

Table S1 UPLC-MS identification of chemical constituents of SYW

Metabolite	m/z	Retention time	Formula	Score
Diallyl Trisulfide	179.0005743	0.03875	C6H10S3	44.1
Dodecamethylcyclohexasiloxane	445.1204113	0.169616667	C12H36O6Si6	53
Maltol	127.0394416	0.193633333	C6H6O3	48.6
Dihydrocarvone	153.127729	0.329816667	C10H16O	52.6
Spermidine	146.165488	0.560866667	C7H19N3	51
Gaba	86.0606727	0.592833333	C4H9NO2	54
Mannosamine	162.0762479	0.592833333	C6H13NO5	53.6
Choline	104.1076568	0.601	C5H14NO+	57.3
2,3-butanedione	104.0713404	0.616816667	C4H6O2	47.3
L-Valine	118.0867886	0.616816667	C5H11NO2	54.7
L-threonine	120.0659642	0.616816667	C4H9NO3	55.4
Glutamic Acid	148.0606047	0.616816667	C5H9NO4	51
Creatine	132.0771185	0.6401	C4H9N3O2	56.5
Trigonelline	138.055124	0.6401	C7H7NO2	50.8
L-proline	116.0711658	0.647916667	C5H9NO2	54.4
Sucrose	365.1055568	0.647916667	C12H22O11	54.5
Ergothioneine	230.0959898	0.655866667	C9H15N3O2S	55.2
Cytosine	112.0511213	0.663833333	C4H5N3O	54.1
D-Pipecolic acid	130.0866469	0.67955	C6H11NO2	55.4
4-guanidinobutanoic acid	146.0926328	0.687283333	C5H11N3O2	57
Adenine	136.0620152	0.711116667	C5H5N5	54.4
2-Phenylacetamide	136.0759357	0.726966667	C8H9NO	56.2
Phloroglucinol	127.0393586	0.774516667	C6H6O3	56
Piperidine	86.09710002	0.790316667	C5H11N	50.2
L-isoleucine	132.1022719	0.790316667	C6H13NO2	51.6
Nicotinic acid	124.0397648	0.806183333	C6H5NO2	56.2
Homoserine	84.04514532	0.829816667	C4H9NO3	54.2
Hypoxanthine	137.0460553	1.092933333	C5H4N4O	55
Uracil	113.0351509	1.28505	C4H4N2O2	55.3
Salicylaldehyde	123.0445844	1.324983333	C7H6O2	51.6
Coumarin	147.044384	1.324983333	C9H6O2	57
L-tyrosine	182.081646	1.324983333	C9H11NO3	57.3
(R)-Nicotine	163.1232815	1.340916667	C10H14N2	46.4
L-Leucine	132.1023429	1.3809	C6H13NO2	54.5
Linalool	137.1328199	1.844966667	C10H18O	46.1
Butanal	73.06549077	1.852966667	C4H8O	46.5
Alpha-methylene-gamma-butyrolactone	99.0447895	1.892966667	C5H6O2	54.6
Thymine	127.0506188	1.90895	C5H6N2O2	53.6
Serotonin	177.1026142	1.90895	C10H12N2O	57.6
5-Hydroxytryptophan	221.0923887	1.90895	C11H12N2O3	53.1

Aromatic aldehyde	107.0498328	2.212966667	C7H6O	51.5
Gamma-glutamylvaline	247.1290908	2.244833333	C10H18N2O5	49
Benzylamine	108.0814741	2.300666667	C7H9N	48.3
5,6-dimethylbenzimidazole	147.091853	2.731266667	C9H10N2	48
Kinetin	216.0869896	2.84925	C10H9N5O	46.8
Benzene-1,2,4-triol	127.039347	2.960583333	C6H6O3	50.7
6-Methyl indole	132.0810909	2.976366667	C9H9N	56.2
Indole-3-carboxyaldehyde	146.0603246	2.976366667	C9H7NO	58.1
D-(+)-Tryptophan	205.0974919	2.976366667	C11H12N2O2	58.8
Securinine	250.1438772	3.0162	C13H15NO2	47.8
Pyridoxine	152.0708085	3.334966667	C8H11NO3	53.5
Gamma-glu-leu	261.1447816	3.341483333	C11H20N2O5	57.8
Ethylmethylmaleimide	140.0707626	3.362783333	C7H9NO2	54.3
2-Acetylpyridine	122.0604967	3.377183333	C7H7NO	47.8
3,4-dihydroxyphenylacetic acid	169.0496529	3.387216667	C8H8O4	48.8
Trans,trans-2,4-Heptadienal	111.0810912	3.434483333	C7H10O	44.2
Antiarol	185.0811295	3.434483333	C9H12O4	55.2
Gamma-glutamylphenylalanine	295.1290206	3.4646	C14H18N2O5	58.2
Sinapic acid	207.0654481	3.470633333	C11H12O5	54.2
Phthalic Anhydride	190.0503258	3.494483333	C8H4O3	47.3
1-naphthylamine	144.0810611	3.568483333	C10H9N	49.7
Norharman	169.0761906	3.589516667	C11H8N2	46.3
Acridin-9-amine	212.1185085	3.6247	C13H10N2	54.4
Pyrrole-2-carboxylic acid	112.0398352	3.6302	C5H5NO2	48.7
(S)-tropic acid	167.0703937	3.6577	C9H10O3	50.8
Phthalic acid	167.0339872	3.754283333	C8H6O4	55.1
L-dopa	162.0550034	3.803383333	C9H11NO4	47.9
3,5-dimethylphenol	123.0808339	3.850283333	C8H10O	52.6
Xanthoxylin	197.0809965	3.862333333	C10H12O4	54.2
Agarotetrol	319.1175324	3.862333333	C17H18O6	48.7
Decaethylene glycol	476.3071386	3.890433333	C20H42O11	51
(R)-(+)-Pulegone	153.1276308	3.99595	C10H16O	48
Ibuprofen	207.1382127	3.999983333	C13H18O2	55.6
N-acetyldopamine	228.1232445	4.03875	C10H13NO3	47.2
Anisole	91.05490979	4.0566	C7H8O	46.8
Trans-Stilbene	181.1014751	4.0566	C14H12	54.4
4-Methylumbelliferone	177.0548218	4.0816	C10H8O3	57.1
Phenylacetone	117.0703281	4.227083333	C9H10O	55.9
4-ethylbenzaldehyde	135.0806394	4.227083333	C9H10O	50.7
6-Methylcoumarin	161.0598006	4.227083333	C10H8O2	51.9
3,5-Dimethoxy-4-hydroxybenzaldehyde	183.0653782	4.331583333	C9H10O4	53.1
Limonene oxide	153.1276286	4.366766667	C10H16O	48.9

2-methylpyridin-3-ol	110.0606643	4.380883333	C6H7NO	54.2
Calycosin-7-O-beta-D-glucoside	447.1281881	4.487583333	C22H22O10	57.1
Isofraxidin	223.0603122	4.50375	C11H10O5	57.3
Beta-guaiene	227.1756753	4.53785	C15H24	46.5
Apigenin 6-C-alpha-L-arabinopyranosyl-8-C-beta-D-xylopyranoside	535.1444021	4.561016667	C25H26O13	54.6
Naringenin	273.0756067	4.680333333	C15H12O5	54
Sulcatone	127.1122134	4.702566667	C8H14O	49.4
Isoliquiritigenin	257.0809549	4.71065	C15H12O4	58.9
N-methylanthranilic acid	152.0706897	4.74105	C8H9NO2	55.5
Fraxidin	223.0602429	4.786383333	C11H10O5	56.5
Pogostone	225.1124807	4.826183333	C12H16O4	53.6
Quinoline	130.065542	4.8883	C9H7N	48.5
Caffeic Acid Methyl Ester	177.0547446	4.987966667	C10H10O4	49.7
4'-O-beta-D-glucosyl-5-O-methylvisaminol	453.1755979	5.1391	C22H28O10	59.4
Alpha-Ionone	193.1588686	5.14265	C13H20O	50.9
Indole-3-carboxaldehyde	146.060384	5.17585	C9H7NO	57.1
Boschnialactone	155.1070112	5.189966667	C9H14O2	48.4
2-Ethylphenol	123.0807217	5.202583333	C8H10O	46.8
Alpha,4-Dimethylstyrene	133.101505	5.202583333	C10H12	55.2
2-buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-	191.1431135	5.202583333	C13H18O	50.6
Dehydrojuncusol	265.1222514	5.205666667	C18H16O2	48.2
Cinnamic acid	131.0495389	5.22615	C9H8O2	56.5
1,4-naphthoquinone	159.0440854	5.233733333	C10H6O2	54.9
2-phenylphenol	171.0805104	5.2562	C12H10O	57.2
Blumenol B	209.1538112	5.313266667	C13H22O3	50.3
Isoquinoline	130.0655411	5.408233333	C9H7N	52.1
Indole-3-acetic acid	176.071083	5.408233333	C10H9NO2	56.7
Pseudoionone	193.1589538	5.418316667	C13H20O	57
Alpha-Cyclogeraniol acetate	211.1694554	5.42285	C13H22O2	54.5
Scytalone	177.0548339	5.6545	C10H10O4	55.7
Baicalein	271.0598898	5.6838	C15H10O5	54.5
Precocene I	191.1067392	5.78685	C12H14O2	48.1
Glycitein	285.0757845	5.857583333	C16H12O5	58.6
Chrysin	255.0652825	5.865916667	C15H10O4	56.7
Caryophyllene	227.1754309	5.950283333	C15H24	43.5
Oleanonic acid	455.3520781	5.957116667	C30H46O3	49.8
4-Hydroxy-2-methylacetophenone	151.0755687	5.97405	C9H10O2	51.5
Benzylideneacetone	147.0806546	5.99915	C10H10O	52.4

Senkyunolide C	205.0862316	6.0112	C12H12O3	53.5
Phytosphingosine	318.3004266	6.04855	C18H39NO3	57.8
Tetradecylamine	214.2532091	6.065866667	C14H31N	52
Epinephrine	166.0865588	6.07385	C9H13NO3	47.5
2(5H)-Furanone	85.02896617	6.08185	C4H4O2	49
Corchorifatty acid F	293.2109664	6.105516667	C18H32O5	54.2
Sphinganine	302.3055028	6.12145	C18H39NO2	56.8
9-Oxo-10,12-octadecadienoic acid	295.2267928	6.153366667	C18H30O3	58.2
Monoolein	398.3266966	6.153366667	C21H40O4	47.7
Tianshic acid	348.2744087	6.1612	C18H34O5	48.5
Sphingosine	300.28981	6.169183333	C18H37NO2	55.3
(-)-gamma-ionone	193.1590822	6.177016667	C13H20O	51.7
Ginsenoside Rb1	453.3362481	6.19295	C30H44O3	51.8
Prostaglandin a1	319.2268326	6.208883333	C20H32O4	51.6
Octadecenedioic acid	313.2371928	6.216883333	C18H32O4	47.7
Sclareolide (Norambreinolide)	251.2005807	6.264533333	C16H26O2	48.9
Alpha-Methylstyrene	119.0860205	6.272533333	C9H10	56.4
Chavicol	135.0807552	6.280533333	C9H10O	54.5
1,3-dicyclohexylurea	225.1964347	6.288533333	C13H24N2O	45.2
Rishitin	223.169465	6.296516667	C14H22O2	51.7
2-(methylthio)benzothiazole	182.009543	6.32845	C8H7NS2	55.1
Testosterone	289.2165421	6.36835	C19H28O2	46.1
Pc(34:2)	758.5706655	6.423883333	C42H80NO8P	58.5
Ginsenoside Rg5	767.4942857	6.4556	C42H70O12	52.6
Notoginsenoside R2	771.4872298	6.486883333	C41H70O13	45.5
Eicosapentaenoic acid	303.2319382	6.510766667	C20H30O2	52.2
Buprenorphine	468.3086893	6.526733333	C29H41NO4	49
Isosteviol	319.2250172	6.558416667	C20H30O3	44.3
4-isopropylbenzoic acid	147.0803853	6.582316667	C10H12O2	45.7
2,6,6-Trimethyl-2-cyclohexene-1,4-dione	153.0910552	6.582316667	C9H12O2	51.6
11-Keto-beta-boswellic acid	471.3466409	6.629916667	C30H46O4	48
Pc(16:0/0:0)	496.3403313	6.752283333	C24H50NO7P	58.9
Erucamide	338.341784	7.2349	C22H43NO	57.7
4-Acetyl-1-methylcyclohexene	139.1119433	7.378	C9H14O	49.8
Sebacic acid	167.1068264	7.378	C10H18O4	54.1
Linolenyl alcohol	282.2792385	7.720683333	C18H32O	49
Taurocholic acid	1031.592704	7.76065	C26H45NO7S	54.2
Dibutyl sebacate	315.2530658	7.378	C18H34O4	55.3
Allyl hexanoate	157.1224654	7.378	C9H16O2	51.8
2-Ethyltoluene	121.1016302	7.378	C9H12	54.4
Farnesyl acetone	280.2636014	6.723733333	C18H30O	55.9
1-Monopalmitin	313.2737769	6.683933333	C19H38O4	49.2

Tetralin	133.1014293	6.582316667	C10H12	57.4
2-Linoleoyl Glycerol	337.2737042	6.5664	C21H38O4	48.1
Dodecanamide	200.2011997	6.49485	C12H25NO	48.4
Levistilide A	381.2058041	6.447633333	C24H28O4	51.6
2,6-Di-tert-butyl-P-benzoquinone	221.1538301	6.4397	C14H20O2	44.4
[8]-Paradol	307.2268927	6.3763	C19H30O3	50.1
Gorlic acid	279.2319661	6.36835	C18H30O2	50.6
Stearidonic acid	277.2163655	6.304516667	C18H28O2	52
Taurohyocholic acid	516.2993004	6.272533333	C26H45NO7S	54.9
Alantolactone	233.1537651	6.264533333	C15H20O2	53.6
Curcumenol	235.1694011	6.248533333	C15H22O2	54.6
4,7-Dimethyl-1-tetralone	175.1118359	6.248533333	C12H14O	54.6
Glycyrrhetic acid	471.3466765	6.19295	C30H46O4	57.6
Biliverdin	583.2555661	6.153366667	C33H34N4O6	53.1
Ectocarpene	149.1325914	6.153366667	C11H16	56.8
3-n-Butylphthalide	191.1067598	6.145366667	C12H14O2	53.1
Bisacumol	219.1744611	6.137383333	C15H22O	49.6
Nandrolone	275.2006199	6.105516667	C18H26O2	48
Corticosterone	347.2217971	6.097683333	C21H30O4	48.1
Hexadecanamide	288.2898269	6.07385	C16H33NO	46.5
6,7,4'-trihydroxyisoflavone	271.0601603	6.025383333	C15H10O5	52.7
Methyl indole-3-acetate	190.0866774	5.927666667	C11H11NO2	52.4
Dihydroactinidiolide	181.1224314	5.78685	C11H16O2	51.4
Senkyunolide F	207.1017835	5.7321	C12H14O3	55
Qing Hau Sau	283.1520101	5.690883333	C15H22O5	46.6
Paulownin	371.11227	5.687333333	C20H18O7	53.6
3-(4-Hydroxy-3-methoxyphenyl)prop anal	181.0860296	5.6838	C10H12O3	47
8-Methylretusin-7-O-glucopyranosid e	461.143742	5.530033333	C23H24O10	57.2
Perillyl alcohol	153.1275607	5.443566667	C10H16O	50.7
Diethyl phthalate	205.0863045	5.418316667	C12H14O4	49.2
O-Cymol	135.1170748	5.418316667	C10H14	54.3
2-aminoacetophenone	136.0759131	5.37465	C8H9NO	47.3
Herniarin	177.0547266	5.29305	C10H8O3	55
Parvisoflavone B	353.1017797	5.251183333	C20H16O6	45.9
Paeoniflorigenone	319.117365	5.202583333	C17H18O6	46.4
N-nornuciferine	282.1487897	5.202583333	C18H19NO2	57.4
7-Methylcoumarin	161.0597647	5.202583333	C10H8O2	47.1
3,4-dimethylbenzoic acid	133.0650238	5.202583333	C9H10O2	50.5
Cis-2,8-Menthadien-1-ol	153.1275298	5.083166667	C10H16O	46.6
Cathinone	132.0811593	5.058416667	C9H11NO	54.1
Tyramine	120.0813879	4.74105	C8H11NO	49.8

Ferulic acid	177.0547044	4.64615	C10H10O4	56.3
Loliolide	197.1174352	4.622833333	C11H16O3	52.2
Epinepetalactone	167.1070464	4.483033333	C10H14O2	46.5
Pelletierine	142.1229828	4.468433333	C8H15NO	48.5
Tryptophol	144.0812213	4.317483333	C10H11NO	50
4-Cresol	109.0653822	4.2321	C7H8O	54.9
Ginsenoside Rg1	151.0754829	4.227083333	C9H10O2	56.1
4-Ethylphenol	123.0807703	4.227083333	C8H10O	55.3
Daidzein	255.0651374	4.208516667	C15H10O4	57.6
2-hydroxyquinoline	146.0603824	4.189466667	C9H7NO	54.9
3-phenylpropionitrile	132.0812269	4.18295	C9H9N	49.6
Ethyl paraben	149.0598566	4.171533333	C9H10O3	51.6
Geranyl acetone	195.1748187	4.113883333	C13H22O	46.7
Coniferyl alcohol	181.0860962	4.0816	C10H12O3	47.2
Hydroxytyrosol	155.0704106	3.983416667	C8H10O3	55.1
Cinnamaldehyde	133.0650542	3.8568	C9H8O	53.6
Fraxinol	223.060248	3.68605	C11H10O5	54.7
5-hydroxyindole	134.0604463	3.6367	C8H7NO	55.8
3-hydroxypicolinic acid	140.034357	3.6247	C6H5NO3	54.7
4-hydroxybenzaldehyde	105.0341803	3.618683333	C7H6O2	56.1
Lycoperodine 1	217.0975894	3.575	C12H12N2O2	57.2
4-Aminobenzoic acid	138.0552406	3.505	C7H7NO2	54.3
Cyclo-(Leu-Thr)	197.1287086	3.494483333	C10H18N2O3	49.3
Indole-3-butyric acid	186.0915766	3.45205	C12H13NO2	47.6
Pseudoprotodioscin	342.1700146	3.341483333	C20H23NO4	48.9
11(13)-dehydroivaxillin	265.1435064	3.304616667	C15H20O4	51.6
Dihydro-alpha-ionone	195.1747056	3.1502	C13H22O	44.1
Indole	118.0656766	3.063733333	C8H7N	55.8
5'-S-Methyl-5'-thioadenosine	298.0970722	2.94475	C11H15N5O3 S	55.3
Noradrenaline	170.0813836	2.801633333	C8H11NO3	50.6
D-pantothenic acid	220.118383	2.7697	C9H17NO5	54.1
H-Glu-Tyr-OH	311.1240016	2.738766667	C14H18N2O6	55.3
2-phenylethylamine	122.0969348	2.603533333	C8H11N	53.3
6-methyluracil	127.0506786	2.57955	C5H6N2O2	56.2
5-hydroxymethyl-2-furancarboxylic acid	125.0237848	2.5052	C6H6O4	55.9
Dioscin	127.039447	2.435666667	C6H6O3	55.3
Panaxynol	120.0813699	2.228916667	C8H9N	53.8
L-phenylalanine	166.0866399	2.220983333	C9H11NO2	57.6
Senecioic acid	101.0604404	1.876966667	C5H8O2	51.7
Adenosine monophosphate	330.0597797	1.86095	C10H14N5O7 P	50.7

6-hydroxy-2-aminopurine	152.056877	1.852966667	C5H5N5O	55.5
Methacrylamide	86.0607317	1.604916667	C4H7NO	45.6
Guanosine-5'-monophosphate	364.0655697	1.3729	C10H14N5O8 P	55.8
M-Coumaric acid	165.0550001	1.324983333	C9H8O3	48.9
Octopamine	136.0760334	1.324983333	C8H11NO2	55.1
Benzofuran	119.049714	1.324983333	C8H6O	51.3
Niacinamide	123.0557954	1.084983333	C6H6N2O	50.6
D-Pyroglutamic acid	130.0503193	0.829816667	C5H7NO3	56.6
3,7-dihydropurin-6-one	137.0459989	0.814016667	C5H4N4O	54.6
4-aminophenol	110.060617	0.790316667	C6H7NO	48.7
Furfural	97.0290369	0.774516667	C5H4O2	54.1
3-hydroxycinnamic acid	165.0548743	0.726966667	C9H8O3	46
L-methionine	150.0586332	0.726966667	C5H11NO2S	53.5
3-Hydroxybenzaldehyde	123.0445214	0.726966667	C7H6O2	50.1
Proline betaine	144.1021286	0.663833333	C7H13NO2	52.6
Acetylcholine	146.1177412	0.624583333	C7H16NO2+	45.3
Levocarnitine	162.1127193	0.616816667	C7H15NO3	53.6
L-arginine	175.1192833	0.608833333	C6H14N4O2	54.8
L-asparagine	133.0610534	0.608833333	C4H8N2O3	57
Sarcosine	90.05564381	0.608833333	C3H7NO2	44.9
Laminine	189.1601693	0.576833333	C9H20N2O2	53.9
D-lysine	147.1130969	0.5052	C6H14N2O2	53.2
Acetophenone	121.065426	0.489683333	C8H8O	48.5
(S)-(+)-alpha-Phellandrene	137.1328184	0.409816667	C10H16	48.4
Isobutyric Acid	89.06043141	0.401816667	C4H8O2	44.7
13-OxoODE	295.2267464	6.486883333	C18H30O3	55.6
6-Hydroxykynurenic acid	206.0452638	3.349716667	C10H7NO4	52.4
Benzyl alcohol	91.05487023	6.582316667	C7H8O	48.2
Beta-eudesmol	245.1859203	3.582983333	C15H26O	48.6
Beta-farnesene	227.1757066	3.2059	C15H24	45.8
Cimifugin	307.1178008	4.89785	C16H18O6	59.5
D-Glucose	203.052996	0.616816667	C6H12O6	54.4
Decursin	329.1382164	6.304516667	C19H20O5	52.7
Dehydroabietic acid	301.2162917	6.4397	C20H28O2	49.4
Diethyl phthalate	391.2838967	7.011966667	C24H38O4	48.2
Farrerol	301.1068524	5.306166667	C17H16O5	54.8
Gibberellin A9	317.1744926	4.1524	C19H24O4	50
Glycitin	447.1280495	4.2715	C22H22O10	57.1
Hydroquinone	111.0446953	2.228916667	C6H6O2	54.3
Isoferulic acid	177.054745	4.771816667	C10H10O4	55.4
Kainic acid	214.1076907	2.857216667	C10H15NO4	49.1
Kobusone	223.1696143	6.04855	C14H22O2	44.4

Ligustilide	191.1068329	6.3444	C ₁₂ H ₁₄ O ₂	57.1
Methyl cinnamate	163.0755554	0.233633333	C ₁₀ H ₁₀ O ₂	49.7
Nicotinamide	123.055745	0.73495	C ₆ H ₆ N ₂ O	53.2
Oxindole	134.0603949	2.857216667	C ₈ H ₇ NO	57.3
P-Tolualdehyde	121.0653265	3.8568	C ₈ H ₈ O	50.9
Phenol	112.0762526	4.396466667	C ₆ H ₆ O	46.1
Riboflavin	377.1456814	3.812966667	C ₁₇ H ₂₀ N ₄ O ₆	54.5
Senkyunolide	193.1225322	6.248533333	C ₁₂ H ₁₆ O ₂	58.2
Sorbose	145.0498636	1.86095	C ₆ H ₁₂ O ₆	50.7
Styrene	105.0704941	4.227083333	C ₈ H ₈	54.1
L-Histidine	154.0612127	3.041483333	C ₆ H ₉ N ₃ O ₂	50.3
L-Glutamate	146.0447627	3.061583333	C ₅ H ₉ NO ₄	55.3
Alpha,beta-trehalose	341.1084222	3.125033333	C ₁₂ H ₂₂ O ₁₁	48.6
D-(+)-Malic acid	133.013117	3.166666667	C ₄ H ₆ O ₅	55.9
D-Arabinono-1,4-lactone	147.0288287	3.382666667	C ₅ H ₈ O ₅	45.6
Phenylacetonitrile	162.0549712	3.61695	C ₈ H ₇ N	45.6
Gallic acid	169.0133235	4.003933333	C ₇ H ₆ O ₅	55.2
Resorcinol	155.0339475	4.123866667	C ₆ H ₆ O ₂	44.1
Itaconic acid	129.0182268	4.129116667	C ₅ H ₆ O ₄	50.7
1h-indol-3-ol	178.0500227	4.155183333	C ₈ H ₇ NO	51.3
Aspirin	179.0340347	4.322016667	C ₉ H ₈ O ₄	46.3
3-methylindole	176.0707426	4.6713	C ₉ H ₉ N	55.4
2-Hydroxycinnamaldehyde	147.0440392	5.176066667	C ₉ H ₈ O ₂	44.6
L-(-)-3-Phenyllactic acid	165.0547033	5.1834	C ₉ H ₁₀ O ₃	53.3
Kojic acid	141.0182534	5.191233333	C ₆ H ₆ O ₄	54
Protocatechuic aldehyde	183.0291003	5.652816667	C ₇ H ₆ O ₃	51.8
2-Methoxybenzaldehyde	135.0440129	5.8784	C ₈ H ₈ O ₂	45.8
7,8-dihydroxyflavone	253.0501577	5.928616667	C ₁₅ H ₁₀ O ₄	46.4
Orcinol	169.0497586	5.988066667	C ₇ H ₈ O ₂	46.8
2-methoxycinnamaldehyde	207.065473	6.057033333	C ₁₀ H ₁₀ O ₂	45.9
Nortricycloekasantalic acid	225.1125854	6.0874	C ₁₁ H ₁₆ O ₂	47.8
3,4-Dihydroxybenzoic acid	153.0183401	6.535	C ₇ H ₆ O ₄	51.4
Ginsenoside Re	165.0183132	6.635133333	C ₈ H ₆ O ₄	46.8
Suberic acid	173.0810207	7.570783333	C ₈ H ₁₄ O ₄	53.1
6-Methyl-7-(3-oxobutyl)-bicyclo[4.1.0]heptan-3-one	239.1284607	7.965316667	C ₁₂ H ₁₈ O ₂	47.7
Azelaic acid	187.0968039	7.979416667	C ₉ H ₁₆ O ₄	49.1
P-Salicylic acid	137.0233392	7.99	C ₇ H ₆ O ₃	57.7
Sorbic acid	93.03352468	7.99	C ₆ H ₈ O ₂	53.1
Isophorone	183.1019032	7.58955	C ₉ H ₁₄ O	55.3
Scopoletin	191.0342102	7.49195	C ₁₀ H ₈ O ₄	50.8
2,3-Dihydroxybenzoic acid	153.0183157	6.984716667	C ₇ H ₆ O ₄	54.8
Syringic acid	197.0447753	6.92795	C ₉ H ₁₀ O ₅	53.7

Cuminaldehyde	193.0861382	6.679666667	C10H12O	54
Pimelic acid	159.0653407	6.679666667	C7H12O4	50.5
(4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-Docosahexaenoic acid	327.2325093	6.5757	C22H32O2	54
3-hydroxy-1-(4-hydroxyphenyl)propan-1-one	165.0548018	6.283516667	C9H10O3	49.6
Salicylic acid	137.0233157	6.197333333	C7H6O3	50.9
Tert-Butylhydroquinone	165.0910903	6.118733333	C10H14O2	44.9
6-Hydroxyindole	178.0500429	5.976216667	C8H7NO	52
Piperonal	195.0291767	5.96125	C8H6O3	48.5
Gentisic acid	153.0182664	5.88305	C7H6O4	55.2
Homogentisic acid	167.0340463	5.85955	C8H8O4	50
5,7-Dimethoxyflavanone	329.1026458	5.825033333	C17H16O4	53
Arecoline	200.0919183	5.820766667	C8H13NO2	52.4
Deoxyvasicinone	231.0768796	5.2501	C11H10N2O	49.3
4-Coumaric acid	163.0390468	5.150533333	C9H8O3	51.7
Patulin	153.0182597	4.85645	C7H6O4	50.4
P-Anisic acid	151.038993	4.713716667	C8H8O3	52.7
Isoquinoline n-oxide	190.0500951	4.706916667	C9H7NO	50.4
4-Pyridoxic acid	182.0449872	4.105033333	C8H9NO4	53.3
Acetosyringone	255.0868564	4.094183333	C10H12O4	47.1
Anthranilic acid	182.0449355	3.87275	C7H7NO2	50.1
Aconitic acid	173.0082318	3.5094	C6H6O6	55.8
Maleic acid	115.0025546	3.166666667	C4H4O4	52.8
Myo-Inositol	179.0551784	3.107383333	C6H12O6	52.6
Dulcitol	181.0708511	3.06875	C6H14O6	49.9
L-Aspartic Acid	132.0290507	3.061583333	C4H7NO4	54.4
Benzoic acid	167.0343023	6.938916667	C7H6O2	55.8
Caffeic acid	179.0341394	6.906416667	C9H8O4	57.8
Malonic acid	163.023824	3.11745	C3H4O4	47.1
Succinic acid	117.0182455	3.5176	C4H6O4	52.4

Table S2 UPLC-MS operating parameters for Shuyu Wan component analysis.

Description	Parameters
Scan type (m/z)	70-1050
Sheath gas flow rate (arb)	50
Aux gas flow rate (arb)	13
Heater temp (°C)	425
Capillary temp (°C)	325
Spray voltage (+) (V)	3500
Spray voltage (-) (V)	-3500
S-Lens RF Level	50
Normalized collision energy (%)	20, 40, 60
Resolution (Full MS)	60000
Resolution (MS2)	7500

Table S3 Sample-level COG functional abundance of gut microbiota (FB_A: ctrl, FB_D: H-SYW+RMPI-14,FB_E: RMPI-14)																				
COG_ID	COG_Description	Function	FB_A1	FB_A2	FB_A3	FB_A4	FB_A5	FB_A6	FB_D1	FB_D2	FB_D3	FB_D4	FB_D5	FB_D6	FB_E1	FB_E2	FB_E3	FB_E4	FB_E5	FB_E6
COG0642	Histidine kinase	T:Signal transduction mechanisms	356631.06	299625.5	365828.2	313430.85	339371	299658.47	276910.11	316363.69	281353.9	373113.64	371255.2	342288.77	293482.08	383963.5	219562.05	380298.36	299429.15	333918.21
COG0745	regulatoR	T:Signal transduction mechanisms	353249.07	341787.96	353064.83	321750.25	333273.75	301786.93	256663.3	320789.7	270089.05	368853.11	355069.79	331444.73	274571.85	379240.83	201435.07	364492.16	290049.45	331061
COG4974	Site-specific tyrosine recombinase, which acts by catalyzing the cutting and rejoining of the recombining DNA molecules. The XerC-XerD complex is essential to convert dimers of the bacterial chromosome into monomers to permit their segregation at cell division. It also contributes to the segregational stability of plasmids (By similarity)	L:Replication, recombination and repair	344851.76	310921.72	364067.35	323625.09	329279.19	275457.73	278990.47	311642	270164.71	360502.29	356328.37	343121.95	284160.05	362910.86	233611.77	358063.9	281161.56	296472.13
COG0534	Mate efflux family protein	V:Defense mechanisms	323629.91	206536.31	362690.09	247556.82	330845.36	235492.89	275489.56	306495.37	270665.93	366396.81	363718.87	340177.12	261601.79	351258.62	221113.96	362663.92	277019.22	275171.13
COG1132	(ABC) transporter	V:Defense mechanisms	327241.67	274650.81	344774.92	277147.79	311881.77	258294.01	240212.15	311970.5	251170.5	353025.37	336059.14	325877.51	254643.83	365429.86	183903.03	356072.18	263806.52	293932.12
COG2207	Transcriptional Regulator AraC Family	K:Transcription	319178.55	213615.89	343567.02	256902.32	326042	230831.22	279593.02	299132.63	268278.73	355435.83	351486.2	331202.68	264476.69	348924.72	240505.06	348622.53	264065.14	243956.69
COG1131	(ABC) transporter	V:Defense mechanisms	320371.17	288343.24	334121.57	283442.46	306194.11	267415.53	238940.41	307319.27	248808.33	339104.18	326504.79	312811.77	257330.5	353672.85	188679.96	339872.88	258568.95	295856.1
COG0438	Glycosyl transferase (Group 1	M:Cell wall/membrane/envelope biogenesis	295644.3	369139.85	293744.03	321078.3	280926.09	286687.74	234632.3	278476.89	237175.39	303642.44	280210.66	292683.95	264812.59	315199.32	230224.06	279108.95	251080.86	290562.7
COG1595	RNA Polymerase	K:Transcription	294484.27	197009.25	341772.82	227953.56	307108.29	223898.86	254138.88	274442.61	258052.33	334289.32	324589.63	319419.16	248476.86	308950.32	232211.96	315935.73	247051.57	240958.2
COG1309	Transcriptional regulator	K:Transcription	303465.76	214246.29	327570.34	248830.6	300072.67	224667.77	234414.5	289957.62	230534.21	333751.02	326733.88	304752.56	238778.12	338301.73	169866.47	331564.48	237629.2	240939.42
COG1136	(ABC) transporter	V:Defense mechanisms	294413.45	293477.51	303722.25	273374.12	283408.04	244893.9	214450.47	272207.44	221496.44	314135.27	293273.65	286537.66	232852.53	327980.75	162741.26	306014.4	232523.07	267393.82
COG0463	Glycosyl transferase, family 2	M:Cell wall/membrane/envelope biogenesis	282140.04	260687.15	293902.61	263914.3	287605.23	223463.34	236816.96	288699.19	229950.24	313116.74	292219.73	287951.13	237442.49	321743.88	206402.4	296996.13	239793.13	240611.75
COG1609	Transcriptional regulator	K:Transcription	284579.11	302901.33	273874.41	281456	274660.25	213386.99	192262.79	270890.06	186272.2	305084.82	284890.56	260164.94	200121.8	327667.37	131187.64	285623.31	200000.59	210289.12
COG0583	Transcriptional regulator	K:Transcription	275833.31	242598.23	246375.67	251897.49	233099.86	206244.72	197526.03	245514	191354.9	260392.72	279180.58	234662.83	216418.55	293297.05	129162.74	297974.68	211469.62	242008.49
COG1476	Transcriptional regulator	K:Transcription	261088.14	188922.16	295152.35	203708.47	257707.98	181824.44	181744.5	242455.97	179293.22	303361.86	290002.76	261410.99	187232.66	293139.79	117386.75	276734.95	195911.47	204400.47
COG1846	Transcriptional regulator	K:Transcription	260241.14	262503.85	227683.83	256973.69	217455.66	197461.18	173326.37	231867.6	170606.31	245563.7	247605.18	211737.22	187932.91	272353.02	126322.67	276055.71	189753.24	228651.97
COG1653	transporter activity	G:Carbohydrate transport and metabolism	255217.37	142561.05	272465.34	186739.71	260741.88	148548.38	182438.99	266318.68	173100.02	296385.51	276988.75	254991.36	186435.93	308512.07	108228.03	286161.97	177549.34	163123.86
COG1028	Dehydrogenase reductase	S:Function unknown	242697.92	204721.49	219830.67	222997.58	221714.71	189474.82	189059.27	234087.53	181075.03	250480.12	246053.91	219587.04	201610.24	253735.21	141591.01	278284.21	194850.83	210774.3
COG1961	Resolvase	L:Replication, recombination and repair	219863.72	121552.69	293656.35	139371.01	235413.93	143547.19	169420.22	212241.16	171178.4	284018.38	258982.8	250758.07	165025.85	254558.95	115854.89	238857.53	183872.09	185845.13
COG0395	Binding-protein-dependent transport systems inner membrane component	G:Carbohydrate transport and metabolism	237628.12	128165.71	249939	175077.46	247748.63	130833.04	169143.58	252689.84	151004.52	280361.85	260906.5	235307.77	171257.02	286160.32	94538.87	259631.63	152204	129153.52
COG3279	Regulator	T:Signal transduction mechanisms	228707.7	181287.94	238206.42	203174	240755.46	140773.83	169969.06	225143.8	151186.61	266126.93	245437.07	226024.91	160316.48	264702.74	97015.21	245294.26	152670.84	151577.22

COG0789	Transcriptional regulator	K:Transcription	238574.25	162347.75	229535.93	196932.66	214411.82	142257.07	165329.9	226520.44	152275.12	245331.97	239806.6	204788.63	174438.01	267083.13	98650.83	270082.93	163707.71	176991.33
COG1175	binding-protein-dependent transport systems inner membrane Component	P:Inorganic ion transport and metabolism	229874.62	125434.09	245041.5	174187.12	244588.63	129326.82	161223.15	246267.58	143015.49	276333.13	256616.17	230560.31	163041.77	282366.48	85790.71	254138.23	145509.5	121791.02
COG2199	Diguanylate cyclase	T:Signal transduction mechanisms	217483.2	154794.21	219186.2	200130.12	205852.53	147385.94	140612.11	216237.56	152363.43	233609.52	236940.58	201152.79	149411.34	270911.42	83036.04	266181.74	165121.49	177604.37
COG1670	acetyltransferase	J:Translation, ribosomal structure and biogenesis	215351.75	155052.79	207528.93	196035.33	207683.39	134433.14	153262.49	211102.98	151676.67	232393.46	222626.41	200543.28	144856.38	242711.4	106036.91	243282.81	148349.37	148992.78
COG0778	nitroreductase	C:Energy production and conversion	199415.32	150788.79	172743.61	190325.5	175780.51	138273.56	158144.77	180706.84	155176.86	187467.83	194877.6	172475.54	152302.56	208262.18	131221.6	220278.59	142855.76	146069.02
COG0524	pfkb domain protein	G:Carbohydrate transport and metabolism	197587.38	181078.01	179102.25	195806.38	181466.99	135157.8	143224.31	184268.13	133006.84	194829.63	194485.02	168328.61	149456.85	216580.84	111219.26	213562.37	141844.47	144980.45
COG2244	Polysaccharide biosynthesis protein	M:Cell wall/membrane/envelope biogenesis	175854.86	189970.61	174418.27	177602.18	167703.19	149821.14	140515.36	158043.65	136141.63	177248.19	170083.27	169492.76	147444.94	187401.71	124322.33	178364.97	148064.36	152806.32
COG0488	(ABC) transporter	S:Function unknown	174122.44	178167.57	174750.33	166986.31	164735.75	149252.66	141526.03	163448.86	136377.91	181832.38	171767.01	167369.48	144916.96	191923.54	118428.68	177602.52	144559.91	155692.31
COG0561	,hydrolase	S:Function unknown	164705.84	164054.77	169775.66	146702.86	162986.41	127160.95	124288.41	166268.21	125211.05	189334.17	169113.1	167213.36	123929.64	204423.46	103802.74	175109.67	136459.78	156560
COG0451	Nad-dependent epimerase dehydratase	M:Cell wall/membrane/envelope biogenesis	156944.74	109750.71	186554.86	131078.35	171146.17	119390.79	142631.12	171925.57	130917.78	190836.45	174282.34	177377.76	143016.81	187958.11	105864.56	177798.95	137955.45	136031.92
COG1879	Periplasmic binding protein LacI transcriptional regulator	G:Carbohydrate transport and metabolism	176027.19	93944.75	188196.68	137656.34	188506.99	85023.69	119740.95	186545.37	111805.22	210481.64	200996.77	178011.52	121951.19	225577.09	53013.59	210006.2	128930.12	108907.17
COG1940	ROK family	G:Carbohydrate transport and metabolism	171060.14	170222.69	158042.91	169483.93	161202.18	122282.92	120271.2	165014.17	115364.81	176186.13	171798.7	149835.1	119471.17	191876.62	86542.19	176418.85	126625.12	128570.47
COG0673	oxidoreductase	S:Function unknown	176247.28	116906.92	151120.09	162480.45	161132.34	105675.61	135278.76	174900.72	122613.28	178123.4	181194.77	146792.14	129216.14	200718.45	85624.03	214936.71	115234.15	112864.53
COG0456	acetyltransferase	S:Function unknown	161144.38	138059.62	176157.11	140172.19	162301.83	122346.46	112348.87	156606.48	118453.31	186096.89	172680.01	167642.99	118012.6	192128.65	77435.23	176128.46	134170.78	145073.12
COG0840	Methyl-accepting chemotaxis	S:Function unknown	143202.3	103899.39	215163.2	110900.19	186151.89	114095.61	99093.09	154943.6	104791.81	224333.3	196338.6	200284.39	97745.99	195482.9	63091.11	166114.2	144079.2	128974.4
COG0436	aminotransferase	E:Amino acid transport and metabolism	148374.57	131047.22	150050.76	134339.27	144428.11	123158.45	129829.75	141935.49	127788.36	155617.53	151602.2	147697.87	134996.46	165297.37	113931.16	159122.89	130678.63	138496.08
COG0366	alpha amylase, catalytic	G:Carbohydrate transport and metabolism	152502.38	155487.65	155260	149314.84	154182.6	111894.33	110336.17	150516.39	102336.42	171323.37	156792.37	148578.8	116417.48	180489.41	83356.08	155350.59	111192.02	109071.93
COG0564	pseudouridine synthase activity	J:Translation, ribosomal structure and biogenesis	139618.9	139175.81	139872.76	132892.15	133823.69	119628.42	111207.86	130180.03	111011.57	146464.93	139650.62	135772.1	114682.77	153169.85	99406.08	142753.76	115201.44	128216.23
COG0664	transcriptional regulator, crp fnr family	T:Signal transduction mechanisms	141720.49	101336.67	138876.62	121890.79	132025.27	107652.61	126963.59	121175.93	116602.03	140891.54	149592.34	129563.06	120387.48	141758.19	107080.88	156064.15	115623.02	116642.71
COG3655	Transcriptional regulator	K:Transcription	145171.4	95657.36	173786.42	105462.22	149014.66	92236.58	107560.31	139433.93	97013.67	170330.18	155720.94	148407.56	108708.61	159052.46	63604.43	147521.6	112143.02	105338.46
COG1307	degv family	S:Function unknown	140020.16	151757.02	136865.5	132750.67	126221.04	109821.09	88207.11	123384.27	93021.6	141254.85	135561.72	124150.95	96702.48	154519.21	62076.31	135048.17	102910.49	122542.6
COG0550	Releases the supercoiling and torsional tension of DNA, which is introduced during the DNA replication and transcription, by	L:Replication, recombination and repair	125043.76	124952.35	138577.42	114652.05	121260.87	96957.93	103535.81	115359.52	99080.81	133204.68	123309.38	127621.67	109028.93	133785.04	86319.07	129150.77	108205.18	108763.98

	transiently cleaving and rejoining one strand of the DNA duplex. Introduces a single-strand break via transesterification at a target site in duplex DNA. The scissile phosphodiester is attacked by the catalytic tyrosine of the enzyme, resulting in the formation of a DNA-(5'-phosphotyrosyl)-enzyme intermediate and the expulsion of a 3'-OH DNA strand. The free DNA strand then undergoes passage around the unbroken strand, thus removing DNA supercoils. Finally, in the religation step, the DNA 3'-OH attacks the covalent intermediate to expel the active-site tyrosine and restore the DNA phosphodiester backbone (By similarity)																			
COG1 191	Sigma factors are initiation factors that promote the attachment of RNA polymerase to specific initiation sites and are then released (By similarity)	K:Transcription	130584.4	79274.68	155089.67	94545.63	133738.6	91368.86	91375.13	121641.02	97222.02	154633.33	146590.12	136824.35	93772.09	147942.83	60382.72	146369.17	99398.92	106435.02
COG1 725	Transcriptional regulator, GntR family	K:Transcription	128926.05	71551.7	154551	88988.38	135885.18	77663.71	93762.38	132902.93	91935.15	160038.76	144409.2	139403.09	94769.65	158395.74	59311.54	147743.81	94812.48	95724.5
COG0 601	Binding-protein-dependent transport systems inner membrane component	P:Inorganic ion transport and metabolism	142875.03	119659.03	116929.17	136588.57	117510.2	92273.95	85218.71	135889.98	83550.8	130803.45	130732.22	107939.69	96380.82	154411.25	47042.27	162530.41	93391.13	103139.39
COG4 753	Transcriptional regulator (AraC family)	T:Signal transduction mechanisms	145743.24	81084.02	117183.18	139108.18	135921.78	71411.74	90839.1	145032.54	76801.44	150704.98	158184.62	115222.6	85554.4	173016.44	37325.02	183798.4	74284.9	68571.46
COG0 860	n-acetylmuramoyl-l-alanine amidase	M:Cell wall/membran e/envelope biogenesis	125343.82	93617.12	135271.23	103971.98	127373.1	89107.3	96089.25	124176.26	95521.42	139487.99	134185.71	124606.29	94631.93	146900.49	74615.73	138920.16	97759.93	100434.03
COG0 628	Membrane	S:Function unknown	124003.15	115492.43	123810.5	113735.55	116850.52	94510.66	94340.22	122020.16	91111.39	132686.69	123817.37	115863.17	98314.93	143346.24	74112.75	129546.6	97294.36	109185.96