Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supplementary Information

Table S1 The ingredients in Kushen and their molecule formulas.

Compound Name	Molecule formula
Formononetin	$C_{16}H_{12}O_4$
2' -methoxykurarinone	$C_{27}H_{32}O_6$
2-n-tricosyl-5,7-dihydroxy-6,8-dimethyl chromone	$C_{34}H_{56}O_4$
2-n-pentacosyl-5,7-dihydroxy-6,8-dimethyl chromone	$C_{36}H_{60}O_4$
2-n-hencosyl-5,7-dihydroxy-6,8-dimethylchromone	$C_{32}H_{52}O_4$
2-n-nonadecyl-5,7-dihydroxy-6,8-dimethyl chromone	$C_{30}H_{48}O_4$
2-n-heptadecyl-5,7-dihydroxy-6,8-dimethyl chromone	$C_{28}H_{44}O_4$
2-n-tridecyl-5,7-dihydroxy-6,8-dimethyl chromone	$C_{24}H_{36}O_4$
2-n-pentadecyl-5,7-dihydroxy-6,8-dimethyl chromone	$C_{26}H_{40}O_4$
Maackiain	$C_{16}H_{12}O_5$
6,8-di(3,3-dimethylally)genistein	$C_{23}H_{24}O_4$
Kushequinone A	$C_{17}H_{22}O_4$
13,14-dehydrosophoridine	$C_{15}H_{22}N_2O$
Sophocarpine	$C_{15}H_{22}N_2O$
9α-hydroxysophoramine	$C_{15}H_{20}N_2O_2$
Matrine	$C_{15}H_{24}N_2O$
Sophoranol	$C_{15}H_{24}N_2O_2$
Isosophocarpine	$C_{15}H_{22}N_2O$
Sophoridine	$C_{15}H_{24}N_2O$
Lehmannine	$C_{15}H_{22}N_2O$
Isoxanthohumol	$C_{21}H_{22}O_5$
Kuraridin	$C_{26}H_{30}O_6$
Δ7-dehydrosophoramine	$C_{15}H_{18}N_2O$
Soyasaponin I	$C_{48}H_{78}O_{18}$
Mamanine	$C_{15}H_{22}N_2O_2$
Lupanine	$C_{15}H_{24}N_2O$

Norkurarinol	$C_{25}H_{30}O_7$
Kuraranine	$C_{12}H_{18}N_2O_2$
Isokuraramine	$C_{12}H_{18}N_2O_2$
Sophoraflavanone G	$C_{25}H_{28}O_6$
7,11-dehydromatrine	$C_{15}H_{22}N_2O$
Sophoramine	$C_{15}H_{20}N_2O$
9α-hydroxymatrine	$C_{15}H_{24}N_2O_2$
5α,9α-dihydroxymatrine	$C_{15}H_{24}N_2O_3$
Norkurarinone	$C_{25}H_{28}O_6$
Biochanin A	$C_{16}H_{12}O_5$
Kuraridinol	$C_{26}H_{32}O_7$
N-allomatrine	$C_{15}H_{24}N_2O$
Anagyrine	$C_{15}H_{20}N_2O$
Trifolirhizin	$C_{22}H_{22}O_{10}$
Kurarinone	$C_{26}H_{30}O_6$
Vkushenol A	$C_{25}H_{28}O_5$
Kushenol B	$C_{30}H_{36}O_6$
Vkushenol C	$C_{25}H_{28}O_6$
Kushenol D	$C_{27}H_{32}O_6$
Kushenol E	$C_{25}H_{28}O_6$
Kushenol F	$C_{25}H_{28}O_6$
Kushenol G	$C_{25}H_{28}O_8$
Kushenol H	$C_{26}H_{32}O_8$
Vkushenol I	$C_{26}H_{28}O_7$
Kushenol J	$C_{27}H_{32}O_{14}$
Xanthohumol	$C_{21}H_{22}O_5$
Vkushenol L	$C_{25}H_{28}O_7$
Kushenol M	$C_{30}H_{36}O_7$
Kushenol N	$C_{26}H_{30}O_7$

Kushenol O	$C_{27}H_{30}O_{13}$
Sophoraflavoside I	$C_{59}H_{96}O_{27}$
Sophoraflavoside II	$C_{48}H_{76}O_{20}$
Sophoraflavoside Ⅲ	$C_{53}H_{84}O_{24}$
Sophoraflavoside Ⅳ	$C_{59}H_{94}O_{29}$
Kurarinol	$C_{26}H_{32}O_{7}$
Oxymatrine	$C_{15}H_{24}N_{2}O_{2}$
luteolin-7-O-glucoside	$C_{21}H_{20}O_{11}$
Cinaroside	$C_{21}H_{20}O_{11}$
Oxysophocarpine	$C_{15}H_{22}N2O_{2}$
Trifolirhizin-6"-O-malonate	$C_{25}H_{24}O1_{3}$
Sophoranol N-oxide	$C_{15}H_{24}N_{2}O_{3}$
N-oxysophocarpine	$C_{15}H_{22}N_{2}O_{2}$
8-prenylkaempferol	$C_{20}H_{18}O_{6}$
9α-hydroxysophocarpine	$C_{15}H_{22}N_{2}O_{2}$
9α-hydroxysophocarpine N-oxide	$C_{15}H_{22}N_{2}O_{3}$
Methylkushenol C	$C_{26}H_{28}O_{7}$
Kushenol K	$C_{26}H_{32}O_{8}$
Rhombifoline	$C_{15}H_{20}N_{2}O$
Isokurarinone	$C_{26}H_{30}O_{6}$
Baptifolin	$C_{15}H_{20}N_{2}O_{2}$
Isomatrine	$C_{15}H_{24}N_{2}O$
Isoanhydroicaritin	$C_{21}H_{22}O_{6}$

Table S2 The detecting parameters for ingredients towards PPARγ through SPR assay.

ID	Name	KD (μM)	Rmax	offset	Chi^2
C6	Matrine	15.34	4.913	-1.540	0.481
C28	Oxymatrine	27.24	17.71	-2.887	0.717
C29	Oxysophocarpine	80.90	25.83	-3.803	1.71
C2	Maackiain	3.094	12.06	-7.955	0.846
C25	Trifolirhizin	190.8	35.72	-0.4447	0.943
C1	Formononetin	181.8	45.62	1.480	0.0175
C22	Biochanin A	52.90	20.82	-4.199	1.09
C11	Isoxanthohumol	31.49	11.60	-2.687	2.37

Table S3 The detecting parameters for ingredients towards ER through SPR assay.

ID	Name	KD (μM)	Rmax	offset	Chi^2
C6	Matrine	10.28	25.40	-15.52	1.55
C28	Oxymatrine	44.93	5.929	-4.595	0.0216
C5	Sophocarpine	113.1	32.47	-5.776	0.826
C29	Oxysophocarpine	28.08	8.191	-1.598	0.598
C2	Maackiain	116.6	87.79	-1.614	0.782
C1	Formononetin	97.95	49.48	-5.138	0.296
C22	Biochanin A	61.36	54.48	-14.84	2.56

Table S4 The detecting parameters for ingredients towards CA2 through SPR assay.

ID	Name	KD (μM)	Rmax	offset	Chi^2
C6	Matrine	155.2	11.26	1.605	0.120
C5	Sophocarpine	93.87	19.37	-0.7353	15.4
C2	Maackiain	22.44	27.96	-3.936	1.97
C25	Trifolirhizin	164.2	53.11	-3.434	7.36
C1	Formononetin	85.84	30.23	-3.655	4.40
C22	Biochanin A	57.47	31.09	-8.904	0.743

Table S5 The detecting parameters for ingredients towards p53 through SPR assay.

ID	Name	KD (μM)	Rmax	offset	Chi^2
C5	Sophocarpine	1.007	34.09	-33.20	0.0885
C29	Oxysophocarpine	3.241	14.96	-12.27	0.157
C2	Maackiain	69.97	33.24	-4.772	2.20
C22	Biochanin A	30.38	52.88	-9.324	0.641
C11	Isoxanthohumol	8.517	59.67	-28.98	0.252

Table S6 The detecting parameters for ingredients towards MIF through SPR assay.

ID	Name	KD (μM)	Rmax	offset	Chi^2
C6	Matrine	67.29	7.114	-0.7330	0.313
C2	Maackiain	56.02	14.90	3.387	0.0833
C25	Trifolirhizin	84.88	32.62	-8.980	2.33
C1	Formononetin	2.069	44.78	-35.07	0.709
C22	Biochanin A	89.94	49.98	-6.461	2.66