

Supplementary Tables and Figures

Supplementary Table S1. A total of 256 chemical ingredients of *Pueraria lobata*

Compounds	m/z	Rt (min)	Formula	Class
L-Histidine	156.08	0.69	C ₆ H ₉ N ₃ O ₂	Carboxylic acids and derivatives
Acacetin	283.06	4.44	C ₁₆ H ₁₂ O ₅	Flavonoids
Traumatic Acid	229.14	5.96	C ₁₂ H ₂₀ O ₄	Fatty Acyls
Caffeic Acid	181.05	3.61	C ₉ H ₈ O ₄	Cinnamic acids and derivatives
1-Kestose	543.13	0.76	C ₁₈ H ₃₂ O ₁₆	Organooxygen compounds
Tyramine	138.09	1.13	C ₈ H ₁₁ NO	Benzene and substituted derivatives
L-Glutamate	295.11	0.76	C ₅ H ₉ NO ₄	Carboxylic acids and derivatives
(+)-Absciscic Acid	247.13	5.18	C ₁₅ H ₂₀ O ₄	Prenol lipids
8-HETE	338.27	8.99	C ₂₀ H ₃₂ O ₃	Fatty Acyls
D-Glutamine	147.08	0.76	C ₅ H ₁₀ N ₂ O ₃	Carboxylic acids and derivatives
Sucrose	381.08	0.76	C ₁₂ H ₂₂ O ₁₁	Organooxygen compounds
Tangeritin	373.13	7.52	C ₂₀ H ₂₀ O ₇	Flavonoids
trans-2,3-Dihydroxycinnamate	181.05	3.82	C ₉ H ₈ O ₄	Cinnamic acids and derivatives
Astragalin	447.09	4.35	C ₂₁ H ₂₀ O ₁₁	Flavonoids
Peonidin 3-O-glucoside	463.12	4.53	C ₂₂ H ₂₂ O ₁₁	Flavonoids
Diosmetin	299.06	5.79	C ₁₆ H ₁₂ O ₆	Flavonoids
Pantothenic Acid	220.12	2.33	C ₉ H ₁₇ NO ₅	Alcohols and polyols
3-Cresotinic acid	151.04	3.77	C ₈ H ₈ O ₃	Benzene and substituted derivatives
Glycitin	447.13	5.08	C ₂₂ H ₂₂ O ₁₀	Isoflavonoids
5' -Deoxy-5'-(methylthio)-adenosine	298.10	3.37	C ₁₁ H ₁₅ N ₅ O ₃ S	5'-deoxyribonucleosides
13R-HODE	297.24	9.72	C ₁₈ H ₃₂ O ₃	Fatty Acyls
Formononetin	267.07	6.26	C ₁₆ H ₁₂ O ₄	Isoflavonoids
KOJIC ACID	143.03	1.16	C ₆ H ₆ O ₄	Pyrans
9-OxoODE	295.23	7.66	C ₁₈ H ₃₀ O ₃	Fatty Acyls
Glechomafuran	249.15	8.19	C ₁₅ H ₂₀ O ₃	Prenol lipids
Linoleic acid	281.25	9.41	C ₁₈ H ₃₂ O ₂	Fatty Acyls
L-trans-5-Hydroxy-2-piperidinecarboxylic acid	146.08	0.78	C ₆ H ₁₁ NO ₃	Carboxylic acids and derivatives
L-Arginine	175.12	0.70	C ₆ H ₁₄ N ₄ O ₂	Carboxylic acids and derivatives
Methylgingerol	309.21	7.72	C ₁₈ H ₂₈ O ₄	Benzene and substituted

				derivatives
Gentisic acid	153.02	2.39	C ₇ H ₆ O ₄	Benzene and substituted derivatives
Colnelenic acid	293.21	6.22	C ₁₈ H ₂₈ O ₃	Fatty Acyls
N-(3S-hydroxy-butanoyl)-homoserine lactone	188.09	1.35	C ₈ H ₁₃ NO ₄	Fatty Acyls
9S-hydroxy-12R,13S-epoxy-10E,15Z-octadecadienoic acid	311.22	6.31	C ₁₈ H ₃₀ O ₄	Fatty Acyls
13-OxoODE	295.23	6.53	C ₁₈ H ₃₀ O ₃	Fatty Acyls
3-Aminosalicylic acid	152.03	3.39	C ₇ H ₇ NO ₃	Benzene and substituted derivatives
Isoquercitrin	465.10	4.19	C ₂₁ H ₂₀ O ₁₂	Flavonoids
(-)-Naringenin	273.08	5.55	C ₁₅ H ₁₂ O ₅	Flavonoids
N-Acetyl-L-glutamic acid	190.07	0.95	C ₇ H ₁₁ NO ₅	Carboxylic acids and derivatives
L-Phenylalanine	164.07	1.93	C ₉ H ₁₁ NO ₂	Carboxylic acids and derivatives
N-ACETYLPROLINE	156.07	2.36	C ₇ H ₁₁ NO ₃	Carboxylic acids and derivatives
L-Lysine	147.11	0.68	C ₆ H ₁₄ N ₂ O ₂	Carboxylic acids and derivatives
ferulic acid	193.05	3.98	C ₁₀ H ₁₀ O ₄	Cinnamic acids and derivatives
12-oxo-5E,8E,10Z-dodecatricenoic acid	209.12	5.10	C ₁₂ H ₁₆ O ₃	Fatty Acyls
Pregabalin	160.13	3.12	C ₈ H ₁₇ NO ₂	Carboxylic acids and derivatives
MG(18:3(6Z,9Z,12Z)/0:0/0:0)	353.27	8.31	C ₂₁ H ₃₆ O ₄	Fatty Acyls
3-Hydroxyanthranilic acid	154.05	2.83	C ₇ H ₇ NO ₃	Benzene and substituted derivatives
9(S)-HpODE	295.23	6.08	C ₁₈ H ₃₂ O ₄	Fatty Acyls
L-Tryptophan	203.08	3.32	C ₁₁ H ₁₂ N ₂ O ₂	Indoles and derivatives
Caryophyllene epoxide	203.18	7.10	C ₁₅ H ₂₄ O	Prenol lipids
Carbendazim	192.08	3.52	C ₉ H ₉ N ₃ O ₂	Benzimidazoles
bicyclo-PGE2	335.22	7.39	C ₂₀ H ₃₀ O ₄	Fatty Acyls
Xanthine	151.03	1.04	C ₅ H ₄ N ₄ O ₂	Imidazopyrimidines
(E)-4-Octenoic acid	143.11	7.58	C ₈ H ₁₄ O ₂	Fatty Acyls
Traumatin	213.15	4.83	C ₁₂ H ₂₀ O ₃	Fatty Acyls
2-Hydroxycinnamic acid	163.04	4.20	C ₉ H ₈ O ₃	Cinnamic acids and derivatives
5-Hydroxykynurenamine	181.10	4.38	C ₉ H ₁₂ N ₂ O ₂	Organooxygen compounds
Corchorifatty acid A	309.21	6.10	C ₁₈ H ₂₈ O ₄	Fatty Acyls
Diplodiatoxin	309.21	7.16	C ₁₈ H ₂₈ O ₄	Keto acids and

				derivatives
Isoleucyl-Lysine	260.20	1.20	C ₁₂ H ₂₅ N ₃ O ₃	Carboxylic acids and derivatives
Nobiletin	403.14	6.99	C ₂₁ H ₂₂ O ₈	Flavonoids
1-(Malonylamino)cyclopropanecarboxylic acid	188.06	1.16	C ₇ H ₉ NO ₅	Carboxylic acids and derivatives
N-Benzoylaspartic acid	238.07	3.91	C ₁₁ H ₁₁ NO ₅	Carboxylic acids and derivatives
MG(0:0/18:3(6Z,9Z,12Z)/0:0)	353.27	9.12	C ₂₁ H ₃₆ O ₄	Fatty Acyls
L-Theanine	175.11	1.40	C ₇ H ₁₄ N ₂ O ₃	Carboxylic acids and derivatives
2,3-Dinor-TXB2	343.21	5.59	C ₁₈ H ₃₀ O ₆	Fatty Acyls
(8)-Gingerol	323.22	8.22	C ₁₉ H ₃₀ O ₄	Phenols
MG(0:0/18:4(6Z,9Z,12Z,15Z)/0:0)	351.25	8.85	C ₂₁ H ₃₄ O ₄	Fatty Acyls
Threoninyl-Isoleucine	233.15	2.31	C ₁₀ H ₂₀ N ₂ O ₄	Carboxylic acids and derivatives
2-tridecene-4,7-diynal	189.13	3.94	C ₁₃ H ₁₆ O	Fatty Acyls
LysoPE(15:0/0:0)	440.28	8.95	C ₂₀ H ₄₂ NO ₇ P	Glycerophospholipids
Megastigmatrienone	381.28	7.99	C ₁₃ H ₁₈ O	Organooxygen compounds
Procyanidin B2	577.14	3.49	C ₃₀ H ₂₆ O ₁₂	Flavonoids
3S-aminodecanoic acid	188.16	4.07	C ₁₀ H ₂₁ NO ₂	Fatty Acyls
12-hydroxy-3Z,6Z-dodecadienoic acid	213.15	5.73	C ₁₂ H ₂₀ O ₃	Fatty Acyls
Hydrocortamate	476.30	5.87	C ₂₇ H ₄₁ NO ₆	Steroids and steroid derivatives
2,3-Dihydroxybenzoic acid	153.02	3.82	C ₇ H ₆ O ₄	Benzene and substituted derivatives
6,8,10,12-pentadecatetraenal	219.17	5.59	C ₁₅ H ₂₂ O	Fatty Acyls
Glycyl-Isoleucine	189.12	2.35	C ₈ H ₁₆ N ₂ O ₃	Carboxylic acids and derivatives
Isoferulic acid	195.07	4.37	C ₁₀ H ₁₀ O ₄	Cinnamic acids and derivatives
6-methyl-5-heptenoic acid	143.11	6.26	C ₈ H ₁₄ O ₂	Fatty Acyls
Corchorifatty acid F	351.21	6.52	C ₁₈ H ₃₂ O ₅	Fatty Acyls
pivaloylcarnitine	246.17	2.93	C ₁₂ H ₂₃ NO ₄	Fatty Acyls
7-Tridecynoic acid	211.17	4.58	C ₁₃ H ₂₂ O ₂	Fatty Acyls
Soyasapogenol C	441.37	9.72	C ₃₀ H ₄₈ O ₂	Prenol lipids
cis,cis-Muconic acid	143.03	3.12	C ₆ H ₆ O ₄	Fatty Acyls
Pimelic acid	159.07	3.86	C ₇ H ₁₂ O ₄	Fatty Acyls
N-Acetylleucine	172.10	4.11	C ₈ H ₁₅ NO ₃	Carboxylic acids and derivatives
(R)-3-Hydroxy-5-phenylpenta	195.10	4.63	C ₁₁ H ₁₄ O ₃	Hydroxy acids and

noic acid				derivatives
Momordicin I	473.36	7.96	C ₃₀ H ₄₈ O ₄	Steroids and steroid derivatives
Isocitrate	191.02	1.04	C ₆ H ₈ O ₇	Carboxylic acids and derivatives
Hydroxyphenylacetyl glycine	210.08	1.64	C ₁₀ H ₁₁ NO ₄	Carboxylic acids and derivatives
4,8 dimethylnonanoyl carnitine	330.26	3.52	C ₁₈ H ₃₅ NO ₄	Fatty Acyls
N-Malonylanthranilate	224.06	4.36	C ₁₀ H ₉ NO ₅	Benzene and substituted derivatives
Dehydrovomifoliol	223.13	6.02	C ₁₃ H ₁₈ O ₃	Prenol lipids
Isovalerylglutamic acid	232.12	4.13	C ₁₀ H ₁₇ NO ₅	Carboxylic acids and derivatives
8-Tridecynoic acid	211.17	5.44	C ₁₃ H ₂₂ O ₂	Fatty Acyls
Gingerol	295.19	8.38	C ₁₇ H ₂₆ O ₄	Phenols
Tocopheronic acid	295.15	4.91	C ₁₆ H ₂₂ O ₅	Prenol lipids
L-Carnitine	162.11	0.78	C ₇ H ₁₅ NO ₃	Organonitrogen compounds
13-Oxo-9,11-tridecadienoic acid	225.15	3.99	C ₁₃ H ₂₀ O ₃	Fatty Acyls
Cinnassiol C3	383.21	4.13	C ₂₀ H ₃₀ O ₇	Prenol lipids
N-Carboxyacetyl-D-phenylalanine	252.09	4.25	C ₁₂ H ₁₃ NO ₅	Carboxylic acids and derivatives
Quercetin	301.04	5.07	C ₁₅ H ₁₀ O ₇	Flavonoids
2-O-(Z-p-Hydroxycinnamoyl)-(x)-glyceric acid	253.07	4.53	C ₁₂ H ₁₂ O ₆	Cinnamic acids and derivatives
6-[5]-ladderane-hexanoic acid	275.20	5.73	C ₁₈ H ₂₆ O ₂	Fatty Acyls
2-Octenoic acid	143.11	7.04	C ₈ H ₁₄ O ₂	Fatty Acyls
Glycyl-L-leucine	189.12	2.72	C ₈ H ₁₆ N ₂ O ₃	Carboxylic acids and derivatives
3-hexenedioic acid	145.05	0.81	C ₆ H ₈ O ₄	Fatty Acyls
Threoninyl-Valine	219.13	1.20	C ₉ H ₁₈ N ₂ O ₄	Carboxylic acids and derivatives
Seriny-Phenylalanine	253.12	3.26	C ₁₂ H ₁₆ N ₂ O ₄	Carboxylic acids and derivatives
beta-Ionone	193.16	9.09	C ₁₃ H ₂₀ O	Prenol lipids
4-Nitrophenol	140.03	1.04	C ₆ H ₅ NO ₃	Phenols
N2-Acetyl-L-ornithine	175.11	1.64	C ₇ H ₁₄ N ₂ O ₃	Carboxylic acids and derivatives
4-Guanidinobutanoic acid	146.09	0.82	C ₅ H ₁₁ N ₃ O ₂	Carboxylic acids and derivatives
Acetylcholine	146.12	0.82	C ₇ H ₁₅ NO ₂	Organonitrogen compounds

Porphobilinogen	227.10	2.15	C ₁₀ H ₁₄ N ₂ O ₄	Organonitrogen compounds
Glycyl-Phenylalanine	223.11	3.38	C ₁₁ H ₁₄ N ₂ O ₃	Carboxylic acids and derivatives
Salicylic acid	137.02	3.50	C ₇ H ₆ O ₃	Benzene and substituted derivatives
9,12,13-trihydroxy-10,15-octadecadienoic acid	329.23	6.75	C ₁₈ H ₃₂ O ₅	Fatty Acyls
Canavanine	177.10	0.89	C ₅ H ₁₂ N ₄ O ₃	Carboxylic acids and derivatives
Asparaginy-Phenylalanine	280.13	3.31	C ₁₃ H ₁₇ N ₃ O ₄	Carboxylic acids and derivatives
DHAP(10:0)	325.14	3.95	C ₁₃ H ₂₅ O ₇ P	Organooxygen compounds
Ononin	431.13	4.86	C ₂₂ H ₂₂ O ₉	Isoflavonoids
7-hexadecynoic acid	275.20	6.22	C ₁₆ H ₂₈ O ₂	Fatty Acyls
Phytosphingosine	318.30	8.17	C ₁₈ H ₃₉ NO ₃	Organonitrogen compounds
ESCULETIN	177.02	3.80	C ₉ H ₆ O ₄	Coumarins and derivatives
6-Undecynoic acid	165.13	5.96	C ₁₁ H ₁₈ O ₂	Fatty Acyls
dexpanthenol	206.14	2.41	C ₉ H ₁₉ NO ₄	Fatty Acyls
Caffeate	163.04	3.11	C ₉ H ₈ O ₄	Cinnamic acids and derivatives
alpha-Ionone	193.16	5.99	C ₁₃ H ₂₀ O	Prenol lipids
Dulcitol	181.07	0.75	C ₆ H ₁₄ O ₆	Organooxygen compounds
Baicalein	269.05	6.01	C ₁₅ H ₁₀ O ₅	Flavonoids
5-L-Glutamyl-L-alanine	219.10	1.06	C ₈ H ₁₄ N ₂ O ₅	Carboxylic acids and derivatives
Eremopetasinorone A	207.14	4.34	C ₁₃ H ₁₈ O ₂	Organooxygen compounds
9S,12S,13S-trihydroxy-10E,15Z-octadecadienoic acid	329.23	6.12	C ₁₈ H ₃₂ O ₅	Fatty Acyls
6E,8E,14E-Hexadecatriene-10,12-diyneic acid	243.14	6.41	C ₁₆ H ₁₈ O ₂	Fatty Acyls
Adipic acid	145.05	3.05	C ₆ H ₁₀ O ₄	Fatty Acyls
1-Phenylethyl formate	151.08	4.15	C ₉ H ₁₀ O ₂	Benzene and substituted derivatives
Helinorbisabone	251.13	5.32	C ₁₄ H ₁₈ O ₄	Prenol lipids
13(S)-HpODE	311.22	7.00	C ₁₈ H ₃₂ O ₄	Fatty Acyls
Indole-3-acetamide	175.09	3.27	C ₁₀ H ₁₀ N ₂ O	Indoles and derivatives
Tyrosyl-Isoleucine	295.17	3.77	C ₁₅ H ₂₂ N ₂ O ₄	Carboxylic acids and derivatives

5,8,12-trihydroxy-9-octadecenoic acid	331.25	5.64	C ₁₈ H ₃₄ O ₅	Fatty Acyls
Uric acid	167.02	0.82	C ₅ H ₄ N ₄ O ₃	Imidazopyrimidines
3-Hydroxyphenyl-valeric acid	195.10	4.84	C ₁₁ H ₁₄ O ₃	Fatty Acyls
Perillic acid	167.11	5.11	C ₁₀ H ₁₄ O ₂	Prenol lipids
Ethyl 4-methylphenoxyacetate	195.10	8.19	C ₁₁ H ₁₄ O ₃	Benzene and substituted derivatives
Guanine	152.06	1.07	C ₅ H ₅ N ₅ O	Imidazopyrimidines
4,4alpha,5,6-Tetrahydro-7-methyl-2(3H)-naphthalenone	163.11	5.46	C ₁₁ H ₁₄ O	Organooxygen compounds
LysoPC(18:1(11Z))	522.36	9.60	C ₂₆ H ₅₂ NO ₇ P	Glycerophospholipids
3-amino-octanoic acid	160.13	3.77	C ₈ H ₁₇ NO ₂	Fatty Acyls
3,4-Dihydroxybenzoic acid	153.02	4.10	C ₇ H ₆ O ₄	Benzene and substituted derivatives
Valyl-Valine	217.15	1.73	C ₁₀ H ₂₀ N ₂ O ₃	Carboxylic acids and derivatives
8-Hydroxy-5,6-octadienoic acid	157.09	3.07	C ₈ H ₁₂ O ₃	Hydroxy acids and derivatives
(-)-Jasmonic acid	211.13	4.34	C ₁₂ H ₁₈ O ₃	Fatty Acyls
capsidiol	219.17	5.22	C ₁₅ H ₂₄ O ₂	Prenol lipids
Glutaryl-glycine	190.07	1.22	C ₇ H ₁₁ NO ₅	Carboxylic acids and derivatives
8-Hydroxy-7-methoxy-2H-1-benzopyran-2-one	193.05	4.10	C ₁₀ H ₈ O ₄	Coumarins and derivatives
O-propanoyl-carnitine	218.14	1.04	C ₁₀ H ₁₉ NO ₄	Fatty Acyls
SerinyI-Isoleucine	219.13	2.04	C ₉ H ₁₈ N ₂ O ₄	Carboxylic acids and derivatives
2-Descarboxy-cyclo-dopa	152.07	3.12	C ₈ H ₉ NO ₂	Indoles and derivatives
Pyridoxamine	169.10	1.78	C ₈ H ₁₂ N ₂ O ₂	Pyridines and derivatives
Metanephrene	198.11	3.57	C ₁₀ H ₁₅ NO ₃	Phenols
Gluconic acid	195.05	0.76	C ₆ H ₁₂ O ₇	Organooxygen compounds
2,8-Dihydroxyadenine	168.05	1.03	C ₅ H ₅ N ₅ O ₂	Imidazopyrimidines
Plantagonine	178.09	2.05	C ₁₀ H ₁₁ NO ₂	Pyridines and derivatives
Isopetasoside	397.22	4.49	C ₂₁ H ₃₂ O ₇	Prenol lipids
(±)-Camphoric acid	201.11	4.56	C ₁₀ H ₁₆ O ₄	Carboxylic acids and derivatives
1,3,5,11-Bisabolatetraen-10-one	217.16	6.87	C ₁₅ H ₂₀ O	Prenol lipids
Ng-L-Glutamyl-L-aspartic acid	263.09	1.04	C ₉ H ₁₄ N ₂ O ₇	Carboxylic acids and derivatives
alpha-Hydroxy-1-methyl-1H-indole-3-propanoic acid	220.10	4.43	C ₁₂ H ₁₃ NO ₃	Indoles and derivatives
Sphinganine	302.31	8.09	C ₁₈ H ₃₉ NO ₂	Organonitrogen

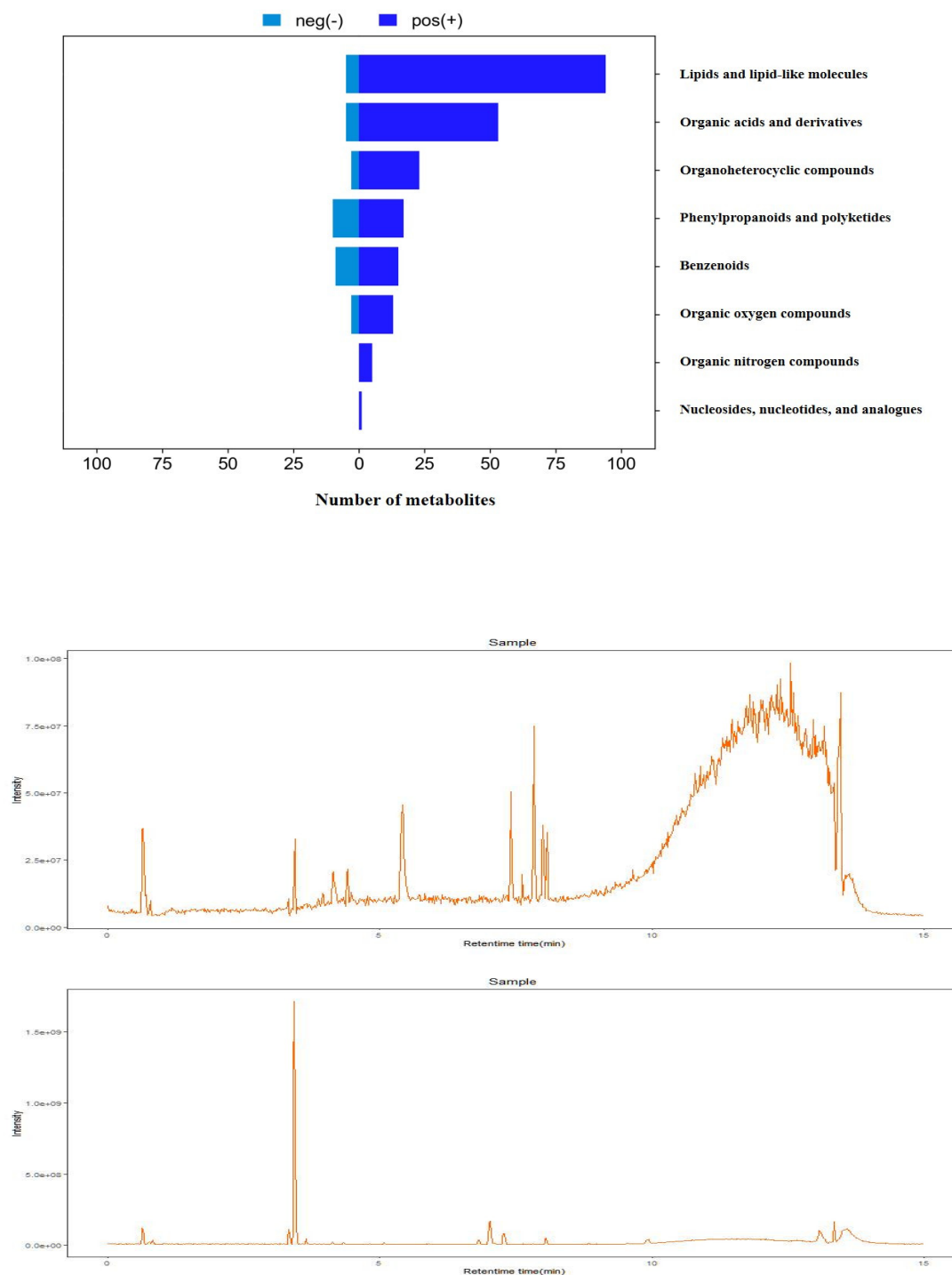
				compounds
5-Acetamidovalerate	160.10	2.04	C ₇ H ₁₃ NO ₃	Fatty Acyls
1,6,9-Farnesatriene-3,11-diol	239.20	5.27	C ₁₅ H ₂₆ O ₂	Prenol lipids
15-Octadecene-9,11,13-triynoic acid	231.14	9.22	C ₁₅ H ₁₈ O ₂	Fatty Acyls
3alpha,7alpha,12alpha,23R-tetrahydroxy-5beta-cholan-24-oic acid	425.29	9.30	C ₂₄ H ₄₀ O ₆	Sterol Lipids
Histidinyl-Proline	253.13	2.56	C ₁₁ H ₁₆ N ₄ O ₃	Carboxylic acids and derivatives
16-iodo-hexadecanoic acid	383.14	3.95	C ₁₆ H ₃₁ IO ₂	Fatty Acyls
Spectinomycin	333.17	4.05	C ₁₄ H ₂₄ N ₂ O ₇	Dioxanes
Indole-3-ethanol	162.09	4.88	C ₁₀ H ₁₁ NO	Indoles and derivatives
Isoleucyl-Valine	231.17	3.07	C ₁₁ H ₂₂ N ₂ O ₃	Carboxylic acids and derivatives
Glycerophosphocholine	258.11	0.78	C ₈ H ₂₀ NO ₆ P	Glycerophospholipids
Alanyl-Leucine	203.14	0.82	C ₉ H ₁₈ N ₂ O ₃	Carboxylic acids and derivatives
7-methyl-3-oxooctanoic acid	173.12	6.14	C ₉ H ₁₆ O ₃	Fatty Acyls
alpha-curcumen	405.35	8.01	C ₁₅ H ₂₂	Prenol lipids
9,10,13-Trihydroxystearic acid	333.26	5.89	C ₁₈ H ₃₆ O ₅	Fatty Acyls
DG(18:4(6Z,9Z,12Z,15Z)/18:3(6Z,9Z,12Z)/0:0)	611.47	10.71	C ₃₉ H ₆₂ O ₅	Fatty Acyls
Dyphylline	255.11	2.07	C ₁₀ H ₁₄ N ₄ O ₄	Imidazopyrimidines
Syringic acid	199.06	3.05	C ₉ H ₁₀ O ₅	Benzene and substituted derivatives
Genistein	271.06	5.51	C ₁₅ H ₁₀ O ₅	Isoflavonoids
ANETHOLE	149.10	8.09	C ₁₀ H ₁₂ O	Benzene and substituted derivatives
2,3-Dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone	213.08	3.14	C ₁₀ H ₁₂ O ₅	Organooxygen compounds
Alpha-N-Phenylacetyl-L-glutamine	265.12	3.83	C ₁₃ H ₁₆ N ₂ O ₄	Carboxylic acids and derivatives
2',4',4'-Trihydroxy-3'-prenylchalcone 4'-O-glucoside	487.19	3.80	C ₂₆ H ₃₀ O ₉	Polyketides
L-isoleucyl-L-proline	229.15	2.72	C ₁₁ H ₂₀ N ₂ O ₃	Carboxylic acids and derivatives
5-Methylquinoxaline	145.08	3.86	C ₉ H ₈ N ₂	Naphthyridines
Folinic acid	474.17	3.19	C ₂₀ H ₂₃ N ₇ O ₇	Pteridines and derivatives
MG(18:4(6Z,9Z,12Z,15Z)/0:0/0:0)	351.25	6.55	C ₂₁ H ₃₄ O ₄	Fatty Acyls

2-Carboxy-4-dodecanolide	243.16	7.44	C ₁₃ H ₂₂ O ₄	Lactones
Rosifoliol	205.20	7.51	C ₁₅ H ₂₆ O	Prenol lipids
3-Oxochohic acid	407.28	8.93	C ₂₄ H ₃₈ O ₅	Steroids and steroid derivatives
Ethyl N-ethylanthranilate	194.12	4.28	C ₁₁ H ₁₅ NO ₂	Benzene and substituted derivatives
2-Hydroxyadenine	152.06	0.81	C ₅ H ₅ N ₅ O	Imidazopyrimidines
Valyl-Proline	215.14	1.38	C ₁₀ H ₁₈ N ₂ O ₃	Carboxylic acids and derivatives
Demethylvestitol	241.09	3.50	C ₁₅ H ₁₄ O ₄	Isoflavonoids
2-[3-Carboxy-3-(methylammonio)propyl]-L-histidine	271.14	1.49	C ₁₁ H ₁₈ N ₄ O ₄	Carboxylic acids and derivatives
(3beta,22R,23R,24S)-3,22,23-Trihydroxystigmastan-6-one	463.38	12.31	C ₂₉ H ₅₀ O ₄	Steroids and steroid derivatives
butalbital	225.12	3.60	C ₁₁ H ₁₆ N ₂ O ₃	Diazines
cis-3-Hexenyl pyruvate	171.10	4.49	C ₉ H ₁₄ O ₃	Keto acids and derivatives
Adenine	136.06	0.81	C ₅ H ₅ N ₅	Imidazopyrimidines
Procaterol	291.17	4.37	C ₁₆ H ₂₂ N ₂ O ₃	Quinolines and derivatives
12-amino-dodecanoic acid	216.20	5.51	C ₁₂ H ₂₅ NO ₂	Fatty Acyls
Ethosuximide	142.09	3.74	C ₇ H ₁₁ NO ₂	Pyrrolidines
Isoleucyl-Isoleucine	245.19	3.92	C ₁₂ H ₂₄ N ₂ O ₃	Carboxylic acids and derivatives
MG(0:0/16:0/0:0)	313.27	9.15	C ₁₉ H ₃₈ O ₄	Glycerolipids
3,6,9,12,15-octadecapentaenoic acid	275.20	5.36	C ₁₈ H ₂₆ O ₂	Fatty Acyls
Ethyl levulinate	145.09	1.92	C ₇ H ₁₂ O ₃	Keto acids and derivatives
2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione	239.13	5.38	C ₁₃ H ₁₈ O ₄	Prenol lipids
2-(Ethylamino)-4,5-dihydroxybenzamide	197.09	3.29	C ₉ H ₁₂ N ₂ O ₃	Benzene and substituted derivatives
Isoferuloyl C1-glucuronide	371.10	5.30	C ₁₆ H ₁₈ O ₁₀	Cinnamic acids and derivatives
9-hydroxy-16-oxo-hexadecanoic acid	287.22	5.69	C ₁₆ H ₃₀ O ₄	Fatty Acyls
Suberylglycine	232.12	2.60	C ₁₀ H ₁₇ NO ₅	Carboxylic acids and derivatives
Hydroxypropyl-Valine	231.13	3.92	C ₁₀ H ₁₈ N ₂ O ₄	Carboxylic acids and derivatives
Succinylacetone	157.05	4.05	C ₇ H ₁₀ O ₄	Keto acids and derivatives

3Z,6Z,9Z,12Z,15Z-octadecapentaenoic acid	275.20	7.10	C ₁₈ H ₂₆ O ₂	Fatty Acyls
Domoic acid	312.14	1.61	C ₁₅ H ₂₁ NO ₆	Carboxylic acids and derivatives
8E,10E-dodecadienoic acid	197.15	4.66	C ₁₂ H ₂₀ O ₂	Fatty Acyls
Emodin	271.06	6.00	C ₁₅ H ₁₀ O ₅	Anthracenes
Nicotinate D-ribonucleoside	256.08	0.81	C ₁₁ H ₁₃ NO ₆	Organooxygen compounds
Kinetin-9-N-glucoside	378.14	3.64	C ₁₆ H ₁₉ N ₅ O ₆	Organooxygen compounds
O-decanoyl-R-carnitine	316.25	4.02	C ₁₇ H ₃₃ NO ₄	Fatty Acyls
2,3-Dinor-6-keto-PGF1a	341.20	7.64	C ₁₈ H ₂₈ O ₆	Fatty Acyls
Glutaminy-Lysine	275.17	1.41	C ₁₁ H ₂₂ N ₄ O ₄	Carboxylic acids and derivatives
Indoleacetaldehyde	160.08	1.62	C ₁₀ H ₉ NO	Indoles and derivatives
Hypoxanthine	137.05	0.83	C ₅ H ₄ N ₄ O	Imidazopyrimidines
Isoleucyl-Alanine	203.14	1.40	C ₉ H ₁₈ N ₂ O ₃	Carboxylic acids and derivatives
3R-aminononanoic acid	174.15	3.76	C ₉ H ₁₉ NO ₂	Fatty Acyls
2-Hydroxymyristic Acid	243.20	9.36	C ₁₄ H ₂₈ O ₃	Fatty Acyls
Tolmetin	258.11	5.32	C ₁₅ H ₁₅ NO ₃	Organooxygen compounds
6-Phosphogluconic acid	275.02	0.79	C ₆ H ₁₃ O ₁₀ P	Organooxygen compounds
Phenylglyoxylic acid	149.02	2.96	C ₈ H ₆ O ₃	Benzene and substituted derivatives
9,10-dihydroxy-Octadecanedioic acid	347.24	5.46	C ₁₈ H ₃₄ O ₆	Fatty Acyls
Glutaminy-Gamma-glutamate	275.13	0.82	C ₁₀ H ₁₈ N ₄ O ₅	Carboxylic acids and derivatives
4-Nitrocatechol	154.01	3.21	C ₆ H ₅ NO ₄	Phenols
2'-Hydroxygenistein	287.06	5.61	C ₁₅ H ₁₀ O ₆	Isoflavonoids
O-octanoyl-R-carnitine	288.22	5.30	C ₁₅ H ₂₉ NO ₄	Fatty Acyls
GLYCYRRHIZIC ACID	821.40	6.30	C ₄₂ H ₆₂ O ₁₆	Prenol lipids
Leucyl-Phenylalanine	279.17	4.10	C ₁₅ H ₂₂ N ₂ O ₃	Carboxylic acids and derivatives
Phosphohydroxypyruvic acid	184.99	10.69	C ₃ H ₅ O ₇ P	Organooxygen compounds
L-Octanoylcarnitine	288.22	4.02	C ₁₅ H ₂₉ NO ₄	Fatty Acyls
PGJ2	357.20	4.80	C ₂₀ H ₃₀ O ₄	Fatty Acyls
Dictyoquinazol C	343.13	5.14	C ₁₈ H ₁₈ N ₂ O ₅	Diazanaphthalenes
Enalapril	377.20	3.57	C ₂₀ H ₂₈ N ₂ O ₅	Carboxylic acids and derivatives
PA(18:3(9Z,12Z,15Z)/18:0)	699.49	11.32	C ₃₉ H ₇₁ O ₈ P	Glycerophospholipids

15-Oxo-ETE	341.21	5.29	C ₂₀ H ₃₀ O ₃	Fatty Acyls
Sulfinpyrazone	403.11	4.41	C ₂₃ H ₂₀ N ₂ O ₃ S	Benzene and substituted derivatives

Supplementary Figure S1. The base peak chromatogram of positive and negative ion and the composition of the chemical metabolites.



Supplementary Figure S2. The common targets of ingredients and DM. The statistical bar chart of proteins with degree value greater than 12

