

Table S2_QikProp ADMET of CP compounds

molecule	#stars	#amine	#amidine	#acid	#amide	#rotor	#rtvFG	CNS	
Scopolin	0	0	0	0	0	0	8	2	-2
Convoline	0	1	0	0	0	0	5	2	1
Convolam	0	1	0	0	0	0	4	1	1
Convolvul	0	1	0	0	0	0	4	1	1
Scopoletin	0	0	0	0	0	0	2	1	0
Hydroxycit	0	0	0	1	0	0	4	1	-2
Kaempferol	0	0	0	0	0	0	4	0	-2
Quercetin	0	0	0	0	0	0	5	0	-2
Ayapanin	1	0	0	0	0	0	1	1	0
Delphinidin	2	0	0	0	0	0	6	4	-2
Taraxerol	5	0	0	0	0	0	1	0	1
β -sitosterol	6	0	0	0	0	0	7	0	0

a#Stars indicates the number of property or descriptor values that fall outside the 95% range

bRule of five indicates the number of violations of Lipinski's rule of five [3]. The rules are: mol_

cRule of three indicates the number of violations of Jorgensen's rule of three. The three rules a

mol_MW	dipole	SASA	FOSA	FISA	PISA	WPSA	volume	donorHB
354.313	4.086	545.048	155.331	237.821	151.896	0	992.725	4
307.346	2.562	569.028	387.354	85.951	95.722	0	992.119	1
305.373	1.731	620.439	488.003	36.735	95.701	0	1059.573	0
291.346	1.348	553.508	403.298	60.676	89.534	0	958.939	1
192.171	7.41	377.41	89.124	116.981	171.304	0	610.457	1
164.16	3.449	376.676	25.371	168.922	182.382	0	585.13	2
286.24	4.588	503.264	0	237.585	265.68	0	839.699	3
302.24	4.899	514.002	0	284.18	229.822	0	860.567	4
176.171	5.261	366.516	91.898	72.055	202.564	0	584.993	0
338.701	1.532	490.29	160.796	247.136	56.973	25.385	720.222	2
426.724	1.906	684.569	634.721	36.439	13.409	0	1383.356	1
414.713	1.903	744.406	666.128	48.445	29.832	0	1444.693	1

of similar values for known drugs (ranging from 0 ? 5). A large number of stars suggests that a
_MW < 500, QPlogPo/w < 5, donor HB ≤5, accptHB ≤10. Compounds that satisfy these rules a
are: QPlogS > -5.7, QP PCaco > 22 nm/s, # Primary Metabolites < 7. Compounds with fewer (a

accptHB	dip^2/V	ACxDN^5glob		QPpolrz	QPlogPC1	QPlogPocl	QPlogPw	QPlogPo/v
12.5	0.016816	0.045868	0.882978	29.889	11.215	22.842	20.088	-0.949
6.7	0.006615	0.011775	0.845423	31.254	8.922	14.822	9.285	1.762
5.5	0.002826	0	0.810127	34.596	8.946	13.518	6.648	2.604
5	0.001895	0.009033	0.849641	30.509	8.391	13.482	7.58	2.368
4	0.089948	0.010599	0.922124	18.628	6.346	10.591	7.552	0.891
2.75	0.020334	0.010325	0.898186	16.436	6.518	9.807	7.771	1.419
4.5	0.025069	0.015487	0.855299	27.42	10.171	16.513	12.297	1.036
5.25	0.027893	0.020428	0.851249	27.27	10.666	18.489	14.379	0.362
3.25	0.047309	0	0.922939	18.55	5.762	7.981	5.45	1.044
1.5	0.003258	0.004327	0.792544	19.361	7.13	9.893	6.06	1.309
1.7	0.002627	0.002483	0.877076	48.694	11.563	18.2	4.624	7.066
1.7	0.002508	0.002284	0.830244	47.453	12.344	17.484	3.638	7.393

a molecule is less drug-like than molecules with few stars. The following properties and descriptors are considered drug-like (maximum is 4) and preferably no) violations of these rules are more likely to be orally available (maximum is 3

QPlogS	CIQPlogS	QPlogHER	QPPCaco	QPlogBB	QPPMDCK	QPlogKp	IP(eV)	EA(eV)
-1.677	-2.342	-4.15	55.036	-1.952	21.535	-4.599	9.572	1.182
-2.234	-2.159	-5.216	378.204	-0.141	191.338	-4.349	9.835	0.517
-3.083	-2.344	-5.787	1107.751	0.348	611.317	-3.538	9.372	0.458
-2.709	-2.494	-5.118	656.771	0.161	347.437	-4.001	9.371	0.493
-1.627	-2.203	-3.609	770.14	-0.474	373.031	-2.88	9.343	0.965
-1.641	-1.812	-2.242	62.749	-1.074	31.561	-3.606	9.13	0.714
-3.09	-4.073	-5.14	55.32	-1.843	21.655	-4.578	9.124	0.643
-2.83	-4.043	-5.035	20	-2.352	7.21	-5.467	9.136	0.657
-1.38	-1.906	-3.745	2054.026	-0.061	1077.06	-2.038	9.264	0.869
-3.486	-4.774	-5.161	44.907	-2.359	23.808	-5.297	5.874	-0.889
-7.983	-7.261	-3.585	4470.446	0.187	2496.332	-2.048	9.48	-1.096
-8.121	-7.033	-4.421	3439.51	-0.327	1880.353	-1.635	9.521	-0.99

tors are included in the determination of #stars: MW, donorHB, accptHB, QPlogPw, QPlogPo/w

)

#metab	QPlogKhsa	HumanOr	PercentHu	SAfluorine	SAamideC	PSA	#NandO	RuleOfFive
5	-0.933	2	52.544	0	0	148.954	9	0
2	-0.18	3	83.398	0	0	76.197	6	0
3	0.053	3	96.685	0	0	52.78	5	0
2	0.102	3	91.236	0	0	62.507	5	0
2	-0.49	3	83.826	0	0	70.484	4	0
1	-0.672	3	67.426	0	0	74.003	3	0
4	-0.201	3	64.205	0	0	120.544	6	0
5	-0.354	2	52.348	0	0	141.943	7	0
1	-0.596	3	92.348	0	0	49.178	3	0
7	-0.129	2	51.222	0	0	100.299	7	1
2	2.06	1	100	0	0	19.72	1	1
3	1.974	1	100	0	0	22.243	1	1

/, QPlogS, QPlogKhsa, QPlogBB, #metabol.

#ringatom	#in34	#in56	#noncon	#nonHatrr	RuleOfThr	Jm
16	0	16	5	25	0	0.188
14	0	14	7	22	0	0.08
14	0	14	7	22	0	0.053
14	0	14	7	21	0	0.056
10	0	10	0	14	0	6.263
6	0	6	0	12	0	1.306
16	0	16	0	21	0	0.006
16	0	16	0	22	1	0.002
10	0	10	0	13	0	81.26
18	14	4	12	23	1	0.001
22	0	22	20	31	1	0
17	0	17	15	30	1	0