

Table S1. Metabolite Detection Information Table and CV Value Statistics of this Project

Compound ID	Compounds	Class	Retention time (min)	m/z	CV_QC (%)	CV_(HS+YS) (%)	CV_HS (%)	CV_YS (%)
Ma086	Moracinflavan F 8-	Flavonoids	3.96	369.17	5.3	12.6	13.9	11.2
Ma150	Azabicyclo[3.2.1]octan-3-ol	DNJ alkaloids	9.96	128.11	2.8	27.1	26.2	16.8
Ma018	Morusignin C.	Flavonoids	1.55	365.04	5.9	23.6	28.9	17.2
Ma146	apigenin-7-O-glucoside	Flavonoids	9.46	433.11	3.8	26.6	25.7	17.5
Ma122	Moracin B	Flavonoids	6.66	269.08	4.5	24.8	27.1	18.8
Ma092	kaempferol	Flavonoids	4.08	287.06	4.2	21.4	21.7	20.2
Ma063	Sanggenol F	Flavonoids	3.35	421.16	10.8	28.9	35.5	20.4
Ma145	Linolenic acid 1-	Lipids-fatty acid	9.26	261.22	25.6	33.6	44.1	20.7
Ma087	Hydroxyanthraquinone	Anthraquinones	4.01	225.05	2.6	38.1	38.6	20.8
Ma051	Sanggenon J 14-	Flavonoids	2.85	527.18	12	27	31	20.9
Ma101	methoxydihydromorusin	Flavonoids	4.69	453.19	3.3	33	34.2	22
Ma068	Moracin C 3,5-dglc	Flavonoids	3.51	635.23	4.6	25.7	23.8	22.3
Ma143	cyanidin-3-sophoroside	Anthocyanin	8.59	594.16	2.6	39.6	49.8	22.5
Ma009	1-deoxynojirimycin 2',4',5,7-	DNJ alkaloids	0.61	146.08	2.7	34.1	31.9	23
Ma053	Tetrahydroxy-3-methoxyflavone.	Flavonoids	3	317.07	3.3	34.1	30.7	23.2
Ma004	2-O- $\alpha$ -D-galactopyranosyl-1-deoxynojirimycin	DNJ alkaloids	0.52	326.15	2.6	25	23.5	23.2

Ma023	2'-hydroxy-4'-methoxyl-2H-(2'',2'''-dimethyl-3''-hydroxy)-pyran-(5'',6''': 8,7)-flavane	Flavonoid derivatives	2.14	339.16	3	26.3	26.5	24
Ma006	(1R,2R,3R,4S,5R,6R)-8-Azabicyclo[3.2.1]octane-1,2,3,4,6-pentol	DNJ alkaloids	0.59	192.09	2.4	28.3	32.2	24.3
Ma077	Dioxycedra flavone A	Flavonoids	3.7	491.11	3.9	29.1	32.1	25.7
Ma001	2-[2-Formyl-5-(hydroxymethyl)-1H-pyrrol-1-yl]propanoic acid	DNJ alkaloids	0.51	198.08	3.3	33.2	39.4	25.7
Ma033	Hesperetin	Flavonoids	2.47	303.09	4	22.6	18.3	25.9
Ma075	2',3,4',5,7-Pentahydroxyflavone	Flavonoids	3.68	303.05	3.3	34.5	31.4	26.1
Ma035	4',7-Dihydroxy-8-prenylflavan	Flavonoid derivatives	2.5	349.12	3.1	25.5	25.1	26.1
Ma097	2',4',7-Trihydroxy-8-(2-hydroxyethyl)flavan 7-me	Flavonoids	4.36	317.14	3.3	29.9	28.2	26.3
Ma003	cyanidin-3-rutinoside	Anthocyanin	0.52	578.16	2.6	29	21.7	26.7
Ma036	Moracinflavan C	Flavonoids	2.5	369.11	4.8	41.2	41.3	26.8
Ma129	Morusyunnansin F.	Flavonoids	7.37	309.15	6.7	27.8	28.6	27.1

Ma015	8-Azabicyclo [3.2.1]octane-2,3,4-triol	DNJ alkaloids	1.02	198.05	2.8	29.7	31.3	27.2
Ma117	Nigrasin J	Flavonoids	5.78	491.17	8.1	35.6	36.9	28.2
Ma065	Moracin Q+	Flavonoids	3.46	393.11	4.7	33.5	37.5	28.9
Ma026	umbelliferone	Coumarins and its derivatives	2.32	163.04	2.6	48.4	45.9	29.7
Ma069	tyrosine	Amino acids	3.52	164.07	2.5	58.9	66.1	29.7
Ma111	Nigrasin A	Flavonoids	5.56	477.15	7.4	35.8	41.2	30
Ma135	Guangsangon B1	Flavonols	7.69	567.2	17.8	34.1	37.8	30
Ma104	2',4',7-Trihydroxy-3-prenylflavone	Flavonoid derivatives	4.84	339.12	2.9	39	35.2	30.2
Ma070	Dihydromorin	Flavonoids	3.64	287.06	15.7	28.2	24.6	31.1
Ma096	Cathayanon I	Flavonoids	4.29	441.19	3.9	32.4	32	31.5
Ma047	Taxifolin	Flavonoids	2.77	287.06	13.8	40.6	45.4	31.6
Ma072	kaempferol-3-O-rutinoside	Flavonoids	3.64	617.15	4.3	37.5	41.2	31.8
Ma014	2',4',7-Trihydroxy-8-(2-hydroxyethyl)flavan 7-me-2-glc	Flavonoids	0.7	517.15	3.4	40.6	42.6	31.8
Ma042	morusin hydroperoxide	Flavonoids	2.71	453.15	6.4	37.7	43.1	32.1
Ma114	Sanggenol E	Flavonoids	5.66	559.31	9.1	54.6	56.3	32.7
Ma022	(2S,5R)-5-Hydroxy-2-piperidinecarboxylic acid	DNJ alkaloids	2.03	593.18	17.9	60.8	85.8	34.4

Ma058	8-Azabicyclo [3.2.1]octane-2,3,6-triol	DNJ alkaloids	3.16	160.1	2.9	59.8	68.1	34.4
Ma113	Dihydroisocycloartomin.	Flavonoids	5.66	473.16	15.6	40.7	46.7	34.6
Ma038	7,2'-dihydroxy-4'-methoxy-8-prenylflavan	Flavonoid derivatives	2.56	379.13	3.1	39.4	43.1	35
Ma130	Morusimic acid B	DNJ alkaloids	7.43	312.25	6.3	29.3	20.5	36.5
Ma080	Sanggenon T.	Flavonoids	3.79	735.24	13.3	34.9	30.7	38
Ma057	Sanggenon K	Flavonoids	3.07	527.18	12.3	40.6	42.9	38.6
Ma094	Mortatarin C	Flavonoids	4.17	441.19	5.8	39.1	39.7	38.6
Ma020	Sanggenon B	Flavonoids	1.87	593.18	10.9	38.3	34.9	40.1
Ma049	5,7,2',4'-tetrahydroxy-3-methoxyflavone	Flavonoids	2.85	317.07	3.5	50.5	47.8	41.3
Ma123	Isobavachalcone	Flavonoids	6.67	307.13	4	42.8	37.9	42.1
Ma095	kaempferol	Flavonoids	4.24	287.06	4.2	39.4	33.9	44.4
Ma011	4-O- $\alpha$ -D-Galactopyranosylcalystegin	Others	0.62	320.13	30.4	45.6	46.6	44.6
Ma074	Moracin M	Flavonoids	3.68	243.06	4.6	46.4	39.4	44.7
Ma071	2',4',7-Trihydroxy-8-(2-hydroxyethyl)flavan-4-me-2-glc	Flavonoids	3.64	479.19	3.3	77.9	78.1	45.8
Ma010	1, 4-dideoxy-1, 4-imino-D-arabinitol	DNJ alkaloids	0.61	134.08	93.6	56.9	64.5	46.1
Ma061	Albocatalol	Flavonoids	3.24	471.14	3.7	44.2	40.7	46.8

Ma133	Moracin I	Flavonoids	7.58	325.14	4.6	48.7	36.5	47.1
Ma137	2',4'- Dihydroxy- 7-methoxy- 8- prenylflava n	Flavonoid derivatives	7.98	323.17	3	69.9	67.9	48.1
Ma013	Mulberrofu ran H	Phenolics	0.67	443.15	48.8	45.7	42.8	48.2
Ma079	6-methoxy- 5,7,4'- trihydroxyi soflavone	Isoflavonoi ds	3.79	301.07	24.1	59.7	63.9	49.9
Ma149	Sanggenof uran A.	Flavonoids	9.81	443.26	8.5	54.3	48.8	51.3
Ma005	(1R,2S,3R, 4S,5S)-8- Azabicyclo [3.2.1]octa ne-1,2,3,4- tetrol	DNJ alkaloids	0.58	363.13	3.2	61.5	71.8	51.7
Ma059	Moracinfla van B	Flavonoids	3.17	313.14	4.8	73.4	71.4	53.4
Ma082	Mulberrofu ran Y (2S)-8- hydroxyeth yl-7,4'-	Phenolics	3.82	391.19	60.4	82	118.1	53.5
Ma105	dimethoxyf lavane-2'- O-β-D- glucopyran oside	Flavonoids	4.95	515.26	3.2	56.7	55.7	54.9
Ma017	Moracinosi de M.	Flavonoids	1.49	441.16	5.5	60.6	62.8	56.4
Ma054	Heneicosan oic acid	Lipids- fatty acid	3	365.28	24.6	59.5	60.1	57.6
Ma028	Ferulic acid	Phenylprop anoids	2.32	177.05	69.6	72.3	87.9	58.3
Ma025	(2R,3S)- guibourtini dol-3-O-α- D- apiofuranos yl-(1→6)- O-β-D- glucopyran oside	Flavonoids	2.28	575.18	3.1	55.3	43.2	59.1

Ma148	Mongolicin C	Stilbenes	9.78	617.12	412.3	92.1	136.7	60.1
Ma083	Sanggenon E	Flavonoids	3.88	815.24	11.6	78	66.1	61.9
Ma067	Wittifuran H.	Others	3.5	517.22	46.7	79.4	90.2	62.3
Ma124	2',4'-dihydroxy-7'-methoxy-8-prenylflavan	Flavonoid derivatives	6.74	323.17	2.9	66.3	56.5	65.6
Ma078	Dihydrocycloartomon.	Flavonoids	3.75	451.18	14.8	70.5	67.7	66.6
Ma084	Morusignin E.	Flavonoids	3.95	413.16	6.1	105.7	141.4	67.5
Ma040	isopropylmalic acid	Organic acid and its derivatives	2.61	199.06	30.2	60.7	48.7	68.2
Ma008	(1RS,3RS,5SR)-8-Azabicyclo[3.2.1]octan-3-ol	DNJ alkaloids	0.59	128.11	5.9	64.4	55	69.4
Ma066	Kuwanol D	Stilbenes	3.49	391.19	113	97.9	131.4	73.1
Ma120	isobavachin	Flavonoids	6.58	307.13	4.1	69.5	42.1	74.2
Ma136	Cycloartomonin.	sterols	7.97	471.14	95.9	102	133.4	74.7
Ma044	DL-arginine	Amino acids	2.75	175.12	2.4	73.9	69.7	76.2
Ma116	Palmitic acid	Lipids-fatty acid	5.74	295.2	27.5	65.8	53.7	76.2
Ma062	Moruslupe noic acid B.	Flavonoids	3.34	477.33	6.4	59	40.7	77
Ma127	Sanggenofuran B	Flavonoids	7.09	307.13	8.5	65.6	48.2	80.9
Ma144	Stearic acid	Lipids-fatty acid	9.05	323.24	29.3	108.9	123.9	84.9
Ma030	methylcaffeate	Others	2.32	195.07	34.7	105.7	127.8	85.7
Ma093	Guangsangon L	Flavonols	4.09	515.11	22.9	91.5	97.6	86

Ma139	(E)-4-isopentenyl-3,5,2',4'-tetrahydroxystilbene	Stilbenes	8.39	335.13	97.3	96	101.6	91.2
Ma016	fagomine	DNJ alkaloids	1.41	130.09	2.7	89.8	64.2	91.8
Ma056	Chaminic acid.	Phenolamides	3.05	149.1	48.4	101.6	111.4	91.9
Ma007	D-glucopyranose	Others	0.59	219.03	35.6	77.6	62.7	93.7
Ma037	3,4',5,7-Tetrahydroxy-6,8-diprenylflavanone	Flavonoids	2.55	425.2	3.4	94.5	72.5	96.1
Ma126	Guangsangon I.	Flavonols	6.9	625.17	20	105.5	85.5	100.9
Ma115	Moracenin D.	Flavonoids	5.73	711.25	4.4	90.5	68.1	102.3
Ma024	artoindonesianin O	Others	2.25	363.1	37	125.4	140.3	103.2
Ma108	2',7-Dihydroxy-4'-methoxy-8-prenylflavan.	Flavonoid derivatives	5.18	341.18	3	343.4	252.8	103.5
Ma019	D-pantothenic acid	Vitamines	1.79	242.1	-	143.5	182.2	112.6
Ma034	p-Coumaric acid	Phenylpropanoids	2.5	147.04	74.7	130.1	143.5	115.6
Ma012	4-Benzyl-1,4-dihydro-3-oxo-3H-pyrrolo[2,1-c][1,4]oxazine-6-carboxaldehyde	DNJ alkaloids	0.63	256.1	3.4	132.8	99.2	120.1
Ma085	Moracinflavan A	Flavonoids	3.96	339.16	4.7	303.9	339.3	122.2
Ma089	quercetin	Flavonoids	4.02	303.05	8.1	119.4	113	122.8
Ma140	m-Hydroxybenzoic acid	Phenylpropanoids	8.44	121.03	82.3	170.7	187.8	122.8

Ma041	Mulberrosi de F.	Stilbenes	2.62	589.15	282.8	127.3	111.8	123.9
Ma039	Mornigrol E.	Flavonoids	2.59	439.18	5.5	101.2	79.3	128.8
Ma099	cis- Mulberrosi de A.	Flavonoids	4.45	569.19	14.2	96.1	68.7	134.2
Ma027	Quinic acid	Phenylprop anoids	2.32	175.06	79.6	183.3	164.3	139.1
Ma106	Dihydroox yresveratro l	Stilbenes	4.97	269.08	111.4	248.9	219.7	150.5
Ma128	3'-O- $\beta$ -D- Glucopyran oside, 4-O- [ $\beta$ -D- glucopyran osyl- (1 $\rightarrow$ 6)- $\beta$ - D- glucopyran oside] mulberr	polysaccha ride	7.28	753.22	88.8	202.6	215.9	150.9
Ma073	Notabilisin D	Flavonoids	3.66	543.2	16.3	163	86.8	152.7
Ma132	3'-O-[ $\beta$ -D- Glucopyran osyl- (1 $\rightarrow$ 6)- $\beta$ - D- glucopyran oside], 4- O- $\beta$ -D- glucopyran oside Mulberry	polysaccha ride	7.54	753.22	88	143.5	135.9	153.1
Ma045	5,7- dihydroxyc hromone	Flavonoids	2.76	179.03	3.6	112.7	83.4	154.4
Ma103	Australone B	Others	4.72	865.3	42.7	109	75	159.8
Ma100	Mulberrofu ran X	Phenolics	4.46	485.23	60.1	188.6	193.3	169.5
Ma029	6,7- dihydroxyc oumarin	Phenylprop anoids	2.32	179.03	68.4	162.7	154	173.5
Ma050	Albafuran A	Stilbenes	2.85	401.17	98.9	209.8	236.7	178.1
Ma110	Rubraflavo ne D	Flavonoids	5.43	511.21	8.3	120	77.4	198.4
Ma043	Yunanenso l A	Others	2.74	441.19	48.4	175.3	148.7	199.5

Ma109	Wittifuran B	Others	5.34	415.15	46.1	179.5	154.5	207.8
Ma055	Guangsang on A.	Flavonols	3.01	705.21	17	169.7	135.9	208.1
Ma088	Soroceal B	Others	4.01	459.15	44.9	194.2	170.4	215.6
Ma131	Mulberrofu ran K	Phenolics	7.54	611.2	51.2	212.5	152.3	223.5
Ma142	Oxyresveratrol	Stilbenes	8.59	245.08	317	281.7	388	224.9
Ma141	7-hydroxyco umarin	Phenylprop anoids	8.44	163.04	68.4	187.3	155.4	226
Ma076	Kuwanon U	Stilbenes	3.68	421.2	183.1	190.8	163.4	230.1
Ma102	Mulberrofu ran R	Phenolics	4.72	457.13	51.5	185.9	151.8	232.9
Ma147	Austrafuran B	Others	9.56	485.12	41.7	185.4	151.1	243.8
Ma048	Mulberrosi de C	Stilbenes	2.79	481.15	233.8	262.6	285.8	244.1
Ma118	Andalasin B.	Stilbenes	5.92	469.13	108.7	235.5	209.7	255.5
Ma138	Atalantoflavone	Flavonoids	8.04	337.11	3.8	132.6	81.4	261.8
Ma098	Kuwanon Q	Stilbenes	4.38	645.25	132.2	264.1	201.8	262.5
Ma090	Kuwanon Z	Stilbenes	4.06	617.14	226.1	350.7	281.8	267.1
Ma002	2-[2-Formyl-5-(hydroxymethyl)-1H-pyrrol-1-yl]butanedioic acid	DNJ alkaloids	0.51	242.07	-	306.5	364.7	268.7
Ma119	Macrouirin G	Stilbenes	6.25	627.2	-	247.7	224.3	279.1
Ma031	p-hydroxybenzaldehyde	Phenylprop anoids	2.33	123.04	77.7	299	301.2	288.4
Ma134	Kuwanon M	Stilbenes	7.6	823.31	122.5	262.6	238.5	296.5
Ma081	protocatechuic acid	Phenolics	3.8	137.02	63.4	168.7	117.3	302.2
Ma121	Yunanensi n E	Others	6.6	611.2	47.8	167.5	113.6	321.1
Ma125	Yunanensi n A	Others	6.74	647.18	47.7	170.7	116.6	323.7
Ma032	eugenyl-O-β-D-glucoside	Phenylprop anoids	2.33	309.13	69.4	158.8	101.1	330.2

Ma046	m-Coumaric acid	Phenylprop anoids	2.77	147.04	70.1	290	260.3	331.9
Ma112	Kuwanon V	Stilbenes	5.63	669.25	222.2	191.6	137.3	338.5
Ma052	sinapic acid	Phenylprop anoids	2.96	225.08	79.7	177	115.6	354.8
Ma060	5-Methoxytryptamine	Tryptamine s and its derivatives	3.19	191.12	-	302.6	234.2	403.1
Ma091	Austrafuran A	Others	4.07	449.13	39.4	239.5	170.2	478.2
Ma107	Mongolicin G.	Stilbenes	5.06	663.26	-	398.2	316.8	571.4
Ma064	Mortatarin B	Flavonoids	3.4	439.18	5.5	172	99.2	830.7
Ma021	(3S,6R)-8-Azabicyclo[3.2.1]octane-3,6-diol	DNJ alkaloids	2.02	205.1	-	667.1	468	-

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