Supplementary data 7

Table S7 Molecular docking results of CA-identified compounds at the RNase H active site of HIV-1 RT

Compound	**Binding energy (kcal/mol)**	**Inhibition constant**
P4Y (original inhibitor)	-5.29	132.5 μM
3β,6α,7α-Trihydroxy-5β-cholan-24-oic acid	-6.77	10.83 μM
27-nor-5β-Cholestane-3α,7α,12α,24,25-pentol	-6.58	15.11 μM
Hydroxyibuprofen	-5.92	45.54 μM
6β,11β,16α,17α,21-Pentahydroxypregna-1,4-diene-3,20-dione-16,17-acetonide	-5.90	47.56 μM
Dihydroergocornine	-5.80	56.02 μM
Lactone of PGF-MUM	-5.57	82.02 μM
Pro Glu	-5.44	103.08 μM
β-Levantenolide	-5.38	114.1 μM
Val Val	-5.34	121.36 μM
6-(3-Hydroxyprop-1-en-2-yl)-4,8a-dimethyl-1,3,5,6,7,8-hexahydronaphthalen-2-one	-5.25	141.74 μM
3-(3,3,8,8-Tetramethyl-5-tricyclo[5.1.0.02,5]oct-5-enyl)propanoic acid	-5.17	161.15 μM
Gemfibrozil M1	-5.16	165.59 μM
Gemfibrozil	-5.13	174.67 μM
Xanthumin	-5.07	193.22 μM
Prostaglandin H1	-5.05	198.21 μM
Cadinol T	-4.89	262.45 μM
Punctaporin B	-4.86	271.97 μM
Ile Thr	-4.80	301.79 μM
Dihydrocostunolide	-4.74	336.3 μM
α-Cadinol	-4.55	465.37 μM
Arglabin	-4.52	485.39 μM
4Z-Decenedioic acid	-4.51	492.23 μM
9-Isopropyl-1-methyl-2-methylene-5-oxatricyclo[5.4.0.03,8]undecane	-4.48	524.49 μM
(4Z)-4-(6,6-dimethyl-2-methylidenecyclohex-3-en-1-ylidene)pentan-2-ol	-4.45	543.19 μM
Gemfibrozil M3	-4.45	545.78 μM
2-Hydroxyethanesulfonate	-4.40	593.72 μM
(E)-2-Methylglutaconic acid	-4.38	612.4 μM
4-(3,3-dimethylbut-1-ynyl)-4-hydroxy-2,6,6-trimethylcyclohex-2-en-1-one	-4.33	667.9 μM
Cycloisolongifolene,8,9-dehydro-9-formyl-	-4.30	709.1 μM
Benzenehexanoic acid, 2,5-dihydroxy-3,4-dimethoxy-6-methyl-	-4.30	704.81 μM

Isoaromadendrene epoxide	-4.25	763.78 µM
Amiloxate	-4.24	782.22 µM
Citronellic acid	-4.22	807.0 µM
Phytosphingosine	-4.21	819.94 µM
4,7,7-Trimethyl-4-(2-methylallyl)tricyclo[3.3.0.02,8]octane-3,6-dione	-4.14	931.07 µM
Ile Leu Leu	-4.14	917.91 µM
13-Hydroxy-tridecanoic acid	-4.12	961.57 µM
4-Hydroxy capric acid	-4.09	1.01 mM
Pantoic acid	-4.08	1.01 mM
QH2	-4.08	1.02 mM
Hexadecasphinganine	-4.00	1.17 mM
α-Terpineol	-3.93	1.32 mM
3-oxo-Tridecanoic acid	-3.71	1.92 mM
3-n-Decyl acrylic acid	-3.66	2.06 mM
Dihydrosphingosine	-3.61	1.98 mM
10-keto Tridecanoic acid	-3.58	2.37 mM
Prostaglandin F1a alcohol	-3.51	2.65 mM
Methyl jasmonate	-3.49	2.78 mM
Taurine	-3.43	3.06 mM
3-Dodecynoic acid	-3.38	3.34 mM
Palmitic acid	-3.37	3.36 mM
Leucine	-3.29	3.85 mM
Oleic Acid	-3.23	4.32 mM
2-oxo-Dodecanoic acid	-3.07	5.62 mM
Deoxyribose	-3.06	5.72 mM
Dihydrojasmonic acid, methyl ester	-3.04	5.93 mM
7E,9Z-Dodecadien-1-ol	-2.78	9.14 mM
Ethyl oxalacetate	-2.74	9.8 mM
9-Dodecen-1-ol	-2.53	14.0 mM
4-Heptanone	-2.52	14.22 mM
4-Methylpentanal	-2.51	14.37 mM
Octanal	-2.33	19.45 mM
Undecanal	-2.18	25.1 mM
Linoleic acid, methyl ester	-1.65	61.56 mM
12-Hydroxy-10-octadecynoic acid	-1.43	89.21 mM
3-Tridecynoic acid	-0.91	213.6 mM
N-(2-hydroxyethyl) icosanamide	-0.49	439.99 mM