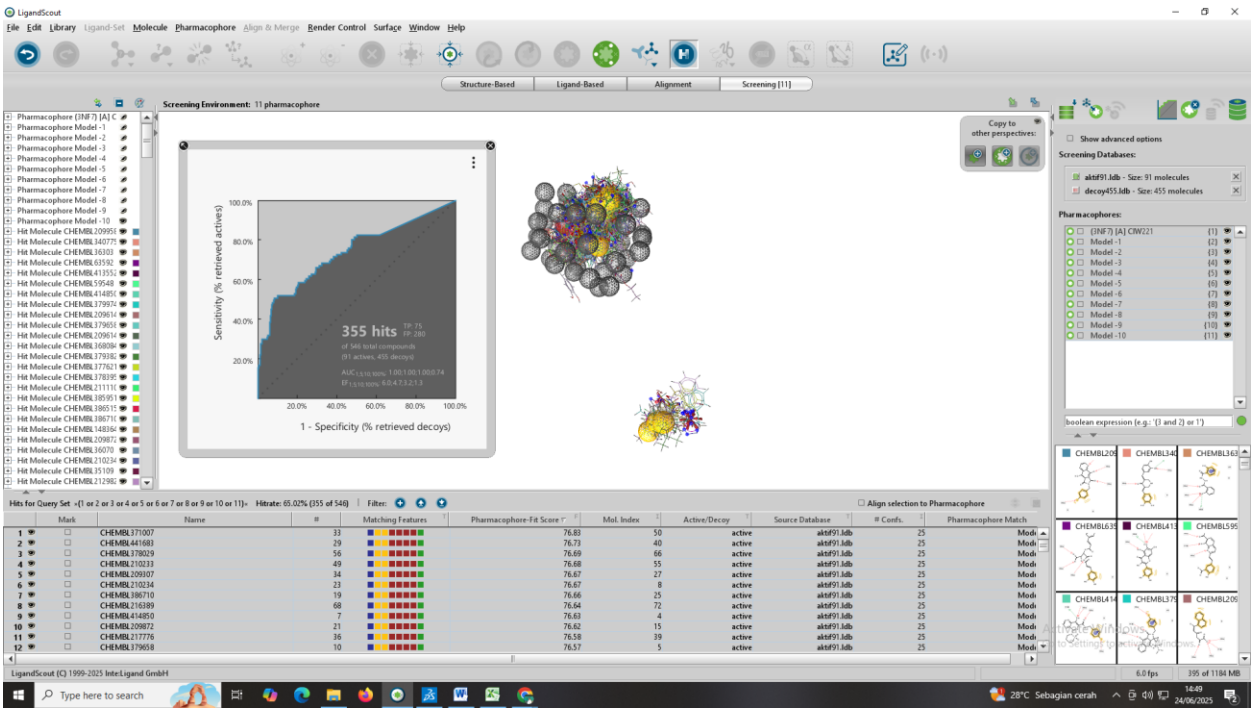
10 model farmakofor dari senyawa tarndar➔pindahkan 10 model farmakofor ke tap screening



Input senyawa aktif dan decoy untuk mencari kurva ROC senyawa hits



Setelah didapat senyawa hits aktif dan decoy akan dilanjutkan untuk screening senyawa uji



Lampiran 4. Hasil skrining database ZINC Netural Products

1. Afronp

No	Name	Smiles	Active/Decoy	ource Databas	Pharmacophore-Fit Score
1	ZINC87493012	:3c(cc1c2cc(O)c(c(O)c2)\C=C\C(C)C)ccc(C	active	afronp_.ldb	75.74
2	ZINC95485973	(OC)cc1c(=O)c4c2c3c(OC(C=C3)(C)C)c(c	active	afronp_.ldb	70.96
3	ZINC14557836	(c(O)c(cc1)C(=O)\C=C\c2ccc(O)cc2)C=CC	active	afronp_.ldb	70.81
4	ZINC95485972	c(OC)cc1c(=O)c4c2c(c3OC(C=Cc3c4O)(C)	active	afronp_.ldb	70.67
5	ZINC95486052	))c1)C(=O)C[C@H]2c4cc(c3OC(CCc3c4)(	active	afronp_.ldb	70.49
6	ZINC01684797	C=Cc12)(C)C)C(=O)[C@H]4c5c(OC[C@H	active	afronp_.ldb	70.16
7	ZINC95486284	1cc(c(O)cc1)C)c(OC)c(=O)c3c2c(c(OC)c(c	active	afronp_.ldb	69.01
8	ZINC13311972	))c(c1)c2c(O)cc(OC)cc2)c(OC)c3c(OC(C=(	active	afronp_.ldb	68.18
9	ZINC43069427	(cc(cc1)\C=C\C(=O)c2c(O)cc(O)cc2)C=CC	active	afronp_.ldb	68.16
10	ZINC15122160	c(c2)[C@@H]3C(=O)c5c(OC3)c4c(OC(C=	active	afronp_.ldb	68.11
11	ZINC14780240	(c(=O)c2c1ccc(O)c2O)c(O)cc4OC(C=Cc34	active	afronp_.ldb	68.06
12	ZINC95486196	]5[C@@H](O[C@H]3O[C@H]([C@H](O	active	afronp_.ldb	67.96
13	ZINC05854599	'1)(C)C)c2)[C@@H]4[C@@H]3c5c(OC4)(	active	afronp_.ldb	65.04
14	ZINC56871274	@]1([C@@H]([C@@H]2[C@@](CO)(CC	active	afronp_.ldb	63.5
15	ZINC95486190	c(OC)cc1c(=O)c3c2c4c(c(c3O)CC=C(C)C)	active	afronp_.ldb	63.45
16	ZINC95486041	@]1([C@H]2[C@@]([C@H](CC2)C\C=C\	active	afronp_.ldb	63.36
17	ZINC95486144	C)=C\C[C@@H]3[C@]2(OC2)CC[C@@H	active	afronp_.ldb	63.3
18	ZINC95485943	)@]3(C[C@@H](O)[C@@H]6[C@]4([C@	active	afronp_.ldb	63.3
19	ZINC13382721	)c3c1cc2OC(C=Cc2c3O)(C)C)cc(O)c(O)c4	active	afronp_.ldb	63.28
20	ZINC95486203	cc(c1cc(c2)CO)c3cc4c(cc3)C[C@H](N[C@	active	afronp_.ldb	63.21
21	ZINC35941652	cc(O)c1)C(=O)C[C@H]2c4cc3c(OC(CC3)(	active	afronp_.ldb	63.17
22	ZINC95485942	(C[C@@H](O)[C@@H]6[C@@]4([C@H	active	afronp_.ldb	63.08
23	ZINC14614051	I](c1c(O)c(O)c(OC)cc1)Cc2cc3)C=C[C@@	active	afronp_.ldb	63.07
24	ZINC95486145	C[C@@H]3[C@]2(OC2)CC[C@@H]4[C@	active	afronp_.ldb	63.02
25	ZINC03978987	)(C)C)ccc2C(=O)[C@H]4c5c(OC[C@@H	active	afronp_.ldb	63
26	ZINC04098748	C)C)ccc2C(=O)[C@@]4(O)c5c(OC[C@@	active	afronp_.ldb	62.98
27	ZINC95486146	)@@H]3[C@]2(OC2)C[C@H](O)[C@@H]4	active	afronp_.ldb	62.88
28	ZINC03978989	'1)(C)C)ccc2C(=O)[C@H]4c5c(OC[C@H]3	active	afronp_.ldb	62.87
29	ZINC95486257	C@H]2O[C@H]([C@H](O)[C@@H](O)[C(	active	afronp_.ldb	62.86
30	ZINC06050191	OC(C=Cc12)(C)C)[C@H]4[C@H]3c5c(OC	active	afronp_.ldb	62.86
31	ZINC05849017	c1C(=N[C@@H](C2)C)C)c4c3c(c(OC)cc(c	active	afronp_.ldb	62.8
32	ZINC95485922	1c(=O)c3c2c(c(O)c(c3O)C\C=C(\CCC=C(C	active	afronp_.ldb	62.73
33	ZINC95486193	O)c(cc1)CC=C(C)C)C(=O)C[C@H]2c3c(O	active	afronp_.ldb	62.67
34	ZINC95486015	C@H](c1c(cc(OC)c(OC)c1)CC2)C(=O)c3cc	active	afronp_.ldb	62.63
35	ZINC14760755	O)cc(OC\C=C(\CCC=C(C)C)/C)cc1cc3c2c(	active	afronp_.ldb	61.8
36	ZINC13481884	(c(O)cc(O)c1)C(=O)[C@H](C2)Cc3cc(O)c	active	afronp_.ldb	61.29
37	ZINC95486261	'(=O)C)c(cc(O)c2[C@H]3O[C@@H]([C@	active	afronp_.ldb	61.25
38	ZINC00001785	1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3ccc(O	active	afronp_.ldb	61.14
39	ZINC02030112	1c(c(O)cc(OC)c1)C(=O)C[C@H]2c3ccc(OC	active	afronp_.ldb	61.12
40	ZINC14819779	1c(OC)c(O)c(cc1c(=O)c3c2cccc3O)CC=C(	active	afronp_.ldb	61.06
41	ZINC95486293	:(Oc1ccc(OC)cc1)c([O-])c(=O)c3c2cc(O)cc	active	afronp_.ldb	61
42	ZINC43079447	C=C1)(C)C)c2CC=C(C)C)C(=O)[C@H](O)	active	afronp_.ldb	60.94
43	ZINC38628344	(C=C1)(C)C)c2CC=C(C)C)C(=O)[C@H](	active	afronp_.ldb	60.94
44	ZINC95485981	C@@H]2c4cc(OCCC=C(C)C)c3OC([C@@	active	afronp_.ldb	60.84
45	ZINC39144622	C=C1)(C)C)c2CC=C(C)C)C(=O)[C@H](O	active	afronp_.ldb	60.83
46	ZINC95486266	c(c(O)cc(O)c1)C(=O)[C@](O)(c2ccc(OC)c	active	afronp_.ldb	60.81
47	ZINC00035526	c3c(OC)c(OC[C@@H](O)C(O)(C)C)ccc3c	active	afronp_.ldb	60.81
48	ZINC95485935	CC[C@H]3[C@]2(OC2)CC[C@H]4[C@@	active	afronp_.ldb	60.8
49	ZINC06404152	c(OC)c(c(O)cc1OC)C(=O)\C=C\c2ccc(OC)(	active	afronp_.ldb	60.77
50	ZINC14645892	c(OC)c(OC)cc(O)c1c(=O)c(c2)c3c(OC)c(O	active	afronp_.ldb	60.75
51	ZINC95486255	OC)c(OC)c(O)c(O)c1c(=O)c(c2)c3c(OC)c(	active	afronp_.ldb	60.73
52	ZINC95486076	)cc(O)c1)C(=O)C[C@H]2c3cc(O)c(OC)c(c	active	afronp_.ldb	60.72
53	ZINC95486014	2)[C@@H]3C(=O)C5C(OC3)=C4COC(C=	active	afronp_.ldb	60.72

54	ZINC14727623	c(O)c1c(=O)c3c2c(c(OC)c(c3O)CC=C(C)C	active	afronp_.ldb	60.71
55	ZINC95486051	)c1)C(=O)C[C@H]2c3c(c(O)c(O)c(c3)C=C	active	afronp_.ldb	60.68
56	ZINC95485931	(c(O)ccc1C(=O)\C=C\c2ccc(O)cc2)CCC=C	active	afronp_.ldb	60.67
57	ZINC95486102	[C@H]([C@@H]2OC(=O)C[C@@H]12)C	active	afronp_.ldb	60.66
58	ZINC95486093	[C@@]([C@@H]1[C@H](C[C@](C=C)(C	active	afronp_.ldb	60.46
59	ZINC95486260	))C)c(cc(O)c2[C@H]3O[C@@H]([C@@H	active	afronp_.ldb	60.44
60	ZINC95485967	lcc3c2C(=O)CC(=O)[C@@H]3CCC=C(C)	active	afronp_.ldb	60.41
61	ZINC95486059	)1c(=O)ccc2c1c(c(OC)cc2C)\C=C\C(O)(C)(	active	afronp_.ldb	60.38
62	ZINC95485921	:1c(O)ccc(O)c1c(=O)c3c2c(ccc3O)CC=C(C	active	afronp_.ldb	60.34
63	ZINC14811038	(c(O)c(O)c(O)c1)C(=O)[C@H](C2)Cc3ccc	active	afronp_.ldb	60.34
64	ZINC95486236	-O)c3c1cc2OC([C@@H](O)Cc2c3O)(C)C)(	active	afronp_.ldb	60.33
65	ZINC95485999	]([C@H](O)[C@H](OCc1ccccc1)[C@@]2(	active	afronp_.ldb	60.33
66	ZINC95486256	)H]([C@@H](O)[C@H](O)[C@H]2O)CO)	active	afronp_.ldb	60.31
67	ZINC04096339	@]1(C(=CC(=O)CC1(C)C)C)\C=C\[C@@H	active	afronp_.ldb	60.2
68	ZINC43121107	c(cc(cc1)\C=C\C(=O)c2c(O)cc(O)cc2)CCC	active	afronp_.ldb	60.18
69	ZINC15150823	c(c1)c2c(OC)cc(O)c(OC)c2)c(O)c3c(OC(C	active	afronp_.ldb	60.07
70	ZINC95485914	cc1O[C@@](C=Cc1c2c(=O)c4c3cccc4O)(C	active	afronp_.ldb	60.04
71	ZINC02004122	C(C=C1)(C)C)c2)[C@@H]4[C@@H]3c5c(	active	afronp_.ldb	57.75
72	ZINC14727631	2c1cc(O)c(OC)c2CC=C(C)C)c(O)c(c(O)c3	active	afronp_.ldb	57.66
73	ZINC95485987	(=O)cc1c2c(O)cc(O)cc2)c(O)c(c(O)c3)CCC	active	afronp_.ldb	56.7
74	ZINC95485899	.O)CO)[C@H]3OC=C[C@H]4[C@H](OC(	active	afronp_.ldb	56.49
75	ZINC15120572	C@@](C(=O)C=C1)(CC(=O)OC)C\C=C(\C	active	afronp_.ldb	56.39
76	ZINC13382495	2c1cc(O)c(OC)c2CC=C(C)C)c(O)c3c(OC(C	active	afronp_.ldb	56.23
77	ZINC95486287	:1cc(OC)c(O)cc1)c(OC)c(=O)c3c2cc(OC)c(	active	afronp_.ldb	56.14
78	ZINC95486004	-C\COC)[C@@H]([C@@H]2c3cc(OC)c(O	active	afronp_.ldb	55.98
79	ZINC95486134	[C@H]2[C@](C1[C@@H](C(=C(O)C(=O	active	afronp_.ldb	55.85
80	ZINC95486151	H]([C@@]1([C@H](C(CCC1)(C)C)CC2)C	active	afronp_.ldb	55.81
81	ZINC14641747	)c(OC)cc1c(=O)c3c2c(c(O)c(c3O)CC=C(C	active	afronp_.ldb	55.79
82	ZINC33831297	@H]([C@@]1([C@H](C(CCC1)(C)C)CC2	active	afronp_.ldb	55.72
83	ZINC33831299	@H]([C@@]1([C@H](C(CCC1)(C)C)CC2)	active	afronp_.ldb	55.7
84	ZINC95486066	@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)	active	afronp_.ldb	55.65
85	ZINC95486262	[C@@](O)(c2c(c(O)ccc2)C3=O)[C@@H]4	active	afronp_.ldb	55.63
86	ZINC95486247	[C@@]2([C@](C[C@H]([C@H](CC/C(/O)=	active	afronp_.ldb	55.6
87	ZINC95485971	c(=O)c2c1cc(O)c(O)c2)c(O)c(c(O)c3)CCC=	active	afronp_.ldb	55.54
88	ZINC14819573	C)c1CC=C(C)C)[C@@]3(O)[C@H]2c4c(C	active	afronp_.ldb	55.53
89	ZINC05854400	:c(O)c1c(=O)c3c2c(c(O)c(c3O)CC=C(C)C)	active	afronp_.ldb	55.52
90	ZINC13485435	C=C(C)C)[C@@H]3[C@@H]2c4c(OC3)c(	active	afronp_.ldb	55.51
91	ZINC15122165	lc(O)c(O)c(OC)cc1)C(=O)c2c(O)c3)C=C[C	active	afronp_.ldb	55.5
92	ZINC28969961	:2c4c(N([C@H](c12)CC(=O)C)C)c3c(cc(O	active	afronp_.ldb	55.49
93	ZINC95486016	@](O)(c1c(cc(OC)c(OC)c1)CC2)C(=O)c3c	active	afronp_.ldb	55.48
94	ZINC01618678	=C(C)C)[C@@H]3[C@@H]2c4c(OC3)c(c	active	afronp_.ldb	55.48
95	ZINC06394172	)(C)C)ccc2C(=O)[C@@]4(O)c5c(OC[C@H	active	afronp_.ldb	55.42
96	ZINC14763066	(c(=O)c2c1cc(O)c(O)c2)c(O)c(c(O)c3)CC=	active	afronp_.ldb	55.36
97	ZINC95486078	]3[C@@H]2c4c(OC3)cc5c(c4)C[C@H]([C	active	afronp_.ldb	55.35
98	ZINC95486269	H]1C2(C)C)ccc3C(=O)[C@@]5(O)c6c(OC	active	afronp_.ldb	55.32
99	ZINC33857007	@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3c(C	active	afronp_.ldb	55.27
100	ZINC95485915	:(c(=O)c2c1ccc(OC)c2)c(O)c(c(O)c3)CC=C	active	afronp_.ldb	55.2
101	ZINC13382725	c(c1c(=O)c4c2c3c(O[C@@H](C3(C)C)C)c	active	afronp_.ldb	55.2
102	ZINC95486259	c(O)ccc2)C3=O)([C@@]4(O[C@H]([C@@	active	afronp_.ldb	55.18
103	ZINC95486276	:(OC)cc(O)c1CC=C(C)C)C(=O)C[C@H]2c	active	afronp_.ldb	55.17
104	ZINC95486010	C@H](c1c(cc(OC)c(OC)c1)CC2)C(=O)c3c	active	afronp_.ldb	55.14
105	ZINC95486258	:c(c(O)ccc2)C3=O)[C@@]4(O[C@H]([C@	active	afronp_.ldb	55.11
106	ZINC95485991	c2c(O)cc(O)c(O)c2)CCC=C(C)C)c(O)cc4C	active	afronp_.ldb	55.06
107	ZINC95486011	C@](O)(c1c(cc(OC)c(OC)c1)CC2)C(=O)c3(	active	afronp_.ldb	54.96
108	ZINC95486050	O)c1)C(=O)C[C@H]2c3cc(c(O)c(c3)CC=C	active	afronp_.ldb	54.91

109	ZINC95486186	=C(O)C(=O)C2(C\C=C\C)C\C=C\C)c(O)c(	active	afronp_.ldb	54.86
110	ZINC95485974	:(OC)cc1c(=O)c3c2c(c(O)c(c3O)CCC=C(C	active	afronp_.ldb	54.69
111	ZINC05430812	c2c1cc(O)c(OC)c2CC=C(C)C)c(O)c(c(O)c:	active	afronp_.ldb	54.53
112	ZINC95486273	C)cc2OC(C=Cc12)(C)C)C(=O)C[C@H]3c-	active	afronp_.ldb	54.52
113	ZINC02026346	c(c(O)c1Cc2c(O)cccc2)C(=O)CCc3ccccc3)	active	afronp_.ldb	54.49
114	ZINC14759061	c3c(c(=O)c(c1)c2cc(O)c(OC)c(O)c2)ccc(O)	active	afronp_.ldb	54.38
115	ZINC01721693	c(c(O)cc(O)c1)C[C@H](O)[C@H]2c3ccc((	active	afronp_.ldb	54.37
116	ZINC14952515	)@H](O)[C@H](O)[C@@H]1O)C)c(=O)c:	active	afronp_.ldb	54.34
117	ZINC00119983	c(O)cc(O)c1)C[C@H](O)[C@H]2c3cc(O)c	active	afronp_.ldb	54.33
118	ZINC14642669	C@@H](OC(=O)c2cc(OC)c(O)c(OC)c2)[(	active	afronp_.ldb	54.16
119	ZINC03978503	[C@@H](OC(=O)c2cc(O)c(O)c(O)c2)[C(	active	afronp_.ldb	54.13
120	ZINC14689062	O)cc1O[C@H]([C@](O)(CO)C)Cc1c4n(c3-	active	afronp_.ldb	54.09
121	ZINC95486286	:1cc(O)c(O)cc1)c(OC)c(=O)c3c2c(c(O)c(c3	active	afronp_.ldb	53.98
122	ZINC95486091	:@@]2([C@H]([C@H](O)C=1)C(C(=O)C(	active	afronp_.ldb	53.89
123	ZINC95485928	(O)c2OC(C=Cc23)(C)C)c(O)c(c(O)c4)C\C=	active	afronp_.ldb	53.87
124	ZINC13480348	(cc1c2)C[C@@](OC(=O)C)(CC3=O)C)C\(	active	afronp_.ldb	53.85
125	ZINC31539795	C@@]3(OC(=O)C2)[C@H](O)[C@H](OC	active	afronp_.ldb	53.79
126	ZINC33831890	H](O)[C@@H](O)[C@@H]1O)CO)c(=O)c	active	afronp_.ldb	53.78
127	ZINC90711737	)H](O)[C@H](O)[C@@H]1O)c(=O)c3c2c(	active	afronp_.ldb	53.77
128	ZINC01663392	c(O)c(OC)c(O)c1)C(=O)[C@H](C2)Cc3cc(	active	afronp_.ldb	53.76
129	ZINC15217320	:1)[C@]4(O)c2c(c(O)cc(c2)C)C(=O)c3c(O)	active	afronp_.ldb	53.7
130	ZINC13365918	On2c1c(nccc1c3c2cccc3)c4nc(ncc4)N	active	afronp_.ldb	53.67
131	ZINC95485961	C@@H]3O[C@H](OCCc2ccc(O)cc2)[C@	active	afronp_.ldb	53.65
132	ZINC06018563	)1c3c(c(=O)c(c1)c2cc(O)c(OC)cc2)ccc(O)c:	active	afronp_.ldb	53.62
133	ZINC05842416	)1c3c(c(=O)cc1c2ccc(O)cc2)c(O)c(O)c(O)c:	active	afronp_.ldb	53.6
134	ZINC00119988	:(O)cc(O)c1)C[C@@H](O)[C@H]2c3cc(O)	active	afronp_.ldb	53.51
135	ZINC14645878	(c(=O)c(c1)c2c(OC)c(O)ccc2)c(OC)c(OC)c	active	afronp_.ldb	53.49
136	ZINC14490611	o1c(c2c(=O)c3c(O)ccc(O)c3c(=O)c2c1)C	active	afronp_.ldb	53.49
137	ZINC95486009	'[C@@H]2c3c(O[C@@H]12)cc(O)cc3)c4)	active	afronp_.ldb	53.48
138	ZINC14644461	c(O)c(=O)c2c1cc(O)cc2)c3cc(OC)c(O)c(O(	active	afronp_.ldb	53.48
139	ZINC01663631	)C)c(OC)cc(OC)c1C(=O)[C@H](C2)Cc3cc	active	afronp_.ldb	53.47
140	ZINC95486081	=O)C[C@H]2c4cc3c(O[C@@H](O)[C@H]	active	afronp_.ldb	53.44
141	ZINC14645874	c(c(=O)c(c1)c2c(OC)c(O)ccc2)c(OC)c(O)c(	active	afronp_.ldb	53.44
142	ZINC95486283	1cc(OC)c(O)cc1)c(OC)c(=O)c3c2c(c(O)c(c	active	afronp_.ldb	53.39
143	ZINC14645890	c(O)c(OC)cc(OC)c1c(=O)c(c2)c3c(OC)c(O	active	afronp_.ldb	53.39
144	ZINC14686464	:1O[C@H]([C@](O)(C(=O)OC)CO)Cc1c4r	active	afronp_.ldb	53.36
145	ZINC15257800	1c(=O)ccc2c1c(c(OC)cc2OC)\C=C\C(O)(C)	active	afronp_.ldb	53.34
146	ZINC95486244	C@@H]([C@@H](O)[C@H](O)[C@H]1O)	active	afronp_.ldb	53.33
147	ZINC18825330	o1c3c(c(=O)c(c1)c2ccc(O)cc2)c(O)cc(O)c3	active	afronp_.ldb	53.32
148	ZINC14645888	1c(O)c(OC)cc(O)c1c(=O)c(c2)c3c(OC)c(O)	active	afronp_.ldb	53.32
149	ZINC14645872	:oc4c1c(O)c2c(occ(c2=O)c3c(OC)c(O)ccc3	active	afronp_.ldb	53.3
150	ZINC95486153	)@]1([C@@](C(CCC1)(C)C)(CC2)C)C(	active	afronp_.ldb	53.26
151	ZINC95486127	:@@H](O)[C@H](O)[C@@H](O)C=O)c1)	active	afronp_.ldb	53.25
152	ZINC95486137	:oc4c1c(O)c2c(occ(c2=O)c3c(O)ccc(OC)c3	active	afronp_.ldb	53.25
153	ZINC95485984	-O)=C\[C@@H]2[C@@]1([C@H](CC(CC	active	afronp_.ldb	53.25
154	ZINC95486189	)c(OC)cc1c(=O)c4c2c(c3OC(C=Cc3c4O)(C	active	afronp_.ldb	53.19
155	ZINC95486194	c(c(c1)C)C(=O)C)C)C(=O)c2c(O)c(c(O)cc:	active	afronp_.ldb	53.16
156	ZINC05158952	:(c(O)c1)CC=C(C)C)C(=O)[C@H](c2c(O)c	active	afronp_.ldb	53.14
157	ZINC02386253	o1c(=O)cc(OC)cc1\C=C\c2ccc(O)cc2	active	afronp_.ldb	53.07
158	ZINC06091807	Oc1c(O)ccc(c1)C#CC\C=C\c2cc(O)c(O)cc2	active	afronp_.ldb	53.06
159	ZINC00608186	)c(c(c1)C)C(=O)OC)C)C(=O)c2c(O)c(c(O)	active	afronp_.ldb	53.05
160	ZINC13327497	c(c(O)cc(O)c1)C(=O)[C@H](C2)Cc3ccc(O	active	afronp_.ldb	53.03
161	ZINC13378640	\C=C(\CCC=C(C)C)/C)C(=O)[C@@H](O)	active	afronp_.ldb	53.02
162	ZINC95486054	C1)(C)C)ccc2C(=O)[C@@H](c3c(OC)cc((	active	afronp_.ldb	53
163	ZINC95485980	:@@H](C=O)C)[C@@H]2OC3C[C@@H]	active	afronp_.ldb	52.98

2. Analyticom

No	Name	Smiles	Active/Decoy	Source Database	Pharmacophore-Fit Score
1	ZINC00477939	=O)ccc3c1cc2occc2c3OC[C@H](O)C(O)	active	acdiscnp_p0.ldb	75.62
2	ZINC00600484	)C)C\C=C(\CC[C@@]2([C@H](C(=O)C	active	acdiscnp_p0.ldb	62.71
3	ZINC00899668	(O)c(c(O)c1)Cc2c(O)cccc2)C(=O)CCc3c	active	acdiscnp_p0.ldb	62.59
4	ZINC00689727	c(c1)c2cc(OC)c(OC)cc2)cc(OC)c4OC(C	active	acdiscnp_p0.ldb	62.57
5	ZINC00058117	(c(O)cc(O)c1)C(=O)C[C@H]2c3cc(O)c(	active	acdiscnp_p0.ldb	61.38
6	ZINC00039092	c(O)cc(O)c1)C(=O)C[C@H]2c3cc(O)c((	active	acdiscnp_p0.ldb	61.37
7	ZINC00156701	1c(c(O)cc(O)c1)C(=O)C[C@H]2c3ccc(C	active	acdiscnp_p0.ldb	61.3
8	ZINC00338284	c(c(O)cc(OC)c1)C(=O)C[C@H]2c3ccc((	active	acdiscnp_p0.ldb	61.23
9	ZINC00058116	c(O)cc(O)c1)C(=O)C[C@@H]2c3cc(O)c	active	acdiscnp_p0.ldb	61.18
10	ZINC00001785	c(c(O)cc(O)c1)C(=O)C[C@@H]2c3ccc(	active	acdiscnp_p0.ldb	61.14
11	ZINC00338283	(c(O)cc(OC)c1)C(=O)C[C@@H]2c3ccc	active	acdiscnp_p0.ldb	61.11
12	ZINC00899370	(O)cc(O)c1)C(=O)C[C@@H]2c3cc(OC)	active	acdiscnp_p0.ldb	60.98
13	ZINC00606754	c(cc1COC(=O)c3c2ccc(c3OC)[C@H](O	active	acdiscnp_p0.ldb	60.92
14	ZINC00105086	)cc(O)c1)C(=O)[C@H](O)[C@H]2c3cc(	active	acdiscnp_p0.ldb	60.87
15	ZINC00900428	O(c1c(c(OC)c(c(c1)CO)CO)C)CC=C(C)C	active	acdiscnp_p0.ldb	60.74
16	ZINC00899915	3c(c(=O)c(c1)c2ccc(O)cc2)c(O)c(OC)c((	active	acdiscnp_p0.ldb	60.62
17	ZINC00477938	O)ccc3c1cc2occc2c3OC[C@@H](O)C(C	active	acdiscnp_p0.ldb	60.49
18	ZINC00338303	1ccc(cc1)[C@H](C(=O)c2c(O)cc(O)cc2)	active	acdiscnp_p0.ldb	60.49
19	ZINC00047553	Oc1c(c(O)cc(O)c1)C(=O)CCc2ccc(O)cc2	active	acdiscnp_p0.ldb	60.48
20	ZINC00898768	c(ccc(O)c1)C(=O)C[C@@H]2c3cc(O)c((	active	acdiscnp_p0.ldb	60.31
21	ZINC00006787	Oc1cc(O)cc(c1)\C=C\c2ccc(O)cc2	active	acdiscnp_p0.ldb	60.31
22	ZINC00899161	Oc1c(ccc(O)c1)\C=C\c2cc(O)cc(O)c2	active	acdiscnp_p0.ldb	60.21
23	ZINC00485799	(cc1)\C=C\C)[C@H]([C@@H](O)c2cc((	active	acdiscnp_p0.ldb	56.05
24	ZINC00012342	cc(c1)C[C@@H]([C@@H](Cc2cc(O)c((	active	acdiscnp_p0.ldb	55.43
25	ZINC00056472	ccc(c1)C[C@@H]([C@H](Cc2cc(O)c(O	active	acdiscnp_p0.ldb	55.35
26	ZINC00113294	(O)cc(O)c1CC=C(C)C)C(=O)C[C@H]2(	active	acdiscnp_p0.ldb	55.13
27	ZINC00011544	cc(OC)c1)[C@H]3[C@@H]2c4c(OC3)c	active	acdiscnp_p0.ldb	54.91
28	ZINC00004749	O)c(c(O)c1C)C)C(=O)C[C@@H]2c3cc((	active	acdiscnp_p0.ldb	54.59
29	ZINC00073693	c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3ccc(	active	acdiscnp_p0.ldb	54.54
30	ZINC00039091	(O)cc(O)c1)C(=O)C[C@@H]2c3cc(O)c	active	acdiscnp_p0.ldb	54.32
31	ZINC00004935	1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3cc(	active	acdiscnp_p0.ldb	54.3
32	ZINC00519174	1c(ccc(O)c1)C(=O)C[C@@H]2c3ccc(O)	active	acdiscnp_p0.ldb	54.26
33	ZINC00898881	)c1CC=C(C)C)CC=C(C)C)C(=O)C[C@(	active	acdiscnp_p0.ldb	54.24
34	ZINC00518554	@@H]2O[C@@H]([C@@H](O)[C@H]	active	acdiscnp_p0.ldb	54.24
35	ZINC00119983	(O)cc(O)c1)C[C@H](O)[C@H]2c3cc(O)	active	acdiscnp_p0.ldb	54.22
36	ZINC00985403	c1c(ccc(O)c1)C(=O)C[C@H]2c3ccc(O)c	active	acdiscnp_p0.ldb	54.15
37	ZINC00968078	:(O)cc(O)c1)C[C@H](O)[C@@H]2c3cc	active	acdiscnp_p0.ldb	54.1
38	ZINC00899922	:1c(ccc(O)c1)C[C@H](c2c(O)cc(OC)cc2	active	acdiscnp_p0.ldb	53.84
39	ZINC00896125	Oc1c(c(O)cc(O)c1)C(=O)c2cc(O)ccc2	active	acdiscnp_p0.ldb	53.84
40	ZINC00968421	[C@]24[C@H](C[C@H]3OC2=O)C(CC	active	acdiscnp_p0.ldb	53.82
41	ZINC01002882	Oc1c(c(O)cc(O)c1)C(=O)CCc2ccccc2	active	acdiscnp_p0.ldb	53.77
42	ZINC01081534	(O)cc(OC)c1)C(=O)C[C@@H]2c3cc(O)	active	acdiscnp_p0.ldb	53.76
43	ZINC00155806	O)ccc1[C@@H]3c2c(cc(O)c(O)c2)C[C@	active	acdiscnp_p0.ldb	53.66
44	ZINC00155803	O)ccc1[C@@H]3c2c(cc(O)c(O)c2)C[C@	active	acdiscnp_p0.ldb	53.64
45	ZINC01484020	)C2[C@](OC(=O)C=2[O-])(C(=O)OC)C	active	acdiscnp_p0.ldb	53.63
46	ZINC00119988	O)cc(O)c1)C[C@@H](O)[C@H]2c3cc((	active	acdiscnp_p0.ldb	53.51
47	ZINC00900254	)C[C@@]2(O)[C@@H](COC2=O)Cc3c	active	acdiscnp_p0.ldb	53.4
48	ZINC01081535	c(O)cc(OC)c1)C(=O)C[C@H]2c3cc(O)c	active	acdiscnp_p0.ldb	53.12
49	ZINC00003968	O(c1c(O)cc(OC)cc1C)c2c(O)c(O)cc(c2)C	active	acdiscnp_p0.ldb	53.06
50	ZINC00899074	OC)c(OC)c(OC)c(O)c1c(=O)cc2c3c(OC)	active	acdiscnp_p0.ldb	53.01
51	ZINC00901461	1c(O)ccc(c1)\C=C\C(=O)NCCc2ccc(O)c	active	acdiscnp_p0.ldb	53
52	ZINC00005789	S(c1c(OC)cc(nc1C=NO)c2ncccc2)C	active	acdiscnp_p0.ldb	52.98
53	ZINC00387872	)=C(N[C@@H](CO)Cc1ccccc1)c2ccccc	active	acdiscnp_p0.ldb	52.97

54	ZINC00485801	:c1)\C=C\C)[C@@H]([C@@H](O)c2cc(	active	acdiscnp_p0.ldb	52.96
55	ZINC00402227	o1coc2c1cc(cc2)C[C@H](O)CO	active	acdiscnp_p0.ldb	52.89
56	ZINC00199444	OC)c1cc2)CC[C@@H](O)[C@@]3(OC	active	acdiscnp_p0.ldb	52.89
57	ZINC00338309	O)ccc2c1c(c(OC)cc2)C[C@@H](O)C(O	active	acdiscnp_p0.ldb	52.88
58	ZINC00387871	O=C(N[C@H](CO)Cc1ccccc1)c2ccccc2	active	acdiscnp_p0.ldb	52.86
59	ZINC00199453	:(OC)c1cc2)CC[C@H](O)[C@@]3(OC)(	active	acdiscnp_p0.ldb	52.79
60	ZINC00898952	:(OC)c(O)c(OC)c(O)c1c(=O)cc2c3ccc(O(	active	acdiscnp_p0.ldb	52.78
61	ZINC00039099	'[C@@H](C(=O)[O-])Cc1c[nH]c2c1cccc	active	acdiscnp_p0.ldb	52.77
62	ZINC00199449	:(OC)c1cc2)CC[C@@H](O)[C@]3(OC)(	active	acdiscnp_p0.ldb	52.75
63	ZINC00265484	O=c1n3c(nc2c1cccc2)[C@H](O)CC3	active	acdiscnp_p0.ldb	52.69
64	ZINC00007602	)@](=O)(c1c(OC)cc(nc1C=NO)c2ncccc	active	acdiscnp_p0.ldb	52.69
65	ZINC00039098	O[C@H](C(=O)[O-])Cc1c[nH]c2c1cccc2	active	acdiscnp_p0.ldb	52.67
66	ZINC00338310	=O)ccc2c1c(c(OC)cc2)C[C@H](O)C(O)(	active	acdiscnp_p0.ldb	52.57
67	ZINC00608130	[C@H](OC(=O)[C@@H](CC)C)[C@@	active	acdiscnp_p0.ldb	51.19
68	ZINC00899936	@@H]2OC3[C@](OC)([C@H]2C)C=C(	active	acdiscnp_p0.ldb	50.17
69	ZINC00895263	c(cc(O)c1)C(=O)OC)C(=O)c2c(O)cc(cc2	active	acdiscnp_p0.ldb	47.28
70	ZINC00056474	ccc(c1)C[C@H]([C@@H](Cc2cc(O)c(O	active	acdiscnp_p0.ldb	47.28
71	ZINC00057677	o1c3c(c(=O)cc1c2ccccc2)cc(O)cc3	active	acdiscnp_p0.ldb	47.11
72	ZINC00605688	C)cc(O)cc1C(=O)OC)c2c(c(O)cc(c2)C)C	active	acdiscnp_p0.ldb	47.01
73	ZINC00199458	(c(OC)c1cc2)CC[C@H](O)[C@]3(OC)C	active	acdiscnp_p0.ldb	46.57
74	ZINC00898293	(cc3c1cc2O[C@H](C(O)(C)C)Cc2c3)C((	active	acdiscnp_p0.ldb	46.4
75	ZINC00397608	Oc1c(cccc1)C(=O)OCCc2ccccc2	active	acdiscnp_p0.ldb	46.4
76	ZINC00506564	Oc1ccc(cc1)CC[C@H](O)C	active	acdiscnp_p0.ldb	46.31
77	ZINC00506563	Oc1ccc(cc1)CC[C@@H](O)C	active	acdiscnp_p0.ldb	46.19
78	ZINC00028038	:1c2c(OC([C@@H](OC(=O)\C(=C/C)\C	active	acdiscnp_p0.ldb	46.19
79	ZINC00025159	O(c1c(O)ccc(c1)CCc2cc(OC)cc(O)c2)C	active	acdiscnp_p0.ldb	46.13
80	ZINC00899897	)c2cc(O)c(O)cc2)c(O)c(c4OC(C=Cc34)(	active	acdiscnp_p0.ldb	46.08
81	ZINC00023222	C(=O)[C@H](C[C@@H](C1)C)C)C[C@	active	acdiscnp_p0.ldb	46.04
82	ZINC00606756	1COC(=O)c3c2ccc(c3OC)[C@H](OC(=(	active	acdiscnp_p0.ldb	45.89
83	ZINC00120273	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3ccccc3	active	acdiscnp_p0.ldb	45.89
84	ZINC00338038	1c(c(OC)cc(O)c1)C(=O)C[C@@H]2c3cc	active	acdiscnp_p0.ldb	45.88
85	ZINC00113287	O)cc(O)c1CC=C(C)C)C(=O)C[C@@H]2	active	acdiscnp_p0.ldb	45.8
86	ZINC00338302	ccc(cc1)[C@@H](C(=O)c2c(O)cc(O)cc2	active	acdiscnp_p0.ldb	45.7
87	ZINC00402623	o2c(=O)c1c(O)cc(O)cc1c3c2cc(O)cc3C	active	acdiscnp_p0.ldb	45.7
88	ZINC00898788	O(c1cc(O)c(c(O)c1)C(=O)CCc2ccccc2)C	active	acdiscnp_p0.ldb	45.47
89	ZINC00086467	C)cc2OC(C=Cc12)(C)C)C(=O)C[C@@H	active	acdiscnp_p0.ldb	45.31
90	ZINC00056555	c(OC)cc1c(c(ncc1)Cc2cc(OC)c(OC)cc2)	active	acdiscnp_p0.ldb	45.26
91	ZINC00897926	O2c1c(cc(c(O)c1)C(=O)C)C=CC2(C)C	active	acdiscnp_p0.ldb	45.12
92	ZINC00338037	:1c(c(OC)cc(O)c1)C(=O)C[C@H]2c3ccc	active	acdiscnp_p0.ldb	45.1
93	ZINC00899093	)2c1c(OC)c(O)cc(O)c1c(=O)cc2c3ccccc3	active	acdiscnp_p0.ldb	45.06
94	ZINC00050703	C(OC)[C@H](NC(=O)c1ccccc1)Cc2ccc(	active	acdiscnp_p0.ldb	45.05
95	ZINC00898098	ccc3c1c(OC[C@@H](O)C(O)(C)C)c2oc(	active	acdiscnp_p0.ldb	45.04
96	ZINC00899429	c(c(O)c1)CC=C(C)C)C(=O)C[C@@H]2(	active	acdiscnp_p0.ldb	45.01
97	ZINC00019047	1cc(OC)c(O)cc1)c(c(c2c3cc(OC)c(O)cc3	active	acdiscnp_p0.ldb	44.47
98	ZINC01081537	3c(c(=O)cc1c2ccc(O)cc2)c(O)c(OC)c(OC	active	acdiscnp_p0.ldb	44.31
99	ZINC00039288	1c3c(c(=O)cc1c2ccccc2)c(O)c(O)c(OC)c	active	acdiscnp_p0.ldb	44.24
100	ZINC01531038	)](=O)(C[C@H]([NH3+])C(=O)[O-])CC	active	acdiscnp_p0.ldb	44.06
101	ZINC00265434	:(c(=O)cc1c2ccc(OC)cc2)c(OC)c(OC)c((	active	acdiscnp_p0.ldb	44
102	ZINC00057676	o1c3c(c(=O)cc1c2ccccc2)c(O)ccc3	active	acdiscnp_p0.ldb	43.95
103	ZINC00005954	o1c3c(c(=O)cc1c2ccccc2)c(OC)ccc3	active	acdiscnp_p0.ldb	43.93
104	ZINC00058120	c(c(OC)cc(OC)c1)C(=O)C[C@@H]2c3c	active	acdiscnp_p0.ldb	43.9
105	ZINC00058119	1c(c(OC)cc(OC)c1)C(=O)C[C@H]2c3cc	active	acdiscnp_p0.ldb	43.81
106	ZINC00338123	3c4c1c2c(cc(O)c(OC)c2)C[C@@H]4[NI	active	acdiscnp_p0.ldb	43.78
107	ZINC00968436	]2[C@@](C@@H]1C(=C[C@@](C=C	active	acdiscnp_p0.ldb	43.7
108	ZINC00898340	1cc2O[C@@H](C(OC(=O)C)(C)C)Cc2c	active	acdiscnp_p0.ldb	43.48

109	ZINC00538127	c1)c2ccc(O)cc2)c(O)c(c4OC(C=Cc34)(C	active	acdiscnp_p0.ldb	43.28
110	ZINC00001758	:2c(O)c(c(OC)c(c2c1)C)C\C=C(\CCC(=(	active	acdiscnp_p0.ldb	43.17
111	ZINC01069090	[C@H]5[NH+](CC2[C@@H]([C@H]4[	active	acdiscnp_p0.ldb	43.07
112	ZINC00518798	O)ccc4c1c(OC[C@@H]2OC2(C)C)c3oc	active	acdiscnp_p0.ldb	43.01
113	ZINC00389626	)H](O)[C@H]2[NH+]3C[C@@H]([C@	active	acdiscnp_p0.ldb	42.82
114	ZINC00689683	O)c(Oc2cc1oc(=O)ccc1cc2)cc4c3cc(O)c(	active	acdiscnp_p0.ldb	42.81
115	ZINC01530575	1c(O)ccc(c1)CNC(=O)CCCC\C=C\C(C)(	active	acdiscnp_p0.ldb	42.79
116	ZINC00080812	[O-])[C@@H](NC(=O)C)Cc1c[nH]c2c1	active	acdiscnp_p0.ldb	42.71
117	ZINC00298413	1c(c(OC)ccc1C(=O)CC(=O)[O-])C=CC2	active	acdiscnp_p0.ldb	42.18
118	ZINC00002209	n2(c1ncnc1c(nc2)N)CC=C(C)C	active	acdiscnp_p0.ldb	42.16
119	ZINC00899870	1)C[C@@H](OC(=O)\C=C\c2cc(O)c(O)(	active	acdiscnp_p0.ldb	42.06
120	ZINC00898031	'@@]24[C@H](C[C@@H]3OC2=O)C((	active	acdiscnp_p0.ldb	42.01
121	ZINC00155804	:(O)ccc1[C@@H]3c2c(cc(O)c(O)c2)C[C	active	acdiscnp_p0.ldb	41.93
122	ZINC00035525	o2c1nc3c(OC)c(OC)ccc3c(OC)c1cc2	active	acdiscnp_p0.ldb	41.93
123	ZINC00080814	'([O-])[C@H](NC(=O)C)Cc1c[nH]c2c1c	active	acdiscnp_p0.ldb	41.86
124	ZINC00519249	H]1[C@](CC[C@H](C1)C(C(=O)[O-])=	active	acdiscnp_p0.ldb	41.74
125	ZINC00388089	O[C@H](C(=O)[O-])Cc1ccccc1	active	acdiscnp_p0.ldb	41.66
126	ZINC00895911	Oc1c(cccc1)\C=C\C(=O)[O-]	active	acdiscnp_p0.ldb	41.53
127	ZINC00135392	O=C([O-])[C@H](NC(=O)C)Cc1ccccc1	active	acdiscnp_p0.ldb	41.5
128	ZINC00898179	:(=O)ccc3c1c2c(O[C@H](C(O)(C)C)C2)	active	acdiscnp_p0.ldb	41.46
129	ZINC00399351	1ccc(cc1)C[C@@H](NC(=O)C)C(=O)[O	active	acdiscnp_p0.ldb	41.45
130	ZINC00388090	O[C@@H](C(=O)[O-])Cc1ccccc1	active	acdiscnp_p0.ldb	41.43
131	ZINC00077999	O(c1ccc(cc1)\C=C\C(=O)[O-])C	active	acdiscnp_p0.ldb	41.41
132	ZINC00116202	O(c1c(OC)ccc(c1)\C=C\C(=O)[O-])C	active	acdiscnp_p0.ldb	41.41
133	ZINC00056981	[O-])[C@@H]([NH2+]C)Cc1c[nH]c2c1	active	acdiscnp_p0.ldb	41.36
134	ZINC00135391	)=C([O-])[C@@H](NC(=O)C)Cc1ccccc	active	acdiscnp_p0.ldb	41.18
135	ZINC00399350	:1ccc(cc1)C[C@H](NC(=O)C)C(=O)[O-	active	acdiscnp_p0.ldb	41.01
136	ZINC00391192	O(c1ccc(cc1)CCC(=O)[O-])C	active	acdiscnp_p0.ldb	41.01
137	ZINC00391893	1c(c(O)cc(OC)c1)C(=O)C[C@@H]2c3cc	active	acdiscnp_p0.ldb	41
138	ZINC00897924	O2c1c(cc(c(OC)c1)C(=O)C)C=CC2(C)C	active	acdiscnp_p0.ldb	40.92
139	ZINC00898337	C([C@@H](OC(=O)C)[C@H]2OC(=O)'	active	acdiscnp_p0.ldb	40.82
140	ZINC00576064	C@H](c3cc(OC)c(O)c(OC)c3)[C@@H]4	active	acdiscnp_p0.ldb	40.79
141	ZINC00399067	[O-])[C@H]1C([C@H](C1)CC(=O)[O-]	active	acdiscnp_p0.ldb	40.75
142	ZINC00156571	O(c1c(O)ccc(c1)CCC(=O)[O-])C	active	acdiscnp_p0.ldb	40.75
143	ZINC00056545	([C@H]2[NH+](CC[C@@]12C)C)Cc	active	acdiscnp_p0.ldb	40.72
144	ZINC00639868	'@H](c3cc(OC)c(O)c(OC)c3)[C@@H]4	active	acdiscnp_p0.ldb	40.71
145	ZINC00156055	O(c1c(O)cc(cc1)\C=C\C(=O)[O-])C	active	acdiscnp_p0.ldb	40.7
146	ZINC00402228	o1coc2c1cc(cc2)C[C@@H](O)CO	active	acdiscnp_p0.ldb	40.69
147	ZINC00028040	3c1c2c(OC([C@H](OC(=O)\C(=C/C)\C)(	active	acdiscnp_p0.ldb	40.63
148	ZINC00057682	o1c(c(O)c(=O)c2c1cc(OC)cc2)c3ccccc3	active	acdiscnp_p0.ldb	40.47
149	ZINC01081322	!)ccc(O[C@@H]3O[C@@H]([C@@H](	active	acdiscnp_p0.ldb	40.3
150	ZINC00018453	o1c(=O)c(O)c(O)c2c1c(O)ccc2	active	acdiscnp_p0.ldb	40.25
151	ZINC00622123	1([C@@H](CC(=O)C=C1OC)C)C(=O)c	active	acdiscnp_p0.ldb	40.18
152	ZINC00518797	=O)ccc4c1c(OC[C@H]2OC2(C)C)c3occ	active	acdiscnp_p0.ldb	40.01
153	ZINC00039119	1c(c(OC)c(=O)c3c1c2c(occ2)cc3)c4cccc	active	acdiscnp_p0.ldb	39.99
154	ZINC00338221	Oc1c(cc(cc1)C(=O)C)CC=C(C)C	active	acdiscnp_p0.ldb	37.33
155	ZINC00000566	o1c(=O)ccc2c1c(c(OC)cc2)CC=C(C)C	active	acdiscnp_p0.ldb	37.3
156	ZINC00155807	)c(O)ccc1[C@H]3c2c(cc(O)c(O)c2)C[C@	active	acdiscnp_p0.ldb	37.18
157	ZINC00586482	Oc1c(O)ccc(c1)CC=C	active	acdiscnp_p0.ldb	36.99
158	ZINC00057954	2c1c(cc(OC)cc1)C(=O)C[C@H]2c3cccc	active	acdiscnp_p0.ldb	36.8
159	ZINC00057966	c1c(cccc1)C(=O)C[C@@H]2c3ccc(OC)(	active	acdiscnp_p0.ldb	36.72
160	ZINC00057922	)2c1c(cccc1)C(=O)C[C@H]2c3ccc(O)cc	active	acdiscnp_p0.ldb	36.61
161	ZINC00057923	2c1c(cccc1)C(=O)C[C@@H]2c3ccc(O)c	active	acdiscnp_p0.ldb	36.61
162	ZINC00057967	2c1c(cccc1)C(=O)C[C@H]2c3ccc(OC)c	active	acdiscnp_p0.ldb	36.51
163	ZINC00689954	·O)c(c1)c2ccc(OC)cc2)cc(OC)c4OC(C=C	active	acdiscnp_p0.ldb	36.34

3. herbal ingredients_In_Vivo_Metabolism

No	Name	Smiles	Active/Decoy	Source Database	nacophore-Fit Score
1	ZINC15115077	:cc1C(=O)C[C@H]2c3ccc(O)cc3)CCC(O)(C)C	active	himnp_p0.ldb	70.71
2	ZINC95099549	O)c1C[C@H](O)C2(C)C)C(=O)\C=C\c3ccc(O)cc	active	himnp_p0.ldb	70.44
3	ZINC34051452	))c(O)c(O)c1)C(=O)[C@H](c2ccc(O)cc2)C3	active	himnp_p0.ldb	68.1
4	ZINC34051453	)c(O)c(O)c1)C(=O)[C@@H](c2ccc(O)cc2)C3	active	himnp_p0.ldb	67.97
5	ZINC65748225	=C(CCCC1(C)C)C)\C)\C)[C@@H](O)[C@H](O)	active	himnp_p0.ldb	64.03
6	ZINC95099191	'1=C\C[C@H]3[C@]2([C@H]([C@@]([C@H]((	active	himnp_p0.ldb	63.11
7	ZINC95099633	O)[C@@H](CC\C=C(\C=C\C1=C(C(=O)CCC1((	active	himnp_p0.ldb	63.03
8	ZINC65748224	'1=C(CCCC1(C)C)C)\C)\C)[C@H](O)[C@H](O)	active	himnp_p0.ldb	63.02
9	ZINC65748226	=C(CCCC1(C)C)C)\C)\C)[C@@H](O)[C@H](C	active	himnp_p0.ldb	62.96
10	ZINC03589221	)C[C@@H]2[C@H](COC2=O)Cc3cc(O)c(O)cc3	active	himnp_p0.ldb	62.9
11	ZINC65748223	=C(CCCC1(C)C)C)\C)\C)[C@H](O)[C@H](O)[(	active	himnp_p0.ldb	62.86
12	ZINC33903076	C1)C)C2)ccc3C(=O)[C@H]5c6c(OC[C@@H]45	active	himnp_p0.ldb	62.85
13	ZINC39560162	c(cc(cc1)C(O)(C)C)CC[C@H]2[C@](C(=O)[O-]	active	himnp_p0.ldb	62.75
14	ZINC95099199	':(=O)/C/1=C\C[C@H]3[C@]2([C@@H]([C@](C	active	himnp_p0.ldb	62.67
15	ZINC95099607	@H]3[C@H]([C@@]2([C@H]([C@H](O)[C@@	active	himnp_p0.ldb	62.56
16	ZINC95099450	:c2)C)C)[C@@H]3O[C@@H]([C@@H](O)[C@	active	himnp_p0.ldb	62.5
17	ZINC95099067	:c(OC)c(O)cc2)[C@H]3O[C@H]([C@@H](O)[C	active	himnp_p0.ldb	61.7
18	ZINC95099533	1)C\C=C\c2ccc(O)cc2)[C@H](OC)[C@@H]3C((	active	himnp_p0.ldb	61.66
19	ZINC95099538	C(=O)\C=C\c2ccc(O)cc2)[C@H](O)[C@H]3C(C	active	himnp_p0.ldb	61.54
20	ZINC95099513	H](O)[C@@H](O)[C@@H]2O)C(=O)[O-])CC=C	active	himnp_p0.ldb	61.54
21	ZINC95099020	@H]2O[C@H]([C@@H](O)[C@@H](O)[C@@H	active	himnp_p0.ldb	61.23
22	ZINC95099339	]2([C@H]([C@H](O)C1)[C@H]([C@](O)(CCC(	active	himnp_p0.ldb	61.15
23	ZINC95099065	:cc(OC)c(O)cc2)[C@H]3O[C@H]([C@@H](O)[(	active	himnp_p0.ldb	61.15
24	ZINC95098987	O[C@H]([C@@H](O)[C@@H](O)[C@@H]2O)(	active	himnp_p0.ldb	61.14
25	ZINC95099017	@H]2O[C@H]([C@@H](O)[C@@H](O)[C@H]	active	himnp_p0.ldb	61.12
26	ZINC95098988	2O[C@H]([C@@H](O)[C@@H](O)[C@@H]2O	active	himnp_p0.ldb	61.03
27	ZINC95099528	1)C\C=C\c2ccc(O)cc2)[C@@H](OC)[C@H]3C((	active	himnp_p0.ldb	61.02
28	ZINC95099019	@H]2O[C@H]([C@@H](O)[C@@H](O)[C@H	active	himnp_p0.ldb	61.02
29	ZINC95099022	@H]2O[C@H]([C@@H](O)[C@@H](O)[C@@	active	himnp_p0.ldb	60.96
30	ZINC95099654	:(O)c2c(c1C)[C@@H](O)[C@](CO)(C2)C)C	active	himnp_p0.ldb	60.66
31	ZINC95099506	(O)c1)C\C=C(/CO)\C)C(=O)\C=C\c2ccc(O)cc2)C	active	himnp_p0.ldb	60.58
32	ZINC95099496	[C@H](O)C[C@@H]2[C@@H](O)C=C(O)C=C	active	himnp_p0.ldb	60.57
33	ZINC95099452	)C)c(O)c(O)c(OC)c1c(=O)cc2c3ccc(O)cc3	active	himnp_p0.ldb	60.57
34	ZINC95098985	]2O[C@H]([C@@H](O)[C@@H](O)[C@H]2O)(	active	himnp_p0.ldb	60.56
35	ZINC95099503	C@H](O)C[C@@H]2[C@@H](O)C=C(O)C=C2(	active	himnp_p0.ldb	60.55
36	ZINC95099498	C[C@H](O)C[C@H]2[C@@H](O)C=C(O)C=C2	active	himnp_p0.ldb	60.45
37	ZINC95099443	c(c3[C@@H]4O[C@H]([C@@H](O)[C@@H]((	active	himnp_p0.ldb	60.39
38	ZINC95099451	c(c(=O)cc1c2ccc(O)cc2)c(O)c(O)c(c3)C	active	himnp_p0.ldb	60.38
39	ZINC14645381	C)c(OC)c(O)c(O)c1c(=O)cc2c3ccc(OC)cc3	active	himnp_p0.ldb	60.37
40	ZINC95099493	C[C@H](O)C[C@@H]2[C@H](O)C=C(O)C=C2	active	himnp_p0.ldb	60.35
41	ZINC71404431	@H](O)[C@H]2[C@H](C(=O)OC2)Cc3cc(OC)c((	active	himnp_p0.ldb	60.35
42	ZINC14645987	(=O)c(c1)c2cc(O)c(O)cc2)c(O)c(O)c(O)c3	active	himnp_p0.ldb	60.34
43	ZINC95099445	(c3[C@@H]4O[C@H]([C@@H](O)[C@@H](O	active	himnp_p0.ldb	60.31
44	ZINC95099099	)H](O)[C@@H]2[C@H](C(=O)OC2)Cc3cc(O)cc	active	himnp_p0.ldb	60.31
45	ZINC40896750	H](O)[C@@H]2[C@H](C(=O)OC2)Cc3cc(OC)c	active	himnp_p0.ldb	60.31
46	ZINC05735437	(ccc(O)c1)C(=O)[C@H](c2ccc(O)cc2)C	active	himnp_p0.ldb	60.28
47	ZINC02561222	:cc(O)c1)C(=O)[C@@H](c2ccc(O)cc2)C	active	himnp_p0.ldb	60.28
48	ZINC00487423	)c1c(ccc(O)c1)C(=O)Cc2ccc(O)cc2	active	himnp_p0.ldb	60.27
49	ZINC95099548	))c1C[C@@H](O)C2(C)C)C(=O)\C=C\c3ccc(O)(	active	himnp_p0.ldb	60.22
50	ZINC95099222	:cc(cc1)[C@@H](CO)C)CC[C@H]2[C@](C(=O)	active	himnp_p0.ldb	60.22
51	ZINC06483745	C[C@@H]2[C@H](COC2=O)Cc3cc(O)c(O)cc3)	active	himnp_p0.ldb	60.21

52	ZINC95099659	2+]CC2)Cc3c4)[C@H]5O[C@H]([C@@H](O)[(	active	himnp_p0.ldb	60.2
53	ZINC71404432	H](O)[C@H]2[C@@H](C(=O)OC2)Cc3cc(OC)c	active	himnp_p0.ldb	60.19
54	ZINC95099479	O)c(O)cc(O)c1c(=O)c(c2)c3cc(c(O)cc3)C	active	himnp_p0.ldb	60.15
55	ZINC95099052	c3c(O)cc(O)cc3c(=O)c2c1c(O)cc(c2)CC	active	himnp_p0.ldb	60.1
56	ZINC14762532	:1)C[C@@H](O)C(=C)C)C(=O)\C=C\c2ccc(O)cc	active	himnp_p0.ldb	59.97
57	ZINC95099594	)CC3[C@@](C@@H]1C2)(CCC(=O)C=3)C)CC	active	himnp_p0.ldb	58.15
58	ZINC95099060	)C)c(O)cc2)[C@@H]3O[C@H]([C@@H](O)[C(	active	himnp_p0.ldb	57.78
59	ZINC95099632	=C\C(=C\C=C\C(=C/C(=O)[O-])\C)\C)C(CC1)(C	active	himnp_p0.ldb	56.1
60	ZINC30731379	C(\C=C\C=C(\C=C\C1=C(CO)CCCC1(C)C)/C)/C	active	himnp_p0.ldb	56.08
61	ZINC95099336	2([C@@H]([C@H](O)C1)[C@@H]([C@](O)(CC	active	himnp_p0.ldb	56.04
62	ZINC13436888	]1O)(C)C)ccc2C(=O)[C@H]4c5c(OC[C@@H]34	active	himnp_p0.ldb	56.03
63	ZINC06394169	C)ccc2C(=O)[C@]4(O)c5c(OC[C@@H]34)cc(OC	active	himnp_p0.ldb	56.03
64	ZINC33903075	)C1)C)C2)ccc3C(=O)[C@H]5c6c(OC[C@@H]4	active	himnp_p0.ldb	55.86
65	ZINC05495779	CO)C)C1)ccc2C(=O)[C@H]4c5c(OC[C@@H]34	active	himnp_p0.ldb	55.85
66	ZINC95099193	.=C\C[C@H]3[C@]2([C@@H]([C@@]([C@H](	active	himnp_p0.ldb	55.79
67	ZINC13436887	H]1O)(C)C)ccc2C(=O)[C@H]4c5c(OC[C@@H]	active	himnp_p0.ldb	55.77
68	ZINC49808411	=C\C(=O)c2c(OC)cc(O)c(c2O)CC=C(C)C)C(=O)	active	himnp_p0.ldb	55.73
69	ZINC01721175	)CCCCC)[C@@H]3[C@@H](C2(C)C)CC=C(C3	active	himnp_p0.ldb	55.72
70	ZINC01721176	1)CCCCC)[C@H]3[C@@H](C2(C)C)CC=C(C3)	active	himnp_p0.ldb	55.71
71	ZINC01721178	c1)CCCCC)[C@H]3[C@H](C2(C)C)CC=C(C3)C	active	himnp_p0.ldb	55.69
72	ZINC22061780	/C=C/C=C(/C=C/C1=C(C(=O)CCC1(C)C)C)\C)\	active	himnp_p0.ldb	55.66
73	ZINC13436891	H]1O)(C)C)ccc2C(=O)[C@H]4c5c(OC[C@@H]3	active	himnp_p0.ldb	55.66
74	ZINC95099631	C=C\C(=C\C=C\C(=C/C(=O)[O-])\C)\C)C(CC1)(	active	himnp_p0.ldb	55.64
75	ZINC05495780	)(CO)C)C1)ccc2C(=O)[C@H]4c5c(OC[C@@H]3	active	himnp_p0.ldb	55.63
76	ZINC95099634	=O)[C@H](CC\C=C(\C=C\C1=C(C(=O)CCC1(C	active	himnp_p0.ldb	55.57
77	ZINC95099526	OC)c1)C\C=C\c2ccc(O)cc2)C[C@@H]3C(O)(C)(	active	himnp_p0.ldb	55.55
78	ZINC95099381	(C([C@@H]1[C@](CC[C@](C(=O)[O-])(C1)C)(	active	himnp_p0.ldb	55.49
79	ZINC13436884	H]1O)(C)C)ccc2C(=O)[C@H]4c5c(OC[C@@H]3	active	himnp_p0.ldb	55.45
80	ZINC03947515	(c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)C[C@@H	active	himnp_p0.ldb	55.4
81	ZINC95099189	=C\C[C@@H]3[C@]2([C@@H]([C@@]([C@H]	active	himnp_p0.ldb	55.39
82	ZINC14758886	)cc(O)c1)C(=O)[C@@H](c2cc(O)c(O)cc2)C3	active	himnp_p0.ldb	55.37
83	ZINC38166908	2(C([C@@H]1[C@](CC[C@](C(=O)[O-])(C1)C)	active	himnp_p0.ldb	55.36
84	ZINC38166909	(C([C@@H]1[C@](CC[C@](C(=O)[O-])(C1)C)(	active	himnp_p0.ldb	55.23
85	ZINC95099590	3[C@@]([C@@H]1C2)(CCC(=O)C=3)C)CC[C@	active	himnp_p0.ldb	55.22
86	ZINC95099551	H](c2c(OC1)cc(OC)c(O)c2)C(=O)c3cc4)C[C@@H	active	himnp_p0.ldb	55.19
87	ZINC95099059	OC)c(O)cc2)[C@H]3O[C@H]([C@@H](O)[C@	active	himnp_p0.ldb	55.18
88	ZINC95099054	(OC)c(O)cc2)[C@H]3O[C@H]([C@@H](O)[C@	active	himnp_p0.ldb	55.14
89	ZINC05158428	O)(c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)C[C@	active	himnp_p0.ldb	55.06
90	ZINC15113812	O)ccc(c1)C[C@H](O)Cc2c(O)cc(O)cc2O	active	himnp_p0.ldb	54.94
91	ZINC02585769	c(O)c(O)ccc1c(=O)c(c2)c3cc(O)c(O)cc3	active	himnp_p0.ldb	54.63
92	ZINC15115078	c1C(=O)C[C@@H]2c3ccc(O)cc3)CCC(O)(C)C	active	himnp_p0.ldb	54.62
93	ZINC00391976	c(c(=O)c(c1)c2cc(O)c(O)cc2)ccc(O)c3	active	himnp_p0.ldb	54.59
94	ZINC95099494	)C[C@H](O)C[C@H]2[C@H](O)C=C(O)C=C2C	active	himnp_p0.ldb	54.4
95	ZINC03589244	[C@@H]2[C@](O)(C(=O)OC2)Cc3cc(OC)c(O)c	active	himnp_p0.ldb	54.39
96	ZINC95099539	C(=O)\C=C\c2ccc(O)cc2)[C@H](O)[C@@H]3C(	active	himnp_p0.ldb	54.37
97	ZINC95099003	@H]2O[C@H]([C@@H](O)[C@@H](O)[C@H]2	active	himnp_p0.ldb	54.32
98	ZINC14762797	=O)c2c1c(c(O)cc2O)CC=C(C)C)c3ccc(OC)cc3	active	himnp_p0.ldb	54.3
99	ZINC14437637	c1)C[C@H]([C@H](CO)Cc2cc(O)c(O)cc2)CO	active	himnp_p0.ldb	54.3
100	ZINC13461250	O)c1C[C@H]2C(O)(C)C)C(=O)\C=C\c3ccc(O)cc	active	himnp_p0.ldb	54.29
101	ZINC95099661	+]CC2)Cc3c4)[C@@H]5O[C@H]([C@@H](O)[	active	himnp_p0.ldb	54.27
102	ZINC14762765	=O)c2c1c(c(O)cc2O)CC=C(C)C)c3ccc(O)cc3	active	himnp_p0.ldb	54.24
103	ZINC95099456	C@@H]([C@@H]([C@@H](O)[C@H]2O)C)C)	active	himnp_p0.ldb	54.15
104	ZINC06093399	1c(O)c(O)ccc1c(=O)c(c2)c3ccc(O)cc3	active	himnp_p0.ldb	54.14

105	ZINC14694406	:1)C[C@H]([C@H](CO)Cc2cc(O)c(O)cc2)CO)C	active	himnp_p0.ldb	54.08
106	ZINC95099006	H]2O[C@H]([C@@H](O)[C@@H](O)[C@@H]	active	himnp_p0.ldb	54.06
107	ZINC13461252	))c1C[C@@H]2C(O)(C)C)C(=O)\C=C\c3ccc(O)c	active	himnp_p0.ldb	54.05
108	ZINC95099535	C(=O)\C=C\c2ccc(O)cc2)[C@@H](O)[C@H]3C(	active	himnp_p0.ldb	54.04
109	ZINC95099473	)c(O)cc(O)c1C(=O)[C@H](c2ccc(O)cc2)C3	active	himnp_p0.ldb	53.97
110	ZINC36470466	c(c1)C[C@H]([C@H](CO)Cc2cc(O)ccc2)CO	active	himnp_p0.ldb	53.97
111	ZINC14646917	C[C@@H]2[C@](O)(C(=O)OC2)Cc3cc(O)c(O)c	active	himnp_p0.ldb	53.91
112	ZINC14758887	O)cc(O)c1)C(=O)[C@H](c2cc(O)c(O)cc2)C3	active	himnp_p0.ldb	53.9
113	ZINC95099419	)[C@H](O)C(=O)N([C@H]2[C@H](O)c3ccccc3	active	himnp_p0.ldb	53.89
114	ZINC14762534	)c1)C[C@H](O)C(=C)C(=O)\C=C\c2ccc(O)cc2	active	himnp_p0.ldb	53.89
115	ZINC95099420	]3[C@H](O)C(=O)N([C@H]3[C@H](O)c2ccccc	active	himnp_p0.ldb	53.79
116	ZINC95099458	C@@H]([C@@H]([C@@H](O)[C@H]2O)C)C)C	active	himnp_p0.ldb	53.67
117	ZINC95099501	C[C@H](O)C[C@H]2[C@H](O)C=C(O)C=C2O	active	himnp_p0.ldb	53.64
118	ZINC15113814	)ccc(c1)C[C@@H](O)Cc2c(O)cc(O)cc2O	active	himnp_p0.ldb	53.63
119	ZINC06018563	c(c(=O)c(c1)c2cc(O)c(OC)cc2)ccc(O)c3	active	himnp_p0.ldb	53.62
120	ZINC95099414	1)[C@H](O)C(=O)N([C@H]2[C@H](O)c3ccccc	active	himnp_p0.ldb	53.61
121	ZINC95099656	]4[NH2+]CC3)[C@@H]5O[C@H]([C@@H](O)[	active	himnp_p0.ldb	53.58
122	ZINC95099465	@@H](O)[C@H](O)[C@H]1O)C(=O)[O-])c2)C	active	himnp_p0.ldb	53.57
123	ZINC95099406	C@@H]3N(C(=O)[C@@H](O)[C@@H]3c2cccc	active	himnp_p0.ldb	53.54
124	ZINC95099655	I]4[NH2+]CC3)[C@H]5O[C@H]([C@@H](O)[(	active	himnp_p0.ldb	53.52
125	ZINC95099519	)CCC(=C)C)C(=O)[C@H]3O[C@@H]3c2ccc(O)	active	himnp_p0.ldb	53.52
126	ZINC95099652	c(c1C)CCO)C)[C@@H](O)[C@](CO)(C2)C	active	himnp_p0.ldb	53.48
127	ZINC95099109	:1)C[C@@H]2[C@H](COC2=O)Cc3cc(O)ccc3	active	himnp_p0.ldb	53.46
128	ZINC14854159	))cc(O[C@H]3O[C@H]([C@@H](O)[C@H](O)[	active	himnp_p0.ldb	53.46
129	ZINC05430816	)ccc1C(=O)C[C@H]2c3ccc(O)cc3)CC=C(C)C	active	himnp_p0.ldb	53.46
130	ZINC95099221	c(cc1)[C@@H](CO)C)CC[C@H]2[C@](C(=O)[	active	himnp_p0.ldb	53.45
131	ZINC39560163	1c(cc(cc1)C(O)(C)C)CC[C@H]2[C@](C(=O)[O-	active	himnp_p0.ldb	53.45
132	ZINC95099478	O-])c(c(=O)c2c1cc(O)cc2O)c3ccc(O)cc3	active	himnp_p0.ldb	53.43
133	ZINC95099000	](O)[C@H]2O)C(=O)[O-])cc(O)c3)[C@H]4O[C(	active	himnp_p0.ldb	53.43
134	ZINC13370550	)cc(O[C@@H]3O[C@H]([C@@H](O)[C@H](O	active	himnp_p0.ldb	53.41
135	ZINC38957372	c(O)c(O)ccc1)C(=O)CCc2cc(O)c(O)cc2	active	himnp_p0.ldb	53.39
136	ZINC95099064	C)c(O)cc2)[C@@H]3O[C@H]([C@@H](O)[C@	active	himnp_p0.ldb	53.38
137	ZINC38420626	1)C[C@@H]2[C@H](C(=O)OC2)Cc3cc(O)ccc3	active	himnp_p0.ldb	53.38
138	ZINC01645462	C[C@H]2[C@@H](C(=O)OC2)Cc3cc(O)c(O)cc	active	himnp_p0.ldb	53.37
139	ZINC95099648	2c1cccc2)c4[nH]c3c(c(O)ccc3)c4[C@H](O)C5	active	himnp_p0.ldb	53.35
140	ZINC95099660	+]CC2)Cc3c4)[C@H]5O[C@H]([C@@H](O)[C	active	himnp_p0.ldb	53.32
141	ZINC71404433	I](O)[C@@H]2[C@@H](C(=O)OC2)Cc3cc(OC)	active	himnp_p0.ldb	53.31
142	ZINC95099662	-]CC2)Cc3c4)[C@@H]5O[C@H]([C@@H](O)[(	active	himnp_p0.ldb	53.29
143	ZINC14759297	c(O)c(O)c(O)cc1c(=O)c(c2)c3ccc(O)cc3	active	himnp_p0.ldb	53.27
144	ZINC95099507	H](O)[C@@H](O)[C@H]2O)C(=O)[O-])CC=C((	active	himnp_p0.ldb	53.25
145	ZINC95099366	]1([C@H]([C@](C@@H](O)CC1)(CO)C)CC2)(	active	himnp_p0.ldb	53.22
146	ZINC95099010	[C@H]([C@@H](O)C3)CO)N)C[C@@H](O)Cc	active	himnp_p0.ldb	53.22
147	ZINC95099218	H]2[C@@](c1c(cc(cc1)[C@@H](CO)C)CC2)(C(	active	himnp_p0.ldb	53.21
148	ZINC95098997	H](O)[C@H]2O)C(=O)[O-])cc(O)c3)[C@H]4O[(	active	himnp_p0.ldb	53.2
149	ZINC95099224	c1c(cc(cc1)C(=C)C)CC[C@H]2[C@](C(=O)[O-]	active	himnp_p0.ldb	53.16
150	ZINC95099220	(cc1)[C@@]2([C@H]([C@](C(=O)[O-])(CCC2)(	active	himnp_p0.ldb	53.16
151	ZINC72131068	c(OC)c(O)cc2)[C@H]3O[C@H]([C@@H](O)[C(	active	himnp_p0.ldb	53.15
152	ZINC33682758	2N(CCC2)C)[C@H](O)[C@H](O)[C@H](O)[C@	active	himnp_p0.ldb	53.15
153	ZINC04097179	O)[C@H]2[NH+]3C[C@@H]([C@@H](C2)CC	active	himnp_p0.ldb	53.15
154	ZINC95099462	C@H]([C@@H]([C@@H](O)[C@H]2O)C)C)C[	active	himnp_p0.ldb	53.14
155	ZINC95099424	O)(C(=O)OCc1cn(cc1)CCCOC(=O)[C@@H]2C)	active	himnp_p0.ldb	53.11
156	ZINC95099436	(C1)CC2)[C@H](O)C3=C4[C@@H](NC(=O)C3	active	himnp_p0.ldb	53.09
157	ZINC95099242	)C(=C1)C)CC(CO)=C[C@@H]2[C@@H](C(=O	active	himnp_p0.ldb	53.07

4. herbal ingredients_targets

No	Name	Smiles	Active/Decoy	Source Database	Fit Score
1	ZINC85737813	COC2=O)Cc3cc(OC)c(OC)cc3)[C@H]4O[C@H]([(	active	hitnp_p0.ldb	70.42
2	ZINC04098334	O)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C[C@]	active	hitnp_p0.ldb	68.24
3	ZINC44699916	CO[C@H]2O[C@H]([C@@H](O)[C@@H](O)[C(	active	hitnp_p0.ldb	68.17
4	ZINC03777403	+]2c1c(c(O)cc(O)c1)C=C(O)[C@H]2c3cc(O)c(O)c(	active	hitnp_p0.ldb	67.81
5	ZINC44699912	CCO[C@H]2O[C@H]([C@@H](O)[C@@H](O)[C	active	hitnp_p0.ldb	67.55
6	ZINC95098872	C@]3([C@@H]2CC=C4[C@@H]3C[C@H](O)[C@	active	hitnp_p0.ldb	64.45
7	ZINC95098803	@H]1O)CO)[C@@H]3OC=C[C@@]4(O)[C@H]((	active	hitnp_p0.ldb	62.93
8	ZINC01702730	2c(O)ccc(O)c2c(=O)cc1[C@H](OC(=O)C(C)C)CC=	active	hitnp_p0.ldb	62.84
9	ZINC02525131	O)ccc(O)c2c(=O)cc1[C@H](OC(=O)CC(O)(C)C)C	active	hitnp_p0.ldb	62.81
10	ZINC85737817	OC2=O)Cc3cc(OC)c(OC)cc3)[C@H]4O[C@H]([C	active	hitnp_p0.ldb	62.63
11	ZINC04268352	](O)[C@H](O)[C@H]1O)CO)[C@H]2OC=C[C@]	active	hitnp_p0.ldb	62.54
12	ZINC95098796	[C@@H](O)[C@@H](O)[C@H]2O)CO)C(=O)[C@	active	hitnp_p0.ldb	61.53
13	ZINC03869685	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3cc(O)c(O)cc3	active	hitnp_p0.ldb	61.3
14	ZINC00156701	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3ccc(O)cc3	active	hitnp_p0.ldb	61.27
15	ZINC33833930	c(c(O)cc(O)c1)C(=O)[C@H]([C@H]2c3cc(O)c(O)c	active	hitnp_p0.ldb	61.22
16	ZINC04097773	]2c3cc(O)c(O)cc3)C(=O)[O-])\C=C\C(O[C@@H](	active	hitnp_p0.ldb	61.22
17	ZINC95098820	@@H]2[C@@H]1[C@@H](OC(=O)C1=C)C=C(C(	active	hitnp_p0.ldb	61.12
18	ZINC00001785	O2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3ccc(O)cc3	active	hitnp_p0.ldb	61.12
19	ZINC33833929	(c(O)cc(O)c1)C(=O)[C@@H]([C@H]2c3cc(O)c(O	active	hitnp_p0.ldb	61.04
20	ZINC02015151	=c1c2c(O)ccc(O)c2c(=O)cc1[C@@H](O)CC=C(C)	active	hitnp_p0.ldb	61
21	ZINC44699918	CO[C@@H]2O[C@H]([C@@H](O)[C@@H](O)[C	active	hitnp_p0.ldb	60.76
22	ZINC01615345	C)ccc(c1)C[C@H]2[C@H](C(=O)OC2)Cc3cc(OC)c	active	hitnp_p0.ldb	60.74
23	ZINC05369365	)[C@@H]2O[C@@H]([C@H](O)[C@H](O)[C@@	active	hitnp_p0.ldb	60.72
24	ZINC02015152	O=c1c2c(O)ccc(O)c2c(=O)cc1[C@H](O)CC=C(C)C	active	hitnp_p0.ldb	60.72
25	ZINC44699914	CO[C@@H]2O[C@H]([C@@H](O)[C@@H](O)[	active	hitnp_p0.ldb	60.71
26	ZINC72186829	([C@H]1[C@]([C@H](C(=O)CO)CC1)(C=O)C2)C	active	hitnp_p0.ldb	60.68
27	ZINC05567588	C\C(O[C@H]2[C@@H](O)[C@H](O)C[C@@](O	active	hitnp_p0.ldb	60.63
28	ZINC03947475	\C(O[C@H]2[C@@H](O)[C@@H](O)C[C@@](C	active	hitnp_p0.ldb	60.56
29	ZINC04268354	](O)[C@H](O)[C@H]1O)CO)[C@H]2OC=C[C@H	active	hitnp_p0.ldb	60.55
30	ZINC00899915	o1c3c(c(=O)c(c1)c2ccc(O)cc2)c(O)c(OC)c(O)c3	active	hitnp_p0.ldb	60.52
31	ZINC06484558	o1c3c(c(=O)c(c1)c2ccc(OC)cc2)c(O)c(OC)c(O)c3	active	hitnp_p0.ldb	60.33
32	ZINC05369366	O[C@@H]2O[C@H]([C@H](O)[C@H](O)[C@@]	active	hitnp_p0.ldb	60.32
33	ZINC04097772	H]2c3cc(O)c(O)cc3)C(=O)[O-])\C=C\C(O[C@@H]	active	hitnp_p0.ldb	60.32
34	ZINC00006787	Oc1cc(O)cc(c1)\C=C\c2ccc(O)cc2	active	hitnp_p0.ldb	60.3
35	ZINC04212683	@@H]1O[C@@H]([C@@H](O)[C@H](O)[C@H]	active	hitnp_p0.ldb	60.19
36	ZINC08234189	C=C[C@@H]3O)C)CC[C@@]5([C@@H]([C@@	active	hitnp_p0.ldb	55.62
37	ZINC95098874	C@]3([C@@H]2CC=C4[C@@H]3C[C@H](O)[C	active	hitnp_p0.ldb	55.57
38	ZINC04097774	]2c3cc(O)c(O)cc3)C(=O)[O-])\C=C\C(O[C@@H](	active	hitnp_p0.ldb	55.18
39	ZINC04963987	O)cc2)c(O)cc(O)c3[C@H]4O[C@H]([C@@H](O)[	active	hitnp_p0.ldb	55.18
40	ZINC13377888	c(O)ccc(c1)CC[C@H](O)CC(=O)CCc2cc(OC)c(O)c	active	hitnp_p0.ldb	54.82
41	ZINC04963990	)cc2)c(O)cc(O)c3[C@H]4O[C@H]([C@@H](O)[C	active	hitnp_p0.ldb	54.58
42	ZINC00901160	)ccc(c1)C[C@H](OC(=O)\C=C\c2cc(O)c(O)cc2)C(	active	hitnp_p0.ldb	54.55
43	ZINC04095807	@@H]1O[C@@H]([C@@H](O)[C@H](O)[C@H]	active	hitnp_p0.ldb	54.35
44	ZINC00058116	2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3cc(O)c(O)c	active	hitnp_p0.ldb	54.3
45	ZINC00119983	c1c(c(O)cc(O)c1)C[C@H](O)[C@H]2c3cc(O)c(O)c	active	hitnp_p0.ldb	54.26
46	ZINC04175638	]([C@H](O)[C@@H](O)[C@H]1O)C)c(=O)c3c2c	active	hitnp_p0.ldb	54.18
47	ZINC95098795	([C@@H](O)[C@@H](O)[C@H]2O)CO)C(=O)[C	active	hitnp_p0.ldb	54.17
48	ZINC08214398	C@H]1O)CO)[C@@H]3OC=C[C@@]4(O)[C@H]	active	hitnp_p0.ldb	54.15
49	ZINC05085286	@H]2c3cc(O)c(O)cc3)[C@@H]5c6c(O[C@H](c4c	active	hitnp_p0.ldb	54.13

50	ZINC95098798	](C@@H](O)[C@@H](O)[C@H]2O)CO)C(=O)[C	active	hitnp_p0.ldb	54.07
51	ZINC00058117	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3cc(O)c(O)cc3	active	hitnp_p0.ldb	54.02
52	ZINC00119978	1c(c(O)cc(O)c1)C[C@H](O)[C@@H]2c3cc(O)c(O	active	hitnp_p0.ldb	53.97
53	ZINC08681509	O)[C@H]2O[C@@H]1O[C@H]([C@@H](O)[C@	active	hitnp_p0.ldb	53.96
54	ZINC04349421	c2)c(O)c(c(O)c3)[C@@H]4O[C@H]([C@@H](O)[	active	hitnp_p0.ldb	53.92
55	ZINC03947432	)cc2)c(O)cc(O[C@@H]3O[C@H]([C@@H](O)[C(	active	hitnp_p0.ldb	53.92
56	ZINC13424725	([C@H](O)[C@@H](O)[C@@H]1O)CO)c(=O)c3c	active	hitnp_p0.ldb	53.8
57	ZINC34933704	cc2)c(O)c(c(O)c3)[C@H]4O[C@H]([C@@H](O)[C	active	hitnp_p0.ldb	53.65
58	ZINC18847034	o1c3c(c(=O)c(c1)c2ccc(O)cc2)ccc(O)c3	active	hitnp_p0.ldb	53.62
59	ZINC05842416	o1c3c(c(=O)cc1c2ccc(O)cc2)c(O)c(O)c(O)c3	active	hitnp_p0.ldb	53.62
60	ZINC54979046	]2N(CC1)CC=C2COC(=O)[C@](O)([C@@](O)([C	active	hitnp_p0.ldb	53.6
61	ZINC05369368	)[C@@H]2O[C@H]([C@@H](O)[C@H](O)[C@@	active	hitnp_p0.ldb	53.54
62	ZINC95098818	C@]2([C@@]3(O)[C@H](OC(=O)[C@H]3C)C4)C	active	hitnp_p0.ldb	53.47
63	ZINC03873123	1c(cc(c(O)c1)C(C=C)(C)C)\C=C\C(=O)c2ccc(O)cc	active	hitnp_p0.ldb	53.47
64	ZINC03947434	cc2)c(O)cc(O[C@@H]3O[C@H]([C@@H](O)[C@	active	hitnp_p0.ldb	53.47
65	ZINC03775158	H+]2c1c(c(O)cc(O)c1)C=C(O)[C@H]2c3cc(O)c(O)	active	hitnp_p0.ldb	53.46
66	ZINC04098633	c2ccc(O)cc2)[C@@H]3O[C@@H]([C@@H](O)[C	active	hitnp_p0.ldb	53.45
67	ZINC04349347	H]([C@H](O)[C@H](O)[C@H]1O)CO)c(=O)c3c2c	active	hitnp_p0.ldb	53.42
68	ZINC05999049	O(c1c(ccc(O)c1)C(=O)\C=C\c2cc(O)c(O)cc2)C	active	hitnp_p0.ldb	53.41
69	ZINC27429758	)H]([C@@H](O)C1)[C@H]2[C@@]([C@@H]([C(	active	hitnp_p0.ldb	53.4
70	ZINC03872686	O(c1c(O)ccc(c1)CCC(=O)C[C@H](O)CCCCC)C	active	hitnp_p0.ldb	53.4
71	ZINC00899931	)ccc(c1)C[C@H]2[C@@H](C(=O)OC2)Cc3cc(OC)	active	hitnp_p0.ldb	53.39
72	ZINC95098819	C@]2([C@@]3(O)[C@H](OC(=O)[C@@H]3C)C4	active	hitnp_p0.ldb	53.38
73	ZINC95098786	([C@]3([C@@H]([C@H](O)C1)[C@@H]([C@]2(	active	hitnp_p0.ldb	53.36
74	ZINC18825330	o1c3c(c(=O)c(c1)c2ccc(O)cc2)c(O)cc(O)c3	active	hitnp_p0.ldb	53.36
75	ZINC05999205	o1c3c(c(=O)c(c1)c2ccc(O)cc2)cc(OC)c(O)c3	active	hitnp_p0.ldb	53.35
76	ZINC00896041	Oc1c(O)cc2c(c1)[C@H]([NH2+]CC2)Cc3ccc(O)cc3	active	hitnp_p0.ldb	53.35
77	ZINC18847036	o1c3c(c(=O)c(c1)c2ccc(OC)cc2)ccc(O)c3	active	hitnp_p0.ldb	53.29
78	ZINC13827980	C@H]1[C@]([C@@H](C(=O)CO)CC1)(C=O)C2)(	active	hitnp_p0.ldb	53.26
79	ZINC03947431	O)cc2)c(O)cc(O[C@H]3O[C@H]([C@@H](O)[C@	active	hitnp_p0.ldb	53.24
80	ZINC95098907	(=O)C[C@H](C(=O)[O-])C)C)CC1=O)(CC(=O)C=(	active	hitnp_p0.ldb	53.23
81	ZINC04098644	O=c1c3c(O)cc(cc3c(=O)c2c1c(O)ccc2)CO	active	hitnp_p0.ldb	53.21
82	ZINC13859683	)@H]2c4ccc(O[C@@H]3O[C@@H]([C@@H](O)[	active	hitnp_p0.ldb	53.19
83	ZINC34933706	c2)c(O)c(c(O)c3)[C@H]4O[C@H]([C@@H](O)[C(	active	hitnp_p0.ldb	53.17
84	ZINC04098556	([C@H](O)[C@@H](O)[C@H]1O)C)c(=O)c3c2cc(	active	hitnp_p0.ldb	53.1
85	ZINC21992916	O)c(O)c(O[C@@H]3O[C@@H]([C@@H](O)[C@	active	hitnp_p0.ldb	53.08
86	ZINC03869608	Oc1c(ccc(O)c1)C(=O)\C=C\c2ccc(O)cc2	active	hitnp_p0.ldb	53.06
87	ZINC33832060	O)[C@H](O)[C@H]1O)CO)[C@H]2OC=C([C@@	active	hitnp_p0.ldb	53.05
88	ZINC00001219	o3c(=O)c1c(oc2c1ccc(O)c2)c4c3cc(O)cc4	active	hitnp_p0.ldb	53.05
89	ZINC06525297	o1c(c(O)c(=O)c2c1c(O)c(O)cc2O)c3cc(O)c(O)cc3	active	hitnp_p0.ldb	53.04
90	ZINC00900233	)=c1n(c2c(OC)cccc2c(OC)c1C[C@@H](O)C(C)C)(	active	hitnp_p0.ldb	53.02
91	ZINC05784821	o1c(c(O)c(O)c2c1cc(=O)c(O)c2O)c3cc(O)c(O)cc3	active	hitnp_p0.ldb	52.98
92	ZINC14488654	O=c1c3c(c(=O)c2c1cccc2)cc(c(O)c3)C	active	hitnp_p0.ldb	52.95
93	ZINC13827986	C@H]1[C@]([C@@H](C(=O)CO)CC1)(C=O)C2)C	active	hitnp_p0.ldb	52.94
94	ZINC08552017	[C@@]2([C@]3(O)[C@@H](OC(=O)[C@H]3C)[(	active	hitnp_p0.ldb	52.89
95	ZINC01702729	O)ccc(O)c2c(=O)cc1[C@@H](OC(=O)CC(O)(C)C)(	active	hitnp_p0.ldb	52.88
96	ZINC95098783	]5([C@@H]([C@H](O)C[C@H]1[C@]2(CC3)C)[C	active	hitnp_p0.ldb	52.87
97	ZINC95098850	([C@H]2[C@H]([C@@]1(C(=CC(=O)CC1)CC2)C	active	hitnp_p0.ldb	52.82
98	ZINC38139712	@H]1O)CO[C@@H]2O[C@@H]([C@@H](O)[C@	active	hitnp_p0.ldb	52.82
99	ZINC26981407	O(c1c(O)cc(cc1)\C=C\c2cc(O)cc(O)c2)C	active	hitnp_p0.ldb	52.79
100	ZINC03874886	c1C=CC2(C)C)Cc3c(O)c(c(O)c(c3O)C)C(=O)C)C(=	active	hitnp_p0.ldb	52.79
101	ZINC86028690	H](C(O[C@H]2O[C@H]([C@@H](O)[C@@H](O)	active	hitnp_p0.ldb	52.78
102	ZINC14818509	)@H]2[C@@H]([C@H]1[C@@]([C@](O)(C(=O)(	active	hitnp_p0.ldb	52.73

103	ZINC04217378	@H]([C@@H](O)[C@H](O)[C@H]1O)CO)c(O)cc	active	hitnp_p0.ldb	52.7
104	ZINC03871358	o1c3c(c(=O)cc1c2ccc(OC)cc2)c(O)cc(O)c3	active	hitnp_p0.ldb	52.68
105	ZINC03871576	o1c3c(c(=O)cc1c2ccc(O)cc2)c(O)cc(O)c3	active	hitnp_p0.ldb	52.67
106	ZINC03871987	lc(c(OC)c(=O)c2c1cc(O)c(OC)c2O)c3cc(O)c(OC)c	active	hitnp_p0.ldb	52.66
107	ZINC40864963	C@@H]2OC[C@@H]3[C@@H](OC[C@H]23)c4	active	hitnp_p0.ldb	52.65
108	ZINC02036574	O=c1n(c2c(OC)cccc2c(OC)c1C[C@H](O)C(C)C)C	active	hitnp_p0.ldb	52.62
109	ZINC03610022	O(c1c(O)ccc(c1)CCC(=O)CCCCCCCCC)C	active	hitnp_p0.ldb	52.6
110	ZINC04492895	OC\C(=C\CNc2ncnc1[nH]cnc12)\C	active	hitnp_p0.ldb	52.59
111	ZINC04349262	cc2)c(O)c(c(O)c3)[C@@H]4O[C@@H]([C@@H](	active	hitnp_p0.ldb	52.55
112	ZINC04098515	]([C@@H](O)[C@H](O)[C@H]1O)CO)c(O)cc(O)c	active	hitnp_p0.ldb	52.31
113	ZINC95098787	]([C@]3([C@@H]([C@H](O)C1)[C@H]([C@]2(C	active	hitnp_p0.ldb	51.88
114	ZINC14727558	=O)c(c1c2c(O)cc(O)cc2)CC=C(C)C)c(O)cc(O)c3C(	active	hitnp_p0.ldb	51.13
115	ZINC01530836	H]1[C@@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4	active	hitnp_p0.ldb	50.75
116	ZINC03947455	]2(C([C@@H]1[C@@H]([C@@H](CC[C@@]1(C	active	hitnp_p0.ldb	50.74
117	ZINC95098851	C@H]([C@H]2[C@]([C@H](O)C1)([C@H]([C@H	active	hitnp_p0.ldb	50.56
118	ZINC95098784	]5([C@@H]([C@H](O)C[C@H]1[C@]2(CC3)C)[	active	hitnp_p0.ldb	49.2
119	ZINC04098201	C@]1(OC1)[C@H]23)([C@H](O)[C@H]5OC(=O)[	active	hitnp_p0.ldb	48.37
120	ZINC00001601	o1c(ccc1)CNc3ncnc2[nH]cnc23	active	hitnp_p0.ldb	48.37
121	ZINC03872070	o1c3c(c(=O)cc1c2ccccc2)c(O)cc(O)c3	active	hitnp_p0.ldb	48.28
122	ZINC08681507	(O)[C@H]2O[C@@H]1O[C@H]([C@H](O)[C@H	active	hitnp_p0.ldb	48.18
123	ZINC06018556	c(c(OC)c(=O)c2c1cc(OC)c(OC)c2O)c3cc(O)c(OC)c	active	hitnp_p0.ldb	48.05
124	ZINC95098792	25[C@@]3(CC[C@H]6[C@]47[C@H](OC([C@@	active	hitnp_p0.ldb	47.96
125	ZINC14764110	o2c1c(OC)cccc1c(=O)c3c2cc(OC)c(OC)c3O	active	hitnp_p0.ldb	47.87
126	ZINC85737808	(COC2=O)Cc3cc(OC)c(OC)cc3)[C@H]4O[C@H](	active	hitnp_p0.ldb	47.85
127	ZINC03869768	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3ccc(O)cc3	active	hitnp_p0.ldb	47.78
128	ZINC14879959	C\C(=C\C=C\C=C(\C=C\C=C(\C=C\C1=C(C[C@H]	active	hitnp_p0.ldb	47.27
129	ZINC14879961	C(=C\C=C\C=C(\C=C\C=C(\C=C\C1=C(C[C@H](	active	hitnp_p0.ldb	47.26
130	ZINC70450846	C\C(=C\C=C\C=C(\C=C\C=C(\C=C\C1=C(CCCC1(	active	hitnp_p0.ldb	47.25
131	ZINC40164432	C(=C\C=C\C=C(\C=C\C=C(\C=C\C1=C(C[C@@H	active	hitnp_p0.ldb	47.2
132	ZINC08221225	(=C\C=C\C=C(\C=C\C=C(\C=C\C1=C(C[C@@H]	active	hitnp_p0.ldb	47.2
133	ZINC04097702	=C\C(=C\C=C\C=C(\C=C\C=C(\C=C\C1=C(CCCC	active	hitnp_p0.ldb	47.19
134	ZINC59872849	]([C@H](O)[C@H](O)[C@@H]1O)CO)c(=O)c3c2	active	hitnp_p0.ldb	47.15
135	ZINC03824868	O=c1c3c(O)cc(O)cc3c(=O)c2c1c(O)cc(c2)C	active	hitnp_p0.ldb	47.06
136	ZINC00119985	c(c(O)cc(O)c1)C[C@@H](O)[C@@H]2c3cc(O)c((	active	hitnp_p0.ldb	47
137	ZINC01532490	C(O[C@@H]2[C@@H](O)[C@@H](O)C[C@@](	active	hitnp_p0.ldb	46.98
138	ZINC03871565	)H]1[NH+]([C@@H]([C@H](O)C1)C2)C)C(=O)[C	active	hitnp_p0.ldb	46.95
139	ZINC00119988	1c(c(O)cc(O)c1)C[C@@H](O)[C@H]2c3cc(O)c(O	active	hitnp_p0.ldb	46.87
140	ZINC14818513	@@H]2[C@@H]([C@H]1[C@@]([C@](O)(C(=O)	active	hitnp_p0.ldb	46.86
141	ZINC01532860	OC\C=C(\CC\C=C(\CCC=C(C)C)/C)/C	active	hitnp_p0.ldb	46.86
142	ZINC00120273	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3ccccc3	active	hitnp_p0.ldb	46.85
143	ZINC05452635	c(O)ccc(O)c2c(=O)cc1[C@@H](OC(=O)C(C)C)CC	active	hitnp_p0.ldb	46.83
144	ZINC13424728	2)c(O)c(c(O)c3)[C@@H]4O[C@H]([C@@H](O)[C	active	hitnp_p0.ldb	46.75
145	ZINC95098781	O)[C@@H]1O)CO)[C@@H]3OC=C[C@H]4[C@(	active	hitnp_p0.ldb	46.71
146	ZINC95098852	C@H]([C@H]2[C@]([C@@H](O)C1)([C@H]([C@	active	hitnp_p0.ldb	46.65
147	ZINC03978460	C@H]1[C@@]([C@H]([C@@H](\C=C\[C@H](C((	active	hitnp_p0.ldb	46.58
148	ZINC04268353	](O)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C[C@	active	hitnp_p0.ldb	46.55
149	ZINC03881558	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3c(O)cc(O)cc3	active	hitnp_p0.ldb	46.53
150	ZINC01529210	OC\C=C(\CCC=C(C)C)/C	active	hitnp_p0.ldb	46.53
151	ZINC95098828	H]4[C@@]3([C@H]([C@@H]2[C@H]([C@@]1([	active	hitnp_p0.ldb	46.47
152	ZINC03871633	o1c3c(c(=O)cc1c2ccccc2)c(O)c(O)c(O)c3	active	hitnp_p0.ldb	46.47
153	ZINC18269545	c1c(OC)c(OC)c(OC)cc1C[C@@H]([C@@H](Cc2c	active	hitnp_p0.ldb	46.32
154	ZINC04097775	2c3cc(O)c(O)cc3)C(=O)[O-])\C=C\C(O[C@@H](C	active	hitnp_p0.ldb	46.32
155	ZINC04349341	]([C@H](O)[C@@H](O)[C@H]1O)CO)c(=O)c3c2	active	hitnp_p0.ldb	46.25

5. IBScreen

No	Name	Smiles	Active/Decoy	Source Database	Fit Score
1	ZINC01856103	c1ccc(cc1)C(=O)[O-])[C@H](O)[C@H](O)[C@@H	active	ibsnp_p0.ldb	76.12
2	ZINC00105086	c(c(O)cc(O)c1)C(=O)[C@H](O)[C@H]2c3cc(O)c((	active	ibsnp_p0.ldb	76.06
3	ZINC00257371	c(ccc(OC)c1)C(=O)C[C@]2(O)c3c(N(C2=O)C)ccc	active	ibsnp_p0.ldb	75.87
4	ZINC01203477	2c(ccc(N[C@@H]1OC[C@@H](O)[C@@H](O)[C	active	ibsnp_p0.ldb	75.85
5	ZINC02091333	)c(c(=O)[nH]1)[C@@H]3OCc2cnc(c(O)c23)C)Cc4	active	ibsnp_p0.ldb	75.83
6	ZINC00120335	c(OC)ccc(c1)C(=O)C[C@]2(O)c3c(N(C2=O)C)ccc	active	ibsnp_p0.ldb	75.56
7	ZINC00526141	c1ccccc1)[C@H]2OC[C@H](O)[C@H](O)[C@H]2	active	ibsnp_p0.ldb	69.22
8	ZINC00870974	O)ccc(c1)[C@H]2N(C(=O)C(O)=C2C(=O)C)Cc3cn	active	ibsnp_p0.ldb	69.18
9	ZINC01099678	c3c(N(C1=O)Cc2ccccc2)cccc3)[C@H]4C(=O)CC((	active	ibsnp_p0.ldb	69.13
10	ZINC01655202	(c(O)c(c(c1)C)C(=O)[O-])C)C(=O)c2c(O)c(c(OC)c	active	ibsnp_p0.ldb	69.04
11	ZINC01322236	1C)C(=O)c2c(OC)c(OC)c(OC)cc2)c(c(O)cc3)C[NH	active	ibsnp_p0.ldb	69
12	ZINC00407264	o1c(ccc1CC(=O)c2c(O)cc(O)cc2O)C(=O)OCC	active	ibsnp_p0.ldb	68.95
13	ZINC02098550	=O)cc(c2c1c(c(O)cc2)C)CC(=O)NCC(=O)NCC(=O	active	ibsnp_p0.ldb	68.91
14	ZINC02090671	I](Cn1c(nc2c1cccc2)[C@@H](O)C)Cn3c5c(c4c3cc	active	ibsnp_p0.ldb	68.87
15	ZINC00141040	O(c1ccc(OC)cc1)CC(=O)c2c(O)cc(O)cc2	active	ibsnp_p0.ldb	68.87
16	ZINC00216909	C@H]2OC[C@]3([C@@H]([C@@H]2C(=C[C@@	active	ibsnp_p0.ldb	68.86
17	ZINC01795912	C)ccc(c1)C(=O)N\C(\C(=O)NCCO)=C/c2cn(c3c2cc	active	ibsnp_p0.ldb	68.85
18	ZINC00519349	C@H]2OC[C@]3([C@H]([C@@H]2C(=C[C@H]	active	ibsnp_p0.ldb	68.85
19	ZINC00487566	c1)[C@@H]3c2c([nH]nc2C[C@](O)([C@@H]3C(	active	ibsnp_p0.ldb	68.77
20	ZINC00358199	c(OC)ccc2c1C(O[C@H]2CC(=O)c3c(O)cc(O)cc3)=	active	ibsnp_p0.ldb	68.77
21	ZINC00518939	=O)ccc2c1cc(OCC(=O)N[C@H](C(=O)[O-])C(C)C	active	ibsnp_p0.ldb	68.75
22	ZINC02091336	O)c(c(=O)[nH]1)[C@H]3OCc2cnc(c(O)c23)C)Cc4c	active	ibsnp_p0.ldb	68.74
23	ZINC01907694	o1c(=O)cc(c2c1cc(OCC(=O)NCC(=O)OCC)cc2)C	active	ibsnp_p0.ldb	68.71
24	ZINC00945242	3c1cc(O[C@H](C(=O)N[C@H](C(=O)[O-])Cc2ccc	active	ibsnp_p0.ldb	68.71
25	ZINC00228787	@H]2OC[C@]3([C@@H]([C@@H]2C(=C[C@@H	active	ibsnp_p0.ldb	68.71
26	ZINC00407252	s1c(nc(c1)CC(=O)c2c(O)cc(O)cc2C)c3ccccc3	active	ibsnp_p0.ldb	68.7
27	ZINC00049255	c1c(cccc1)C(=O)C[C@@]2(O)c3c(N(C2=O)C)ccc	active	ibsnp_p0.ldb	68.68
28	ZINC02090877	O=c3n(cnc1c3[nH]c2c1cc(OC)cc2)CCCO	active	ibsnp_p0.ldb	68.67
29	ZINC00462588	O[C@H](c1n(c2c(n1)cccc2)C\C=C\c3ccccc3)C	active	ibsnp_p0.ldb	68.67
30	ZINC00407265	Oc1c(ccc(O)c1)C(=O)Cc2ncccc2	active	ibsnp_p0.ldb	68.67
31	ZINC00395509	C@]3(N([C@H]([C@H]1c2ccccc2)CO)C(=O)CCC	active	ibsnp_p0.ldb	68.67
32	ZINC00187153	c(cc1)[C@H]2OC[C@@]3(CO)C[C@@H]2C(=C(	active	ibsnp_p0.ldb	68.66
33	ZINC00189266	OC[C@H]1[C@@H]([NH2+]Cc2c(OC)cc(OC)cc2)	active	ibsnp_p0.ldb	68.62
34	ZINC00064468	Oc1c(cc(c(O)c1)CC)C(=O)Cc2ncccc2	active	ibsnp_p0.ldb	68.62
35	ZINC01821760	c1)CC[NH2+]C[C@@H](O)Cn2c4c(c3c2C(=O)N(	active	ibsnp_p0.ldb	68.61
36	ZINC00489005	o1c(=O)cc(c2c1cc(OCC(=O)NCC(=O)[O-])cc2)CC	active	ibsnp_p0.ldb	68.61
37	ZINC00408754	Oc1c(cc(c(O)c1)CC)C(=O)Cc2nc3c(cc2)cccc3	active	ibsnp_p0.ldb	68.6
38	ZINC00457763	O=c/1[nH]c3c(c(=O)c/1=C(\O)/C=C/c2ccccc2)cccc	active	ibsnp_p0.ldb	68.6
39	ZINC02098358	:1c(c(O[C@H](C(=O)N[C@@H](C(=O)[O-])CCC)	active	ibsnp_p0.ldb	68.58
40	ZINC00268013	:(=O)cc(c3c1cc(OCC(=O)NC[C@@H]2OCCC2)cc	active	ibsnp_p0.ldb	68.57
41	ZINC00519526	[C@H]2OC[C@]3([C@H]([C@@H]2C(=C[C@@	active	ibsnp_p0.ldb	68.56
42	ZINC00517322	O=C([O-])[C@H](NC(=O)c1cnccc1)CC(=O)[O-]	active	ibsnp_p0.ldb	68.56
43	ZINC00199427	:3c(c(OC)c1cc2)CC[C@@H](O)[C@]3(OC)CCC((	active	ibsnp_p0.ldb	68.56
44	ZINC00519737	1c(OC)cccc1)[C@H]([C@H](O)c2cc(OC)c(OC)cc2	active	ibsnp_p0.ldb	68.55
45	ZINC00519740	(OC)cccc1)[C@@H]([C@@H](O)c2cc(OC)c(OC)c	active	ibsnp_p0.ldb	68.54
46	ZINC01742967	c2c1cc(O[C@H](C(=O)N[C@@H](C(=O)OC)C(C	active	ibsnp_p0.ldb	68.52
47	ZINC01714349	O-])c1cc(ccc1)[C@@H](O)[C@@H](NC(=O)C(	active	ibsnp_p0.ldb	68.52
48	ZINC00519452	C@H]2OC[C@]3([C@H]([C@@H]2C(=C[C@@H	active	ibsnp_p0.ldb	68.52
49	ZINC00358200	(OC)ccc2c1C(O[C@@H]2CC(=O)c3c(O)cc(O)cc3	active	ibsnp_p0.ldb	68.5
50	ZINC00488953	=O)cc(c2c1cc(OCC(=O)N[C@H](C(=O)[O-])C)cc2	active	ibsnp_p0.ldb	68.49
51	ZINC01317976	)C)c3c(c2)CC[N+]([C@H]3C[C@@H](O)Cc4c(OC	active	ibsnp_p0.ldb	68.44

52	ZINC01020371	C(=O)[C@]23c1nc4c(nc1[C@](C2(C)C)(CC3)C)c	active	ibsnp_p0.ldb	68.44
53	ZINC00491126	[C@@H]1C(=O)N(C(=O)C1)Cc2ccccc2)C(=O)CC	active	ibsnp_p0.ldb	68.43
54	ZINC00366225	O(c1ccc(cc1)[C@@]2(NC(=O)N(C2=O)C)C)C(C)C	active	ibsnp_p0.ldb	68.43
55	ZINC01737557	cc(O[C@@H](C(=O)N[C@@H](C(=O)[O-])CCC)	active	ibsnp_p0.ldb	68.42
56	ZINC00236293	C(F)(F)[C@]3(Oc2c(OC)c1occc1c(OC)c2C(=O)C3)	active	ibsnp_p0.ldb	68.42
57	ZINC00207109	O(c1c(OC)ccc(c1)C2(CNC(=O)C)CCOCC2)C	active	ibsnp_p0.ldb	68.42
58	ZINC02091500	c(=O)cc(c2c1c(c(OCC(=O)NCCC(=O)[O-])cc2)C)C	active	ibsnp_p0.ldb	68.39
59	ZINC00216904	[C@H]2OC[C@]3([C@H]([C@@H]2C(=C[C@H]	active	ibsnp_p0.ldb	68.39
60	ZINC00268018	c(=O)cc(c3c1cc(OCC(=O)NC[C@H]2OCCC2)cc3)	active	ibsnp_p0.ldb	68.38
61	ZINC01014247	NC(=O)[C@@H]1N(C(=O)OCC(C)C)C[C@H](O)C	active	ibsnp_p0.ldb	68.33
62	ZINC00206896	O2c1c(cccc1)C(=O)N[C@H]2c3ccc(OC)cc3	active	ibsnp_p0.ldb	68.32
63	ZINC00050920	O(c1ccc(cc1)[C@]2(C(=O)NC(=O)C2)C)C	active	ibsnp_p0.ldb	68.32
64	ZINC02098499	c2c1c(c(OCC(=O)N[C@H](C(=O)[O-])CC(C)C)cc	active	ibsnp_p0.ldb	68.31
65	ZINC00035529	2c1nc3c(c(OC)c1C[C@@H]2[C@@](O)(CO)C)ccc	active	ibsnp_p0.ldb	68.3
66	ZINC01700876	[C@@]2(O)C(=O)c1c(cccc1)C2(O)O)C(=O)c3c(cc	active	ibsnp_p0.ldb	68.29
67	ZINC01770024	H](NC(=O)[C@@H](Oc2cc1oc(=O)cc(c1cc2)C)C)	active	ibsnp_p0.ldb	68.27
68	ZINC00316454	(ccc(OC)c1)C(=O)C[C@@]2(O)c3c(NC2=O)ccc(c	active	ibsnp_p0.ldb	68.26
69	ZINC00098467	=C([O-])c2ccc(NC(=O)c1c(NC(=O)C(C)C)cccc1)c	active	ibsnp_p0.ldb	68.25
70	ZINC00035532	=c1n(c2c(OC[C@@H](O)C(O)(C)C)cccc2c(OC)c1	active	ibsnp_p0.ldb	68.25
71	ZINC02095148	=O)c(c(c3c1cc(cc3OC(=O)CNC(=O)OCc2ccccc2)C	active	ibsnp_p0.ldb	68.21
72	ZINC00945236	cc(c3c1cc(OCC(=O)N[C@H](C(=O)[O-])Cc2ccccc	active	ibsnp_p0.ldb	68.2
73	ZINC00941338	(=O)cc1c2ccccc2)c(O)cc(OC(=O)CNC(=O)OCc3cc	active	ibsnp_p0.ldb	68.2
74	ZINC02090267	3c4c(c(=O)c(Oc2cc1OCCCOc1cc2)c3C)ccc(OCC)c	active	ibsnp_p0.ldb	68.19
75	ZINC00720431	)c5n1c(n(c(c1)c2ccc(OC)cc2)C[C@@H](O)c3cccc	active	ibsnp_p0.ldb	68.14
76	ZINC00120338	(OC)ccc(c1)C(=O)C[C@@]2(O)c3c(N(C2=O)C)cc	active	ibsnp_p0.ldb	68.1
77	ZINC00374813	O(c1ccc(cc1)[C@@]2(NC(=O)NC2=O)C)C	active	ibsnp_p0.ldb	68.09
78	ZINC00061169	Oc2c(cc(\N=C\c1c(O)cccc1)cc2)C(=O)[O-]	active	ibsnp_p0.ldb	68.09
79	ZINC02091769	(c2c1cc(O[C@H](C(=O)N[C@H](C(=O)[O-])CCC	active	ibsnp_p0.ldb	68.08
80	ZINC01052224	O-])c2c(ccc(N[C@H]1O[C@@H]([C@@H](O)C1	active	ibsnp_p0.ldb	68.04
81	ZINC02094504	)cc(c2c1c(c(OCC(=O)N[C@H](C(=O)[O-])CCC)cc	active	ibsnp_p0.ldb	67.96
82	ZINC00084867	O2c1c(ccc(OCC(=O)[O-])c1)C(=O)CC2(C)C	active	ibsnp_p0.ldb	67.96
83	ZINC00519432	O2c1c3c(nc(c1C[C@H]2CO)C)ccc(c3)C	active	ibsnp_p0.ldb	67.92
84	ZINC02090247	4c(OC)c(OC[C@H]1OC(OC1(C)C)(C)C)ccc4c(OC	active	ibsnp_p0.ldb	67.84
85	ZINC02095973	N[C@H](C(Oc2c(c1oc(=O)c(c(c1cc2)C)C)C)=O)C)	active	ibsnp_p0.ldb	67.77
86	ZINC00035531	)2c1nc3c(c(OC)c1C[C@H]2[C@@](O)(CO)C)cccc	active	ibsnp_p0.ldb	67.72
87	ZINC00487792	C(NN2[C@@H](c1cnccc1)CCCC2)NC(=O)c3cncc	active	ibsnp_p0.ldb	66.82
88	ZINC01742890	cccc1)c2C)ccc(OC(=O)[C@H](NC(=O)OCc3ccccc	active	ibsnp_p0.ldb	65.81
89	ZINC02097948	[C@@H](C(=O)N[C@H](C(=O)[O-])Cc2c[nH]c3c	active	ibsnp_p0.ldb	65.75
90	ZINC01321570	ln(c(=O)c2n(cnc2n1C)C[C@@H](O)CO)CC[NH+]	active	ibsnp_p0.ldb	63.44
91	ZINC02091870	C@H](C(Oc2c(c1oc(=O)c3c(c1cc2)CCCC3)C)=O)	active	ibsnp_p0.ldb	63.37
92	ZINC01838637	n(c2nc(n(c2c(=O)[nH]1)CCOC)N3CCC(C(=O)N)C	active	ibsnp_p0.ldb	62.92
93	ZINC01745911	C(F)(F)C(F)(F)[C@]3(Oc2c(OC)c1occc1c(OC)c2C(	active	ibsnp_p0.ldb	62.8
94	ZINC01280328	(F)(F)C(F)(F)[C@]3(Oc2c(OC)c1occc1c(OC)c2C(=O)	active	ibsnp_p0.ldb	62.71
95	ZINC00958910	H](Cn1c(nc2c1cccc2)C)Cn3c5c(c4c3C(=O)N(CC4	active	ibsnp_p0.ldb	62.21
96	ZINC00519316	@H](O)C[NH+]2C[C@H]3c1n(c(=O)ccc1)C[C@@	active	ibsnp_p0.ldb	62.19
97	ZINC01831741	ccc(cc1)C[NH2+]CC[C@]2(O)C[C@](OCC2)(CC	active	ibsnp_p0.ldb	62.06
98	ZINC01831740	cc(cc1)C[NH2+]CC[C@]2(O)C[C@@](OCC2)(CC	active	ibsnp_p0.ldb	62.05
99	ZINC01774011	OC)ccc(c1)C[NH2+]CC[C@]2(O)C[C@](OCC2)(C	active	ibsnp_p0.ldb	62.05
100	ZINC01821346	([O-])[C@@H](NC(=O)C(NC(=O)c1ccccc1)=C(C)	active	ibsnp_p0.ldb	62.04
101	ZINC01821761	(c1)CC[NH2+]C[C@H](O)Cn2c4c(c3c2C(=O)N(C	active	ibsnp_p0.ldb	62.03
102	ZINC01550030	c2n(cnc12)[C@@H]3O[C@@H]([C@@H](O)[C@	active	ibsnp_p0.ldb	62.01
103	ZINC00518612	c(cccc1)C(=O)C[C@H]2c3c(c(OC)c(OC)cc3)C(=O	active	ibsnp_p0.ldb	61.99
104	ZINC00803232	C[NH2+]C[C@H](O)Cn1c3c(c2c1C(=O)N(CC2)C	active	ibsnp_p0.ldb	61.97

105	ZINC00056584	c1c(O)cc2c(c1)[C@H]([NH2+]CC2)Cc3cc(O)c(O)c	active	ibsnp_p0.ldb	61.96
106	ZINC01729470	O=c1n(c(nc2c1cccc2)C)CCc3cc(O)c(O)cc3	active	ibsnp_p0.ldb	61.94
107	ZINC01774013	C)ccc(c1)C[NH2+]CC[C@@]2(O)C[C@@](OCC2)	active	ibsnp_p0.ldb	61.93
108	ZINC00171760	(c1ccc(cc1)C[NH2+]C[C@@]2(O)CC(OCC2)(C)C)	active	ibsnp_p0.ldb	61.93
109	ZINC01427668	c1c(OC(=O)C[C@@H]1c2c(OC)cc(OC)c(OC)c2)c4	active	ibsnp_p0.ldb	61.91
110	ZINC02094442	4c(c3c1c(c(OC(=O)CCNC(=O)OCc2ccccc2)cc3)C)c	active	ibsnp_p0.ldb	61.9
111	ZINC02092689	:(c3c1c(c(OC(=O)CCNC(=O)OCc2ccccc2)cc3)C)C)	active	ibsnp_p0.ldb	61.9
112	ZINC02090622	c(c1)c3cc2OCCOc2cc3)ccc(OC(=O)CCNC(=O)OC	active	ibsnp_p0.ldb	61.9
113	ZINC00407682	:1n(c2nc([nH]c2c(=O)[nH]1)NCCc3cc(OC)c(OC)cc	active	ibsnp_p0.ldb	61.9
114	ZINC00105086	(c(O)cc(O)c1)C(=O)[C@@H](O)[C@H]2c3cc(O)c	active	ibsnp_p0.ldb	61.9
115	ZINC02093252	(OC)[C@H](NC(=O)NCCc1c[nH]c2c1cccc2)Cc3cc	active	ibsnp_p0.ldb	61.88
116	ZINC02092701	c(c3c1cc(OC(=O)CCNC(=O)OCc2ccccc2)cc3)c4cc	active	ibsnp_p0.ldb	61.86
117	ZINC01774009	)C)ccc(c1)C[NH2+]CC[C@]2(O)C[C@@](OCC2)(	active	ibsnp_p0.ldb	61.86
118	ZINC02097684	=O)c4c(c3c1cc(OC(=O)CCNC(=O)OCc2ccccc2)cc3	active	ibsnp_p0.ldb	61.83
119	ZINC02093402	(c(c3c1cc(OC(=O)CCNC(=O)OCc2ccccc2)cc3)C)C	active	ibsnp_p0.ldb	61.81
120	ZINC02091983	(=O)cc(c3c1cc(cc3OC(=O)CCNC(=O)OCc2ccccc2)	active	ibsnp_p0.ldb	61.81
121	ZINC00727945	@H]([C@H]3[C@H](c12)c4c(OC3=O)cccc4)C(=O	active	ibsnp_p0.ldb	61.8
122	ZINC01857640	))cc(c3c1cc(OC(=O)CCNC(=O)OCc2ccccc2)cc3)c4	active	ibsnp_p0.ldb	61.79
123	ZINC01830842	=O)[C@@H]4O[C@@H]2OC(O[C@@H]2[C@H]	active	ibsnp_p0.ldb	61.79
124	ZINC01654345	'C[C@H](NC(=O)N[C@@H](c1ccccc1)C)C(=O)O	active	ibsnp_p0.ldb	61.79
125	ZINC01280329	F)C(F)(F)[C@@]3(Oc2c(OC)c1occc1c(OC)c2C(=C	active	ibsnp_p0.ldb	61.79
126	ZINC02004083	)(=O)c2c1c(c(OC)cc2C)C=O)c(c(O)c4c3[C@H](OC	active	ibsnp_p0.ldb	61.77
127	ZINC00286970	H](c1[nH]c2c(n1)cccc2)[C@@H](O)[C@H](O)[C@	active	ibsnp_p0.ldb	61.77
128	ZINC01279974	c(c(=O)c(c1)c2ccc(OC)cc2)c(OC(=O)C)cc(OC(=O)	active	ibsnp_p0.ldb	61.76
129	ZINC02094004	:(=O)cc(c3c1cc(cc3OC(=O)CNC(=O)OCc2ccccc2)C	active	ibsnp_p0.ldb	61.75
130	ZINC01099281	:(cc2c1cccc2)C(O[C@H](c3ccccc3)C(=O)c4ccc(OC	active	ibsnp_p0.ldb	61.75
131	ZINC00089370	c(OC)cc2c(c1)[C@H]([NH2+]CC2)c3cc(OC)c(O)c	active	ibsnp_p0.ldb	61.75
132	ZINC02093737	O)cc(c3c1c(c(OC(=O)CCNC(=O)OCc2ccccc2)cc3)	active	ibsnp_p0.ldb	61.74
133	ZINC00344091	c1c(OC)ccc(c1)C3(C[NH2+]Cc2ccc(O)cc2)CCCC3	active	ibsnp_p0.ldb	61.74
134	ZINC02097986	S(CC[C@H](NC(=O)NCCc1ccccc1)C(=O)OC)C	active	ibsnp_p0.ldb	61.72
135	ZINC02094097	)cc(c3c1c(c(OC(=O)CCNC(=O)OCc2ccccc2)cc3)C	active	ibsnp_p0.ldb	61.72
136	ZINC02093009	=O)c(c(c3c1cc(OC(=O)CCNC(=O)OCc2ccccc2)cc3	active	ibsnp_p0.ldb	61.72
137	ZINC00395508	'@]3(N([C@@H]([C@H]1c2ccccc2)CO)C(=O)CC	active	ibsnp_p0.ldb	61.72
138	ZINC00057631	[C@H]([C@H](O)CO)[C@H](O)CNc1cc(c(cc1)C)	active	ibsnp_p0.ldb	61.72
139	ZINC01225597	c(OC[C@@H]1[C@H](NC(=O)\C=C\c2ccccc2)C)	active	ibsnp_p0.ldb	61.71
140	ZINC00517614	[C@@H]3[C@H]4OC[C@H](OC(=O)c2occc2)[C(	active	ibsnp_p0.ldb	61.71
141	ZINC01749975	O)c4c(c3c1cc(OC(=O)CCNC(=O)OCc2ccccc2)cc3)	active	ibsnp_p0.ldb	61.7
142	ZINC00488978	1c(=O)cc(c2c1c(c(OCC(=O)NCC(=O)[O-])cc2)C)C	active	ibsnp_p0.ldb	61.7
143	ZINC00518611	(cccc1)C(=O)C[C@@H]2c3c(c(OC)c(OC)cc3)C(=	active	ibsnp_p0.ldb	61.68
144	ZINC00282377	(OC)cc2c(c1)[C@@H](OC(=O)C2)c3cc(OC)c(OC)	active	ibsnp_p0.ldb	61.66
145	ZINC00106051	'@H](Nc1nc2c(cn1)C(=O)CC(C2)(C)C)c3c(cccc3)(	active	ibsnp_p0.ldb	61.66
146	ZINC02093320	c(c3c1cc(cc3OC(=O)[C@H](NC(=O)OCc2ccccc2)(	active	ibsnp_p0.ldb	61.65
147	ZINC01321211	)@H]([C@H]([C@H]1C=C2)C(=O)[O-])C(=O)N(c	active	ibsnp_p0.ldb	61.63
148	ZINC02092145	=C([O-])[C@@H](NC(=O)NCCc1ccccc1)Cc2cccc	active	ibsnp_p0.ldb	61.62
149	ZINC00283778	O[C@@]1(c2c(NC1=O)cccc2)CC(=O)c3ccc(N)cc3	active	ibsnp_p0.ldb	61.62
150	ZINC00519077	o1nc(c(c1c2c(O)cc(O)cc2)c4cc3OCCOc3cc4)C	active	ibsnp_p0.ldb	61.6
151	ZINC00281476	C@@H](c1[nH]c2c(n1)cccc2)[C@@H](O)C(=O)[(	active	ibsnp_p0.ldb	61.6
152	ZINC00517969	Oc1c(ccc(O)c1)C(=O)Cc3cc2ncccc2cc3	active	ibsnp_p0.ldb	61.59
153	ZINC00488823	)([C@@H]([C@H]1C=C2)C(=O)OCC)C(=O)N([C(	active	ibsnp_p0.ldb	61.59
154	ZINC00186764	o1c(=O)cc(c2c1cc(O)c(O)c2)c3ccccc3	active	ibsnp_p0.ldb	61.59
155	ZINC00758691	])c3c(NC(=O)c1cc(ccc1)C(=O)Nc2c(cccc2)C(=O)[(	active	ibsnp_p0.ldb	61.58
156	ZINC00265532	:(N)ccc2c1c(OC)c(OC)c(OC)cc1CC[C@H]([NH3+)	active	ibsnp_p0.ldb	61.58
157	ZINC00282254	O(c1c(OC)ccc(c1)C(=O)Cc2cc(OC)c(OC)cc2)C	active	ibsnp_p0.ldb	61.58

7 NPACT_natural products

No	Name	Smiles	Active/Decoy	Source Database	Fit Score
1	ZINC01585585	O(c1c(O)c(O)cc(c1)CC=C)c2ccc(cc2)CC=C	active	npactnp_p0.ldb	75.64
2	ZINC15120713	2c1c(O)cccc1c(=O)c3c2cc(O)c(c3O)C\C=C(\CCC=C(C)C)/	active	npactnp_p0.ldb	70.67
3	ZINC08221377	O)[C@@]3([C@H]2CC=C4[C@H]3C[C@@H](O)[C@@]	active	npactnp_p0.ldb	70.52
4	ZINC14768752	=O)c2c1[C@H](Oc3c2cc(OC)c(OC)c3)O)c(O)cc5OC(C=C	active	npactnp_p0.ldb	70.11
5	ZINC95099374	o1c(c(OC)c(=O)c2c1c(OC)c(O)cc2O)c3ccc(cc3)C	active	npactnp_p0.ldb	68.82
6	ZINC04098334	H](O)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C[C@H]3	active	npactnp_p0.ldb	68.27
7	ZINC14644239	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3c(O)cccc3O	active	npactnp_p0.ldb	68.13
8	ZINC00899915	o1c3c(c(=O)c(c1)c2ccc(O)cc2)c(O)c(OC)c(O)c3	active	npactnp_p0.ldb	67.93
9	ZINC03777403	OH+]2c1c(c(O)cc(O)c1)C=C(O)[C@H]2c3cc(O)c(O)c(O)c	active	npactnp_p0.ldb	67.81
10	ZINC14768876	1c(O)c(O)ccc1c(=O)c4c2c(c3OC(C=Cc3c4O)(C)C)CC=C(	active	npactnp_p0.ldb	64.11
11	ZINC58598789	:cc2)C3=O)[C@@H]4O[C@@H](OC(=O)C)[C@H](O)[C	active	npactnp_p0.ldb	63.74
12	ZINC15251982	=O)c2c1cc(O)c(c2O)C\C=C(\CCC=C(C)C)/C)c(c(O)c(O)c3	active	npactnp_p0.ldb	63.61
13	ZINC02008850	cc(O)c1C[C@H](C(=C)C)CC=C(C)C)C(=O)C[C@H]2c3c	active	npactnp_p0.ldb	63.53
14	ZINC00039452	)2c1c(c(O)cc(O)c1CC=C(C)C)C(=O)C[C@H]2c3ccc(O)cc	active	npactnp_p0.ldb	63.52
15	ZINC49793204	@@H]1[C@@H](OC)C=C3[C@]([C@@H](O)CC[C@H]	active	npactnp_p0.ldb	63.46
16	ZINC00899892	c(ccc2OC(C=Cc12)(C)C)[C@H]4[C@@H]3c5c(OC4)cc(	active	npactnp_p0.ldb	63.43
17	ZINC64416996	C@@](C[C@H]2[C@]([C@H]1C(C([C@@H](O)CC1)(C)C	active	npactnp_p0.ldb	63.41
18	ZINC13382721	4c(c(=O)c3c1cc2OC(C=Cc2c3O)(C)C)cc(O)c(O)c4CC=C(	active	npactnp_p0.ldb	63.26
19	ZINC14586284	1cc(O)c(OC)c2CC=C(C)C)c(O)c3c(O[C@@H]([C@@H]3	active	npactnp_p0.ldb	63.26
20	ZINC49881394	2c1c3c(O[C@H](C(OO)(C)C)C2)cc(O)cc3)c(O)c(c(OC)c4	active	npactnp_p0.ldb	63.21
21	ZINC13382497	)c2c1cc(O)c(OC)c2CC=C(C)C)c(O)c3c(OC([C@@H](O)(	active	npactnp_p0.ldb	63.2
22	ZINC14690604	1)[C@]5(Oc2c(c(O)cc3OC(C=Cc23)(C)C)C(=O)[C@@]4	active	npactnp_p0.ldb	63.11
23	ZINC14781062	c1c(O)cccc1c(=O)c3c2c(c(OC)c(c3O)CC=C(C)C)CC=C(C	active	npactnp_p0.ldb	63.08
24	ZINC14645645	)cc(O)c1Cc2ccc(O)cc2)C(=O)[C@H](O)[C@@H]3c4cc(	active	npactnp_p0.ldb	63.05
25	ZINC40897166	C@H]1[C@@]([C@@H]2C(C(=O)C1)=C[C@@](C=C)(	active	npactnp_p0.ldb	63.03
26	ZINC95098931	O)C1)(C3[C@@]([C@H]([C@@H]2[C@H](O[C@@H]([	active	npactnp_p0.ldb	63.01
27	ZINC34097920	))([C@H]1[C@@](O)(C(=O)C(=C1)C)CC(CO)=C2)[C@@	active	npactnp_p0.ldb	63
28	ZINC14727633	(c(=O)c2c1cc(O)c(OC)c2CCC(O)(C)C)c(O)c(c(O)c3)CC=(	active	npactnp_p0.ldb	62.97
29	ZINC15203440	OC(C=Cc12)(C)C)[C@H]4[C@@H]3c5c(OC4)c(c(O)cc5)	active	npactnp_p0.ldb	62.95
30	ZINC13436907	)[C@@H]1OC)(C)C)cc(O)c2C(=O)[C@@]4(O)c5c(OC[C	active	npactnp_p0.ldb	62.94
31	ZINC04098748	C=C1)(C)C)ccc2C(=O)[C@@]4(O)c5c(OC[C@@H]34)cc	active	npactnp_p0.ldb	62.93
32	ZINC95099511	O)c(c1)c2ccc(cc2)C)c(O)c(c(O)c3C[C@@H](O)C(=C)C)C	active	npactnp_p0.ldb	62.92
33	ZINC06483531	c1c(OC)c(O)ccc1C[C@@H](c2c(OC)c(O)c(OC)c(OC)c2)(	active	npactnp_p0.ldb	62.88
34	ZINC04102356	@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2O)CC	active	npactnp_p0.ldb	62.88
35	ZINC15217330	OC(C=Cc12)(C)C)[C@H]4[C@@H]3c5c(OC4)cc(O)c(c5)	active	npactnp_p0.ldb	62.87
36	ZINC01530850	@H]1c2cc(OC)c(O)cc2)CO)ccc(c3)[C@H]5Oc4c(c(O)cc(O	active	npactnp_p0.ldb	62.7
37	ZINC95099120	)c2c1cc(O)c(c2O)CC\C=C(\CCCC(O)(C)C)/C)c(c(O)c(O)(	active	npactnp_p0.ldb	62.69
38	ZINC14727636	)c2c1cc(O)c(OC)c2C[C@@H](O)C(O)(C)C)c(O)c(c(O)c3)	active	npactnp_p0.ldb	62.53
39	ZINC05998557	o1c3c(c(=O)cc1c2cc(O)c(O)cc2)c(O)c(OC)c(O)c3	active	npactnp_p0.ldb	62.52
40	ZINC33955327	)C=C[C@@H]1OC(=O)C)[C@@H]2\C=C\[C@@H](OC(	active	npactnp_p0.ldb	62.43
41	ZINC14728446	O2c1c(O)c(O)cc(O)c1C(=O)C[C@@H]2c3ccc(O)cc3	active	npactnp_p0.ldb	61.86
42	ZINC13480350	c2cc(O)c1c(O)c3c(cc1c2)C[C@@](O)(CC3=O)C)CC=C(C	active	npactnp_p0.ldb	61.76
43	ZINC05854400	:1c(O)ccc(O)c1c(=O)c3c2c(c(O)c(c3O)CC=C(C)C)CC=C((	active	npactnp_p0.ldb	61.75
44	ZINC14512219	O)OC[C@H]3O[C@@H](OCCc2cc(O)c(O)cc2)[C@H](O)	active	npactnp_p0.ldb	61.63
45	ZINC95099219	)H](O)[C@H]1O)CO[C@@H]2O[C@@H]([C@@H](O)[(	active	npactnp_p0.ldb	61.46
46	ZINC03869685	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3cc(O)c(O)cc3	active	npactnp_p0.ldb	61.3
47	ZINC14883290	c(c(O)c1c(O)c3c(cc1c2)C[C@@](O)(CC3=O)C)\C=C\C(C	active	npactnp_p0.ldb	61.28
48	ZINC95099040	@@H](OC(=O)[C@@H](OC(=O)\C=C(\C(C)C)/C)[C@H	active	npactnp_p0.ldb	61.24
49	ZINC00105086	c1c(c(O)cc(O)c1)C(=O)[C@@H](O)[C@H]2c3cc(O)c(O)c	active	npactnp_p0.ldb	61.17
50	ZINC00001785	O2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3ccc(O)cc3	active	npactnp_p0.ldb	61.12
51	ZINC14643592	2c1c(c(O)cc(O)c1)C(=O)[C@H](O)[C@H]2c3cc(OC)c(O)c	active	npactnp_p0.ldb	61.08

52	ZINC01561069	O2c1c(c(O)cc(OC)c1)C(=O)C[C@@H]2c3ccc(OC)cc3	active	npactnp_p0.ldb	61.08
53	ZINC00039092	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3cc(O)c(OC)cc3	active	npactnp_p0.ldb	60.97
54	ZINC95099031	(OC(=O)c1ccccc1)[C@@H](O)[C@H](O)[C@@H](O)[C@	active	npactnp_p0.ldb	60.95
55	ZINC02004123	:(cc1c(OC(C=C1)(C)C)c2)[C@@H]4[C@H]3c5c(OC4)cc(	active	npactnp_p0.ldb	60.95
56	ZINC95099587	O=c3c1c(OC)c(OC)c(OC)c(OC)c1cc(c2ccccc2)c3	active	npactnp_p0.ldb	60.92
57	ZINC06482465	l)\C=C\C(O[C@H]2[C@H](O)[C@H](O)C[C@@](O)(C(=	active	npactnp_p0.ldb	60.87
58	ZINC11682415	](n1c2ncnc(NCC=C(C)C)c2nc1)[C@@H](O)[C@H](O)[C	active	npactnp_p0.ldb	60.86
59	ZINC04098740	O3c1c(ccc(O)c1)C[C@@H](c2c(OC)c(O)c(OC)cc2)C3	active	npactnp_p0.ldb	60.85
60	ZINC04098725	c(c1)\C=C\C(O[C@H]2[C@H](O)[C@H](O)C=C(C(=O)[(	active	npactnp_p0.ldb	60.77
61	ZINC49033278	O(c1c(OC)c(ccc1O)C\C=C\c2cc(O)c(OC)cc2)C	active	npactnp_p0.ldb	60.75
62	ZINC00899074	o2c1c(OC)c(OC)c(OC)c(O)c1c(=O)cc2c3c(OC)cccc3O	active	npactnp_p0.ldb	60.71
63	ZINC05854691	c(O)cc(O)c1CC=C(C)C)C(=O)C[C@H]2c3cc(c(O)cc3)CC=	active	npactnp_p0.ldb	60.69
64	ZINC87529332	O(c1c(O)cc(O)cc1CCCCCCC\C=C/CCCCCC)C(=O)C	active	npactnp_p0.ldb	60.65
65	ZINC95099409	)C[C@@H]2[C@@H]1C(=O)C[C@H]3[C@H]2CC=C4[C	active	npactnp_p0.ldb	60.63
66	ZINC39013243	H]1[C@](CC=C(C(=O)[C@H]1CC(=O)C)CO)(C\C=C\C(	active	npactnp_p0.ldb	60.63
67	ZINC14758833	O3c1c(ccc(O)c1)C(=O)[C@H](c2c(OC)c(OC)c(OC)cc2)C3	active	npactnp_p0.ldb	60.63
68	ZINC31156700	[C@H]2[C@H](O)[C@@H](O)[C@@H](O[C@@H]2CO	active	npactnp_p0.ldb	60.55
69	ZINC14505475	O(c1c(c(OC)cc(O)c1)CCC(=O)c2ccc(O)cc2)C	active	npactnp_p0.ldb	60.45
70	ZINC36471304	)cc3O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H	active	npactnp_p0.ldb	60.44
71	ZINC13327787	O=c1c3c(O)c(c(OC)cc3c(=O)c2c1cccc2)CO	active	npactnp_p0.ldb	60.44
72	ZINC03198912	O3c1c(OC)c(O)ccc1C[C@@H](c2c(OC)c(O)c(OC)cc2)C3	active	npactnp_p0.ldb	60.43
73	ZINC04245692	-]5[C@@H]3C[C@@H]4[C@@H]([C@@H](OC)[C@H](	active	npactnp_p0.ldb	60.42
74	ZINC00006787	Oc1cc(O)cc(c1)\C=C\c2ccc(O)cc2	active	npactnp_p0.ldb	60.3
75	ZINC38816510	O2c1c(ccc(O)c1)C(=O)\C(\C2)=C/c3ccc(OC)cc3	active	npactnp_p0.ldb	60.26
76	ZINC06483567	O(c1cc(O)cc(c1)\C=C\c2ccc(O)cc2)C	active	npactnp_p0.ldb	60.26
77	ZINC49051452	c(O)c(ccc1C([C@@H](OC(=O)\C(=C/C)\C)CC=C(C)C)=(	active	npactnp_p0.ldb	60.25
78	ZINC14680748	3c(OC(=O)c2c1c(c(O)cc2C)C=O)c(c(O)c(c3C)C(=O)[O-])(	active	npactnp_p0.ldb	60.21
79	ZINC05195808	c(=O)c(c1c2c(O)cc(O)cc2)CC=C(C)C)c(O)cc4OC(C=Cc3-	active	npactnp_p0.ldb	58.49
80	ZINC95099012	@H]([C@H]2[C@H](C(OC2=O)(C)C)C3)C(=O)C)c(O)cc	active	npactnp_p0.ldb	58.16
81	ZINC42807974	H]([C@@]3([C@@H](C[C@@H](O[C@@H]2O[C@@H]	active	npactnp_p0.ldb	57.7
82	ZINC95098912	c(=O)c2c1cc(O)c(OC)c2CCC=C(C)C)c(O)c3c(OC(C=C3)(	active	npactnp_p0.ldb	56.67
83	ZINC06018601	C=C\C(=O)OC\C=C/3/[C@H]([C@]2([C@]([C@@H](CC2	active	npactnp_p0.ldb	56.39
84	ZINC95099123	c(=O)c2c1cc(O)c(O)c2CCCC(O)(C)C)c(O)c(c(O)c3)CCC=	active	npactnp_p0.ldb	56.25
85	ZINC66099308	@H](OC(=O)[C@H](OC(=O)[C@H](CC)C)[C@@H]12)(	active	npactnp_p0.ldb	56.22
86	ZINC01618680	(O)c1CC=C(C)C)[C@@H]3[C@H]2c4c(OC3)c(c(O)cc4)(	active	npactnp_p0.ldb	56.18
87	ZINC01531823	C(C=C1)(C)C)ccc2C(=O)[C@@H]4c5c(OC[C@H]34)cc((	active	npactnp_p0.ldb	56.14
88	ZINC49771186	:@@H]1[C@@H](O)C=C3[C@]([C@@H](O)CC[C@H]3	active	npactnp_p0.ldb	56.13
89	ZINC95099072	CC(=O)[C@]3([C@@H]2CC=C4[C@H]3C[C@H](O)[C@	active	npactnp_p0.ldb	56.11
90	ZINC03645834	=O)c(c1)c2ccc(O)cc2)c(O)c3c(O[C@H](C(O)(C)C)C3)c4C	active	npactnp_p0.ldb	56.02
91	ZINC95099205	:c1)C(=O)[C@@H](C[C@@H]2[C@@H](C2(C)C)CCC(=	active	npactnp_p0.ldb	55.95
92	ZINC95099615	O[C@H]1[C@H](c2c(OC1)cc(OC)c(OC)c2)[C@@H](O)c	active	npactnp_p0.ldb	55.93
93	ZINC14504352	Oc1ccc(cc1)CC[C@H](O)C[C@H](OC)\C=C\c2ccccc2	active	npactnp_p0.ldb	55.87
94	ZINC95098941	1C)(CC[C@@H]5[C@@]2([C@]([C@H]3[C@@](C(=O)	active	npactnp_p0.ldb	55.84
95	ZINC13382494	4c(c(=O)c2c1ccc(O)c2CC=C(C)C)c(O)c3c(OC(C=C3)(C)C	active	npactnp_p0.ldb	55.82
96	ZINC02561287	c1c(c(OC)cc(O)c1CC=C(C)C)C(=O)C[C@@H]2c3ccc(O)(	active	npactnp_p0.ldb	55.82
97	ZINC49802668	@@]2([C@]([C@@H]1[C@@H](O)C=C3[C@]([C@@H	active	npactnp_p0.ldb	55.8
98	ZINC05854592	OC(C=C1)(C)C)c2)[C@@H]4[C@H]3c5c(OC4)c(c(O)cc5	active	npactnp_p0.ldb	55.79
99	ZINC13459665	=O)c(c1)c2ccc(O)cc2)ccc4O[C@@H](OC)[C@@H](O)C((	active	npactnp_p0.ldb	55.74
100	ZINC13373147	ic3c1c2c(O)cc(O)c(O)c2[C@H](C3)C(=C)C)c(O)cc5OC(C	active	npactnp_p0.ldb	55.73
101	ZINC84154372	C@@H]1O[C@]1(CC[C@H]4[C@@H](C[C@H](C(=O)C	active	npactnp_p0.ldb	55.72
102	ZINC13485433	(O)c1CC=C(C)C)[C@@H]3[C@H]2c4c(OC3)cc(O)c(c4)(	active	npactnp_p0.ldb	55.67
103	ZINC64415809	]2([C@H]([C@]1([C@@]([C@@H]([C@@H](CC(=O)C)	active	npactnp_p0.ldb	55.64
104	ZINC01684799	:2OC(C=Cc12)(C)C)C(=O)[C@H]4c5c(OC[C@@H]34)cc	active	npactnp_p0.ldb	55.55

105	ZINC82157267	][C@@H]1[C@@H](O)C=C3[C@H]([C@@]1(CC2)C)C	active	npactnp_p0.ldb	55.52
106	ZINC05849312	2c1c(O)cccc1c(=O)c3c2c(c(O)c(c3O)CC=C(C)C)CC=C(C)	active	npactnp_p0.ldb	55.52
107	ZINC15120982	1c(c(O)c(c(O)c1)C(C=C)(C)C)C(=O)C[C@H]2c3cc(O)c(O	active	npactnp_p0.ldb	55.51
108	ZINC13382495	(c(=O)c2c1cc(O)c(OC)c2CC=C(C)C)c(O)c3c(OC(C=C3)(C	active	npactnp_p0.ldb	55.5
109	ZINC03979083	H]1[C@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3c(O)c4)C[C	active	npactnp_p0.ldb	55.49
110	ZINC13384106	C)ccc(c1)[C@@H]3[C@@H](\C=C\c2cc(OC)c(OC)cc2)C(	active	npactnp_p0.ldb	55.45
111	ZINC38296656	c4c(c1)[C@@H]3[C@@H](O[C@@H](c2ccc(O)cc2)C=C	active	npactnp_p0.ldb	55.44
112	ZINC15052537	)(c1c(O)ccc(c1)C[C@H]([C@H](Cc2cc(OC)c(O)cc2)C)C)(	active	npactnp_p0.ldb	55.41
113	ZINC15120983	c(c(O)c(c(O)c1)C(C=C)(C)C)C(=O)C[C@H]2c3cc(OC)c(C	active	npactnp_p0.ldb	55.38
114	ZINC03860715	@H]1[C@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)C[C@	active	npactnp_p0.ldb	55.37
115	ZINC04098734	)H]1[C@](O)(c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)C[C@	active	npactnp_p0.ldb	55.35
116	ZINC14455726	O)c2c1cc(O)c(OC)c2CC=C(C)C)c3OC([C@@H](O)Cc3c(	active	npactnp_p0.ldb	55.28
117	ZINC00039111	o1c(c(O)c(=O)c2c1cc(O)cc2)c3cc(O)c(O)cc3	active	npactnp_p0.ldb	55.28
118	ZINC14711635	cc(O)c1C[C@H](C(=C)C)CC=C(C)C)C(=O)C[C@H]2c3c	active	npactnp_p0.ldb	55.27
119	ZINC03873123	O(c1c(cc(c(O)c1)C(C=C)(C)C)\C=C\C(=O)c2ccc(O)cc2)C	active	npactnp_p0.ldb	55.26
120	ZINC95099300	=O)c3c1cc(O)c2O[C@H](C(O)(C)C)Cc23)c(O)c(c(O)c4)C	active	npactnp_p0.ldb	55.25
121	ZINC15115190	1c(ccc(O)c1)[C@@H]3[C@H]2c4c(OC3)c(c(O)cc4)CC=C	active	npactnp_p0.ldb	55.23
122	ZINC14760181	:1c(OC)ccc(c1)C[C@@H]([C@H](Cc2cc(OC)c(O)cc2)C)C	active	npactnp_p0.ldb	55.19
123	ZINC05854680	(O)c1)CC=C(C)C)[C@@H]3[C@H]2c4c(OC3)c(c(O)cc4)	active	npactnp_p0.ldb	55.19
124	ZINC13414433	c4c1c3c(O)cc(O)c2OC([C@H](c23)C4)(C)C)c(O)cc6OC(C	active	npactnp_p0.ldb	55.18
125	ZINC14645822	c1c(c(O)cc(O)c1)C(=O)[C@@H](c2c(OC)c(O)c(OC)cc2)(	active	npactnp_p0.ldb	55.15
126	ZINC08234300	@H](O)[C@H]1O)CO[C@@H]2O[C@H]([C@H](O)[C@	active	npactnp_p0.ldb	55.15
127	ZINC00056474	Oc1c(O)ccc(c1)C[C@H]([C@@H](Cc2cc(O)c(O)cc2)C)C	active	npactnp_p0.ldb	55.12
128	ZINC14727537	)c(c(O)c1CC=C(C)C)CC=C(C)C)C(=O)C[C@@H]2c3cc(C	active	npactnp_p0.ldb	55.09
129	ZINC04098325	O(c1c(c(O)cc(O)c1Cc2c(O)cccc2)C(=O)CCc3ccccc3)C	active	npactnp_p0.ldb	55.01
130	ZINC13327407	O2c1c(ccc(O)c1)C[C@@H](C2)Cc3ccc(O)cc3	active	npactnp_p0.ldb	54.58
131	ZINC04164596	c2c1c(c(O)cc2C)C=O)c(c(O)c(c3C)C(=O)[O-])COC(=O)\C	active	npactnp_p0.ldb	54.51
132	ZINC14728095	O2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3c(O)cccc3O	active	npactnp_p0.ldb	54.42
133	ZINC00004935	O2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3ccccc3	active	npactnp_p0.ldb	54.31
134	ZINC00895707	O2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3ccc(OC)cc3	active	npactnp_p0.ldb	54.3
135	ZINC00073693	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3ccccc3	active	npactnp_p0.ldb	54.3
136	ZINC00119983	O2c1c(c(O)cc(O)c1)C[C@H](O)[C@H]2c3cc(O)c(O)cc3	active	npactnp_p0.ldb	54.26
137	ZINC33832943	ccc(c1)[C@@H]3O[C@H](c2cc(OC)c(O)cc2)[C@H]([C@	active	npactnp_p0.ldb	54.25
138	ZINC04098249	O2c1c(ccc(O)c1)CC[C@H]2c3ccc(O)cc3	active	npactnp_p0.ldb	54.24
139	ZINC08234345	(O)[C@@H](O[C@@H]2CO[C@@H]3O[C@H]([C@H](	active	npactnp_p0.ldb	54.2
140	ZINC13485961	Oc1ccc(cc1)[C@H]3O[C@@H](c2ccc(O)cc2)C(=C3C)C	active	npactnp_p0.ldb	54.19
141	ZINC95099030	:1ccccc1)[C@@H](O)[C@H](O)[C@H]2O)[C@@H]3O[C	active	npactnp_p0.ldb	54.18
142	ZINC04098252	O2c1c(c(O)ccc1CC[C@H]2c3ccc(O)cc3)C	active	npactnp_p0.ldb	54.15
143	ZINC00985403	O2c1c(ccc(O)c1)C(=O)C[C@H]2c3ccc(O)cc3	active	npactnp_p0.ldb	54.12
144	ZINC59729351	)c1CC=C(C)C)[C@@]3(O)[C@]2(O)c5c(OC3)cc4OC(C=	active	npactnp_p0.ldb	54.1
145	ZINC38883997	:(cc2)[C@H]4O[C@@H](c3cc(OC)c(O)cc3)[C@@H]([C@	active	npactnp_p0.ldb	54.04
146	ZINC00058117	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3cc(O)c(O)cc3	active	npactnp_p0.ldb	54.02
147	ZINC14690574	)[C@]5(Oc3c(c(O)c2c(OC(C=C2)(C)C)c3)C(=O)[C@@]4	active	npactnp_p0.ldb	54
148	ZINC13515283	H](O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H	active	npactnp_p0.ldb	54
149	ZINC00119978	O2c1c(c(O)cc(O)c1)C[C@H](O)[C@@H]2c3cc(O)c(O)cc3	active	npactnp_p0.ldb	53.97
150	ZINC04098747	)cc2)c(O)c(OC)c(O[C@@H]3O[C@@H]([C@@H](O)[C(	active	npactnp_p0.ldb	53.9
151	ZINC14806385	O2c1c(c(O)cc(O)c1)C(=O)[C@H](O)[C@@H]2c3ccccc3	active	npactnp_p0.ldb	53.87
152	ZINC04097913	(O)cc2)c(O)cc(O[C@@H]3O[C@@H]([C@@H](O)[C@H	active	npactnp_p0.ldb	53.86
153	ZINC49052423	(c(O)cc1C([C@@H](OC(=O)\C(=C/C)\C)CC=C(C)C)=C)(	active	npactnp_p0.ldb	53.84
154	ZINC14814150	O=c1c3c(O)c(c(O)cc3c(=O)c2c1ccc(O)c2)C	active	npactnp_p0.ldb	53.84
155	ZINC08214484	)H]([C@@H](O)[C@H](O)[C@H]2O)CO[C@@H]3O[C@	active	npactnp_p0.ldb	53.84
156	ZINC95098947	c3c2cc(O)cc3O)=C)CO[C@H]4O[C@H]([C@H](O)[C@(	active	npactnp_p0.ldb	53.79
157	ZINC14642031	[C@@H]2OC[C@H]([C@H]2COC(=O)c3ccc(O)cc3)Cc4c	active	npactnp_p0.ldb	53.76

8. Nubbe Natural Products

No	Name	Smiles	Active/Decoy	Source Database	Fit Score
1	ZINC13460804	:(O)c(c(c1CC=C(C)C)C)C(=O)[O-])CC[C@@]2(\C=C\C=C	active	nubbenp_p0.ldb	71.37
2	ZINC84154056	(O)[C@H]1O)CO)[C@H]2OC=C([C@H]([C@H]2[C@H](	active	nubbenp_p0.ldb	70.56
3	ZINC84153764	)[C@H]1O)CO)[C@@H]2OC=C([C@H]([C@H]2[C@@H	active	nubbenp_p0.ldb	64.04
4	ZINC84154167	)@H]([C@@]1([C@@H](C([C@@H](O)[C@H](O)C1)(C	active	nubbenp_p0.ldb	63.57
5	ZINC15120545	Oc1c(cc(cc1)C(=O)[O-])C(=O)\C=C(/CCC=C(C)C)\C	active	nubbenp_p0.ldb	63.5
6	ZINC15120543	O(c1c(cc(cc1)C(=O)[O-])C\C=C(\CCC=C(C)C)/C)C	active	nubbenp_p0.ldb	63.21
7	ZINC13340428	Oc1c(cc(O)cc1)C(=O)\C=C(/CCC=C(C)C)\C	active	nubbenp_p0.ldb	63.16
8	ZINC84153891	C(=O)C)[C@H]([C@@](C@@H]([C@@H](OC(=O)CC(	active	nubbenp_p0.ldb	62.91
9	ZINC84153961	)[C@@H](O)[C@H](O)[C@H]2CO[C@H]3O[C@@H]([C	active	nubbenp_p0.ldb	62.81
10	ZINC33832113	'@@H]([C@H](O)[C@H](O)[C@H]1O)CO)c(=O)c3c2cc(	active	nubbenp_p0.ldb	61.5
11	ZINC06067050	:cc(c1)[C@@H]3O[C@H](c2cc(OC)c(O)cc2)[C@H]([C@	active	nubbenp_p0.ldb	61.5
12	ZINC03869685	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3cc(O)c(O)cc3	active	nubbenp_p0.ldb	61.3
13	ZINC84154296	](O[C@@H]2O[C@@H]([C@@H](O)[C@@H](O)[C@H	active	nubbenp_p0.ldb	61.28
14	ZINC15120547	Oc1c(cc(cc1)C(=O)[O-])C(=O)C[C@@](O)(CCC=C(C)C)C	active	nubbenp_p0.ldb	61.18
15	ZINC00105086	!c1c(c(O)cc(O)c1)C(=O)[C@@H](O)[C@H]2c3cc(O)c(O)c	active	nubbenp_p0.ldb	61.17
16	ZINC04098290	2[C@@]1(C(=O)C=C3[C@]2([C@H]([C@H](O)CC3)C)C	active	nubbenp_p0.ldb	61.12
17	ZINC03978792	C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C@H	active	nubbenp_p0.ldb	61.11
18	ZINC01081535	O2c1c(c(O)cc(OC)c1)C(=O)C[C@H]2c3cc(O)c(O)cc3	active	nubbenp_p0.ldb	61.11
19	ZINC84154291	O)[C@H](O[C@@H]2OC[C@H](O)[C@H](O)[C@H]2O)	active	nubbenp_p0.ldb	60.92
20	ZINC15120545	Oc1c(cc(cc1)C(=O)[O-])C(=O)\C=C(\CCC=C(C)C)/C	active	nubbenp_p0.ldb	60.92
21	ZINC84154079	:1)\C=C\C(O[C@H]2[C@H](O)[C@H](O)C[C@@](O)(C(	active	nubbenp_p0.ldb	60.85
22	ZINC84154300	](C[C@H](O)C[C@@H](O)C[C@@H](O)\C=C\c1ccccc1)	active	nubbenp_p0.ldb	60.84
23	ZINC01561070	O2c1c(c(O)cc(OC)c1)C(=O)C[C@@H]2c3cc(OC)c(O)cc3	active	nubbenp_p0.ldb	60.82
24	ZINC03779261	OC)\C=C\CO)[C@@H]2O[C@@H]([C@@H](O)[C@H](	active	nubbenp_p0.ldb	60.72
25	ZINC05973246	Oc1c(O)cc(cc1O)C(=O)OCCCCC	active	nubbenp_p0.ldb	60.68
26	ZINC36471042	)C)ccc(c1)\C=C\C(O[C@H]2[C@@H](O)[C@@H](O)CC	active	nubbenp_p0.ldb	60.66
27	ZINC09292114	C@H]1[C@@]2([C@H]([C@H](O)CCC2=CC3=O)C)C)[C	active	nubbenp_p0.ldb	60.56
28	ZINC14455534	o1c2c(c(=O)cc1C[C@H](O)C)c(O)ccc2	active	nubbenp_p0.ldb	60.42
29	ZINC84154330	'@H](C[C@H]3OC(=O)C([C@@H]3[C@@H](OC(=O)[C	active	nubbenp_p0.ldb	60.38
30	ZINC49877356	](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]([C@H]2C	active	nubbenp_p0.ldb	60.3
31	ZINC01729187	Oc1c(O)cc(cc1O)C(=O)OCC(C)C	active	nubbenp_p0.ldb	59.91
32	ZINC84154280	O(c1ccc(cc1)C(=O)[O-])C\C=C(\CCC=C(C)C)/C	active	nubbenp_p0.ldb	56.88
33	ZINC38750914	]2(CC[C@]4([C@H]3[C@](C(=O)[C@H](O)[C@@](C(=	active	nubbenp_p0.ldb	56.24
34	ZINC84154635	S(c1nc(SCC(=O)OCCC)ccc1[N+](=O)[O-])CC(=O)OCCC	active	nubbenp_p0.ldb	55.8
35	ZINC84154372	C@@H]1O[C@]1(CC[C@H]4[C@@H](C[C@H](C(=O)C	active	nubbenp_p0.ldb	55.72
36	ZINC15252691	c1c(cc(cc1CC=C(C)C)C(=O)[O-])C=C[C@]2(CCC=C(C)C	active	nubbenp_p0.ldb	55.71
37	ZINC84154694	O(c1c(O)ccc(c1)C(=O)[O-])C\C=C(\CCC=C(C)C)/C	active	nubbenp_p0.ldb	55.7
38	ZINC13340428	Oc1c(cc(O)cc1)C(=O)\C=C(\CCC=C(C)C)/C	active	nubbenp_p0.ldb	55.49
39	ZINC34210843	([C@H]2[C@]([C@H](O)[C@H](O)[C@@](C(=O)OC)(C	active	nubbenp_p0.ldb	55.32
40	ZINC01530286	Oc1c(cc(cc1)C(=O)[O-])C\C=C(\CCC=C(C)C)/C	active	nubbenp_p0.ldb	55.27
41	ZINC84154407	@H](O)[C@H](O)[C@H]1\C=C\c2ccccc2)C\C=C\[C@@H	active	nubbenp_p0.ldb	55.08
42	ZINC14728348	O2c1c(c(O)cc(OC)c1)C(=O)C[C@@H]2c3cc(OC)c(OC)cc3	active	nubbenp_p0.ldb	54.66
43	ZINC84154015	@H]([C@H](O)[C@@H](O)[C@H]1O)C)c(=O)c3c2cc(OC	active	nubbenp_p0.ldb	54.59
44	ZINC00073693	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3ccccc3	active	nubbenp_p0.ldb	54.3
45	ZINC00058116	O2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3cc(O)c(O)cc3	active	nubbenp_p0.ldb	54.3
46	ZINC31156436	C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@H]3[C@H]	active	nubbenp_p0.ldb	54.29
47	ZINC84153777	C@H](O)[C@@H](O)[C@H](O)[C@H]1O)c(=O)c3c2cc(O	active	nubbenp_p0.ldb	54.28
48	ZINC00119983	O2c1c(c(O)cc(O)c1)C[C@H](O)[C@H]2c3cc(O)c(O)cc3	active	nubbenp_p0.ldb	54.26
49	ZINC00338284	O2c1c(c(O)cc(OC)c1)C(=O)C[C@H]2c3ccc(O)cc3	active	nubbenp_p0.ldb	54.24
50	ZINC04175638	C@H]([C@H](O)[C@@H](O)[C@H]1O)C)c(=O)c3c2cc(O	active	nubbenp_p0.ldb	54.18

51	ZINC02146973	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3ccc(OC)cc3	active	nubbenp_p0.ldb	54.11
52	ZINC25763680	1OC[C@@H](O)[C@H](O)[C@H]1O)c(=O)c3c2cc(O)cc3(	active	nubbenp_p0.ldb	54.08
53	ZINC44405113	:(O)c(c(O)c3)[C@@H]5O[C@@H]([C@@H](O)[C@H](O(	active	nubbenp_p0.ldb	53.96
54	ZINC14951522	c(O)ccc(c1)\C=C\C(O[C@@H]2[C@H](O)[C@H](O)CC2	active	nubbenp_p0.ldb	53.93
55	ZINC04102166	I](O)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H].	active	nubbenp_p0.ldb	53.92
56	ZINC27310265	Oc1c(O)ccc(c1)C(=O)OC\C=C(\CCC=C(C)C)/C	active	nubbenp_p0.ldb	53.89
57	ZINC14436844	o1c(c(O)c(=O)c2c1cc(OC)c(O)c2O)c3cc(O)c(O)cc3	active	nubbenp_p0.ldb	53.84
58	ZINC00105086	)2c1c(c(O)cc(O)c1)C(=O)[C@H](O)[C@H]2c3cc(O)c(O)cc	active	nubbenp_p0.ldb	53.79
59	ZINC84154643	(c1nc(SCC(=O)OCCCC)ccc1[N+](=O)[O-])CC(=O)OCCC(	active	nubbenp_p0.ldb	53.69
60	ZINC34098825	S(c1ncccc1[N+](=O)[O-])CC(=O)OCC	active	nubbenp_p0.ldb	53.65
61	ZINC84154241	Oc1c(O)ccc(c1)\C=C\C(=O)OC[C@H](CCO)C	active	nubbenp_p0.ldb	53.62
62	ZINC01645304	:1c(OC)cc(cc1[C@H]([C@@H]2c3cc(OC)c(O)cc3)CO)CC	active	nubbenp_p0.ldb	53.62
63	ZINC14644928	o1c(c(O)c(=O)c2c1cc(OC)c(O)c2O)c3ccc(O)cc3	active	nubbenp_p0.ldb	53.6
64	ZINC15657732	[C@H]([C@H](O)[C@@H](O)[C@H]1O)C)c(=O)c3c2cc(	active	nubbenp_p0.ldb	53.56
65	ZINC04096845	)@H]([C@@H](O)[C@H](O)[C@H]1O)CO)c(=O)c3c2cc(	active	nubbenp_p0.ldb	53.53
66	ZINC84154716	@H]1C[C@@H]5[NH+]3[C@H](c2[nH]c4c(c2CC3)cccc4	active	nubbenp_p0.ldb	53.48
67	ZINC13459832	Oc1c(O)ccc2c1C(O[C@@H](C2)C)=O	active	nubbenp_p0.ldb	53.48
68	ZINC84154479	)C(=CC(=O)CC1(C)C)C)C)[C@H]2O[C@H]([C@H](O)[C(	active	nubbenp_p0.ldb	53.47
69	ZINC36337239	Clc1nc(SCC(=O)OCC)c([N+](=O)[O-])cc1	active	nubbenp_p0.ldb	53.46
70	ZINC01532172	Oc1c(O)cc(cc1O)C(=O)OCCC	active	nubbenp_p0.ldb	53.44
71	ZINC39213584	@@H]([C@@H](O)[C@H](O)[C@H]1O)CO)c(=O)c3c2cc	active	nubbenp_p0.ldb	53.39
72	ZINC13339550	Oc1c(c(cc(O)c1)\C=C\C=C\C)C=O	active	nubbenp_p0.ldb	53.36
73	ZINC00897734	o/1c3c(c(=O)c/1=C\c2cc(O)c(O)cc2)ccc(O)c3	active	nubbenp_p0.ldb	53.36
74	ZINC84154564	O[C@H](C1(O)CCC(CC1)CC)C	active	nubbenp_p0.ldb	53.33
75	ZINC84154598	S(c1nc(SCC(=O)OCC)ccc1[N+](=O)[O-])CC(=O)OCC	active	nubbenp_p0.ldb	53.3
76	ZINC84154451	)ccc(c1)\C=C\C(=O)OC2[C@H](O)CC(O)(C(=O)OC)C[C(	active	nubbenp_p0.ldb	53.23
77	ZINC84153966	)@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2O)COC(	active	nubbenp_p0.ldb	53.21
78	ZINC01665979	Oc1c(O)cc(cc1O)C(=O)OCCCC	active	nubbenp_p0.ldb	53.18
79	ZINC84154417	)H](O)[C@@H](O)[C@@H]1\C=C\c2ccccc2)C\C=C\[C@(	active	nubbenp_p0.ldb	53.16
80	ZINC13411368	:@H](C[C@@H](O)\C=C\c1ccccc1)C[C@H]2OC(=O)C=C(	active	nubbenp_p0.ldb	53.16
81	ZINC03914680	@H]1[C@@]2([C@H]([C@H](O)CCC2=CC3=O)C)C)[C(	active	nubbenp_p0.ldb	53.14
82	ZINC04098339	O)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C	active	nubbenp_p0.ldb	53.13
83	ZINC84154672	H]2[C@@H](OC(=O)C)C(C(=O)OC)=CCCC(=C[C@H]3(	active	nubbenp_p0.ldb	53.11
84	ZINC04098556	@H]([C@H](O)[C@@H](O)[C@H]1O)C)c(=O)c3c2cc(O)c	active	nubbenp_p0.ldb	53.1
85	ZINC17263588	\C=C\C(O[C@@H]2[C@H](O)[C@H](O)C[C@@](O)(C(	active	nubbenp_p0.ldb	53.09
86	ZINC12428433	Oc1c(O)ccc(c1)\C=C\C(=O)c2c(O)cc(O)cc2	active	nubbenp_p0.ldb	53.09
87	ZINC36471041	)[C@@H]3[C@@H]2O[C@@H](O[C@@H]2CC3)c5ccc(	active	nubbenp_p0.ldb	53.07
88	ZINC13462817	O2c1c(c(O)ccc1)[C@H](O)C[C@@H]2C	active	nubbenp_p0.ldb	53.06
89	ZINC13377758	S(SCSSSCc1ccccc1)SCc2ccccc2	active	nubbenp_p0.ldb	53.05
90	ZINC84154086	]([C@]1(C([C@@H]2[C@](C[C@H](O)C1)(CO)CC[C@H]	active	nubbenp_p0.ldb	53.03
91	ZINC04098352	)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@H]3[C@I	active	nubbenp_p0.ldb	53
92	ZINC14807486	o1c3c(c(=O)cc1c2cc(O)c(OC)cc2)ccc(OC)c3	active	nubbenp_p0.ldb	52.97
93	ZINC84154210	)\C=C\C(=O)OCC2[C@@H]3[C@H]([C@@H](OC=2)O)[	active	nubbenp_p0.ldb	52.94
94	ZINC84153771	@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@H]3[C@H](O	active	nubbenp_p0.ldb	52.93
95	ZINC44404940	)c(c(O)c3)[C@@H]5O[C@@H]([C@@H](O)[C@H](O)[C	active	nubbenp_p0.ldb	52.9
96	ZINC33833252	O)cc2)c(O)c(O[C@@H]3O[C@@H]([C@@H](O)[C@H](	active	nubbenp_p0.ldb	52.9
97	ZINC71316232	1)\C=C/C(O[C@H]2[C@H](O)[C@H](O)C[C@@](O)(C(=	active	nubbenp_p0.ldb	52.89
98	ZINC00407934	Oc1c(O)cc(cc1O)C(=O)OC(C)C	active	nubbenp_p0.ldb	52.83
99	ZINC31161968	Oc1c(O)ccc2c1C(O[C@@H]([C@@H]2O)C)=O	active	nubbenp_p0.ldb	52.81
100	ZINC84153980	)[C@H]1O)CO[C@H]2O[C@@H]([C@@H](O)[C@H](O)	active	nubbenp_p0.ldb	52.73
101	ZINC40933411	@H]2[C@]1(C[C@H](OC(=O)CC(=O)[O-])[C@@H]3[C@	active	nubbenp_p0.ldb	52.69
102	ZINC05640267	o1c(c(OC)c(=O)c2c1cc(O)cc2O)c3cc(O)c(OC)cc3	active	nubbenp_p0.ldb	52.69
103	ZINC03871576	o1c3c(c(=O)cc1c2ccc(O)cc2)c(O)cc(O)c3	active	nubbenp_p0.ldb	52.67

104	ZINC84154134	O2c1c(OC)cc(cc1C[C@@H]2c3cc(OC)c(OC)cc3)CCCO	active	nubbenp_p0.ldb	52.62
105	ZINC04098238	O2c1c(ccc(O)c1)C(=O)C[C@H]2c3cc(O)c(O)cc3	active	nubbenp_p0.ldb	52.62
106	ZINC36471040	\C(O[C@@H]3[C@@H]2O[C@@H](O[C@@H]2CC3)c5	active	nubbenp_p0.ldb	52.6
107	ZINC84154474	H]3[C@H]1[C@](C(=O)[O-])(CC([C@@H]1CC2)(C)C)C(	active	nubbenp_p0.ldb	52.55
108	ZINC14952519	@H]([C@@H](O)[C@H](O)[C@@H]1O)C)c(=O)c3c2cc((	active	nubbenp_p0.ldb	52.49
109	ZINC67903244	:@@H]([C@@]2([C@H]([C@@]([C@@H](O)[C@H](O)	active	nubbenp_p0.ldb	52.39
110	ZINC40875672	@@H]2[C@@H](C1=O)C(C=O)=CCC3[C@](C2)(CCC=3	active	nubbenp_p0.ldb	52.34
111	ZINC35324701	O=C([O-])\C(=C/CC\C(=C\CCC(=O)C)\C)\CCC=C(C)C	active	nubbenp_p0.ldb	51.52
112	ZINC84154348	C[C@H]4[C@@H](C[C@H](C(=O)[C@]3(O)[C@H]2C(=	active	nubbenp_p0.ldb	51.4
113	ZINC84153842	=O)cc1C)C\C=C(\CC\C=C(\CC\C=C(/C(=O)[O-])\CCC=C(	active	nubbenp_p0.ldb	51.37
114	ZINC84154387	.OC(=O)C=CC1)C[C@@H](OC(=O)C)[C@H](OC(=O)C)|	active	nubbenp_p0.ldb	51.31
115	ZINC14947575	@H](\C=C\C[C@H](O)C[C@@H](O)\C=C\c1ccccc1)CC=	active	nubbenp_p0.ldb	51.24
116	ZINC26545142	O2c1c(cc(cc1)C(=O)OC)CCC2(C)C	active	nubbenp_p0.ldb	50.76
117	ZINC13411177	O2[C@@H](C[C@H](O)\C=C\c1ccccc1)CC=CC2=O	active	nubbenp_p0.ldb	50.74
118	([C@]2(C([C@H]1[C@H]([C@@H](CC[C@]1(C(=O)[O-	active	nubbenp_p0.ldb	50.73
119	ZINC84154656	Clc1nc(SCC(=O)OCCC)cnc1	active	nubbenp_p0.ldb	50.41
120	ZINC33832012	:@H](C[C@@H]4[NH+](C1)CC[C@@]24c3c(NC2=O)ccc	active	nubbenp_p0.ldb	48.64
121	ZINC84153978	.C@H]1O)CO[C@@H]2O[C@@H]([C@H](O)[C@H](O)|	active	nubbenp_p0.ldb	48.63
122	ZINC84154674	@@H]2[C@H]4OC(=O)[C@@]2([C@H]3[C@H]([C@@	active	nubbenp_p0.ldb	48.5
123	ZINC38139774	H](O)[C@H]1O)CO)[C@@H]2OC=C([C@H]([C@H]2[C(	active	nubbenp_p0.ldb	48.48
124	ZINC03872070	o1c3c(c(=O)cc1c2ccccc2)c(O)cc(O)c3	active	nubbenp_p0.ldb	48.28
125	ZINC84154026	2c1c(c(O)cc(c1CC=C(C)C)C)CC[C@@]2(\C=C\C=C(C)C)	active	nubbenp_p0.ldb	48.25
126	ZINC84154553	c(O)ccc(c1)[C@H]3c2c(cc(OC)c(O)c2)C[C@H]([C@H]3C	active	nubbenp_p0.ldb	48.23
127	ZINC72320407	[C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C@	active	nubbenp_p0.ldb	48.22
128	ZINC00001083	Oc1c(O)ccc(c1)\C=C\C(=O)OCCc2ccccc2	active	nubbenp_p0.ldb	48.22
129	ZINC84154194	@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C@H	active	nubbenp_p0.ldb	48.14
130	ZINC38321681	[C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@H]3[C@@	active	nubbenp_p0.ldb	48.14
131	ZINC28703364	)C(=O)C)[C@@H](O)C[C@H]([C@]([C@@H]2C[C@@H	active	nubbenp_p0.ldb	47.99
132	ZINC13484870	Oc1c(c(c(c(O)c1)C)C)C(=O)OCC	active	nubbenp_p0.ldb	47.97
133	ZINC84154233	1OC(=O)C)[C@@H](O)C[C@H]([C@]([C@@H]2C[C@@	active	nubbenp_p0.ldb	47.91
134	ZINC31156118	@H](O[C@@H]2O[C@H]([C@H](O)[C@@H](O)[C@H]2	active	nubbenp_p0.ldb	47.79
135	ZINC03869768	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3ccc(O)cc3	active	nubbenp_p0.ldb	47.78
136	ZINC84153871	o1coc5c1c3c2c(cccc2)C[C@H]4N(C(=O)[O-])CCc(c34)c5	active	nubbenp_p0.ldb	47.75
137	ZINC84154100	[C@@](C2[C@](C1C(C(=C(O)C(=O)C=1)C)=CC=2)(CC3	active	nubbenp_p0.ldb	47.68
138	ZINC06483721	o1coc4c1cc(c3oc2c(OC)cc(cc2c3)CCCO)cc4	active	nubbenp_p0.ldb	47.66
139	ZINC84154064	@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@H]([C@H]2[C	active	nubbenp_p0.ldb	47.47
140	ZINC84153856	@H]1[C@@]([C@H](CC[C@]1(C(=C2)C)C)C)(CC[C@@	active	nubbenp_p0.ldb	47.25
141	ZINC03882101	-H](O)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]	active	nubbenp_p0.ldb	47.23
142	ZINC84154195	I](O)[C@H]1O)CO)[C@@H]2O[C@H](O)[C@H]([C@@	active	nubbenp_p0.ldb	47.22
143	ZINC14947607	:=C\C[C@H](O)C[C@@H](O)C[C@@H](O)\C=C\c1cccc	active	nubbenp_p0.ldb	47.21
144	ZINC84154128	o1coc2c1cc(cc2)[C@@H]4Oc3c(OC)cc(cc3C4)CCCO	active	nubbenp_p0.ldb	46.99
145	ZINC84154556	C@@H]2c3cc(O)c(O)cc3)[C@]4(O[C@@H]([C@@H](O	active	nubbenp_p0.ldb	46.94
146	ZINC33833868	)@H](O)[C@H](O)[C@H]1O)CO)[C@H]2OC=C3[C@@H	active	nubbenp_p0.ldb	46.8
147	ZINC84154205	(@H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C@H	active	nubbenp_p0.ldb	46.79
148	ZINC84154649	S(c1ncccc1[N+](=O)[O-])CC(=O)OCCCC	active	nubbenp_p0.ldb	46.7
149	ZINC84154617	Clc1nc(SCC(=O)OCC)ccc1[N+](=O)[O-]	active	nubbenp_p0.ldb	46.7
150	ZINC84154365	)]([O-])(C(=O)[C@@H](C[C@@H]1[C@@H](C1(C)C)C(	active	nubbenp_p0.ldb	46.67
151	ZINC84154469	C=C[C@H]3[C@H](O)C(=C([C@H]4[C@@H](NC(=O)[(	active	nubbenp_p0.ldb	46.66
152	ZINC00021790	Oc1c(O)cc(cc1O)C(=O)OCC	active	nubbenp_p0.ldb	46.66
153	ZINC84153787	)c(O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]	active	nubbenp_p0.ldb	46.64
154	ZINC84154646	S(c1ncccc1[N+](=O)[O-])CC(=O)OCCC	active	nubbenp_p0.ldb	46.62
155	ZINC02008803	)@H]([C@@H](O)[C@H](O)[C@@H]1O)C)c(=O)c3c2cc	active	nubbenp_p0.ldb	46.54
156	ZINC84154472	C@H]3[C@H]1[C@](C(=O)[O-])(CC([C@@H]1CC2)(C)C(	active	nubbenp_p0.ldb	46.46

10.specs natural products

No	Name	Smiles	Active/Decoy	Source Database	Fit Score
1	ZINC04104885	C@H]1O[C@@H](O)[C@H](O)[C@@H](O)[C@H]1	active	specsnp_p0.ldb	78.78
2	ZINC01559620	:c(O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C(	active	specsnp_p0.ldb	78.21
3	ZINC00518554	cc1)[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C(	active	specsnp_p0.ldb	78.2
4	ZINC85340755	(O)[C@H](O)[C@H]1O)CO)cccc2cc3C)[C@@H]4O|	active	specsnp_p0.ldb	75.98
5	ZINC02561268	o1c3c(c(=O)cc1c2ccc(OC)cc2)c(O)c(OC)c(OC)c3	active	specsnp_p0.ldb	74.34
6	ZINC96316253	([O-])nc(=O)c2nc1)[C@@H]3O[C@@H]([C@H](O)[	active	specsnp_p0.ldb	74.24
7	ZINC33594115	O-])nc(=O)c2nc1)[C@@H]3O[C@@H]([C@@H](O)[	active	specsnp_p0.ldb	73.83
8	ZINC00338044	)2c1c(c(OC(=O)C)cc(OC)c1)C(=O)C[C@H]2c3ccccc	active	specsnp_p0.ldb	73.83
9	ZINC05733763	c(c(OC)c(=O)c2c1cc(OC)c(OC)c2O)c3cc(OC)c(OC)c	active	specsnp_p0.ldb	73.74
10	ZINC05037436	O-])nc(=O)c2nc1)[C@@H]3O[C@@H]([C@@H](O)	active	specsnp_p0.ldb	73.27
11	ZINC00338046	2c1c(c(OC(=O)C)cc(OC)c1)C(=O)C[C@@H]2c3cccc	active	specsnp_p0.ldb	73.07
12	ZINC96316254	O-])nc(=O)c2nc1)[C@@H]3O[C@@H]([C@H](O)[C	active	specsnp_p0.ldb	72.14
13	ZINC85341087	1)[C@H](O)C(=O)c2c(O)c3)[C@@H]4O[C@H]([C@	active	specsnp_p0.ldb	71.08
14	ZINC05037452	)[C@H]3O[C@@H]([C@@H]4OC(O[C@@H]34)(C	active	specsnp_p0.ldb	66.15
15	ZINC96316334	C@@H](CNC(=[NH2+])N)C[C@H]([NH2+]Cc1ccc	active	specsnp_p0.ldb	65.85
16	ZINC06017650	o1c(c(OC)c(=O)c2c1cc(OC)c(OC)c2O)c3cc(O)c(O)cc3	active	specsnp_p0.ldb	65.77
17	ZINC08672998	2)[C@H]3O[C@H]([C@@H]4OC(O[C@@H]34)(C)	active	specsnp_p0.ldb	65.75
18	ZINC08672997	12)[C@H]3O[C@H]([C@H]4OC(O[C@@H]34)(C)C	active	specsnp_p0.ldb	65.74
19	ZINC05037524	@H](O[C@@H]2O[C@@H]([C@H](O)[C@H](O)[C	active	specsnp_p0.ldb	63.12
20	ZINC04104826	H](O)[C@@H]1O)CO)[C@@H]2OC=C([C@@H]3[C	active	specsnp_p0.ldb	62.85
21	ZINC05037522	@H](O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[	active	specsnp_p0.ldb	62.68
22	ZINC96316284	C@H]2O[C@@H]1O[C@H]([C@H](O)[C@@H](O)	active	specsnp_p0.ldb	62.65
23	ZINC04257488	2c3ncnc(NCc1ccccc1)c3nc2)[C@@H](O)[C@H](O)[C	active	specsnp_p0.ldb	59.16
24	ZINC05783606	O=c1c3c([O-])c(OC)c(OC)cc3n(c2c1cccc2)C	active	specsnp_p0.ldb	58.64
25	ZINC96316280	@H]1O)CO[C@@H]2O[C@H]([C@H](O)[C@@H](	active	specsnp_p0.ldb	58.09
26	ZINC04104789	O(c1c(cccc1)\C=C\C(=O)c2c(O)cc(O)cc2)Cc3ccccc3	active	specsnp_p0.ldb	58.02
27	ZINC05037523	C@H](O[C@@H]2O[C@@H]([C@H](O)[C@H](O)[	active	specsnp_p0.ldb	56.57
28	ZINC03984048	([C@H]2[C@@H]([C@@]1(C(=CC(=O)CC1)CC2)C	active	specsnp_p0.ldb	56.17
29	ZINC39929324	)H]([C@H](O)[C@H](O)[C@@H]1O)CO)c(=O)c3c2	active	specsnp_p0.ldb	56.11
30	ZINC85341114	H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C@	active	specsnp_p0.ldb	56.03
31	ZINC04098340	@H](O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)	active	specsnp_p0.ldb	56
32	ZINC04104827	H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C@	active	specsnp_p0.ldb	55.95
33	ZINC19800830	C[C@@H]2[C@](O)(C(=O)C(C(=O)N)=C([O-])[C@	active	specsnp_p0.ldb	55.91
34	ZINC04104727	C@@H]1[C@](O)(C[C@H](O)[C@@H]2[C@@]1(C	active	specsnp_p0.ldb	55.89
35	ZINC70708070	)@H](O)[C@H](O)[C@H]2O)CO[C@@H]3O[C@H]	active	specsnp_p0.ldb	55.87
36	ZINC03973253	@H]([C@H](O)[C@H](O)[C@H]1O)CO)c(=O)c3c2c	active	specsnp_p0.ldb	55.86
37	ZINC04104889	H]2[C@H]([C@]1(O)[C@@](C@@H]([C@@H](O)(	active	specsnp_p0.ldb	55.74
38	ZINC03978792	)H](O)[C@H]1O)CO)[C@@H]2OC=C([C@@H]3[C(	active	specsnp_p0.ldb	55.43
39	ZINC04096845	)H]([C@@H](O)[C@H](O)[C@H]1O)CO)c(=O)c3c2	active	specsnp_p0.ldb	55.42
40	ZINC04104934	(O)[C@@](C@H]1[C@@H]([C@H]2[C@](CC1)(C	active	specsnp_p0.ldb	55.37
41	ZINC00338209	Oc1c(ccc(O)c1)C(=O)OCC	active	specsnp_p0.ldb	55.27
42	ZINC03869685	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3cc(O)c(O)cc3	active	specsnp_p0.ldb	55.21
43	ZINC04104677	)cc1)[C@@H]2O[C@@H]([C@H](O)[C@H](O)[C@	active	specsnp_p0.ldb	54.97
44	ZINC02138728	C=C\C(O[C@H]2[C@H](O)[C@H](O)C[C@@](O)(C	active	specsnp_p0.ldb	54.44
45	ZINC04104676	c1)[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@	active	specsnp_p0.ldb	54.13
46	ZINC04257487	(n2c3ncnc(NCc1ccccc1)c3nc2)[C@H](O)[C@H](O)[C	active	specsnp_p0.ldb	54.06
47	ZINC04104687	O(c1cc(O)c(cc1)C(=O)\C=C\c2ccccc2)C	active	specsnp_p0.ldb	54.06
48	ZINC04257486	n2c3ncnc(NCc1ccccc1)c3nc2)[C@H](O)[C@H](O)[C	active	specsnp_p0.ldb	53.98
49	ZINC04257489	n2c3ncnc(NCc1ccccc1)c3nc2)[C@@H](O)[C@H](O)	active	specsnp_p0.ldb	53.98
50	ZINC04104678	cc1)[C@@H]2O[C@@H]([C@H](O)[C@H](O)[C@	active	specsnp_p0.ldb	53.89
51	ZINC85340873	C@@H]5[C@@H](O[C@@H]3O[C@@H]([C@@H	active	specsnp_p0.ldb	53.64

52	ZINC04792350	)[C@@]3([C@@H]([C@H](O)C[C@H]2C)[C@@]((	active	specsnp_p0.ldb	53.56
53	ZINC08382359	@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2O	active	specsnp_p0.ldb	53.53
54	ZINC04104869	[C@H]2[C@@H]([C@@]1([C@@H](C[C@@H](O(	active	specsnp_p0.ldb	53.53
55	ZINC08382348	C@H]5[C@H](O[C@@H]3O[C@@H]([C@@H](O)	active	specsnp_p0.ldb	53.5
56	ZINC96316333	)[C@H](CNC(=[NH2+])N)C[C@H]([NH2+]Cc1cccc(	active	specsnp_p0.ldb	53.42
57	ZINC00621833	OC)cc2c(c1)[C@@H]([NH+](CC2)C)Cc3cc(OC)c(OC	active	specsnp_p0.ldb	53.25
58	ZINC29482909	Oc1c(c(O)c(c(O)c1/C(/[O-])=C\C(=O)c2ccccc2)C)C=C	active	specsnp_p0.ldb	53.23
59	ZINC00345846	c(O)cc2c(c1)CC[N+]([C@@H]2Cc3cc(O)c(OC)cc3)(C	active	specsnp_p0.ldb	53.17
60	ZINC26187321	c(O)cc2)c(O)cc(O)c3[C@@H]5[C@H](Oc4c(c(O)cc(	active	specsnp_p0.ldb	53.15
61	ZINC14951118	H]([C@@H](O)[C@H](O)[C@@H]1O)CO)c(=O)c3c	active	specsnp_p0.ldb	53.13
62	ZINC01760775	O=C([O-])[C@@H]([NH+](Cc1ccccc1)C)C(C)C	active	specsnp_p0.ldb	53.08
63	ZINC08385324	))([C@H]2[C@]([C@@H](O)C1)([C@H]([C@@H](	active	specsnp_p0.ldb	52.87
64	ZINC00895630	1c(O)cc2c(c1)CC[NH+]([C@H]2Cc3cc(O)c(OC)cc3)(	active	specsnp_p0.ldb	52.81
65	ZINC00338225	(OC)cc2c(c1)[C@@H]([NH+](CC2)C)Cc3cc(O)c(OC	active	specsnp_p0.ldb	52.8
66	ZINC00056555	O(c3c(OC)cc1c(c(ncc1)Cc2cc(OC)c(OC)cc2)c3)C	active	specsnp_p0.ldb	52.08
67	ZINC08382305	@H]([C@H]1[C@@]([C@@H]([C@@H](CCCC(C)(	active	specsnp_p0.ldb	51.98
68	ZINC02138831	-]c3c(OC)c(OC[C@@H](OC(=O)C)C(O)(C)C)ccc3c(	active	specsnp_p0.ldb	51.27
69	ZINC85341071	O=c1c(O)c(c(=O)c([O-])c1)CCCCCCCCC	active	specsnp_p0.ldb	51.18
70	ZINC19795890	[C@@H]2C3)[C@]4([C@@H]([C@@]5(C(=C(O)C4	active	specsnp_p0.ldb	51.01
71	ZINC06556397	o1c2c(c(=O)c(OC)c1C)c(OC)cc(O)c2CC=C	active	specsnp_p0.ldb	51.01
72	ZINC33831305	)]2(O)[C@@](OC(=O)C)(C(=O)C[C@@H]3[C@@]2	active	specsnp_p0.ldb	50.9
73	ZINC00338128	O=c3c1nccc2c(OC)c(OC)c(OC)c(c12)c4c3cccc4	active	specsnp_p0.ldb	50.88
74	ZINC19800831	C[C@H]2[C@](O)(C(=O)C(C(=O)N)=C([O-])[C@@	active	specsnp_p0.ldb	50.84
75	ZINC85341151	C@@]2(C[C@@]([C@H](OC(=O)C)C1)(COC(=O)C	active	specsnp_p0.ldb	50.7
76	ZINC03872132	(OC)ccc2c1c(OC)c(OC)c(OC)cc1CC[C@H]([NH2+](	active	specsnp_p0.ldb	50.69
77	ZINC00000052	c4c1c2c(c([N+](=O)[O-])cc3c(OC)cccc23)c(c4)C(=O)	active	specsnp_p0.ldb	50.66
78	ZINC05037451	2)[C@H]3O[C@@H]([C@H]4OC(O[C@@H]34)(C)	active	specsnp_p0.ldb	50.4
79	ZINC96316401	@H]2[C@]6(OC)[C@H](C(=O)OCC)C[C@@]5([C@	active	specsnp_p0.ldb	50.38
80	ZINC71404303	C@H](OC(=O)[C@@]2(O[C@H]2C)C)[C@@H](OC	active	specsnp_p0.ldb	50.33
81	ZINC85341117	1c(c(OCC)c(=O)c2c1cc(OC)cc2OC)c3cc(OC)c(OC)cc	active	specsnp_p0.ldb	50.21
82	ZINC85341120	(OCC(=O)[O-])c(=O)c2c1cc(OC)cc2OC)c3cc(OC)c(O	active	specsnp_p0.ldb	50.21
83	ZINC03978794	O=c1c3c(O)cc(OC)cc3c(=O)c2c1c(O)cc(c2)C	active	specsnp_p0.ldb	49.75
84	ZINC38205978	(OC)c(=O)c2c1cc(OC)cc2O)c4cc(OCOC)c(OCc3cccc(	active	specsnp_p0.ldb	49.35
85	ZINC85340611	o1c(c(OC)c(=O)c2c1cc(OC)cc2O)c3cc(OCOC)c(O)cc3	active	specsnp_p0.ldb	49.15
86	ZINC85340865	[C@H]5[C@@H](O[C@@H]3O[C@@H]([C@@H](	active	specsnp_p0.ldb	49.15
87	ZINC14807307	o1c3c(c(=O)cc1c2c(O)cccc2)c(O)cc(OC)c3	active	specsnp_p0.ldb	49.12
88	ZINC85340879	Oc2c(O)cc1nc3c(nc1c2CCCCCCCCCCC)cc(c(c3)C)C	active	specsnp_p0.ldb	49.03
89	ZINC40163554	3([C@H]([C@@H]1[C@@H]([C@]2(OC[C@@]1(C	active	specsnp_p0.ldb	48.99
90	ZINC00338216	o1c3c(c(=O)cc1c2ccccc2)c(O)cc(O)c3C	active	specsnp_p0.ldb	48.99
91	ZINC13334942	O2c1c(c(O)cc(O)c1C)C(=O)C[C@H]2c3ccccc3	active	specsnp_p0.ldb	48.97
92	ZINC06070415	O=c1c3c(O)cc(OC)cc3c(=O)c2c1cc(O)c(c2)C	active	specsnp_p0.ldb	48.89
93	ZINC00338222	o1c3c(c(=O)cc1c2ccccc2)c(O)c(c(OC)c3)C	active	specsnp_p0.ldb	48.88
94	ZINC03875425	@@](O)([C@H]3[C@@H]([C@@]2([C@@](O)(C[C(	active	specsnp_p0.ldb	48.86
95	ZINC96316355	OC)[C@H](C(=O)N[C@@H](C(=O)OCC)CC(C)C)C	active	specsnp_p0.ldb	48.81
96	ZINC05037520	:1)[C@@H]2OC[C@@H]3[C@H](OC[C@H]23)c4cc	active	specsnp_p0.ldb	48.81
97	ZINC04104828	](O)[C@@H]1O)CO)[C@@H]2OC=C([C@@H]3[C(	active	specsnp_p0.ldb	48.75
98	ZINC96316433	@H]2[C@]6(OC)[C@@](C(O)(C)C)(C[C@@]5([C@I	active	specsnp_p0.ldb	48.7
99	ZINC34406449	@H]2[C@]6(OC)[C@@H](C(O)(C)C)C[C@@]5([C@	active	specsnp_p0.ldb	48.7
100	ZINC49022543	@]3([C@@](C2[C@@H]([C@@]1([C@H](C(C(=O)(	active	specsnp_p0.ldb	48.66
101	ZINC03984051	([C@@H]2[C@H]([C@@]1(C(=CC(=O)CC1)CC2)C	active	specsnp_p0.ldb	48.63
102	ZINC14611785	2c(OC)c3c1c(O)ccc(c1)CC[C@@H](O)CCCCc(c2O)c	active	specsnp_p0.ldb	48.62
103	ZINC08382372	O=c1c(OC(=O)C)cc(=O)c(O)c1CCCCCCCCCCC	active	specsnp_p0.ldb	48.61
104	ZINC96316418	4c1[C@]35C2=C(OC)[C@H](C(O)(C)C)C=C5[C@H	active	specsnp_p0.ldb	48.57

105	ZINC08382349	:@H]5[C@H](O[C@@H]3O[C@@H]([C@@H](O)[(	active	specsnp_p0.ldb	48.56
106	ZINC04104758	C@@H]([C@@H]1[C@@]([C@@H]([C@@H](CC(	active	specsnp_p0.ldb	48.55
107	ZINC04098812	O=c2c4c(OC)cc1OC(C=Cc1c4n(c3c2cccc3)C)(C)C	active	specsnp_p0.ldb	48.55
108	ZINC00001785	O2c1c(c(O)cc(O)c1)C(=O)C[C@@H]2c3ccc(O)cc3	active	specsnp_p0.ldb	48.49
109	ZINC85340557	[C@H]([C@H]2[C@]([C@@H](O)C1)([C@@H]([C	active	specsnp_p0.ldb	48.45
110	ZINC04104741	]([C@H]2[C@H]([C@]1(C(C[C@@H](OC(=O)C)C(	active	specsnp_p0.ldb	48.42
111	ZINC02008843	:(O)c1)C(=O)C[C@@H]2c3c(c(O)c(O)c(c3)CC=C(C)	active	specsnp_p0.ldb	48.42
112	ZINC04104864	C@H]([C@@H]1[C@@]([C@H]([C@@H](O)C1)C(	active	specsnp_p0.ldb	48.41
113	ZINC04104740	H]([C@H]2[C@H]([C@]1(C(C[C@H](OC(=O)C)CC	active	specsnp_p0.ldb	48.41
114	ZINC01704333	:(O)c2c1c(cc(O)c(OC)c1)C[C@H]3[NH+](CCc(c23)c<	active	specsnp_p0.ldb	48.39
115	ZINC85340876	'@@H]5[C@@H](O[C@@H]3O[C@@H]([C@@H](	active	specsnp_p0.ldb	48.38
116	ZINC04314604	)@H]([C@H]2[C@@]([C@@]1(OC(O[C@@H]1C2)	active	specsnp_p0.ldb	48.36
117	ZINC00057657	o2c1c(O)c(O)ccc1c(=O)cc2c3ccccc3	active	specsnp_p0.ldb	48.36
118	ZINC03594859	c5c1c3c2c(OC)c(O)ccc2C[C@@H]4[NH+](CCc(c34)	active	specsnp_p0.ldb	48.33
119	ZINC04104879	2O[C@@]25[C@@]3(CC[C@@H]6[C@@]4([C@@	active	specsnp_p0.ldb	48.32
120	ZINC13482688	oc5c1c3c2c(OC)c(O)ccc2C[C@H]4[NH+](CCc(c34)c	active	specsnp_p0.ldb	48.28
121	ZINC00338392	O(c1c(OC)cc2c(c1)C(=[N+]([O-])CC2)c3ccccc3)C	active	specsnp_p0.ldb	48.28
122	ZINC13334943	O2c1c(c(O)cc(OC)c1C)C(=O)C[C@H]2c3ccccc3	active	specsnp_p0.ldb	48.27
123	ZINC96316399	C@@H]6[C@H]([C@H]([C@@]5([C@H]([NH+](CC	active	specsnp_p0.ldb	48.26
124	ZINC01627642	O2c1c(c(O)c(c(OC)c1)C)C(=O)C[C@H]2c3ccccc3	active	specsnp_p0.ldb	48.26
125	ZINC00896218	c1c(O)cc2c(c1)CC[NH2+][C@H]2Cc3cc(O)c(OC)cc3	active	specsnp_p0.ldb	48.24
126	ZINC96316432	)H]2[C@]6(O)[C@@H](C(=O)OCC)C[C@@]5([C@	active	specsnp_p0.ldb	48.22
127	ZINC32123758	Cc2ccc(OC)cc2)[C@@H]3O[C@H]([C@@H](O)[C@	active	specsnp_p0.ldb	48.21
128	ZINC02149675	o1c3c(c(=O)c(c1)c2ccccc2)c(O)cc(O)c3	active	specsnp_p0.ldb	48.19
129	ZINC19897755	@H]([C@H]2[C@@]([C@@]1(O[C@@H]1C2)[C@	active	specsnp_p0.ldb	48.18
130	ZINC18825330	o1c3c(c(=O)c(c1)c2ccc(O)cc2)c(O)cc(O)c3	active	specsnp_p0.ldb	48.17
131	ZINC18269677	(c1)[C@@H]3O[C@H](c2cc(OC)c(OC)cc2)[C@H]([	active	specsnp_p0.ldb	48.17
132	ZINC00689737	\NC(=O)c2ccccc2)/C(=O)N4C[C@@H]5c3n(c(=O)cc	active	specsnp_p0.ldb	48.14
133	ZINC19800833	3C[C@H]2[C@](O)(C(=O)C(C(=O)N)=C([O-])[C@	active	specsnp_p0.ldb	48.1
134	ZINC71404298	)[C@@H]([C@@H]1[C@@H](O)[C@@H](O)C(C(=	active	specsnp_p0.ldb	48.09
135	ZINC05037538	]3[C@H]([C@]1(CCCC2)C)CC[C@]4([C@H]3CC[C	active	specsnp_p0.ldb	48.09
136	ZINC04104704	@]2([C@H]([C@@H]1[C@@H](C1(C)C)CC2)[C@@	active	specsnp_p0.ldb	48.09
137	ZINC04104757	[C@@H]([C@H]1[C@@]([C@@H]([C@@H](CCC	active	specsnp_p0.ldb	48.08
138	ZINC02585423	(OC)c(=O)c2c1c(OC)c(OC)cc2OC)c3cc(OC)c(OC)c(C	active	specsnp_p0.ldb	48.08
139	ZINC96316388	2([C@]6(OC)[C@H]([C@](O)(CCC)C)C[C@@]5([C	active	specsnp_p0.ldb	48.07
140	ZINC71404299	))[C@H]([C@@H]1[C@@H](O)[C@@H](O)C(C(=C	active	specsnp_p0.ldb	48.07
141	ZINC00689660	OC(=O)C)c2c1c(c3OC(C=Cc3c2OC)(C)C)CC=C(C)C	active	specsnp_p0.ldb	48.07
142	ZINC05809705	O2c1c(c(O)c(c(OC)c1)C)C(=O)C[C@@H]2c3ccccc3	active	specsnp_p0.ldb	48.06
143	ZINC00399556	O=C([O-])[C@@H](NC(=O)c1ccccc1)CC(C)C	active	specsnp_p0.ldb	48.06
144	ZINC01870371	o1coc2c1cc(cc2)\C=C\C=C\C(=O)[O-]	active	specsnp_p0.ldb	48.05
145	ZINC96316376	C@]6(OC)[C@@H]([C@](O)(CCCC)C)C[C@@]5([C	active	specsnp_p0.ldb	48.01
146	ZINC08382367	H]([C@]1(CC2)C)CC[C@]4([C@@H]3CC[C@@H]4	active	specsnp_p0.ldb	48
147	ZINC85341198	C@H]([C@H]1[C@@]([C@@H]([C@](O)(COC(=O)	active	specsnp_p0.ldb	47.98
148	ZINC32038000	5[C@@]3([C@H](OC(=O)C)C[C@H]6[C@@]([C@(	active	specsnp_p0.ldb	47.94
149	ZINC00338283	O2c1c(c(O)cc(OC)c1)C(=O)C[C@@H]2c3ccc(O)cc3	active	specsnp_p0.ldb	47.93
150	ZINC13334944	O2c1c(c(O)cc(OC)c1C)C(=O)C[C@@H]2c3ccccc3	active	specsnp_p0.ldb	47.91
151	ZINC85340973	c1c2CCCCCCCCCCC)ccc(c3)C(=O)N[C@H](C(=O)	active	specsnp_p0.ldb	47.9
152	ZINC85340936	Oc2c(O)cc1nc3c(nc1c2CCCCCCCCCCC)cc(cc3)C	active	specsnp_p0.ldb	47.83
153	ZINC03978408	C@@]4(O)[C@@]2(CC[C@@H]5[C@@]3([C@@H]	active	specsnp_p0.ldb	47.82
154	ZINC00338220	o1c3c(c(=O)c(OC)c1C)c(OC)cc(OCc2ccccc2)c3	active	specsnp_p0.ldb	47.79
155	ZINC04104746	C@H]3[C@H]([C@]1(CC2)C)CC[C@]4([C@H]3CC	active	specsnp_p0.ldb	47.78
156	ZINC71404297	I]3OC(=O)[C@@H]([C@H]3[C@@H](O)[C@@H]((	active	specsnp_p0.ldb	47.76
157	ZINC02106086	)2c5c(c(=[NH+]/c1ccccc1)cc2c4cc3OCCOc3cc4)cccc	active	specsnp_p0.ldb	47.76

11. tcmnp

No	Name	Smiles	Active/Decoy	Source Database	Fit Score
1	ZINC00022210	Oc1c(cc(cc1CC=C(C)C)\C=C\C(=O)[O-])CC=C(C)C	active	tcmnp_p0.ldb	46.35
2	ZINC00004749	O2c1c(c(O)c(c(O)c1C)C)C(=O)C[C@@H]2c3cc(O)c(O)cc3	active	tcmnp_p0.ldb	64.21
3	ZINC00001382	Clc1c(Cl)c(ccc1OCC(=O)[O-])C(=O)C(=C)CC	active	tcmnp_p0.ldb	55.27
4	ZINC00189892	o1c3c(c(=O)c(c1C)c2ccccc2)ccc(OC(=O)C)c3	active	tcmnp_p0.ldb	45.26
5	ZINC00105309	O=c4n2c(c1nc3c(cc1c2)cccc3)cc5c4COC(=O)[C@]5(O)CC	active	tcmnp_p0.ldb	60.93
6	ZINC00057143	Clc1c(OCC(=O)[O-])ccc(Cl)c1	active	tcmnp_p0.ldb	55.25
7	ZINC00012342	Oc1c(O)ccc(c1)C[C@H]([C@H](Cc2cc(O)c(O)cc2)C)C	active	tcmnp_p0.ldb	53.38
8	ZINC00035527	o2c1[nH+]c3c(OC)c(OC[C@H](O)C(O)(C)C)ccc3c(OC)c1cc2	active	tcmnp_p0.ldb	63.74
9	ZINC00485801	:1c(OC)cc(cc1)\C=C\C)[C@@H]([C@@H](O)c2cc(OC)c(O)cc2	active	tcmnp_p0.ldb	45.9
10	ZINC00608186	O(c1c(c(O)c(c(c1)C)C(=O)OC)C)C(=O)c2c(O)c(c(O)cc2C)C=C	active	tcmnp_p0.ldb	72.38
11	ZINC00537805	(c(OC)cc1)C(=O)NCCc3ccc(S(=O)(=O)\N=C(\[O-])/NC2CCCC	active	tcmnp_p0.ldb	55.15
12	ZINC00897912	(O)c(c(O)c1C=CC2(C)C)Cc3c(OC)c(c(O)c(c3O)C(=O)C)C)C(=	active	tcmnp_p0.ldb	45.55
13	ZINC00899897	c(c(=O)c(c1)c2cc(O)c(O)cc2)c(O)c(c4OC(C=Cc34)(C)C)CC=C	active	tcmnp_p0.ldb	53.77
14	ZINC00899911	:1c(c(O)cc(O)c1)C(=O)[C@@H](c2c(OC)c(c(O)cc2)CC=C(C)C	active	tcmnp_p0.ldb	63.83
15	ZINC00897714	[OH+]2c1c(c(O)cc(O)c1)C=C(O)[C@H]2c3cc(OC)c(O)c(OC)c3	active	tcmnp_p0.ldb	63.82
16	ZINC00689691	c(O)cc(O)c1)C(=O)C[C@H]2c3c(c(O)c(O)c(c3)CC=C(C)C)CC=	active	tcmnp_p0.ldb	54.37
17	ZINC00901095	c(ccc(O)c1)[C@@]3(O)[C@@H]2c5c(OC3)c4c(OC(C=C4)(C)(	active	tcmnp_p0.ldb	63.47
18	ZINC00897961	o1c3c(c(=O)cc1C)c(O)c2c(OC[C@](O)(CO)C=C2)c3	active	tcmnp_p0.ldb	63.66
19	ZINC00898642	Oc1c(ccc(O)c1)CCCc2cc(c(O)cc2)CC=C(C)C	active	tcmnp_p0.ldb	53.93
20	ZINC00898941	CC=C(C)C)C(=O)C6[C@@]34[C@]5(OC([C@@H]4C[C@H]	active	tcmnp_p0.ldb	55.04
21	ZINC00898291	o1c(=O)c(cc3c1cc2O[C@@H](C(O)(C)C)Cc2c3)C(C=C)(C)C	active	tcmnp_p0.ldb	62.13
22	ZINC00898792	O2c1c(c(O)ccc1CC[C@@H]2c3cc(O)c(OC)cc3)C	active	tcmnp_p0.ldb	55.28
23	ZINC00898340	(=O)c(cc3c1cc2O[C@@H](C(OC(=O)C)(C)C)Cc2c3)C(C=C)(	active	tcmnp_p0.ldb	45.69
24	ZINC00899656	2c1c(O)c(c(cc1ccc2c4c(O)c3c(O)c(c(cc3cc4)C)C(=O)C)C)C(=C	active	tcmnp_p0.ldb	55.94
25	ZINC00899892	c1c(ccc2OC(C=Cc12)(C)C)[C@H]4[C@@H]3c5c(OC4)cc(O)c	active	tcmnp_p0.ldb	45.53
26	ZINC01531702	Oc1c(c(O)cc(c1)\C=C\c2c(O)cc(O)cc2)C\C=C(\CCC=C(C)C)/C	active	tcmnp_p0.ldb	54.41
27	ZINC00897931	O)c(c(O)c1C=CC2(C)C)Cc3c(OC)c(c(O)c(c3O)C(=O)C)C)C(=	active	tcmnp_p0.ldb	64.1
28	ZINC00900482	)H]1[C@H](O)[C@@H]2[NH+]([C@H]1CC(OC(=O)\C(=C\C)	active	tcmnp_p0.ldb	53.2
29	ZINC00968436	@]3([C@H]2[C@@]([C@@H]1C(=C[C@@](C=C)(CC1)C)C	active	tcmnp_p0.ldb	45.2
30	ZINC01531062	O=C([O-])CCCCCCC\C=C\CCCC	active	tcmnp_p0.ldb	45.15
31	ZINC00899894	O4c1c(ccc(O)c1)C[C@@H](c3c(O)c2c(OC(C=C2)(C)C)cc3)C4	active	tcmnp_p0.ldb	71.97
32	ZINC00899651	)c1)CC2C(=O)C(C(=O)C(C)C)=C(O)C(C=2O)(C)C)C(=O)c3cc	active	tcmnp_p0.ldb	60.93
33	ZINC01530575	O(c1c(O)ccc(c1)CNC(=O)CCCC\C=C\C(C)C)C	active	tcmnp_p0.ldb	45.72
34	ZINC01617235	Oc1c3c(c(O)cc1)C(=O)[C@H]2O[C@]2(C3=O)CC=C(C)C	active	tcmnp_p0.ldb	55.59
35	ZINC01856370	c3c(ccc1C(C)C)[C@@]2([C@H](C(=C(C(=O)[O-])CC2)C)CC3	active	tcmnp_p0.ldb	45.53
36	ZINC01531300	o2c(c1c(c(O)cc(O)c1)C\C=C(\CCC=C(C)C)/C)cc3c2cc(O)cc3	active	tcmnp_p0.ldb	45.96
37	ZINC01530836	C@@H]1[C@@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)C[C(	active	tcmnp_p0.ldb	45.67
38	ZINC00898942	CC=C(C)C)C(=O)C6[C@@]34[C@]5(OC([C@@H]4C[C@H]	active	tcmnp_p0.ldb	53.8
39	ZINC01531861	Oc1c(O)ccc(c1)\C=C\C(=O)OCC=C(C)C	active	tcmnp_p0.ldb	53.71
40	ZINC01531348	o2c(c1c(c(OC)cc(O)c1)C\C=C(\CCC=C(C)C)/C)cc3c2cc(O)cc3	active	tcmnp_p0.ldb	53.95
41	ZINC01631509	O[C@H]([C@H](O)\C=C\CCCO)C#CC#C\C=C\C	active	tcmnp_p0.ldb	55.66
42	ZINC01858796	c1c(ccc(O)c1)[C@H]3[C@@H]2c4c(OC3)cc(OC)c(c4)CC=C(C	active	tcmnp_p0.ldb	63.59
43	ZINC01531633	(C(=O)C1)C\C=C\C=C)C(=O)[C@H]2[C@@H](C2(C)C)\C=	active	tcmnp_p0.ldb	46.84
44	ZINC01653303	Oc1c(O)ccc(c1)[C@](C=C)(CC\C=C(\CCC=C(C)C)/C)C	active	tcmnp_p0.ldb	53.34
45	ZINC01684797	O)cc2OC(C=Cc12)(C)C)C(=O)[C@H]4c5c(OC[C@H]34)cc(OC	active	tcmnp_p0.ldb	53.41
46	ZINC01531956	O)cc(c1C(=O)[O-])CCCCC)[C@@H]2[C@@H](C(=C)C)CCC	active	tcmnp_p0.ldb	54.96
47	ZINC01655202	O(c1c(c(O)c(c(c1)C)C(=O)[O-])C)C(=O)c2c(O)c(c(OC)cc2C)C	active	tcmnp_p0.ldb	73.6
48	ZINC01856367	1c3c(ccc1C(C)C)[C@]2([C@H](C(=C(C(=O)[O-])CC2)C)CC3)	active	tcmnp_p0.ldb	46.06
49	ZINC02008845	cc(O)c1C[C@@H](C(=C)C)CC=C(C)C)C(=O)C[C@@H]2c3c(	active	tcmnp_p0.ldb	54.56
50	ZINC01687273	O(c1c(c(O)c(c(c1)C)C(=O)[O-])C)C(=O)c2c(OC)c(c(OC)cc2C)C	active	tcmnp_p0.ldb	73.92
51	ZINC01664038	o1c(=O)ccc2c1c(OC)c(OC\C=C(\CCC=C(C)C)/C)cc2	active	tcmnp_p0.ldb	56.27

52	ZINC01653285	2c1c(ccc(OC)c1CC=C(C)C)[C@H]3[C@@H]2c4c(OC3)cc(O)c	active	tcmnp_p0.ldb	45.82
53	ZINC01532039	c(OC)cc(cc1)\C=C\C)[C@@H]([C@H](O)c2cc(OC)c(OC)c(OC	active	tcmnp_p0.ldb	65.66
54	ZINC01856358	c1c3c(ccc1C(C)C)[C@]2([C@H](C(=C(C(=O)[O-])CC2)C)CC3	active	tcmnp_p0.ldb	46.19
55	ZINC02036848	]c(=O)c2nc3c(n(c2n1)C[C@H](O)[C@H](O)[C@H](O)CO)cc(	active	tcmnp_p0.ldb	64.1
56	ZINC01725698	O=c1c2c(O)ccc(O)c2c(=O)cc1[C@H](OC(=O)C)CC=C(C)C	active	tcmnp_p0.ldb	64.22
57	ZINC02015151	O=c1c2c(O)ccc(O)c2c(=O)cc1[C@@H](O)CC=C(C)C	active	tcmnp_p0.ldb	72.47
58	ZINC01730009	O=c1c2c(O)ccc(O)c2c(=O)cc1CCC=C(C)C	active	tcmnp_p0.ldb	55.47
59	ZINC01531848	@@H]1[C@@](O)(c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)C[C	active	tcmnp_p0.ldb	45.54
60	ZINC02037148	O=C([O-])CCCCCC[C@H](CC)C	active	tcmnp_p0.ldb	53.66
61	ZINC02033588	'@@H]1c2cc(OC)c(O)cc2)CO)ccc(c3)[C@H]5Oc4c(c(O)cc(O)c	active	tcmnp_p0.ldb	53.96
62	ZINC02033589	C@H]1c2cc(OC)c(O)cc2)CO)ccc(c3)[C@H]5Oc4c(c(O)cc(O)c4	active	tcmnp_p0.ldb	54.29
63	ZINC02097389	))C[C@@H]2c4ccc(O[C@H]3O[C@H]([C@H](O)[C@@H](O	active	tcmnp_p0.ldb	45.34
64	ZINC02525131	c1c2c(O)ccc(O)c2c(=O)cc1[C@H](OC(=O)CC(O)(C)C)CC=C(	active	tcmnp_p0.ldb	56.15
65	ZINC03648307	o2c1c(c(OC)c(c(O)c1)CC=C(C)C)cc2c3c(O)cc(O)cc3	active	tcmnp_p0.ldb	53.92
66	ZINC03630060	2c1c(c(O)c(c(O)c1)CC=C(C)C)C(=O)C[C@@H]2c3c(O)cc(O)c	active	tcmnp_p0.ldb	72.92
67	ZINC01863457	O(c1c(O)ccc(c1)C[C@H]([C@@H](Cc2cc(OC)c(O)cc2)C)C)C	active	tcmnp_p0.ldb	46.47
68	ZINC02526482	c(O)cc2)c(O)c(OC)c(O[C@H]3O[C@H]([C@H](O)[C@@H](C	active	tcmnp_p0.ldb	53.92
69	ZINC02563650	o2c(=O)c(c1c(O)cc(O)cc1)cc3c2cc4OC(CCc4c3OC)(C)C	active	tcmnp_p0.ldb	63.55
70	ZINC03651079	)1c3c(O[C@H]([C@@H]1c2cc(O)c(O)cc2)CO)cc(cc3)\C=C\C(	active	tcmnp_p0.ldb	84.56
71	ZINC03644977	o2c(=O)c(c1c(O)cc(O)cc1)cc4c2cc3O[C@](CO)(CCc3c4OC)C	active	tcmnp_p0.ldb	59.15
72	ZINC01856355	c(O)cc1C(C)C)[C@@]2([C@@H](C(=C(C(=O)[O-])CC2)C)C	active	tcmnp_p0.ldb	55.44
73	ZINC03203022	c(c3O[C@H]1[C@@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4	active	tcmnp_p0.ldb	46.11
74	ZINC03645200	(O[C@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H]1O)CO)c	active	tcmnp_p0.ldb	63.68
75	ZINC03831000	Ic2c(Oc1cc(I)c(O)cc1)c(I)cc(c2)C[C@@H]([NH3+])C(=O)[O-]	active	tcmnp_p0.ldb	45.84
76	ZINC02008848	)cc(O)c1C[C@@H](C(=C)C)CC=C(C)C)C(=O)C[C@H]2c3c((	active	tcmnp_p0.ldb	54.39
77	ZINC03644943	(OC)c(c(OC)c1)CC=C(C)C)C[C@@H](c2c(O)c(c(O)cc2)CC=C	active	tcmnp_p0.ldb	54.46
78	ZINC02015152	O=c1c2c(O)ccc(O)c2c(=O)cc1[C@H](O)CC=C(C)C	active	tcmnp_p0.ldb	63.88
79	ZINC03830994	c2c(Oc1cc(I)c(O)c(I)c1)c(I)cc(c2)C[C@@H]([NH3+])C(=O)[O-	active	tcmnp_p0.ldb	53.66
80	ZINC03197725	1c(OC(C=C1)(C)C)c2)C(=O)[C@@H]4c5c(OC[C@@H]34)cc(	active	tcmnp_p0.ldb	65.19
81	ZINC03870707	)3c1c(ccc(O)c1)C(=O)[C@@H](c2c(O)c(c(O)cc2)CC=C(C)C)C	active	tcmnp_p0.ldb	60.56
82	ZINC03871182	c(c(O)c(=O)c2c1c(c(O)c(c2O)CC=C(C)C)CC=C(C)C)c3ccc(O)c	active	tcmnp_p0.ldb	64.19
83	ZINC03775158	[OH+]2c1c(c(O)cc(O)c1)C=C(O)[C@H]2c3cc(O)c(O)cc3	active	tcmnp_p0.ldb	63.83
84	ZINC03777403	[OH+]2c1c(c(O)cc(O)c1)C=C(O)[C@H]2c3cc(O)c(O)c(O)c3	active	tcmnp_p0.ldb	55.56
85	ZINC03831425	O)[C@@H](O)[C@@H](O)Cn1c3nc(=O)[nH]c(=O)c3nc2c1cc	active	tcmnp_p0.ldb	55.66
86	ZINC02584002	Oc1c(O)c(c(c(c1O)C\C=C(\CC\C=C(\CCC=C(C)C)/C)/C)C)C=C	active	tcmnp_p0.ldb	62.7
87	ZINC03978768	C=C\c2ccc(OC)cc2)[C@@H]3O[C@@H]([C@@H](O)[C@H]	active	tcmnp_p0.ldb	63.79
88	ZINC04016718	'@H]1c2cc(OC)c(O)cc2)CO)ccc(c3)[C@@H]5Oc4c(c(O)cc(O)c	active	tcmnp_p0.ldb	62.33
89	ZINC04097595	O[C@@H](CO)C#CC#CC#CC#C\C=C\C	active	tcmnp_p0.ldb	55.24
90	ZINC04026149	)H]([C@H]3[C@@H]2C[C@H]4[C@@]3(CC[C@H]5[C@H]-	active	tcmnp_p0.ldb	52.21
91	ZINC03978987	OC(C=C1)(C)C)ccc2C(=O)[C@H]4c5c(OC[C@@H]34)cc(OC	active	tcmnp_p0.ldb	60.43
92	ZINC03954302	[OH+]2c1c(c(O)cc(O)c1)C=C(O)[C@H]2c3cc(OC)c(O)c(O)c3	active	tcmnp_p0.ldb	63.79
93	ZINC04097766	c2c(ccc(O)c2)[C@@H]6[C@@H]3[C@@H](c4c(O)c5)C=C(C(	active	tcmnp_p0.ldb	63.69
94	ZINC04023706	([O-])[C@]3([C@H]2[C@@](c1c(cc(cc1)C(C)C)CC2)(CCC3)	active	tcmnp_p0.ldb	44.61
95	ZINC04082065	[C@@H]([C@H](O)C1)[C@@H]2[C@@]([C@@H]([C@@H	active	tcmnp_p0.ldb	53.37
96	·3c(c(=O)c2c1cc(O)c(OC)c2CC=C(C)C)c(O)c(c(OC)c3)CC=C(	active	tcmnp_p0.ldb	61.99
97	'=C(O[C@@H]2O[C@@H]([C@H](O)[C@H](O)[C@H]2O)C	active	tcmnp_p0.ldb	63.56
98	ZINC04096342	@H](OC\C=C\c1ccccc1)[C@H](O)[C@@H](O)[C@H](O)[C@	active	tcmnp_p0.ldb	72.46
99	ZINC03979083	@H]1[C@H](c2c(OC1)cc(OC)c(OC)c2)C(=O)c3c(O)c4)C[C@	active	tcmnp_p0.ldb	67.05
100	ZINC04097826	c2)[C@H]4[C@H]([C@H](c3c(O)cc(O)cc3)CC(=C4)C)C(=O)c	active	tcmnp_p0.ldb	62.93
101	ZINC04097724	[C@@]2([C@]([C@H]([C@H]1CO[C@H]([C@H](O)C1)C(O	active	tcmnp_p0.ldb	45.83
102	ZINC04097602	O[C@H](CO)\C=C\C#CC#CC#C\C=C\C	active	tcmnp_p0.ldb	54.59
103	ZINC04097596	O1[C@H]([C@H](O)CCC1)\C=C\C#CC#CC	active	tcmnp_p0.ldb	46.07
104	ZINC04096993	C)c(O)cc2)c(O)c(O[C@@H]3O[C@@H]([C@@H](O)[C@H]((	active	tcmnp_p0.ldb	53.6

105	ZINC04097839	C(=O)C)c(cc(O)c2[C@@H]3O[C@@H]([C@@H](O)[C@H](C	active	tcmnp_p0.ldb	64.25
106	ZINC04098003	@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2O)CO)c3O[C	active	tcmnp_p0.ldb	53.63
107	ZINC04098004	O2c1c(ccc(O)c1)C(=O)C[C@H]2c4cc3c(OC(C=C3)(C)C)cc4	active	tcmnp_p0.ldb	61.89
108	ZINC04097840	1C)c(O)c(c(O)c2)[C@@H]3O[C@@H]([C@@H](O)[C@H](O	active	tcmnp_p0.ldb	70.39
109	ZINC04098251	O2c1c(c(O)ccc1CC[C@H]2c3cc(O)c(OC)cc3)C	active	tcmnp_p0.ldb	55.16
110	ZINC04097986	C@@H]1[C@H](OC(=O)C1=C)[C@H]3[C@@]2(OC2)[C@@	active	tcmnp_p0.ldb	46.44
111	ZINC04097908	@]3([C@H]2[C@@](C@@H]1C(C[C@@](C=C)(CC1)C)=CC	active	tcmnp_p0.ldb	45.04
112	ZINC04097890	C@H]1[C@@](O)(C(=O)C(=C1)C)CC(COC(=O)C)=C2)[C@@	active	tcmnp_p0.ldb	56.73
113	ZINC04097941	12[C@@H]([C@@](C@@H](C1)C)(CO)CC/C(/CO)=C/CO)C	active	tcmnp_p0.ldb	54.35
114	ZINC04098456	O)c(c(O)c1C)Cc2c(O)c(c(O)c(c2O)C=O)C(=O)CC(C)C)C(=O)	active	tcmnp_p0.ldb	63.5
115	ZINC04098720	2c1c(OC(C=C1)(C)C)ccc2C[C@H](c3c(O)c(c(O)cc3)CC=C(C)	active	tcmnp_p0.ldb	63.58
116	ZINC04098453	CC[C@H](O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@@	active	tcmnp_p0.ldb	54.76
117	ZINC04098466	(O)c1c(O)c3c(cc1c2)C[C@@](O)(CC3=O)C)C\C=C(\CCC=C(	active	tcmnp_p0.ldb	73.5
118	ZINC04098622	'=C\c2cc(O)c(O)cc2)[C@@H]3O[C@@H]([C@@H](O)[C@H	active	tcmnp_p0.ldb	64.38
119	ZINC04098325	O(c1c(c(O)cc(O)c1Cc2c(O)cccc2)C(=O)CCc3ccccc3)C	active	tcmnp_p0.ldb	62.09
120	ZINC04098633	\C=C\c2ccc(O)cc2)[C@@H]3O[C@@H]([C@@H](O)[C@H](	active	tcmnp_p0.ldb	64.06
121	ZINC04098603	)c(O)cc2)c(O)c(c(OC)c3)[C@@H]4O[C@@H]([C@@H](O)[C	active	tcmnp_p0.ldb	53.42
122	ZINC04098320	)2c1c(c(O)cc(O)c1CC=C(C)C)C(=O)[C@H](O)[C@H]2c3ccccc	active	tcmnp_p0.ldb	55.38
123	ZINC04098611	O)C[C@@H]1c2cc(O)c(O)cc2)cc(O)c3C[C@@H](O)[C@H]4c	active	tcmnp_p0.ldb	60.98
124	ZINC04098719	O4c2c1c(OC(C=C1)(C)C)ccc2C[C@H](c3c(O)cc(O)cc3)C4	active	tcmnp_p0.ldb	63.62
125	ZINC04098334	)@H](O)[C@H](O)[C@H]1O)CO)[C@@H]2OC=C[C@H]3[C	active	tcmnp_p0.ldb	55.64
126	ZINC04199939	o1c(c(O)c(=O)c2c1c(c(O)cc2OC)CC=C(C)C)c3ccc(O)cc3	active	tcmnp_p0.ldb	55.36
127	ZINC04098362	2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3cc(OC)c(O)c(c3)CC=C(C)	active	tcmnp_p0.ldb	64.31
128	ZINC05139518	s1c(nnc1c2ccccc2)c3c(oc4c(c3)ccc(N(CC)CC)c4)=O	active	tcmnp_p0.ldb	45.07
129	ZINC05158123	s2c(c1sc(cc1)C#CC)ccc2C(=O)[O-]	active	tcmnp_p0.ldb	45.97
130	ZINC04098822	O2c1c(OC)cc(cc1[C@@H]([C@H]2c3cc(OC)c(O)cc3)C)\C=C\(	active	tcmnp_p0.ldb	44.99
131	ZINC04642622	o1c(ccc1\C=C\C(=O)[O-])C(=O)C#C\C=C/CC	active	tcmnp_p0.ldb	46.37
132	ZINC04098688	O=c1c3c(O)c(O)ccc3c(=O)c2c(O)c(ccc12)C	active	tcmnp_p0.ldb	72.41
133	ZINC04098629	=C\c2cc(OC)c(O)cc2)[C@@H]3O[C@@H]([C@@H](O)[C@H	active	tcmnp_p0.ldb	55.66
134	ZINC04654881	O1[C@H]([C@H](O)CCC1)\C=C\C#CC#CC#CC	active	tcmnp_p0.ldb	46.08
135	ZINC04098734	C@H]1[C@](O)(c2c(OC1)cc(OC)c(OC)c2)C(=O)c3cc4)C[C@@	active	tcmnp_p0.ldb	52.25
136	ZINC04102354	(O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2O)CO	active	tcmnp_p0.ldb	53.31
137	ZINC04716494	O2c1c(ccc(O)c1)C(=O)C[C@H]2c3cc(c(O)cc3)CC=C(C)C	active	tcmnp_p0.ldb	55.66
138	ZINC05158979	(O)c1c(OC(C=C1)(C)C)c2CC=C(C)C)C(=O)[C@H](c3c(O)cc(	active	tcmnp_p0.ldb	63.86
139	ZINC04102357	(O[C@@H]2O[C@@H]([C@@H](O)[C@H](O)[C@H]2O)CO	active	tcmnp_p0.ldb	63.65
140	ZINC04273377	C@H](O)C(=O)c2c(O)c3)CC=C(C)C)[C@@H]4O[C@@H]([C	active	tcmnp_p0.ldb	53.65
141	ZINC05104405	-C([O-])[C@]3([C@H]2[C@](c1c(cc(cc1)C(C)C)CC2)(CCC3)C	active	tcmnp_p0.ldb	45.74
142	ZINC05114532	o3c2[nH+]c4c(OC)c(OC[C@H]1OC1(C)C)ccc4c(OC)c2cc3	active	tcmnp_p0.ldb	44.78
143	ZINC04474613	O=C([O-])CCCCCCC\C=C/C\C=C/CCCCC	active	tcmnp_p0.ldb	45.79
144	ZINC04349491	]3O[C@@H]([C@@H](O)[C@H](O)[C@H]3O)CO[C@@H]4(	active	tcmnp_p0.ldb	53.41
145	ZINC05521326	c(cc3c(c1)[C@@]2([C@H](C(CCC2)(C)C)CC3)C)[C@@H](C	active	tcmnp_p0.ldb	53.26
146	ZINC04349262	)c(O)cc2)c(O)c(c(O)c3)[C@@H]4O[C@@H]([C@@H](O)[C(	active	tcmnp_p0.ldb	45.22
147	ZINC05037517	-H]([C@]1([C@@H]([C@]([C@H](O)CC1)(COC(=O)C)C)C2)(	active	tcmnp_p0.ldb	62.12
148	ZINC05158589	O(c1c(OC)cc(cc1OC)\C=C\CO)C\C=C(\CCC=C(C)C)/C	active	tcmnp_p0.ldb	45.99
149	ZINC04716495	O2c1c(ccc(O)c1)C(=O)C[C@@H]2c3cc(c(O)cc3)CC=C(C)C	active	tcmnp_p0.ldb	53.62
150	ZINC04646295	C@](C@@]3(O[C@@H]2O[C@@H]([C@H](O)[C@@H](O)	active	tcmnp_p0.ldb	53.47
151	ZINC05158963	o1c3c(c(=O)c(c1)c2c(O)c(c(O)cc2)CC=C(C)C)c(O)cc(O)c3	active	tcmnp_p0.ldb	64.66
152	ZINC05162835	O=c4n2c(c1nc3c(cc1c2)cccc3)cc5c4COC(=O)[C@]5(O)CCO	active	tcmnp_p0.ldb	84.11
153	ZINC05158048	C@@H]([C@@H](O)[C@H](O)[C@H]2O)CO[C@@H]3OC[(	active	tcmnp_p0.ldb	63.96
154	ZINC05158566	1c(=O)c(c([O-])c2c1cccc2)C\C=C(\CC\C=C(\CCC=C(C)C)/C)/(	active	tcmnp_p0.ldb	45.02
155	ZINC05639632	c1c(OC)cc(cc1)\C=C\CO)[C@H]([C@H](O)c2cc(OC)c(O)cc2)(	active	tcmnp_p0.ldb	64.24
156	ZINC05159013	o1c(c(O)c2c1cc(OC)c(OC)c2)c3cc(c(O)cc3)CC=C(C)C	active	tcmnp_p0.ldb	53.4
157	ZINC05158077	CO[C@]2([C@@H]1O[C@@H]1C(OC#CC#CC)=C2)CC3)C(=	active	tcmnp_p0.ldb	55.75

12. UENF_np

No	Name	Smiles	Active/Decoy	Source Database	Fit Score
1	ZINC06092198	o1c3c(c(=O)cc1c2cc(O)c(O)cc2)c(O)c(O)c(O)c3	active	uefsnp_p0.ldb	78.83
2	ZINC00058118	o1c3c(c(=O)cc1c2ccccc2)c(OC)c(OC)c(OC)c3	active	uefsnp_p0.ldb	74.21
3	ZINC69482230	o1c3c(c(=O)cc1c2ccccc2)c(O)c(OC)c(O)c3CC=C(C)C	active	uefsnp_p0.ldb	73.86
4	ZINC05733763	1c(c(OC)c(=O)c2c1cc(OC)c(OC)c2O)c3cc(OC)c(OC)c(	active	uefsnp_p0.ldb	73.74
5	ZINC14438231	c(OC)c(O)c1CC=C(C)C)C(=O)[C@H](O)[C@H]2c3c(	active	uefsnp_p0.ldb	73.65
6	ZINC05842416	o1c3c(c(=O)cc1c2ccc(O)cc2)c(O)c(O)c(O)c3	active	uefsnp_p0.ldb	72.11
7	ZINC69481935	]2O[C@@H]([C@@H](O)[C@@H](O)[C@H]2O)CO	active	uefsnp_p0.ldb	71.04
8	ZINC14775976	o2c(Oc1ccc(O)cc1)cc(=O)c3c2cc(O)cc3O	active	uefsnp_p0.ldb	70.91
9	ZINC69481932	:O[C@@H]([C@@H](O)[C@@H](O)[C@H]2O)CO)(	active	uefsnp_p0.ldb	70.81
10	ZINC14644952	o1c(c(OC)c(=O)c2c1cc(OC)c(OC)c2O)c3ccc(O)cc3	active	uefsnp_p0.ldb	67.04
11	ZINC69482338	o1c3c(c(=O)cc1c2c(O)ccc(O)c2)c(O)c(OC)c(OC)c3	active	uefsnp_p0.ldb	66.3
12	ZINC69481931	:[C@H]2c3ccc(O)cc3)[C@H]4O[C@H]([C@H](O)[C(	active	uefsnp_p0.ldb	65.63
13	ZINC69482447	[C@@H](O)[C@H]2[C@@H](O[C@@](O)([C@]2(C	active	uefsnp_p0.ldb	64.22
14	ZINC69482313	1c(c(O)cc(OC(=O)CN)c1)C(=O)C[C@H]2c3cc(O)c(O	active	uefsnp_p0.ldb	58.16
15	ZINC69482068	)@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H]1O)(	active	uefsnp_p0.ldb	57.05
16	ZINC04963674	O=c1c3c(O)ccc(O)c3c(=O)c2c1c(O)cc(c2)C	active	uefsnp_p0.ldb	56.63
17	ZINC05733766	o1c(c(OC)c(=O)c2c1cc(OC)cc2O)c3cc(OC)c(OC)cc3	active	uefsnp_p0.ldb	56.15
18	ZINC29037474	:(c(O)cc(OC)c1)C(=O)[C@H](OC)[C@H]2c3cc(O)c(O	active	uefsnp_p0.ldb	56.14
19	ZINC06403375	o1c(c(O)c(=O)c2c1cc(OC)cc2O)c3cc(OC)c(O)cc3	active	uefsnp_p0.ldb	56.05
20	ZINC69482027	o1c(c(O)c(=O)c2c1cc(cc2O)C)c3ccc(cc3)C	active	uefsnp_p0.ldb	56.03
21	ZINC01645590	o1c(c(O)c(=O)c2c1cc(OC)cc2O)c3cc(O)c(OC)cc3	active	uefsnp_p0.ldb	55.93
22	ZINC03875620	o1c(c(O)c(=O)c2c1cc(OC)cc2O)c3cc(O)c(O)cc3	active	uefsnp_p0.ldb	55.86
23	ZINC69482028	1c(c(OC)c(=O)c2c1c(OC)c(OC)cc2O)c3cc(c(OC)cc3)(	active	uefsnp_p0.ldb	55.81
24	ZINC15117446	1c(c(OC)c(=O)c2c1c(OC)c(OC)cc2O)c3cc(O)c(OC)cc	active	uefsnp_p0.ldb	55.81
25	ZINC69482277	o1c(c(OC(=O)CN)c(=O)c2c1cc(O)cc2O)c3ccc(O)cc3	active	uefsnp_p0.ldb	55.8
26	ZINC00898006	o1c3c(c(=O)cc1C)c(O)c2c(O)cc(OC)cc2c3	active	uefsnp_p0.ldb	55.72
27	ZINC03869685	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3cc(O)c(O)cc3	active	uefsnp_p0.ldb	55.21
28	ZINC05733537	o1c(c(OC)c(=O)c2c1cc(O)cc2O)c3ccc(OC)cc3	active	uefsnp_p0.ldb	55.18
29	ZINC15149439	O=c1n(c2c(c(OC)c1C[C@@H](O)C(=C)C)cccc2)C	active	uefsnp_p0.ldb	54.99
30	ZINC14436305	:(c(O)c(OC)c(O)c1)C(=O)[C@H](O)[C@H]2c3c(O)ccc	active	uefsnp_p0.ldb	53.41
31	ZINC15119278	2c1cc(cc2)C[C@@H]/3COC(=O)/C/3=C/c4cc(OC)c(O	active	uefsnp_p0.ldb	53.18
32	ZINC06041137	cc(O)cc2)c(O)c(c(O)c3)c6c5O[C@@H](c4ccc(O)cc4)(	active	uefsnp_p0.ldb	53.18
33	ZINC14762732	)C)c(O)c(c(O)c1C(=O)[C@H](O)[C@H]2c3ccccc3)CC	active	uefsnp_p0.ldb	53.1
34	ZINC69482479	:(O)c(O)c(OC)c1)C(=O)[C@H](OC)[C@H]2c3cc(O)c(	active	uefsnp_p0.ldb	52.46
35	ZINC14639505	O=c1c3c(O)c(OC)c(OC)cc3c(=O)c2c1c(O)c(O)cc2	active	uefsnp_p0.ldb	51.82
36	ZINC14647423	O=c1c3c(O)c(OC)c(OC)cc3c(=O)c2c1c(O)c(O)c(c2)C	active	uefsnp_p0.ldb	51.68
37	ZINC69482118	O=c1c3c(OC)cccc3c(=O)c2c1c(O)c(OC)c(O)c2	active	uefsnp_p0.ldb	51.61
38	ZINC69482124	)=c1c3c(OC)c(OC)c(OC)cc3c(=O)c2c1c(OC)c(c(c2)C)(	active	uefsnp_p0.ldb	51.52
39	ZINC14647417	O=c1c3c(O)c(OC)c(O)cc3c(=O)c2c1c(O)c(O)c(c2)C	active	uefsnp_p0.ldb	51.46
40	ZINC14647433	O=c1c3c(OC)c(OC)c(OC)cc3c(=O)c2c1c(O)c(O)c(c2)C	active	uefsnp_p0.ldb	51.45
41	ZINC06070307	O=c1c3c(OC)c(O)c(cc3c(=O)c2c1c(O)c(OC)c(O)c2)C	active	uefsnp_p0.ldb	51.45
42	ZINC40836221	O=c1c3c(OC)cc(O)cc3c(=O)c2c1c(OC)cc(c2)C	active	uefsnp_p0.ldb	51.44
43	ZINC14764105	o2c1c(O)cccc1c(=O)c3c2cc(OC)c(OC)c3O	active	uefsnp_p0.ldb	51.43
44	ZINC06070308	O=c1c3c(OC)c(O)c(cc3c(=O)c2c1c(O)c(OC)c(OC)c2)C	active	uefsnp_p0.ldb	51.43
45	ZINC14652116	)=c1[nH]c2c(OC)c(OC)c(O)c(c2c1=O)CCCCCc3ccccc	active	uefsnp_p0.ldb	51.06
46	ZINC14652112	O=c1[nH]c2c(c1=O)c(ccc2)CCCCCc3ccc(OC)cc3	active	uefsnp_p0.ldb	51.04
47	ZINC00899122	Oc1cc(O)cc(c1)CCc2ccccc2	active	uefsnp_p0.ldb	50.94
48	ZINC13365912	O=c3c1nccc2c1c(c(O)c(OC)c2)c4c3c(OC)c(OC)cc4	active	uefsnp_p0.ldb	50.72
49	ZINC69482541	c2c(O)c(c1c(O)c(OC)cc(c1)\C=C\CO)cc(c2)\C=C\C=C	active	uefsnp_p0.ldb	50.7
50	ZINC14728327	)2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3cc(OC)c(OC)cc	active	uefsnp_p0.ldb	50.68
51	ZINC14807483	o1c3c(c(=O)cc1c2cc(O)c(OC)cc2)ccc(O)c3	active	uefsnp_p0.ldb	50.61

52	ZINC13374352	1c(=O)ccc2c1cc(OC\C=C(\C[C@H](O)C=C(C)C)/C)cc	active	uefsnp_p0.ldb	50.58
53	ZINC00895662	:(ccc(O)c1CC=C(C)C)[C@H]3[C@@H]2c4c(OC3)cc(	active	uefsnp_p0.ldb	50.57
54	ZINC69482464	c(=O)cc1c2ccccc2)c(OC)c(c(O)c3)[C@H]4[NH+](CC(	active	uefsnp_p0.ldb	50.48
55	ZINC69482316	@H](C[C@@H]2C(=O)[C@@]3([C@@H](C(CC3=O)	active	uefsnp_p0.ldb	50.15
56	ZINC69482132	O(c2c(c(O)c1c(O)c3c(cc1c2)CC(CC3=O)(C)C)C)C	active	uefsnp_p0.ldb	49.96
57	ZINC03978794	O=c1c3c(O)cc(OC)cc3c(=O)c2c1c(O)cc(c2)C	active	uefsnp_p0.ldb	49.86
58	ZINC03861630	O=c1c3c(O)cc(cc3c(=O)c2c1c(O)ccc2)C	active	uefsnp_p0.ldb	49.81
59	ZINC69482290	S[C@@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H	active	uefsnp_p0.ldb	49.61
60	ZINC05940186	O=c1c3c(O)cc(OCC=C(C)C)cc3c(=O)c2c1c(O)cc(c2)C	active	uefsnp_p0.ldb	49.49
61	ZINC14728236	c1c(c(O)cc(OC)c1)C(=O)[C@H](O)[C@H]2c3ccc(O)c	active	uefsnp_p0.ldb	49.44
62	ZINC69482139	:(OC)cc2c1C(C3=C(O)[C@H](O)[C@@H](C=C3C2=(	active	uefsnp_p0.ldb	49.4
63	ZINC03869768	o1c(c(O)c(=O)c2c1cc(O)cc2O)c3ccc(O)cc3	active	uefsnp_p0.ldb	49.39
64	ZINC05998596	o1c(c(OC)c(=O)c2c1cc(O)cc2O)c3cc(O)c(O)cc3	active	uefsnp_p0.ldb	49.1
65	ZINC14779932	O=c1c3c(O)c(c(OC)cc3c(=O)c2c1c(O)cc(c2)C)C	active	uefsnp_p0.ldb	49.06
66	ZINC69482243	:(O)c(cc1)[C@@H]3[C@@H](OC)C(=O)c2c(O)cc(OC	active	uefsnp_p0.ldb	48.99
67	ZINC69482539	-c1c3c(O)c(c(OC)cc3c(=O)c2c1c(O)cc(OC)c2)CC=C(C	active	uefsnp_p0.ldb	48.98
68	ZINC69482300	H]2[C@H](O)C[C@H]4[C@](][C@@H]2CC3=O)(CC	active	uefsnp_p0.ldb	48.83
69	ZINC03871358	o1c3c(c(=O)cc1c2ccc(OC)cc2)c(O)cc(O)c3	active	uefsnp_p0.ldb	48.77
70	ZINC69482235	@@H]2OC[C@@H](O)[C@@H](O)[C@H]2O)[C@H	active	uefsnp_p0.ldb	48.66
71	ZINC06017938	O(c2cc(O)c1c(O)c3c(cc1c2)CC(OC3=O)=C)C	active	uefsnp_p0.ldb	48.62
72	ZINC05421170	O=c1c3c(n(c2O[C@H](C(O)(C)C)Cc12)C)c(OC)ccc3	active	uefsnp_p0.ldb	48.55
73	ZINC69482249	C)c(OC)c(OC)c1)C(=O)[C@H](OC)[C@H]2c3cc(O)c(	active	uefsnp_p0.ldb	48.54
74	ZINC69481952	[C@@H]([C@]([C@@H](C1)C)(CC/C(/CO)=C/CO)C	active	uefsnp_p0.ldb	48.47
75	ZINC14437230	1c(c(OC)c(=O)c2c1c(OC)c(OC)c(OC)c2O)c3ccc(O)cc	active	uefsnp_p0.ldb	48.44
76	ZINC13384038	O(c2cc(O)c1c(O)c3c(cc1c2)C[C@](OC3=O)(CO)C)C	active	uefsnp_p0.ldb	48.39
77	ZINC69482142	)c2c(cc1O)C(=O)C3=C[C@H]([C@@H](O)C(O)=C3(	active	uefsnp_p0.ldb	48.32
78	ZINC69482032	@@](][C@@H]2[C@@H](O[C@@]1(OC[C@@H](C[	active	uefsnp_p0.ldb	48.29
79	ZINC28536305	C@@]3([C@@H]2[C@](C(C(=O)[O-])=CCC2)(CC[(	active	uefsnp_p0.ldb	48.29
80	ZINC04097525	)C=CCC1)[C@@H]2O[C@@H]([C@@H](O)[C@H](	active	uefsnp_p0.ldb	48.21
81	ZINC13401794	:(\CC[C@@]2([C@@H]1[C@](C(=CCC1)C)(CC[C@	active	uefsnp_p0.ldb	48.18
82	ZINC00105086	1c(c(O)cc(O)c1)C(=O)[C@@H](O)[C@H]2c3cc(O)c(C	active	uefsnp_p0.ldb	48.16
83	ZINC00105086	:1c(c(O)cc(O)c1)C(=O)[C@H](O)[C@H]2c3cc(O)c(O)	active	uefsnp_p0.ldb	48.15
84	ZINC59149142	1c(=O)c2c(c1=O)cc5c3c(oc4c(c23)cc(O)c(O)c4)c(O)cc	active	uefsnp_p0.ldb	48.14
85	ZINC69482193	[O-])C[C@H]2[C@H]1[C@@H](C(CCC1)(C)C)CC=(	active	uefsnp_p0.ldb	48.06
86	ZINC69482340	(O)cc2c(c1C(C)C)C(C[C@H]3[C@@]2(CCCC3(C)C)	active	uefsnp_p0.ldb	48
87	ZINC69482526	C@@]3([C@@H](C[C@H]2O[C@@H]4O[C@@H]((	active	uefsnp_p0.ldb	47.98
88	ZINC00900257	O=c1c(OC)c([nH]c2c1c4c(cc2)C(c3ccccc3)=CCCC4)C	active	uefsnp_p0.ldb	47.91
89	ZINC69482307	3[C@H]([C@]2([C@@H](C1)C(CCC2)(C)C)C)CC(=(	active	uefsnp_p0.ldb	47.88
90	ZINC69482018	C[C@H]2[C@]([C@H](O)[C@H](O)C=C2C)([C@H]	active	uefsnp_p0.ldb	47.86
91	ZINC69482170	(O)([C@@H]3[C@@H]([C@@]2([C@](C[C@@H]((	active	uefsnp_p0.ldb	47.82
92	ZINC69481950	@H]([C@@]([C@@H](C1)C)(CO)CC/C(/CO)=C/CO)	active	uefsnp_p0.ldb	47.65
93	ZINC69482026	o1c(c(O)c(=O)c2c1cc(cc2O)C)c3ccc(O)cc3	active	uefsnp_p0.ldb	47.65
94	ZINC69482253	O)c(O)c(OC)c1)C(=O)[C@H](OC)[C@H]2c3c(O)c(O)	active	uefsnp_p0.ldb	47.57
95	ZINC69481928	C@H]2c3cc(O)c(O)cc3)[C@H]4O[C@H]([C@H](O)[(	active	uefsnp_p0.ldb	47.47
96	ZINC00338284	O2c1c(c(O)cc(OC)c1)C(=O)C[C@H]2c3ccc(O)cc3	active	uefsnp_p0.ldb	47.47
97	ZINC00156701	O2c1c(c(O)cc(O)c1)C(=O)C[C@H]2c3ccc(O)cc3	active	uefsnp_p0.ldb	47.47
98	ZINC69482210	])(O)C[C@@]3([C@H]2[C@](C(C(=O)[O-])=CCC2)(	active	uefsnp_p0.ldb	47
99	ZINC69482418	2[C@@H]3[NH+](CC2)CC[C@H]3COC(=O)[C@@]	active	uefsnp_p0.ldb	46.98
100	ZINC14556518	H+](CC1)CC[C@H]2COC(=O)[C@@](O)([C@@H](	active	uefsnp_p0.ldb	46.78
101	ZINC69481972	([C@H]([C@@](C1)(CC)C)CC[C@@]34[C@@H]2C	active	uefsnp_p0.ldb	46.31
102	ZINC00035525	o2c1nc3c(OC)c(OC)ccc3c(OC)c1cc2	active	uefsnp_p0.ldb	46.27
103	ZINC69481958	[C@H]([C@H]1[C@H]3[C@@](O)(C=C1)CC[C@H]	active	uefsnp_p0.ldb	46.12
104	ZINC69481941	o1c(=O)ccc2c1c(c(OC)cc2)[C@@H](O)\C=C(\CO)/C	active	uefsnp_p0.ldb	46.09

105	ZINC69482165	[C@](O)(C2[C@H]([C@H](O)C1)[C@@]3([C@@H	active	uefsnp_p0.ldb	46.06
106	ZINC15113633	o1c(=O)cc(c2c1c(O)c(OC)cc2OC)c3cc(O)c(O)cc3	active	uefsnp_p0.ldb	45.74
107	ZINC01721695	o1coc4c1cc3c2n(c(=O)c5c(c2ccc3c4)cc(OC)c(OC)c5)C	active	uefsnp_p0.ldb	45.72
108	ZINC69482017	C@@](C@H]1[C@@]4([C@H](OC(=O)C1)C[C@@	active	uefsnp_p0.ldb	45.63
109	ZINC69482106	O(c1c(O)cc(cc1O)C\C=C\c2cc(cc(c2)C)C)C	active	uefsnp_p0.ldb	44.25
110	ZINC69482145	cc(OC)c2c1C(C3=C(O)[C@@H]([C@H](O)C=C3C2=	active	uefsnp_p0.ldb	44.15
111	ZINC69482473	c(OC)cc(=O)c3c1C[C@@]2([C@H](O)CC=C(CO)C2=	active	uefsnp_p0.ldb	44.07
112	ZINC69482435	1cc(cc2)\C=C(\C(=O)OC)/C(/C(=O)OC)=C\c3cc(OC)c	active	uefsnp_p0.ldb	43.98
113	ZINC15104854	o1c3c(c(=O)c2c1ccc(O)c2C(=O)OC)c(O)cc(c3)C	active	uefsnp_p0.ldb	43.91
114	ZINC69482521	C@]5(O[C@@H]5[C@H]2OC(=O)[C@H]([C@@H]2	active	uefsnp_p0.ldb	43.6
115	ZINC69482256	))c(O)c(OC)c1)C(=O)[C@H](OC)[C@H]2c3cc(OC)c((	active	uefsnp_p0.ldb	43.55
116	ZINC14684940	o1c3c(c(=O)cc1C)c(O)c2c(O)cc(OC)c(c2c3)C	active	uefsnp_p0.ldb	43.55
117	ZINC01531431	O=c1[nH]c2c(OC)c(OC)cc(c2c1=O)CCCCCc3ccccc3	active	uefsnp_p0.ldb	43.43
118	ZINC69482082	)c(c(O)c1)[C@H]2[NH+](CCCC2)C)C(=O)C[C@H]3c	active	uefsnp_p0.ldb	43.32
119	ZINC69482433	O=C([O-])CC1(C=CC(C=C1)C)C	active	uefsnp_p0.ldb	43.31
120	ZINC69481889	@@H]2[C@@H]([C@@H]1[C@@]([C@H](C(=O)C1	active	uefsnp_p0.ldb	43.3
121	ZINC13384042	=O)(=O)(Oc3c2c1oc(cc(=O)c1c(O)cc2c(c(OC)c3)C)C)[	active	uefsnp_p0.ldb	43.28
122	ZINC69481997	@@]3([C@@]12[C@H](C[C@@H](C1)C(CC2)(C)C	active	uefsnp_p0.ldb	43.24
123	ZINC14762765	)1c(c(O)c(=O)c2c1c(c(O)cc2O)CC=C(C)C)c3ccc(O)cc3	active	uefsnp_p0.ldb	43.2
124	ZINC69482302	C@@]3([C@@H](C[C@H](O)[C@H]1C(C(=O)OC)=	active	uefsnp_p0.ldb	43.13
125	ZINC13400223	ccc3c1c2O[C@H]([C@@H](Oc2c(OC)c3)c4cc(OC)c(	active	uefsnp_p0.ldb	43.13
126	ZINC69482103	O(c1c(O)cc(cc1O)\C=C\c2cc(cc(c2)C)C)C	active	uefsnp_p0.ldb	43.12
127	ZINC01530416	O=C([O-])CCCCCCC	active	uefsnp_p0.ldb	43.08
128	ZINC69482092	))c(OC)c(OC)c1)C(=O)[C@H](OC)[C@H]2c3c(O)cc((	active	uefsnp_p0.ldb	43.05
129	ZINC13523214	(c1c(O)ccc4c1CN3[C@H](c2c(cc(O)c(OC)c2)CC3)C4	active	uefsnp_p0.ldb	43.01
130	ZINC69482184	O(c1c(cc(cc1)C)C(\C=C\C)=C)C=O	active	uefsnp_p0.ldb	42.97
131	ZINC69481901	C[C@H](O)C[C@@H](O)C[C@@H](O)CCCCC)CC(	active	uefsnp_p0.ldb	42.93
132	ZINC69482212	@@H]3[C@]([C@H]2[C@]1(C[C@H](C(C1=C)=C)C	active	uefsnp_p0.ldb	42.92
133	ZINC69482055	C@H](C(=O)C(=C1)C)CC(OC(=O)C)=C[C@H]2C(C(	active	uefsnp_p0.ldb	42.84
134	ZINC13451751	Clc2c1occ(c(=O)c1c(O)c(Cl)c2OC)c3cc(Cl)c(O)cc3	active	uefsnp_p0.ldb	42.8
135	ZINC69482385	c1cc(c2coc4c(c2=O)c(O)c3c(OC([C@@H](C3)C)(C)C	active	uefsnp_p0.ldb	42.78
136	ZINC69481945	3C([C@H]2[C@@]([C@H]1[C@H](O)COC1=CC2)((	active	uefsnp_p0.ldb	42.78
137	ZINC69482325	)C)cc4c(c1O)c2c(OC)c(OC)cc3c2[C@H]([NH+](CC3)	active	uefsnp_p0.ldb	42.74
138	ZINC01580260	cc3c1c2O[C@@H]([C@H](Oc2c(OC)c3)c4cc(OC)c((	active	uefsnp_p0.ldb	42.62
139	ZINC13374022	O(c1c(O)cc(c2c1c3c(cc2)cccc3)CC[NH+](C)C)C	active	uefsnp_p0.ldb	42.62
140	ZINC69482450	H]3[C@@](C1C(C(=C(O)C(=O)C=1)C(C)C)=C2)(CC(	active	uefsnp_p0.ldb	42.43
141	ZINC69481985	H]([C@](CO)(C=C1O)C)CC[C@@]34[C@H]2CC[C(	active	uefsnp_p0.ldb	42.43
142	ZINC01626261	c(O)cc(O)c1CC=C(C)C)C(=O)[C@H](O)[C@H]2c3cc(	active	uefsnp_p0.ldb	42.38
143	ZINC69482424	]2[C@H]3[NH+](CC2)CC[C@@H]3COC(=O)[C@]((	active	uefsnp_p0.ldb	42.35
144	ZINC69482509	(=O)c4c(OC)ccc3oc(=O)c2c(OC)cc(c1c2c34)C[NH+](	active	uefsnp_p0.ldb	42.08
145	ZINC69482286	:1C2=CC[C@@H](O)C=C2)c(O)c(c(O)c3)[C@H]4[NH	active	uefsnp_p0.ldb	42.02
146	ZINC05733652	o1c3c(c(=O)cc1c2cc(O)c(OC)cc2)c(O)cc(O)c3	active	uefsnp_p0.ldb	41.88
147	ZINC14646949	2c1cc(cc2)C[C@]3(O)[C@@H](COC3=O)Cc5cc4oco	active	uefsnp_p0.ldb	41.82
148	ZINC13459886	Oc1c2c(ccc1)[C@@H](O)[C@@H](CC2=O)C	active	uefsnp_p0.ldb	41.77
149	ZINC04654690	Oc1c2c(ccc1)[C@H](O)[C@@H](CC2=O)C	active	uefsnp_p0.ldb	41.77
150	ZINC06037073	o2c1c(=O)c3c(c(=O)c1cc2[C@H](O)C)c(O)ccc3	active	uefsnp_p0.ldb	41.67
151	ZINC06037435	@]12[C@](C(=O)CC[C@@H]1C)(CC[C@H](C2)C(=	active	uefsnp_p0.ldb	41.66
152	ZINC01531432	O=c1[nH]c2c(c1=O)c(ccc2)CCCCCc3ccccc3	active	uefsnp_p0.ldb	41.64
153	ZINC69482501	C@@H](O)[C@]3([C@@H]2[C@](C(OC(=O)C)=CC(	active	uefsnp_p0.ldb	41.63
154	ZINC13485082	c(c(OC)c(=O)c3c1c2c(OC(C=C2)(C)C)c(OC)c3)c4ccc(	active	uefsnp_p0.ldb	41.63
155	ZINC14694264	O=c1c(c(cc1)C)C[C@@H](C(=C)C)CCC(=O)C	active	uefsnp_p0.ldb	41.61
156	ZINC14643827	2c1c(c(O)cc(OC)c1)C(=O)C[C@H]2c3cc(OC)c(O)c(O)	active	uefsnp_p0.ldb	41.54
157	ZINC00113309	o1c(=O)ccc2c1c(O)c(O)c(OC)c2	active	uefsnp_p0.ldb	41.54

Lampiran 5

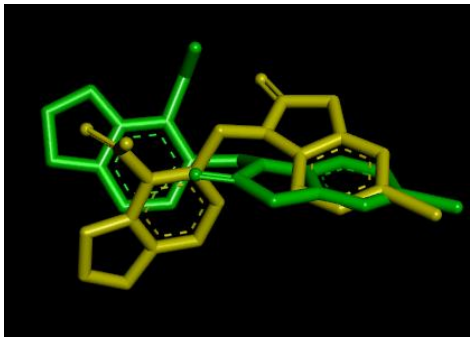
Validasi Docking Enzim HIV Integrase

Tabel Parameter Validasi Penambatan Molekul Enzim HIV Integrase

Grid Box			*Grid Spacing*	*Grid Center*		
X	***Y***	***Z***	0.375 Å	***X center***	***Y center***	***Z center***
40	40	40		10.156	-26.763	-10.901

Number of Runs: 100
Number of Evals: Medium
Metode Algoritma: Lamarckian Genetic Algorith
RMSD :1.688 Å
Energi ikatan : - 8.79 kcal/mol
Konstanta inhiisi : 357.73 nm (nanomolar)

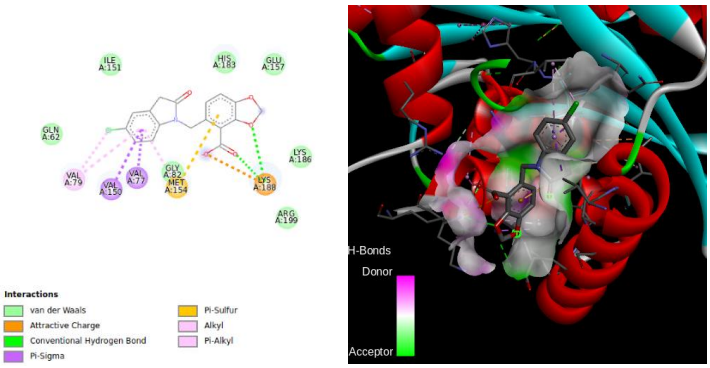
```
MODEL       76
USER    Run = 76
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 42
USER
USER    RMSD from reference structure       = 1.688 A
USER
USER    Estimated Free Energy of Binding    =   -8.79 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  357.73 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -9.69 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -7.76 kcal/mol
USER        Electrostatic Energy            =   -1.93 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.20 kcal/mol
USER    (3) Torsional Free Energy           =   +0.89 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   +0.20 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig.pdbqt
USER    NEWDPF about    10.153000 -27.000700 -10.168300
USER    NEWDPF tran0    10.802392 -26.853435 -10.223021
USER    NEWDPF axisangle0       0.774621 0.597084 0.208456 -75.517002
USER    NEWDPF quaternion0      0.474327 0.365615 0.127645 -0.790599
USER    NEWDPF dihe0    -22.98 -103.26 -76.89
```



Gambar Visualisasi tumpang tindih ligan alami HIV integrase (kuning) dan ligan redocking (hijau).

Tabel 5. Hasil interaksi senyawa uji dengan residu asam amino

Komplek	ΔG (kJ/mol)	Ki (konstanta Inhibisi)	Interaksi	Residu asam amino
Ligan alami	-8.79	357.73 nM	**Ikatan Hidrogen** LYS A:188 **Ikatan Hidrofobik** MET A:154, VAL A:150. VAL A:77 **Ikatan Van Der Waals** VAL A:79, GLN A:62, SER A:81, ARG A:199, GLY A:82, ALA A:196	**LYS188** **MET154** **VAL150** **VAL77** **VAL79** **GLN62** **SER81** **ARG199** **GLY82** **ALA196**



Gambar Visualisasi interaksi Enzim HIV Integrase dengan Ligan Alami

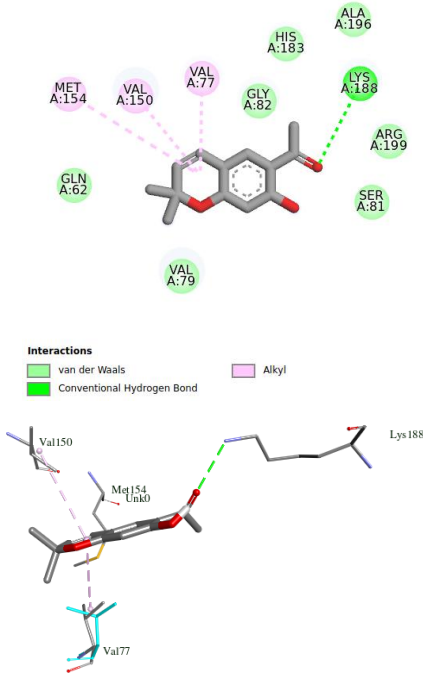
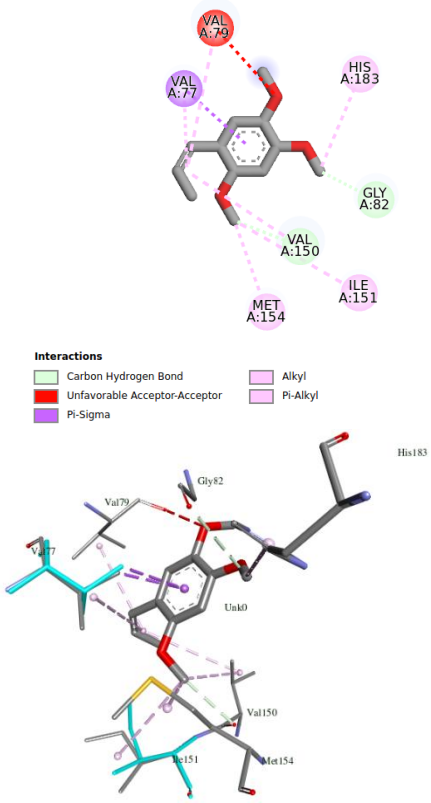
Lampiran 6: Hasil Penembatan Senyawa Uji

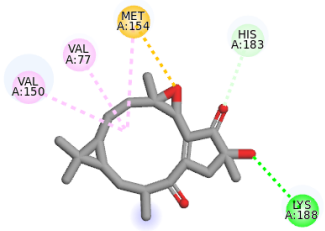
Tabel 5. Hasil interaksi senyawa uji dengan residu asam amino

Komplek	ΔG (kJ/mol)	Ki (konstanta Inhibisi)	Interaksi	Residu asam amino
Ligan alami	-8.79	357.73 nM	**Ikatan Hidrogen** LYS A:188 **Ikatan Hidrofobik** MET A:154, VAL A:150. VAL A:77 **Ikatan Van Der Waals** VAL A:79, GLN A:62, SER A:81, ARG A:199, GLY A:82, ALA A:196	**LYS188** **MET154** **VAL150** **VAL77** **VAL79** **GLN62** **SER81** **ARG199** **GLY82** **ALA196**
ZINC00897926	-5.54	86.98 uM	**Ikatan Hidrogen** LYS A:188 **Ikatan Hidrofobik** VAL A:77, VAL A:150, MET A :154 **Ikatan Van Der Waals** GLN A:62, VAL A:79, SER A:81, GLY A:82, HIS A:183, ALA A:196, ARG A:199	**LYS188** **VAL77** **VAL150** **MET154** **GLN62** **VAL79** **SER81** **GLY82** HIS183 **ALA196** ARG199
ZINC13424754	-4.78	311.10 uM	**Ikatan Hidrogen** GLY A:82 **Ikatan Hidrofobik** VAL A:77, VAL A:150, ILE A:151, MET A:154, HIS A:183 VAL A:79 **Ikatan Van Der Waals** VAL A:79	**GLY82** **VAL77,** **VAL150,** ILE151, **MET154,** HIS183 **VAL79**
ZINC84154372	**-7.75**	**2.75 uM**	**Ikatan Hidrogen** LYS A:188, HIS A 183 **Ikatan Hidrofobik** VAL A:77, VAL A:150 **Ikatan Van Der Waals** MET A:154	**LYS188,** **HIS183** **VAL77,** **VAL150** **MET154**

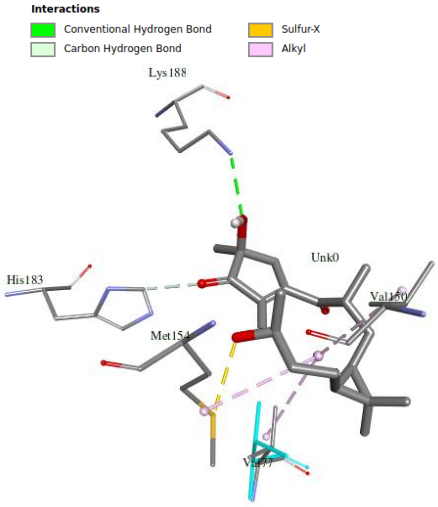
ZINC84154348	-7.22	5.10 uM	**Ikatan Hidrogen** LYS A:188, HIS A:183, GLY A:82 **Ikatan Hidrofobik** **Ikatan Van Der Waals** MET A:154, VAL A:77, VAL A:150, VAL A:79, LEU A:158, GLU A:157, ILE A:84, ARG A:199, SER A:81	**LYS188,** HIS183, **GLY82** **MET154, VAL77, VAL150, VAL79,** LEU158, GLU157, ILE84, **ARG199, SER81**
ZINC26545142	-6.20	28.44 uM	**Ikatan Hidrogen** GLY A:82, GLN A: 62 **Ikatan Hidrofobik** MET A:154, VAL A:150, VAL A:79, VAL A:77 **Ikatan Van Der Waals** ILE A:151, SER A:147, HIS A:183	**GLY82, GLN62** **MET154, VAL150, VAL79, VAL77** ILE151, SER147, HIS183
ZINC69482080	-7.46	3.41 uM	**Ikatan Hidrogen** VAL A:79 **Ikatan Hidrofobik** MET A:154, VAL A:77 **Ikatan Van Der Waals** HIS A:183, VAL A:150, ILE A:151, GLN A:62, SER A:147, GLY A:82	VAL79 **MET154, VAL77** HIS183, **VAL150,** ILE151, **GLN62,** SER147, **GLY82**
ZINC69482354	-7.00	7.36 uM	**Ikatan Hidrogen** LYS A:188 **Ikatan Hidrofobik** VAL A:77, VAL A:150, VAL A:79 **Ikatan Van Der Waals** GLU A:157, HIS A:183, ARG A:199, GLY A:82, MET A:154, ILE A:151, GLN A:62, SER A: 147	**LYS188** **VAL77, VAL150, VAL79** GLU157, HIS183, **ARG199, GLY82, MET154,** ILE151, **GLN62**, SER147

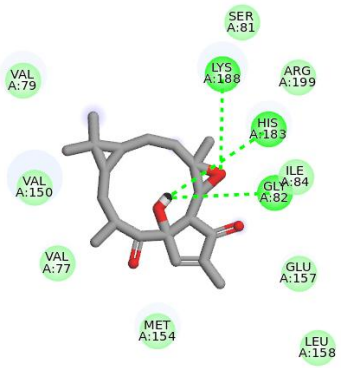
Tabel 6. Hasil Visualisasi Interaksi Senyawa Uji

No	Senyawa	Interaksi
1	ZINC00897926	
2	ZINC13424754	

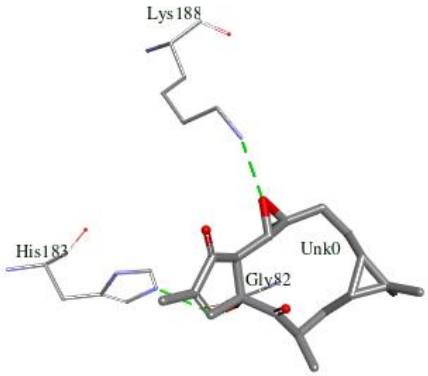


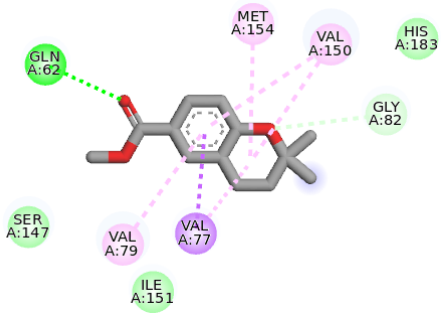
3 **ZINC84154372**



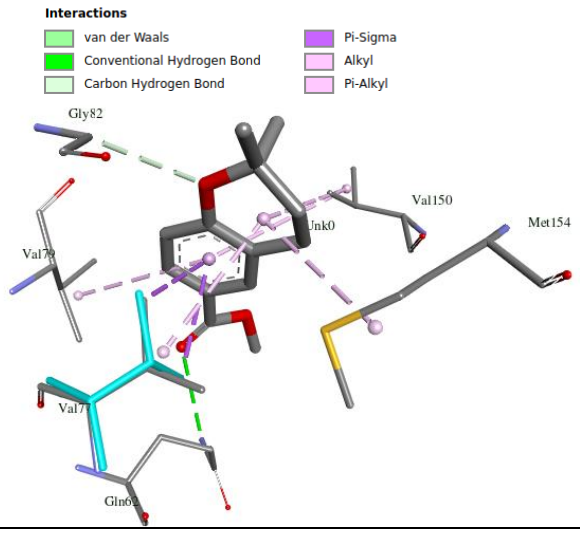


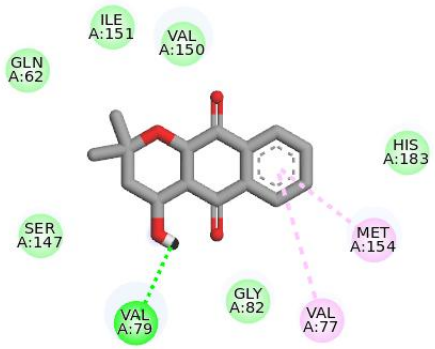
4 ZINC84154348



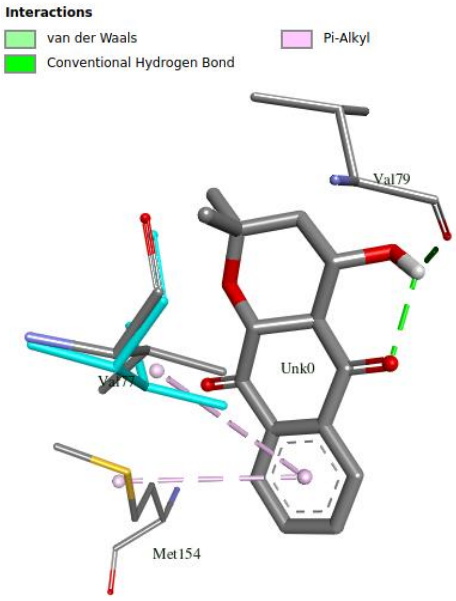


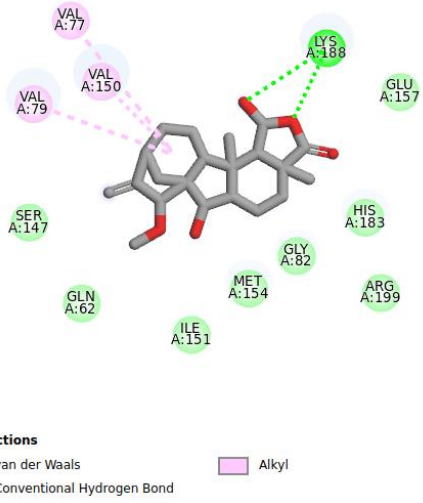
5 ZINC26545142



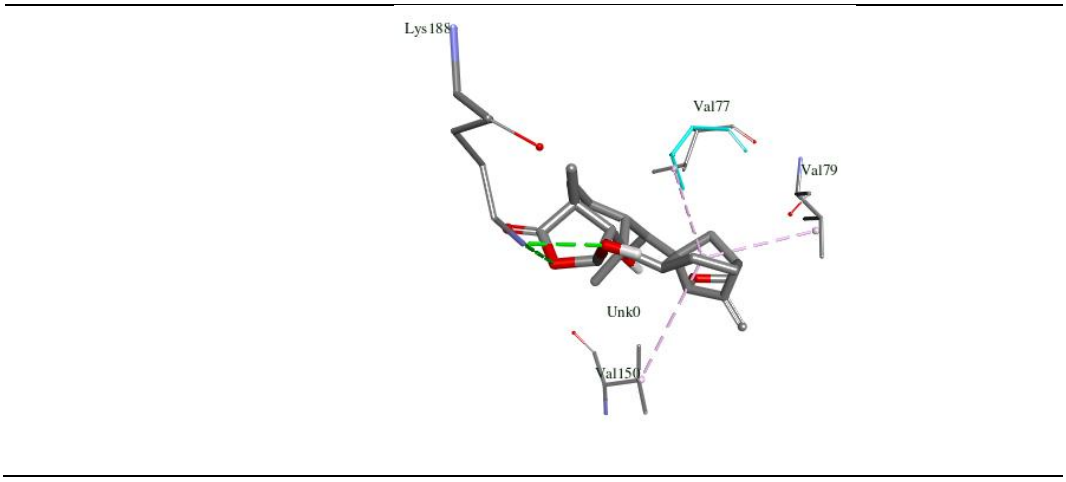


6 ZINC69482080





7 ZINC69482354



LIGAN ALAMI

```
MODEL        76
USER    Run = 76
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 42
USER
USER    RMSD from reference structure       = 1.688 A
USER
USER    Estimated Free Energy of Binding    =   -8.79 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  357.73 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -9.69 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -7.76 kcal/mol
USER        Electrostatic Energy            =   -1.93 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.20 kcal/mol
USER    (3) Torsional Free Energy           =   +0.89 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   +0.20 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig.pdbqt
USER    NEWDPF about    10.153000 -27.000700 -10.168300
USER    NEWDPF tran0    10.802392 -26.853435 -10.223021
USER    NEWDPF axisangle0       0.774621 0.597084 0.208456 -75.517002
USER    NEWDPF quaternion0      0.474327 0.365615 0.127645 -0.790599
USER    NEWDPF dihe0    -22.98 -103.26 -76.89
```

SENYAWA UJI

ZINC00897926

```
MODEL       48
USER    Run = 48
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 88
USER
USER    RMSD from reference structure       = 27.120 A
USER
USER    Estimated Free Energy of Binding    =   -5.54 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   86.98 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -6.14 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.96 kcal/mol
USER        Electrostatic Energy            =   -0.17 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.70 kcal/mol
USER    (3) Torsional Free Energy           =   +0.60 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.70 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     liganalitycom.pdbqt
USER    NEWDPF about    0.121700 -0.180500 0.000100
USER    NEWDPF tran0    7.638392 -25.812514 -9.101269
USER    NEWDPF axisangle0       -0.877877 -0.462408 0.124541 -170.239153
USER    NEWDPF quaternion0      -0.874694 -0.460732 0.124090 -0.085076
USER    NEWDPF dihe0    -152.04 -54.71
```

ZINC13424754

```
MODEL       37
USER    Run = 37
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 71
USER
USER    RMSD from reference structure       = 27.879 A
USER
USER    Estimated Free Energy of Binding    =   -4.78 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  311.10 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -5.98 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -5.97 kcal/mol
USER        Electrostatic Energy            =   -0.00 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.66 kcal/mol
USER    (3) Torsional Free Energy           =   +1.19 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.66 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig.pdbqt
USER    NEWDPF about    -0.144500 -0.042300 -0.180300
USER    NEWDPF tran0    6.991131 -27.272525 -8.718016
USER    NEWDPF axisangle0       0.389981 0.194797 0.899983 -77.310615
USER    NEWDPF quaternion0      0.243595 0.121677 0.562160 -0.780918
USER    NEWDPF dihe0    -33.42 -120.86 -170.46 43.13
```

ZINC84154372

```
MODEL       82
USER    Run = 82
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 100
USER
USER    RMSD from reference structure       = 27.735 A
USER
USER    Estimated Free Energy of Binding    =   -7.59 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    2.75 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -7.88 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -7.72 kcal/mol
USER        Electrostatic Energy            =   -0.16 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.22 kcal/mol
USER    (3) Torsional Free Energy           =   +0.30 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.22 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig1.pdbqt
USER    NEWDPF about    0.197600 -0.019000 0.051600
USER    NEWDPF tran0    8.298900 -26.460391 -9.634716
USER    NEWDPF axisangle0       -0.920563 -0.366803 0.134236 -168.988963
USER    NEWDPF quaternion0      -0.916316 -0.365111 0.133617 -0.095942
USER    NEWDPF dihe0    55.82
USER
```

ZINC84154348

```
MODEL       88
USER    Run = 88
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 100
USER
USER    RMSD from reference structure       = 27.029 A
USER
USER    Estimated Free Energy of Binding    =   -7.22 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    5.10 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -7.52 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -6.94 kcal/mol
USER        Electrostatic Energy            =   -0.58 kcal/mol
USER    (2) Final Total Internal Energy     =   +0.03 kcal/mol
USER    (3) Torsional Free Energy           =   +0.30 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   +0.03 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig.pdbqt
USER    NEWDPF about    -0.067000 0.049500 0.099900
USER    NEWDPF tran0    9.187217 -25.780620 -10.277940
USER    NEWDPF axisangle0       -0.067078 -0.100028 -0.992721 175.642012
USER    NEWDPF quaternion0      -0.067029 -0.099956 -0.992003 0.038021
USER    NEWDPF dihe0    44.22
```

ZINC26545142

```
MODEL       89
USER    Run = 89
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 38
USER
USER    RMSD from reference structure       = 29.491 A
USER
USER    Estimated Free Energy of Binding    =   -6.20 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   28.44 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -6.80 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -6.76 kcal/mol
USER        Electrostatic Energy            =   -0.04 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.16 kcal/mol
USER    (3) Torsional Free Energy           =   +0.60 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.16 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig.pdbqt
USER    NEWDPF about    0.000100 -0.009100 -0.060200
USER    NEWDPF tran0    6.595065 -28.486629 -8.868947
USER    NEWDPF axisangle0       -0.229334 0.259910 -0.938005 -154.108965
USER    NEWDPF quaternion0      -0.223505 0.253304 -0.914164 -0.224024
USER    NEWDPF dihe0    -19.32 137.87
```

ZINC69482080

```
MODEL       18
USER    Run = 18
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 100
USER
USER    RMSD from reference structure       = 28.298 A
USER
USER    Estimated Free Energy of Binding    =   -7.46 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    3.41 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -7.76 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -7.79 kcal/mol
USER        Electrostatic Energy            =   +0.03 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.62 kcal/mol
USER    (3) Torsional Free Energy           =   +0.30 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.62 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig.pdbqt
USER    NEWDPF about    -0.049900 -0.157500 0.031200
USER    NEWDPF tran0    7.240644 -27.682400 -9.248428
USER    NEWDPF axisangle0       0.967595 0.205893 -0.146179 164.437332
USER    NEWDPF quaternion0      0.958685 0.203997 -0.144833 0.135393
USER    NEWDPF dihe0    -14.95
```

ZINC69482354

```
MODEL       22
USER    Run = 22
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 42
USER
USER    RMSD from reference structure       = 27.386 A
USER
USER    Estimated Free Energy of Binding    =   -7.00 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    7.36 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -7.90 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -7.61 kcal/mol
USER        Electrostatic Energy            =   -0.28 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.33 kcal/mol
USER    (3) Torsional Free Energy           =   +0.89 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.33 kcal/mol
USER
USER
USER
USER    DPF = ./dock.dpf
USER    NEWDPF move     lig.pdbqt
USER    NEWDPF about    0.071000 -0.018100 0.042700
USER    NEWDPF tran0    8.327976 -26.592980 -10.132930
USER    NEWDPF axisangle0       -0.949939 -0.289941 0.116408 171.964083
USER    NEWDPF quaternion0      -0.947604 -0.289228 0.116122 0.070069
USER    NEWDPF dihe0    88.44 112.38 -106.95
```

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