

Table 2. The information of key ingredients

MOL ID	Name	Average Shortest Path Length	Between ness Centrali ty	Closeness Centrality	Deg ree
MOL00 0098	quercetin	1.979798	0.130149	0.505102	100
MOL00 0006	luteolin	2.410774	0.021713	0.414804	38
MOL00 0422	kaempferol	2.3367	0.030765	0.427954	37
MOL00 0358	beta-sitosterol	2.451178	0.014165	0.407967	24
MOL00 4328	naringenin	2.545455	0.011223	0.392857	22
MOL00 0392	formononetin	2.538721	0.003915	0.393899	19
MOL00 0497	licochalcone a	2.531987	0.00575	0.394947	19
MOL00 3896	7-Methoxy-2-methyl isoflavone	2.538721	0.003108	0.393899	19
MOL00 2565	Medicarpin	2.552189	0.004666	0.391821	18
MOL00 4978	2-[(3R)-8,8-dimethyl- 3,4-dihydro-2H- pyrano[6,5-f]chromen- 3-yl]-5- methoxyphenol	2.538721	0.002232	0.393899	18
MOL00	Vestitol	2.552189	0.002592	0.391821	17

0500					
MOL00	bicuculline	2.558923	0.007969	0.390789	17
0791					
MOL00	shinpterocarpin	2.552189	0.003206	0.391821	17
4891					
MOL00	1-	2.558923	0.001332	0.390789	16
4959	Methoxyphaseollidin				
MOL00	Licoagrocarpin	2.552189	0.001357	0.391821	16
5003					
MOL00	Stigmasterol	2.478114	0.013133	0.403533	15
0449					
MOL00	Fumarine	2.585859	0.002985	0.386719	15
0787					
MOL00	HMO	2.565657	0.00134	0.389764	15
4957					
MOL00	3'-Hydroxy-4'-O-	2.565657	0.001284	0.389764	15
4966	Methylglabridin				
MOL00	3'-Methoxyglabridin	2.565657	0.001221	0.389764	15
4974					
MOL00	Glypallichalcone	2.572391	0.001208	0.388743	14
4835					
MOL00	Glyasperins M	2.579125	0.001144	0.387728	14
5007					
MOL00	isorhamnetin	2.592593	7.30E-04	0.385714	13
0354					
MOL00	Glyasperin C	2.579125	5.99E-04	0.387728	13
4811					
MOL00	Glepidotin A	2.579125	7.62E-04	0.387728	13
4828					

MOL00 4833	Phaseolinisoflavan	2.572391	8.08E-04	0.388743	13
MOL00 4912	Glabrone	2.579125	5.53E-04	0.387728	13
MOL00 4991	7-Acetoxy-2-methylisoflavone	2.585859	7.06E-04	0.386719	13
MOL00 4824	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one	2.592593	5.07E-04	0.385714	12
MOL00 4849	3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin	2.592593	5.39E-04	0.385714	12
MOL00 4908	Glabridin	2.585859	6.65E-04	0.386719	12
MOL00 4911	Glabrene	2.585859	4.75E-04	0.386719	12
MOL00 0417	Calycosin	2.599327	3.69E-04	0.384715	11
MOL00 0737	morin	2.606061	0.00326	0.383721	11
MOL00 3656	Lupiwighteone	2.592593	3.48E-04	0.385714	11
MOL00 4808	glyasperin B	2.599327	4.45E-04	0.384715	11

MOL00 4810	glyasperin F	2.599327	3.52E-04	0.384715	11
MOL00 4815	(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one	2.599327	3.52E-04	0.384715	11
MOL00 4820	kanzonols W	2.599327	3.52E-04	0.384715	11
MOL00 4856	Gancaonin A	2.592593	3.92E-04	0.385714	11
MOL00 4857	Gancaonin B	2.592593	4.78E-04	0.385714	11
MOL00 4864	5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone	2.599327	3.94E-04	0.384715	11
MOL00 4885	licoisoflavanone	2.599327	3.98E-04	0.384715	11
MOL00 4907	Glyzaglabrin	2.606061	4.27E-04	0.383721	11
MOL00 4915	Eurycarpin A	2.592593	3.48E-04	0.385714	11
MOL00 4961	Quercetin der.	2.599327	3.36E-04	0.384715	11
MOL00 5000	Gancaonin G	2.599327	4.44E-04	0.384715	11
MOL00 5012	Licoagroisoflavone	2.592593	3.48E-04	0.385714	11

MOL00 5016	Odoratin	2.599327	3.36E-04	0.384715	11
MOL00 4805	(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyrano[2,3-f]chromen-4-one	2.612795	3.13E-04	0.382732	10
MOL00 4841	Licochalcone B	2.606061	2.93E-04	0.383721	10
MOL00 4848	licochalcone G	2.612795	3.21E-04	0.382732	10
MOL00 4879	Glycyrin	2.606061	4.15E-04	0.383721	10
MOL00 4990	7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin	2.612795	2.55E-04	0.382732	10
MOL00 5020	dehydroglyasperins C	2.599327	3.34E-04	0.384715	10
MOL00 0049	3 β - acetoxylatractylone	2.612795	8.12E-04	0.382732	9
MOL00 0296	hederagenin	2.552189	0.005173	0.391821	9
MOL00 4827	Semilicoisoflavone B	2.612795	2.69E-04	0.382732	9
MOL00 4883	Licoisoflavone	2.612795	3.04E-04	0.382732	9
MOL00 4884	Licoisoflavone B	2.619529	2.36E-04	0.381748	9

MOL00 4980	Inflacoumarin A	2.606061	3.27E-04	0.383721	9
MOL00 5008	Glycyrrhiza flavonol A	2.612795	2.67E-04	0.382732	9
MOL00 5321	Frutinone A	2.612795	3.88E-04	0.382732	9
MOL00 1484	Inermine	2.639731	7.44E-04	0.378827	8
MOL00 3370	Onjixanthone I	2.632997	4.67E-04	0.379795	8
MOL00 4814	Isotrifoliol	2.632997	2.38E-04	0.379795	8
MOL00 4855	Licoricone	2.626263	2.82E-04	0.380769	8
MOL00 4863	3-(3,4- dihydroxyphenyl)-5,7- dihydroxy-8-(3- methylbut-2- enyl)chromone	2.626263	1.62E-04	0.380769	8
MOL00 4904	licopyranocoumarin	2.626263	2.64E-04	0.380769	8
MOL00 4945	(2S)-7-hydroxy-2-(4- hydroxyphenyl)-8-(3- methylbut-2- enyl)chroman-4-one	2.619529	2.34E-04	0.381748	8
MOL00 0239	Jaranol	2.626263	1.58E-04	0.380769	7
MOL00 2311	Glycyrol	2.646465	1.59E-04	0.377863	7

MOL00 3648	Inermin	2.653199	5.29E-04	0.376904	7
MOL00 4609	Areapillin	2.619529	1.69E-04	0.381748	7
MOL00 4806	euchrenone	2.632997	1.88E-04	0.379795	7
MOL00 4866	2-(3,4- dihydroxyphenyl)-5,7- dihydroxy-6-(3- methylbut-2- enyl)chromone	2.619529	2.06E-04	0.381748	7
MOL00 4910	Glabranin	2.632997	2.48E-04	0.379795	7
MOL00 4949	Isolicoflavonol	2.632997	1.27E-04	0.379795	7
MOL00 5017	Phaseol	2.639731	1.70E-04	0.378827	7
MOL00 5344	ginsenoside rh2	2.666667	0.001238	0.375	7
MOL00 5384	suchilactone	2.646465	3.86E-04	0.377863	7
MOL00 0490	petunidin	2.653199	8.98E-05	0.376904	6
MOL00 0522	arctiin	2.653199	2.05E-04	0.376904	6
MOL00 1792	DFV	2.639731	2.51E-04	0.378827	6
MOL00 2844	Pinocembrin	2.639731	2.51E-04	0.378827	6

MOL00 3330	(-)-Phillygenin	2.646465	2.60E-04	0.377863	6
MOL00 4598	3,5,6,7-tetramethoxy- 2-(3,4,5- trimethoxyphenyl)chro mone	2.639731	1.35E-04	0.378827	6
MOL00 4829	Glepidotin B	2.639731	2.04E-04	0.378827	6
MOL00 4898	(E)-3-[3,4-dihydroxy- 5-(3-methylbut-2- enyl)phenyl]-1-(2,4- dihydroxyphenyl)prop -2-en-1-one	2.646465	8.07E-05	0.377863	6
MOL00 4941	(2R)-7-hydroxy-2-(4- hydroxyphenyl)chrom an-4-one	2.639731	2.51E-04	0.378827	6
MOL00 4948	Isoglycyrol	2.639731	9.81E-05	0.378827	6
MOL00 5308	Aposiopolamine	2.936027	2.52E-04	0.340596	6
MOL00 3322	FORSYTHINOL	2.659933	1.23E-04	0.375949	5
MOL00 4798	delphinidin	2.659933	1.19E-04	0.375949	5
MOL00 4913	1,3-dihydroxy-9- methoxy-6- benzofurano[3,2- c]chromenone	2.835017	2.48E-05	0.352732	5
MOL00	1,3-dihydroxy-8,9-	2.814815	2.76E-05	0.355263	5

4914	dimethoxy-6-benzofurano[3,2-c]chromenone				
MOL004988	Kanzonol F	2.646465	7.90E-05	0.377863	5
MOL004989	6-prenylated eriodictyol	2.646465	7.86E-05	0.377863	5
MOL005001	Gancaonin H	2.646465	1.23E-04	0.377863	5
MOL005018	Xambioona	2.653199	6.59E-05	0.376904	5
MOL005356	Girinimbin	2.666667	1.17E-04	0.375	5
MOL000492	(+)-catechin	2.666667	4.64E-04	0.375	4
MOL000493	campesterol	2.606061	0.002357	0.383721	4
MOL003347	hyperforin	3.420875	4.16E-05	0.292323	4
MOL004653	(+)-Anomalin	2.673401	8.38E-05	0.374055	4
MOL004838	8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol	2.666667	7.98E-05	0.375	4
MOL004882	Licocoumarone	2.814815	1.86E-05	0.355263	4
MOL004903	liquiritin	2.680135	3.34E-04	0.373116	4
MOL00	Sigmoidin-B	2.659933	8.24E-05	0.375949	4

4935					
MOL00	8-prenylated	2.653199	5.73E-05	0.376904	4
4993	eriodictyol				
MOL01	Cubebin	2.666667	7.38E-05	0.375	4
3187					
MOL00	sitosterol	3.313131	1.71E-04	0.301829	2
0359					
MOL00	CLR	3.313131	1.71E-04	0.301829	2
0953					
MOL00	Linoleyl acetate	2.700337	6.26E-06	0.370324	2
1645					
MOL00	(3S,5R,8R,9R,10S,14S	3.313131	1.71E-04	0.301829	2
1919)-3,17-dihydroxy- 4,4,8,10,14- pentamethyl- 2,3,5,6,7,9-hexahydro- 1H- cyclopenta[a]phenanth rene-15,16-dione				
MOL00	paeoniflorin	3.441077	1.22E-05	0.290607	2
1924					
MOL00	Diop	3.003367	4.50E-06	0.33296	2
2879					
MOL00	Spinasterol	3.313131	1.71E-04	0.301829	2
4355					
MOL00	Longikaurin A	3.313131	1.84E-05	0.301829	2
4624					
MOL00	α -spinasterol	3.313131	1.71E-04	0.301829	2
4718					

MOL00 4924	(-)-Medicocarpin	2.700337	1.89E-05	0.370324	2
MOL00 5317	Deoxyharringtonine	2.888889	9.56E-04	0.346154	2
MOL00 5318	Dianthramine	2.700337	6.26E-06	0.370324	2
MOL00 5320	arachidonate	2.700337	6.26E-06	0.370324	2
MOL00 6767	Vulgaxanthin-I	2.700337	5.70E-06	0.370324	2
MOL00 0022	14-acetyl-12-senecioyl-2E,8Z,10E-atractylentriol	2.707071	0	0.369403	1
MOL00 0033	(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yl]octan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	3.353535	0	0.298193	1
MOL00 0072	8 β -ethoxyatractylenolide III	2.707071	0	0.369403	1
MOL00 0211	Mairin	3.353535	0	0.298193	1
MOL00 0273	(2R)-2-[(3S,5R,10S,13R,14R,	3.393939	0	0.294643	1

	16R,17R)-3,16-dihydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-enoic acid				
MOL00 0275	trametenolic acid	3.393939	0	0.294643	1
MOL00 0279	Cerevisterol	3.393939	0	0.294643	1
MOL00 0282	ergosta-7,22E-dien-3beta-ol	3.353535	0	0.298193	1
MOL00 0283	Ergosterol peroxide	3.353535	0	0.298193	1
MOL00 2776	Baicalin	3.043771	0	0.32854	1
MOL00 3315	3beta-Acetyl-20,25-epoxydammarane-24alpha-ol	3.454545	0	0.289474	1
MOL00 5348	Ginsenoside-Rh4_qt	3.393939	0	0.294643	1
MOL00 5376	Panaxadiol	3.454545	0	0.289474	1
MOL00 5399	alexandrin_qt	3.353535	0	0.298193	1

MOL00	poriferasterol	3.353535	0	0.298193	1
6772	monoglucoside_qt				
MOL00	stigmast-7-enol	3.353535	0	0.298193	1
6774					
