Supplementary information

Table S1 GC-MS assignments of metabolites identified in rat urine *via* GC/MS post silylation

Peak	Metabolites	KI	RT(min)	*m/z*
1	Hydorgen sulfide -TMS	940	8.64	146
U2	Unknown	947	8.86	151
U3	Silanamine TMS	955	9.06	174
U4	Unkown	956	9.11	171
U5	Lysine, 4-hydroxy TMS	962	9.28	144
U6	Borate-TMS	972	9.58	221
U7	Nicotinic acid, 4-amino-, methyl ester TMS	1032	11.28	152
U8	Lactic acid TMS	1047	11.72	117
U9	Glycolic acid-TMS	1064	12.21	147
U10	L-alanine-TMS	1093	13.03	116
U11	N-butylamine TMS	1102	13.28	174
U12	Fumaric acid TMS	1111	13.58	245
U13	Glycine, N TMS	1113	13.62	102
U14	Oxalic acid TMS	1121	13.86	147
U15	Malonic acid TMS	1132	14.19	133
U16	Phenol, 3-(1,1-dimethylethyl)-4-methoxy-TMS	1151	14.77	165
U17	Unknown	1201	16.29	131
U18	Lvaline TMS	1207	16.45	144
U19	Urea TMS	1237	17.37	147
U20	Benzoic acid TMS	1248	17.71	179
U21	Oxamic acid TMS	1251	17.77	147
U22	Glycerol TMS	1261	18.06	205
U23	Phosphate TMS	1262	18.11	299
U24	Glycine TMS	1299	19.23	174
U25	Succinic acid TMS	1306	19.41	147
U26	Glyceric acid TMS	1317	19.75	292
U27	Uracil TMS	1331	20.15	241
U28	O-Methyl methylphenylthiophosphinate TMS	1354	20.81	188
U29	Phenylamine TMS	1362	21.05	224
U30	N-hydroxysuccinimide TMS	1411	22.44	172
U31	Malic acid TMS	1475	24.19	233
U32	Threitol TMS	1483	24.4	217
U33	Erythritol TMS	1490	24.62	147
U34	Aspartic acid TMS	1508	25.08	232
U35	Pyroglutamic acid TMS	1517	25.33	156
U36	Ribose TMS	1522	25.45	117
U37	5-MethylcytosineTMS	1533	25.73	254
U38	Threonic Acid TMS	1543	25.98	292

U39	Creatinine enol TMS	1550	26.17	115
U40	Suberic acid 2 TMS	1574	26.79	303
U41	Citramalic acid TMS	1591	27.23	247
U42	Cadaverine TMS	1622	28.01	174
U43	Fructose TMS	1643	28.55	103
U44	Ribitol TMS	1687	29.61	217
U45	Putrescine TMS	1733	30.69	174
U46	2-Keto-glconic acid-TMS	1761	31.37	292
U47	Arabinofuranose TMS	1792	32.09	217
U48	Citric Acid TMS		32.31	273
U49	Pinitol TMS	1813	32.57	260
U50	Ribonic acid TMS	1829	32.98	292
U51	Fumaric acid TMS	1839	33.14	245
U52	Tagatose methoxyamine TMS	1851	33.4	307
U53	Fructose TMS	1861	33.61	307
U54	Ascorbic Acid TMS	1867	33.75	274
U55	Mannose TMS	1871	33.85	205
U56	Allantoin TMS	1874	33.9	331
U57	Glucose TMS	1878	33.99	319
U58	Glucose TMS	1899	34.44	319
U59	Methyl citric acid TMS	1906	34.61	287
U60	Glucosamine TMS	1922	34.95	319
U61	Inositol TMS	1939	35.29	318
U62	Ribonic acid TMS	1949	35.51	333
U63	Glucose TMS	1951	35.57	204
U64	Myo-Inositol TMS	2077	38.12	318
U65	Uric acid-TMS	2083	38.25	456
U66	Mannose- TMS	2129	39.70	204
U67	Sucrose TMS	2340	47.56	361

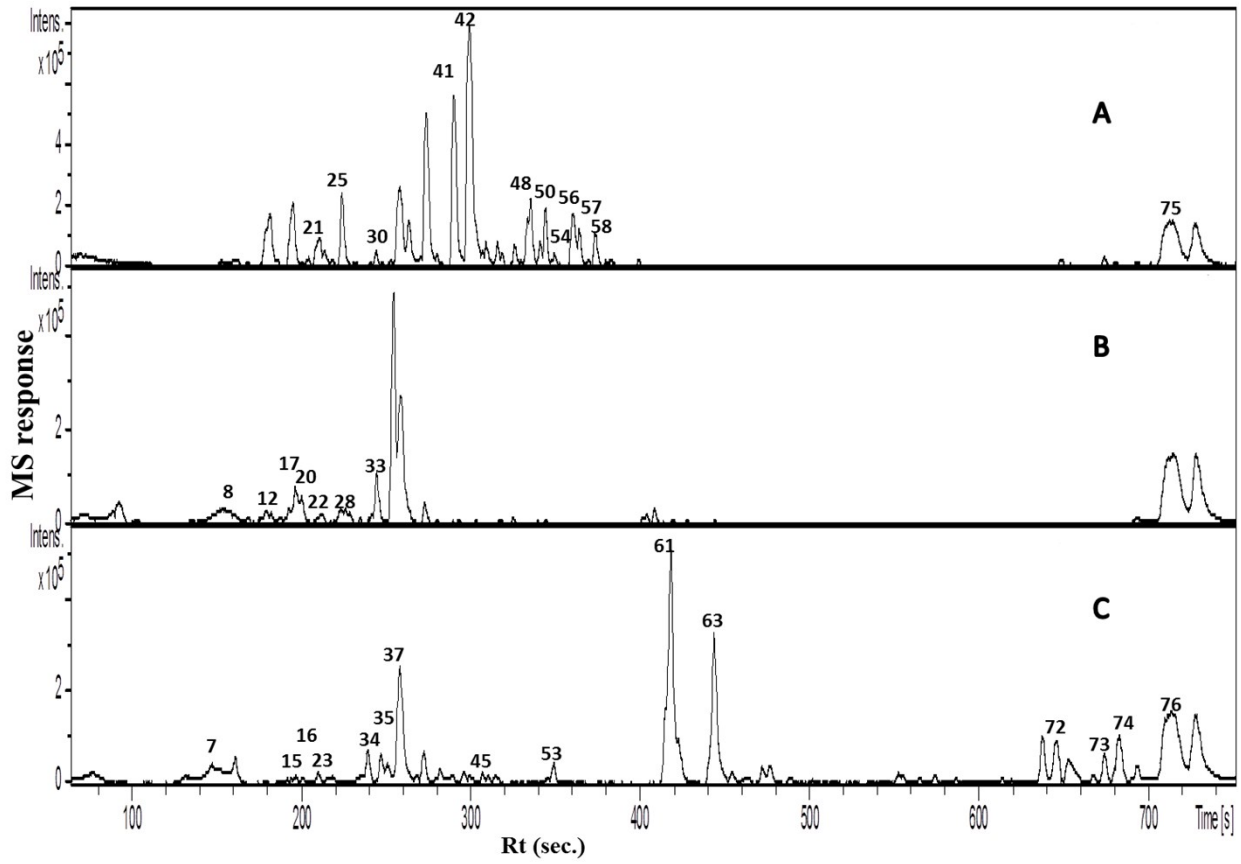

Figure S1 Base peak chromatogram (BPC) for water extract of grapefruit (A), pomegranate (B) and red cabbage (C) analyzed by UPLC-qTOF-(-)ESI-MS showing the most significant peaks. Peak numbers follow those listed in **Table S2** for metabolite identification using UPLC-PDA-MS.

Figure S2 Diagram sketch representing experimental design and results showing chemical biomarkers found elevated in rat obese urine *i.e*, phosphate and oxalate versus *i.e*., lactate in healthy ones as revealed from analysis of rat urine samples using GC-MS coupled to OPLS-DA

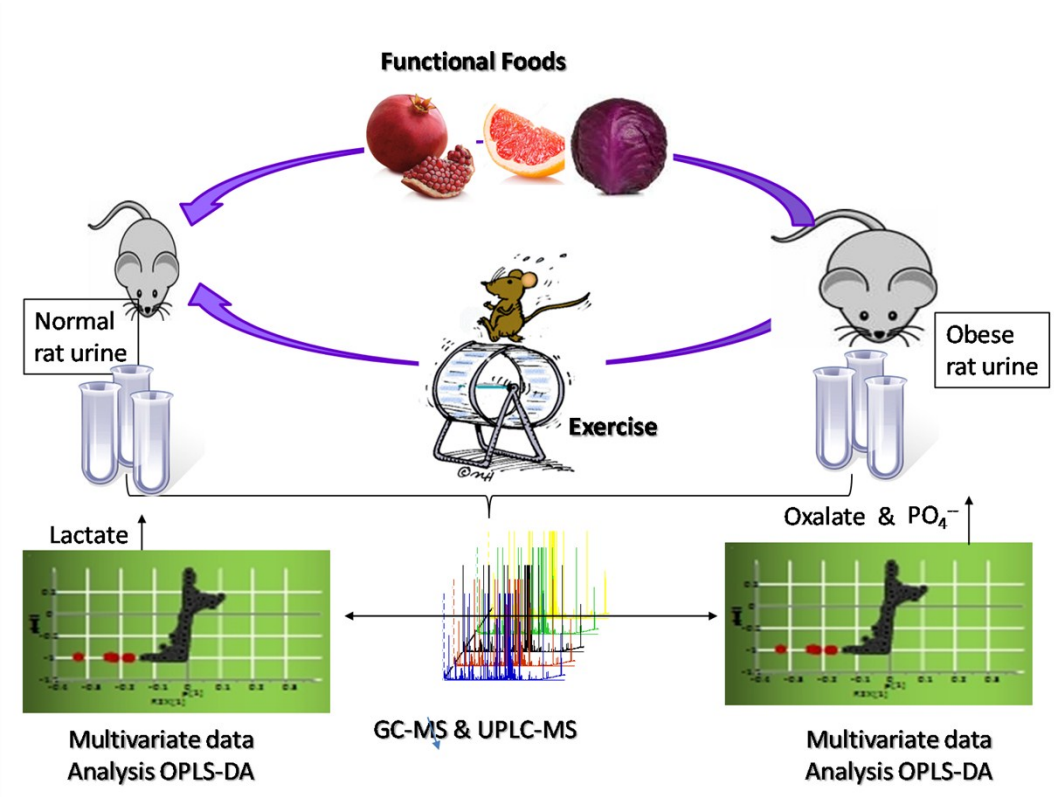

Table S2 Metabolites identified in pomegranate, red cabbage, grapefruit juice extracts via UPLC–PDA–MS in negative ionization mode.

Peak	RT (sec.)	UV(nm)	$[M-H]^-$	Mol. Formula	Error (pm)	MS fragments	Name	Class	Red cabbage	pomegranate	Grapefruit
1.	25.6	265.5	341.108	$C_{12}H_{21}O_{11}$	2.9	179	Unknown sugar	Sugar	-	-	+
2.	29	270, 325 shd.	191.02	$C_6H_7O_7$	1.2	133, 111	(iso)citric acid	Organic acid	+	+	-
3.	71.8	258, 290 shd.	353.145	$C_{14}H_{25}O_{10}$	7	191	Propanol-*O*-pentosyl-hexoside	Alcohol glycoside	-	+	-
4.	102.6	273.5	299.077	$C_{13}H_{15}O_8$	8.1	279, 137	Hydroxybenzoyl hexoside	Aromatic	-	+	-
5.	131.8	287, 326	375.0689	$C_{25}H_{11}O_4$	7.1	353, 275, 203	Unknown		+	-	-
6.	146.9	292, 325	789.2104	$C_{33}H_{41}O_{22}$	1.1	415, 353, 191	Unknown		+	-	-
7.	149	289, 322	771.201	$C_{33}H_{39}O_{21}$	-2.7	695, 547, 415, 375, 353, 285, 191	Kaempferol-*O*-sophoroside -*O*-glucoside	Flavonol acylated glycoside	+	-	-
8.	153.5	278, 323 shd.	341.087	$C_{15}H_{17}O_9$	2.1	299, 179, 161	*O*-Caffeoyl-hexoside	Phenolic acid	-	+	-
9.	160.8	289, 328	789.2112	$C_{33}H_{41}O_{22}$	2.1	389, 315	Unknown		+	-	-
10.	160.9	299, 330	341.0892	$C_{15}H_{17}O_9$	4.1	263, 179, 161	*O*-Caffeoyl-hexoside	Phenolic acid	-	-	+
11.	168	277	359.0976	$C_{15}H_{19}O_{10}$	2.2	315, 197	*O*-Syringoyl-hexoside	Phenolic acid	-	+	-
12.	179.2	275	783.0712	$C_{34}H_{23}O_{22}$	3.3	631, 621, 481, 470	Granatin A	Tannin	-	+	-
13.	187.6	276	323.1333	$C_{13}H_{23}O_9$	4.5	281	Unknown sugar		-	+	-
14.	192.7	275, 301 shd.	363.1071	$C_{18}H_{19}O_8$	4	145	Unknown lignin		-	+	-
15.	196.6	288	353.0872	$C_{16}H_{17}O_9$	1.8	291, 191, 161	*O*-Caffeoylquinic acid	Phenolic acid	+	-	-
16.	200.3	282, 314 shd.	977.2594	$C_{44}H_{49}O_{25}$	-2.6	771, 577, 385, 285, 223	Kaempferol -*O*-sinapoylglucoside-*O*-sophoroside	Flavonol acylated glycoside	+	-	-
17.	208.2	279	481.098	$C_{21}H_{21}O_{13}$	1.6	465, 423, 387, 335, 325, 265, 207	Granatum flavanyl xyloside	Flavanone glycoside	-	+	-
18.	210.2	295, 330	355.1025	$C_{16}H_{19}O_9$	2.6	325, 221	Unknown		-	-	+

				Mol.	Erro				Red	Pomegran	

Peak	RT (sec.)	UV(nm)	[M-H]$^-$	Formula	r (ppm)	MS fragments	Name	Class	cabbage	ate	Grapefruit
19.	211.5	280, 323 shd.	393.1754	$C_{17}H_{29}O_{10}$	3	372, 355, 99	Hexen-1-ol-pentosyl hexoside	Alcohol glycoside	-	+	-
20.	212.2	276	785.086	$C_{34}H_{25}O_{22}$	2.1	633, 483, 481, 321	Di-*O*-galloyl-hexahydroxydiphenoyl-glucopyranose (Tercatain)	Tannin	-	+	-
21.	213.5	289, 329	519.1685	$C_{22}H_{31}O_{14}$	6.7	497, 423, 355, 175	Citrusin F	Cinnamate	-	-	+
22.	216.9	272	633.0724	$C_{27}H_{21}O_{18}$	1.4	331,481, 265, 179	Punicacortein A/B	Tannin	-	+	-
23.	217.5	284, 324 shd.	1109.304	$C_{49}H_{57}O_{29}$	-4	995, 885, 771, 683, 555, 487, 443, 285	Kaempferol-*O*-feruloylsophoroside-di-hexoside	flavonol acylated glycoside	+	-	-
24.	223.4	281	449.1085	$C_{21}H_{21}O_{11}$	1	415, 385, 329	Unknown		-	+	-
25.	223.7	271, 334	593.1509	$C_{27}H_{29}O_{15}$	0.5	575, 503, 473, 311	3,8-*C,C*-Diglucosylapigenin	*C*-Flavone glycoside.	-	-	+
26.	225.4	-	623.1565	$C_{28}H_{31}O_{16}$	8.4	605, 533, 503, 413, 329	*C,C*-Diglucosyldiosmetin	*C*-Flavone glycoside	-	+	-
27.	225.7	279	393.1178	$C_{19}H_{21}O_9$	3	329	Unknown		-	+	-
28.	228.4	254, 289 shd.	463.0515	$C_{20}H_{15}O_{13}$	0.7	301, 283	Ellagic acid-*O*-hexoside	Tannin	-	+	-
29.	238.7	303	935.2496	$C_{35}H_{51}O_{29}$	2.7	625, 467, 287	Unknown		+	-	-
30.	240.5	286, 322	741.2241	$C_{33}H_{41}O_{19}$	3.9	625, 577, 509, 417, 341	Naringenin 4′- *O* – glucoside-7-*O*-rutinoside (Narirutin 4′-glucoside)	Flavanone glycoside	-	-	+
31.	244.3	277	415.1605	$C_{19}H_{27}O_{10}$	1.2	393	Unknown		-	+	-
32.	246.8	290, 330	965.2617	$C_{54}H_{45}O_{17}$	4.6	657	Unknown		+	-	-
33.	248.3	274.5	951.0788	$C_{41}H_{27}O_{27}$	4.5	799, 771, 649, 507, 415	Granatin B	Tannin	-	+	-
34.	249.2	289, 324	753.227	$C_{34}H_{41}O_{19}$	-2.9	609, 223, 175	Disinapoylgentiobiose	Phenolic acid	+	-	-

Peak	RT (sec.)	UV(nm)	[M-H]$^-$	Mol. Formula	Error	MS fragments	Name	Class	Red cabbage	pomegranate	Grapefruit

					(ppm)						
35.	255.6	322, 288 shd.	917.2371	$C_{42}H_{45}O_{23}$	-1.5	285, 161	Kaempferol-*O*-*p*-coumaroylsophoroside-*O*-glucoside	Flavonol acylated glycoside	+	-	-
36.	257.7	324	497.1303	$C_{22}H_{25}O_{13}$	0.5	427, 161	Unknown		-	-	+
37.	261	322, 289 shd.	947.2511	$C_{43}H_{47}O_{24}$	-5.1	285, 161	Kaempferol-*O*-feruloylsophoroside-*O*-hexoside	Flavonol acylated glycoside	+	-	-
38.	263.1	325	413.2176	$C_{21}H_{33}O_{8}$	1.3	367, 161	Unknown		-	-	+
39.	272.6	279, 300 shd.	507.1507	$C_{24}H_{27}O_{12}$	0.1	489, 345,327	Unknown		-	+	-
40.	273.3	288, 326	649.2513	$C_{32}H_{41}O_{14}$	1.8	413, 341	Unknown		-	-	+
41.	289.8	284, 328 shd.	579.1749	$C_{27}H_{31}O_{14}$	-5.2	459, 413, 341, 271, 191	Naringin	*O*-Flavanone glycoside	-	-	+
42.	305.7	287, 327	623.1622	$C_{28}H_{31}O_{16}$	-0.7	605, 533, 503, 579, 443	6,8-*C,C*-Diglucosyldiosmetin isomer	*C*-flavone glyc.	-	-	+
43.	306.5	313	229.1437	$C_{12}H_{21}O_{4}$	3.4	211	Unknown		+	-	
44.	308.7	294	507.1147	$C_{23}H_{23}O_{13}$	-0.6	463, 305, 201	Unknown flavonoid glycoside		-	-	+
45.	309.9	322	723.2177	$C_{33}H_{39}O_{18}$	-4.9	427, 341, 223, 193	Feruloyl-sinapoylgentiobiose	Phenolic acid	+	-	-
46.	315.4	287, 323 shd.	609.1846	$C_{46}H_{25}O_{2}$	3.3	507, 425, 341	Unknown		-	-	+
47.	317.2	275	409.2058	$C_{18}H_{33}O_{10}$	5.2	279	Unknown		-	+	-
48.	333	287, 321	693.2775	$C_{34}H_{45}O_{15}$	-1.6	531, 443, 341	Nomilinic acid-4-*O*-glucoside	Limonoid	-	-	+
49.	335	290, 320	711.2883	$C_{34}H_{47}O_{16}$	-1.9	693, 549, 341	Nomilinic acid -17-*O*-glucoside	Limonoid	-	-	+
50.	340.7	308	651.1583	$C_{29}H_{31}O_{17}$	-2.5	507, 417, 341	Kaempferol acetyl dihexoside		-	-	+
51.	343.8	294, 318	843.1994	$C_{39}H_{39}O_{21}$	-0.6	651, 507, 341, 201	Unknown		-	-	+

Peak	RT (sec.)	UV(nm)	$[M-H]^-$	Mol. Formula	Error	MS fragments	Name	Class	Red cabbage	pomegranate	Grapefruit

					(ppm)						
52.	345	286, 324	537.167	$C_{18}H_{33}O_{18}$	0.5	343, 299	Unknown		+	-	-
53.	348.7	326	959.2868	$C_{45}H_{51}O_{23}$	-4.3	753, 537, 411, 343, 223	Trisinapoylgentiobiose	Phenolic acid	+	-	-
54.	351.9	291, 320	633.2545	$C_{32}H_{41}O_{13}$	1.2	463, 341, 261, 193	Obacunone 17-*O*-glucoside	Limonoid	-	-	+
55.	356.5	289, 322	929.2749	$C_{44}H_{49}O_{22}$	-3	641, 537, 489, 343, 223	Feruloyl-disinapoylgentiobiose	Phenolic acid	+	-	-
56.	360	268, 314	201.0186	$C_{11}H_{5}O_{4}$	3.5	-	Bergaptol	Furanocoumarin	-	-	+
57.	367.1	292, 319	399.2375	$C_{21}H_{35}O_{7}$	3.4	341, 330, 201	Citrusoside A	Prenylated sugar	-	-	+
58.	373.1	286, 326	593.1872	$C_{28}H_{33}O_{14}$	0.7	341	(Neo)poncirin	*O*-flavanone glycoside	-	-	+
59.	403.2	286	481.1134	$C_{25}H_{21}O_{10}$	1.3	-	Unknown		-	+	-
60.	407.9	261, 288 shd.	269.0434	$C_{15}H_{9}O_{5}$	7.8	-	Unknown		-	+	-
61.	417.9	N.D.	327.2196	$C_{18}H_{31}O_{5}$	5.9	291, 309	Trihydroxy-octadecadienoic acid	Fatty acid	+	-	-
62.	420.4	301	371.1488	$C_{21}H_{23}O_{6}$	3.3	341	6′,7′-Dihydroxybergamotin	Furanocoumarin	-	-	+
63.	443.2	N.D.	329.234	$C_{18}H_{33}O_{5}$	1.8	311, 293	Trihydroxy-octadecenoic acid	Fatty acid	+	-	-
64.	444	N.D.	329.2312	$C_{18}H_{33}O_{5}$	6.6	-	Unknown		-	+	-
65.	489.5	N.D.	469.186	$C_{26}H_{29}O_{8}$	1.6	341	Limonin/17-Epilimonin.	Limonoid	-	-	+
66.	501.2	N.D.	307.1895	$C_{18}H_{27}O_{4}$	6.5	289, 235	Hydroxy-oxo-octadecatrienoic acid	Fatty acid	+	-	-
67.	552.2	N.D.	311.2214	$C_{18}H_{31}O_{4}$	4.5	293, 265	Hydroxy-oxo-octadecenoic acid	Fatty acid	+	-	-
68.	555	N.D.	487.3411	$C_{30}H_{47}O_{5}$	3.8	447	Unknown		-	+	-
69.	564.4	N.D.	309.2063	$C_{18}H_{29}O_{4}$	2.8	291, 197	Hydroxy-oxo-octadecadienoic acid	Fatty acid	+	-	-

Peak	RT (sec.)	UV(nm)	[M-H]$^-$	Mol. Formula	Error (ppm	MS fragments	Name	Class	Red cabbage	pomegranate	Grapefruit

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70.	586.3	N.D.	313.2373	$C_{18}H_{33}O_4$	3.6	-	Dihydroxy-octadecenoic acid	Fatty acid	+	-	-
71.	618.7	N.D.	291.1966	$C_{18}H_{27}O_3$	0.1	-	Hydroxy-octadecatetraenoic acid	Fatty acid	+	-	-
72.	645.3	N.D.	293.212	$C_{18}H_{29}O_3$	0.8	275, 171	Hydroxy-octadecatrienoic acid	Fatty acid	+	-	-
73.	673.3	278	291.1967	$C_{18}H_{27}O_3$	0.5	273	Oxo-octadecatrienoic acid	Fatty acid	+	-	-
74.	682.1	N.D.	295.228	$C_{18}H_{31}O_3$	0.4	277	Hydroxy-octadecadienoic acid	Fatty acid	+	-	-
75.	711.9	N.D.	297.1519	$C_{19}H_{21}O_3$	-7.7	265	Geranyloxycoumarin	Coumarin	-	-	+
76.	713.2	N.D.	297.1527	$C_{12}H_{25}O_8$	9.5	279, 175	Hydroxy-octadecenoic acid	Fatty acid	+	-	-
77.	727.5	N.D.	297.1522	$C_{19}H_{21}O_3$	8.6	-	Unknown		-	+	-
78.	782.1	N.D.	311.1678	$C_{20}H_{23}O_3$	8	-	Unknown		-	+	-
79.	823.2	N.D.	277.2167	$C_{18}H_{29}O_2$	2.2	251, 211	Linolenic acid	Fatty acid	+	-	-
80.	916.3	N.D.	255.232	$C_{16}H_{31}O_2$	3.5	-	Palmitic acid	Fatty acid	+	-	-
81.	931.8	N.D.	281.2485	$C_{18}H_{33}O_2$	0.5	-	Oleic acid	Fatty acid	+	+	-
82.	1008.9	N.D.	339.1993	$C_{22}H_{27}O_3$	8.1	-	Unknown		-	+	-

+ and – denotes the presence or absence of a metabolite in a certain functional food juice extract. N.D.= not detected