

**Supplemental Table-2. Full ADME properties in silico of 121 candidate compounds via admetSAR Prediction**

Compounds	Absorption		Metabolism (CYP450 isoforms Inhibitor)						Herbs
	HIA	Caco-2	1A2	2C9	2D6	2C19	3A4	score	
Majudin	0.9933	0.6835	0.9774	0.8257	0.8931	0.9296	0.7959	3.48407919	Notopterygium
									incisum
									K.C.Ting ex
									H.T.Chang
Bergaptin	0.9964	0.5379	0.9107	0.8949	0.8931	0.8994	0.8123	3.47147818	Notopterygium
									incisum
									K.C.Ting ex
									H.T.Chang
sesamin	1	0.5774	0.9106	0.8949	0.8932	0.8994	0.796	3.46096872	Stemona
									sessilifolia
									(Miq.) Miq.
									Stemona
suchilactone	0.9884	0.7833	0.6598	0.9399	0.8096	0.9801	0.9591	3.39143188	sessilifolia
									(Miq.) Miq.
isorhamnetin	0.9783	0.8866	0.9218	0.756	0.6993	0.8648	0.7348	3.12557861	Ginkgobiloba.
									Notopterygium
Ammidin	0.9962	0.5187	0.8503	0.7199	0.7115	0.8977	0.7497	3.08492296	incisum
									K.C.Ting ex
									H.T.Chang
									Notopterygium
8-geranoxo-5-methoxypsoralen	0.9924	0.5556	0.8058	0.7084	0.788	0.8398	0.7848	3.0808701	incisum
									K.C.Ting ex
									H.T.Chang
									Notopterygium
Cnidilin	0.9925	0.5243	0.8169	0.5477	0.641	0.8984	0.6951	2.82470425	incisum
									K.C.Ting ex
									H.T.Chang
naringenin	0.967	0.7533	0.9106	0.8949	-0.7463	0.8994	0.8988	2.12533827	Smilax glabra Roxb.
Genkwanin	0.9921	0.929	0.9378	0.9385	-0.8253	0.9012	0.7232	2.00309141	Ginkgobiloba.
Diosmetin	0.9783	0.8866	0.9218	0.756	-0.6993	0.8648	0.7348	1.92963575	Ginkgobiloba.
Chryseriol	0.9783	0.8866	0.9218	0.756	-0.6993	0.8648	0.7348	1.92963575	Ginkgobiloba.
Kaempferid	0.9783	0.8866	0.9218	0.756	-0.6993	0.8648	0.7348	1.92963575	Smilax china L.
Syringetin	0.9719	0.8896	0.8668	0.6258	-0.6249	0.8187	0.7817	1.83717389	Ginkgobiloba.
4'-methylpinosylvins	0.9968	0.9191	0.9614	0.903	-0.8899	0.886	0.5	1.78240889	Stemona
									sessilifolia
									(Miq.) Miq.
Dehydrodieug	0.9721	0.8004	0.744	0.797	-0.7521	0.9261	0.6365	1.75847413	Eucommia

enol									ulmoides Oliv.
Moracin M	0.9964	0.6043	0.9061	0.7842	-0.8215	0.7031	0.804	1.74936332	Smilax china L. Eucommia ulmoides Oliv.; Moutan officinalis (L.)
kaempferol	0.9855	0.7447	0.9108	0.8948	-0.9083	0.6434	0.7241	1.66803093	Lindl. & Paxton, cortex; Morus alba L., twig, dry; Ginkgobiloba.
morin	0.9855	0.7447	0.9108	0.8948	-0.9083	0.6434	0.7241	1.66803093	Morus alba L., twig, dry Notopterygium
notoptol	0.9762	0.5537	0.7233	0.7758	-0.6654	0.7588	0.6368	1.66419893	incisum K.C.Ting ex H.T.Chang
Dihydroresveratrol	0.9503	0.8604	0.7749	0.742	-0.8326	0.8434	0.7201	1.65802923	Smilax glabra Roxb. Smilax china L.;
cis-resveratrol	0.9952	0.8915	0.9106	0.7068	-0.9226	0.8052	0.7539	1.65443638	Reynoutria japonica Houtt.
cis-pinosylvin	0.9948	0.9014	0.9177	0.6648	-0.9171	0.8322	0.6678	1.5974595	Eucommia ulmoides Oliv.
Oxysanguinarine	0.9841	0.7216	0.8373	-0.8557	0.5126	0.7982	0.669	1.50874759	Morus alba L., twig, dry Paeonia anomala L.; Moutan officinalis (L.)
$\alpha$ -Viniferin	1	0.6216	0.9277	0.9497	-0.7239	0.8042	-0.6358	1.13587144	Lindl. & Paxton, cortex; Reynoutria japonica Houtt.; Ginkgobiloba.
AIDS214634	0.5176	0.6408	0.6819	0.5427	-0.8266	0.5876	0.542	1.10669817	Eucommia ulmoides Oliv.
Isoflavon	1	0.8727	0.9662	0.7441	-0.9436	0.9213	-0.6675	0.88838768	Ginkgobiloba.
4,7-Dihydroxy-5-methoxyl-6-methyl-8-formyl-flavan	0.9889	0.9077	0.7694	0.565	-0.6802	0.7659	-0.6223	0.71368052	Smilax glabra Roxb.
6,8-Dihydroxy-7-methoxyxanthone	0.9306	0.9044	0.9724	-0.6549	-0.6476	0.6923	0.6321	0.67863562	Reynoutria japonica Houtt.

40957-99-1	0.9944	0.763	-0.538 1	0.6912	-0.8313	0.7443	0.5296	0.34602068	Eucommia ulmoides Oliv.
(+)-medioresinol	0.9944	0.763	-0.538 1	0.6912	-0.8313	0.7443	0.5296	0.34602068	Eucommia ulmoides Oliv.
Torachrysone	0.9803	0.92	0.9469	-0.7326	-0.8119	0.5056	0.5459	0.2491008	Reynoutria japonica Houtt.
palmidin A	0.9932	0.6209	0.7561	0.7273	-0.7856	-0.5209	-0.5122	-0.22252461	Rheum palmatum L.
aloe-emodin	0.9815	0.5847	0.7957	0.6696	-0.766	-0.5	-0.7395	-0.34954203	Rheum palmatum L.
Morkit	1	0.8682	0.9357	0.5919	-0.6483	-0.6245	-0.9241	-0.41647792	Reynoutria japonica Houtt.
EUPATIN	0.9854	0.8992	0.8642	-0.6863	-0.8329	0.6566	-0.7237	-0.49638525	Rheum palmatum L.
Xanthotoxol	0.9811	0.6754	0.8392	-0.7372	-0.5847	-0.6555	0.627	-0.53089239	Notopterygium incisum K.C.Ting ex H.T.Chang
Pterostilbene	0.9974	0.8911	0.8736	-0.9304	-0.9249	0.7583	-0.5979	-0.60006547	Notopterygium incisum K.C.Ting ex H.T.Chang
Toralactone	0.808	0.9237	0.7076	-0.6892	-0.7022	-0.7325	0.6957	-0.71779906	Rheum palmatum L.
Laricitrin	0.9482	0.6824	0.9091	-0.7982	-0.8687	-0.6361	0.633	-0.7462083	Ginkgobiloba.
didehydrotuberostemonine	1	0.6682	0.7281	-0.5909	-0.8438	-0.6156	0.5101	-0.76892367	Stemona sessilifolia (Miq.) Miq.
luteolin	0.965	0.8957	0.9106	-0.5823	-0.9287	-0.9025	0.6951	-0.79768769	Reynoutria japonica Houtt.; Ginkgobiloba.
quercetin	0.965	0.8957	0.9106	-0.5823	-0.9287	-0.9025	0.6951	-0.79768769	Eucommia ulmoides Oliv.; Reynoutria japonica Houtt.; Moutan officinalis (L.) Lindl. & Paxton, cortex; Smilax glabra Roxb.; Ginkgobiloba
(-)-taxifolin	0.965	0.8957	0.9106	-0.5823	-0.9287	-0.9025	0.6951	-0.79768769	Smilax glabra Roxb.
taxifolin	0.965	0.8957	0.9106	-0.5823	-0.9287	-0.9025	0.6951	-0.79768769	Smilax china L.

									Smilax glabra Roxb. Smilax china L.;
cis-Dihydroquercetin	0.965	0.8957	0.9106	-0.5823	-0.9287	-0.9025	0.6951	-0.79768769	Smilax glabra Roxb.
2-(4-hydroxyphenyl)ethyl 4-methoxybenzoate	0.913	0.8278	0.6793	-0.647	-0.9494	0.6062	-0.8666	-0.84789435	Notopterygium incisum K.C.Ting ex H.T.Chang
Procyanidin B-5,3'-O-gallate	0.6772	0.8786	-0.9306	-0.6236	-0.9414	0.5937	0.8413	-1.04234896	Rheum palmatum L.
Erythraline	0.9903	0.7737	-0.6103	-0.9082	0.6973	-0.7351	-0.6481	-1.63921898	Eucommia ulmoides Oliv.
bisdehydroneotuberostemonine	1	0.7947	0.8351	-0.7972	-0.8819	-0.7283	-0.5961	-1.684009	Stemona sessilifolia (Miq.) Miq. Notopterygium
Demethylfuropinnarin	0.986	0.5274	-0.757	-0.5341	-0.7866	-0.6967	0.8551	-1.72717362	incisum K.C.Ting ex H.T.Chang
(2R,8aS)-2,5,5,8a-tetramethyl-3,6-dihydro-2H-chromene	1	0.7072	-0.6951	-0.541	-0.896	0.6473	-0.782	-1.74929595	Ginkgobiloba.
bisdehydrostemoninine A	1	0.6195	0.5846	-0.6855	-0.8956	-0.6526	-0.693	-1.81177688	Stemona sessilifolia (Miq.) Miq.
bisdehydrostemoninine B	1	0.6195	0.5846	-0.6855	-0.8956	-0.6526	-0.693	-1.81177688	Stemona sessilifolia (Miq.) Miq.
Dipropylphthalate	0.976	0.7171	0.6006	-0.6511	-0.8898	-0.5322	-0.9319	-1.82332052	Paeonia anomala L.
Picralinal	0.9523	0.5762	-0.6662	0.5	-0.8749	-0.5633	-0.7786	-1.84585895	Reynoutria japonica Houtt. Notopterygium
Guaiol	0.9971	0.6777	-0.6113	0.5515	-0.9198	-0.5347	-0.9156	-1.86356377	incisum K.C.Ting ex H.T.Chang
(Z)-1,3-di(phenyl)prop-2-en-1-one	0.9868	0.7267	-0.6793	0.7477	-0.9424	-0.6922	-0.8629	-1.87383447	Ginkgobiloba.
Mutatochrome	1	0.6964	-0.5529	-0.7813	-0.9208	0.5353	-0.8346	-1.97145643	Rheum palmatum L.

Moutan officinalis (L.) Lindl. & Paxton, cortexoside-h _qt 2	1	0.8465	0.7765	-0.9292	-0.9619	-0.5912	-0.9796	-2.04293318	Moutan officinalis (L.) Lindl. & Paxton, cortex
cis-Verbenyl acetate	1	0.7257	-0.819 8	-0.8266	-0.8985	0.624	-0.8518	-2.14580769	Notopterygium incisum K.C.Ting ex H.T.Chang
rhein	0.9689	0.6092	-0.649 7	0.5	-0.868	-0.9233	-0.9258	-2.21140421	Rheum palmatum L.; Reynoutria japonica Houtt.
stemonine	0.9969	0.6647	0.561	-0.8532	-0.9112	-0.8372	-0.832	-2.21713706	Stemona sessilifolia (Miq.) Miq.
stemoninine B	0.9969	0.6647	0.561	-0.8532	-0.9112	-0.8372	-0.832	-2.21713706	Stemona sessilifolia (Miq.) Miq.
Enhydrin	0.9483	0.5168	-0.532 8	-0.8902	-0.9273	-0.8657	0.6247	-2.23507203	Smilax glabra Roxb.
dihydrostemo ninine	0.7795	0.7545	0.7434	-0.9321	-0.9603	-0.8954	-0.9422	-2.29173649	Stemona sessilifolia (Miq.) Miq.
Physovenine	0.9963	0.5936	-0.607 2	-0.7115	-0.7206	-0.6225	-0.61	-2.5761631	Reynoutria japonica Houtt.
Isogoycycrol	0.9421	0.5174	-0.636 2	-0.6707	-0.7755	-0.7514	-0.7693	-2.82058551	Ginkgobiloba.
2H-3,9a-Meth ano-1-benzox epin-9-methan ol, octahydro-2,2, 5a-trimethyl-, (3R-(3alpha,5 aalpha,9alpha, 9aalpha)) bis[(2S)-2-eth ylhexyl] benzene-1,2-d icarboxylate (1R,2R)-1,2-D iphenylethyle	1	0.596	-0.773 6	-0.5085	-0.9158	-0.5554	-0.9291	-2.86765646	Smilax glabra Roxb.
	0.9797	0.7003	-0.653 9	-0.7448	-0.8432	-0.631	-0.8309	-2.89507119	Ginkgobiloba.
	0.935	0.6935	-0.723 3	-0.5862	-0.9209	-0.6888	-0.7833	-2.90673728	Ginkgobiloba.

nediamine									
olivil	0.9607	0.5748	-0.746	-0.7071	-0.9041	-0.6443	-0.7101	-2.92474861	Eucommia ulmoides Oliv.
6'-Feruloylnod akenin	0.593	0.8264	-0.735 6	-0.6762	-0.8667	-0.5911	-0.9088	-2.94483359	Notopterygium incisum K.C.Ting ex H.T.Chang
DBP	0.9941	0.6564	-0.592	-0.897	-0.5245	-0.9265	-0.8539	-2.94698555	Ginkgobiloba.
PIT	0.7874	0.5717	-0.641 6	-0.7426	-0.8602	-0.7117	-0.8345	-2.9651409	Rheum palmatum L.
Marmesin	0.9881	0.7636	-0.671 7	-0.7486	-0.827	-0.7313	-0.8285	-2.97800069	Notopterygium incisum K.C.Ting ex H.T.Chang
(8S)-8-(2-hydr oxypropan-2- yl)-8,9-dihydr ofuro[2,3-h]ch romen-2-one	0.9881	0.7636	-0.671 7	-0.7486	-0.827	-0.7313	-0.8285	-2.97800069	Notopterygium incisum K.C.Ting ex H.T.Chang
nodakenetin	0.9881	0.7636	-0.671 7	-0.7486	-0.827	-0.7313	-0.8285	-2.97800069	Notopterygium incisum K.C.Ting ex H.T.Chang
copaene	1	0.6705	-0.824 4	-0.6794	-0.9197	-0.5547	-0.8317	-2.98601895	Notopterygium incisum K.C.Ting ex H.T.Chang
DIBP	0.9745	0.7151	-0.566 6	-0.6604	-0.9218	-0.7906	-0.8983	-2.99550166	Ginkgobiloba.
isoengelitin	0.9051	0.7493	-0.530 6	-0.8538	-0.9547	-0.8339	-0.7109	-3.06337419	Smilax china L.;
Engelitin	0.9051	0.7493	-0.530 6	-0.8538	-0.9547	-0.8339	-0.7109	-3.06337419	Smilax glabra Roxb.
astilbin	0.9051	0.7493	-0.530 6	-0.8538	-0.9547	-0.8339	-0.7109	-3.06337419	Smilax china L.
Neoastilbin	0.9051	0.7493	-0.530 6	-0.8538	-0.9547	-0.8339	-0.7109	-3.06337419	Smilax china L.;
β-cedrene	0.9954	0.6484	-0.761 3	-0.7311	-0.9271	-0.7087	-0.8805	-3.13789978	Smilax glabra Roxb.
diversoside_qt	0.6685	0.8787	-0.687	-0.7973	-0.9165	-0.7401	-0.918	-3.17110414	Smilax glabra Roxb. Notopterygium incisum K.C.Ting ex H.T.Chang

			3						incisum K.C.Ting ex H.T.Chang
hirsutin_qt	0.8588	0.5	-0.694 8	-0.8465	-0.8465	-0.7712	-0.964	-3.21152389	Eucommia ulmoides Oliv.
Daucosterol_q t	0.8788	0.8336	-0.805 2	-0.7682	-0.9187	-0.8388	-0.7938	-3.24509009	Rheum palmatum L.
(-)-alpha-cedr ene	1	0.6555	-0.797 6	-0.7774	-0.929	-0.7584	-0.8897	-3.2521838	Paeonia anomala L.
nodakenin	0.7967	0.8705	-0.693 2	-0.868	-0.9033	-0.8343	-0.8892	-3.27860349	Notopterygium incisum K.C.Ting ex H.T.Chang
benzoylpaeoni florin	0.6197	0.8556	-0.873 2	-0.8869	-0.9338	-0.7759	-0.8118	-3.3695257	Paeonia anomala L.
Torachrysone- 8-O-beta-D-(6 '-oxayl)-gluco side	0.7886	0.7989	-0.688 2	-0.8912	-0.917	-0.9199	-0.908	-3.38591486	Rheum palmatum L.; Reynoutria japonica Houtt.
albiflorin_qt	0.7098	0.8668	-0.892 7	-0.8984	-0.9399	-0.8197	-0.8046	-3.43048168	Paeonia anomala L.
paeoniflorin	0.8238	0.8487	-0.883 4	-0.9006	-0.9314	-0.7995	-0.8545	-3.433317	Paeonia anomala L.
paeoniflorin_q t	0.8238	0.8487	-0.883 4	-0.9006	-0.9314	-0.7995	-0.8545	-3.433317	Paeonia anomala L.; Moutan officinalis (L.) Lindl. & Paxton, cortex Moutan
4-O-methylpa eoniflorin_qt	0.6133	0.8067	-0.881 6	-0.8915	-0.9323	-0.8	-0.8696	-3.43546595	officinalis (L.) Lindl. & Paxton, cortex
(3S,5R,8R,9R, 10S,14S)-3,17 -dihydroxy-4, 4,8,10,14-pent amethyl-2,3,5, 6,7,9-hexahyd ro-1H-cyclope nta[a]phenant hrene-15,16-di one	0.997	0.6592	-0.882 5	-0.8505	-0.9601	-0.8399	-0.8531	-3.44859012	Paeonia anomala L.
paeonidanin_q t	0.6484	0.8203	-0.894 5	-0.88	-0.9411	-0.8085	-0.868	-3.45009366	Moutan officinalis (L.)

									Lindl. & Paxton, cortex
paeoniflorgen one	0.9811	0.6976	-0.887 2	-0.8919	-0.9494	-0.8415	-0.8208	-3.4569193	Paeonia anomala L.
diosgenin	0.9961	0.5872	-0.863 8	-0.8878	-0.9107	-0.9127	-0.8309	-3.46533455	Smilax china L.; Smilax glabra Roxb.
Lactiflorin	0.5395	0.8577	-0.899 7	-0.8963	-0.9457	-0.7886	-0.9046	-3.47891244	Paeonia anomala L.
L-Bornyl acetate	0.9969	0.7743	-0.931 7	-0.9218	-0.9606	-0.7031	-0.9384	-3.49110903	Notopterygium incisum K.C.Ting ex H.T.Chang; Smilax glabra Roxb.
gallic acid-3-O-(6'- O-galloyl)-glu coside	0.8558	0.898	-0.931 5	-0.7955	-0.9425	-0.9121	-0.8723	-3.49989554	Rheum palmatum L.
(-)-Tabernemo ntanine	1	0.5706	-0.904 5	-0.907	-0.9231	-0.9025	-0.8309	-3.51627556	Eucommia ulmoides Oliv.
ent-Epicatechi n	0.9654	0.8956	-0.904 6	-0.9071	-0.9231	-0.9041	-0.8309	-3.51772585	Eucommia ulmoides Oliv.
(-)-catechin	0.9654	0.8956	-0.904 6	-0.9071	-0.9231	-0.9041	-0.8309	-3.51772585	Rheum palmatum L.; Ginkgobiloba Paeonia anomala L.; Moutan officinalis (L.)
(+)-catechin	0.9654	0.8956	-0.904 6	-0.9071	-0.9231	-0.9041	-0.8309	-3.51772585	Lindl. & Paxton, cortex; Reynoutria japonica Houtt.; Ginkgobiloba. Smilax china L.; Paeonia anomala L.; Rheum
beta-sitosterol	1	0.7953	-0.929 1	-0.9125	-0.9346	-0.9025	-0.8309	-3.55056073	palmatum L.; Reynoutria japonica Houtt.; Smilax glabra Roxb.
sitosterol	1	0.7953	-0.929 1	-0.9125	-0.9346	-0.9025	-0.8309	-3.55056073	Smilax china L.; Paeonia anomala



									L.; Moutan officinalis (L.) Lindl. & Paxton, cortex; Notopterygium incisum K.C.Ting ex H.T.Chang; Smilax glabra Roxb. Smilax glabra Roxb.;
Stigmasterol	1	0.7953	-0.929 1	-0.9125	-0.9346	-0.9025	-0.8309	-3.55056073	Ginkgobiloba. Paeonia anomala L.; Moutan officinalis (L.) Lindl. & Paxton, cortex Smilax china L.; Paeonia anomala L.; Moutan officinalis (L.) Lindl. & Paxton, cortex
Mairin	0.9952	0.8835	-0.916 7	-0.9071	-0.9554	-0.9025	-0.8309	-3.55391481	Smilax china L.; Paeonia anomala L.; Moutan officinalis (L.) Lindl. & Paxton, cortex
oleanolic acid	1	0.8353	-0.916 9	-0.9071	-0.9485	-0.9025	-0.8695	-3.57307456	Smilax china L.
pseudoprotodi oscin_qt	0.6254	0.8883	-0.884 8	-0.9118	-0.936	-0.9113	-0.946	-3.59643242	Smilax china L.
methylprotodi oscin_qt	0.5247	0.8488	-0.892 1	-0.9148	-0.9364	-0.8976	-0.9573	-3.60138169	Rheum palmatum L. Rheum palmatum L.; Reynoutria japonica Houtt.
1-O-Galloyl-g lycerol	0.7501	0.8336	-0.764 2	-0.973	-0.9622	-0.9726	-0.9526	-3.6232814	Ginkgobiloba. Smilax china L.;
Physciondiglu coside	0.7916	0.8674	-0.916 7	-0.9167	-0.9519	-0.9109	-0.9311	-3.6300136	Morus alba L., twig, dry Rheum palmatum L.
Luteolin-4'-gl ucoside	0.7855	0.9398	-0.908 4	-0.9296	-0.9513	-0.9289	-0.9193	-3.63996795	Rheum palmatum L.
Cudranin	0.7855	0.9398	-0.908 4	-0.9296	-0.9513	-0.9289	-0.9193	-3.63996795	Rheum palmatum L.
Sennoside E_qt	0.5493	0.9338	-0.932	-0.9171	-0.9596	-0.9032	-0.9365	-3.64666492	Rheum palmatum L.
Sennoside D_qt	0.5493	0.9338	-0.932	-0.9171	-0.9596	-0.9032	-0.9365	-3.64666492	Ginkgobiloba.
6-Hydroxykyn	0.9193	0.6778	-0.897	-0.9167	-0.9492	-0.9641	-0.9666	-3.67756296	

