

Characterization and valorization of ‘Sulmona red garlic’ peels and small bulbs

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Table S1. Retention time, calibration curve and correlation coefficient of reference compounds.

	Retention time (min)	Calibration curve (µg/mL)	Correlation coefficient
Gallic acid	4.86	$y = 15.51x + 37.06$	0.9987
Alliin	6.89	$y = 6.35x + 50.34$	0.9987
Catechin	15.48	$y = 5.18x - 24.29$	0.9961
Chlorogenic acid	18.01	$y = 12.02x - 3.95$	0.9991
Caffeic acid	19.01	$y = 35.23x - 28.86$	0.9989
Epicatechin	20.98	$y = 2.47x + 58.32$	0.9982
<i>p</i> -Coumaric acid	24.71	$y = 42.12x - 19.25$	0.9987
Cyanidin-3-rutinoside	27.01	$y = 16.58x + 34.53$	0.9987
Ferulic acid	27.38	$y = 20.65x + 22.96$	0.9993
Sinapic acid	27.91	$y = 11.37x + 9.92$	0.9987
Myricetin	32.40	$y = 21.51x - 5.93$	0.9991
Quercetin	37.78	$y = 21.69x + 24.12$	0.9995
Kaempferol	42.25	$y = 25.94x + 27.50$	0.9988

Figure S1. Chromatogram of standard compounds. Panel A: 1. Gallic acid; 2. Alliin; 3. Catechin; 4. Chlorogenic acid; 5. Caffeic acid; 6. Epicatechin; 7. *p*-Coumaric acid; 8. Cyanidin-3-rutinoside; 9. Ferulic acid; 10. Sinapic acid; Panel B 11. Myricetin; 12. Quercetin; 13. Kaempferol.

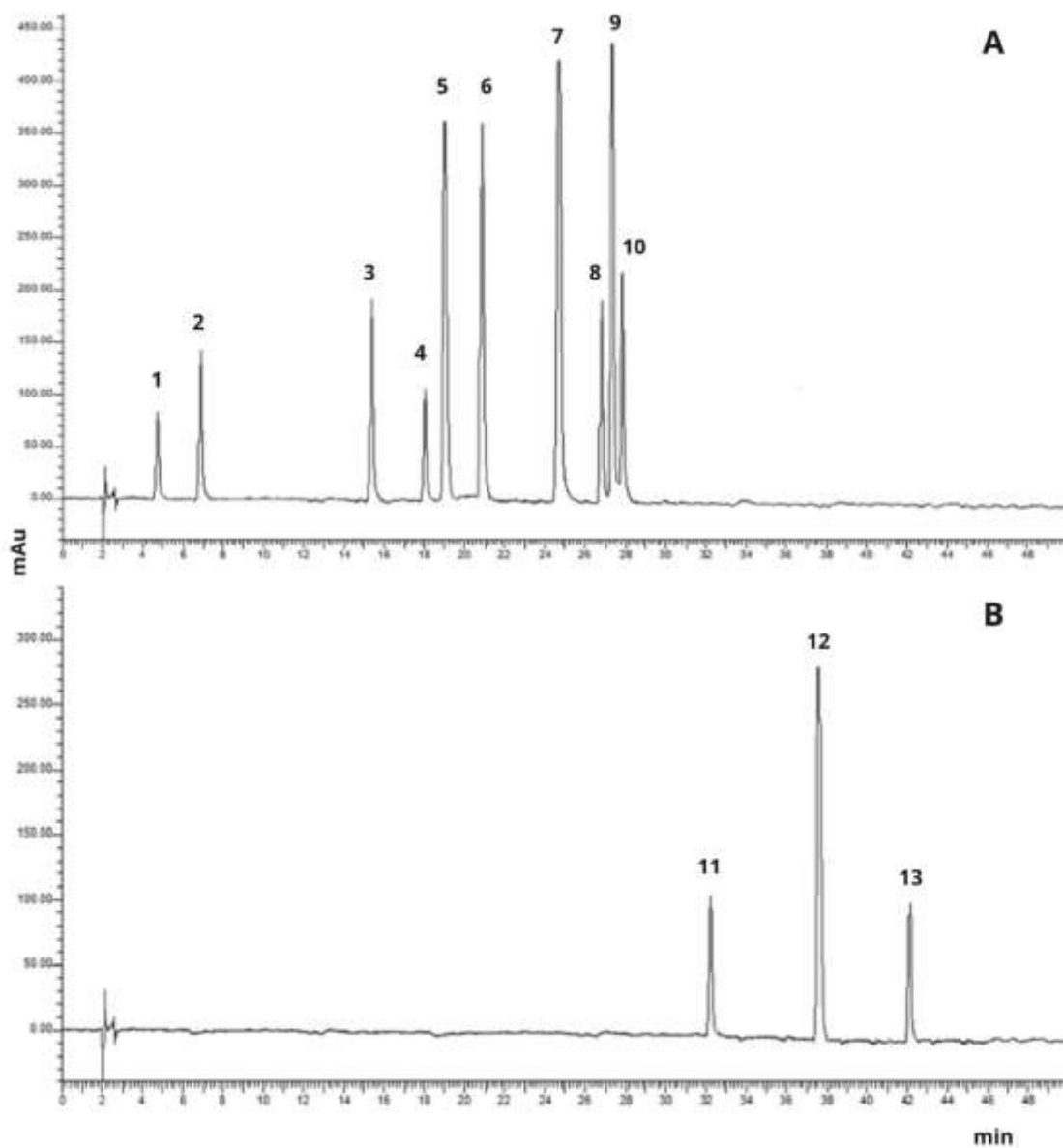


Table S2. Extraction yield of obtained hydroalcoholic extracts (p value < 0.002).

Harvest date	2020	2021
Sample	Yield %	
W	2.2 ± 0.5	3.3 ± 0.1
R	3.9 ± 0.5	5.2 ± 0.4
B	14.9 ± 1.9	17.9 ± 0.7

Table S3. CIEL*a*b parameters of the hydroalcoholic dried extracts. ^a p value ≤ 0.002 ; ^b p value ≤ 0.01 ; ^c p value ≤ 0.001 ; ^{a,b} p value ≤ 0.02 ; ^{a,c} p value ≤ 0.05 ; ^{a,c} p value ≤ 0.001 .

Sample	Harvest	L*	a*	b*	C* _{ab}	h _{ab}
W^a	2020	73.1 ± 0.9	-0.5 ± 0.7	21.3 ± 5.4	21.4 ± 5.4	91.3 ± 1.6
	2021	70.8 ± 0.3	-2.2 ± 0.1	16.0 ± 0.4	16.1 ± 0.4	97.8 ± 0.7
R^b	2020	61.8 ± 4.6	17.1 ± 2.6	6.5 ± 1.2	18.8 ± 1.6	23.2 ± 1.7
	2021	66.1 ± 0.1	8.3 ± 0.1	5.5 ± 0.1	10.0 ± 0.1	33.6 ± 0.1
B^c	2020	72.4 ± 4.8	-1.7 ± 0.2	9.4 ± 2.3	9.5 ± 2.4	101.7 ± 5.1
	2021	76.1 ± 0.1	-1.7 ± 0.1	2.4 ± 0.1	2.97 ± 0.1	125.0 ± 2.3

Figure S2. Reflectance curves. Panel A, white tunica, 2020 and 2021; Panel B, red tunica, 2020 and 2021; Panel C; bulb, 2020 and 2021.

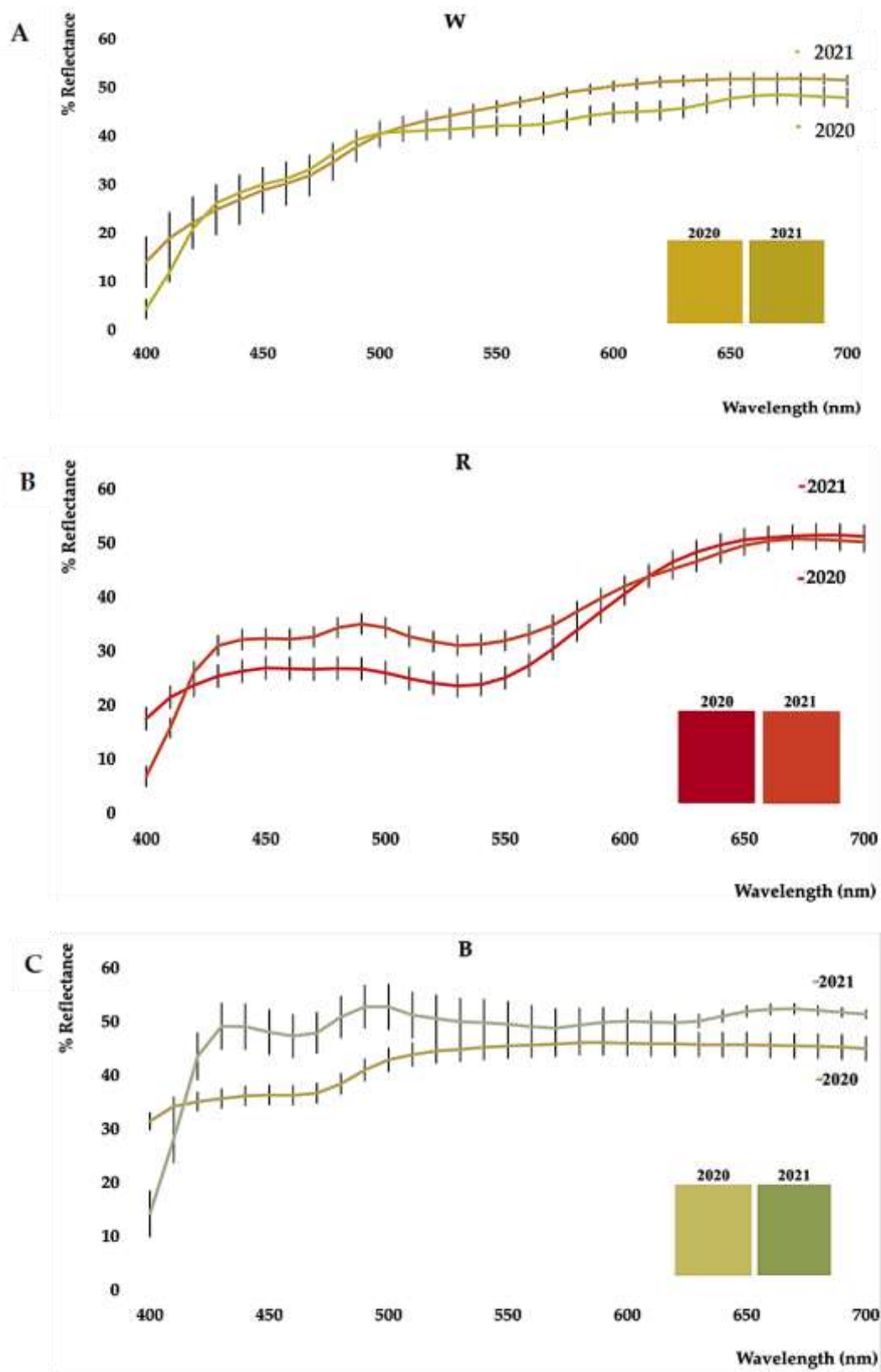


Table S4. DPPH analysis of the obtained extracts expressed as Inhibition % calculated as: Control Abs – Sample Abs/Control Abs x 100. *p* value ≤ 0.05 .

Harvest date	July 2020	July 2021
Sample	DPPH (Inhibition %)	
W	24.19 \pm 0.09	39.21 \pm 2.50
R	19.76 \pm 0.16	16.70 \pm 1.14
B	3.25 \pm 0.12	2.19 \pm 0.04

Figure S3. Chromatograms related the different analyzed samples. Panel A (W-2020, W-2021); Panel B (R-2020; R-2021); Panel C (R-2020, R-2021 and B-2020, B-2021). Identified peaks: 1. Gallic acid; 2. Alliin; 3. Catechin; 4. Chlorogenic acid; 5. Caffeic acid; 6. Epicatechin; 7. *p*-coumaric acid; 8. Ferulic acid; 9. Sinapic acid; 10. Myricetin; 11. Quercetin; a. cinnamic acid derivative; b. kaempferol derivative; c,d,e. anthocyanins.

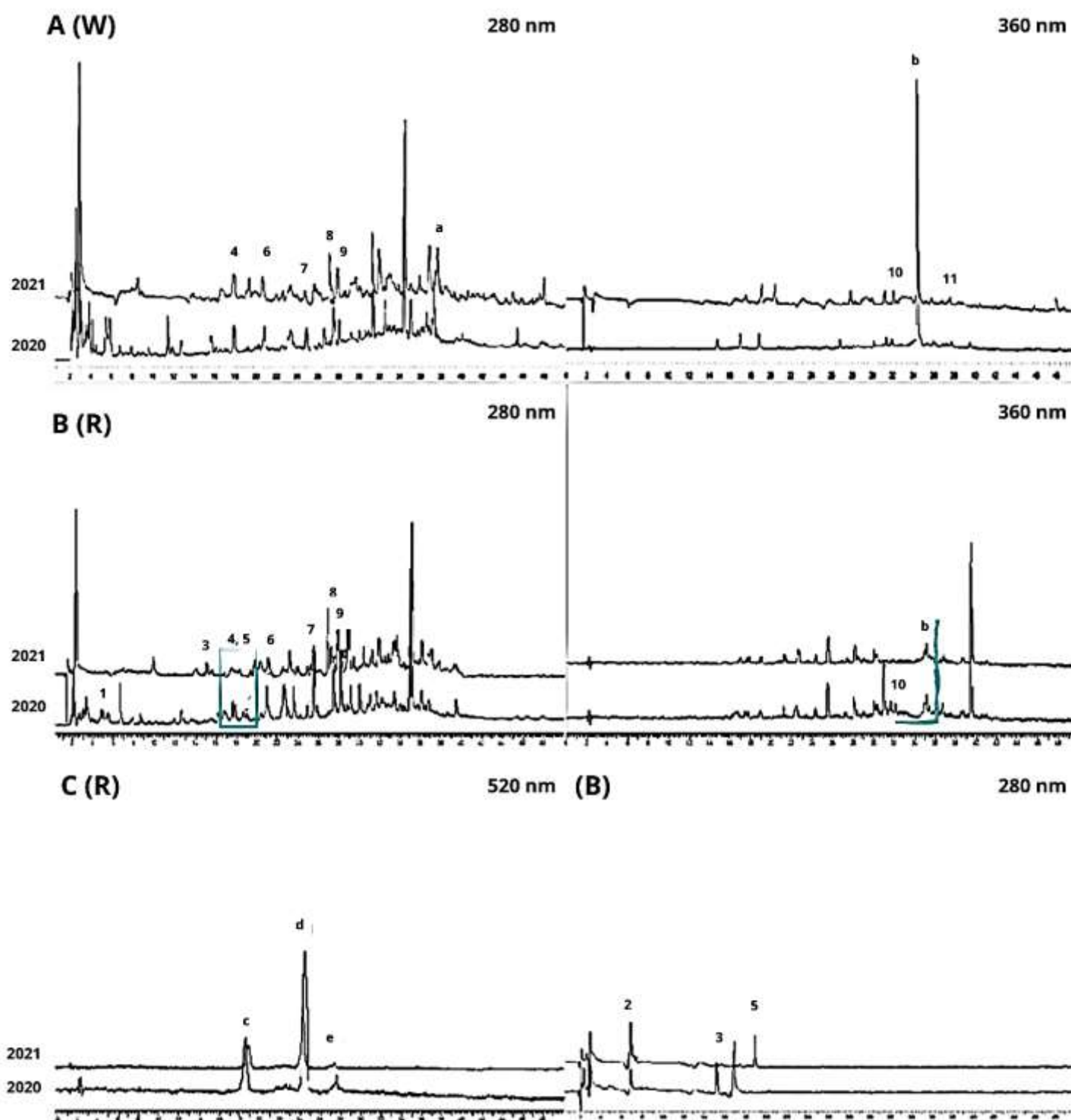


Table S5. HPLC-DAD quantitative analysis. Values are expressed as mg/g dry extract \pm SD; NI: not identified; ---: not searched; *expressed as equivalents of cyanidin-3-rutinoside; **expressed as equivalents of Kaempferol; ***expressed as equivalents of *p*-coumaric acid. ^a*p* value \leq 0.002; ^b*p* value \leq 0.001; ^c*p* value \leq 0.87; ^{a,b}*p* value \leq 0.03; ^{a,c}*p* value \leq 0.002; ^{b,c}*p* value \leq 0.009.

	White tunica (W) ^a		Red tunica (R) ^b		Bulb (B) ^c	
	2020	2021	2020	2021	2020	2021
Gallic acid	NI	NI	0.03 \pm 0.01	NI	NI	NI
Alliin	NI	NI	NI	NI	0.20 \pm 0.03	0.26 \pm 0.08
Catechin	NI	NI	NI	0.84 \pm 0.02	2.05 \pm 0.06	NI
Chlorogenic acid	0.32 \pm 0.02	0.58 \pm 0.03	NI	NI	NI	NI
Caffeic acid	NI	NI	0.21 \pm 0.02	NI	NI	0.20 \pm 0.06
Epicatechin	2.08 \pm 0.10	1.56 \pm 0.08	5.95 \pm 0.07	2.29 \pm 0.2	NI	NI
<i>p</i>-Coumaric acid	0.10 \pm 0.01	0.14 \pm 0.01	0.08 \pm 0.01	NI	NI	NI
Anthocyanins*	---	---	2.50 \pm 0.07	0.67 \pm 0.02	---	---
Ferulic acid	0.29 \pm 0.01	0.43 \pm 0.02	0.92 \pm 0.01	0.37 \pm 0.03	NI	NI
Sinapic acid	0.32 \pm 0.02	0.63 \pm 0.03	0.40 \pm 0.03	0.67 \pm 0.003	NI	NI
Myricetin	0.08 \pm 0.01	0.16 \pm 0.01	0.10 \pm 0.01	NI	NI	NI
Kaempferol derivative**	1.64 \pm 0.08	1.97 \pm 0.15	0.80 \pm 0.01	0.15 \pm 0.01	NI	NI
Quercetin	0.04 \pm 0.01	0.08 \pm 0.01	NI	NI	NI	NI
Cinnamic acid derivative***	0.55 \pm 0.03	0.54 \pm 0.03	NI	NI	NI	NI

SD: standard deviation.

Figure S4. Comparison between experimental ESI(+) CID assay performed by using LTQ XL ion trap and reference data obtained from Metlin database has allowed to confirm the assignments of the following peaks: Panel A) anethole m/z 149; Panel B) ferulic acid m/z 195.

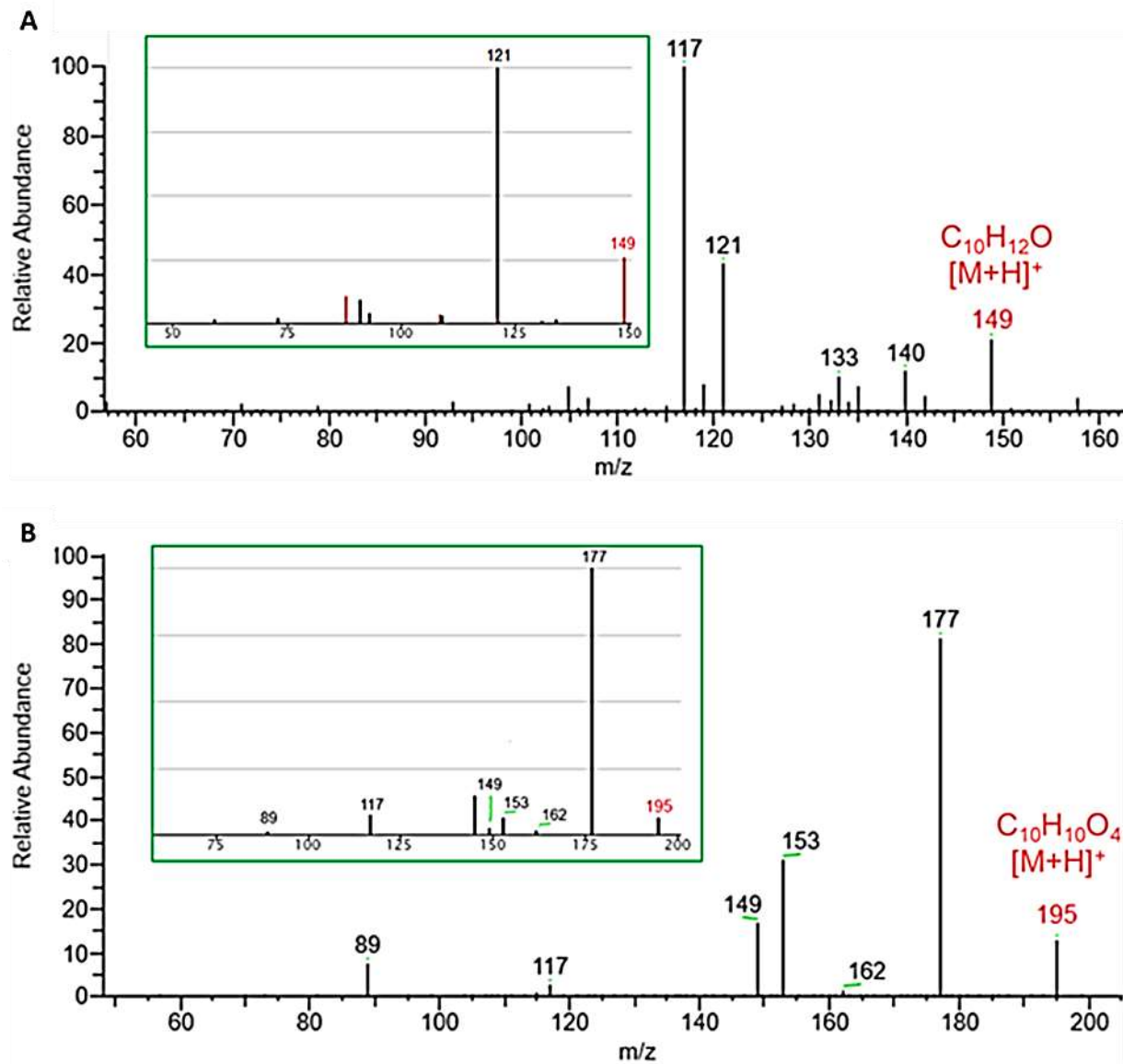


Figure S5. Van Krevelen diagram obtained by ESI FT-ICR MS analysis of hydroalcoholic extracts from ‘Sulmona red garlic’. The diagrams show broken lines with the following meaning: (A) lines related to (de)hydrogenation paths; (B) lines associated to oxidation or reduction reactions; (C) lines that describe hydration and condensation processes; (D) lines that correspond to (de)methylation paths. Noteworthy, peaks along A-lines include myristoleic ($C_{14}H_{26}O_2$)/myristic acids ($C_{14}H_{28}O_2$) for $O/C = 0.14$, palmitoleic ($C_{16}H_{30}O_2$)/palmitic ($C_{16}H_{32}O_2$) acids for $O/C = 0.12$; carnosol ($C_{20}H_{26}O_4$)/carnosic acid ($C_{20}H_{28}O_4$) for $O/C = 0.2$; items along B-lines encompass cysteine ($C_3H_7NO_2S$)/cysteic acid ($C_3H_7NO_5S$) for $H/C = 2.3$, oleic acid ($C_{18}H_{34}O_2$)/octadecadienoic acid ($C_{18}H_{34}O_4$) for $H/C = 1.8$, abscisic alcohol ($C_{15}H_{22}O_3$)/xanthoxic acid ($C_{15}H_{22}O_4$) for $H/C = 1.4$, ferulaldehyde ($C_{10}H_{10}O_3$)/ferulic acid ($C_{10}H_{10}O_4$) for $H/C = 1$; hits along D-lines include myristic ($C_{14}H_{28}O_2$)/palmitoleic ($C_{16}H_{30}O_2$)/linoleic ($C_{18}H_{32}O_2$) acids.

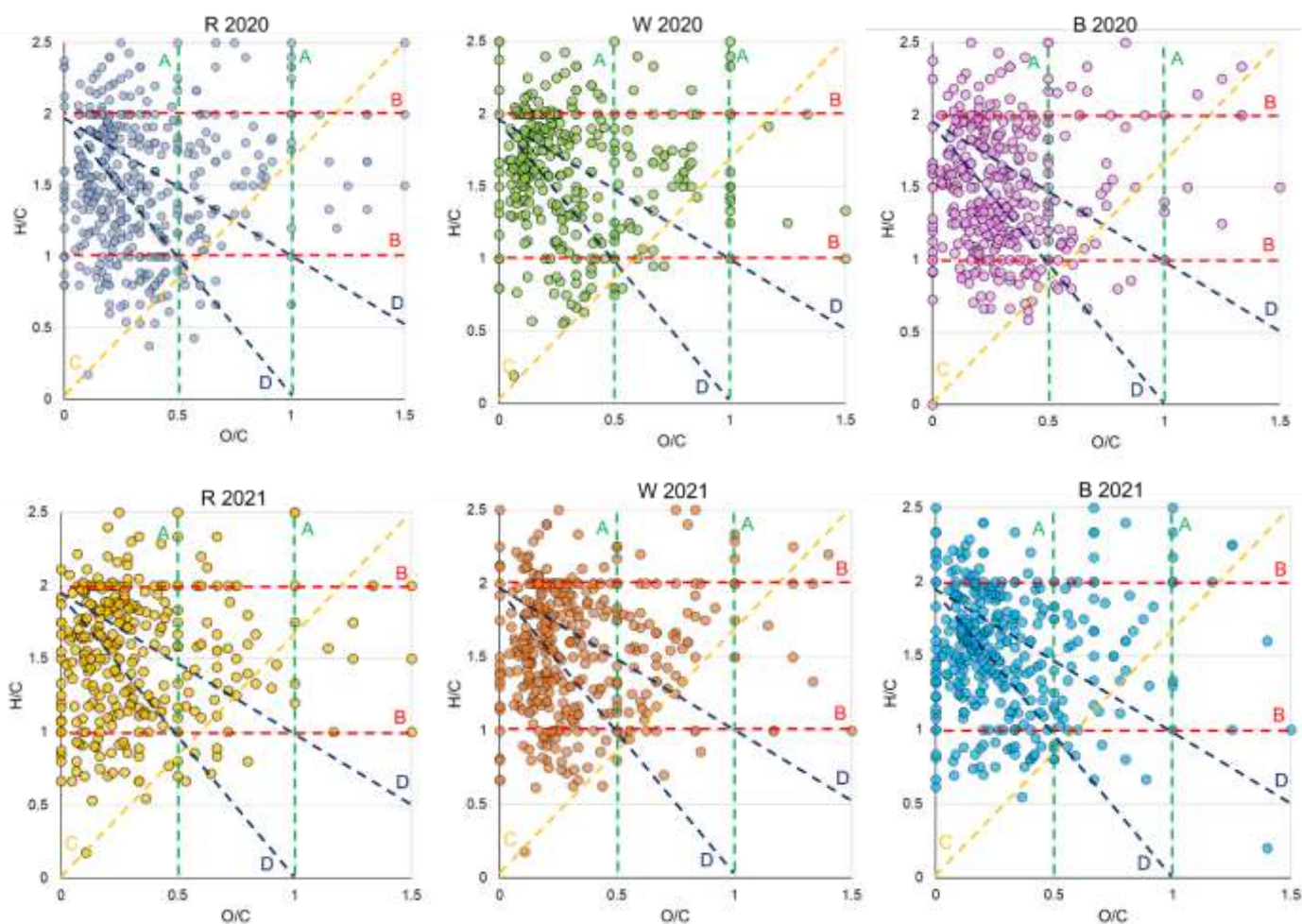


Figure S6. Enlargement of ESI(+) FT-ICR MS of red tunica 2021 extract. Spectrum shows protonated (m/z 178.05310) and sodiated (m/z 200.03512) adducts of metabolite with molecular formula $C_6H_{11}NO_3S$.

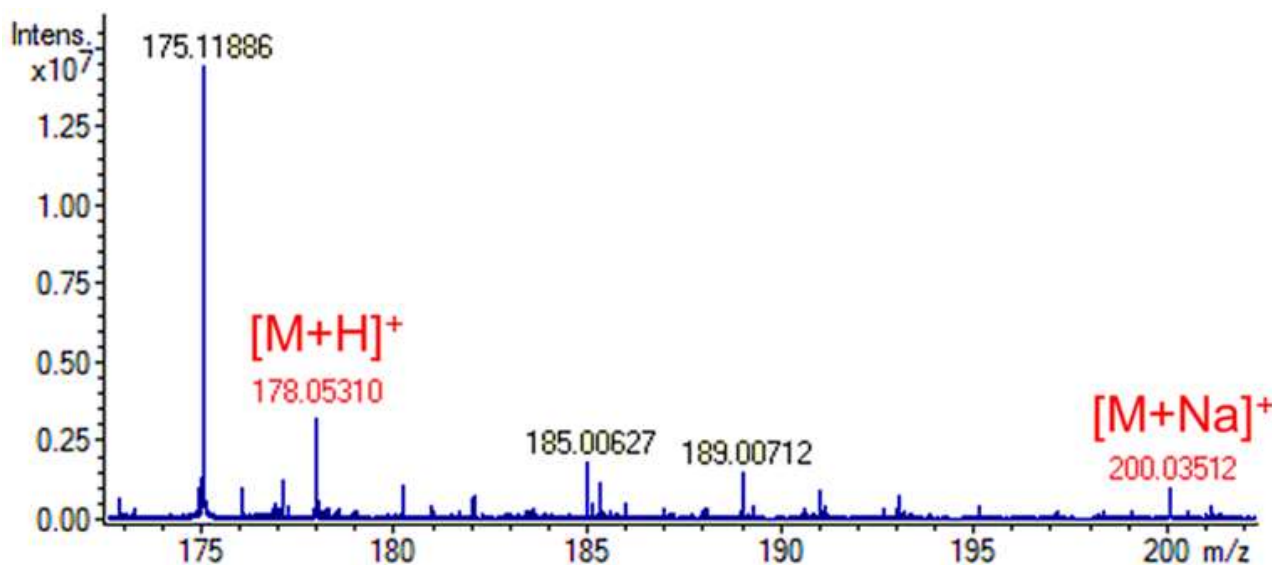


Figure S7. Comparison between experimental ESI(+) CID assay of peaks at m/z 178.0 performed by using LTQ XL ion trap and reference data obtained from Metlin database (green panel). Red fragments belonging to *N*-formylmethionine and blue fragments fit to $[C_3H_5NO_2+H]^+$ fragment present in both alliin and 1-PeCSO spectra.

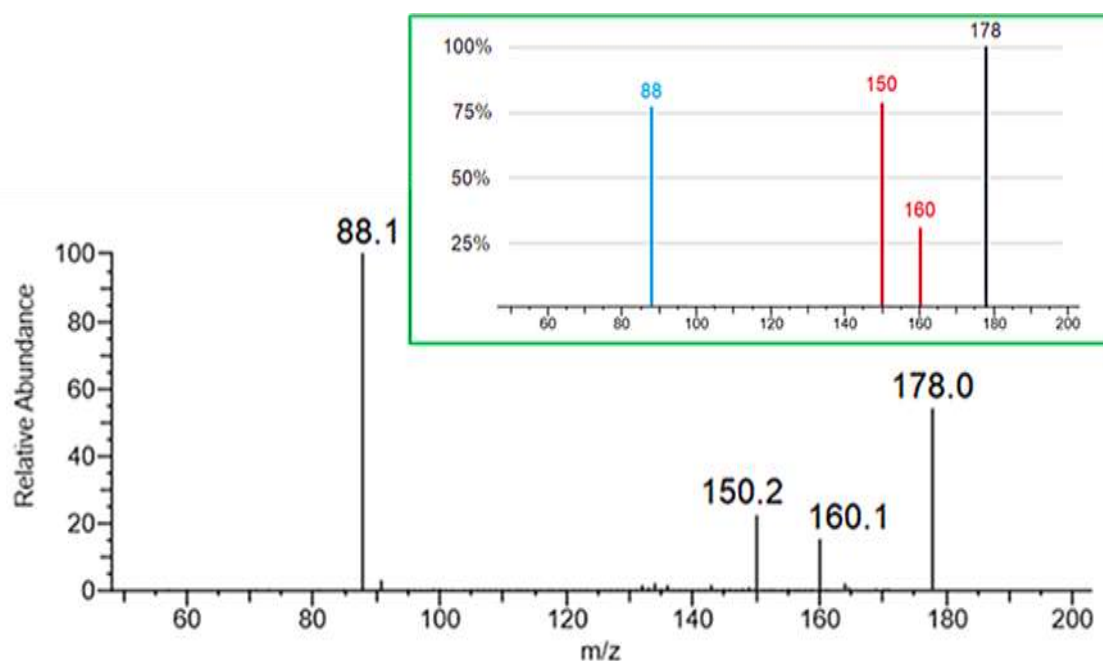


Figure S8. Panel A: Scores plot of the PCA analyses of the FT-ICR MS data for white and red tunica, and bulb of ‘Sulmona red garlic’ extracts. The firsts two components retain close to 70% of variation. in both cases. Dendograms, obtained on Pearson distances, are reported in panel B.

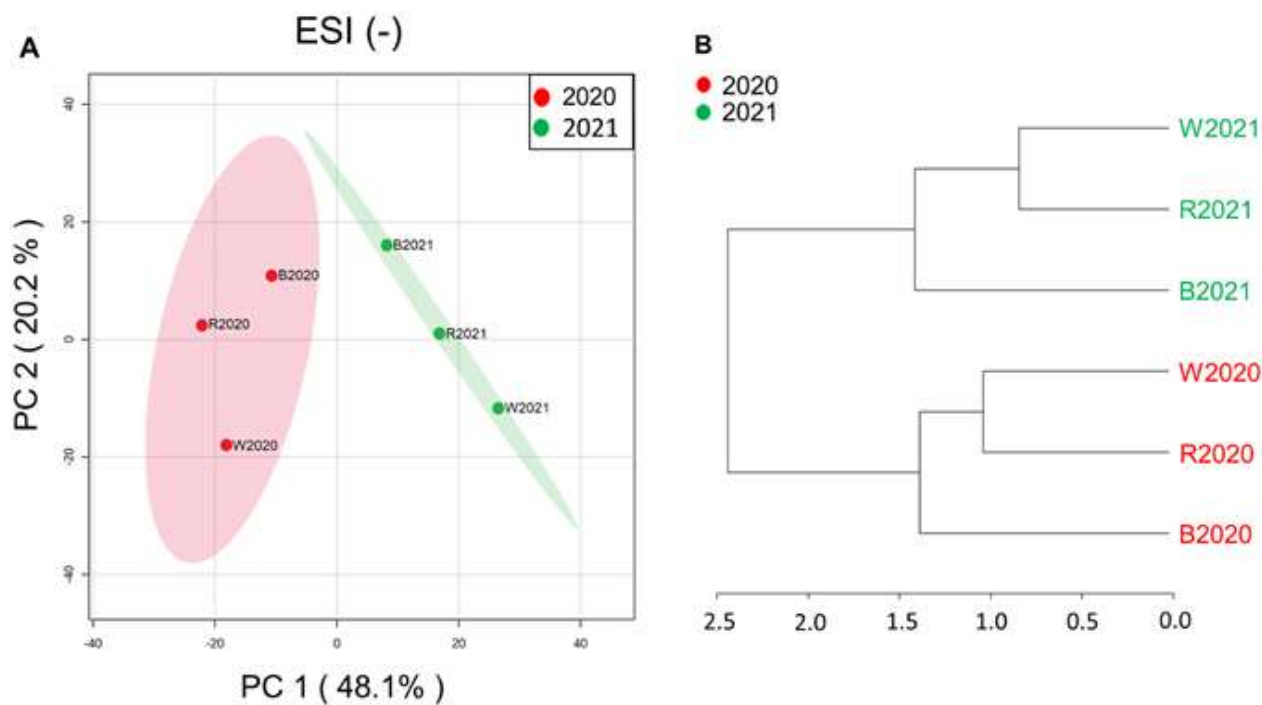


Figure S9. Box plots of most statistically relevant features discovered in ESI(-) data set. Box plots summarize the normalized concentrations and display that stearic and palmitic acids are variables more relevant for vintage 2020, as well as phosphatidic acid is more relevant for 2021. Positive polarity mode underlined (4-aminobutyl)guanidine ($[C_5H_{14}N_4+Na]^+$), isopropylmaleate ($[C_7H_{10}O_4+Na]^+$), fraxetin ($[C_{10}H_8O_5+H]^+$), butenylcarnitine ($[C_{11}H_{19}NO_4+H]^+$), faltarindiol ($[C_{17}H_{24}O_2+K]^+$) as the most significant features.

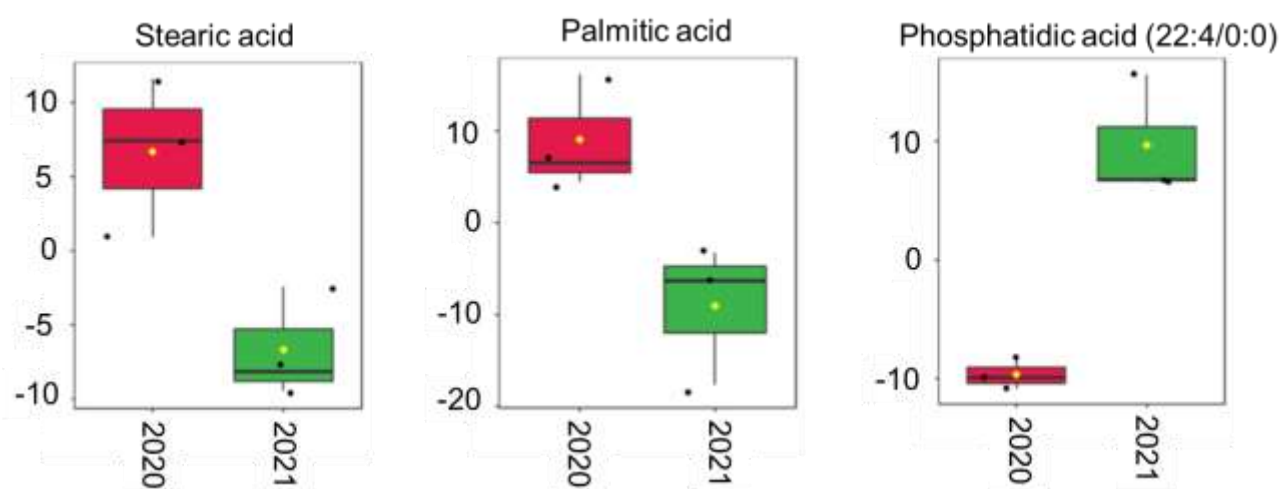


Figure S10. Cell metabolic activity (MTS assay) of undifferentiated (monocytes) and differentiated (macrophages), after 24 h and 48 h. THP-1 cells were assayed without differentiation or after differentiation as described in Materials and Methods. Undifferentiated and differentiated cells were untreated or treated with different doses (5, 10, 25, 50, 100 µg/mL) of garlic extracts (W: White Tunica; B: Bulb; R: Red Tunica). (Panel A) undifferentiated THP-1 cells at 24 h; (Panel B) differentiated THP-1 cells at 24 h; (Panel C) undifferentiated THP-1 cells and (Panel D) differentiated THP-1 cells at 48 h. The cells were stimulated with H₂O₂ as cytotoxicity model at concentration of 1 mM for 8 h. Data are expressed as the mean ± SD (*n*=3) and are represented as percentages of the untreated control (100% viability); **p*<0.05 vs untreated cells (control); #*p*<0.05 vs H₂O₂ stimulation.

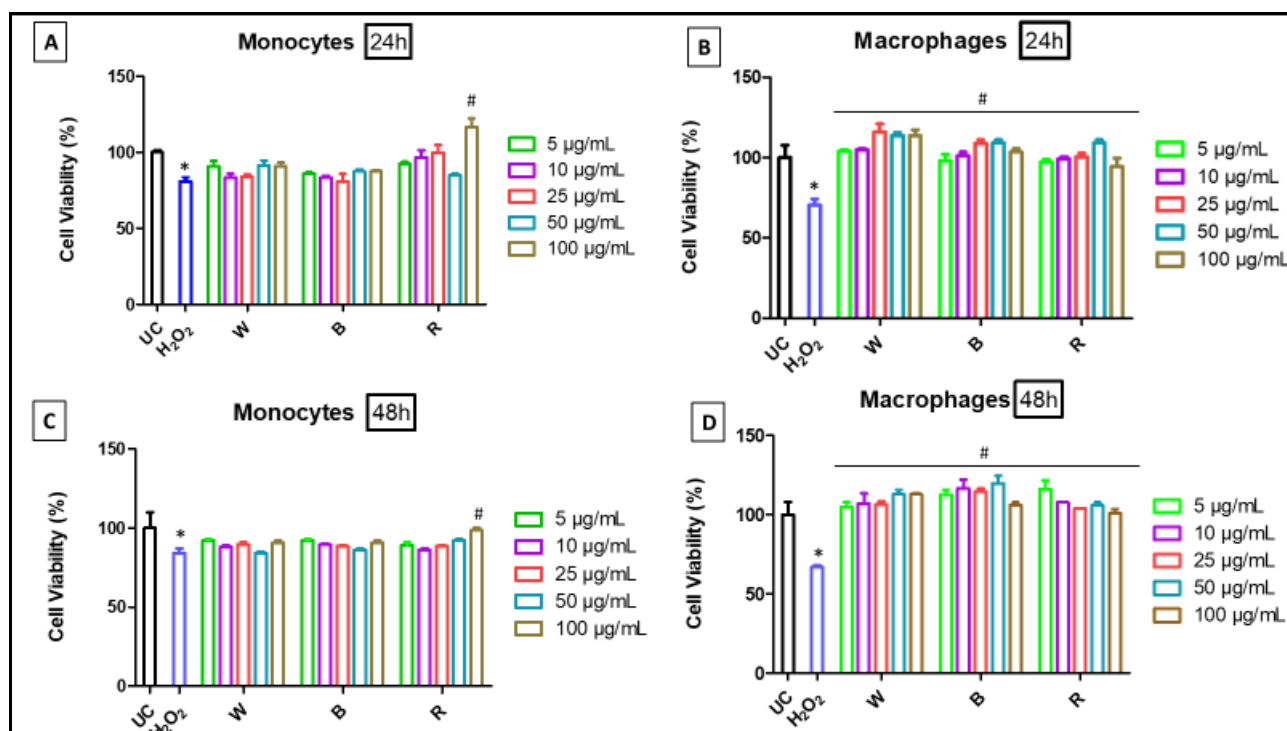


Figure S11. Generation of peroxynitrite by monocytes and macrophages after 24 h exposure. (Panels A, D) Histograms were obtained by flow cytometry and are generated by plotting the cell count (y-axis) and the FITC fluorescence emission (x-axis). (Panels B, C) Bar graphs show the fold increase of the mean fluorescence intensities (MFIs) related to the emissions in the FL-1/FITC channel which are proportional to the generation of peroxynitrite. Values are the ratios of the MFI generated from each sample on the unstained control (negative). $a = p < 0.01$, $b = p < 0.001$ and $c = p < 0.0001$ between treated samples and UC; $d = p < 0.01$, $e = p < 0.001$ and $f = p < 0.0001$ between samples and H_2O_2 . UC = untreated control.

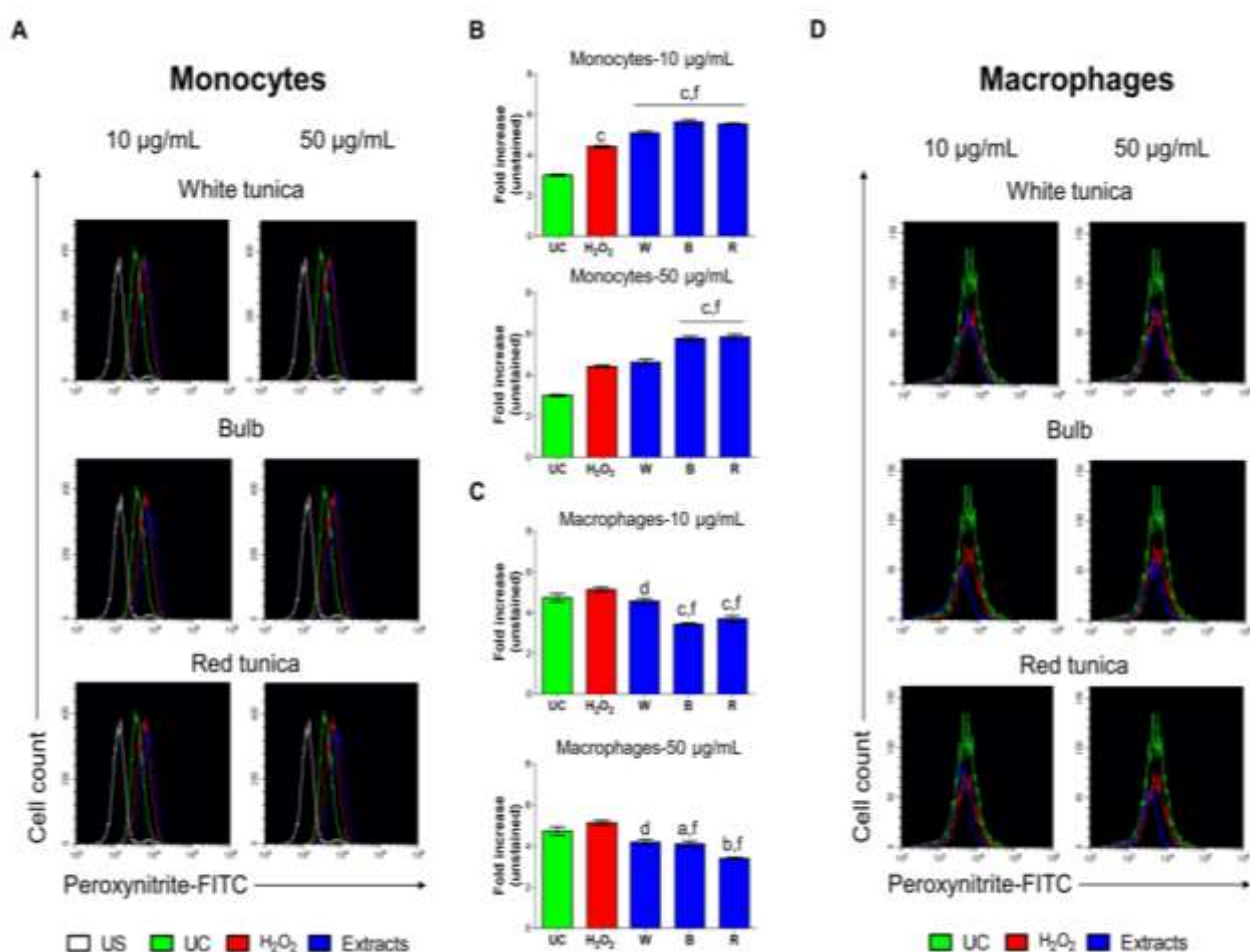


Table S6: Untargeted metabolic profiling of *Sulmona red garlic* hydroalcoholic extracts by ESI(+) FT-ICR MS

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1 Dimethylamine	[M+K] ⁺	C2H7N	84.02125			1.3E+05	-2.9			
2 Butyrate	[M+H] ⁺	C4H8O2	85.02877			9.8E+04	-4.3			
3 Methanethiol	[M+K] ⁺	CH4S	86.96611				1.2E+05	4.8		1.2E+05 3.2
4 Pentan-2-one	[M+H] ⁺	C5H10O	87.08046				1.1E+05	-0.2		
5 Piperazine	[M+H] ⁺	C4H10N2	87.09169		1.1E+05	-0.2				
6 Methylbutanamine	[M+H] ⁺	C5H13N	88.11185							1.1E+05 2.6
7 Pyruvic acid	[M+H] ⁺	C3H4O3	89.02329		1.2E+05	0.3	1.1E+05	4.8		
8 N,N'-Dimethylurea	[M+H] ⁺	C3H8N2O	89.07051						1.6E+05	4.8
9 Pentanol	[M+H] ⁺	C5H12O	89.09632						1.7E+05	-2.6
10 Oxamic acid	[M+H] ⁺	C2H3NO3	90.01857	1.1E+05	-3.4		1.1E+05	-3.0		
11 Alanine	[M+H] ⁺	C3H7NO2	90.05519		1.2E+05	-2.6				1.7E+05 5.0
12 N-(Aminomethyl)urea	[M+H] ⁺	C2H7N3O	90.06611				8.1E+04	0.9		
13 Oxalic acid	[M+H] ⁺	C2H2O4	91.00290							1.6E+05 -3.5
14 Propanethial S-oxide	[M+H] ⁺	C3H6OS	91.02151		1.3E+05	-3.3			1.4E+05	2.1
15 Imidazole	[M+Na] ⁺	C3H4N2	91.02623							1.4E+05 4.8
16 Lactate	[M+H] ⁺	C3H6O3	91.03855							1.6E+05 4.6
17 Diethyl sulfide	[M+H] ⁺	C4H10S	91.05774		1.5E+05	-1.6				
18 Butanediol	[M+H] ⁺	C4H10O2	91.07502		1.5E+05	3.7	8.5E+04	-2.7		
19 3-Aminopropane-1,2-diol	[M+H] ⁺	C3H9NO2	92.07072				1.1E+05	-1.2	1.9E+05	-1.3
20 Propynoic acid	[M+Na] ⁺	C3H2O2	92.99443				7.6E+05	2.9		1.1E+05 0.5
21 Thioglycolic acid	[M+H] ⁺	C2H4O2S	93.00057		2.3E+05	-1.0				
22 Butadiene	[M+K] ⁺	C4H6	93.01011	9.6E+04	4.8				2.1E+05	4.8
23 alpha-Aminopropionitrile	[M+Na] ⁺	C3H6N2	93.04197		1.2E+05	3.7				
24 3-Buten-1-amine	[M+Na] ⁺	C4H9N	94.06277						9.6E+04	-0.5
25 Aniline	[M+H] ⁺	C6H7N	94.06507						1.0E+05	0.6
26 Acrolein	[M+K] ⁺	C3H4O	94.98940							1.4E+05 -0.3
27 Malondialdehyde	[M+Na] ⁺	C3H4O2	95.00998				1.2E+05	3.9		
28 Butanal	[M+Na] ⁺	C4H8O	95.04674	1.0E+05	3.6	1.5E+05	3.2			
29 Phenol	[M+H] ⁺	C6H6O	95.04870						9.0E+04	4.6
30 Aminopyridine	[M+H] ⁺	C5H6N2	95.05993				2.1E+05	4.7		
31 N-Methylpyridinium	[M+H] ⁺	C6H8N	95.07304							1.2E+05 -0.9
32 Iminoglycine	[M+Na] ⁺	C2H3NO2	96.00542		1.6E+05	1.9			3.4E+05	-3.6
33 Cyclopropylamine	[M+K] ⁺	C3H7N	96.02115							1.3E+05 -1.5
34 Glyoxal	[M+K] ⁺	C2H2O2	96.96886		2.7E+05	-2.3				
35 Glyoxylic acid	[M+Na] ⁺	C2H2O3	96.99042							3.3E+05 -4.6
36 Methanesulfonic acid	[M+H] ⁺	CH4SO3	96.99513		1.5E+05	2.7				
37 Lactaldehyde	[M+Na] ⁺	C3H6O2	97.02574							1.8E+05 2.7
38 Propanoic acid	[M+Na] ⁺	C3H6O2	97.02600	1.5E+05	-2.9					
39 Furfural	[M+H] ⁺	C5H4O2	97.02841	1.3E+05	4.8					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
40 2-Cyclohexen-1-one	[M+H] ⁺	C6H8O	97.06512		1.6E+05	-3.4				
41 Aminoacetaldehyde	[M+K] ⁺	C2H5NO	98.00039				1.4E+05	-1.2		
42 Guanidine	[M+K] ⁺	CH5N3	98.01158				9.1E+04	-0.7		
43 Glycine	[M+Na] ⁺	C2H5NO2	98.02139		1.8E+05	-1.4	1.2E+05	-2.9		
44 Isopropylamine	[M+K] ⁺	C3H9N	98.03671				3.4E+05	-0.5	1.1E+05	4.6
45 Deoxycytosine	[M+H] ⁺	C4H7N3	98.07093						1.4E+05	3.5
46 Sulfuric acid	[M+H] ⁺	H2SO4	98.97540		1.3E+05	-0.4				
47 Thiourea	[M+Na] ⁺	CH4N2S	98.99878						1.2E+05	-0.4
48 Glycolic acid	[M+Na] ⁺	C2H4O3	99.00483				8.7E+04	4.4		
49 Hydroxyurea	[M+Na] ⁺	CH4N2O2	99.01650	2.3E+05	0.3					
50 Propan-2-ol	[M+K] ⁺	C3H8O	99.02067	8.7E+04	3.2					
51 Propyl mercaptan	[M+Na] ⁺	C3H8S	99.02396		1.2E+05	-0.7				
52 Propane-1,2-diol	[M+Na] ⁺	C3H8O2	99.04128				1.9E+05	3.7		
53 Imidazole-4-methanol	[M+H] ⁺	C4H6N2O	99.05536						1.3E+05	-0.7
54 Guanidine	[M+K41] ⁺	CH5N3	100.00917				1.2E+05	4.5		
55 Ethanolamine	[M+K] ⁺	C2H7NO	100.01592	8.7E+04	1.4					
56 2-Piperidinone	[M+H] ⁺	C5H9NO	100.07573						1.7E+05	-0.4
57 Cyclohexylamine	[M+H] ⁺	C6H13N	100.11204						1.1E+05	0.4
58 Glycol	[M+K] ⁺	C2H6O2	100.99994	6.8E+04	0.7					
59 Tiglic acid	[M+H] ⁺	C5H8O2	101.05931		1.8E+05	3.9	4.4E+05	-4.6		
60 Hexanal	[M+H] ⁺	C6H12O	101.09590					8.7E+04	1.9	
61 Pyridine	[M+Na] ⁺	C5H5N	102.03137		1.5E+05	0.5	1.4E+05	-2.7	8.3E+04	-3.3
62 1-Aminocyclopropane-1-carboxylate	[M+H] ⁺	C4H7NO2	102.05460					1.3E+05	3.5	1.6E+05
63 5-Aminopentanal	[M+H] ⁺	C5H11NO	102.09071						1.1E+05	5.0
64 Ethylenethiourea	[M+H] ⁺	C3H6N2S	103.03287					8.5E+04	-4.1	
65 Succinic acid semialdehyde	[M+H] ⁺	C4H6O3	103.03856						1.2E+05	4.0
66 N-Nitrosodiethylamine	[M+H] ⁺	C4H10N2O	103.08690					9.4E+04	-3.0	
67 Hexanol	[M+H] ⁺	C6H14O	103.11149					8.6E+04	2.4	
68 Cadaverine	[M+H] ⁺	C5H14N2	103.12283				1.0E+05	1.4		
69 Sulfite	[M+Na] ⁺	H2SO3	104.96205		1.6E+05	-3.5				
70 Allophanic acid	[M+H] ⁺	C2H4N2O3	105.02947	7.6E+04	-1.9					
71 Cyanopyridine	[M+H] ⁺	C6H4N2	105.04454					2.2E+05	1.8	9.5E+04
72 Hydroxybutanoic acid	[M+H] ⁺	C4H8O3	105.05468				8.8E+04	-0.6		
73 Styrene	[M+H] ⁺	C8H8	105.06979				1.3E+05	0.8		
74 3-Butyn-1-al	[M+K] ⁺	C4H4O	106.98937	8.1E+04	1.5					
75 Isoprene	[M+K] ⁺	C5H8	107.02576	9.0E+04	1.5				9.0E+04	0.0
76 Aminoimidazole	[M+Na] ⁺	C2H4N4	107.03329				1.2E+05	-4.4		
77 Glyceric acid	[M+H] ⁺	C3H6O4	107.03381		1.0E+05	0.7	1.2E+05	4.6		
78 Cyclohexane	[M+Na] ⁺	C6H12	107.08337						1.3E+05	-2.3
79 Iso-Valeraldehyde	[M+Na] ⁺	C5H10O	109.06202		2.6E+05	3.4				

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
80 3-Buten-1-amine	[M+K] ⁺	C4H9N	110.03670					8.7E+04	-0.4	
81 Malondialdehyde	[M+K] ⁺	C3H4O2	110.98346		1.6E+05	5.0				
82 Resorcinol	[M+H] ⁺	C6H6O2	111.04365		1.9E+05	3.7	4.3E+06	-3.5		
83 Putrescine	[M+Na] ⁺	C4H12N2	111.08907					9.9E+04	1.8	
84 N-(Aminomethyl)urea	[M+Na] ⁺	C2H7N3O	112.04786			2.9E+05	2.4			
85 Lactic acid	[M+Na] ⁺	C3H6O3	113.02089		2.0E+05	0.2				
86 Furoic acid	[M+H] ⁺	C5H4O3	113.02314			3.0E+05	1.6			
87 Butanol	[M+K] ⁺	C4H10O	113.03625				8.1E+04	0.7	8.3E+04	5.0
88 Butanediol	[M+Na] ⁺	C4H10O2	113.05782		2.7E+05	-4.6				
89 Aleprolic acid	[M+H] ⁺	C6H8O2	113.05971	1.1E+05	0.7					
90 2-heptenal	[M+H] ⁺	C7H12O	113.09599		1.1E+05	0.9				1.1E+05 -4.5
91 epsilon-Caprolactam	[M+H] ⁺	C6H11NO	114.09109		1.9E+05	2.2				
92 Glycerol	[M+Na] ⁺	C3H8O3	115.03653		3.2E+05	0.3				
93 3-oxo-4-pentenoic acid	[M+H] ⁺	C5H6O3	115.03917			3.1E+05	-1.7			
94 Hydrosorbic acid	[M+H] ⁺	C6H10O2	115.07540		1.1E+05	-0.4				
95 3-Amino-2-piperidone	[M+H] ⁺	C5H10N2O	115.08707				9.0E+04	-4.2		
96 Maleamic acid	[M+H] ⁺	C4H5NO3	116.03413				9.2E+04	0.8	1.0E+05	-4.9
97 Proline	[M+H] ⁺	C5H9NO2	116.07060	4.8E+05	2.3	1.6E+05	-3.4			
98 Aminopentanamide	[M+H] ⁺	C5H12N2O	117.10176					9.8E+04	4.1	1.4E+05 -3.0
99 Valine	[M+H] ⁺	C5H11NO2	118.08626	1.9E+05	2.2	2.2E+05	2.4			
100 Pyrimidine	[M+K] ⁺	C4H4N2	119.00065			1.3E+05	-0.4			
101 Sorbaldehyde	[M+Na] ⁺	C6H8O	119.04662			1.1E+05	1.0			
102 Hydroxy-isovaleric acid	[M+H] ⁺	C5H10O3	119.07118						1.0E+05	-1.9
103 2-Phenylpropene	[M+H] ⁺	C9H10	119.08520						9.0E+04	2.7
104 Aminomalonic acid	[M+H] ⁺	C3H5NO4	120.02913	7.9E+04	-1.6					
105 Hexenal	[M+Na] ⁺	C6H10O	121.06195			2.6E+05	3.6			
106 Phenylethylamine	[M+H] ⁺	C8H11N	122.09592					1.5E+06	4.1	2.3E+06 -4.4
107 Mercaptolactic acid	[M+H] ⁺	C3H6O3S	123.01104	8.8E+04	-4.8					
108 Tiglic acid	[M+Na] ⁺	C5H8O2	123.04165	7.0E+04	2.9	1.1E+05	3.7	4.5E+06	-4.8	
109 Benzoic acid	[M+H] ⁺	C7H6O2	123.04455					1.7E+05	-4.0	
110 Erythritol	[M+H] ⁺	C4H10O4	123.06519	1.0E+05	-3.0					
111 Nicotinic acid	[M+H] ⁺	C6H5NO2	124.03930	8.7E+04	-3.3				1.5E+05	-3.1
112 Aminopentanal	[M+Na] ⁺	C5H11NO	124.07361				7.5E+04	-2.6		
113 Valeric acid	[M+Na] ⁺	C5H10O2	125.05650			9.4E+05	5.0			
114 Methylimidazole acetaldehyde	[M+H] ⁺	C6H8N2O	125.07112		1.1E+05	-1.4				
115 Maltol	[M+H] ⁺	C6H6O3	127.03937					2.1E+05	-3.1	
116 Thymine	[M+H] ⁺	C5H6N2O2	127.05020	1.1E+05	1.2					
117 Pentanol	[M+K] ⁺	C5H12O	127.05196						1.1E+05	0.1
118 5-Amino-4-imidazolecarboxamide	[M+H] ⁺	C4H6N4O	127.06206					9.5E+04	-4.9	
119 2-octenal	[M+H] ⁺	C8H14O	127.11140				7.8E+04	2.7		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
120 Coniine	[M+H] ⁺	C8H17N	128.14338	7.4E+04	1.4					
121 6-hydroxy-2-hexynoic acid	[M+H] ⁺	C6H8O3	129.05461					3.4E+05	0.1	
122 Azulene	[M+H] ⁺	C10H8	129.07017			2.0E+05 -2.3				
123 3-isopropyl-3-butenic acid	[M+H] ⁺	C7H12O2	129.09132				7.5E+04 -2.4			
124 3-Aminopropane-1,2-diol	[M+K] ⁺	C3H9NO2	130.02649	1.2E+05	3.6					
125 Oxoproline	[M+H] ⁺	C5H7NO3	130.04987	4.1E+05	0.6					
126 Pipecolic acid	[M+H] ⁺	C6H11NO2	130.08626	1.6E+05	0.2					
127 Dimethylbiguanide	[M+H] ⁺	C4H11N5	130.10874				8.9E+04 -0.1			
128 Octylamine	[M+H] ⁺	C8H19N	130.15860			2.8E+05 3.3				
129 Leucine	[M+H] ⁺	C6H13NO2	132.10191	8.0E+05	1.0	2.5E+05 -1.3				
130 Resorcinol	[M+Na] ⁺	C6H6O2	133.02522				9.3E+04 5.0			
131 Imidazole acetaldehyde	[M+Na] ⁺	C5H6N2O	133.03699					2.0E+06	1.8	
132 Asparagine	[M+H] ⁺	C4H8N2O3	133.06077	3.7E+05	-0.3					
133 Dicyclopentadiene	[M+H] ⁺	C10H12	133.10118	1.2E+05	-2.8					
134 Aminomethylphosphonic acid	[M+Na] ⁺	CH6NO3P	133.99754					7.5E+04	1.6	
135 Hydroxypyridine	[M+K] ⁺	C5H5NO	134.00012						1.0E+05	1.1
136 Methylthiobutanaldoxime	[M+H] ⁺	C5H11NOS	134.06341	1.2E+05	-1.5					
137 Tetrahydroisoquinoline	[M+H] ⁺	C9H11N	134.09636						8.5E+04	0.5
138 Malic acid	[M+H] ⁺	C4H6O5	135.02885				1.6E+05 -0.4	1.7E+05	-4.8	
139 Ureidoglycolate	[M+H] ⁺	C3H6N2O4	135.04042			1.0E+05 -2.9				
140 Adenine	[M+H] ⁺	C5H5N5	136.06177	6.9E+04	2.6					
141 epsilon-Caprolactam	[M+Na] ⁺	C6H11NO	136.07338				7.0E+04 -0.7			
142 Phenylacetamide	[M+H] ⁺	C8H9NO	136.07543					2.1E+05	1.9	
143 Hydrosorbic acid	[M+Na] ⁺	C6H10O2	137.05679			1.6E+05 3.7				
144 Vinylcatechol	[M+H] ⁺	C8H8O2	137.05930					2.7E+05	3.0	
145 Tetrahydropteridine	[M+H] ⁺	C6H8N4	137.08217	7.6E+04 -0.2						
146 Myrcene	[M+H] ⁺	C10H16	137.13305				7.6E+05 -4.2			
147 Succinimide	[M+K] ⁺	C4H5NO2	137.99560			1.0E+05 -3.0				
148 Proline	[M+Na] ⁺	C5H9NO2	138.05177			1.3E+05 1.8				
149 Trigonelline	[M+H] ⁺	C7H7NO2	138.05495	1.1E+05	3.9			1.4E+05	0.8	
150 Tyramine	[M+H] ⁺	C8H11NO	138.09120					2.6E+05	1.0	
151 Tiglic acid	[M+K] ⁺	C5H8O2	139.01474				8.5E+04 1.8			
152 Levulinic acid	[M+Na] ⁺	C5H8O3	139.03652	1.6E+05	0.3		1.2E+05 -3.9			
153 Hydroxybenzoic acid	[M+H] ⁺	C7H6O3	139.03869					8.3E+05	2.0	
154 Urocanic acid	[M+H] ⁺	C6H6N2O2	139.05020	1.1E+06	0.7	5.8E+05 2.6				
155 Caproaldehyde	[M+K] ⁺	C6H12O	139.05144				1.4E+05 3.8			
156 Aspartate-semialdehyde	[M+Na] ⁺	C4H7NO3	140.03144			2.0E+05 2.7				
157 Methylaminoethylphosphonate	[M+H] ⁺	C3H10NO3P	140.04714						7.5E+04	-0.2
158 Aminopentanal	[M+K] ⁺	C5H11NO	140.04790			1.4E+05 -4.8				
159 Valine	[M+Na] ⁺	C5H11NO2	140.06776			3.2E+05 3.1				

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
160 Succinic acid	[M+Na] ⁺	C4H6O4	141.01619		1.3E+05	-2.6				
161 N-Nitrosodiethylamine	[M+K] ⁺	C4H10N2O	141.04247	7.8E+04	1.5					
162 Hydroxymethylcatechol	[M+H] ⁺	C7H8O3	141.05430		1.7E+05	2.3				
163 Octadienoic acid	[M+H] ⁺	C8H12O2	141.09065					3.9E+06	2.5	
164 Diaminopropanoate	[M+K] ⁺	C3H8N2O2	143.02174	7.0E+04	-1.0					
165 Erythrose	[M+Na] ⁺	C4H8O4	143.03145						7.3E+04	0.2
166 Purine	[M+Na] ⁺	C5H4N4	143.03281				7.1E+04	0.1	3.1E+05	-0.6
167 7-hydroxy-5-heptynoic acid	[M+H] ⁺	C7H10O3	143.07027	1.1E+05	-1.8					
168 Octenoic acid	[M+H] ⁺	C8H14O2	143.10736				1.7E+05	-4.9		
169 Proline betaine	[M+H] ⁺	C7H13NO2	144.10147		1.4E+05	3.0	8.3E+04	-3.4		
170 Glyceric acid	[M+K] ⁺	C3H6O4	144.98936		1.6E+05	2.8	9.8E+04	4.1	1.1E+05	-3.1
171 Mercaptolactic acid	[M+Na] ⁺	C3H6O3S	144.99299	1.9E+05	-4.4					
172 Nicotinamide	[M+Na] ⁺	C6H6N2O	145.03666				9.8E+04	4.0		
173 Erythritol	[M+Na] ⁺	C4H10O4	145.04713	8.3E+04	4.9		1.1E+05	-4.1	1.9E+05	0.6
174 n-valeryl acetic acid	[M+H] ⁺	C7H12O3	145.08636				9.4E+04	-3.0		
175 4-Amino-1-piperidinecarboxylic acid	[M+H] ⁺	C6H12N2O2	145.09683						7.3E+04	2.2
176 Guanidinobutanamide	[M+H] ⁺	C5H12N4O	145.10792				8.0E+04	3.2		
177 1-(3-Aminopropyl)-4-aminobutanal	[M+H] ⁺	C7H16N2O	145.13295						7.8E+04	4.1
178 Allysine	[M+H] ⁺	C6H11NO3	146.08079						8.2E+04	2.6
179 Orcinol	[M+Na] ⁺	C7H8O2	147.04204				9.4E+04	-2.7		
180 N-Propanoylimidazole	[M+Na] ⁺	C6H8N2O	147.05218					4.9E+05	4.8	
181 Glutamine	[M+H] ⁺	C5H10N2O3	147.07642	1.3E+06	0.5					
182 2,4-octadienal	[M+Na] ⁺	C8H12O	147.07795				6.3E+04	0.6		
183 Lysine	[M+H] ⁺	C6H14N2O2	147.11280	6.2E+05	0.2	1.2E+05	-0.5	3.3E+05	3.8	
184 Glutamic acid	[M+H] ⁺	C5H9NO4	148.06043	4.3E+05	1.5					
185 Dihydroxyfumaric acid	[M+H] ⁺	C4H4O6	149.00745				1.7E+06	4.1	2.5E+06	-2.7
186 Anethole	[M+H] ⁺	C10H12O	149.09609						1.1E+05	2.2
187 Trihydroxypyridine	[M+Na] ⁺	C5H5NO3	150.01602		1.9E+05	1.0				
188 Methionine	[M+H] ⁺	C5H11NO2S	150.05893						1.7E+05	-4.0
189 Triethanolamine	[M+H] ⁺	C6H15NO3	150.11247	2.8E+05	1.5					
190 Sorbic acid	[M+K] ⁺	C6H8O2	151.01550		1.5E+05	0.6				
191 Ribose	[M+H] ⁺	C5H10O5	151.06010	2.5E+05	4.1					
192 Dipropyl disulfide	[M+H] ⁺	C6H14S2	151.06091	2.5E+05	-1.6		4.6E+04	0.5	7.6E+04	0.4
193 Methylhypoxanthine	[M+H] ⁺	C6H6N4O	151.06208				3.5E+05	-4.3		
194 3-isopropyl-3-butenic acid	[M+Na] ⁺	C7H12O2	151.07271		1.3E+05	1.6				
195 Hydrocinnamic acid	[M+H] ⁺	C9H10O2	151.07536	1.9E+05	3.7					
196 Carvacrol	[M+H] ⁺	C10H14O	151.11174	1.7E+05	-2.9	1.5E+05	1.7			
197 Sulfinylpyruvic acid	[M+H] ⁺	C3H3O5S	151.97715				1.0E+05	1.6		
198 Cyanuric acid	[M+Na] ⁺	C3H3N3O3	152.00666	8.9E+04	2.6					
199 Pyroglutamic acid	[M+Na] ⁺	C5H7NO3	152.03181	1.4E+05	-3.6	1.0E+05	-2.3			

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
200 epsilon-Caprolactam	[M+K] ⁺	C6H11NO	152.04756					1.4E+05	-2.2	
201 Guanine	[M+H] ⁺	C5H5N5O	152.05669	1.0E+05	3.1					
202 Phenylpropanolamine	[M+H] ⁺	C9H13NO	152.10699	1.1E+05	1.0					
203 2-Hydroxy-2,4-pentadienoate	[M+K] ⁺	C5H6O3	152.99512			1.1E+05	-1.7			
204 Allyl sulfide	[M+K] ⁺	C6H10S	153.01305			9.2E+04	2.8			
205 Alloxanthine	[M+H] ⁺	C5H4N4O2	153.04002							1.2E+05 4.5
206 3-Amino-2-piperidone	[M+K] ⁺	C5H10N2O	153.04290				8.9E+04	-2.8		
207 2-keto-n-caproic acid	[M+Na] ⁺	C6H10O3	153.05204		1.8E+05	1.1	9.2E+04	-0.1		8.2E+04 -2.1
208 Vanillin	[M+H] ⁺	C8H8O3	153.05405				2.5E+06	3.7		
209 (4-Aminobutyl) guanidine	[M+Na] ⁺	C5H14N4	153.11045				6.2E+05	4.0	6.9E+05	2.9 5.0E+05 2.9
210 Myrtenol	[M+H] ⁺	C10H16O	153.12752				9.2E+05	-0.8		
211 Thiocysteine	[M+H] ⁺	C3H7NO2S2	153.99877							9.1E+04 2.1
212 Creatine	[M+Na] ⁺	C4H9N3O2	154.05864				1.6E+05	0.4	7.2E+04	3.0
213 N-Dimethyl-2-aminoethylphosphonate	[M+H] ⁺	C4H12NO3P	154.06276	1.8E+05	4.6					3.8E+05 -4.4
214 Leucine	[M+Na] ⁺	C6H13NO2	154.08385	7.0E+04	-4.6	1.3E+05	3.4			
215 Vanillylamine	[M+H] ⁺	C8H11NO2	154.08595							1.1E+05 2.0
216 N-Carbamoylputrescine	[M+Na] ⁺	C5H13N3O	154.09538				6.0E+05	-1.9		
217 N-Guanylhistamine	[M+H] ⁺	C6H11N5	154.10839							1.9E+05 2.2
218 Glutaric acid	[M+Na] ⁺	C5H8O4	155.03177		1.6E+05	-1.9				6.2E+04 -4.1
219 Gentisic acid	[M+H] ⁺	C7H6O4	155.03307				4.4E+05	4.2	9.0E+04	4.7
220 Pteridine	[M+Na] ⁺	C6H4N4	155.03310						3.1E+05	-1.8
221 Leucinic acid	[M+Na] ⁺	C6H12O3	155.06839				7.5E+04	-3.4		
222 Ornithine	[M+Na] ⁺	C5H12N2O2	155.07815				8.2E+05	4.9		
223 Boschnialactone	[M+H] ⁺	C9H14O2	155.10666	8.8E+04	4.9				1.2E+05	3.3
224 Indole	[M+K] ⁺	C8H7N	156.02142				6.1E+04	-2.6		
225 Valine	[M+K] ⁺	C5H11NO2	156.04214	7.1E+04	0.1					
226 Indolin-2-one	[M+Na] ⁺	C8H7NO	156.04215			9.4E+04	-1.1			
227 Valine	[M+K] ⁺	C5H11NO2	156.04215			9.4E+04	-0.1			
228 Histidine	[M+H] ⁺	C6H9N3O2	156.07675	2.6E+05	1.2					
229 Ketomalonic acid	[M+K] ⁺	C3H2O5	156.95338	6.8E+04	2.1					
230 Phosphoglycolic acid	[M+H] ⁺	C2H5O6P	156.98929				7.4E+04	2.3		
231 Malic acid	[M+Na] ⁺	C4H6O5	157.01074	1.3E+05	-3.2					
232 S-Dimethylsulfonium propionic acid	[M+Na] ⁺	C5H10O2S	157.02990				6.9E+04	-3.4	1.3E+05	-0.4
233 Dihydropteridine	[M+Na] ⁺	C6H6N4	157.04804			1.2E+05	2.7			
234 Nonane-4,6-dione	[M+H] ⁺	C9H16O2	157.12248						8.5E+04	-1.1
235 Nitrosonaphthalene	[M+H] ⁺	C10H7NO	158.05933				6.2E+04	4.5		
236 Purine	[M+K] ⁺	C5H4N4	159.00676	1.3E+05	2.2					
237 Maleylacetate	[M+H] ⁺	C6H6O5	159.02848						8.7E+04	2.0
238 1,4-Naphthoquinone	[M+H] ⁺	C10H6O2	159.04406	8.5E+04	-1.3					
239 Methylerythritol	[M+Na] ⁺	C5H12O4	159.06278	1.5E+05	4.7					1.5E+05 -3.0

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
240 Tetrahydropteridine	[M+Na] ⁺	C6H8N4	159.06409				1.9E+05	0.2		
241 Nonatrienal	[M+Na] ⁺	C9H12O	159.07804	9.7E+04	-1.0					
242 1-decanol	[M+H] ⁺	C10H22O	159.17427						1.5E+05	0.5
243 Cysteine	[M+K] ⁺	C3H7NO2S	159.98244			8.0E+04	2.9			
244 Trigonelline	[M+Na] ⁺	C7H7NO2	160.03690	9.2E+04	0.6					
245 Phenylethylamine	[M+K] ⁺	C8H11N	160.05232		9.5E+04	-0.1				
246 4-Methylene-L-glutamate	[M+H] ⁺	C6H9NO4	160.06033					6.0E+04	0.7	
247 Dimethylaniline-N-oxide	[M+Na] ⁺	C8H11NO	160.07328	9.1E+04	1.8					
248 Aminopropylcadaverine	[M+H] ⁺	C8H21N3	160.18115						7.2E+04	-2.0
249 Isonicotineamide	[M+K] ⁺	C6H6N2O	161.01117	3.4E+05	2.7					
250 Urocanic acid	[M+Na] ⁺	C6H6N2O2	161.03157				8.4E+04	3.6		
251 Hydroxypurine	[M+Na] ⁺	C5H6N4O	161.04272					1.1E+05	4.1	
252 Diaminotoluene	[M+K] ⁺	C7H10N2	161.04756	2.5E+05	-2.6					
253 Dehydrocarnitine	[M+H] ⁺	C7H14NO3	161.10453			3.0E+05	0.7			
254 S-Allyl-L-cysteine	[M+H] ⁺	C6H11NO2S	162.05833	1.4E+05	-4.1					
255 Carnitinamide	[M+H] ⁺	C7H17N2O2	162.13692			1.5E+05	-4.0			
256 Methylimidazole acetaldehyde	[M+K] ⁺	C6H8N2O	163.02682	9.6E+05	4.2					
257 Umbelliferone	[M+H] ⁺	C9H6O3	163.03897	2.1E+06	0.9					
258 Octadienoic acid	[M+Na] ⁺	C8H12O2	163.07348		1.5E+05	-3.2	8.4E+04	-1.2	1.8E+05	-1.6
259 Safrole	[M+H] ⁺	C10H10O2	163.07545			1.3E+06	-0.6			
260 Nicotine	[M+H] ⁺	C10H14N2	163.12297	1.1E+06	1.5					
261 Taurine	[M+K] ⁺	C2H7NO3S	163.97782	3.9E+05	-4.9					
262 2-Aminoethylphosphonate	[M+K] ⁺	C2H8NO3P	163.98721		7.1E+05	0.8				
263 Aminomuconate semialdehyde	[M+Na] ⁺	C6H7NO3	164.03181	9.1E+04	-4.1		6.5E+04	3.9	1.2E+05	2.8
264 Histidinol	[M+Na] ⁺	C6H11N3O	164.07994			1.6E+05	-3.1			
265 N-Methylconiine	[M+Na] ⁺	C9H19N	164.14109				1.1E+05	-0.7	1.0E+05	-1.1
266 5-Amino-4-imidazolecarboxamide	[M+K] ⁺	C4H6N4O	165.01732	1.1E+05	-2.7					
267 Coumaric acid	[M+H] ⁺	C9H8O3	165.05462	2.3E+05	-1.4	6.3E+05	3.2	2.0E+06	4.6	4.2E+05
268 2,4-Dimethyl-2E,4E-hexadien-1-ol	[M+K] ⁺	C8H14O	165.06790					4.7E+05	-1.7	
269 Trihydroxypyridine	[M+K] ⁺	C5H5NO3	165.98975		2.0E+05	2.1				
270 Guvacine	[M+K] ⁺	C6H9NO2	166.02649	8.9E+04	1.5					
271 Tetrazolyl-glycine	[M+Na] ⁺	C3H5N5O2	166.03355	2.0E+05	-1.8			1.5E+05	-2.0	1.2E+05
272 Methylguanine	[M+H] ⁺	C6H7N5O	166.07178				9.9E+04	-1.8		1.2E+05
273 Phenylalanine	[M+H] ⁺	C9H11NO2	166.08626	1.3E+06	1.1		1.7E+05	-2.7	9.3E+04	-1.4
274 Coniine	[M+K] ⁺	C8H17N	166.09968					2.6E+05	-2.5	
275 Azulene	[M+K] ⁺	C10H8	167.02569		5.4E+05	0.4				
276 Methylmercaptapurine	[M+H] ⁺	C6H6N4S	167.03793		1.6E+05	4.0				
277 Hydroxy-3-nitrosobenzamide	[M+H] ⁺	C7H6N2O3	167.04512	1.7E+05	0.5					
278 Noradrenochrome o-semiquinone	[M+H] ⁺	C8H8NO3	167.05769	1.4E+05	-3.4					
279 Lysine 1,6-lactam	[M+K] ⁺	C6H12N2O	167.05808		3.5E+05	0.3			3.1E+05	2.4

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
280 Caffeyl alcohol	[M+H] ⁺	C9H10O3	167.07021			4.8E+06	0.4			
281 Guanidinobutanamide	[M+Na] ⁺	C5H12N4O	167.09033	1.5E+05	-2.7					
282 Caprylic acid	[M+Na] ⁺	C8H16O2	167.10425	8.7E+04	-1.4			1.8E+05	-4.2	
283 1-(3-Aminopropyl)-4-aminobutanal	[M+Na] ⁺	C7H16N2O	167.11548	7.1E+04	-0.4					
284 Keto-glutaramic acid	[M+Na] ⁺	C5H7NO4	168.02658				1.5E+05	0.9		9.8E+04 -3.0
285 Thioguanine	[M+H] ⁺	C5H5N5S	168.03444				6.9E+04	-3.6		
286 Guanidinobutanal	[M+K] ⁺	C5H11N3O	168.05397						6.9E+04	-3.6
287 Allysine	[M+Na] ⁺	C6H11NO3	168.06337			2.2E+05	-1.5			
288 Dihydrophenylalanine	[M+H] ⁺	C9H13NO2	168.10191	1.0E+05	-0.1					
289 Lysinamide	[M+Na] ⁺	C6H15N3O	168.11130			3.9E+05	-3.4			
290 Sulfopyruvic acid	[M+H] ⁺	C3H4O6S	168.98014	3.7E+05	1.6	3.6E+05	0.5		7.1E+04	-0.6
291 Mevaldic acid	[M+Na] ⁺	C6H10O4	169.04713	1.5E+05	0.5	2.7E+05	2.0	2.3E+05	-4.1	1.0E+05 -0.2
292 Vanillic acid	[M+H] ⁺	C8H8O4	169.04928			3.3E+06	1.5			
293 Glutamine	[M+Na] ⁺	C5H10N2O3	169.05836	1.3E+05	0.3					
294 Hydroxyisoheptanoic acid	[M+Na] ⁺	C7H14O3	169.08312				8.1E+04	2.3	2.4E+05	-2.2
295 Agmatine	[M+K] ⁺	C5H14N4	169.08546							5.3E+04 -2.7
296 Trimethylaminoethylphosphonate	[M+H] ⁺	C5H15NO3P	169.08546							5.3E+04 4.6
297 Lysine	[M+Na] ⁺	C6H14N2O2	169.09491			2.9E+06	-1.0			
298 Geranic acid	[M+H] ⁺	C10H16O2	169.12229				7.7E+04	0.1		
299 Cysteic acid	[M+H] ⁺	C3H7NO5S	170.01141	1.2E+05	4.3		7.2E+04	2.1	1.0E+05	-4.1
300 Methylindole	[M+K] ⁺	C9H9N	170.03666	9.9E+04	-3.0					
301 Pyridoxine	[M+H] ⁺	C8H11NO3	170.08117	5.5E+05	2.0					
302 Oxaluric acid	[M+K] ⁺	C3H4N2O4	170.98108					6.6E+04	-4.8	
303 4-Methylthio-2-oxobutanoic acid	[M+Na] ⁺	C5H8O3S	171.00864	7.6E+04	4.2		8.1E+04	2.0		
304 Asparagine	[M+K] ⁺	C4H8N2O3	171.01665	9.6E+04	-2.9		9.8E+04	4.3	8.1E+04	0.7
305 Citramalic acid	[M+Na] ⁺	C5H8O5	171.02691			1.5E+05	-3.0			
306 Methylenediurea	[M+K] ⁺	C3H8N4O2	171.02788	8.3E+04	-2.4					
307 Dicyclopentadiene	[M+K] ⁺	C10H12	171.05690				2.3E+05	0.9		
308 Mevalonic acid	[M+Na] ⁺	C6H12O4	171.06283			1.3E+05	-0.3			
309 Dihydroxyphenylethyleneglycol	[M+H] ⁺	C8H10O4	171.06532							5.1E+04 -0.8
310 Furfural diethyl acetal	[M+H] ⁺	C9H14O3	171.10109							8.0E+04 2.8
311 Citronellic acid	[M+H] ⁺	C10H18O2	171.13796	1.0E+05	-3.5		1.9E+05	-1.9		
312 2-Undecanone	[M+H] ⁺	C11H22O	171.17405				8.4E+04	1.7		
313 Aspartate	[M+K] ⁺	C4H7NO4	172.00165				6.2E+04	-4.7		
314 Ureidoglycine	[M+K] ⁺	C3H7N3O3	172.01190	6.5E+04	-3.1					
315 Phenylpropionaldoxim	[M+Na] ⁺	C9H11NO	172.07385							2.4E+05 -3.3
316 6E-Octene-2,4-diyonic acid	[M+K] ⁺	C8H6O2	173.00003							4.9E+04 -0.5
317 S,S-Dimethyl-beta-propiothetin	[M+K] ⁺	C5H10O2S	173.00331	1.2E+05	0.1					
318 Benzenamine sulfate	[M+H] ⁺	C6H6NO3S	173.01347					8.8E+04	3.7	
319 Cinnamyl alcohol	[M+K] ⁺	C9H10O	173.03571				3.4E+05	3.6		

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm			
320	Ribose	[M+Na] ⁺	C5H10O5	173.04134		2.2E+05	4.1		3.4E+05	-4.1				
321	(Hydroxyphosphinyl)pyruvate	[M+Na] ⁺	C3H5O5P	174.97641					1.2E+05	1.6				
322	Sulfinoalanine	[M+Na] ⁺	C3H6NO4S	174.99097	1.0E+06	-0.3		2.3E+05	-5.0					
323	Threonic acid	[M+K] ⁺	C4H8O5	174.99995					7.9E+04	2.2				
324	Mercaptopurine	[M+Na] ⁺	C5H4N4S	175.00478		1.2E+05	0.6							
325	N-Methylnicotinamide	[M+K] ⁺	C7H8N2O	175.02732					1.6E+05	-2.8				
326	Arabitol	[M+Na] ⁺	C5H12O5	175.05794		2.5E+05	-1.4							
327	Shikimic acid	[M+H] ⁺	C7H10O5	175.05933					1.1E+05	4.4				
328	Suberic acid	[M+H] ⁺	C8H14O4	175.09727				9.0E+04	-4.5					
329	N-Acetylornithine	[M+H] ⁺	C7H14N2O3	175.10703		1.3E+05	3.9							
330	Dodecapentaenal	[M+H] ⁺	C12H14O	175.11174	3.4E+06	-1.6								
331	Arginine	[M+H] ⁺	C6H14N4O2	175.11895	1.4E+07	0.3	2.1E+05	0.1	1.2E+07	-0.2	1.6E+05	0.0	3.6E+05	-0.2
332	N-Acetylhistamine	[M+Na] ⁺	C7H11N3O	176.07868				9.8E+04	4.3					
333	Citrulline	[M+H] ⁺	C6H13N3O3	176.10312						5.8E+04	-0.9			
334	Debrisoquine	[M+H] ⁺	C10H13N3	176.11902						1.2E+05	-4.5			
335	Urocanic acid	[M+K] ⁺	C6H6N2O2	177.00693		5.7E+05	-4.8		6.0E+05	-4.1			1.5E+05	-3.4
336	Imidazole pyruvic acid	[M+Na] ⁺	C6H6N2O3	177.02668		1.6E+05	2.2							
337	Tyrosol	[M+K] ⁺	C8H10O2	177.03124	1.4E+05	3.3								
338	Vanillyl alcohol	[M+Na] ⁺	C8H10O3	177.05296				9.6E+04	-4.2					
339	4-Methylumbelliferone	[M+H] ⁺	C10H8O3	177.05462	3.0E+05	-2.0								
340	Allantoic acid	[M+H] ⁺	C4H8N4O4	177.06101	1.7E+05	-2.9	3.2E+05	4.6			1.8E+05	4.1		
341	Nonadienal	[M+K] ⁺	C9H14O	177.06762	2.5E+05	3.4					1.5E+05	-3.9		
342	Propylmalate	[M+H] ⁺	C7H12O5	177.07575	1.3E+05	-3.7	1.1E+05	0.0						
343	Boschnialactone	[M+Na] ⁺	C9H14O2	177.08869					4.6E+04	-0.5	1.8E+05	-4.9		
344	Cinnamyl acetate	[M+H] ⁺	C11H12O2	177.09096				3.3E+06	0.3					
345	3-Aminopropanesulfonate	[M+K] ⁺	C3H9NO3S	177.99347	3.4E+05	1.2								
346	Methylaminoethylphosphonate	[M+K] ⁺	C3H10NO3P	178.00300		3.0E+05	-0.1							
347	Nitrocatechol	[M+Na] ⁺	C6H5NO4	178.01163					4.4E+04	-3.1				
348	S-(1-propenyl)-L-cysteine sulfoxide	[M+H] ⁺	C6H11NO3S	178.05324	6.4E+06	0.0		8.3E+04	1.1	8.5E+05	-0.8		5.9E+04	-1.0
349	N-Formyl-L-methionine	[M+H] ⁺	C6H11NO3S	178.05324	6.4E+06	0.0		8.3E+04	1.1	8.5E+05	-0.8		5.9E+04	-1.0
350	Alliin	[M+H] ⁺	C6H11NO3S	178.05324	6.4E+06	0.0		8.3E+04	1.1	8.5E+05	-0.8		5.9E+04	-1.0
351	Histidine	[M+Na] ⁺	C6H9N3O2	178.05840		1.0E+05	1.7							
352	Phosphoglycolic acid	[M+Na] ⁺	C2H5O6P	178.97138					8.1E+04	1.2	7.5E+04	-3.3		
353	Uracil 5-carbaldehyde	[M+K] ⁺	C5H4N2O3	178.98535	1.4E+05	3.0								
354	Imidazolepropionic acid	[M+K] ⁺	C6H8N2O2	179.02241					1.8E+05	-3.8	1.6E+05	-4.4		
355	Imidazolelactic acid	[M+Na] ⁺	C6H8N2O3	179.04271	8.3E+04	1.2								
356	Octadienoic acid	[M+K] ⁺	C8H12O2	179.04684		1.5E+05	0.3		9.8E+04	1.8				
357	Indoleacetonitrile	[M+Na] ⁺	C10H8N2	179.05797	1.5E+05	-0.8								
358	5-oxo-7-octenoic acid	[M+Na] ⁺	C8H12O3	179.06786	1.1E+05	1.5								
359	Ferulaldehyde	[M+H] ⁺	C10H10O3	179.06964				4.2E+06	3.5					

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm				
360	2-aminomuconic acid semialdehyde	[M+K] ⁺	C6H7NO3	180.00550		8.0E+04	1.4								
361	Isoxanthopterin	[M+H] ⁺	C6H5N5O2	180.05230		1.0E+05	-3.9								
362	Glucosamine	[M+H] ⁺	C6H13NO5	180.08688		1.0E+05	-1.3								
363	Homophenylalanine	[M+H] ⁺	C10H13NO2	180.10212				3.3E+05	-1.2	1.4E+05	0.7	1.6E+05	-2.3	1.7E+05	3.1
364	Hydroxymethyluracil	[M+K] ⁺	C5H6N2O3	181.00100	4.4E+05	-2.7									
365	Isopropylmaleate	[M+Na] ⁺	C7H10O4	181.04626				2.0E+06	4.8	2.3E+06	1.3	1.6E+06	4.9		
366	Caffeic acid	[M+H] ⁺	C9H8O4	181.04954	2.8E+05	0.6		1.4E+06	2.8						
367	Coniferyl alcohol	[M+H] ⁺	C10H12O3	181.08538				7.4E+06	3.0						
368	3-tert-Butyl-5-methylcatechol	[M+H] ⁺	C11H16O2	181.12231	8.5E+04	2.0									
369	4-Methyl-5-(2-hydroxyethyl)-thiazole	[M+K] ⁺	C6H9NOS	182.00361				2.0E+05	0.2						
370	Tet-glycine	[M+K] ⁺	C3H5N5O2	182.00807		8.2E+04	-3.2								
371	4-Methylene-L-glutamate	[M+Na] ⁺	C6H9NO4	182.04246						3.9E+05	-0.5	2.8E+05	1.2		
372	Valerylglycine	[M+Na] ⁺	C7H13NO3	182.07902				2.0E+05	-1.4						
373	Tyrosine	[M+H] ⁺	C9H11NO3	182.08117	7.6E+05	-0.2									
374	Dicyclohexylamine	[M+H] ⁺	C12H23N	182.19053				1.9E+05	-1.1	1.1E+05	0.8				
375	Oxadipic acid	[M+Na] ⁺	C6H8O5	183.02585				6.2E+04	3.0						
376	aceto valeric acid	[M+K] ⁺	C7H12O3	183.04239				7.3E+04	-3.2			8.1E+04	-4.0		
377	Pimelic acid	[M+Na] ⁺	C7H12O4	183.06241		3.0E+05	2.0			4.6E+05	-1.1				
378	Dihydrocaffeic acid	[M+H] ⁺	C9H10O4	183.06421				5.5E+06	0.3						
379	5-Oxo-1,2-campholide	[M+H] ⁺	C10H14O3	183.10185				1.5E+05	-1.5						
380	Butyro-betaine	[M+K] ⁺	C8H18NO	183.10200	8.0E+04	0.1	1.5E+05	-3.3	4.2E+06	-3.4		6.8E+04	-4.3		
381	Dihydrostilbene	[M+H] ⁺	C14H14	183.11683	8.3E+04	-4.5									
382	Keto-glutaramic acid	[M+K] ⁺	C5H7NO4	183.99987								4.6E+04	4.3		
383	4-Amino-2-hydroxylamino-6-nitrotoluene	[M+H] ⁺	C7H9N3O3	184.07130		8.6E+04	2.0								
384	Carnitinamide	[M+Na] ⁺	C7H17N2O2	184.11822	1.2E+05	3.1	1.5E+05	-0.1							
385	Carnitinamide	[M+Na] ⁺	C7H17N2O2	184.11824											
386	4-Hydroxy-2-oxoglutarate	[M+Na] ⁺	C5H6O6	185.00566	1.8E+06	4.1									
387	Allicin	[M+Na] ⁺	C6H10OS2	185.00653	1.8E+06	-0.6		1.6E+06	0.4	1.6E+05	1.5		1.6E+06	0.3	
388	Thiouric acid	[M+H] ⁺	C5H4N4O2S	185.01259								6.0E+04	1.0		
389	Methyleneoxindole	[M+K40] ⁺	C9H7NO	185.01546				6.5E+04	4.1						
390	Hydroxycoumarin	[M+Na] ⁺	C9H6O3	185.02077		1.1E+05	0.8								
391	Hydroxyisourate	[M+H] ⁺	C5H4N4O4	185.03114				2.2E+05	-3.3			1.4E+05	-1.1		
392	Glutamine	[M+K] ⁺	C5H10N2O3	185.03194						2.8E+05	2.0				
393	Hydroxymethyl-glutaric acid	[M+Na] ⁺	C6H10O5	185.04181		9.6E+04	1.3								
394	3-O-Methylgallate	[M+H] ⁺	C8H8O5	185.04522						1.4E+05	-4.2				
395	Oleandrose	[M+Na] ⁺	C7H14O4	185.07880		1.2E+05	-2.0								
396	Oxo-decenoic acid	[M+H] ⁺	C10H16O3	185.11748				4.9E+05	-1.4						
397	Citronellyl formate	[M+H] ⁺	C11H20O2	185.15428		9.8E+04	-3.6	2.0E+05	-4.0						
398	Laurylaldehyde	[M+H] ⁺	C12H24O	185.19018								7.2E+04	-1.0		
399	Fucosamine	[M+Na] ⁺	C6H13NO4	186.07398								7.0E+04	-1.6		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
400 N-Acetylphenylethylamine	[M+Na] ⁺	C10H13NO	186.08967					1.5E+05	-4.0	
401 Sulfolbenzaldehyde	[M+H] ⁺	C7H6O4S	187.00683			2.9E+05	-4.7			
402 O-Carbamoyl-L-serine	[M+K] ⁺	C4H8N2O4	187.01157	9.9E+04	1.1					
403 Cinnamic acid	[M+K] ⁺	C9H8O2	187.01601			9.3E+04	-2.3			
404 Angelicin	[M+H] ⁺	C11H6O3	187.03897	1.0E+05	2.9					
405 Quercitol	[M+Na] ⁺	C6H12O5	187.05825		1.4E+05	-3.0		2.4E+05	-0.7	
406 p-Cumate	[M+Na] ⁺	C10H12O2	187.07292					1.2E+05	0.2	
407 Carboxycyclohexyl-acetic acid	[M+H] ⁺	C9H14O4	187.09621					8.2E+04	1.5	
408 Oxo-decanoic acid	[M+H] ⁺	C10H18O3	187.13358						4.5E+04	-3.8
409 Pyridoxolactone	[M+Na] ⁺	C8H7NO3	188.03181	1.5E+05	0.6					
410 Methyladenine	[M+K] ⁺	C6H7N5	188.03384		9.8E+04	-2.8				
411 L-Methionine S-oxide	[M+Na] ⁺	C5H11NO3S	188.03440					9.6E+04	4.2	
412 Indoleacrylic acid	[M+H] ⁺	C11H9NO2	188.07060	3.7E+05	0.9					
413 N-Heptanoylglycine	[M+H] ⁺	C9H17NO3	188.12725		1.8E+05	4.6				
414 Tartaric acid	[M+K] ⁺	C4H6O6	188.97889				4.7E+04	3.7		
415 Phenylglyoxylic acid	[M+K] ⁺	C8H6O3	188.99514						4.7E+04	-1.5
416 Ribose	[M+K] ⁺	C5H10O5	189.01598	3.4E+05	1.5					
417 Dipropyl disulfide	[M+K] ⁺	C6H14S2	189.01685	3.4E+05	-3.1					
418 Hydrocinnamic acid	[M+K] ⁺	C9H10O2	189.03097			1.3E+05	1.4			
419 Caffeyl alcohol	[M+Na] ⁺	C9H10O3	189.05268					3.2E+05	-2.5	
420 Ramentaceone	[M+H] ⁺	C11H8O3	189.05531				4.2E+04	-3.7		
421 2-tridecene-4,7-diynal	[M+H] ⁺	C13H16O	189.12685					6.1E+04	2.9	
422 Homoarginine	[M+H] ⁺	C7H16N4O2	189.13460	1.8E+05	4.5					
423 Guanine	[M+K] ⁺	C5H5N5O	190.01257	9.9E+04	0.7					
424 2-Dimethylamino-5,6-dimethylpyrimidin-4-ol	[M+Na] ⁺	C8H13N3O	190.09516			8.2E+04	-0.4			
425 3-Mercapto-2-mercaptomethylpropanoate	[M+K] ⁺	C4H8O2S2	190.95892				5.9E+04	4.3	1.2E+05	-3.7
426 Phosphoenolpyruvic acid	[M+Na] ⁺	C3H5O6P	190.97160	1.1E+05	-2.0		4.5E+04	-4.7		
427 Butanoylphosphate	[M+Na] ⁺	C4H9O5P	191.00815						4.7E+04	-0.9
428 N1-Methyl-2-pyridone-5-carboxamide	[M+K] ⁺	C7H8N2O2	191.02261				4.2E+05	-4.6		
429 Arabitol	[M+K] ⁺	C5H12O5	191.03256		2.2E+05	-4.9				
430 Dehydroquinic acid	[M+H] ⁺	C7H10O6	191.05556		1.2E+05	-2.9				
431 Ethoxycoumarin	[M+H] ⁺	C11H10O3	191.06940			4.8E+06	4.6			
432 Chrysanthemic acid	[M+Na] ⁺	C10H16O2	191.10389	3.8E+05	-2.0	3.6E+05	1.9	9.9E+04	-0.5	2.4E+05 -0.9
433 Hydroxydebrisoquine	[M+H] ⁺	C10H13N3O	192.11256		9.1E+04	3.0				
434 N-Butyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine	[M+H] ⁺	C9H13N5	192.12426					5.0E+04	0.6	
435 Diethylphosphoric acid	[M+K] ⁺	C4H11O4P	193.00265	3.4E+05	2.3					
436 Thiourocanic acid	[M+Na] ⁺	C6H6N2O2S	193.00456						2.1E+05	-1.8
437 Furfural diethyl acetal	[M+Na] ⁺	C9H14O3	193.08352	1.2E+05	4.2				4.7E+04	0.2
438 Myristicin	[M+H] ⁺	C11H12O3	193.08494		2.1E+05	0.9	1.3E+07	4.7		
439 Citronellic acid	[M+Na] ⁺	C10H18O2	193.11990	1.2E+05	4.7		8.6E+04	4.9	2.5E+05	3.3

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
440 2,4,7-tridecatrienal	[M+H] ⁺	C13H20O	193.15849					9.4E+04	1.0	
441 Salsoline	[M+H] ⁺	C11H15NO2	194.11763							2.0E+05 -0.4
442 Glucuronic acid	[M+H] ⁺	C6H10O7	195.04993	7.5E+04	1.0					
443 Ferulic acid	[M+H] ⁺	C10H10O4	195.06519	1.9E+05	4.3	2.9E+05	3.6	2.7E+06	3.9	4.9E+05 3.5
444 4-n-valeryl butyric acid	[M+Na] ⁺	C9H16O3	195.09954						6.2E+05	-1.9 1.5E+05 0.6
445 Zingerone	[M+H] ⁺	C11H14O3	195.10157	6.3E+04	2.1		6.5E+06	1.6		
446 Aminomuconic acid	[M+K] ⁺	C6H7NO4	196.00078							3.9E+04 -0.6
447 Orthanic acid	[M+Na] ⁺	C6H7NO3S	196.00388	3.7E+05	-2.1	9.7E+05	4.5			
448 Deoxy-5-aminoshikimic acid	[M+Na] ⁺	C7H11NO4	196.05787					7.7E+04	0.8	
449 Glucosaminic acid	[M+H] ⁺	C6H13NO6	196.08237							4.0E+04 -4.1
450 N-Acetyl-L-leucine	[M+Na] ⁺	C8H15NO3	196.09453				2.1E+05	-0.6		8.1E+04 -0.4
451 Tyrosine methyl ester	[M+H] ⁺	C10H13NO3	196.09633				6.1E+04	2.5		
452 Phenolic phosphate	[M+Na] ⁺	C6H7O4P	196.99677					8.6E+04	3.3	
453 Allantoin	[M+K] ⁺	C4H6N4O3	197.00773		9.2E+04	-2.9				
454 1-Naphthalenemethanol	[M+K] ⁺	C11H10O	197.03620				6.3E+04	0.6		
455 N-Acetylasparagine	[M+Na] ⁺	C6H10N2O4	197.05272							4.0E+04 2.8
456 Suberic acid	[M+Na] ⁺	C8H14O4	197.07843	1.8E+05	0.8	3.6E+05	-0.3	2.2E+05	0.8	4.9E+05 -2.3 1.1E+05 0.6
457 Xanthoxyl	[M+H] ⁺	C10H12O4	197.08010				6.2E+06	3.7		
458 N-Acetylornithine	[M+Na] ⁺	C7H14N2O3	197.08883							6.9E+04 4.2
459 Hydroxy pelargonic acid	[M+Na] ⁺	C9H18O3	197.11482	2.4E+05	3.4	2.6E+05	-0.5		1.6E+06	-1.6 2.5E+05 -0.3
460 Coryneine	[M+H] ⁺	C11H18NO2	197.14103	9.3E+04	-3.0					
461 Indole-3-acetaldehyde	[M+K] ⁺	C10H9NO	198.03093					5.9E+04	3.3	
462 Dihydroxy-L-phenylalanine	[M+H] ⁺	C9H11NO4	198.07608	6.6E+04	0.3					
463 Citrulline	[M+Na] ⁺	C6H13N3O3	198.08491	6.6E+04	2.8					
464 N-Formimino-L-aspartate	[M+K] ⁺	C5H8N2O4	199.01157	9.0E+04	-0.1	4.2E+05	0.4	1.7E+05	-1.4	1.1E+05 -2.5 8.3E+04 -0.8
465 Ascorbic acid	[M+Na] ⁺	C6H8O6	199.02174					6.1E+04	-2.2	4.6E+04 -2.9
466 Vanillylmandelic acid	[M+H] ⁺	C9H10O5	199.05932			8.2E+05	3.9			
467 Dehydrocarnitine	[M+K] ⁺	C7H14NO3	199.06086					4.8E+04	-1.7	
468 5-Acetylamino-6-amino-3-methyluracil	[M+H] ⁺	C7H10N4O3	199.08188							4.8E+04 3.4
469 Dihydroxy-octanoic acid	[M+Na] ⁺	C8H16O4	199.09440		2.1E+05	-1.6		9.1E+04	3.9	2.0E+05 0.5
470 Trimethyl-L-histidine	[M+H] ⁺	C9H16N3O2	199.13143				2.5E+05	0.5		
471 Linderic acid	[M+H] ⁺	C12H22O2	199.16921					9.9E+04	0.2	9.8E+04 -4.0
472 Alliin	[M+Na] ⁺	C6H11NO3S	200.03518	9.4E+05	0.4					
473 S-(1-propenyl)-L-cysteine sulfoxide	[M+Na] ⁺	C6H11NO3S	200.03518	9.4E+05	0.4					
474 N-Formyl-L-methionine	[M+Na] ⁺	C6H11NO3S	200.03518	9.4E+05	0.4					
475 Methylthiohexanaldoxime	[M+K] ⁺	C7H15NOS	200.05115				8.7E+04	-2.8		
476 Dodecanamide	[M+H] ⁺	C12H25NO	200.20084							3.9E+04 0.3
477 Umbelliferone	[M+K] ⁺	C9H6O3	200.99554		1.2E+05	-3.4				
478 Cysteinylglycine	[M+Na] ⁺	C5H10N2O3S	201.03043	8.7E+04	-4.4					
479 Safrole	[M+K] ⁺	C10H10O2	201.03129					2.0E+05	-0.3	

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
480	Hydroxy-L-lysine	[M+K] ⁺	C6H14N2O3	201.06406				5.7E+04	-2.3		
481	Nicotine	[M+K] ⁺	C10H14N2	201.07851						5.1E+04	1.7
482	Eugenol methyl ether	[M+Na] ⁺	C11H14O2	201.08860	3.7E+05	-3.0	1.6E+05	3.9	1.2E+05	3.9	
483	Isoxanthopterin	[M+Na] ⁺	C6H5N5O2	202.03355	5.9E+04	-1.7		5.2E+04	3.8		
484	Amino-undecanoic acid	[M+H] ⁺	C11H23NO2	202.17940						3.9E+04	3.7
485	5-Hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate	[M+H] ⁺	C5H6N4O5	203.04120				9.8E+04	-0.5		
486	Glucose	[M+Na] ⁺	C6H12O6	203.05261	1.7E+06	-1.4	4.0E+06	0.2		5.6E+06	0.0
487	alpha-Curcumene	[M+H] ⁺	C15H22	203.17943	1.1E+05	1.8					
488	Methionine sulfoxide	[M+K] ⁺	C5H11NO3S	204.00916				7.8E+04	-0.2		
489	2-Methyl-3-hydroxy-5-formylpyridine-4-carboxylate	[M+Na] ⁺	C8H7NO4	204.02663						3.8E+04	0.5
490	Acetylcarnitine	[M+H] ⁺	C9H17NO4	204.12359				1.5E+05	-2.7	4.4E+04	0.5
491	Succimer	[M+Na] ⁺	C4H6O4S2	204.95927			9.4E+04	3.4			
492	Mannitol	[M+Na] ⁺	C6H14O6	205.06814			3.9E+05	0.6		1.8E+05	1.5
493	Dihydroconiferyl alcohol	[M+Na] ⁺	C10H14O3	205.08348						4.0E+04	0.2
494	3-Butylidene-7-hydroxyphthalide	[M+H] ⁺	C12H12O3	205.08531				1.1E+06	3.0		
495	Tryptophan	[M+H] ⁺	C11H12N2O2	205.09715	5.7E+05	2.9					
496	Diethyl-2-methyl-3-hydroxysuccinate	[M+H] ⁺	C9H16O5	205.10637			9.0E+04	3.3			
497	Isocaryophyllene	[M+H] ⁺	C15H24	205.19510			8.8E+04	-0.1	4.5E+05	-4.6	
498	Homocysteinesulfinic acid	[M+K] ⁺	C4H9NO4S	205.98839	8.9E+04	2.5					
499	Nalpha,Nalpha-Dimethyl-histidine	[M+Na] ⁺	C8H13N3O2	206.08927				2.4E+05	3.5		
500	2-Acetamido-2,6-dideoxy-D-galactose	[M+H] ⁺	C8H15NO5	206.10230	8.1E+04	-2.1					
501	Pantothenol	[M+H] ⁺	C9H19NO4	206.13801			8.2E+04	3.3			
502	Diaminosalicylic acid	[M+K] ⁺	C7H8N2O3	207.01665	1.1E+06	4.3		1.8E+06	-4.6		
503	N-Cyclopropylammelide	[M+K] ⁺	C6H8N4O2	207.02788	2.5E+05	2.6					
504	Homocitric acid	[M+H] ⁺	C7H10O7	207.05035			1.2E+05	-2.0			
505	Lipoic acid	[M+H] ⁺	C8H14O2S2	207.05035			1.2E+05	2.2			
506	Phosphorylcholine	[M+Na] ⁺	C5H15NO4P	207.06320						1.7E+05	-0.5
507	Geranic acid	[M+K] ⁺	C10H16O2	207.07819	2.3E+05	0.0					
508	Withasomnine	[M+Na] ⁺	C12H12N2	207.08864						6.5E+04	3.0
509	5-exo-Hydroxy-1,2-campholide	[M+Na] ⁺	C10H16O3	207.09882			1.6E+05	1.7		2.3E+05	2.5
510	Methoxycinnamic acid ethyl ester	[M+H] ⁺	C12H14O3	207.10150				2.6E+06	0.3		4.7E+04
511	Citronellyl formate	[M+Na] ⁺	C11H20O2	207.13555						1.6E+05	0.0
512	11-dodecen-1-ol	[M+Na] ⁺	C12H24O	207.17258			1.2E+05	-3.1			
513	Octylphenol	[M+H] ⁺	C14H22O	207.17434	9.8E+04	0.3					
514	2-Amino-3-carboxymuconate semialdehyde	[M+Na] ⁺	C7H7NO5	208.02153				9.2E+04	0.5		
515	2-Deoxy-2-dimethylamino-alpha-D-Glucose	[M+H] ⁺	C8H17NO5	208.11756				4.5E+04	1.9		
516	Phospho-D-glycerate	[M+Na] ⁺	C3H7O7P	208.98136				1.7E+05	3.8		
517	Fraxetin	[M+H] ⁺	C10H8O5	209.04500			1.1E+05	-2.6	2.7E+05	1.3	2.4E+05
									-0.5	1.7E+05	1.4

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
518 cis-2-Carboxycyclohexyl-acetic acid	[M+Na] ⁺	C9H14O4	209.07793					3.1E+05	2.4	
519 Benzylsuccinate	[M+H] ⁺	C11H12O4	209.08009			9.7E+06	3.6			
520 Oxodecanoate	[M+Na] ⁺	C10H18O3	209.11481					3.8E+05	0.0	1.0E+05 1.4
521 Benzyl -2-methyl-3-hydroxybutanoate	[M+H] ⁺	C12H16O3	209.11706		1.3E+05	0.8				
522 Methyl-decanoic acid	[M+Na] ⁺	C11H22O2	209.15208		1.7E+05	-4.2				
523 Heptyloxyphenol	[M+H] ⁺	C13H20O2	209.15316				1.8E+05	2.1		9.6E+04 4.1
524 Ammodendrine	[M+H] ⁺	C12H20N2O	209.16484	9.5E+04	0.0					
525 2-(Acetamidomethylene)succinate	[M+Na] ⁺	C7H9NO5	210.03721				7.3E+04	0.4		
526 Hydroxyiminostilbene	[M+H] ⁺	C14H11NO	210.09099						4.7E+04	1.7
527 8-Amino-7-oxononanoic acid	[M+Na] ⁺	C9H17NO3	210.10935		6.0E+05	3.4				
528 Decanamide	[M+K] ⁺	C10H21NO	210.12611					4.8E+04	-3.0	
529 Hydantoin-propionate	[M+K] ⁺	C6H8N2O4	211.01157	8.0E+04	1.2		3.5E+05	-0.4	2.5E+05	-2.8 3.5E+05 -0.7
530 Glucaric acid	[M+H] ⁺	C6H10O8	211.04484	9.1E+04	2.2					
531 Glycylproline	[M+K] ⁺	C7H12N2O3	211.04894				1.6E+05	-4.7		
532 Sedoheptulose	[M+H] ⁺	C7H14O7	211.08185					1.5E+05	-2.9	
533 1,3,7-Trimethyluric acid	[M+H] ⁺	C8H10N4O3	211.08312				8.2E+04	-2.6		
534 Azelaic acid	[M+Na] ⁺	C9H16O4	211.09408	1.5E+05	-1.6	4.1E+05 -0.3	2.4E+05	-1.2	5.8E+05	-0.8 1.6E+05 -1.3
535 Acetylglutamine	[M+K] ⁺	C7H16N4O	211.09569			5.2E+06 -0.6				
536 Jasmonic acid	[M+H] ⁺	C12H18O3	211.13220					2.0E+05	3.2	
537 Undecanol	[M+K] ⁺	C11H24O	211.14578					7.8E+04	0.5	
538 Aminobenzenesulfonate	[M+K] ⁺	C6H7NO3S	211.97722						4.9E+04	2.8
539 Quinaldinic acid	[M+K] ⁺	C10H7NO2	212.01102						7.2E+04	-0.9
540 N-Acetyl-L-glutamate	[M+Na] ⁺	C7H11NO5	212.05294				4.8E+04	0.0		
541 Menadiol	[M+K] ⁺	C11H10O2	213.03169					6.4E+04	-2.1	
542 N-Carbamyl-L-glutamate	[M+Na] ⁺	C6H10N2O5	213.04914						5.7E+04	-4.4
543 N-Acetylornithine	[M+K] ⁺	C7H14N2O3	213.06450				6.2E+04	-4.2		1.7E+05 -1.7
544 Arginine	[M+K] ⁺	C6H14N4O2	213.07484	2.0E+05	0.4			1.1E+05	2.1	
545 Propyl gallate	[M+H] ⁺	C10H12O5	213.07543			9.3E+05	1.5			
546 Arginine	[M+K] ⁺	C6H14N4O2	213.07576						7.8E+04	-4.3
547 Pinosylvin	[M+H] ⁺	C14H12O2	213.09101	9.7E+04	-3.6					
548 Perseitol	[M+H] ⁺	C7H16O7	213.09696					6.1E+04	-0.4	
549 p-Cumylphenol	[M+H] ⁺	C15H16O	213.12697				4.0E+04	2.0		
550 Citric acid	[M+Na] ⁺	C6H8O7	215.01622	2.4E+05	-0.4					
551 Dinitroguaiacol	[M+H] ⁺	C7H6N2O6	215.03066					8.2E+04	-3.7	
552 2-Deoxy-D-ribose 1-phosphate	[M+H] ⁺	C5H11O7P	215.03066					8.2E+04	4.0	
553 Amino-3-(3-carboxy-5-methyl-4-isoxazolyl)porionic acid	[M+H] ⁺	C8H10N2O5	215.06656					9.0E+04	-1.5	
554 Methyl 2-diazoacetamidohexonate	[M+H] ⁺	C9H16N3O3	215.12644	1.9E+05	-1.3			2.4E+05	3.8	2.3E+05 4.6
555 N-Formyl-L-methionine	[M+K] ⁺	C6H11NO3S	216.00912	1.2E+06	2.0					
556 Alliin	[M+K] ⁺	C6H11NO3S	216.00912	1.2E+06	2.0					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
557 S-(1-propenyl)-L-cysteine sulfoxide	[M+K] ⁺	C6H11NO3S	216.00912	1.2E+06	2.0					
558 Methyl beta-D-galactoside	[M+Na] ⁺	C7H14O6	217.06840			1.3E+05	-0.7			
559 Hydroxynicotine	[M+K] ⁺	C10H14N2O	217.07377	1.4E+05	0.5					
560 Tetradecadiene-diyonic acid	[M+H] ⁺	C14H16O2	217.12321			8.2E+05	-4.2			
561 Undecanedioic acid	[M+H] ⁺	C11H20O4	217.14346				7.3E+04	-0.1		
562 Isoxanthopterin	[M+K] ⁺	C6H5N5O2	218.00748	1.4E+05	-1.5					
563 Cyclohexylsulfamate	[M+K] ⁺	C6H13NO3S	218.02388			1.2E+05	4.1			
564 Pyridarone	[M+Na] ⁺	C13H9NO	218.05783						3.7E+04	-0.9
565 L-Homophenylalanine	[M+K] ⁺	C10H13NO2	218.05783						3.7E+04	-0.2
566 2-(Hydroxymethyl)-3-(acetamidomethylene)succinate	[M+H] ⁺	C8H11NO6	218.06677					7.7E+04	-3.9	
567 Tyrosine methyl ester	[M+Na] ⁺	C10H13NO3	218.07920					1.7E+05	-2.0	
568 3-Methylindolepyruvate	[M+H] ⁺	C12H11NO3	218.08101						3.9E+04	0.7
569 Sulfosalicylic acid	[M+H] ⁺	C7H6O6S	218.99632			1.5E+05	-2.4			
570 Caffeic acid	[M+K] ⁺	C9H8O4	219.00542	3.1E+05	1.7				4.0E+04	4.2
571 Isonicotinylglycine	[M+K] ⁺	C8H8N2O3	219.01583				1.0E+05	3.8		
572 Glucose	[M+K] ⁺	C6H12O6	219.02655	1.4E+06	4.3	2.2E+06	-0.4		5.2E+05	-0.6
573 Aminophenylalanine	[M+K] ⁺	C9H12N2O2	219.05372					1.4E+05	-3.1	
574 1,2,3-triacetyl-glycerol	[M+H] ⁺	C9H14O6	219.08556				5.0E+04	3.4		
575 5-L-Glutamyl-L-alanine	[M+H] ⁺	C8H14N2O5	219.09670						7.0E+04	3.9
576 Geranyl acetate	[M+Na] ⁺	C12H20O2	219.13470					1.6E+05	3.9	
577 Tetradecapentaenoic acid	[M+H] ⁺	C14H18O2	219.13733				8.0E+04	2.9		
578 Guanidinoethyl methyl phosphate	[M+Na] ⁺	C4H12N3O4P	220.04626				4.4E+04	-2.3		
579 N-Hydroxy-L-tyrosine	[M+Na] ⁺	C9H11NO4	220.05863				3.6E+04	-2.7		
580 Amidino-3-keto-scylo-inosamine	[M+H] ⁺	C7H13N3O5	220.09348						4.0E+04	-3.1
581 Succimer	[M+K] ⁺	C4H6O4S2	220.93457					9.2E+05	-3.0	
582 Dihydrocaffeic acid	[M+K] ⁺	C9H10O4	221.02107	2.7E+05	1.9	2.2E+05	-3.5		1.7E+05	1.5
583 Imidazole acetol-phosphate	[M+H] ⁺	C6H9N2O5P	221.03218	7.5E+05	3.1	3.2E+05	-2.3		3.7E+05	-4.1
584 Diisopropyl phosphate	[M+K] ⁺	C6H15O4P	221.03340						1.9E+05	2.5
585 Purpurogallin	[M+H] ⁺	C11H8O5	221.04445	3.5E+05	2.0					
586 N-Nitrosodiphenylamine	[M+Na] ⁺	C12H10N2O	221.06758						7.0E+04	4.3
587 cis-2,3-Dihydroxy-2,3-dihydro-p-cumate	[M+Na] ⁺	C10H14O4	221.07891						3.6E+04	-2.2
588 N-Acetyl-beta-D-glucosaminylamine	[M+H] ⁺	C8H16N2O5	221.11348					1.3E+05	-1.3	
589 Linderic acid	[M+Na] ⁺	C12H22O2	221.15120	1.7E+05	2.7	1.9E+05	-3.4			
590 Caryophyllene epoxide	[M+H] ⁺	C15H24O	221.19020				5.2E+05	-0.9		
591 p-Hydroxyphenylacetothiohydroximate	[M+K] ⁺	C8H9NO2S	221.99879				4.2E+04	-1.0		
592 Pyridoxic acid	[M+K] ⁺	C8H9NO4	222.01680			7.8E+04	-2.2			
593 Dictamnine	[M+Na] ⁺	C12H9NO2	222.05323				4.6E+04	-3.1		
594 3-(3,4-Dihydroxypyridin-1-yl)-L-alanine	[M+Na] ⁺	C8H11N2O4	222.06087				1.2E+05	1.0		
595 Nalpha,Nalpha-Dimethyl-L-histidine	[M+K] ⁺	C8H13N3O2	222.06397				3.6E+04	-0.2		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
596 Erythrose 4-phosphate	[M+Na] ⁺	C4H9O7P	222.99879					6.7E+04	-4.4	
597 3-(3'-Methylthio)propylmalic acid	[M+H] ⁺	C8H14O5S	223.06347	1.0E+05	-3.9					
598 Decenedioic acid	[M+Na] ⁺	C10H16O4	223.09408	1.4E+05	-2.8			7.4E+05	-0.9	2.4E+05 -2.4
599 Apiole	[M+H] ⁺	C12H14O4	223.09572		5.6E+05	3.4	7.4E+06	3.4	3.7E+05	2.0
600 Lauric acid	[M+Na] ⁺	C12H24O2	223.16685	6.1E+04	3.7					
601 Capryloylglycine	[M+Na] ⁺	C10H19NO3	224.12669						4.0E+04	-4.4
602 Sulfolobenzaldehyde	[M+K] ⁺	C7H6O4S	224.96247				2.1E+05	-2.8		
603 Bergaptol	[M+Na] ⁺	C11H6O4	225.01539				1.6E+05	2.0		
604 Dimethoxy-4-hydroxycinnamic acid	[M+H] ⁺	C11H12O5	225.07671						1.3E+05	-4.3
605 3-Hydroxykynurenine	[M+H] ⁺	C10H12N2O4	225.08643				9.6E+04	2.5		
606 Sebacic acid	[M+Na] ⁺	C10H18O4	225.10973	1.2E+05	2.4	2.8E+05	-3.7	1.9E+05	-2.6	5.4E+05 -0.1
607 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine	[M+H] ⁺	C13H12N4	225.11253				3.7E+06	4.2		
608 4-Amino-4-deoxychorismate;ADC	[M+H] ⁺	C10H11NO5	226.07028				3.9E+04	3.2		
609 N-Heptanoylglycine	[M+K] ⁺	C9H17NO3	226.08416		1.0E+05	-0.7				
610 L-beta-aspartyl-L-alanine	[M+Na] ⁺	C7H12N2O5	227.06477		1.0E+05	-4.1				
611 Dimethylenetriurea	[M+Na] ⁺	C5H12N6O3	227.08681		1.5E+05	-2.2				
612 Genipin	[M+H] ⁺	C11H14O5	227.09077				1.8E+06	2.8		
613 O-Acetylcarnitine	[M+Na] ⁺	C9H18NO4	227.11221				5.9E+04	2.6		
614 Tuberonic acid	[M+H] ⁺	C12H18O4	227.12779	2.5E+05	-2.4					
615 1,8-Diazacyclotetradecane-2,9-dione	[M+H] ⁺	C12H22N2O2	227.17588						3.7E+04	-2.1
616 S-Prenyl-L-cysteine	[M+K] ⁺	C8H15NO2S	228.04576						5.5E+04	-1.1
617 1-Methyl-4-phenyl-1,2,3,6-tetrahydropyridine N-oxide	[M+K] ⁺	C12H15NO	228.07950				1.2E+05	-4.3		
618 Methylthiooctanaldoxime	[M+K] ⁺	C9H19NOS	228.08174		7.9E+04	0.7		6.0E+04	-0.3	
619 Deoxycytidine	[M+H] ⁺	C9H13N3O4	228.09693						4.5E+04	4.2
620 Oxalosuccinic acid	[M+K] ⁺	C6H6O7	228.97532					4.8E+04	-3.5	
621 4-Nitroquinoline N-oxide	[M+K] ⁺	C9H6N2O3	229.00041				5.1E+04	2.6		
622 Serine phosphoethanolamine	[M+H] ⁺	C5H13N2O6P	229.05879				2.6E+05	-1.7		
623 Resveratrol	[M+H] ⁺	C14H12O3	229.08655		1.4E+05	-2.7				
624 trans,trans-1,4-Diphenyl-1,3-butadiene	[M+Na] ⁺	C16H14	229.09877	1.0E+05	-0.9					
625 Monoethylglycinexylidide	[M+Na] ⁺	C12H18N2O	229.13128				1.7E+05	-0.6		
626 Dodecenedioic acid	[M+H] ⁺	C12H20O4	229.14350						5.5E+04	-0.3
627 L-isoleucyl-L-proline	[M+H] ⁺	C11H20N2O3	229.15515		8.8E+04	-2.1				
628 Octylphenol	[M+Na] ⁺	C14H22O	229.15629	1.2E+05	2.0					
629 N-Acetyl-L-methionine	[M+K] ⁺	C7H13NO3S	230.02431						3.7E+04	2.0
630 S-(2-Hydroxyethyl)-N-acetyl-L-cysteine	[M+Na] ⁺	C7H13NO4S	230.04546				1.0E+05	1.3		
631 Dihydroliipoamide	[M+Na] ⁺	C8H17NOS2	230.06377		1.4E+05	2.6				
632 Hydroxydebrisoquine	[M+K] ⁺	C10H13N3O	230.06838					5.7E+04	2.8	
633 Anthocyanin	[M+Na] ⁺	C15H11O	230.07021				5.4E+04	0.0		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
634 N-Acetyl-D-phenylalanine	[M+Na] ⁺	C11H13NO3	230.07810						5.6E+04	2.9
635 N-Butyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine	[M+K] ⁺	C9H13N5	230.08027					6.1E+04	-0.1	
636 Butenylcarnitine	[M+H] ⁺	C11H19NO4	230.13938				1.8E+05	-3.0	1.9E+05	3.2 2.3E+05 -3.9
637 Decanoylglycine	[M+H] ⁺	C12H23NO3	230.17507	3.4E+05	0.1				8.8E+04	-1.2
638 Xestostanol C	[M+H] ⁺	C14H31NO	230.24784	1.2E+05	-3.1		3.9E+05	-1.3	4.2E+05	1.3 1.2E+05 -1.1
639 Citric acid	[M+K] ⁺	C6H8O7	230.99016	2.9E+05	-1.7					
640 Myristicin	[M+K] ⁺	C11H12O3	231.04087			1.9E+05	4.0			
641 Chalcone	[M+Na] ⁺	C15H12O	231.07834				9.1E+04	-1.3		
642 12-oxo-5E,8E,10Z-dodecatricienoic acid	[M+Na] ⁺	C12H16O3	231.09917	1.6E+05	3.2					
643 Diphenylcyclobutane	[M+Na] ⁺	C16H16	231.11442	9.7E+04	-1.1					
644 Linderenol	[M+H] ⁺	C15H18O2	231.13724					1.4E+05	3.1	
645 Dodecanedioic acid	[M+H] ⁺	C12H22O4	231.15878				4.0E+04	1.3		
646 Hydroxy-tridecanoic acid	[M+H] ⁺	C13H26O3	231.19636			1.3E+05	-3.8			
647 Hydroxypseudoxyntocine	[M+K] ⁺	C10H14N2O2	233.06801						6.4E+04	2.9
648 Dihydrochalcone	[M+Na] ⁺	C15H14O	233.09416				9.2E+04	-2.0		
649 Apotaxene	[M+H] ⁺	C17H28	233.22686			2.5E+05	-2.1			
650 Hydroxypropionylcarnitine	[M+H] ⁺	C10H19NO5	234.13401		1.1E+05	-1.8				
651 Deoxynupharidine	[M+H] ⁺	C15H23NO	234.18470					9.6E+04	2.3	
652 (Homo)3-citrate	[M+H] ⁺	C9H14O7	235.08202					8.7E+05	-3.4	
653 Harmine	[M+Na] ⁺	C13H12N2O	235.08483				8.0E+05	-2.8		
654 Acetoxychavicol acetate	[M+H] ⁺	C13H14O4	235.09678						3.4E+05	-1.3
655 3,7-Dimethyl-8,11-dioxo-2E,6E,9E-dodecatricenal	[M+H] ⁺	C14H18O3	235.13261			3.5E+06	1.1			
656 2-methyl-2-dodecenoic acid	[M+Na] ⁺	C13H24O2	235.16668		2.1E+05	0.7				
657 2-methyl-2-dodecenoic acid	[M+Na] ⁺	C13H24O2	235.16685	1.5E+05	2.8					
658 Myristaldehyde	[M+Na] ⁺	C14H28O	235.20403		2.4E+05	-3.4				
659 Hexadecatrienal	[M+H] ⁺	C16H26O	235.20564	2.4E+05	-0.6					
660 Benzenedisulfonamide	[M+H] ⁺	C6H8N2O4S2	236.99893			1.1E+06	3.8			
661 Capillarin	[M+K] ⁺	C13H10O2	237.03124	1.4E+05	3.2					
662 Trimethoxycoumarin	[M+H] ⁺	C12H12O5	237.07498		1.3E+06	3.2				
663 Trimethoxycoumarin	[M+H] ⁺	C12H12O5	237.07575	2.3E+05	-0.2					
664 N-(Phenylmethyl)-N-methyl-2-pyridinamine	[M+K] ⁺	C13H14N2	237.07828				6.0E+04	2.4		4.5E+04 4.2
665 Coryneine	[M+K41] ⁺	C11H18NO2	237.09452							4.1E+04 2.2
666 Dimethylallyl-hydroxymandelic acid	[M+H] ⁺	C13H16O4	237.11171			9.6E+06	1.8	1.5E+05	0.3	
667 Heptyloxybenzoic acid	[M+H] ⁺	C14H20O3	237.14754							8.1E+04 4.1
668 Capsidiol	[M+H] ⁺	C15H24O2	237.18476							4.6E+04 0.6
669 Hexadecynal	[M+H] ⁺	C16H28O	237.22129	9.0E+04	-0.1					
670 N-Nonanoylglycine	[M+Na] ⁺	C11H21NO3	238.14136	6.6E+04	1.6		6.1E+04	1.9		
671 Trimethylallantoin	[M+K] ⁺	C7H12N4O3	239.05410	7.4E+04	3.7					
672 Decenedioic acid	[M+K] ⁺	C10H16O4	239.06832		8.4E+04	-1.3				

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
673 Flavonol	[M+H] ⁺	C15H10O3	239.07027	9.9E+04	2.9					
674 Trimethoxycinnamic acid	[M+H] ⁺	C12H14O5	239.09061			6.1E+06	3.3			
675 Tetrahydrozoline	[M+K] ⁺	C13H16N2	239.09451						1.0E+05	0.0
676 Methoxychalcone	[M+H] ⁺	C16H14O2	239.10709			1.3E+06	-1.8			
677 7-hydroxy-dodecanoic acid	[M+Na] ⁺	C12H24O3	239.16226						1.5E+05	-2.1
678 Hydroxy lauric acid	[M+Na] ⁺	C12H24O3	239.16270					4.4E+05	-3.9	
679 Sundiversifolide	[M+H] ⁺	C14H22O3	239.16417	1.2E+05	-2.5	1.9E+05	0.6	1.2E+05	-2.6	
680 2-(Acetamidomethylene)-3-(hydroxymethyl)succinate	[M+Na] ⁺	C8H11NO6	240.04845				7.4E+04	-2.5		
681 Methylindolepyruvate	[M+Na] ⁺	C12H11NO3	240.06313				6.4E+04	-0.1	3.6E+04	-1.9
682 beta-Alanyl-L-lysine	[M+Na] ⁺	C9H19N3O3	240.13128			3.2E+05	2.4			
683 Amino-undecanoic acid	[M+K] ⁺	C11H23NO2	240.13648						3.6E+04	-1.8
684 Bergaptol	[M+K] ⁺	C11H6O4	240.99028						9.6E+04	-2.1
685 Dihydroxyanthraquinone	[M+H] ⁺	C14H8O4	241.04923		9.4E+04	1.3				
686 Sebacic acid	[M+K] ⁺	C10H18O4	241.08367	1.2E+05	-1.0					
687 Hydroxysebacic acid	[M+Na] ⁺	C10H18O5	241.10515		9.9E+04	-2.1		1.6E+05	-2.9	
688 Dimethyl-L-arginine	[M+K] ⁺	C8H18N4O2	241.10614	2.4E+05	-1.9	2.1E+06	-3.0			
689 O-Succinyl-L-homoserine	[M+Na] ⁺	C8H13NO6	242.06448					5.3E+04	-4.0	
690 L-Acetylcarnitine	[M+K] ⁺	C9H17NO4	242.07966					7.4E+04	-3.1	
691 N-Phenyl-1-naphthylamine	[M+Na] ⁺	C16H13N	242.09370						4.9E+04	1.3
692 Pantothenic acid	[M+Na] ⁺	C9H17NO5	242.10015		1.1E+05	-1.1				
693 Pentahomomethionine	[M+Na] ⁺	C10H21NO2S	242.11783					5.9E+04	2.9	
694 Diethyl-2-methyl-3-hydroxysuccinate	[M+K] ⁺	C9H16O5	243.06386					5.2E+04	-3.8	
695 gamma-Hydroxy-L-homoarginine	[M+K] ⁺	C7H16N4O3	243.08463				4.8E+04	3.2		
696 Caulophylline	[M+K] ⁺	C12H16N2O	243.08945			2.7E+05	-0.1			
697 Lipoamide	[M+K] ⁺	C8H15NOS2	244.02347						6.6E+04	-3.3
698 Pantothenol	[M+K] ⁺	C9H19NO4	244.09399					1.1E+05	2.4	
699 N-Undecanoylglycine	[M+H] ⁺	C13H25NO3	244.19072	1.4E+05	-1.3	1.8E+05	-3.1			
700 2-amino-tetradecanoic acid	[M+H] ⁺	C14H29NO2	244.22720					5.9E+04	-0.4	
701 Sulfolactone	[M+Na] ⁺	C6H6O7S	244.97270				5.3E+04	-0.2		
702 6-Acetyl-D-glucose	[M+Na] ⁺	C8H14O7	245.06332					3.3E+05	-0.6	8.8E+04 -1.8
703 Apiole	[M+Na] ⁺	C12H14O4	245.07843	5.5E+05	3.4	7.1E+05	-2.0	1.2E+06	0.1	3.2E+05 -2.1
704 Piceatannol	[M+H] ⁺	C14H12O4	245.08143			2.2E+05	-2.4	3.9E+05	1.7	
705 Osthol	[M+H] ⁺	C15H16O3	245.11740			3.6E+05	-0.7			
706 Dodecatrienyl acetate	[M+Na] ⁺	C14H22O2	245.15120	9.5E+04	-3.8					
707 6E,8E,12E-Hexadecatrien-10-ynoic acid	[M+H] ⁺	C16H20O2	245.15435						4.6E+04	-3.0
708 Kynurenine	[M+K] ⁺	C10H12N2O3	247.04839				7.0E+04	-1.8		
709 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine	[M+Na] ⁺	C13H12N4	247.09514			7.1E+05	1.1			
710 Methyl jasmonate	[M+Na] ⁺	C13H20O3	247.13047	2.9E+05	-2.5			2.1E+05	-2.2	

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm	
711	alpha-Santonin	[M+H] ⁺	C15H18O3	247.13315						5.3E+04	-1.1	
712	Tetradecadienal	[M+K] ⁺	C14H24O	247.14587	8.6E+04	-1.7						
713	Pentadecenal	[M+Na] ⁺	C15H28O	247.20324	8.2E+04	-3.2						
714	Proflavine	[M+K] ⁺	C13H11N3	248.05943				5.0E+04	-3.9			
715	Lycopodine	[M+H] ⁺	C16H25NO	248.20063				4.2E+04	1.1			
716	Tryptanthrine	[M+H] ⁺	C15H8N2O2	249.06638				1.3E+05	-2.1			
717	Dihydrochalcone	[M+K] ⁺	C15H14O	249.06762	8.6E+04	-1.2						
718	Beta-aspartyl-aspartic acid	[M+H] ⁺	C8H12N2O7	249.07103			7.6E+05	2.8				
719	Prenyl caffeate	[M+H] ⁺	C14H16O4	249.11157			4.8E+06	2.3				
720	Hydroxymelatonin	[M+H] ⁺	C13H16N2O3	249.12337	1.1E+05	-1.6						
721	Canellal	[M+H] ⁺	C15H20O3	249.14852	1.9E+05	-3.1						
722	Myristoleic acid	[M+Na] ⁺	C14H26O2	249.18250	8.3E+04	-0.8	2.7E+05	-1.2				
723	Hexadecadiynoic acid	[M+H] ⁺	C16H24O2	249.18411						8.0E+04	3.2	
724	5-(2'-Formylethyl)-4,6-dihydroxypicolinate	[M+K] ⁺	C9H9NO5	250.01066					7.3E+04	2.3		
725	1-(4-Methoxyphenyl)-3-(4-morpholinyl)-1-propanone	[M+H] ⁺	C14H19NO3	250.14316					9.4E+04	2.4		
726	Serine-phosphoethanolamine	[M+Na] ⁺	C5H13N2O6P	251.04026					1.2E+05	0.3		
727	Deoxyuridine	[M+Na] ⁺	C9H12N2O5	251.06470						5.4E+04	-3.4	
728	L-prolyl-L-proline	[M+K] ⁺	C10H16N2O3	251.07863				1.2E+05	2.5	7.8E+04	-2.3	
729	3-(5'-Methylthio)pentylmalic acid	[M+H] ⁺	C10H18O5S	251.09386						6.5E+04	3.6	
730	Ubiquinone Q1	[M+H] ⁺	C14H18O4	251.12791			6.8E+06	-0.5	1.5E+05	2.4	9.7E+04	3.8
731	2-methyl-2-dodecenoic acid	[M+K] ⁺	C13H24O2	251.14108					1.6E+05	-1.2		
732	2-keto tridecanoic acid	[M+Na] ⁺	C13H24O3	251.16103				7.6E+04	2.9			
733	Arbusculin A	[M+H] ⁺	C15H22O3	251.16372					2.0E+05	1.8	6.2E+04	1.0
734	Myristic acid	[M+Na] ⁺	C14H28O2	251.19807		3.2E+05	0.3					
735	4-Phospho-L-aspartate	[M+K] ⁺	C4H8NO7P	251.96788				4.3E+04	-3.5			
736	N-Decanoylglycine	[M+Na] ⁺	C12H23NO3	252.15701	4.9E+05	-1.8			6.1E+05	-0.2		
737	Dodecanedioic acid	[M+Na] ⁺	C12H22O4	253.14126				1.5E+05	-0.9			
738	Tetramethyl-undecan-1,10-diol	[M+Na] ⁺	C14H30O2	253.21307		1.8E+05	2.9					
739	2,2,9,9-tetramethyl-undecan-1,10-diol	[M+Na] ⁺	C14H30O2	253.21380	1.1E+05	-1.4						
740	Robustine	[M+K] ⁺	C12H9NO3	254.02052			1.7E+05	3.5				
741	N-Nonanoylglycine	[M+K] ⁺	C11H21NO3	254.11618						6.7E+04	-3.5	
742	Solenopsin A	[M+H] ⁺	C17H35N	254.28423	1.3E+05	-3.9						
743	Bisnorbiotin	[M+K] ⁺	C8H12N2O3S	255.02064						1.2E+05	-2.4	
744	7,4'-Dihydroxyflavone	[M+H] ⁺	C15H10O4	255.06519	7.0E+04	-0.8						
745	Arginine phosphate	[M+H] ⁺	C6H15N4O5P	255.08432			1.6E+06	3.8	1.0E+05	2.4		
746	N2-Succinyl-L-ornithine	[M+Na] ⁺	C9H16N2O5	255.09429						5.1E+04	3.3	
747	Methyl 4-[2-(2-formyl-vinyl)-3-hydroxy-5-oxo-cyclopentyl]-butanoate	[M+H] ⁺	C13H18O5	255.12356			2.4E+06	-3.4				
748	Hydroxydodecanoic acid	[M+K] ⁺	C12H24O3	255.13634					7.1E+04	-2.5		

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
749	2-(Acetamidomethylene)-3-(hydroxymethyl)succinate	[M+K] ⁺	C8H11NO6	256.02156				5.7E+04	0.9		
750	Methylphenidate	[M+Na] ⁺	C14H19NO2	256.13004						7.4E+04	3.0
751	Palmitic amide	[M+H] ⁺	C16H33NO	256.26349	5.8E+04	0.4					
752	2-Oxo-9-methylthiononanoic acid	[M+K] ⁺	C10H18O3S	257.06082	8.6E+04	3.1					
753	N-Acetylserotonin	[M+K] ⁺	C12H14N2O2	257.06868				8.0E+04	0.0		
754	Abrine	[M+K] ⁺	C12H14N2O2	257.06877						7.2E+04	-0.3
755	Hydroxysebacic acid	[M+K] ⁺	C10H18O5	257.07858	2.7E+05	-2.8					
756	Phenylglucoside	[M+H] ⁺	C12H16O6	257.10216			3.6E+05	-0.8		1.5E+05	3.6
757	Benzoylagmatine	[M+Na] ⁺	C12H18N4O	257.13641						4.7E+04	3.4
758	Curcumenol	[M+Na] ⁺	C15H22O2	257.15154					1.7E+05	-1.3	
759	3,3'-Dimethylbisphenol A	[M+H] ⁺	C17H20O2	257.15361	1.3E+05	1.5		4.4E+04	1.5		
760	Hexadecatrienal	[M+Na] ⁺	C16H26O	257.18733			1.8E+05	1.0		2.1E+05	-1.1
761	4-Nitrophenyl phosphate	[M+K] ⁺	C6H6NO6P	257.95623						4.0E+04	0.8
762	Pentahomomethionine	[M+K] ⁺	C10H21NO2S	258.09246	6.0E+04	3.7					
763	Glycerophosphocholine	[M+H] ⁺	C8H20NO6P	258.11010	1.7E+05	3.1			1.1E+05	3.8	
764	Glycosminine	[M+Na] ⁺	C15H12N2O	259.08418	1.1E+05	-0.2					
765	Capsidiol	[M+Na] ⁺	C15H24O2	259.16664			1.2E+05	0.8			
766	Tetradecanedioic acid	[M+H] ⁺	C14H26O4	259.19097				1.6E+05	-2.3		
767	Apiole	[M+K] ⁺	C12H14O4	261.05237	5.5E+05	0.7					
768	7E,9E,11-Dodecatrienyl acetate	[M+K] ⁺	C14H22O2	261.12514	1.6E+05	0.0					
769	1-(4-Hydroxyphenyl)-1-decene-3,5-dione	[M+H] ⁺	C16H20O3	261.14841						2.3E+05	0.4
770	3-Hydroxykynurenine	[M+K] ⁺	C10H12N2O4	263.04208				1.3E+05	3.0		
771	Beta-aspartyl-glutamic acid	[M+H] ⁺	C9H14N2O7	263.08720			1.4E+06	0.7			
772	L-beta-aspartyl-L-glutamic acid	[M+H] ⁺	C9H14N2O7	263.08798			2.2E+05	-2.3			
773	Ornaline	[M+H] ⁺	C10H18N2O6	263.12444					2.8E+05	-2.6	
774	Marmasmic acid	[M+H] ⁺	C15H18O4	263.12725			2.9E+06	2.0			
775	Acutifolane A	[M+H] ⁺	C16H22O3	263.16484					1.4E+05	-2.5	
776	Pentadecenoic acid	[M+Na] ⁺	C15H28O2	263.19859			3.9E+05	-1.7			
777	Heptadecadiynoic acid	[M+H] ⁺	C17H26O2	263.20046					1.3E+05	0.4	
778	Dihydroxy-N-benzoyl-L-serine	[M+Na] ⁺	C10H11NO6	264.04693				5.5E+04	3.5		
779	4-(Dimethylamino)azobenzene	[M+K] ⁺	C14H15N3	264.08919				6.6E+04	2.2		
780	3-(Phosphoacetylamido)-L-alanine	[M+Na] ⁺	C5H11N2O7P	265.02047						5.4E+04	-3.3
781	Nitrotyrosine	[M+K] ⁺	C9H10N2O5	265.02213	7.4E+05	3.5					
782	Thymidine	[M+Na] ⁺	C10H14N2O5	265.07955						7.3E+04	-0.2
783	N-Acetylcystathionine	[M+H] ⁺	C9H16N2O5S	265.08527	8.0E+05	0.1					
784	2'-Hydroxyfurano[2'',3'':4',3']chalcone	[M+H] ⁺	C17H12O3	265.08605			1.0E+06	-0.5			
785	2-(6'-Methylthio)hexylmalate	[M+H] ⁺	C11H20O5S	265.11040				7.5E+04	0.1		
786	Abscisic acid	[M+H] ⁺	C15H20O4	265.14264			1.2E+05	3.0			
787	Keto myristic acid	[M+Na] ⁺	C14H26O3	265.17759			2.7E+05	-0.7		5.6E+05	-3.6

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
788 Dehydrojuvabione	[M+H] ⁺	C16H24O3	265.17963				1.6E+05	0.7	1.8E+05	-1.0
789 Aroenate	[M+K] ⁺	C10H13NO5	266.04253	8.8E+04	-0.5					
790 Dehydroadenosine	[M+H] ⁺	C10H11N5O4	266.08875						4.6E+04	-1.4
791 Annonaine	[M+H] ⁺	C17H15NO2	266.11702						5.6E+04	2.0
792 N-Undecanoylglycine	[M+Na] ⁺	C13H25NO3	266.17266	7.7E+05	0.5					
793 Amino-tetradecanoic acid	[M+Na] ⁺	C14H29NO2	266.20916					5.9E+04	-0.4	
794 Deoxyuridine	[M+K] ⁺	C9H12N2O5	267.03820						5.8E+04	-1.6
795 Resveratrol	[M+K] ⁺	C14H12O3	267.04130				6.2E+04	1.9		
796 Methyl-dodecanedioic acid	[M+Na] ⁺	C13H24O4	267.15614		1.8E+05	2.0	1.4E+05	3.3	2.9E+05	1.2
797 Myristic acid	[M+K] ⁺	C14H28O2	267.17237				7.1E+04	-1.1	1.5E+05	3.4
798 Pentadecanol	[M+K] ⁺	C15H32O	267.20932			6.4E+05	-3.2			
799 2-Amino-4-oxo-6-(1',2'-dioxopropyl)-7,8-dihydroxypteridine	[M+H] ⁺	C9H9N5O5	268.06794						4.8E+04	-1.1
800 S-Ribosyl-L-homocysteine	[M+H] ⁺	C9H17NO6S	268.08432						4.7E+04	2.3
801 Acetylcarnosine	[M+H] ⁺	C11H15N4O4	268.11561		1.2E+05	3.7				
802 N-Decanoylglycine	[M+K] ⁺	C12H23NO3	268.13095	4.6E+05	0.5					
803 Aspartyl-L-proline	[M+K] ⁺	C9H14N2O5	269.05293					8.4E+04	1.9	7.3E+04 -2.3
804 Saphenic acid	[M+H] ⁺	C15H12N2O3	269.09207	8.0E+04	-3.0					
805 Linderenol	[M+K] ⁺	C15H18O2	269.09383				6.0E+04	0.0		
806 3-oxo-2-pentyl-cyclopentanehexanoic acid	[M+H] ⁺	C16H28O3	269.21042						1.3E+05	2.6
807 7-methyl-6E-hexadecenoic acid	[M+H] ⁺	C17H32O2	269.24751	1.2E+05	2.0					
808 N-Succinyl-L-glutamate 5-semialdehyde	[M+K] ⁺	C9H13NO6	270.03671		1.1E+05	2.7				
809 N-Acetyl-L-glutamyl 5-phosphate	[M+H] ⁺	C7H12NO8P	270.03725					7.7E+04	0.3	
810 Benzoyldehydro-2,3-dihydroxy-benzene	[M+K] ⁺	C13H13NO3	270.05246					6.5E+04	0.9	
811 Isovalerylglutamic acid	[M+K] ⁺	C10H17NO5	270.07427			1.5E+05	-1.6			
812 O-Butanoylcarnitine	[M+K] ⁺	C11H21NO4	270.10988			3.1E+05	1.2			
813 2,3-Dimethoxy-[2-(4-Pyridinyl)-1-butenyl]phenol	[M+H] ⁺	C17H19NO2	270.14796						8.1E+04	3.3
814 3,5-Dinitro-4-hydroxyphenylpyruvate	[M+H] ⁺	C9H6N2O8	271.02038						4.5E+04	-2.5
815 Melatonin	[M+K] ⁺	C13H16N2O2	271.08434	8.0E+04	3.5					
816 Aphylline	[M+Na] ⁺	C15H24N2O	271.17794			2.4E+05	0.5			
817 Sterol	[M+Na] ⁺	C17H28O	271.20369		2.7E+05	-1.7				
818 Hypusine	[M+K] ⁺	C10H23N3O3	272.13791				5.1E+04	-3.0		
819 2-amino-hexadecanoic acid	[M+H] ⁺	C16H33NO2	272.25939						2.1E+05	-3.6
820 2-Hydroxy-6-oxo-6-(2-hydroxyphenyl)-hexa-2,4-dienoate	[M+K] ⁺	C12H10O5	273.01598	6.3E+04	1.2				7.3E+04	3.6
821 Gamma-Glutamylcysteine	[M+Na] ⁺	C8H14N2O5S	273.05096				7.6E+04	2.2		
822 2,2-Dimethyl-8-prenylchromene 6-carboxylic acid	[M+H] ⁺	C17H20O3	273.14833					2.2E+05	0.7	
823 Hexadecatrienoic acid	[M+Na] ⁺	C16H26O2	273.18278		4.4E+05	-1.0				

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
824 Retamine	[M+Na] ⁺	C15H26N2O	273.19306			1.7E+05	2.5			
825 Methylhexadecane-1,2-diol	[M+H] ⁺	C17H36O2	273.27876					1.0E+05	0.2	
826 Hexadecaspinganine	[M+H] ⁺	C16H35NO2	274.27350					2.9E+05	2.0	2.0E+05 1.9
827 S-(Phenylacetothiohydroximoyl)-L-cysteine	[M+Na] ⁺	C11H14N2O3S	277.06132		1.7E+05	1.5				
828 4'-Hydroxy-2'-methoxychalcone	[M+Na] ⁺	C16H14O3	277.08358						4.4E+05	-0.2
829 Biotin sulfone	[M+H] ⁺	C10H16N2O5S	277.08443			5.9E+05	3.0			
830 methyl 4-[2-(2-formyl-vinyl)-3-hydroxy-5-oxo-cyclopentyl]-butanoate	[M+Na] ⁺	C13H18O5	277.10464	4.0E+05	0.8					
831 Palmitoleic acid	[M+Na] ⁺	C16H30O2	277.21380	4.0E+05	1.7	2.0E+06	0.1			
832 1,2-Dihydroxynaphthalene-6-sulfonate	[M+K] ⁺	C10H8O5S	278.97192						1.5E+05	1.7
833 Ascorbate 2-sulfate	[M+Na] ⁺	C6H8O9S	278.97825		2.1E+05	-0.5				
834 Dihydroflavonol	[M+K] ⁺	C15H12O3	279.04220					2.2E+05	-1.4	
835 alhpa-tocopheronolactone	[M+H] ⁺	C16H22O4	279.15921		4.1E+06	-0.4			1.8E+06	-1.7
836 4-keto pentadecanoic acid	[M+Na] ⁺	C15H28O3	279.19319				5.6E+05	-0.5		
837 Palmitic acid	[M+Na] ⁺	C16H32O2	279.22945	1.7E+05	-0.3					
838 alpha-linolenic acid	[M+H] ⁺	C18H30O2	279.23125		8.5E+05	2.2				
839 Glycerophosphocholine	[M+Na] ⁺	C8H20NO6P	280.09204	1.5E+05	-2.0					
840 Apigeniflavan	[M+Na] ⁺	C15H14O4	281.07828			9.9E+05	0.5			
841 Glycerophosphocholine	[M+Na] ⁺	C8H21NO6P	281.10076			4.0E+06	-3.2			
842 Falcarinone	[M+K] ⁺	C17H22O	281.13014		9.5E+04	0.3			6.9E+04	-3.3
843 Phaseic acid	[M+H] ⁺	C15H20O5	281.13875			4.4E+06	-1.4			
844 1-(3,4-Dihydroxyphenyl)-5-hydroxy-3-decanone	[M+H] ⁺	C16H24O4	281.17488				4.2E+05	-0.5	3.1E+05	2.9
845 N-Undecanoylglycine	[M+K] ⁺	C13H25NO3	282.14660	8.2E+05	0.3					
846 Uridine	[M+K] ⁺	C9H12N2O6	283.03186					9.2E+04	3.0	
847 Piceatannol	[M+K] ⁺	C14H12O4	283.03682				6.3E+04	-0.4		
848 Biotin	[M+K] ⁺	C10H16N2O3S	283.05159		8.9E+04	-0.9				
849 Corylinal	[M+H] ⁺	C16H10O5	283.06091					8.5E+04	-2.9	
850 Hemigossypol	[M+Na] ⁺	C15H16O4	283.09455			8.6E+05	-1.7			
851 Dihydrophaseic acid	[M+H] ⁺	C15H22O5	283.15497			2.4E+06	-3.4			
852 Cadamine	[M+H] ⁺	C15H26N2O3	283.20162	7.3E+04	-2.4					
853 Oleic acid	[M+H] ⁺	C18H34O2	283.26316	1.3E+05	2.4					
854 Guanosine	[M+H] ⁺	C10H13N5O5	284.09881			1.8E+05	0.5			
855 Homovanillic acid sulfate	[M+Na] ⁺	C9H10O7S	285.00449						7.0E+04	-1.9
856 Maclurin	[M+Na] ⁺	C13H10O6	285.03715				1.3E+05	-0.7		
857 7,4',5'-Trihydroxy-5,2'-oxido-4-phenylcoumarin	[M+H] ⁺	C15H8O6	285.03936	9.7E+04	-2.7					
858 Aromaticin	[M+K] ⁺	C15H18O3	285.08917			4.3E+05	-1.5			
859 Caffeic acid phenethyl ester	[M+H] ⁺	C17H16O4	285.11214	1.7E+05	-2.3					
860 Cernuine	[M+Na] ⁺	C16H26N2O	285.19373	1.4E+05	-2.5					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
861 L-beta-aspartyl-L-aspartic acid	[M+K] ⁺	C8H12N2O7	287.02761	6.9E+04	-3.3					
862 Hydroxyindoleacetyl glycine	[M+K] ⁺	C12H12N2O4	287.04287	6.6E+04	3.0					
863 5'-Phosphoribosylglycinamide	[M+H] ⁺	C7H15N2O8P	287.06463			3.0E+05	-2.6			
864 1'-Acetoxyeugenol acetate	[M+Na] ⁺	C14H16O5	287.08870				5.6E+04	1.0		
865 4-(Hydroxymethyl)phenyl-beta-D-glucopyranoside	[M+H] ⁺	C13H18O7	287.11263				5.5E+04	-0.4		
866 N-Acetyl-leucyl-leucine	[M+H] ⁺	C14H26N2O4	287.19743		2.9E+05	-3.1				
867 3,7,11-Trimethyl-2,6,10-dodecatrienyl acetate	[M+Na] ⁺	C17H28O2	287.19891				5.9E+04	-2.6	1.6E+05	-0.4
868 Pyridoxine 5'-phosphate	[M+K] ⁺	C8H12NO6P	288.00406						7.1E+04	-2.4
869 C17 Sphinganine	[M+H] ⁺	C17H37NO2	288.29012					1.0E+06	-1.4	
870 Xanthoxic acid	[M+Na] ⁺	C15H22O4	289.14103	2.7E+05	-1.9					
871 Karwinaphthol B	[M+H] ⁺	C17H20O4	289.14363			5.5E+05	-0.7			
872 Methyl 2-(4-isopropyl-4-methyl-5-oxo-2-imidazolin-2-yl)-p-toluate	[M+H] ⁺	C16H20N2O3	289.15473						1.9E+05	-0.2
873 4,7,10-hexadecatrienoic acid	[M+K] ⁺	C16H26O2	289.15548					1.9E+05	3.3	
874 Elaeocarpidine	[M+Na] ⁺	C17H21N3	290.16276			4.4E+05	0.0			
875 Azaadenosine	[M+Na] ⁺	C9H12N6O4	291.08039						3.4E+05	2.9
876 Aurin	[M+H] ⁺	C19H14O3	291.10155						1.4E+06	0.1
877 5-O-Methylvisamminol	[M+H] ⁺	C16H18O5	291.12173			1.7E+06	3.3			
878 Shikimate 3-phosphate	[M+K] ⁺	C7H11O8P	292.98199				7.2E+04	1.1		
879 Gingerdione	[M+H] ⁺	C17H24O4	293.17513				7.5E+04	-1.3	9.0E+04	0.5
880 Dihydrobunolol	[M+H] ⁺	C17H27NO3	294.20676					1.2E+05	-1.3	
881 N-Glycosyl-L-asparagine	[M+H] ⁺	C10H18N2O8	295.11347					1.1E+05	0.4	
882 Aspartame	[M+H] ⁺	C14H18N2O5	295.12885	2.6E+06	-1.0				4.0E+05	-2.7
883 Methyl-tetradecanedioic acid	[M+Na] ⁺	C15H28O4	295.18836		2.4E+05	-1.3				
884 Dimethyladenosine	[M+H] ⁺	C12H17N5O4	296.13446						6.5E+04	2.9
885 Apigeniflavan	[M+K] ⁺	C15H14O4	297.05177				6.1E+04	2.0		
886 hydroxy-linoleic acid	[M+H] ⁺	C18H32O3	297.24297				2.9E+05	-1.9	2.3E+05	-1.5
887 Thiomethyladenosine	[M+H] ⁺	C11H15N5O3S	298.09690			2.2E+05	-0.2			
888 Hexanoylcarnitine	[M+K] ⁺	C13H25NO4	298.14172					8.7E+04	-0.7	
889 Demethylbellidifolin	[M+K] ⁺	C13H8O6	298.99525	7.5E+04	0.6					
890 Prephenyllactate	[M+H] ⁺	C13H14O8	299.07572					1.7E+05	1.4	
891 Falcarindiol	[M+K] ⁺	C17H24O2	299.14154				1.9E+05	-2.5	2.5E+05	0.2
892 Dihydroxy myristic acid	[M+K] ⁺	C14H28O4	299.16106				3.9E+05	2.9		
893 Stearidonic acid	[M+Na] ⁺	C18H28O2	299.19724					4.1E+05	3.0	
894 Pyrimidine 5'-deoxynucleotide	[M+Na] ⁺	C9H14N2O6P	300.04861				6.4E+04	-1.5		
895 Palmitoylethanolamide	[M+H] ⁺	C18H37NO2	300.28971	2.1E+05	-1.7	3.2E+05	-1.9			
896 Artecanin	[M+Na] ⁺	C15H18O5	301.10431			1.8E+05	1.1			
897 alhpa-tocopheronolactone	[M+Na] ⁺	C16H22O4	301.14103	1.7E+06	0.8	5.6E+06	-0.6		6.3E+06	-2.3
898 Trimethoxyflavan	[M+H] ⁺	C18H20O4	301.14386				2.4E+06	-1.4		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
899 Pinolenic acid	[M+Na] ⁺	C18H30O2	301.21385			2.3E+05	-0.2			
900 Hydroxy stearic acid	[M+H] ⁺	C18H36O3	301.27465		4.2E+05	-3.1				
901 Sphinganine	[M+H] ⁺	C18H39NO2	302.30536	9.2E+04	2.1				1.8E+05	-2.6
902 3-Methoxy-4-Hydroxyphenylglycol sulfate	[M+K] ⁺	C9H12O7S	302.99329					7.3E+04	0.8	
903 Ellagic acid	[M+H] ⁺	C14H6O8	303.01354	7.8E+04	-0.9					
904 2-(6'-Methylthio)hexylmalic acid	[M+K] ⁺	C11H20O5S	303.06716					1.2E+05	-2.8	
905 2-(4-Methoxyphenethyl)chromone	[M+Na] ⁺	C18H16O3	303.09917	7.5E+04	0.6					
906 Absciscic acid	[M+K] ⁺	C15H20O4	303.09957					1.4E+05	-0.8	
907 Subaphyllin	[M+K] ⁺	C14H20N2O3	303.11066						1.0E+05	-0.4
908 Phaseic acid	[M+Na] ⁺	C15H20O5	303.12029	8.9E+04	-2.2	4.0E+05	-0.4	1.3E+05	1.3	
909 Eicosapentaenoic acid	[M+H] ⁺	C20H30O2	303.23186	4.4E+05	-1.9					
910 Methyladenosine	[M+Na] ⁺	C11H15N5O4	304.10074		1.6E+05	2.9				
911 Arachidonoyl amine	[M+H] ⁺	C20H33NO	304.26439				3.2E+05	-3.0		
912 Methylinosine	[M+Na] ⁺	C11H14N4O5	305.08565						1.0E+05	0.0
913 Catechin 4'-methyl ether	[M+H] ⁺	C16H16O6	305.10196	1.2E+05	-3.1					
914 Oleic acid	[M+Na] ⁺	C18H34O2	305.24525		1.6E+06	-0.5				
915 Matricin	[M+H] ⁺	C17H22O5	307.15445			3.3E+06	-1.5			
916 3-oxo-2-pentyl-cyclopentanehexanoic acid	[M+K] ⁺	C16H28O3	307.16700	7.8E+04	2.1					
917 Retinal	[M+Na] ⁺	C20H28O	307.20327		1.5E+05	-0.1				
918 Eicosatrienoic acid	[M+H] ⁺	C20H34O2	307.26320		4.6E+05	-0.1				
919 Leu-Gly-Pro	[M+Na] ⁺	C13H23N3O4	308.15785			4.8E+05	0.7			
920 4-Hydrocinnamoyl-2,2,5-trimethyl-4-cyclopentene-1,3-dione	[M+K] ⁺	C17H18O3	309.08899			1.2E+06	-0.8			
921 Fructoselysine	[M+H] ⁺	C12H24N2O7	309.16591				9.7E+04	-0.9		
922 O-Methylembelin	[M+H] ⁺	C18H28O4	309.20604	2.3E+05	-2.5				1.2E+05	-2.2
923 Tridecanoylglycine	[M+K] ⁺	C15H29NO3	310.17700			4.3E+05	2.9			
924 Gamma-Glutamyltyrosine	[M+H] ⁺	C14H18N2O6	311.12376	1.8E+05	0.7			8.2E+04	-1.6	
925 Cupreine	[M+H] ⁺	C19H22N2O2	311.17540	1.0E+05	2.1					
926 9-hydroperoxy-10E,12,15Z-octadecatrienoic acid	[M+H] ⁺	C18H30O4	311.22229				6.3E+04	-1.9		
927 Thyronine	[M+K] ⁺	C15H15NO4	312.06260						1.1E+05	2.1
928 Taxiphyllin	[M+H] ⁺	C14H17NO7	312.10849					1.0E+05	-2.3	
929 Hydroxycinnamyl alcohol 4-D-glucoside	[M+H] ⁺	C15H20O7	313.12852					1.4E+05	-1.1	
930 Sauroxine	[M+K] ⁺	C17H26N2O	313.16700			1.2E+06	2.1		1.5E+05	-2.4
931 Hydroperoxylinoic acid	[M+H] ⁺	C18H32O4	313.23814					4.9E+05	-2.6	
932 Beta-D-Glucopyranuronic acid	[M+H] ⁺	C13H14O9	315.07106	6.9E+04	0.5					
933 Coumatetralyl	[M+Na] ⁺	C19H16O3	315.09951			3.1E+05	-1.1			
934 Grevillol	[M+Na] ⁺	C19H32O2	315.23037						7.8E+04	-2.9
935 Octadecanedioic acid	[M+H] ⁺	C18H34O4	315.25299	7.0E+05	-0.7	1.3E+06	-1.4			
936 Rosinidin	[M+H] ⁺	C17H15O6	316.09414	6.8E+04	2.9					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
937 Melosatin B	[M+Na] ⁺	C19H19NO2	316.13098				9.5E+04	-0.6		
938 Dehydrophytosphingosine	[M+H] ⁺	C18H37NO3	316.28462	9.1E+05	-0.3				3.0E+05	-0.9
939 L-phenylalanyl-L-hydroxyproline	[M+K] ⁺	C14H18N2O4	317.08985				1.1E+05	-0.1	1.6E+05	2.9
940 alhpa-tocopheronolactone	[M+K] ⁺	C16H22O4	317.11479		1.5E+06	0.6			2.9E+05	1.8
941 2-Butyl-3-(4-hydroxybenzoyl)benzofuran	[M+Na] ⁺	C19H18O3	317.11482	2.7E+06	-0.7					
942 alhpa-tocopheronolactone	[M+K] ⁺	C16H22O4	317.11500				1.2E+05	-0.1		
943 4-Hydroxy-5,7,4'-trimethoxyflavan	[M+H] ⁺	C18H20O5	317.13903			2.4E+05	-2.1		2.8E+05	2.4
944 Gibberellin A9	[M+H] ⁺	C19H24O4	317.17486						3.5E+05	-0.4
945 2-hydroxy-9Z,12Z,15Z-octadecatrienoic acid	[M+Na] ⁺	C18H30O3	317.20794						1.2E+05	2.4
946 Eicosenal	[M+Na] ⁺	C20H38O	317.28081		1.1E+05	2.1				
947 Dimethyladenosine	[M+Na] ⁺	C12H17N5O4	318.11762		2.9E+05	-1.1				
948 Phytosphingosine	[M+H] ⁺	C18H39NO3	318.30027	1.0E+06	0.6					
949 L-beta-aspartyl-L-phenylalanine	[M+K] ⁺	C13H16N2O5	319.06830			2.7E+05	2.4			
950 Methylaminoadenosine	[M+Na] ⁺	C11H16N6O4	319.11168		1.7E+05	2.6				
951 Linoleic acid	[M+K] ⁺	C18H32O2	319.20334		2.7E+05	0.2				
952 Oleamide	[M+K] ⁺	C18H35NO	320.23580						8.6E+04	-2.4
953 2,3-Diphenyl-1-indanone	[M+K] ⁺	C21H14O	321.06736				8.2E+04	0.8		
954 Methylguanosine	[M+Na] ⁺	C11H16N5O5	321.10436	1.3E+05	2.9					
955 Mugineic acid	[M+H] ⁺	C12H20N2O8	321.12968						3.0E+05	-1.4
956 Dehydroretinal	[M+K] ⁺	C20H26O	321.16073		1.2E+05	2.5				
957 Quebrachamine	[M+K] ⁺	C19H26N2	321.17220						2.7E+05	1.7
958 Hydroxy-arachidonic acid	[M+H] ⁺	C20H32O3	321.24320		2.3E+05	-2.4				
959 8-Anilino-1-naphthalene sulfonic acid	[M+Na] ⁺	C16H13NO3S	322.05083	8.4E+04	-1.1					
960 Digallic acid	[M+H] ⁺	C14H10O9	323.03997				7.4E+04	-0.7		
961 2'-Hydroxy-4',6'-dimethoxy-3'-methylidihydrochalcone	[M+Na] ⁺	C18H20O4	323.12538	1.7E+05	0.7					
962 Tetranor-PGF1alpha	[M+Na] ⁺	C16H28O5	323.18336				7.4E+04	-1.4		
963 Retinoic acid	[M+Na] ⁺	C20H28O2	323.19815	1.1E+05	-1.5	9.9E+04	0.8			
964 Gingerol	[M+H] ⁺	C19H30O4	323.22086						1.7E+05	2.6
965 Stearic acid	[M+K] ⁺	C18H36O2	323.23451			9.5E+05	0.6			
966 Hydroxystearate	[M+Na] ⁺	C18H36O3	323.25616			5.3E+05	-1.5			
967 Myristoylglycine	[M+K] ⁺	C16H31NO3	324.19355	7.7E+04	0.0					
968 Galactosylhydroxylysine	[M+H] ⁺	C12H24N2O8	325.16132						2.2E+05	-2.4
969 12-oxo-14,18-dihydroxy-9Z,13E,15Z-octadecatrienoic acid	[M+H] ⁺	C18H28O5	325.20095	1.1E+05	-1.0					
970 Alchornoic acid	[M+H] ⁺	C20H36O3	325.27453						4.4E+05	-2.5
971 Farnesylcysteine	[M+H] ⁺	C18H31NO2S	326.21406		1.3E+05	2.4				
972 Dihydrokaempferol	[M+K] ⁺	C15H12O6	327.02709		1.1E+05	-1.7				
973 Hydroxyflemichapparin C	[M+H] ⁺	C17H10O7	327.05057			3.3E+05	-2.0			
974 Hinokitiol glucoside	[M+H] ⁺	C16H22O7	327.14355			1.1E+06	0.9			

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
975 Acutifolin A	[M+H] ⁺	C20H22O4	327.15980				1.6E+05	-2.2		
976 Capsaicin	[M+Na] ⁺	C18H27NO3	328.18836				7.6E+04	-0.1		
977 Lonchocarpin	[M+Na] ⁺	C20H18O3	329.11480			3.0E+05	0.0			
978 Eicosatrienoic acid	[M+Na] ⁺	C20H34O2	329.24577		9.6E+04	-2.0				
979 Adenosine 2',3'-cyclic phosphate	[M+H] ⁺	C10H12N5O6P	330.05980	1.2E+05	0.7					
980 Stealthin C	[M+Na] ⁺	C18H13NO4	330.07322				1.2E+05	1.4		
981 Glutathione	[M+Na] ⁺	C10H17N3O6S	330.07400					1.3E+05	-3.0	
982 Gingerdione	[M+K] ⁺	C17H24O4	331.13139				1.2E+05	-2.3		
983 Cinnamodial	[M+Na] ⁺	C17H24O5	331.15159	1.9E+05	-1.6					
984 5'-O-beta-D-Glucosylpyridoxine	[M+H] ⁺	C14H21NO8	332.13399	2.4E+05	-1.9					
985 Megastachine	[M+H] ⁺	C20H29NO3	332.22188				8.5E+04	0.4		
986 Ovalitenin B	[M+Na] ⁺	C19H18O4	333.10918					2.1E+05	1.7	
987 Gibberellin A20	[M+H] ⁺	C19H24O5	333.17003			6.5E+05	-1.1			
988 Hydroxylinolenic acid	[M+K] ⁺	C18H30O3	333.18265	1.2E+05	-1.7					
989 9-hydroperoxy-10E,12,15Z-octadecatrienoic acid	[M+Na] ⁺	C18H30O4	333.20300				8.3E+04	1.9		
990 Tintinnadiol	[M+H] ⁺	C21H32O3	333.24282					1.5E+05	-1.2	
991 18-hydroxy-9S,10R-dihydroxy-stearic acid	[M+H] ⁺	C18H36O5	333.26324						8.0E+04	0.9
992 Spiradine A	[M+Na] ⁺	C20H25NO2	334.17688			1.7E+05	2.6			
993 Arabino-galactose	[M+Na] ⁺	C11H20O10	335.09487	1.2E+05	-0.8					
994 alhpa-tocopheronic acid	[M+K] ⁺	C16H24O5	335.12613				1.2E+05	-1.8	3.9E+05	-2.3
995 Oxo-nonadecanoic acid	[M+Na] ⁺	C19H36O3	335.25641		1.7E+05	-2.2				
996 Palmitoleoyl Ethanolamide	[M+K] ⁺	C18H35NO2	336.22935			2.6E+05	1.8			
997 2-amino-14,16-dimethyloctadecan-3-ol	[M+Na] ⁺	C20H43NO	336.32272						7.2E+04	2.9
998 Epihydroxymugineic acid	[M+H] ⁺	C12H20N2O9	337.12339			1.5E+06	2.3			
999 Astrophylline	[M+K] ⁺	C19H26N2O	337.16767	9.8E+04	1.7					
1000 Apovincamine	[M+H] ⁺	C21H24N2O2	337.19025					3.8E+05	2.4	
1001 Octadecanedioic acid	[M+Na] ⁺	C18H34O4	337.23532		2.7E+06	-1.2				
1002 Belladine	[M+Na] ⁺	C19H25NO3	338.17266	1.4E+05	-2.1					
1003 Pentadecanoylglycine	[M+K] ⁺	C17H33NO3	338.20919			2.8E+05	0.0			
1004 Peroxyferolide	[M+H] ⁺	C17H22O7	339.14283			2.9E+06	2.9			
1005 2,3-dihydroxy stearic acid	[M+Na] ⁺	C18H36O4	339.25077					1.5E+05	-0.6	
1006 Ormosanine	[M+Na] ⁺	C20H35N3	340.27158				1.8E+05	2.2		
1007 Cellobiono-1,5-lactone	[M+H] ⁺	C12H20O11	341.10784	8.6E+04	-1.0					
1008 2-Phenethylsulfanyl-5,6,7,8-tetrahydro-benzo[4,5]thieno[2,3-d]pyrimidin-4-ylamine	[M+H] ⁺	C18H19N3S2	342.10901			1.9E+05	0.9			
1009 Caffeic acid 3-glucoside	[M+H] ⁺	C15H18O9	343.10230					1.0E+05	0.2	
1010 Coniferin	[M+H] ⁺	C16H22O8	343.13874	8.2E+04	0.2					
1011 Phellodendrine	[M+H] ⁺	C20H24NO4	343.17749			9.3E+05	0.9			
1012 Arachidonic acid	[M+K] ⁺	C20H32O2	343.20344		1.3E+05	-0.1				

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1013	4-Carboxy-4'-sulfoazobenzene	[M+K] ⁺	C13H10N2O5S	344.99420	8.9E+04	1.7					
1014	Ovalitenin C	[M+Na] ⁺	C19H14O5	345.07259					8.6E+04	2.2	
1015	6-O-alpha-D-Galactosyl-D-glucitol	[M+H] ⁺	C12H24O11	345.13883			1.9E+05	0.9			
1016	Hydroxyeicosatrienoic acid	[M+Na] ⁺	C20H34O3	345.24069				2.5E+05	-2.0		
1017	1alpha-hydroxy-22-oxo-23,24,25,26,27-pentano- <i>vitamin D3</i>	[M+H] ⁺	C22H32O3	345.24154					2.1E+05	2.6	
1018	Fructose 1,6-bisphosphate	[M+Na] ⁺	C6H14O11P2	346.99036	8.8E+04	-2.8					
1019	Dimethoxy-furanoflavanone	[M+Na] ⁺	C19H16O5	347.08933			1.1E+05	-1.0			
1020	Cinnamodial	[M+K] ⁺	C17H24O5	347.12558			1.2E+05	-0.1			
1021	Tetraneurin E	[M+Na] ⁺	C17H24O6	347.14668				8.4E+04	-0.5		
1022	Gibberellin A24	[M+H] ⁺	C20H26O5	347.18530	1.8E+05	-1.7					
1023	5-(Heptadec-12-enyl)resorcinol	[M+H] ⁺	C23H38O2	347.29444				7.1E+04	0.1		
1024	Hydroxysanguinarine	[M+H] ⁺	C20H13NO5	348.08665	6.8E+04	1.4					
1025	N-(3-Hydroxy-7-cis-tetradecenoyl)homoserine lactone	[M+Na] ⁺	C18H31NO4	348.21437					1.0E+05	0.5	
1026	Carboxy-alpha-chromanol	[M+H] ⁺	C21H31O4	348.22874			1.5E+05	2.2			
1027	O-Arachidonoyl Ethanolamine	[M+H] ⁺	C22H37NO2	348.28918			1.5E+05	1.5			
1028	Inosinic acid	[M+H] ⁺	C10H13N4O8P	349.05438	6.8E+04	2.5					
1029	Calopogoniumisoflavone B	[M+H] ⁺	C21H16O5	349.10664			1.3E+05	1.2			
1030	Apigenin 7-sulfate	[M+H] ⁺	C15H10O8S	351.01621				8.0E+04	2.0		
1031	Desmosdumotin C	[M+K] ⁺	C19H20O4	351.09932	3.1E+05	-1.7					
1032	Jatrophone	[M+K] ⁺	C20H24O3	351.13637					1.3E+05	-1.9	
1033	Rhododendrin	[M+Na] ⁺	C16H24O7	351.14120			1.5E+06	0.6			
1034	Gibberellin A2	[M+H] ⁺	C19H26O6	351.18064			2.5E+06	-1.2			
1035	9,12,13-trihydroxy-10,15-octadecadienoic acid	[M+Na] ⁺	C18H32O5	351.21389				2.0E+05	0.9		
1036	Coumestrol diacetate	[M+H] ⁺	C19H12O7	353.06612		1.6E+05	-1.5				
1037	Carnosol	[M+Na] ⁺	C20H26O4	353.17290				9.4E+04	-1.6		
1038	Jasmolin I	[M+Na] ⁺	C21H30O3	353.20872	5.9E+05	-1.2					
1039	Geranylgeranylacetone	[M+Na] ⁺	C23H38O	353.28192				1.4E+05	-1.2		
1040	N,N-dimethyl arachidonoyl amine	[M+Na] ⁺	C22H37NO	354.27633		9.8E+04	1.1				
1041	8,12,16,19-docosatetraenoic acid	[M+Na] ⁺	C22H36O2	355.26063				3.2E+05	0.3		
1042	Spirasine I	[M+H] ⁺	C22H29NO3	356.22237				1.1E+05	-1.0		
1043	Feruloyl-D-glucose	[M+H] ⁺	C16H20O9	357.11858					2.2E+05	-1.6	
1044	Ubiquinone Q2	[M+K] ⁺	C19H26O4	357.14568						1.2E+05	1.6
1045	Vinorine	[M+Na] ⁺	C21H22N2O2	357.15691			4.8E+05	1.2			
1046	Estradiol valerate	[M+H] ⁺	C23H32O3	357.24242	2.7E+05	-0.8					
1047	1-Carbazol-9-yl-3-(3,5-dimethylpyrazol-1-yl)-propan-2-ol	[M+K] ⁺	C20H21N3O	358.13162	6.8E+04	2.4					
1048	Bakankoside	[M+H] ⁺	C16H23NO8	358.15011					1.7E+05	-1.3	
1049	Leucyl-leucyl-norleucine	[M+H] ⁺	C18H35N3O4	358.27086						1.1E+05	-2.3

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1050	Coumeroic acid	[M+H] ⁺	C17H14N2O7	359.08714						8.3E+04	0.7
1051	Docosapentaynoic acid	[M+K] ⁺	C22H24O2	359.14079	7.0E+04	1.6					
1052	Ficine	[M+Na] ⁺	C20H19NO4	360.12063	8.3E+04	-1.2					
1053	Thymidylc acid	[M+K] ⁺	C10H15N2O8P	361.01981			1.3E+05	-0.1			
1054	Peroxyferolide	[M+Na] ⁺	C17H22O7	361.12507			2.3E+05	1.9			
1055	N-Arachidonoyl glycine	[M+H] ⁺	C22H35NO3	362.26982						8.1E+04	-2.3
1056	5,7,3'-Trihydroxy-6,4',5'-trimethoxyflavanone	[M+H] ⁺	C18H18O8	363.10744	2.1E+05	2.2					
1057	Gibberellin A19	[M+H] ⁺	C20H26O6	363.18012			1.5E+06	0.3			
1058	Docosanoic acid	[M+Na] ⁺	C22H44O2	363.32371				1.1E+05	-1.0		
1059	Lactosamine	[M+Na] ⁺	C12H23NO10	364.12053			2.5E+05	2.4			
1060	PC(0:0/5:0)	[M+Na] ⁺	C13H28NO7P	364.14985			2.5E+05	-0.8			
1061	N-Oleoylethanolamine	[M+K] ⁺	C20H39NO2	364.26168				1.7E+05	-1.2		
1062	Xanthylic acid	[M+H] ⁺	C10H13N4O9P	365.04974						7.6E+04	-1.2
1063	Lactose	[M+Na] ⁺	C12H22O11	365.10543	3.0E+06	-1.3			4.2E+05	2.0	
1064	Brosimacutin C	[M+Na] ⁺	C20H22O5	365.13632			9.8E+05	-1.0			
1065	Gibberellin A8	[M+H] ⁺	C19H24O7	365.15901						2.6E+05	1.3
1066	Gibberellin A37	[M+H] ⁺	C20H28O6	365.19606			2.1E+06	-0.5			
1067	Homophytanic acid	[M+K] ⁺	C21H42O2	365.28191				1.1E+05	-0.7		
1068	PC(O-2:0/2:0)	[M+K] ⁺	C12H26NO7P	366.10785	4.4E+05	-1.7	2.1E+05	0.3			
1069	2-(acetylamino)-1,5-anhydro-2-deoxy-3-O-b-D-galactopyranosyl-D-arabino-Hex-1-enitol	[M+H] ⁺	C14H23NO10	366.13961			3.0E+05	-0.4			
1070	Dolichyl diphosphate	[M+Na] ⁺	C12H26O7P2	367.10460	8.9E+04	-0.2					
1071	Deoxyelephantopin	[M+Na] ⁺	C19H20O6	367.11550					8.9E+04	-0.8	
1072	Rhododendrin	[M+K] ⁺	C16H24O7	367.11550					8.9E+04	-0.4	
1073	Boschnaloside	[M+Na] ⁺	C16H24O8	367.13570			1.2E+06	1.7			
1074	12,13-dihydroxy-11-methoxy-9-octadecenoic acid	[M+Na] ⁺	C19H36O5	367.24605						1.1E+05	-1.5
1075	Prostaglandin G2	[M+H] ⁺	C20H32O6	369.22747					1.1E+05	-0.8	
1076	Mahanimbine	[M+K] ⁺	C23H25NO	370.15776			2.8E+05	-2.7			
1077	Prostaglandin G1	[M+H] ⁺	C20H33O6	370.23421			2.1E+05	2.1			
1078	Fraxin	[M+H] ⁺	C16H18O10	371.09736					1.6E+05	-0.2	
1079	Leonuridine	[M+Na] ⁺	C15H24O9	371.13116						1.2E+05	0.3
1080	Carnosic acid	[M+K] ⁺	C20H28O4	371.16219				2.1E+05	-0.7		
1081	Naphthylacetylspermine	[M+H] ⁺	C22H34N4O	371.28066						6.6E+05	-0.3
1082	N-Acetylphenylalanine beta-naphthyl ester	[M+K] ⁺	C21H19NO3	372.09965	8.3E+04	-0.5		8.9E+04	1.4		
1083	Eicosatrienoylethanolamide	[M+Na] ⁺	C22H39NO2	372.28808				1.4E+05	-2.1		
1084	Calopogoniumisoflavone A	[M+K] ⁺	C21H18O4	373.08367	1.0E+05	1.9					
1085	Cathenamine	[M+Na] ⁺	C21H22N2O3	373.15241					9.2E+04	-0.4	
1086	Gingerol	[M+Na] ⁺	C21H34O4	373.23484				4.2E+05	0.2	2.0E+05	-1.9
1087	5,7,4'-Trihydroxyflavanone 7-sulfate	[M+Na] ⁺	C15H12O8S	375.01451	8.6E+04	0.5	9.5E+04	0.2			

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1088 Umbellatine	[M+K] ⁺	C20H18NO4	375.08708					1.3E+05	-0.9	
1089 Myricetin 3,7,3',4'-tetramethyl ether	[M+H] ⁺	C19H18O8	375.10701			1.8E+05	1.2			
1090 Phantomolin	[M+H] ⁺	C21H26O6	375.17948			3.1E+05	2.0			
1091 Picrasin B	[M+H] ⁺	C21H28O6	377.19516			7.6E+05	1.9			
1092 Methyl-docosanoic acid	[M+Na] ⁺	C23H46O2	377.33887		1.2E+05	0.3				
1093 Feruloyl-D-glucose	[M+Na] ⁺	C16H20O9	379.09981		1.1E+05	0.4				
1094 gibberellin A17	[M+H] ⁺	C20H26O7	379.17455			2.0E+06	1.5			
1095 Arachidonoylglycerol	[M+H] ⁺	C23H38O4	379.28423		2.3E+05	0.1				
1096 Lactosamine	[M+K] ⁺	C12H23NO10	380.09536	1.8E+05	1.4					
1097 Lactose	[M+K] ⁺	C12H22O11	381.07937	3.9E+06	-0.4					
1098 Brosimacutin C	[M+K] ⁺	C20H22O5	381.11071		2.4E+05	-2.2				
1099 PA(14:1(9Z)/0:0)	[M+H] ⁺	C17H33O7P	381.20344				3.3E+05	0.6		
1100 Nogalonic acid	[M+H] ⁺	C20H14O8	383.07614	3.3E+05	-0.5	4.2E+05	0.9			
1101 Brosimacutin H	[M+Na] ⁺	C20H24O6	383.14651	2.1E+05	-1.9					
1102 1α,23-dihydroxy-24,25,26,27-tetranorvitamin D3	[M+Na] ⁺	C23H36O3	383.25547		1.2E+05	0.5				
1103 10,11-dihydroxy-4Z,7Z,13Z,16Z,19Z-docosapentaenoic acid	[M+Na] ⁺	C22H34O4	385.23416						9.9E+04	2.0
1104 MG(0:0/20:1(11Z)/0:0)	[M+H] ⁺	C23H44O4	385.33099		1.6E+05	0.6				
1105 8-Cinnamoyl-3,4-dihydro-5,7-dihydroxy-4-phenylcoumarin	[M+H] ⁺	C24H18O5	387.12215					8.4E+04	1.4	
1106 4-O-beta-D-Glucosyl-sinapate	[M+H] ⁺	C17H22O10	387.12857	7.0E+04	-2.3					
1107 DG(18:0e/2:0/0:0)	[M+H] ⁺	C23H46O4	387.34742					9.0E+04	-1.4	
1108 Quassin	[M+H] ⁺	C22H28O6	389.19597			3.3E+05	-0.3	1.4E+05	-1.5	
1109 5-Hydroxy-4'-methoxy-6'',6''-dimethylpyrano	[M+K] ⁺	C21H20O5	391.09343					1.3E+05	2.1	
1110 Apocholic acid	[M+H] ⁺	C24H38O4	391.28520		1.8E+06	-2.3				
1111 Deoxyvitamin D3	[M+Na] ⁺	C27H44	391.33349			2.5E+05	0.1			
1112 Prostaglandin G1	[M+Na] ⁺	C20H33O6	392.21693	7.7E+04	2.4					
1113 Heteratisine	[M+H] ⁺	C22H33NO5	392.24329						1.2E+05	-0.4
1114 Chlorogenic acid	[M+K] ⁺	C16H18O9	393.05894			4.8E+05	-1.8			
1115 Fraxin	[M+Na] ⁺	C16H18O10	393.07922	1.6E+05	-0.8			7.2E+05	2.1	
1116 Picrasin G	[M+H] ⁺	C21H28O7	393.19065			1.5E+06	0.3			
1117 Docosanedioic acid	[M+Na] ⁺	C22H42O4	393.29832		5.2E+05	-2.0				
1118 Murocholic acid	[M+H] ⁺	C24H40O4	393.29994	4.9E+05	-2.4					
1119 Spirasine I	[M+K] ⁺	C22H29NO3	394.17752					1.8E+05	1.0	
1120 Syringin	[M+Na] ⁺	C17H24O9	395.13100			7.4E+05	0.6			
1121 3-Geranyl-4,2',4'-trihydroxydihydrochalcone	[M+H] ⁺	C25H30O4	395.22239					1.5E+05	-1.8	
1122 MG(0:0/18:1(11Z)/0:0)	[M+K] ⁺	C21H40O4	395.25582	1.5E+05	0.7					
1123 Conessine	[M+K] ⁺	C24H40N2	395.28194			4.6E+05	0.9			
1124 Phenylaminoadenosine	[M+K] ⁺	C16H18N6O4	397.10211	3.4E+05	0.3					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1125 Icaceine	[M+Na] ⁺	C22H33NO4	398.22933			2.5E+05	2.1			
1126 Myricetin 7,3',4'-trimethyl ether	[M+K] ⁺	C18H16O8	399.04768	1.6E+05	-0.6					
1127 Calicoferol E	[M+H] ⁺	C27H42O2	399.32513		1.1E+05	1.6				
1128 5,7,3',4',5'-Pentahydroxy-3,6-dimethoxyflavone	[M+K] ⁺	C17H14O9	401.02607			1.7E+05	2.2			
1129 MG(0:0/20:4(8Z,11Z,14Z,17Z)/0:0)	[M+Na] ⁺	C23H38O4	401.26642				3.9E+05	-0.5		
1130 Xanthylic acid	[M+K] ⁺	C10H13N4O9P	403.00503				9.8E+04	0.4		
1131 Cinn cassiol C1	[M+Na] ⁺	C20H28O7	403.17243			2.8E+05	0.7			
1132 delta-Tocopherol	[M+H] ⁺	C27H46O2	403.35706	1.4E+05	1.7					
1133 Cinn cassiol C3	[M+Na] ⁺	C20H30O7	405.18837	1.2E+05	1.6					
1134 Alpha-Linoleoylcholine	[M+K] ⁺	C23H44NO2	405.30058						1.4E+05	-0.5
1135 Pentacosanal	[M+K] ⁺	C25H50O	405.35023			3.3E+05	-2.2			
1136 Rhyncophylline	[M+Na] ⁺	C22H28N2O4	407.19388					6.8E+05	0.6	
1137 Picrasin E	[M+H] ⁺	C22H30O7	407.20626			1.5E+06	0.4			
1138 MG(0:0/20:1(11Z)/0:0)	[M+Na] ⁺	C23H44O4	407.31303						8.0E+04	0.4
1139 Ovatine	[M+Na] ⁺	C24H35NO3	408.25012					9.7E+04	2.0	
1140 Geranylgeranylecysteine	[M+H] ⁺	C23H37NO3S	408.25600						7.8E+04	1.7
1141 Isorobustin 4-methyl ether	[M+H] ⁺	C23H20O7	409.12837						1.6E+05	-0.5
1142 Docosanedioic acid	[M+K] ⁺	C22H42O4	409.27147	6.3E+05	-0.7					
1143 Hydroxy-tricosanoic acid	[M+K] ⁺	C23H46O3	409.30883		1.6E+05	-2.4				
1144 Carboxy-gama-tocotrienol	[M+K] ⁺	C23H31O4	410.18546			3.0E+05	-0.2			
1145 N-palmitoyl methionine	[M+Na] ⁺	C21H41NO3S	410.27008			2.1E+05	-0.4			
1146 Bensulfuron methyl	[M+H] ⁺	C16H18N4O7S	411.09690	9.5E+04	1.1					
1147 Spinoflavanone A	[M+Na] ⁺	C25H24O4	411.15745				8.1E+04	-1.9		
1148 5-Methoxy-7,8-diprenylflavone	[M+Na] ⁺	C26H28O3	411.19273						8.2E+04	0.8
1149 Rehmanioside C	[M+Na] ⁺	C19H32O8	411.19966				1.4E+05	-1.8		
1150 Vitamin D6	[M+H] ⁺	C29H46O	411.36300						7.2E+04	-2.1
1151 Curacin A	[M+K] ⁺	C23H35NOS	412.20611			3.6E+05	2.4			
1152 N-oleoyl taurine	[M+Na] ⁺	C20H39NO4S	412.24919			2.0E+05	0.0			
1153 11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside	[M+Na] ⁺	C18H30O9	413.17767			7.9E+05	1.3			
1154 Apocholic acid	[M+Na] ⁺	C24H38O4	413.26690		3.2E+06	-1.6			3.3E+05	-2.2
1155 N-stearoyl glutamine	[M+H] ⁺	C23H44N2O4	413.33825					6.6E+05	-2.1	
1156 Hexacosatrienoic acid	[M+Na] ⁺	C26H46O2	413.33981				1.0E+06	-2.0		
1157 Hydroxy-hexacosanoic acid	[M+H] ⁺	C26H52O3	413.39892	2.6E+05	2.0					
1158 Anguvin	[M+Na] ⁺	C24H24O5	415.15103			3.2E+05	1.4			
1159 Phytol phosphate	[M+K] ⁺	C20H41O4P	415.23813			3.5E+05	-1.7			
1160 Lupulone	[M+H] ⁺	C26H38O4	415.28429	1.8E+05	1.1					
1161 MG(0:0/22:0/0:0)	[M+H] ⁺	C25H50O4	415.37792		1.7E+05	0.6				
1162 Spironolactone	[M+H] ⁺	C24H32O4S	417.20941	2.2E+05	-1.6					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1163 Calcitriol	[M+H] ⁺	C27H44O3	417.33556						5.8E+05	1.8
1164 PGF2alpha isopropyl ester	[M+Na] ⁺	C23H40O5	419.27699					3.0E+05	-0.5	
1165 1alpha,25-dihydroxy-22-oxavitamin D3	[M+H] ⁺	C26H42O4	419.31566		1.3E+05	-0.2			1.3E+05	-2.0
1166 8'-apo-beta-Carotenol	[M+H] ⁺	C30H42O	419.33163				1.3E+05	-1.9		
1167 Hexacosanal	[M+K] ⁺	C26H52O	419.36417			2.5E+05	1.9			
1168 Lisetin	[M+K] ⁺	C21H18O7	421.06808			2.8E+05	0.8			
1169 N-Benzoyl-D-arginine-4-nitroanilide	[M+Na] ⁺	C19H22N6O4	421.15998					1.0E+05	-1.2	
1170 C17 Sphingosine-1-phosphate	[M+K] ⁺	C17H39N2O5P	421.22284				1.1E+06	-0.1		
1171 8-(2-Carboxy-1-phenylethyl)-3,5,7-trihydroxyflavone delta-lactone	[M+Na] ⁺	C24H16O6	423.08292				3.7E+05	2.3		
1172 Carboxy-alpha-tocotrienol	[M+K] ⁺	C24H33O4	424.20155				3.3E+05	-1.2	1.0E+05	-2.4
1173 Myxalamid B	[M+Na] ⁺	C25H39NO3	424.28221	2.3E+05	0.7					
1174 N-(2-phenoxy-ethyl) arachidonoyl amine	[M+H] ⁺	C28H41NO2	424.32164		1.3E+05	-1.5			8.3E+04	0.6
1175 Diferulic acid	[M+K] ⁺	C20H18O8	425.06246				3.9E+05	2.0		
1176 delta-Tocopherol	[M+Na] ⁺	C27H46O2	425.33807				7.6E+04	2.2		
1177 Chitobiose	[M+H] ⁺	C15H26N2O12	427.15601		2.0E+05	-0.4				
1178 MG(0:0/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	[M+Na] ⁺	C25H40O4	427.28247				4.5E+05	-1.4		
1179 Hydroxy-gama-tocotrienol	[M+H] ⁺	C28H42O3	427.32021				2.6E+05	1.1		
1180 3-Deoxy-3-azido-25-hydroxyvitamin D3	[M+H] ⁺	C27H44N3O	427.35528				5.1E+05	1.0		
1181 Rubraflavone A	[M+Na] ⁺	C25H26O5	429.16814				3.4E+05	-2.1		
1182 Aliarin 4'-methyl ether	[M+H] ⁺	C23H26O8	431.16945				2.2E+05	1.4		
1183 Dimethamine	[M+Na] ⁺	C24H32N4O2	431.24175	5.1E+05	1.3					
1184 Cholic acid	[M+Na] ⁺	C24H40O5	431.27657						1.8E+05	0.5
1185 Hexacosadienoic acid	[M+K] ⁺	C26H48O2	431.32840				1.5E+05	0.4		
1186 Dihydroxycampesterol	[M+H] ⁺	C28H46O3	431.35277					9.0E+05	-1.9	5.1E+05 -2.2
1187 Undecylprodigiosin	[M+K] ⁺	C25H35N3O	432.24049					2.0E+05	1.6	
1188 Veratramine	[M+Na] ⁺	C27H39NO2	432.28730	9.8E+04	-1.3					
1189 Sphingofungin C	[M+H] ⁺	C22H41NO7	432.29496				6.3E+05	1.4		
1190 Quercetin 3,7-dimethyl ether 4'-sulfate	[M+Na] ⁺	C17H14O10S	433.01929						7.7E+04	1.6
1191 Geranyl-4,2',4'-trihydroxydihydrochalcone	[M+K] ⁺	C25H30O4	433.17852				3.9E+05	-2.2		
1192 25-hydroxy-16,17,23,23,24,24-hexadehydrovitamin D3	[M+K] ⁺	C27H38O2	433.25129					1.3E+05	-2.2	8.7E+04 -0.4
1193 1alpha,25-dihydroxy-24-oxo-22-oxavitamin D3	[M+H] ⁺	C26H40O5	433.29421					2.5E+05	1.5	
1194 Vitamin D6	[M+Na] ⁺	C29H46O	433.34309				2.2E+05	2.3		
1195 Dalpanol	[M+Na] ⁺	C23H24O7	435.14130		1.8E+05	0.3				
1196 alpha,4,2'-Trihydroxy-4-O-geranyldihydrochalcone	[M+K] ⁺	C24H28O5	435.15683	1.0E+05	-0.4					
1197 (9S,10S)-10-Hydroxy-9-(phosphonoxy)octadecanoate	[M+K] ⁺	C18H37O7P	435.19131						1.2E+05	-1.1
1198 Deoxoteasterone	[M+H] ⁺	C28H50O3	435.38327	8.3E+04	0.2					
1199 PC(4:0/4:0)	[M+K] ⁺	C16H32NO8P	436.15005					1.1E+05	-0.8	

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1200	(22E,24E)-1alpha,26-dihydroxy-22,23,24,25-tetradehydro-27-norvitamin D3	[M+K] ⁺	C26H38O3	437.24483					3.4E+06	1.0	
1201	Tetracosanedioic acid	[M+K] ⁺	C24H46O4	437.30324			5.2E+05	-1.1			
1202	Palmitoylcarnitine	[M+K] ⁺	C23H45NO4	438.29860					2.2E+05	-1.3	
1203	Lupinisoflavone J	[M+K] ⁺	C25H26O7	439.17513	1.8E+05	1.2					
1204	PA(18:0/0:0)	[M+H] ⁺	C21H43O7P	439.28126				1.2E+05	1.5		
1205	LysoPE(0:0/15:0)	[M+H] ⁺	C20H42NO7P	440.27652					1.9E+05	1.5	
1206	Carboxy-alpha-chromanol	[M+Na] ⁺	C26H41O4	440.28960			2.2E+05	0.2			
1207	Kaempferol 3-arabinopyranoside	[M+Na] ⁺	C20H18O10	441.07922	2.6E+05	0.5					
1208	Chalconaringenin 2'-xyloside	[M+K] ⁺	C20H20O9	443.07389	1.7E+05	0.9					
1209	4,4'-Diapo-zeta-carotene	[M+K] ⁺	C30H44	443.30731						1.1E+05	0.3
1210	Lepidissipyron	[M+Na] ⁺	C24H22O7	445.12677			2.2E+05	-2.2			
1211	1-Octen-3-ol-3-o-beta-D-xylopyranosyl(1->6)-beta-D-glucopyranoside	[M+Na] ⁺	C19H34O10	445.20455					2.4E+05	-0.3	
1212	Quassin	[M+Na] ⁺	C23H34O7	445.21955				1.2E+05	0.3		
1213	11alpha-ethyl-1alpha,25-dihydroxyvitamin D3	[M+H] ⁺	C29H48O3	445.36841						6.5E+05	-1.8
1214	N-oleoyl tyrosine	[M+H] ⁺	C27H43NO4	446.32564					2.7E+05	1.9	
1215	PA(16:1(9Z)/0:0)	[M+K] ⁺	C19H37O7P	447.19178			3.1E+05	-2.1	1.0E+05	1.5	
1216	PA(8:0/8:0)	[M+Na] ⁺	C19H37O8P	447.21137						1.3E+05	1.0
1217	2-Geranyl-3,4,2',4'-tetrahydroxydihydrochalcone	[M+K] ⁺	C25H30O5	449.17164					1.2E+05	1.9	
1218	1alpha-hydroxy-24-methylvitamin D2	[M+Na] ⁺	C29H46O2	449.33935			3.5E+05	-0.8			
1219	Catechin 3-O-(1-hydroxy-6-oxo-2-cyclohexene-1-carboxylate)	[M+Na] ⁺	C22H20O9	451.09999			3.7E+05	-0.1			
1220	Tephrocin	[M+H] ⁺	C25H22O8	451.13790						8.7E+04	1.9
1221	Cinchonin 1a	[M+H] ⁺	C24H20O9	453.11835			5.1E+05	-0.8			
1222	2,2-Dimethyl-3,4-bis(4-methoxyphenyl)-2H-1-benzopyran-7-ol acetate	[M+Na] ⁺	C27H26O5	453.16818					2.1E+05	-2.1	
1223	Oxo-leukotriene E4	[M+H] ⁺	C23H34NO6S	453.21761					4.6E+05	0.8	
1224	MG(0:0/24:6(6Z,9Z,12Z,15Z,18Z,21Z)/0:0)	[M+Na] ⁺	C27H42O4	453.29746						1.2E+05	0.2
1225	Phyllanthin	[M+K] ⁺	C24H34O6	457.19957			5.7E+05	-1.9			
1226	Deoxytyphasterol	[M+Na] ⁺	C28H50O3	457.36522	1.5E+05	-2.0			8.0E+05	1.5	
1227	N-(4-benzenesulfonamide) arachidonoyl amine	[M+H] ⁺	C26H38N2O3S	459.26759	1.4E+05	0.7					
1228	Salvisyriacalide	[M+Na] ⁺	C25H40O6	459.27091				1.8E+05	1.7		
1229	1-(3-methylpentadecyl)-3-nonylcyclopentane	[M+K] ⁺	C30H60	459.43216						2.3E+05	1.1
1230	Militarinone A	[M+H] ⁺	C26H37NO6	460.27030				9.6E+04	-2.0		
1231	N-stearoyl histidine	[M+K] ⁺	C24H43N3O3	460.29344			1.9E+05	0.4			
1232	Apigenin 5,7-dimethyl ether 4'-galactoside	[M+H] ⁺	C23H24O10	461.14461				9.5E+04	-0.8		
1233	PA(P-18:0/0:0)	[M+K] ⁺	C21H43O6P	461.24344				2.1E+05	-1.2		
1234	Ophirasterol	[M+Na] ⁺	C31H50O	461.37521			2.7E+05	0.4			

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1235 Linoelaidyl carnitine	[M+K] ⁺	C25H45NO4	462.29773					1.2E+05	0.6	
1236 Flemiflavanone D	[M+K] ⁺	C25H28O6	463.15075		1.4E+05	2.2				
1237 Retinyl beta-glucuronide	[M+H] ⁺	C26H38O7	463.26933						1.3E+05	-0.6
1238 PA(20:2(11Z,14Z)/0:0)	[M+H] ⁺	C23H43O7P	463.28226				1.1E+05	-0.7		
1239 Pfaffic acid	[M+Na] ⁺	C29H44O3	463.31861			3.8E+05	-0.7	2.4E+05	1.2	
1240 1-O-alpha-D-glucopyranosyl-1,2-nonadecandiol	[M+H] ⁺	C25H50O7	463.36241			3.2E+05	1.1			
1241 N-arachidonoyl histidine	[M+Na] ⁺	C26H39N3O3	464.28830		1.2E+05	0.1				
1242 PA(20:1(11Z)/0:0)	[M+H] ⁺	C23H45O7P	465.29770			6.1E+05	-0.3			
1243 PGF2alpha-dihydroxypropylamine	[M+K] ⁺	C23H41NO6	466.25654						8.0E+04	0.0
1244 N-Adenylylanthranilate	[M+H] ⁺	C17H19N6O8P	467.10673					2.5E+05	1.6	
1245 dihydrophaseic acid 4-O-beta-D-glucoside	[M+Na] ⁺	C21H32O10	467.18870						1.0E+05	0.1
1246 Ercalcitriol	[M+K] ⁺	C28H44O3	467.29219		1.5E+05	0.0				
1247 LysoSM(d18:0)	[M+H] ⁺	C23H51N2O5P	467.36084	1.1E+05	0.6					
1248 Phthioceranic acid	[M+H] ⁺	C31H62O2	467.48226	1.1E+05	-1.0					
1249 Apigenin 7-glucuronide	[M+Na] ⁺	C21H18O11	469.07413	9.7E+04	-0.2					
1250 1alpha,25-dihydroxy-11-(3-hydroxy-1-propynyl)-9,11-didehydrovitamin D3	[M+H] ⁺	C30H44O4	469.33062		8.2E+05	1.3				
1251 Vitamin E	[M+K] ⁺	C29H50O2	469.34405			3.8E+05	0.4			
1252 Glutathionylspermidine	[M+K] ⁺	C17H34N6O5S	473.19430	8.6E+04	1.9					
1253 Euchrenone a14	[M+H] ⁺	C30H32O5	473.23267				1.2E+05	-0.9		
1254 PA(O-20:0/0:0)	[M+Na] ⁺	C23H49O6P	475.31590	1.4E+05	-1.2					
1255 (20S)-1alpha,25-dihydroxy-20-methoxy-26,27-dimethylvitamin D3	[M+H] ⁺	C30H50O4	475.37906						1.4E+05	-1.8
1256 N-docosahexaenoyl phenylalanine	[M+H] ⁺	C31H41NO3	476.31676						4.3E+05	-1.8
1257 Rhodojaponin IV	[M+Na] ⁺	C24H38O8	477.24574			4.3E+05	0.3			
1258 Moronic acid	[M+Na] ⁺	C30H46O3	477.33379				1.7E+05	0.3		
1259 triacontan-1,14-diol	[M+Na] ⁺	C30H62O2	477.46344						8.5E+04	1.6
1260 PS(13:0/0:0)	[M+Na] ⁺	C19H38NO9P	478.21863					1.4E+05	-2.1	
1261 PA(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	[M+Na] ⁺	C23H37O7P	479.21679			6.8E+05	0.3			
1262 Soyasapogenol C	[M+K] ⁺	C30H48O2	479.32838					3.1E+05	0.4	
1263 Lythramine	[M+H] ⁺	C29H37NO5	480.27445	1.0E+05	1.1					
1264 Exiguaflavanone M	[M+K] ⁺	C25H30O7	481.16245		1.3E+05	-0.3				
1265 N-palmitoyl tryptophan	[M+K] ⁺	C27H42N2O3	481.28207				4.4E+05	1.3		
1266 sn-3-O-(Geranylgeranyl)glycerol 1-phosphate	[M+K] ⁺	C23H41O6P	483.22682					1.2E+05	0.9	
1267 1alpha,25-dihydroxy-24a,24b-didihomo-22-thia-20-epivitamin D3	[M+Na] ⁺	C28H46O3S	485.30599	3.1E+05	1.9					
1268 S-Decyl GSH	[M+K] ⁺	C20H37N3O6S	486.20347	9.1E+04	-1.1					
1269 Quercitrin	[M+K] ⁺	C21H20O11	487.06372	1.3E+05	0.4					
1270 Glucosylgalactosyl hydroxylysine	[M+H] ⁺	C18H34N2O13	487.21365				1.2E+05	-0.6		

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1271	N-(2'-(4-benzenesulfonamide)-ethyl)arachidonoyl amine	[M+H] ⁺	C28H42N2O3S	487.29889	4.0E+05	0.3					
1272	Fucosyllactose	[M+H] ⁺	C18H32O15	489.18087			1.2E+05	1.1			
1273	Vitamin K1 epoxide	[M+Na] ⁺	C31H46O3	489.33309			2.3E+05	1.7	1.6E+05	0.7	
1274	4'-Apo-3,4-didehydrolycopene	[M+Na] ⁺	C35H46	489.34972						2.0E+05	-1.1
1275	alpha-Hydroxy-castasterone	[M+Na] ⁺	C28H50O5	489.35470					8.9E+05	0.7	
1276	(17E)-1alpha,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydro-24a-homovitamin D3	[M+K] ⁺	C30H44O3	491.29281						1.2E+05	-1.2
1277	PA(22:2(13Z,16Z)/0:0)	[M+H] ⁺	C25H47O7P	491.31370					1.3E+05	-1.0	
1278	Palmatoside G	[M+H] ⁺	C25H32O10	493.20683					1.6E+05	0.0	
1279	TG(8:0/8:0/8:0)	[M+Na] ⁺	C27H50O6	493.35001			3.6E+05	-0.1			
1280	Eburicoic acid	[M+Na] ⁺	C31H50O3	493.36514		1.8E+05	0.2				
1281	24R-Ethyl-26,26,27-trimethyl-3beta-hydroxycholesta-7,26-(30)-diene	[M+K] ⁺	C32H54O	493.38043				1.3E+05	0.4		
1282	3,5,8,3',4'-Pentamethoxy-7-prenyloxyflavone	[M+K] ⁺	C25H28O8	495.14252						8.2E+04	-1.9
1283	Atocalcitol	[M+H] ⁺	C32H46O4	495.34665				1.1E+05	0.5		
1284	Deoxypumiloside	[M+H] ⁺	C26H28N2O8	497.19234					1.7E+05	-1.0	
1285	Palmitoylglycerophosphocholine	[M+H] ⁺	C24H51NO7P	497.34759	1.7E+05	0.6					
1286	Soyasapogenol A	[M+Na] ⁺	C30H50O4	497.35975		1.6E+05	0.8				
1287	1alpha,25-dihydroxy-24a-homo-26,27-dimethyl-22-thiavitamin D3	[M+Na] ⁺	C29H48O3S	499.32189				1.2E+05	-0.5		
1288	6-methylvitamin D3 6,19-sulfur dioxide adduct	[M+K] ⁺	C28H46O3S	501.27967					2.8E+05	0.5	
1289	LysoPE(0:0/18:1(11Z))	[M+Na] ⁺	C23H46NO7P	502.29130					1.4E+05	-1.8	
1290	Cycloheterophyllin	[M+H] ⁺	C30H30O7	503.20574			2.8E+05	1.4			
1291	Castasterone	[M+K] ⁺	C28H48O5	503.31323					2.6E+05	0.2	
1292	Hexaprenylphenol	[M+H] ⁺	C36H54O	503.42541						2.5E+05	-1.3
1293	3,4,2',3',4',6',alpha-Heptahydroxychalcone 2'-glucoside	[M+Na] ⁺	C21H22O13	505.09526	1.1E+05	0.2					
1294	11-beta-hydroxyandrosterone-3-glucuronide	[M+Na] ⁺	C25H38O9	505.24041					1.2E+05	0.8	
1295	Eudesobovatol A	[M+H] ⁺	C33H44O4	505.33212					2.2E+05	-1.8	1.2E+05 -1.7
1296	Methyl-triacontanoic acid	[M+K] ⁺	C31H62O2	505.43757		1.5E+05	1.1				
1297	Artoindonesianin B	[M+K] ⁺	C26H28O8	507.14152					1.3E+05	0.1	
1298	Stigmatellin X	[M+K] ⁺	C28H38O6	509.23029			7.2E+05	-0.6			
1299	PA(20:4(5Z,8Z,11Z,14Z)e/2:0)	[M+Na] ⁺	C25H43O7P	509.26303				1.4E+05	1.6		
1300	N-(2'-(4-benzenesulfonamide)-ethyl)arachidonoyl amine	[M+Na] ⁺	C28H42N2O3S	509.27994		8.6E+05	1.8				
1301	PS(17:1(9Z)/0:0)	[M+H] ⁺	C23H44NO9P	510.28265	2.7E+05	-0.6					
1302	PS(8:0/8:0)	[M+H] ⁺	C22H42NO10P	512.26285		1.4E+05	-1.8				
1303	DG(14:0/14:0/0:0)	[M+H] ⁺	C31H60O5	513.45084						1.6E+05	1.0

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1304 N-docosahexaenoyl phenylalanine	[M+K] ⁺	C31H41NO3	514.27230			2.7E+05	-1.0			
1305 Taurocholic acid	[M+H] ⁺	C26H45NO7S	516.29925			1.9E+05	-0.6			
1306 Leukotriene D4	[M+Na] ⁺	C25H40N2O6S	519.24952			3.0E+05	0.8			
1307 Linoleoylglycerophosphocholine 1alpha,22,25-trihydroxy-26,27-dimethyl-	[M+H] ⁺	C26H51NO7P	521.34825						1.5E+05	-1.3
1308 23,23,24,24-tetradehydro-24a,24b,24c- trihomovitamin D3	[M+Na] ⁺	C32H50O4	521.35994					1.4E+05	0.4	
1309 Taurodeoxycholic acid	[M+Na] ⁺	C26H45NO6S	522.28631			2.2E+05	-0.6			
1310 Frangulanine	[M+Na] ⁺	C28H44N4O4	523.32530						8.7E+04	0.3
1311 Docosanediol-1,14-disulfate	[M+Na] ⁺	C22H46O8S2	525.25263	1.9E+06	-1.7					
1312 N-(2'-(4-benzenesulfonamide)-ethyl) arachidonoyl amine	[M+K] ⁺	C28H42N2O3S	525.25563				1.9E+05	-1.6		
1313 PG(19:1(9Z)/0:0)	[M+H] ⁺	C25H49O9P	525.31929				3.4E+05	-1.1		
1314 Retinyl palmitate	[M+H] ⁺	C36H60O2	525.46611						1.3E+05	0.9
1315 6-Hydroxykaempferol 3,5,7,4'-tetramethyl ether 6-rhamnoside	[M+Na] ⁺	C25H28O11	527.15296						8.9E+04	-1.1
1316 PG(18:3(6Z,9Z,12Z)/0:0)	[M+Na] ⁺	C24H43O9P	529.25369	1.1E+05	-1.2					
1317 Curcumin monoglucoside	[M+H] ⁺	C27H30O11	531.18596		1.4E+05	0.2				
1318 Caryoptin	[M+K] ⁺	C26H36O9	531.19922						1.2E+05	-0.2
1319 PI(13:0/0:0)	[M+H] ⁺	C22H43O12P	531.25632						1.4E+05	0.3
1320 Uscharidin	[M+H] ⁺	C29H38O9	531.25956		3.7E+05	-1.3				
1321 PG(18:2(9Z,12Z)/0:0)	[M+Na] ⁺	C24H45O9P	531.26936					4.9E+05	0.0	
1322 LysoPC(18:4(6Z,9Z,12Z,15Z))	[M+Na] ⁺	C26H46NO7P	538.28948						9.7E+04	1.7
1323 zeta-Carotene	[M+H] ⁺	C40H60	541.47656						1.6E+05	0.4
1324 PC(O-16:1(11Z)/2:0)	[M+Na] ⁺	C26H52NO7P	544.33736	3.9E+05	-1.4					
1325 Quercetin 3-(3''-sulfatoglucoside)	[M+H] ⁺	C21H20O15S	545.05992		1.4E+05	-0.6				
1326 Phytoene	[M+H] ⁺	C40H64	545.50808	2.4E+05	0.2					
1327 Guanosine triphosphate	[M+Na] ⁺	C10H16N5O14P3	545.98084						2.5E+05	-1.8
1328 Hirsutidin 3-glucoside	[M+K] ⁺	C24H27O12	546.11317					4.3E+05	0.4	
1329 Deacetylipecoside	[M+Na] ⁺	C25H33NO11	546.19426				2.0E+05	0.6		
1330 PG(P-20:0/0:0)	[M+Na] ⁺	C26H53O8P	547.33686					2.9E+05	0.3	
1331 N3'-Acetyltobramycin	[M+K] ⁺	C20H39N5O10	548.23285	1.6E+05	-1.5					
1332 PS(20:3(8Z,11Z,14Z)/0:0)	[M+H] ⁺	C26H46NO9P	548.29731			1.9E+05	1.8			
1333 Cholesteryl-beta-D-glucoside	[M+H] ⁺	C33H56O6	549.41497	2.1E+05	-1.1					
1334 PC(16:0/3:1(2E))	[M+H] ⁺	C27H52NO8P	550.35105					1.4E+05	-1.3	
1335 L-Oleandrosyl-oleandolide	[M+Na] ⁺	C27H46O10	553.29762			6.6E+05	1.3			
1336 6,8a-Seco-6,8a-deoxy-5-oxoavermectin "1b" aglycone	[M+H] ⁺	C33H46O7	555.33163	5.2E+05	0.7					
1337 Cucurbitacin F	[M+K] ⁺	C30H46O7	557.28838			4.5E+05	-1.6			
1338 PC(O-16:0/2:0)	[M+K] ⁺	C26H54NO7P	562.32709			1.8E+05	-0.3			

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1339	Cortolone-3-glucuronide	[M+Na] ⁺	C27H42O11	565.26267			4.1E+05	-1.3			
1340	dTDP-L-oleandrose	[M+Na] ⁺	C17H28N2O14P2	569.09121		1.2E+05	-0.7				
1341	Sarmentoloside	[M+H] ⁺	C29H44O11	569.29595			6.7E+05	-0.5			
1342	12alpha-Hydroxyamoorstatin	[M+K] ⁺	C28H36O10	571.19407		1.3E+05	-0.1				
1343	2-Hexaprenyl-6-methoxyphenol	[M+K] ⁺	C37H56O2	571.39211		1.4E+05	-1.6				
1344	Adonitoxigenin 3-O-alpha-L-rhamnoside	[M+Na] ⁺	C29H42O10	573.26772						1.5E+05	-1.2
1345	PI(16:0/0:0)	[M+H] ⁺	C25H49O12P	573.30344	1.5E+05	-0.2					
1346	beta-Carotene	[M+K] ⁺	C40H56	575.40210					5.2E+05	-1.3	
1347	PA(P-16:0/12:0)	[M+H] ⁺	C31H61O7P	577.42196					7.1E+05	1.4	
1348	Cucurbitacin E	[M+Na] ⁺	C32H44O8	579.29225						1.1E+05	1.0
1349	Prorepensin	[M+K] ⁺	C35H44O5	583.28185			5.0E+05	0.3			
1350	Ouabain	[M+H] ⁺	C29H44O12	585.29104			4.8E+05	-0.8			
1351	Apigenin 7-alpha-L-arabinofuranosyl-(1->6)-glucoside	[M+Na] ⁺	C26H28O14	587.13740						1.3E+05	-0.5
1352	PC(10:0/10:0)	[M+Na] ⁺	C28H56NO8P	588.36358	3.7E+05	0.9					
1353	PC(O-16:0/4:0)	[M+K] ⁺	C28H58NO7P	590.35908			1.8E+05	-1.4			
1354	Lithocholate 3-O-glucuronide	[M+K] ⁺	C30H48O9	591.29398					2.8E+05	-1.7	
1355	Spheroidene	[M+Na] ⁺	C41H60O	591.45291				2.7E+05	1.2		
1356	Agavoside A	[M+H] ⁺	C33H52O9	593.36912						1.5E+05	-1.2
1357	PI(P-16:0/0:0);	[M+K] ⁺	C25H49O11P	595.26456						9.9E+04	-0.3
1358	7,8-Didehydroastaxanthin	[M+H] ⁺	C40H50O4	595.37800						9.7E+04	0.3
1359	PG(22:4(7Z,10Z,13Z,16Z)/0:0)	[M+K] ⁺	C28H49O9P	599.27363						1.3E+05	1.6
1360	PI(18:0/0:0)	[M+H] ⁺	C27H53O12P	601.33412			2.7E+05	1.0			
1361	Quercetin 3-rhamnosyl-(1->2)-alpha-L-arabinopyranoside	[M+Na] ⁺	C26H28O15	603.13180			1.5E+05	0.4			
1362	alpha,alpha'-Trehalose 6-palmitate	[M+Na] ⁺	C28H52O12	603.33569		1.4E+05	-1.0		4.7E+05	-0.7	
1363	1-(O-alpha-D-glucopyranosyl)-3-keto-(1,27R)-octacosanediol	[M+H] ⁺	C34H66O8	603.48262					4.3E+05	0.7	
1364	5-Oxoavermectin "1a" aglycone	[M+Na] ⁺	C34H46O8	605.30813					3.2E+05	0.6	
1365	Avermectin B2b aglycone	[M+Na] ⁺	C33H48O9	611.31880			5.4E+05	0.4			
1366	PC(18:1(9Z)/4:0)	[M+Na] ⁺	C30H58NO8P	614.37959					2.6E+05	-0.6	
1367	Cytidine monophosphate N-acetylneuraminic acid	[M+H] ⁺	C20H31N4O16P	615.15453		2.7E+05	0.0				
1368	PA(P-16:0/12:0)	[M+K] ⁺	C31H61O7P	615.37823						1.1E+05	0.7
1369	CE(14:1(9Z))	[M+Na] ⁺	C41H70O2	617.52603					1.7E+05	1.3	
1370	Catechin 3-O-rutinoside	[M+Na] ⁺	C27H34O15	621.17899	1.8E+05	1.5					
1371	Dihydrospirilloxanthin	[M+Na] ⁺	C42H62O2	621.46388				3.5E+05	0.5		
1372	Rodiasine	[M+H] ⁺	C38H42N2O6	623.31090			5.5E+05	1.1			
1373	Leukotriene C4	[M+H] ⁺	C30H47N3O9S	626.30959			2.1E+05	1.6			
1374	Agavoside A	[M+K] ⁺	C33H52O9	631.32479			2.7E+05	-0.8			

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1375	DG(14:0/20:2(11Z,14Z)/0:0)	[M+K] ⁺	C37H68O5	631.46994		1.5E+05	-0.2				
1376	PA(12:0/19:0)	[M+H] ⁺	C34H67O8P	635.46528						2.3E+05	-1.0
1377	Ansatrienin A	[M+H] ⁺	C36H48N2O8	637.34786				4.0E+05	0.8		
1378	PG(12:0/14:1(9Z))	[M+H] ⁺	C32H61O10P	637.40751	1.5E+05	0.7					
1379	dolichyl beta-D-glucosyl phosphate	[M+K] ⁺	C31H55O9P	641.32115			4.5E+05	0.6			
1380	Pentacosanyl oleate	[M+K] ⁺	C41H80O2	643.57905				5.9E+05	-0.1		
1381	Rhizochalinin D	[M+H] ⁺	C35H70N2O8	647.52100					5.1E+05	-0.8	
1382	5-O-Methylesteriodictyol 7-glucosyl-(1->4)-galactoside	[M+Na] ⁺	C28H34O16	649.17469		1.4E+05	-1.2				
1383	PI(20:1(11Z)/0:0)	[M+Na] ⁺	C29H55O12P	649.33220			3.3E+05	0.2			
1384	PE(14:0/15:0)	[M+H] ⁺	C34H68NO8P	650.47592				2.0E+05	-0.6		
1385	DG(17:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	[M+H] ⁺	C42H66O5	651.49923		1.8E+05	-1.4				
1386	Hydroxymytiloxanthin	[M+K] ⁺	C40H54O5	653.36084					2.6E+05	-0.9	
1387	Hirsutidin 3-O-(6-O-p-coumaroyl)glucoside	[M+H] ⁺	C33H33O14	654.19431	1.3E+05	0.3					
1388	Cer(d18:1/22:1(13Z))	[M+K] ⁺	C40H77NO3	658.55417						2.9E+05	-1.0
1389	Peonidin 3-(6''-caffeyl)glucoside)	[M+K] ⁺	C31H29O14	664.11810					1.3E+05	1.2	
1390	PI(21:0/0:0)	[M+Na] ⁺	C30H59O12P	665.36434					2.0E+05	-1.1	
1391	PA(12:0/20:2(11Z,14Z))	[M+Na] ⁺	C35H65O8P	667.42993				1.4E+05	1.5		
1392	DG(15:0/22:4(7Z,10Z,13Z,16Z)/0:0)	[M+K] ⁺	C40H70O5	669.48461		1.3E+05	1.3				
1393	SM(d18:0/12:0)	[M+Na] ⁺	C35H73N2O6P	671.50988		1.5E+05	-0.1				
1394	Decaprenoxanthin	[M+H] ⁺	C50H72	673.57059						1.6E+05	0.1
1395	CerP(d18:1/20:0)	[M+H] ⁺	C38H76NO6P	674.54820					3.1E+05	0.2	
1396	Octaprenylcatechol	[M+Na] ⁺	C46H70O2	677.52696					8.0E+05	-0.2	
1397	PS(O-16:0/13:0)	[M+H] ⁺	C35H70NO9P	680.48553		1.2E+06	0.8				
1398	DG(16:0/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	[M+K] ⁺	C41H70O5	681.48561		6.0E+05	-0.2				
1399	PA(O-20:0/14:1(9Z))	[M+Na] ⁺	C37H73O7P	683.49791					1.7E+05	1.0	
1400	Cyanidin 3-(6''-malonylsambubioside)	[M+Na] ⁺	C29H31O18	690.14065		1.4E+05	-0.6				
1401	Diphytanyl-sn-glycerol	[M+K] ⁺	C43H88O3	691.63600		1.7E+05	0.7				
1402	Octaprenylcatechol	[M+K] ⁺	C46H70O2	693.50086				2.1E+05	-0.2		
1403	PC(10:0/18:2(9Z,12Z))	[M+Na] ⁺	C36H68NO8P	696.45798						1.3E+05	-0.7
1404	PS(14:1(9Z)/14:1(9Z))	[M+Na] ⁺	C34H62NO10P	698.40080		1.8E+05	-0.6				
1405	PE(14:0/16:1(9Z))	[M+K] ⁺	C35H68NO8P	700.43122				1.3E+05	0.3		
1406	PA(13:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M+Na] ⁺	C38H63O8P	701.41607						1.2E+05	-1.1
1407	1-Palmitoyl-2-(5-keto-6-octendioyl)-sn-glycero-3-phosphatidylcholine	[M+K] ⁺	C32H58NO11P	702.33696				1.1E+05	1.3		
1408	PS(P-16:0/12:0)	[M+K] ⁺	C34H66NO9P	702.41006		1.8E+05	0.9				
1409	Anthenoside A	[M+Na] ⁺	C38H65NO9	702.45446					1.6E+05	1.0	
1410	Bruceoside A	[M+Na] ⁺	C32H42O16	705.23585					1.3E+05	0.9	
1411	PA(15:0/20:3(8Z,11Z,14Z))	[M+Na] ⁺	C38H69O8P	707.46170				1.6E+05	0.7		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1412 Kaempferol 3-(6''-sulfatogetiobioside)	[M+Na] ⁺	C27H30O19S	713.09959			1.2E+05	-0.2			
1413 DG(21:0/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	[M+H] ⁺	C46H80O5	713.60740						1.0E+05	0.6
1414 PE(14:0/20:2(11Z,14Z))	[M+H] ⁺	C39H74NO8P	716.52248	1.5E+05	-1.2					
1415 CE(20:1(11Z))	[M+K] ⁺	C47H82O2	717.59518						2.2E+05	-0.8
2',4'-Dihydroxy-6'-methoxy-3'-(2-hydroxybenzyl)-5'-(3 x 2-hydroxybenzyl)dihydrochalcone	[M+Na] ⁺	C44H40O8	719.26239			1.4E+05	-1.2			
1417 PA(O-18:0/18:4(6Z,9Z,12Z,15Z))	[M+K] ⁺	C39H71O7P	721.45623				2.3E+05	0.9		
1418 PE(18:2(9Z,12Z)/P-18:1(11Z))	[M+H] ⁺	C41H76NO7P	726.54277		2.1E+05	0.6				
1419 Chivosazole F	[M+K] ⁺	C41H57NO8	730.37070					1.3E+05	1.2	
1420 Diguanosine diphosphate	[M+Na] ⁺	C20H26N10O15P2	731.09465	1.3E+05	1.2					
1421 Ubiquinol 8	[M+H] ⁺	C49H78O4	731.59798			1.0E+05	-0.9			
1422 PE(15:0/18:4(6Z,9Z,12Z,15Z))	[M+K] ⁺	C38H68NO8P	736.43215			1.2E+05	-1.0			
1423 PG(O-20:0/14:0)	[M+H] ⁺	C40H81O9P	737.56969		2.0E+05	-0.8				
1424 PA(15:0/22:1(11Z))	[M+Na] ⁺	C40H77O8P	739.52510						1.5E+05	-0.4
1425 PA(17:1(9Z))	[M+H] ⁺	C42H77O8P	741.54296					1.3E+05	-0.1	
1426 PI(12:0/14:1(9Z))	[M+Na] ⁺	C35H65O13P	747.40624					1.6E+05	-1.0	
1427 PA(O-20:0/20:0)	[M+H] ⁺	C43H87O7P	747.62622	9.1E+04	0.0					
1428 PC(o-16:0/18:0)	[M+H] ⁺	C42H86NO7P	748.62215					1.3E+05	-0.9	
1429 Quercetin 3-(2'''-galloylglucosyl)-(1->2)-alpha-L-arabinofuranoside	[M+H] ⁺	C33H32O20	749.15558			1.5E+05	0.5			
1430 PG(O-18:0/17:0)	[M+H] ⁺	C41H83O9P	751.58485				3.0E+05	-0.1		
1431 PE(20:2(11Z,14Z))	[M+H] ⁺	C43H80NO7P	754.57533					1.2E+05	-1.1	
1432 DG(22:4(7Z,10Z,13Z,16Z)/24:1(15Z)/0:0)	[M+H] ⁺	C49H86O5	755.65443				1.5E+05	0.5		
1433 PC(10:0/22:0)	[M+Na] ⁺	C40H80NO8P	756.55091						1.1E+05	0.6
1434 PC(14:0/20:1(11Z))	[M+H] ⁺	C42H82NO8P	760.58508	1.7E+05	-0.8					
1435 Ophiopogonin B	[M+K] ⁺	C39H62O12	761.38729	1.7E+05	0.7					
1436 Malvidin 3-O-(6-O-(4-O-malonyl-alpha-rhamnopyranosyl)-beta-glucopyranoside	[M+K] ⁺	C32H37O19	764.15606	8.4E+05	-1.0					
1437 Lampranthin II	[M+K] ⁺	C34H34N2O16	765.15436						1.5E+05	-0.5
1438 PG(P-16:0/18:4(6Z,9Z,12Z,15Z))	[M+K] ⁺	C40H71O9P	765.44669			1.2E+05	0.1			
1439 Quercetin 3-(2'''-galloylglucosyl)-(1->2)-alpha-L-arabinofuranoside	[M+Na] ⁺	C33H32O20	771.13789			8.3E+04	0.0			
1440 Myxochromide S3	[M+Na] ⁺	C40H56N6O8	771.40430			1.2E+05	1.1			
1441 PA(17:2(9Z,12Z))	[M+K] ⁺	C42H71O8P	773.45132					1.6E+05	0.6	
1442 Loropetalin D	[M+Na] ⁺	C35H28O19	775.11186			6.2E+04	-0.2			
1443 PI(12:0/18:4(6Z,9Z,12Z,15Z))	[M+H] ⁺	C39H67O13P	775.43844					1.3E+05	1.0	
1444 2-Methyl-6-solanyl-1,4-benzoquinol	[M+K] ⁺	C52H80O2	775.57968			5.8E+04	-0.9			
1445 PG(14:0/20:5(5Z,8Z,11Z,14Z,17Z))	[M+K] ⁺	C40H69O10P	779.42646						1.5E+05	-0.6
1446 PC(14:0/20:1(11Z))	[M+Na] ⁺	C42H82NO8P	782.56703	6.1E+05	-0.1					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1447 PA(O-18:0/22:1(11Z))	[M+K] ⁺	C43H85O7P	783.56652						1.1E+05	-0.1
1448 PC(O-16:0/19:0)	[M+Na] ⁺	C43H88NO7P	784.61933						1.2E+05	-0.3
1449 PA(20:0/22:1(11Z))	[M+H] ⁺	C45H87O8P	787.62147					1.4E+05	-0.4	
1450 PA(20:4)/(22:6)	[M+Na] ⁺	C45H69O8P	791.46314						9.6E+04	-1.2
Quercetin 7-methyl ether 3-[3-hydroxy-3-methylglutaryl-(1->6)]-[apiosyl-(1->2)-galactoside]	[M+K] ⁺	C33H38O20	793.15866					1.3E+05	0.2	
1452 PG(15:0/20:3(8Z,11Z,14Z))	[M+K] ⁺	C41H75O10P	797.47294	1.5E+05	0.8					
1453 MGDG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	[M+Na] ⁺	C45H76O10	799.53266						8.8E+04	0.5
1454 PS(15:0/20:3(8Z,11Z,14Z))	[M+K] ⁺	C41H74NO10P	810.46737				1.4E+05	1.0		
1455 GalCer(d18:2/23:0)	[M+Na] ⁺	C47H89NO8	818.64804	1.2E+05	1.2					
1456 Thalicoside A	[M+Na] ⁺	C42H70O14	821.46641					1.1E+05	-0.8	
1457 GalCer(d18:0/22:0)	[M+K] ⁺	C46H91NO8	824.63808						1.7E+05	-0.5
1458 Yiamoloside B	[M+H] ⁺	C43H68O15	825.46292					1.8E+05	0.2	
1459 PA(21:0/22:0)	[M+Na] ⁺	C46H91O8P	825.63437				1.9E+05	0.0		
1460 TG(16:0/16:1(9Z)/16:1(9Z))	[M+Na] ⁺	C51H94O6	825.69420		6.6E+05	0.1				
1461 TG(16:1(9Z)/16:1(9Z)/16:1(9Z))	[M+K] ⁺	C51H92O6	839.65286					1.5E+05	-0.4	
1462 PG(17:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M+K] ⁺	C45H73O10P	843.45784					1.7E+05	-0.7	
1463 Acetyl coenzyme A	[M+K] ⁺	C23H38N7O17P3S	848.08874					1.0E+05	0.2	
1464 TG(16:1(9Z)/16:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	[M+H] ⁺	C55H92O6	849.69590						1.6E+05	0.9
1465 Chrysoeriol 7-(2'''-feruloylglucuronosyl)-(1->2)-glucuronide	[M+Na] ⁺	C38H36O21	851.16422					1.1E+05	-0.1	
1466 PG(O-18:0/22:1(11Z))	[M+K] ⁺	C46H91O9P	857.60291				5.2E+04	0.4		
1467 PI(O-16:0/19:1(9Z))	[M+Na] ⁺	C44H85O12P	859.56732				1.1E+05	-0.3		
1468 TG(17:2(9Z,12Z))	[M+Na] ⁺	C54H92O6	859.67769					9.5E+04	1.1	
1469 PI(16:0/20:2(11Z,14Z))	[M+H] ⁺	C45H83O13P	863.56377				1.2E+05	0.7		
1470 PG(20:4(5Z,8Z,11Z,14Z))	[M+Na] ⁺	C48H75O10P	865.49899					1.1E+05	0.0	
1471 PG(22:4(7Z,10Z,13Z,16Z))	[M+Na] ⁺	C48H77O10P	867.51495					1.4E+05	-0.3	
1472 TG(17:1(9Z)/18:1(9Z)/18:1(9Z))	[M+H] ⁺	C56H102O6	871.77588				1.5E+05	-1.1		
1473 PG(19:1(9Z)/22:2(13Z,16Z))	[M+K] ⁺	C47H87O10P	881.56685	1.1E+05	-0.7					
1474 TG(16:0/18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	[M+H] ⁺	C57H100O6	881.75927	1.8E+05	0.5	1.9E+06	-0.7			
1475 PI(16:0/20:2(11Z,14Z))	[M+Na] ⁺	C45H83O13P	885.54568					9.7E+04	0.8	
1476 PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M+Na] ⁺	C50H79O10P	893.53108					1.3E+05	-0.9	
1477 TG(17:2(9Z,12Z)/18:0/18:0)	[M+Na] ⁺	C56H104O6	895.77239					8.1E+04	0.1	
1478 TG(18:3(9Z,12Z,15Z))	[M+H] ⁺	C59H94O6	899.71292					8.5E+04	-0.7	
1479 TG(17:1/20:5/20:5)	[M+H] ⁺	C60H94O6	911.71274						1.5E+05	-0.5
1480 3-O-Sulfogalactosylceramide	[M+Na] ⁺	C48H91NO11S	912.62065				5.5E+04	-0.2		
1481 TG(16:0/18:1/20:4)	[M+K] ⁺	C57H100O6	919.71482		3.1E+06	0.4				
1482 PC(22:4/24:0)	[M+H] ⁺	C54H100NO8P	922.72690		1.4E+06	-1.0				
1483 Cassiaside B2	[M+Na] ⁺	C39H52O25	943.26946				7.1E+04	-0.5		

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1484	Delphinidin 3,3'-di-glucoside-5-(6-caffeoylglucoside)	[M+H] ⁺	C42H47O25	952.24853			5.7E+04	-0.6			
1485	PI(19:0/22:1(11Z))	[M+Na] ⁺	C50H95O13P	957.64122			5.7E+04	-1.0			
1486	TG(17:2/20:5/22:4)	[M+Na] ⁺	C62H98O6	961.72556	1.4E+05	0.3					
1487	TG(18:2(9Z,12Z)/20:1(11Z)/20:4(5Z,8Z,11Z,14Z))	[M+K] ⁺	C61H104O6	971.74713		2.1E+05	-0.7				
1488	1-O-[(6'-O-hexadecanoyl)-α-D-glucopyranosyl]- (2-hexadecanoyloxy)-eicosan-1-ol	[M+Na] ⁺	C58H112O9	975.81998		1.5E+05	-0.1				
1489	Malvidin 3-O-(6-O-(4-O-feruloyl-α- rhamnopyranosyl)-β-D-glucopyranoside)-5- β-D-glucopyranoside	[M+H] ⁺	C45H53O24	978.30085			8.4E+04	-0.9			
1490	D-Mannosylphosphodecaprenol	[M+K] ⁺	C56H93O9P	979.61813		2.0E+05	0.8				
1491	Magnoloside C	[M+K] ⁺	C41H56O25	987.27493			9.3E+04	-0.7			

^a CE Cholesteryl ester; Cer Ceramide; Galcer Galactosylceramide; DG Diacylglycerol; MG Monoacylglycerol; MGDG Monogalactosyldiacylglycerol; PA Phosphatidic acid; PC Phosphatidylcholine; PE Phosphatidylethanolamine; PG Glycerophospholipids; PGF2 Prostaglandin F2; PI Phosphatidylinositol; PS Phosphatidylserine; SM Sphingomyelin; TG Triacylglycerol.

^b Theoretical mass

^c R stands for red tunica, W stands for white tunica and B stands for bulb.

Table S7: Untargeted metabolic profiling of *Sulmona red garlic* hydroalcoholic extracts by ESI(-) FT-ICR MS

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
1 Pyruvic acid	[M-H]-	C3H4O3	87.00812			3.4E+04	4.7			
2 Butyric acid	[M-H]-	C4H8O2	87.04546						6.9E+04	-3.5
3 Pentanol	[M-H]-	C5H12O	87.08154	6.3E+04	3.7					
4 2-Propyn-1-al	[M+Cl]-	C3H2O	88.98055			3.7E+04	-2.1			
5 Propanethial S-oxide	[M-H]-	C3H6OS	89.00663			2.9E+04	0.3			
6 1,3-Butadiene	[M+Cl]-	C4H6	89.01609			2.9E+04	2.9			
7 Diethyl sulfide	[M-H]-	C4H10S	89.04343						8.1E+04	-4.3
8 3-Aminopropane-1,2-diol	[M-H]-	C3H9NO2	90.05639				5.0E+04	-3.8		
9 Thioglycolate	[M-H]-	C2H4O2S	90.98537			2.9E+04	1.6			
10 Dimethyl sulfone	[M-H]-	C2H6O2S	93.00157	6.2E+04	1.7				8.1E+04	0.8
11 Thiocyanate	[M+Cl]-	CHNS	93.95237		8.2E+04	0.9				
12 Hexadienal	[M-H]-	C6H8O	95.05029			4.1E+04	-0.5			
13 Carbamic acid	[M+Cl]-	CH3NO2	95.98567					5.3E+04	1.2	
14 Maleimide	[M-H]-	C4H3NO2	96.00910		8.2E+04	2.9				
15 Ethanolamine	[M+Cl]-	C2H7NO	96.02217		4.6E+04	-2.8				
16 Beta-vinyl acrylic acid	[M-H]-	C5H6O2	97.02883			3.0E+04	4.8			
17 Succinimide	[M-H]-	C4H5NO2	98.02475		9.3E+04	2.8				
18 Piperidinone	[M-H]-	C5H9NO	98.06144			3.2E+04	-3.1			
19 Tiglic acid	[M-H]-	C5H8O2	99.04515	7.0E+04	2.6				8.3E+04	4.0
20 Aminocyclopropane-carboxylate	[M-H]-	C4H7NO2	100.04040	5.4E+04	-2.2					
21 Succinate semialdehyde	[M-H]-	C4H6O3	101.02442	1.2E+05	-0.5	6.8E+04	-4.8		1.2E+05	4.6
22 Betaine aldehyde	[M-H]-	C5H12NO	101.08511					5.6E+04	-4.9	
23 Imidazole	[M+Cl]-	C3H4N2	103.00694						6.6E+04	-0.9
24 Choline	[M-H]-	C5H14NO	103.10052					3.4E+04	-2.5	
25 S-Methylthioglycolate	[M-H]-	C3H6O2S	105.00119				4.7E+04	3.7		
26 Glyceric acid	[M-H]-	C3H6O4	105.01976				4.1E+04	-4.1		
27 N-Methylaniline	[M-H]-	C7H9N	106.06652			3.2E+04	-2.8			
28 2-Methylpropanamine	[M+Cl]-	C4H11N	108.05855		3.5E+04	0.5				
29 Furoic acid	[M-H]-	C5H4O3	111.00877	7.4E+04	4.3					
30 Allyl sulfide	[M-H]-	C6H10S	113.04358				4.5E+04	-4.7		
31 Octane	[M-H]-	C8H18	113.13405			2.9E+04	-4.2			
32 Pyridine	[M+Cl]-	C5H5N	114.01204			2.4E+04	-3.9			
33 Methylthiopropionic acid	[M-H]-	C4H8O2S	119.01745						5.5E+04	-1.9
34 3-Methyl-2-butenal	[M+Cl]-	C5H8O	119.02746				3.0E+04	-4.6		
35 D-Erythrose	[M-H]-	C4H8O4	119.03498		4.0E+04	2.1				
36 Purine	[M-H]-	C5H4N4	119.03599					6.6E+04	2.8	
37 Cysteine	[M-H]-	C3H7NO2S	120.01247	4.9E+04	-4.8					
38 Piperidine	[M+Cl]-	C5H11N	120.05881						3.9E+04	-2.2
39 1,4-Lactone	[M+Cl]-	C4H6O2	121.00618	5.0E+04	-4.3					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
40 Nicotinamide	[M-H]-	C6H6N2O	121.04046			3.8E+04	2.3			
41 Sulfoacetaldehyde	[M-H]-	C2H4O4S	122.97575	5.9E+04	0.6					
42 Selenocysteine	[M+Cl]-	C3H6NO2Se	123.00894						9.0E+05	2.6
43 2,4-octadienal	[M-H]-	C8H12O	123.08154	7.5E+04	-1.6					
44 Taurine	[M-H]-	C2H7NO3S	124.00739		5.3E+04	2.0				
45 Maltol	[M-H]-	C6H6O3	125.02375				4.2E+04	3.7		
46 Dihydrophloroglucinol	[M-H]-	C6H8O3	127.03966				2.7E+04	3.2		
47 L-Lysine 1,6-lactam	[M-H]-	C6H12N2O	127.08775						4.8E+04	-0.5
48 Aniline	[M+Cl]-	C6H7N	128.02733				3.3E+04	-0.6		
49 Guanidinobutanal	[M-H]-	C5H11N3O	128.08251			2.9E+04	3.3			
50 Octylamine	[M-H]-	C8H19N	128.14381			4.1E+04	4.8			
51 Dimethyl valeric acid	[M-H]-	C7H14O2	129.09293					4.2E+04	-3.1	
52 2-Hydroxypyridine	[M+Cl]-	C5H5NO	130.00652		5.9E+04	-1.5				
53 Hydroxy-L-proline	[M-H]-	C5H9NO3	130.05097	6.7E+04	0.3					
54 4-Guanidino-1-butanol	[M-H]-	C5H13N3O	130.09763			4.9E+04	4.8			
55 Furfural	[M+Cl]-	C5H4O2	130.99053	3.8E+04	-1.5					
56 Oxalacetic acid	[M-H]-	C4H4O5	130.99856						3.7E+04	0.3
57 Pteridine	[M-H]-	C6H4N4	131.03613				2.4E+04	1.5	5.2E+04	-3.7
58 Asparagine	[M-H]-	C4H8N2O3	131.04622		8.0E+04	2.4				
59 Aspartic acid	[M-H]-	C4H7NO4	132.03023	3.4E+04	-3.0					
60 Ureidoglycine	[M-H]-	C3H7N3O3	132.04232						4.9E+04	-2.7
61 Hydroxyindole	[M-H]-	C8H7NO	132.04580			2.7E+04	-2.4			
62 Malic acid	[M-H]-	C4H6O5	133.01389				3.5E+04	2.7		
63 Imidazole-4-methanol	[M+Cl]-	C4H6N2O	133.01672					1.3E+05	5.2	
64 Cinnamyl alcohol	[M-H]-	C9H10O	133.06589		9.7E+04	0.3				
65 2-Phenylacetamide	[M-H]-	C8H9NO	134.06114		5.8E+04	-1.0				
66 Caproaldehyde	[M+Cl]-	C6H12O	135.05822	5.0E+04	2.5					
67 Hydroxypurine	[M-H]-	C5H6N4O	137.04627			3.7E+04	4.5			
68 Hexan-1-ol	[M+Cl]-	C6H14O	137.07387	5.0E+04	0.3					
69 Cadaverine	[M+Cl]-	C5H14N2	137.08433					3.8E+04	2.7	
70 Malonic acid	[M+Cl]-	C3H4O4	138.98036	5.2E+04	4.5					
71 5-Phenyl-1,3-pentadiyne	[M-H]-	C11H8	139.05589			4.9E+04	-4.1			
72 Methylthiopropylamine	[M+Cl]-	C4H11NS	140.03090					3.2E+04	-2.0	
73 Muconic acid	[M-H]-	C6H6O4	141.01869					3.3E+04	4.6	
74 4-Oxocyclohexanecarboxylate	[M-H]-	C7H10O3	141.05572		6.1E+04	1.3				
75 Octenoic acid	[M-H]-	C8H14O2	141.09210	4.1E+04	3.0					
76 Pyridine-3-aldehyde	[M+Cl]-	C6H5NO	142.00618						7.0E+04	2.4
77 Quinone	[M+Cl]-	C6H4O2	142.98986				3.2E+04	4.7		
78 n-valeryl acetic acid	[M-H]-	C7H12O3	143.07108				2.5E+04	2.0		
79 Dehydroxycarnitine	[M-H]-	C7H15NO2	144.10336				2.8E+04	-2.5		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
80 Resorcinol	[M+Cl]-	C6H6O2	145.00701						3.8E+04	-2.5
81 Oxoglutarate	[M-H]-	C5H6O5	145.01425	9.3E+04	-4.7					
82 Coumarin	[M-H]-	C9H6O2	145.03000			1.7E+05	-3.4			
83 Glutamine	[M-H]-	C5H10N2O3	145.06193					4.4E+04	-0.4	
84 Cytosine	[M+Cl]-	C4H5N3O	146.01266	8.3E+04	-4.9	2.7E+04	-4.8			
85 Dihydroxyfumarate	[M-H]-	C4H4O6	146.99351		5.7E+04	-1.8				
86 Heptenal	[M+Cl]-	C7H12O	147.05904			2.4E+04	-4.6			
87 1-Pyrroline-2-carboxylate	[M+Cl]-	C5H7NO2	148.01644			1.9E+05	4.3			
88 threo-3-Hydroxy-L-aspartate	[M-H]-	C4H7NO5	148.02450				2.8E+04	4.4		
89 epsilon-Caprolactam	[M+Cl]-	C6H11NO	148.05336			4.8E+04	0.7			
90 Phenylglyoxylic acid	[M-H]-	C8H6O3	149.02427					4.3E+04	1.0	3.0E+04 2.4
91 Dipropyl disulfide	[M-H]-	C6H14S2	149.04642	6.2E+04	-4.9					
92 3-Amino-2-piperidone	[M+Cl]-	C5H10N2O	149.04815					1.4E+05	3.8	
93 Sulfinyipyruvic acid	[M-H]-	C3H3O5S	149.96284	3.4E+04	-0.9					
94 Sulfinyipyruvic acid	[M-H]-	C3H3O5S	149.96357			2.9E+04	-4.8			
95 6-Imino-5-oxocyclohexa-1,3-dienecarboxylate	[M-H]-	C7H5NO3	150.01967	4.4E+04	-2.8					
96 N3-Metyladenine	[M-H]-	C6H9N5	150.07852		7.4E+04	1.0	4.5E+04	1.1		
97 Fumaric acid	[M+Cl]-	C4H4O4	150.98052			4.7E+04	-1.1			
98 Sulfinoalanine	[M-H]-	C3H6NO4S	150.99448	4.0E+04	-4.0					
99 Arabitol	[M-H]-	C5H12O5	151.06120	7.1E+04	4.5					
100 5-Aminopentanamide	[M+Cl]-	C5H12N2O	151.06436		4.5E+04	1.0				
101 Myrtenol	[M-H]-	C10H16O	151.11381			3.5E+04	-4.0			
102 N-(4,6-diaminopyrimidin-5-yl)formamide	[M-H]-	C5H7N5O	152.05812			4.0E+04	-2.2			
103 Oxomalonate	[M+Cl]-	C3H2O5	152.95962		6.3E+04	0.7				
104 Imidazole pyruvic acid	[M-H]-	C6H6N2O3	153.03057	3.2E+04	-0.8	1.7E+04	-3.3			
105 Diaminobutyric acid	[M+Cl]-	C4H10N2O2	153.04462			3.1E+04	-4.6			
106 S-Acetylthioethanolamine	[M+Cl]-	C4H9NOS	154.00989		1.0E+05	1.3				
107 Nitrocatechol	[M-H]-	C6H5NO4	154.01458	3.7E+04	1.2					
108 Histidine	[M-H]-	C6H9N3O2	154.06220	8.0E+04	-4.9					
109 Dimethylsulfonioacetate	[M+Cl]-	C4H9O2S	156.00125					1.1E+05	3.1	
110 Selenocysteine seleninic acid	[M+Cl]-	C3H7NO4Se	156.00662			4.0E+04	1.9			
111 Phenylethylamine	[M+Cl]-	C8H11N	156.05885						2.8E+04	-1.9
112 Mercaptolactic acid	[M+Cl]-	C3H6O3S	156.97303				3.4E+04	0.9		
113 Nicotinamide	[M+Cl]-	C6H6N2O	157.01713			2.7E+04	1.8			
114 Allantoin	[M-H]-	C4H6N4O3	157.03721				3.4E+04	-3.2		
115 (+)-6-methyl caprylic acid	[M-H]-	C9H18O2	157.12340		4.2E+04	-2.2				
116 Guaiacol	[M+Cl]-	C7H8O2	159.02183	7.3E+04	1.0					
117 Pimelic acid	[M-H]-	C7H12O4	159.06628	8.4E+04	-0.3				4.2E+04	-4.4
118 D-Alanyl-D-alanine	[M-H]-	C6H12N2O3	159.07848					1.4E+05	-4.8	
119 Hydroxy-L-glutamic acid	[M-H]-	C5H7NO5	160.02542	3.1E+04	-1.7					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
120 gamma-Coniceine	[M+Cl]-	C8H15N	160.08986				3.6E+04	-0.1		
121 Safrole	[M-H]-	C10H10O2	161.05984			7.0E+04	4.9			
122 Oleandrose	[M-H]-	C7H14O4	161.08232						2.9E+04	-2.4
123 3-Methyldioxyindole	[M-H]-	C9H9NO2	162.05663					1.7E+04	-3.6	
124 Octanal	[M+Cl]-	C8H16O	163.08873					2.7E+04	4.8	
125 Goitrin	[M+Cl]-	C5H7NOS	163.99351					2.1E+04	4.4	
126 Methionine S-oxide	[M-H]-	C5H11NO3S	164.03943				3.4E+04	-4.5		
127 D-Pipecolic acid	[M+Cl]-	C6H11NO2	164.04838		5.2E+04	-0.5				
128 Cucurbitine	[M+Cl]-	C5H10N2O2	165.04338					4.2E+04	1.5	
129 Agmatine	[M+Cl]-	C5H14N4	165.09131						9.8E+04	-0.4
130 4-Trimethylammoniobutanol	[M+Cl]-	C7H16NO	165.09323					3.5E+04	-3.9	
131 Iminoaspartate	[M+Cl]-	C4H5NO4	165.99126		7.2E+04	2.4				
132 Dihydroxyadenine	[M-H]-	C5H5N5O2	166.03668						3.0E+04	2.2
133 Guanidinopropanoate	[M+Cl]-	C4H9N3O2	166.03888	5.2E+04	-4.9		7.4E+04	5.0		
134 N-Carbamoylputrescine	[M+Cl]-	C5H13N3O	166.07554				2.2E+04	-1.7		
135 2-Dimethylamino-5,6-dimethylpyrimidin-4-ol	[M-H]-	C8H13N3O	166.09917						7.4E+04	-3.5
136 Oxaluric acid	[M+Cl]-	C3H4N2O4	166.98570					1.7E+04	4.8	
137 Glutaric acid	[M+Cl]-	C5H8O4	167.01156					1.7E+04	0.6	
138 Aspartic acid	[M+Cl]-	C4H7NO4	168.00723					1.5E+04	-1.9	
139 Piperidione	[M-H]-	C9H15NO2	168.10376						2.2E+04	-4.5
140 Dodecane	[M-H]-	C12H26	169.19617		3.1E+04	-1.0				
141 Decanamide	[M-H]-	C10H21NO	170.15471					1.8E+04	1.9	
142 Methylerythritol	[M+Cl]-	C5H12O4	171.04364					2.6E+04	-4.0	
143 Capric acid	[M-H]-	C10H20O2	171.13905	2.5E+05	1.6		1.0E+05	2.1		
144 Trigonelline	[M+Cl]-	C7H7NO2	172.01722						4.8E+04	-0.8
145 Quinaldic acid	[M-H]-	C10H7NO2	172.03969				2.0E+04	4.1		
146 N-Acetyl-L-leucine	[M-H]-	C8H15NO3	172.09799						2.3E+04	-0.4
147 2,4-nonadienal	[M+Cl]-	C9H14O	173.07387		3.8E+04	2.0				
148 Echinorine	[M-H]-	C11H12NO	173.08518				2.9E+04	-3.3		
149 Hydroxy pelargonic acid	[M-H]-	C9H18O3	173.11785					1.5E+04	2.7	
150 Histidinal	[M+Cl]-	C6H9N3O	174.04410						2.7E+04	-0.8
151 Acetyl phosphate	[M+Cl]-	C2H5O5P	174.95686	2.5E+04	-1.4					
152 Hydroxymethylcatechol	[M+Cl]-	C7H8O3	175.01759				1.8E+04	-4.8		
153 2-Oxo-6-methylthiohexanoic acid	[M-H]-	C7H12O3S	175.04286			2.8E+04	3.3			
154 Nonenal	[M+Cl]-	C9H16O	175.08909				2.0E+04	2.4		
155 O-Phosphoethanolamine	[M+Cl]-	C2H8NO4P	175.98846				2.9E+04	0.2		
156 Guvacoline	[M+Cl]-	C7H11NO2	176.04765			3.0E+04	4.1			
157 Valerianine	[M-H]-	C11H15NO	176.10747			2.0E+04	3.5			
158 Thiopheneacetic acid	[M+Cl]-	C6H6O2S	176.97885						4.9E+04	-3.4
159 Cysteinylglycine	[M-H]-	C5H10N2O3S	177.03328				2.1E+04	3.7		

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
160 Vinylacetyl glycine	[M+Cl]-	C6H9NO3	178.02764	3.2E+04	0.5					
161 Glucose	[M-H]-	C6H12O6	179.05599					3.4E+05	0.7	
162 Dicyclohexylamine	[M-H]-	C12H23N	180.17521			1.8E+04	3.1			
163 Dodecenal	[M-H]-	C12H22O	181.15966						1.9E+04	0.7
164 Glutamic acid	[M+Cl]-	C5H9NO4	182.02344				2.3E+04	-4.8		
165 Thiouric acid	[M-H]-	C5H4N4O2S	182.99888						2.7E+04	-3.6
166 Chamazulene	[M-H]-	C14H16	183.11784					5.5E+04	0.5	
167 L-Serine O-sulfate	[M-H]-	C3H7NO6S	183.99213	3.2E+04	-2.2					
168 2-Formylaminobenzaldehyde	[M+Cl]-	C8H7NO2	184.01708		2.7E+05	-0.2				
169 D-Methionine	[M+Cl]-	C5H11NO2S	184.02045		2.7E+05	0.1				
170 Methyladenine	[M+Cl]-	C6H7N5	184.04000					1.4E+04	-2.5	
171 cis-2-Carboxycyclohexyl-acetic acid	[M-H]-	C9H14O4	185.08273				2.7E+04	-4.3		
172 2-Phenylglycine	[M+Cl]-	C8H9NO2	186.03273		4.3E+04	-0.6				
173 2-(Acetamidomethylene)succinate	[M-H]-	C7H9NO5	186.04143					2.1E+04	-3.4	
174 p-Cresol sulfate	[M-H]-	C7H8O4S	187.00632				2.3E+04	3.9		
175 Ngamma-Monomethyl-L-arginine	[M-H]-	C7H16N4O2	187.12005		5.3E+04	-1.0				
176 Thiocysteine	[M+Cl]-	C3H7NO2S2	187.96062				1.5E+04	3.2		
177 N-Amidino-L-glutamate	[M-H]-	C6H11N3O4	188.06768	2.8E+04	-3.0					
178 Sulfocatechol	[M-H]-	C6H6O5S	188.98635					2.2E+04	-0.2	
179 Ethoxycoumarin	[M-H]-	C11H10O3	189.05531				2.0E+04	2.2		
180 2-Oxo-7-methylthioheptanoic acid	[M-H]-	C8H14O3S	189.05909	3.1E+04	-0.5					
181 N-Methylpelletierine	[M+Cl]-	C9H17NO	190.10042		4.0E+04	-1.3			2.2E+05	4.3
182 Orotic acid	[M+Cl]-	C5H4N2O4	190.98568			4.2E+04	4.3			
183 Methylmuconolactone	[M+Cl]-	C7H8O4	191.01166	2.7E+04	0.6					
184 Quinic acid	[M-H]-	C7H12O6	191.05611	3.0E+04	3.3					
185 (-)-Citronellol	[M+Cl]-	C10H20O	191.12082		5.5E+04	-1.3				
186 Maleylacetate	[M+Cl]-	C6H6O5	192.99131					1.4E+04	-2.0	
187 Methyl beta-D-galactoside	[M-H]-	C7H14O6	193.07088					2.6E+04	4.6	
188 Glucosaminic acid	[M-H]-	C6H13NO6	194.06614					1.4E+04	4.5	
189 Aminopropylcadaverine	[M+Cl]-	C8H21N3	194.14363				2.3E+04	-3.5		
190 Dihydroxyphenylpyruvate	[M-H]-	C9H8O5	195.02968						1.8E+04	1.1
191 Benzocoumarin	[M-H]-	C13H8O2	195.04444					2.2E+04	3.7	
192 Guanidinoethyl methyl phosphate	[M-H]-	C4H12N3O4P	196.04975			2.3E+04	-2.5			
193 Hydroxymethyl-glutaric acid	[M+Cl]-	C6H10O5	197.02180				1.3E+04	2.2		
194 Hydroxylysine	[M+Cl]-	C6H14N2O3	197.06961				1.7E+04	1.2		
195 Threonine phosphate	[M-H]-	C4H10NO6P	198.01730	2.4E+04	-2.3					
196 3-Methyldioxyindole	[M+Cl]-	C9H9NO2	198.03273		3.7E+04	1.0				
197 4-(3-Pyridyl)-3-butenic acid	[M+Cl]-	C9H9NO2	198.03283						1.3E+04	-0.5
198 Homomethionine	[M+Cl]-	C6H13NO2S	198.03610		3.7E+04	-2.0				
199 N-Acetylphenylethylamine	[M+Cl]-	C10H13NO	198.06884						2.1E+04	1.4

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
200 Mephentermine	[M+Cl]-	C11H17N	198.10531						1.7E+04	1.0
201 Hydroxycinnamate	[M+Cl]-	C9H8O3	199.01723				2.4E+04	-2.4		
202 Phenylheptatriyne	[M+Cl]-	C13H8	199.03228						2.1E+04	-1.4
203 Propionyl caprylic acid	[M-H]-	C11H20O3	199.13467			2.6E+04	-3.5			
204 Lauric acid	[M-H]-	C12H24O2	199.17035	4.4E+05	2.4	2.6E+04	-0.7	2.0E+05	-2.4	
205 Hydroxy hendecanoic acid	[M-H]-	C11H22O3	201.14957					1.9E+04	0.2	
206 Butanoylphosphate	[M+Cl]-	C4H9O5P	202.98900			2.2E+04	-4.1			
207 Pyridoxamine	[M+Cl]-	C8H12N2O2	203.05928	2.4E+04	4.8					
208 N6-Acetyl-N6-hydroxy-L-lysine	[M-H]-	C8H16N2O4	203.10286			3.0E+04	4.3			
209 Bellendine	[M-H]-	C12H15NO2	204.10387				1.6E+04	-4.3		
210 Methoxycinnamic acid ethyl ester	[M-H]-	C12H14O3	205.08702	1.9E+04	4.5					
211 Actinamine	[M-H]-	C8H18N2O4	205.11897					2.7E+04	2.0	
212 Octylphenol	[M-H]-	C14H22O	205.15979	5.6E+04	-4.5					
213 4-(1,2-Epoxyethyl)-8,9-epoxy-enediyne	[M-H]-	C14H8O2	207.04515		1.0E+05	-2.9				
214 Dihydrolipoic acid	[M-H]-	C8H16O2S2	207.05171					8.3E+04	0.9	
215 Glycylproline	[M+Cl]-	C7H12N2O3	207.05462				2.9E+04	-2.1		
216 Undecan-1-ol	[M+Cl]-	C11H24O	207.15174			4.0E+04	1.8			
217 5-Deoxy-5-aminoshikimic acid	[M+Cl]-	C7H11NO4	208.03821	1.8E+04	-2.4				1.4E+04	-4.4
218 1,3-Dimethyl-8-isoquinolinol	[M+Cl]-	C11H11NO	208.05284				2.4E+04	3.0		
219 Benzimidazolylguanidine	[M+Cl]-	C8H9N5	210.05515			2.9E+04	0.2			
220 Perseitol	[M-H]-	C7H16O7	211.08145					1.4E+04	4.2	
221 Myristaldehyde	[M-H]-	C14H28O	211.20607				1.2E+04	3.2		
222 2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate	[M-H]-	C9H10O6	213.03988				2.4E+04	2.7		
223 Methyl lauric acid	[M-H]-	C13H26O2	213.18619				1.7E+05	-0.9		
224 5-Methyl-3-isoxazolyl sulfate	[M+Cl]-	C4H5NO5S	213.95786			4.4E+04	1.8			
225 Kinetin	[M-H]-	C10H9N5O	214.07419						3.0E+04	-3.5
226 3-Phospho-D-erythronate	[M-H]-	C4H9O8P	214.99623		2.1E+05	-1.6				
227 Bergapten	[M-H]-	C12H8O4	215.03587				5.7E+04	-4.1	3.1E+05	0.6
228 2-Methyl-3-hydroxy-5-formylpyridine-4-carboxylate	[M+Cl]-	C8H7NO4	216.00666						7.8E+04	1.2
229 2-(Hydroxymethyl)-3-(acetamidomethylene)succinate	[M-H]-	C8H11NO6	216.05057			2.0E+04	3.7			
230 O-Propanoylcarnitine	[M-H]-	C10H19NO4	216.12413		3.8E+04	-1.6				
231 cis-1,2-Dihydroxy-1,2-dihydrodibenzothiophene	[M-H]-	C12H10O2S	217.03205				3.0E+04	3.8		
232 Diisopropyl phosphate	[M+Cl]-	C6H15O4P	217.04020	3.3E+04	4.0					
233 Xanthan	[M+Cl]-	C13H10O	217.04257		1.1E+05	2.3				
234 5-Methoxydimethyltryptamine	[M-H]-	C13H18N2O	217.13464		4.1E+04	0.3				
235 L-Homocysteic acid	[M+Cl]-	C4H9NO5S	217.98967						1.4E+04	-0.6
236 4-Amino-5-phosphomethyl-2-methylpyrimidine	[M-H]-	C6H10N3O4P	218.03385					1.2E+04	-1.1	
237 Ngamma-Nitro-L-arginine	[M-H]-	C6H13N5O4	218.08906			1.8E+04	1.9			

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
238 N-Phenyl-1-naphthylamine	[M-H]-	C16H13N	218.09776					1.5E+04	-1.1	
239 Tecostanine	[M+Cl]-	C11H21NO	218.13207			1.7E+04	-1.6			1.4E+04 -3.5
240 Polygonolide	[M-H]-	C12H12O4	219.06628	1.8E+04	2.8					
241 Chamazulene	[M+Cl]-	C14H16	219.09499					1.6E+04	-1.8	2.5E+04 0.0
242 Dihydroxykynurenate	[M-H]-	C10H7NO5	220.02507				1.3E+04	0.3		
243 Sulfomuconate	[M-H]-	C6H6O7S	220.97563					1.6E+04	2.3	
244 Undecanoic acid	[M+Cl]-	C11H22O2	221.13076			2.0E+04	2.8			
245 n-Decanohydroxamic acid	[M+Cl]-	C10H21NO2	222.12604			2.0E+04	2.7			
246 Methylnaconitate	[M+Cl]-	C7H8O6	223.00149	2.3E+04	-2.7					
247 Dihydroflavone	[M-H]-	C15H12O2	223.07702					1.4E+04	-2.5	
248 Prenyl-L-cysteine	[M+Cl]-	C8H15NO2S	224.05259				1.3E+04	-3.7	1.3E+04	-4.4
249 Homocitrulline	[M+Cl]-	C7H15N3O3	224.08074		3.3E+04	-2.9				
250 Methylthiooctanaldoxime	[M+Cl]-	C9H19NOS	224.08801				1.3E+04	0.6		
251 Myristoleic acid	[M-H]-	C14H26O2	225.18600	3.2E+04	1.7					
252 Myristic acid	[M-H]-	C14H28O2	227.20176					1.3E+06	-0.5	
253 N-Decanoylglycine	[M-H]-	C12H23NO3	228.16100					3.4E+05	-2.1	
254 Ferulic acid	[M+Cl]-	C10H10O4	229.02731		1.9E+05	2.1				
255 Zingerone	[M+Cl]-	C11H14O3	229.06384					2.7E+04	-0.6	
256 Hydroxypseudooxynicotine	[M+Cl]-	C10H14N2O2	229.07493	2.9E+04	3.8	5.9E+04	4.5			
257 Xanthine-8-carboxylate	[M+Cl]-	C6H4N4O4	230.99266	2.4E+04	-1.8					
258 Gluconic acid	[M+Cl]-	C6H12O7	231.02840						2.8E+04	-3.0
259 Hydroxyatrazine	[M+Cl]-	C8H15N5O	232.09700				2.5E+04	0.3		
260 Curcumenol	[M-H]-	C15H22O2	233.15472						1.9E+04	-0.1
261 Benzoxazolate	[M-H]-	C11H9NO5	234.04018			1.8E+04	2.6			
262 D-Erythrose 4-phosphate	[M+Cl]-	C4H9O7P	234.97857						1.3E+04	-2.5
263 Indolepyruvic acid	[M+Cl]-	C11H9NO3	238.02764	2.0E+04	3.9					
264 Dehydrofalcarnone	[M-H]-	C17H20O	239.14451				4.2E+04	-1.6	4.3E+04	1.4
265 Tridecenyl acetate	[M-H]-	C15H28O2	239.20131				1.3E+05	1.4		
266 N-(2,3-Dihydroxybenzoyl)-L-serine	[M-H]-	C10H11NO6	240.05131				2.1E+04	0.2		
267 4-(Dimethylamino)phenylazoxybenzene	[M-H]-	C14H15N3O	240.11424	1.8E+04	1.0					
268 Methyl myristic acid	[M-H]-	C15H30O2	241.21730	3.4E+05	1.0	1.6E+06	0.5	3.0E+05	-2.4	
269 Methyl 5-hydroxy-2-benzimidazole carbamate	[M+Cl]-	C9H9N3O3	242.03363						2.1E+04	0.7
270 N-Undecanoylglycine	[M-H]-	C13H25NO3	242.17628				1.8E+05	-0.5	8.4E+04	-2.2
271 Jasmonic acid	[M+Cl]-	C12H18O3	245.09446						1.3E+04	2.2
272 3-(2-Carboxyethenyl)-cis,cis-muconate	[M+Cl]-	C9H8O6	247.00120				8.2E+04	1.2		
273 Confertin	[M-H]-	C15H20O3	247.13400			1.6E+04	-0.1			
274 N-Caffeoylputrescine	[M-H]-	C13H18N2O3	249.12477			2.2E+04	-1.2			
275 Absciscic alcohol	[M-H]-	C15H22O3	249.15051					1.4E+04	-3.6	
276 Glycerylphosphorylethanolamine	[M+Cl]-	C5H14NO6P	250.02528	2.7E+04	2.8					
277 cis-Hinokiresinol	[M-H]-	C17H16O2	251.10854			3.0E+04	-3.1			

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm				
278	Vulgraon B	[M+Cl]-	C16H24	251.15795				7.1E+04	-3.0						
279	S-(Phenylacetothiohydroximoyl)-L-cysteine	[M-H]-	C11H14N2O3S	253.06524	3.2E+04	-2.3									
280	Palmitoleic acid	[M-H]-	C16H30O2	253.21719					3.6E+05	0.5					
281	Nicotinate D-ribonucleoside	[M-H]-	C11H14NO6	255.07484	2.0E+05	-0.6									
282	N-Acetyl-beta-D-glucosaminylamine	[M+Cl]-	C8H16N2O5	255.07532	2.0E+05	-2.5									
283	Palmitic acid	[M-H]-	C16H32O2	255.23295	1.3E+06	-0.4	4.5E+06	-0.2	5.3E+05	-1.1	7.4E+05	2.8	3.2E+05	1.0	
284	Benzythioguanine	[M-H]-	C12H11N5S	256.06568				2.6E+04	2.2						
285	Hydroxykynurenine	[M+Cl]-	C10H12N2O4	259.04857							1.9E+04	2.1			
286	Hemigossypol	[M-H]-	C15H16O4	259.09758		3.2E+04	1.1								
287	1-Hydroxy-2-methyl-2-butenyl 4-diphosphate	[M-H]-	C5H12O8P2	260.99314				1.6E+04	1.2						
288	Chorismic acid	[M+Cl]-	C10H10O6	261.01660							7.5E+04	2.1			
289	N-acetyl-S-(3-oxo-3-carboxy-n-propyl)cysteine	[M-H]-	C9H13NO6S	262.03969					2.8E+04	-2.3					
290	Serine phosphoethanolamine	[M+Cl]-	C5H13N2O6P	263.02052				2.1E+04	0.0						
291	Myristic acid	[M+Cl]-	C14H28O2	263.17833	2.7E+04	2.1	2.6E+06	0.4	1.4E+06	-2.1	1.3E+04	1.9			
292	Xanthoxic acid	[M-H]-	C15H22O4	265.14385							7.4E+04	2.6			
293	Pentadecadienyl acetate	[M-H]-	C17H30O2	265.21730	6.7E+04	3.7									
294	N-Succinyl-L-glutamate 5-semialdehyde	[M+Cl]-	C9H13NO6	266.04416					1.6E+04	-1.8					
295	Hexadecatrienal	[M+Cl]-	C16H26O	269.16777	6.1E+04	-2.8		2.1E+04	4.2						
296	2,4'-Dihydroxy-4-methoxydihydrochalcone	[M-H]-	C16H16O4	271.09697						3.1E+04	2.3				
297	Glutaconylcarnitine	[M-H]-	C12H19NO6	272.11442				2.2E+04	-1.7						
298	Methoxychalcone	[M+Cl]-	C16H14O2	273.06888						3.3E+04	-0.4				
299	Ranunculin	[M-H]-	C11H16O8	275.07640				4.5E+04	3.1						
300	Cyperaquinone	[M+Cl]-	C14H10O4	277.02652						3.4E+04	2.9				
301	Thymidine	[M+Cl]-	C10H14N2O5	277.06028				2.3E+04	-2.2						
302	Pantetheine	[M-H]-	C11H22N2O4S	277.12275	2.3E+04	2.4									
303	Linoleic acid	[M-H]-	C18H32O2	279.23357							4.7E+04	-2.2			
304	7-N,N-Dimethylamino-1,2,3,4,5-pentathiocyclooctane	[M+Cl]-	C5H11NS5	279.91979							1.5E+04	-3.2			
305	Oleamide	[M-H]-	C18H35NO	280.26471							2.1E+04	-0.4			
306	Oleic acid	[M-H]-	C18H34O2	281.24860	1.8E+05	1.1		1.9E+05	1.2	1.3E+05	-0.3	2.0E+05	-0.1	6.0E+04	-2.0
307	Stearic acid	[M-H]-	C18H36O2	283.26425	7.9E+05	-1.2	1.6E+06	-0.4	1.9E+05	-0.5	3.4E+05	0.9			
308	C17 Sphingosine	[M-H]-	C17H35NO2	284.25933				3.7E+04	0.6						
309	4'-O-Methylisoflavone	[M+Cl]-	C16H12O3	287.04708							4.6E+04	3.4			
310	Dihydroxy palmitic acid	[M-H]-	C16H32O4	287.22210				2.3E+05	2.4	2.3E+05	1.1				
311	All-trans-13,14-dihydroretinol	[M-H]-	C20H32O	287.23804		1.1E+05	1.2								
312	5-(3'-Carboxy-3'-oxopropenyl)-4,6-dihydroxypicolinate	[M+Cl]-	C10H7NO7	287.99126						2.1E+04	1.4				
313	methyl 4-[2-(2-formyl-vinyl)-3-hydroxy-5-oxo-cyclopentyl]-butanoate	[M+Cl]-	C13H18O5	289.08580				2.3E+05	-3.4						
314	N-(4-Aminobutyl)-L-histidine	[M+Cl]-	C11H18N4O3	289.10760							1.2E+05	-1.1			

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
315 5-O-Methylvisamminol	[M-H]-	C16H18O5	289.10760						1.2E+05	1.9
316 2-Deoxy-2,3-dehydro-N-acetylneuraminic acid	[M-H]-	C11H17NO8	290.08789					2.0E+04	0.9	
317 Phenylbutyrylglutamine	[M-H]-	C15H20N2O4	291.13500						2.0E+04	0.1
318 Tutin	[M-H]-	C15H18O6	293.10396				7.0E+04	-3.1		
319 Gingerol	[M-H]-	C17H26O4	293.17675						3.3E+04	-3.1
320 Khellin	[M+Cl]-	C14H12O5	295.03788	2.9E+04	0.5					
321 L-gamma-glutamyl-L-isoleucine	[M+Cl]-	C11H20N2O5	295.10724						1.7E+04	-2.1
322 Methylaminoadenosine	[M-H]-	C11H16N6O4	295.11639					1.8E+04	-1.2	
323 Beta-Acetoxy-4-oplopanone	[M-H]-	C17H28O4	295.19148	5.2E+04	-3.1					
324 Phosphotyrosine	[M+Cl]-	C9H12NO6P	296.00963	3.0E+04	-2.5					
325 Longifolnine	[M-H]-	C17H15NO4	296.09379					2.1E+04	-3.2	
326 3-Methoxy-4-Hydroxyphenylglycol sulfate	[M+Cl]-	C9H12O7S	299.00001						1.8E+04	-0.8
327 Kaempferol 4'-methyl ether	[M-H]-	C16H12O6	299.05611	3.8E+04	1.3					
328 MG(0:0/14:1(9Z)/0:0)	[M-H]-	C17H32O4	299.22214				1.8E+05	2.2		
329 Methoxybrassinin	[M+Cl]-	C12H14N2OS2	301.02389					2.2E+04	0.9	
330 MG(0:0/14:0/0:0)	[M-H]-	C17H34O4	301.23867					1.2E+05	-0.8	
331 2-Amino-4-oxo-6-(1',2'-dioxopropyl)-7,8-dihydroxypteridine	[M+Cl]-	C9H9N5O5	302.03041					1.7E+04	-2.1	
332 Coumestrol	[M+Cl]-	C15H8O5	303.00657	8.6E+04	-1.1					
333 3',4'-Methylenedioxymurone	[M-H]-	C18H10O5	305.04555		1.7E+05	0.1				
334 Gallocatechin	[M-H]-	C15H14O7	305.06669			2.7E+04	0.0			
335 Isolochocarpin	[M-H]-	C20H18O3	305.11798				4.7E+04	1.1		
336 Eicosatrienoic acid	[M-H]-	C20H34O2	305.24929			3.7E+04	-2.2			
337 Octadecatrienoic acid	[M+Cl]-	C18H24O2	307.14613				2.1E+04	2.9		
338 Cinmethylin	[M+Cl]-	C18H26O2	309.16357						3.2E+04	-2.9
339 Botrydial	[M-H]-	C17H26O5	309.17075	1.8E+05	-1.4					
340 Sauroxine	[M+Cl]-	C17H26N2O	309.17392			4.2E+05	0.0			
341 PC(0:0/3:1(2E))	[M-H]-	C11H22NO7P	310.10524			3.5E+04	2.8			
342 Epsilon-(gamma-Glutamyl)-lysine	[M+Cl]-	C11H21N3O5	310.11752	1.0E+05	-0.2					
343 Jatrophone	[M-H]-	C20H24O3	311.16444						4.7E+04	2.7
344 10,12-octadecadienoic acid	[M+Cl]-	C18H28O2	311.17833		9.5E+05	1.7				
345 Phosphoribosylformylglycineamide	[M-H]-	C8H16N3O8P	312.06018						4.4E+04	0.1
346 4-Oxo-13-cis-retinoate	[M-H]-	C20H25O3	312.17309		1.6E+05	0.8				
347 Octadecanedioic acid	[M-H]-	C18H34O4	313.23799			8.2E+04	1.4			
348 MG(15:0/0:0/0:0)	[M-H]-	C18H36O4	315.25477				5.2E+04	-2.2		
349 Caffeic acid phenethyl ester	[M+Cl]-	C17H16O4	319.07426	4.9E+04	0.8					
350 gamma-L-Glutamyl-L-cysteinyl-beta-alanine	[M-H]-	C11H19N3O6S	320.09218	3.5E+04	2.1					
351 Cytidine-5'-monophosphate	[M-H]-	C9H14N3O8P	322.04457	4.4E+04	2.3					
352 Fructose 1,6-bisphosphate	[M-H]-	C6H14O11P2	322.99386	9.7E+04	0.3					
353 Portulacaxanthin I	[M-H]-	C14H16N2O7	323.08920						1.5E+04	-2.2

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
354 Karwinaphthol B	[M+Cl]-	C17H20O4	323.10463				1.6E+04	2.9		
355 Isoacitretin	[M-H]-	C21H26O3	325.18178			2.9E+05	-2.7			
356 Colnelenic acid	[M+Cl]-	C18H28O3	327.17325	5.8E+05	0.0					
357 3,7,11,15-Tetramethyl-6,10,14-hexadecatrien-1-ol	[M+Cl]-	C20H36O	327.24670					3.2E+04	-2.1	
358 MG(0:0/16:0/0:0)	[M-H]-	C19H38O4	329.27043							
359 Gibberellin A12	[M-H]-	C20H28O4	331.19140				7.0E+04	0.3		
360 Longifolonine	[M+Cl]-	C17H15NO4	332.06971					2.6E+04	-0.6	
361 Heptahydroxyflavone	[M-H]-	C15H10O9	333.02521	5.2E+04	-2.7					
362 Kaempferol 4'-methyl ether	[M+Cl]-	C16H12O6	335.03279		7.9E+04	-0.4				
363 Umbellatine	[M-H]-	C20H18NO4	335.11574						3.0E+04	1.7
364 Maximaisoflavone J	[M-H]-	C21H20O4	335.12986					2.3E+04	-2.9	
365 6-hydroperoxy-4E,8Z,11Z,14Z-eicosatetraenoic acid	[M-H]-	C20H32O4	335.22247						2.3E+04	0.9
366 N-Acetyl-D-glucosamine 6-phosphate	[M+Cl]-	C8H16NO9P	336.02567	6.2E+04	-1.4					
367 S-(Hydroxymethyl)glutathione	[M-H]-	C11H19N3O7S	336.08700					3.5E+04	0.3	
368 (Ac)2-L-lysyl-D-alanine	[M+Cl]-	C13H23N3O5	336.13295			2.7E+04	0.7			
369 Neotenone	[M-H]-	C19H14O6	337.07117					2.9E+04	1.8	
370 5,7-Dimethoxy-8-prenylflavan	[M-H]-	C22H26O3	337.18092	1.8E+05	2.3					
371 Eicosapentaenoic acid	[M+Cl]-	C20H30O2	337.19389				4.0E+04	0.3		
372 1beta,3beta,5alpha,6beta-tetrahydroxyandrostane-17-one	[M-H]-	C19H30O5	337.20205		3.9E+05	-1.1				
373 Disopyramide	[M-H]-	C21H29N3O	338.22294						2.2E+04	2.5
374 Oleoyl glycine	[M-H]-	C20H37NO3	338.27007	1.4E+05	1.6					
375 Aristolochic acid	[M-H]-	C17H11NO7	340.04591			3.2E+04	1.1			
376 Lactosamine	[M-H]-	C12H23NO10	340.12500					1.7E+04	-0.2	
377 Lupinate	[M+Cl]-	C13H18N6O3	341.11344		2.1E+05	2.1				
378 Matricin	[M+Cl]-	C17H22O5	341.11706						5.4E+04	-2.7
379 11,14-eicosadienoic acid	[M+Cl]-	C20H36O2	343.24093		1.3E+05	1.2				
380 Ovalifolin	[M-H]-	C22H18O4	345.11386					1.6E+04	-1.8	
381 O-Arachidonoyl Ethanolamine	[M-H]-	C22H37NO2	346.27515		3.7E+04	-0.9				
382 Triphenyl-1-hexene	[M+Cl]-	C24H24	347.15785			2.6E+04	-1.9			
383 Hydroxybowdichione	[M+Cl]-	C16H10O7	349.01284					2.2E+04	-2.3	
384 N-Acetylthienamycin	[M+Cl]-	C13H18N2O5S	349.06262						2.2E+04	1.2
385 Vincamine	[M-H]-	C21H26N2O3	353.18699					5.8E+04	0.2	
386 5-hydroperoxy-7-[3,5-epidioxy-2-(2-octenyl)-cyclopentyl]-6-heptenoic acid	[M-H]-	C19H30O6	353.19603			2.8E+05	2.6	1.7E+05	-2.1	
387 Spirasine I	[M-H]-	C22H29NO3	354.20707			6.9E+04	1.1			
388 5-O-(1-Carboxyvinyl)-3-phosphoshikimate	[M+Cl]-	C10H13O10P	358.99336						2.1E+04	1.9
389 Dityrosine	[M-H]-	C18H20N2O6	359.12403				2.6E+04	2.3		
390 p-Coumaroyl-D-glucose	[M+Cl]-	C15H18O8	361.07042						1.7E+04	-2.4

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
391 Shikodonin	[M-H]-	C20H26O6	361.16566		3.8E+04	2.5				
392 Europine	[M+Cl]-	C16H27NO6	364.15385				1.4E+05	-1.7		
393 Palmitoyl Serinol	[M+Cl]-	C19H39NO3	364.26289				3.7E+04	-1.4		
394 7'-carboxy-gama-tocotrienol	[M+Cl]-	C20H27O4	366.16107						1.9E+04	-2.0
395 Catechin 5,7,3'-trimethyl ether	[M+Cl]-	C18H20O6	367.09570						3.6E+04	-0.8
396 Hydroxy-PGE1	[M-H]-	C20H34O6	369.22818				2.6E+04	0.2		
397 Docosanedioic acid	[M-H]-	C22H42O4	369.30103		7.0E+04	2.4				
398 10,11-dihydro-12-oxo-LTB4	[M+Cl]-	C20H31O4	370.19125						1.9E+04	1.0
399 3-Epihydroxymugineic acid	[M+Cl]-	C12H20N2O9	371.08548						1.5E+04	2.2
400 1-Acetylaspidoalbidine	[M+Cl]-	C21H26N2O2	373.16869							2.2E+04 0.4
401 9'-Carboxy-gama-chromanol	[M-H]-	C23H35O4	374.24626		3.8E+04	-2.6				
402 Riboflavin	[M-H]-	C17H20N4O6	375.13087				3.4E+04	0.4		
403 PGE1 alcohol	[M+Cl]-	C20H36O4	375.23076	2.9E+04	1.3					
404 Brosimacutin C	[M+Cl]-	C20H22O5	377.11641						2.0E+04	-0.8
405 Eicosanedioic acid	[M+Cl]-	C20H38O4	377.24641		2.8E+05	-1.5				
406 N-(7-Mercaptoheptanoyl)threonine 3-O-phosphate	[M+Cl]-	C11H22NO7PS	378.05459				3.5E+04	0.7		
407 Gibberellic acid	[M+Cl]-	C19H22O6	381.11053						3.3E+04	1.3
408 5-(Heptadec-12-enyl)resorcinol	[M+Cl]-	C23H38O2	381.25658	9.8E+04	1.6					
409 Trihydroxy-7,3',4'-trimethoxyisoflavan	[M+Cl]-	C18H20O7	383.08988				1.5E+04	1.1		
410 24-hydroxy-tetracosanoic acid	[M-H]-	C24H48O3	383.35307		4.9E+04	0.3				
411 S-(Formylmethyl)glutathione	[M+Cl]-	C12H19N3O7S	384.06340				2.4E+04	1.0		
412 O-Feruloylgalactarate	[M-H]-	C16H18O11	385.07727						2.0E+04	0.9
413 5,3',4',5'-Tetramethoxy-6,7-methylenedioxyflavone	[M-H]-	C20H18O8	385.09289		3.1E+04	-2.1				
414 Mercaptoacetyl-Phe-Leu	[M+Cl]-	C17H24N2O4S	387.11573						5.1E+04	-1.7
415 Palmatine	[M+Cl]-	C21H22NO4	387.12471				3.9E+04	-1.1		
416 5-Hydroxy-6-methoxy-3',4'-methylenedioxyfurano[2'',3''':7,8]flavanone	[M+Cl]-	C19H14O7	389.04335		6.0E+04	-2.4				
417 Latifoline	[M-H]-	C20H27NO7	392.17086						2.7E+04	1.6
418 2,2-Dimethyl-3-(4-methoxyphenyl)-4-ethyl-6-(1-pyrrolidinylmethyl)-2H-1-benzopyran-7-ol	[M-H]-	C25H31NO3	392.22312		5.4E+04	0.2				
419 PA(15:0/0:0)	[M-H]-	C18H37O7P	395.22057				6.6E+04	-0.4		
420 N-Arachidonoyl glycine	[M+Cl]-	C22H35NO3	396.23016				2.6E+04	2.4		
421 Hexadecenoylcarnitine	[M-H]-	C23H43NO4	396.31193	2.6E+04	1.5					
422 Gibberellin A19	[M+Cl]-	C20H26O6	397.14172						2.1E+04	1.6
423 Erythronolide B	[M-H]-	C21H38O7	401.25403						2.1E+04	1.1
424 Glucoiberverin	[M-H]-	C11H21NO9S3	406.02982							2.3E+04 1.8
425 Ginkgolide A	[M-H]-	C20H24O9	407.13396						1.9E+04	2.0
426 Cholic acid	[M-H]-	C24H40O5	407.27960						3.0E+04	1.7

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
427	4Z,7Z,10Z,13Z,16Z,19Z,22Z,25Z-octacosaoctaenoic acid	[M-H]-	C28H40O2	407.29555		1.6E+05	-2.4				
428	N-oleoyl glutamine	[M-H]-	C23H42N2O4	409.30718	4.8E+04	0.6					
429	Ovaliflavanone A	[M+Cl]-	C25H28O3	411.17391						1.3E+05	-1.6
430	Trimethyl-5Z,9Z,19Z-docosatrenoic acid	[M+Cl]-	C25H44O2	411.30383			4.3E+04	-0.7			
431	Cryptopleurine	[M+Cl]-	C24H27NO3	412.16779					7.8E+04	1.7	
432	22:2(5Z,9Z)(13Me,17Me,21Me)	[M+Cl]-	C25H46O2	413.31918		3.8E+04	2.8				
433	4-Deoxy-beta-D-gluc-4-enuronosyl-(1,3)-N-acetyl-D-galactosamine	[M+Cl]-	C14H21NO11	414.08086	7.0E+04	-1.6					
434	Briantheine W	[M-H]-	C24H32O6	415.21178			2.5E+04	2.0			
435	Dihydroxycholecalciferol	[M-H]-	C27H44O3	415.32177		5.2E+04	-2.1				
436	beta-Tocopherol	[M-H]-	C28H48O2	415.35786						1.9E+04	0.7
437	Syringaresinol	[M-H]-	C22H26O8	417.15579			2.3E+04	-0.7			
438	N-stearoyl valine	[M+Cl]-	C23H45NO3	418.30941			2.5E+04	-0.2			
439	Lamioside	[M-H]-	C18H28O11	419.15580					2.6E+04	0.2	
440	N-stearoyl histidine	[M-H]-	C24H43N3O3	420.32317					1.8E+04	0.0	
441	8-Cinnamoyl-3,4-dihydro-5,7-dihydroxy-4-phenylcoumarin	[M+Cl]-	C24H18O5	421.08506			2.2E+04	-0.6			
442	Militarinone C	[M-H]-	C26H33NO4	422.23299					5.5E+04	1.6	
443	Quassin	[M+Cl]-	C22H28O6	423.15799		3.8E+04	1.3				
444	Chitobiose	[M-H]-	C16H28N2O11	423.16203		3.8E+04	-1.0				
445	Didrovaltratum	[M-H]-	C22H32O8	423.20244	6.7E+04	-0.6					
446	1alpha,25-dihydroxy-26,27-dinorvitamin D3	[M+Cl]-	C25H40O3	423.26685						2.4E+04	0.7
447	Montanic acid	[M-H]-	C28H56O2	423.42075	4.3E+04	-1.9					
448	Jervine	[M-H]-	C27H39NO3	424.28496				3.0E+04	1.8		
449	Bispyribac acid	[M-H]-	C19H18N4O8	429.10432						2.5E+04	2.0
450	PA(P-16:0/O:0)	[M+Cl]-	C19H39O6P	429.21783		5.3E+04	-1.3				
451	Stanolone benzoate	[M+Cl]-	C26H34O3	429.22020		5.3E+04	0.3				
452	Heptacosanol	[M+Cl]-	C27H56O	431.40174				2.1E+04	1.8		
453	Echimidine	[M+Cl]-	C20H31NO7	432.17893				1.6E+04	1.2		
454	PC(O-12:0/O-1:0)	[M-H]-	C21H46NO6P	438.29833				2.8E+04	1.5		
455	Bleekerine	[M+Cl]-	C23H24N2O5	443.13780				2.1E+04	0.3		
456	(22E)-1alpha-hydroxy-24-oxo-26,27-cyclo-22,23-didehydrovitamin D3	[M+Cl]-	C27H38O3	445.25150		5.0E+04	-1.9				
457	Calophyllolide	[M+Cl]-	C26H24O5	451.13172			2.5E+04	0.1			
458	Calcitriol	[M+Cl]-	C27H44O3	451.29889						1.7E+04	-1.0
459	8-Caffeoyl-3,4-dihydro-5,7-dihydroxy-4-phenylcoumarin	[M+Cl]-	C24H18O7	453.07465		4.8E+04	-2.7				
460	Lactose 6-phosphate	[M+Cl]-	C12H23O14P	457.05194		1.2E+05	-1.8				
461	Eruberin A	[M-H]-	C25H30O8	457.18679	1.8E+04	-0.9					

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
462 CDP-N-methylethanolamine	[M-H]-	C12H22N4O11P2	459.06802						2.9E+04	1.6
463 Rutarin	[M+Cl]-	C20H24O10	459.10544			2.4E+04	2.0			
464 PA(20:3(8Z,11Z,14Z)/0:0)	[M-H]-	C23H41O7P	459.25171		4.8E+04	1.2				
3,7-Dihydroxy-2-[3-(4-hydroxy-3-methylbutyl)-4-methoxyphenyl]-5,6-dimethoxy-4H-1-benzopyran-4-one	[M+Cl]-	C23H26O8	465.13232				2.3E+04	-0.3		
466 PC(0:0/14:0)	[M-H]-	C22H46NO7P	466.29391		4.8E+04	-1.6				
467 Lupinisoflavone N	[M-H]-	C25H28O9	471.16621				1.9E+04	-0.3		
468 Parsonsine	[M+Cl]-	C23H37NO7	474.22706					2.4E+04	-1.4	
469 (-)-Asbestinine 2	[M-H]-	C28H44O6	475.30651		5.2E+04	0.0				
470 Bidenoside B	[M-H]-	C24H30O10	477.17567					6.2E+04	2.0	
471 PG(13:0/0:0)	[M+Cl]-	C19H39O9P	477.20257	3.5E+04	-0.1					
472 Guanosine diphosphate	[M+Cl]-	C10H15N5O11P2	477.99279			4.2E+04	2.0			
473 Delcorine	[M-H]-	C26H41NO7	478.28103		7.2E+04	1.0				
474 sn-3-O-(Geranylgeranyl)glycerol 1-phosphate	[M+Cl]-	C23H41O6P	479.23329					1.9E+04	0.4	
475 Ceramide (d18:1/12:0)	[M-H]-	C30H59NO3	480.44261			3.9E+04	-0.8	1.9E+04	-1.4	
476 Coenzyme M 7-mercaptoheptanoylthreonine-phosphate heterodisulfide	[M-H]-	C13H26NO10PS3	482.03910			6.3E+04	-1.5			
477 17beta-Estradiol 17-(beta-D-glucuronide)	[M+Cl]-	C24H31O8	482.17129		9.9E+04	1.3				
478 PA(20:4(5Z,8Z,11Z,14Z)e/2:0)	[M-H]-	C25H43O7P	485.26829				1.5E+06	-1.9	7.2E+05	0.0
479 Acacetin 7-(2''-acetylglucoside)	[M-H]-	C24H24O11	487.12459		1.2E+05	-1.5				
480 Fucosyllactose	[M-H]-	C18H32O15	487.16744					2.9E+04	-1.2	
481 1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole	[M+Cl]-	C13H19N4O12P	489.04284				3.3E+04	0.6		
482 Deoxylimonic acid D-ring-lactone	[M-H]-	C26H34O9	489.21309			4.1E+04	-0.2			
483 PC(O-16:0/O-1:0)	[M-H]-	C25H54NO6P	494.36082				2.4E+04	1.6		
484 LysoPE(0:0/20:5(5Z,8Z,11Z,14Z,17Z))	[M-H]-	C25H42NO7P	498.26356						2.5E+04	-1.9
485 Pumilaisoflavone B	[M+Cl]-	C27H28O7	499.15227					2.0E+04	1.3	
486 6-Hydroxykaempferol 3,5,7,4'-tetramethyl ether 6-rhamnoside	[M-H]-	C25H28O11	503.15589	2.6E+04	0.7					
487 N-oleoyl tryptophan	[M+Cl]-	C29H44N2O3	503.30375					1.6E+04	1.7	
488 N3'-Acetylto bramycin	[M-H]-	C20H39N5O10	508.26154			3.3E+04	1.7			
489 PC(14:0/2:0)	[M-H]-	C24H48NO8P	508.30435						1.8E+04	0.3
490 Cer(d18:1/14:0)	[M-H]-	C32H63NO3	508.47412				1.7E+04	-1.2		
491 Flemiphyllin	[M+Cl]-	C30H34O5	509.21003	2.4E+04	0.3					
492 6'',6''-Dimethylpyraono[2'',3'':7,8]kaempferol 4'-methyl ether 3-rhamnoside	[M-H]-	C27H28O10	511.16035						1.9E+04	1.2
493 Raucaffricine	[M-H]-	C27H32N2O8	511.20814				2.2E+04	0.9		
494 Luteolin 7-(2''-glucosyllactate)	[M-H]-	C24H24O13	519.11396			3.9E+04	0.9			
495 Cer(d18:0/15:0)	[M-H]-	C33H67NO3	524.50427			4.0E+04	1.0			

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
496 Kaempferol 3,7,4'-tri-O-sulfate	[M-H]-	C15H10O15S3	524.91091	2.6E+04	-0.9					
497 Quercetin 3-rhamnoside-3'-sulfate	[M-H]-	C21H20O14S	527.05010			3.0E+05	1.4			
498 dTDP-L-olivose	[M-H]-	C16H26N2O14P2	531.07865	2.1E+04	-0.2					
499 13-Deoxycarminomycin	[M+Cl]-	C26H29NO9	534.15328						2.0E+04	0.7
500 Lappaol A	[M-H]-	C30H32O9	535.19736	6.1E+04	-0.2					
501 Phytofluene	[M-H]-	C40H62	541.47784				2.3E+04	0.1		
502 2,5-Diaminopyrimidine nucleoside triphosphate	[M+Cl]-	C9H18N5O14P3	547.97622			3.9E+04	-0.9			
503 Phoslactomycin B	[M+Cl]-	C25H40NO8P	548.21866					2.1E+04	-0.2	
504 Quercetin 3-sulfate-7-alpha-arabinopyranoside	[M+Cl]-	C20H18O14S	549.01038						2.1E+04	1.4
505 all-trans-retinyl stearate	[M-H]-	C38H64O2	551.48335		3.7E+05	0.3				
506 Pantethine	[M-H]-	C22H42N4O8S2	553.23713	2.4E+04	-1.8					
507 PI(P-16:0/0:0)	[M-H]-	C25H49O11P	555.29397		2.8E+06	0.9				
508 Cucurbitacin E	[M-H]-	C32H44O8	555.29634		2.8E+06	1.6				
509 Cucurbitacin P	[M+Cl]-	C30H48O7	555.31034				2.7E+04	-1.7		
510 Linoleoylglycerophosphocholine	[M+Cl]-	C26H51NO7P	555.31034				2.7E+04	-1.1		
511 5,7,2',3',4'-Pentahydroxy-3,6-dimethoxyflavone 7-glucoside	[M+Cl]-	C23H24O14	559.08601	2.9E+04	-0.5					
512 PG(P-20:0/0:0)	[M+Cl]-	C26H53O8P	559.31735					2.4E+04	-0.3	
513 3-Hydroxy-L-tyrosyl-AMP	[M+Cl]-	C19H23N6O10P	561.09073		1.9E+05	1.7				
514 Musaroside	[M-H]-	C30H44O10	563.28617		1.2E+05	-0.5				
515 N-[(3a,5b,7b)-7-hydroxy-24-oxo-3-(sulfoxy)cholan-24-yl]-Glycine	[M+Cl]-	C26H43NO8S	564.24034	2.4E+04	-1.4					
516 Ginkgetin	[M-H]-	C32H22O10	565.11402		9.2E+04	1.0				
517 dTDP-L-olivose	[M+Cl]-	C16H26N2O14P2	567.05533	4.7E+04	-1.3					
518 Apigenin 7-methyl ether 5-(6''-malonylglucoside)	[M+Cl]-	C25H24O13	567.09088					3.4E+04	0.4	
519 Corotoxigenin-3-o-alpha-L-rhamnopyranoside	[M+Cl]-	C29H42O9	569.25228	3.3E+04	-0.3					
520 PS(22:4(7Z,10Z,13Z,16Z)/0:0)	[M-H]-	C28H48NO9P	572.29924						3.4E+04	0.3
521 Cer(d18:1/19:0)	[M-H]-	C37H73NO3	578.55105						4.9E+04	1.2
522 Vitamin K2	[M-H]-	C41H56O2	579.41991						2.8E+04	1.5
523 Dihydrozeatin-9-N-glucoside-O-glucoside	[M+Cl]-	C22H35N5O11	580.20307				1.9E+04	-0.6		
524 Cer(t18:0/16:0)	[M+Cl]-	C34H69NO4	590.49206		1.3E+05	1.0				
525 Ceramide (d18:1/20:0)	[M-H]-	C38H75NO3	592.56705				2.0E+04	0.6	3.1E+04	1.5
526 Dalpanol O-glucoside	[M+Cl]-	C29H34O12	609.17443	2.5E+04	0.3					
527 DG(15:0/18:4(6Z,9Z,12Z,15Z)/0:0)	[M+Cl]-	C36H62O5	609.42987						2.8E+04	-1.2
528 Myricetin 3-sambubioside	[M-H]-	C26H28O17	611.12457			3.0E+04	1.3			
529 Naringenin 7-(2-p-Coumaroylglucoside)	[M+Cl]-	C30H28O12	615.12748		8.4E+04	2.8				
530 Apigenin 5-rhamnosyl-(1->2)-(6''-acetylglucoside)	[M-H]-	C29H32O15	619.16661						2.8E+04	0.4
531 Cer(d18:0/22:0)	[M-H]-	C40H81NO3	622.61437		5.2E+04	-2.0				
532 Glycochenodeoxycholic acid 3-glucuronide	[M-H]-	C32H51NO11	624.33942			7.9E+04	-0.8			
533 Ubiquinone-6	[M+Cl]-	C39H58O4	625.40219						3.2E+04	1.2

# Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm W2020 ^c	ppm B2020 ^c	ppm R2021 ^c	ppm W2021 ^c	ppm B2021 ^c	ppm
534 Quercetin 3-(4''-acetylramnoside)-7-rhamnoside	[M-H]-	C29H32O16	635.16251			3.9E+04	-1.2			
535 Cer(t18:0/24:0)	[M-H]-	C42H85NO4	666.64024				2.1E+04	0.5		
536 Acacetin 7-(4'''-acetylrutinoside)	[M+Cl]-	C30H34O15	669.15973			2.8E+04	-0.8			
537 PE(14:1(9Z)/P-18:1(11Z))	[M-H]-	C37H70NO7P	670.48163				3.2E+04	0.1		
538 Purpureacin-1	[M+Cl]-	C37H66O8	673.44517	4.1E+04	0.7					
539 Gnididin	[M+Cl]-	C37H44O10	683.26330					1.9E+04	-0.7	
540 DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	[M-H]-	C45H66O5	685.48341			3.9E+04	0.5			
541 PG(14:0/16:0)	[M-H]-	C36H71O10P	693.47087					3.4E+05	0.5	
542 Tauroolithocholic acid 3-glucuronide	[M+Cl]-	C32H53NO11S	694.30269					4.4E+04	0.9	
543 Ecdysone palmitate	[M-H]-	C43H74O7	701.53534				2.4E+04	1.2		
544 CE(19:0)	[M+Cl]-	C46H82O2	701.60088		4.1E+04	1.1				
545 PA(16:1(9Z)/22:4(7Z,10Z,13Z,16Z))	[M-H]-	C41H71O8P	721.48213					3.0E+04	-1.0	
546 Kaempferol 3-rhamnosyl-(1->4)-rhamnoside-7-rhamnoside	[M-H]-	C33H40O18	723.21460			3.6E+04	-0.6			
547 Naringenin 7-O-(2'',6''-di-O-alpha-rhamnopyranosyl)-beta-glucopyranoside	[M-H]-	C33H42O18	725.22936				3.5E+04	0.7		
548 PG(12:0/18:2(9Z,12Z))	[M+Cl]-	C36H67O10P	725.41754			5.6E+04	-1.3			
549 Ubiquinone-8	[M-H]-	C49H74O4	725.55191					3.6E+04	-0.7	
550 DG(19:0/22:2(13Z,16Z)/0:0)[iso2]	[M+Cl]-	C44H82O5	725.58563		1.0E+05	-1.9				
551 Scillarenin 3-O-glucosylrhamnoside	[M+Cl]-	C36H52O13	727.31118			1.6E+05	-1.4			
552 PG(13:0/20:4(5Z,8Z,11Z,14Z))	[M-H]-	C39H69O10P	727.45651				1.6E+05	-1.3		
553 PA(17:0/21:0)	[M-H]-	C41H81O8P	731.55963	5.7E+04	-0.3					
554 PC(16:0/16:0)	[M-H]-	C40H80NO8P	732.55538					2.3E+04	-0.7	
555 PE(O-16:1(1Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M-H]-	C43H74NO7P	746.51325						4.9E+04	-0.3
556 19'-Hexanoyloxyisomytiloxanthin	[M+Cl]-	C46H64O6	747.43969		4.2E+04	0.5				
557 UDP-N-acetylmuramoyl-L-alanine	[M-H]-	C23H36N4O20P2	749.13254	7.2E+04	-0.8					
558 Luteolin 7-glucuronide-3',4'-dirhamnoside	[M-H]-	C33H38O20	753.18916			5.2E+04	-1.1			
559 SM(d18:0/20:2(11Z,14Z))	[M-H]-	C43H83N2O6P	753.59160		3.4E+04	1.4				
560 PA(16:0/22:1(11Z))	[M+Cl]-	C41H79O8P	765.52066	7.0E+04	0.1					
561 PC(O-16:0/O-18:1(9Z))	[M+Cl]-	C42H86NO6P	766.58966						3.0E+04	-1.3
562 PC(15:0/20:3(5Z,8Z,11Z))	[M-H]-	C43H80NO8P	768.55557						3.0E+04	-0.9
563 PA(20:3(8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M-H]-	C45H71O8P	769.48176						3.1E+04	-0.5
564 1-(6-[3]-ladderane-hexanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycero-3-phospho-(1'-sn-glycerol)	[M-H]-	C44H73O9P	775.49259						2.6E+04	-0.8
565 Patellamide A	[M+Cl]-	C35H50N8O6S2	777.29953						1.3E+05	-0.8
566 Cyanidin 3,5-di-(6-malonylglucoside)	[M-H]-	C33H35O22	782.15472		3.0E+04	-0.6				
567 Pfaffoside A	[M+Cl]-	C40H60O13	783.37374			3.0E+04	-1.2			
568 PI(P-16:0/16:1(9Z))	[M-H]-	C41H77O12P	791.50893			3.0E+04	-1.2			
569 Delphinidin 3-(2-xylosylgalactoside)-5-glucoside	[M+Cl]-	C32H39O21	794.16791				2.7E+04	-0.2		

#	Putative Annotation ^a	Ion	Formula	m/z _{Theo.} ^b	R2020 ^c	ppm	W2020 ^c	ppm	B2020 ^c	ppm	R2021 ^c	ppm	W2021 ^c	ppm	B2021 ^c	ppm
570	PA(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M+Cl]-	C45H69O8P	803.44198											4.3E+04	0.5
571	PS(13:0/22:4(7Z,10Z,13Z,16Z))	[M+Cl]-	C41H72NO10P	804.45879			2.5E+04	-0.8								
572	PG(O-18:0/21:0)	[M-H]-	C45H91O9P	805.63279			2.4E+04	0.5								
573	PG(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M-H]-	C45H77O10P	807.51816			2.0E+04	-2.0								
574	PG(15:0/22:4(7Z,10Z,13Z,16Z))	[M+Cl]-	C43H77O10P	819.49529									1.9E+04	-0.6		
575	PG(17:0/22:0)	[M-H]-	C45H89O10P	819.61206			9.2E+04	-1.5								
576	PG(O-18:0/20:3(8Z,11Z,14Z))	[M+Cl]-	C44H83O9P	821.54601							3.3E+04	1.1				
577	5-Methyl-5,6,7,8-tetrahydromethanopterin	[M+Cl]-	C31H47N6O16P	825.24802			2.1E+04	0.6								
578	PG(18:1(9Z)/22:2(13Z,16Z))	[M-H]-	C46H85O10P	827.58076	3.6E+04	0.5										
579	PG(16:0/22:1(11Z))	[M+Cl]-	C44H85O10P	839.55744			2.9E+04	2.4								
580	Bayogenin 3-O-cellobioside	[M+Cl]-	C42H68O15	847.42499											1.7E+04	0.3
581	PS(O-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M-H]-	C48H84NO9P	848.58109			3.3E+04	-2.1								
582	Palargonidin 3-(6''-ferulylglucoside)-5-(6'''-malonylglucoside)	[M-H]-	C40H41O21	856.20695											2.4E+04	-0.2
583	PS(O-18:0/22:4(7Z,10Z,13Z,16Z))	[M+Cl]-	C46H84NO9P	860.55854							4.4E+04	-0.9				
584	PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	[M+Cl]-	C48H84NO8P	868.56286			2.0E+04	2.2								
585	PI(O-18:0/20:5(5Z,8Z,11Z,14Z,17Z))	[M-H]-	C47H83O12P	869.55453											1.8E+04	0.5
586	PG(19:0/22:4(7Z,10Z,13Z,16Z))	[M+Cl]-	C47H85O10P	875.55744			2.0E+04	-2.5								
587	Guanosine tetraphosphate adenosine	[M+Cl]-	C20H28N10O20P	887.01258			2.9E+04	2.2								
588	PC(20:2(11Z,14Z))	[M+Cl]-	C50H84NO8P	892.56338							4.8E+04	-0.6				
589	Pelargonidin 3-glucoside-7-(6-(4-(glucosyl)-p-hydroxybenzoyl)glucoside)	[M+Cl]-	C40H45O22	912.20966									4.8E+04	0.0		
590	4-Isopropenyl-2-oxy-cyclohexanecarboxyl-CoA	[M-H]-	C31H48N7O18P3	930.19201									2.0E+04	-0.4		
591	TG(17:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z)/20:5(5Z,8Z,11Z,14Z,17Z))	[M+Cl]-	C60H92O6	943.65879			3.1E+04	-2.2								
592	Pentaglutamyl folate	[M-H]-	C39H47N11O18	956.30308							3.4E+04	-0.3				
593	PI(20:1(11Z)/22:4(7Z,10Z,13Z,16Z))	[M+Cl]-	C51H89O13P	975.57287							3.7E+04	0.6				
594	Isorhamnetin 3-rhamnosyl-(1->2)-gentiobiosyl-(1->6)-glucoside	[M+Cl]-	C40H52O26	983.24408	6.3E+04	-0.4										

^a CE Cholesteryl ester; Cer Ceramide; DG Diacylglycerol; MG Monoacylglycerol; PA Phosphatidic acid; PC Phosphatidylcholine; PE Phosphatidylethanolamine; PG Glycerophospholipids; PGE1 Prostaglandin E1; PI Phosphatidylinositol; PS Phosphatidylserine; SM Sphingomyelin; TG Triacylglycerol.

^b Theoretical mass

^c R stands for red tunica, W stands for white tunica and B stands for bulb.