

Supplementary Materials

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Table S1 Metabolites identified in the root of *Ailanthus altissima*

Molecular weight (Da)	Formula	Compounds	Class I	Class II	CAS	Repeat 1	Repeat 2	Repeat 3	Average
376.15	C20H24O7	Ailanthone	Terpenoids	Diterpenoids	981-15-7	14382251.45	11776154.64	8679388.40	11612598.16
388.16	C21H24O7	Ailantinol E	Terpenoids	Diterpenoids	-	210246.83	141213.65	174487.43	175315.97
364.19	C20H28O6	Amarolide	Terpenoids	Diterpenoids	29913-86-8	130990.39	125277.55	148619.78	134962.57
528.26	C26H40O11	Shinjuglycoside E	Terpenoids	Diterpenoids	112667-45-5	81742.59	125664.02	127265.02	111557.21
104.11	C5H14NO+	Choline	Alkaloids	Alkaloids	62-49-7	52980012.03	57544454.67	51093268.29	53872578.33
220.06	C14H8N2O	Canthin-6-one	Alkaloids	Plumerane	479-43-6	13279024.61	10512992.15	13856279.42	12549432.06
581.26	C33H35N5O5	Ergotamine	Alkaloids	Plumerane	113-15-5	14800859.18	6010230.11	12610148.45	11140412.58
204.09	C11H12N2O2	1-Methoxy-indole-3-acetamide	Alkaloids	Plumerane	-	10066015.40	14531911.18	7142445.30	10580123.96
181.07	C9H11NO3	N-(2-Hydroxy-4-methoxyphenyl)acetamide	Alkaloids	Phenolamine	58469-06-0	5261728.00	5342848.39	5948862.64	5517813.01
202.22	C10H26N4	Spermine	Alkaloids	Alkaloids	71-44-3	1843872.30	3256558.62	3678646.62	2926359.18
149.05	C8H7NO2	4-Hydroxymandelonitrile	Alkaloids	Phenolamine	13093-65-7	2670774.98	3166475.29	2161332.37	2666194.21
119.07	C8H9N	N-Benzylmethylene isomethylamine	Alkaloids	Alkaloids	-	2863350.55	2986009.28	1768473.50	2539277.78
141.09	C6H11N3O	Histidinol	Alkaloids	Alkaloids	501-28-0	1621750.04	2535370.05	3417357.58	2524825.89
184.07	C5H15NO4P+	O-Phosphocholine	Alkaloids	Alkaloids	107-73-3	2385230.05	2555490.52	2309089.62	2416603.39
250.08	C15H10N2O2	1-Methoxycanthin-6-one	Alkaloids	Plumerane	-	1570913.72	2540038.04	2373929.34	2161627.03
250.08	C15H10N2O2	5-Methoxycanthin-6-one	Alkaloids	Plumerane	15071-56-4	1555189.53	2621726.88	2275595.56	2150837.32
324.18	C20H24O2N2	Quinine	Alkaloids	Quinoline alkaloids	130-95-0	2661506.59	1191353.22	2283569.15	2045476.32
187.06	C11H9O2N	3-amino-2-naphthoic acid	Alkaloids	Alkaloids	-	1744774.39	2495545.88	1349571.68	1863297.32
187.06	C11H9NO2	naphthisoxazol A	Alkaloids	Alkaloids	-	1571236.17	1793326.88	984984.33	1449849.13
131.09	C6H13NO2	6-Deoxyfagomine	Alkaloids	Piperidine alkaloids	197449-09-5	1764343.62	1173726.54	1345603.69	1427891.28

187.06	C11H9NO2	3-Indoleacrylic acid	Alkaloids	Plumerane	1204-06-4	1025411.56	1417997.27	790450.77	1077953.20
85.09	C5H11N	Piperidine	Alkaloids	Piperidine alkaloids	110-89-4	988314.50	1012587.24	986042.40	995648.05
218.14	C13H18N2O	N,N-Dimethyl-5-methoxytryptamine	Alkaloids	Plumerane	1019-45-0	1010655.52	863251.10	929505.01	934470.54
266.08	C15H10N2O3	Picrasidine Q; 4-Hydroxy-5-Methoxy-Canthin-6-One	Alkaloids	Plumerane	101219-61-8	184312.64	551469.32	690554.58	475445.51
192.13	C11H16N2O	N-(4-Aminobutyl)benzamide	Alkaloids	Alkaloids	5692-23-9	508403.31	273638.91	387621.13	389887.78
557.27	C29H39N3O8	N1,N8-Bis(sinapoyl)spermidine	Alkaloids	Phenolamine	-	290958.36	344114.36	403380.62	346151.11
340.18	C20H24N2O3	Lochneridine	Alkaloids	Plumerane	5980-01-8	250357.15	267033.27	242562.13	253317.51
575.31	C32H41N5O5	α -Ergocryptine	Alkaloids	Plumerane	511-09-1	439021.78	120556.47	168233.21	242603.82
205.07	C11H11NO3	Methoxyindoleacetic acid	Alkaloids	Plumerane	3471-31-6	164152.10	307632.55	170521.55	214102.07
117.06	C8H7N	Indole	Alkaloids	Plumerane	120-72-9	110361.06	109165.12	100753.88	106760.02
145.05	C9H7NO	Indole-3-carboxaldehyde	Alkaloids	Plumerane	487-89-8	111990.78	134193.00	67395.33	104526.37
497.25	C27H35N3O6	N',N''-Diferuloylspermidine	Alkaloids	Phenolamine	-	116257.50	87507.50	94151.28	99305.43
240.09	C14H12N2O2	β -Carboline-1-propanoic acid	Alkaloids	Plumerane	89915-39-9	151480.99	50595.90	74267.07	92114.65
141.02	C2H8NO4P	O-Phosphorylethanolamine	Alkaloids	Alkaloids	1071-23-4	87021.68	86822.49	89916.44	87920.20
473.15	C20H27NO12	Dhurrin-6'-O-Glucoside	Alkaloids	Phenolamine	-	88027.34	98020.04	68689.17	84912.18
105.08	C4H11NO2	Diethanolamine	Alkaloids	Alkaloids	111-42-2	88530.28	73791.18	68157.57	76826.34
352.18	C21H24N2O3	Lochnericine	Alkaloids	Plumerane	72058-36-7	73241.20	56257.50	86516.27	72004.99
102.12	C5H14N2	Cadaverine	Alkaloids	Alkaloids	462-94-2	55696.29	82742.30	65578.26	68005.62
236.06	C14H8N2O2	11-Hydroxycanthin-6-One; Amalorin*	Alkaloids	Plumerane	75969-83-4	55105.01	54130.70	88497.15	65910.95
236.06	C14H8N2O2	9-Hydroxycanthin-6-one*	Alkaloids	Plumerane	138544-91-9	57856.51	44274.29	73483.38	58538.06
236.06	C14H8N2O2	1-Hydroxycanthin-6-One*	Alkaloids	Plumerane	80787-59-3	62154.09	52617.20		57385.65
447.19	C23H29NO8	3'-Glucosyl-6,7-dihydroxy-N-methyl-benzyltetrahydroisoquinoline	Alkaloids	Isoquinoline alkaloids	-	83151.91	28924.06		56037.99

248.12	C13H16N2O3	6-Hydroxymelatonin	Alkaloids	Plumerane	2208-41-5	76573.63	48513.93	37417.72	54168.43
236.06	C14H8N2O2	2-Hydroxycanthin-6-one	Alkaloids	Plumerane	86293-43-8	63675.21	16842.54	77304.14	52607.29
233.14	C14H19NO2	Paniculidine B	Alkaloids	Plumerane	97399-94-5	44085.30	52410.55	40239.12	45578.32
221.07	C11H11NO4	Methyl dioxindole-3-acetate	Alkaloids	Plumerane	57061-18-4	28642.78	37194.39	25049.66	30295.61
544.21	C27H32N2O10	Cadambine	Alkaloids	Plumerane	54422-49-0	24274.85	30342.35	34688.78	29768.66
327.15	C19H21NO4	Stepholidine	Alkaloids	Isoquinoline alkaloids	16562-13-3	29236.53	23061.35	13915.90	22071.26
130.11	C6H14N2O	N-Acetylputrescine	Alkaloids	Alkaloids	18233-70-0	19151.96	21584.64	21584.64	20773.75
303.14	C12H21N3O6	Nicotianamine	Alkaloids	Alkaloids	34441-14-0	20564.29	21740.05	19325.87	20543.40
202.11	C12H14N2O	Acetryptine	Alkaloids	Plumerane	3551-18-6	19811.53	20695.53	20952.66	20486.58
583.27	C34H37N3O6	N',N'',N'''-p-Coumaroyl-cinnamoyl-caffeoyl spermidine	Alkaloids	Phenolamine	-	26114.61	22274.88	13040.94	20476.81
147.03	C8H5NO2	Isatin	Alkaloids	Plumerane	91-56-5	18659.31	15007.50	6282.52	13316.44
281.27	C18H35NO	Laurocapram	Alkaloids	Alkaloids	59227-89-3	16288.07	11830.68	11030.59	13049.78
130.12	C5H14N4	Agmatine	Alkaloids	Alkaloids	306-60-5	11527.89	12180.83	11592.00	11766.91
161.05	C9H7NO2	Indole-5-carboxylic acid*	Alkaloids	Plumerane	1670-81-1	8675.56	12330.16	13443.33	11483.01
161.05	C9H7NO2	Indole-3-carboxylic acid*	Alkaloids	Plumerane	771-50-6	8675.56	12330.16	13443.33	11483.01
189.04	C10H7NO3	N-Acetylisatin	Alkaloids	Plumerane	574-17-4	16469.98	9483.83	7562.16	11171.99
394.19	C23H26N2O4	Akuammiline	Alkaloids	Plumerane	1897-26-3	5358.56	8694.86	6291.29	6781.57
165.07	C9H11NO2	L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	63-91-2	111797783.70	120303517.00	96778093.10	109626464.60
147.05	C5H9NO4	L-Glutamic acid	Amino acids and derivatives	Amino acids and derivatives	56-86-0	47670907.13	46911873.23	50903606.00	48495462.12
131.09	C6H13NO2	L-Isoleucine*	Amino acids and derivatives	Amino acids and derivatives	73-32-5	30418208.12	30820546.27	32379795.86	31206183.42

188.13	C7H16N4O2	N-Monomethyl-L-arginine	Amino acids and derivatives	Amino acids and derivatives	17035-90-4	34513868.47	42506128.70	12850522.30	29956839.82
131.09	C6H13NO2	L-Leucine*	Amino acids and derivatives	Amino acids and derivatives	61-90-5	28787330.76	29815032.72	29878220.88	29493528.12
131.09	C6H13NO2	L-Norleucine*	Amino acids and derivatives	Amino acids and derivatives	327-57-1	28864088.57	29050263.36	29774997.03	29229782.99
146.11	C6H14N2O2	L-Lysine	Amino acids and derivatives	Amino acids and derivatives	56-87-1	34464887.39	43215725.24	5518466.17	27733026.27
188.13	C7H16N4O2	Arginine methyl ester	Amino acids and derivatives	Amino acids and derivatives	-	31936911.81	39435692.76	11728309.84	27700304.80
117.08	C5H11NO2	L-Valine	Amino acids and derivatives	Amino acids and derivatives	72-18-4	7535669.43	8491029.94	10304292.14	8776997.17
146.07	C5H10N2O3	L-Glutamine	Amino acids and derivatives	Amino acids and derivatives	56-85-9	7195541.00	8280626.11	5378700.83	6951622.65
103.06	C4H9NO2	Methyl 3-aminopropanoate	Amino acids and derivatives	Amino acids and derivatives	4138-35-6	6294674.88	6366024.35	6125574.34	6262091.19
133.04	C4H7NO4	L-Aspartic Acid	Amino acids and derivatives	Amino acids and derivatives	56-84-8	6373727.70	6928876.53	4592102.92	5964902.38
129.08	C6H11NO2	Cycloleucine	Amino acids and derivatives	Amino acids and derivatives	52-52-8	6255942.26	7105135.84	4326891.13	5895989.74
181.07	C9H11NO3	L-Tyrosine	Amino acids and derivatives	Amino acids and derivatives	60-18-4	5950608.49	5850789.18	5032079.81	5611159.16
202.14	C8H18N4O2	NG,NG-Dimethyl-L-arginine	Amino acids and derivatives	Amino acids and derivatives	30315-93-6	6133605.29	5924935.74	3210917.74	5089819.59
457.14	C16H27NO14	L-Aspartic acid-O-diglucoside	Amino acids and derivatives	Amino acids and derivatives	-	3194807.87	4680611.36	4854820.13	4243413.12

103.06	C4H9NO2	N,N-Dimethylglycine	Amino acids and derivatives	Amino acids and derivatives	1118-68-9	3652433.56	3176460.60	2994291.65	3274395.27
149.05	C5H11NO2S	L-Methionine	Amino acids and derivatives	Amino acids and derivatives	63-68-3	1842140.38	2218676.98	1611442.12	1890753.16
131.06	C5H9NO3	Trans-4-Hydroxy-L-proline	Amino acids and derivatives	Amino acids and derivatives	51-35-4	1898569.44	1734672.70	1614231.93	1749158.02
174.10	C7H14N2O3	N- α -Acetyl-L-ornithine	Amino acids and derivatives	Amino acids and derivatives	6205-08-9	1534708.27	2316576.14	850436.91	1567240.44
204.09	C11H12N2O2	L-Tryptophan	Amino acids and derivatives	Amino acids and derivatives	73-22-3	1264106.27	1989500.18	1123930.50	1459178.98
165.05	C5H11NO3S	L-Methionine Sulfoxide	Amino acids and derivatives	Amino acids and derivatives	3226-65-1	1402160.10	1220457.00	1592622.14	1405079.75
175.10	C6H13N3O3	L-Citrulline	Amino acids and derivatives	Amino acids and derivatives	372-75-8	1428562.73	1857302.10	746646.61	1344170.48
119.06	C4H9NO3	L-Homoserine	Amino acids and derivatives	Amino acids and derivatives	672-15-1	908599.68	1285992.74	899816.45	1031469.63
119.06	C4H9NO3	L-Threonine	Amino acids and derivatives	Amino acids and derivatives	72-19-5	811079.46	1178117.76	852752.98	947316.73
115.06	C5H9NO2	L-Proline	Amino acids and derivatives	Amino acids and derivatives	147-85-3	845132.18	1014647.16	856435.57	905404.97
147.05	C5H9NO4	L-threo-3-Methylaspartate	Amino acids and derivatives	Amino acids and derivatives	6061-13-8	840788.83	767946.51	780620.36	796451.90
132.05	C4H8N2O3	L-Asparagine	Amino acids and derivatives	Amino acids and derivatives	70-47-3	779476.98	900301.98	633685.30	771154.75
105.04	C3H7NO3	L-Serine	Amino acids and derivatives	Amino acids and derivatives	56-45-1	763570.36	742477.91	741138.00	749062.09

307.08	C10H17N3O6 S	Glutathione reduced form	Amino acids and derivatives	Amino acids and derivatives	70-18-8	467160.97	757348.79	183438.64	469316.13
207.09	C11H13NO3	N-Acetyl-L-phenylalanine	Amino acids and derivatives	Amino acids and derivatives	2018-61-3	502670.14	430240.14	449634.43	460848.24
612.15	C20H32N6O1 2S2	Oxiglutatione	Amino acids and derivatives	Amino acids and derivatives	27025-41-8	389899.41	350326.41	349915.25	363380.36
162.05	C6H10O5	3-Hydroxy-3-methylpentane-1,5- dioic acid	Amino acids and derivatives	Amino acids and derivatives	503-49-1	202064.21	235671.41	172674.30	203469.97
121.02	C3H7NO2S	L-Cysteine	Amino acids and derivatives	Amino acids and derivatives	52-90-4	165430.42	199101.26	192549.68	185693.79
321.10	C11H19N3O6 S	S-(Methyl)glutathione	Amino acids and derivatives	Amino acids and derivatives	2922-56-7	204953.86	157812.03	170135.99	177633.96
135.04	C4H9NO2S	S-Methyl-L-cysteine	Amino acids and derivatives	Amino acids and derivatives	1187-84-4	158131.74	143908.11	174029.52	158689.79
223.08	C11H13NO4	N-Acetyl-L-tyrosine	Amino acids and derivatives	Amino acids and derivatives	537-55-3	146821.06	115798.73	115195.67	125938.49
230.16	C11H22N2O3	L-Valyl-L-Leucine	Amino acids and derivatives	Amino acids and derivatives	3989-97-7	134325.18	123260.99	111178.37	122921.51
169.09	C7H11N3O2	3-Methyl-L-Histidine	Amino acids and derivatives	Amino acids and derivatives	368-16-1	117662.04	113053.80	98873.37	109863.07
308.12	C11H20N2O8	L-Glutamine-O-glycoside	Amino acids and derivatives	Amino acids and derivatives	-	115625.80	93930.79	92643.71	100733.43
188.12	C8H16N2O3	N-Glycyl-L-leucine	Amino acids and derivatives	Amino acids and derivatives	869-19-2	102093.51	94505.02	91879.93	96159.49
189.11	C7H15N3O3	L-Homocitrulline	Amino acids and derivatives	Amino acids and derivatives	1190-49-4	56535.96	149957.30	75763.96	94085.74

161.07	C6H11NO4	N-Acetyl-L-threonine	Amino acids and derivatives	Amino acids and derivatives	17093-74-2	94989.72	91802.88	78385.99	88392.87
220.08	C11H12N2O3	5-Hydroxy-L-tryptophan	Amino acids and derivatives	Amino acids and derivatives	56-69-9	62406.62	66107.25	52762.26	60425.38
244.18	C12H24N2O3	L-Leucyl-L-Leucine	Amino acids and derivatives	Amino acids and derivatives	3303-31-9	67924.25	28479.16	55562.20	50655.20
280.11	C13H16N2O5	L-Aspartyl-L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	13433-09-5	45035.70	60564.52	41637.34	49079.19
264.15	C14H20N2O3	L-Valyl-L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	3918-92-1	59208.36	42916.07	33809.03	45311.15
278.16	C15H22N2O3	L-Leucyl-L-phenylalanine	Amino acids and derivatives	Amino acids and derivatives	56217-82-4	41563.64	47672.11	33767.18	41000.98
218.09	C8H14N2O5	5-L-Glutamyl-L-amino acid	Amino acids and derivatives	Amino acids and derivatives	5875-41-2	43603.60	35885.88	40522.36	40003.94
276.13	C11H20N2O6	L-Saccharopine	Amino acids and derivatives	Amino acids and derivatives	997-68-2	44835.54	39586.54	35279.84	39900.64
132.09	C5H12N2O2	L-Ornithine	Amino acids and derivatives	Amino acids and derivatives	70-26-8	51887.40	43426.92	16060.51	37124.94
174.06	C6H10N2O4	N-Alpha-Acetyl-L-Asparagine	Amino acids and derivatives	Amino acids and derivatives	4033-40-3	30991.08	53340.56	26838.08	37056.57
240.02	C6H12N2O4S 2	L-Cystine	Amino acids and derivatives	Amino acids and derivatives	56-89-3	23215.20	16325.68	29087.40	22876.09
323.21	C18H29NO4	Jasmonoyl-L-Isoleucine	Amino acids and derivatives	Amino acids and derivatives	120330-93-0	18071.77	7987.48	18393.21	14817.49
309.11	C11H19NO9	L-Glutamic acid-O-glycoside	Amino acids and derivatives	Amino acids and derivatives	-	5568.08	10070.63	14149.92	9929.54

312.15	C18H20N2O3	L-Phenylalanyl-L-phenylalanine	Amino acids and derivatives	Amino acids and derivatives	2577-40-4	6303.30	1076.29	8511.63	5297.07
300.10	C17H16O5	4'-Hydroxy-5,7-dimethoxyflavanone	Flavonoids	Flavanones	-	32891933.19	28202792.11	33295320.84	31463348.71
522.10	C23H22O14	Tricin-7-O-saccharic acid	Flavonoids	Flavones	-	10856389.91	12937127.08	12034911.94	11942809.64
340.13	C20H20O5	2,4,2',4'-tetrahydroxy-3'-prenylchalcone	Flavonoids	Chalcones	-	1313855.42	1124540.90	1269839.62	1236078.65
448.10	C21H20O11	Kaempferol-3-O-galactoside (Trifolin)	Flavonoids	Flavonols	23627-87-4	964697.72	1236608.44	1107996.09	1103100.75
300.06	C16H12O6	6-methyl luteolin	Flavonoids	Flavones	-	981843.71	954348.71	834471.58	923554.67
450.12	C21H22O11	6-C-Glucosyl-2-Hydroxynaringenin	Flavonoids	Flavanones	-	580811.70	454592.98	493573.98	509659.56
418.13	C21H22O9	O-MethylNaringenin-8-C-arabinoside	Flavonoids	Flavanones	-	362392.78	336121.10	398925.31	365813.07
626.18	C28H34O16	Hesperetin-5,7-di-O-glucoside	Flavonoids	Flavanones	-	371741.82	346894.32	322991.25	347209.13
508.12	C23H24O13	5,6,3',4'-Tetrahydroxy-3,7-dimethoxyflavone-6-O-glucoside	Flavonoids	Flavones	-	390937.47	275298.44	304926.44	323720.78
450.12	C21H22O11	Aromadendrin-7-O-glucoside	Flavonoids	Flavanonols	28189-90-4	268656.15	262279.42	346123.20	292352.92
450.12	C21H22O11	3,4,2',4',6'-Pentahydroxychalcone-4'-O-glucoside	Flavonoids	Chalcones	-	251149.27	294647.46	314813.18	286869.97
638.15	C28H30O17	Chrysoeriol-7-O-(2''-O-glucuronyl)glucoside	Flavonoids	Flavones	-	182928.25	275396.99	184145.02	214156.76
450.12	C21H22O11	Eriodictyol-8-C-glucoside	Flavonoids	Flavanones	1023271-51-3	206156.22	213617.28	210657.28	210143.59
436.14	C21H24O10	Dihydrocharcone-4'-O-glucoside	Flavonoids	Chalcones	-	242655.65	127386.21	178901.52	182981.13
436.14	C21H24O10	Phloretin-2'-O-glucoside (Phlorizin)	Flavonoids	Chalcones	60-81-1	259908.82	122325.00	163885.72	182039.85
466.11	C21H22O12	Taxifolin-3'-O-glucoside	Flavonoids	Flavanonols	31106-05-5	125649.95	154161.11	233806.94	171206.00
640.16	C28H32O17	Isorhamnetin-3,7-O-diglucoside	Flavonoids	Flavonols	6758-51-6	154563.36	156149.87	174900.79	161871.34
452.13	C21H24O11	Epicatechin-3'-O-β-D-glucopyranoside*	Flavonoids	Flavanols	-	167295.24	64091.24	239305.30	156897.26
464.09	C21H20O12	Isohyperoside*	Flavonoids	Flavonols	35589-21-0	112428.78	192727.23	163379.66	156178.56

550.13	C25H26O14	Hesperetin-7-O-(6''-malonyl)glucoside	Flavonoids	Flavanones	-	144201.27	159850.13	154161.80	152737.73
464.10	C21H20O12	Quercetin-5-O-β-D-glucoside*	Flavonoids	Flavonols	-	122840.73	190318.23	125269.77	146142.91
418.09	C20H18O10	Luteolin-8-C-arabinoside	Flavonoids	Flavones	-	137291.73	144394.10	149454.31	143713.38
452.13	C21H24O11	Epicatechin-6-C-β-D-glucopyranoside*	Flavonoids	Flavanols	-	77443.76	192270.46	134896.65	134870.29
464.10	C21H20O12	Quercetin-3-O-glucoside (Isoquercitrin)*	Flavonoids	Flavonols	482-35-9	92096.78	159006.28	140778.77	130627.28
448.10	C21H20O11	Kaempferol-7-O-glucoside	Flavonoids	Flavonols	16290-07-6	90302.72	158511.26	132888.43	127234.13
448.10	C21H20O11	Carthamone	Flavonoids	Chalcones	86579-00-2	90302.72	158511.26	132888.43	127234.13
452.13	C21H24O11	Epicatechin-4'-O-β-D-glucopyranoside*	Flavonoids	Flavanols	-	85854.76	176589.75	71204.75	111216.42
624.17	C28H32O16	Rhamnetin-3-O-Rutinoside*	Flavonoids	Flavonols	-	125798.90	117209.77	53051.64	98686.77
434.12	C21H22O10	Choerospondin	Flavonoids	Flavanones	81202-36-0	128208.39	64962.32	94859.00	96009.90
624.17	C28H32O16	Isorhamnetin-3-O-rutinoside (Narcissin)*	Flavonoids	Flavonols	604-80-8	143064.40	95594.84	44386.30	94348.51
594.16	C27H30O15	5,7-Dihydroxy-4-methoxyflavone-3-O-xylose-(1-6)-glucose	Flavonoids	Flavones	-	87703.47	117248.97	75345.93	93432.79
254.06	C15H10O4	Chrysin	Flavonoids	Flavones	480-40-0	55528.83	78011.05	134703.72	89414.53
624.17	C28H32O16	Isorhamnetin-3-O-neohesperidoside*	Flavonoids	Flavonols	55033-90-4	102367.15	109884.77	45692.77	85981.56
756.21	C33H40O20	Apigenin-8-C-glucoside-7-O-Sophoroside	Flavonoids	Flavones	-	108275.25	110223.55	23186.90	80561.90
624.17	C28H32O16	Sexangularetin-3-O-glucoside-7-O-rhamnoside	Flavonoids	Flavonols	-	100434.84	85420.22	40305.61	75386.89
306.07	C15H14O7	Gallocatechin	Flavonoids	Flavanols	970-73-0	89021.12	114492.28	20165.60	74559.67
624.17	C28H32O16	6-C-Methylquercetin-3-O-rutinoside	Flavonoids	Flavonols	-	99224.84	75796.22	39120.36	71380.47
594.16	C27H30O15	Kaempferol-3-O-neohesperidoside*	Flavonoids	Flavonols	32602-81-6	105551.03	61036.97	34244.34	66944.11
642.16	C31H30O15	Luteolin-7-O-(6''-eudesmyl)glucoside	Flavonoids	Flavones	-	69863.55	54350.45	73817.99	66010.66
626.15	C27H30O17	Quercetin-3,7-Di-O-glucoside	Flavonoids	Flavonols	-	48031.19	80425.25	64227.91	64228.12

594.16	C27H30O15	Vitexin-2''-O-galactoside	Flavonoids	Flavones	-	50009.28	80351.32	59225.08	63195.23
610.19	C28H34O15	Hesperetin-7-O-neohesperidoside(Neohesperidin)*	Flavonoids	Flavanones	13241-33-3	59207.70	75377.20	40064.56	58216.49
594.16	C27H30O15	Kaempferol-3-O-rutinoside(Nicotiflorin)*	Flavonoids	Flavonols	17650-84-9	71000.97	56054.97	43416.19	56824.05
594.16	C27H30O15	Luteolin-7-O-neohesperidoside(Lonicerin)*	Flavonoids	Flavones	25694-72-8	85447.03	51430.74	27292.94	54723.57
464.10	C21H20O12	6-Hydroxyluteolin 5-glucoside	Flavonoids	Flavones	-	72743.10	42851.27	45071.34	53555.24
300.06	C16H12O6	Diosmetin (5,7,3'-Trihydroxy-4'-methoxyflavone)	Flavonoids	Flavones	520-34-3	50879.15	35713.15	67382.02	51324.77
594.16	C27H30O15	Kaempferol-3-O-glucorhamnoside*	Flavonoids	Flavonols	40437-72-7	85946.97	30161.03	37384.98	51164.33
610.19	C28H34O15	Hesperetin-7-O-rutinoside(Hesperidin)*	Flavonoids	Flavanones	520-26-3	51187.19	60303.10	38968.63	50152.97
402.13	C21H22O8	Nobiletin (5,6,7,8,3',4'-Hexamethoxyflavone)	Flavonoids	Flavones	478-01-3	58043.65	52877.22	38307.24	49742.70
594.16	C27H30O15	Luteolin-7-O-rutinoside*	Flavonoids	Flavones	3563-98-2	69112.53	52654.99	22331.94	48033.15
452.13	C21H24O11	Epicatechin glucoside	Flavonoids	Flavanols	-	41451.52	45840.98	47480.00	44924.16
594.16	C27H30O15	Kaempferol-3-O-robinobioside(Biorobin)	Flavonoids	Flavonols	17297-56-2	56967.84	41878.87	24845.41	41230.71
450.12	C21H22O11	Dihydrokaempferol-3-O-glucoside	Flavonoids	Flavanonols	1049-08-8	48111.43	24674.93	39863.00	37549.79
504.13	C24H24O12	Pinocembrin-7-O-(6''-O-malonyl)glucoside	Flavonoids	Flavanones	-	35645.71	52887.91	20159.06	36230.90
652.16	C29H32O17	Limocitrin-3-O-(3-hydroxy-3-methylglutarate)glucoside	Flavonoids	Flavonols	-	40341.25	40739.68	22009.38	34363.44
452.13	C21H24O11	Sieboldin	Flavonoids	Chalcones	18777-73-6	22213.33	35744.30	33170.79	30376.14
476.10	C22H20O12	Diosmetin-7-O-glucuronide	Flavonoids	Flavones	35110-20-4	34401.53	16619.98		25510.75
742.23	C33H42O19	Naringenin-7-O-Rutinoside-4'-O-glucoside	Flavonoids	Flavanones	-	20538.77	21531.30	31550.26	24540.11
610.15	C27H30O16	Quercetin-3-O-glucoside-7-O-rhamnoside*	Flavonoids	Flavonols	-	17234.05	28448.99	19511.31	21731.45
448.10	C21H20O11	Luteolin-8-C-glucoside (Orientin)	Flavonoids	Flavones	28608-75-5	27300.30		14453.95	20877.12

464.10	C21H20O12	Quercetin-3-O-galactoside (Hyperin)	Flavonoids	Flavonols	482-36-0	29940.40	22611.36	9346.34	20632.70
610.15	C27H30O16	Luteolin-7-O-gentiobioside	Flavonoids	Flavones	-	25264.53	21688.23	14356.78	20436.51
504.13	C24H24O12	Chrysoeriol-7-O-(6''-acetyl)glucoside	Flavonoids	Flavones	-	17843.35	20762.61	21745.85	20117.27
442.09	C22H18O10	Epicatechin gallate*	Flavonoids	Flavanols	1257-08-5	26613.84	10795.30	19310.89	18906.68
442.09	C22H18O10	Catechin gallate*	Flavonoids	Flavanols	130405-40-2	23930.04	18681.98	12463.59	18358.54
962.26	C40H50O27	Isorhamnetin-3-O-rutinoside-7-O-(2''-O-glucosyl)glucuronate	Flavonoids	Flavonols	-	19792.36	22273.42	12197.31	18087.70
610.15	C27H30O16	Quercetin-3-O-robinobioside	Flavonoids	Flavonols	52525-35-6	22367.36	15528.45	13844.86	17246.89
372.12	C20H20O7	Tangeretin (4',5,6,7,8-Pentamethoxyflavone)	Flavonoids	Flavones	481-53-8	23246.47	17425.55	10232.18	16968.07
594.14	C30H26O13	Kaempferol-3-O-(6''-p-Coumaroyl)galactoside*	Flavonoids	Flavonols	-	13779.80	18330.69	15414.62	15841.70
594.14	C30H26O13	Kaempferol-3-O-(6''-p-Coumaroyl)glucoside (Tiliroside)*	Flavonoids	Flavonols	20316-62-5	13779.80	18330.69	15414.62	15841.70
610.15	C27H30O16	Quercetin-3-O-neohesperidoside*	Flavonoids	Flavonols	117611-67-3	16098.18	18634.97	12197.31	15643.49
610.15	C27H30O16	Luteolin-7,3'-di-O-glucoside	Flavonoids	Flavones	52187-80-1	15668.98	15665.73	11859.61	14398.11
478.07	C21H18O13	Quercetin-4'-O-glucuronide	Flavonoids	Flavonols	201463-36-7	10765.77	14974.36	14948.49	13562.87
594.16	C27H30O15	Apigenin-6,8-di-C-glucoside (Vicenin-2)	Flavonoids	Flavones	23666-13-9	14461.90	7698.42	15885.97	12682.10
594.14	C30H26O13	Luteolin-7-O-(6''-caffeoyl)rhamnoside	Flavonoids	Flavones	-	7739.45	15705.87	8017.11	10487.48
594.19	C28H34O14	Poncirin (Isosakuranetin-7-O-neohesperidoside)	Flavonoids	Flavanones	14941-08-3	6264.95	12739.27	12083.12	10362.44
610.15	C27H30O16	Quercetin-3-O-rutinoside (Rutin)	Flavonoids	Flavonols	153-18-4	9179.44	11988.49	9755.24	10307.72
448.10	C21H20O11	Luteolin-6-C-glucoside (Isoorientin)	Flavonoids	Flavones	4261-42-1	9206.87	9515.11	9572.32	9431.43
918.21	C41H42O24	Quercetin-3-O-(6''-O-sinapoyl)glucoside-7-O-(6''-O-malonyl)glucoside	Flavonoids	Flavonols	-	9873.40	4989.47	10697.00	8519.96
594.19	C28H34O14	Didymin (Isosakuranetin-7-O-rutinoside)	Flavonoids	Flavanones	14259-47-3	8483.00	9999.65	6090.73	8191.13

468.11	C23H16O11	Isorhamnetin-3-O-gallate	Flavonoids	Flavonols	-	15540.98	4292.29	3209.77	7681.01
814.16	C37H34O21	Luteolin-7-O-glucuronide-(2→1)-(2''-Feruloyl)glucuronide	Flavonoids	Flavones	-	7225.22	3634.84	11714.68	7524.91
844.17	C38H36O22	Luteolin-7-O-glucuronide-(2→1)-(2''-Sinapoyl)glucuronide	Flavonoids	Flavones	-	3592.78	2424.84	4688.68	3568.77
520.19	C26H32O11	Dehydrodiconiferyl alcohol-4-O-glucoside	Lignans and Coumarins	Lignans	107870-88-2	52795513.29	51955343.60	51249932.27	52000263.05
520.19	C26H32O11	saikolignanose D	Lignans and Coumarins	Lignans	-	48751828.39	52984706.97	50674381.09	50803638.82
520.19	C26H32O11	Pittogoside B	Lignans and Coumarins	Lignans	-	48958002.07	50280261.53	47985069.03	49074444.21
524.23	C26H36O11	Secoisolariciresinol 4-O-glucoside	Lignans and Coumarins	Lignans	-	27780142.75	34320069.17	40621064.89	34240425.60
146.04	C9H6O2	Coumarin	Lignans and Coumarins	Coumarins	91-64-5	18249154.58	25569558.43	22354228.17	22057647.06
522.21	C26H34O11	Lariciresinol-4'-O-glucoside	Lignans and Coumarins	Lignans	143663-00-7	16821282.41	17854877.04	16965125.09	17213761.51
522.21	C26H34O11	Manglieside D	Lignans and Coumarins	Lignans	-	12106214.80	16232419.94	15539053.87	14625896.20
580.22	C28H36O13	Syringaresinol-4'-O-glucoside	Lignans and Coumarins	Lignans	7374-79-0	10648518.58	8790587.91	8482688.85	9307265.11
700.26	C32H44O17	Olivil-4,4'-Di-O-glucoside	Lignans and Coumarins	Lignans	-	7536803.55	6852910.02	11673232.32	8687648.63
356.13	C20H20O6	(-)-dihydrosesamin	Lignans and Coumarins	Lignans	-	2789359.49	2230127.15	3261050.21	2760178.95
356.13	C20H20O6	Horsfieldin	Lignans and Coumarins	Lignans	-	3173530.23	1782335.11	3267715.80	2741193.72
552.22	C27H36O12	5'-Methoxyisolariciresinol-9'-O-glucoside	Lignans and Coumarins	Lignans	-	2778354.52	2293269.77	2616154.14	2562592.81
278.15	C16H22O4	Methylillicinone F	Lignans and Coumarins	Coumarins	-	2524784.18	2699142.94	2350242.56	2524723.22
682.25	C32H42O16	Pinoresinol-4,4'-O-di-O-glucoside	Lignans and Coumarins	Lignans	63902-38-5	2584745.75	2638456.92	1988816.10	2404006.26
522.21	C26H34O11	Isolariciresinol-9'-O-glucoside	Lignans and Coumarins	Lignans	63358-12-3	1929228.63	1814320.58	2628275.81	2123941.67
522.21	C26H34O11	Dihydrodehydrodiconiferyl alcohol-4-O-glucoside	Lignans and Coumarins	Lignans	-	1929228.63	1814320.58	2628275.81	2123941.67
538.21	C26H34O12	(-)-olivil 4'-O-bate-D-glucopyranoside	Lignans and Coumarins	Lignans	-	1456897.44	2284405.83	2358498.78	2033267.35

370.14	C21H22O6	Fargesin	Lignans and Coumarins	Lignans	31008-19-2	2029791.95	1771271.20	2256555.70	2019206.28
412.13	C19H24O10	Methylpicraquassioside A	Lignans and Coumarins	Coumarins	-	1756432.30	1186666.77	1356939.64	1433346.24
538.21	C26H34O12	Olivil-4'-O-glucoside	Lignans and Coumarins	Lignans	76880-93-8	917980.49	832510.85	1275567.18	1008686.17
520.17	C26H32O11	Matairesinol-4'-O-glucoside (Matairesinoside)	Lignans and Coumarins	Lignans	23202-85-9	840125.13	1075092.46	1101708.70	1005642.09
712.26	C33H44O17	Medioresinol-4,4'-di-O-glucoside	Lignans and Coumarins	Lignans	88142-63-6	945500.39	986840.60	796655.64	909665.55
522.21	C26H34O11	Saikolignanose A	Lignans and Coumarins	Lignans	-	507397.56	1121331.26	1063614.86	897447.89
426.04	C17H14O13	Ditartaroyl-hydroxycoumarin	Lignans and Coumarins	Coumarins	-	1023930.40	931995.23	717705.45	891210.36
176.05	C10H8O3	7-Methoxycoumarin	Lignans and Coumarins	Coumarins	531-59-9	1365165.68	399003.18	563552.93	775907.26
520.19	C26H32O11	Pinoresinol-4-O-glucoside	Lignans and Coumarins	Lignans	41607-20-9	463492.22	428536.96	521099.71	471042.96
536.19	C26H32O12	1-Hydroxypinoresinol-4'-O-Glucoside	Lignans and Coumarins	Lignans	-	366911.39	349370.91	347122.22	354468.17
358.14	C20H22O6	Pinoresinol*	Lignans and Coumarins	Lignans	487-36-5	313455.04	252253.25	394214.17	319974.15
222.05	C11H10O5	Isofraxidin	Lignans and Coumarins	Coumarins	486-21-5	376923.36	215090.20	312981.88	301665.15
550.21	C27H34O12	Eucommin A	Lignans and Coumarins	Lignans	99633-12-2	400485.64	259299.06	214215.38	291333.36
418.16	C22H26O8	Lirioresinol A	Lignans and Coumarins	Lignans	-	280010.81	242822.12	309675.71	277502.88
358.14	C20H22O6	Epipinoresinol*	Lignans and Coumarins	Lignans	24404-50-0	269387.37	196237.64	340059.14	268561.38
222.05	C11H10O5	Umckalin (7-hydroxy-5,6-dimethoxycoumarin)	Lignans and Coumarins	Coumarins	43053-62-9	264449.40	311727.17	221829.67	266002.08
392.15	C20H24O8	Massoniresinol; Vladinol A	Lignans and Coumarins	Lignans	96087-10-4	195235.83	228590.07	243140.24	222322.04
532.14	C22H28O15	Fraxetin-7,8-di-O-glucoside	Lignans and Coumarins	Coumarins	-	185212.40	213746.24	201000.39	199986.34
354.10	C16H18O9	Scopoletin-7-O-glucoside (Scopolin)	Lignans and Coumarins	Coumarins	531-44-2		108371.75	289529.70	198950.72
486.14	C21H26O13	Scopoletin-7-O-xylosyl(1→6)glucoside	Lignans and Coumarins	Coumarins	-	225435.06	86566.66	268928.09	193643.27

486.14	C21H26O13	Zanthoxyloside	Lignans and Coumarins	Coumarins	-	171293.62	118643.62	263725.78	184554.34
360.16	C20H24O6	Isolariciresinol	Lignans and Coumarins	Lignans	548-29-8	204737.14	147094.52	125699.64	159177.10
622.23	C30H38O14	Syringaresinol-4'-O-(6''-acetyl)glucoside	Lignans and Coumarins	Lignans	-	117678.18	160777.73	122315.22	133590.37
536.19	C26H32O12	1-Hydroxypinoresinol-1-O-Glucoside	Lignans and Coumarins	Lignans	81495-71-8	117100.78	132634.58	120642.58	123459.31
370.09	C16H18O10	Fraxetin-8-O-glucoside (Fraxin)	Lignans and Coumarins	Coumarins	524-30-1	115842.31	110387.18	130811.53	119013.68
222.05	C11H10O5	Fraxidin (8-Hydroxy-6,7-dimethoxycoumarin)	Lignans and Coumarins	Coumarins	525-21-3	88199.83	89345.16	142691.24	106745.41
384.11	C17H20O10	Fraxidin-8-O-glucoside	Lignans and Coumarins	Coumarins	-	113118.93	54927.96	47798.95	71948.61
208.04	C10H8O5	Isofraxetin	Lignans and Coumarins	Coumarins	50656-75-2	85256.71	73229.55	49056.54	69180.93
352.13	C21H20O5	1-Methoxyphaseollin	Lignans and Coumarins	Coumarins	157226-48-7	80716.54	57201.99	66306.87	68075.14
384.11	C17H20O10	Mandshurin	Lignans and Coumarins	Coumarins	32451-87-9	58313.49	70639.03	53382.86	60778.46
400.15	C22H24O7	(7R,8S)-9-acetyl-dehydrodiconiferyl alcohol	Lignans and Coumarins	Lignans	-	72062.05	58961.05	43606.54	58209.88
374.14	C20H22O7	8-Hydroxypinoresinol	Lignans and Coumarins	Lignans	81426-17-7	51591.36	54898.34	63062.29	56517.33
418.16	C22H26O8	Syringaresinol	Lignans and Coumarins	Lignans	21453-71-4	53020.37	44682.06	53962.52	50554.98
192.04	C10H8O4	Isoscopoletin (6-Hydroxy-7-Methoxycoumarin)	Lignans and Coumarins	Coumarins	776-86-3	47362.20		52672.95	50017.58
360.16	C20H24O6	(-)-Lariciresinol	Lignans and Coumarins	Lignans	-	44907.74	55700.26	36467.44	45691.82
360.16	C20H24O6	(7S,8R)-dihydrodehydrodiconferyl alcohol	Lignans and Coumarins	Lignans	-	44907.74	55700.26	36467.44	45691.82
188.04	C11H8O3	Ayapin	Lignans and Coumarins	Coumarins	494-56-4	44280.59	41804.68	50381.70	45488.99
384.11	C17H20O10	Isofraxidin-7-O-glucoside	Lignans and Coumarins	Coumarins	483-91-0	21290.91	52802.42	29868.87	34654.07
236.07	C12H12O5	Dimethylfraxetin; 6,7,8-Trimethoxycoumarin*	Lignans and Coumarins	Coumarins	6035-49-0	10947.69	26603.94	37979.29	25176.97

236.07	C12H12O5	5,6,7-Trimethoxycoumarin*	Lignans and Coumarins	Coumarins	55085-47-7	5955.87	31967.18	34732.75	24218.60
516.15	C22H28O14	Scopoletin 7-O-β-D-Sophoroside	Lignans and Coumarins	Coumarins	-	4752.25	4689.24	5417.59	4953.03
282.26	C18H34O2	Petroselinic acid*	Lipids	Free fatty acids	593-39-5	73122204.72	58645133.21	71223424.97	67663587.63
282.26	C18H34O2	11-Octadecanoic acid(Vaccenic acid)*	Lipids	Free fatty acids	506-17-2	73122204.72	58645133.21	71223424.97	67663587.63
521.35	C26H52NO7P	LysoPC 18:1(2n isomer)	Lipids	LPC	-	88677217.08	23869892.59	75574081.17	62707063.61
280.24	C18H32O2	Linoleic acid	Lipids	Free fatty acids	60-33-3	50165117.25	39369581.59	60502855.53	50012518.12
278.22	C18H30O2	γ-Linolenic Acid*	Lipids	Free fatty acids	506-26-3	54669496.36	32437137.72	52174642.75	46427092.28
278.22	C18H30O2	α-Linolenic Acid*	Lipids	Free fatty acids	463-40-1	54669496.36	32437137.72	52174642.75	46427092.28
312.30	C20H40O2	Arachidic acid	Lipids	Free fatty acids	506-30-9	33065232.24	29126348.65	23707153.92	28632911.60
495.33	C24H50NO7P	LysoPC 16:0(2n isomer)	Lipids	LPC	-	12564253.67	13163367.46	8206174.95	11311265.36
484.28	C22H45O9P	LysoPG 16:0	Lipids	Glycerol ester	-	12583453.26	8440175.03	10357841.22	10460489.84
240.25	C16H32O	Palmitaldehyde	Lipids	Free fatty acids	629-80-1	9882744.09	9663455.41	10353169.63	9966456.38
495.33	C24H50NO7P	LysoPC 16:0	Lipids	LPC	17364-16-8	11792821.10	10317855.12	7285253.70	9798643.31
273.27	C16H35NO2	Hexadecylsphingosine	Lipids	Sphingolipids	-	5662055.91	4848524.27	7831823.49	6114134.56
356.29	C21H40O4	1-Oleoyl-Sn-Glycerol	Lipids	Glycerol ester	129784-87-8	8743755.28	2596132.39	4661629.15	5333838.94
517.32	C26H48NO7P	LysoPC 18:3(2n isomer)	Lipids	LPC	-	4792162.39	2387671.95	4534990.86	3904941.73
519.33	C26H50NO7P	LysoPC 18:2(2n isomer)	Lipids	LPC	-	2555973.60	854138.32	2245315.35	1885142.42
453.29	C21H44NO7P	LysoPE 16:0	Lipids	LPE	53862-35-4	1744472.43	2411722.93	947274.62	1701156.66
330.24	C18H34O5	9,10,13-Trihydroxy-11-Octadecenoic Acid	Lipids	Free fatty acids	29907-57-1	1848609.41	1672240.71	1364838.50	1628562.87
475.27	C23H42NO7P	LysoPE 18:3(2n isomer)	Lipids	LPE	-	1822773.91	851160.98	1812216.98	1495383.96
240.21	C15H28O2	Cis-10-Pentadecenoic Acid(C15:1)	Lipids	Free fatty acids	84743-29-3	1682105.92	1174408.72	1321141.07	1392551.90
278.22	C18H30O2	Punicic acid (9Z,11E,13Z-octadecatrienoic acid)	Lipids	Free fatty acids	544-72-9	1106579.31	796723.87	858681.73	920661.64

296.24	C18H32O3	13(S)-HODE;13(S)-Hydroxyoctadeca-9Z,11E-dienoic acid*	Lipids	Free fatty acids	10219-69-9	1015152.91	761769.32	847362.30	874761.51
296.24	C18H32O3	9S-Hydroxy-10E,12Z-octadecadienoic acid*	Lipids	Free fatty acids	15514-85-9	1015152.91	761769.32	847362.30	874761.51
354.28	C21H38O4	1-Linoleoylglycerol*	Lipids	Glycerol ester	2277-28-3	992480.72	540171.92	1022935.85	851862.83
354.28	C21H38O4	2-Linoleoylglycerol*	Lipids	Glycerol ester	3443-82-1	711308.18	384223.45	923665.83	673065.82
292.24	C19H32O2	Methyl linolenate	Lipids	Free fatty acids	301-00-8	1004315.49	307513.21	657444.93	656424.55
310.21	C18H30O4	13(s)-hydroperoxy-(9z,11e,15z)-octadecatrienoic acid	Lipids	Free fatty acids	67597-26-6	795462.74	593810.26	566311.78	651861.59
312.23	C18H32O4	9-Hydroxy-13-oxo-10-octadecenoic Acid	Lipids	Free fatty acids	-	898909.90	308792.85	532164.51	579955.75
516.33	C27H48O9	2-Linoleoylglycerol-1-O-glucoside	Lipids	Glycerol ester	-	588832.94	455091.31	543885.41	529269.89
302.25	C17H34O4	1-Monomyristin	Lipids	Free fatty acids	589-68-4	424035.24	501280.59	584966.61	503427.48
499.27	C25H42NO7P	LysoPE 20:5	Lipids	LPE	-	667793.26	324200.88	476654.19	489549.44
352.26	C21H36O4	1- α -Linolenoyl-glycerol*	Lipids	Glycerol ester	-	608877.81	256341.66	581013.68	482077.72
493.32	C24H48NO7P	LysoPC 16:1(2n isomer)	Lipids	LPC	-	425407.29	429287.90	557831.01	470842.06
257.10	C8H20NO6P	Choline Alfoscerate	Lipids	PC	28319-77-9	648034.07	322237.69	392142.44	454138.06
523.36	C26H54NO7P	LysoPC 18:0(2n isomer)	Lipids	LPC	-	480113.87	338932.96	327483.31	382176.71
523.36	C26H54NO7P	LysoPC 18:0	Lipids	LPC	19420-57-6	377999.27	276503.82	319094.91	324532.67
352.26	C21H36O4	2- α -Linolenoyl-glycerol*	Lipids	Glycerol ester	55268-58-1	320323.11	164807.37	426789.67	303973.38
507.33	C25H50NO7P	LysoPC 17:1	Lipids	LPC	-	289574.64	174733.07	406961.25	290422.99
296.24	C18H32O3	9(10)-EpOME;(9R,10S)-(12Z)-9,10-Epoxyoctadecenoic acid	Lipids	Free fatty acids	16833-56-0	369169.75	195526.62	272681.45	279125.94
254.22	C16H30O2	Palmitoleic Acid*	Lipids	Free fatty acids	373-49-9	250820.28	256864.41	248146.46	251943.72
276.21	C18H28O2	9,12-Octadecadien-6-Ynoic Acid	Lipids	Free fatty acids	61481-29-6	312867.53	162666.14	249140.36	241558.01
254.22	C16H30O2	(7Z)-Hexadecenoic acid*	Lipids	Free fatty acids	2416-19-5	230754.04	234199.33	239839.19	234930.86
278.22	C18H30O2	Crepenynic acid	Lipids	Free fatty acids	2277-31-8	273360.18	160567.54	259518.91	231148.88

280.24	C18H32O2	(9Z,11E)-Octadecadienoic acid	Lipids	Free fatty acids	2540-56-9	208341.26	162933.73	264088.25	211787.74
308.27	C20H36O2	Eicosadienoic acid	Lipids	Free fatty acids	5598-38-9	198360.55	214989.79	196091.33	203147.22
509.35	C25H52NO7P	LysoPC 17:0*	Lipids	LPC	50930-23-9	176947.94	252344.07	85104.96	171465.66
547.36	C28H54NO7P	LysoPC 20:2	Lipids	LPC	-	237346.79	83544.12	183438.12	168109.68
300.27	C18H36O3	2R-Hydroxyoctadecanoic Acid	Lipids	Free fatty acids	26633-48-7	237196.00	136546.73	94071.48	155938.07
338.25	C20H34O4	5,6-DiHETrE [(±)5,6-dihydroxy-8Z,11Z,14Z-eicosatrienoic acid]	Lipids	Free fatty acids	213382-49-1	220977.63	80049.09	154708.81	151911.84
509.35	C25H52NO7P	LysoPC 17:0(2n isomer)*	Lipids	LPC	-	123470.41	209566.64	114281.40	149106.15
314.25	C18H34O4	Hydroxy ricinoleic acid	Lipids	Free fatty acids	-	209484.99	96585.92	139570.16	148547.02
317.29	C18H39NO3	4-Hydroxysphinganine	Lipids	Sphingolipids	554-62-1	131529.89	157636.97	139887.27	143018.05
481.32	C23H48NO7P	LysoPC 15:0(2n isomer)*	Lipids	LPC	-	115546.78	143610.30	106723.60	121960.23
514.31	C27H46O9	1-α-Linolenoyl-glycerol-3-O-glucoside	Lipids	Glycerol ester	-	108501.33	112270.20	144502.23	121757.92
678.38	C33H58O14	2-Linoleoylglycerol-1,3-di-O-glucoside	Lipids	Glycerol ester	-	106631.87	105580.46	149452.83	120555.05
465.29	C22H44NO7P	LysoPE 17:1(2n isomer)*	Lipids	LPE	-	144217.98	44395.29	168112.91	118908.72
505.32	C25H48NO7P	LysoPC 17:2	Lipids	LPC	-	144442.34	58569.12	139468.26	114159.90
200.18	C12H24O2	Dodecanoic acid (Lauric acid)	Lipids	Free fatty acids	143-07-7	134826.02	120880.80	86536.20	114081.01
256.24	C16H32O2	Palmitic acid	Lipids	Free fatty acids	57-10-3	109985.34	106370.78	120100.83	112152.32
481.32	C23H48NO7P	LysoPC 15:0*	Lipids	LPC	108273-89-8	113317.26	130043.14	93045.83	112135.41
676.37	C33H56O14	2-α-Linolenoyl-glycerol-1,3-di-O-glucoside	Lipids	Glycerol ester	-	94332.12	69979.20	170791.66	111700.99
296.23	C18H32O3	15(R)-Hydroxylinoleic Acid	Lipids	Free fatty acids	177931-23-6	173103.98	60163.56	73830.70	102366.08
296.23	C18H32O3	9-Oxo-12Z-Octadecenoic acid	Lipids	Free fatty acids	112543-32-5	173103.98	60163.56	73830.70	102366.08
330.24	C18H34O5	9,10,11-Trihydroxy-12-octadecenoic acid	Lipids	Free fatty acids	61911-67-9	108812.93	93981.51	79610.57	94135.00
330.24	C18H34O5	9,12,13-TriHOME; 9(S),12(S),13(S)-Trihydroxy-10(E)-octadecenoic acid	Lipids	Free fatty acids	97134-11-7	117839.36	81306.36	71222.81	90122.84

294.22	C18H30O3	13-Hydroxy-6,9,11-octadecatrienoic acid	Lipids	Free fatty acids	74784-20-6	85331.91	88956.89	93173.71	89154.17
501.29	C25H44NO7P	LysoPE 20:4	Lipids	LPE	-	126828.26	49990.02	73027.52	83281.93
298.32	C20H42O	1-Eicosanol	Lipids	Free fatty acids	629-96-9	86314.81	71954.07	71726.96	76665.28
312.23	C18H32O4	9-Hydroperoxy-9Z,11E-Octadecadienoic Acid	Lipids	Free fatty acids	-	67049.33	79239.73	82629.38	76306.15
467.30	C22H46NO7P	LysoPC 14:0	Lipids	LPC	20559-16-4	82138.90	77992.88	65889.15	75340.31
479.30	C23H46NO7P	LysoPC 15:1	Lipids	LPC	-	72091.79	72769.07	72623.05	72494.63
328.23	C18H32O5	9,12,13-Trihydroxy-10,15-octadecadienoic acid	Lipids	Free fatty acids	-	89431.16	65623.54	59844.10	71632.93
298.25	C18H34O3	Ricinoleic acid	Lipids	Free fatty acids	141-22-0	76065.68	67788.87	64564.26	69472.94
296.24	C18H32O3	12,13-Epoxy-9-Octadecenoic Acid	Lipids	Free fatty acids	6799-85-5	81182.93	43280.83	67742.46	64068.74
244.17	C13H24O4	Tridecanedioic acid	Lipids	Free fatty acids	505-52-2	58033.09	50728.87	49831.66	52864.54
184.11	C10H16O3	(E)-Linalool-1-oic acid	Lipids	Free fatty acids	-	61360.80	49541.19	40258.15	50386.71
286.25	C17H34O3	3-Hydroxy-palmitic acid methyl ester	Lipids	Free fatty acids	51883-36-4	60925.31	38952.48	34205.31	44694.37
294.22	C18H30O3	9-Oxo-10E,12Z-octadecadienoic acid	Lipids	Free fatty acids	54232-59-6	45375.89	23802.01	34235.96	34471.29
310.10	C18H30O4	9-Hydroperoxy-10E,12,15Z-octadecatrienoic acid	Lipids	Free fatty acids	111004-08-1	33454.40	25449.30	38219.39	32374.36
491.30	C24H46NO7P	LysoPC 16:2(2n isomer)	Lipids	LPC	-	35819.53	25658.50	30787.19	30755.08
286.21	C16H30O4	Hexadecanedioic acid	Lipids	Free fatty acids	505-54-4	28130.01	25198.09	28410.45	27246.18
286.29	C18H38O2	1,18-Octadecanediol	Lipids	Free fatty acids	3155-43-9	45878.40	19898.64	13765.10	26514.05
437.25	C20H40NO7P	LysoPE 15:1(2n isomer)*	Lipids	LPE	-	30334.87	13720.86	20776.31	21610.68
439.27	C20H42NO7P	LysoPE 15:0	Lipids	LPE	-	25890.70	28031.25	7914.35	20612.10
226.19	C14H26O2	Myristoleic acid	Lipids	Free fatty acids	544-64-9	26405.25	10115.43	19524.87	18681.85
439.27	C20H42NO7P	LysoPE 15:0(2n isomer)	Lipids	LPE	-	20067.79	18739.43	10450.75	16419.32
437.25	C20H40NO7P	LysoPE 15:1*	Lipids	LPE	-	16768.85	11653.19	19857.87	16093.30

425.25	C19H40NO7P	LysoPE 14:0*	Lipids	LPE	-	16597.97	15685.99	13268.16	15184.04
425.25	C19H40NO7P	LysoPE 14:0(2n isomer)*	Lipids	LPE	-	18114.54	15520.89	11167.52	14934.32
294.22	C18H30O3	13-KODE; (9Z,11E)-13-Oxo-octadeca-9,11-dienoic acid	Lipids	Free fatty acids	54739-30-9	15289.65	7390.62	10476.91	11052.39
294.22	C18H30O3	9-Hydroxy-10,12,15-octadecatrienoic acid	Lipids	Free fatty acids	89886-42-0	15289.65	7390.62	10476.91	11052.39
310.21	C18H30O4	9-Hydroxy-12-oxo-10(E),15(Z)-octadecadienoic acid	Lipids	Free fatty acids	-	11296.75	4233.10	5475.30	7001.72
230.15	C12H22O4	Dodecanedioic acid	Lipids	Free fatty acids	693-23-2	2124.54	1608.29	1001.08	1577.97
267.10	C10H13N5O4	Adenosine	Nucleotides and derivatives	Nucleotides and derivatives	58-61-7	35729731.11	25204794.59	21455754.04	27463426.58
166.03	C6H6N4S	6-Methylmercaptopurine	Nucleotides and derivatives	Nucleotides and derivatives	50-66-8	11250234.94	13340053.56	6862915.89	10484401.46
332.05	C10H13N4O7P	2'-Deoxyinosine-5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	3393-18-8	9823463.00	6025572.69	4983122.98	6944052.89
383.11	C14H17N5O8	Succinyladenosine	Nucleotides and derivatives	Nucleotides and derivatives	4542-23-8	5996380.58	6782308.67	5219452.76	5999380.67
283.09	C10H13N5O5	Guanosine	Nucleotides and derivatives	Nucleotides and derivatives	118-00-3	3020169.18	2288837.63	2272976.09	2527327.63
297.09	C11H15N5O3S	5'-Deoxy-5'-(methylthio)adenosine	Nucleotides and derivatives	Nucleotides and derivatives	2457-80-9	2292718.75	2571223.00	2455033.80	2439658.52
365.17	C16H23N5O5	Isopentenyladenine-7-N-glucoside	Nucleotides and derivatives	Nucleotides and derivatives	-	1234947.95	1203699.75	1277516.00	1238721.23
566.06	C15H24N2O17P2	Uridine 5'-diphospho-D-glucose	Nucleotides and derivatives	Nucleotides and derivatives	133-89-1	1014252.27	1222834.02	981827.65	1072971.31
111.04	C4H5N3O	Cytosine	Nucleotides and derivatives	Nucleotides and derivatives	71-30-7	559852.82	537891.37	609434.62	569059.60

331.07	C10H14N5O6 P	2'-Deoxyadenosine-5'- monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	653-63-4	491176.26	576480.26	265025.11	444227.21
295.06	C8H14N3O7P	5-Aminoimidazole ribonucleotide	Nucleotides and derivatives	Nucleotides and derivatives	25635-88-5	326000.44	192974.80	219118.40	246031.21
284.08	C10H12N4O6	Xanthosine	Nucleotides and derivatives	Nucleotides and derivatives	146-80-5	258265.65	252322.53	161986.51	224191.57
663.11	C21H27N7O1 4P2	Nicotinic acid adenine dinucleotide	Nucleotides and derivatives	Nucleotides and derivatives	53-84-9	252514.83	223356.79	146915.40	207595.67
347.06	C10H14N5O7 P	Adenosine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	61-19-8	185535.06	161970.67	160252.80	169252.84
283.09	C10H13N5O5	Crotonoside; 2- Hydroxyadenosine	Nucleotides and derivatives	Nucleotides and derivatives	1818-71-9	182145.50	153463.30	155986.07	163864.96
114.04	C4H6N2O2	5,6-Dihydrouracil	Nucleotides and derivatives	Nucleotides and derivatives	504-07-4	119516.13	108823.04	119235.22	115858.13
345.05	C10H12N5O7 P	Guanosine 3',5'-cyclic monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	7665-99-8	140218.25	100716.94	104905.89	115280.36
244.07	C9H12N2O6	Uridine	Nucleotides and derivatives	Nucleotides and derivatives	58-96-8	112598.46	116479.47	113320.95	114132.96
243.09	C9H13N3O5	Cytidine	Nucleotides and derivatives	Nucleotides and derivatives	65-46-3	104147.61	82440.82	78046.15	88211.53
311.12	C12H17N5O5	2-(Dimethylamino)guanosine	Nucleotides and derivatives	Nucleotides and derivatives	2140-67-2	74162.76	93141.50	93604.83	86969.70
743.08	C21H28N7O1 7P3	NADP (Nicotinamide adenine dinucleotide phosphate)	Nucleotides and derivatives	Nucleotides and derivatives	53-59-8	78259.20	90131.83	74465.10	80952.04
427.03	C10H15N5O1 0P2	Adenosine 5'-diphosphate	Nucleotides and derivatives	Nucleotides and derivatives	58-64-0	89767.20	76822.53	62822.73	76470.82

251.10	C10H13N5O3	2'-Deoxyadenosine	Nucleotides and derivatives	Nucleotides and derivatives	958-09-8	72195.48	44741.29	56100.79	57679.19
785.16	C27H33N9O15P2	Riboflavin 5'-Adenosine Diphosphate	Nucleotides and derivatives	Nucleotides and derivatives	146-14-5	49460.89	42522.33	46190.68	46057.97
324.04	C9H13N2O9P	Uridine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	58-97-9	48227.74	33737.49	50707.27	44224.17
149.07	C6H7N5	1-Methyladenine	Nucleotides and derivatives	Nucleotides and derivatives	5142-22-3	34601.01	46132.26	32059.25	37597.51
244.07	C9H12N2O6	β -Pseudouridine	Nucleotides and derivatives	Nucleotides and derivatives	1445-07-4	38852.07	11046.80	47804.12	32567.66
112.03	C4H4N2O2	Uracil	Nucleotides and derivatives	Nucleotides and derivatives	66-22-8	35107.80	34571.82	22106.11	30595.24
214.02	C5H11O7P	2-Deoxyribose-1-phosphate	Nucleotides and derivatives	Nucleotides and derivatives	17210-42-3	37622.56	34688.90	18588.22	30299.89
404.00	C9H14N2O12P2	Uridine 5'-diphosphate	Nucleotides and derivatives	Nucleotides and derivatives	27821-45-0	26990.88	28686.37	33997.29	29891.51
267.10	C10H13N5O4	2'-Deoxyguanosine	Nucleotides and derivatives	Nucleotides and derivatives	961-07-9	35442.83	24139.12	28891.66	29491.20
268.08	C10H12N4O5	9-(Arabinosyl)hypoxanthine	Nucleotides and derivatives	Nucleotides and derivatives	7013-16-3	35620.97	20765.38	30057.83	28814.73
214.02	C5H11O7P	2-Deoxyribose-5'-phosphate	Nucleotides and derivatives	Nucleotides and derivatives	102916-66-5	35260.08	27693.81	22021.47	28325.12
227.09	C9H13N3O4	2'-Deoxycytidine	Nucleotides and derivatives	Nucleotides and derivatives	951-77-9	32914.12	25219.13	19771.83	25968.36
363.06	C10H14N5O8P	Guanosine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	85-32-5	24814.21	15383.52	19083.03	19760.25

297.11	C11H15N5O5	N7-Methylguanosine	Nucleotides and derivatives	Nucleotides and derivatives	20244-86-4	14176.47	20659.87	18768.61	17868.32
134.02	C4H6O5	L-Malic acid	Organic acids	Organic acids	97-67-6	35040038.34	37484507.26	41538291.12	38020945.57
192.03	C6H8O7	Citric Acid	Organic acids	Organic acids	77-92-9	21054809.24	21107799.10	23687683.62	21950097.32
192.03	C6H8O7	Isocitric Acid	Organic acids	Organic acids	320-77-4	15361145.54	19107938.40	13473021.71	15980701.88
142.03	C6H6O4	Muconic acid	Organic acids	Organic acids	1119-72-8	11097220.36	13830047.07	16162036.18	13696434.54
103.06	C4H9NO2	2-Aminoisobutyric acid	Organic acids	Organic acids	62-57-7	7084533.51	6830301.10	6418667.55	6777834.05
118.03	C4H6O4	Succinic acid*	Organic acids	Organic acids	110-15-6	6135433.34	6671740.86	4440645.27	5749273.16
118.03	C4H6O4	Methylmalonic acid*	Organic acids	Organic acids	516-05-2	6135433.34	6671740.86	4440645.27	5749273.16
129.08	C6H11NO2	L-Pipecolic Acid	Organic acids	Organic acids	3105-95-1	5207612.09	6131165.54	3688007.73	5008928.45
131.09	C6H13NO2	6-Aminocaproic acid	Organic acids	Organic acids	60-32-2	4806302.43	4958982.51	5141279.75	4968854.90
103.06	C4H9NO2	γ-Aminobutyric acid	Organic acids	Organic acids	56-12-2	5079589.27	4309073.94	4050043.22	4479568.81
145.09	C5H11N3O2	4-Guanidinobutyric acid	Organic acids	Organic acids	463-00-3	1524867.82	1569623.88	1632930.31	1575807.34
192.06	C7H12O6	Quinic Acid	Organic acids	Organic acids	77-95-2	1003886.05	1155064.67	1011937.08	1056962.60
133.04	C4H7NO4	Iminodiacetic acid	Organic acids	Organic acids	142-73-4	780951.21	722646.98	561563.73	688387.31
188.10	C9H16O4	Azelaic acid	Organic acids	Organic acids	123-99-9	681472.76	550841.12	529060.83	587124.90
104.06	C3H4O4	Malonic acid	Organic acids	Organic acids	141-82-2	699992.57	596935.73	435441.43	577456.58
132.04	C5H8O4	Glutaric acid	Organic acids	Organic acids	110-94-1	538983.98	519153.35	513199.31	523778.88
272.24	C16H32O3	2-Hydroxyhexadecanoic acid	Organic acids	Organic acids	764-67-0	690008.87	233545.94	178155.32	367236.71
174.02	C6H6O6	Trans-Citridic acid	Organic acids	Organic acids	4023-65-8	200693.67	311558.79	312780.80	275011.09
116.01	C4H4O4	Fumaric acid	Organic acids	Organic acids	110-17-8	286549.10	323780.81	211890.86	274073.59
176.07	C7H12O5	2-Isopropylmalic Acid	Organic acids	Organic acids	49601-06-1	232246.88	285597.29	150736.10	222860.09
176.07	C7H12O5	3-Isopropylmalic Acid*	Organic acids	Organic acids	921-28-8	229348.71	223962.30	167487.12	206932.71

176.07	C7H12O5	2-Propylmalic Acid*	Organic acids	Organic acids	-	229348.71	223962.30	167487.12	206932.71
146.02	C5H6O5	α -Ketoglutaric acid	Organic acids	Organic acids	328-50-7	204522.58	201890.77	197121.04	201178.13
119.02	C3H5NO4	Aminomalonic acid	Organic acids	Organic acids	1068-84-4	185529.09	268432.79	128280.30	194080.73
118.06	C5H10O3	β -Hydroxyisovaleric acid	Organic acids	Organic acids	625-08-1	165379.18	160868.53	111773.47	146007.06
132.05	C4H8N2O3	3-Ureidopropionic Acid	Organic acids	Organic acids	462-88-4	133428.10	183463.78	81208.66	132700.18
148.04	C5H8O5	2-Hydroxyglutaric Acid	Organic acids	Organic acids	13095-48-2	109097.08	129392.87	106523.52	115004.49
148.04	C5H8O5	3-Methylmalic acid	Organic acids	Organic acids	152204-30-3	119542.70	124872.55	89100.47	111171.91
170.00	C3H7O6P	DL-Glyceraldehyde-3-phosphate	Organic acids	Organic acids	591-59-3	67536.91	81603.43	49623.53	66254.62
167.98	C3H5O6P	Phosphoenolpyruvate	Organic acids	Organic acids	138-08-9	69083.43	65587.73	59316.18	64662.45
123.03	C6H5NO2	2-Picolinic acid	Organic acids	Organic acids	98-98-6	76698.06	47707.70	41985.81	55463.86
150.02	C4H6O6	L-Tartaric acid	Organic acids	Organic acids	87-69-4	68200.87	60043.32	35959.69	54734.63
174.09	C8H14O4	Suberic Acid	Organic acids	Organic acids	505-48-6	66631.43	27521.73	54142.62	49431.93
290.12	C10H18N4O6	Argininosuccinic acid	Organic acids	Organic acids	2387-71-5	42583.91	45011.60	44671.71	44089.08
148.04	C5H8O5	L-Citramalic acid	Organic acids	Organic acids	6236-09-5	31429.11	35720.99	41655.00	36268.37
101.05	C4H7NO2	1-Aminocyclopropane-1-carboxylic acid	Organic acids	Organic acids	22059-21-8	43998.56	25473.13	34102.72	34524.80
130.03	C5H6O4	Methylenesuccinic acid	Organic acids	Organic acids	97-65-4	37659.85	25603.23	38500.35	33921.14
146.06	C6H10O4	2,2-Dimethylsuccinic acid	Organic acids	Organic acids	597-43-3	22806.18	47624.53	19307.22	29912.64
544.13	C19H28O18	Quinic acid O-di-glucuronic acid	Organic acids	Organic acids	-	35748.83	19708.71	25486.02	26981.18
132.04	C5H8O4	2-Hydroxy-2-methyl-3-oxobutanoic acid	Organic acids	Organic acids	71698-08-3	29004.56	27537.04	20171.87	25571.16
190.10	C7H14N2O4	2,6-Diaminoimelic acid	Organic acids	Organic acids	583-93-7	20993.28	22622.34	22334.62	21983.42
146.02	C5H6O5	2-Methyl-3-oxosuccinic acid	Organic acids	Organic acids	-	21434.47	18925.73	18203.19	19521.13
104.01	C3H4O4	Hydroxypyruvic acid	Organic acids	Organic acids	1113-60-6	17588.84	16127.54	18193.67	17303.35
104.01	C3H4O4	Tartronate semialdehyde	Organic acids	Organic acids	2480-77-5	17588.84	16127.54	18193.67	17303.35

159.09	C7H13NO3	5-Acetamidopentanoic Acid	Organic acids	Organic acids	1072-10-2	11968.57	18255.02	17805.37	16009.65
144.04	C6H8O4	2,3-Dimethylsuccinic acid	Organic acids	Organic acids	13545-04-5	9380.58	15705.05	6254.22	10446.62
131.07	C4H9N3O2	Creatine	Organic acids	Organic acids	57-00-1	8413.02		9661.72	9037.37
342.12	C12H22O11	Galactinol	Others	Saccharides	3687-64-7	30856895.01	29647759.25	25992880.00	28832511.42
134.02	C4H6O5	3-Dehydro-L-Threonic Acid	Others	Saccharides	-	23087043.25	24488290.69	27158096.87	24911143.60
342.12	C12H22O11	D-Sucrose*	Others	Saccharides	57-50-1	12062614.01	15920510.64	11115694.59	13032939.75
342.12	C12H22O11	Isomaltulose*	Others	Saccharides	13718-94-0	8530914.44	7144711.96	7709333.20	7794986.53
290.00	C6H11PO11	Glucarate O-Phosphoric acid	Others	Saccharides	-	6770144.44	7050864.14	8392677.31	7404561.96
332.11	C14H20O9	2,6-Dimethoxy-4-hydroxyphenol- 1-O-β-D-glucopyranoside	Others	Others	-	5939667.72	6068964.24	10115001.42	7374544.46
330.13	C15H22O8	Bartsioside	Others	Alcohol compounds	62133-72-6	8682681.93	5471078.07	7540288.48	7231349.49
342.12	C12H22O11	D-Maltose*	Others	Saccharides	69-79-4	4695746.96	7965693.00	5689236.71	6116892.22
192.08	C11H12O3	Eugenyl formate	Others	Others	-	5055543.00	3716127.67	3938694.35	4236788.34
129.02	C5H7NOS	Epigoitrin	Others	Others	1072-93-1	3046701.26	4002315.38	4904991.12	3984669.25
342.12	C12H22O11	D-Trehalose*	Others	Saccharides	99-20-7	3576380.70	4195844.90	3907905.35	3893376.98
290.04	C7H15O10P	D-Sedoheptuiose 7-phosphate	Others	Saccharides	2646-35-7	4052575.39	3477315.58	3986375.53	3838755.50
256.08	C11H14NO6+	Nicotinate D-ribonucleoside	Others	Vitamin	17720-18-2	3108359.74	3720847.15	3688813.98	3506006.96
342.12	C12H22O11	Melibiose	Others	Saccharides	585-99-9	3692257.34	3696966.70	3079849.35	3489691.13
356.13	C20H20O6	6,7-dimethoxy-2-[2-(4'-hydroxy- 3'-methoxyphenyl)ethyl]chromone	Others	Others	-	2535546.45	1935374.91	3236543.23	2569154.86
180.06	C6H12O6	D-Fructose	Others	Saccharides	57-48-7	2633817.41	2089177.81	1453908.06	2058967.76
180.06	C6H12O6	D-Glucose	Others	Saccharides	50-99-7	2128796.60	2305956.07	1246775.27	1893842.65
180.06	C6H12O6	Inositol	Others	Saccharides	87-89-8	2129975.63	2013674.47	1315886.77	1819845.62
278.15	C16H22O4	Senkyunolide M	Others	Lactones	146986-60-9	1542331.73	1640315.02	1368396.03	1517014.26

260.03	C6H13O9P	Glucose-1-phosphate*	Others	Saccharides	59-56-3	1312979.08	1520055.93	1078638.17	1303891.06
331.13	C14H21NO8	Pyridoxine-5'-O-glucoside	Others	Vitamin	-	1626823.48	1289382.45	974240.21	1296815.38
260.03	C6H13O9P	D-Glucose 6-phosphate*	Others	Saccharides	56-73-5	1176916.92	1472484.35	1197008.69	1282136.65
219.11	C9H17NO5	D-Pantothenic Acid	Others	Vitamin	79-83-4	1034937.41	1175688.04	981492.72	1064039.39
122.05	C6H6N2O	Nicotinamide	Others	Vitamin	98-92-0	940772.14	784896.94	848694.56	858121.21
488.17	C18H32O15	Solatriose	Others	Saccharides	528-40-5	753930.93	981872.93	436501.66	724101.84
260.03	C6H13O9P	D-Fructose 6-phosphate*	Others	Saccharides	643-13-0	618497.87	729988.29	487992.13	612159.43
504.17	C18H32O16	Maltotriose	Others	Saccharides	1109-28-0	569434.06	460221.96	732523.66	587393.23
504.17	C18H32O16	Raffinose	Others	Saccharides	512-69-6	514943.02	413141.44	695441.01	541175.16
204.08	C12H12O3	Senkyunolide B*	Others	Lactones	93236-67-0	490716.53	432468.03	356513.19	426565.92
196.06	C6H12O7	Gluconic acid	Others	Saccharides	526-95-4	399572.99	427714.70	263689.19	363658.96
179.08	C6H13NO5	D-Glucosamine	Others	Saccharides	3416-24-8	75253.44	748571.18	263837.19	362553.94
210.04	C6H10O8	D-Galactaric acid	Others	Saccharides	526-99-8	275707.61	302156.18	323658.27	300507.35
210.04	C6H10O8	D-Saccharic acid	Others	Saccharides	87-73-0	250951.48	305879.02	246372.49	267734.33
493.18	C20H31NO13	Pyridoxine-5'-O-diglucoside	Others	Vitamin	-	185300.53	229853.65	272388.82	229181.00
182.08	C6H14O6	Dulcitol	Others	Saccharides	608-66-2	227133.58	144613.56	310043.07	227263.40
185.99	C3H7O7P	3-Phospho-D-glyceric acid	Others	Saccharides	820-11-1	218556.32	168983.17	232225.23	206588.24
310.12	C19H18O4	6,7-dimethoxy-2-[2-phenylethyl]chromone	Others	Others	-	185511.96	174551.35	241723.89	200595.73
169.07	C8H11NO3	Pyridoxine	Others	Vitamin	65-23-6	234369.63	187777.97	134852.38	185666.66
210.07	C7H14O7	Sedoheptulose	Others	Saccharides	3019-74-7	195939.47	185222.06	175156.51	185439.35
221.09	C8H15NO6	N-Acetyl-D-glucosamine	Others	Saccharides	7512-17-6	76699.02	184555.98	258017.12	173090.71
342.12	C12H22O11	D-Cellobiose	Others	Saccharides	528-50-7	190450.87	143465.24	144394.11	159436.74
174.02	C6H6O6	Dehydroascorbic acid	Others	Vitamin	490-83-5	164657.36	186517.87	125204.26	158793.16

182.08	C6H14O6	D-Sorbitol	Others	Saccharides	50-70-4	155994.20	106636.95	201669.17	154766.77
666.22	C24H42O21	Stachyose	Others	Saccharides	470-55-3	159406.64	112381.64	150238.12	140675.47
666.22	C24H42O21	Nystose	Others	Saccharides	13133-07-8	176420.28	77544.13	158204.89	137389.76
334.07	C9H19O11P	1-(sn-Glycero-3-phospho)-1D-myo-inositol	Others	Saccharides	-	124711.68	138681.94	105314.59	122902.73
166.05	C5H10O6	D-Xylonic acid	Others	Saccharides	526-91-0	127878.55	139960.67	54645.90	107495.04
422.08	C12H23O14P	Trehalose 6-phosphate	Others	Saccharides	4484-88-2	90537.71	107154.57	102554.50	100082.26
148.04	C5H8O5	D-Arabinono-1,4-lactone	Others	Saccharides	2782-09-4	110662.57	71338.30	89672.92	90557.93
123.03	C6H5NO2	Nicotinic acid (Vitamin B3)	Others	Vitamin	59-67-6	111701.83	76854.54	75839.01	88131.79
136.04	C4H8O5	D-Threonic Acid	Others	Saccharides	3909-12-4	97556.93	79172.45	82824.34	86517.90
150.05	C5H10O5	D-Arabinose	Others	Saccharides	10323-20-3	90645.09	88471.94	71938.40	83685.14
504.17	C18H32O16	D-Melezitose	Others	Saccharides	597-12-6	59053.50	87561.21	102599.11	83071.27
194.03	C6H10O7	D-Galacturonic acid*	Others	Saccharides	685-73-4	94612.37	61974.82	76415.33	77667.51
504.17	C18H32O16	D-Panose	Others	Saccharides	33401-87-5	74499.48	62851.57	91797.49	76382.85
123.03	C6H5NO2	Isonicotinic acid	Others	Vitamin	55-22-1	98085.90	64980.61	47754.33	70273.61
650.23	C24H42O20	DMelezitose O-rhamnoside	Others	Saccharides	-	57602.55	96779.21	55417.92	69933.23
188.10	C9H16O4	Eucommiol	Others	Alcohol compounds	55930-44-4	73558.74	74412.60	51684.37	66551.90
301.06	C8H16NO9P	N-Acetyl-D-glucosamine-1-phosphate	Others	Saccharides	6866-69-9	59112.32	70714.95	58984.45	62937.24
194.04	C6H10O7	D-Glucuronic acid*	Others	Saccharides	6556-12-3	60960.45	65950.79	56097.84	61003.02
164.07	C6H12O5	1,5-Anhydro-D-glucitol	Others	Saccharides	154-58-5	55263.86	50028.03	64118.53	56470.14
170.00	C3H7O6P	Dihydroxyacetone phosphate	Others	Saccharides	57-04-5	50750.58	60978.52	55439.82	55722.97
182.08	C6H14O6	D-Mannitol	Others	Saccharides	69-65-8	48476.04	42352.94	71959.47	54262.82
345.11	C14H19NO9	4-Pyridoxic acid-O-glucoside	Others	Vitamin	-	49626.24	34799.38	44384.74	42936.79
230.02	C5H11O8P	Ribulose-5-phosphate	Others	Saccharides	4300-28-1	49184.01		29696.63	39440.32

120.04	C4H8O4	D-Threose	Others	Saccharides	95-43-2	46815.01	23904.04		35359.53
450.35	C31H46O2	Phylloquinone (Vitamin K1)	Others	Vitamin	84-80-0	37028.64	30459.82	30110.48	32532.98
666.22	C24H42O21	D-Maltotetraose	Others	Saccharides	34612-38-9	25275.79	27026.92	44216.50	32173.07
205.13	C9H19NO4	D-Panthenol	Others	Saccharides	81-13-0	27424.05	33365.68		30394.87
382.21	C24H30O4	(Z)-3,8-Dihydro 6,6';7,3'a-diligustilide	Others	Others	-	34026.45	29151.07	25924.62	29700.71
340.00	C6H14O12P2	D-Fructose-1,6-biphosphate	Others	Saccharides	488-69-7	18560.69	35026.67	17666.15	23751.17
194.08	C7H14O6	D-Pinitol	Others	Saccharides	10284-63-6	25648.98	16870.15	28707.33	23742.15
507.17	C24H29NO11	Pyridoxine-5'-O-(6''-feruloyl)glucoside	Others	Vitamin	-	17163.91	25978.00	22553.50	21898.47
259.05	C6H14NO8P	D-Glucosamine 1-phosphate	Others	Saccharides	2152-75-2	20807.65	12191.02	17041.63	16680.10
200.01	C4H9O7P	D-Erythrose-4-phosphate	Others	Saccharides	585-18-2	18278.58	16682.63	14509.61	16490.27
262.05	C6H15O9P	Sorbitol-6-phosphate	Others	Saccharides	20479-58-7	12792.36	12551.09	6468.54	10604.00
340.00	C6H14O12P2	D-Glucose 1,6-bisphosphate	Others	Saccharides	10139-18-1	3564.04	4584.21	3576.41	3908.22
520.19	C26H32O11	Dehydrodiconiferyl alcohol-gamma'-O-glucoside	Phenolic acids	Phenolic acids	-	51716935.06	56508164.44	49393249.57	52539449.69
368.11	C17H20O9	3-O-Caffeoylquinic acid methyl ester	Phenolic acids	Phenolic acids	123483-19-2	38390882.17	36602493.28	28762039.66	34585138.37
338.10	C16H18O8	3-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	87099-71-6	30848517.91	29904437.83	27005272.01	29252742.58
500.15	C22H28O13	5-O-p-Coumaroylquinic acid O-glucoside	Phenolic acids	Phenolic acids	-	18035696.26	18976405.00	16753327.35	17921809.54
368.11	C17H20O9	1-O-Feruloylquinic acid	Phenolic acids	Phenolic acids	-	16652724.25	16108036.84	16220831.55	16327197.55
338.10	C16H18O8	1-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	-	17222652.72	16168227.60	14063990.87	15818290.40
278.15	C16H22O4	Dibutyl phthalate*	Phenolic acids	Phenolic acids	84-74-2	15385283.11	14599739.11	13730504.97	14571842.40
278.15	C16H22O4	Diisobutyl phthalate*	Phenolic acids	Phenolic acids	84-69-5	14540764.16	13373721.53	13066017.54	13660167.74
166.06	C9H10O3	4'-Hydroxy-3'-methoxyacetophenone (Acetovanillone)	Phenolic acids	Phenolic acids	498-02-2	14302184.06	11216180.11	11953325.06	12490563.08
272.09	C12H16O7	Arbutin	Phenolic acids	Phenolic acids	497-76-7	4554143.42	4509662.48	7493020.47	5518942.12

338.10	C16H18O8	4-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	32451-86-8	6176807.13	5746997.33	4477741.64	5467182.04
332.11	C14H20O9	Leonuriside A	Phenolic acids	Phenolic acids	121748-12-7	3945143.20	3902009.89	6665442.28	4837531.79
368.11	C17H20O9	5-O-Feruloylquinic acid	Phenolic acids	Phenolic acids	-	5366301.27	3858366.70	2957389.71	4060685.89
368.11	C17H20O9	3-O-Feruloylquinic acid	Phenolic acids	Phenolic acids	1899-29-2	3664564.79	3494071.25	3399478.35	3519371.47
368.11	C17H20O9	Chlorogenic acid methyl ester	Phenolic acids	Phenolic acids	29708-87-0	2860536.45	3120434.74	2838149.33	2939706.84
300.08	C13H16O8	4-O-Glucosyl-4-hydroxybenzoic acid	Phenolic acids	Phenolic acids	-	3527180.47	2928118.78	2041620.16	2832306.47
354.10	C16H18O9	4-O-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	-	3094624.12	3819393.27	1207368.77	2707128.72
300.08	C13H16O8	Salicylic acid-2-O-glucoside	Phenolic acids	Phenolic acids	10366-91-3	2323824.52	2312037.34	3458000.66	2697954.17
354.10	C16H18O9	5-O-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	-	3065846.36	3314526.09	1614347.49	2664906.65
461.15	C19H27NO12	Anthranilate-1-O-Sophoroside	Phenolic acids	Phenolic acids	-	2544147.34	3426691.38	1769954.95	2580264.56
139.03	C6H5NO3	4-Nitrophenol	Phenolic acids	Phenolic acids	100-02-7	2711136.11	2433552.12	2394995.32	2513227.85
300.09	C13H16O8	Glucosyloxybenzoic acid	Phenolic acids	Phenolic acids	-	2871280.65	2599282.06	2026485.85	2499016.19
354.10	C16H18O9	3-O-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	-	2831799.57	3043729.58	1611059.27	2495529.47
300.08	C13H16O8	1-O-Salicyloyl- β -D-glucose	Phenolic acids	Phenolic acids	60517-74-0	2811395.44	2620105.65	1823819.04	2418440.04
354.10	C16H18O9	1-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	1241-87-8	2360749.49	2545072.96	1296815.38	2067545.94
482.14	C22H26O12	5-O-p-Coumaroylshikimic acid O-glucoside	Phenolic acids	Phenolic acids	-	1723340.67	1764035.58	2090094.03	1859156.76
338.10	C16H18O8	5-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	1899-30-5	2303223.55	1454011.38	1586191.11	1781142.01
152.05	C8H8O3	Vanillin; 4-Hydroxy-3-Methoxybenzaldehyde	Phenolic acids	Phenolic acids	121-33-5	1693002.87	1168017.04	2139343.13	1666787.68
280.06	C13H12O7	p-Coumaroylmalic acid	Phenolic acids	Phenolic acids	-	1953532.09	1360119.72	1571519.91	1628390.57
316.08	C13H16O9	Protocatechuic acid-4-O-glucoside	Phenolic acids	Phenolic acids	-	2088310.69	1265761.89	1209407.88	1521160.16
316.08	C13H16O9	1-O-Gentisoyl- β -D-glucoside	Phenolic acids	Phenolic acids	23445-11-6	2088310.69	1265761.89	1209407.88	1521160.16
500.15	C22H28O13	3-O-p-Coumaroylquinic acid-O-glucoside	Phenolic acids	Phenolic acids	-	1314658.61	1629937.33	1117518.68	1354038.21

238.05	C11H10O6	Benzoylmalic acid	Phenolic acids	Phenolic acids	22138-51-8	848135.35	1066635.35	1098835.35	1004535.35
302.10	C13H18O8	Tachioside	Phenolic acids	Phenolic acids	109194-60-7	782791.41	695571.77	1003216.43	827193.20
356.11	C16H20O9	Ferulic acid-4-O-glucoside	Phenolic acids	Phenolic acids	117405-51-3	727321.79	1042556.79	639109.89	802996.16
332.11	C14H20O9	Koaburaside	Phenolic acids	Phenolic acids	41653-73-0	798939.21	764881.28	571982.61	711934.37
386.10	C17H22O10	1-O-Eudesmoylquinic acid	Phenolic acids	Phenolic acids	-	682695.95	388039.61	670649.67	580461.74
286.11	C13H18O7	Salicin	Phenolic acids	Phenolic acids	138-52-3	572176.11	569005.29	499001.68	546727.69
400.10	C17H20O11	Sinapoylglucuronic acid	Phenolic acids	Phenolic acids	-	397250.33	484201.82	605915.32	495789.15
122.04	C7H6O2	4-Hydroxybenzaldehyde	Phenolic acids	Phenolic acids	123-08-0	549722.70	388481.39	528551.49	488918.53
138.03	C7H6O3	4-Hydroxybenzoic acid	Phenolic acids	Phenolic acids	99-96-7	452533.08	373189.83	556926.84	460883.25
342.10	C15H18O9	1-O-Caffeoyl- β -D-glucose*	Phenolic acids	Phenolic acids	14364-08-0	503072.05	480668.45	353938.13	445892.87
530.16	C23H30O14	3-O-Feruloylquinic acid-O-glucoside*	Phenolic acids	Phenolic acids	-	434745.31	505271.29	357458.15	432491.58
530.16	C23H30O14	5-O-Feruloyl quinic acid glucoside*	Phenolic acids	Phenolic acids	-	434745.31	505271.29	357458.15	432491.58
464.12	C18H24O14	mudanoside B	Phenolic acids	Phenolic acids	203511-37-9	525504.64	378646.69	378320.86	427490.73
204.08	C12H12O3	Senkyunolide C*	Phenolic acids	Phenolic acids	-	490716.53	432468.03	356513.19	426565.92
332.07	C13H16O10	1-O-Galloyl- β -D-glucose	Phenolic acids	Phenolic acids	58511-73-2	492886.88	516508.04	201218.56	403537.83
318.10	C13H18O9	4,6-dimethoxy-2-methoxyphenyl-1-O-beta-D-glucopyranoside	Phenolic acids	Phenolic acids	-	394321.74	347974.39	464224.35	402173.49
342.10	C15H18O9	6-O-Caffeoyl-D-glucose*	Phenolic acids	Phenolic acids	-	421348.59	453695.40	295824.87	390289.62
332.11	C14H20O9	2,6-dimethoxy-hydroquinone-4-O- β -D-glucopyranoside	Phenolic acids	Phenolic acids	-	401169.15	410982.26	333158.41	381769.94
320.09	C16H16O7	Trans-5-O-(p-Coumaroyl)shikimate	Phenolic acids	Phenolic acids	-	501257.50	208757.50	416750.53	375588.51
182.06	C9H10O4	Syringaldehyde; 4-Hydroxy-3,5-Dimethoxybenzaldehyde	Phenolic acids	Phenolic acids	134-96-3	333903.18	287228.99	436810.24	352647.47
326.10	C15H18O8	Phenylpropionic acid-O- β -D-glucopyranoside	Phenolic acids	Phenolic acids	-	369432.51	350437.87	328165.38	349345.25
326.10	C15H18O8	p-Coumaric acid-4-O-glucoside	Phenolic acids	Phenolic acids	117405-48-8	326588.84	377651.18	305532.57	336590.87

326.10	C15H18O8	1-O-p-Coumaroyl- β -D-glucose	Phenolic acids	Phenolic acids	7139-64-2	326588.84	377651.18	305532.57	336590.87
344.11	C15H20O9	Syringaldehyde-4-O-glucoside	Phenolic acids	Phenolic acids	-	332576.17	360559.98	316082.66	336406.27
342.13	C16H22O8	Coniferin	Phenolic acids	Phenolic acids	531-29-3	297632.16	334328.53	321482.18	317814.29
164.05	C9H8O3	2-Hydroxycinnamic acid*	Phenolic acids	Phenolic acids	583-17-5	346735.35	284635.35	320934.61	317435.10
164.05	C9H8O3	α -Hydroxycinnamic Acid*	Phenolic acids	Phenolic acids	5801-57-0	346735.35	284635.35	320934.61	317435.10
1172.38	C52H68O30	Oleoechinacoside	Phenolic acids	Phenolic acids	122960-94-5	232266.55	320855.05	336133.70	296418.44
344.11	C15H20O9	Dihydrocaffeoylglucose	Phenolic acids	Phenolic acids	-	371717.44	242146.53	207077.90	273647.29
208.07	C11H12O4	Sinapinaldehyde	Phenolic acids	Phenolic acids	4206-58-0	261926.58	192331.97	363411.26	272556.60
226.08	C11H14O5	3,4'-Dihydroxy-3',5'-dimethoxypropiofenone	Phenolic acids	Phenolic acids	136196-47-9	284854.75	274295.12	183211.14	247453.67
356.11	C16H20O9	1-O-Feruloyl- β -D-glucose	Phenolic acids	Phenolic acids	7196-71-6	190071.26	229308.78	177186.16	198855.40
180.08	C10H12O3	Coniferyl alcohol	Phenolic acids	Phenolic acids	458-35-5	187039.39	150095.39	173185.39	170106.72
194.06	C10H10O4	Ferulic acid	Phenolic acids	Phenolic acids	537-98-4	157636.21	157737.34	161605.21	158992.92
402.15	C18H26O10	Benzyl β -primeveroside	Phenolic acids	Phenolic acids	130622-31-0	59384.48	201006.00	166316.90	142235.79
254.08	C12H14O6	1-O-Caffeoylglycerol	Phenolic acids	Phenolic acids	-	163864.94	82266.09	126634.39	124255.14
434.12	C21H22O10	6-O-Caffeoylarbutin	Phenolic acids	Phenolic acids	136172-60-6	120865.36	160381.82	83394.90	121547.36
370.13	C17H22O9	Sinapaldehyde-4-O-Glucoside	Phenolic acids	Phenolic acids	154461-65-1	115842.31	110387.18	130811.53	119013.68
402.15	C18H26O10	Benzyl-(2''-O-xylosyl)glucoside	Phenolic acids	Phenolic acids	-	119565.38	109771.05	119472.82	116269.75
444.20	C21H32O10	(1'R,3R,5R,8'S)-Dihydrophaseic acid-O- β -D-glucoside	Phenolic acids	Phenolic acids	-	131636.17	107749.57	109243.23	116209.66
494.11	C22H22O13	1-O-Caffeoyl-4-O-galloyl- β -D-glucose	Phenolic acids	Phenolic acids	-	110169.84	160875.34	70356.30	113800.49
194.06	C10H10O4	Dimethyl phthalate	Phenolic acids	Phenolic acids	131-11-3	107086.24	107975.35	104272.44	106444.67
678.18	C31H34O17	Dicaffeoylquinic acid-O-glucoside	Phenolic acids	Phenolic acids	-	109977.06	89044.94	91289.83	96770.61
284.05	C12H12O8	Vnilloylmalic acid	Phenolic acids	Phenolic acids	-	101629.78	67996.39	113862.02	94496.06
418.09	C20H18O10	Salvianolic Acid D	Phenolic acids	Phenolic acids	-	55246.68	90083.22	95569.54	80299.81

198.05	C9H10O5	4-Hydroxy-3-methoxymandelate	Phenolic acids	Phenolic acids	55-10-7	78660.82	82804.36	69714.26	77059.81
165.04	C8H7NO3	2-(Formylamino)benzoic acid	Phenolic acids	Phenolic acids	3342-77-6	75052.89	67036.05	86020.64	76036.53
624.21	C29H36O15	Acteoside; Verbascoside	Phenolic acids	Phenolic acids	61276-17-3	68808.72	79208.31	76318.61	74778.55
316.12	C14H20O8	5-(2-Hydroxyethyl)-2-O-glucosylphenol	Phenolic acids	Phenolic acids	-	78582.10	79151.40	61463.25	73065.58
316.12	C14H20O8	Cimidahurinine	Phenolic acids	Phenolic acids	142542-89-0	78582.10	79151.40	61463.25	73065.58
206.17	C14H22O	2,4-Di-Tert-Butylphenol*	Phenolic acids	Phenolic acids	96-76-4	67965.91	75258.92	74585.79	72603.54
168.04	C8H8O4	Vanillic acid	Phenolic acids	Phenolic acids	121-34-6	83296.62	46049.69	88352.17	72566.16
206.17	C14H22O	2,6-Di-tert-butylphenol*	Phenolic acids	Phenolic acids	128-39-2	73726.51	71770.62	69321.18	71606.10
314.10	C14H18O8	Mandelic acid- β -glucoside	Phenolic acids	Phenolic acids	-	56301.57	76695.93	64926.08	65974.53
316.12	C14H20O8	Vanilloside	Phenolic acids	Phenolic acids	74950-96-2	71262.97	51981.70	67417.04	63553.90
478.15	C23H26O11	3,5-Digalloylshikimic acid	Phenolic acids	Phenolic acids	95753-52-9	49018.20	85179.77	47965.70	60721.22
194.06	C10H10O4	Vanillin acetate	Phenolic acids	Phenolic acids	881-68-5	71926.53	60768.29	39223.85	57306.22
530.14	C26H26O12	3,4-O-Dicaffeoylquinic Acid Methyl Ester	Phenolic acids	Phenolic acids	-	73021.27	63354.54	33361.73	56579.18
496.09	C21H20O14	3-O-Digalloyl quinic acid	Phenolic acids	Phenolic acids	-	31326.89	87209.54	43845.46	54127.30
150.07	C9H10O2	p-Coumaryl alcohol	Phenolic acids	Phenolic acids	3690-05-9	54538.74	33329.22	71900.51	53256.16
458.08	C22H18O11	p-Coumaroylcaffeoyltartaric acid	Phenolic acids	Phenolic acids	-	43622.19	41792.68	69639.19	51684.69
268.09	C13H16O6	2-Feruloyl-sn-glycerol	Phenolic acids	Phenolic acids	-	59637.12	41750.45	53551.58	51646.38
386.12	C17H22O10	4-O-Glucosyl-sinapate	Phenolic acids	Phenolic acids	-	61080.27	46312.43	37750.04	48380.91
178.06	C10H10O3	4-Methoxycinnamic acid	Phenolic acids	Phenolic acids	830-09-1	53514.90	40713.80	46725.65	46984.78
482.14	C22H26O12	3-O-p-Coumaroylshikimic acid-O-glucoside	Phenolic acids	Phenolic acids	-	42543.68	43702.78	54481.75	46909.40
452.09	C20H20O12	2-O-Salicyl-6-O-Galloyl-D-Glucose	Phenolic acids	Phenolic acids	-	47246.12	42941.57	41193.25	43793.65
372.11	C16H20O10	Quinacyl syringic acid	Phenolic acids	Phenolic acids	-	49392.92	40435.90	41384.33	43737.72
332.07	C13H16O10	Gallic acid-4-O-glucoside	Phenolic acids	Phenolic acids	84274-52-2	33636.30	28217.42	63216.58	41690.10

198.05	C9H10O5	Syringic acid	Phenolic acids	Phenolic acids	530-57-4	35679.01	29351.34	56716.95	40582.43
398.12	C18H22O10	4-O-Sinapoylquinic acid	Phenolic acids	Phenolic acids	-	38052.57	36372.32	45689.08	40037.99
372.11	C16H20O10	Trihydroxycinnamoylquinic acid	Phenolic acids	Phenolic acids	-	33029.29	45403.68	40760.97	39731.31
148.05	C9H8O2	p-Coumaraldehyde	Phenolic acids	Phenolic acids	2538-87-6	32504.72	22627.31	39744.41	31625.48
504.15	C21H28O14	1-O-Caffeoyl-(6-O-glucosyl)- β -D-glucose	Phenolic acids	Phenolic acids	-	25552.79	23232.33	28729.00	25838.04
634.08	C27H22O18	1-O-Galloyl-4,6-hexahydroxydiphenoyl-D-glucose	Phenolic acids	Phenolic acids	126721-55-9	19198.82	40998.83	14225.78	24807.81
300.05	C12H12O9	Vnilloyltartaric acid	Phenolic acids	Phenolic acids	-	22596.56	20522.55	25412.06	22843.72
326.10	C15H18O8	(2E)-3-[4-(β -D-glucopyranoside)-phenylacrylic]-acid	Phenolic acids	Phenolic acids	-	35252.38	21274.29	9549.67	22025.45
210.09	C11H14O4	Sinapyl alcohol	Phenolic acids	Phenolic acids	537-33-7	19215.95	28411.78	17449.65	21692.46
666.22	C31H38O16	2'-Acetylacteoside	Phenolic acids	Phenolic acids	94492-24-7	13931.63	30728.40	20001.45	21553.83
518.16	C22H30O14	6'-O-Feruloyl-D-sucrose	Phenolic acids	Phenolic acids	118230-77-6	24613.20	23806.88	15338.18	21252.75
756.25	C34H44O19	Forsythoside B	Phenolic acids	Phenolic acids	81525-13-5	8868.63	23138.26	14836.18	15614.36
208.07	C11H12O4	3,4-Dimethoxycinnamic acid	Phenolic acids	Phenolic acids	2316-26-9	17801.85	6393.55	17279.87	13825.09
212.07	C10H12O5	Eudesmic acid (3,4,5-trimethoxybenzoic acid)	Phenolic acids	Phenolic acids	118-41-2		10425.19	12018.51	11221.85
514.10	C21H22O15	1,7-Di-O-galloyl-D-sedoheptulose	Phenolic acids	Phenolic acids	-	11887.85	13836.42	7476.34	11066.87
414.39	C29H50O	β -Sitosterol	Steroids	Steroid	83-46-5	12715938.01	12319283.66	12449578.70	12494933.46
416.33	C27H44O3	Tigogenin	Steroids	Steroid	77-60-1	318449.97	210418.79	255540.88	261469.88
316.02	C15H8O8	3-O-Methylellagic acid	Tannins	Tannin	-	40013.62	43791.42	34234.82	39346.62
434.05	C19H14O12	Ellagic acid-4-O-Xyloside	Tannins	Tannin	139163-18-1	10756.26	23658.24	26451.27	20288.59
634.08	C27H22O18	Corilagin	Tannins	Tannin	23094-69-1	7861.37	22513.67	10808.15	13727.73
470.34	C30H46O4	4,4,8-Trimethyl-3 β ,7 α ,23-trihydroxy-chola-14,24-dien-21-oic acid-21,23-lactone	Terpenoids	Triterpene	-	20621034.70	4675529.55	11060155.06	12118906.44
344.15	C16H24O8	illicinolide A	Terpenoids	Sesquiterpenoids	-	4738440.78	5254002.50	4522610.58	4838351.28

538.21	C26H34O12	Sinenoside	Terpenoids	Monoterpenoids	-	1456897.44	2284405.83	2358498.78	2033267.35
406.15	C17H26O11	8-O-Acetylharpagide	Terpenoids	Monoterpenoids	6926-14-3	1445005.76	1055929.72	704301.66	1068412.38
462.23	C25H34O8	Kumulactone K	Terpenoids	Diterpenoids	-	1165809.91	729423.21	444429.09	779887.40
456.36	C30H48O3	24,30-Dihydroxy-12(13)-ene-lupeol	Terpenoids	Triterpene	-	974157.93	526639.29	838563.66	779786.96
374.17	C21H26O6	12-Norquassin	Terpenoids	Diterpenoids	23460-59-5	265368.51	745421.68	799543.63	603444.61
346.13	C15H22O9	Aucubin	Terpenoids	Sesquiterpenoids	479-98-1	405064.77	468036.29	351548.38	408216.48
362.14	C19H22O7	6-O-p-Coumaroyl-3-methoxy-7-deoxyrehmaglutin A	Terpenoids	Monoterpenoids	-	325583.64	231311.41	250546.04	269147.03
478.22	C25H34O9	Ailanthinone	Terpenoids	Diterpenoids	53683-73-1	356306.74	238129.89	154795.91	249744.18
390.12	C16H22O11	Deacetylasperulosidic acid	Terpenoids	Monoterpenoids	14259-55-3	211082.51	274305.38	208756.33	231381.41
454.34	C30H46O3	Ursonic acid	Terpenoids	Triterpene	6246-46-4	202404.35	230647.35	230100.87	221050.86
470.34	C30H46O4	Semimoronic acid	Terpenoids	Triterpene	102053-38-3	246301.16	135747.31	240630.95	207559.80
538.17	C25H30O13	5-Hydroxy-10-O-(p-methoxycinnamoyl)adoxosidic acid	Terpenoids	Monoterpenoids	-	191951.90	178813.95	227153.28	199306.38
250.12	C14H18O4	13-Nor-desacylcynaropicrin	Terpenoids	Sesquiterpenoids	-	271198.83	180498.94	145802.89	199166.89
302.22	C20H30O2	Levopimaric acid*	Terpenoids	Diterpenoids	79-54-9	174401.09	185203.23	130665.15	163423.16
302.22	C20H30O2	Isopimaric acid*	Terpenoids	Diterpenoids	5835-26-7	173673.30	177695.24	128689.70	160019.41
536.15	C25H28O13	10-O-[(E)-Caffeoyl]-geniposidic acid	Terpenoids	Monoterpenoids	-	117605.96	178937.92	136916.09	144486.66
476.39	C30H52O4	Hispidol B	Terpenoids	Triterpene	78739-39-6	209990.70	92811.78	110050.54	137617.67
610.21	C25H38O17	6'-O- α -D-galactosylbarlerin*	Terpenoids	Monoterpenoids	927691-89-2	99537.96	134701.96	84986.07	106408.66
346.18	C20H26O5	Epirosmanol	Terpenoids	Diterpenoids	-	228943.96	21380.40	65584.68	105303.01
234.16	C15H22O2	7 β -H-9(10)-ene-11,12-Epoxy-8-oxoeremophilane	Terpenoids	Sesquiterpenoids	-	88505.57	107142.28	90363.24	95337.03

610.21	C25H38O17	6'-O- β -D-glucosylbarlerin*	Terpenoids	Monoterpenoids	927691-88-1	113841.96	95961.96	75159.86	94987.93
194.13	C12H18O2	Carvylacetate	Terpenoids	Monoterpenoids	97-42-7	129388.86	62794.29	66531.05	86238.07
456.36	C30H48O3	Oleanolic acid	Terpenoids	Triterpene	508-02-1	76398.03	67584.40	92167.05	78716.49
234.16	C15H22O2	polygodial	Terpenoids	Sesquiterpenoids	6754-20-7	89106.50	73278.51	71771.06	78052.03
456.36	C30H48O3	(23S)-3 β -hydroxydammar-21-oic acid 21,23-lactone	Terpenoids	Triterpene	-	76156.07	71673.28	78275.30	75368.22
388.14	C17H24O10	Vogeloside	Terpenoids	Monoterpenoids	60077-47-6	59637.12	39778.70	98782.78	66066.20
414.23	C21H34O8	Dendronobiloside E-iso-1	Terpenoids	Sesquiterpenoids	-	100153.11	47943.03	25535.64	57877.26
456.36	C30H48O3	Ursolic acid	Terpenoids	Triterpene	77-52-1	57697.51	54222.82	46962.79	52961.04
404.13	C17H24O11	Oleoside 11-methyl ester	Terpenoids	Monoterpenoids	60539-23-3	42917.96	60630.32	48142.57	50563.62
454.34	C30H46O3	Moronic acid	Terpenoids	Triterpene	6713-27-5	48599.14	23836.58	59974.72	44136.82
454.34	C30H46O3	3-Ketoursolic acid	Terpenoids	Triterpene	-	48599.14	23836.58	59974.72	44136.82
394.20	C21H30O7	Nigakilactone M	Terpenoids	Diterpenoids	37812-54-7	85917.10	31013.27	13337.11	43422.49
454.34	C30H46O3	Betulonic acid	Terpenoids	Triterpene	4481-62-3	41112.23	25173.22	62381.75	42889.07
440.37	C30H48O2	Glochidonol	Terpenoids	Triterpene	23963-54-4	67964.98	26745.19	31723.28	42144.49
520.18	C22H32O14	Genipin-1-O-(2''-O-apiosyl)glucoside	Terpenoids	Monoterpenoids	-	44645.95	35717.95		40181.95
312.17	C20H24O3	Triptophenolide	Terpenoids	Diterpenoids	74285-86-2	76370.17	17628.53	24975.18	39657.96
454.34	C30H46O3	Urs-12(13)-en-3-one-28-oic acid	Terpenoids	Triterpene	-	46869.36	28125.09	42995.75	39330.07
458.38	C30H50O3	12,13-Dihydroursolic acid	Terpenoids	Triterpene	-	53631.27	19499.22	34585.95	35905.48
470.38	C31H50O3	Ambolic acid	Terpenoids	Triterpene	13878-93-8	43485.65	28992.14	34511.42	35663.07
390.15	C17H26O10	ajugoside	Terpenoids	Monoterpenoids	52916-96-8	10040.87	51122.68	41379.59	34181.05
498.30	C30H42O6	Cucurbitacin S	Terpenoids	Triterpene	60137-06-6	45430.37	12644.46	38205.76	32093.53

550.19	C23H34O15	Genipin-1-O-gentiobioside	Terpenoids	Monoterpenoids	29307-60-6	29957.74	28657.21	30981.51	29865.49
432.13	C18H24O12	Asperulosidic acid	Terpenoids	Monoterpenoids	25368-11-0	19846.84	23072.91	29169.12	24029.62
530.36	C32H50O6	Viburnenone B1 methyl ester*	Terpenoids	Triterpene	-	29930.88	12117.91	17508.41	19852.40
530.36	C32H50O6	Viburnenone B2 methyl ester*	Terpenoids	Triterpene	-	29930.88	12117.91	17508.41	19852.40
292.20	C18H28O3	JiangxiBaiyingsu I	Terpenoids	Sesquiterpenoids	-	15766.61	9847.99	13739.78	13118.13
456.36	C30H48O3	3,4-Cycloopen-cycloaltin-4(29),25-diene-24(R)-hydroxy-3-carboxylic acid	Terpenoids	Triterpene	-	14194.37	7140.27	17406.33	12913.66
426.39	C30H50O	Cycloartenol	Terpenoids	Triterpene	469-38-5	11561.65	12010.50	12916.81	12162.98
550.28	C29H42O10	Ajugamarin B1	Terpenoids	Diterpenoids	121521-88-8	13320.20		9311.48	11315.84
506.18	C25H30O11	2'-Cinnamoyl mussaenosidic acid	Terpenoids	Monoterpenoids	-	8495.54	7095.80	11744.21	9111.85
408.21	C22H32O7	Picrasinol D	Terpenoids	Diterpenoids	164416-31-3		4520.01	3519.51	4019.76

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Table S2 Metabolites identified in the trunk of *Ailanthus altissima*

Molecular weight (Da)	Formula	Compounds	Class I	Class II	CAS	B1	B2	B3	b-average
376.15	C20H24O7	Ailanthone	Terpenoids	Diterpenoids	981-15-7	151926.33	1805526.32	1497642.80	1151698.48
528.26	C26H40O11	Shinjuglycoside E	Terpenoids	Diterpenoids	112667-45-5	281835.94	623028.52	368333.39	424399.28
388.16	C21H24O7	Ailantinol E	Terpenoids	Diterpenoids	-	232677.02	336283.40	153621.74	240860.72
364.19	C20H28O6	Amarolide	Terpenoids	Diterpenoids	29913-86-8	30446.76	65389.97	62834.96	52890.56
408.21	C22H32O7	Shinjulactone K	Terpenoids	Diterpenoids	94451-22-6	8074.46	7794.15	3727.96	6532.19
104.11	C5H14NO+	Choline	Alkaloids	Alkaloids	62-49-7	89628678.28	110617579.1	103813555.7	101353271.0
204.09	C11H12N2O2	1-Methoxy-indole-3-acetamide	Alkaloids	Plumerane	-	28909126.46	19649523.29	44892442.99	31150364.25
220.06	C14H8N2O	Canthin-6-one	Alkaloids	Plumerane	479-43-6	67345341.97	225783.60	248309.99	22606478.52
181.07	C9H11NO3	N-(2-Hydroxy-4-methoxyphenyl)acetamide	Alkaloids	Phenolamine	58469-06-0	10361198.45	11802569.95	13252380.46	11805382.95
141.09	C6H11N3O	Histidinol	Alkaloids	Alkaloids	501-28-0	5431704.97	5302443.11	5369837.76	5367995.28
187.06	C11H9O2N	3-amino-2-naphthoic acid	Alkaloids	Alkaloids	-	4555257.50	3598759.08	7927627.94	5360548.17
202.22	C10H26N4	Spermine	Alkaloids	Alkaloids	71-44-3	3573645.05	4785855.06	5177235.43	4512245.18
187.06	C11H9NO2	naphthisoxazol A	Alkaloids	Alkaloids	-	3736218.50	3259419.10	6394438.68	4463358.76
187.06	C11H9NO2	3-Indoleacrylic acid	Alkaloids	Plumerane	1204-06-4	3081622.46	2231874.11	4864141.63	3392546.07
266.08	C15H10N2O3	Picrasidine Q; 4-Hydroxy-5-Methoxy-Canthin-6-One	Alkaloids	Plumerane	101219-61-8	6412597.98	1879435.33	516481.06	2936171.45
149.05	C8H7NO2	4-Hydroxymandelonitrile	Alkaloids	Phenolamine	13093-65-7	2228474.46	2434922.98	3617320.02	2760239.15
184.07	C5H15NO4P+	O-Phosphocholine	Alkaloids	Alkaloids	107-73-3	2981746.90	3182579.96	1813764.66	2659363.84
581.26	C33H35N5O5	Ergotamine	Alkaloids	Plumerane	113-15-5	2501022.70	1740318.22	2624364.99	2288568.63
218.14	C13H18N2O	N,N-Dimethyl-5-methoxytryptamine	Alkaloids	Plumerane	1019-45-0	2346282.97	1901188.86	1025139.16	1757537.00
192.13	C11H16N2O	N-(4-Aminobutyl)benzamide	Alkaloids	Alkaloids	5692-23-9	1293308.38	2061255.95	1526808.06	1627124.13

131.09	C6H13NO2	6-Deoxyfagomine	Alkaloids	Piperidine alkaloids	197449-09-5	1131860.41	1187841.99	1466804.85	1262169.08
119.07	C8H9N	N-Benzylmethylene isomethylamine	Alkaloids	Alkaloids	-	856427.15	853140.11	1570959.64	1093508.97
240.09	C14H12N2O2	β -Carboline-1-propanoic acid	Alkaloids	Plumerane	89915-39-9	2275877.65	20697.90	33390.20	776655.25
236.06	C14H8N2O2	2-Hydroxycanthin-6-one	Alkaloids	Plumerane	86293-43-8	2249876.08	19118.04	28124.23	765706.11
85.09	C5H11N	Piperidine	Alkaloids	Piperidine alkaloids	110-89-4	600142.58	596205.96	867445.27	687931.27
236.06	C14H8N2O2	11-Hydroxycanthin-6-One; Amalorin*	Alkaloids	Plumerane	75969-83-4	1787043.88	42798.90	23392.75	617745.18
236.06	C14H8N2O2	9-Hydroxycanthin-6-one*	Alkaloids	Plumerane	138544-91-9	1754561.84	47033.70	12779.43	604791.65
236.06	C14H8N2O2	1-Hydroxycanthin-6-One*	Alkaloids	Plumerane	80787-59-3	1587236.66	20176.13	16234.90	541215.90
205.07	C11H11NO3	Methoxyindoleacetic acid	Alkaloids	Plumerane	3471-31-6	384391.27	275405.61	695527.77	451774.89
557.27	C29H39N3O8	N1,N8-Bis(sinapoyl)spermidine	Alkaloids	Phenolamine	-	411462.73	378032.84	414719.61	401405.06
324.18	C20H24O2N2	Quinine	Alkaloids	Quinoline alkaloids	130-95-0	217100.93	368931.43	246269.93	277434.10
145.05	C9H7NO	Indole-3-carboxaldehyde	Alkaloids	Plumerane	487-89-8	230873.83	171732.08	352750.27	251785.40
340.18	C20H24N2O3	Lochneridine	Alkaloids	Plumerane	5980-01-8	227988.39	237900.39	208385.28	224758.02
141.02	C2H8NO4P	O-Phosphorylethanolamine	Alkaloids	Alkaloids	1071-23-4	200560.95	170383.71	175634.76	182193.14
117.06	C8H7N	Indole	Alkaloids	Plumerane	120-72-9	176902.75	144142.34	173914.75	164986.61
189.04	C10H7NO3	N-Acetylisatin	Alkaloids	Plumerane	574-17-4	171622.94	125993.08	150040.61	149218.88
135.07	C8H9NO	N-benzylformamide	Alkaloids	Alkaloids	6343-54-0	104911.95	161472.74	163629.41	143338.03
250.08	C15H10N2O2	1-Methoxycanthin-6-one	Alkaloids	Plumerane	-	377604.41	6130.05	32891.78	138875.41
250.08	C15H10N2O2	5-Methoxycanthin-6-one	Alkaloids	Plumerane	15071-56-4	376377.64	4342.57	27048.34	135922.85
438.21	C20H30O7N4	N'-p-Coumaroylagmatine-glucoside	Alkaloids	Phenolamine	-	139036.16	133416.69	124390.35	132281.07
221.07	C11H11NO4	Methyl dioxindole-3-acetate	Alkaloids	Plumerane	57061-18-4	126837.96	131281.46	134647.20	130922.21

447.19	C23H29NO8	3'-Glucosyl-6,7-dihydroxy-N-methyl-benzyltetrahydroisoquinoline	Alkaloids	Isoquinoline alkaloids	-	102986.43	54493.56	160666.30	106048.76
473.15	C20H27NO12	Dhurrin-6'-O-Glucoside	Alkaloids	Phenolamine	-	100985.28	117308.00	98320.45	105537.91
105.08	C4H11NO2	Diethanolamine	Alkaloids	Alkaloids	111-42-2	101161.42	104282.51	82553.50	95999.14
352.18	C21H24N2O3	Lochnericine	Alkaloids	Plumerane	72058-36-7	43317.45	75477.06	148709.80	89168.11
236.06	C14H8N2O2	Canthin-6-one N-oxide	Alkaloids	Plumerane	60755-87-5	173865.25		693.64	87279.44
303.14	C12H21N3O6	Nicotianamine	Alkaloids	Alkaloids	34441-14-0	59559.26	98777.40	68600.63	75645.77
233.14	C14H19NO2	Paniculidine B	Alkaloids	Plumerane	97399-94-5	38522.56	43878.56	62976.30	48459.14
102.12	C5H14N2	Cadaverine	Alkaloids	Alkaloids	462-94-2	41407.84	55765.44	46505.70	47892.99
497.25	C27H35N3O6	N',N''-Diferuloylspermidine	Alkaloids	Phenolamine	-	13661.20	52507.50	44859.97	37009.55
575.31	C32H41N5O5	α -Ergocryptine	Alkaloids	Plumerane	511-09-1	39395.22	30946.74	18742.13	29694.70
130.11	C6H14N2O	N-Acetylputrescine	Alkaloids	Alkaloids	18233-70-0	28784.49	29606.67	29209.49	29200.22
130.12	C5H14N4	Agmatine	Alkaloids	Alkaloids	306-60-5	17567.49	40372.17	28586.97	28842.21
327.15	C19H21NO4	Stepholidine	Alkaloids	Isoquinoline alkaloids	16562-13-3	8495.85	26500.73	50913.30	28636.63
442.18	C21H32NO9+	Feruloylcholine glucoside	Alkaloids	Phenolamine	-	12635.28	27354.54	16005.07	18664.96
202.11	C12H14N2O	Acetryptine	Alkaloids	Plumerane	3551-18-6	10564.22	23764.18	21062.37	18463.59
210.08	C13H10N2O	1-Acetyl- β -carboline	Alkaloids	Plumerane	-	36974.33	2655.41	4211.24	14613.66
147.03	C8H5NO2	Isatin	Alkaloids	Plumerane	91-56-5	18697.47	11209.98	11193.80	13700.42
544.21	C27H32N2O10	Cadambine	Alkaloids	Plumerane	54422-49-0		14464.23	12144.86	13304.54
156.07	C10H8N2	3-Indoleacetonitrile	Alkaloids	Plumerane	771-51-7	14735.60	9397.44	8752.25	10961.76
281.27	C18H35NO	Laurocapram	Alkaloids	Alkaloids	59227-89-3	8722.06	13812.88	10332.06	10955.67
248.12	C13H16N2O3	6-Hydroxymelatonin	Alkaloids	Plumerane	2208-41-5	7941.95	14695.80	5221.67	9286.47
280.08	C16H12N2O3	Picrasidine O	Alkaloids	Alkaloids	101219-63-0	15704.83	1511.94	808.64	6008.47

165.07	C9H11NO2	L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	63-91-2	60972710.85	58931867.49	87255940.54	69053506.29
147.05	C5H9NO4	L-Glutamic acid	Amino acids and derivatives	Amino acids and derivatives	56-86-0	57427271.73	65715891.60	19304560.64	47482574.66
131.09	C6H13NO2	L-Leucine*	Amino acids and derivatives	Amino acids and derivatives	61-90-5	22325334.69	25281369.33	34263316.23	27290006.75
146.11	C6H14N2O2	L-Lysine	Amino acids and derivatives	Amino acids and derivatives	56-87-1	20746646.75	22263607.45	27112035.20	23374096.47
131.09	C6H13NO2	L-Isoleucine*	Amino acids and derivatives	Amino acids and derivatives	73-32-5	14642271.18	11019708.61	37902604.21	21188194.67
131.09	C6H13NO2	L-Norleucine*	Amino acids and derivatives	Amino acids and derivatives	327-57-1	21622041.83	7603778.33	33675055.82	20966958.66
146.07	C5H10N2O3	L-Glutamine	Amino acids and derivatives	Amino acids and derivatives	56-85-9	18365343.31	18309213.40	21368577.35	19347711.35
103.06	C4H9NO2	Methyl 3-aminopropanoate	Amino acids and derivatives	Amino acids and derivatives	4138-35-6	10318672.90	13475228.09	12423212.39	12072371.13
181.07	C9H11NO3	L-Tyrosine	Amino acids and derivatives	Amino acids and derivatives	60-18-4	8680816.39	13052942.22	13257507.25	11663755.29
117.08	C5H11NO2	L-Valine	Amino acids and derivatives	Amino acids and derivatives	72-18-4	8531312.78	8792844.65	9616779.28	8980312.23
457.14	C16H27NO14	L-Aspartic acid-O-diglucoside	Amino acids and derivatives	Amino acids and derivatives	-	8450639.31	8362907.59	8458885.46	8424144.12
103.06	C4H9NO2	N,N-Dimethylglycine	Amino acids and derivatives	Amino acids and derivatives	1118-68-9	6402163.00	4436735.84	4209909.48	5016269.44
129.08	C6H11NO2	Cycloleucine	Amino acids and derivatives	Amino acids and derivatives	52-52-8	4003437.37	4629634.91	5111572.53	4581548.27

133.04	C4H7NO4	L-Aspartic Acid	Amino acids and derivatives	Amino acids and derivatives	56-84-8	3584654.50	3947303.50	5727220.76	4419726.25
204.09	C11H12N2O2	L-Tryptophan	Amino acids and derivatives	Amino acids and derivatives	73-22-3	3862594.85	2583508.74	6352743.97	4266282.52
165.05	C5H11NO3S	L-Methionine Sulfoxide	Amino acids and derivatives	Amino acids and derivatives	3226-65-1	2898798.83	3313178.16	3818706.44	3343561.14
115.06	C5H9NO2	L-Proline	Amino acids and derivatives	Amino acids and derivatives	147-85-3	3456416.62	3273078.03	3143534.64	3291009.76
202.14	C8H18N4O2	NG,NG-Dimethyl-L-arginine	Amino acids and derivatives	Amino acids and derivatives	30315-93-6	2469562.79	3511235.67	3710378.14	3230392.20
188.13	C7H16N4O2	N-Monomethyl-L-arginine	Amino acids and derivatives	Amino acids and derivatives	17035-90-4	2621295.57	3451634.80	3567786.12	3213572.16
188.13	C7H16N4O2	Arginine methyl ester	Amino acids and derivatives	Amino acids and derivatives	-	2514258.18	3618842.21	3398974.33	3177358.24
149.05	C5H11NO2S	L-Methionine	Amino acids and derivatives	Amino acids and derivatives	63-68-3	1660736.95	1708325.41	2811252.59	2060104.98
105.04	C3H7NO3	L-Serine	Amino acids and derivatives	Amino acids and derivatives	56-45-1	906186.81	2146106.04	1092510.11	1381600.99
131.06	C5H9NO3	Trans-4-Hydroxy-L-proline	Amino acids and derivatives	Amino acids and derivatives	51-35-4	1279905.88	915061.81	1630886.21	1275284.63
147.05	C5H9NO4	L-threo-3-Methylaspartate	Amino acids and derivatives	Amino acids and derivatives	6061-13-8	1148091.22	1333700.00	1235811.79	1239201.01
132.05	C4H8N2O3	L-Asparagine	Amino acids and derivatives	Amino acids and derivatives	70-47-3	1317361.29	1006662.44	836467.63	1053497.12
174.10	C7H14N2O3	N- α -Acetyl-L-ornithine	Amino acids and derivatives	Amino acids and derivatives	6205-08-9	861784.78	1179420.70	957215.25	999473.58

175.10	C6H13N3O3	L-Citrulline	Amino acids and derivatives	Amino acids and derivatives	372-75-8	563291.20	784295.60	724437.38	690674.72
307.08	C10H17N3O6S	Glutathione reduced form	Amino acids and derivatives	Amino acids and derivatives	70-18-8	562263.50	698125.24	699475.22	653287.99
119.06	C4H9NO3	L-Threonine	Amino acids and derivatives	Amino acids and derivatives	72-19-5	578340.61	611893.41	767136.65	652456.89
119.06	C4H9NO3	L-Homoserine	Amino acids and derivatives	Amino acids and derivatives	672-15-1	577810.12	642948.63	719873.15	646877.30
216.12	C8H16N4O3	N-Acetyl-L-Arginine	Amino acids and derivatives	Amino acids and derivatives	155-84-0	461932.31	328785.20	422756.04	404491.18
207.09	C11H13NO3	N-Acetyl-L-phenylalanine	Amino acids and derivatives	Amino acids and derivatives	2018-61-3	249432.44	509068.69	433711.19	397404.11
135.04	C4H9NO2S	S-Methyl-L-cysteine	Amino acids and derivatives	Amino acids and derivatives	1187-84-4	256282.89	283148.26	282552.83	273994.66
612.15	C20H32N6O12S 2	Oxiglutathione	Amino acids and derivatives	Amino acids and derivatives	27025-41-8	277341.77	233879.46	284815.12	265345.45
169.09	C7H11N3O2	3-Methyl-L-Histidine	Amino acids and derivatives	Amino acids and derivatives	368-16-1	215133.95	234023.24	243403.24	230853.48
162.05	C6H10O5	3-Hydroxy-3-methylpentane-1,5-dioic acid	Amino acids and derivatives	Amino acids and derivatives	503-49-1	284421.21	171215.85	226229.59	227288.88
223.08	C11H13NO4	N-Acetyl-L-tyrosine	Amino acids and derivatives	Amino acids and derivatives	537-55-3	135070.75	180488.35	158974.75	158177.95
121.02	C3H7NO2S	L-Cysteine	Amino acids and derivatives	Amino acids and derivatives	52-90-4	167767.47	143373.48	139070.07	150070.34
321.10	C11H19N3O6S	S-(Methyl)glutathione	Amino acids and derivatives	Amino acids and derivatives	2922-56-7	160381.60	138325.60	150324.70	149677.30

308.12	C11H20N2O8	L-Glutamine-O-glycoside	Amino acids and derivatives	Amino acids and derivatives	-	122008.14	135761.03	83830.39	113866.52
230.16	C11H22N2O3	L-Valyl-L-Leucine	Amino acids and derivatives	Amino acids and derivatives	3989-97-7	130186.37	61444.48	129034.37	106888.41
276.13	C11H20N2O6	L-Saccharopine	Amino acids and derivatives	Amino acids and derivatives	997-68-2	86618.79	104563.30	88258.23	93146.77
280.11	C13H16N2O5	L-Aspartyl-L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	13433-09-5	78464.26	77356.39	117093.04	90971.23
161.07	C6H11NO4	N-Acetyl-L-threonine	Amino acids and derivatives	Amino acids and derivatives	17093-74-2	59242.17	66977.79	79029.81	68416.59
218.09	C8H14N2O5	5-L-Glutamyl-L-amino acid	Amino acids and derivatives	Amino acids and derivatives	5875-41-2	58943.63	69413.13	62944.70	63767.15
188.12	C8H16N2O3	N-Glycyl-L-leucine	Amino acids and derivatives	Amino acids and derivatives	869-19-2	84199.21	32423.67	71154.24	62592.37
244.18	C12H24N2O3	L-Leucyl-L-Leucine	Amino acids and derivatives	Amino acids and derivatives	3303-31-9	50412.15	43389.14	81976.25	58592.51
220.08	C11H12N2O3	5-Hydroxy-L-tryptophan	Amino acids and derivatives	Amino acids and derivatives	56-69-9	45678.69	53096.73	60934.28	53236.57
132.09	C5H12N2O2	L-Ornithine	Amino acids and derivatives	Amino acids and derivatives	70-26-8	32491.35	36208.41	39986.87	36228.88
309.11	C11H19NO9	L-Glutamic acid-O-glycoside	Amino acids and derivatives	Amino acids and derivatives	-	46460.33	33015.54	27672.50	35716.12
278.16	C15H22N2O3	L-Leucyl-L-phenylalanine	Amino acids and derivatives	Amino acids and derivatives	56217-82-4	46995.13	19266.64	31664.88	32642.21
264.15	C14H20N2O3	L-Valyl-L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	3918-92-1	34485.28	16552.94	39054.14	30030.79

240.02	C6H12N2O4S2	L-Cystine	Amino acids and derivatives	Amino acids and derivatives	56-89-3	20312.52	17938.69	42728.19	26993.13
174.06	C6H10N2O4	N-Alpha-Acetyl-L-Asparagine	Amino acids and derivatives	Amino acids and derivatives	4033-40-3	24043.62	21731.09	19444.82	21739.84
312.15	C18H20N2O3	L-Phenylalanyl-L-phenylalanine	Amino acids and derivatives	Amino acids and derivatives	2577-40-4	28237.11	8694.86		18465.98
300.10	C17H16O5	4'-Hydroxy-5,7-dimethoxyflavanone	Flavonoids	Flavanones	-	24327341.11	19947404.33	24119032.26	22797925.90
522.10	C23H22O14	Tricin-7-O-saccharic acid	Flavonoids	Flavones	-	2398442.21	4302383.84	2204399.63	2968408.56
450.12	C21H22O11	6-C-Glucosyl-2-Hydroxynaringenin	Flavonoids	Flavanones	-	2033607.65	2287951.96	2282768.21	2201442.61
448.10	C21H20O11	Kaempferol-3-O-galactoside (Trifolin)	Flavonoids	Flavonols	23627-87-4	2135037.02	942270.83	348766.59	1142024.82
340.13	C20H20O5	2,4,2',4'-tetrahydroxy-3'-prenylchalcone	Flavonoids	Chalcones	-	959278.61	664840.61	689945.11	771354.77
638.15	C28H30O17	Chrysoeriol-7-O-(2''-O-glucuronyl)glucoside	Flavonoids	Flavones	-	335523.21	679223.21	730626.81	581791.08
626.18	C28H34O16	Hesperetin-5,7-di-O-glucoside	Flavonoids	Flavanones	-	522587.50	468085.23	564788.75	518487.16
418.13	C21H22O9	O-MethylNaringenin-8-C-arabinoside	Flavonoids	Flavanones	-	334072.95	534694.23	376079.11	414948.76
464.09	C21H20O12	Isohyperoside*	Flavonoids	Flavonols	35589-21-0	179111.94	162938.06	217319.94	186456.65
742.23	C33H42O19	Naringenin-7-O-Rutinoside-4'-O-glucoside	Flavonoids	Flavanones	-	154974.05	227915.33	139560.89	174150.09
464.10	C21H20O12	Quercetin-5-O-β-D-glucoside*	Flavonoids	Flavonols	-	183864.61	107185.48	218513.94	169854.68
448.10	C21H20O11	Kaempferol-7-O-glucoside	Flavonoids	Flavonols	16290-07-6	273783.04	129082.16	47573.99	150146.40
448.10	C21H20O11	Carthamone	Flavonoids	Chalcones	86579-00-2	273783.04	129082.16	47573.99	150146.40
418.09	C20H18O10	Luteolin-8-C-arabinoside	Flavonoids	Flavones	-	68663.73	178236.23	146925.73	131275.23
464.10	C21H20O12	Quercetin-3-O-glucoside (Isoquercitrin)*	Flavonoids	Flavonols	482-35-9	132502.23	70539.28	161376.73	121472.74
594.16	C27H30O15	5,7-Dihydroxy-4-methoxyflavone-3-O-xylose-(1-6)-glucose	Flavonoids	Flavones	-	146415.60	77338.51	118716.60	114156.90

550.13	C25H26O14	Hesperetin-7-O-(6''-malonyl)glucoside	Flavonoids	Flavanones	-	116420.53	90062.08	130172.63	112218.41
436.14	C21H24O10	Dihydrocharcone-4'-O-glucoside	Flavonoids	Chalcones	-	81682.30	141224.88	107177.52	110028.23
436.14	C21H24O10	Phloretin-2'-O-glucoside (Phlorizin)	Flavonoids	Chalcones	60-81-1	78654.24	131579.15	112538.16	107590.52
466.11	C21H22O12	Taxifolin-3'-O-glucoside	Flavonoids	Flavanonols	31106-05-5	21841.93	108586.95	123276.38	84568.42
594.16	C27H30O15	Vitexin-2''-O-galactoside	Flavonoids	Flavones	-	44924.28	64551.49	78891.09	62788.95
450.12	C21H22O11	Eriodictyol-8-C-glucoside	Flavonoids	Flavanones	1023271-51-3	20482.50	135140.37	14059.01	56560.63
640.16	C28H32O17	Isorhamnetin-3,7-O-diglucoside	Flavonoids	Flavonols	6758-51-6	22942.16	63656.79	75538.12	54045.69
452.13	C21H24O11	Epicatechin-3'-O-β-D-glucopyranoside*	Flavonoids	Flavanols	-	52956.15	68776.97	37133.64	52955.59
594.16	C27H30O15	Apigenin-6,8-di-C-glucoside (Vicenin-2)	Flavonoids	Flavones	23666-13-9	59170.89	66030.09	30558.79	51919.92
450.12	C21H22O11	3,4,2',4',6'-Pentahydroxychalcone-4'-O-glucoside	Flavonoids	Chalcones	-	26357.12	69066.92	57346.68	50923.57
450.12	C21H22O11	Aromadendrin-7-O-glucoside	Flavonoids	Flavanonols	28189-90-4	46380.81	61613.69	36903.08	48299.19
652.16	C29H32O17	Limocitrin-3-O-(3-hydroxy-3-methylglutarate)glucoside	Flavonoids	Flavonols	-	42414.84	69034.25	21244.25	44231.11
452.13	C21H24O11	Epicatechin-6-C-β-D-glucopyranoside*	Flavonoids	Flavanols	-	20413.22	68853.31	41421.15	43562.56
452.13	C21H24O11	Sieboldin	Flavonoids	Chalcones	18777-73-6	37847.57	49154.70	31056.44	39352.90
918.21	C41H42O24	Quercetin-3-O-(6''-O-sinapoyl)glucoside-7-O-(6''-O-malonyl)glucoside	Flavonoids	Flavonols	-	38238.15	41636.74	30621.62	36832.17
464.10	C21H20O12	6-Hydroxyluteolin 5-glucoside	Flavonoids	Flavones	-	67952.07	16751.88	25221.94	36641.96
450.12	C21H22O11	Dihydrokaempferol-3-O-glucoside	Flavonoids	Flavanonols	1049-08-8	33309.43	49344.93	19740.93	34131.77
300.06	C16H12O6	6-methyl luteolin	Flavonoids	Flavones	-	46862.91	25882.27	28219.02	33654.73
452.13	C21H24O11	Epicatechin-4'-O-β-D-glucopyranoside*	Flavonoids	Flavanols	-	17623.02	61507.63	20042.02	33057.56
626.15	C27H30O17	Quercetin-3,7-Di-O-glucoside	Flavonoids	Flavonols	-	10475.93	45882.80	33356.75	29905.16

610.15	C27H30O16	Luteolin-7-O-gentiobioside	Flavonoids	Flavones	-	35672.26	25045.04	22719.28	27812.19
504.13	C24H24O12	Chrysoeriol-7-O-(6''-acetyl)glucoside	Flavonoids	Flavones	-	22862.86	38412.41	22096.40	27790.55
610.15	C27H30O16	Luteolin-7,3'-di-O-glucoside	Flavonoids	Flavones	52187-80-1	39763.98	20328.28	14350.78	24814.35
402.13	C21H22O8	Nobiletin (5,6,7,8,3',4'-Hexamethoxyflavone)	Flavonoids	Flavones	478-01-3	34648.43	32729.34	6960.69	24779.49
448.10	C21H20O11	Luteolin-8-C-glucoside (Orientin)	Flavonoids	Flavones	28608-75-5	25116.80	26928.73	19658.05	23901.19
508.12	C23H24O13	5,6,3',4'-Tetrahydroxy-3,7-dimethoxyflavone-6-O-glucoside	Flavonoids	Flavones	-	18678.72	13810.02	32479.66	21656.13
962.26	C40H50O27	Isorhamnetin-3-O-rutinoside-7-O-(2''-O-glucosyl)glucuronate	Flavonoids	Flavonols	-	25984.42		14902.97	20443.69
468.11	C23H16O11	Isorhamnetin-3-O-gallate	Flavonoids	Flavonols	-	9988.99	30164.89	14889.70	18347.86
624.17	C28H32O16	Isorhamnetin-3-O-neohesperidoside*	Flavonoids	Flavonols	55033-90-4		24497.24	9875.40	17186.32
624.17	C28H32O16	Sexangularetin-3-O-glucoside-7-O-rhamnoside	Flavonoids	Flavonols	-	12026.28	16727.94	15533.94	14762.72
478.07	C21H18O13	Quercetin-4'-O-glucuronide	Flavonoids	Flavonols	201463-36-7	9067.66	15391.44	19258.16	14572.42
624.17	C28H32O16	6-C-Methylquercetin-3-O-rutinoside	Flavonoids	Flavonols	-	12049.54	13573.15	17078.19	14233.63
442.09	C22H18O10	Catechin gallate*	Flavonoids	Flavanols	130405-40-2	13025.48	15405.24	14166.88	14199.20
448.10	C21H20O11	Luteolin-6-C-glucoside (Isorientin)	Flavonoids	Flavones	4261-42-1	16184.86	9570.19	13160.29	12971.78
624.17	C28H32O16	Rhamnetin-3-O-Rutinoside*	Flavonoids	Flavonols	-	8438.73	10834.22	17078.19	12117.05
300.06	C16H12O6	Diosmetin (5,7,3'-Trihydroxy-4'-methoxyflavone)	Flavonoids	Flavones	520-34-3	16954.53	11978.40	7183.45	12038.79
624.17	C28H32O16	Isorhamnetin-3-O-rutinoside (Narcissin)*	Flavonoids	Flavonols	604-80-8	6287.53	19514.19	9641.04	11814.25
594.16	C27H30O15	Kaempferol-3-O-rutinoside(Nicotiflorin)*	Flavonoids	Flavonols	17650-84-9	14779.56	9965.47	9965.47	11570.17
642.16	C31H30O15	Luteolin-7-O-(6''-eudesmyl)glucoside	Flavonoids	Flavones	-	8691.77	14597.68	10101.97	11130.47
594.16	C27H30O15	Luteolin-7-O-neohesperidoside (Lonicerin)*	Flavonoids	Flavones	25694-72-8		7544.03	13584.44	10564.23

594.16	C27H30O15	Kaempferol-3-O-neohesperidoside*	Flavonoids	Flavonols	32602-81-6		13240.22	7411.94	10326.08
372.12	C20H20O7	Tangeretin (4',5,6,7,8-Pentamethoxyflavone)	Flavonoids	Flavones	481-53-8	13763.50	12279.40	4761.30	10268.07
610.15	C27H30O16	Quercetin-3-O-neohesperidoside*	Flavonoids	Flavonols	117611-67-3		8680.86	8639.43	8660.15
610.15	C27H30O16	Quercetin-3-O-glucoside-7-O-rhamnoside*	Flavonoids	Flavonols	-	4867.05	4938.93	6212.47	5339.48
328.09	C18H16O6	5-Hydroxy-3,7,4'-trimethoxyflavone	Flavonoids	Flavones	-	7984.15	5274.43	943.71	4734.10
610.15	C27H30O16	Quercetin-3-O-robinobioside	Flavonoids	Flavonols	52525-35-6	5234.61	2888.46	4007.09	4043.39
814.16	C37H34O21	Luteolin-7-O-glucuronide-(2→1)-(2''-Feruloyl)glucuronide	Flavonoids	Flavones	-	2507.50	1163.94	1240.90	1637.45
700.26	C32H44O17	Olivil-4,4'-Di-O-glucoside	Lignans and Coumarins	Lignans	-	34338278.52	48704220.54	36382886.94	39808462.00
520.19	C26H32O11	Dehydrodiconiferyl alcohol-4-O-glucoside	Lignans and Coumarins	Lignans	107870-88-2	16147633.97	25277045.17	18077437.51	19834038.88
520.19	C26H32O11	saikolignanose D	Lignans and Coumarins	Lignans	-	15284937.40	24220321.89	17840030.02	19115096.44
520.19	C26H32O11	Pittogside B	Lignans and Coumarins	Lignans	-	14362057.03	22851644.96	18046398.88	18420033.62
682.25	C32H42O16	Pinoresinol-4,4'-O-di-O-glucoside	Lignans and Coumarins	Lignans	63902-38-5	5236272.32	10991240.01	5034266.43	7087259.59
222.05	C11H10O5	Umckalin (7-hydroxy-5,6-dimethoxycoumarin)	Lignans and Coumarins	Coumarins	43053-62-9	7447878.40	3593911.87	4594886.19	5212225.49
712.26	C33H44O17	Medioresinol-4,4'-di-O-glucoside	Lignans and Coumarins	Lignans	88142-63-6	4934190.73	4543572.65	5599197.73	5025653.70
524.23	C26H36O11	Secoisolariciresinol 4-O-glucoside	Lignans and Coumarins	Lignans	-	3551457.81	5968719.65	2961827.12	4160668.19
580.22	C28H36O13	Syringaresinol-4'-O-glucoside	Lignans and Coumarins	Lignans	7374-79-0	1387028.37	6767724.40	3582089.54	3912280.77
278.15	C16H22O4	Methylillicinone F	Lignans and Coumarins	Coumarins	-	3503805.03	3821929.96	2961022.79	3428919.26
522.21	C26H34O11	Manglieside D	Lignans and Coumarins	Lignans	-	1666907.70	3587965.06	1867673.57	2374182.11
236.07	C12H12O5	Dimethylfraxetin; 6,7,8-Trimethoxycoumarin*	Lignans and Coumarins	Coumarins	6035-49-0	4864476.18	1442978.13	227832.86	2178429.05
522.21	C26H34O11	Lariciresinol-4'-O-glucoside	Lignans and Coumarins	Lignans	143663-00-7	2075935.40	2245175.26	1813658.29	2044922.98

552.22	C27H36O12	5'-Methoxysolariciresinol-9'-O-glucoside	Lignans and Coumarins	Lignans	-	1737669.69	2385133.44	1694101.75	1938968.29
236.07	C12H12O5	5,6,7-Trimethoxycoumarin*	Lignans and Coumarins	Coumarins	55085-47-7	4062620.82	1251990.54	206713.64	1840441.66
426.04	C17H14O13	Ditartaroyl-hydroxycoumarin	Lignans and Coumarins	Coumarins	-	1881940.11	2071526.79	1553684.90	1835717.27
370.14	C21H22O6	Fargesin	Lignans and Coumarins	Lignans	31008-19-2	2811244.86	1217614.98	1374484.98	1801114.94
412.13	C19H24O10	Methylpicraquassioside A	Lignans and Coumarins	Coumarins	-	1770880.49	1822521.05	1800165.00	1797855.52
522.21	C26H34O11	Saikolignanose A	Lignans and Coumarins	Lignans	-	1242767.10	3096311.99	1032342.60	1790473.89
146.04	C9H6O2	Coumarin	Lignans and Coumarins	Coumarins	91-64-5	1656657.28	2104099.11	1519594.88	1760117.09
356.13	C20H20O6	(-)-dihydrosesamin	Lignans and Coumarins	Lignans	-	1647564.04	1758999.22	634458.77	1347007.34
356.13	C20H20O6	Horsfieldin	Lignans and Coumarins	Lignans	-	1684424.49	1545223.90	544311.78	1257986.72
384.11	C17H20O10	Mandshurin	Lignans and Coumarins	Coumarins	32451-87-9	1250104.49	1144639.29	902761.24	1099168.34
384.11	C17H20O10	Isofraxidin-7-O-glucoside	Lignans and Coumarins	Coumarins	483-91-0	1127884.79	1108628.49	696219.09	977577.46
538.21	C26H34O12	Olivil-4'-O-glucoside	Lignans and Coumarins	Lignans	76880-93-8	489166.73	1551968.43	490342.98	843826.05
522.21	C26H34O11	Isolariciresinol-9'-O-glucoside	Lignans and Coumarins	Lignans	63358-12-3	531527.47	919659.55	620445.72	690544.24
522.21	C26H34O11	Dihydrodehydrodiconiferyl alcohol-4-O-glucoside	Lignans and Coumarins	Lignans	-	531527.47	919659.55	620445.72	690544.24
222.05	C11H10O5	Isofraxidin	Lignans and Coumarins	Coumarins	486-21-5	1338655.94	397594.57	300826.94	679025.82
176.05	C10H8O3	7-Methoxycoumarin	Lignans and Coumarins	Coumarins	531-59-9	747636.32	553589.18	286422.32	529215.94
418.16	C22H26O8	Lirioresinol A	Lignans and Coumarins	Lignans	-	505216.23	631289.40	385355.20	507286.94
400.15	C22H24O7	(7R,8S)-9-acetyl-dehydrodiconiferyl alcohol	Lignans and Coumarins	Lignans	-	327116.79	590734.05	373234.29	430361.71
192.04	C10H8O4	isoscopoletin	Lignans and Coumarins	Coumarins	-	347465.94	445372.77	387907.17	393581.96
538.21	C26H34O12	(-)-olivil 4'-O-bate-D-glucopyranoside	Lignans and Coumarins	Lignans	-	250863.72	430687.22	321786.02	334445.65

358.14	C20H22O6	Pinoresinol*	Lignans and Coumarins	Lignans	487-36-5	331500.43	410439.35	233937.50	325292.43
358.14	C20H22O6	Epipinoresinol*	Lignans and Coumarins	Lignans	24404-50-0	297005.44	394781.42	207142.82	299643.23
222.05	C11H10O5	Fraxidin (8-Hydroxy-6,7-dimethoxycoumarin)	Lignans and Coumarins	Coumarins	525-21-3	538762.04	139292.47	121854.56	266636.36
532.14	C22H28O15	Fraxetin-7,8-di-O-glucoside	Lignans and Coumarins	Coumarins	-	393534.58	198451.67	204060.63	265348.96
536.19	C26H32O12	1-Hydroxypinoresinol-4'-O-Glucoside	Lignans and Coumarins	Lignans	-	219068.16	243963.20	247609.86	236880.41
486.14	C21H26O13	Scopoletin-7-O-xylosyl(1→6)glucoside	Lignans and Coumarins	Coumarins	-	535681.18	26868.83	93433.39	218661.13
486.14	C21H26O13	Zanthoxyloside	Lignans and Coumarins	Coumarins	-	555794.61	74471.68	22287.30	217517.86
360.16	C20H24O6	Isolariciresinol	Lignans and Coumarins	Lignans	548-29-8	185326.91	189477.95	244756.03	206520.30
550.21	C27H34O12	Eucommin A	Lignans and Coumarins	Lignans	99633-12-2	75512.52	375262.90	112970.23	187915.22
520.19	C26H32O11	Pinoresinol-4-O-glucoside	Lignans and Coumarins	Lignans	41607-20-9	91795.01	209991.66	188089.38	163292.02
622.23	C30H38O14	Syringaresinol-4'-O-(6''-acetyl)glucoside	Lignans and Coumarins	Lignans	-	52377.23	219125.69	155470.44	142324.45
354.10	C16H18O9	Scopoletin-7-O-glucoside (Scopolin)	Lignans and Coumarins	Coumarins	531-44-2	183163.04	119220.57	100421.40	134268.34
360.16	C20H24O6	(-)-Lariciresinol	Lignans and Coumarins	Lignans	-	35552.74	182428.25	147534.98	121838.66
360.16	C20H24O6	(7S,8R)-dihydrodehydrodiconferyl alcohol	Lignans and Coumarins	Lignans	-	35552.74	182428.25	147534.98	121838.66
534.19	C23H34O14	Isosyringinoside	Lignans and Coumarins	Lignans	152686-85-6	102234.79	178992.35	61673.04	114300.06
520.17	C26H32O11	Matairesinol-4'-O-glucoside (Matairesinoside)	Lignans and Coumarins	Lignans	23202-85-9	117842.67	122759.86	92660.40	111087.64
392.15	C20H24O8	Massoniresinol; Vladinol A	Lignans and Coumarins	Lignans	96087-10-4	75845.07	140890.46	107483.58	108073.04
418.16	C22H26O8	Syringaresinol	Lignans and Coumarins	Lignans	21453-71-4	93888.69	125366.93	51816.23	90357.28
536.19	C26H32O12	1-Hydroxypinoresinol-1-O-Glucoside	Lignans and Coumarins	Lignans	81495-71-8	101029.14	73965.82	82566.08	85853.68

192.04	C10H8O4	Isoscopoletin (6-Hydroxy-7-Methoxycoumarin)	Lignans and Coumarins	Coumarins	776-86-3	137321.94	26305.78	34637.94	66088.55
188.04	C11H8O3	Ayapin	Lignans and Coumarins	Coumarins	494-56-4	74602.19	43094.92	58739.71	58812.27
208.04	C10H8O5	Isofraxetin	Lignans and Coumarins	Coumarins	50656-75-2		38828.55	60998.56	49913.55
384.11	C17H20O10	Fraxidin-8-O-glucoside	Lignans and Coumarins	Coumarins	-	67695.05		23613.61	45654.33
696.23	C32H40O17	Sesamolinal 4'-O- β -D-Glucosyl (1->6)-O- β -D-Glucoside	Lignans and Coumarins	Lignans	-		17380.93	11345.81	14363.37
374.14	C20H22O7	8-Hydroxypinoresinol	Lignans and Coumarins	Lignans	81426-17-7	2923.50	12686.46	12188.73	9266.23
280.24	C18H32O2	Linoleic acid	Lipids	Free fatty acids	60-33-3	62185693.76	36222369.07	38683690.68	45697251.17
282.26	C18H34O2	Petroselinic acid*	Lipids	Free fatty acids	593-39-5	62283679.67	35385759.28	37285398.12	44984945.69
282.26	C18H34O2	11-Octadecanoic acid(Vaccenic acid)*	Lipids	Free fatty acids	506-17-2	62283679.67	35385759.28	37285398.12	44984945.69
278.22	C18H30O2	γ -Linolenic Acid*	Lipids	Free fatty acids	506-26-3	36533471.16	30642149.76	22588457.12	29921359.35
278.22	C18H30O2	α -Linolenic Acid*	Lipids	Free fatty acids	463-40-1	36533471.16	30642149.76	22588457.12	29921359.35
312.30	C20H40O2	Arachidic acid	Lipids	Free fatty acids	506-30-9	18567939.95	34306795.54	24127803.03	25667512.84
495.33	C24H50NO7P	LysoPC 16:0(2n isomer)	Lipids	LPC	-	11690198.96	10089547.19	16421493.78	12733746.64
495.33	C24H50NO7P	LysoPC 16:0	Lipids	LPC	17364-16-8	9099030.25	9017636.22	13297525.06	10471397.18
240.25	C16H32O	Palmitaldehyde	Lipids	Free fatty acids	629-80-1	10797258.73	8916194.69	9766262.81	9826572.08
521.35	C26H52NO7P	LysoPC 18:1(2n isomer)	Lipids	LPC	-	10093207.01	4971267.90	9397850.73	8154108.55
273.27	C16H35NO2	Hexadecylsphingosine	Lipids	Sphingolipids	-	5058590.14	5520324.49	3697408.30	4758774.31
453.29	C21H44NO7P	LysoPE 16:0	Lipids	LPE	53862-35-4	3264930.37	2574978.47	3367085.73	3068998.19
240.21	C15H28O2	Cis-10-Pentadecenoic Acid(C15:1)	Lipids	Free fatty acids	84743-29-3	1569520.89	1410385.05	1269828.66	1416578.20
257.10	C8H20NO6P	Choline Alfoscerate	Lipids	PC	28319-77-9	1332884.28	770495.97	1937153.72	1346844.66
278.22	C18H30O2	Punicic acid (9Z,11E,13Z-octadecatienoic acid)	Lipids	Free fatty acids	544-72-9	2820648.10	592026.72	534144.97	1315606.60

330.24	C18H34O5	9,10,13-Trihydroxy-11-Octadecenoic Acid	Lipids	Free fatty acids	29907-57-1	1318589.46	639727.70	1399020.56	1119112.57
493.32	C24H48NO7P	LysoPC 16:1(2n isomer)	Lipids	LPC	-	1251241.65	799854.44	1141668.87	1064254.98
286.21	C16H30O4	Hexadecanedioic acid	Lipids	Free fatty acids	505-54-4	2260997.62	510510.79	83468.95	951659.12
302.25	C17H34O4	1-Monomyristin	Lipids	Free fatty acids	589-68-4	526439.18	1025725.14	837574.68	796579.67
517.32	C26H48NO7P	LysoPC 18:3(2n isomer)	Lipids	LPC	-	503806.76	694263.28	844384.59	680818.21
296.24	C18H32O3	13(S)-HODE;13(S)-Hydroxyoctadeca-9Z,11E-dienoic acid*	Lipids	Free fatty acids	10219-69-9	1383363.53	294144.82	231077.31	636195.22
296.24	C18H32O3	9S-Hydroxy-10E,12Z-octadecadienoic acid*	Lipids	Free fatty acids	15514-85-9	1383363.53	294144.82	231077.31	636195.22
484.28	C22H45O9P	LysoPG 16:0	Lipids	Glycerol ester	-	747590.30	368906.80	763647.07	626714.73
310.21	C18H30O4	13(s)-hydroperoxy-(9z,11e,15z)-octadecatrienoic acid	Lipids	Free fatty acids	67597-26-6	600896.00	667305.38	601329.43	623176.94
354.28	C21H38O4	1-Linoleoylglycerol*	Lipids	Glycerol ester	2277-28-3	475374.59	493372.64	414959.33	461235.52
354.28	C21H38O4	2-Linoleoylglycerol*	Lipids	Glycerol ester	3443-82-1	344030.00	495051.91	366468.02	401849.98
523.36	C26H54NO7P	LysoPC 18:0(2n isomer)	Lipids	LPC	-	388561.70	311542.78	322544.96	340883.15
300.27	C18H36O3	2R-Hydroxyoctadecanoic Acid	Lipids	Free fatty acids	26633-48-7	573491.78	225631.18	210765.26	336629.41
523.36	C26H54NO7P	LysoPC 18:0	Lipids	LPC	19420-57-6	275777.84	224304.31	337783.20	279288.45
254.22	C16H30O2	Palmitoleic Acid*	Lipids	Free fatty acids	373-49-9	269486.31	249025.26	243044.05	253851.87
254.22	C16H30O2	(7Z)-Hexadecenoic acid*	Lipids	Free fatty acids	2416-19-5	263992.43	242070.78	214864.69	240309.30
509.35	C25H52NO7P	LysoPC 17:0*	Lipids	LPC	50930-23-9	228007.94	225004.22	233777.24	228929.80
296.23	C18H32O3	15(R)-Hydroxylinoleic Acid	Lipids	Free fatty acids	177931-23-6	461195.36	89811.78	69127.39	206711.51
296.23	C18H32O3	9-Oxo-12Z-Octadecenoic acid	Lipids	Free fatty acids	112543-32-5	461195.36	89811.78	69127.39	206711.51
509.35	C25H52NO7P	LysoPC 17:0(2n isomer)*	Lipids	LPC	-	168090.06	161378.46	256553.04	195340.52
280.24	C18H32O2	(9Z,11E)-Octadecadienoic acid	Lipids	Free fatty acids	2540-56-9	263885.31	160215.09	149812.39	191304.26
317.29	C18H39NO3	4-Hydroxysphinganine	Lipids	Sphingolipids	554-62-1	178873.60	163271.72	230681.16	190942.16

352.26	C21H36O4	1- α -Linolenoyl-glycerol*	Lipids	Glycerol ester	-	156746.00	239675.24	141151.93	179191.06
308.27	C20H36O2	Eicosadienoic acid	Lipids	Free fatty acids	5598-38-9	195225.65	178402.93	141923.61	171850.73
479.30	C23H46NO7P	LysoPC 15:1	Lipids	LPC	-	137329.71	114906.56	242056.63	164764.30
481.32	C23H48NO7P	LysoPC 15:0*	Lipids	LPC	108273-89-8	141863.78	121881.11	226456.82	163400.57
481.32	C23H48NO7P	LysoPC 15:0(2n isomer)*	Lipids	LPC	-	138781.13	115162.82	217681.46	157208.47
475.27	C23H42NO7P	LysoPE 18:3(2n isomer)	Lipids	LPE	-	125897.81	167055.28	168844.41	153932.50
352.26	C21H36O4	2- α -Linolenoyl-glycerol*	Lipids	Glycerol ester	55268-58-1	149777.77	202994.75	106732.31	153168.28
200.18	C12H24O2	Dodecanoic acid (Lauric acid)	Lipids	Free fatty acids	143-07-7	162100.51	145767.46	125198.21	144355.39
467.30	C22H46NO7P	LysoPC 14:0	Lipids	LPC	20559-16-4	175573.06	94470.81	157814.81	142619.56
278.22	C18H30O2	Crepennic acid	Lipids	Free fatty acids	2277-31-8	174120.13	140459.23	107743.56	140774.31
356.29	C21H40O4	1-Oleoyl-Sn-Glycerol	Lipids	Glycerol ester	129784-87-8	127442.97	74889.30	209922.34	137418.20
519.33	C26H50NO7P	LysoPC 18:2(2n isomer)	Lipids	LPC	-	170045.82	77957.14	149424.79	132475.92
276.21	C18H28O2	9,12-Octadecadien-6-Ynoic Acid	Lipids	Free fatty acids	61481-29-6	223336.73	73649.64	37163.22	111383.20
298.32	C20H42O	1-Eicosanol	Lipids	Free fatty acids	629-96-9	146244.10	94880.46	79159.19	106761.25
296.24	C18H32O3	9(10)-EpOME;(9R,10S)-(12Z)-9,10-Epoxyoctadecenoic acid	Lipids	Free fatty acids	16833-56-0	177303.87	71211.70	70068.88	106194.82
256.24	C16H32O2	Palmitic acid	Lipids	Free fatty acids	57-10-3	109008.29	101907.38	88754.58	99890.08
294.22	C18H30O3	13-Hydroxy-6,9,11-octadecatrienoic acid	Lipids	Free fatty acids	74784-20-6	88556.38	116728.34	93526.50	99603.74
298.25	C18H34O3	Ricinoleic acid	Lipids	Free fatty acids	141-22-0	129217.62	87537.64	68504.43	95086.56
312.23	C18H32O4	9-Hydroperoxy-9Z,11E-Octadecadienoic Acid	Lipids	Free fatty acids	-	101842.20	86010.59	74872.50	87575.10
286.25	C17H34O3	3-Hydroxy-palmitic acid methyl ester	Lipids	Free fatty acids	51883-36-4	136431.75	53209.82	54513.13	81384.90
493.32	C24H48NO7P	LysoPC 16:1	Lipids	LPC	76790-27-7	74787.12	52698.62	93353.57	73613.10
499.27	C25H42NO7P	LysoPE 20:5	Lipids	LPE	-	89081.60	40162.83	86250.30	71831.58

330.24	C18H34O5	9,10,11-Trihydroxy-12-octadecenoic acid	Lipids	Free fatty acids	61911-67-9	99176.47	37557.38	77307.95	71347.27
477.29	C23H44NO7P	LysoPE 18:2(2n isomer)	Lipids	LPE	-	96538.56	32434.32	65130.08	64700.98
314.25	C18H34O4	Hydroxy ricinoleic acid	Lipids	Free fatty acids	-	112622.01	39995.70	35087.54	62568.42
439.27	C20H42NO7P	LysoPE 15:0	Lipids	LPE	-	55941.27	44054.10	65529.31	55174.89
437.25	C20H40NO7P	LysoPE 15:1*	Lipids	LPE	-	47165.39	43958.36	69983.40	53702.39
296.24	C18H32O3	12,13-Epoxy-9-Octadecenoic Acid	Lipids	Free fatty acids	6799-85-5	92906.30	34684.40	31589.73	53060.14
439.27	C20H42NO7P	LysoPE 15:0(2n isomer)	Lipids	LPE	-	57326.67	35351.93	63725.97	52134.85
425.25	C19H40NO7P	LysoPE 14:0(2n isomer)*	Lipids	LPE	-	55711.36	37783.08	52438.05	48644.16
425.25	C19H40NO7P	LysoPE 14:0*	Lipids	LPE	-	57575.27	39862.71	46228.22	47888.73
244.17	C13H24O4	Tridecanedioic acid	Lipids	Free fatty acids	505-52-2	44572.75	47808.76	50840.85	47740.79
330.24	C18H34O5	9,12,13-TriHOME; 9(S),12(S),13(S)-Trihydroxy-10(E)-octadecenoic acid	Lipids	Free fatty acids	97134-11-7	68966.79	18149.70		43558.25
491.30	C24H46NO7P	LysoPC 16:2(2n isomer)	Lipids	LPC	-	39855.34	36915.87	35970.86	37580.69
516.33	C27H48O9	2-Linoleoylglycerol-1-O-glucoside	Lipids	Glycerol ester	-	38697.19	15550.95	37851.01	30699.72
310.10	C18H30O4	9-Hydroperoxy-10E,12,15Z-octadecatrienoic acid	Lipids	Free fatty acids	111004-08-1	30028.67	34752.46	24607.28	29796.13
465.29	C22H44NO7P	LysoPE 17:1*	Lipids	LPE	-	28717.39	19819.44	28566.28	25701.04
465.29	C22H44NO7P	LysoPE 17:1(2n isomer)*	Lipids	LPE	-	29040.16	18300.94	25574.38	24305.16
547.36	C28H54NO7P	LysoPC 20:2	Lipids	LPC	-	22835.34	19986.55	29758.48	24193.46
328.23	C18H32O5	9,12,13-Trihydroxy-10,15-octadecadienoic acid	Lipids	Free fatty acids	-	24471.30	17825.30	27304.86	23200.49
505.32	C25H48NO7P	LysoPC 17:2	Lipids	LPC	-	24495.67	14460.06	29622.71	22859.48
226.19	C14H26O2	Myristoleic acid	Lipids	Free fatty acids	544-64-9	12193.31	28310.89	11289.35	17264.52
481.32	C23H48NO7P	LysoPE 18:0	Lipids	LPE	69747-55-3	16582.42	12296.35	13241.00	14039.92
310.21	C18H30O4	9-Hydroxy-12-oxo-10(E),15(Z)-octadecadienoic acid	Lipids	Free fatty acids	-	15018.30	12737.10	5609.80	11121.73

501.29	C25H44NO7P	LysoPE 20:4	Lipids	LPE	-	8630.93	3431.87	7838.24	6633.68
437.25	C20H40NO7P	LysoPE 15:1(2n isomer)*	Lipids	LPE	-	8430.62	4710.27	6452.80	6531.23
676.37	C33H56O14	2- α -Linolenoyl-glycerol-1,3-di-O-glucoside	Lipids	Glycerol ester	-	8261.05	4109.19	6250.36	6206.87
294.22	C18H30O3	13-KODE; (9Z,11E)-13-Oxo-octadeca-9,11-dienoic acid	Lipids	Free fatty acids	54739-30-9	4025.56	3179.92	1910.51	3038.66
294.22	C18H30O3	9-Hydroxy-10,12,15-octadecatrienoic acid	Lipids	Free fatty acids	89886-42-0	4025.56	3179.92	1910.51	3038.66
467.30	C22H46NO7P	LysoPE 17:0	Lipids	LPE	-	3069.29		1805.17	2437.23
230.15	C12H22O4	Dodecanedioic acid	Lipids	Free fatty acids	693-23-2	2245.94	1701.97	1095.96	1681.29
267.10	C10H13N5O4	Adenosine	Nucleotides and derivatives	Nucleotides and derivatives	58-61-7	5660764.86	13262117.98	43284148.52	20735677.12
383.11	C14H17N5O8	Succinyladenosine	Nucleotides and derivatives	Nucleotides and derivatives	4542-23-8	10370447.66	13693198.01	10000662.86	11354769.51
332.05	C10H13N4O7P	2'-Deoxyinosine-5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	3393-18-8	8126866.79	6830831.59	6896126.54	7284608.30
166.03	C6H6N4S	6-Methylmercaptopurine	Nucleotides and derivatives	Nucleotides and derivatives	50-66-8	3963360.22	3731793.85	6397602.20	4697585.42
297.09	C11H15N5O3S	5'-Deoxy-5'-(methylthio)adenosine	Nucleotides and derivatives	Nucleotides and derivatives	2457-80-9	3392864.32	4108948.46	4273914.38	3925242.38
283.09	C10H13N5O5	Guanosine	Nucleotides and derivatives	Nucleotides and derivatives	118-00-3	1599070.50	2891642.65	4152889.91	2881201.02
566.06	C15H24N2O17P2	Uridine 5'-diphospho-D-glucose	Nucleotides and derivatives	Nucleotides and derivatives	133-89-1	1829012.47	2498323.30	2516808.98	2281381.59
295.06	C8H14N3O7P	5-Aminoimidazole ribonucleotide	Nucleotides and derivatives	Nucleotides and derivatives	25635-88-5	579615.80	477553.46	875041.95	644070.41
284.08	C10H12N4O6	Xanthosine	Nucleotides and derivatives	Nucleotides and derivatives	146-80-5	410535.45	554296.70	669164.11	544665.42

111.04	C4H5N3O	Cytosine	Nucleotides and derivatives	Nucleotides and derivatives	71-30-7	465759.21	416688.89	408112.04	430186.71
365.17	C16H23N5O5	Isopentenyladenine-7-N-glucoside	Nucleotides and derivatives	Nucleotides and derivatives	-	263718.41	419238.97	306364.43	329773.94
347.06	C10H14N5O7P	Adenosine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	61-19-8	416719.27	240154.29	245296.13	300723.23
244.07	C9H12N2O6	Uridine	Nucleotides and derivatives	Nucleotides and derivatives	58-96-8	256033.27	282480.95	353363.06	297292.43
311.12	C12H17N5O5	2-(Dimethylamino)guanosine	Nucleotides and derivatives	Nucleotides and derivatives	2140-67-2	198237.65	190754.15	253423.76	214138.52
251.10	C10H13N5O3	2'-Deoxyadenosine	Nucleotides and derivatives	Nucleotides and derivatives	958-09-8	434482.34	78938.32	74807.93	196076.20
283.09	C10H13N5O5	Crotonoside; 2-Hydroxyadenosine	Nucleotides and derivatives	Nucleotides and derivatives	1818-71-9	126315.84	144578.82	212293.73	161062.79
663.11	C21H27N7O14P ₂	Nicotinic acid adenine dinucleotide	Nucleotides and derivatives	Nucleotides and derivatives	53-84-9	133412.98	167611.73	142049.00	147691.24
114.04	C4H6N2O2	5,6-Dihydrouracil	Nucleotides and derivatives	Nucleotides and derivatives	504-07-4	133086.20	117953.21	107367.55	119468.99
404.00	C9H14N2O12P2	Uridine 5'-diphosphate	Nucleotides and derivatives	Nucleotides and derivatives	27821-45-0	106741.01	95221.93	144485.80	115482.91
331.07	C10H14N5O6P	2'-Deoxyadenosine-5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	653-63-4	33493.75	103105.72	117701.24	84766.90
427.03	C10H15N5O10P ₂	Adenosine 5'-diphosphate	Nucleotides and derivatives	Nucleotides and derivatives	58-64-0	67606.29	67923.96	90419.33	75316.53
242.09	C10H14N2O5	Thymidine	Nucleotides and derivatives	Nucleotides and derivatives	50-89-5	104665.89	58549.36	56103.33	73106.19

166.05	C6H6N4O2	3-Methylxanthine	Nucleotides and derivatives	Nucleotides and derivatives	1076-22-8	68674.90	88979.22	57189.12	71614.41
243.09	C9H13N3O5	Cytidine	Nucleotides and derivatives	Nucleotides and derivatives	65-46-3	45743.60	64608.67	99810.63	70054.30
267.10	C10H13N5O4	2'-Deoxyguanosine	Nucleotides and derivatives	Nucleotides and derivatives	961-07-9	110945.68	36019.00	36997.15	61320.61
743.08	C21H28N7O17P3	NADP (Nicotinamide adenine dinucleotide phosphate)	Nucleotides and derivatives	Nucleotides and derivatives	53-59-8	50540.41	68184.09	53658.99	57461.16
244.07	C9H12N2O6	β -Pseudouridine	Nucleotides and derivatives	Nucleotides and derivatives	1445-07-4	57115.75	30312.02	77676.26	55034.68
345.05	C10H12N5O7P	Guanosine 3',5'-cyclic monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	7665-99-8	51015.84	57371.76	51113.34	53166.98
149.07	C6H7N5	1-Methyladenine	Nucleotides and derivatives	Nucleotides and derivatives	5142-22-3	39680.99	49230.79	58764.39	49225.39
297.11	C11H15N5O5	N7-Methylguanosine	Nucleotides and derivatives	Nucleotides and derivatives	20244-86-4	61429.57	45539.66	38178.63	48382.62
785.16	C27H33N9O15P2	Riboflavin 5'-Adenosine Diphosphate	Nucleotides and derivatives	Nucleotides and derivatives	146-14-5	22782.81	57520.18	61491.70	47264.90
227.09	C9H13N3O4	2'-Deoxycytidine	Nucleotides and derivatives	Nucleotides and derivatives	951-77-9	41590.22	39283.88	28628.76	36500.95
112.03	C4H4N2O2	Uracil	Nucleotides and derivatives	Nucleotides and derivatives	66-22-8	35541.73	22291.22	47077.82	34970.26
324.04	C9H13N2O9P	Uridine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	58-97-9	37953.61	17898.43	15113.45	23655.16
214.02	C5H11O7P	2-Deoxyribose-5'-phosphate	Nucleotides and derivatives	Nucleotides and derivatives	102916-66-5	21655.04	14541.97	14615.35	16937.45

363.06	C10H14N5O8P	Guanosine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	85-32-5	25045.42	10392.05	10475.64	15304.37
214.02	C5H11O7P	2-Deoxyribose-1-phosphate	Nucleotides and derivatives	Nucleotides and derivatives	17210-42-3	16278.10	12576.12		14427.11
165.07	C6H7N5O	7-Methylguanine	Nucleotides and derivatives	Nucleotides and derivatives	578-76-7	4277.75	5918.31	5701.05	5299.04
192.03	C6H8O7	Citric Acid	Organic acids	Organic acids	77-92-9	44238306.94	36347510.24	37432089.33	39339302.17
192.03	C6H8O7	Isocitric Acid	Organic acids	Organic acids	320-77-4	20609221.53	22134805.86	28531531.19	23758519.53
134.02	C4H6O5	L-Malic acid	Organic acids	Organic acids	97-67-6	7858550.71	15186485.91	21187888.78	14744308.47
103.06	C4H9NO2	2-Aminoisobutyric acid	Organic acids	Organic acids	62-57-7	11526821.88	15475804.70	13757355.00	13586660.53
103.06	C4H9NO2	γ -Aminobutyric acid	Organic acids	Organic acids	56-12-2	9465114.02	1764223.79	5674255.97	5634531.26
129.08	C6H11NO2	L-Pipecolic Acid	Organic acids	Organic acids	3105-95-1	2792036.39	4045395.32	4418186.89	3751872.87
131.09	C6H13NO2	6-Aminocaproic acid	Organic acids	Organic acids	60-32-2	2795779.96	3062943.67	4462881.35	3440534.99
118.03	C4H6O4	Succinic acid*	Organic acids	Organic acids	110-15-6	2754233.76	3210943.20	3768920.20	3244699.05
118.03	C4H6O4	Methylmalonic acid*	Organic acids	Organic acids	516-05-2	2754233.76	3210943.20	3768920.20	3244699.05
142.03	C6H6O4	Muconic acid	Organic acids	Organic acids	1119-72-8	1416910.72	4083868.98	2012928.11	2504569.27
192.06	C7H12O6	Quinic Acid	Organic acids	Organic acids	77-95-2	1567561.65	1736749.39	1747737.65	1684016.23
272.24	C16H32O3	2-Hydroxyhexadecanoic acid	Organic acids	Organic acids	764-67-0	1276753.86	463128.56	426864.25	722248.89
145.09	C5H11N3O2	4-Guanidinobutyric acid	Organic acids	Organic acids	463-00-3	699325.29	804968.21	649168.20	717820.57
188.10	C9H16O4	Azelaic acid	Organic acids	Organic acids	123-99-9	983680.11	664009.91	505659.30	717783.11
133.04	C4H7NO4	Iminodiacetic acid	Organic acids	Organic acids	142-73-4	377851.81	503771.93	717820.17	533147.97
104.06	C3H4O4	Malonic acid	Organic acids	Organic acids	141-82-2	494168.40	455168.56	324186.36	424507.78
132.04	C5H8O4	Glutaric acid	Organic acids	Organic acids	110-94-1	248002.87	319939.99	314321.43	294088.10
146.02	C5H6O5	α -Ketoglutaric acid	Organic acids	Organic acids	328-50-7	200802.56	221374.66	309701.14	243959.45

116.01	C4H4O4	Fumaric acid	Organic acids	Organic acids	110-17-8	309109.20	119538.68	209319.75	212655.88
174.02	C6H6O6	Trans-Citridic acid	Organic acids	Organic acids	4023-65-8	154244.87	220210.43	214673.83	196376.38
148.04	C5H8O5	3-Methylmalic acid	Organic acids	Organic acids	152204-30-3	136691.47	146884.61	143382.71	142319.59
118.06	C5H10O3	β -Hydroxyisovaleric acid	Organic acids	Organic acids	625-08-1	153457.12	134097.47	123520.11	137024.90
119.02	C3H5NO4	Aminomalonic acid	Organic acids	Organic acids	1068-84-4	99983.98	132072.95	140859.79	124305.57
123.03	C6H5NO2	2-Picolinic acid	Organic acids	Organic acids	98-98-6	131192.32	117081.99	101677.39	116650.57
148.04	C5H8O5	2-Hydroxyglutaric Acid	Organic acids	Organic acids	13095-48-2	100499.74	113338.22	99856.48	104564.81
101.05	C4H7NO2	1-Aminocyclopropane-1-carboxylic acid	Organic acids	Organic acids	22059-21-8	79361.08	88875.12	76660.20	81632.13
148.04	C5H8O5	L-Citramalic acid	Organic acids	Organic acids	6236-09-5	81149.19	72866.30	85242.23	79752.57
146.06	C6H10O4	2,2-Dimethylsuccinic acid	Organic acids	Organic acids	597-43-3	67788.23	75162.32	81723.26	74891.27
132.05	C4H8N2O3	3-Ureidopropionic Acid	Organic acids	Organic acids	462-88-4	79824.10	75556.47	63428.14	72936.23
184.11	C10H16O3	Oleuropeic acid	Organic acids	Organic acids	5027-76-9	64800.34	81285.21	31909.45	59331.67
176.07	C7H12O5	3-Isopropylmalic Acid*	Organic acids	Organic acids	921-28-8	52674.77	62461.66	61862.43	58999.62
176.07	C7H12O5	2-Propylmalic Acid*	Organic acids	Organic acids	-	52674.77	62461.66	61862.43	58999.62
176.07	C7H12O5	2-Isopropylmalic Acid	Organic acids	Organic acids	49601-06-1	80167.16	61741.07	28866.23	56924.82
290.12	C10H18N4O6	Argininosuccinic acid	Organic acids	Organic acids	2387-71-5	43324.19	62536.82	57038.48	54299.83
130.03	C5H6O4	Methylenesuccinic acid	Organic acids	Organic acids	97-65-4	46860.48	59655.86	50742.81	52419.72
150.02	C4H6O6	L-Tartaric acid	Organic acids	Organic acids	87-69-4	43261.54	31171.72	63906.84	46113.37
167.98	C3H5O6P	Phosphoenolpyruvate	Organic acids	Organic acids	138-08-9	45031.06	56093.51	22028.71	41051.09
170.00	C3H7O6P	DL-Glyceraldehyde-3-phosphate	Organic acids	Organic acids	591-59-3	49035.20	34842.89	30378.62	38085.57
190.10	C7H14N2O4	2,6-Diaminooimelic acid	Organic acids	Organic acids	583-93-7	22120.09	22264.39	29877.90	24754.13
104.05	C4H8O3	2-Hydroxybutyric Acid*	Organic acids	Organic acids	3347-90-8	64162.41	5383.74	3499.44	24348.53
104.05	C4H8O3	2-Hydroxyisobutyric acid*	Organic acids	Organic acids	594-61-6	64162.41	5383.74	3499.44	24348.53

544.13	C19H28O18	Quinic acid O-di-glucuronic acid	Organic acids	Organic acids	-	27288.39	18513.70	16507.12	20769.74
146.02	C5H6O5	2-Methyl-3-oxosuccinic acid	Organic acids	Organic acids	-	19163.87	22269.32	19757.41	20396.87
132.04	C5H8O4	2-Hydroxy-2-methyl-3-oxobutanoic acid	Organic acids	Organic acids	71698-08-3	15427.89	16774.44	22456.65	18219.66
159.09	C7H13NO3	5-Acetamidopentanoic Acid	Organic acids	Organic acids	1072-10-2	13246.85	15829.89	7731.93	12269.56
342.12	C12H22O11	Galactinol	Others	Saccharides	3687-64-7	34378478.19	33062391.34	34744563.18	34061810.90
342.12	C12H22O11	D-Sucrose*	Others	Saccharides	57-50-1	14728599.20	18013108.08	16216971.91	16319559.73
342.12	C12H22O11	D-Maltose*	Others	Saccharides	69-79-4	11191263.17	10997757.65	11773290.47	11320770.43
342.12	C12H22O11	Isomaltulose*	Others	Saccharides	13718-94-0	9823080.88	5435569.42	11242558.14	8833736.14
290.00	C6H11PO11	Glucarate O-Phosphoric acid	Others	Saccharides	-	9594092.80	7865657.72	7724463.11	8394737.87
134.02	C4H6O5	3-Dehydro-L-Threonic Acid	Others	Saccharides	-	3939671.61	8468764.25	10886804.15	7765080.00
342.12	C12H22O11	D-Trehalose*	Others	Saccharides	99-20-7	5737545.71	7229085.31	5750160.11	6238930.38
342.12	C12H22O11	Melibiose	Others	Saccharides	585-99-9	7155575.14	5773907.33	4849033.19	5926171.89
290.04	C7H15O10P	D-Sedoheptuiose 7-phosphate	Others	Saccharides	2646-35-7	4430570.54	5109546.50	3955260.06	4498459.03
192.08	C11H12O3	Eugenyl formate	Others	Others	-	2232314.77	3622381.97	2937250.52	2930649.09
256.08	C11H14NO6+	Nicotinate D-ribonucleoside	Others	Vitamin	17720-18-2	2891583.00	3199138.94	2672016.19	2920912.71
330.13	C15H22O8	Bartsioside	Others	Alcohol compounds	62133-72-6	2725292.93	3038865.38	2304270.55	2689476.29
180.06	C6H12O6	D-Glucose	Others	Saccharides	50-99-7	1755520.72	2220704.15	2926354.52	2300859.80
260.03	C6H13O9P	D-Glucose 6-phosphate*	Others	Saccharides	56-73-5	1792249.12	2365642.27	2696215.14	2284702.18
180.06	C6H12O6	Inositol	Others	Saccharides	87-89-8	1490952.33	2096919.11	3068884.29	2218918.58
180.06	C6H12O6	D-Fructose	Others	Saccharides	57-48-7	1279827.85	2359267.76	2880783.50	2173293.03
488.17	C18H32O15	Solatriose	Others	Saccharides	528-40-5	2109575.01	2322702.52	1962759.62	2131679.05
260.03	C6H13O9P	Glucose-1-phosphate*	Others	Saccharides	59-56-3	1721105.77	2199043.76	2296580.53	2072243.35
278.15	C16H22O4	Senkyunolide M	Others	Lactones	146986-60-9	1900116.23	2135667.24	1521906.32	1852563.26

356.13	C20H20O6	6,7-dimethoxy-2-[2-(4'-hydroxy-3'-methoxyphenyl)ethyl]chromone	Others	Others	-	1585683.38	1399673.24	531688.82	1172348.48
219.11	C9H17NO5	D-Pantothenic Acid	Others	Vitamin	79-83-4	931378.97	1117570.60	1415028.62	1154659.40
122.05	C6H6N2O	Nicotinamide	Others	Vitamin	98-92-0	1010233.84	1137067.06	1148359.21	1098553.37
129.02	C5H7NOS	Epigoitrin	Others	Others	1072-93-1	768430.52	910730.07	941136.50	873432.36
504.17	C18H32O16	Raffinose	Others	Saccharides	512-69-6	1127542.22	685271.35	708499.88	840437.82
260.03	C6H13O9P	D-Fructose 6-phosphate*	Others	Saccharides	643-13-0	696507.39	834822.04	914621.67	815317.03
182.08	C6H14O6	Dulcitol	Others	Saccharides	608-66-2	822865.40	521692.79	422098.56	588885.58
204.08	C12H12O3	Senkyunolide B*	Others	Lactones	93236-67-0	543016.19	635611.87	450707.99	543112.02
210.04	C6H10O8	D-Galactaric acid	Others	Saccharides	526-99-8	412513.20	477341.35	486287.05	458713.87
210.04	C6H10O8	D-Saccharic acid	Others	Saccharides	87-73-0	342884.12	448396.20	411590.47	400956.93
182.08	C6H14O6	D-Sorbitol	Others	Saccharides	50-70-4	540488.43	384743.89	260016.72	395083.01
334.07	C9H19O11P	1-(sn-Glycero-3-phospho)-1D-myo-inositol	Others	Saccharides	-	382537.69	225073.11	459220.53	355610.44
650.23	C24H42O20	DMelezitose O-rhamnoside	Others	Saccharides	-	373083.05	242963.25	267556.03	294534.11
332.11	C14H20O9	2,6-Dimethoxy-4-hydroxyphenol-1-O-β-D-glucopyranoside	Others	Others	-	197230.10	416389.87	183449.50	265689.82
221.09	C8H15NO6	N-Acetyl-D-glucosamine	Others	Saccharides	7512-17-6	203065.19	207303.56	377993.18	262787.31
342.12	C12H22O11	D-Cellobiose	Others	Saccharides	528-50-7	262753.78	142302.88	315375.01	240143.89
331.13	C14H21NO8	Pyridoxine-5'-O-glucoside	Others	Vitamin	-	86295.83	334514.32	284986.13	235265.42
210.07	C7H14O7	Sedoheptulose	Others	Saccharides	3019-74-7	213208.31	272410.62	211835.45	232484.79
196.06	C6H12O7	Gluconic acid	Others	Saccharides	526-95-4	188623.84	232451.88	218413.98	213163.23
174.02	C6H6O6	Dehydroascorbic acid	Others	Vitamin	490-83-5	170928.57	249797.46	207797.84	209507.95
504.17	C18H32O16	Maltotriose	Others	Saccharides	1109-28-0	191137.87	234825.00	168247.08	198069.98
123.03	C6H5NO2	Nicotinic acid (Vitamin B3)	Others	Vitamin	59-67-6	170583.76	160496.30	185190.00	172090.02

493.18	C20H31NO13	Pyridoxine-5'-O-diglucoside	Others	Vitamin	-	166769.87	156005.05	163594.62	162123.18
123.03	C6H5NO2	Isonicotinic acid	Others	Vitamin	55-22-1	139675.83	169038.02	169260.39	159324.74
310.12	C19H18O4	6,7-dimethoxy-2-[2-phenylethyl]chromone	Others	Others	-	175585.54	153227.65	120571.97	149795.05
182.08	C6H14O6	D-Mannitol	Others	Saccharides	69-65-8	166839.45	124435.61	126428.15	139234.40
166.05	C5H10O6	D-Xylonic acid	Others	Saccharides	526-91-0	85406.23	128670.19	186984.42	133686.95
504.17	C18H32O16	D-Panose	Others	Saccharides	33401-87-5	154661.71	85508.36	108271.63	116147.23
179.08	C6H13NO5	D-Glucosamine	Others	Saccharides	3416-24-8	95338.74	150645.61	80342.99	108775.78
185.99	C3H7O7P	3-Phospho-D-glyceric acid	Others	Saccharides	820-11-1	86117.06	110142.86	102691.93	99650.62
504.17	C18H32O16	D-Melezitose	Others	Saccharides	597-12-6	122743.42	87198.27	83188.73	97710.14
150.05	C5H10O5	D-Arabinose	Others	Saccharides	10323-20-3	81797.05	86591.07	109027.53	92471.89
301.06	C8H16NO9P	N-Acetyl-D-glucosamine-1-phosphate	Others	Saccharides	6866-69-9	103151.25	87705.72	81574.71	90810.56
148.04	C5H8O5	D-Arabinono-1,4-lactone	Others	Saccharides	2782-09-4	75461.94	79550.74	70750.48	75254.39
188.10	C9H16O4	Eucommiol	Others	Alcohol compounds	55930-44-4	99409.65	54318.99	54790.35	69506.33
136.04	C4H8O5	D-Threonic Acid	Others	Saccharides	3909-12-4	53496.54	74415.08	66665.02	64858.88
422.08	C12H23O14P	Trehalose 6-phosphate	Others	Saccharides	4484-88-2	58341.77	61692.97	58370.35	59468.36
194.03	C6H10O7	D-Galacturonic acid*	Others	Saccharides	685-73-4	44286.76	57416.53	64766.45	55489.91
194.04	C6H10O7	D-Glucoronic acid*	Others	Saccharides	6556-12-3	24577.72	58675.92	61548.71	48267.45
167.06	C8H9NO3	Pyridoxal	Others	Vitamin	66-72-8	47370.97	27473.51	57908.72	44251.07
230.02	C5H11O8P	Ribulose-5-phosphate	Others	Saccharides	4300-28-1	40120.36	40119.30	50958.74	43732.80
205.13	C9H19NO4	D-Panthenol	Others	Saccharides	81-13-0	46272.31	37669.68	32694.84	38878.94
170.00	C3H7O6P	Dihydroxyacetone phosphate	Others	Saccharides	57-04-5	43171.40	25857.99	40890.24	36639.88
194.08	C7H14O6	D-Pinitol	Others	Saccharides	10284-63-6	31073.20	35205.51	39972.07	35416.93

382.21	C24H30O4	(Z)-3,8-Dihydro 6,6';7,3'a-diligustilide	Others	Others	-	30021.13	35716.84	36200.40	33979.45
376.14	C17H20N4O6	Riboflavin (Vitamin B2)	Others	Vitamin	83-88-5	46143.61	21520.24	28843.33	32169.06
164.07	C6H12O5	1,5-Anhydro-D-glucitol	Others	Saccharides	154-58-5	25565.28	31774.72	29193.22	28844.41
666.22	C24H42O21	D-Maltotetraose	Others	Saccharides	34612-38-9	19486.57	21787.73	44755.30	28676.53
450.35	C31H46O2	Phylloquinone (Vitamin K1)	Others	Vitamin	84-80-0	24876.10	27779.21	29269.04	27308.11
666.22	C24H42O21	Stachyose	Others	Saccharides	470-55-3	25691.76	17631.18	28045.47	23789.47
340.00	C6H14O12P2	D-Fructose-1,6-biphosphate	Others	Saccharides	488-69-7	17986.27	34143.63	18240.93	23456.95
200.01	C4H9O7P	D-Erythrose-4-phosphate	Others	Saccharides	585-18-2	15789.19	13584.21	28842.58	19405.33
259.05	C6H14NO8P	D-Glucosamine 1-phosphate	Others	Saccharides	2152-75-2	20826.11	17920.05	19257.25	19334.47
507.17	C24H29NO11	Pyridoxine-5'-O-(6''-feruloyl)glucoside	Others	Vitamin	-	19471.12	15979.99	17866.45	17772.52
666.22	C24H42O21	Nystose	Others	Saccharides	13133-07-8	20717.62	17266.53	13781.19	17255.11
262.05	C6H15O9P	Sorbitol-6-phosphate	Others	Saccharides	20479-58-7	11051.37	19190.79	13530.88	14591.01
150.05	C5H10O5	D-Ribose	Others	Saccharides	50-69-1	4619.27	6549.36	12585.81	7918.15
340.00	C6H14O12P2	D-Glucose 1,6-bisphosphate	Others	Saccharides	10139-18-1	6488.87	6684.84	6820.62	6664.77
520.19	C26H32O11	Dehydrodicoumaroyl alcohol-gamma'-O-glucoside	Phenolic acids	Phenolic acids	-	16471646.96	26484920.19	19121269.68	20692612.28
278.15	C16H22O4	Dibutyl phthalate*	Phenolic acids	Phenolic acids	84-74-2	17342252.60	18855428.90	15448909.24	17215530.25
278.15	C16H22O4	Diisobutyl phthalate*	Phenolic acids	Phenolic acids	84-69-5	17471809.46	18186369.17	14812306.25	16823494.96
356.11	C16H20O9	Ferulic acid-4-O-glucoside	Phenolic acids	Phenolic acids	117405-51-3	15383861.58	13338062.81	8742809.16	12488244.52
300.08	C13H16O8	Salicylic acid-2-O-glucoside	Phenolic acids	Phenolic acids	10366-91-3	11895424.10	5535858.55	9252427.09	8894569.91
166.06	C9H10O3	4'-Hydroxy-3'-methoxyacetophenone (Acetovanillone)	Phenolic acids	Phenolic acids	498-02-2	8329750.33	7458718.05	4518799.08	6769089.15
368.11	C17H20O9	3-O-Caffeoylquinic acid methyl ester	Phenolic acids	Phenolic acids	123483-19-2	3932294.18	5134266.77	2817970.97	3961510.64
368.11	C17H20O9	1-O-Feruloylquinic acid	Phenolic acids	Phenolic acids	-	2570903.68	2919139.00	2106469.26	2532170.65

461.15	C19H27NO12	Anthranilate-1-O-Sophoroside	Phenolic acids	Phenolic acids	-	2254949.13	2286324.21	2287471.41	2276248.25
338.10	C16H18O8	3-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	87099-71-6	2445359.95	2384497.92	1666403.53	2165420.47
139.03	C6H5NO3	4-Nitrophenol	Phenolic acids	Phenolic acids	100-02-7	1824404.41	2630185.97	1786640.35	2080410.25
356.11	C16H20O9	1-O-Feruloyl- β -D-glucose	Phenolic acids	Phenolic acids	7196-71-6	1613767.35	1093882.85	1439135.20	1382261.80
500.15	C22H28O13	5-O-p-Coumaroylquinic acid O-glucoside	Phenolic acids	Phenolic acids	-	1703099.74	1268496.26	1171591.74	1381062.58
300.08	C13H16O8	4-O-Glucosyl-4-hydroxybenzoic acid	Phenolic acids	Phenolic acids	-	2065567.61	1037230.36	839381.40	1314059.79
300.09	C13H16O8	Glucosyloxybenzoic acid	Phenolic acids	Phenolic acids	-	2054140.01	1024405.42	837799.75	1305448.39
300.08	C13H16O8	1-O-Salicyloyl- β -D-glucose	Phenolic acids	Phenolic acids	60517-74-0	1918324.97	960089.75	800281.50	1226232.07
338.10	C16H18O8	1-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	-	1083264.90	1270248.32	918423.68	1090645.63
464.12	C18H24O14	mudanoside B	Phenolic acids	Phenolic acids	203511-37-9	1411906.08	825294.28	561285.40	932828.58
152.05	C8H8O3	Vanillin; 4-Hydroxy-3-Methoxybenzaldehyde	Phenolic acids	Phenolic acids	121-33-5	944244.67	1209100.06	385226.92	846190.55
368.11	C17H20O9	Chlorogenic acid methyl ester	Phenolic acids	Phenolic acids	29708-87-0	928652.44	824197.48	418803.94	723884.62
482.14	C22H26O12	5-O-p-Coumaroylshikimic acid O-glucoside	Phenolic acids	Phenolic acids	-	431690.21	893597.71	626074.25	650454.05
204.08	C12H12O3	Senkyunolide C*	Phenolic acids	Phenolic acids	-	543016.19	635611.87	450707.99	543112.02
530.16	C23H30O14	3-O-Feruloylquinic acid-O-glucoside*	Phenolic acids	Phenolic acids	-	673884.26	494526.57	361037.08	509815.97
530.16	C23H30O14	5-O-Feruloyl quinic acid glucoside*	Phenolic acids	Phenolic acids	-	673884.26	494526.57	361037.08	509815.97
208.07	C11H12O4	Sinapinaldehyde	Phenolic acids	Phenolic acids	4206-58-0	444337.39	714221.86	370460.58	509673.28
326.10	C15H18O8	Phenylpropionic acid-O- β -D-glucopyranoside	Phenolic acids	Phenolic acids	-	370127.44	457847.70	448621.33	425532.16
338.10	C16H18O8	4-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	32451-86-8	419786.23	527779.15	310185.65	419250.34
332.07	C13H16O10	1-O-Galloyl- β -D-glucose	Phenolic acids	Phenolic acids	58511-73-2	471787.50	393291.67	364928.50	410002.56
286.11	C13H18O7	Salicin	Phenolic acids	Phenolic acids	138-52-3	420120.68	369746.01	438837.82	409568.17
332.11	C14H20O9	Koaburaside	Phenolic acids	Phenolic acids	41653-73-0	316287.89	447468.68	353949.75	372568.77

402.15	C18H26O10	Benzyl-(2''-O-xylosyl)glucoside	Phenolic acids	Phenolic acids	-	82597.92	569523.56	449322.56	367148.01
316.08	C13H16O9	Protocatechuic acid-4-O-glucoside	Phenolic acids	Phenolic acids	-	280555.47	338655.95	447119.74	355443.72
316.08	C13H16O9	1-O-Gentisoyl-β-D-glucoside	Phenolic acids	Phenolic acids	23445-11-6	280555.47	338655.95	447119.74	355443.72
326.10	C15H18O8	p-Coumaric acid-4-O-glucoside	Phenolic acids	Phenolic acids	117405-48-8	287605.79	383999.90	363536.91	345047.53
326.10	C15H18O8	1-O-p-Coumaroyl-β-D-glucose	Phenolic acids	Phenolic acids	7139-64-2	287605.79	383999.90	363536.91	345047.53
122.04	C7H6O2	4-Hydroxybenzaldehyde	Phenolic acids	Phenolic acids	123-08-0	351435.99	526749.91	148337.99	342174.63
342.13	C16H22O8	Coniferin	Phenolic acids	Phenolic acids	531-29-3	303085.34	267121.31	427752.23	332652.96
342.10	C15H18O9	1-O-Caffeoyl-β-D-glucose*	Phenolic acids	Phenolic acids	14364-08-0	386082.96	229956.06	351719.75	322586.26
180.08	C10H12O3	Coniferyl alcohol	Phenolic acids	Phenolic acids	458-35-5	371460.35	344960.94	235785.98	317402.42
226.08	C11H14O5	3,4'-Dihydroxy-3',5'-dimethoxypropiophenone	Phenolic acids	Phenolic acids	136196-47-9	223029.45	294655.17	367499.64	295061.42
344.11	C15H20O9	Dihydrocaffeoylglucose	Phenolic acids	Phenolic acids	-	245598.37	345486.01	281665.46	290916.61
342.10	C15H18O9	6-O-Caffeoyl-D-glucose*	Phenolic acids	Phenolic acids	-	328334.72	247830.19	296295.55	290820.15
182.06	C9H10O4	Syringaldehyde; 4-Hydroxy-3,5-Dimethoxybenzaldehyde	Phenolic acids	Phenolic acids	134-96-3	302854.16	402845.09	155693.60	287130.95
354.10	C16H18O9	1-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	1241-87-8	154419.94	315287.76	295886.26	255197.98
354.10	C16H18O9	4-O-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	-	274858.70	235302.28	254925.21	255028.73
368.11	C17H20O9	3-O-Feruloylquinic acid	Phenolic acids	Phenolic acids	1899-29-2	278352.62	282331.55	200248.31	253644.16
344.11	C15H20O9	Syringaldehyde-4-O-glucoside	Phenolic acids	Phenolic acids	-	224130.48	266677.51	234477.46	241761.82
296.05	C13H12O8	Cis-Coutaric acid	Phenolic acids	Phenolic acids	67920-37-0	276609.74	220603.48	220584.14	239265.78
402.15	C18H26O10	Benzyl β-primeveroside	Phenolic acids	Phenolic acids	130622-31-0	132372.98	380887.04	179504.65	230921.55
194.06	C10H10O4	Ferulic acid	Phenolic acids	Phenolic acids	537-98-4	116216.26	215051.74	340691.49	223986.49
444.20	C21H32O10	(1'R,3R,5R,8'S)-Dihydrophaseic acid-O-β-D-glucoside	Phenolic acids	Phenolic acids	-	159448.03	212001.54	211873.99	194441.19
138.03	C7H6O3	4-Hydroxybenzoic acid	Phenolic acids	Phenolic acids	99-96-7	169360.74	226975.32	151139.37	182491.81

272.09	C12H16O7	Arbutin	Phenolic acids	Phenolic acids	497-76-7	71089.69	286000.66	136255.87	164448.74
332.11	C14H20O9	Leonuriside A	Phenolic acids	Phenolic acids	121748-12-7	123839.51	260265.98	102301.32	162135.60
302.10	C13H18O8	Tachioside	Phenolic acids	Phenolic acids	109194-60-7	98795.47	158424.62	218492.27	158570.78
354.10	C16H18O9	5-O-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	-	166997.45	163791.71	138949.51	156579.56
678.16	C34H30O15	3,4,5-Tricaffeoylquinic acid	Phenolic acids	Phenolic acids	86632-03-3	171602.15	83673.30	205111.65	153462.37
354.10	C16H18O9	3-O-Caffeoylquinic acid*	Phenolic acids	Phenolic acids	-	155781.48	161296.19	143221.16	153432.94
332.11	C14H20O9	2,6-dimethoxy-hydroquinone-4-O- β -D-glucopyranoside	Phenolic acids	Phenolic acids	-	378003.54	35974.38	31711.78	148563.23
500.15	C22H28O13	3-O-p-Coumaroylquinic acid-O-glucoside	Phenolic acids	Phenolic acids	-	173868.06	122720.45	123738.11	140108.87
478.15	C23H26O11	3,5-Digalloylshikimic acid	Phenolic acids	Phenolic acids	95753-52-9	88227.47	111637.58	171000.43	123621.82
338.10	C16H18O8	5-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	1899-30-5	126357.96	105782.01	133741.42	121960.46
254.08	C12H14O6	1-O-Caffeoylglycerol	Phenolic acids	Phenolic acids	-	137887.23	106543.94	116788.44	120406.54
194.06	C10H10O4	Dimethyl phthalate	Phenolic acids	Phenolic acids	131-11-3	97077.62	98175.88	92837.08	96030.19
206.17	C14H22O	2,6-Di-tert-butylphenol*	Phenolic acids	Phenolic acids	128-39-2	90117.43	89322.26	87395.90	88945.19
206.17	C14H22O	2,4-Di-Tert-Butylphenol*	Phenolic acids	Phenolic acids	96-76-4	83415.31	80029.08	79964.91	81136.44
238.05	C11H10O6	Benzoylmalic acid	Phenolic acids	Phenolic acids	22138-51-8	67336.65	86363.42	72479.65	75393.24
284.05	C12H12O8	Vnilloylmalic acid	Phenolic acids	Phenolic acids	-	73642.78	79956.46	58419.09	70672.78
164.05	C9H8O3	2-Hydroxycinnamic acid*	Phenolic acids	Phenolic acids	583-17-5	80052.38	57179.43	70197.15	69142.99
164.05	C9H8O3	α -Hydroxycinnamic Acid*	Phenolic acids	Phenolic acids	5801-57-0	80052.38	57179.43	70197.15	69142.99
314.10	C14H18O8	Mandelic acid- β -glucoside	Phenolic acids	Phenolic acids	-	53253.46	87906.46	61897.64	67685.85
318.10	C13H18O9	4,6-dimethoxy-2-methoxyphenyl-1-O-beta-D-glucopyranoside	Phenolic acids	Phenolic acids	-	46633.67	98649.94	44014.59	63099.40
514.10	C21H22O15	1,7-Di-O-galloyl-D-sedoheptulose	Phenolic acids	Phenolic acids	-	55671.84	57577.70	67012.20	60087.25
386.12	C17H22O10	4-O-Glucosyl-sinapate	Phenolic acids	Phenolic acids	-		54737.00	62521.31	58629.15

268.09	C13H16O6	2-Feruloyl-sn-glycerol	Phenolic acids	Phenolic acids	-	61405.62	44472.95	54380.00	53419.52
368.11	C17H20O9	5-O-Feruloylquinic acid	Phenolic acids	Phenolic acids	-	46723.62	69795.27	43078.02	53198.97
168.04	C8H8O4	Vanillic acid	Phenolic acids	Phenolic acids	121-34-6	72553.70	47092.16	31113.70	50253.19
150.07	C9H10O2	p-Coumaryl alcohol	Phenolic acids	Phenolic acids	3690-05-9	64538.44	54653.85	29694.40	49628.90
198.05	C9H10O5	4-Hydroxy-3-methoxymandelate	Phenolic acids	Phenolic acids	55-10-7	33204.76	33226.16	78676.88	48369.27
198.05	C9H10O5	Syringic acid	Phenolic acids	Phenolic acids	530-57-4	55421.14	47842.19	34110.68	45791.34
210.09	C11H14O4	Sinapyl alcohol	Phenolic acids	Phenolic acids	537-33-7	38178.53	60791.45	33507.73	44159.24
194.06	C10H10O4	Vanillin acetate	Phenolic acids	Phenolic acids	881-68-5	45379.69	24269.30	61928.16	43859.05
332.07	C13H16O10	Gallic acid-4-O-glucoside	Phenolic acids	Phenolic acids	84274-52-2	91685.07	19767.39	16640.97	42697.81
386.10	C17H22O10	1-O-Eudesmoylquinic acid	Phenolic acids	Phenolic acids	-	42677.74	48071.87	33396.00	41381.87
666.22	C31H38O16	2'-Acetylacteoside	Phenolic acids	Phenolic acids	94492-24-7	46334.02	29118.53	47543.30	40998.62
530.14	C26H26O12	3,4-O-Dicaffeoylquinic Acid Methyl Ester	Phenolic acids	Phenolic acids	-	27831.09	50293.95	42253.03	40126.03
320.09	C16H16O7	Trans-5-O-(p-Coumaroyl)shikimate	Phenolic acids	Phenolic acids	-	35007.50	41089.98	40968.70	39022.06
756.25	C34H44O19	Forsythoside B	Phenolic acids	Phenolic acids	81525-13-5	36676.69	34695.59	43295.27	38222.51
316.12	C14H20O8	5-(2-Hydroxyethyl)-2-O-glucosylphenol	Phenolic acids	Phenolic acids	-	51026.76	33015.01	23564.32	35868.70
316.12	C14H20O8	Cimidahurinine	Phenolic acids	Phenolic acids	142542-89-0	51026.76	33015.01	23564.32	35868.70
316.12	C14H20O8	Vanilloloside	Phenolic acids	Phenolic acids	74950-96-2	47921.18	24856.34	23410.15	32062.56
165.04	C8H7NO3	2-(Formylamino)benzoic acid	Phenolic acids	Phenolic acids	3342-77-6	27647.76	44462.26	19007.81	30372.61
624.21	C29H36O15	Acteoside; Verbascoside	Phenolic acids	Phenolic acids	61276-17-3	16243.36	36503.53	37274.31	30007.07
300.05	C12H12O9	Vnilloyltartaric acid	Phenolic acids	Phenolic acids	-	31218.12	27888.69	28678.23	29261.68
372.11	C16H20O10	Trihydroxycinnamoylquinic acid	Phenolic acids	Phenolic acids	-	12925.98	36742.94	34635.74	28101.55
1172.38	C52H68O30	Oleoechinacoside	Phenolic acids	Phenolic acids	122960-94-5	19631.23	38658.03	12386.13	23558.46

326.10	C15H18O8	(2E)-3-[4-(β-D-glucopyranoside)-phenylacrylic]-acid	Phenolic acids	Phenolic acids	-	15218.06	20177.84	16964.67	17453.52
482.14	C22H26O12	3-O-p-Coumaroylshikimic acid-O-glucoside	Phenolic acids	Phenolic acids	-		19509.90	14562.02	17035.96
452.09	C20H20O12	2-O-Salicyl-6-O-Galloyl-D-Glucose	Phenolic acids	Phenolic acids	-	11708.00	16704.68	14874.26	14428.98
458.08	C22H18O11	p-Coumaroylcaffeoyltartaric acid	Phenolic acids	Phenolic acids	-	17156.28	9484.52	16272.01	14304.27
280.06	C13H12O7	p-Coumaroylmalic acid	Phenolic acids	Phenolic acids	-	7139.32	17247.55	12546.27	12311.05
148.05	C9H8O2	p-Coumaraldehyde	Phenolic acids	Phenolic acids	2538-87-6	15743.27	16348.53	4086.81	12059.54
678.18	C31H34O17	Dicaffeoylquinic acid-O-glucoside	Phenolic acids	Phenolic acids	-	15628.80		7736.89	11682.85
634.08	C27H22O18	1-O-Galloyl-4,6-hexahydroxydiphenoyl-D-glucose	Phenolic acids	Phenolic acids	126721-55-9	1957.96	26541.50	6368.07	11622.51
398.12	C18H22O10	4-O-Sinapoylquinic acid	Phenolic acids	Phenolic acids	-	12355.27	9364.40	5043.36	8921.01
178.06	C10H10O3	4-Methoxycinnamic acid	Phenolic acids	Phenolic acids	830-09-1	5201.09	3517.69	4992.89	4570.55
238.08	C12H14O5	3,4,5-Trimethoxycinnamic acid	Phenolic acids	Phenolic acids	90-50-6	3801.63	3267.49	1902.89	2990.67
414.39	C29H50O	β-Sitosterol	Steroids	Steroid	83-46-5	18464148.40	15839489.65	14815587.54	16373075.20
416.33	C27H44O3	Tigogenin	Steroids	Steroid	77-60-1	251417.58	268789.29	189157.73	236454.87
464.06	C20H16O13	Ellagic acid-4-O-glucoside	Tannins	Tannin	-	41272.34	33433.48	23800.99	32835.61
316.02	C15H8O8	3-O-Methylellagic acid	Tannins	Tannin	-	14448.66	15412.52	17130.96	15664.05
634.08	C27H22O18	Corilagin	Tannins	Tannin	23094-69-1	969.94	25886.96	4908.53	10588.47
434.05	C19H14O12	Ellagic acid-4-O-Xyloside	Tannins	Tannin	139163-18-1	16815.36		3398.26	10106.81
374.17	C21H26O6	12-Norquassin	Terpenoids	Diterpenoids	23460-59-5	7361306.87	293910.93	79403.90	2578207.23
250.12	C14H18O4	13-Nor-desacylcynaropicrin	Terpenoids	Sesquiterpenoids	-	1002431.60	1029652.10	981499.53	1004527.74
344.15	C16H24O8	ilicininolide A	Terpenoids	Sesquiterpenoids	-	703581.23	848809.78	428898.23	660429.75
406.15	C17H26O11	8-O-Acetylharpagide	Terpenoids	Monoterpenoids	6926-14-3	363860.64	665198.98	944863.01	657974.21
362.14	C19H22O7	6-O-p-Coumaroyl-3-methoxy-7-deoxyrehmaglutin A	Terpenoids	Monoterpenoids	-	380104.74	557842.91	477379.08	471775.58

610.21	C25H38O17	6'-O- β -D-glucosylbarlerin*	Terpenoids	Monoterpenoid s	927691-88- 1	418467.38	366860.57	219479.97	334935.97
538.21	C26H34O12	Sinenoside	Terpenoids	Monoterpenoid s	-	250863.72	430687.22	321786.02	334445.65
610.21	C25H38O17	6'-O- α -D-galactosylbarlerin*	Terpenoids	Monoterpenoid s	927691-89- 2	410662.50	351676.20	234902.30	332413.67
538.17	C25H30O13	5-Hydroxy-10-O-(p-methoxycinnamoyl)adoxosidic acid	Terpenoids	Monoterpenoid s	-	309991.49	378664.64	247958.35	312204.83
346.13	C15H22O9	Aucubin	Terpenoids	Sesquiterpenoid s	479-98-1	211533.43	379374.69	245196.90	278701.67
414.23	C21H34O8	Dendronobiloside E-iso-1	Terpenoids	Sesquiterpenoid s	-	183909.42	329406.18	223688.60	245668.07
456.36	C30H48O3	24,30-Dihydroxy-12(13)-ene-lupeol	Terpenoids	Triterpene	-	248053.91	217824.27	212941.80	226273.33
550.19	C23H34O15	Genipin-1-O-gentiobioside	Terpenoids	Monoterpenoid s	29307-60-6	126139.80	260922.95	165418.55	184160.43
536.15	C25H28O13	10-O-[(E)-Caffeoyl]-geniposidic acid	Terpenoids	Monoterpenoid s	-	137593.75	183394.19	156277.94	159088.63
302.22	C20H30O2	Levopimaric acid*	Terpenoids	Diterpenoids	79-54-9	208088.39	168669.91	89863.60	155540.63
302.22	C20H30O2	Isopimaric acid*	Terpenoids	Diterpenoids	5835-26-7	215310.67	165279.69	78146.01	152912.12
234.16	C15H22O2	7 β -H-9(10)-ene-11,12-Epoxy-8-oxoeremophilane	Terpenoids	Sesquiterpenoid s	-	109750.75	119262.42	115056.96	114690.04
234.16	C15H22O2	polygodial	Terpenoids	Sesquiterpenoid s	6754-20-7	100750.07	113066.25	111057.05	108291.12
486.33	C30H46O5	27,28-Dicarboxyl ursolic acid	Terpenoids	Triterpene	-	302557.36	7728.14	3778.35	104687.95
550.28	C29H42O10	Ajugamarin B1	Terpenoids	Diterpenoids	121521-88- 8	292194.76	8338.56	3196.00	101243.11
456.36	C30H48O3	Oleanolic acid	Terpenoids	Triterpene	508-02-1	110616.70	105693.98	48919.10	88409.93
194.13	C12H18O2	Carvylacetate	Terpenoids	Monoterpenoid s	97-42-7	91468.36	47907.77	98917.18	79431.10
520.16	C25H28O12	10-O-[(E)-p-Coumaroyl]-geniposidic acid	Terpenoids	Monoterpenoid s	-	56421.88	143184.14	37107.13	78904.38
456.36	C30H48O3	(23S)-3 β -hydroxydammara-21-oic acid 21,23-lactone	Terpenoids	Triterpene	-	103233.85	53668.22	46287.24	67729.77
472.36	C30H48O4	2,3-Dihydroxy-12-ursen-28-oic acid	Terpenoids	Triterpene	-	130909.82	26439.17	25892.61	61080.53

390.15	C17H26O10	ajugoside	Terpenoids	Monoterpenoids	52916-96-8	58713.69	57997.33	61582.84	59431.29
390.12	C16H22O11	Deacetylasperulosidic acid	Terpenoids	Monoterpenoids	14259-55-3	27843.08	45086.40	41431.08	38120.19
456.36	C30H48O3	3-Epiursolic acid	Terpenoids	Triterpene	989-30-0	39991.09	42822.26	18066.83	33626.73
470.34	C30H46O4	4,4.8-Trimethyl-3 β ,7 α ,23-trihydroxy-chola-14,24-dien-21-oic acid-21,23-lactone	Terpenoids	Triterpene	-	10816.83	4770.62	64110.45	26565.96
456.36	C30H48O3	Ursolic acid	Terpenoids	Triterpene	77-52-1		26333.91	22779.33	24556.62
292.20	C18H28O3	JiangxiBaiyingsu I	Terpenoids	Sesquiterpenoids	-	43294.38	20204.53	6828.62	23442.51
470.38	C31H50O3	Ambolic acid	Terpenoids	Triterpene	13878-93-8	23081.53	26022.28	19228.31	22777.37
432.13	C18H24O12	Asperulosidic acid	Terpenoids	Monoterpenoids	25368-11-0	29056.15	23866.60	14702.32	22541.69
478.22	C25H34O9	Ailanthinone	Terpenoids	Diterpenoids	53683-73-1	10976.15	17898.61	13372.29	14082.35
456.36	C30H48O3	3,4-Cycloopen-cycloaltin-4(29),25-diene-24(R)-hydroxy-3-carboxylic acid	Terpenoids	Triterpene	-	14413.33	11935.64	5818.17	10722.38
424.21	C22H32O8	Nigakilactone H	Terpenoids	Diterpenoids	30248-06-7	2179.35		16586.32	9382.83
426.39	C30H50O	Cycloartenol	Terpenoids	Triterpene	469-38-5	11227.64	4541.03	4702.67	6823.78
462.23	C25H34O8	Kumulactone K	Terpenoids	Diterpenoids	-	3048.46	8334.96	6555.02	5979.48
506.18	C25H30O11	2'-Cinnamoyl mussaenosidic acid	Terpenoids	Monoterpenoids	-	7017.72	5956.02	2413.54	5129.09

60 **Table S3** Summary of sequencing data for genome assembly of *Eucryptorrhynchus scrobiculatus*, *E. brandti* and *Ailanthus altissima*

Type of library	Peak insert size of the library (bp)	Sequencing data (Gb)			Coverage (X)			Usage
		<i>E. scrobiculatus</i>	<i>E. brandti</i>	<i>A. altissima</i>	<i>E. scrobiculatus</i>	<i>E. brandti</i>	<i>A. altissima</i>	
Illumina NovaSeq	500	51.7	89.2	33.11	129.2	223.0	35.79	Survey and correction
PacBio Sequel/Hifi	20Kb/15Kb	38.0	87.9	545.65	95.0	219.8	589.89	Draft assembly
Hi-C	100-500	57.9	131.0	136.68	144.6	327.5	147.76	Chromosomal-level assembly
Total	-	147.6	308.1	715.44	369.0	770.3	773.44	-

Table S4 Features of genome assembly of *Eucryptorrhynchus scrobiculatus*, *E. brandti* and *Ailanthus altissima*

	<i>A. altissima</i>	<i>E. scrobiculatus</i>	<i>E. brandti</i>
Assembly level	Chr.	Chr.	Chr.
Genome size (Mb)	925	318	401
No. chromosomes	32	18	21
Scaf. N50 (Mb)	29.664	17.6	21.024
No. of contigs	1184	389	228
Contig N50 (Mb)	25.202	4.215	4.009
Completeness (%)	94.3	98.6	97.8
Single copy gene (%)	66.9	97.8	96.6
Duplicated (%)	27.4	0.8	1.2
Fragmented (%)	1.4	0.5	0.7
No. genes	43139	22059	17928

Table S5 Information for genome assemblies in coleopteran species

Species	Assembly level	Genome size (Mb)	No. Sequences	Scaf. N50 (Mb)	No. of contigs	Contig N50 (Mb)	Completeness (%)	Duplicated (%)	No. genes
<i>Eucryptorrhynchus brandti</i>	Chr.	401	21	21.024	228	4.009	97.6	0.9	17928
<i>Eucryptorrhynchus scrobiculatus</i>	Chr.	318	18	17.6	389	4.215	98.2	0.4	22059
<i>Abscondita terminalis</i>	Scaf.	499	3187	1.22	3273	1.22	98.3	2.1	
<i>Adranes taylori</i>	Scaf.	888	113285	0.583	123425	0.027	74.8	0.3	
<i>Aenictocupidus jacobsonorum</i>	Scaf.	178	77446	0.445	89330	0.005	87	0.4	
<i>Aethina tumida</i>	Cont.	234	-	-	3063	0.298	96.3	7.3	14076
<i>Agrilus planipennis</i>	Scaf.	353	3613	1.11	23186	0.028	97.7	6.7	14922
<i>Alaus oculatus</i>	Scaf.	188	222737	1.329	222850	0.002	9.3	2.3	
<i>Aleochara bilineata</i>	Scaf.	85	33003	0.054	40224	0.012	93.2	0.4	
<i>Aquatica lateralis</i>	Scaf.	908	5388	0.693	38880	0.045	99	1	14285
<i>Anoplophora glabripennis</i>	Scaf.	707	9867	0.68	26749	0.08	98.7	1.9	22035
<i>Asbolus verrucosus</i>	Scaf.	249	135581	0.005	155593	0.004	93.5	1	
<i>Callosobruchus maculatus</i>	Cont.	1.007 Gb	-	-	15778	0.212	87.2	4	21264
<i>Chrysina resplendens</i>	Scaf.	611	113068	0.02	114419	0.02	79.0	0.5	
<i>Coccinella septempunctata</i>	Scaf.	514	55573	0.067	66468	0.021	95.4	5.7	
<i>Dendroctonus ponderosae</i>	Scaf.	253	8188	0.63	59583	0.008	96.2	4	13088
	Scaf.	261	6520	0.465	40744	0.01	98.4	1.6	
<i>Diabrotica virgifera</i>	Scaf.	2.4 Gb	87712	0.489	585680	0.006	92.3	2	
<i>Harmonia axyridis</i>	Scaf.	417	2183	2.054	2785	1.254	97.5	2.3	
<i>Hycleus cichorii</i>	Scaf.	111.7	13823	0.099	16072	0.086	92.51	2.01	13813
<i>Hycleus phaleratus</i>	Scaf.	106.7	12877	0.078	13783	0.075	92.59	2.62	13725
<i>Hypothenemus hampei</i>	Scaf.	162	8198	0.34	14837	0.036	96.8	0.2	20301
<i>Ignelater luminosus</i>	Scaf.	842	91322	0.095	106630	0.031	96.8	1.5	27557
<i>Lamprigera yunnana</i>	Cont.	1.05 Gb	-	-	2684	3.5	99.1	1.4	
<i>Leptinotarsa decemlineata</i>	Scaf.	642	26908	0.139	45556	0.046	92.1	0.9	24671
<i>Marronus borbonicus</i>	Scaf.	407	1023	16.8	8169	0.107	96.1	1.8	
<i>Nicrophorus vespilloides</i>	Scaf.	195	4650	0.122	8129	0.067	99.5	1.5	13562
<i>Onthophagus taurus</i>	Scaf.	267	5821	0.337	10620	0.101	99.6	2.7	17483
<i>Ophraella communa</i>	Cont.	774	-	-	7003	0.195	95.6	8.4	

<i>Oryctes borbonicus</i>	Scaf.	388	523	8.4	5214	0.171	91.2	1.3	20504
<i>Oryzaephilus surinamensis</i>	Scaf.	104	10890	0.021	11864	0.019	97.9	0.4	
<i>Photinus pyralis</i>	Scaf.	471	2160	50.6	7909	0.17	98.7	8.8	15773
<i>Pogonus chalceus</i>	Chr.	280	29168	0.066	84614	0.005	93.5	0.7	
<i>Popillia japonica</i>	Scaf.	531	75144	0.015	81484	0.013	85.6	2.9	
<i>Pyrocoelia pectoralis</i>	Scaf.	760.4	474	3.04	474	3.04	98.7	36.7	23092
<i>Propylaea japonica</i>	Scaf.	851	1074	100	4779	0.813	94.3	6.2	18018
<i>Protaetia brevitarsis</i>	Scaf.	1.14 Gb	5266	1.955	7277	0.318	96	32	34110
<i>Rhynchophorus ferrugineus</i>	Scaf.	782	4807	64	48516	0.023	93.4	40.6	25567
<i>Sitophilus oryzae</i>	Scaf.	770	2025	2.86	4474	1.04	98.4	1.9	23498
<i>Tribolium castaneum</i>	Chr.	166	91221	4.456	7059	0.073	99.2	0.4	16404
<i>Lycorma delicatula</i>	-	2.25Gb	-	-	2927	1.52	96.8	2.4	-

Species	Family	Assembly version	Public date	Reference/Accession no.
<i>Eucryptorrhynchus brandti</i>	Curculionidae			This study
<i>Eucryptorrhynchus scrobiculatus</i>	Curculionidae			This study
<i>Abscondita terminalis</i>	Lampyridae	Ate		GCA_013368085.1
<i>Adranes taylori</i>	Staphylinidae	ASM986724v1		GCA_009867245.1
<i>Aenictocupidus jacobsonorum</i>	Staphylinidae	ASM1001476v1		GCA_010014765.1
<i>Aethina tumida</i>	Nitidulidae	Atum_1.0	2017-01-05	¹⁵⁴
<i>Agrilus planipennis</i>	Buprestidae	Apla_2.0	2018-01-03	²⁸
<i>Alaus oculatus</i>	Elateridae	ASM985246v1		GCA_009852465.1
<i>Aleochara bilineata</i>	Staphylinidae	ASM305499v1	2018-04-17	GCA_003054995.1
<i>Aquatica lateralis</i>	Lampyridae	Alat1.3	2019-10-02	⁴⁵
<i>Anoplophora glabripennis</i>	Cerambycidae	Agla_2.0	2017-12-12	²⁷
<i>Asbolus verrucosus</i>	Tenebrionidae	BDFB_1.0	2019-02-13	GCA_004193795.1
<i>Callosobruchus maculatus</i>	Chrysomelidae	ASM90065972v1	2019-11	¹⁵⁵
<i>Chrysina resplendens</i>	Scarabaeidae	ASM1009189v1		GCA_010091895.1
<i>Coccinella septempunctata</i>	Coccinellidae	Csep_MD8_v1	2018-08-24	GCA_003568925.1

<i>Dendroctonus ponderosae</i>	Scolytidae	DendPond_male_1.0	2013-04-10	26
	Scolytidae	DendPond_female_1.0	2013-09-23	26
<i>Diabrotica virgifera</i>	Chrysomelidae	Dvir_v2.0	2018-10-15	GCA_003013835.2
<i>Harmonia axyridis</i>	Coccinellidae	Haxy_hC_F2.3_v1	2018-07-25	GCA_003402655.1
<i>Hycleus cichorii</i>	Meloidae	ASM1384121v1	2018-02-10	156
<i>Hycleus phaleratus</i>	Meloidae	ASM1384118v1	2018-02-10	156
<i>Hypothenemus hampei</i>	Scolytidae	ASM101285v1	2015-05-22	157
<i>Ignelater luminosus</i>	Lampyridae	Ilumi1.2	2019-10-02	45
<i>Lamprigera yunnana</i>	Lampyridae	ASM1336807v1		GCA_013368075.1
<i>Leptinotarsa decemlineata</i>	Chrysomelidae	Ldec_2.0	2017-10-31	158
<i>Marronus borbonicus</i>	Scarabaeidae	Marronus_mpgtue_10X		GCA_902655005.1
<i>Nicrophorus vespilloides</i>	Silphidae	Nicve_v1.0	2015-10-23	159
<i>Onthophagus taurus</i>	Scarabaeidae	Otau_2.0	2017-10-31	160
<i>Ophraella communa</i>	Chrysomelidae	Ophraella_communra_draft_assembly		GCA_902651945.1
<i>Oryctes borbonicus</i>	Scarabaeidae	ASM144370v1	2015-11-13	161
<i>Oryzaephilus surinamensis</i>	Silvanidae	ASM479650v1	2019-04-16	GCA_004796505.1
<i>Photinus pyralis</i>	Lampyridae	Ppyr1.3	2019-10-02	45
<i>Pogonus chalceus</i>	Carabidae	Pchal_1.0	2017-09-15	GCA_002278615.1
<i>Popillia japonica</i>	Scarabaeidae	GSC_JBeet_1.0	2019-03-29	GCA_004785975.1
<i>Pyrocoelia pectoralis</i>	Lampyridae	-	2017-11-24	162
<i>Propylaea japonica</i>	Coccinellidae	ASM1342104v1	2019-10-09	163
<i>Protaetia brevitarsis</i>	Scarabaeidae	ASM414364v1	2019-02-07	46
<i>Rhynchophorus ferrugineus</i>	Curculionidae	ASM1297910v1		99
<i>Sitophilus oryzae</i>	Curculionidae	Soryzae_2.0	2019-09-09	164
<i>Tribolium castaneum</i>	Tenebrionidae	Tcas5.2	2016-03-10	25
<i>Lycorma delicatula</i>	Fulgoridae	-	2019-10-10	165

67 **Table S6** Summary of repeat elements in genomes of *Eucryptorrhynchus scrobiculatus*, *E. brandti* and *Ailanthus altissima*

Item	No. of elements			Length (bp)			Percentage of sequence (%)		
	<i>E. scrobiculatus</i>	<i>E. brandti</i>	<i>A. altissima</i>	<i>E. scrobiculatus</i>	<i>E. brandti</i>	<i>A. altissima</i>	<i>E. scrobiculatus</i>	<i>E. brandti</i>	<i>A. altissima</i>
Retroelements	14757	20454	240411	2526638	4288707	197746037	0.79	1.07	21.37
SINEs	49	56	19	2999	3524	1263	0	0	0
LINEs	11406	15157	15622	1896388	2499778	5213150	0.60	0.62	0.56
LTR elements	3302	5241	224770	627251	1785405	192531624	0.20	0.44	20.81
DNA transposons	47525	68493	31058	10963315	17944899	7620087	3.44	4.47	0.82
Total interspersed repeats	-	-		13593625	22319520	206059973	4.27	5.55	22.27
Small RNA	168	163	2625	18865	28500	3053422	0.01	0.01	0.33
Satellites	17	35	425	1383	2036	56930	0	0	0.01
Simple repeats	36752	44401	383427	1531918	1917016	20230208	0.48	0.48	2.19
Low complexity	10792	14199	99096	501260	662018	5832302	0.16	0.16	0.63

68 SINEs: short interspersed nuclear elements; LINEs: long interspersed nuclear elements; LTR: long terminal repeat.

69

70 **Table S7** Summary of non-coding RNAs in genomes of *Eucryptorrhynchus scrobiculatus*, *E. brandti* and *Ailanthus altissima*

Classes	Type	<i>E. scrobiculatus</i>	<i>E. brandti</i>	<i>A. altissima</i>
rRNA count	8s_rRNA	85	20	223
	28s_rRNA	26	2	564
	18s_rRNA	20	4	559
Cove/Infernal Stats	Candidate tRNAs read	1471	1472	1351
	Cove/Infernal-confirmed tRNAs	381	384	1067
	Bases scanned by Cove/Infernal	169671	173462	128576
	tRNAs decoding Standard 20 AA	371	376	894
	Selenocysteine tRNAs (TCA)	1	0	0
tRNA Count	Possible suppressor tRNAs (CTA, TTA)	0	0	5
	tRNAs with undetermined/ unknown isotypes	1	0	5
	Predicted pseudogenes	8	8	163
	Total tRNAs	381	384	1067
	tRNAs with intron	23	29	46

Table S8 Summary of annotated protein-coding genes in *Eucryptorrhynchus scrobiculatus* and *E. brandti* genome

Database	<i>E. scrobiculatus</i>		<i>E. brandti</i>	
	Number	Percentage %	Number	Percentage %
Nr terms	14371	65	13848	77
UniRef50 terms	14553	66	13965	78
NCBI RefSeq terms	14355	65	13927	78
KO terms	12977	59	12657	71
InterPro domains	10171	46	10225	57
GO terms	5635	26	5667	32
Uniprot/Swissprot terms	9871	45	9929	55
CDD terms	11103	50	11028	62
COG/KOG	10547	48	10628	59

Percentage, percentage of each item in all genes.

76 **Table S9** Overall statistics of the orthogroups among twelve plants in this study

Number of species	12
Number of genes	450871
Number of genes in orthogroups	430628
Number of unassigned genes	20243
Percentage of genes in orthogroups	95.5
Percentage of unassigned genes	4.5
Number of orthogroups	26279
Number of species-specific orthogroups	7992
Number of genes in species-specific orthogroups	41464
Percentage of genes in species-specific orthogroups	9.2
Mean orthogroup size	16.4
Median orthogroup size	14
G50 (assigned genes)	25
G50 (all genes)	24
O50 (assigned genes)	4925
O50 (all genes)	5332
Number of orthogroups with all species present	8597
Number of single-copy orthogroups	20

78 **Table S10** Per-species statistics of the orthogroups among twelve plants in this study

	Aalt	Athal	Atric	Atrun	Ayang	Csine	Dlong	Ptric	Pvera	Tsine	Vvini	Xsorb
Number of genes	42775	48265	31494	28438	28320	39056	39282	51717	41299	34345	41208	24672
Number of genes in orthogroups	38773	45410	30529	26884	27446	38422	36396	50512	40191	31587	40257	24221
Number of unassigned genes	4002	2855	965	1554	874	634	2886	1205	1108	2758	951	451
Percentage of genes in orthogroups	90.6	94.1	96.9	94.5	96.9	98.4	92.7	97.7	97.3	92	97.7	98.2
Percentage of unassigned genes	9.4	5.9	3.1	5.5	3.1	1.6	7.3	2.3	2.7	8	2.3	1.8
Number of orthogroups containing species	15754	14770	12874	14976	14635	14690	15402	14477	15171	14449	14651	14398
Percentage of orthogroups containing species	59.9	56.2	49	57	55.7	55.9	58.6	55.1	57.7	55	55.8	54.8
Number of species-specific orthogroups	552	2113	806	288	300	441	840	787	620	444	707	94
Number of genes in species-specific orthogroups	2572	9335	3487	984	1115	2055	8610	4401	2943	1090	4627	245
Percentage of genes in species-specific orthogroups	6	19.3	11.1	3.5	3.9	5.3	21.9	8.5	7.1	3.2	11.2	1
Number of orthogroups	7992	2475	880	501	349	348	337	425	565	1090	2720	8597

79 Note: Aalt: *Ailanthus altissima*; Athal: *Arabidopsis thaliana*; Atric: *Amborella trichopoda*; Atrun: *Acer truncatum*; Ayang: *Acer yangbiense*; Csine: *Citrus sinensis*;
80 Dlong: *Dimocarpus longan*; Ptric: *Populus trichocarpa*; Pvera: *Pistacia vera*; Tsine: *Toona sinensis*; Vvini: *Vitis vinifera*; Xsorb: *Xanthoceras sorbifolium*.

81

82 **Table S11** Overall statistics of the orthogroups among sixteen Coleopteran insects

Number of species	16
Number of genes	340982
Number of genes in orthogroups	320887
Number of unassigned genes	20095
Percentage of genes in orthogroups	94.1
Percentage of unassigned genes	5.9
Number of orthogroups	22655
Number of species-specific orthogroups	6787
Number of genes in species-specific orthogroups	30541
Percentage of genes in species-specific orthogroups	9
Mean orthogroup size	14.2
Median orthogroup size	8
G50 (assigned genes)	23
G50 (all genes)	22
O50 (assigned genes)	3891
O50 (all genes)	4333
Number of orthogroups with all species present	4340
Number of single-copy orthogroups	87

83

84 **Table S12** Per-species statistics of the orthogroups among sixteen Coleopteran insects in this study

Species	Agla	Alat	Apla	Atum	Bmor	Dpon	Dvir	Ebra	Escr	Ilum	Ldec	Otau	Pbre	Ppec	Ppyr	Tcas
Number of genes	20632	14284	22159	17463	14623	20551	28061	17289	22059	27557	19038	21668	34123	23092	15773	22610
Number of genes in orthogroups	20224	13756	21556	16667	11806	20255	26970	14985	19072	25824	18549	21066	31077	21719	15262	22099
Number of unassigned genes	408	528	603	796	2817	296	1091	2304	2987	1733	489	602	3046	1373	511	511
Percentage of genes in orthogroups	98	96.3	97.3	95.4	80.7	98.6	96.1	86.7	86.5	93.7	97.4	97.2	91.1	94.1	96.8	97.7
Percentage of unassigned genes	2	3.7	2.7	4.6	19.3	1.4	3.9	13.3	13.5	6.3	2.6	2.8	8.9	5.9	3.2	2.3
Number of orthogroups containing species	9877	9672	9508	9463	8250	9591	10934	10790	11347	11289	9693	9815	11142	10518	9789	9803
Percentage of orthogroups containing species	43.6	42.7	42	41.8	36.4	42.3	48.3	47.6	50.1	49.8	42.8	43.3	49.2	46.4	43.2	43.3
Number of species-specific orthogroups	225	83	415	333	253	177	773	149	288	924	216	408	1342	644	161	396
Number of genes in species-specific orthogroups	1130	279	1507	1043	1198	535	3680	497	2705	4581	842	1402	6634	2519	484	1505
Percentage of genes in species-specific orthogroups	5.5	2	6.8	6	8.2	2.6	13.1	2.9	12.3	16.6	4.4	6.5	19.4	10.9	3.1	6.7

85 Note: Agla: *Anoplophora glabripennis* (Cerambycidae); Alat: *Aquatica lateralis* (Lampyridae); Apla: *Agrilus planipennis* (Buprestidae); Atum: *Aethina tumida*
86 (Nitidulidae); Bmor: *Bombyx mori* (Lepidoptera: Bombycidae); Dpon: *Dendroctonus ponderosae* (Scolytinae); Dvir: *Diabrotica virgifera* (Chrysomelidae);
87 Ebra: *Eucryptorrhynchus brandti* (Curculionidae); Escr: *Eucryptorrhynchus scrobiculatus* (Curculionidae); Ilum: *Ignelater luminosus* (Lampyridae); Ldec:
88 *Leptinotarsa decemlineata* (Chrysomelidae); Otau: *Onthophagus taurus* (Scarabaeidae); Pbre: *Protaetia brevitarsis* (Scarabaeidae); Ppec: *Pyrocoelia*
89 *pectoralis* (Lampyridae); Ppyr: *Photinus pyralis* (Lampyridae); Tcas: *Tribolium castaneum* (Tenebrionidea)

90

91 **Table S13** Summary of annotated Carbohydrate-Active Enzymes in eight coleopteran insects and *Lycorma delicatula*

	Auxiliary Activities	Carbohydrate- Binding Modules	Carbohydrate Esterases	Glycoside Hydrolases	Glycosyl Transferases	Polysaccharide Lyases
<i>Eucryptorrhynchus scrobiculatus</i>	30	157	9	139	110	9
<i>Eucryptorrhynchus brandti</i>	31	163	13	150	105	6
<i>Tribolium castaneum</i>	101	143	19	260	224	-
<i>Dendroctonus ponderosae</i>	104	117	32	252	235	73
<i>Anoplophora glabripennis</i>	99	117	30	361	222	-
<i>Agrilus planipennis</i>	150	125	19	441	285	79
<i>Photinus pyralis</i>	96	73	10	133	192	-
<i>Sitophilus oryzae</i>	79	118	25	268	243	-
<i>Lycorma delicatula</i>	26	57	6	114	136	-

92

93

Table S14 Genetics distance matrix of glutathione-s transferases (GSTs)

	EB_00925	ES_09938	EB_00927	ES_09936	EB_00928	ES_09935	EB_00929	ES_09934	EB_00930	ES_09933	ES_09932	EB_00931	ES_09931	EB_00932	ES_09930	EB_00933	ES_09929	EB_00934	ES_09928	ES_09926	EbGSTs1	EsGSTs1	EbGSTt1	EsGSTt1	EbGSTo1	EsGSTo1	EsGSTu1	EbGSTu1	EsGSTz1	EbGSTz1	EbGSTm1	TmGSTm1	
EB_00925-RA	0.013																																
ES_09938-RA	2.295	2.105																															
EB_00927-RA	2.293	2.140	0.106																														
ES_09936-RA	2.250	2.092	1.203	1.345																													
EB_00928-RA	2.005	1.963	0.250	0.302	1.020																												
ES_00929-RA	2.304	2.143	1.787	1.730	2.038	1.741																											
EB_00934-RA	2.344	2.139	1.820	1.782	2.143	1.792	0.041																										
ES_00930-RA	2.244	2.196	1.527	1.564	2.133	1.677	0.826	0.848																									
EB_00933-RA	2.356	2.293	1.534	1.570	2.105	1.697	0.864	0.893	0.130																								
ES_09932-RA	2.310	2.253	1.850	1.836	2.128	1.705	0.772	0.796	0.323	0.353																							
EB_00931-RA	2.127	2.016	1.995	1.995	2.125	2.035	0.769	0.783	0.434	0.447	0.409																						
ES_09931-RA	2.009	2.015	1.899	1.898	2.143	1.913	0.779	0.805	0.394	0.385	0.386	0.106																					
EB_00932-RA	2.092	2.054	1.761	1.833	2.254	1.835	0.592	0.604	0.343	0.403	0.318	0.381	0.365																				
ES_09930-RA	2.069	2.031	1.637	1.703	2.145	1.705	0.665	0.684	0.351	0.385	0.324	0.376	0.370	0.107																			
EB_00933-RA	2.500	2.287	2.211	2.214	2.768	2.334	1.354	1.348	1.414	1.373	1.555	1.449	1.400	1.224	1.237																		
ES_09929-RA	2.526	2.282	2.223	2.226	2.772	2.346	1.351	1.345	1.395	1.355	1.535	1.418	1.370	1.207	1.234	0.020																	
EB_00934-RA	2.603	2.377	2.099	2.105	2.927	2.303	1.349	1.344	1.393	1.373	1.499	1.390	1.356	1.108	1.124	0.171	0.170																
ES_09928-RA	2.615	2.388	2.270	2.210	3.004	2.330	1.351	1.345	1.393	1.430	1.496	1.340	1.315	1.112	1.111	0.192	0.191	0.120															
ES_09926-RA	2.274	2.104	2.116	1.973	2.695	1.999	1.260	1.228	1.414	1.393	1.431	1.398	1.391	1.101	1.156	0.825	0.843	0.835	0.844														
EbGSTs1	8.313	8.449	5.542	5.561	6.845	6.237	5.708	5.735	4.997	5.106	5.737	4.755	5.237	5.462	5.437	5.948	5.973	6.021	5.570	6.281													
EsGSTs1	8.647	8.721	5.423	5.441	7.010	5.992	5.826	5.855	5.006	5.079	5.784	4.900	5.249	5.401	5.588	5.988	6.014	6.030	5.576	6.366	0.048												
EbGSTt1	5.228	5.200	5.417	5.851	6.713	6.096	5.980	5.731	5.562	5.616	5.203	5.005	5.660	5.002	5.007	4.823	4.863	4.494	4.789	4.307	7.542	7.644											
EsGSTt1	5.476	5.279	5.240	5.707	6.567	5.877	6.352	6.078	5.955	6.019	5.638	5.218	5.565	5.404	5.476	5.118	5.164	4.755	5.079	4.610	7.536	7.637	0.038										
EbGSTo1	6.731	6.220	5.347	5.080	4.797	5.409	7.012	7.269	5.751	5.936	5.932	5.483	6.039	5.557	5.515	8.276	8.177	8.376	8.724	6.774	9.231	8.807	7.337	7.175									
EsGSTo1	6.667	6.174	5.469	5.194	4.904	5.535	7.210	7.480	5.891	6.085	6.079	5.613	6.193	5.691	5.646	8.213	8.116	8.312	8.657	6.723	9.611	9.157	7.578	7.404	0.005								
EbGSTu1	4.416	5.334	3.694	3.349	3.629	3.789	3.870	3.867	4.015	4.127	4.093	3.619	3.568	3.999	4.138	5.357	5.307	5.498	5.288	3.733	7.443	7.660	8.423	8.217	4.025	4.025							
EsGSTu1	4.967	5.396	4.159	3.999	3.819	4.205	4.111	4.115	4.016	4.060	4.076	3.784	3.808	4.046	4.342	5.611	5.567	5.378	5.366	3.972	8.909	9.652	7.617	7.816	4.212	4.197	0.019						
EbGSTz1	6.847	7.192	6.038	5.763	5.000	5.854	5.647	5.591	5.190	5.308	5.144	5.056	5.071	4.759	4.567	5.303	5.424	5.269	5.606	4.399	8.910	9.044	6.135	5.695	5.171	5.290	4.305	5.270					
EbGSTz1	6.049	6.356	5.288	5.243	4.892	5.372	5.289	5.238	4.684	4.795	4.797	4.724	4.712	4.362	4.241	5.399	5.523	5.345	5.775	4.187	8.868	8.976	6.087	5.674	5.202	5.322	4.244	5.256	0.092				
EbGSTm1	-1.000	-1.000	-1.000	-1.000	74.345	68.966	63.516	68.448	91.770	67.957	-1.000	66.890	45.238	-1.000	93.824	44.323	72.685	-1.000	-1.000	73.469	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	
TmGSTm1	-1.000	97.683	63.309	82.419	48.853	48.601	34.133	36.620	27.459	19.961	36.049	25.763	21.509	46.305	49.659	31.997	44.044	73.242	-1.000	64.246	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	0.737		
AgGSTm1	53.337	81.693	30.162	33.935	25.086	24.471	21.394	22.532	23.630	22.956	21.823	23.152	23.159	28.562	26.410	20.735	24.705	30.503	30.741	21.513	53.202	40.806	29.058	29.977	-1.000	-1.000	-1.000	-1.000	-1.000	48.342	55.151	0.867	0.806

97 **Table S15** Summary of annotated transient receptor potential (TRP) ion channels genes in insects

Species Name		Channel type																Total
		TRPC				TRPA				TRPN		TRPV		TRPM	TRPP		TRPML	
		TRP	TRPL	TRPy	TRPA1	TRPA5	HsTRPA	Pain	Pyx	Wtrw	NompC	lav	Nan	TRPM	Brv	Pkd2	TRPML	
	<i>B. mori</i>	1	1	1	1	1	0	1	1	2	1	1	1	1	0	0	1	14
	<i>D. plexippus</i>	1	1	1	1	1	0	1	1	2	1	1	1	1	0	0	1	14
Lepidoptera	<i>M. sexta</i>	1	1	1	1	2	0	1	1	2	1	1	1	1	0	0	1	15
	<i>P. Xuthus</i>	1	1	1	1	1	0	1	1	2	1	1	1	1	0	0	1	14
	<i>P. rapae</i>	1	1	1	1	1	0	1	1	2	1	1	1	1	0	0	1	14
Isoptera	<i>Z. nevadensis</i>	1	1	1	1	1	0	7	1	1	1	1	1	1	1	2	1	22
Blattodea	<i>B. germanica</i>	1	1	1	1	2	0	7	1	1	1	1	1	1	0	2	1	22
Hemiptera	<i>N. lugens</i>	1	1	1	1	0	0	1	0	1	1	1	1	1	0	1	1	14
Hymenoptera	<i>A. mellifera</i>	1	1	1	0	2	1	1	1	1	1	1	1	1	0	0	1	13
	<i>A. gambiae</i>	1	1	1	1	0	0	1	1	1	1	1	1	1	0	0	1	13
Diptera	<i>D. melanogaster</i>	1	1	1	1	0	0	1	1	1	1	1	1	1	3	1	1	16
	<i>T. castaneum</i>	1	1	1	1	0	0	1	0	1	1	1	1	1	1	1	1	15
Coleoptera	<i>E. scrobiculatus</i>	2	1	1	1	0	0	0	1	3	1	1	1	1	1	0	1	15
	<i>E. brandti</i>	2	1	1	1	0	0	1	1	3	1	1	1	0	1	1	1	16

Table S16 Reference organisms used in KAAS webserver annotation

Code	Organism	Number of sequences
dme	<i>Drosophila melanogaster</i> (fruit fly)	13,933
dpo	<i>Drosophila pseudoobscura</i>	14,574
dnv	<i>Drosophila navojoa</i>	10,673
dhe	<i>Drosophila hydei</i>	13,105
mde	<i>Musca domestica</i> (house fly)	14,896
aga	<i>Anopheles gambiae</i> (mosquito)	12,600
aag	<i>Aedes aegypti</i> (yellow fever mosquito)	14,626
cqu	<i>Culex quinquefasciatus</i> (southern house mosquito)	18,896
ame	<i>Apis mellifera</i> (honey bee)	9,922
bim	<i>Bombus impatiens</i> (common eastern bumble bee)	10,557
soc	<i>Solenopsis invicta</i> (red fire ant)	14,825
aec	<i>Acromyrmex echinator</i> (Panamanian leafcutter ant)	11,219
dqu	<i>Dinoponera quadriceps</i>	11,048
cfo	<i>Camponotus floridanus</i> (Florida carpenter ant)	12,512
lhu	<i>Linepithema humile</i> (Argentine ant)	11,623
pgc	<i>Pseudomyrmex gracilis</i>	11,572
obo	<i>Ooceraea biroi</i> (clonal raider ant)	11,927
pcf	<i>Polistes canadensis</i>	9,876
nvi	<i>Nasonia vitripennis</i> (jewel wasp)	13,358
mdl	<i>Microplitis demolitor</i>	12,144
tca	<i>Tribolium castaneum</i> (red flour beetle)	12,881
dpa	<i>Dendroctonus ponderosae</i> (mountain pine beetle)	13,021
nvl	<i>Nicrophorus vespilloides</i>	12,642
dpl	<i>Danaus plexippus</i> (monarch butterfly)	15,245
haw	<i>Helicoverpa armigera</i> (cotton bollworm)	13,836
tnl	<i>Trichoplusia ni</i> (cabbage looper)	15,089
pxy	<i>Plutella xylostella</i> (diamondback moth)	18,119
api	<i>Acyrtosiphon pisum</i> (pea aphid)	18,277
dnx	<i>Diuraphis noxia</i> (Russian wheat aphid)	12,390
ags	<i>Aphis gossypii</i> (cotton aphid)	12,828
zne	<i>Zootermopsis nevadensis</i>	12,381
fcd	<i>Folsomia candida</i>	20,251
bter	<i>Bombus terrestris</i> (buff-tailed bumblebee)	10,581
mpha	<i>Monomorium pharaonis</i> (pharaoh ant)	12,651
acep	<i>Atta cephalotes</i> (leaf cutting ant)	10,491
pbar	<i>Pogonomyrmex barbatus</i> (red harvester ant)	11,317
bmor	<i>Bombyx mori</i> (domestic silkworm)	13,743
pmac	<i>c</i> (common yellow swallowtail)	13,871
prap	<i>Pieris rapae</i> (cabbage white)	12,484
clec	<i>Cimex lectularius</i> (bed bug)	11,949
Total		527,933

Table S17 qPCR primers used in this study

Genes	Forward primer (5'-3')	Reverse primer (5'-3')
<i>EbraSNMP1a</i>	ACGTTGAAGATGGCGAAGGT	GCAGTCAGGACCATCAGCTT
<i>EbraSNMP1b</i>	CAGTTCTGGCGGTTGCTCTA	AGCTGCTGCATGTCGTTACT
<i>EbraSNMP2</i>	CAACCAGTGAGGACGACGAA	ACCTGATCCAGACCAGACGA
<i>EbraSNMP5a</i>	TGAACCGAAAACGGGTATGC	ATATTGGCGGCACTTTCTCG
<i>EbraSNMP5b</i>	ATGCCACTGCTGTAGG	AAGCCACTTGCTCTTATCTG
<i>EbraSNMP5c</i>	GATGAATCCGAACCCA	AAACGCAGCATAAACG
<i>EbraSNMP5d</i>	AACCACAGGCCAAAATGGGA	TGCAATCAGCCCCAACTCCT
<i>EbraSNMP5e</i>	CGCCACCTCGCAGTCCAAA	TCAGCAGCGGGTCCTCGTAG
<i>EbraSNMP5f</i>	GGAATCTGGAGCTTGGCCTT	GTCCGCTGCTCACTCTAGAC
<i>EbraSNMP5g</i>	ATGGGCCTTCTGATCCTCCT	TCGCTGTTTCGTCACATTCCA
<i>EbraSNMP5h</i>	GCCTCTCTCAACCCCACTTC	TTGTGGTTGGCCTTGGTTCT
<i>EbraSNMP5j</i>	TAGGGAACGAGCACGGAAAC	TTAGCTGACAACTGGGCTCG
<i>EscrSNMP1</i>	GATTCAAGGCGGCGGAATTC	GCAGTCAGGACCATCAGCTT
<i>EscrSNMP2</i>	AACGTTTCCAATCCGGACGA	TCGCCATAAGAACCGGGTTC
<i>EscrSNMP5a</i>	TCCAGCGCAGTATCAGCAAA	TACTTGCCAGCTGTGTGAG
<i>EscrSNMP5b</i>	CTCAGTGTTCTCAGCCGGTT	CACGAGTTTTGCCTGCTTCC
<i>EscrSNMP5c</i>	CCATCAGTTTGTTGCCACG	TCCCTGACGCGAAACATGAA
<i>EscrSNMP5d</i>	GGAACGCTTCCCGAAGTACA	ACGACCCTTCACTCGCTTTT
<i>EscrSNMP5e</i>	GGCGAACGACAGTTACAGGA	AGGCCTGTCATTTCTGTCTGG
<i>EscrSNMP5f</i>	GAAATATGGCGCCCGTTCAC	AAAATCGGTTTTTCGCGGCA
<i>EscrSNMP5g</i>	TGGGCCTTTCGATCCTCCTA	TCGCTGTTTCGTCACATTCCA
<i>EscrSNMP5h</i>	CAGACCTGTTCCCTTGCACT	CAGTCCGTTGACCGTCTTCA
<i>EscrSNMP5j</i>	CGATCCTGTATTGGGTCCCG	CAAATGCGGCAGGTATTTCGG
<i>EbraActin</i>	GCTATGTACGTCGCCATCCA	GACCTGCCAAGTCCAATCGA
<i>RPS11</i>	GCTTCAGGGATGTAGAGATTGG	TGCCCTTCGTAACCTTCAAC
<i>EscrActin</i>	TCGTGTGGCTCCAGAAGAAC	GGATGGCGACGTACATAGCA
<i>α-Tublin</i>	GTTTTGAGCCAGCCAACCAG	AGTAGGACACCAGTCGACGA

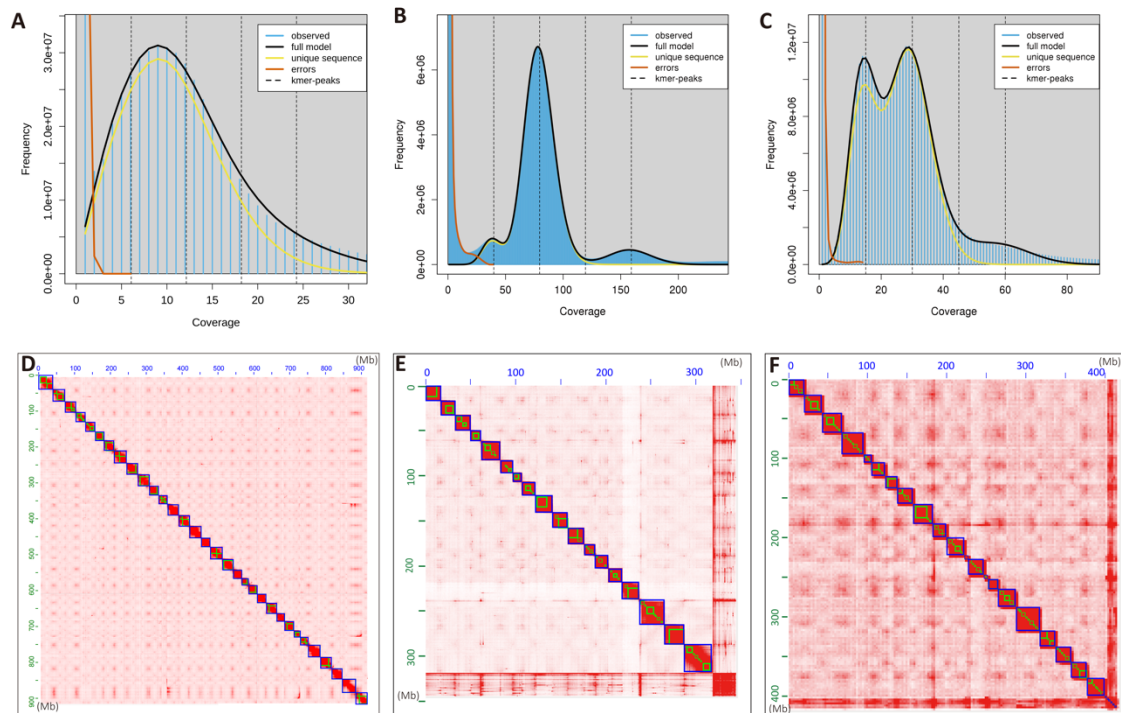


Fig. S1 K-mer estimate, contig contact matrix of tree of heaven *Ailanthus altissima*, root weevil *Eucryptorrhynchus scrobiculatus* and trunk weevil *E. brandti*. 17-mer was used to estimate the genome size, heterozygosity and duplication rate for *A. altissima* (A), *E. scrobiculatus* (B) and *E. brandti* (C). The blue area is the observed *k*-mer distribution; the area under the red line is the *k*-mers whose occurrence frequency was very low and is regarded as sequencing error; the area under the yellow line is the *k*-mer distribution of the nonrepeating region; the vertical dotted lines are peaks of the chart; the area under the black line is the reliably *k*-mer counts, which was used to estimate the genome size. There are three observed peaks for each species. The first peak presents at about half of the depth of the second main peak is a heterozygous peak; the second peak is the main peak of estimated species; the third peak whose coverage is about twice the main peak is a repetitive peak. The formula $G = N_{17\text{-mer}}/D_{17\text{-mer}}$, where the $N_{17\text{-mer}}$ is the total number of 17-mer, and $D_{17\text{-mer}}$ denotes the peak frequency of 17-mer, was used to estimate the genome size. D-F: contig contact matrix of root and trunk weevils and tree of heaven assembled using the Juicer grouped using 3D-DNA based on Hi-C data, the blue squares represent the clustered contig group. Only sequences anchored on chromosomes are shown in the plot.

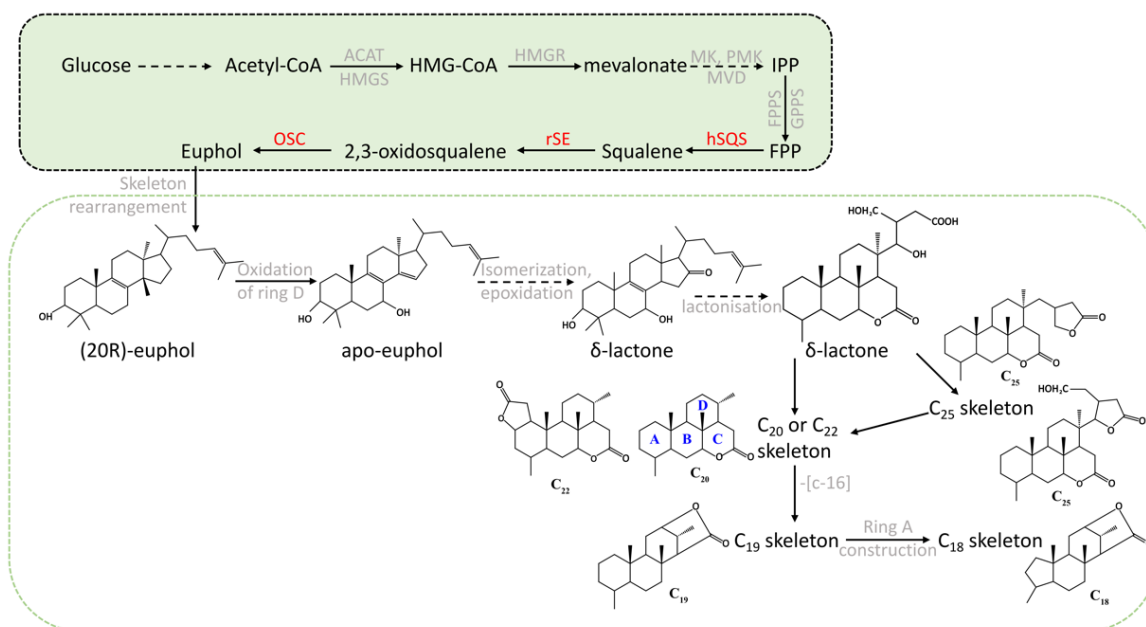


Fig. S2 Predicted schematic diagram of the quassinoids biosynthesis pathway in Simaroubaceae plants. The red enzymes of SQS, SE and OSC represent three crucial enzymes in the biosynthesis pathway. ACAT, acetyl-CoA acetyltransferase; HMGS, hydroxymethylglutaryl-CoA synthase; HMGR, hydroxymethylglutaryl-CoA reductase; MK, mevalonate kinase; PMK, phosphomevalonate kinase; MVD, mevalonate diphosphate diphosphatase; GPPS, geranyl diphosphate synthase; FPPS, farnesyl diphosphate synthase; SQS, squalene synthase; SE, squalene epoxidase; and OSC, oxidosqualene cyclase.



Fig. S3 Synteny blocks between root weevil *Eucryptorrhynchus scrobiculatus* and trunk weevil *E. brandti* based on MUMmer. X-axis represents *E. scrobiculatus*, Y-axis represents *E. brandti*. Each grid represents a single chromosome, the relative width of the grid represents the relative length of chromosome. There is obvious synteny between the two weevils' genomes.

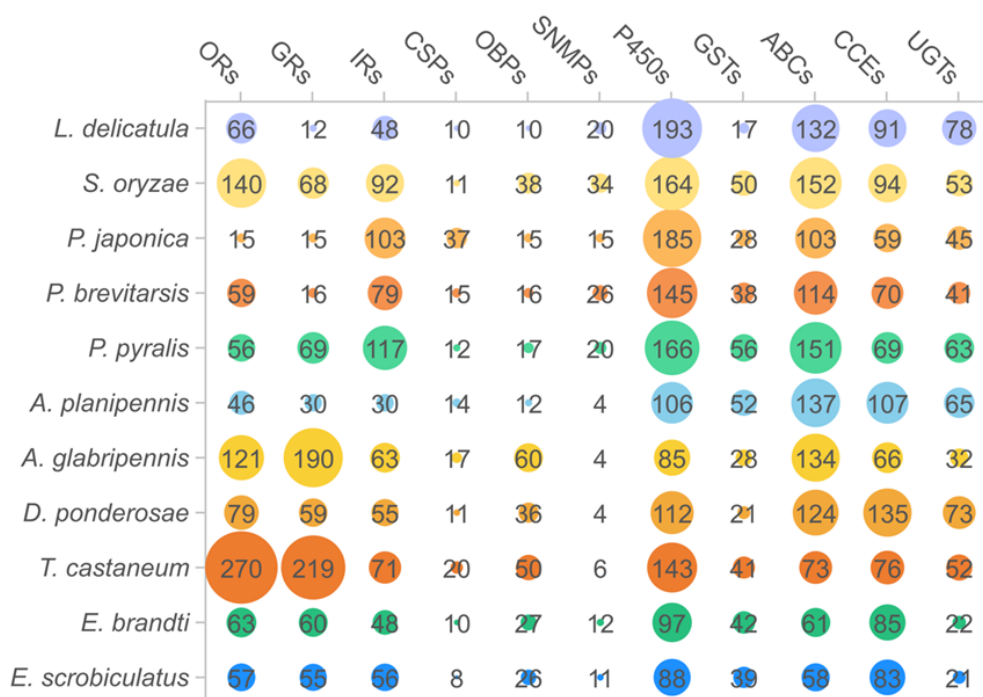


Fig. S4 Numbers of putatively functional proteins of root weevil *Eucryptorrhynchus scrobiculatus*, trunk weevil *E. brandti* and nine other insects. Monophagous: *E. scrobiculatus*, *E. brandti*; Oligophagous: *D. ponderosae*, *A. planipennis*; Polyphagous: *A. glabripennis*, *T. castaneum*, *P. brevitarsis*, *S. oryzae*; Predatist: *P. pyralis*, *P. japonica*.

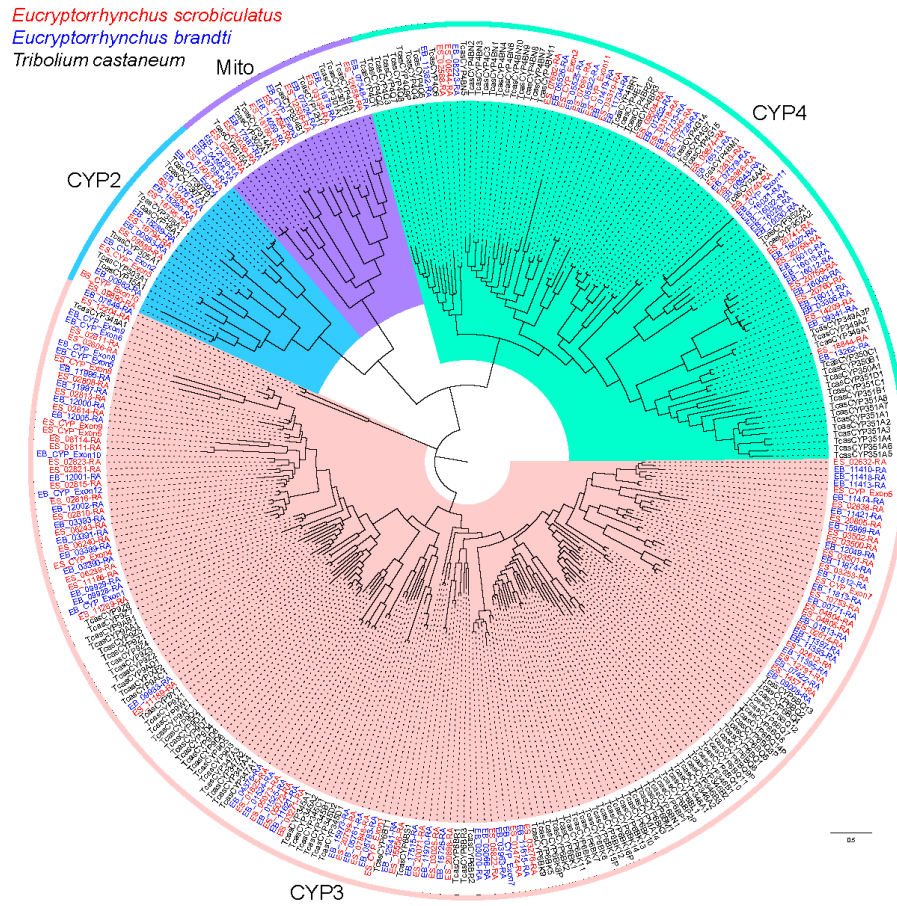


Fig. S5 Phylogenetic tree of the cytochrome P450 monooxygenases (P450s) family. The receptor sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *Eucryptorrhynchus brandti* (EB, blue) and *Tribolium castaneum* (Tcas, black). The tree is constructed using Maximum-Likelihood method in MEGA7 and unrooted. P450s are found clearly in four clades, CYP2, CYP3, CYP4, and mitochondrial, and are grouped further into families and subfamilies. There were several lineage-specific expansions ('blooms') in the CYP4 and CYP3 clans, respectively. Mainly orthologous P450s between weevils and *T. castaneum* were clade in CYP2 and mitochondrial CYPs, the CYPs of *T. castaneum* were displayed as outgroups of root weevil and trunk weevil at each branch' ends. Sources of sequence data and explanation of receptor classification are detailed in the Methods and Results section.

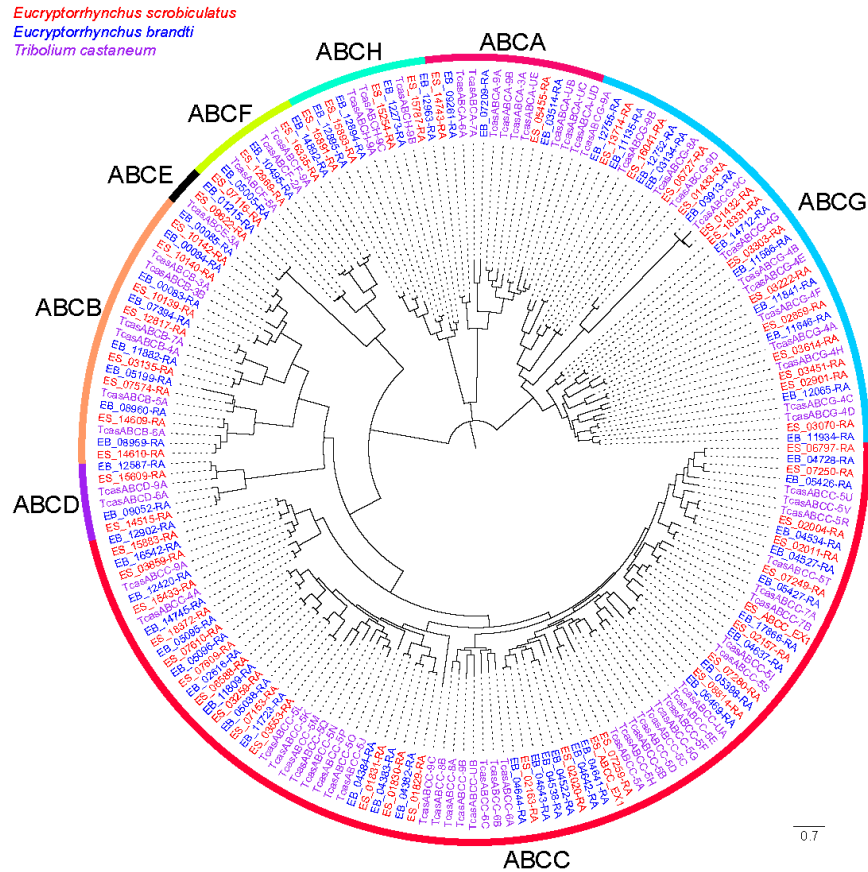


Fig. S6 Phylogenetic tree of the ATP-binding cassette transporters (ABCs) family. The enzymes sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *Eucryptorrhynchus brandti* (EB, blue) and *Tribolium castaneum* (Tcas, purple). The tree is constructed using Neighbor-Joining method in MEGA 7 and unrooted. All the ABCs of trunk weevil and root weevil could be divided into eight subfamilies, with the major group placed in ABCC subfamily followed by ABCG, ABCB, ABCA, ABCH, ABCF, ABCD and ABCE, showing that ABC transporter genes are highly conserved in insects. Approximately half of the ABCs were occupied by the ABCC subfamily in both trunk weevil and root weevil genomes, indicating that the ABCC subfamily appears to have undergone a recent expansion in Curculionidae weevils. Sources of sequence data and explanation of receptor classification are detailed in the Methods and Results section.

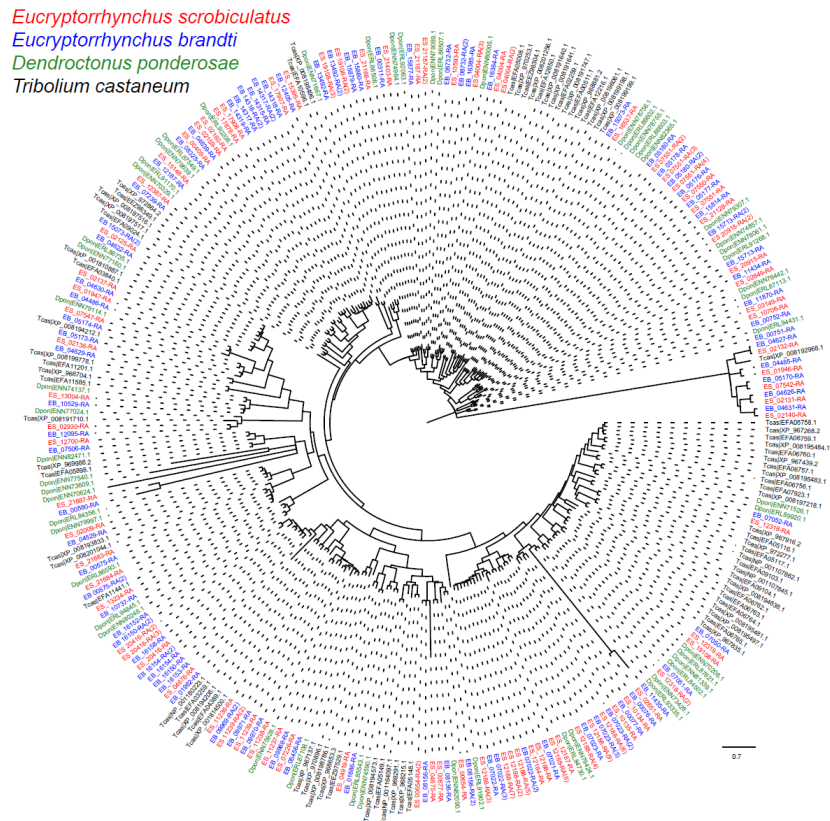


Fig. S7 Phylogenetic tree of the carboxyl/cholinesterases (CCEs) family. The receptor sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *Eucryptorrhynchus brandti* (EB, blue), *Dendroctonus ponderosae* (Dpon, green) and *Tribolium castaneum* (Tcas, black). The tree is constructed using Maximum-Likelihood method in MEGA 7 and unrooted. The phylogeny analysis showed the genes of each subclade mostly appeared in pairs, there is an item identified in ES genome, there is always an orthology gene found in EB genome, and vice versa. There are several species-specific expansions in CCEs. Sources of sequence data and explanation of sequences classification are detailed in the Methods and Results section.

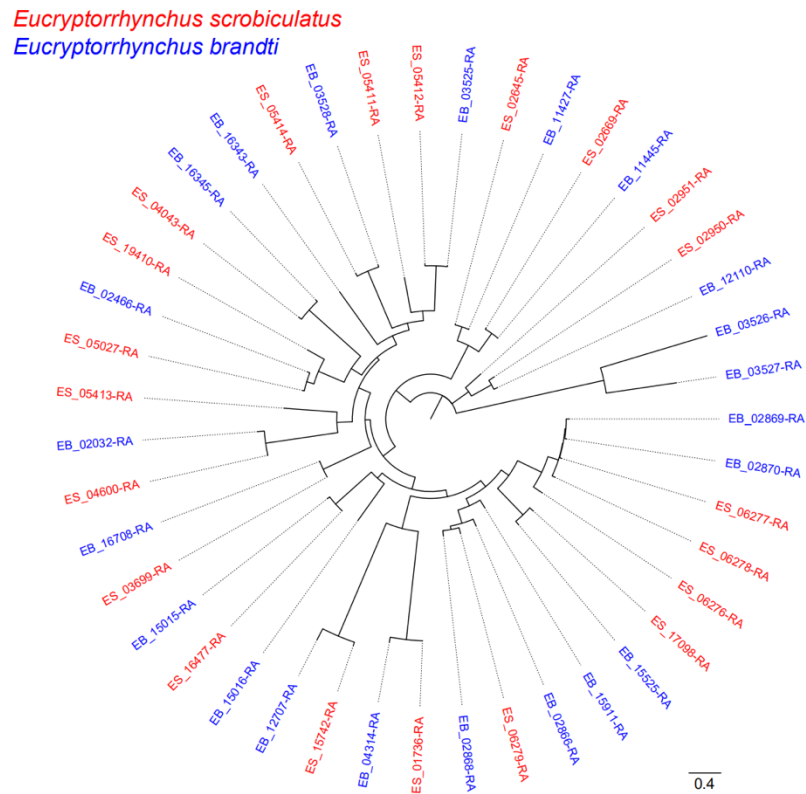


Fig. S8 Phylogenetic tree of the UDP-glycosyltransferases (UGTs) family. The enzyme sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red) and *Eucryptorrhynchus brandti* (EB, blue). The tree is constructed using Neighbor-Joining method in MEGA 7 and unrooted. The phylogeny analysis showed the same results that the genes of each subclade mostly appeared in pairs, there is an item identified in ES genome, there is always an orthology gene found in EB genome, and vice versa. Sources of sequence data and explanation of sequences classification are detailed in the Methods and Results section.

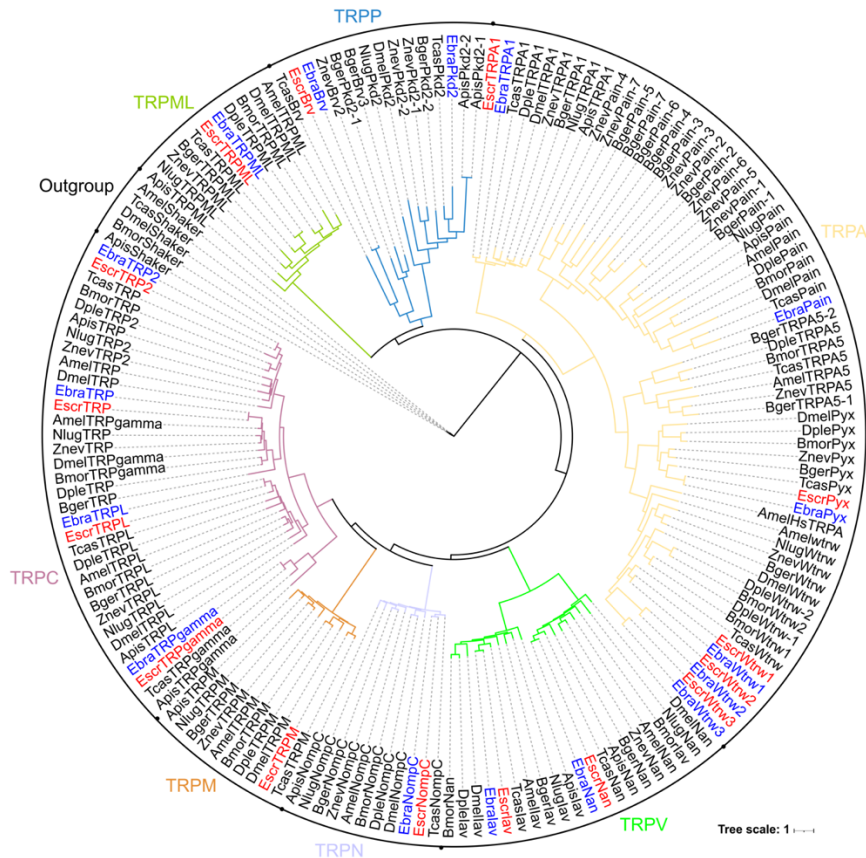


Fig. S10 Phylogenetic tree of the transient receptor potential (TRP) ion channels family. The enzymes sequences included were from *Eucryptorrhynchus scrobiculatus* (Escr, red), *Eucryptorrhynchus brandti* (Ebra, blue) and other reported insects. The tree is constructed using IQ-tree and the Shaker genes were used as outgroups. A total of 15 genes encoding putative proteins were identified in root weevil and 16 genes were identified in root weevil. The branches in different colors represent the corresponding subfamilies of this superfamily. Seven subfamilies were classified according to the topological structure. Sources of sequence data are detailed in the Methods and Results section.

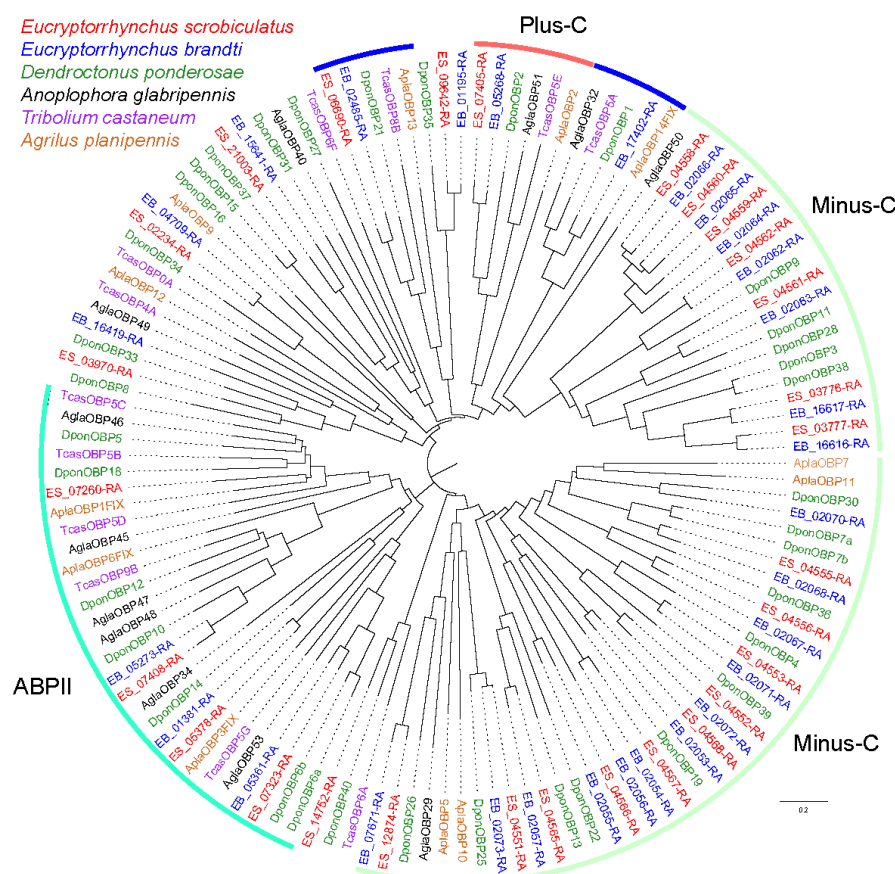


Fig. S11 Phylogenetic tree of the Odorant-binding proteins (OBPs) family. The receptor sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *Eucryptorrhynchus brandti* (EB, blue), *Dendroctonus ponderosae* (Dpon, green), *Anoplophora glabripennis* (Apla, black), *Tribolium castaneum* (Tcas, purple) and *Agrilus planipennis* (Apla, orange). The tree is constructed using the Maximum-Likelihood method in MEGA 7 and unrooted. One root weevil (ES_06690-RA) and two trunk weevils (EB_02485-RA and EB_17402-RA) are grouped in the clade of classic OBPs, which include one member from each of the four species in the analysis. A single paralogue of the Plus-C gene was recognized in both the trunk weevil and root weevil genomes and only seven Curculionidae genes fell into the ABPII clade. The remaining OBPs were clustered as Minus-C groups, with no major species-specific lineage expansions observed. Sources of sequence data and explanation of receptor classification are detailed in the Methods and Results section.

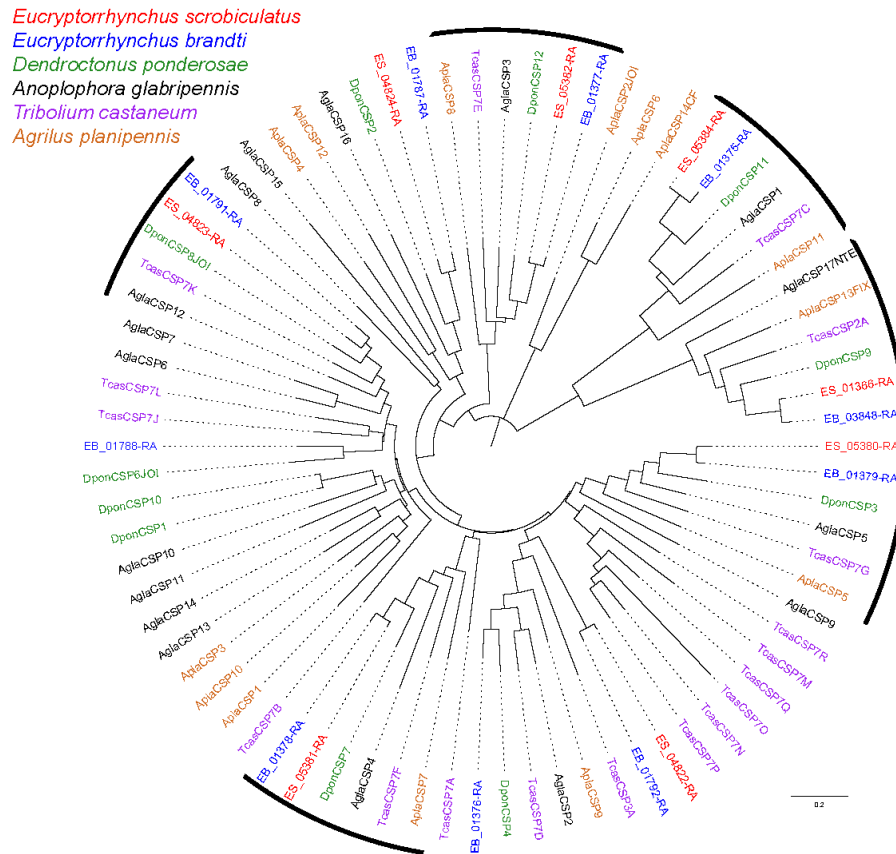


Fig. S12 Phylogenetic tree of the chemosensory protein (CSP) family. The receptor sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *Eucryptorrhynchus brandti* (EB, blue), *Dendroctonus ponderosae* (Dpon, green), *Anoplophora glabripennis* (Apla, black), *Tribolium castaneum* (Tcas, purple) and *Agrilus planipennis* (Apla, orange). The tree is constructed using Maximum-Likelihood method in MEGA 7 and unrooted. The phylogenetic analysis revealed the presence of several highly-supported clades with one CSPs from each of the six species (black arcs), which suggests the existence of several simple orthologous relationships in this gene family. There was no other species-specific gene expansion in CSPs. Sources of sequence data and explanation of receptor classification are detailed in the Methods and Results section.



Fig. S13 Phylogenetic tree of the odorant receptor (ORs) family. The receptor sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *Eucryptorrhynchus brandti* (EB, blue), *Dendroctonus ponderosae* (Dpon, black) and *Agrilus planipennis* (Apla, blue). The tree is constructed using Maximum-Likelihood method in MEGA 7 and unrooted. There are some subfamilies loss and expansion in trunk weevil and root weevil genomes. Only one *Orco* gene in trunk weevil (EB_09319-RA) and root weevil (ES_14186-RA) genome respectively. All of the identified ORs, except for three trunk weevil (ES_21494-RA, ES_12018-RA and ES_12180-RA) and three root weevil (EB_02996-RA, EB_07014-RA and EB_00537-RA) genes, are divided into five subfamilies (Groups 1, 2A, 2B, 5A and 7). The distribution of the ORs subfamilies was similar in trunk weevil and root weevil genomes. Most ORs fell into Group 7 (light blue circular arc), which occupied half of the total ORs recognized, followed by Group 5A, 1, 2A and 2B. There were no items of Group 3, 4, 5B and 6 in trunk weevil or root weevil genome. Genes of Group 7 in the beetles' genome greatly expanded during the evolution process. Sources of sequence data and explanation of receptor classification are detailed in the Methods and Results section.

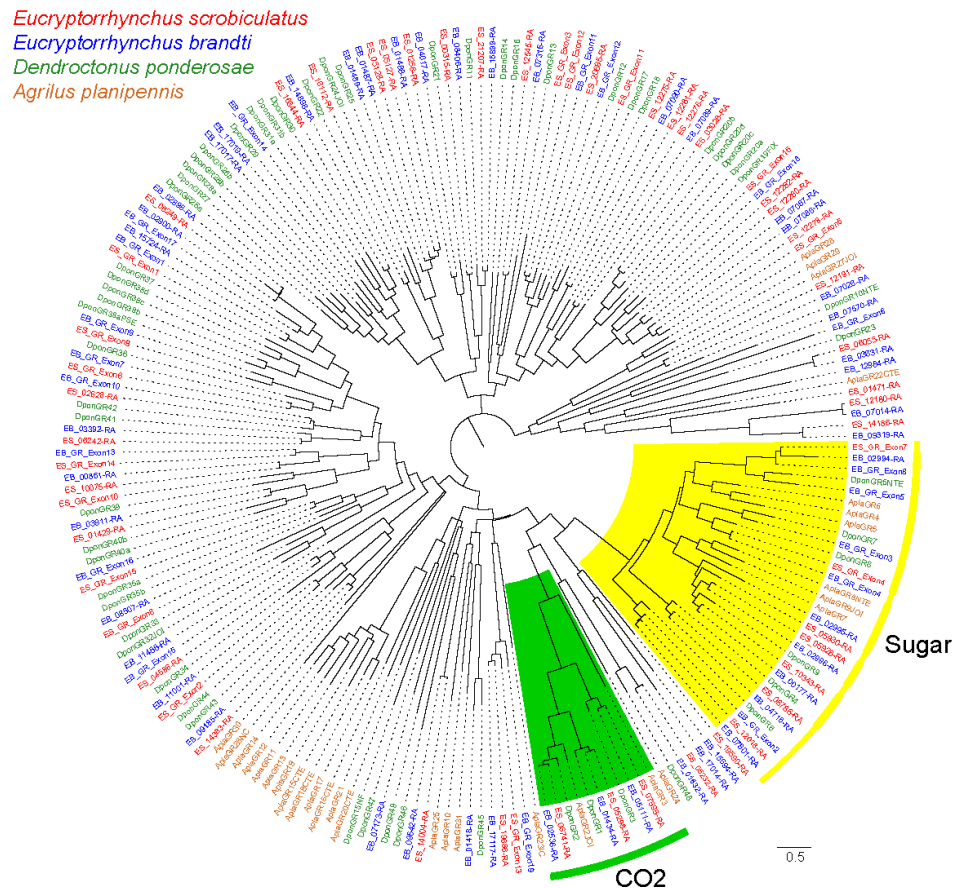


Fig. S14 Phylogenetic tree of the gustatory receptor (GRs) family. The receptor sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *Eucryptorrhynchus brandti* (EB, blue), *Dendroctonus ponderosae* (Dpon, green) and *Agrilus planipennis* (Apla, orange). The tree is constructed using Neighbor-Joining method in MEGA 7 and unrooted. The GRs from trunk weevil and root weevil were phylogenetically analyzed together with the DponOR and AplaOR, showing that the three conserved GRs for carbon dioxide (GR1–3) (green part) are all present, except for GR1 of Apla, in the four species genome and all single-copied. Both trunk weevil and root weevil have six GRs (GR4–9) (yellow part) grouped within the clade of conserved sugar receptors. Three GR groups (GR4, GR8 and GR9) were single-copied, while GR5 and GR7 were lost in root weevil genome. The other sugar receptors genes could not clearly placed into any subfamilies of GRs; most of the remaining GRs (putative bitter-taste GRs) of all four species were uniformly distributed in the branches and have no species-specific gene expansion found. Sources of sequence data and explanation of receptor classification are detailed in the Methods and Results section.

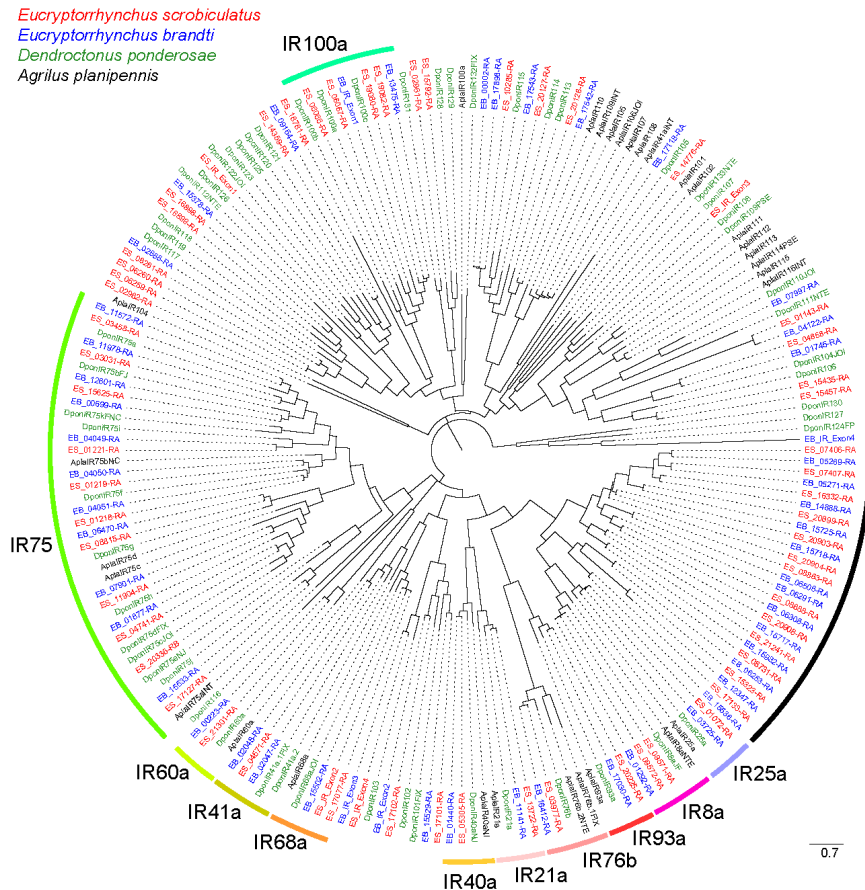


Fig. S15 Phylogenetic tree of the Ionotropic receptors (IRs) family. The receptor sequences included were from *Eucryptorrhynchus scrobiculatus* (ES, red), *E. brandti* (EB, blue), *Dendroctonus ponderosae* (Dpon, green) and *Agrilus planipennis* (Apla, black). The tree is constructed using Maximum-Likelihood method in MEGA7 and unrooted. The conserved antennal IR25a, IR8a, IR93a, IR76b, IR21a, IR40a, IR68a, and IR41a were identified in trunk weevil and root weevil. Eleven IRs fell within the IR75 clade were annotated for both root weevil and root weevil, representing the largest number of this clade reported from a beetle genome. The black arcs indicate a species-specific expansion of the two Curculionidae weevils in the IRs gene family. Sources of sequence data and explanation of receptor classification are detailed in the Methods and Results section.

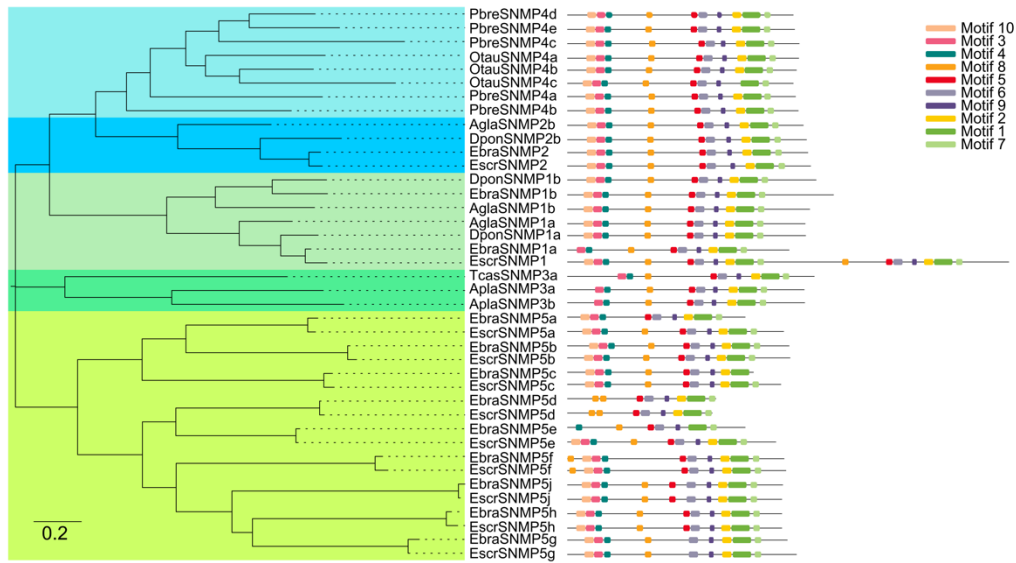


Fig. S16 Phylogenetic tree of the Sensory neuron membrane proteins (SNMPs) family among Coleoptera. There was a novel subfamily SNMP5 expanded in the root weevil and the trunk weevil. The two weevils' genes were displayed in pair except for the SNMP1, two SNMP1 genes were found in the trunk weevil genome, while only one with a doubled domain in root weevil genome.

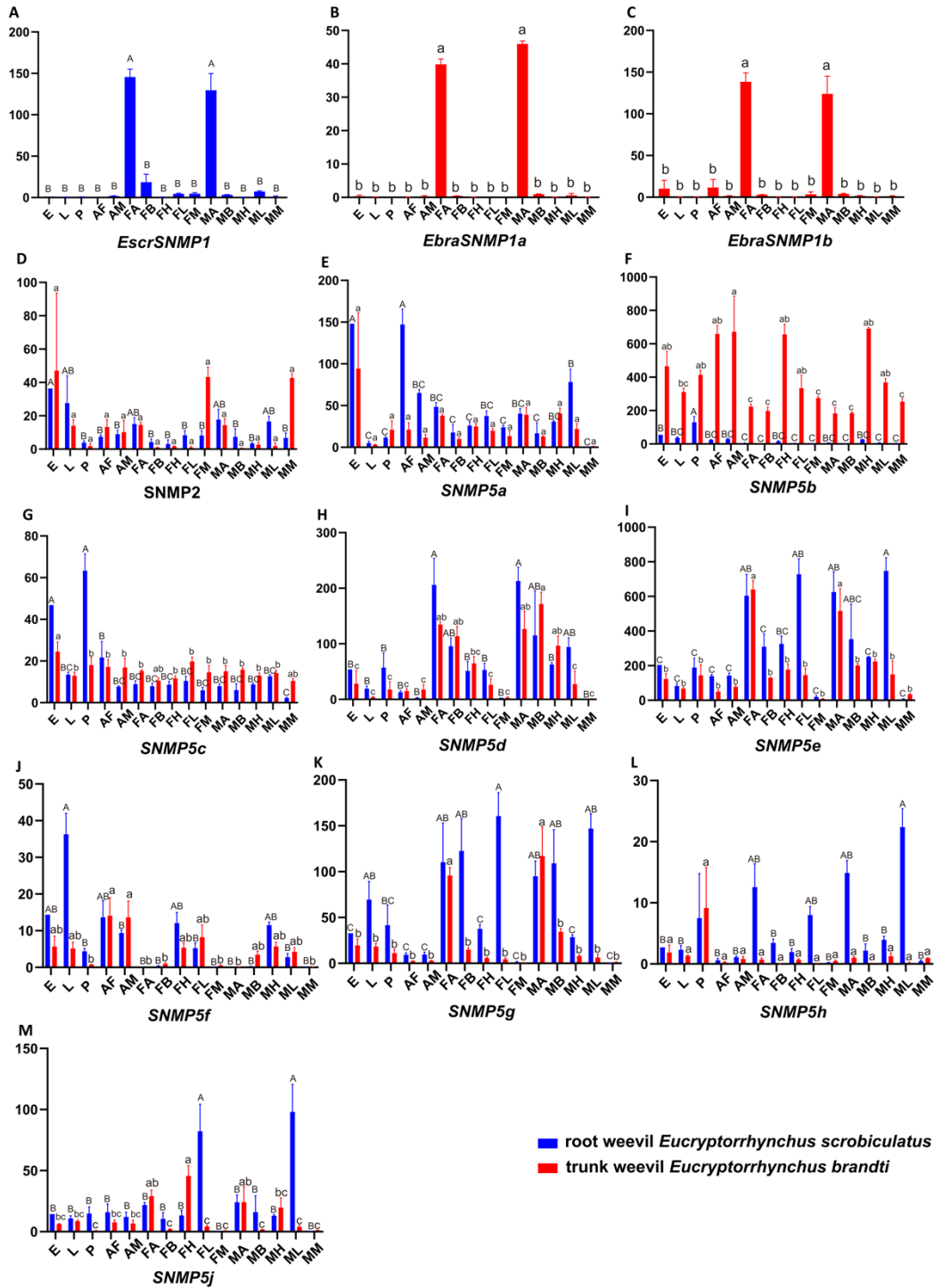


Fig. S17 Expression levels of *Eucryptorrhynchus brandti* and *E. scrobiculatus* SNMP family genes in fifteen samples based on transcriptome. A histogram represents one gene of the SNMP family. X-axes represent five development stages and ten adult tissues. Y-axes represent expression levels of the corresponding gene. E: egg; L: larva; P: pupa; AF: adult female; AM: adult male; FA: female antenna; FB: female beak; FH: female head; FL: female leg; FM: female midgut; MA: male antenna; MB: male beak; MH: male head; ML: male leg; MM: male midgut.

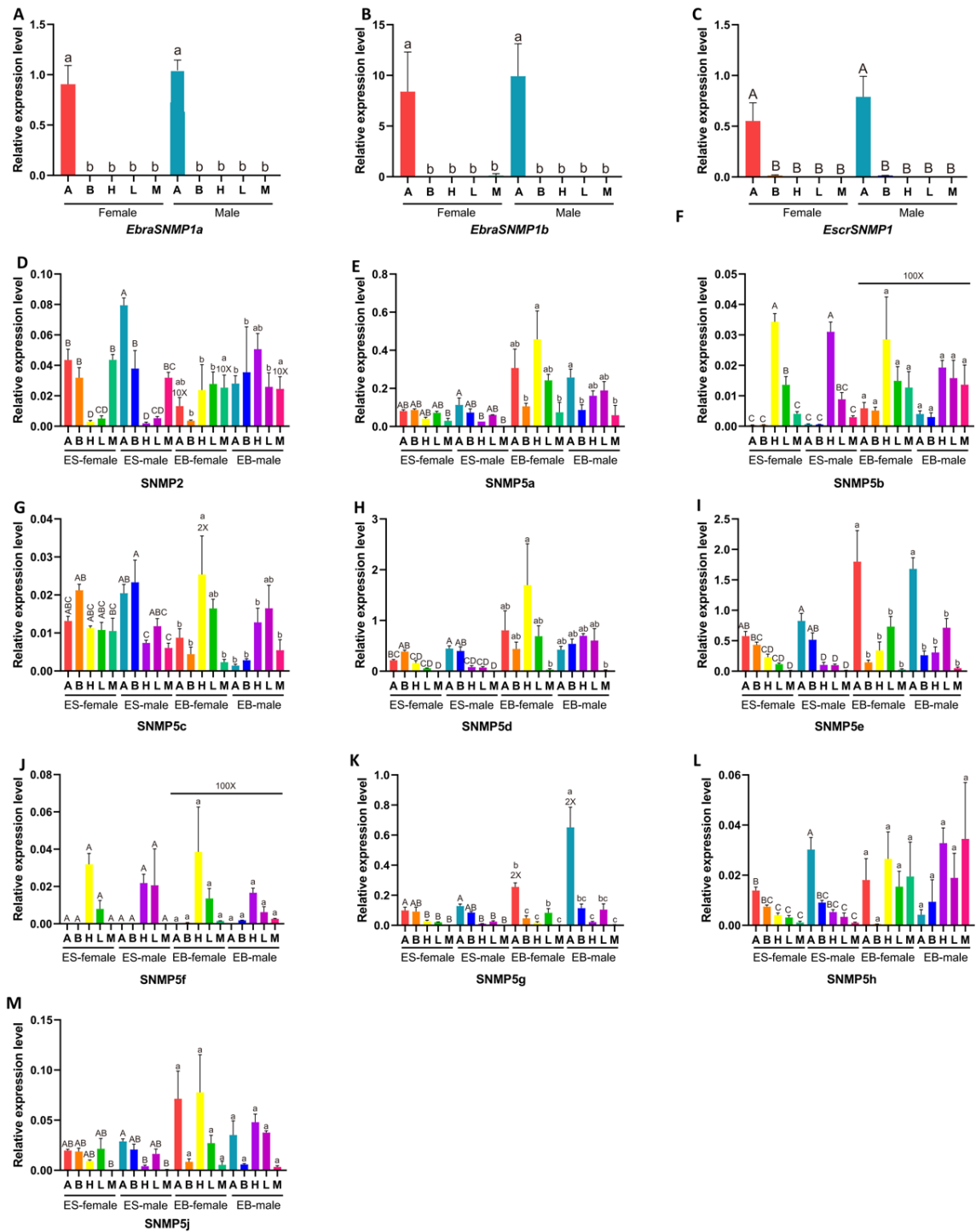


Fig. S18 Expression levels of *Eucryptorrhynchus brandti* and *E. scrobiculatus* SNMP family genes in fifteen samples based on qPCR. The columns in different colors represent different tissues in this study. A: antenna; B: beak; H: head (remove antenna and beak); L: leg; M: midgut.