

**S9 Table.** Anti-HIV activities of top 20 predicted candidates based on the evidence from literatures.

Predicted drug names	p-value	Adjusted p-value	Refs of Anti-HIV activity	Ranks
camptothecin	0.0000609	0.003715	[1,2]	Top1
sertaconazole	0.0000939	0.005728	NA	Top2
alsterpaullone	0.0001745	0.010642	[3]	Top3
lycorine	0.0002327	0.014195	[4]	Top4
sanguinarine	0.000319	0.01946	[5]	Top5
testosterone	0.0006199	0.037815	NA	Top6
amylocaine	0.000741	0.045201	NA	Top7
2,6-dimethylpiperidine	0.0007523	0.04589	NA	Top8
triprolidine	0.0009069	0.055322	NA	Top9
fursultiamine	0.0009652	0.058877	[6]	Top10
trichostatin A	0.0011253	0.068646	[7]	Top11
doxorubicin	0.0011878	0.071269	[8]	Top12
cobalt chloride	0.0012114	0.073893	NA	Top13
fulvestrant	0.0012775	0.07793	NA	Top14
promethazine	0.0013481	0.080886	[9,10]	Top15
viomycin	0.0013504	0.082375	NA	Top16
8-azaguanine	0.0016932	0.103283	[11]	Top17
0179445-0000	0.0019612	0.119631	NA	Top18
chlorphenesin	0.0022216	0.135518	NA	Top19
staurosporine	0.0023821	0.145307	[12,13]	Top20

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