

Table S6: List of differential non-volatile compounds between RC-R vs. RC-L

Number	Class	Subclass	Compounds	Biomarkers	Fold change	P-value	VIP	Type
1	Flavonoids	Quercetin and derivatives	Quercetin 3-beta-D-sophoroside	Yes	1.07E+05	3.95E-05	1.04E+00	up
2			Azaleatin (5-O-Methylquercetin)	Yes	4.60E+04	4.95E-04	1.03E+00	up
3			Quercetin-3-O-(2"-O-galactosyl)glucoside	Yes	3.34E+04	2.47E-04	1.04E+00	up
4			Quercetin-7-O-glucoside	Yes	1.83E+04	4.43E-04	1.03E+00	up
5			Isorhamnetin-3-O-rutinoside (Narcissin)	Yes	1.11E+04	4.90E-06	1.04E+00	up
6			Rhamnetin-3-O-Rutinoside	Yes	1.10E+04	9.32E-07	1.04E+00	up
7			Quercetin-3-O-(2"-O-Rhamnosyl)rutinoside		1.70E+02	5.33E-08	1.04E+00	up
8			Quercetin-3-O-robinobioside		3.52E+01	7.15E-07	1.04E+00	up
9			Quercetin-3-O-glucosyl(1→4)rhamnoside-7-O-rutinoside		3.37E+01	1.06E-07	1.04E+00	up
10			Quercetin-3-O-rutinoside-7-O-glucoside		1.42E+01	3.28E-06	1.04E+00	up
11			Quercetin-3-O-neohesperidoside		1.02E+01	1.41E-04	1.04E+00	up
12			Quercetin-3-O-(2"-O-rhamnosyl)galactoside		9.70E+00	2.96E-05	1.04E+00	up
13			Quercetin-3',4'-dimethyl ether		3.42E+00	1.02E-03	1.03E+00	up
14			Quercetin-7-O-rutinoside		9.29E-02	7.35E-07	1.04E+00	down
15			Quercetin-3-O-(2"-O-glucosyl)glucuronide		9.02E-02	7.61E-06	1.04E+00	down
16			Quercetin-3-O-rutinoside (Rutin)		4.90E-02	2.70E-05	1.04E+00	down
17			Quercetin-3-O-xyloside (Reynoutrin)		3.29E-02	5.47E-07	1.04E+00	down
18			Quercetin		2.26E-02	7.40E-08	1.04E+00	down
19			Quercetin-3-O-glucoside (Isoquercitrin)		1.90E-02	2.34E-07	1.04E+00	down
20			Quercetin-3-O-(6"-galloyl)galactoside		9.96E-03	2.62E-05	1.04E+00	down
21			Quercetin-3-O-sophoroside (Baimaside)		4.38E-03	2.10E-07	1.04E+00	down
22			Quercetin-3-O-apiosyl(1→2)galactoside		8.91E-04	1.19E-05	1.04E+00	down
23			Quercetin-3-O-xylosyl(1→2)glucoside		7.67E-04	6.80E-06	1.04E+00	down
24			Quercetin-3-O-(6"-O-arabinosyl)glucoside		5.34E-04	3.20E-08	1.04E+00	down
25			Rhamnetin (7-O-Methyl Quercetin)	Yes	6.07E-04	6.21E-04	1.02E+00	down
26			Quercetin-3-O-sophorotrioside-7-O-arabinoside	Yes	3.21E-06	1.99E-06	1.04E+00	down
27			Quercetin-3-O-xylosyl(1→2)glucosyl(1→2)glucoside	Yes	9.80E-07	2.29E-07	1.04E+00	down
28		Kaempferol and derivatives	6-Hydroxykaempferol-3-O-rutinoside-6-O-glucoside	Yes	1.58E+04	4.93E-06	1.04E+00	up
29			Kaempferol-3-O-robinoside-7-O-rhamnoside (Robinin)		5.31E+01	9.97E-05	1.04E+00	up
30			Kaempferol-3-O-rhamnoside (Afzelin)(Kaempferin)		1.08E+01	8.18E-07	1.04E+00	up
31			6-C-MethylKaempferol-3-glucoside		7.93E+00	7.20E-04	1.03E+00	up
32			Dihydrokaempferol		6.68E+00	1.23E-05	1.04E+00	up
33			Rhamnocitrin (7-Methylkaempferol)		5.34E+00	7.60E-08	1.04E+00	up
34			Kaempferol-3-O-neohesperidoside		4.85E+00	3.91E-05	1.04E+00	up
35			Kaempferol-6,8-di-C-glucoside-7-O-glucoside		3.70E+00	1.70E-04	1.03E+00	up
36			8-Prenylkaempferol		2.91E-01	2.95E-03	1.02E+00	down
37			Dihydrokaempferol-7-O-glucoside		1.89E-01	2.98E-04	1.03E+00	down
38			Kaempferol-4'-O-glucoside		5.53E-02	4.10E-06	1.04E+00	down
39			6-Hydroxykaempferol-7-O-glucoside		4.89E-02	1.18E-03	1.02E+00	down
40			6-Hydroxykaempferol-3,6-O-Diglucoside		4.88E-03	5.30E-07	1.04E+00	down
41			Kaempferol-3-O-sambubioside		4.44E-03	1.15E-10	1.04E+00	down
42		Luteolin and derivatives	Luteolin-7-O-(2"-O-rhamnosyl)rutinoside		4.10E+01	1.91E-04	1.03E+00	up

43		Luteolin-7-O-neohesperidoside (Lonicerin)		2.37E+00	3.42E-06	1.04E+00	up
44		Luteolin-7-O-rutinoside		2.18E+00	1.15E-04	1.04E+00	up
45		Isoluteolin (Orobol)(5,7,3',4'-tetrahydroxyisoflavone)		4.68E-01	2.65E-05	1.04E+00	down
46		Luteolin-3'-O-glucoside		5.31E-02	1.44E-07	1.04E+00	down
47		Luteolin-7-O-glucoside (Cynaroside)		1.77E-02	5.65E-05	1.04E+00	down
48	Catechin and derivatives	Gallocatechin 3-O-gallate	Yes	1.71E+03	2.00E-04	1.03E+00	up
49		Epicatechin		3.79E+01	1.09E-09	1.04E+00	up
50		Catechin gallate		2.44E+01	1.02E-07	1.04E+00	up
51		Epicatechin gallate		2.24E+01	2.29E-06	1.04E+00	up
52		Procyanidin B2		1.61E+01	4.92E-05	1.04E+00	up
53		Procyanidin C1 3'-O-gallate		9.49E+00	5.67E-05	1.04E+00	up
54		Procyanidin B4		9.12E+00	1.33E-05	1.04E+00	up
55		Procyanidin B1		3.56E+00	2.37E-04	1.03E+00	up
56		Catechin		2.47E+00	1.73E-04	1.03E+00	up
57		(-)-Epicatechin-3-(3"-O-methyl)gallate		2.45E+00	2.57E-03	1.02E+00	up
58		Epigallocatechin		1.73E-01	5.04E-04	1.03E+00	down
59		Sexangularetin-3-O-glucoside-7-O-rhamnoside	Yes	1.09E+04	7.49E-07	1.04E+00	up
60		2'-Hydoxy,5-methoxyGenistein-O-rhamnosyl-glucoside	Yes	1.07E+04	2.78E-06	1.04E+00	up
61		Petunidin-3-O-(6"-O-p-Coumaroyl)glucoside	Yes	1.06E+04	1.42E-07	1.04E+00	up
62	Other flavonoids	Rhodiogidin		1.47E+01	2.09E-05	1.04E+00	up
63		Sachaloside IV		1.38E+01	1.55E-04	1.03E+00	up
64		Phloretin		1.20E+01	5.56E-08	1.04E+00	up
65		Rhodianidin		1.01E+01	8.10E-06	1.04E+00	up
66		Pinocembrin (Dihydrochrysin)		7.18E+00	2.19E-06	1.04E+00	up
67		Aromadendrin-7-O-glucoside		6.19E+00	4.37E-07	1.04E+00	up
68		6,7,8-Tetrahydroxy-5-methoxyflavone		5.69E+00	3.26E-06	1.04E+00	up
69		Hispidulin (5,7,4'-Trihydroxy-6-methoxyflavone)		5.45E+00	2.24E-06	1.04E+00	up
70		Rhodosin		4.22E+00	2.65E-06	1.04E+00	up
71		Hesperetin-7-O-rutinoside (Hesperidin)		4.02E+00	5.54E-05	1.04E+00	up
72		2,4,2',4'-tetrahydroxy-3'-prenylchalcone		3.94E+00	2.78E-04	1.03E+00	up
73		3',4',7-Trihydroxyflavone		3.32E+00	4.22E-03	1.01E+00	up
74		Naringenin chalcone		3.26E+00	6.55E-07	1.04E+00	up
75		Rhodiolin		3.17E+00	2.24E-06	1.04E+00	up
76		Naringenin (5,7,4'-Trihydroxyflavanone)		2.77E+00	8.33E-07	1.04E+00	up
77		Pinobanksin		2.71E+00	1.02E-05	1.04E+00	up
78		Phloretin-2'-O-glucoside (Phlorizin)		2.01E+00	1.48E-03	1.01E+00	up
79		Naringenin-7-O-glucoside (Prunin)		4.45E-01	1.26E-05	1.04E+00	down
80		Eriodictyol-7-O-glucoside		1.87E-01	6.28E-06	1.04E+00	down
81		Isosalipurposide (Phlorizin Chalcone)		1.31E-01	1.41E-06	1.04E+00	down
82		Rhodioglin		5.28E-02	4.60E-07	1.04E+00	down
83		Cyanidin-3-O-sophoroside-5-O-glucoside		4.13E-02	1.43E-05	1.04E+00	down
84		Herbacetin		2.85E-02	1.41E-03	1.02E+00	down
85		Spiraeoside		2.09E-02	8.88E-06	1.04E+00	down
86		Rhodioflavonoside		7.46E-03	1.03E-08	1.04E+00	down

87		Delphinidin-3-O-glucoside (Mirtillin)	Yes	1.44E-06	1.34E-05	1.04E+00	down
88		Methyl 6-O-galloyl-glucoside	Yes	2.11E+03	5.75E-05	1.04E+00	up
89		Ethyl gallate		2.98E+01	3.96E-07	1.04E+00	up
90		1-O-Galloyl-rhamnose		5.61E+00	1.62E-04	1.03E+00	up
91		2-O-Salicyl-6-O-Galloyl-D-Glucose		4.10E+00	3.12E-05	1.04E+00	up
92		2,3-Di-O-Galloyl-D-Glucose		4.02E+00	1.88E-03	1.01E+00	up
93		1,2,3-Tri-O-galloyl-D-glucose		3.91E+00	4.77E-06	1.04E+00	up
94		1,3,6-Tri-O-galloyl-D-glucose		3.79E+00	1.91E-04	1.04E+00	up
95		Monogalloyl-digluco		3.35E+00	9.84E-06	1.04E+00	up
96	Gallic acid derivatives	2,4,6-Tri-O-galloyl-D-glucose		2.50E+00	6.37E-05	1.04E+00	up
97		6-O-Galloyl-glucose		4.02E-01	2.99E-05	1.04E+00	down
98		Digallic Acid		3.90E-01	2.58E-05	1.04E+00	down
99		2,3-O-Digalloyl-1,4,6-tri-O-galloyl-glucose		2.47E-01	7.74E-06	1.04E+00	down
100		Galloyl Methyl gallate		2.20E-01	6.04E-06	1.04E+00	down
101		p-Dimeric galloyl methyl ester		1.85E-01	8.51E-06	1.04E+00	down
102		Di-O-galloyl Methyl gallate		1.00E-01	1.38E-06	1.04E+00	down
103		1,3-Trigallic acid		2.77E-02	1.17E-05	1.04E+00	down
104		1,4-Trigallic acid		2.61E-02	5.33E-05	1.04E+00	down
105		3-O-p-Coumaroylquinic acid	Yes	1.20E+03	1.33E-03	1.01E+00	up
106		2-Hydroxycinnamic acid		3.22E+01	7.05E-10	1.04E+00	up
107		p-Coumaryl alcohol		2.13E+01	1.63E-07	1.04E+00	up
108		p-Coumaric acid		1.13E+01	8.25E-07	1.04E+00	up
109		3,4-Dimethoxycinnamic acid		9.30E+00	2.34E-05	1.04E+00	up
110		p-Coumaroylquinic acid-4'-O-glucuronide		5.75E+00	7.72E-05	1.04E+00	up
111		3-O-p-Coumaroylquinic acid O-glucoside		5.41E+00	2.41E-04	1.04E+00	up
112	Cinnamic acid-Coumaroyl	p-Coumaraldehyde		2.96E+00	2.83E-05	1.04E+00	up
113	and derivatives	4-Methoxycinnamic acid		4.92E-01	1.02E-07	1.04E+00	down
114		Ditartaroyl-hydroxycoumarin		3.46E-01	1.42E-04	1.03E+00	down
115		Coumarin		3.09E-01	1.59E-04	1.03E+00	down
116		7-Methoxy-5-Prenyloxycoumarin		2.32E-01	2.90E-04	1.03E+00	down
117	Phenylpropanoids	p-Coumaric acid-4-O-glucoside		1.26E-01	3.56E-07	1.04E+00	down
118		Scopoletin (7-Hydroxy-5-methoxycoumarin)		8.37E-02	6.23E-07	1.04E+00	down
119		5,7-Dimethoxycoumarin (Limettin)(Citropten)	Yes	8.16E-05	1.86E-07	1.04E+00	down
120		p-Coumaroylmalic acid	Yes	4.53E-06	9.86E-06	1.04E+00	down
121		3-hydroxybenzaldehyde	Yes	6.37E+03	2.47E-04	1.04E+00	up
122		4-Hydroxybenzoic acid		1.04E+01	2.37E-09	1.04E+00	up
123		Protocatechuic aldehyde		9.91E+00	5.02E-06	1.04E+00	up
124		3-O-Digalloyl quinic acid		9.40E+00	4.16E-05	1.04E+00	up
125	Phenylmethanes	Vanillic acid		9.30E+00	5.49E-08	1.04E+00	up
126		Salicin		9.03E+00	6.62E-05	1.04E+00	up
127		3,4,5-Trimethoxyphenyl-1-O-Glucoside		6.75E+00	2.83E-05	1.04E+00	up
128		Salicylic acid		6.02E+00	1.33E-05	1.04E+00	up
129		Syringaldehyde-4-O-glucoside		5.82E+00	6.66E-05	1.04E+00	up
130		Vanillin		4.85E+00	3.05E-05	1.04E+00	up

131	Salicylic acid-2-O-glucoside		4.18E+00	7.68E-07	1.04E+00	up
132	Vanillic acid-4-O-glucoside		2.93E+00	1.52E-04	1.03E+00	up
133	4-O-Glucosyl-4-hydroxybenzoic acid		2.24E+00	7.26E-04	1.02E+00	up
134	Terephthalic acid		3.82E-01	3.82E-04	1.03E+00	down
135	2,5-Dihydroxybenzoic acid O-glucoside		2.73E-01	4.24E-06	1.04E+00	down
136	Syringic acid		2.43E-01	4.72E-05	1.04E+00	down
137	Protocatechuic acid-4-O-glucoside		2.23E-01	2.68E-07	1.04E+00	down
138	4-O-Glucosyl-3,4-dihydroxybenzyl alcohol		1.53E-01	1.56E-05	1.04E+00	down
139	Syringaldehyde (4-Hydroxy-3,5-Dimethoxybenzaldehyde)		1.10E-01	1.79E-05	1.04E+00	down
140	1-O-Vanilloyl-D-Glucose		6.25E-02	4.06E-05	1.04E+00	down
141	1-O-(3,4-Dihydroxy-5-methoxy-benzoyl)-glucoside		4.24E-02	3.72E-08	1.04E+00	down
142	4-Methylcatechol	Yes	3.19E-04	1.86E-03	1.02E+00	down
143	4-Hydroxybenzyl Alcohol	Yes	1.30E-04	5.53E-05	1.04E+00	down
144	4-O-(6'-O-Glucosylcaffeoylglucosyl)-4-hydroxybenzyl alcohol	Yes	2.50E+05	4.94E-05	1.04E+00	up
145	1'-O-(3,4-Dihydroxyphenethyl)-O-caffeoyl-glucoside	Yes	5.83E+03	2.06E-06	1.04E+00	up
146	Isoeugenol	Yes	1.90E+03	8.45E-04	1.03E+00	up
147	Phenylpyruvic acid		2.13E+01	5.45E-05	1.04E+00	up
148	3-(4-Hydroxyphenyl)-propionic acid		1.80E+01	6.93E-06	1.04E+00	up
149	Ferulic acid		1.78E+01	1.06E-05	1.04E+00	up
150	1-O-[(E)-Caffeoyl]-D-glucose		1.24E+01	5.30E-05	1.04E+00	up
151	6-O-Caffeoyl-D-glucose		1.11E+01	3.59E-06	1.04E+00	up
152	Methyl ferulate		1.06E+01	4.97E-06	1.04E+00	up
153	1-O-Feruloylquinic acid		6.33E+00	6.12E-07	1.04E+00	up
154	Scopoletin-7-O-glucuronide		6.25E+00	9.67E-08	1.04E+00	up
155	3-O-Feruloylquinic acid		6.18E+00	8.28E-04	1.03E+00	up
156	Caffeic acid		6.10E+00	1.04E-06	1.04E+00	up
157	Dihydrocaffeoylglucose		5.04E+00	1.64E-05	1.04E+00	up
158	6-O-Caffeoylarbutin		4.96E+00	2.62E-04	1.03E+00	up
159	Phenylpropanes					
159	Dicaffeoylquinic acid-O-glucoside		2.16E+00	2.75E-03	1.00E+00	up
160	Scopoletin-7-O-glucoside (Scopolin)		4.37E-01	9.25E-04	1.02E+00	down
161	Rhododendrol		4.08E-01	1.74E-04	1.03E+00	down
162	Osthole		3.12E-01	1.72E-04	1.04E+00	down
163	Methyl caffeate		3.10E-01	1.42E-03	1.02E+00	down
164	Isoimperatorin		1.93E-01	2.08E-08	1.04E+00	down
165	6-O-Feruloyl-D-glucose		1.79E-01	1.60E-03	1.02E+00	down
166	Sinapic acid		1.17E-01	5.36E-05	1.04E+00	down
167	1-O-Glucosyl sinapate		3.40E-02	5.23E-06	1.04E+00	down
168	Feruloylmalic acid		5.99E-03	5.80E-11	1.04E+00	down
169	Sinapoyl malate	Yes	8.03E-04	5.32E-05	1.04E+00	down
170	Cis-Coutaric acid	Yes	7.33E-04	1.86E-03	1.01E+00	down
171	6'-O-Feruloyl-D-sucrose	Yes	4.57E-04	5.12E-04	1.02E+00	down
172	1,2-O-Diferuloylglycerol	Yes	3.43E-04	6.47E-06	1.04E+00	down
173	Caffeoylbenzoyltartaric acid	Yes	1.92E-04	5.71E-04	1.02E+00	down
174	Chlorogenic acid methyl ester	Yes	7.67E-05	7.11E-06	1.04E+00	down

175		Caffeic aldehyde	Yes	1.77E-05	4.91E-08	1.04E+00	down
176		3,4-Dihydroxybenzeneacetic acid	Yes	9.88E+04	7.97E-07	1.04E+00	up
177		Tyrosol		1.44E+01	8.79E-08	1.04E+00	up
178		4-Hydroxyacetophenone		8.39E+00	1.11E-06	1.04E+00	up
179		Salidroside		6.00E+00	4.70E-05	1.04E+00	up
180		2-phenylethyl- D-β- glucopyranoside		3.73E+00	1.22E-04	1.04E+00	up
181	Phenylethanes	Mandelic acid		2.55E+00	2.69E-05	1.04E+00	up
182		2-Acetyl-3-hydroxyphenyl-1-O-glucoside		4.45E-01	1.94E-03	1.01E+00	down
183		2',4'-Dihydroxy-6'-methoxyacetophenone		3.48E-01	1.36E-07	1.04E+00	down
184		5-(2-Hydroxyethyl)-2-O-glucosylphenol		1.58E-01	3.35E-05	1.04E+00	down
185		Picein (4-Acetylphenyl-glucoside)		4.11E-02	1.29E-03	1.02E+00	down
186		3-Hydroxy-4-isopropylbenzylalcohol-3-O-glucoside		2.67E-02	4.49E-06	1.04E+00	down
187		4-Hydroxy-3,5-diisopropylbenzaldehyde	Yes	2.44E-04	1.12E-06	1.04E+00	down
188		3,4-Digalloylshikimic acid		2.10E+01	2.08E-08	1.04E+00	up
189		Trans-5-O-(p-Coumaroyl)shikimate		5.70E+00	8.74E-05	1.04E+00	up
190	Shikimic acids	3-O-p-Coumaroylshikimic acid		3.58E+00	1.12E-03	1.02E+00	up
191		Shikimic acid		3.23E-01	4.69E-04	1.03E+00	down
192		3,5-Di-O-galloylshikimic acid		2.62E-01	1.94E-05	1.04E+00	down
193		Matairesinol	Yes	1.23E+04	1.19E-05	1.04E+00	up
194		5'-Methoxysolariciresinol-9'-O-glucoside		2.22E+01	1.10E-05	1.04E+00	up
195		Isolariciresinol-9'-O-glucoside		1.94E+01	2.19E-07	1.04E+00	up
196	Lignans	Epipinoresinol		5.42E+00	1.84E-06	1.04E+00	up
197		Pinoresinol		5.07E+00	7.56E-06	1.04E+00	up
198		Pinoresinol-4-O-glucoside		3.23E+00	7.85E-05	1.04E+00	up
199		Syringaresinol		4.51E-01	6.03E-04	1.02E+00	down
200		Olivil-4,4'-Di-O-glucoside		1.29E-01	4.39E-05	1.04E+00	down
201		Coniferyl alcohol	Yes	2.27E+04	3.76E-09	1.04E+00	up
202	Lignins	Coniferin		1.29E+01	1.70E-06	1.04E+00	up
203		Coniferaldehyde		7.94E+00	1.08E-06	1.04E+00	up
204		4,7,9,9'-Tetrahydroxy-3,3'-dimethoxy-8-O-4'-neolignan		6.16E+00	4.43E-05	1.04E+00	up
205		D-Glucuronic acid	Yes	8.09E+04	1.48E-05	1.04E+00	up
206		1,10-Decanediol	Yes	7.67E+03	7.22E-07	1.04E+00	up
207		N-Acetyl-D-glucosamine-1-phosphate	Yes	1.70E+03	1.74E-04	1.04E+00	up
208		Glucose-1-phosphate		5.28E+01	1.25E-05	1.04E+00	up
209		D-Glucose 6-phosphate		5.06E+01	1.07E-06	1.04E+00	up
210		Trehalose 6-phosphate		7.91E+00	2.69E-05	1.04E+00	up
211	Saccharides	Glucarate O-Phosphoric acid		5.25E+00	1.11E-05	1.04E+00	up
212		D-Sedoheptuose 7-phosphate		4.77E+00	1.66E-04	1.03E+00	up
213		Mannitol		4.24E+00	1.47E-06	1.04E+00	up
214		D-Sorbitol		3.76E+00	6.08E-05	1.04E+00	up
215		D-(+)-Sucrose		2.42E+00	4.87E-04	1.03E+00	up
216		Gluconic acid		2.28E+00	3.81E-06	1.04E+00	up
217		D-Saccharic acid		2.14E+00	1.50E-05	1.04E+00	up
218		D-Galactaric acid		2.11E+00	5.71E-05	1.04E+00	up

219		D-Ribose		3.55E-01	1.89E-05	1.04E+00	down
220		Solatriose		2.16E-01	3.72E-05	1.04E+00	down
221		LysoPC 19:2	Yes	2.12E+04	2.75E-12	1.04E+00	up
222		LysoPC 20:1	Yes	1.23E+04	8.62E-06	1.04E+00	up
223		LysoPC 18:2(2n isomer)		5.12E+01	6.13E-07	1.04E+00	up
224		LysoPC 18:1(2n isomer)		4.44E+01	1.18E-07	1.04E+00	up
225		LysoPC 17:2		3.46E+01	3.15E-06	1.04E+00	up
226		LysoPC 16:1		3.37E+01	4.72E-08	1.04E+00	up
227		LysoPC 16:1(2n isomer)		3.13E+01	4.77E-09	1.04E+00	up
228		LysoPC 18:1		2.50E+01	1.51E-06	1.04E+00	up
229		LysoPC 16:0(2n isomer)		2.12E+01	6.36E-11	1.04E+00	up
230		LysoPC 20:3		1.87E+01	9.79E-07	1.04E+00	up
231		LysoPC 18:2		1.46E+01	1.18E-05	1.04E+00	up
232		LysoPC 18:0(2n isomer)		1.41E+01	1.14E-04	1.04E+00	up
233		LysoPC 20:2		1.33E+01	2.02E-04	1.03E+00	up
234		Choline Alfoscerate		1.06E+01	2.26E-06	1.04E+00	up
235		LysoPC 17:1		1.03E+01	1.03E-05	1.04E+00	up
236	Phospholipids	LysoPE 18:2		8.39E+00	2.15E-05	1.04E+00	up
237		LysoPE 16:1(2n isomer)		6.15E+00	2.85E-06	1.04E+00	up
238		LysoPC 15:1		5.89E+00	1.89E-05	1.04E+00	up
239		LysoPE 16:1		5.56E+00	8.90E-07	1.04E+00	up
240		LysoPE 15:0		3.98E+00	9.73E-07	1.04E+00	up
241		LysoPC 18:3(2n isomer)		3.61E+00	1.49E-06	1.04E+00	up
242		LysoPE 17:1(2n isomer)		3.54E+00	6.39E-05	1.04E+00	up
243		LysoPC 14:0		3.49E+00	9.92E-07	1.04E+00	up
244		LysoPE 16:0(2n isomer)		3.27E+00	1.54E-07	1.04E+00	up
245		LysoPE 20:2		2.85E+00	9.10E-04	1.03E+00	up
246		LysoPC 19:2(2n isomer)		4.85E-01	1.17E-03	1.03E+00	down
247		LysoPC 19:1		2.70E-01	4.13E-06	1.04E+00	down
248		LysoPE 14:0		2.67E-01	1.93E-06	1.04E+00	down
249		LysoPC 19:0		8.66E-02	1.85E-06	1.04E+00	down
250		LysoPC 17:0		3.35E-02	8.03E-08	1.04E+00	down
251		LysoPC 17:0(2n isomer)	Yes	2.67E-05	1.59E-06	1.04E+00	down
252		L- α -Glutamyl-L-Glutamic Acid	Yes	7.99E+03	7.35E-08	1.04E+00	up
253		N-Acetyl-L-Aspartic Acid	Yes	7.59E+03	6.46E-06	1.04E+00	up
254		N- α -Acetyl-L-ornithine		3.75E+01	7.35E-06	1.04E+00	up
255		Oxiglutatione		1.16E+01	8.66E-06	1.04E+00	up
256		L-Arginine		1.05E+01	7.98E-06	1.04E+00	up
257	Amino acids	L-Aspartic Acid		7.12E+00	9.34E-08	1.04E+00	up
258		L-Prolyl-L-Phenylalanine		4.09E+00	7.55E-05	1.04E+00	up
259		L-Aspartic acid-O-diglucoside		2.92E+00	3.47E-05	1.04E+00	up
260		N-Acetyl-L-tyrosine		2.85E+00	1.01E-04	1.03E+00	up
261		L-Citrulline		2.61E+00	3.21E-05	1.04E+00	up
262		N-Acetyl-L-glutamic acid		2.11E+00	1.22E-03	1.03E+00	up

263		S-(Methyl)glutathione		2.05E+00	1.31E-03	1.03E+00	up
264		N-(3-Indolylacetyl)-L-alanine		2.05E+00	9.07E-05	1.04E+00	up
265		L-Valyl-L-Phenylalanine		4.46E-01	4.98E-05	1.04E+00	down
266		L-Leucyl-L-phenylalanine		3.99E-01	1.76E-05	1.04E+00	down
267		L-Phenylalanyl-L-phenylalanine		3.87E-01	5.92E-04	1.03E+00	down
268		L-Histidine		3.78E-01	6.82E-05	1.04E+00	down
269		N-Acetyl-L-threonine		3.68E-01	4.49E-05	1.04E+00	down
270		3-Hydroxy-3-methylpentane-1,5-dioic acid		3.56E-01	3.18E-06	1.04E+00	down
271		L-Glutamic acid-O-glycoside		3.54E-01	1.79E-03	1.01E+00	down
272		L-Methionine		2.35E-01	5.47E-08	1.04E+00	down
273		L-Phenylalanine		2.25E-01	2.07E-07	1.04E+00	down
274		Trans-4-Hydroxy-L-proline		2.21E-01	7.52E-05	1.04E+00	down
275		N-Acetyl-L-Arginine		2.16E-01	3.69E-04	1.03E+00	down
276		L-Threonine		1.99E-01	1.24E-06	1.04E+00	down
277		L-Homoserine		1.88E-01	5.69E-06	1.04E+00	down
278		L-Valine		1.85E-01	1.14E-06	1.04E+00	down
279		Cycloleucine		1.83E-01	1.15E-05	1.04E+00	down
280		L-Lysine		1.37E-01	1.15E-06	1.04E+00	down
281		L-Glutamine		1.33E-01	1.30E-06	1.04E+00	down
282		L-Leucine		1.32E-01	3.25E-06	1.04E+00	down
283		5-Hydroxy-L-tryptophan		1.24E-01	9.81E-04	1.03E+00	down
284		L-Isoleucine		1.22E-01	2.61E-06	1.04E+00	down
285		4-Acetamidobutyric acid		1.19E-01	3.57E-07	1.04E+00	down
286		3,4-Dihydroxy-L-phenylalanine		8.95E-02	4.35E-05	1.04E+00	down
287		L-Cystine		8.91E-02	6.19E-06	1.04E+00	down
288		L-Glutaminyl-L-valyl-L-valyl-L-cysteine		3.93E-02	6.84E-06	1.04E+00	down
289		3-Methyl-L-Histidine		2.89E-02	7.00E-05	1.04E+00	down
290		L-Glutamine-O-glycoside		1.56E-02	3.84E-05	1.04E+00	down
291		N-Phenylacetyl glycine	Yes	5.37E-04	2.39E-03	1.01E+00	down
292		D-Galacturonic acid	Yes	6.19E+04	3.68E-05	1.04E+00	up
293		Argininosuccinic acid		7.71E+01	1.16E-06	1.04E+00	up
294		Propyl 2-(trimethylammonio)ethyl phosphate		3.13E+01	4.48E-06	1.04E+00	up
295		β -Hydroxyisovaleric acid		1.22E+01	5.58E-08	1.04E+00	up
296		3-Hydroxybutyric acid		5.98E+00	2.65E-07	1.04E+00	up
297		Muconic acid		5.45E+00	3.25E-06	1.04E+00	up
298		L-Citramalic acid		4.23E+00	2.29E-04	1.03E+00	up
299	Organic acids	Malonic acid		3.06E+00	3.34E-06	1.04E+00	up
300		Isocitric Acid		2.56E+00	5.75E-05	1.04E+00	up
301		4-Hydroxy-2-oxoglutaric acid		2.48E+00	4.51E-04	1.03E+00	up
302		4-Guanidinobutyric acid		2.41E+00	1.80E-05	1.04E+00	up
303		Citric Acid		2.24E+00	1.02E-04	1.04E+00	up
304		Quinic Acid		2.22E+00	2.95E-05	1.04E+00	up
305		2-Hydroxyhexadecanoic acid		4.79E-01	3.83E-05	1.04E+00	down
306		2-Hydroxy-4-methylpentanoic acid		3.46E-01	3.72E-03	1.01E+00	down

307		2-Hydroxybutyric Acid		3.46E-01	8.70E-06	1.04E+00	down
308		2-Hydroxyisobutyric acid		3.40E-01	1.97E-03	1.02E+00	down
309		Phthalic acid		3.18E-01	8.77E-04	1.02E+00	down
310		2-Aminoethanesulfonic acid		3.11E-01	2.14E-04	1.03E+00	down
311		Lauric acid		2.71E-01	2.99E-05	1.04E+00	down
312		2-Furanoic acid		2.56E-01	5.01E-03	1.00E+00	down
313		1-Aminocyclopropane-1-carboxylic acid		2.43E-01	9.97E-06	1.04E+00	down
314		Acetoxyacetic acid		2.26E-01	5.43E-06	1.04E+00	down
315		Anchoic Acid		2.01E-01	2.15E-07	1.04E+00	down
316		Succinic anhydride		1.40E-01	5.76E-05	1.04E+00	down
317		6-Aminocaproic acid		1.28E-01	1.98E-06	1.04E+00	down
318		Ethylmalonic acid		1.21E-01	1.08E-05	1.04E+00	down
319		3-Dehydro-L-Threonic Acid		1.09E-01	4.18E-07	1.04E+00	down
320		Dodecanedioic acid		1.05E-01	2.35E-06	1.04E+00	down
321		Glutaric acid		1.05E-01	1.28E-06	1.04E+00	down
322		2,2-Dimethylsuccinic acid		1.02E-01	6.12E-05	1.04E+00	down
323		Succinic acid		1.01E-01	3.59E-07	1.04E+00	down
324		α -Ketoglutaric acid		1.01E-01	7.61E-08	1.04E+00	down
325		Methylmalonic acid		1.00E-01	4.52E-07	1.04E+00	down
326		Aminomalonic acid		9.64E-02	2.33E-06	1.04E+00	down
327		L-(-)-Malic acid		9.54E-02	4.89E-07	1.04E+00	down
328		3-Hydroxypropanoic acid		7.13E-02	2.19E-05	1.04E+00	down
329		(-)-Jasmonoyl-L-Isoleucine		1.47E-02	9.22E-09	1.04E+00	down
330		D-Pantothenic Acid		4.12E-01	1.33E-06	1.04E+00	down
331		Riboflavin		3.30E-01	5.95E-04	1.02E+00	down
332		Pyridoxine		2.42E-01	8.46E-07	1.04E+00	down
333	Vitamins	4-Pyridoxic acid		2.12E-01	1.80E-07	1.04E+00	down
334		Pyridoxine-5'-O-glucoside		1.06E-01	1.00E-05	1.04E+00	down
335		L-Ascorbic acid		7.65E-02	2.67E-06	1.04E+00	down
336		4-Pyridoxic acid-O-glucoside	Yes	2.53E-04	2.61E-06	1.04E+00	down
337		2-Aminopurine	Yes	1.36E+04	1.03E-04	1.04E+00	up
338		Heptadecanoic acid	Yes	9.85E+03	4.75E-08	1.04E+00	up
339		1-O-Feruloyl-3-O-caffeoylglycerol	Yes	7.11E+03	9.41E-06	1.04E+00	up
340		3,5-Dihydroxy-2,4-dimethoxy-9H-fluoren-9-one	Yes	1.34E+03	6.31E-05	1.04E+00	up
341		Ursolic acid	Yes	1.19E+03	2.75E-04	1.03E+00	up
342		Rosiridin	Yes	9.88E+02	3.11E-06	1.04E+00	up
343		27,28-Dicarboxyl ursolic acid	Yes	8.34E+02	2.54E-03	1.00E+00	up
344	Others	9,10-Epoxyoctadecanoic Acid	Yes	7.97E+02	1.15E-06	1.04E+00	up
345		2'-Deoxyinosine-5'-monophosphate		3.99E+02	4.72E-06	1.04E+00	up
346		8,15-Dihydroxy-5,9,11,13-eicosatetraenoic acid		1.88E+02	7.27E-09	1.04E+00	up
347		2-(Formylamino)benzoic acid		3.25E+01	7.05E-07	1.04E+00	up
348		Sarmentosin		2.97E+01	6.68E-08	1.04E+00	up
349		Cyclic 3',5'-Adenylic acid		2.82E+01	7.19E-07	1.04E+00	up
350		β -Nicotinamide mononucleotide		2.60E+01	2.65E-05	1.04E+00	up

351	Adenosine 5'-monophosphate	1.97E+01	8.57E-06	1.04E+00	up
352	Guanosine 3',5'-cyclic monophosphate	1.94E+01	3.66E-06	1.04E+00	up
353	2-Deoxyribose-5'-phosphate	1.74E+01	1.64E-06	1.04E+00	up
354	Guanosine 5'-monophosphate	1.51E+01	2.29E-04	1.03E+00	up
355	O-Phosphocholine	1.51E+01	1.10E-06	1.04E+00	up
356	Eicosadienoic acid	1.07E+01	2.67E-08	1.04E+00	up
357	Uridine 5'-monophosphate	1.03E+01	1.84E-05	1.04E+00	up
358	5-Aminoimidazole ribonucleotide	9.79E+00	6.25E-06	1.04E+00	up
359	O-Phosphorylethanolamine	8.79E+00	6.03E-06	1.04E+00	up
360	Cinidilide	8.49E+00	5.49E-05	1.04E+00	up
361	Uridine 5'-diphospho-D-glucose	8.14E+00	4.98E-05	1.04E+00	up
362	2-Deoxyribose-1-phosphate	7.32E+00	1.83E-03	1.02E+00	up
363	2-Linoleoylglycerol	6.91E+00	3.08E-06	1.04E+00	up
364	Cytidine 5'-monophosphate(Cytidylic acid)	6.69E+00	2.82E-04	1.04E+00	up
365	1-Linoleoylglycerol	6.01E+00	2.19E-07	1.04E+00	up
366	N6-Isopentenyladenine	5.86E+00	9.86E-05	1.03E+00	up
367	Cis-10-Heptadecenoic Acid	5.72E+00	2.26E-08	1.04E+00	up
368	5-Hydroxymethylfurfural	4.69E+00	1.42E-03	1.02E+00	up
369	5,6-Dihydroxyindole-5-O- β -glucoside	4.54E+00	4.24E-05	1.04E+00	up
370	N1,N8-Bis(sinapoyl)spermidine	4.34E+00	2.04E-04	1.03E+00	up
371	2-Linoleoylglycerol-1-O-glucoside	4.21E+00	2.13E-04	1.03E+00	up
372	Sodium Valproate	4.11E+00	1.11E-08	1.04E+00	up
373	1-Oleoyl-Sn-Glycerol	3.76E+00	1.61E-05	1.04E+00	up
374	Rosiridoside A	3.69E+00	6.48E-03	1.00E+00	up
375	β -Pseudouridine	3.57E+00	2.25E-03	1.02E+00	up
376	9-Hydroxy-13-oxo-10-octadecenoic Acid	3.56E+00	2.98E-05	1.04E+00	up
377	11-Octadecanoic acid(Vaccenic acid)	3.35E+00	3.61E-06	1.04E+00	up
378	Uridine 5'-diphospho-N-acetylglucosamine	3.11E+00	1.86E-05	1.04E+00	up
379	NADP (Nicotinamide adenine dinucleotide phosphate)	3.11E+00	1.51E-03	1.02E+00	up
380	9(10)-EpOME;(9R,10S)-(12Z)-9,10-Epoxyoctadecenoic acid	3.02E+00	2.39E-06	1.04E+00	up
381	Uridine	2.87E+00	1.63E-04	1.03E+00	up
382	Adenosine	2.74E+00	1.55E-04	1.03E+00	up
383	1-Linoleoylglycerol-2,3-di-O-glucoside	2.67E+00	6.47E-05	1.04E+00	up
384	Nicotinic acid adenine dinucleotide	2.63E+00	9.37E-05	1.04E+00	up
385	L-Tyramine	2.61E+00	1.73E-04	1.04E+00	up
386	Oleamide (9-Octadecenamide)	2.60E+00	1.08E-03	1.03E+00	up
387	7S,8S-DiHODE; (9Z,12Z)-(7S,8S)-Dihydroxyoctadeca-9,12-dienoic acid	2.58E+00	7.62E-05	1.04E+00	up
388	1-Eicosanol	2.28E+00	4.08E-06	1.04E+00	up
389	Phenylethanolamine	2.20E+00	8.57E-07	1.04E+00	up
390	12,13-Epoxy-9-Octadecenoic Acid	2.16E+00	6.18E-05	1.04E+00	up
391	Cytidine	4.82E-01	1.54E-03	1.01E+00	down
392	Cytosine	4.45E-01	1.89E-05	1.04E+00	down
393	Isoguanine	4.29E-01	1.35E-04	1.04E+00	down

394	Undecylic Acid	4.15E-01	1.22E-04	1.04E+00	down
395	Guanine	3.86E-01	1.46E-04	1.04E+00	down
396	Histamine	3.68E-01	1.51E-05	1.04E+00	down
397	2-(Dimethylamino)guanosine	3.25E-01	4.14E-07	1.04E+00	down
398	Xanthine	3.22E-01	7.53E-03	1.00E+00	down
399	1-Linolenoyl-rac-glycerol-diglucoiside	2.95E-01	8.15E-05	1.04E+00	down
400	9,12-Octadecadien-6-Ynoic Acid	2.89E-01	4.49E-05	1.04E+00	down
401	DL-2-Aminoadipic acid	2.86E-01	1.38E-05	1.04E+00	down
402	Indole-3-carboxylic acid	2.63E-01	5.59E-04	1.03E+00	down
403	7-Methylguanine	2.58E-01	6.99E-05	1.04E+00	down
404	6-Methylmercaptapurine	2.46E-01	5.06E-07	1.04E+00	down
405	N-Benzylmethylene isomethylamine	2.37E-01	1.15E-08	1.04E+00	down
406	4-Hydroxymandelonitrile	2.32E-01	7.49E-05	1.04E+00	down
407	1-methylguanidine	2.25E-01	2.49E-04	1.03E+00	down
408	N-Oleoylethanolamine	2.25E-01	1.93E-04	1.04E+00	down
409	Clove chromone	2.08E-01	2.18E-04	1.03E+00	down
410	Cadaverine	2.06E-01	1.10E-07	1.04E+00	down
411	Myristic Acid	1.97E-01	1.98E-07	1.04E+00	down
412	Eucommiol	1.82E-01	9.40E-08	1.04E+00	down
413	2'-Deoxyadenosine	1.76E-01	8.45E-07	1.04E+00	down
414	2- α -Linolenoyl-glycerol-1-O-glucoside	1.66E-01	2.32E-03	1.02E+00	down
415	N7-Methylguanosine	1.59E-01	3.78E-05	1.04E+00	down
416	Indole-5-carboxylic acid	1.56E-01	6.21E-05	1.04E+00	down
417	1-Stearidonoyl-Glycerol	1.55E-01	3.30E-08	1.04E+00	down
418	1- α -Linolenoyl-glycerol-3-O-glucoside	1.55E-01	4.91E-04	1.02E+00	down
419	3-Hydroxypropyl palmitate glc-glucosamine	1.43E-01	7.15E-07	1.04E+00	down
420	1- α -Linolenoyl-glycerol-2,3-di-O-glucoside	1.42E-01	1.05E-04	1.04E+00	down
421	1-Methyladenine	1.35E-01	8.54E-04	1.03E+00	down
422	9,12,13-Trihydroxy-10,15-octadecadienoic acid	1.32E-01	1.24E-07	1.04E+00	down
423	2'-Deoxyadenosine-5'-monophosphate	1.22E-01	5.77E-06	1.04E+00	down
424	domesticoside	1.20E-01	6.23E-06	1.04E+00	down
425	Piperidine	1.19E-01	9.89E-07	1.04E+00	down
426	Oleoside 11-methyl ester	1.16E-01	9.64E-04	1.02E+00	down
427	6-Deoxyfagomine	1.16E-01	1.87E-07	1.04E+00	down
428	Methyl 7,10-hexadecadienoate	9.37E-02	7.31E-09	1.04E+00	down
429	3-Aminosalicylic acid	7.71E-02	3.79E-06	1.04E+00	down
430	9-Hydroperoxy-10E,12,15Z-octadecatrienoic acid	7.46E-02	6.13E-09	1.04E+00	down
431	9-Oxo-10E,12Z-octadecadienoic acid	7.16E-02	9.19E-08	1.04E+00	down
432	3,5,7,4'-Tetrahydroxy-Coumaronochromone	6.54E-02	3.19E-03	1.02E+00	down
433	9-Hydroxy-12-oxo-15(Z)-octadecenoic acid	5.98E-02	5.09E-10	1.04E+00	down
434	9-Hydroxy-10,12,15-octadecatrienoic acid	5.78E-02	8.50E-07	1.04E+00	down
435	Thymidine	5.66E-02	8.29E-06	1.04E+00	down
436	13-KODE; (9Z,11E)-13-Oxo-octadeca-9,11-dienoic acid	5.44E-02	1.01E-09	1.04E+00	down
437	5-Methylcytosine	4.84E-02	1.75E-04	1.04E+00	down

438	2'-Deoxycytidine		4.38E-02	1.14E-05	1.04E+00	down
439	2'-Deoxyguanosine		4.36E-02	2.26E-07	1.04E+00	down
440	Rosiridoside B		4.34E-02	1.46E-05	1.04E+00	down
441	Cis-4,7,10,13,16,19-Docosahexaenoic Acid		9.51E-03	1.36E-04	1.04E+00	down
442	Eucommioside		2.91E-03	4.38E-06	1.04E+00	down
443	D-erythro-sphinganine	Yes	3.96E-04	2.00E-04	1.03E+00	down
444	2'-Deoxyuridine	Yes	2.70E-04	1.12E-04	1.04E+00	down
445	N-Hydroxytryptamine	Yes	2.30E-04	1.64E-04	1.04E+00	down
446	Serotonin	Yes	2.06E-04	6.65E-06	1.04E+00	down
447	Pyrocatechol	Yes	2.01E-04	7.68E-04	1.03E+00	down
448	Tryptamine	Yes	8.77E-05	9.01E-07	1.04E+00	down
449	1-Methylpiperidine-2-carboxylic acid	Yes	8.51E-05	2.85E-06	1.04E+00	down
450	2-Aminoethylphosphonate	Yes	1.63E-05	7.55E-07	1.04E+00	down