

Supplementary material:

Table 1: Enrichment Factor and Area Under Curve of HIV-1 Protease DUD Database Virtual Screening using AutoDock. The best EF1% and AUC was indicated by bold text.

HIV-1 Condition	Protease	Macromolecule	Grid (units)	Box	Maximum Evaluations	Number of Energy	EF 1%	EF 10%	EF 20%	AUC
Without water molecule on binding site			50x50x50		250.000		0	1,45	1,53	0.6551
					1.000.000		6,45	1,77	1,53	0.6152
			60x60x60	250.000		1,61	1,13	0,81	0.4492	
				1.000.000		1,61	1,45	1,45	0.5574	
Retaining water molecules on binding site			50x50x50		250.000		3,23	2,74	1,61	0.5654
					1.000.000		11,29	3,55	2,34	0.6992
			60x60x60	250.000		1,61	3,23	2,66	0,7275	
				1.000.000		1,61	1,13	1,21	0,6055	

Table 2: Top ten compounds of HIV-1 Protease virtual screening result using AutoDock

Rank	Name	ΔG (kcal/mol)	N	SD	CV (%)	Plant(s) Source
1	8-Hydroxyapigenin (2'',4''-disulfatoglucuronide)	-18,74	5	2,89	15,41	<i>Helicteres isora</i>
2	Isoscutellarein 4'-methyl ether 8-(2'',4''-disulfatoglucuronide)	-17,83	5	1,20	6,72	<i>Helicteres isora</i>
3	Amaranthin	-17,72	5	1,58	8,91	<i>Amaranthus caudatus</i> , <i>Amaranthus tricolor</i> , <i>Celosia argentea</i> var.cristata (L.) Kuntze, <i>Celosia argentea</i> var.plumosa (Burvenich) Voss, <i>Celosia cristata</i> , <i>Atriplex hortensis</i> , <i>Chenopodium amaranticolor</i>
4	Torvanol A	-14,58	5	0,59	4,04	<i>Solanum torvum</i>
5	Ursonic acid	-12,46	5	0,03	0,28	<i>Angelica ursina</i> Maxim, <i>Cordia multispicata</i> , <i>Myrica rubra</i> , <i>Lantana camara</i> LINN.
6	5-Carboxypyranocyanidin 3-O-(6''-O-malonyl-beta-glucopyranoside)	-12,39	4	0,35	2,82	<i>Allium cepa</i>
7	Oleoside	-12,04	5	0,46	3,79	<i>Chionanthus retusus</i> Lindl.& Paxton, <i>Forestiera acuminata</i> (Michx.) Poir., <i>Fraxinus</i> sp., <i>Jasminum</i> sp., <i>Ligustrum</i> sp., <i>Nestegis sandwicensis</i> (Gray) O.& I.Deg.& Johnson, <i>Olea</i> sp., <i>Osmanthus</i> sp., <i>Phillyrea latifolia</i> L., <i>Picconia excelsa</i> (Aiton) DC., <i>Syringa</i> sp
8	Jacoumaric acid	-11,95	4	0,06	0,47	<i>Jacaranda caucana</i> , <i>Psidium guajava</i>
9	Platanic acid	-11,91	5	0,19	1,56	<i>Platanus occidentalis</i>
10	5-Carboxypyranocyanidin 3-O-beta-glucopyranoside	-11,79	3	0,55	4,63	<i>Allium cepa</i>