Table S1. New and reduced secondary metabolites in the comparison group SD3 vs. CP

Index	Compounds	Class I	Class II	Formula	Level	CAS	SD3a	SD3b	SD3c	CPa	CPb	CPc
3,4-Dihydroxybenzoic Acid Ethyl Ester (Protocatechuic acid ethyl ester)												
nmw01160		Phenolic acids	Phenolic acids	C9H10O4	3	3943-89-3	1.02E+04	2.47E+04	1.46E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmat6298	3-Hydroxypyridine	Alkaloids	Pyridine alkaloids	C5H5NO	3	109-00-2	4.35E+05	6.76E+05	4.07E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Limn003111	1-O-β-Coumaroyl-β-D-glucose*	Phenolic acids	Phenolic acids	C15H18O8	2	7139-64-2	3.33E+04	9.11E+04	5.41E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmp0031973	Syringaldehyde, 4-[1-hydroxy-2-[2-(4-hydroxyphenyl)ethyl]ethoxy]-	Alkaloids	Phenylamines	C19H23NO5	2	94-07-5	2.32E+04	4.35E+04	2.58E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
ML01179402	4-Aminoacrylic acid	Phenolic acids	Phenolic acids	C7H7NO3	3	65-49-6	4.93E+04	5.45E+04	5.32E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MWSH1201668	Methyl cumulate	Phenolic acids	Phenolic acids	C10H10O4	3	6011-41-3	1.57E+05	2.52E+05	1.43E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
1,10-dimethoxy-6-demethyl-2,9-dioxo-2,9-dihydropyran-2-yloxy)-5,6,6a,7,8,9,10,10a-octahydro-6,9-epoxybenzo[b]oxepin-3-yl ester												
Wbmp006077		Alkaloids	Alkaloids	C26H36NO4+	3		1.49E+05	2.26E+05	3.77E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmw01444	3-Acetylpyridine	Alkaloids	Pyridine alkaloids	C7H7NO	3	570-23-0	1.79E+05	1.52E+05	2.04E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Hmdb0000626	Folpropanone A	Alkaloids	Alkaloids	C9H11NO2	3		1.51E+06	1.31E+06	1.63E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmw01588	2,4-Dihydroxybenzoic acid	Phenolic acids	Phenolic acids	C7H6O4	3	89-86-1	1.60E+06	1.41E+06	1.62E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmb2795	4-Methoxycinnamic acid	Phenolic acids	Phenolic acids	C10H10O3	3	830-09-1	7.40E+04	5.57E+04	7.67E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmn01394	2,3,5,4'-Tetrahydroxystilbene-2-O-glucoside	Others	Stilbene	C20H22O9	3	82373-94-2	1.21E+04	4.62E+04	1.68E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
2Hp397704	deruxtecan	Quinones	PhenAnthrazines	C15H10O4	3		1.79E+05	1.49E+05	1.42E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wbc0056513	1,2-dihydro-1-oxo-β-carboline	Alkaloids	Alkaloids	C11H9N2O	3		7.59E+05	4.61E+05	6.35E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Limn003151	4-coumaroyl	Phenolic acids	Phenolic acids	C9H7O2	3	121745-12-7	1.79E+05	1.74E+05	1.90E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW2mer1339	2-Methoxycinnamic acid	Phenolic acids	Phenolic acids	C10H10O3	3	6099-03-2	5.59E+04	7.01E+04	6.30E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmw01183	3,4-Dihydroxybenzeneacetic acid (Protocatechuic acid-3*)	Phenolic acids	Phenolic acids	C8H8O4	3	99-50-3	1.94E+04	1.92E+04	1.91E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wbda004126	Javanacoside C	Terpenoids	Diterpenoids	C26H36O11	3		4.38E+04	4.66E+04	6.62E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Hmdb0000437	Ellagenol C	Terpenoids	Monoterpenoids	C17H16O11	3	36151-82-7	1.36E+04	2.13E+04	5.47E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmw01064	Quercetin	Flavonoids	Isoflavones	C15H10O7	3	40246-10-4	9.91E+04	1.25E+05	8.03E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
2-(3-β-D-glucopyranosyloxy-4-hydroxyphenyl)ethanol-1-O-β-D-glucopyranoside												
Jnnwn002057		Phenolic acids	Phenolic acids	C20H30O13	3		3.43E+05	3.73E+05	5.15E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmse3200	1-Methylguanidine	Alkaloids	Alkaloids	C2H7N3	3	471-29-4	1.51E+05	1.12E+05	1.33E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmpg001670	Salicin	Phenolic acids	Phenolic acids	C13H18O7	3	69-27-2	2.47E+05	3.44E+05	4.66E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmpg003569	(R)-Mandelamide	Alkaloids	Alkaloids	C8H9NO2	3	24003-62-6	1.17E+05	1.23E+05	1.39E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wbc0040275	Luxamune oxide	Others	Others	C14H13NO	3	1643-20-5	2.88E+04	2.69E+04	3.92E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
1-(4'-Hydroxy-3'-methoxyphenyl)-2-[4''-(3-hydroxypropyl)-2',6''-dimethoxyphenoxy]-propane-1,3-Diol												
Wcha005575		Others	Others	C21H28O8	3		9.91E+04	9.29E+04	1.57E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmse0428	3,4,5-Trimethoxycinnamic acid	Phenolic acids	Phenolic acids	C12H14O5	3	90-50-6	1.44E+04	1.06E+04	2.17E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW2H70163	Aromadendrin (Dihydrokaempferol)	Flavonoids	Flavanonols	C15H12O6	3	480-20-6	1.50E+04	1.37E+04	1.85E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmb3056	Homovanillylglycine	Phenolic acids	Phenolic acids	C11H13NO4	3		3.29E+04	3.79E+04	7.64E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmds005852	Gramenone A	Lignans and Coumarins	Lignans	C20H20O7	3	161497-72-3	2.91E+04	2.19E+04	3.77E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wbmp011422	5,8-Epidoxyergosta-6,22-dien-3-ol (Ergosterol peroxide)	Steroids	Sterol	C28H44O3	2	2061-64-5	1.85E+04	4.84E+04	2.55E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
1-(3-hydroxyphenyl)-N,N,3-tris[4-hydroxyphenethyl)-(5-(1-dimethyl-2,3-dihydroxyphenethyl)-2,3-dicarbonamide												
pmp001187		Alkaloids	Phenolamines	C36H36N2O6	1		4.25E+04	2.29E+04	4.37E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW01139	Ethylparaben	Phenolic acids	Phenolic acids	C9H10O3	3	120-47-8	2.60E+04	1.55E+04	2.45E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnn004685	Nectandrin B	Lignans and Coumarins	Lignans	C20H24O5	2	74683-16-2	1.63E+04	3.58E+04	2.23E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Sleg000054	3,5-Dimethoxy-4-hydroxycinnamaldehyde	Others	Aldehydic compounds	C11H12O4	3	51-41-2	7.72E+04	5.68E+04	8.38E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmn01399	2,4,6,4'-Tetrahydroxy-stilbene-2-O-glucoside	Others	Stilbene	C20H22O9	3		2.14E+04	2.40E+04	2.50E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Znmp002356	3-Hydroxymorphinan	Phenolic acids	Phenolic acids	C7H8O2	3	620-24-6	7.57E+04	9.11E+04	9.47E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmp000601	Aurantio-obtusin-6-O-glucoside	Quinones	Anthraquinone	C28H32O14	3	129925-96-2	2.32E+05	2.24E+05	2.47E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Xmnn0004568	Mutagiosuide F	Terpenoids	Monoterpenoids	C16H24O8	3		2.66E+04	3.17E+04	6.03E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW2kf6188	8-O-Acetylshanzhiside	Terpenoids	Monoterpenoids	C17H26O11	3	6926-14-3	1.20E+04	9.88E+03	1.47E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wcp008839	5-methylbutiral	Others	Others	C6H6O2	2	620-02-0	4.17E+05	3.19E+05	4.49E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmb4797	4-Hydroxy-7-methoxycoumarin-8-diamonoside	Lignans and Coumarins	Coumarins	C11H10O5	3		1.76E+03	1.10E+04	5.57E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Znmp000758	1-(Hydroxymethyl)tetrahydro-1h-pyrrolizin-2-ol	Alkaloids	Pyrrole alkaloids	C8H15NO2	2		1.68E+07	1.81E+07	1.49E+07	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmwp110273	(3S)-Fraxidiol	Lignans and Coumarins	Coumarins	C14H16O5	2		2.26E+04	5.91E+04	6.95E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wcha005594	4-hydroxy-2,4-pyridinedicarboxylic acid	Alkaloids	Pyridine alkaloids	C7H5NO5	3		1.21E+04	2.04E+04	2.42E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
NR10253223	2-Amino-3-methoxybenzoic acid	Phenolic acids	Phenolic acids	C8H9NO3	3	3177-80-8	3.09E+05	2.70E+05	3.00E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmw01026	Pyrocatechol	Phenolic acids	Phenolic acids	C6H6O2	3	87-66-1	4.40E+05	3.68E+05	4.15E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnn002288	1-O-Caffeoyl-(4-O-glucosyl)-β-D-glucose	Phenolic acids	Phenolic acids	C21H28O14	3	20316-62-5	2.03E+05	2.27E+05	1.46E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW5206	4-Hydroxyphenylacetic Acid	Phenolic acids	Phenolic acids	C9H10O4	3	306-23-0	3.29E+04	3.06E+04	4.02E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Znmp003001	3,4-Dimethoxybenzoic acid, 2-Veratric acid	Phenolic acids	Phenolic acids	C9H10O4	3	93-07-2	2.28E+04	1.81E+04	2.62E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Spiro5'-ene-3,3'7'-tri-O-methyl-2'-oxo-1'-oxaspiro[cyclohexane-4,4'-cyclopenta[c]pyran]-6-ol												
Hmdb0034403	(Neoisothiocaside D)*	Steroids	Steroidal saponin	C45H72O18	2	2.29E+05	4.95E+05	4.53E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
3,17-epoxy-1,22-dioxo-spirost-5-en-3-yl-O-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranosyl-(1→4)-β-D-galactopyranoside (Neosolaniocaside D)*				C45H72O18	2	880152-67-0	2.29E+05	4.95E+05	4.53E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnn011818	lactone (Sensilactone)	Terpenoids	Triterpene	C30H44O4	3	366450-66-6	2.98E+04	2.44E+04	3.20E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Znmp005324	Dihydrodehydrodiconiferyl alcohol	Lignans and Coumarins	Lignans	C20H24O6	3	126253-61-8	1.18E+04	2.18E+04	2.44E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmdp002153	N-p-Coumaroyltryptophyranose	Alkaloids	Phenolamine	C31H31N3O10	3		9.34E+04	1.43E+05	7.70E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
mgp112328	Pyridine-4-thiocarboxylic acid	Others	Others	C6H5NOS	3		1.77E+05	2.23E+05	2.31E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wcp006751	Flumbagin, 5-Hydroxy-2-Methyl-1,4-Naphthoquinone	Quinones	Quinones	C11H8O3	3	481-42-5	2.17E+04	2.23E+04	5.12E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW2mer355	Methyl Syringate	Phenolic acids	Phenolic acids	C10H12O5	3	884-35-5	2.42E+04	1.55E+04	1.87E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp110110	Pyranoidin F(pin-01)	Others	Others	C22H24O7	3		2.67E+04	2.87E+04	2.27E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
N-(4-hydroxyphenyl)-2-(2-aminoacyl-4-((E)-2-(4-hydroxybenzylidene)-6-carboxy)ethenyl)phenoxy)-2-[(2)-2-(2-methoxy-4-((E)-2-(4-hydroxyphenylidene)-6-carboxy)ethenyl)phenoxy)-2-(4-hydroxybenzylidene)-3-carboxamide												
Wbp006749		Alkaloids	Alkaloids	C54H53N3O12	2		1.31E+04	1.02E+04	7.72E+03	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmw01098	Indole-2-carboxylic acid	Alkaloids	Pharmarane	C9H7NO2	3	1477-50-5	7.01E+04	6.84E+04	6.71E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wbda005691	3-(4-methoxy-9H-pyrido[3,4-b]indol-1-yl)propanoic acid	Alkaloids	Alkaloids	C15H14N2O3	3		6.18E+05	6.37E+05	7.49E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Ymcp002388	4-O-Methylsinapoylcholine	Alkaloids	Alkaloids	C16H23NO5	2	4579-60-4	7.60E+04	1.31E+05	1.14E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW01154	4-aminophenol	Alkaloids	Phenolamine	C6H7NO	3	123-30-8	5.62E+04	4.62E+04	8.66E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW3tz201	β-Carboline-1-propionic acid	Alkaloids	Pharmarane	C14H12N2O2	3	89915-39-9	4.90E+05	3.91E+05	3.24E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Cmpb002794	Folicanthine	Alkaloids	Alkaloids	C21H30N4	3	6879-55-6	2.12E+05	2.57E+05	1.93E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmb0752	3-O-Feruloylquinic acid*	Phenolic acids	Phenolic acids	C17H20O9	3	1899-29-2	1.36E+06	1.26E+06	2.33E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmw01055	Terpinolene	Terpenoids	Monoterpenoids	C10H16	3	586-62-9	1.61E+05	1.16E+05	3.42E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmn01311	6-Hydroxykaempferol-7,6-O-Diglucoside	Flavonoids	Flavonols	C27H30O17	3	1.00E+07	1.53E+07	7.14E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW2mer713	3-(4-Hydroxyphenyl)-1-propanol	Phenolic acids	Phenolic acids	C9H12O2	3	10210-17-0	1.89E+04	1.18E+04	2.19E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
5-formyl-4,7-dihydroxy-1,6-dimethoxy-9,10-dihydrophenanthrene-2-carboxylic acid												
Sdd000819		Diterpenoids	Diterpenoids	C17H16O3	2	-	8.45E+04	6.18E+04	1.01E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Cmpb004621	Machilin H(1C3)	Lignans and Coumarins	Lignans	C21H26O6	2	-	7.12E+05	2.83E+05	4.09E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Znmp003044	7-Hydroxycoumarin,Umbelliferone	Lignans and Coumarins	Coumarins	C9H6O3	3	93-35-6	9.83E+03	7.29E+03	8.09E+03	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wafn003423	Isoquercitrin	Phenolic acids	Phenolic acids	C21H20O12	3	-	5.91E+04	5.56E+04	6.03E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Cmcp002990	Lochrovidine	Alkaloids	Alkaloids	C22H26N2O6	3	1359-09-7	7.79E+05	7.72E+05	1.59E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
Hmdb0011288	Methyl 2,4-dihydroxyphenylacetate	Phenolic acids	Phenolic acids	C9H10O4	3	67828-42-6	3.88E+04	2.45E+04	4.59E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wbmp004939	3-Demethoxyubiquinol	Alkaloids	Pharmarane	C19H22O4N2	3		1.61E+05	1.45E+05	1.44E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW1133785	4'-Methoxyflavone	Flavonoids	Flavones	C16H12O3	3	4143-74-2	5.47E+03	3.91E+03	6.97E+03	**0.00E+00**	**0.00E+00**	**0.00E+00**
Smilp002161	4-ethylcatechol	Alkaloids	Phenylamines	C9H13NO2	3		1.44E+04	1.03E+04	1.84E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
4'-(Trans)-acetal-3,6,8-trihydroxy-3-methyl-dihydronaphtalene-1-one												
Lmp004059		Others	Chromone	C11H10O5	2	-	1.49E+05	1.79E+05	2.31E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmpb005841		Others	Chromone	C11H10O4	2	-	1.64E+05	2.28E+05	3.09E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Ymnn000116		Phenolic acids	Phenolic acids	C14H18O8	2	10338-88-2	1.13E+05	1.72E+05	2.68E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
HJAP041		Phenolic acids	Phenolic acids	C14H18O8	2	-	1.15E+04	4.69E+04	5.35E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmr1014		Phenolic acids	Phenolic acids	C10H8O5	2	-	1.88E+05	4.43E+05	1.38E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Fraxetin (7,8-Dihydroxy-6-methoxycoumarin)												
11R,14S,19R,20R,21S,24R)-7-ethyl-3,3,4,9,19,20,21,24-octamethyl-2,6,8,10,13,18,23-heptaoxo-1,4,4a,7-tetrahydro-2,3,4,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25-icosahydro-11,14-epoxybenzo[b]cyclohepta[g]pyrido[2,3-k][1,4,7,10,13,16,19]heptaoxacyclohenicosine-20-carboxylic acid												
Lmnn002603	Lignans and Coumarins	Coumarins	C10H8O5	2	-	1.53E+05	2.02E+05	3.36E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Hmdb0001179	Lanosterol-3-O-α-glucoside*	Terpenoids	Triterpene	C36H60O7	3	-	2.84E+05	2.45E+05	3.43E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Ldlp111278	Corypanstanine A	Alkaloids	Alkaloids	C16H16N2O5	2	-	1.42E+05	6.23E+04	1.38E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmb3661	7-Hydroxycoumarin-6-Oxanoside	Lignans and Coumarins	Coumarins	C15H16O7	3	-	4.44E+04	5.12E+04	5.95E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp002933	Piloine	Alkaloids	Alkaloids	C16H11N2O3	2	13640-28-5	5.31E+05	4.05E+05	4.54E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW05739	Dunnyxanthon	Alkaloids	Other Flavonoids	C18H9O4	2	-	3.86E+04	6.12E+04	5.29E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmn01505	Oleanolic acid-3-O-[xylosyl-(1→2)-glucosyl-(1→2)]-arabinoside	Terpenoids	Triterpene Saponin	C46H74O16	3	-	1.17E+04	1.19E+04	1.81E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Cmnn004016	Dihydrorunanin	Phenolic acids	Chalcones	C12H14O11	3	-	3.23E+03	7.62E+03	1.96E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmr1019	Gossypitrin acid	Terpenoids	Monoterpenoids	C10H12O3	3	27741-01-1	9.34E+04	1.22E+05	5.14E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp002942	Apigenin-6,8-di-C-arabinoside*	Flavonoids	Flavones	C25H26O13	3	-	1.45E+06	9.47E+05	1.69E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
Znmb003227	4-O-Glucosyl-sinapate	Phenolic acids	Phenolic acids	C17H22O10	3	-	4.16E+04	4.69E+04	6.49E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp003442	Aureusin	Flavonoids	Flavonols	C21H20O11	3	-	1.99E+04	1.23E+05	1.26E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmp004442	3,4-Dihydro-4-(4'-hydroxyphenyl)-5,7-dihydroxycoumarin	Lignans and Coumarins	Coumarins	C15H12O5	3	-	3.54E+03	7.33E+03	9.16E+03	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp002434	Apigenin-6-C-(2''-glucuronide)-glucoside	Flavonoids	Flavones	C26H28O18	3	-	4.29E+05	4.39E+05	6.35E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW5H120155	1-ketopuerarin	Lignans and Coumarins	Lignans	C21H20O7	3	66288-89-9	2.34E+04	1.24E+04	1.34E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Yamp002097	1-[2-(Furan-2-yl)-2-methyltetrahydrofuran-3-yl]-2-methylpropane-1,2-diol	Alkaloids	Alkaloids	C13H18NO3	2	-	4.08E+05	5.12E+05	5.06E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmr01028	9-Fluorenanthrone	Alkaloids	Alkaloids	C15H9NO2	2	59-49-4	8.38E+04	1.87E+05	8.05E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
(5-8)-Hydroxy-1-hydroxymethyl-3-methoxycarbonyl-N1,N3-bis(4-hydroxyphenethyl)-(5-1)-dimethoxy-1,2-dihydronaphthalene-2,3-dicarboxamide												
pmn01189		Alkaloids	Phenolamine	C38H40N2O10	2	-	7.64E+03	5.89E+03	8.54E+03	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW2mer632	Vasalin acetate	Alkaloids	Alkaloids	C10H10O4	3	881-68-5	8.60E+03	5.52E+03	1.31E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW03020	N-Acetylcadaverine	Alkaloids	Alkaloids	C7H16N2O	3	32343-75-8	2.68E+05	2.56E+05	2.54E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnb001501	Gardoside*	Terpenoids	Monoterpenoids	C16H22O10	3	54835-76-6	2.69E+04	2.94E+04	5.36E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
3-Hydroxy-3-(6-methyl-2-pyridinyl)-methyl]-5-methoxyindolone-2-one												
Wbp003603		Alkaloids	Alkaloids	C14H16N2O2	2	-	4.47E+05	3.83E+05	5.03E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp002832	Apigenin-6-C-arabinoside-8-C-xyloside*	Flavonoids	Flavones	C25H26O13	3	-	1.18E+06	9.15E+05	2.03E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
Hmdb0031950	2'-O-Glucosyl-3',4'-dimethoxyflavonol	Flavonoids	Other Flavonoids	C29H36O16	3	52250-35-3	1.98E+07	1.09E+07	1.84E+07	**0.00E+00**	**0.00E+00**	**0.00E+00**
pmb3074	5-O-Caffeoylquinic acid	Phenolic acids	Phenolic acids	C16H18O9	3	1899-30-5	6.09E+04	9.72E+04	1.72E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
nmr1429	Vomifoliol (Blumenol A)	Terpenoids	Monoterpenoids	C13H20O2	3	109351-15-5	9.34E+03	6.19E+03	8.36E+03	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW02011	2-Methoxy-1,4-naphthalenedione (2-methoxy-1,4-naphthoquinone; methyl ether)	Quinones	Quinones	C11H8O3	3	2348-82-5	2.20E+04	1.51E+04	1.86E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Wcb003984	1,4,8-Trihydroxynaphthalene-1-O-glucoside	Quinones	Naphthol	C16H18O8	3	39015-63-9	3.84E+04	3.51E+04	1.54E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Zgcp100331	mangiferin-2G-Glc	Steroids	Steroidal saponin	C45H72O19	3		5.48E+04	3.18E+05	1.24E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lhdp110832	Paraserotenpalline	Terpenoids	Seroquetrenoids	C18H22O	3	6750-13-6	5.36E+04	4.79E+04	7.26E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp004855	Tricin (5,7,4'-Trihydroxy-3',5'-dimethoxyflavone)	Flavonoids	Flavones	C17H14O7	3	520-32-1	3.75E+04	4.13E+04	4.13E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp122302	Dehydrocrepenynylacetonide	Terpenoids	Seroquetrenoids	C17H22O7	3	-	7.41E+04	6.56E+04	6.04E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Zmdp110730	6-Hydroxykaempferol-3,6-O-Diglucoside*	Flavonoids	Flavonols	C27H30O17	3	-	1.05E+05	1.49E+05	6.35E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Hmdb0031628	Lanosterol-3,17,21-triol-3-O-α-glucoside	Terpenoids	Triterpene	C36H62O8	3	-	2.99E+05	2.95E+05	4.01E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW03149	3-Methoxybenzoic acid	Phenolic acids	Phenolic acids	C8H8O3	3	586-38-9	5.47E+03	5.08E+03	3.20E+03	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW02094	Cimaroside A	Steroids	Sterol	C39H62O	3	140-10-3	7.66E+04	6.34E+04	1.06E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp003558	3,4,5-Trimethoxycinnamoyl-1-O-β-D-glucoside	Phenolic acids	Phenolic acids	C18H22O9	3	-	1.75E+05	2.59E+05	3.25E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnn004665	Triacanthinagoside*	Alkaloids	Alkaloids	C15H21N5O4	3	-	3.27E+04	4.63E+04	5.76E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
3-[(3,4-dihydroxyphenyl)methoxy]-5,7-dihydroxy-6-methoxy-2h-1-benzopyran-4-one glucoside												
Lmpb006064		Flavonoids	Other Flavonoids	C22H24O13	3	-	1.52E+06	1.12E+06	3.37E+06	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmpb005645		Flavonoids	Flavonols	C21H20O13	3	33429-83-3	6.37E+04	1.32E+05	1.47E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp005753	5,3'-dihydroxy-6,7,4'-trimethoxyflavone-3-O-β-D-glucoside	Flavonoids	Flavones	C23H24O12	3	-	1.24E+05	2.32E+05	4.75E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**
Smnp003454	Alion B	Quinones	Anthraquinone	C21H22O9	3	28371-16-6	1.92E+04	1.42E+04	3.52E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
MW03470057	Biacalin	Flavonoids	Flavones	C21H18O11	3	21967-41-9	3.08E+04	3.52E+04	2.35E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Hmdb0001194	N-Cis-Feruloyl-5-O-methyldopamine*	Phenolic acids	Phenolic acids	C19H21NO5	3	-	2.10E+04	1.94E+04	2.46E+04	**0.00E+00**	**0.00E+00**	**0.00E+00**
Lmnp002642	Apigenin-8-C-(2''-glucuronide)-glucoside	Flavonoids	Flavones	C26H28O18	3	-	4.70E+05	4.63E+05	7.70E+05	**0.00E+00**	**0.00E+00**	**0.00E+00**