

Supplementary Table 1: Results of 36 compounds satisfying Lipinski rule and ADMET analysis

s.no	compound s/drugs	pubchem id	Molecular Weight	Log P	#Rotatable Bonds	#Acceptors	#Donors	Water solubility	Intestinal absorption (human)	hERG I inhibitor	hERG II inhibitor	Hepato toxicity	AMES toxicity
1	Castanospermine	54445	189.211	-2.4821	0	5	4	-1.696	52.418	No	No	No	No
2	Australine	442628	189.211	-2.4821	1	5	4	-1.72	52.388	No	No	No	No
3	Glycycomarin	5317756	368.385	4.0941	4	6	3	-3.609	85.365	No	No	No	No
4	Licochalcone A	5318998	338.403	4.4661	6	4	2	-4.528	91.243	No	No	No	No
5	Isolicoflavanol	5318585	354.358	3.7911	3	6	4	-3.046	76.365	No	No	No	No
6	Protolichesterinic acid	468953	324.461	4.8699	13	3	1	-3.927	95.589	No	No	No	No
7	Thiarubrine A	441551	228.341	3.3653	0	2	0	-5.199	97.053	No	No	No	No
8	Coriandrin	119586	230.219	2.8562	1	4	0	-3.019	97.144	No	No	No	No
9	Ellagic acid	5281855	302.194	1.3128	0	8	4	-3.181	86.684	No	No	No	No
10	1-deoxynojirimycin	29435	163.173	-2.9668	1	5	5	-0.747	42.869	No	No	No	No
11	1-deoxyrhamnnojirimycin	452001	163.173	-2.9668	1	5	5	-0.747	42.869	No	No	No	No
12	Berberine	12457	433.438	2.1009	2	7	1	-3.202	72.74	No	No	No	No
13	nateglinide	5311309	317.429	3.2609	6	2	2	-2.996	100	No	No	No	No
14	treprostinil	6918140	390.52	3.5832	10	4	3	-4.15	93.217	No	No	No	No
15	clemastine	5281069	459.97	4.8162	8	4	2	-2.891	91.193	No	No	No	No
16	misoprostol	5282381	382.541	3.9536	13	5	2	-4.544	92.248	No	No	No	No
17	Toxifolin	439533	304.254	1.1863	1	7	5	-3.042	64.709	No	No	No	No
18	andrographolide	5318517	350.455	1.9626	3	5	3	-3.494	95.357	No	No	No	No
19	Flutimide	6443207	238.287	1.7714	3	4	1	-2.739	93.088	No	No	No	No
20	Trenbolone acetate	66359	312.409	3.9001	1	3	0	-4.414	98.605	No	No	No	No
21	NAPROXEN	156391	230.263	3.0365	3	2	1	-3.144	97.941	No	No	No	No
22	Kaempferol	5280	286.	2.2	1	6	4	-3.04	74.29	No	No	No	No

23	Quercetin	863 5280 343	239 302. 238	824 1.9 88	1	7	5	-2.925	77.20 7	No	No	No	No
24	Baicalein	5281 605	270. 24	2.5 768	1	5	3	-3.375	94.16 4	No	No	No	No
25	6-Hydroxylut eolin	5281 642	302. 238	1.9 88	1	7	5	-2.941	71.60 2	No	No	No	No
26	Pedalitin	3116 1	316. 265	2.2 91	2	7	4	-3.168	79.87 7	No	No	No	No
27	Scutellarein	5281 697	286. 239	2.2 824	1	6	4	-3.081	71.65 6	No	No	No	No
28	6-Hydroxyka empferol	5281 638	302. 238	1.9 88	1	7	5	-2.922	67.73 3	No	No	No	No
29	(-)- Arctigenin	6498 1	372. 417	2.9 924	7	6	1	-4.261	94.41 6	No	No	No	No
30	Tracheloge nin	4528 55	388. 416	2.1 073	7	7	2	-3.689	74.31 3	No	No	No	No
31	Ribavirin	3754 2	244. 207	- 3.0 115	3	8	4	-1.712	54.98 8	No	No	No	No
32	Npc A	1080 99	279. 273	1.1 626	6	3	4	-2.89	39.50 3	No	No	No	No
33	favipiravir	4924 05	157. 104	- 0.9 921	1	3	2	-2.121	91.69	No	No	No	No
34	Leupeptin	7242 9	426. 562	- 0.1 946	14	5	5	-2.869	40.31 2	No	No	No	No
35	Genistein	5280 961	270. 24	2.5 768	1	5	3	-3.595	93.38 7	No	No	No	No
36	Colchicine	6167 443	399. 716	2.8 716	5	6	1	-3.929	97.24 5	No	No	No	No
