

Table S1. Screened ADMET properties for 49 *Piper betle* compounds

Molecule	Stars	mol_MW	donor HB	accpt HB	QPlog Po/w	QPlogS	QPP Caco	QPlogBB	QPP MDCK	Human Oral Absorption	QPlog Khsa	#metab	QPlog HERG	Rule Of Five	Rule Of Three
IMPHY001368	0	344.407	1	5.95	3.438	-4.196	2284.676	-0.549	1557.521	100	1.035	5	-4.797	1	1
IMPHY002191	0	358.433	1	5.95	3.745	-4.43	2858.892	-0.413	1208.361	100	0.228	7	-4.481	0	1
IMPHY005374	0	234.251	0	5	1.972	-2.576	1565.198	-0.318	1539.734	100	0.33	7	-4.454	0	1
IMPHY006709	0	206.241	0	3.25	2.67	-2.956	3873.461	-0.384	746.792	93.286	-0.389	3	-3.845	0	0
IMPHY007615	0	234.251	0	5	1.894	-2.164	1755.31	0.89	5899.293	100	0.879	3	-3.965	1	1
IMPHY008892	0	400.471	0	6.25	4.098	-4.803	1961.3	0.868	5899.293	100	0.4	4	-3.859	0	0
IMPHY017327	0	172.267	2	2.45	1.747	-2.172	1694.628	-0.129	1647.426	100	-0.108	3	-3.954	0	0
IMPHY001073	0	386.444	1	6.25	3.347	-4.471	509.281	1.076	5899.293	100	0.973	6	-2.896	1	1
IMPHY001240	0	141.169	1	4	-1.495	-0.77	54.287	0.036	1844.599	100	1.65	3	-4.292	1	1
IMPHY003129	1	150.177	2	1.5	1.654	-1.336	1463.748	1.113	5899.293	100	0.997	7	-3.032	1	2
IMPHY005639	1	155.196	0	4	0.442	-0.174	605.79	1.059	5899.293	100	0.938	2	-3.21	1	1
IMPHY006362	1	176.126	4	7.9	-1.851	-0.64	36.244	0.849	5899.293	100	0.402	4	-3.407	0	0
IMPHY006593	1	150.177	2	1.5	1.593	-1.376	1069.106	1.086	5899.293	100	0.949	4	-3.445	1	1
IMPHY009708	1	176.215	0	2.5	2.281	-2.526	3609.328	-0.127	5899.293	100	-0.194	1	-3.269	0	0
IMPHY011519	1	196.2	0	2	3.206	-3.77	4011.929	-1.641	134.684	91.918	0.788	1	-3.61	1	1

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IMPHY000846	1	376.3 68	5	12.3	-0.982	-2.718	10.817	-0.451	802.891	95.668	-0.425	1	-4.547	0	0
IMPHY001308	2	286.4 56	1	1.7	5.424	-6.073	2889.433	1.029	5899.293	100	0.998	5	-2.929	1	1
IMPHY003536	2	164.2 04	1	1.5	2.661	-2.387	3043.414	0.365	318.38	79.332	-0.7	3	-4.107	0	0
IMPHY003681	2	414.6 27	1	3.2	6.136	-7.338	3378.96	0.702	5899.293	100	0.343	2	-3.714	0	0
IMPHY004631	2	284.4 81	1	2	6.033	-6.388	240.229	-0.13	1648.664	100	-0.106	3	-3.982	0	0
IMPHY006297	2	164.2 04	1	1.5	2.667	-2.405	3045.528	-0.049	1088.858	96.881	-0.203	2	-2.795	0	0
IMPHY006325	2	150.2 2	0	2	1.805	-2.057	2074.833	-1.809	13.711	44.013	-0.947	5	-2.827	0	0
IMPHY006946	2	222.3 7	1	0.75	3.929	-4.135	5517.682	0.922	5899.293	100	0.427	4	-3.807	0	0
IMPHY006970	2	156.2 67	0	2	2.749	-2.712	2164.94	-1.933	1785.814	100	2.535	1	-6.85	1	1
IMPHY007840	2	220.3 54	1	0.75	3.932	-4.228	4917.97	-0.512	531.763	90.488	-0.377	3	-3.881	0	0
IMPHY011521	2	170.2 94	0	2	3.298	-3.334	3953.378	0.102	5899.293	100	0.069	3	-3.928	0	0
IMPHY011542	2	222.3 7	1	0.75	4.012	-4.191	5034.539	-0.069	2138.039	100	-0.151	2	-4.496	0	0
IMPHY011640	2	164.2 04	1	1.5	2.818	-2.501	3043.83	0.258	5899.293	100	0.081	2	-4.018	0	0
IMPHY014847	2	196.2 89	0	2	2.898	-3.308	3748.856	0.296	3134.016	100	0.669	1	-2.686	0	0
IMPHY014857	2	222.3 7	1	0.75	3.738	-3.823	5372.81	-0.56	1140.059	100	-0.077	1	-3.94	0	0
IMPHY014986	2	222.3 7	1	0.75	3.964	-4.15	6008.905	-0.059	1625.784	100	-0.17	2	-3.965	0	0
IMPHY015022	2	222.3 7	1	0.75	4.94	-5.161	5461.821	-0.505	72.584	69.038	-0.903	2	-1.496	0	0

IMPHY015042	2	152.2 36	0	2	2.174	-2.133	4055.026	1.082	5899.293	100	1.005	2	-3.337	1	1
IMPHY015128	2	222.3 7	1	0.75	4.091	-4.493	4939.358	-1.128	2.271	34.379	-1.22	0	1.514	0	1
IMPHY007317	3	134.1 77	1	0.75	2.207	-1.365	3006.405	1.115	5899.293	100	0.987	4	-3.078	1	1
IMPHY007357	3	123.1 11	1	3.5	0.671	-0.714	135.594	1.142	5899.293	100	1.011	0	-3.04	1	1
IMPHY011396	3	154.2 52	1	0.75	2.978	-2.625	5690.09	-0.364	908.799	96.106	-0.485	1	-4.25	0	0
IMPHY011558	3	222.2 4	0	3	2.538	-3.033	9906.038	0.25	2767.507	100	0.67	3	-2.99	0	0
IMPHY012036	3	152.2 36	0	2	1.945	-1.99	3964.568	-0.508	1024.603	100	0.358	6	-4.699	0	0
IMPHY012058	3	154.2 52	1	0.75	3.14	-2.959	5247.419	2.502	5899.293	100	3.263	0	-6.91	1	1
IMPHY012104	3	156.2 67	1	1.7	2.714	-2.603	3373.526	1.102	5899.293	100	1.021	6	-3.476	1	1
IMPHY012160	3	154.2 52	1	0.75	2.962	-2.67	4922.657	-0.641	2571.893	100	2.375	5	-5.755	1	1
IMPHY012265	3	152.2 36	1	1.7	2.14	-2.266	4048.342	2.761	5899.293	100	3.789	0	-7.242	1	1
IMPHY012712	3	296.5 35	1	1.7	6.366	-7.075	2842.463	-0.026	1980.897	100	-0.145	1	-4.526	0	0
IMPHY013133	3	154.2 52	1	0.75	2.958	-2.709	4250.74	0.875	5899.293	100	0.401	1	-3.436	0	0
IMPHY013835	3	152.2 36	0	2	2.07	-2.035	4878.541	0.605	5899.293	100	0.224	1	-2.597	0	0
IMPHY000099	3	152.2 36	1	1.7	2.11	-2.178	3780.468	0.995	5899.293	100	0.948	4	-3.725	1	1
IMPHY001144	3	222.2 4	0	3	2.216	-2.751	9906.038	1.014	5899.293	100	0.979	6	-3.616	1	