

Supplementary Figure 1 HQD can reshape the intestinal tissue microenvironment of loperamide-induced STC mice. **A:** Comparison of the average optical density of Claudin-1 in mice between the CON, STC, and HQD groups. ^a*P* < 0.0001, STC vs CON; ^b*P* < 0.001, STC vs HQD; **B:** Representative images of the immunohistochemical expression levels of Claudin-1 in the colonic mucosa of patients from the CON and STC groups were shown. The black scale bar represents 50 μm; **C:** Comparison of the average optical density of Claudin-1 in patients between the CON and STC groups. ^a*P* < 0.0001, STC vs CON; **D:** Comparison of the average optical density of MUC2 in mice between the CON, STC, and HQD groups. ^a*P* < 0.0001, STC vs CON; ^b*P* < 0.001, STC vs HQD; **E:** Representative images of the immunohistochemical expression levels of MUC2 in the colonic mucosa of patients from the CON and STC groups were shown. The black scale bar represents 50 μm; **F:** Comparison of the average optical density of MUC2 in patients between the CON and STC groups. ^a*P* < 0.0001, STC vs CON; **G:** The UMAP plot illustrates the dynamic changes of major cell types among the CON, STC, and HQD groups; **H:** The stacked bar chart illustrates the dynamic changes of major cell types between the CON, STC, and HQD groups; **I:** GSEA enrichment for gene sets in epithelial cells comparing STC vs. HQD group. NES, normalize enrichment score.; **J:** GSEA enrichment for gene sets in different cell types comparing STC vs. HQD group. NES, normalize enrichment score.

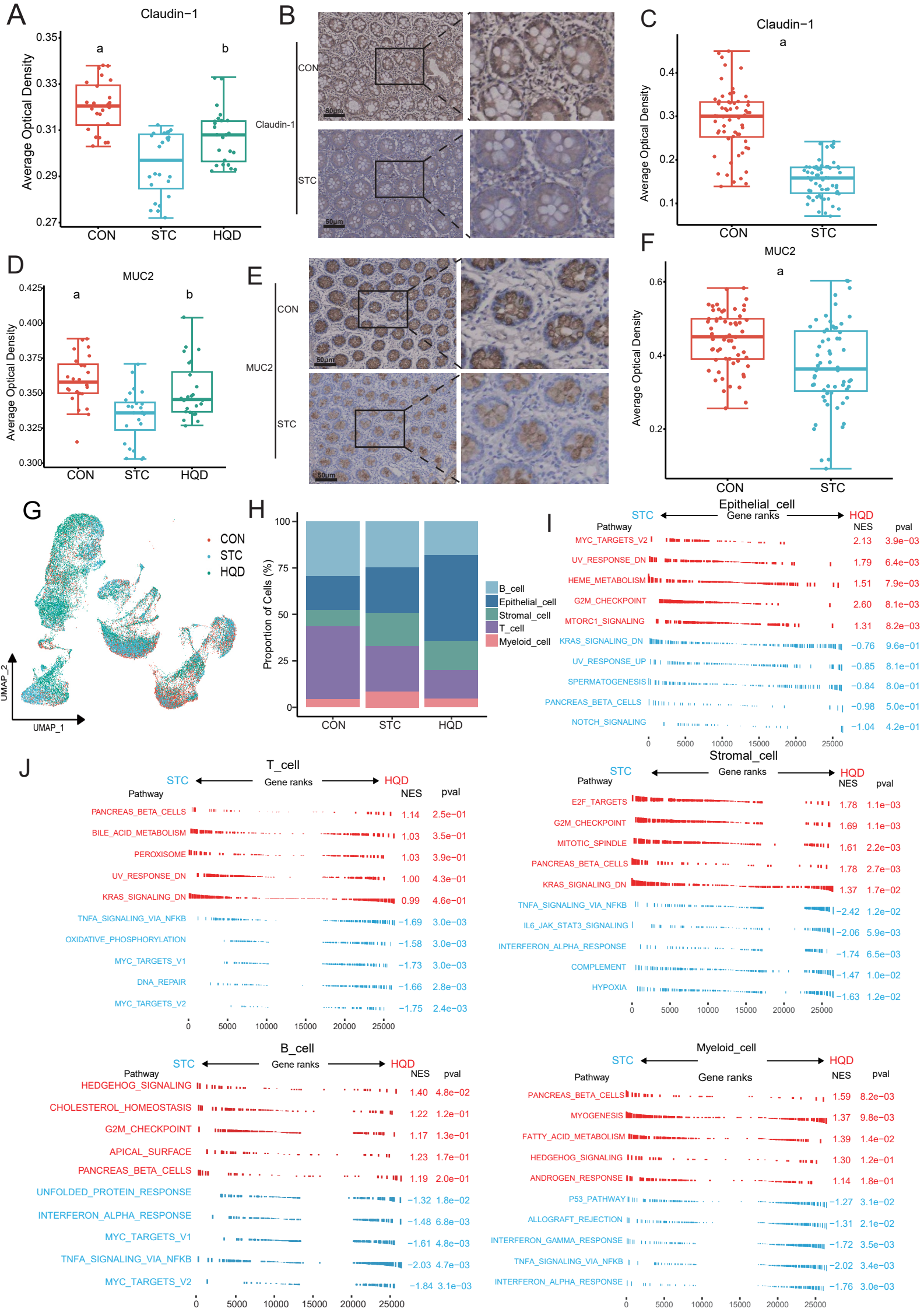
Supplementary Figure 2 Heterogeneity of epithelial cells. **A:** The cell distribution of the epithelial cell in ST-seq data. There are three ST-seq samples from CON, STC, and HQD groups; **B:** Violin plots showing the MP score in all epithelial subtypes.

Supplementary Figure 3 HQD treatment enhances the proliferative activity of goblet cells. **A:** Spatial expression of the E2F targets pathway in epithelial cell regions of a CON sample (left), an STC sample (middle), and an HQD sample (right); **B:** Violin plots showing the E2F targets pathway score in goblet cells regions from three ST-seq samples; **C:** Representative images of the immunohistochemical expression levels of P65 in the colonic mucosa of patients from the CON and STC groups were shown. The black scale bar represents 50 μm; **D:** Comparison of the average optical density of P65 in patients between the CON and STC groups. ^a*P* < 0.0001, STC vs CON.

Supplementary Figure 4 Regulating the differentiation pathway of intestinal stem cells. **A:**

DEGs of ISC_C1 cells between STC and HQD group. Blue dot: DEGs in STC group; Red dot: DEGs in HQD group. DEGs were defined as those with a P -value < 0.05 from the Wilcoxon Rank Sum test and a log2 fold change > 0.25 ; **B**: Violin plots showing the E2F TARGETS, WNT BETA CATENIN SIGNALING, and HALLMARK NOTCH SIGNALING pathway score in ISC cells regions from three ST-seq samples; **C**: Pseudotime trajectory analysis of epithelial cell. Trajectory is colored by CytoTRACE scores; **D**: Violin plots showing the WNT and NOTCH pathway score in ISC cell from scRNA-seq data.

Supplementary Figure 5 High expression of aquaporin in STC group. **A**: DEGs between enterocyte_C1 and enterocyte_C3. Blue dot: DEGs in enterocyte_C3 cells; Red dot: DEGs in enterocyte_C1 cells. DEGs were defined as those with a P -value < 0.05 from the Wilcoxon Rank Sum test and a log2 fold change > 0.25 ; **B**: Representative images of the immunohistochemical expression levels of AQP3 in the colonic mucosa of patients from the CON and STC groups were shown. The black scale bar represents 50 μm ; **C**: Comparison of the average optical density of AQP3 in patients between the CON and STC groups. $^aP < 0.0001$, STC vs CON.

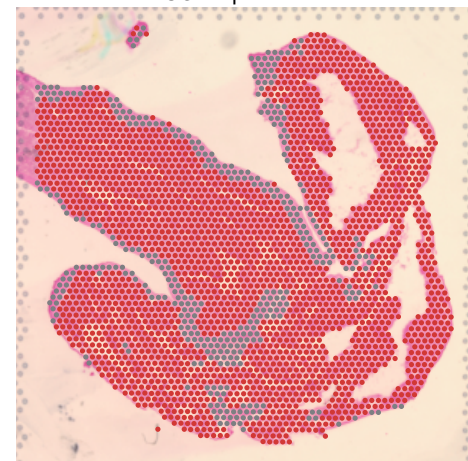


A

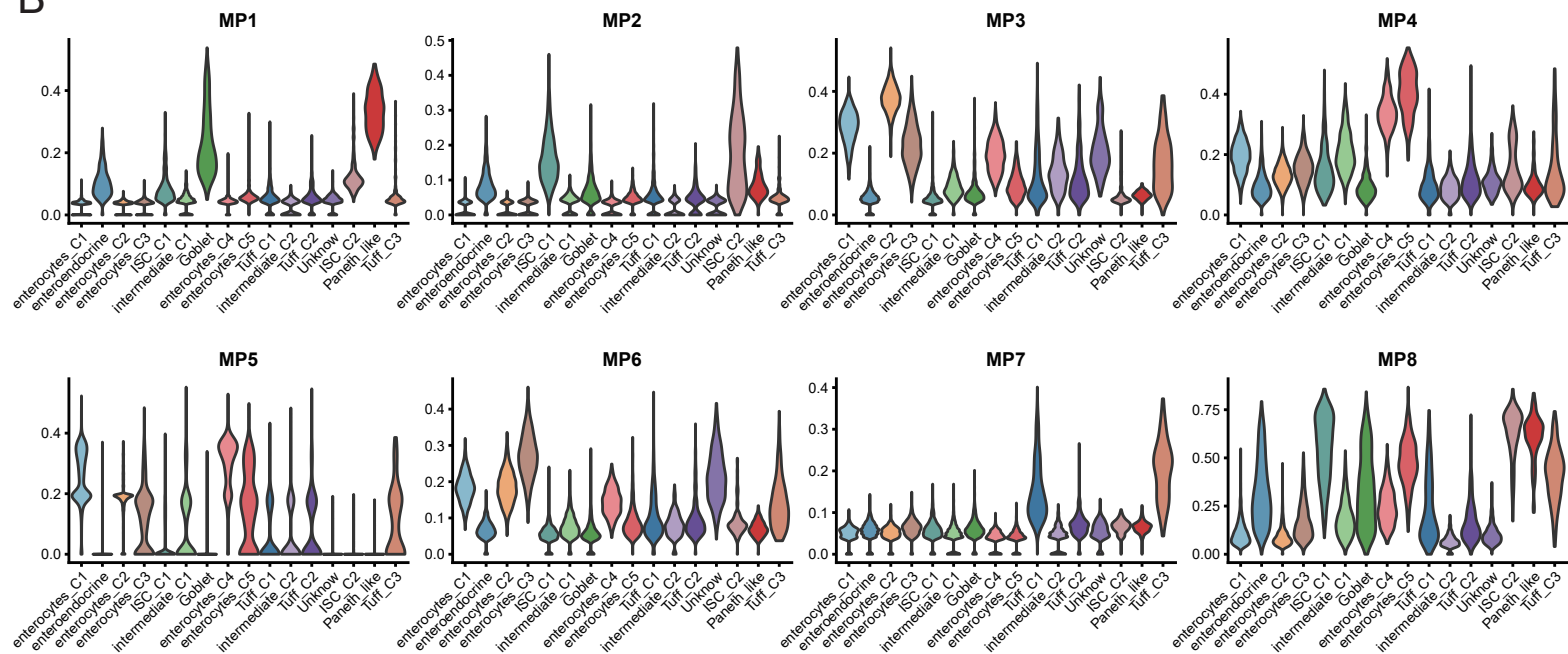
CON Epithelial-cell

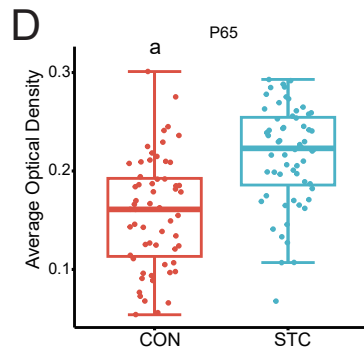
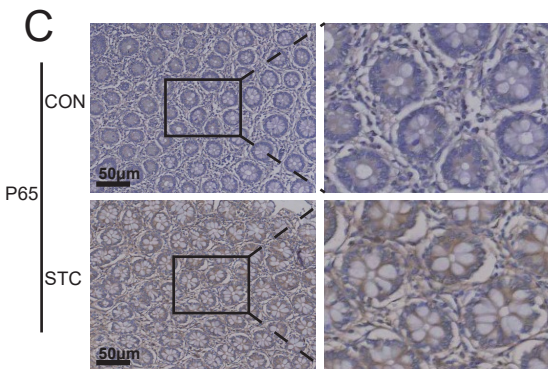
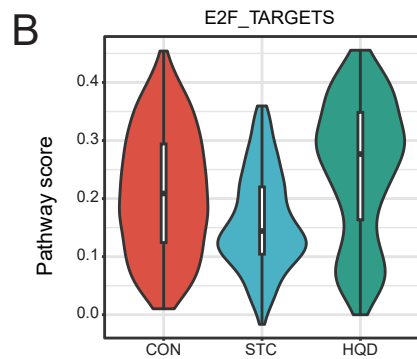
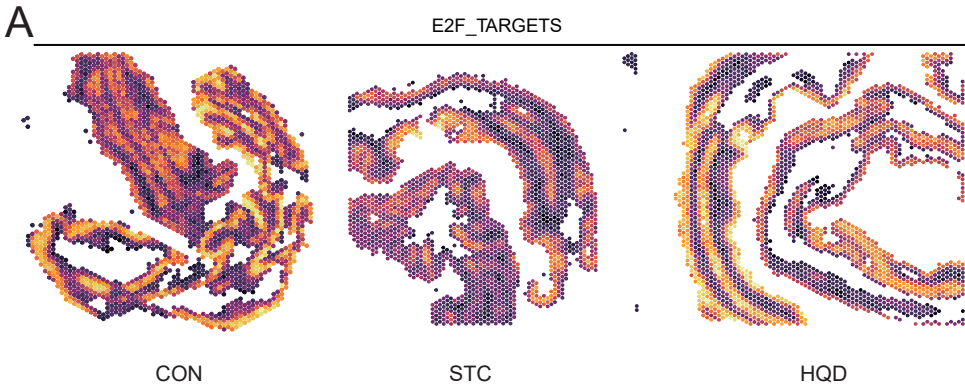
STC Epithelial-cell

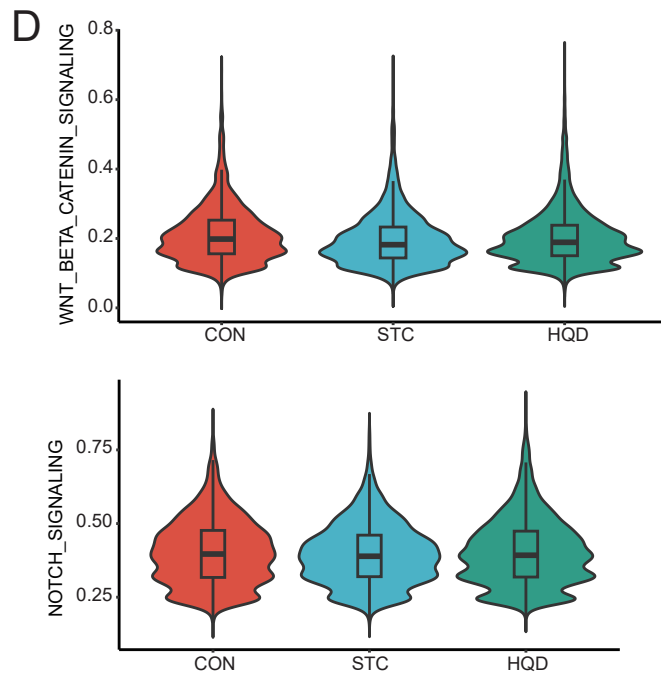
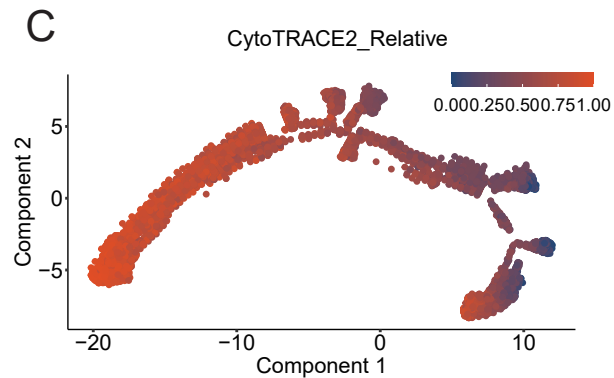
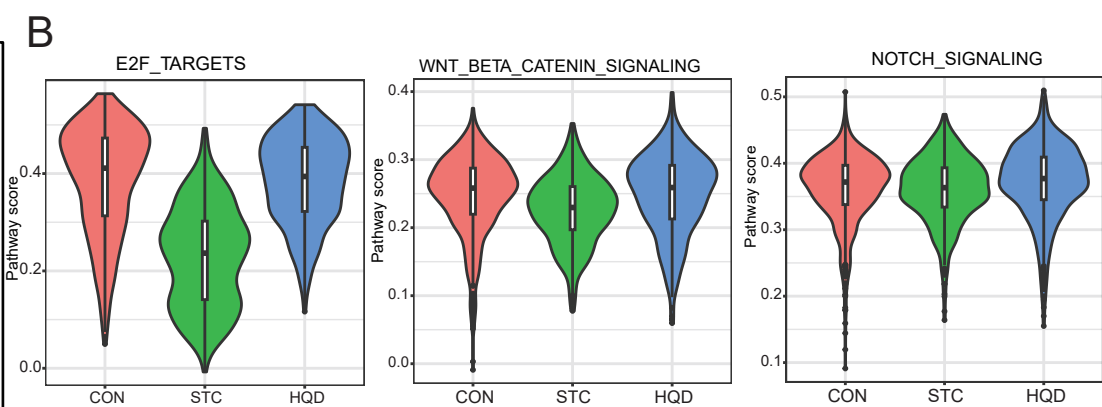
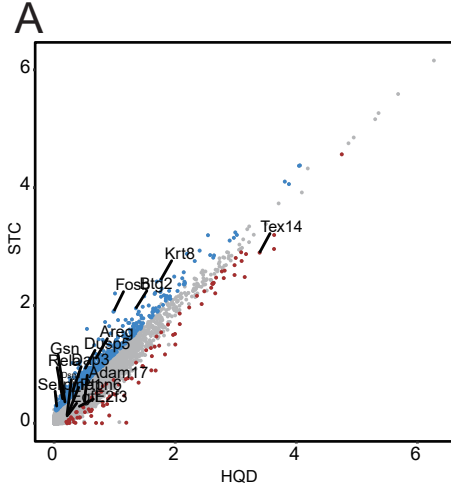
HQD Epithelial-cell

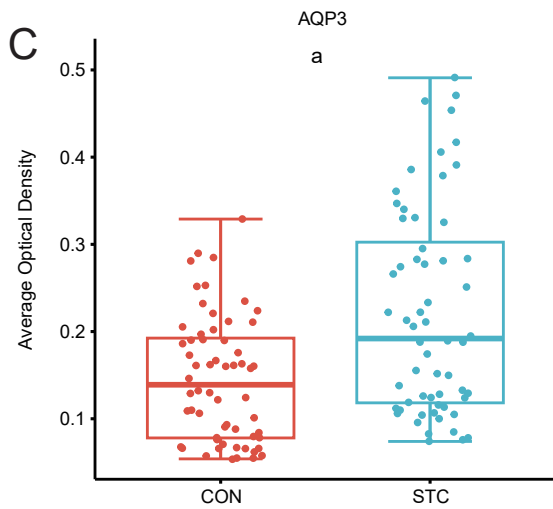
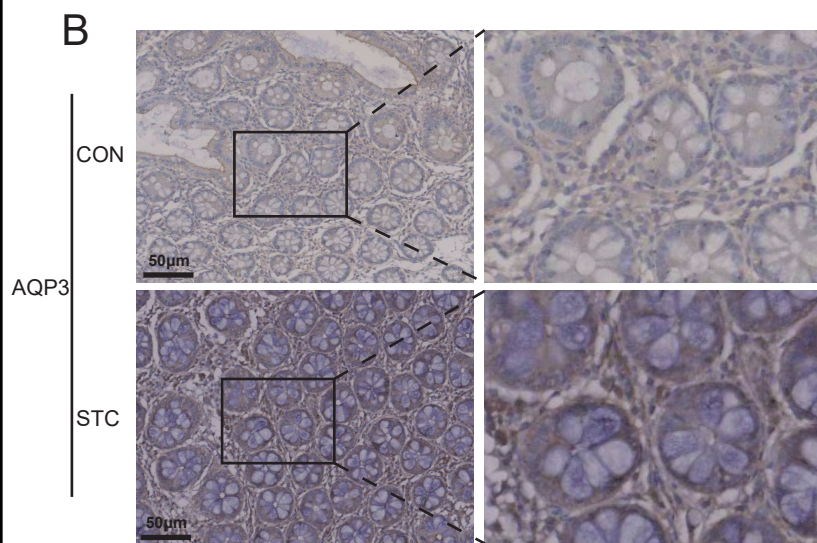
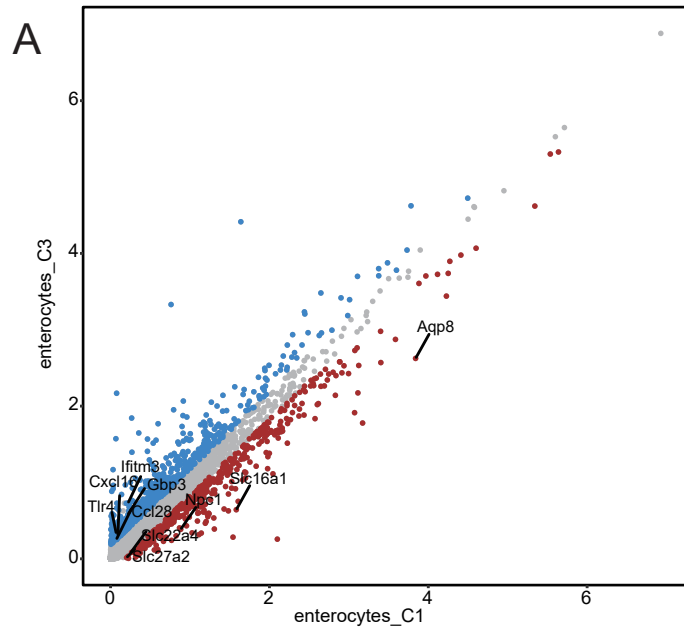


B









Tabel S1 HQD Substances detected by LC-MS in positive and negative modes.

Peak Num ber	m/z	RT mi n	Formula	pp m	compound name	adduct
1	166.0 857	2.2 6	C ₁₀ H ₁₂ N ₂ O ₃	0. 6	N-Carbamoyl-L-phenylalanine	[M+H-CHNO] ⁺
2	188.0 702	2.9 6	C ₁₁ H ₁₁ NO ₃	0. 3	3-Indolylactic acid	[M+H-H ₂ O] ⁺
3	177.0 544	3.1 6	C ₂₆ H ₃₃ NO ₁₂	0. 5	Simmondsin 2'-ferulate	[M+H-C ₁₆ H ₂₅ NO ₉] ⁺
4	177.0 545	3.6 1	C ₂₁ H ₂₀ O ₁₀	0. 2	Cimicifuga acid A	[M+H-C ₁₁ H ₁₂ O ₇] ⁺
5	153.1 274	3.9 7	C ₁₀ H ₁₆ O	0. 1	(1S)-Pulegone	[M+H] ⁺
6	491.1 196	4.5 5	C ₂₂ H ₂₂ O ₁₀	0. 3	Calycosin-7-o-beta-d-glucoside	[M+HCO ₂] ⁻
7	289.1 757	4.7 4	C ₁₆ H ₂₆ O ₃	5. 8	Tetranor-12(R)-HETE	[M+Na] ⁺
8	533.1 288	5.3 1	C ₂₅ H ₂₄ O ₁₃	0. 7	6''-O-Malonylglycitin	[M+H] ⁺
9	475.1 245	6.1 8	C ₂₂ H ₂₂ O ₉	0. 2	Ononin	[M+HCO ₂] ⁻
10	263.1 289	7.0 4	C ₁₅ H ₂₀ O ₄	0. 1	(+)-Absciscic acid	[M-H] ⁻
11	283.0 612	7.2 7	C ₁₆ H ₁₂ O ₅	1. 4	Calycosin	[M-H] ⁻
12	267.0 662	9.7 1	C ₁₆ H ₁₂ O ₄	1. 2	Formononetin	[M-H] ⁻
13	403.1	10.	C ₂₁ H ₂₂ O ₈	0	Nobiletin	[M+H] ⁺

	386	63				
14	433.1 492	10. 99	C22H24O9	0. 5	Hibiscetin heptamethyl ether	[M+H] ⁺
15	373.1 281	11. 38	C20H20O7	2	Tangeritin	[M+H] ⁺
16	189.0 761	4.7 9	C8H14O5	2. 1	3-Hydroxysuberic acid	[M-H] ⁻
17	579.1 72	5.0 4	C27H32O14	0. 1	Narirutin	[M-H] ⁻
18	609.1 825	5.3 3	C28H34O15	0	Hesperidin	[M-H] ⁻
19	298.1 083	5.5 8	C17H17NO4	0. 8	N-trans- Coumaroyloctopamine	[M-H] ⁻
20	187.0 97	6.1 4	C9H16O4	2. 6	Azelaic acid	[M-H] ⁻
21	137.0 234	6.4 4	C10H12O3	6. 7	Isopropyl m- hydroxybenzoate	[M-H- C3H6] ⁻
22	593.1 876	6.8 8	C28H34O14	0. 6	Didymin	[M-H] ⁻
23	329.2 332	9.9 4	C18H34O5	0	9-Octadecenoic acid, 5,8,11-trihydroxy-	[M-H] ⁻
24	871.4 692	11. 29	C43H70O15	1. 3	Astragaloside II	[M+HCO2] -
25	311.2 227	11. 87	C18H32O4	0. 3	(9Z,12E)-15,16- Dihydroxyoctadeca-9,12- dienoic acid	[M-H] ⁻
26	295.2 277	13. 45	C18H32O3	1. 3	9(S)-HODE	[M-H] ⁻
	91.05 47	1.3 5	C7H8O	5. 3	Phenylcarbinol	[M+H- H2O] ⁺
	91.05	9.2	C7H9N	5.	m-Toluidine	[M+H- H2O] ⁺

47	1		1		NH3]+
95.04	1.3	C6H8O2	5	Sorbic acid	[M+H-H2O]+
96	4				
95.08	3.9	C7H12O	4.9	exo-Norborneol	[M+H-H2O]+
6	7				
96.05	1.1	C4H5N3	4.1	2-Aminopyrazine	[M+H]+
61	4				
100.0	2.2	C16H23NO3	3.6	1-(2-Allylphenoxy)-3-morpholinopropan-2-ol	[M+H-C11H14O2]+
763	9				
100.0	2.5	C5H9NO	4.6	6-Paradol	[M+H]+
764	3				
101.0	0.5	C5H8O2	4	3-Methyl-.gamma.-butyrolactone	[M+H]+
602	7				
101.0	4.5	C5H8O2	4.1	3,3-Dimethylacrylic acid	[M+H]+
602					
102.1	7.9	C6H15N	3.9	Ethyl(sec-butyl)amine	[M+H]+
281	1				
103.0	2.2	C9H8FN3	3.9	1-Cyclopropyl-6-fluorobenzotriazole	[M+H-CH2FN3]+
547	6				
104.1	0.8	C5H13NO	3.4	2-(Dimethylamino)propanol	[M+H]+
073	2				
105.0	2.9	C13H13N3OS	3.6	Ketone, 2-(allylamino)-4-amino-5-thiazolyl phenyl	[M+H-C6H9N3S]+
337					
105.0	3.6	C17H15N3OS	4	N-(5-Phenethyl-[1,3,4]thiadiazol-2-yl)benzamide	[M+H-C10H11N3S]+
342	1				
105.0	2.6	C22H25NO	4.2	JWH 251 3-methylphenyl isomer	[M+H-C14H17NO]+
702	5				

105.0 702	7.0 5	C8H10O3S	3. 5	3,4-Xylenesulfonic acid	[M+H- H2SO3]+
105.0 702	9.9 5	C10H11N3S	3. 2	4-(2-Phenylethyl)-4H- 1,2,4-triazole-3-thiol	[M+H- C2H3N3S] +
105.0 703	3.9 7	C16H16O4	3. 5	2',6'-Dihydroxy 4'- methoxydihydrochalcone	[M+H- C8H8O4]+
105.0 704	9.7 9	C15H16O2	3. 8	3-Methoxy-5-(2- phenylethyl)phenol	[M+H- C7H8O2]+
107.0 495	2.2 6	C19H22O4	4. 4	1-(3,4-Dihydroxyphenyl)- 7-(4- hydroxyphenyl)heptan-3- one	[M+H- C12H16O3] +
107.0 495	3.2 1	C13H12FNO	4	2-[(4- Fluoroanilino)methyl]pheno l	[M+H- C6H6FN]+
107.0 611	18. 37	C6H6N4	4. 3	1H-Benzotriazol-6-amine	[M+H- N2]+
107.0 857	10. 72	C9H10O	3. 9	3,4-Dimethylbenzaldehyde	[M+H- CO]+
107.0 859	7.0 5	C10H16O	3. 5	Carveol	[M+H- C2H6O]+
107.0 86	3.9 7	C10H16O	4. 5	.alpha.,.beta.-Thujone	[M+H- C2H6O]+
107.0 861	4.6	C10H16O	3. 7	1,2-Epoxy limonene	[M+H- C2H6O]+
108.0 689	18. 38	C12H12N2O2S	2. 7	Benzenesulfonanilide, 3'- amino-	[M+H- C6H5SO2] +
109.0 289	1.1 7	C6H10O5	3. 5	3-Hydroxy-3- methylglutaric acid	[M+H- 3H2O]+
109.0	7.0	C8H8O3	3	3,2-Cresotic acid	[M+H-

651	5				CO2]+
109.0 774	17. 8	C13H13N3O	3. 4	Benzanilide, 3,4'-diamino-	[M+H- C7H5NO]+
109.0 785	18. 52	C6H8N2	1. 5	Phenylhydrazine	[M+H]+
109.1 014	10. 92	C14H26O	3. 4	3- Oxabicyclo[10.3.0]pentadecane	[M+H- C6H14O]+
109.1 015	4.6 8	C8H16O2	3. 7	2-(3-Methyloxan-4-yl)ethanol	[M+H- 2H2O]+
109.1 015	9.9	C12H22O	3. 1	1-(3,3-Dimethylnorbornan-2-yl)propan-1-ol	[M+H- C4H10O]+
109.1 017	4.4 3	C9H14O2	2. 8	4-Oxo-2-nonenal	[M+H- CH2O2]+
110.0 604	4.3 7	C13H11NO2	4. 3	4-(2-Pyridinylmethoxy)benzaldehyde	[M+H- C7H4O]+
110.0 716	0.7 5	C11H17N3O4	3	N-.alpha.-(tert-Butoxycarbonyl)-L-histidine	[M+H- C6H10O4] +
111.0 446	2.2 2	C7H6O3	2. 8	2,6-Dihydroxybenzaldehyde	[M+H- CO]+
112.0 51	0.9 9	C9H13N3O5	3. 5	Cytidine	[M+H- C5H8O4]+
112.0 762	4.7 4	C10H18N2O	3	1-(4-Piperidinylcarbonyl)pyrrolidine	[M+H- C4H9N]+
112.0 873	2.0 4	C12H12Cl2N4O	3. 8	N-(3,4-Dichlorophenyl)-N'-[2-(1H-imidazol-4-yl)ethyl]urea	[M+H- C7H3Cl2NO]+
112.0 874	1.4 1	C12H20N4O	3	N-Cyclohexyl-N'-[2-(1H-imidazol-4-yl)ethyl]urea	[M+H- C7H11NO]

					+
113.0 237	1.7 1	C5H4O3	3. 3	2-Furoic acid	[M+H] ⁺
113.0 353	1.2 5	C4H4N2O2	2. 5	Uracil	[M+H] ⁺
113.0 605	2.1	C6H10O3	3. 3	4-Methyl-2-oxovaleric acid	[M+H- H2O] ⁺
114.0 665	0.9 9	C4H7N3O	2. 8	Creatinine	[M+H] ⁺
114.0 92	18. 59	C6H12FNO	3. 4	4-Piperidinemethanol, 4-fluoro-	[M+H- HF] ⁺
114.0 925	19. 16	C6H11NO	3. 4	3,3-Dimethyl-2-pyrrolidone	[M+H] ⁺
115.0 393	2.1 1	C5H6O3	2. 9	Methyl tetronate	[M+H] ⁺
115.0 394	3.5 8	C5H10O5	2. 7	D-Xylulose	[M+H- 2H2O] ⁺
115.0 545	2.9 6	C9H8N2S	3. 1	4-Phenyl-5-methyl-1,2,3-thiadiazole	[M+H- H2N2S] ⁺
115.0 546	4.4 7	C12H7F3O3	3. 3	5-[3-(Trifluoromethoxy)phenyl]furfural	[M+H- C3HF3O3] ⁺
115.0 87	2.5 2	C5H12N2O2	3. 5	4,5-Diaminovaleric acid	[M+H- H2O] ⁺
116.0 534	12. 8	C11H15N3O2S	3. 5	N,N-Diethyl-N'-(4-nitrophenyl)thiourea	[M+H- C6H6N2O2]] ⁺
116.0 711	1.8 2	C6H11NO4	2. 9	N-Methyl-L-glutamic acid	[M+H- CH2O2] ⁺
116.1 073	4.9 6	C6H13NO	2. 3	4-Aminomethyltetrahydropyr	[M+H] ⁺

				an	
116.1 437	18. 08	C7H17N	1. 5	Heptylamine	[M+H] ⁺
117.0 568	2.9 6	C10H13CIN2	1. 9	Chlordimeform	[M+H- C2H7CIN] ⁺
118.0 322	14. 72	C4H9NO2S	0. 8	DL-Homocysteine	[M+H- H2O] ⁺
118.0 654	2.2 6	C9H10N2	3. 4	2-(Aminomethyl)indole	[M+H- CH3N] ⁺
118.0 655	2.9 6	C12H11NO3	2. 5	.gamma.-Oxoindole-3- butyric acid	[M+H- C4H4O3] ⁺
118.0 655	9.9 6	C8H7N	2. 6	Indole	[M+H] ⁺
118.0 868	1	C5H11NO2	1. 4	Betaine	[M+H] ⁺
119.0 355	1.3 2	C8H6N2O3	8. 8	o-Anisonitrile, 6-nitro-	[M+H- CH2NO2] ⁺
119.0 494	1.3 2	C9H10OS	2. 4	Phenacyl methyl sulfide	[M+H- CH4S] ⁺
119.0 495	2.9	C8H10O3	3. 2	2-(2- Hydroxyethoxy)phenol	[M+H- 2H2O] ⁺
119.0 495	3.4 2	C9H12O3	3. 1	Homovanillyl alcohol	[M+H- CH6O2] ⁺
119.0 857	7.0 4	C12H16O2	2. 2	4-Ethylbenzenebutanoic acid	[M+H- C3H6O2] ⁺
119.0 858	3.9 7	C10H15N	2. 1	N-(4-Ethylbenzyl)-N- methylamine	[M+H- CH5N] ⁺
120.0 446	4.7 3	C8H9NO2	2. 5	Methyl 2-methylnicotinate	[M+H- CH4O] ⁺
120.0 657	0.9 8	C4H9NO3	2. 2	L-.beta.-Homoserine	[M+H] ⁺

120.0 808	4.6 9	C ₁₁ H ₁₈ N ₂	1. 6	N-Ethyl-4-(dimethylamino)benzylamine	[M+H-C ₃ H ₉ N] ⁺
120.0 81	2.2 6	C ₉ H ₁₁ NO ₃	1. 5	3-Phenylserine	[M+H-CH ₂ O ₃] ⁺
120.0 81	4.4 5	C ₁₉ H ₁₈ N ₂ O ₃	2. 1	N-(1H-Indol-3-ylacetyl)phenylalanine	[M+H-C ₁₁ H ₉ NO ₃] ⁺
120.0 811	4.1 9	C ₂₀ H ₂₃ N ₃ O ₄	2. 3	Gly-Phe-Phe	[M+H-C ₁₂ H ₁₄ N ₂ O ₄] ⁺
120.0 811	2.8	C ₉ H ₉ NO ₂	2. 5	Resedine	[M+H-CO ₂] ⁺
120.0 811	3.2 4	C ₁₆ H ₁₇ NO ₂	2. 2	1-Phenyl-2,3,4,5-tetrahydro-1H-3-benzazepine-7,8-diol	[M+H-C ₈ H ₈ O ₂] ⁺
121.0 283	13. 67	C ₇ H ₇ NO ₃	2. 2	N,3-Dihydroxybenzamide	[M+H-H ₃ NO] ⁺
121.0 287	3.2 3	C ₈ H ₆ O ₄	2. 5	Pisolithin A	[M+H-CH ₂ O ₂] ⁺
121.0 649	2.2 6	C ₈ H ₈ O	0. 6	4-Vinylphenol	[M+H] ⁺
121.0 65	7.0 5	C ₁₂ H ₁₆ O ₃	1. 5	Thymoxyacetic acid	[M+H-C ₄ H ₈ O ₂] ⁺
121.0 65	1.3 7	C ₉ H ₁₀ O ₃	2	Dihydro-m-coumaric acid	[M+H-CH ₂ O ₂] ⁺
121.1 014	4.5 1	C ₁₅ H ₂₆ O	2	Patchouli alcohol	[M+H-C ₆ H ₁₄ O] ⁺
122.0 967	2.7 9	C ₁₀ H ₁₆ N ₂	2. 9	4,5,7-Trimethyl-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridine	[M+H-C ₂ H ₅ N] ⁺
122.0	2.6	C ₈ H ₁₁ N	2.	Phenylethylamine	[M+H] ⁺

968	5		8		
123.0	7.2	C13H16O7	1.	Helicid	[M+H-
441	6		2		C6H10O5] +
123.0	6.9	C7H6O2	1.	Salicylaldehyde	[M+H]+
442	2		2		
123.0	9.4	C14H11NO3	1.	4-Formylphenyl phenylcarbamate	[M+H- C7H5NO]+
444	9		5		
123.0	7.6	C9H12O4	1.	Asperlactone	[M+H- C2H6O2]+
446			8		
123.0	18.	C12H14N4O	2.	Bis(3,4-diaminophenyl) ether	[M+H- C6H8N2]+
555	39		1		
123.0	1.2	C6H6N2O	1.	Picolinamide	[M+H]+
559	2		9		
124.0	1.2	C6H5NO2	1.	Nicotinic acid	[M+H]+
395	2		9		
124.0	0.9	C6H5NO2	1.	Isonicotinic acid	[M+H]+
395	7		5		
124.0	2.1	C7H7NO4	2.	Didox	[M+H- CH2O2]+
397	9		4		
124.0	3.3	C8H14N2O	2.	(.+/-.)-Loline	[M+H- CH5N]+
76	8		8		
124.0	12.	C6H9N3	2.	2,5-Dimethyl-4- pyrimidinamine	[M+H]+
874	48		6		
125.0	2.3	C7H8F2N2O	2.	[6-(Difluoromethoxy)-3- pyridyl]methylanine	[M+H- CF2]+
707	6		7		
125.0	6.1	C8H14O2	1.	.gamma.-Octalactone	[M+H- H2O]+
963	3		9		
125.0	12.	C11H18O	1.	Dihydrojasmane	[M+H- C3H6]+
963	27		1		
125.0	13.	C23H24FNO	1.	FUB-144	[M+H-

964	02		5		C15H12FN] +
126.0 552	2.3 6	C7H10N2O3S	1. 6	3-Amino-4-hydroxy-N-methylbenzenesulfonamide	[M+H- CH3NOS]+
126.0 552	2.7 3	C6H7NO2	1. 9	6-(Hydroxymethyl)pyridin-3-ol	[M+H]+
128.0 193	0.7 1	C6H8N2OS	23 .1	4H,5H,6H,7H-[1,2]Thiazolo[5,4-c]pyridin-3-ol	[M+H- CH3N]+
128.1 071	18. 08	C14H28N2O	1. 1	N-(Cyclohexylmethyl)-4-morpholinepropanamine	[M+H- C7H15N]+
128.1 072	4.1 7	C17H27NO3	2. 2	Pramacort	[M+H- C10H14O2] +
129.0 55	3.0 5	C6H10O4	2	Monomethyl glutarate	[M+H- H2O]+
129.1 388	0.6 9	C7H16N2	1. 3	4-Piperidinemethanamine, 1-methyl-	[M+H]+
130.0 863	2.0 9	C6H11NO2	1. 4	(1S,3R)-3-aminocyclopentanecarboxylic acid	[M+H]+
131.0 492	2.2 6	C9H10O3	1. 5	Tropic acid	[M+H- 2H2O]+
131.0 494	4.5 6	C18H19NO2	0. 7	N-[2-(4-Methoxyphenyl)ethyl]-3-phenylacrylamide	[M+H- C9H13NO] +
131.0 705	2.1	C6H10O3	1. 4	DL-Mevalonic acid lactone	[M+H]+
132.0 769	0.8 8	C4H9N3O2	0. 4	Guanidinepropanoic acid	[M+H]+
132.0 807	2.9 6	C10H13NO2S	0. 7	3-(Phenylamino)sulfolane	[M+H- CH4SO2]+

132.1 017	0.9 8	C13H24N2O3	1	6- [(Cyclohexylcarbamoyl)ami no]hexanoic acid	[M+H- C7H11NO] +
132.1 019	1.5 6	C6H15NO3	0. 4	Triethylolamine	[M+H- H2O]+
133.0 487	19. 65	C16H13NO3	19	PD 98059	[M+H- C8H7O2]+
133.0 65	3.2 5	C12H14N2O3	1. 2	4-Hydroxymephenytoin	[M+H- C3H6N2O2]+
133.0 65	4.4 7	C16H16O3	1. 1	Pterostilbene	[M+H- C7H8O2]+
133.0 652	3.6 8	C9H10O2	1	(2S,3S)-(-)-3- Phenylglycidol	[M+H- H2O]+
133.0 652	3.5 3	C13H21NO2	1. 2	1-(Butylamino)-3- phenoxy-2-propanol	[M+H- C4H13NO] +
133.0 654	2.8 3	C11H12N2O3	1. 4	(S)-5-(4-Hydroxyphenyl)- 5-ethylhydantoin	[M+H- C2H4N2O2]+
133.0 762	18. 4	C15H19N3	0. 6	3-(2-Methyl-1H- benzimidazol-1-yl)-8- azabicyclo[3.2.1]octane	[M+H- C7H11N]+
133.1 011	5.6 9	C13H20O	0. 5	4-(2,4,6-Trimethyl-3- cyclohexen-1-yl)-3-buten- 2-one	[M+H- C3H8O]+
133.1 012	7.0 5	C14H22O	0. 4	(1S,5S)-2,4,9-Trimethyl-6- [(E)-prop-1-enyl]-7- oxabicyclo[3.3.1]non-3-ene	[M+H- C4H10O]+
133.1 014	4	C11H12O2	1. 2	7-Methylindane-4- carboxylic acid	[M+H- CO2]+
133.1	6.3	C15H22O2	0.	Polygodial	[M+H- C5H10O2]

014	8		9		+
133.1 014	11. 88	C12H18O3	0. 9	Jasmonic acid	[M+H- C2H6O3]+
134.0 607	7.0 2	C16H18N2O	1. 1	Glycoamide A	[M+H- C8H11N]+
134.0 96	2.3 7	C20H21N2	1. 5	2-[4-(Dimethylamino)styryl]-1-methylquinolinium cation	[Cat- C11H9N]+
135.0 441	6.6 9	C14H12N2O5	0. 4	N-(2-Hydroxy-4-nitrophenyl)-4-methoxybenzamide	[M+H- C6H6N2O3]+
135.0 442	5.2	C10H11NO4	0. 8	Hippuric acid, o-methoxy-	[M+H- C2H5NO2] +
135.0 803	6.4 3	C15H20O2	0. 9	6-(4-Hydroxy-3-methylphenyl)-2-methylhept-2-en-4-one	[M+H- C6H10O]+
135.0 807	7.0 5	C9H13NO	0. 5	4-Amino-2,3,6-trimethylphenol	[M+H- NH3]+
135.0 809	5.6 9	C16H26O8	1. 1	(4E,6E)-8-(.beta.-D-Glucopyranosyloxy)-2,7-dimethylocta-4,6-dienoic acid	[M+H- C7H16O7] +
135.1 168	4.5 9	C10H16O	1	Absinthol	[M+H- H2O]+
135.1 168	3.9 7	C10H16O	1. 2	2,3-Epoxy-pinane	[M+H- H2O]+
135.1 17	4.3 3	C10H16O	1. 6	Fenchone	[M+H- H2O]+
135.1 172	6.4 3	C15H26O2	0. 8	[(9R)-8-Isopropyl-2,4,9-trimethyl-7-oxabicyclo[3.3.1]non-2-en-	[M+H- C5H12O2] +

				5-yl]methanol	
136.0 618	1.3 2	C8H11N5O	0. 1	3-Denin-9-ylpropan-1-ol	[M+H- C3H6O]+
136.0 619	0.9 7	C5H5N5	0. 1	Adenine	[M+H]+
136.0 756	2.8 7	C10H13NO3	0. 8	Nigelline	[M+H- C2H4O2]+
136.0 758	5.0 9	C5H10FNO2	7. 8	4-Amino-5-fluorovaleric acid	[M+H]+
136.0 758	1.3 2	C11H15NO3	2. 8	Ethyl L-tyrosinate	[M+H- C3H6O2]+
136.0 759	3.5	C9H10N2OS	1. 1	4'- Thioureidoacetophenone	[M+H- CHNS]+
137.0 598	4.3 6	C21H34O4	0. 7	(R)-[10]Gingerol	[M+H- C13H26O2] +
137.0 598	3.4 8	C18H29NO3	0. 9	Dihydrocapsaicin	[M+H- C10H21NO]+
137.0 599	2.6 1	C20H22O6	1. 4	Matairesinol	[M+H- C12H14O4] +
137.0 962	5.6 9	C11H15NO2	0. 5	3,4,5-Trimethacarb	[M+H- C2H3NO]+
137.1 326	5.2 5	C10H18O	0. 6	Chrysanthemyl alcohol	[M+H- H2O]+
138.0 548	2.2 3	C8H7NO4	0. 6	4-Carbomethoxynicotinic acid	[M+H- CO2]+
138.0 549	6.9 9	C7H7NO2	0. 8	3-Acetoxy pyridine	[M+H]+
138.0	4.7	C7H7NO2	0.	5-Methylpicolinic acid	[M+H]+

55	3		6		
138.0	2.7		1.		
553	2	C7H7NO2	1	3-Aminobenzoic acid	[M+H]+
138.0	1.3		0.		
914	6	C10H13NO2	6	N-Acetyltyramine	[M+H-C2H2O]+
138.0	2.2		0.		
914	9	C17H20N2O2	3	N,N'-Bis(4-ethoxyphenyl)formamidine	[M+H-C9H9NO]+
139.0	3.2		1.		
391	4	C9H10O3	4	Ethyl salicylate	[M+H-C2H4]+
139.0	2.4		1.		
391	1	C13H16O3	1	4-Cyclohexyloxybenzoic acid	[M+H-C6H10]+
140.0	1.2		0.		
347	6	C6H5NO3	9	3-Hydroxypicolinic acid	[M+H]+
140.0	15.		16		
673	38	C8H11NO4	.4	Eglumetad	[M+H-CH2O2]+
140.0	15.		16		
681	91	C7H9NO2	.7	2-Methoxycarbonyl-N-methylpyrrole	[M+H]+
140.0	4.0		1.		
705	5	C7H9NO2	1	3-Amino-2,3-dihydrobenzoic acid	[M+H]+
141.0	4.2		0.		
913	8	C8H12O2	4	4,4-Dimethyl-1,3-cyclohexanedione	[M+H]+
142.0	2.7		21		
5	9	C5H5BFNO2	.1	6-Fluoro-3-pyridinylboronic acid	[M+H]+
142.0	2.2		0.		
863	8	C9H15NO4	5	Methyl 1-(2-Methoxyethyl)-2-oxopyrrolidine-4-carboxylate	[M+H-C2H4O2]+
142.1	17.				
227	04	C8H17NO2	1	2-(2,6-Dimethylmorpholino)ethanol	[M+H-H2O]+
143.0	2.9		21		
		C6H7ClN2		4-Chlorobenzene-1,2-	[M+H]+

342	8		.1	diamine	
144.0 651	2.0 8	C6H9NO3	0. 3	2-Pyrrolidinoneacetic acid	[M+H] ⁺
144.0 654	2.8 4	C6H9NO3	1. 4	(2R)-6-Ketopipicolinic acid	[M+H] ⁺
144.0 799	2.9 6	C11H14N2	0. 1	N-Methyltryptamine	[M+H-CH5N] ⁺
144.0 802	17. 18	C10H12N2	0. 1	Tryptamine	[M+H-NH3] ⁺
144.0 803	3.7	C12H14N2	0. 7	Azepindole	[M+H-C2H5N] ⁺
144.1 019	0.8 8	C7H13NO2	1. 4	Stachydrine	[M+H] ⁺
144.1 02	1.3 3	C7H13NO2	0. 7	4-Methylpipercolinic acid	[M+H] ⁺
145.0 492	1.5	C6H8O4	0. 5	(3E)-3-Hexenedioic acid	[M+H] ⁺
146.0 237	5.0 9	C8H4ClNO2	0. 4	N-Chlorophthalimide	[M+H-HCl] ⁺
146.0 6	3.1 7	C10H9NO2	0. 7	Gentianine	[M+H-CH2O] ⁺
146.0 6	4.3 6	C9H7NO	1	Quinolin-2-ol	[M+H] ⁺
146.0 6	2.9 6	C9H7NO	0. 4	7-Formylindole	[M+H] ⁺
146.0 602	3.5 7	C9H9NO2	0. 9	3,4-Dihydro-6-hydroxycarbostyryl	[M+H-H2O] ⁺
146.0 924	0.9	C5H11N3O2	0. 3	4-Guanidinobutyric acid	[M+H] ⁺
147.0 434	2.9	C9H8O3	0. 4	trans-3-Coumaric acid	[M+H-H2O] ⁺

147.0 441	6.5 9	C ₁₄ H ₁₇ NO ₃	0. 2	MDPPP	[M+H- C ₅ H ₁₁ NO] +
147.0 443	1.3 2	C ₉ H ₈ O ₃	0	p-Coumaric acid	[M+H- H ₂ O] ⁺
147.1 129	0.7 4	C ₆ H ₁₄ N ₂ O ₂	0. 3	Lysine	[M+H] ⁺
147.1 166	9.7 9	C ₁₁ H ₁₈ O ₂	0. 4	10-Undecynoic acid	[M+H- 2H ₂ O] ⁺
149.0 233	13. 67	C ₈ H ₆ O ₄	0. 2	4-Formyl-2- hydroxybenzoic acid	[M+H- H ₂ O] ⁺
149.0 597	2.2 6	C ₉ H ₁₀ O ₃	0. 1	(+)-2-Phenyllactic acid	[M+H- H ₂ O] ⁺
149.0 6	3.6 1	C ₉ H ₈ O ₂	0	trans-Cinnamic acid	[M+H] ⁺
149.0 958	7.0 5	C ₁₀ H ₁₄ O ₂	0. 1	(1S)-(+)-Camphorquinone	[M+H- H ₂ O] ⁺
150.0 912	1.9 6	C ₉ H ₁₁ NO	0. 6	Cyclopropyl(3- pyridyl)methanol	[M+H] ⁺
150.0 912	6.3 3	C ₁₀ H ₁₁ NO ₂	0. 5	2,6-Dimethyl-2H-1,4- benzoxazin-3(4H)-one	[M+H- CO] ⁺
150.0 913	1.2 2	C ₉ H ₁₃ NO ₂	0. 5	Synephrine	[M+H- H ₂ O] ⁺
150.0 914	6.9 7	C ₉ H ₁₃ NO ₂	1. 3	5-Acetyl-2,6-dimethyl-2,3- dihydropyridin-4(1H)-one	[M+H- H ₂ O] ⁺
151.0 372	4.6 7	C ₁₀ H ₁₀ O ₅	0. 1	4-Acetoxyvanillic acid	[M+H- C ₂ H ₄ O ₂] ⁺
151.1 115	7.0 5	C ₁₀ H ₁₄ O	0. 6	(-)-Myrtenal	[M+H] ⁺
151.1 118	11. 92	C ₁₀ H ₁₇ NO	1. 1	1-Amino-3- hydroxyadamantane	[M+H- NH ₃] ⁺

151.1 118	3.6 2	C ₁₀ H ₁₆ O ₂	1	Jasminlactone	[M+H- H ₂ O] ⁺
151.1 118	9.8 5	C ₁₀ H ₁₄ O	0. 5	2-Adamantanone	[M+H] ⁺
152.0 334	3.1 1	C ₇ H ₇ NO ₄	0. 9	3-Methylpyrrole-2,4- dicarboxylic Acid	[M+H- H ₂ O] ⁺
152.0 563	1.4 5	C ₁₀ H ₁₃ N ₅ O ₅	0. 1	Guanosine	[M+H- C ₅ H ₈ O ₄] ⁺
152.0 706	7.0 2	C ₈ H ₉ NO ₂	0. 4	N-Methylantranilic acid	[M+H] ⁺
152.0 812	4.1 3	C ₉ H ₁₂ N ₄ O ₂	1. 3	Methylcaffeine	[M+H- C ₂ H ₃ NO] ⁺
153.0 407	2	C ₁₀ H ₁₂ N ₄ O ₆	0. 3	Xanthosine	[M+H- C ₅ H ₈ O ₄] ⁺
153.0 543	5.2	C ₈ H ₈ O ₃	0. 5	2,4-Cresotic acid	[M+H] ⁺
153.0 547	4.2 5	C ₈ H ₈ O ₃	0. 8	Methyl salicylate	[M+H] ⁺
153.0 547	4.6 2	C ₈ H ₈ O ₃	0. 9	Vanillin	[M+H] ⁺
153.0 911	19. 92	C ₉ H ₁₂ O ₂	0. 2	3-Phenoxy-1-propanol	[M+H] ⁺
153.1 274	6.6 6	C ₁₀ H ₁₆ O	0. 6	(+)-Dihydrocervone	[M+H] ⁺
153.1 274	5.9 1	C ₁₁ H ₂₀ O ₄	0. 6	2-Hexylglutaric acid	[M+H- CH ₄ O ₃ - H ₂ O] ⁺
154.0 499	1.6 5	C ₇ H ₇ NO ₃	0. 8	3-Amino-4- hydroxybenzoate	[M+H] ⁺
154.0 503	2.3 8	C ₇ H ₇ NO ₃	0. 5	3-Methoxypicolinic acid	[M+H] ⁺

154.0 624	5.8 5	C ₁₀ H ₁₂ O ₄	0. 1	Asarylaldehyde	[M+H- C ₂ H ₃ O] ⁺
154.0 976	3.1	C ₇ H ₁₁ N ₃ O	0. 4	6-Propylisocytosine	[M+H] ⁺
154.1 333	5.0 8	C ₈ H ₁₅ N ₃	0. 4	5-Methyl-2-tert-butyl-2H-pyrazol-3-ylamine	[M+H] ⁺
155.1 066	9.9	C ₉ H ₁₆ O ₃	0	8-Oxononanoic acid	[M+H- H ₂ O] ⁺
156.0 769	0.7 5	C ₉ H ₁₄ N ₄ O ₃	0. 5	L-Carnosine	[M+H- C ₃ H ₅ NO] ⁺
156.1 02	3.1 9	C ₉ H ₁₅ NO ₃	1	PRIMA-1	[M+H- CH ₂ O] ⁺
157.0 488	12. 27	C ₁₀ H ₁₂ O ₅	0. 7	Prohexadione	[M+H- C ₃ H ₄ O] ⁺
158.0 601	3.6 1	C ₁₀ H ₉ NO ₂	1	4-Methylquinoline-2,7-diol	[M+H- H ₂ O] ⁺
158.0 813	3.0 6	C ₇ H ₁₃ NO ₄	0. 7	Spermidic acid	[M+H- H ₂ O] ⁺
158.0 813	2.4 6	C ₇ H ₁₁ NO ₃	1. 9	Acetylproline	[M+H] ⁺
158.0 924	1.2 3	C ₁₈ H ₃₆ N ₄ O ₃	0. 1	N-Lauroyl-L-arginine	[M+H- C ₁₂ H ₂₅ NO] ⁺
158.1 29	2.7 5	C ₇ H ₁₅ N ₃ O	0. 7	3-Amino-1-cyclohexylurea	[M+H] ⁺
158.1 552	10. 4	C ₂₄ H ₄₀ O ₅	0. 2	Hyocholic acid	[M+H] ⁺
159.0 76	2.0 1	C ₆ H ₁₃ N ₃ O ₃	0. 8	L-Citrulline	[M+H- NH ₃] ⁺
159.0 913	2.9 6	C ₁₈ H ₁₅ ClN ₂ O 3	0	Benzotript	[M+H- C ₈ H ₅ ClO ₃]

					+
159.1	9.9	C ₁₅ H ₁₈ O ₃	0.	Tourneforin	[M+H-
172	6		7		C ₃ H ₄ O ₃]+
160.0	0.7	C ₁₀ H ₉ NO	24	1-Acetylindole	[M+H]+
718	5		.6		
160.1	1.2	C ₈ H ₁₈ NO ₂	0.	Methacholine cation	[Cat]+
332	2		3		
161.0	4.4	C ₁₀ H ₁₀ O ₃	0.	Mellein	[M+H-
597	7		4		H ₂ O]+
161.0	1.2	C ₆ H ₁₂ N ₂ O ₃	0.	L-.beta.-Homoglutamine	[M+H]+
921	3		4		
161.0	5.4	C ₁₁ H ₁₆ O ₃	0.	1-Carboxy-3-adamantanol	[M+H-
954	6		7		2H ₂ O]+
162.0	4.7	C ₁₁ H ₁₃ NO ₃	0.	N-Acetyl-D-phenylalanine	[M+H-
913	4		5		CH ₂ O ₂]+
163.0	3.3	C ₂₄ H ₂₈ O ₁₃	0.	Verminoside	[M+H-
38	8		3		C ₁₅ H ₂₂ O ₁₀]+
163.0	4.2	C ₁₅ H ₁₂ O ₄	0.	Dihydrodaidzein	[M+H-
386	7		6		C ₆ H ₆ O]+
163.0	7.7	C ₉ H ₈ O ₄	0.	3-Hydroxy-7-methoxyphthalide	[M+H-
391	9		4		H ₂ O]+
163.0	2.8	C ₁₈ H ₁₉ NO ₄	0.	N-Caffeoyl-O-methyltyramine	[M+H-
394	4		5		C ₉ H ₁₃ NO]
					+
163.0	4.5	C ₁₀ H ₁₂ O ₃	0.	Coniferyl alcohol	[M+H-
757	6		2		H ₂ O]+
163.1	7.6	C ₁₁ H ₂₀ O ₄	0.	5-(Hydroxymethyl)-3-(1-hydroxy-4-methylpentyl)oxolan-2-one	[M+H-
11	4		7		3H ₂ O]+
163.1	6.1	C ₁₅ H ₂₂ O	0.	.alpha.-Cyperone	[M+H-

118	3		7		C4H8]+
164.0 703	3.9 7	C9H12N2O2	0. 2	L-Tyrosinamide	[M+H- NH3]+
165.0 543	7.6	C22H26O12	0. 1	Catalposide	[M+H- C13H18O9] +
165.0 546	1.3 2	C13H19NO3	0. 4	L-Tyrosine, O-(1,1- dimethylethyl)-	[M+H- C4H11N]+
165.1 142	18. 14	C18H20N6	0. 4	NGD 94-1	[M+H- C10H8N2] +
165.1 275	5.2 1	C11H16O	0. 4	cis-Jasmone	[M+H]+
166.0 5	2.7 1	C12H17NO4	1	Diethyl 2,4- dimethylpyrrole-3,5- dicarboxylate	[M+H- C4H10O]+
166.0 857	2.5 6	C9H11NO2	18 .9	Phenylalanine	[M+H]+
166.0 863	4.1 9	C13H17N3O4	0. 4	Gly-Gly-Phe	[M+H- C4H6N2O2]+
166.0 864	3.4 5	C9H11NO2	0. 7	2-Amino-4'- methoxyacetophenone	[M+H]+
166.1 228	1.7 7	C10H15NO	0. 1	Hordenine	[M+H]+
166.1 336	5.3 7	C9H15N3	0. 3	2-Cyclopentyl-5- methylpyrazol-3-amine	[M+H]+
167.0 339	13. 67	C8H4O3	0. 3	Phthalic anhydride	[M+H+H2 O]+
167.0 699	6.5 9	C17H18O5	0. 1	Isomucronulatol	[M+H- C8H8O2]+
167.0	5.9	C19H23ClN2O	0.	4-({4-[(4-	[M+H-

703	6	5S	4	Chlorophenyl)sulfonyl]-1-piperazinyl)methyl)-2,6-dimethoxyphenol	C10H13ClN2O2S]+
167.0703	9.2	C9H10O3	0.3	2'-Hydroxy-6'-methoxyacetophenone	[M+H]+
167.0703	16.46	C24H30O11	0.3	Harpagoside	[M+H-C15H20O8]+
167.1067	4.51	C10H16O3	0.1	cis-Pinonic acid	[M+H-H2O]+
168.0764	2.07	C7H9N3O2	0.2	2-Nitro-4,6-diaminotoluene	[M+H]+
168.0767	1.55	C7H9N3O2	0.2	3-Amino-5,6-dimethyl-2-pyrazinecarboxylic acid	[M+H]+
168.1013	2.12	C9H13NO2	0.6	dl-p-Hydroxynorephedrine	[M+H]+
168.1132	4.23	C8H13N3O	0.9	2-Dimethylamino-5,6-dimethylpyrimidin-4-ol	[M+H]+
169.0614	3.11	C7H8N2O3	0.3	4-Hydroxy-2-keto-6-methyl-1H-pyridine-3-carboxamide	[M+H]+
169.1218	5.2	C16H26O7	0.3	Jasminoside A	[M+H-C6H10O5]+
169.1225	3.49	C10H18O3	0.4	4-Hydroxy-6-pentyloxan-2-one	[M+H-H2O]+
170.0585	2.96	C11H11N3O	0.2	2-(1H-Pyrrol-1-yl)benzohydrazide	[M+H-N2H4]+
170.0812	2.49	C8H13NO4	0.4	4-Hydroxy-1-propionylproline	[M+H-H2O]+
170.1539	9.23	C10H19NO	0.5	Lupinine	[M+H]+

171.0 288	5.3 3	C7H6O5	0. 4	Phloroglucinolcarboxylic acid	[M+H] ⁺
171.1 129	3.2	C14H27N3O2	0. 3	N-Cyclohexyl-N'-[3-(4- morpholinyl)propyl]urea	[M+H- C6H13N] ⁺
171.1 38	15. 03	C10H18O2	0. 5	cis-2-Decenoic acid	[M+H] ⁺
171.1 38	4.3 2	C10H18O2	1. 1	xi-5-Hexyldihydro-2(3H)- furanone	[M+H] ⁺
171.1 38	4.6 1	C10H20O3	0. 2	3,7-Dimethyloct-6-ene- 1,2,3-triol	[M+H- H2O] ⁺
172.1 081	1.2 9	C13H17N3S	23 .6	2-Phenyl-1,2,4- triazaspiro[4.5]decane-3- thione	[M+H- CH4N2S] ⁺
172.1 692	11. 46	C10H21NO	0. 1	1,2,2,6,6-Pentamethyl-4- piperidinol	[M+H] ⁺
173.1 325	7.0 5	C21H28O5	0. 3	4-(Hydroxymethyl)- 4,6a,9,12b-tetramethyl- 4a,6,6a,12,12a,12b- hexahydro-4H,9H- benzo[f]pyrano[2,3- b]chromene-1,11(5H,10H)- dione	[M+H- C8H12O5] +
174.0 915	3.8 8	C11H11NO	1	1,6-Dimethyl-2-quinolone	[M+H] ⁺
174.1 238	2.8 5	C12H17NO	21 .8	Pentedrone	[M+H- H2O] ⁺
174.1 487	1.6 7	C9H20NO2	0. 3	(+)-Muscarine cation	[Cat] ⁺
175.0 599	11. 74	C7H12O6	0. 8	Sedoheptulosan	[M+H- H2O] ⁺
175.1 188	0.7 7	C12H25N5O3	0. 3	D-Leucyl-L-arginine	[M+H- C6H11NO]

					+
175.1 482	5.7 2	C ₁₃ H ₂₀ O	0. 7	(E)-.alpha.-Ionone	[M+H- H ₂ O]+
176.0 707	3.8 4	C ₅ H ₉ N ₃ O ₄	23 .4	Guanidinosuccinic acid	[M+H]+
176.0 816	6.1 5	C ₁₂ H ₁₆ O ₃	0. 1	6-Methoxy-2,2- dimethylchroman-4-ol	[M+H- CH ₅ O]+
177.0 539	4.1 8	C ₁₆ H ₁₄ O ₆	0. 5	(-)-Homoeriodictyol	[M+H- C ₆ H ₆ O ₃]+
177.0 891	5.8 7	C ₂₇ H ₃₆ N ₂ O ₅	1	Ivabradine	[M+H- C ₁₆ H ₂₄ N ₂ O ₃]+
177.0 981	0.7 5	C ₅ H ₁₂ N ₄ O ₃	0. 1	L-Canavanine	[M+H]+
177.1 274	9.9 6	C ₁₂ H ₂₂ O ₄	0. 2	Dodecanedioic acid	[M+H- 3H ₂ O]+
178.0 867	2.0 7	C ₁₁ H ₁₃ NO ₄	0	Phenylalanine, 4- (carboxymethyl)-	[M+H- CH ₂ O ₂]+
179.0 703	3.0 5	C ₁₀ H ₁₀ O ₃	0	Methyl 4-coumarate	[M+H]+
180.0 88	2.3 8	C ₁₂ H ₁₇ N ₅ O ₅	0. 3	N,N-Dimethylguanosine	[M+H- C ₅ H ₈ O ₄]+
180.1 008	1.7 2	C ₁₀ H ₁₃ NO ₂	0. 3	L-Benzylalanine	[M+H]+
180.1 019	2.7	C ₁₀ H ₁₃ NO ₂	0. 5	Pgaba	[M+H]+
180.1 02	3.8 9	C ₁₀ H ₁₃ NO ₂	0. 3	N-Phenylglycine ethyl ester	[M+H]+
180.1 02	4.4 5	C ₁₀ H ₁₃ NO ₂	0. 2	2',6'-Glycoloxylidide	[M+H]+
181.0	9.1	C ₂₀ H ₁₄ N ₂ O	0.	N-(4-Cyanophenyl)[1,1'-	[M+H-

648	3		7	biphenyl]-4-carboxamide	C7H6N2]+
181.0	6.9	C12H19NO3	0.	Escaline	[M+H- C2H7N]+
859	2		4		
181.0	6.4	C10H16O5	0	Tuckolide	[M+H- 2H2O]+
859	3				
181.0	9.9	C19H32N2O3	0.	1-(1-Ethylpropyl)-4-(2,3,4-trimethoxybenzyl)piperazine	[M+H- C9H20N2] +
859	6		3		
181.1	9.5	C11H20O4	0	Undecanedioic acid	[M+H- 2H2O]+
216	6				
181.1	7.6	C11H20O4	0.	3-(1-Hydroxyhexyl)-4-(hydroxymethyl)oxolan-2-one	[M+H- 2H2O]+
224	4		4		
182.0	0.8	C7H13NOS	17	6-Methylsulfinylhexanenitrile	[M+Na]+
578	5		.3		
182.0	1.3	C9H11NO3	0.	L-Tyrosine	[M+H]+
812	2		2		
182.0	2.0	C9H11NO3	0.	DL-o-Tyrosine	[M+H]+
813	8		8		
182.1	6.2	C11H18N4O2	0.	Pirimicarb	[M+H- C2H3NO]+
289	7		4		
182.1	4.3	C13H24N3O3PS	0.	Pirimiphos-ethyl	[M+H- C4H9O2PS] +
289	3		6		
183.0	4.6	C9H10O4	0.	Syringaldehyde	[M+H]+
653	9		5		
183.0	6.1	C6H15O4P	1	Triethyl phosphate	[M+H]+
776	9				
184.1	5.8	C9H17N3O	0.	1-Piperazineacetamide, N-cyclopropyl-	[M+H]+
445	8		9		
185.0	4.8	C11H14O5	1.	3,4,5-Trimethoxyphenyl	[M+H-

81			3	acetate	C2H2O]+
185.1	7.0			(9,9b-Dihydroxy-6,6,9a-	
325	5	C21H32O6	0.	trimethyl-1-oxo-	[M+H-
			1	3,5,5a,7,8,9-	C7H16O6]
				hexahydrobenzo[e][2]benz	+
				ofuran-5-yl) hexanoate	
186.0	3.6	C20H19F3N2O	13	Trifloxystrobin	[M+H-
551	1	4	.7		C11H13NO
					4]+
186.1	3.9	C21H22ClNO2	20	JWH 203 N-(5-	[M+H-
238	7		.7	hydroxypentyl) metabolite	C8H7ClO2]
					+
187.1	7.0	C17H24O3	0.	Antibiotic NFAT 133	[M+H-
117	5		2		C4H10O2]
					+
188.0	2.3	C10H8N2O3	18	Tyrphostin 46	[M+H-
376	2		.2		NH3]+
188.0	3.6	C11H9NO2	0.	3-Indoleacrylic acid	[M+H]+
707	7		3		
188.1	3.9	C24H26N2O	20	N-[1-(2-Phenylethyl)-4-	[M+H-
394	7		.8	piperidinyl]-2-	C11H9NO]
				naphthamide	+
188.1	2.7	C10H21NO2	0.	10-Aminocapric acid	[M+H]+
647	3		9		
189.0	6.3	C15H16O5	0.	8-(1,2-Dihydroxy-3-	[M+H-
547	9		4	methylbut-3-enyl)-7-	C4H8O2]+
				methoxycoumarin	
189.1	2.4	C8H16N2O3	0.	Glycyl-L-norleucine	[M+H]+
235	4		8		
189.1	2.6	C8H16N2O3	2	Glycylleucine	[M+H]+
235					
189.1	3.9	C13H20O3	0	4-(1-Hydroxy-4-keto-	[M+H-
				2,6,6-trimethyl-2-	

271	8			cyclohexen-1-yl)-3-buten-2-ol	[2H ₂ O]+
189.1 279	4.4 7	C ₁₅ H ₂₀ O ₃	0. 2	Tetrahydro-2,2-dimethyl-4-phenyl-2H-pyran-4-acetic acid	[M+H-C ₂ H ₄ O ₂]+
189.1 598	0.7 6	C ₉ H ₂₀ N ₂ O ₂	1	Nepsilon,nepsilon,nepsilon-trimethyllysine	[M+H]+
190.0 5	3.2 7	C ₁₀ H ₉ NO ₄	0. 7	2,3-Dihydro-3-oxo-4H-1,4-benzoxazine-4-acetic acid	[M+H-H ₂ O]+
190.0 61	5.0 1	C ₉ H ₇ N ₃ O ₂	7. 6	6-(1H-Pyrazol-1-yl)nicotinic acid	[M+H]+
191.0 698	6.5 9	C ₁₁ H ₁₂ O ₄	0. 2	trans-2,4-Dimethoxycinnamic acid	[M+H-H ₂ O]+
191.0 701	7.0 5	C ₁₇ H ₁₈ O ₄	0. 2	7-(2-Ketocyclohexoxy)-4,8-dimethylcoumarin	[M+H-C ₆ H ₈ O]+
191.1 066	6.6 6	C ₁₂ H ₂₀ O ₅	0. 3	4-Oxododecanedioic acid	[M+H-3H ₂ O]+
191.1 431	7.6 9	C ₁₃ H ₂₂ O ₃	0. 6	1,2,3-Cyclohexanetriol, 5-(1,3-heptadien-1-yl)-	[M+H-2H ₂ O]+
192.0 655	2.9 3	C ₁₀ H ₁₁ NO ₄	0. 4	Phenoxyacetyl glycine	[M+H-H ₂ O]+
192.1 02	2.0 4	C ₁₁ H ₁₃ NO ₂	0. 8	L-.beta.-indanylglycine	[M+H]+
192.9 986	0.7 9	C ₈ H ₇ ClF ₃ N	20 .7	1-(4-Chlorophenyl)-2,2,2-trifluoroethan-1-amine	[M+H-NH ₃]+
193.0 494	4.8 6	C ₁₀ H ₈ O ₄	1. 3	Isoscopoletin	[M+H]+
193.0 86	6.9 8	C ₂₃ H ₃₀ O ₇	0. 3	2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4,5-trimethoxyphenyl)propan-	[M+H-C ₁₂ H ₁₈ O ₄]+

				1-ol	
193.0 86	4.4 7	C ₁₁ H ₁₄ O ₄	0. 4	Sinapyl alcohol	[M+H- H ₂ O] ⁺
193.0 861	3.6 8	C ₁₁ H ₁₂ O ₃	1. 2	Methyl 4- methoxycinnamate	[M+H] ⁺
193.1 224	13. 07	C ₂₁ H ₃₀ O ₂	1	exo-THC	[M+H- C ₉ H ₁₄] ⁺
193.1 225	3.4 5	C ₁₂ H ₂₀ O ₄	1. 2	4-(5,6-Dihydroxyheptyl)-3- methylfuran-2(5H)-one	[M+H- 2H ₂ O] ⁺
193.1 587	19. 7	C ₁₃ H ₂₀ O	0. 2	.beta.-Damascone	[M+H] ⁺
193.1 7	5.6 6	C ₁₂ H ₂₀ N ₂	0. 8	(S)-Amiflamine	[M+H] ⁺
194.0 811	1.3 2	C ₁₄ H ₁₉ NO ₃	0. 5	3-(3-Methylbut-2-en-1- yl)tyrosine	[M+H- C ₄ H ₈] ⁺
194.1 151	6.5 2	C ₂₁ H ₃₀ N ₂ O ₄	12 .9	Diethyl 5,5'- methylenebis(4-ethyl-3- methyl-1H-pyrrole-2- carboxylate)	[M+H- C ₁₀ H ₁₅ NO 2] ⁺
194.1 176	6.9 8	C ₁₁ H ₁₅ NO ₂	0. 3	4-(Butylamino)benzoic acid	[M+H] ⁺
194.1 177	2.3 2	C ₁₁ H ₁₅ NO ₂	0. 8	Alanine, 2-methyl-N-p- tolyl-	[M+H] ⁺
194.1 289	9.7 5	C ₁₀ H ₁₇ N ₃ O ₂	0. 2	Isouron	[M+H- H ₂ O] ⁺
195.0 289	5.3 3	C ₁₅ H ₁₂ O ₇	0	Taxifolin	[M+H- C ₆ H ₆ O ₂] ⁺
195.0 653	7.7 9	C ₁₀ H ₁₀ O ₄	1. 3	Caffeic acid methylester	[M+H] ⁺
195.1 016	5.8 4	C ₁₁ H ₁₄ O ₃	0. 6	6-Methoxyeugenol	[M+H] ⁺

195.1 13	2.7 1	C10H14N2O2	1. 1	(5aR,10aR)- Octahydrodipyrrolo[1,2- a:1',2'-d]pyrazine-5,10- dione	[M+H] ⁺
195.1 371	9.9 6	C12H22O4	0. 1	4-(Hydroxymethyl)-3-(1- hydroxy-5- methylhexyl)oxolan-2-one	[M+H- 2H2O] ⁺
196.0 96	2.1 3	C10H15NO4	3. 3	(-)-Kainic acid	[M+H- H2O] ⁺
197.0 809	9.4 9	C20H22O7	0. 2	2,3,8,9,10-Pentamethoxy- 6a,11a-dihydro-6H- [1]benzofuro[3,2- c]chromene	[M+H- C10H10O3] +
197.0 81	3.7 8	C10H12O4	1. 2	Ethyl 2,4-dihydroxy-6- methylbenzoate	[M+H] ⁺
197.0 948	18. 39	C16H12O3	5. 9	(2Z)-2-Benzal-6- methoxycoumaran-3-one	[M+H- C2O2] ⁺
197.1 173	5.4 6	C11H16O3	1. 2	Loliolide	[M+H] ⁺
197.1 286	3.4 5	C10H18N2O3	0. 8	5-(4-Methylpiperazin-1- yl)-5-oxopentanoic acid	[M+H- H2O] ⁺
197.1 65	2.0 3	C13H27N3O	0. 9	N-[3-(Dimethylamino)-2,2- dimethylpropyl]-4- piperidinecarboxamide	[M+H- C2H7N] ⁺
198.0 528	0.8 2	C7H7N3O4	8. 6	3,5-Dinitro-p-toluidine	[M+H] ⁺
198.1 119	1.7 2	C10H15NO3	0	Deglymidodrine	[M+H] ⁺
198.1 126	7.7 1	C10H15NO3	0. 5	Tenuazonic acid	[M+H] ⁺
198.1 126	2.4 3	C10H15NO3	0	Metanephrene	[M+H] ⁺

198.1 489	7.8 9	C ₁₁ H ₁₉ NO ₂	0. 1	L-Proline, 4-cyclohexyl-, (4S)-	[M+H] ⁺
199.0 965	7.6 5	C ₈ H ₁₄ N ₄ S	23 .1	Norburimamide	[M+H] ⁺
199.1 918	1.6 2	C ₁₀ H ₂₂ N ₄	0. 3	1,2-Di(1-piperazinyl)ethane	[M+H] ⁺
200.1 282	5.3 2	C ₁₀ H ₁₇ NO ₃	0. 2	N-Hexanoyl-L-homoserine lactone	[M+H] ⁺
200.1 282	5.7 7	C ₁₀ H ₁₇ NO ₃	0. 1	Methylecgonine	[M+H] ⁺
200.1 283	2.5 1	C ₁₀ H ₁₇ NO ₃	0. 7	APR-246	[M+H] ⁺
200.1 394	5.1 2	C ₉ H ₁₇ N ₃ O ₂	0	Vinyl-L-NIO	[M+H] ⁺
200.1 758	6.2 9	C ₁₀ H ₂₁ N ₃ O	0. 7	Diethylcarbamazine	[M+H] ⁺
201.1 276	7.0 5	C ₁₆ H ₂₂ O ₄	0	trans-Abscisin	[M+H- C ₂ H ₆ O ₃] ⁺
202.0 711	2.1 6	C ₉ H ₉ F ₂ NO ₂	18 .4	3,5-Difluoro-L- phenylalanine	[M+H] ⁺
202.1 075	2.4 7	C ₉ H ₁₇ NO ₅	1	Pantothenic acid	[M+H- H ₂ O] ⁺
202.1 55	5.0 8	C ₁₄ H ₂₁ NO	19 .8	Valerophenone, 2- (propylamino)-	[M+H- H ₂ O] ⁺
203.0 517	18. 21	C ₆ H ₁₂ O ₆	1. 5	beta-D-Fructose	[M+Na] ⁺
203.0 519	0.8 2	C ₆ H ₁₂ O ₆	1. 7	Psicose	[M+Na] ⁺
203.1 392	2.5 8	C ₉ H ₁₈ N ₂ O ₃	1. 2	L-Alanyl-L-norleucine	[M+H] ⁺
203.1	7.0	C ₁₅ H ₂₂ O ₄	0.	2-((1S,3aR,4S,6S,7R,8aR)-1-	[M+H-

43	5		2	Hydroxy-4,8a-dimethyloctahydro-1H-3a,6-epoxyazulen-7-yl)prop-2-enoic acid	CH4O3]+
203.1 432	12. 5	C15H24O4	0. 9	4,6-Dihydroxy-4-(hydroxymethyl)-3,4a,8,8-tetramethyl-5,6,7,8a-tetrahydronaphthalen-1-one	[M+H-CH6O3]+
203.1 795	13. 67	C15H26O2	0. 5	Jaeskeanadiol	[M+H-2H2O]+
204.0 867	6.9 9	C8H15NO6	0. 2	2-Acetamido-D-glucose	[M+H-H2O]+
204.0 868	3.0 6	C12H15N5O	5. 6	4-Methyl-N-(2-propyl-2H-tetraazol-5-yl)benzamide	[M+H-C3H6-H2O]+
205.0 82	1.2 3	C18H16F3NO4	18 .7	Picoxystrobin	[M+H-C6H4F3NO] +]
205.0 863	13. 67	C12H14O4	0. 5	Terephthalic acid, butyl ester	[M+H-H2O]+
205.0 972	2.9 6	C11H12N2O2	0. 4	L-Tryptophan	[M+H]+
206.0 813	2.4 1	C17H23NO7	0. 2	4-[2-[(2-Ethyl-2,3-dihydroxybutanoyl)oxymethyl]anilino]-4-ketobutyric acid	[M+H-C6H12O4] +
207.0 644	4.8 8	C11H12O5	1. 1	Sinapic acid	[M+H-H2O]+
207.0 652	5.9 3	C11H10O4	0	O-Methylscopoletin	[M+H]+
207.0 653	3.8 9	C13H16O5	0. 5	Ethyl (2E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-2-	[M+H-C2H6O]+

				propenoate	
207.1 016	6.1 5	C12H18O5	0. 1	p-Methoxytodadiol	[M+H- 2H2O]+
207.1 13	2.4 5	C11H14N2O2	1. 1	1-(2-Methyl-4-nitrophenyl)pyrrolidine	[M+H]+
207.1 38	4.7 3	C19H30O8	0. 1	Opuntiside B	[M+H- C6H12O6] +
207.1 381	4.4 7	C13H18O2	0. 5	Aureonitol	[M+H]+
208.1 082	2.3 7	C12H14FNO	23 .9	A-967079	[M+H]+
208.1 329	2.5 1	C12H17NO2	0. 8	Phenylalanine betaine	[M+H]+
208.9 726	0.7 9	C6H4Cl2N2O2	15 .2	Botran	[M+H+2i]+
209.0 809	5.4 9	C11H12O4	1	trans-3,5-Dimethoxy-4-hydroxycinnamaldehyde	[M+H]+
209.1 173	6.1 3	C20H24O6	0. 8	3-Methoxy-4-[1-methyl-2-(3,4,5-trimethoxyphenyl)ethoxy]benzaldehyde	[M+H- C8H8O3]+
209.1 173	11. 24	C12H16O3	0. 3	cis-Asarone	[M+H]+
209.1 537	4.4	C13H22O3	3. 4	Ncgc00385600-01_c13h22o3_2-cyclohexen-1-one, 4-hydroxy-4-(3-hydroxybutyl)-3,5,5-trimethyl-	[M- H2O+H]+
210.0 763	2.6 1	C10H11NO4	0. 7	2-[(2-Methoxy-2-oxoethyl)amino]benzoic	[M+H]+

				acid	
210.0 875	2.4 7	C14H11NO	18 .3	4-Methylacridin-9-ol	[M+H] ⁺
210.1 126	3.3	C11H15NO3	1. 2	L-Tyrosine, N,O-dimethyl-	[M+H] ⁺
210.1 232	5.4 8	C10H15N3O2	0. 3	N-(3-Aminopropyl)-4-methyl-2-nitroaniline	[M+H] ⁺
210.1 239	6.6 8	C8H20NO3P	7. 6	Diethyl tert-butylamidophosphate	[M+H] ⁺
211.0 947	6.1 4	C17H26O10	11 .8	Methyl (1S)-1-(.beta.-D-glucopyranosyloxy)-6-hydroxy-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[c]pyran-4-carboxylate	[M+H- C6H12O6] +
211.1 305	3.9 7	C11H18N2S	20 .1	4-Isopropyl-3,4,5,6,7,8-hexahydro-2(1H)-quinazolinethione	[M+H] ⁺
211.1 442	4.6 4	C11H18N2O2	0. 5	Cyclo(proline-leucine)	[M+H] ⁺
211.1 693	5.7 3	C26H36O11	0. 3	4-(2,6,6-Trimethyl-4-oxocyclohex-2-en-1-yl)butan-2-yl 6-O-(3,4,5-trihydroxybenzoyl)hexopyranoside	[M+H- C13H14O9] +
212.1 03	1.5	C11H14FNO2	24	4-Fluoro-N-(2-hydroxy-1,1-dimethylethyl)benzamide	[M+H] ⁺
213.0 983	0.8 9	C13H12N2O	18 .4	1-Phenyl-6,7-dihydro-5H-indazol-4-one	[M+H] ⁺
214.1 439	4.4	C11H19NO3	0. 5	Ethyl ecgonine	[M+H] ⁺

214.1 552	3.7 7	C ₁₀ H ₁₉ N ₃ O ₂	0. 7	Propenyl-L-NIO	[M+H] ⁺
215.0 163	1.2 5	C ₆ H ₁₀ Cl ₂ N ₂ O 2	0. 1	2-Chloro-N-{2- [(chloroacetyl)amino]ethyl}a cetamide	[M+H+2i] ⁺
215.1 392	2.0 5	C ₁₀ H ₁₈ N ₂ O ₃	0. 6	Val-Pro	[M+H] ⁺
216.0 98	1.3	C ₁₃ H ₁₃ NO ₂	18 .1	TC-E 5008	[M+H] ⁺
216.1 022	3.9 2	C ₁₃ H ₁₃ NO ₂	2. 4	Phenopyrrozin	[M+H] ⁺
216.1 234	3.4 2	C ₁₁ H ₁₅ F ₂ NO	17 .9	N-(2,6-Difluorobenzyl)-1- methoxy-2-propanamine	[M+H] ⁺
216.9 507	0.6 9	C ₈ H ₂ Cl ₂ O ₃	24 .7	3,6-Dichlorophthalic anhydride	[M+H] ⁺
217.0 708	12. 27	C ₁₄ H ₁₇ N ₅ O ₆	0. 4	Adenosine, 2',3'-diacetate	[M+H- C ₅ H ₅ N ₅] ⁺
217.0 973	3.7	C ₁₂ H ₁₂ N ₂ O ₂	15 .2	L-1,2,3,4-Tetrahydro-beta- carboline-3-carboxylic acid	[M+H] ⁺
218.1 379	5.0 6	C ₁₀ H ₁₉ NO ₄	0. 1	N-(2-Hydroxy-3- methylbutanoyl)valine	[M+H] ⁺
218.1 389	4.9	C ₁₄ H ₂₇ NO ₄	0. 5	tert-Butyl [(4R,6R)-6-(2- aminoethyl)-2,2-dimethyl- 1,3-dioxan-4-yl]acetate	[M+H- C ₄ H ₈] ⁺
218.9 837	0.7	C ₅ H ₇ BrN ₄ O	17 .9	4-Bromo-1-methyl-1H- pyrazole-5-carbohydrazide	[M+H] ⁺
219.0 652	7.5 2	C ₁₆ H ₂₀ O ₆	0. 2	Toddalolactone	[M+H- C ₄ H ₁₀ O ₂] +
219.0 654	2.6 3	C ₁₆ H ₁₈ O ₄	0. 3	Rutacultin	[M+H- C ₄ H ₈] ⁺

219.1 001	5.4 8	C ₁₁ H ₁₁ FN ₄	21 .7	N4- benzyl- 6- fluoropyrimidine- 2,4- diamine	[M+H] ⁺
219.1 341	2.4 8	C ₉ H ₁₈ N ₂ O ₄	0. 8	Ser-Leu	[M+H] ⁺
219.1 389	6.4 3	C ₁₄ H ₂₂ O ₄	0. 5	trans-C 75	[M+H- 2H ₂ O] ⁺
219.1 74	13. 09	C ₁₅ H ₂₄ O ₂	0. 5	8-Hydroxyageraphorone	[M+H- H ₂ O] ⁺
219.1 744	12. 93	C ₁₅ H ₂₂ O	0. 7	Nootkatone	[M+H] ⁺
220.0 968	5.6 3	C ₁₂ H ₁₃ NO ₃	0. 7	{4- [(Cyclopropylcarbonyl)amin o]phenyl}acetic acid	[M+H] ⁺
220.1 333	9.4 7	C ₉ H ₁₃ N ₇	12 .8	Epicure MI 2AZ	[M+H] ⁺
221.1 149	7.9 9	C ₁₃ H ₁₆ O ₃	10 .6	3-Allyl-4-ethoxy-5- methoxybenzaldehyde	[M+H] ⁺
221.1 286	4.2 2	C ₁₂ H ₁₆ N ₂ O ₂	0. 4	4-(4- Methylpiperazino)benzoic acid	[M+H] ⁺
221.1 538	19. 87	C ₁₄ H ₂₀ O ₂	0. 4	2,6-Di-tert- butylbenzoquinone	[M+H] ⁺
222.1 124	3.2 2	C ₁₂ H ₁₅ NO ₃	0. 5	Butylone	[M+H] ⁺
223.0 965	10. 04	C ₁₂ H ₁₄ O ₄	0. 2	Diethyl phthalate	[M+H] ⁺
223.0 966	3.6 2	C ₁₂ H ₁₄ O ₄	0. 3	1,3-Benzodioxole, 4,5- dimethoxy-6-(1-propen- 1-yl)-	[M+H] ⁺
223.0 966	7.6 6	C ₁₂ H ₁₄ O ₄	0. 8	3,4,5- Trimethoxycinnamaldehyde	[M+H] ⁺

223.1 078	2.9 1	C ₁₁ H ₁₄ N ₂ O ₃	1	Gly-Phe	[M+H] ⁺
223.1 329	5.2	C ₁₃ H ₂₀ O ₄	0. 1	Cyclopentanecarboxylic acid, 5-(1,3-heptadien-1- yl)-2,3-dihydroxy-	[M+H- H ₂ O] ⁺
224.1 128	0.8 1	C ₈ H ₁₇ NO ₆	0. 1	N-Acetyl-D- galactosaminitol	[M+H] ⁺
224.1 257	5.8 7	C ₁₀ H ₁₉ NO ₃	0. 5	N-Boc-D-prolinol	[M+Na] ⁺
225.0 395	2.6 9	C ₁₀ H ₉ ClN ₂ O ₂	12 .9	6-Chloro-1H- benzimidazole-2- propanoic acid	[M+H] ⁺
225.1 1	4.5	C ₁₂ H ₁₇ ClN ₂	24 .9	4-(1-Azepanyl)-3- chloroaniline	[M+H] ⁺
226.0 824	2.0 8	C ₇ H ₁₆ NO ₅ P	6. 6	L-2-Amino-7- phosphonoheptanoic acid	[M+H] ⁺
226.1 55	4.5 3	C ₁₆ H ₁₉ N	17 .5	Polycain	[M+H] ⁺
226.1 802	9.3 8	C ₁₃ H ₂₃ NO ₂	0. 7	2,2,6,6-Tetramethyl-4- piperidiny methacrylate	[M+H] ⁺
227.1 027	2.3 1	C ₁₀ H ₁₄ N ₂ O ₄	0. 1	PyroGlu-Pro	[M+H] ⁺
227.1 255	3.6 1	C ₁₁ H ₁₈ N ₂ OS	18 .5	4-(Ethylaminomethyl)-2- methyl-5- [(methylthio)methyl]pyridin -3-ol	[M+H] ⁺
227.1 257	3.8 2	C ₁₁ H ₁₈ N ₂ OS	19 .4	4-(2-Ethyltetrahydro-2- methyl-2H-pyran-4-yl)-2- thiazolamine	[M+H] ⁺
227.1 278	5.5 1	C ₁₂ H ₂₀ O ₅	0. 2	3,8,9-Trihydroxy-10- propyl-3,4,5,8,9,10- hexahydro-2H-oxecin-2-	[M+H- H ₂ O] ⁺

				one	
227.1 279	4.4 2	C12H18O4	0. 1	Tuberonic acid	[M+H] ⁺
229.1 435	12. 13	C10H22O4	11 .3	Tri(propylene glycol) methyl ether	[M+Na] ⁺
229.1 547	1.3 1	C11H20N2O3	0. 2	4- (Cyclohexylcarbamoylamino)butyric acid	[M+H] ⁺
229.1 548	2.7 9	C11H20N2O3	0. 9	Leu-Pro	[M+H] ⁺
230.1 024	1.5 4	C18H17F3N6O	4. 5	1-(7H-Purin-6-yl)-N-[3- (trifluoromethyl)phenyl]ison ipcotamide	[M+H- C7H6F3N] ⁺
230.1 135	2.2 5	C14H15NO2	17 .9	4-(2,5-Dimethyl-1- pyrryl)phenylacetic acid	[M+H] ⁺
230.1 501	4.0 5	C15H22N2O	16 .3	Milnacipran	[M+H- NH3] ⁺
230.2 479	10. 91	C14H31NO	0. 4	N,N- Dimethyldodecylamine N- oxide	[M+H] ⁺
231.1 088	0.9 7	C13H14N2O2	16 .8	5-(2-Hydroxyethyl)-6- methyl-2-phenyl-4(3H)- pyrimidinone	[M+H] ⁺
231.1 339	0.8 8	C5H9NO2	0. 1	3-Pyrrolidinecarboxylic acid	[2M+H] ⁺
231.1 705	3.1 3	C11H22N2O3	1. 1	Val-Ile	[M+H] ⁺
232.0 928	1.2 2	C13H13NO3	16 .8	1,4-Dihydro-4-oxo-1- propyl-3- quinolinecarboxylic acid	[M+H] ⁺
232.0 969	1.9 8	C13H15NO4	0. 7	4'- Carbethoxyacetoacetanilide	[M+H- H2O] ⁺

232.1 656	4.5 2	C ₁₅ H ₂₁ NO	18 .7	bk-EABDI	[M+H] ⁺
233.0 593	2.7 3	C ₁₃ H ₂₁ N ₃ O ₈ S	0. 8	S-Lactoylglutathione	[M+H- C ₅ H ₉ NO ₄] +
233.1 245	0.8 1	C ₁₃ H ₁₆ N ₂ O ₂	17 .6	Aminoglutethimide	[M+H] ⁺
233.1 537	12. 58	C ₁₅ H ₂₀ O ₂	0. 2	Atractylenolide II	[M+H] ⁺
234.0 738	3.9 2	C ₁₂ H ₁₁ NO ₄	9. 3	6-Ethoxy-4-hydroxy-3-quinolinecarboxylic acid	[M+H] ⁺
234.9 612	0.6 8	C ₈ H ₆ BrFO ₂	9. 8	2-Bromo-6-fluoro-3-methylbenzoic acid	[M+H+2i] ⁺
235.0 941	6.2 3	C ₁₃ H ₁₄ O ₄	10 .4	6,7-Dimethoxy-4-ethylcoumarin	[M+H] ⁺
235.1 442	2.8 6	C ₂₂ H ₂₄ N ₂ O ₄	1	Di-p-coumarylputrescin	[M+H- C ₉ H ₆ O ₂] ⁺
235.1 693	9.3 6	C ₂₂ H ₃₀ CINO ₄ S	0. 5	ONO-8711	[M+H- C ₇ H ₈ CINO 2S] ⁺
235.1 693	5.2 1	C ₁₅ H ₂₄ O ₃	0. 5	Ageratriol	[M+H- H ₂ O] ⁺
235.1 694	13. 17	C ₁₅ H ₂₂ O ₂	0. 1	3,5-Di-tert-butylsalicylaldehyde	[M+H] ⁺
236.0 796	0.7 9	C ₉ H ₁₁ N ₅ O ₄	8. 2	D-(+)-Neopterin	[M+H- H ₂ O] ⁺
236.1 258	7.4 6	C ₁₃ H ₁₇ NO ₃	9. 6	2,3-Pentylone isomer	[M+H] ⁺
237.1 234	2.9 7	C ₁₂ H ₁₆ N ₂ O ₃	0	Ala-Phe	[M+H] ⁺
237.1	4.4	C ₁₇ H ₁₈ O ₂	16	Cyclopropyl(4-methoxyphenyl)phenylmeth	[M+H-]

234	6		.9	anol	H ₂ O]+
237.1	2.4	C ₁₂ H ₁₆ N ₂ O ₃	0.	Phe-Ala	[M+H] ⁺
235	4		7		
237.1	7.7	C ₁₄ H ₂₂ O ₄	0.	(3E,5E)-2-(4-Methoxy-4-oxobutyl)nona-3,5-dienoic acid	[M+H-H ₂ O] ⁺
486	1		1		
237.1	11.	C ₁₅ H ₂₈ O ₄	0.	6-Hydroxy-6-(3-hydroxy-2,3-dimethylcyclopentyl)-2-methylenanthic acid	[M+H-2H ₂ O] ⁺
85	87		4		
238.1	4.6	C ₁₄ H ₂₀ FNO	21	4-Fluoro IPV	[M+H] ⁺
551	3		.4		
239.1	3.4	C ₁₃ H ₁₈ O ₄	0.	1-(3-ethyl-2,4-dihydroxy-6-methoxyphenyl)butan-1-one	[M+H] ⁺
279	5		4		
239.1	14.	C ₁₀ H ₂₂ O ₆	0.	Pentaethylene glycol	[M+H] ⁺
489	54		5		
240.1	1.9	C ₁₃ H ₁₃ N ₅	5.	N-Benzyl-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine	[M+H] ⁺
23	3		1		
240.1	4.0	C ₁₁ H ₁₇ N ₃ O ₃	1.	2-Oxazolidinone, 4-hydroxy-3-[2-(1H-imidazol-4-yl)ethyl]-4,5,5-trimethyl-	[M+H] ⁺
342	7		1		
241.1	1.5	C ₁₂ H ₂₀ N ₂ O ₃	0	Ethyl 4-(1-hydroxy-1-methylethyl)-2-propyl-1H-imidazole-5-carboxylate	[M+H] ⁺
546	1		0		
241.1	11.	C ₂₁ H ₃₂ O ₂	0	3,20-Allopregnanedione	[M+H-C ₃ H ₈ O ₂] ⁺
951	88		0		
242.0	1.7	C ₁₄ H ₁₃ NO ₄	16	CCX 1959	[M+H-H ₂ O] ⁺
772	9		.3		
242.0	9.0	C ₉ H ₁₄ N ₄ O ₅	17	Acadesine	[M+H-NH ₃] ⁺
811	5		.1		

242.1 136	2.2 3	C15H18N2O2	16 .7	N-[2-(5-Methoxy-1H-indol-3-yl)ethyl]cyclopropanecarboxamide	[M+H-NH3]+
242.1 746	5.9	C13H23NO3	0. 2	N-Nonanoyl-L-homoserine lactone	[M+H]+
243.0 654	4.0 1	C15H12O6	1. 1	(-)-Aromadendrin	[M+H-CH2O2]+
243.1 016	8.5	C15H16O4	1. 6	Auraptanol	[M-H2O+H]+
243.1 342	2.6 7	C11H18N2O4	0. 7	2-Piperazinepropionic acid, 5-isobutyl-3,6-dioxo-	[M+H]+
244.1 293	2.3 6	C16H18N2O2S	15 .9	Dimethylenastron	[M+H-CHNS]+
244.1 294	2.8 1	C10H17N3O4	0. 2	Gln-Pro	[M+H]+
244.1 294	2.5 7	C13H16F3N	5. 5	4-[3-(Trifluoromethyl)benzyl]piperidine	[M+H]+
244.1 544	4.1 8	C12H21NO4	0. 9	N-3-Hydroxyoctanoyl-L-homoserine lactone	[M+H]+
245.1 383	6.1 3	C13H16N4O	5. 1	1,3,5-Trimethyl-N-2-pyridinyl-1H-pyrazole-4-acetamide	[M+H]+
245.1 86	3.9 8	C12H24N2O3	0. 5	6-(6-Aminohexanamido)hexanoic acid	[M+H]+
246.1 084	2.3 2	C12H14F3NO	5. 5	4-[3-(Trifluoromethyl)phenyl]-4-piperidinol	[M+H]+
246.1 45	2.4 9	C10H19N3O4	0. 7	Asn-Ile	[M+H]+

247.1 038	1.2 3	C13H14N2O3	15 .9	N-(1H-Indol-3-ylacetyl)alanine	[M+H] ⁺
247.1 289	2.1 7	C10H18N2O5	0. 1	gamma-l-glutamyl-l-valine	[M+H] ⁺
247.1 329	7.4 3	C15H20O4	0. 1	2-cis-4-trans-Absciscic acid	[M+H-H2O] ⁺
247.1 331	3.1 3	C15H22O5	0. 8	Dihydrophaseic acid	[M+H-2H2O] ⁺
247.1 658	18. 16	C16H24O3	10 .1	Oxacyclohexadeca-3,11,13-trien-2-one, 6-hydroxy-16-methyl-	[M-H2O+H] ⁺
247.2 42	15. 28	C19H36O2	0. 2	(12Z)-Octadecenoic acid, methyl ester	[M+H-CH6O2] ⁺
248.1 128	0.8 6	C10H17NO6	0. 1	Linamarin	[M+H] ⁺
249.1 098	7.6 4	C13H16N2OS	16 .8	1-(2-Hydroxyphenyl)-4,4,6-trimethyl-3,4-dihydro-2(1H)-pyrimidinethione	[M+H] ⁺
249.1 119	4.5 7	C14H18O5	0. 1	(+)-2,5-epi-Goniothalesdiol	[M+H-H2O] ⁺
249.1 85	13. 21	C20H32O2	0. 4	Methyl 2,4,6-tri-tert-butylbenzoate	[M+H-C4H8] ⁺
249.2 213	13. 68	C17H32O3	0. 4	5,16-Heptadecadiene-1,2,4-triol	[M+H-2H2O] ⁺
250.1 777	10. 39	C15H23NO2	9. 8	Alprenolol	[M+H] ⁺
251.1 254	8.1 8	C14H18O4	9. 2	Trolox	[M+H] ⁺
251.1 601	0.7	C21H36O6	16	[4,5-Dihydroxy-3,4-bis(hydroxymethyl)-4a,8,8-trimethyl-5,6,7,8a-	[M+H-C6H14O3] ⁺

				tetrahydro-1H-naphthalen-1-yl]hexanoate	
252.0729	2.43	C ₁₄ H ₁₈ N ₅ O ₁₁ P	0.6	Adenylsuccinic acid	[M+H-C ₅ H ₉ O ₇ P] +
252.1091	1.4	C ₁₀ H ₁₃ N ₅ O ₃	0.3	Cordycepin	[M+H] ⁺
252.1231	4.22	C ₁₃ H ₁₇ NO ₄	0.1	Acetyl tyrosine ethylester	[M+H] ⁺
252.1706	5.66	C ₂₄ H ₃₉ N ₅ O ₆	0.4	Syringolin A	[M+H-C ₁₁ H ₁₈ N ₂ O ₄] ⁺
253.01	0.79	C ₁₂ H ₁₅ N ₃ O ₃ S ₂	0.5	N-(2-Hydroxyethyl)-2-[(4-keto-5,6-dimethyl-3H-thieno[2,3-d]pyrimidin-2-yl)thio]acetamide	[M+H-C ₂ H ₇ NO] ⁺
253.1296	2.44	C ₁₃ H ₁₇ FN ₂ O ₂	20.1	4-Fluoro-N-[2-(4-morpholinyl)ethyl]benzamide	[M+H] ⁺
253.1799	12.5	C ₁₅ H ₂₄ O ₃	0.4	(+)-Sydonol	[M+H] ⁺
254.1387	2.31	C ₁₁ H ₂₁ NO ₄	10.3	Methyl N-(2-hydroxy-3-methylbutanoyl)valinate	[M+Na] ⁺
254.15	5.24	C ₁₇ H ₁₉ NO	15.3	(R)-.alpha.,.alpha.-Diphenyl-2-pyrrolidinemethanol	[M+H] ⁺
255.0651	6.88	C ₁₅ H ₁₀ O ₄	0.9	Daidzein	[M+H] ⁺
255.1203	5.78	C ₁₃ H ₁₉ ClN ₂ O	21.6	2-Chloro-N-[2-(diethylamino)ethyl]benzamide	[M+H] ⁺

256.0 928	1.2 9	C ₁₇ H ₁₆ N ₂ O ₆	15 .5	Dehydronifedipine	[M+H- C ₂ H ₃ NO ₃] +
256.1 292	2.8	C ₁₁ H ₂₀ FNO ₃	10 .5	tert-Butyl 4-fluoro-4-(hydroxymethyl)piperidine-1-carboxylate	[M+Na] ⁺
256.2 634	15. 13	C ₁₆ H ₃₃ NO	0	Palmitamide	[M+H] ⁺
257.0 808	6.8 3	C ₁₅ H ₁₂ O ₄	1. 6	Pinocembrin	[M+H] ⁺
257.0 808	4.7 8	C ₁₅ H ₁₂ O ₄	0. 5	Liquiritigenin	[M+H] ⁺
257.1 359	4.6 3	C ₁₂ H ₂₀ N ₂ O ₂ S	16 .4	Sulfanilamide, N1-hexyl-	[M+H] ⁺
257.1 609	2.4 1	C ₁₆ H ₂₀ N ₂ O	15 .4	Fordimine	[M+H] ⁺
257.1 9	11. 96	C ₁₈ H ₂₈ O ₃	0. 2	4-Hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one	[M+H- 2H ₂ O] ⁺
257.1 9	11. 59	C ₁₉ H ₂₈ O ₃	0. 2	19-Hydroxytestosterone	[M+H- CH ₄ O ₂] ⁺
258.1 449	3.3 1	C ₁₈ H ₂₁ NO ₄	15 .8	1,8-Diethyl-1,3,4,9-tetrahydro-4-oxo-pyrano[3,4-b]indole-1-acetic acid methyl ester	[M+H- C ₂ H ₂ O ₂] ⁺
258.1 449	3.9 3	C ₁₆ H ₁₉ NO ₂	15	BB-22 3-carboxyindole metabolite	[M+H] ⁺
259.0 925	1.2 5	C ₅ H ₇ NO ₃	0. 1	D-Pyroglutamic acid	[2M+H] ⁺
259.1 766	5.9 4	C ₁₆ H ₂₄ N ₂ O ₂	15 .9	Norsufentanil	[M+H- H ₂ O] ⁺

260.1 282	5.8 9	C ₁₅ H ₁₇ NO ₃	0. 7	3-Acetyl-7- diethylaminocoumarin	[M+H] ⁺
260.1 607	2.5	C ₁₁ H ₂₁ N ₃ O ₄	0. 8	Gln-Leu	[M+H] ⁺
260.1 969	1.3 8	C ₁₂ H ₂₅ N ₃ O ₃	0. 8	Lys-Ile	[M+H] ⁺
261.1 122	6.3 9	C ₁₅ H ₁₆ O ₄	1. 5	Isomeranzin	[M+H] ⁺
261.1 194	2.0 6	C ₁₆ H ₁₂ N ₄	23 .2	MMV023233	[M+H] ⁺
261.1 309	18. 38	C ₁₃ H ₁₆ N ₄ O ₂	14 .2	Diaveridine	[M+H] ⁺
261.1 446	2.6 7	C ₁₁ H ₂₀ N ₂ O ₅	0. 4	Glu-Ile	[M+H] ⁺
261.1 462	11. 07	C ₁₁ H ₂₀ N ₂ O ₅	6. 2	Leu-Glu	[M+H] ⁺
262.0 688	0.8	C ₁₃ H ₁₂ ClN ₃ O	20 .3	N-(4-Chlorophenyl)-N'-(5- methyl-2-pyridinyl)urea	[M+H] ⁺
262.1 285	1.2 2	C ₁₁ H ₁₉ NO ₆	2. 2	Mycosporine	[M+H] ⁺
262.1 414	8.6 2	C ₁₄ H ₁₉ N ₃ S	16 .1	Methapyrilene	[M+H] ⁺
263.1 278	7.6 9	C ₂₀ H ₂₆ O ₆	0. 1	3',5a'-Dimethyl-2'- oxodecahydro-2'H- spiro[oxirane-2,8'- oxireno[6,7]naphtho[1,2- b]furan]-6'-yl (2Z)-2- methylbut-2-enoate	[M+H- C ₅ H ₈ O ₂] ⁺
263.1 392	3.2 1	C ₁₄ H ₁₈ N ₂ O ₃	0. 8	Phe-Pro	[M+H] ⁺
263.1 754	5.0 5	C ₂₂ H ₃₀ O ₄	15 .4	Cafestol acetate	[M+H- C ₂ H ₈ O ₄] ⁺

263.2 369	14. 69	C18H32O2	0. 5	Linoelaidic acid	[M+H- H2O]+
265.1 071	5.0 1	C34H46O18	0. 1	Syngaresinol diglucoside	[M+H- C20H30O1 3]+
265.1 295	2.4 7	C18H23FN2O2	19	NAD 299	[M+H- C4H6]+
265.1 433	7.0 5	C15H20O4	0. 3	Peruvinine	[M+H]+
265.1 434	8.3 2	C15H20O4	0. 5	2,2a,6,6a,7a,8,9,9a- Octahydro-1a,5,7a- trimethylbisoxireno[4,5:8,9] cyclodeca[1,2-b]furan- 4(1aH)-one	[M+H]+
265.1 435	4.1 4	C21H32O10	0. 7	1-O-((2E,4E)-5- ((1R,3S,5S,8S)-3,8- Dihydroxy-1,5-dimethyl-6- oxabicyclo[3.2.1]octan-8- yl)-3-methylpenta-2,4- dienoyl)-.beta.-D- glucopyranose	[M+H- C6H12O6] +
265.1 547	3.6	C14H20N2O3	4. 3	Phenylalanyl-Valine	[M+H]+
265.1 548	3.2 4	C14H20N2O3	0. 1	Phe-Val	[M+H]+
265.1 551	3.0 9	C14H20N2O3	0. 5	Triamcinolone diacetate	[M+H]+
265.2 518	15. 29	C21H40O4	0. 1	Monoelaidin	[M+H- C3H8O3]+
266.1 176	6.9 7	C17H17NO3	0. 7	3-Phenyl-N- (phenylacetyl)-.beta.- alanine	[M+H- H2O]+
266.1	5.4	C14H19NO4	8.	Anisomycin	[M+H]+

364			5		
266.1 727	9.3 8	C15H23NO3	9. 2	Oxprenolol	[M+H] ⁺
267.1 089	1.9 6	C16H14N2O2	14 .6	1H-1,4-Benzodiazepine- 2,5-dione, 3-benzyl-3,4- dihydro-, L-	[M+H] ⁺
267.1 203	6.6 6	C14H18O5	8. 8	3',4'-Dihydroinfectopyrone	[M+H] ⁺
267.1 339	2.9 7	C13H18N2O4	0. 3	Phe-Thr	[M+H] ⁺
268.0 929	3.3 6	C16H13NO3	15 .1	2-Indolinone, 3-hydroxy- 3-phenacyl-	[M+H] ⁺
268.0 929	2.4 5	C16H15NO4	14 .3	2-[[2- Methylphenoxy)acetyl]amin o}benzoic acid	[M+H- H2O] ⁺
268.1 039	1.3 2	C10H13N5O4	0. 8	Adenosine	[M+H] ⁺
269.1 148	9.1 3	C17H16O3	8. 5	2'-Hydroxy-5'-methyl-2- methoxychalcone	[M+H] ⁺
269.1 36	5.9 6	C17H22N4O2	13 .2	Resiquimod	[M+H- C2H6O] ⁺
269.1 609	3.4 7	C12H20N4O3	0. 3	His-Leu	[M+H] ⁺
270.1 124	5.9 8	C16H17NO4	0. 2	Panracine	[M+H- H2O] ⁺
270.1 812	5.9 3	C18H23NO	14 .5	Orphenadrine	[M+H] ⁺
270.1 925	2.5 9	C24H29N3O2	14 .5	FK-866	[M+H- C7H6O2] ⁺
271.0 6	6.8 3	C15H10O5	0. 2	3'-Hydroxydaidzein	[M+H] ⁺

271.0 965	7.2 9	C16H14O4	0. 4	(.+/-)-Medicarpin	[M+H] ⁺
271.1 038	2.0 6	C15H14N2O3	14 .3	6-(1-Naphthyl)-5-nitro-2-piperidinone	[M+H] ⁺
271.1 154	3.5 5	C14H14N4O2	13 .5	N,N'-Ethylenebis(nicotinamide)	[M+H] ⁺
271.1 651	4.7 4	C18H22O2	15 .1	Trenbolone	[M+H] ⁺
271.1 765	3.2 2	C17H22N2O	14 .8	5-Methoxy DALT	[M+H] ⁺
272.0 917	10. 55	C14H13N3OS	24 .5	N-Benzoyl-N'-(6-methyl-2-pyridinyl)thiourea	[M+H] ⁺
272.1 492	4.7 4	C14H17N5O	4. 9	N-(4,6-Dimethyl-2-pyrimidinyl)-N'-(4-methoxyphenyl)guanidine	[M+H] ⁺
272.1 604	4.5 7	C11H21N5OS	24 .1	Methoprotrotryne	[M+H] ⁺
272.1 606	4.7 9	C24H27NO4	13 .9	Adaphostin	[M+H- C7H6O2] ⁺
272.1 968	5.2 9	C18H25NO	14 .6	Dextromethorphan	[M+H] ⁺
273.0 757	5.0 5	C15H12O5	0. 5	Naringenin chalcone	[M+H] ⁺
273.1 193	0.9	C13H18N2O3	6	N'-Caproyl-2-hydroxybenzohydrazide	[M+Na] ⁺
273.1 558	2.4 8	C16H22N2O3	14 .8	8-Hydroxy-5-[1-hydroxy-2-(isopropylamino)butyl]-2(1H)-quinolinone	[M+H- H2O] ⁺
273.1 849	10. 78	C20H28O4	0. 3	Foetidin	[M+H- C2H4O2] ⁺
274.0	7.3	C12H13NO5	8.	2-Carboxymalonanilic acid,	[M+Na] ⁺

709	7		4	ethyl ester	
274.1 033	1.3	C17H13N3O2	21	N-(4-Phenoxyphenyl)-2-pyrazinecarboxamide	[M+H-H2O]+
274.1 398	2.3 8	C14H21NO3	6	Furmecyclox	[M+Na]+
274.1 398	2.0 7	C15H16FN3O	17 .6	N-Acetylretigabine	[M+H]+
274.1 438	3.6 9	C13H23NO3S	11 .9	N-[(4-Methylcyclohexyl)carbonyl]methionine	[M+H]+
274.1 761	4.4 6	C17H23NO2	14 .9	Tilidine	[M+H]+
275.1 601	3.9 7	C15H24O3	6. 1	Sydonol	[M+Na]+
275.1 618	12. 5	C15H24O3	0. 1	Illicic acid	[M+Na]+
275.1 713	1.5 3	C11H22N4O4	0. 5	Gln-Lys	[M+H]+
276.1 232	3.0 8	C15H17NO4	0. 8	Dubinidine	[M+H]+
276.1 806	4.1 4	C13H22O5	1	Octyl .alpha.-ketoglutarate	[M+NH4]+
277.2 162	11. 88	C18H34O5	0. 1	15-Octadecenoic acid, 9,12,13-trihydroxy-	[M+H-3H2O]+
277.2 162	12. 93	C18H30O3	0. 1	9-Oxo-10(E),12(E)-octadecadienoic acid	[M+H-H2O]+
279.1 59	13. 67	C16H22O4	0. 4	Butyl terephthalate	[M+H]+
279.1 704	4.4 7	C15H22N2O3	0. 1	Phe-Leu	[M+H]+
279.1	4.2	C15H22N2O3	0.	Phe-Ile	[M+H]+

704	3		1		
279.2	13.		0.		
319	47	C18H32O3	3	Laetisaric acid	[M+H-H2O]+
279.2	12.		0.		
319	39	C18H32O3	2	9(10)-EpOME	[M+H-H2O]+
280.1	7.2		12		
522	5	C16H17N5	.3	MLS000061860	[M+H]+
281.1	3.1		0.		
133	9	C13H16N2O5	3	Aspartylphenylalanine	[M+H]+
281.1	2.4		0.		
497	2	C14H20N2O4	2	Tyr-Val	[M+H]+
282.1	2.0		0		
197	5	C11H15N5O4	0	2'-O-Methyladenosine	[M+H]+
282.1	7.0		0.		
699	5	C15H23NO4	2	Cycloheximide	[M+H]+
282.2	15.		0.		
791	29	C18H35NO	2	Oleamide	[M+H]+
283.0	9.7		8.		
942	1	C17H14O4	2	7,3'-Dimethoxyflavone	[M+H]+
283.1	3.3		14		
289	7	C18H20O4	.1	1-(3,4-Dihydroxyphenyl)-2,3-dimethyltetralin-6,7-diol	[M+H-H2O]+
283.1	1.7		13		
401	5	C17H18N2O2	.9	p-Malonotoluidide	[M+H]+
283.1	6.5		13		
516	3	C16H21N5O	.1	2-Amino-5-guanidino-N-(2-naphthyl)valeramide	[M+H-NH3]+
283.1	5.9		0.		
54	6	C15H24O6	2	Zinndiol	[M+H-H2O]+
283.1	4.4		5		
765	3	C12H26O7	5	Hexaethylene glycol	[M+H]+
284.0	2.1		14		
		C16H13NO4	14	2-	[M+H]+

878	8		.3	(Phenacylcarbamoyl)benzoic acid	
284.1 214	1.9 4	C17H17NO3	13 .7	3,4-Methylenedioxy-N-benzylcathinone	[M+H] ⁺
284.1 28	6.4 2	C17H17NO3	0. 2	Paprazine	[M+H] ⁺
284.2 947	16	C18H37NO	0. 2	Stearamide	[M+H] ⁺
285.0 757	7.5 6	C16H12O5	1. 9	Biochanin A	[M+H] ⁺
285.1 193	1.9 6	C11H16N4O5	0	Glu-His	[M+H] ⁺
285.1 194	2.7 5	C11H16N4O5	0. 5	His-Glu	[M+H] ⁺
285.1 308	5.5 1	C15H16N4O2	12 .7	N-{2-[(3-Pyridinylcarbonyl)amino]propyl}nicotinamide	[M+H] ⁺
285.1 922	4.1 7	C13H24N4O3	0. 1	MIF, amide	[M+H] ⁺
286.1 649	6.2 5	C13H23N3O2S	23 .7	Benzenamine, N,N-dimethyl-4-(1-piperidinylmethyl)-	[M+H] ⁺
286.1 762	5.4	C18H20O2	13 .8	3,6-Diphenylcyclohexane-1,2-diol	[M+NH4] ⁺
287.0 55	5.2	C15H10O6	0. 7	Kaempferol	[M+H] ⁺
287.0 877	10. 82	C16H14O5	20 .3	Sakuranetin	[M+H] ⁺
287.0 909	6.8 8	C16H14O5	0. 4	Ponciretin	[M+H] ⁺
287.1	7.0	C16H18N2OS	13	Pifithrin- α .	[M+H] ⁺

246	5		.3		
287.1 714	3.3 7	C18H22O3	24 .9	4-Hydroxyestrone	[M+H] ⁺
287.1 715	2.8 6	C17H22N2O2	13 .7	N-(2,6-Diisopropylphenyl)- 5-methyl-3- isoxazolecarboxamide	[M+H] ⁺
287.2 006	14. 22	C19H26O2	0. 1	Tetrahydrocannabivarin	[M+H] ⁺
288.0 866	9.2 6	C9H14N5O4P	4	Tenofovir	[M+H] ⁺
288.1 23	5.0 5	C16H17NO4	0. 1	Lycorine	[M+H] ⁺
288.1 666	2.0 7	C16H23N3O3	13 .7	N-Acetyl-.beta.-alanyl-N- (2-phenylethyl)-.beta.- alaninamide	[M+H- H2O] ⁺
288.1 917	5.2 9	C16H21NO2	18 .9	2-Heptyl-3-hydroxy- quinolone	[M+H] ⁺
289.0 706	4.4 8	C15H12O6	0. 4	Eriodictyol	[M+H] ⁺
289.0 708	4.0 1	C15H12O6	0. 5	Maesopsin	[M+H] ⁺
289.0 917	2.1 9	C12H16O8	0. 7	Dianthoside	[M+H] ⁺
289.1 07	10. 22	C22H27ClO10	0. 4	4,5-Epoxy-8,9-dihydroxy- 1(10),11(13)- germacradien-12,6-olid- 14-oic acid, 8-(3-Chloro- 2-hydroxy-2- methylpropanoyl), 9-A	[M+H- C6H11ClO5] ⁺
289.1 798	11. 24	C18H28O5	0. 2	Hymeglusin	[M+H- 2H2O] ⁺
290.1	2.1	C16H19NO4	14	Zephyranthine	[M+H] ⁺

345	1				
291.0 627	9.7 1	C14H14N2OS2	2. 6	N-(2,6-Dimethylphenyl)- N'-(2- thienylcarbonyl)thiourea	[M+H] ⁺
291.0 863	4.6 4	C15H18O8	0. 2	3-[5-(3,4-dihydroxy-4- methyl-5-oxooxolan-2-yl)- 2-hydroxy-4- methoxyphenyl]propanoic acid	[M+H- 2H2O] ⁺
291.0 863	3.3 8	C15H14O6	1. 3	Epicatechin	[M+H] ⁺
291.0 974	5.0 4	C14H14N2O5	0. 1	N-Malonyltryptophan	[M+H] ⁺
291.1 815	1.9 6	C21H24O2	24 .9	Gestrinone	[M+H- H2O] ⁺
291.1 955	10. 78	C20H30O5	0. 5	4-Acetoxy-8-(3-keto-2- pent-2-enylcyclopenten-1- yl)caprylic acid	[M+H- C2H4O2] ⁺
292.1 178	2.2 5	C19H27NO7	0. 2	Bruceolline F	[M+H- C4H10O2] +
292.1 292	3.4	C14H17N3O4	0. 4	Ser-Trp	[M+H] ⁺
292.1 519	8.3 6	C13H22O4S	20	Isopropyl (1S)-(+)-10- camphorsulfate	[M+NH4] ⁺
293.2 103	12. 59	C18H28O3	0. 1	Tetrahydrodicranenone B	[M+H] ⁺
293.2 111	11. 51	C19H34O5	0. 7	Methyl (9Z,14Z)-12,13,16- trihydroxyoctadeca-9,14- dienoate	[M+H- CH6O2] ⁺
294.1 546	1.5 2	C12H23NO7	3. 7	N-fructosyl isoleucine	[M+H] ⁺

294.1 812	2.0 4	C15H23N3O3	0. 4	Phe-Lys	[M+H] ⁺
295.1 289	3.9 3	C19H18O3	13 .3	Dianisalacetone	[M+H] ⁺
295.1 289	2.3	C14H18N2O5	0. 6	Phe-Glu	[M+H] ⁺
295.1 29	3.4 7	C14H18N2O5	0	gamma- Glutamylphenylalanine	[M+H] ⁺
295.1 516	6.9 8	C27H25ClN4O 2	12 .6	MK2 Inhibitor IV	[M+H- C10H7ClO] +
295.1 654	3.5	C15H22N2O4	0. 7	Tyr-Leu	[M+H] ⁺
295.2 267	13. 59	C18H30O3	0. 5	13-Oxo-ODE	[M+H] ⁺
296.0 66	0.7 9	C8H20NO6P	0. 5	Glycerophosphocholine	[M+K] ⁺
297.0 349	0.7 5	C13H10N2O3S	15 .9	2-Phenyl-5- sulfobenzimidazole	[M+Na] ⁺
297.0 582	12. 8	C10H20N2S4	0	Disulfiram	[M+H] ⁺
297.1 672	7.3 3	C16H25ClN2O	18 .9	N,N-Dibutyl-N'-(3-chloro- 2-methylphenyl)urea	[M+H] ⁺
297.2 213	11. 3	C21H34O4	0. 3	Allotetrahydro compound B	[M+H- 3H2O] ⁺
297.2 213	12. 56	C21H32O3	0. 2	21-Hydroxypregnenolone	[M+H- 2H2O] ⁺
298.0 97	2.7 8	C11H15N5O3S	0. 3	5'-S-Methyl-5'- thioadenosine	[M+H] ⁺
298.1 146	2.0 7	C11H15N5O5	0. 8	2-Methylguanosine	[M+H] ⁺

298.1 762	6	C19H23NO2	13 .6	N-(2,3-Dimethoxybenzyl)- 1,2,3,4-tetrahydro-1- naphthalenamine	[M+H] ⁺
299.0 914	8.4 1	C17H14O5	0. 4	3',4'-Dimethoxyflavonol	[M+H] ⁺
299.0 914	9.8 3	C17H14O5	0. 2	Galangin-5,7-dimethyl ether	[M+H] ⁺
299.1 465	6.6 7	C16H18N4O2	12 .3	Nialamide	[M+H] ⁺
299.2 077	5.0 7	C20H26O2	23 .5	Norethindrone	[M+H] ⁺
299.2 078	4.9 1	C20H28O3	24 .1	Polyalthic acid	[M+H- H2O] ⁺
300.1 229	5.5 8	C16H17N3OS	21 .9	N-Benzoyl-N'-[4- (dimethylamino)phenyl]thio urea	[M+H] ⁺
300.1 417	8.1 5	C15H17N5O2	12 .3	2-[(6-Ethoxy-4-methyl-2- quinazolinyl)amino]-5,6- dihydro-4-pyrimidinol	[M+H] ⁺
300.1 918	6.9 3	C19H25NO2	13 .3	Nylidrin	[M+H] ⁺
301.0 706	8.7 4	C21H20O6	0. 1	5'-Prenylpratensein	[M+H- C5H8] ⁺
301.0 706	9.5 2	C22H22O11	0. 2	5-Hydroxy-2-(5-hydroxy- 7-methoxy-4-oxo-4H- chromen-3- yl)phenyl .beta.-D- glucopyranoside	[M+H- C6H10O5] +
301.0 708	4.1	C16H12O6	1. 2	3-(2,3-dihydroxy-4- methoxyphenyl)-7- hydroxy-4H-chromen-4- one	[M+H] ⁺

301.1 409	13. 67	C ₁₈ H ₂₀ O ₄	8. 1	2,3',4,5'- Tetramethoxystilbene	[M+H] ⁺
301.1 87	2.1 1	C ₁₉ H ₂₄ O ₃	23 .9	Adrenosterone	[M+H] ⁺
301.1 871	4.3 8	C ₁₉ H ₂₄ O ₃	24 .5	19-Oxoandrostenedione	[M+H] ⁺
302.2 073	6.1 2	C ₁₉ H ₂₇ NO ₂	13 .6	2'-Piperidinoethyl 1- phenylcyclopentanecarboxy late	[M+H] ⁺
302.3 053	11. 9	C ₁₈ H ₃₉ NO ₂	0. 1	Sphinganine (d18:0)	[M+H] ⁺
303.0 499	4.6 9	C ₁₅ H ₁₀ O ₇	0. 8	Morin	[M+H] ⁺
303.0 991	7.0 5	C ₂₀ H ₁₄ O ₃	8. 1	2'-Methoxy-7,8- benzoflavone	[M+H] ⁺
303.1 299	1.2 2	C ₁₆ H ₁₈ N ₂ O ₄	13 .5	4-[formyl(6- methoxyquinolin-8- yl)amino]pentanoic acid	[M+H] ⁺
303.2 027	3.6 3	C ₁₉ H ₂₆ O ₃	23 .7	6.beta.-Hydroxyboldenone	[M+H] ⁺
304.1 138	1.2 2	C ₁₃ H ₂₂ NO ₃ PS	2. 8	Fenamiphos	[M+H] ⁺
305.1 57	18. 2	C ₂₁ H ₂₈ O ₆	11 .4	16.alpha.- Hydroxyprednisolone	[M+H- 4H ₂ O] ⁺
305.1 572	3.0 4	C ₂₀ H ₂₀ N ₂ O	24 .8	4-Butyl-N-(3- quinolyl)benzamide	[M+H] ⁺
305.1 819	3.1 9	C ₁₈ H ₂₄ O ₄	23 .6	6-Amyl-2-isopropenyl-4- methoxycoumaran-7- carboxylic acid	[M+H] ⁺
306.1 338	2.4 7	C ₁₆ H ₁₉ NO ₅	0. 8	m- Hydroxybenzoylecgonine	[M+H] ⁺

306.2 791	14. 4	C20H35NO	0. 1	(2E,4E,10Z)-N- Isobutylhexadeca-2,4,10- trienamide	[M+H] ⁺
307.0 576	7.2 8	C20H16CIN3O 2	18 .7	CPI-0610	[M+H- C2H5NO] ⁺
307.1 176	5.2	C18H14N4O4	4. 7	4,4'-(Pyrimidine-2,4- diyl-diimino)dibenzoic acid	[M+H- CO2] ⁺
307.2 267	15. 14	C19H30O3	0. 3	17-Epioxandrolone	[M+H] ⁺
307.2 267	12. 93	C19H30O3	0. 7	Oxandrolone	[M+H] ⁺
308.1 524	12. 17	C16H22CIN3O	0. 3	Tebuconazol	[M+H] ⁺
308.2 179	0.6 8	C18H29NO3	12 .8	Gabapentin related compound D	[M+H] ⁺
309.1 557	2.0 2	C19H20N2O2	13	Phenylbutazone	[M+H] ⁺
309.2 059	10. 95	C18H30O5	0. 4	2-Furanacetic acid, 5- (2,12-dihydroxy-3,6- dodecadien-1- yl)tetrahydro-	[M+H- H2O] ⁺
310.3 103	16. 08	C20H39NO	0. 6	Oleoyl ethylamide	[M+H] ⁺
311.0 737	2.1 4	C12H14N4O4S	23 .1	Sulfadimethoxine	[M+H] ⁺
311.1 465	7.4 4	C15H17F3N4	4. 7	4-(4-Methyl-1,4-diazepan- 1-yl)-2- (trifluoromethyl)quinazoline	[M+H] ⁺
312.1 44	1.2 2	C22H19NO2	18 .8	Phthalimidine, 2,3- dibenzyl-3-hydroxy-	[M+H- H2O] ⁺
312.1 552	6.9 7	C17H23NO3	5. 8	L-Hyoscyamin	[M+Na] ⁺

312.1 651	1.5 5	C13H21N5O4	4. 4	Xanthinol	[M+H] ⁺
313.1 069	10. 61	C18H16O5	0. 4	2',5,6-Trimethoxyflavone	[M+H] ⁺
313.1 543	4.7 1	C18H20N2O3	0. 1	Phe-Phe	[M+H] ⁺
313.1 797	14. 85	C20H26O4	0. 6	Carnosol	[M+H- H2O] ⁺
313.1 869	5.1 8	C17H23F3N2	5. 6	1-Cyclopentyl-4-[2-(trifluoromethyl)benzyl]piperazine	[M+H] ⁺
313.2 351	13. 58	C20H28N2O	24 .8	1-(1-Piperidiny)-3-(1,2,3,4-tetrahydro-9H-carbazol-9-yl)-2-propanol	[M+H] ⁺
314.1 709	5.4 4	C19H23NO3	13 .3	Codethyline	[M+H] ⁺
314.1 962	5.0 1	C16H27NO5	0. 4	Heliotrine	[M+H] ⁺
315.0 69	3.2 2	C12H14N2O6S	13 .8	1-[(4-Nitrophenyl)sulfonyl]piperidine-4-carboxylic acid	[M+H] ⁺
315.0 71	2.9 1	C13H19BrN2O 2	2. 4	2C-B-BZP	[M+H] ⁺
315.0 862	8.4 1	C17H14O6	2	7,8-dihydroxy-6-methoxy-3-(4-methoxyphenyl)-4H-chromen-4-one	[M+H] ⁺
315.0 862	7.3 9	C17H14O6	0. 8	Odoratin	[M+H] ⁺
315.2 028	3.5 7	C20H26O3	23 .2	6-Oxirane boldenone	[M+H] ⁺
315.2 028	3.7 6	C20H28O4	23 .4	7,15-Dihydroxyabieta-8,11,13-trien-18-oic acid	[M+H- H2O] ⁺

315.2 028	4.0 4	C20H29FO4	23 .9	6.beta.- Hydroxyfluoxymesterone	[M+H- H3FO]+
315.2 318	11. 3	C21H36O5	0	Cortol	[M+H- 3H2O]+
316.1 867	5.9 3	C19H25NO3	12 .5	2-Benzyl-4-(octahydro- 2H-isoindol-2-yl)-4- oxobutanoic acid	[M+H]+
316.1 868	4.8	C19H25NO3	12	Piperolein A	[M+H]+
316.2 847	11. 85	C18H37NO3	0. 3	Dehydrophytosphingosine (not validated, isomer of 1677)	[M+H]+
317.1 209	3.5 3	C18H17FO4	7. 3	4-Fluoro-2',4',6'- trimethoxychalcone	[M+H]+
317.2 068	6.6 9	C20H29FO3	13	Testoral	[M+H- HF]+
317.2 087	12. 96	C20H30O4	7. 6	1,10a-Dihydroxy- 4,4,7,11b-tetramethyl- 1,2,3,4a,5,6,6a,7,11,11a- decahydronaphtho[2,1- f][1]benzofuran-9-one	[M+H- H2O]+
318.1 465	11. 48	C19H21NO2	0. 2	URB 602	[M+Na]+
318.1 813	4.4	C17H23N3O3	0. 1	Leu-Trp	[M+H]+
318.2 024	3.6 8	C19H27NO3	12 .7	PRE-084	[M+H]+
318.3 002	10. 85	C18H39NO3	0. 5	Phytosphingosine	[M+H]+
319.0 812	6.2 7	C16H14O7	0. 4	Lecanoric acid	[M+H]+
319.1	3.0	C18H26O7	8	Propofol glucuronide	[M+H-

514	4				2H ₂ O]+
319.2	13.		7.		
244	93	C ₂₀ H ₃₀ O ₃	8	15-OxoETE	[M+H]+
320.1	3.0		0.		
242	7	C ₁₅ H ₁₇ N ₃ O ₅	3	Asp-Trp	[M+H]+
320.2	13.		7.		
56	92	C ₂₀ H ₃₅ NO ₃	7	Linoleoylglycine	[M+H-H ₂ O]+
322.1	5.5		7.		
049	8	C ₁₉ H ₁₅ NO ₄	1	Berberrubine	[M+H]+
322.1	2.0				
874	8	C ₁₅ H ₂₃ N ₅ O ₃	0	Phe-Arg	[M+H]+
323.0	3.2		23		
738	4	C ₁₇ H ₁₂ N ₂ O ₆	.8	2-Isoindolinepropionic acid, .beta.-(m-nitrophenyl)-1,3-dioxo-	[M+H-H ₂ O]+
323.0	9.6				
889	5	C ₁₇ H ₁₆ O ₅	0	1-(3,4-Dihydroxy-2,6-dimethoxyphenyl)-3-phenylprop-2-en-1-one	[M+Na]+
323.1	6.7		4.		
465	1	C ₁₂ H ₂₄ N ₂ O ₉	7	Chitobiose	[M+H-H ₂ O]+
324.1	2.0		19		
442	7	C ₁₉ H ₁₈ FN ₃ O	.8	Rucaparib	[M+H]+
324.2	14.		0.		
897	48	C ₂₀ H ₃₉ NO ₃	1	C-2 Ceramide	[M+H-H ₂ O]+
325.1	6.5		0.		
069	7	C ₂₇ H ₃₀ O ₁₂	5	1,3,4-Trihydroxy-5-(((2E)-3-(2-(4-hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-methoxy-2,3-dihydro-1-benzofuran-5-yl)prop-2-enoyl)oxy)cyclohexanecarboxylic acid	[M+H-C ₈ H ₁₄ O ₇]+
325.1	0.9	C ₁₂ H ₂₂ O ₁₁	0.	D-Turanose	[M+H-

128	4		2		H ₂ O]+
325.1	3.9	C ₁₅ H ₂₀ N ₂ O ₆	0.	SCHEMBL22285878	[M+H] ⁺
393	8		5		
325.1	7.1	C ₁₂ H ₂₄ N ₂ O ₈	4.	5-(Galactosylhydroxy)-L-lysine	[M+H] ⁺
621	7		9		
325.2	15.	C ₂₀ H ₃₈ O ₄	6.	Prostaglandin F ₁ .alpha. alcohol	[M+H- H ₂ O] ⁺
713	63		9		
326.1	3.7	C ₂₀ H ₂₃ NO ₃	12	(E)-N-Homoveratryl-N-methyl-3-phenylacrylamide	[M+H] ⁺
711	1		.1		
327.0	11.	C ₉ H ₁₈ Cl ₃ O ₄ P	0.	Tri(3-chloropropyl) phosphate	[M+H] ⁺
081	44		1		
327.0	12.	C ₁₈ H ₁₅ O ₄ P	0.	Triphenyl phosphate	[M+H] ⁺
78	87		7		
327.1	5.9	C ₂₀ H ₂₂ O ₄	22	Dehydrodiisoeugenol	[M+H] ⁺
663	8		.1		
328.1	2.2	C ₁₅ H ₂₁ NO ₇	0.	N-Fructosyl phenylalanine	[M+H] ⁺
39	4		8		
328.1	3.2	C ₁₇ H ₂₉ NO ₃ S	22	Sethoxydim	[M+H] ⁺
868	7		.2		
329.0	11.	C ₉ H ₁₈ Cl ₃ O ₄ P	1	Tris(2-chloroisopropyl) phosphate	[M+H+2i] ⁺
051	44				
329.1	11.	C ₂₉ H ₃₄ O ₁₅	0.	7,8-Dimethoxy-3-(4-methoxyphenyl)-4-oxo-4H-chromen-5-yl 2-O-pentopyranosylhexopyranoside	[M+H- C ₁₁ H ₁₈ O ₉] +
02	8		4		
329.1	11.	C ₂₀ H ₂₄ O ₄	7.	5-Geranoxy-7-methoxycoumarin	[M+H] ⁺
724	54		1		
329.1	3.4	C ₂₀ H ₂₄ O ₄	22	4-[5-(3,4-Dimethoxyphenyl)-3,4-dimethyloxolan-2-yl]phenol	[M+H] ⁺
82	8		.3		

329.2 07	7.5 6	C ₂₁ H ₂₈ O ₃	12	10.beta.- Hydroxy-.DELTA.4-tibolone	[M+H] ⁺
329.2 183	4.9 7	C ₁₅ H ₂₈ N ₄ O ₄	0	Peramivir	[M+H] ⁺
330.0 596	1.2 2	C ₁₀ H ₁₂ N ₅ O ₆ P	0. 8	cAMP	[M+H] ⁺
330.1 658	5.5 7	C ₁₉ H ₂₃ NO ₄	12 .6	G 642	[M+H] ⁺
330.1 659	4.4 3	C ₁₉ H ₂₃ NO ₄	11 .2	Sinomenine	[M+H] ⁺
331.1 152	7.5 2	C ₁₆ H ₂₀ O ₆	0. 4	3-(2,4-Dihydroxypentyl)- 6,8-dimethoxyisocoumarin	[M+Na] ⁺
331.1 862	6.8 7	C ₁₉ H ₂₆ FN ₃ O ₂	14 .5	5-Fluoro ABICA	[M+H- NH ₃] ⁺
331.1 903	14. 84	C ₂₀ H ₂₆ O ₄	0. 3	7-[2-(3-Furyl)ethyl]-5- hydroxy-7,8-dimethyl- 5,6,6a,8,9,10-hexahydro- 1H-benz[d]isobenzofuran- 3-one	[M+H] ⁺
332.1 816	5.1 3	C ₁₈ H ₂₅ FN ₄ O ₂	14 .6	5-Fluoro AB-PINACA	[M+H- NH ₃] ⁺
332.2 18	3.6 7	C ₁₅ H ₂₉ N ₃ O ₅	0. 2	Thr-Val-Leu	[M+H] ⁺
333.0 604	4.9 8	C ₂₂ H ₂₂ O ₁₂	0. 1	Mearnsitrin	[M+H- C ₆ H ₁₀ O ₄] +
333.0 693	0.8	C ₁₂ H ₁₄ N ₄ O ₄ S	20 .4	Sulfadoxin	[M+Na] ⁺
333.1 826	13. 58	C ₂₀ H ₂₅ FO ₃	10 .4	17-Oxodexamethasone	[M+H] ⁺
333.2 036	11. 96	C ₂₀ H ₃₀ O ₅	7. 5	Andrographolide	[M+H- H ₂ O] ⁺

333.2 132	3.8 2	C20H28O4	20 .9	5-[2-(3-Furyl)ethyl]-8-hydroxy-5,6,8a-trimethyl-3,4,4a,6,7,8-hexahydronaphthalene-1-carboxylic acid	[M+H] ⁺
333.2 133	3.3 2	C20H28O4	21 .7	Hautriwaic acid	[M+H] ⁺
334.1 396	3.9 4	C16H19N3O5	0	Glu-Trp	[M+H] ⁺
334.1 647	5.0 6	C18H23NO5	1. 3	Seneciophylline	[M+H] ⁺
335.1 6	6.6 5	C17H22N2O5	0. 8	TDP-2	[M+H] ⁺
335.1 827	10. 15	C21H22N2O2. 1/2H2SO4	21 .2	Strychnine sulfate	[M+H] ⁺
336.1 917	4.9 3	C18H25N3O6	0. 4	Carbobenzyloxyglycylglycyl-L-norleucine	[M+H-CO2] ⁺
336.3 26	16. 22	C22H41NO	0. 3	Pipericine	[M+H] ⁺
337.0 53	2.9 1	C4H9O5P	24 .2	2-Phosphonobutyric acid	[2M+H] ⁺
337.0 681	7.3 9	C21H20O10	7. 3	4H-1-Benzopyran-4-one, 6-hexopyranosyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-	[M+H-C2H8O4] ⁺
337.1 717	0.7 8	C15H26N2O5	4. 3	Loxistatin acid	[M+Na] ⁺
338.1 234	3.8 4	C16H19NO7	0. 1	3-(Carboxymethyl)-1-.beta.-D-glucopyranosyl-1H-indole	[M+H] ⁺
338.3 417	17. 05	C22H43NO	0. 1	Erucamide	[M+H] ⁺

339.1 075	5.4 9	C22H30O14	0. 1	Sibiricose A5	[M+H- C6H12O6] +
339.1 076	3.5 2	C25H31NO12	0. 7	4-Demethylsimmondsin 2'- ferulate	[M+H- C9H13NO4]+
340.1 178	11. 87	C19H17NO5	0. 4	Mofezolac	[M+H]+
341.1 383	6.1 6	C26H32O11	0. 8	4-((2S,3S)-3- (Hydroxymethyl)-5-((1E)- 3-hydroxyprop-1-en-1- yl)-7-methoxy-2,3- dihydro-1-benzofuran-2- yl)-2-methoxyphenyl hexopyranoside	[M+H- C6H12O6] +
341.2 662	14. 72	C22H32N2O	22 .2	1-(Cyclohexylamino)-3-(6- methyl-1,2,3,4- tetrahydrocarbazol-9- yl)propan-2-ol	[M+H]+
342.1 062	3.0 7	C19H21N3O5	6. 6	6,7-Dimethoxy-N-(3,4,5- trimethoxyphenyl)quinazoli n-4-amine	[M+H- C2H6]+
342.1 548	2.1 9	C17H19N5O3	3. 5	His-Trp	[M+H]+
343.0 807	11. 38	C17H14N2O4S	18	Oxamflatin	[M+H]+
343.1 176	10. 01	C19H18O6	1. 1	6-Demethoxytangeretin	[M+H]+
343.1 176	10. 76	C19H18O6	0. 1	5-Methoxysalvigenin	[M+H]+
343.1 724	2.5 9	C13H22N6O5	0. 4	PyroGlu-Gly-Arg	[M+H]+
344.1	1.2	C15H21NO8	2	N-Fructosyl tyrosine	[M+H]+

34	6				
344.2	3.3		15		
279	5	C20H29N3O2	.6	ADBICA	[M+H] ⁺
345.1	2.6		7.	2'-Hydroxy-2,4,5,6'-	
307	7	C19H20O6	1	tetramethoxychalcone	[M+H] ⁺
345.2	3.7		11	L-Valine, N-[(1-pentyl-1H-	
133	1	C20H28N2O3	.9	indol-3-yl)carbonyl]-, methyl ester	[M+H] ⁺
346.0	1.2		0.		
546	3	C10H12N5O7P	5	Cyclic GMP	[M+H] ⁺
346.2	14.		6.	Leukotriene B4	
717	48	C22H37NO3	9	dimethylamide	[M+H-H2O] ⁺
347.0	5.6		0.		
761	5	C31H36O18	1	Haploside C	[M+H-C14H22O10] ⁺
347.1	9.3		10		
829	2	C21H22N4O	.4	PF-622	[M+H] ⁺
347.1	3.6		21	9,11,18-Trihydroxy-6,18-	
926	7	C20H26O5	.4	epoxypimara-5,8(14),15-trien-7-one	[M+H] ⁺
347.2	12.		6.		
195	93	C21H30O4	5	Corticosterone	[M+H] ⁺
348.0	1.2		0.		
703	5	C10H14N5O7P	1	Adenosine monophosphate	[M+H] ⁺
349.1	6.1		10	Glycine, N-2-naphthyl-, (p-	
257	3	C19H16N4O3	.7	nitrobenzylidene)hydrazide	[M+H] ⁺
349.1	18.		19		
833	19	C18H24N2O5	.3	Enalaprilat	[M+H] ⁺
351.1	11.		11	Citroside A or B	
84	87	C19H30O8			[M+H-2H2O] ⁺
351.2	8.8		7.	6,10a-Dihydroxy-4-(hydroxymethyl)-4,7,11b-	
		C20H30O5			[M+H] ⁺

141	3		3	trimethyl- 1,2,3,4a,5,6,6a,7,11,11a- decahydronaphtho[2,1- f][1]benzofuran-9-one	
351.2	10.		7.	5-(4-Carboxy-3- methylbutyl)-5,6,8a- trimethyl-3-oxo-4a,6,7,8- tetrahydro-4H- naphthalene-1-carboxylic acid	[M+H] ⁺
141	19	C20H30O5	2		
351.2	9.9		20	Vinpocetine	[M+H] ⁺
142	1	C22H26N2O2	.6		
352.2	13.		6.	N-Oleoyl-L-serine	[M+H- H2O] ⁺
821	72	C21H39NO4	5		
353.0	9.6		0.	Griseofulvin	[M+H] ⁺
786	1	C17H17ClO6	4		
353.1	4.2		21	Chroma Dye 88	[M+H] ⁺
572	2	C20H20N2O4	.6		
353.2	9.9		20	Anileridine	[M+H] ⁺
296	5	C22H28N2O2	.8		
353.2	12.		0.	1-Monolinolenin	[M+H] ⁺
685	83	C21H36O4	2		
355.1	4.5		0.	MCULE-9958171223	[M+Na] ⁺
727	9	C16H28O7	1		
355.2	15.		6.	1-Monolinolein	[M+H] ⁺
818	03	C21H38O4	8		
357.1	5.2		20	Isophthaloylbiscaprolactam	[M+H] ⁺
884	5	C20H24N2O4	.8		
359.1	11.		0.	3'-Hydroxy-5,6,7,4'- tetramethoxyflavone	[M+H] ⁺
124	39	C19H18O7	6		
359.1	11.		3.	2-(2,4-dimethoxyphenyl)- 5-hydroxy-7,8-	[M+H] ⁺
125	07	C19H18O7	1		

				dimethoxyflavone	
359.1 126	12. 19	C19H18O7	0. 6	Gardenin B	[M+H] ⁺
359.1 925	3.3 1	C21H27FO5	20 .1	Isoflupredone	[M+H- HF] ⁺
359.1 925	4.1 7	C21H26O5	20 .6	4-Hydroxy-6-[1-[1-(2-hydroxyethyl)-4,7-dimethylisochroman-3-yl]ethyl]-3-methylpyran-2-one	[M+H] ⁺
359.1 931	2.9 7	C21H26O5	19 .1	Prednisone	[M+H] ⁺
360.1 65	1.2 2	C19H22FN3O3	19 .1	Enrofloxacin	[M+H] ⁺
361.2 081	2.9	C21H28O5	20 .1	Aldosterone	[M+H] ⁺
362.1 96	4.2 9	C27H23N	16 .4	(9,9-Dimethylfluoren-2-yl)-(4-phenylphenyl)amine	[M+H] ⁺
362.2 076	4.2 9	C19H27N3O4	0. 7	Semagacestat	[M+H] ⁺
363.2 124	4.2 5	C21H30O5	11 .2	5.beta.-Dihydrocortisone	[M+H] ⁺
363.2 126	4.4 3	C19H27FN4O2	17 .5	5-Fluoro-ADB-PINACA isomer 2	[M+H] ⁺
363.3 105	14. 71	C20H42O5	0. 2	3,6,9,12-tetraoxatetracosan-1-ol	[M+H] ⁺
364.1 005	0.8	C16H17N3O5S	11 .6	N-(4-Morpholin-4-ylphenyl)-2-nitrobenzenesulfonamide	[M+H] ⁺
365.0 993	10. 01	C19H18O6	0. 8	Zapotin	[M+Na] ⁺

365.1 207	3.0 7	C16H22O8	0. 5	9,15-Dihydroxy-4,10,16-trimethyl-1,5,11-trioxacyclohexadeca-7,13-diene-2,6,12-trione	[M+Na] ⁺
365.1 821	2.7 4	C18H25ClN4O2	21 .9	5-Chloro AB-PINACA	[M+H] ⁺
365.1 935	8.2 9	C18H30O6	0. 2	(2E,4E)-12-Hydroxy-3,5,7-trimethyl-13-methyltetradeca-2,4-dienedioic acid	[M+Na] ⁺
367.1 53	11. 9	C20H24O5	1. 4	ZINC106754735	[M+Na] ⁺
367.2 093	7.7 4	C22H26N2O3	18 .8	Hirsuteine	[M+H] ⁺
369.2 976	15. 62	C11H20O2	6. 1	.delta.-Undecalactone	[2M+H] ⁺
371.2 064	5.6 9	C19H32O8	1. 6	6-Hydroxy-2,4,4-trimethyl-3-(3-oxobutyl)cyclohex-2-en-1-yl .beta.-D-glucopyranoside	[M-H2O+H] ⁺
371.2 29	4.4 7	C22H30N2O3	10 .8	Aspidocarpine	[M+H] ⁺
372.2 129	6.1 5	C16H29N5O3S	17 .3	Biocytinamide	[M+H] ⁺
373.0 912	10. 63	C20H17FO4S	2	Sulindac sulfone	[M+H] ⁺
373.1 281	8.9	C20H20O7	0. 1	Isosinensetin	[M+H] ⁺
373.1 281	10. 05	C20H20O7	0. 5	3,5,7,3',4'-Pentamethoxyflavone	[M+H] ⁺
373.1 835	3.7 4	C16H28N4O4S	18 .4	Biocytin	[M+H] ⁺

373.2 082	4.0 5	C22H28O5	19 .1	Betamethasone 9,11- epoxide	[M+H] ⁺
373.2 22	5.7 2	C19H32O7	0. 5	MCULE-1861643007	[M+H] ⁺
374.1 923	4.3 7	C21H27NO5	10	Spirotetramat	[M+H] ⁺
375.1 074	10. 76	C19H18O8	0. 2	Neobaicalein	[M+H] ⁺
375.1 276	0.7 9	C14H24O10	3. 5	Ethyl 4-O-(4-carboxy-3- hydroxy-3- methylbutanoyl)-.beta.-D- glucopyranoside	[M+Na] ⁺
375.2 239	3.5 7	C22H30O5	19 .9	6.alpha.- Methylprednisolone	[M+H] ⁺
376.2 595	11. 6	C16H33N5O5	10 .9	Thr-Lys-Lys	[M+H] ⁺
376.3 187	15. 37	C24H41NO2	6	Docosatetraenoyl ethanolamide	[M+H] ⁺
377.0 866	5.5 9	C18H16O9	0. 4	3',4',5,7-Tetrahydroxy- 3,6,8-trimethoxyflavone	[M+H] ⁺
377.1 07	0.7 9	C19H21ClN2O 2S	3. 7	Capsazepine	[M+H] ⁺
377.1 457	3.8 1	C17H20N4O6	0. 2	Vitamin B2	[M+H] ⁺
377.2 663	14. 9	C21H38O4	0. 2	2-Linoleoylglycerol	[M+Na] ⁺
379.1 363	5.8 5	C21H18N2O5	19 .4	9-Methoxycamptothecin	[M+H] ⁺
379.2 075	4.9 7	C21H30O6	10 .9	2a,11-Dihydroxy- 2,2,4a,7,10b-pentamethyl- 1a,2a,3,4,4a,7,8,10,10a,10b, 11,11a-dodecahydro-	[M+H] ⁺

				2H,9H-[1]benzoxireno[3,4-f]pyrano[2,3-b]chromen-9-one	
380.1 705	3.3	C19H22O7	0. 5	Janerin	[M+NH4]+
381.0 793	0.9 6	C12H22O11	0	Sucrose	[M+K]+
382.1 713	2.4 4	C16H23N5O6	2. 6	O-beta-D-Glucopyranosyl-cis-zeatin	[M+H]+
383.2 039	6.4 3	C22H26N2O4	20 .5	Corynoxine	[M+H]+
384.2 282	4.0 7	C27H29NO	10 .1	JWH 182	[M+H]+
385.2 081	5.7 9	C22H28N2O4	10 .4	Rhyncophylline	[M+H]+
385.2 197	5.4 8	C22H28N2O4	19 .1	Voacristine	[M+H]+
385.2 925	14. 71	C22H42O6	6	Sorbitan monopalmitate	[M+H-H2O]+
386.2 285	6.8 5	C23H31NO4	9. 1	Stachybotrylactam	[M+H]+
387.1 399	2.5	C19H24O7	3. 9	6-Hydroxyeurycomalactone	[M+Na]+
387.2 239	3.7 7	C23H30O5	19	Corticosterone, 11-deoxy-16.alpha.,17-epoxy-, acetate	[M+H]+
388.2 078	4.5	C22H29NO5	9. 8	Guan-fu base y	[M+H]+
389.1 231	10. 69	C20H20O8	0. 8	Artemetin	[M+H]+
389.1	12.	C20H20O8	1.	5-O-Demethylnobiletin	[M+H]+

231	01		4		
389.1 784	3.5	C ₂₀ H ₂₅ ClN ₄ O 2	11 .5	ML-180	[M+H] ⁺
389.2 393	4.5 7	C ₁₇ H ₃₂ N ₄ O ₆	0. 9	Glu-Leu-Lys	[M+H] ⁺
389.2 395	4.2 2	C ₁₇ H ₃₂ N ₄ O ₆	0. 3	Glu-Ile-Lys	[M+H] ⁺
391.1 023	7.5 1	C ₁₉ H ₁₈ O ₉	0. 5	4',5,7-Trihydroxy 3,3',6,8-tetramethoxyflavone	[M+H] ⁺
391.1 824	2.1 3	C ₂₃ H ₂₈ O ₄	11 .8	Isooctyl benzyl phthalate	[M+Na] ⁺
391.2 842	16. 43	C ₂₄ H ₃₈ O ₄	0. 1	Dioctyl phthalate	[M+H] ⁺
393.1 883	5.6 9	C ₁₄ H ₂₈ N ₆ O ₅ S	7. 4	Ser-Met-Arg	[M+H] ⁺
393.2 096	3.6 1	C ₂₄ H ₂₈ N ₂ O ₃	19 .5	Ivacaftor	[M+H] ⁺
393.2 611	12. 87	C ₂₅ H ₃₂ N ₂ O ₂	19 .2	Racemoramide	[M+H] ⁺
395.1 315	3.2 6	C ₂₀ H ₂₅ ClO ₇	14 .7	18-Chloro-17-hydroxy-5,15-dimethoxy-11-methyl-12-oxabicyclo[12.4.0]octadeca-1(18),14,16-triene-3,8,13-trione	[M+H-H ₂ O] ⁺
395.2 025	3.3 4	C ₂₁ H ₃₀ O ₇	10 .3	2,3,4a-Trihydroxy-4,4,6a,9,12b-pentamethyl-3,4,4a,6,6a,12,12a,12b-octahydro-2H,9H-benzo[f]pyrano[2,3-b]chromene-1,11(5H,10H)-dione	[M+H] ⁺

395.2 042	5.7 3	C23H26N2O4	19 .4	Brucine	[M+H] ⁺
395.2 178	3.2	C23H32O4	3. 3	Deoxycorticosterone acetate	[M+Na] ⁺
398.2 415	11. 6	C21H35NO4S	14 .7	14(15)-EET-SI	[M+H] ⁺
399.3 082	15. 01	C23H42O5	5. 6	1-Oleoyl-2-acetyl-sn- glycerol	[M+H] ⁺
401.1 594	5.0 1	C22H26O8	0	Syringaresinol	[M+H- H2O] ⁺
401.2 032	3.5	C22H28N2O5	9. 4	Reserpine acid	[M+H] ⁺
401.2 875	3.7 3	C18H36N6O4	1. 2	Ile-Leu-Arg	[M+H] ⁺
403.1 016	10. 99	C19H19ClN4O 2S	6. 6	MMV658993	[M+H] ⁺
403.1 388	10. 27	C21H22O8	0. 4	Hexamethylquercetin	[M+H] ⁺
403.2 189	4.4 2	C23H30O6	18 .2	Prednisolone 21-acetate	[M+H] ⁺
403.2 552	4.6 6	C24H34O5	18 .6	Gambogin	[M+H] ⁺
405.1 181	11. 64	C23H20N2O3S	21 .2	Sulfinpyrazone	[M+H] ⁺
406.2 531	15. 48	C29H39N3O2	10 .4	Echinulin	[M+H- C4H8] ⁺
407.2 39	3.9 4	C18H34N2O8	0. 1	N- deoxyfructosylleucylisoleuci ne	[M+H] ⁺
407.2 404	10. 85	C9H17NO4	3. 3	Acetyl-L-carnitine	[2M+H] ⁺

409.1 833	3.9 8	C20H28N2O5S	10 .2	(-)-Tamsulosin	[M+H] ⁺
411.1 052	12. 01	C20H20O8	0. 6	3-O-Methylfunicone	[M+Na] ⁺
412.2 231	5.7 7	C21H33NO7	24 .3	Lasiocarpine	[M+H] ⁺
413.1 417	3	C15H20N6O8	0. 6	N6-threonylcarbamoyladenosine	[M+H] ⁺
417.1 544	8.6 5	C20H26O8	5. 8	(2E)-5-(4-(Carboxymethyl)-4-(methoxycarbonyl)-3-methyl-6-methylidene-2-oxooctahydro-1-benzofuran-5-yl)-3-methylpent-2-enoic acid	[M+Na] ⁺
419.1 336	11. 24	C21H22O9	0. 3	Gardenin	[M+H] ⁺
419.1 45	4.4 6	C10H11NO4	0	N-[2-(4-Hydroxyphenyl)acetyl]glycine	[2M+H] ⁺
419.3 309	10. 72	C32H50O5	0. 3	Alisol B acetate	[M+H-C2H8O4] ⁺
421.1 47	7.7 2	C21H24O9	5. 4	Rhapontin	[M+H] ⁺
423.1 628	3.4 5	C21H24N2O6	24 .1	N,N'-Dicarbobenzyloxy-L-ornithine	[M+Na] ⁺
423.3 623	11. 02	C36H62O9	0. 6	Ginsenoside F1	[M+H-C6H16O8] ⁺
425.1 206	10. 63	C21H22O8	0. 6	3',4',5',5,6,7-Hexamethoxyflavone	[M+Na] ⁺
425.2	14.	C22H32O8	5	3-Methylbutyric acid [(1S,6S,7R)-6-acetoxy-1-	[M+H] ⁺

147	27			isovaleryloxyspiro[4a,5,6,7a -tetrahydro-1H- cyclopenta[c]pyran-7,2'- oxirane]-4-yl]methyl ester	
425.2 51	8.4	C21H38O7	0. 1	Caperatic acid	[M+Na]+
427.2 055	6.1 6	C23H32O6	7. 8	3-[5-Hydroxy-4-keto-7- methoxy-2,3-dimethyl-6- (3-methylbut-2- enyl)chroman-8- yl]hexanoic acid	[M+Na]+
427.2 304	9.5 1	C22H32N2O5	23 .5	Enalaprilat tert-butyl ester	[M+Na]+
427.2 668	9.0 4	C18H39N2O7P	23 .7	Methylcarbamyl PAF C-8	[M+H]+
431.2 389	1.9 7	C25H34O6	9	Budesonide	[M+H]+
433.1 931	3.3 1	C21H30O8	22 .7	2-(1,2- Dihydroxyethyl)acrylic acid [2-(1-carbomethoxyvinyl)- 3-hydroxy-5-methyl-4-(1- methylolvinyl)-5- vinylcyclohexyl] ester	[M+Na]+
433.2 295	4.6 8	C24H32O7	16 .9	Gelomulide N	[M+H]+
435.1 286	5.0 5	C21H22O10	1. 4	Naringenin 7-O-beta-D- glucoside	[M+H]+
435.2 028	14. 74	C16H30N6O6S	1. 7	Met-Glu-Arg	[M+H]+
437.2 361	3.8 6	C21H32N4O6	7. 4	(6R,9S,14aR)-3,6R- Dimethyl-9S-(7-((S)- oxiran-2-yl)-7- oxoheptyl)decahydropyrrol o[1,2-	[M+H]+

				a][1,4,7,10]tetraazacyclodo decine-1,4,7,10-tetranone	
437.3 415	10. 72	C42H68O13	0	Saikosaponin D	[M+H- C12H24O1 1]+
439.2 303	6.5 7	C25H30N2O5	17 .5	Quinapril	[M+H]+
439.3 571	10. 44	C32H50O4	0	Acetyl lupeolic acid	[M+H- C2H4O2]+
441.1 157	11. 24	C21H22O9	0. 7	Likviritin	[M+Na]+
441.2 097	9.3 1	C17H28N8O6	24 .5	His-Glu-Arg	[M+H]+
				(3.beta.,6.alpha.,12.beta.,20 Z)-3,12- Dihydroxydammara- 20(22),24-dien-6-yl 2-O- (6-deoxy-.alpha.-L- mannopyranosyl)-.beta.-D- glucopyranoside	[M+H- C12H22O1 0]+
443.1 79	4.1 4	C24H26O8	21 .5	2,5a,11,11,13a- Pentamethyl- 5a,6,6a,13a,13b,13c- hexahydro-9H- spiro[furo[4,3,2- ij]pyrano[4',3':4,5]cyclohept a[1,2-f]isochromene-7,2'- oxirane]- 1,5,9,13(2H,3aH,11H)- tetrone	[M+H]+
443.3 344	15	C30H50O2	1. 1	Cycloart-23-ene-3_, 25 diol	[M+H]+
447.3 065	7.4 3	C27H44O6	8. 3	Ecdysone	[M+H- H2O]+

448.1 943	2.7 8	C24H25N5O4	8. 6	Trp-Gly-Trp	[M+H] ⁺
449.1 443	6.8 8	C22H24O10	1. 1	Isosakuranin	[M+H] ⁺
449.1 784	4.9 7	C21H20N8O4	23 .6	Dg-c8-aac	[M+H] ⁺
451.2 664	2.7 9	C21H34N6O5	0. 5	Leu-Tyr-Arg	[M+H] ⁺
455.1 312	10. 99	C18H28N2O6S 2	7	Captopril disulfide	[M+Na] ⁺
455.2 063	6.4 5	C26H30O7	0. 1	Obacunone	[M+H] ⁺
455.2 252	9.9 8	C23H46N6O13	21	Neomycin	[M+H- C6H12N2O 3] ⁺
455.3 52	10. 72	C41H66O13	0. 1	Bacoside A	[M+H- C11H20O1 0] ⁺
455.3 521	12. 04	C30H46O3	0. 5	Wilforlide A	[M+H] ⁺
457.2 326	15. 13	C25H32N2O6	1. 2	Vindolin	[M+H] ⁺
457.3 501	15. 44	C27H44N4O2	7. 7	2,2',6,6'- Tetrakis[(dimethylamino)me thyl]bisphenol A	[M+H] ⁺
463.1 235	5.3 6	C28H33O15	0. 8	Peonidin 3-O-rutinoside cation	[Cat- C6H10O4] +
463.1 238	4.1	C27H30O15	0. 6	4-(3,4-Dihydroxyphenyl)- 7-methoxy-2-oxo-2H- chromen-5-yl 6-O-.beta.- D-xylopyranosyl-.beta.-D-	[M+H- C5H8O4] ⁺

				glucopyranoside	
463.1 599	6.5 9	C23H26O10	1. 8	Methylnissolin-3-O-glucoside	[M+H] ⁺
463.2 764	4	C30H44O7	16 .6	Ganoderic acid A	[M+H-3H2O] ⁺
463.3 031	14. 27	C27H44O7	4. 4	Ecdysterone	[M+H-H2O] ⁺
465.1 028	4.6 9	C27H30O17	0. 7	Quercetin 3,4'-diglucoside	[M+H-C6H10O5] ⁺
467.1 891	3.1 3	C27H28N2O4	10 .5	Asperglaucide	[M+Na] ⁺
467.3 158	12. 89	C36H58O12	0	2,3,16,20,25-Pentahydroxycucurbita-5-ene-11,22-dione-3-O-glucoside	[M+H-C6H16O8] ⁺
469.1 105	4.5 5	C22H22O10	0. 6	3'-Methoxydaidzin	[M+Na] ⁺
469.2 547	6.5 2	C24H32N6O4	2. 7	Phe-Phe-Arg	[M+H] ⁺
469.3 315	12. 74	C30H44O4	1. 1	Glabrolide	[M+H] ⁺
473.3 451	14. 67	C31H46O2	12 .9	Phylloquinone	[M+Na] ⁺
475.2 401	6.0 2	C21H30N8O5	2. 8	Asn-Trp-Arg	[M+H] ⁺
476.2 239	4.7	C21H29N7O6	2. 1	Trp-Asp-Arg	[M+H] ⁺
477.1 393	4.6 1	C29H34O15	0. 4	Pectolinarin	[M+H-C6H10O4] ⁺

478.2 929	13. 53	C20H36N4O8	12 .2	Desferrioxamine H	[M+NH4] ⁺
479.1 185	5.2 5	C22H23O12	0. 4	Petunidin 3-glucoside cation	[Cat] ⁺
479.1 55	5.4 1	C23H28O12	0. 6	6-(Benzoyloxy)-1- (hexopyranosyloxy)-5- hydroxy-7-methyl- 1,4a,5,6,7,7a- hexahydrocyclopenta[c]pyr an-4-carboxylic acid	[M+H- H2O] ⁺
479.2 289	14. 72	C25H33N7O4	23 .2	21-Deacetoxy-11- oxodeflazacort-3,20- hydrazinecarboxamide	[M+H- NH3] ⁺
485.1 419	6.5 9	C34H56N2O27	1. 7	Glycan MC=h2a2	[M+2Na] ²⁺
487.1 575	6.9 2	C25H26O10	5. 3	Fridamycin A	[M+H] ⁺
487.2 652	7.8 9	C28H38O7	8. 8	Andrastin A	[M+H] ⁺
489.1 392	5.9 5	C24H24O11	0. 8	6''-O-Acetylglycitin	[M+H] ⁺
489.2 121	4.9 7	C26H32O9	0	Clausenarin	[M+H] ⁺
489.2 806	8.6 5	C26H42O7	3. 6	4-Hydroxy-1,4a-dimethyl- 7-(propan-2-yl)- 1,2,3,4,4a,5,8,8a- octahydronaphthalen-1-yl 6-deoxy-2-O-((2Z)-2- methylbut-2- enoyl)hexopyranoside	[M+Na] ⁺
495.1 262	7.9 7	C24H23ClN6O 2S	21 .1	MMV688283	[M+H] ⁺
496.2	4.2	C26H40ClN5	12	AGELASINE	[M+K] ⁺

539	5		.6	(stereochemistry of diterpene unknown)	
496.3 398	13. 93	C24H50NO7P	0. 5	Lyso-PC(16:0)	[M+H] ⁺
501.1 158	6.5 9	C22H22O12	24 .7	Nepetin 7-glucoside	[M+Na] ⁺
505.2 504	4.2 8	C28H37FO7	18 .3	Betamethasone dipropionate	[M+H] ⁺
509.1 291	5.3 2	C23H24O13	0. 2	Syringetin 3-glucoside	[M+H] ⁺
509.3 24	12. 74	C30H46O5	0. 2	Ncg00384869-01!4,4,8,10,14-pentamethyl-17-(4,5,6-trihydroxy-6-methylheptan-2-yl)-2,5,6,7,9,15-hexahydro-1h-cyclopenta[a]phenanthrene-3,16-dione	[M+Na] ⁺
511.1 21	5.9 5	C21H24N6O4S 2	4. 1	Dendroamide a	[M+Na] ⁺
511.3 396	13. 15	C30H48O5	0. 4	Asiatic acid	[M+Na] ⁺
513.3 553	12. 59	C30H50O5	1. 4	Cycloastragenol	[M+Na] ⁺
517.1 339	7.0 5	C25H24O12	0. 2	3-(4-Methoxyphenyl)-4-oxo-4H-chromen-7-yl 6-O-(carboxyacetyl)-.beta.-D-glucopyranoside	[M+H] ⁺
517.3 714	14. 64	C29H50N4O5	6. 8	N6-Carbamimidoyl-N2-((4E,6E,12E,14E)-3-hydroxy-2-(hydroxymethyl)-8,10,16-trimethyloctadeca-	[M-H2O+H] ⁺

				4,6,12,14-tetraenoyl)lysine	
519.1 132	5.8	C24H22O13	0. 9	Malonylgenistin	[M+H] ⁺
520.3 399	13. 28	C26H50NO7P	0. 5	LPC 18:2	[M+H] ⁺
523.2 551	14. 69	C33H36N2O5	7. 6	Defluoroatorvastatin	[M+H- H2O] ⁺
527.1 523	8.2 2	C18H32O16	11	Maltotriose	[M+Na] ⁺
529.1 68	8.5 8	C27H30O12	4. 1	2-Hydroxy-2-[2-[(Z)-2-hydroxy-2,6-dimethyl-8-(7-oxofuro[3,2-g]chromen-4-yl)oxyoct-6-en-3-yl]oxy-2-oxoethyl]butanedioic acid	[M+H- H2O] ⁺
531.3 868	14. 96	C30H52N4O5	5. 7	Arginine conjugated chenodeoxycholic acid	[M- H2O+H] ⁺
535.2 704	15. 94	C30H40O7	8. 7	3-DEOXO-3beta-ACETOXYDEOXYDIHYDRO GEDUNIN	[M+Na] ⁺
542.3 217	13. 47	C26H50NO7P	0. 1	.beta.-Linoleoyl-.alpha.-glycerophosphorylcholine	[M+Na] ⁺
547.2 61	5.1 6	C24H44O12	21 .1	Hypocrealesate	[M+Na] ⁺
549.1 238	6.1 6	C25H24O14	3. 9	Flavone base + 3O, 1MeO, O-MalonylHex	[M+H] ⁺
551.2 615	7.0 5	C15H20O4	2. 8	Umbellifolide	[2M+Na] ⁺
563.5 512	15. 28	C18H35NO	0. 3	Elaidamide	[2M+H] ⁺
569.3 839	10. 72	C35H58O9	0. 3	Bafilomycin A1	[M+H- 3H2O] ⁺

571.1 425	7.2 6	C26H28O13	3. 1	5,7-dihydroxy-2-phenyl-6-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-8-(3,4,5-trihydroxyoxan-2-yl)-4H-chromen-4-one	[M+Na] ⁺
573.1 581	7.6	C26H30O13	0. 4	Jasminoside	[M+Na] ⁺
574.2 286	5.5 6	C27H35N5O7S	7. 7	MET-enkephalin	[M+H] ⁺
575.4 135	14. 93	C15H29NO4	23	Octanoylcarnitine	[2M+H] ⁺
581.1 983	3.6 7	C27H32O14	20	Glucoliquiritin	[M+H] ⁺
593.2 765	15. 39	C35H36N4O5	1. 6	Pheophorbide a	[M+H] ⁺
595.1 661	5.2	C27H30O15	0. 7	Scolymoside	[M+H] ⁺
595.1 661	4.6	C27H30O15	0. 9	Loniceroside	[M+H] ⁺
601.2 597	4.8	C29H42N2O10	21 .7	4,5-Dihydro-19-hydroxygeldanamycin	[M+Na] ⁺
609.1 454	5.1 5	C27H28O16	0. 8	6''-O-(3-Hydroxy-3-methylglutaroyl)hyperin	[M+H] ⁺
609.3 224	4.8 7	C26H46N6O9	4. 5	MLS000863563	[M+Na] ⁺
611.1 611	4.6 9	C27H31O16	1. 7	Tulipanin	[M] ⁺
611.1 975	5.3 3	C28H34O15	1. 1	MCULE-9952557572	[M+H] ⁺
611.3 078	14. 64	C35H46O9	21 .8	Asperphenalenone E	[M+H] ⁺

611.3 949	12. 04	C37H50N6O2	19 .1	Demethyltirilazad	[M+H] ⁺
617.1 844	6.8 8	C28H34O14	0. 4	Poncirin	[M+Na] ⁺
625.1 767	2.8 6	C28H32O16	0. 3	5-Hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-oxo-4H-chromen-3-yl 2-O-.beta.-D-galactopyranosyl-.beta.-D-glucopyranoside	[M+H] ⁺
655.3 339	14. 61	C38H48O8	15 .5	TETRAHYDROGAMBOGIC ACID	[M+Na] ⁺
662.3 992	14. 7	C33H57N3O9	0. 7	Enniatin B	[M+Na] ⁺
668.4 482	15. 32	C35H61N3O9	0	Cyclo[(2R)-2-hydroxy-3-methylbutanoyl-N-methyl-L-valyl-(2R)-2-hydroxy-3-methylbutanoyl-N-methyl-L-valyl-(2R)-2-hydroxy-4-methylpentanoyl-N-methyl-L-isoleucyl]	[M+H] ⁺
675.1 533	5.6 5	C54H82O25	13 .1	29-Hydroxy-29-oxoolean-12-en-3-yl 6-deoxy-.alpha.-L-mannopyranosyl-(1->2)-.beta.-D-glucopyranuronosyl-(1->2)-.beta.-D-galactopyranuronosyl-(1->2)-.beta.-D-glucopyranosiduronic acid	[M+H-C30H48O3] ⁺
676.4 147	15. 01	C34H59N3O9	1. 2	Enniatin b1	[M+Na] ⁺
687.4	12.	C37H60O10	0	SCHEMBL18334795	[M+Na] ⁺

081	09				
690.4	15.		1.		
303	32	C35H61N3O9	3	Enniatin a1	[M+Na]+
				3,7,8-Trihydroxy-2-(4-hydroxy-3-methoxyphenyl)-4-oxo-4H-chromen-5-yl 6-O-acetyl-2-O-(6-deoxy-.alpha.-L-mannopyranosyl)-.beta.-D-glucopyranoside	
705.1	5.5		0.		
633	9	C30H34O18	1		[M+Na]+
707.2	10.		17	Glycan MC=h2	[2M+Na]+
098	01	C12H22O11			
728.3	8		21	Fumonisin B3	[M+Na]+
979		C34H59NO14	.7		
740.5	16.		1.		
225	09	C41H74NO8P	4	18:2 PE	[M+H]+
747.2	8.1		1.		
106	1	C33H40O18	3	Melitidin	[M+Na]+
				Kaempferol 3-O-.beta.-D-(6"-p-coumaroyl)glucopyranosyl(1->2)-.alpha.-L-rhamnopyranoside	
763.1	8.1		7.		
806	1	C36H36O17	5		[M+Na]+
785.4	10.		0.	Astragaloside IV	[M+H]+
682	73	C41H68O14	1		
851.4	12.		1.	Astragaloside I	[M+H-H2O]+
791	27	C45H72O16	2		
941.5	11.		0.	MCULE-8825599956	[M+H]+
109	68	C48H76O18	4		
93.03	6.4		10		
38	4	C6H6O	.6	Phenol	[M-H]-

101.0 234	10. 62	C ₄ H ₈ O ₄	9. 7	D-(-)-Erythrose	[M-H- H ₂ O]-
101.0 234	1.7 9	C ₄ H ₆ O ₃	9. 5	Butanoic acid, 4-oxo-	[M-H]-
103.0 027	0.9 3	C ₃ H ₄ O ₄	9. 7	Malonic acid	[M-H]-
103.0 393	1.8 7	C ₄ H ₈ O ₃	9. 6	(R)-2-Hydroxybutyric acid	[M-H]-
104.0 343	0.8	C ₃ H ₇ NO ₃	9. 2	Serine	[M-H]-
105.0 186	0.8 7	C ₃ H ₆ O ₄	9	D-Glycerate	[M-H]-
107.0 492	3.0 3	C ₈ H ₈ O ₃	9. 2	3-Hydroxyphenylacetic acid	[M-H- CO ₂]-
109.0 285	2.8 4	C ₆ H ₆ O ₂	8. 7	Hydroquinone	[M-H]-
111.0 078	1.2 3	C ₆ H ₄ O ₅	9. 2	2,5-Furandicarboxylic acid	[M-H- CO ₂]-
113.0 226	9.6	C ₅ H ₈ O ₄	8. 4	Glutaric acid	[M-H- H ₂ O]-
114.0 181	0.8	C ₄ H ₇ NO ₄	8. 4	Iminodiacetic acid	[M-H- H ₂ O]-
114.0 549	0.9 9	C ₅ H ₉ NO ₂	8. 2	D-Proline	[M-H]-
115.0 028	1.1 6	C ₄ H ₇ NO ₄	8. 8	D-Aspartic acid	[M-H- NH ₃]-
117.0 184	1.4 6	C ₄ H ₆ O ₄	7. 8	Succinic acid	[M-H]-
118.0 5	0.8	C ₄ H ₉ NO ₃	7. 8	L-Homoserine	[M-H]-
121.0	4.3	C ₇ H ₆ O ₂	8.	4-Formylphenol	[M-H]-

285	5		8		
121.0	3.8	C7H6O5S	7.	1-Phenol-2-sulfonic acid,	[M-H-
286	7		4	4-formyl-	SO3]-
122.0	7.0	C14H14O4S	7.	o-Cresol, 4,4'-sulfonyldi-	[M-H-
364	4		3		C7H7SO2]-
124.0	2.5	C8H9NO3	7.	3-Hydroxyacetaminophen	[M-H-
395	3		4		C2H2O]-
125.0	6.1	C10H18O4	7	Methyl hydrogen azelate	[M-H-
963	4				C2H4O3]-
128.0	1.2	C5H7NO3	6.	Pidolic acid	[M-H]-
344	6		6		
129.0	1.2	C5H6O4	6.	Mesaconic acid	[M-H]-
185	8		5		
129.0	3.3	C6H10O3	6.	2-Ketohexanoic acid	[M-H]-
548	3		9		
130.0	4.2	C6H13NO2	3.	Leucine	[M-H]-
865	1		7		
130.0	1.5	C6H13NO2	3.	L-Norleucine	[M-H]-
867	6		7		
131.0	0.8	C4H8N2O3	6.	D-Asparagine	[M-H]-
451			1		
131.0	3.1	C6H12O3	6	5-Hydroxyhexanoic acid	[M-H]-
705	7				
131.0	4.5	C6H12O3	6.	2-Ethyl-2-hydroxybutyric	[M-H]-
706	9		4	acid	
133.0	1.5	C4H6O5	5.	(S)-Malate	[M-H]-
132	3		4		
133.0	1.6	C5H10O4	2	Deoxyribose	[M-H]-
497	4				
134.0	4.9	C6H5N3O	3.	4-hydroxybenzotriazole	[M-H]-
364	9		9		

134.0 463	1.3 2	C15H23N7O5	6. 2	Sinefungin	[M-H- C10H18N2 O5]-
135.0 288	0.8 5	C4H8O5	6. 3	Threonic acid	[M-H]-
135.0 443	4.7	C9H8O4	6. 7	3-(4-Hydroxyphenyl)-3-oxopropanoic acid	[M-H- CO2]-
135.0 443	3.9 6	C16H14O6	6. 5	7-O-Methyleleriodictyol	[M-H- C8H6O4]-
135.0 443	6.2 4	C9H8O4	6. 5	5-Formyl-2-hydroxy-3-methylbenzoic acid	[M-H- CO2]-
136.0 394	5.0 9	C8H9NO4S	6. 7	2- [(Methylsulfonamido)benzoic acid	[M-H- CH2SO2]-
136.0 521	7.0 4	C5H12NO4P	8. 6	Glufosinate	[M-H- CO2]-
136.0 759	3.0 3	C8H11NO	6. 8	L-Dopa	[M-H]-
137.0 234	3.7 1	C15H22O5	5. 9	Hydroxysydonic acid	[M-H- C8H16O2]-
137.0 235	3.4 6	C7H6O3	4. 6	3,4-Dihydroxybenzaldehyde	[M-H]-
137.0 235	3.2 3	C7H6O3	6. 1	Salicylic acid	[M-H]-
137.0 238	2.1 2	C17H24O3	6. 2	Menthyl salicylate	[M-H- C10H18]-
138.0 188	1.2 7	C6H5NO3	6	5-Hydroxynicotinic acid	[M-H]-
138.0 552	3.3 7	C8H9NO4	6. 4	4-Pyridoxic acid	[M-H- CO2]-
139.0	7.0	C9H12O4	6.	Spiro[3.3]heptane-2,2-	[M-H-

756	4		3	dicarboxylic acid	CO2]-
141.0	2.3	C8H8O9	5.	Furantetracarboxylic acid,	[M-H-
183	5		7	tetrahydro-	C2H2O5]-
141.0	9.5	C8H14O2	5.	2-Propyl-4-pentenoic acid	[M-H]-
906	1		8		
141.0	7.4	C8H14O2	5.	2-Octenoic acid	[M-H]-
907	7		6		
143.0	9.5	C12H22O11	5.	Lactose	[M-H-
337	9		7		C6H14O7]-
143.0	5.1	C16H22O6	5.	Tetranor-PGJM	[M-H-
695	5		9		C9H10O3]-
144.0	5.6	C10H7NO3	5.	4-(5-Oxazolyl)benzoic acid	[M-H-
44	4		4		CO2]-
144.0	2.0	C6H11NO3	2	4-Acetamidobutanoate	[M-H]-
651	2				
145.0	3.7	C6H10O4	4.	2,2-Dimethylsuccinic acid	[M-H]-
497	1		7		
145.0	5.4	C7H14O3	4.	3-Hydroxy-3,4-	[M-H]-
859	5		9	dimethylvaleric acid	
146.0	0.8	C5H9NO4	6.	Glutamic acid	[M-H]-
447	1		1		
147.0	1.4	C5H8O5	4.	L-2-Hydroxyglutaric acid	[M-H]-
295	8		9		
147.0	5.4	C18H22O11	5.	Asperuloside	[M-H-
44	5		3		C9H14O9]-
147.0	6	C10H8O3	5.	Hymecromone	[M-H-CO]-
441			7		
147.0	2.2	C9H8O2	5.	4-Hydroxycinnamyl	[M-H]-
444	5		1	aldehyde	
147.0	2.0	C6H12O4	5.	Mevalonic acid	[M-H]-
657	9		5		

149.0 237	2.9 1	C ₁₄ H ₁₁ FO ₄	4. 7	1-(2,4-Dihydroxyphenyl)- 2-(4-fluorophenoxy)ethanone	[M-H- C ₆ H ₅ FO]-
149.0 255	2.5	C ₈ H ₈ O ₄	17 .5	Homogentisic acid	[M-H- H ₂ O]-
149.0 265	2.6 6	C ₁₆ H ₁₁ NO ₅	17 .9	N-(2,4-Dihydroxyphenacyl)phthalimide	[M-H- C ₈ H ₅ NO ₂]-
149.0 447	0.8 9	C ₁₄ H ₁₆ O ₈	4. 7	4-[3-(3,4-Dihydroxyphenyl)acryloyloxy]-2,3-dihydroxy-2-methylbutyric acid	[M-H- C ₉ H ₆ O ₃]-
150.0 414	1.4 4	C ₉ H ₁₃ N ₅ O ₄	4. 4	Ganciclovir	[M-H- C ₄ H ₈ O ₃]-
151.0 393	5.0 7	C ₈ H ₈ O ₃	5. 1	4-Formyl-3-methoxyphenol	[M-H]-
151.0 393	3.1	C ₂₃ H ₃₂ O ₅	4. 6	2,4-Dihydroxy-3-[(6-hydroxy-1,2,5,5-tetramethyl-2,3,4,4a,6,7-hexahydronaphthalen-1-yl)methyl]-6-methylolbenzaldehyde	[M-H- C ₁₅ H ₂₄ O ₂]-
151.0 393	3.7 1	C ₈ H ₈ O ₃	5	2-Hydroxy-3-methoxybenzaldehyde	[M-H]-
151.0 393	8.9 7	C ₈ H ₈ O ₃	5. 5	Cresotinic acid	[M-H]-
151.0 394	4.6 2	C ₈ H ₈ O ₃	4. 9	2-Hydroxy-5-methoxybenzaldehyde	[M-H]-
151.0 394	5.8 6	C ₈ H ₈ O ₃	5	2-Acetylresorcinol	[M-H]-
151.0 41	3.3 8	C ₈ H ₈ O ₃	16 .7	2-Hydroxy-4-methoxybenzaldehyde	[M-H]-

152.0 108	2.7 6	C ₈ H ₈ O ₄	4. 9	o-Vanillic acid	[M-H- CH ₃]-
152.0 346	8.4 1	C ₈ H ₇ NO ₄	4. 9	3-Methyl-5-nitrosalicylaldehyde	[M-H-CO]-
152.0 346	2.3 7	C ₇ H ₇ NO ₃	4. 5	3-Hydroxyanthranilic acid	[M-H]-
152.0 836	7.0 4	C ₇ H ₁₁ N ₃ O	3. 8	2-Amino-5-ethyl-6-methyl-4(3H)-pyrimidinone	[M-H]-
153.0 186	3.6 8	C ₇ H ₆ O ₄	4	Gentisic acid	[M-H]-
153.0 186	4.2 3	C ₇ H ₆ O ₄	5	3,4-Dihydroxybenzoic acid	[M-H]-
153.0 549	5.1 5	C ₁₄ H ₁₆ ClNO ₃	4. 4	(1R,2S)-2-[(4-Chloroanilino)carbonyl]cyclohexanecarboxylic acid	[M-H- C ₆ H ₆ ClN]-
154.0 138	5.1	C ₆ H ₅ NO ₄	2. 3	4-Nitrocatechol	[M-H]-
154.0 613	0.7 8	C ₆ H ₉ N ₃ O ₂	4. 4	His	[M-H]-
154.0 628	11. 77	C ₁₁ H ₁₀ N ₂ O ₂	22 .2	3-(2-Nitro-1-propenyl)indole	[M-H- HNO ₂]-
154.9 98	1.2 2	C ₆ H ₆ O ₆	4	Isocitric acid lactone	[M-H- H ₂ O]-
155.0 706	7.5 1	C ₈ H ₁₄ O ₄	5	2-Propylglutaric acid	[M-H- H ₂ O]-
155.1 076	7	C ₉ H ₁₆ O ₂	4. 9	4-Methylcyclohexanecarboxylic acid	[M-H]-
157.0 5	4.2 5	C ₇ H ₁₀ O ₄	4. 1	Isopropylfumaric acid	[M-H]-
157.0 61	1.9 9	C ₁₀ H ₂₀ N ₂ O ₄	4. 8	N-.delta.-BOC-L-Ornithine	[M-H- C ₄ H ₁₀ O]-

157.0 859	8.5 5	C8H14O3	4	2-Oxooctanoic acid	[M-H]-
157.0 864	8.8 9	C8H14O3	4. 3	2-((2R)-2-Hydroxycyclohexyl)acetic acid	[M-H]-
158.0 801	3.0 6	C7H13NO3	4. 5	N-Acetylvaline	[M-H]-
158.0 816	4.4 1	C15H18N2O5	4. 3	IDE1	[M-H- C8H5NO2] -
159.0 652	3.8 7	C7H12O4	4. 6	Pimelic acid	[M-H]-
159.1 02	7.2 4	C8H16O3	4. 7	5-Hydroxyvalproic acid	[M-H]-
160.0 609	1.2 9	C6H11NO4	3. 9	3-Aminoadipic acid	[M-H]-
161.0 232	4.2 7	C15H12O6	3. 4	2',5,6',7-Tetrahydroxyflavanone	[M-H- C6H6O3]-
163.0 394	4.8	C24H30O12	4. 5	8-O-4-Hydroxycinnamoylharpagide	[M-H- C15H22O9] -
164.0 347	5.1 5	C8H7NO3	3. 7	2-Formamidobenzoic acid	[M-H]-
165.0 187	4.5 1	C8H8O5	3. 8	3,4-Dihydroxymandelic acid	[M-H- H2O]-
165.0 193	1.7 1	C8H6O4	4. 3	3-Formyl-2-hydroxybenzoic acid	[M-H]-
165.0 398	0.8 2	C5H8O5	4. 5	D-(+)-Ribono-1,4-lactone	[M+OH]-
165.0 55	5.2 3	C9H10O3	3. 3	3-Phenoxypropionic acid	[M-H]-

165.0 551	4.9 9	C ₉ H ₁₀ O ₃	3. 4	L-(-)-3-Phenyllactic acid	[M-H]-
165.0 551	3.5 3	C ₉ H ₁₀ O ₃	3. 5	3,4'- Dihydroxypropiophenone	[M-H]-
166.0 5	9.5	C ₈ H ₉ NO ₃	4. 3	2,4-Dimethyl-6- nitrophenol	[M-H]-
167.0 343	2.7 6	C ₈ H ₈ O ₄	4. 1	Vanillic acid	[M-H]-
168.0 296	6.5 9	C ₇ H ₇ NO ₄	3. 2	2-Methoxy-5-nitrophenol	[M-H]-
168.0 658	2.4 8	C ₈ H ₁₃ NO ₄	3. 7	5-Acetamido-4- oxohexanoic acid	[M-H- H ₂ O]-
168.1 02	6.8	C ₉ H ₁₅ NO ₂	3. 6	(2S,3aS,7aS)-Octahydro- 1H-indole-2-carboxylic acid	[M-H]-
169.0 861	9.5 1	C ₉ H ₁₆ O ₄	3. 9	3-Isobutylglutaric acid	[M-H- H ₂ O]-
169.0 863	6.1 4	C ₉ H ₁₄ O ₃	3. 3	2- Oxocyclohexanepropanoic acid	[M-H]-
169.1 225	8.4	C ₁₀ H ₁₈ O ₂	4	(6E)-8-Methyl-6-nonenic acid	[M-H]-
171.0 656	4.5 7	C ₈ H ₁₂ O ₄	3. 7	1,3- Cyclohexanedicarboxylic acid	[M-H]-
171.0 656	5.3 9	C ₈ H ₁₂ O ₄	3. 6	1,4- cyclohexanedicarboxylic acid	[M-H]-
171.1 02	7.8 3	C ₉ H ₁₆ O ₃	3. 5	(2E)-4-Hydroxynon-2- enoic acid	[M-H]-
173.0 085	0.9 4	C ₁₅ H ₁₄ O ₉	4	1-[(E)-3-(4- Hydroxyphenyl)acryloyl]oxy	[M-H- C ₉ H ₈ O ₃]-

				propane-1,2,3-tricarboxylic acid	
173.0085	1.29	C6H6O6	3.9	trans-Aconitic acid	[M-H]-
173.0085	5.22	C6H8O7	3.4	Isocitric acid	[M-H-H2O]-
173.045	2.47	C7H10O5	3.2	4-Ketopimelic acid	[M-H]-
173.0814	4.9	C8H14O4	3.2	Suberic acid	[M-H]-
173.1039	0.79	C6H14N4O2	2.8	DL-Arginine	[M-H]-
173.177	7.85	C9H18O3	3.7	9-Hydroxynonanoic acid	[M-H]-
173.177	6.37	C9H18O3	2.5	3-hydroxy-nonanoic acid	[M-H]-
174.0765	1.37	C7H13NO4	3.9	2-Aminopimelate	[M-H]-
175.0606	3.57	C7H12O5	3.6	2-Isopropylmalic acid	[M-H]-
175.0606	2.86	C7H12O5	3.4	3-Hydroxy-5-keto-5-methoxy-3-methylvaleric acid	[M-H]-
175.0831	0.78	C5H12N4O3	1.4	Canavanine	[M-H]-
175.097	5.38	C8H16O4	3.8	(2-Butoxyethoxy)acetic acid	[M-H]-
177.0399	0.97	C6H10O6	3.4	L-Gulono-1,4-lactone	[M-H]-
177.0551	5.61	C10H10O3	3.6	Coniferyl aldehyde	[M-H]-

177.0 552	3.9 7	C10H10O3	3	4-Methoxycinnamic acid	[M-H]-
177.0 915	10. 81	C11H14O2	3. 1	5-Phenylvaleric acid	[M-H]-
179.0 344	3.9 6	C9H8O4	1. 9	Caffeate	[M-H]-
181.0 137	2.1 1	C8H6O5	2. 7	4-(2-Furyl)-2,4-dioxobutanoic acid	[M-H]-
181.1 228	9.0 1	C12H18O4	3	3-[(1E,3E)-Hepta-1,3-dienyl]glutaric acid	[M-H-CO2]-
183.1 017	7.5 3	C10H18O4	3. 3	Hexylsuccinic acid	[M-H-H2O]-
183.1 384	9.5 5	C11H20O2	3. 6	10-Undecenoic acid	[M-H]-
184.0 973	4.2	C9H15NO3	2. 6	5-Oxo-1-propyl-2-pyrrolidineacetic acid	[M-H]-
185.0 814	7.4 7	C9H14O4	2. 6	Gabapentin related compound E	[M-H]-
186.1 131	4.4 4	C9H17NO3	2. 6	8-Amino-7-oxononanoic acid	[M-H]-
187.1 083	2.6	C8H16N2O3	2. 1	Glycyl-leucine	[M-H]-
187.1 334	10. 64	C10H20O3	3. 1	10-Hydroxydecanoic acid	[M-H]-
188.0 348	10. 4	C10H7NO3	2. 7	4-Nitro-1-naphthol	[M-H]-
188.0 56	1.3 1	C7H11NO5	2. 8	N-acetyl-dl-glutamic acid	[M-H]-
188.0 924	2.0 7	C12H12FN	22 .8	6-Fluoro-1,2,3,4-tetrahydrocarbazole	[M-H]-
189.0	0.9	C6H6O7	2.	Garcinia lactone	[M-H]-

036	9		6		
189.0	3.2	C9H10N4O	10	6-(3,5-Dimethyl-1H-pyrazol-1-yl)-3(2H)-pyridazinone	[M-H]-
763	9				
191.0	1.2	C6H8O7	2.8	Citric acid	[M-H]-
191	3				
191.0	6.7	C11H12O3	15.1	1-(4-Methoxyphenyl)cyclopropanecarboxylic acid	[M-H]-
743	6				
193.0		C25H30O13	2.5	Picroside III	[M-H-C15H20O9]-
5	5				
193.0	3.7	C22H30O14	2.6	Arillatose B	[M-H-C12H20O10]-
501	2				
193.0	5.2	C10H10O4	3.2	Ferulate	[M-H]-
504	8				
193.0	10.	C19H30O4	2.5	8-Gingerol	[M-H-C8H16O]-
865	57				
195.0	2.8	C9H8O5	2.1	HAEMATOMMIC ACID	[M-H]-
294	1				
195.0	0.8	C6H12O7	2.6	Dextronic acid	[M-H]-
505	1				
195.0		C10H12O4	14.9	.alpha.,4-Dihydroxybenzenebutanoic acid	[M-H]-
634	4.9				
195.1	4.0	C12H20O2	2.7	Dodeca-2(E),4(E)-dienoic acid	[M-H]-
386	3				
197.0	5.6	C9H10O5	3	3,4-Dimethoxysalicylic acid	[M-H]-
451	8				
199.1	8.3	C11H20O3	2.1	(2E)-5-Hydroxyundec-2-enoic acid	[M-H]-
336	1				

201.0 764	3.5 6	C15H24O10	2. 1	Harpagide	[M-H- C6H10O5]-
201.1 128	7.5 3	C10H18O4	1. 8	Sebacic acid	[M-H]-
201.1 28	7.0 4	C9H18N2O3	17 .5	Ala-Leu	[M-H]-
202.0 505	10. 99	C11H9NO3	2. 1	Indole-3-pyruvic acid	[M-H]-
202.1 081	9.3 4	C10H13N5	8. 6	Isopentenyladenine	[M-H]-
203.0 921	4.2 8	C10H12N4O	8. 7	3-(1H-Benzimidazol-2-yl)propanohydrazide	[M-H]-
203.1 284	5.0 8	C10H20O4	2	3,5-Dihydroxycapric acid	[M-H]-
205.0 347	2.0 8	C7H10O7	1. 9	3-Carbomethoxy-3-hydroxyglutaric acid	[M-H]-
205.0 349	1.0 2	C7H10O7	2. 3	(R)-2-Hydroxybutane-1,2,4-tricarboxylate	[M-H]-
206.0 819	4.6 9	C11H13NO3	2	N-Acetyl-L-phenylalanine	[M-H]-
207.0 293	3.1 1	C9H9FN4S	10 .4	4-Amino-5-[(4-fluorophenyl)methyl]-2,4-dihydro-3H-1,2,4-triazole-3-thione	[M-H- NH2]-
207.0 656	5.4 9	C11H12O4	2. 5	Sinapoyl aldehyde	[M-H]-
208.0 611	3.0 3	C10H11NO4	1. 4	[2-(Acetylamino)phenoxy]acetic acid	[M-H]-
209.0 298	3.6 1	C6H8O7	2. 1	Saccharo-1,4-lactone	[M+OH]-

209.0 663	0.8 8	C8H10N4O3	8. 3	1,3,7-Trimethyluric acid	[M-H]-
209.0 791	6.1 4	C11H14O4	13 .7	Preleptospermone	[M-H]-
209.1 179	8.5 9	C12H18O3	2	(-)-Jasmonic acid	[M-H]-
210.0 762	3.9 1	C10H13NO4	1	3-Methoxytyrosine	[M-H]-
211.0 067	2.7 8	C6H8O6	24 .9	.beta.-D- Glucurono-.gamma.- lactone	[M+Cl]-
211.0 641	5.0 6	C10H12O5	14 .2	Methyl syringate	[M-H]-
211.0 721	2	C9H14N2O5	1. 3	Pro-Asp	[M-H- H2O]-
211.1 336	11. 92	C12H20O3	2. 1	(-)-Dihydrojasmonic acid	[M-H]-
213.0 514	1.9 7	C13H10O3	20 .4	3-Phenoxybenzoic acid	[M-H]-
213.1 493	10. 03	C12H22O3	0. 3	12-hydroxydodec-3-enoic acid	[M-H]-
215.0 324	0.8 2	C6H12O6	2	D-Psicose	[M+Cl]-
215.0 823	3.6 9	C12H12N2O2	1. 7	5-Phenethyl-1H-pyrazole- 3-carboxylic acid	[M-H]-
215.0 922	5.0 9	C11H12N4O	7. 6	4,7-Dihydro-5-methyl-6- (1-methylethyl)-7- oxopyrazolo[1,5- a]pyrimidine-3-carbonitrile	[M-H]-
215.0 922	4.4 1	C10H16O5	1. 7	Decanedioic acid, 4-oxo-	[M-H]-

215.1 075	6.1	C ₂₃ H ₂₄ O ₇	1. 7	11b,13-Dihydrolactucopicrin	[M-H-C ₉ H ₈ O ₅]-
215.1 286	6.2 6	C ₁₁ H ₂₀ O ₄	1. 4	Homononactinic acid	[M-H]-
215.1 398	3.6 1	C ₁₀ H ₂₀ N ₂ O ₃	1. 5	Val-Val	[M-H]-
215.1 649	10. 53	C ₁₂ H ₂₄ O ₃	1. 8	4-Hydroxylauric acid	[M-H]-
215.1 65	12. 42	C ₁₂ H ₂₄ O ₃	1. 7	12-Hydroxylauric acid	[M-H]-
217.1 079	5.2 9	C ₁₀ H ₁₈ O ₅	0. 3	3-Hydroxysebacic acid	[M-H]-
217.1 231	6.1	C ₁₆ H ₂₂ O ₅	1. 2	(E)-7-(4-Methoxy-5-methyl-6-oxopyran-2-yl)-5-methyloct-6-enoic acid	[M-H-C ₂ H ₄ O ₃]-
217.1 442	5.6 2	C ₁₂ H ₂₀ N ₄ S	7. 9	N-Cyclohexyl-N'-(3,5-dimethyl-1H-pyrazol-4-yl)thiourea	[M-H-H ₂ S]-
218.1 031	2.4 5	C ₉ H ₁₇ NO ₅	3. 9	Pantothenate	[M-H]-
219.1 388	8.3 1	C ₁₅ H ₂₀ O ₄	1. 3	Spirodionic acid	[M-H-CO ₂]-
220.1 466	11. 92	C ₁₅ H ₂₄ O ₂	1. 3	NSC 14451	[M-H-CH ₃]-
221.0 663	0.8	C ₁₂ H ₂₂ O ₁₁	1. 3	Palatinose	[M-H-C ₄ H ₈ O ₄]-
221.0 792	7	C ₁₂ H ₁₄ O ₄	12	Tetramethylterephthalic acid	[M-H]-
221.0 817	10. 04	C ₁₂ H ₁₄ O ₄	1. 3	4-(Boc)benzoic acid	[M-H]-
221.0	7.3	C ₂₄ H ₂₆ O ₇	1.	6-[(E)-But-2-en-2-yl]-4-[6-[(Z)-but-2-en-2-yl]-	[M-H-C ₁₂ H ₁₂ O ₃

817	3		4	2,4-dihydroxy-3-methylbenzoyl]oxy-2-hydroxy-3-methylbenzoic acid	-CO2]-
223.0 246	2.6 8	C12H12FN3OS	11 .6	4-Allyl-3-[(4-fluorophenoxy)methyl]-1H-1,2,4-triazole-5-thione	[M-H-C3H5]-
223.0 949	7.5 3	C12H16O4	12 .1	4-Isobutoxy-3-methoxybenzoic acid	[M-H]-
223.1 701	11. 87	C14H24O2	1. 3	5-Tetradecynoic acid	[M-H]-
227.1 033	2.9 3	C10H16N2O4	1. 6	PyroGlu-Val	[M-H]-
227.1 285	9.7 8	C12H20O4	1. 8	trans-Traumatic acid	[M-H]-
228.1 238	8.4	C11H19NO4	1. 5	N-(tert-Butyloxycarbonyl)isonipecotic acid	[M-H]-
229.1 079	6.8 3	C11H18O5	1	2-(6-Hydroxyhexyl)-3-methylenesuccinic acid	[M-H]-
230.1 395	4.3 9	C11H21NO4	0. 9	N-(2-Hydroxy-3-methylbutanoyl)leucine	[M-H]-
231.1 347	2.5 8	C10H20N2O4	1	Thr-Leu	[M-H]-
233.1 543	18. 13	C15H24O3	0. 8	(E)-5-(3-Hydroxy-2,3-dimethylnorbornan-2-yl)-2-methylpent-2-enoic acid	[M-H-H2O]-
235.0 644	5.6 8	C18H22O10	13 .4	Picraquassioside A	[M-H-C6H10O5]-
235.0 949	8.4	C13H16O4	13 .2	Q63392268	[M-H]-
235.1	2.9	C12H16N2O3	0.	.beta.-Ala-Phe	[M-H]-

086	7		9		
235.1	6.1	C ₁₄ H ₂₀ O ₃	0.	1-Naphthalenepropanoic acid, 1,2,3,5,6,7,8,8a-octahydro-2-methyl-3-oxo-	[M-H]-
337			9		
235.1	12.	C ₁₅ H ₂₄ O ₂	2.	Dihydroartemisinic acid	[M-H]-
701	92		2		
236.0	2.2	C ₁₂ H ₁₅ NO ₄	0.	2-((3aR,4S,7R,7aS)-1,3-Dioxohexahydro-1H-4,7-methanoisoindol-2(3H-yl)propanoic acid	[M-H]-
926	3		9		
236.1	11.	C ₁₃ H ₁₆ FNO ₂	17	1-(2-Fluorobenzyl)-4-piperidinecarboxylic acid	[M-H]-
052	61		.3		
237.0	5.4	C ₁₁ H ₁₀ O ₆	1.	Benzoylmalic acid	[M-H]-
403	6		2		
237.0	4.1	C ₁₂ H ₁₄ O ₅	14	3,4,5-Trimethoxycinnamic acid	[M-H]-
802			.2		
237.1	11.	C ₁₄ H ₂₂ O ₃	0.	MCULE-2036056204	[M-H]-
494	06		6		
239.0	3.6	C ₁₁ H ₁₂ O ₆	1	Acetylsyringic acid	[M-H]-
559	2				
239.0	4.3	C ₁₂ H ₁₆ O ₅	1.	Propylurofuranic acid	[M-H]-
921	9		8		
239.1	11.	C ₁₃ H ₂₀ O ₄	1.	3-(Hepta-1,3-dienyl)adipic acid	[M-H]-
286	77		4		
239.1	5.6	C ₁₄ H ₁₈ N ₄ S	6.	N-[2-(1H-Imidazol-5-yl)ethyl]-N'-(2-phenylethyl)thiourea	[M-H-H ₂ S]-
287	1		4		
239.1	5.5	C ₁₄ H ₂₆ O ₄	1.	Tetradecanedioic acid	[M-H-H ₂ O]-
65	2		2		
240.0	9.0	C ₁₄ H ₁₁ NO ₃	0.	1,3-Dihydroxy-N-methylacridone	[M-H]-
665	5		6		

240.1 24	6.7 4	C13H15N5	6. 2	Spiro[cyclopentane- 1,4'(1'H)-[1,3,5]triazino[1,2- a]benzimidazol]-2'-amine	[M-H]-
241.0 022	2.6 8	C6H14O7P2	5. 9	(E)-C-HDMAPP	[M-H- H2O]-
241.0 828	2.1 6	C10H14N2O5	1. 1	Thymidine	[M-H]-
241.1 08	7.3 2	C18H30O10	0. 6	1-O-((2E,4E)-9-Carboxy- 8-hydroxy-2,7- dimethylnona-2,4- dienoyl)hexitol	[M-H- C6H12O5]-
241.1 08	5.7 6	C18H28O10	0. 8	1-O-((2E,4E)-9-Carboxy- 8-hydroxy-2,7- dimethylnona-2,4- dienoyl)-.beta.-D- glucopyranose	[M-H- C6H10O5]-
241.1 192	4.2 1	C11H20N2O5	1. 1	L-.gamma.-Glutamyl-L- leucine	[M-H- H2O]-
241.1 442	5.7 2	C13H22O4	0. 7	2-Oct-7-enylglutaric acid	[M-H]-
241.1 444	4.7 2	C13H22O4	0. 5	2-Pentenedioic acid, 2- octyl-	[M-H]-
243.0 621	1.2 6	C9H12N2O6	1. 6	Uridine	[M-H]-
243.1 6	11. 15	C13H24O4	0. 4	Brassylic acid	[M-H]-
243.1 712	3.7 5	C12H24N2O3	0. 8	Leu-Leu	[M-H]-
243.1 964	13. 7	C14H28O3	0. 8	14-Hydroxymyristic acid	[M-H]-
244.1 302	2.4 9	C10H19N3O4	0. 4	Asn-Leu	[M-H]-

245.0 431	0.7 8	C ₁₄ H ₁₁ ClO ₂	23 .1	2'-Chloro-2-hydroxy-5-methylbenzophenone	[M-H]-
245.0 93	5.0 4	C ₁₃ H ₁₄ N ₂ O ₃	1. 3	N-Acetyltryptophan	[M-H]-
245.1 143	2.6 9	C ₁₀ H ₁₈ N ₂ O ₅	0. 3	Asp-Ile	[M-H]-
246.0 771	2.9 8	C ₈ H ₁₃ N ₃ O ₆	16	Asn-Asp	[M-H]-
247.1 186	4.6 1	C ₁₂ H ₁₆ N ₄ O ₂	5. 4	8-Cyclopentyltheophylline	[M-H]-
247.1 55	6	C ₁₃ H ₂₀ N ₄ O	5. 7	2-(4-Methyl-1-piperazinyl)-5,6,7,8-tetrahydro-4-quinazolinol	[M-H]-
247.1 702	13. 19	C ₁₇ H ₂₄ O ₄	1. 3	Lasiodiplodin	[M-H-CO ₂]-
249.1 107	9.7 8	C ₃₅ H ₅₆ O ₈	9. 9	Lasalocid C	[M-H-C ₂₁ H ₃₈ O ₄]-
249.1 494	14. 28	C ₁₅ H ₂₂ O ₃	1. 2	2-((1S,2S,4aR,8aS)-1-hydroxy-4a-methyl-8-methylenedecahydronaphthalen-2-yl)acrylic acid	[M-H]-
250.0 72	4.2 1	C ₁₂ H ₁₃ NO ₅	2. 3	N-Phenylacetylaspatic acid	[M-H]-
250.1 447	13. 88	C ₁₅ H ₂₁ NO ₅	0. 7	2-[(2-Ethylbutanoyl)amino]-4,5-dimethoxybenzoic acid	[M-H-CO ₂]-
251.0 56	4.4 7	C ₁₂ H ₁₄ O ₇	0. 7	Phenol glucuronide	[M-H-H ₂ O]-
251.1 036	2.8	C ₁₂ H ₁₆ N ₂ O ₄	0	Ser-Phe	[M-H]-
251.1	10.	C ₁₅ H ₂₀ O ₆	9.	1-Hydroxy-1-	[M-H-

265	27		9	(hydroxymethyl)-8,8-dimethyl-2-oxo-4a,6a,7,9-tetrahydro-4H-pentaleno[1,6a-c]pyran-5-carboxylic acid	CO2]-
251.1	7.6		0.	(2E,4E)-5-(3,8-Dihydroxy-1,5-dimethyl-7-oxo-6-oxabicyclo[3.2.1]octan-8-yl)-3-methylpenta-2,4-dienoic acid	[M-H- CO2]-
288	1	C15H20O6	7		
251.1	11.		0.	2-(8-Hydroxy-4a,8-dimethyldecalin-2-yl)acrylic acid	[M-H]-
651	96	C15H24O3	8		
252.0	7.0		0.	6-Hydroxy-5-methoxyflavone	[M-H- CH3]-
427	5	C16H12O4	3		
252.0			9.	5-(Trifluoromethyl)deoxyuridine	[M-H- CHNO]-
513	2	C10H11F3N2O5	8		
254.0	5.7		13	Methyl N-(2,3-dihydroxybenzoyl)serinate	[M-H]-
704	2	C11H13NO6			
255.0	2.5		10	1,3-Dimethyl-2-hydroxythioxanthone	[M-H]-
51	4	C15H12O2S			
255.0	6.9		0.	Isoliquiritigen	[M-H]-
67	1	C15H12O4	8		
255.2	15.		0.	PG(16:0/18:2(9Z,12Z))	[M-H- C24H43O8 P]-
328	91	C40H75O10P	3		
256.1	7.2		0.	cis-2-tert-Butoxycarbonylamino-2-methylcyclohexanecarboxylic acid	[M-H]-
554	3	C13H23NO4	2		
257.0			15	Lactupicrin	[M-H- C8H8O3]-
779	2.1	C23H22O7	.6		

257.1 394	3.4	C ₁₉ H ₃₀ O ₉	0	5-[4-[(E)-3-Carboxy-3-hydroxy-prop-1-enyl]-4-hydroxy-3,3,5-trimethylcyclohexoxy]-3-hydroxy-5-keto-3-methylvaleric acid	[M-H-C ₆ H ₈ O ₄]-
257.1 394	7.4 4	C ₁₃ H ₂₀ O ₄	0. 5	(Z)-2-Oct-7-enylpent-2-enedioic acid	[M+OH]-
257.2 121	14. 58	C ₁₅ H ₃₀ O ₃	0. 1	3-Lauryloxypropionic acid	[M-H]-
259.0 225	0.7 6	C ₆ H ₁₃ O ₉ P	0. 2	D-Fructose 6-phosphate	[M-H]-
259.0 724	3.6 7	C ₁₄ H ₁₂ N ₂ O ₆	0. 2	9-Nitro-3a,4,5,9b-tetrahydro-3H-cyclopenta[c]quinoline-4,6-dicarboxylic acid	[M-H-CO ₂]-
259.1 187	5.1 9	C ₁₆ H ₁₈ FN ₃ O ₃	24	Norfloxacin	[M-H-C ₂ H ₃ O ₂]-
259.1 3	2.6 6	C ₁₁ H ₂₀ N ₂ O ₅	0. 1	Glu-Leu	[M-H]-
261.0 075	2.5 2	C ₉ H ₁₀ O ₇ S	0. 2	Homovanillic acid sulfate	[M-H]-
261.0 881	3.7 2	C ₁₃ H ₁₄ N ₂ O ₄	0. 1	1-[4-(Acetylamino)phenyl]-5-oxo-3-pyrrolidinecarboxylic acid	[M-H]-
261.1 108	10. 28	C ₁₅ H ₁₈ O ₄	9	Pentalenolactone E	[M-H]-
261.1 343	5.5 1	C ₁₂ H ₂₂ O ₆	0. 4	9-Glyceryloxy-9-ketopelargonic acid	[M-H]-
262.1 448	10. 23	C ₁₅ H ₂₁ NO ₃	0. 4	N-(4-Methylpentanoyl)phenylalanine	[M-H]-

263.0 959	5.6 5	C ₁₄ H ₁₆ O ₅	13	Peucedanol	[M-H]-
263.1 288	12. 33	C ₁₅ H ₂₀ O ₄	0. 7	(3aS,6Z,10E,11aS)-3,10-Dimethyl-2-oxo-3a,4,5,8,9,11a-hexahydro-3H-cyclodeca[b]furan-6-carboxylic acid	[M-H]-
263.1 289	7.6 5	C ₁₅ H ₂₀ O ₄	0. 1	Peruvic acid	[M-H]-
263.1 29	8.2 9	C ₁₅ H ₂₀ O ₄	0. 2	2-(6-Hydroxy-2-keto-3,8-dimethyl-4,5,6,7,8,8a-hexahydro-1H-azulen-5-yl)acrylic acid	[M-H]-
263.1 293	8	C ₁₅ H ₂₀ O ₄	0. 2	Abscisate	[M-H]-
264.0 877	2.9 6	C ₁₇ H ₁₆ N ₂ O ₂	9. 9	3,5-Bis(3-methoxyphenyl)-1H-pyrazole	[M-H-CH ₃]-
264.1 031	6.9 6	C ₁₇ H ₁₅ NO ₂	0. 1	2-Phenyl-1H-indole-1-propanoic acid	[M-H]-
264.1 335	7.5 5	C ₁₃ H ₁₉ N ₃ O ₃	0. 2	Pyroxamide	[M-H]-
265.0 718	4.4 7	C ₁₉ H ₂₄ O ₈	0. 1	5-[2-[(E)-4-Carboxybut-1-enyl]-6-hydroxy-4-methoxybenzoyl]oxyhexanoic acid	[M-H-C ₆ H ₁₀ O ₂]-
265.0 929	1.7 8	C ₁₇ H ₁₄ O ₃	22. .3	2-HBA	[M-H]-
265.1 058	6.1 4	C ₂₀ H ₂₈ O ₁₀	8. 9	Hyuganoside V	[M-H-C ₆ H ₁₀ O ₅]-
265.1 194	2.9 7	C ₁₃ H ₁₈ N ₂ O ₄	0. 5	Thr-Phe	[M-H]-
265.1	13.	C ₁₂ H ₂₆ O ₄ S	0.	Laurylsulfuric acid	[M-H]-

479	68		1		
266.1	3.4	C13H17NO5	0.	2-(4-Morpholinyl)ethyl 2,4-dihydroxybenzoate	[M-H]-
034	3		2		
267.0	1.1	C4H6O5	0.	DL-Malic acid	[2M-H]-
358	5		2		
267.1	11.	C15H24O4	0.	2-(9-Decenyl)glutaconic acid	[M-H]-
601	54		5		
268.0	7.2	C16H12O5	0.	4',6-Dihydroxy-3'-methoxyaurone	[M-H-CH3]-
378	7		4		
268.1	7.6	C14H23NO4	0.	N-(3-Oxodecanoyl)-DL-homoserine lactone	[M-H]-
555			5		
269.0	6.8	C15H10O5	0.	Sulfuretin	[M-H]-
456	2		8		
269.0	8.3	C15H10O5	1.	Genistein	[M-H]-
457	8		5		
269.0	7.6	C16H14O4	0.	Isoimperatorin	[M-H]-
82	4		4		
269.0	8.9	C15H14N2OS	23	2-(2-Phenoxyethylthio)-1H-benzimidazole	[M-H]-
828	2		.9		
269.0	8.2	C16H14O4	0.	Echinatin	[M-H]-
832	2		7		
269.2	12.	C16H30O3		(z)-3-hydroxyhexadec-7-enoic acid (nmr)	[M-H]-
122	7		0		
270.0	2.9	C14H9NO5	12	o-(m-Nitrobenzoyl)benzoic acid	[M-H]-
442	3		.9		
270.0	10.	C15H13NO4	0.	Benzoic acid, p-(p-anisamido)-	[M-H]-
772	55		1		
271.0	9.8	C15H12O5	0.	Butin	[M-H]-
613	1		3		
271.0	8.2	C15H12O5	0.	Naringenin	[M-H]-
615			2		

271.0 977	8.9 8	C16H16O4	0. 5	p-Anisic acid, 2-hydroxy- 6-phenethyl-	[M-H]-
271.1 915	11. 51	C28H43NO6	0. 2	Borrelidin	[M-H- C13H15NO 2]-
271.2 279	15. 03	C16H32O3	0. 2	Juniperic acid	[M-H]-
271.2 279	14. 04	C16H32O3	0. 5	2-Hydroxypalmitic acid	[M-H]-
271.2 279	14. 7	C16H32O3	0. 6	3-Hydroxypalmitic acid	[M-H]-
272.0 566	7.3 7	C14H11N3O6S 2	24 .7	5'-Carboxymeloxicam	[M-H- CSO4]-
272.0 93	7.2	C10H14N2O6	15 .1	1-methylpseudouridine	[M-H]-
273.0 769	6.1 8	C15H14O5	0. 5	Phloretin	[M-H]-
275.2 017	12. 91	C18H28O2	0. 1	9,12-Octadecadiynoic acid	[M-H]-
276.0 99	3.0 8	C10H19N3O4S	11 .9	Gln-Met	[M-H]-
277.1 293	4.3 9	C11H22N2O4S	23 .6	Pantetheine	[M-H]-
277.1 444	13. 07	C16H22O4	0. 5	Mono-2-ethylhexyl phthalate	[M-H]-
277.1 558	4.4 7	C15H22N2O3	0. 4	Leu-Phe	[M-H]-
277.2 172	13. 47	C18H30O2	0	Pinolenic acid	[M-H]-
277.2 173	14. 89	C18H30O2	0. 4	(9Z,12Z,15Z)- Octadecatrienoic acid	[M-H]-

279.0722	2.02	C16H12N2O3	18.6	N-(1,3-Dioxo-2,3-dihydro-1H-isoindol-5-yl)-2-phenylacetamide	[M-H]-
279.1087	2.58	C17H16N2O2	18.8	Cyclopeptine	[M-H]-
279.1238	6.1	C15H22O6	0.4	Hydroheptelidic acid	[M-H-H2O]-
279.1601	12.6	C16H26O5	0.6	13,14-Dihydro-15-ketotetranorprostaglandin E2	[M-H-H2O]-
279.1965	12.87	C17H28O3	0.4	12(S)-HHTrE	[M-H]-
279.2329	15.38	C18H32O2	0.1	Linoleate	[M-H]-
281.0304	2.96	C10H10ClF3N2O2	2.3	2-[4-Chloro-5-cyclopropyl-3-(trifluoromethyl)pyrazol-1-yl]propionic acid	[M-H]-
281.1395	10.82	C15H22O5	0.4	3-((3aS,6S,8aR)-8-Hydroxy-6,8-dimethyl-3-methylidene-2-oxooctahydro-2H-cyclohepta[b]furan-7-yl)propanoic acid	[M-H]-
281.2122	12.96	C17H30O3	0	12(S)-Hydroxy-16-heptadecynoic acid	[M-H]-
281.2485	16.01	C18H34O2	0.5	Oleic acid	[M-H]-
282.1136	6.42	C18H17NO5	0.1	N-trans-p-Coumaroyltyrosine	[M-H-CO2]-
283.0612	7.55	C16H12O5	1.7	Genkwanin	[M-H]-

283.0 685	2	C10H12N4O6	2. 2	9-.beta.-D- Ribofuranosylxanthine	[M-H]-
283.1 551	9.1 3	C15H24O5	0. 3	2,3-Dihydroxy-3-(2- hydroxypropan-2-yl)-8a- methyl-1,2,3a,4,5,8- hexahydroazulene-6- carboxylic acid	[M-H]-
285.0 406	7.3 5	C15H10O6	1. 6	Luteolin	[M-H]-
285.0 565	2.5 6	C15H10N2O7	12 .2	5-(4- Nitrobenzoylamino)isophth alic acid	[M-H- CO2]-
285.0 617	3.0 2	C12H14O8	4. 3	Uralenneoside	[M-H]-
285.0 769	6.8 8	C16H14O5	0	Isosakuranetin	[M-H]-
285.0 769	5.4 2	C16H14O5	0. 5	Melilotocarpan B	[M-H]-
285.2 071	13. 01	C16H30O4	0. 1	Hexadecanedioic acid	[M-H]-
285.2 072	10. 48	C16H32O5	0. 1	Aleuritic acid	[M-H- H2O]-
286.1 523	2.0 6	C16H21N3O2	13 .2	Zolmitriptan	[M-H]-
287.0 676	4.1 1	C11H16N2O5S	10 .7	1-(3,5-Dimethylisoxazol-4- yl)sulfonylisonipecotic acid	[M-H]-
287.1 501	5.7 8	C14H24O6	0. 3	(E)-3,10-Dihydroxy-4,9- dimethyldodec-6-enedioic acid	[M-H]-
287.1 653	11. 54	C19H24O5	0	Gibberellin A4	[M-H- CO2]-
288.0	2.3	C15H12FNO4	16	2-[[4-	[M-H]-

726	7		.5	Fluorophenoxy)acetyl]amin o}benzoic acid	
288.1 454	4.3 8	C13H23NO6	0. 6	Adipoyl-L-carnitine	[M-H]-
289.0 719	3.3 8	C15H14O6.H2 O	0. 7	(+)-catechin hydrate	[M-H]-
289.0 72	3.8 9	C15H14O6	1. 6	Catechin	[M-H]-
290.0 881	0.9	C11H17NO8	3. 4	N-Fructosyl pyroglutamate	[M-H]-
291.0 875	3.8 8	C15H16O6	0. 7	Altenuene	[M-H]-
291.1 451	4.8 5	C19H20N2O	17 .9	N-(1-Methyl-3- phenylpropyl)-1H-indole- 6-carboxamide	[M-H]-
291.1 966	13. 09	C18H28O3	0. 2	9-OxoOTrE	[M-H]-
293.1 243	2.6 1	C19H18O3	20 .4	Alnusone	[M-H]-
293.1 244	3.5 2	C14H18N2O5	2. 2	H-gamma-glu-phe-oh	[M-H]-
293.1 759	11. 61	C17H26O4	1. 2	[6]-Gingerol	[M-H]-
293.2 122	12. 91	C18H30O3	1. 7	(9S,10E,12Z,15Z)-9- Hydroxy-10,12,15- octadecatrienoic acid	[M-H]-
293.2 122	14. 2	C18H30O3	0. 4	13-HOTE	[M-H]-
293.2 122	13. 58	C18H32O4	0. 5	9-HpODE	[M-H- H2O]-
295.1	2.0	C18H16O4	20	6-Ethoxy-3-(4- hydroxyphenyl)-4-	[M-H]-

035	6		.2	methylcoumarin	
295.1	4.7	C15H20O6	11	Deoxynivalenol	[M-H]-
221	7		.2		
295.2	14.	C18H32O3	1	12(13)-EpOME	[M-H]-
277	1				
297.0	9.8	C17H14O5	0.	7-hydroxy-2',4'- dimethoxyisoflavone	[M-H]-
767	2		4		
297.0	8.4	C17H14O5	0.	Cladrin	[M-H]-
768	1		6		
297.0	7	C17H14O5	0.	7-O-Methylbiochanin A	[M-H]-
768			4		
297.1	1.9	C18H18O4	20	2,4-Dimethoxy-2'- hydroxy-5'-methylchalcone	[M-H]-
192	4				
297.1	3.7	C15H22O6	0.	2-(Hydroxy(7a-hydroxy-3- oxo-5-(propan-2- yl)octahydro-2- benzofuran-4- yl)methyl)prop-2-enoic acid	[M-H]-
343	2		4		
297.2	11.	C17H30O4	0.	Nephrosteranic acid	[M-H]-
07	23		2		
297.2	13.	C18H34O3	0.	Oleic acid epoxide	[M-H]-
434	91		5		
299.0	9.5	C15H14N2O4S	15	Belinostat	[M-H- H2O]-
449	1		.7		
299.0	6.1	C16H12O6	0.	Tectorigenin	[M-H]-
561	6		3		
299.0	8.7	C27H30O15	0.	Tectorigenin, 7-O- β - D-apiofuranosyl-(1- 6)- β -D- glucopyranosid]	[M-H- C11H18O9] -
561	4		3		
299.0	6.8	C16H12O6	2.	Luteolin 7-methyl ether	[M-H]-

562	1		1		
299.0	8.5	C16H12O6	0.	Isokaempferide	[M-H]-
562	8		4		
299.0	2.1	C13H16O8	1	Salicylic acid beta-D-glucoside	[M-H]-
773	2				
299.0	8.2	C17H16O5	0.	2',4'-Dihydroxy-3,4-dimethoxychalcone	[M-H]-
923	4		4		
299.1	7.5	C17H28O7	0.	4-(Acetyloxy)-6-hydroxy-2-(2-hydroxypropan-2-yl)-4a,6-dimethyloctahydro-2H-chromene-5-carboxylic acid	[M-H-CO2]-
866	3		2		
299.2	11.	C17H32O4	0.	Roccellic acid	[M-H]-
227	79		1		
299.2	14.	C18H36O3	0.	(R)-2-Hydroxystearate	[M-H]-
59	3		7		
300.1	12.	C18H23NO3	0.	Ractopamine	[M-H]-
604	75		1		
300.1	3.7	C14H27N3O4	0.	Leu-Gly-Leu	[M-H]-
929	3		1		
301.1	14.	C18H24O5	0.	Zearalanone	[M-H-H2O]-
444	11		7		
301.2	7.8	C12H26N6O3	9	Lys-Arg	[M-H]-
021					
302.1	4.1	C15H17N3O4	0.	Glutamine, N2-(indol-3-ylacetyl)-	[M-H]-
148	1		1		
305.0	3.7	C12H18O7S	4.	2-[3-oxo-2-(5-sulfooxy-pent-2-enyl)cyclopentyl]acetic acid	[M-H]-
702	5		8		
305.1	5.2	C26H32O4	19	Amorfrutin C	[M-H-C5H10O2]-
606	5		.2		

305.1 758	11. 23	C18H26O4	4. 3	9,16-dioxooctadec- 10,12,14-trienoic acid	[M-H]-
305.1 759	10. 52	C18H26O4	0. 2	Amorfrutin 2	[M-H]-
307.0 858	4.8 8	C21H22O9	11 .6	Robustaside A	[M-H- C6H6O2]-
307.1 399	4.5 8	C19H20N2O2	17 .3	Vincanidine	[M-H]-
307.1 552	7.1 2	C19H20N4O2	3. 9	Plinabulin	[M-H-CO]-
307.1 915	12. 21	C18H28O4	1. 4	16-hydroxy-9- oxooctadeca-10,12,14- trienoic acid	[M-H]-
309.1 193	1.8 8	C18H18N2O3	16 .9	Orantinib	[M-H]-
309.1 344	6.4 3	C15H20O4	1. 4	Pentalenolactone D	[M+FA-H]-
309.1 433	4.7 4	C23H26O7	20 .6	Purpactin A	[M-H- C3H4O4]-
309.1 742	15. 26	C18H32N8O4	19 .5	Gly-Pro-Arg-Pro-amide	[M-H- C5H10N2O]-
309.2 071	12. 93	C18H30O4	0. 4	trans-EKODE-(E)-Ib	[M-H]-
309.2 072	10. 51	C18H30O4	0. 1	9-HpOTrE	[M-H]-
310.0 358	5.2 2	C16H9NO6	0. 4	5-Phthalimidoisophthalic acid	[M-H]-
310.1 661	8.3 6	C12H21N7O3	9. 4	Arg-His	[M-H]-
311.0	2.9	C14H11F3N2O	19	XAV 939	[M-H]-

411	9	S	.3		
311.0 925	6.4 7	C18H16O5	0. 1	3-(3,4-Dimethoxyphenyl)- 6-hydroxy-4- methylcoumarin	[M-H]-
311.1 097	0.8	C17H16N4	9. 3	1,3-Bis(2- benzimidazolyl)propane	[M+Cl]-
311.1 687	15. 71	C20H24O3	11	Hypolide	[M-H]-
311.2 227	13. 43	C18H32O4	2. 2	FA 18:2+2o	[M-H]-
311.2 228	12. 51	C18H32O4	4	9(S)-HPODE	[M-H]-
312.1 242	6.5 6	C18H19NO4	0. 1	Moupinamide	[M-H]-
313.0 719	7.3 9	C17H14O6	0. 3	Cirsimaritin	[M-H]-
313.0 719	8.4 1	C17H14O6	0. 1	Hortensin	[M-H]-
313.0 931	2.5 8	C14H18O8	1	4-(.beta.-D- Glucopyranosyloxy)benzen eacetic acid	[M-H]-
313.0 958	3.9 4	C18H19N3O3S	16 .8	Rosiglitazone	[M-H- CHNO]-
313.2 383	12. 51	C18H34O4	0	12,13-DiHOME	[M-H]-
313.2 384	11. 7	C18H34O4	0. 1	Oxiraneoctanoic acid, .eta.- hydroxy-3-octyl-	[M-H]-
313.2 385	11. 45	C18H34O4	2. 4	(+/-)12(13)-DiHOME	[M-H]-
314.2 087	4.4 3	C20H29NO2	12 .4	2,4-Dodecadienamide, N- (p-hydroxyphenethyl)-,	[M-H]-

				(E,E)-	
315.0 512	8.7 7	C16H12O7	1	Isorhamnetol	[M-H]-
315.0 723	2.4 2	C13H16O9	4. 4	Benzoic acid + 2O, O-Hex	[M-H]-
315.0 933	0.8 4	C19H22O6	17 .9	3-(3,4-Dimethoxyphenyl)- 1-(2-hydroxy-4,6- dimethoxyphenyl)propan- 1-one	[M-H- C2H6]-
315.1 563	5.7 1	C19H24O4	12 .4	Heminordihydroguaiaretic acid	[M-H]-
315.2 539	13. 08	C17H34O2	0. 5	Methyl palmitate	[M+HCO2] -
316.1 878	3.6 8	C19H27NO3	13 .1	Nateglinide	[M-H]-
317.1 606	4.9 8	C13H26N4O3S	15 .2	GLM(Amide)	[M-H]-
317.1 757	11. 58	C19H26O4	0. 7	Ubiquinone	[M-H]-
319.1 187	6.8 3	C15H17FN4O3	7. 6	Penetrex	[M-H]-
320.0 904	5.5 8	C19H15NO4	7. 8	Cinnamyl 3,4- dihydroxy-.alpha.- cyanocinnamate	[M-H]-
321.0 729	2.5 5	C19H14O5	12 .1	Tetrangomycin	[M-H]-
321.1 556	4.3 3	C20H22N2O2	16 .2	Gelsemine	[M-H]-
322.1 084	12. 65	C13H17N5O5	22 .9	Anorexigenic Peptide	[M-H]-
322.2	10.	C22H32O8	1.	HT-2 Toxin	[M-H]-

025	65		7		
323.0 286	1.2 2	C9H13N2O9P	0. 4	1-.beta.-D-Arabinofuranosyluracil 5'-monophosphate	[M-H]-
323.0 984	1.3 2	C12H22O11	0. 1	D-(+)-Cellobiose	[M-H-H2O]-
323.0 985	1.6 3	C6H10O5	0. 3	Levoglucosan	[2M-H]-
323.1 348	2.9 6	C20H20O4	18	Corylifolinin	[M-H]-
323.2 228	13. 27	C19H32O4	0. 2	TOFA	[M-H]-
325.0 93	3.4 6	C15H18O8	0. 1	4-O-D-Glucopyranosyl-p-coumaric acid	[M-H]-
325.2 021	9.6 8	C18H30O5	4. 5	FA 18:3+3o	[M-H]-
325.2 173	14. 82	C22H32O3	0. 1	(.+/-.)20-HDoHE	[M-H-H2O]-
326.1 398	7.2 5	C19H21NO4	0. 2	(.+/-.)-Laurotetanine	[M-H]-
327.0 875	4.6 5	C18H16O6	0	2,4-Bis(4-hydroxyphenyl)cyclobutane-1,3-dicarboxylic acid	[M-H]-
327.1 086	3.9 5	C15H20O8	0. 2	3,4'-Dihydroxypropiophenone 3-glucoside	[M-H]-
327.2 177	9.3 2	C18H32O5	4. 5	FA 18:2+3o	[M-H]-
327.2 177	10. 18	C18H32O5	0. 2	12,15-Octadecadienoic acid, 7,9,10-trihydroxy-	[M-H]-
327.2	8.2	C18H32O5	0.	9,10,11-Trihydroxy-12(Z),15(Z)-	[M-H]-

178	2		1	octadecadienoic acid	
327.2	6.9	C18H32O5	0.	(10E,15Z)-9,12,13-	[M-H]-
178	5		1	Trihydroxyoctadeca-10,15-dienoic acid	
328.0	1.2	C10H12N5O6P	0.	2',3'-cAMP	[M-H]-
454	2		2		
328.1	5.5	C15H23NO5S	9.	Metolachlor esa	[M-H]-
191			6		
329.0	4.2	C16H10O8	0.	3,3',4,4' -	[M-H]-
304	8		9	Biphenyltetracarboxylic acid	
329.0	8.3	C17H14O7	0.	Jaceosidin	[M-H]-
667	9		2		
329.0	6.9	C17H14O7	0.	3,4' -Dimethylquercetin	[M-H]-
668	8		2		
329.0	2.4	C14H18O9	0.	4-(Hexopyranosyloxy)-3-	[M-H]-
879	3		1	methoxybenzoic acid	
329.1	6.0	C19H22O5	2.	Muricarpone B	[M-H]-
396	6		7		
329.1	14.	C20H26O4	0.	(6E,10Z,14E)-2-Keto-6,14-	[M-H]-
758	84		4	dimethyl-3-methylene-3a,4,5,8,9,12,13,15a-octahydrocyclotetradeca[b]furan-10-carboxylic acid	
329.1	13.	C20H28O5	0.	Ingenol	[M-H-H2O]-
758	45		1		
329.2	10.	C18H34O5	2.	FA 18:1+3o	[M-H]-
332	65		1		
329.2	11.	C18H34O5	0.	(Z)-9,10,11-Trihydroxy-12-	[M-H]-
333	2		1	octadecenoic acid	
331.0	2.1	C18H18Cl2O4	21	4-Chloro-6-(6-chloro-7-	[M-H-HCl]-
673			.4	hydroxy-2,4,4-trimethylchroman-2-	

				yl)resorcinol	
333.0 595	0.7 6	C16H14O8	6. 4	6,6'-Dihydroxy-5,5'- dimethoxybiphenyl-3,3'- dicarboxylic acid	[M-H]-
335.0 523	10. 39	C19H14O7	11 .9	WS 5995C	[M-H- H2O]-
335.1 713	4.6	C21H26N2O3	15 .6	Rauwolscine	[M-H- H2O]-
337.1 082	7.1 8	C20H18O5	0. 6	Terphenyllin	[M-H]-
337.1 505	2.9 7	C21H22O4	17	Licochalcone A	[M-H]-
339.1 812	9.3 3	C14H24N6O4	7. 9	Gly-His-Lys	[M-H]-
339.2 328	15. 02	C23H32O2	0. 6	2,2'-Methylene-bis(4- methyl-6-tert-butylphenol)	[M-H]-
341.0 878	3.3 8	C15H18O9	2. 5	Caffeic acid hexoside	[M-H]-
341.1 088	0.8 6	C10H18O9	0. 3	Glycan 1,4-D-Xylobiose	[M+C2H3O 2]-
341.1 089	1.5 7	C12H22O11	0. 2	Galactinol	[M-H]-
341.1 089	3.5	C12H22O11	2. 3	Isomaltose	[M-H]-
343.0 822	10. 68	C18H16O7	1. 7	Eupatilin	[M-H]-
343.1 915	14. 72	C21H28O4	0. 1	(.+/-)-11-Nor-9- carboxy-.DELTA.9-THC	[M-H]-
343.2 126	7.0 9	C18H32O6	0. 2	2,3-Dinorthromboxane B1	[M-H]-
343.2	6.0	C18H32O6	1.	FA 18:2+4o	[M-H]-

126	4		3		
344.0 401	1.2 3	C10H12N5O7P	0. 7	3',5'-Cyclic GMP	[M-H]-
345.0 616	8.6 2	C17H14O8	0	Syringetin	[M-H]-
345.1 191	2.9 4	C14H20O7	0. 2	Salidroside	[M+HCOO] -
345.2 07	12. 95	C21H30O4	0. 3	21-Deoxycortisol	[M-H]-
345.2 07	15. 07	C21H30O4	1. 3	NCGC00380281-01	[M-H]-
345.2 283	7.8 4	C18H32O5	0	(11E,15Z)-9,10,13-Trihydroxy-11,15-octadecadienoic acid	[M+OH]-
346.0 932	10. 32	C16H17N3O4S	18 .7	PFI-1	[M-H]-
347.0 985	2.0 5	C13H18O8	0. 4	4-Hydroxy-3-methoxyphenyl .beta.-D-glucopyranoside	[M+HCOO] -
347.1 499	11. 24	C19H24O6	0. 5	Eurycomalactone	[M-H]-
348.0 878	8.5 5	C16H16FN3O3 S	15 .8	Ulifloxacin	[M-H]-
350.1 609	5.0 6	C18H25NO6	0. 1	Boc-N-methyl-L-glutamic acid .gamma.-benzyl ester	[M-H]-
351.0 873	12. 51	C20H16O6	2	Ncgc00169972-02!3,6-dihydroxy-8-methoxy-3-methyl-2,4-dihydrobenzo[a]anthracene-1,7,12-trione	[M-H]-
353.0 727	1.2 2	C12H18O12	3	6:3+6O fatty acyl hexoside	[M-H]-

353.0 879	2.7 6	C16H18O9	3	Caffeoyl quinic acid	[M-H]-
353.2 003	16. 52	C19H30O6	9. 9	(E)-3-(4-Acetoxy-2,3-dihydroxy-2,5,5,8a-tetramethyldecalin-1-yl)acrylic acid	[M-H]-
354.2 036	5.8 7	C24H33NO4	11	Altersetin	[M-H-C2H4O]-
355.0 671	2.9	C15H16O10	4. 1	Coumaroyl + c6h9o8 (isomer of 844, 845, 846)	[M-H]-
355.1 035	3.7	C16H20O9	3. 7	1-O-Feruloylglucose	[M-H]-
356.1 868	14. 67	C15H27N5O5	20 .3	trans-Epoxy succinyl-L-leucylamido(4-guanidino)butane	[M-H]-
357.0 797	2.2 9	C17H20N6O4S	6. 3	Bromosporine	[M-H-C2H6O]-
357.1 04	0.8	C12H22O12	0. 9	Lactobionic acid	[M-H]-
357.1 192	3.3 8	C16H22O9	0. 1	2-O-.beta.-D-Glucosyloxy-4-methoxybenzenepropanoic acid	[M-H]-
357.1 192	3.0 4	C16H22O9	0. 3	3-(3-(.beta.-D-Glucopyranosyloxy)-2-methoxyphenyl)propanoic acid	[M-H]-
357.1 192	2.8 2	C15H20O7	0. 3	Juniperoside III	[M+HCOO]-
357.2 071	15. 57	C22H30O4	0. 4	Cannabidiolic acid	[M-H]-
359.0	2.6	C15H20O10	2.	Benzoic acid + 1o, 2meo,	[M-H]-

985	6		7	o-hex	
359.1 195	0.8 3	C6H12O6	0	Quercinitol	[2M-H]-
359.1 351	4.6 4	C16H24O9	0. 4	1-(.beta.-D-Glucopyranosyloxy)-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[c]pyran-4-carboxylic acid	[M-H]-
359.2 077	6.2 3	C19H28N4O3	3. 8	ADB-PINACA N-(4-hydroxypentyl) metabolite	[M-H]-
361.1 504	3.1 8	C16H26O9	0. 1	2-(2-((Hexopyranosyloxy)methyl)-3-methylcyclopent-2-en-1-yl)-3-hydroxypropanoic acid	[M-H]-
361.1 657	11. 46	C20H26O6	0	Secoisolariciresinol	[M-H]-
361.1 983	4.4 3	C20H27FN2O3	13 .8	5-Fluoro-Amb-Pica	[M-H]-
362.0 509	1.3 7	C10H14N5O8P	0. 2	GMP	[M-H]-
363.1 663	3.9	C23H24O4	14	Clusiacyclol A	[M-H]-
363.1 815	4.1 3	C21H24N4O2	3. 7	Pelanserine	[M-H]-
363.2 39	8.6 3	C25H32O2	16 .6	2-[(2E)-3,7-Dimethylocta-2,6-dienyl]-3-methoxy-5-phenethylphenol	[M-H]-
364.1 613	3.2 3	C18H19N7O2	23 .4	LY2606368	[M-H]-
367.1 035	4.1 7	C17H20O9	0. 2	3-O-Feruloylquinic acid	[M-H]-

369.1 225	4.8 9	C21H23NO6	1. 7	Colchicine	[M-H- CH3]-
371.2 3	4.5 3	C23H32O4	19 .6	LL-Z 1272.epsilon.	[M-H]-
373.0 928	10. 75	C19H18O8	0. 1	Casticin	[M-H]-
373.1 141	2.5 3	C16H22O10	0. 4	Ketologanic acid	[M-H]-
373.1 292	11. 45	C20H22O7	0. 3	(-)-Hydroxymatairesinol	[M-H]-
373.1 69	9.7 9	C21H26O6	7. 5	1,7-Bis(3,4-dihydroxyphenyl)heptan-3-yl acetate	[M-H]-
373.1 787	10. 82	C24H23FN2O	17	5-Fluoro NNEI	[M-H]-
373.1 869	6.2 5	C18H30O8	0. 5	(3-(Hexopyranosyloxy)-2-((2Z)-pent-2-en-1-yl)cyclopentyl)acetic acid	[M-H]-
373.2 384	15. 67	C23H34O4	4. 3	SCHEMBL16224903	[M-H]-
375.1 846	10. 48	C17H24N6O4	16 .1	[3-Me-His2] TRH	[M-H]-
377.1 818	5.9 1	C16H28O7	0. 1	2-Hydroxy-1,8-cineole glucoside	[M+HCOO] -
377.1 819	4.7 5	C16H28O7	0. 1	4-(Hydroxymethyl)-1-(propan-2-yl)cyclohex-3-en-1-yl .beta.-D-glucopyranoside	[M+FA-H]-
378.1 56	5.3 9	C14H25N3O9	10 .6	Kasugamycin	[M-H]-
378.1 77	4.3 8	C23H25NO4	11 .9	Atalaphylline	[M-H]-

380.1 564	2.4 3	C22H21NO4	16 .1	CAY10581	[M+OH]-
381.1 768	4.2 1	C16H30O10	0. 2	Foliachinenoside I	[M-H]-
383.1 196	2.3 2	C7H12O6	0. 5	(-)-Quinic acid	[2M-H]-
387.1 661	3.8 1	C18H28O9	1. 4	CHEBI:139442	[M-H]-
389.1 64	7.2 9	C23H22N4O5	4. 7	3-(4-Hydroxy-2,2-dimethyl-1-oxo-3,3a-dihydroimidazo[1,2-a]indol-4-yl)-2-(4-oxoquinazolin-3-yl)propanoic acid	[M-H-CO2]-
389.1 818	3.9 9	C23H31ClO3	22	5-Chloro-2,4-dihydroxy-6-methyl-3-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trienyl]benzaldehyde	[M-H]-
389.1 97	12. 82	C22H30O6	0. 2	14-Hydroxy-7-O-methylrosmanol	[M-H]-
391.1 975	6.2 8	C25H28O4	14 .9	3-[(2E)-3,7-Dimethylocta-2,6-dienyl]-2,4-dihydroxy-6-[(E)-styryl]benzoic acid	[M-H]-
392.1 716	5.5 7	C24H24FNO3	12 .8	NFPS	[M-H]-
393.1 954	9.1 3	C21H26N6O2	22 .9	Quisinostat	[M-H]-
395.0 29	2.3	C8H6O6	8. 2	4,5-Dihydroxyphthalic acid	[2M-H]-
395.0 443	5.8 7	C16H16N2O6S 2	16 .8	Cephalothin	[M-H]-
395.1	9.7	C23H24O6	4.	.gamma.-Mangostin	[M-H]-

508	8		1		
395.1 923	5.3 9	C17H32O10	0. 2	Hexyl 6-O- pentopyranosylhexopyrano side	[M-H]-
395.1 923	3.7 4	C16H30O8	5	(1R,2R,4S)-p-Menthane- 1,2,8-triol 8-glucoside	[M+HCOO] -
396.2 001	11. 87	C20H31NO7	6. 9	Tapentadol-.beta.-D- glucuronide	[M-H]-
397.0 598	5.5 9	C18H14N4O5S	3. 9	Sulfasalazine	[M-H]-
397.1 666	10. 48	C24H22N4O2	1. 1	Ro 31-7549	[M-H]-
399.1 66	3.4 4	C19H28O9	0. 9	Hexose + c13h17o3	[M-H]-
401.1 606	12. 93	C16H26N4O8	17 .9	CAY10679	[M-H]-
401.1 818	4.8 7	C19H30O9	0. 6	6-(3-(.beta.-D- Glucopyranosyloxy)butyl)- 5,5-dimethyl-3- oxocyclohex-1-ene-1- carboxylic acid	[M-H]-
401.2 039	3.3 1	C24H31FO4	23 .2	(S)-AL 8810	[M-H]-
403.1 034	11. 12	C20H20O9	5. 9	CHEMBL3407503	[M-H]-
403.2 086	6.1 6	C23H32O6	9. 7	Hydrocortisone 21-acetate	[M-H]-
403.2 642	15. 77	C21H41O5P	6	C18:1 Cyclic LPA	[M-H]-
404.1 045	0.8 6	C24H20ClNO3	3. 2	JWH 398 N-pentanoic acid metabolite	[M-H]-

405.1 559	6.0 6	C20H24O6	0. 3	Lariciresinol	[M+FA-H]-
405.1 587	5.5 9	C24H41N3O16	17 .7	Oligosaccharides-DP3- Chitin	[M-H- C8H15NO6]-
407.1 559	3.7 8	C24H24O6	14 .6	Xanthone I	[M-H]-
407.1 725	2.9 5	C11H12N2O2	0. 2	Tryptophan	[2M-H]-
409.1 65	4.8 1	C24H26O6	0. 5	3-Isomangostin	[M-H]-
409.3 112	17. 01	C28H42O2	0	.beta.-Tocotrienol	[M-H]-
411.1 873	3.1 8	C12H14O3	12 .9	2-(2,3-Dihydro-1H-inden- 5-yloxy)propanoic acid	[2M-H]-
413.1 454	4.7	C19H26O10	0. 5	Benzyl 6-O-(4-carboxy-3- hydroxy-3- methylbutanoyl)hexopyran oside	[M-H]-
415.1 248	4.6 7	C20H21ClN4O 4	16 .5	KRN 633	[M-H]-
415.2 2	4.0 7	C23H32N2O5	9. 3	Ramipril	[M-H]-
417.1 192	4.7 7	C21H22O9	1. 1	Liquiritin	[M-H]-
417.1 404	3.6 7	C17H24O9	0. 9	Syringin	[M+HCO2] -
417.1 993	2.9 9	C38H44N2O6	11 .1	Dauricine	[M-H- C12H16NO 2]-
419.1 35	4.5	C21H24O9	0. 1	4-Deoxyphloridzin	[M-H]-

421.076	0.76	C ₁₂ H ₂₃ O ₁₄ P	0.8	Trehalose, 6-(dihydrogen phosphate)	[M-H]-
421.2081	6.93	C ₁₉ H ₃₄ O ₁₀	0.3	Oct-1-en-3-yl 6-O-((2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-.beta.-D-glucopyranoside	[M-H]-
425.1665	3.69	C ₁₆ H ₂₈ O ₁₀	0.6	2-Methylbut-3-en-2-yl 6-O-((2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-.beta.-D-glucopyranoside	[M+HCOO] -
427.1609	5.76	C ₂₁ H ₂₅ ClN ₆ O ₂	11	AZD 5363	[M-H]-
427.161	5.53	C ₂₀ H ₂₈ O ₁₀	0.2	2-Phenylethyl 3-O-(4-carboxy-3-hydroxy-3-methylbutanoyl)-.beta.-D-glucopyranoside	[M-H]-
428.1562	2.55	C ₂₄ H ₂₃ N ₅ O ₅ S	2.3	StemRegenin 1	[M-H]-
429.1249	1.31	C ₂₁ H ₂₀ O ₇	13.8	(5-Benzoyloxy-1,2,6-trihydroxycyclohex-3-en-1-yl)methyl benzoate	[M+HCOO] -
431.0984	5.48	C ₂₁ H ₂₀ O ₁₀	0.9	Sophoricoside	[M-H]-
431.0984	4.71	C ₂₁ H ₂₀ O ₁₀	0.6	Vitexin	[M-H]-
431.1194	3.42	C ₁₈ H ₂₄ O ₁₂	0.1	Licoagroside B	[M-H]-
431.1922	3.97	C ₁₉ H ₃₀ O ₈	0.4	(3E)-4-((1S)-1-Hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-	[M+HCOO] -

				yl)but-3-en-2-yl .beta.-D-glucopyranoside	
431.1 923	6.4 1	C19H30O8	0. 5	3-Hydroxy-3,5,5-trimethyl-4-(3-oxobut-1-en-1-ylidene)cyclohexyl .beta.-D-glucopyranoside	[M+HCOO] -
433.1 141	6.6 9	C21H22O10	0. 3	Prunin	[M-H]-
433.2 082	4.3 9	C19H32O8	0. 2	(3E)-4-(1-Hydroxy-2,2,6-trimethyl-4-oxocyclohexyl)but-3-en-2-yl hexopyranoside	[M+HCOO] -
435.1 298	4.4 7	C21H24O10	2. 4	Dihydrostilbene base + 3O, 1carboxy, O-Hex	[M-H]-
435.1 426	3.4 5	C17H26O10	19 .4	Secologanol	[M+HCOO] -
437.1 666	4.8 7	C24H26N2O6	12 .3	Suxibuzone	[M-H]-
441.1 768	4.7 1	C21H30O10	0. 1	(2E,4E)-5-(6-((.beta.-D-Glucopyranosyloxy)methyl)-1-hydroxy-2,6-dimethyl-4-oxocyclohex-2-en-1-yl)-3-methylpenta-2,4-dienoic acid	[M-H]-
441.1 808	11. 87	C20H28O8	8. 9	14,15-Dihydroxyklaineanone	[M+FA-H]-
443.1 922	3.1 2	C21H32O10	0. 1	1'R,3'S,5'R,8'S,2E,4E)-Dihydrophaseic acid 3'-O-.beta.-D-glucopyranoside	[M-H]-
443.2 288	9.4 7	C23H30N2O4	22 .5	Mitragynine	[M+FA-H]-
445.1	3.4	C25H24N2O3	12	JWH 200 7-hydroxyindole	[M+HCOO]

716	4		.1	metabolite	-
445.1 717	6.7	C20H30O11	0. 4	Mongrghoside	[M-H]-
445.2 08	6.8 2	C21H34O10	2. 4	MCULE-1479479024	[M-H]-
447.0 934	4.3 5	C21H20O11	2. 3	Orientin	[M-H]-
447.0 936	5.4 8	C21H20O11	0. 1	Astragalin	[M-H]-
447.1 51	3.7 8	C18H26O10	1. 5	Benzyl alcohol + hex-pen	[M+HCOO] -
447.2 06	8.9 2	C18H32N4O9	8. 1	3-[5- [Acetyl(hydroxy)amino]pent ylcarbamoyl]-5-[3- [acetyl(hydroxy)amino]prop ylamino]-3-hydroxy-5- ketovaleric acid	[M-H]-
449.1 091	4.0 1	C21H22O11	0. 4	Hovetrichoside C	[M-H]-
449.1 091	5.4 1	C21H22O11	1. 9	Eriodictyol-7-O-glucoside	[M-H]-
449.1 092	4.8 7	C21H22O11	0. 2	Miscanthoside	[M-H]-
449.1 456	6.5 1	C22H26O10	0. 6	4-Methoxyphlorizin	[M-H]-
452.2 784	13. 99	C21H44NO7P	0. 1	16:0 Lyso PE	[M-H]-
455.3 532	17. 53	C30H48O3	0. 2	Oleanolic acid	[M-H]-
461.1 092	7.6 3	C22H22O11	0. 8	Tectoridin	[M-H]-

461.1 092	4.9	C22H22O11	4. 4	Scoparin	[M-H]-
461.1 093	4.1 1	C22H22O11	1	Diosmetin 7-O-beta-D-glucopyranoside	[M-H]-
461.1 301	3.2 2	C19H26O13	0. 1	Sibiricose A3	[M-H]-
461.1 667	4.3 8	C19H28O10	0. 5	Icariside D1	[M+HCOO] -
461.2 395	9.3 2	C27H31FN4O2	7. 6	AGI-5198	[M-H]-
463.0 886	4.9 3	C21H20O12	0. 7	Hirsutrin	[M-H]-
463.1 248	5.6 5	C22H24O11	0. 8	Protogenkwanin 4'-glucoside	[M-H]-
463.1 611	6.9 1	C23H28O10	1	Isomucronulatol 7-o-glucoside	[M-H]-
469.1 927	3.4 8	C18H32O11	0. 2	(2E)-4-Hydroxy-3,4-dimethylpent-2-en-1-yl 6-O-((2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-.beta.-D-glucopyranoside	[M+HCOO] -
469.2 08	3.7 7	C24H34O7	15 .5	MCULE-6411503838	[M+Cl]-
469.3 323	14. 77	C30H46O4	0	18.beta.-Glycyrrhetic acid	[M-H]-
469.3 324	15. 06	C30H46O4	0. 1	Colubrinic acid	[M-H]-
471.2 025	10. 73	C26H32O8	0. 2	Ethynylestradiol 3-.beta.-D-glucuronide	[M-H]-
471.3	15.	C30H48O4	0.	Echinocystic acid	[M-H]-

48	19		6		
471.3	15.	C30H48O4	0.	Maslinic acid	[M-H]-
481	04		1		
472.1	2.6	C20H23N7O7	0.	Folinic acid	[M-H]-
588			4		
475.0	5.5	C22H20O12	0.	6-O-Methylscutellarin	[M-H]-
881	9		3		
475.1	1.1	C21H28O10	15	Grandidentoside	[M+Cl]-
305	4		.3		
475.1	4.5	C20H30O10	0.	Phenethyl rutinoside	[M+HCOO] -
821	4		1		
476.2	14.	C23H44NO7P	1.	LPE 18:2	[M-H]-
783	38		4		
477.1	5.5	C22H23O12	0.	Petunidin 3-galactoside	[M-2H]-
039	1		8		
477.1	4.9	C21H20O10	0.	Genistin	[M+HCOO] -
04	6		4		
477.1	3.0	C19H28O11	1	Osmanthuside h	[M+FA-H]-
616	4				
477.2	8.5	C29H38N2O4	11	Ikarugamycin	[M-H]-
705	7		.2		
478.1	5.9	C26H29N3O6	0.	Nicardipine	[M-H]-
986	3		1		
				4-((1E)-3-Hydroxyprop-1-en-1-yl)-2-methoxyphenyl	
485.1	4.0	C22H30O12	0.	6-O-(4-carboxy-3-hydroxy-3-methylbutanoyl)-.beta.-D-glucopyranoside	[M-H]-
666	5		6		
485.3	15.	C48H76O19	0.	6-Deoxy-.alpha.-L-mannopyranosyl-(1->3)-[.beta.-D-glucopyranosyl-	[M-H-C18H30O14]-
274	1		5		

				(1->6)]-1-O-(3,27-dihydroxy-27,28-dioxolup-20(29)-en-28-yl)-.beta.-D-glucopyranose	
487.1 46	3.0 6	C21H28O13	0. 3	(2E)-3-(4-((2-O-((2S,3R,4R)-3,4-Dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-.beta.-D-glucopyranosyl)oxy)-3-methoxyphenyl)prop-2-enoic acid	[M-H]-
487.1 975	9.4 5	C26H32O9	0. 2	Methyl (4aR,4bR,10aR,12aS)-6,10-dihydroxy-3,4b,7,7,10a,12a-hexamethyl-12-methylidene-1,4,5,8-tetraoxo-9,10,10b,11-tetrahydronaphtho[2,1-f]isochromene-4a-carboxylate	[M-H]-
487.3 43	14. 5	C30H48O5	0	(3.beta.,5.xi.,9.xi.)-3,6,19-Trihydroxyurs-12-en-28-oic acid	[M-H]-
489.1 615	2.7 9	C20H28O11	0. 7	4-(.beta.-D-Glucopyranosyloxy)benzyl methyl 3-hydroxy-3-methylpentanedioate	[M+HCOO] -
491.1 197	7.5 5	C22H22O10	0. 1	Sissotrin	[M+HCOO] -
493.0 991	4.7 6	C22H22O13	0. 2	2-(3,5-Dihydroxy-4-methoxyphenyl)-5,7-dihydroxy-4-oxo-4H-chromen-3-yl .beta.-D-	[M-H]-

				glucopyranoside	
497.1 224	6.5 9	C22H26O13	15 .7	Verproside	[M-H]-
500.1 565	5.4 8	C25H27NO10	1. 3	CHEBI:139464	[M-H]-
501.3 225	11. 55	C42H66O16	0. 1	6-O-.beta.-D- Glucopyranosyl-1-O- ((3.beta.,5.xi.,9.xi.)-3,19,24- trihydroxy-24,28-dioxours- 12-en-28-yl)-.beta.-D- glucopyranose	[M-H- C12H20O1 0]-
503.1 54	4.0 7	C18H32O16	15 .3	Glycan MC=h3	[M-H]-
503.1 62	2.1 9	C18H32O16	0. 6	Maltodextrin	[M-H]-
503.1 62	1.6 3	C18H32O16	0. 6	3-Fucosylated Blood Group A tetraose	[M-H]-
503.3 381	11. 4	C30H48O6	0. 8	(2.alpha.,3.alpha.)- 2,3,19,23-Tetrahydroxyurs- 12-en-28-oic acid	[M-H]-
505.1 353	6.2 3	C23H24O10	9. 3	Wistin	[M+FA-H]-
505.2 083	5.6 5	C20H38O12	4. 4	3-Hydroxy-6-methylheptyl 2-O-.beta.-D- glucopyranosyl-.beta.-D- glucopyranoside	[M+Cl]-
506.2 297	9.3 6	C27H33N5O5	22 .2	3,15-dibenzyl-1,4,12- trimethyl-1,4,7,10,13- pentazacyclopentadecane- 2,5,8,11,14-pentone	[M-H]-
507.1 143	5.3 6	C22H22O11	1	4-(3,4-Dihydroxyphenyl)- 7-methoxy-2-oxo-2H- chromen-5-yl .beta.-D-	[M+FA-H]-

				glucopyranoside	
507.2 811	7.7 9	C33H44O8	11 .4	Fumigacin	[M-H- C2H4O2]-
509.2 24	5.4 4	C21H36O11	0. 2	5-Hydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 6-O-(3,4-dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)hexopyranoside	[M+HCOO] -
509.2 241	4.4 1	C21H36O11	0. 1	(2E)-6-Hydroxy-2,6-dimethylocta-2,7-dien-1-yl 6-O-.alpha.-L-arabinopyranosyl-.beta.-D-glucopyranoside	[M+HCOO] -
515.1 922	9.6 9	C26H30O8	0. 4	Evodin	[M+HCO2] -
517.2 308	5.8 9	C26H34N4O5	16 .6	Calpain Inhibitor XII	[M+Cl]-
519.3 328	10. 84	C30H48O7	0. 1	Bellericagenin B	[M-H]-
522.2 248	7.4	C47H85O19P3	24 .8	18:0-20:4 PI(4,5)P2	[M-2H]2-
527.2 862	13. 49	C14H20N2O3	2. 3	Suberoylanilide hydroxamic acid	[2M-H]-
529.3 019	14. 06	C28H42N4O6	2. 4	Kukoamine B	[M-H]-
531.1 148	5.3	C25H24O13	1. 7	6'-Malonyltrifolirhizin	[M-H]-
531.2 085	3.4 9	C29H27F3N6O	7. 6	Iclusig	[M-H]-
531.2 237	10. 51	C28H36O10	0. 1	Nomilinic acid	[M-H]-

533.1 667	4.7 6	C26H30O12	1. 2	Aegineoside	[M-H]-
533.2 031	8.8 2	C30H46O8	0	Periplocymarin	[M-H]-
535.1 4	9.7 1	C9H16O9	21 .9	3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid	[2M-H]-
540.3 31	13. 92	C24H50NO7P	0. 4	LPC 16:0	[M+HCOO] -
543.2 251	9.1 9	C33H33FO6	11 .4	Etalocib	[M-H]-
549.1 677	0.8	C18H32O16	0. 9	Erlose	[M+HCOO] -
549.1 677	1	C18H32O16	1. 5	Gentianose	[M+HCOO] -
549.3 074	7.5	C36H56O14	1. 2	Acobioside A	[M-H- C6H10O5]-
553.3 75	11. 15	C30H52O6	2. 3	Fasciculol C	[M+FA-H]-
559.3 125	13. 45	C27H46O9	0. 7	CHEBI:139416	[M+FA-H]-
561.1 617	5.8 6	C27H30O13	0. 3	Formononetin 7-O-.beta.-D-apiofuranosyl-(1->6)-.beta.-D-glucopyranoside	[M-H]-
561.2 357	8.3 3	C34H34N4O4	24 .5	Protoporphyrin	[M-H]-
561.3 283	14. 04	C27H48O9	1	MGMG 18:2	[M+HCOO] -
562.3 152	12. 85	C26H48NO7P	4	LPC 18:3	[M+HCOO] -
562.3	12.	C26H48NO7P	4.	1-Hydroxy-2-(9Z,12Z,15Z-octadecatrienoyl)-sn-	[M+FA-H]-

153	66		1	glycero-3-phosphocholine	
				(1S)-1,5-Anhydro-2-O-.alpha.-L-	
563.1	4.5	C26H28O14	0.	arabinopyranosyl-1-(5,7-	[M-H]-
407	4		5	dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-6-yl)-D-glucitol	
563.1	3.8	C22H30O14	0.	6-O-((2E)-3-(4-Hydroxy-3-methoxyphenyl)prop-2-enoyl)hex-2-ulofuranosyl	[M+HCOO] -
62	4		2	hexopyranoside	
564.3	13.	C26H50NO7P	0	1-Linoleoyl-sn-glycero-3-phosphorylcholine	[M+HCOO] -
309	28				
567.2	4.3	C26H34O11	0.	Indigoticoside A	[M+HCOO] -
085	2		8		
567.2	9.2	C27H36O13	24	Gallomyrtucommulone C	[M-H]-
228	8		.3		
577.1	5.1	C27H30O14	0.	Isorhoifolin	[M-H]-
567	5		5		
577.2	4.8	C30H42O11	4.	Hellebrigenin-3-O-.beta.-glucoside	[M-H]-
629			6		
579.1	4.2	C26H28O15	0.	Adonivernithol	[M-H]-
358	6		7		
579.1	3.1	C30H28O12	10	3''-p-Coumaroylprunin	[M-H]-
568	3				
579.2		C28H36O13		(-)-Syringaresinol-4-O-.beta.-D-glucopyranoside	[M-H]-
086	5		1		
582.2	7.7	C34H37N3O6	0.	Cumaroylspermidine	[M-H]-
612	8		3		
585.3	4.8	C31H46N4O7	6.	6-Benzyl-3-butan-2-yl-9-(7,8-dihydroxy-6-oxooctyl)-1,4,7,10-	[M-H]-
256	7		9		

				tetrazabicyclo[10.4.0]hexadecane-2,5,8,11-tetrone	
593.1 512	3.7 9	C27H30O15	0. 4	Vicenin-2	[M-H]-
593.1 515	5.1 9	C27H30O15	0. 2	Datiscin	[M-H]-
593.1 515	4.6 1	C27H30O15	0. 7	Biorobin	[M-H]-
593.1 516	4.4 1	C27H30O15	1. 9	4'-o-glucosylvitexin	[M-H]-
593.1 528	6.1 3	C27H30O15	6. 2	Quercetin 3,7-dirhamnoside	[M-H]-
593.1 896	6.0 5	C28H34O14	8. 9	2',6'-dihydroxy-4-methoxychalcone-4'-o-neohesperid	[M-H]-
593.2 735	13. 48	C30H42O12	23	5-(4-Hydroxyphenyl)-1-[2-(4-hydroxyphenyl)ethyl]pentyl 2-O-D-apio-.beta.-D-furanosyl-.beta.-D-glucopyranoside	[M-H]-
593.2 982	9.2 8	C35H46O8	22 .6	2-[(2E,6E,10E)-14,15-Dihydroxy-3,7,11,15-tetramethylhexadeca-2,6,10-trienyl]-2,4,6,9-tetrahydroxy-5,7-dimethylphenalene-1,3-dione	[M-H]-
595.1 671	4.4 9	C27H32O15	0	Eriocitrin	[M-H]-
595.1 672	3.5 4	C27H32O15	0. 8	2,6-Dihydroxy-2-(4-hydroxybenzyl)-3-oxo-2,3-dihydro-1-benzofuran-4-yl 6-O-(6-deoxy-.alpha.-L-	[M-H]-

				mannopyranosyl)-.beta.-D-glucopyranoside	
595.1 881	2.2	C29H36O11	13 .3	Detigloylswietenine, 2-Hydroxy, 8,30-epoxide, 3-acetate	[M+Cl]-
595.2 893	14. 97	C27H49O12P	0. 8	D-myo-Inositol, 1-[2-hydroxy-3-[(1-oxo-9,12-octadecadienyl)oxy]propyl hydrogen phosphate], [S-(Z,Z)]-	[M-H]-
597.1 83	4.7 5	C27H34O15	0. 5	3',5'-Di-.beta.-D-glucopyranosylphloretin	[M-H-C4H8O4]-
597.2 243	5.5 8	C17H17NO4	0. 6	4-[4-(Benzyloxy)anilino]-4-oxobutanoic acid	[2M-H]-
607.1 672	5.1 8	C28H32O15	2. 6	Diosmin	[M-H]-
607.1 672	5.8 6	C27H30O13	0. 2	3-(4-Methoxyphenyl)-4-oxo-4H-chromen-7-yl 2-O-((2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)hexopyranoside	[M+HCOO] -
607.1 673	6.6 9	C28H32O15	1. 4	7-((6-Deoxy-.alpha.-L-mannopyranosyl)oxy)-5-hydroxy-2-(4-methoxyphenyl)-4-oxo-4H-chromen-3-yl .beta.-D-glucopyranoside	[M-H]-
609.1 462	4.6 9	C27H30O16	0. 1	Rutin	[M-H]-
609.1 464	3.4 5	C27H30O16	0. 2	4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-6,8-dihexopyranosyl-5,7-dihydroxy-	[M-H]-

609.1 466	4.4 9	C27H30O16	0. 4	Multinoside A	[M-H]-
609.1 828	5.6 7	C28H34O15	1. 6	Neohesperidin	[M-H]-
611.1 447	1.2 2	C20H32N6O12 S2	0. 3	Glutathione disulfide	[M-H]-
614.3 31	9.5 9	C27H54NO12P	4. 9	Hexosyl LPE 16:0	[M-H]-
615.1 486	5.0 4	C27H32O14	0. 2	Naringin	[M+Cl]-
615.1 7	6.0 4	C30H32O14	3. 3	Methyl (1S,4aS,7aS)-1-(.beta.-D-glucopyranosyloxy)-4'-((1S)-1-(((2E)-3-(4-hydroxyphenyl)prop-2-enoyl)oxy)ethyl)-5'-oxo-4a,7a-dihydro-1H,5'H-spiro[cyclopenta[c]pyran-7,2'-furan]-4-carboxylate	[M-H]-
623.1 621	5.2 5	C28H32O16	0. 7	Narcissin	[M-H]-
623.1 622	3.9 7	C28H32O16	0. 3	Isorhamnetin-3-o-rutinoside	[M-H]-
623.1 987	6.0 1	C29H36O15	0. 6	Methyl hesperidin	[M-H]-
623.2 404	9.2 1	C36H36N2O8	3. 2	Grossamide	[M-H]-
627.1 207	3.2 5	C13H14O9	0. 7	Salicyl glucuronide	[2M-H]-
633.4 016	12. 02	C36H58O9	0. 5	Echinocystic acid-3-o-glucoside	[M-H]-
637.1	5.8	C28H32O14	0.	Isoflavone base + 1O,	[M+HCOO]

784	5		5	1MeO, O-Hex-Hex	-
639.1 934	6.8 8	C28H34O14	0. 7	MEGxp0_001204	[M+FA-H]-
639.1 939	4.1 5	C29H36O16	0. 9	Purpureaside A	[M-H]-
645.1 892	1.5 4	C28H38O17	22 .5	Haploperoside E	[M-H]-
				(4aS,8aR,9R,10S,12bR)-10- ((S)-Furan-3- yl(hexopyranosyloxy)methyl)-6,6,8a,10-tetramethyl- 3,8-dioxodecahydro- 3H,6H- spiro[naphtho[1',2':3,4]furo[3,2-c]pyran-9,2'-oxirane]- 3'-carboxylic acid	[M-H]-
651.2 664	5.3 1	C32H44O14	1	Crocin 3	[M-H]-
655.1 886	5.3 3	C28H34O15	0. 6	Hesperetin 7-O-rutinoside	[M+FA-H]-
				12-[13-Carboxy-3- hydroxy-2- (hydroxymethyl)-8,10,12- trimethyltrideca-10,12- dienoyl]oxy-13- (hydroxymethyl)-3,5,7- trimethyltetradeca-2,4- dienedioic acid	[M-H]-
665.3 916	11. 18	C36H58O11	1. 6	3''-O-Caffeoyl-6-O- rhamnopyranosylcatalpol	[M-H]-
669.2 047	4.6 2	C30H38O17	1. 7	Kanokoside D	[M+HCOO] -
669.2 762	4.9 6	C27H44O16	24	Monensin	[M-H]-
669.4	10.	C36H62O11	1.		

23	07		7		
681.2	4.1	C31H38O17	0.	Tenuifoliside A	[M-H]-
045	3		4		
683.2	5.6	C33H48O15	0.	Methyl deacetyl nomilinate 17-glucoside	[M-H]-
923	1		1		
685.2	4.3	C32H46O16	0.	Secoisolariciresinol diglucoside	[M-H]-
723	5		8		
695.4	11.	C36H58O10	1.	1-O-(3,19,23-Trihydroxy- 28-oxours-12-en-28- yl)hexopyranose	[M+HCOO] -
021	11		6		
711.2	6.0	C34H48O16	0.	Nomilinic acid 17-glucoside	[M-H]-
877	8		9		
741.2	3.8	C33H42O19	1.	Narirutin 4'-O-glucoside	[M-H]-
257	5		1		
755.2	2.9	C33H41O20	2.	Cyanidin 3-(2g- glucosylrutinoside)	[M-2H]-
047	2		2		
755.2	4.1	C33H40O20		2-(3,4-Dihydroxyphenyl)- 5,7-dihydroxy-4-oxo-4H- chromen-3-yl 6- deoxy-.alpha.-L- mannopyranosyl-(1->2)- [6-deoxy-.alpha.-L- mannopyranosyl- (1->6)]-.beta.-D- galactopyranoside	[M-H]-
049	6		1		
771.2	3.2	C33H40O21		3-((6-Deoxy-4-O-.beta.- D-glucopyranosyl-.alpha.- L-mannopyranosyl)oxy)-2- (3,4-dihydroxyphenyl)-5- hydroxy-4-oxo-4H- chromen-7-yl hexopyranoside	[M-H]-
	5		1.		
			5		
779.2	1.9	C20H22O8	10	Polydatin	[2M-H]-

467	8		.7		
783.4	10.	C41H68O14	1.	Astragaloside III	[M-H]-
536	74		2		
787.2	4.0	C34H46O18	2.	Liriodendrin	[M+FA-H]-
675	7		3		
793.4	11.	C42H66O14	0.	Chikusetsu saponin 4a	[M-H]-
389	96		9		
795.4	11.	C42H68O14	4.	Soyasaponin III	[M-H]-
542	33		1		
809.4	11.	C42H66O15	1.	Soyasapogenol B base + O-HexA-HexA	[M-H]-
338	2		7		
				6-O-((2E)-2-Methylbut-2-enoyl)-.beta.-D-glucopyranosyl-(1->2)-6-O-((2E)-2-methylbut-2-enoyl)-.alpha.-D-glucopyranosyl .beta.-D-glucopyranosyl-(1->2)-6-O-((2E)-2-methylbut-2-enoyl)-.alpha.-D-glucopyranoside	
811.3	4.5	C39H60O24	20		[M-H-C5H8O2]-
039	4				
				1-O-((2.beta.,3.beta.,5.Xi.,9.Xi.,18.Xi.)-3-(.beta.-D-Glucopyranuronosyloxy)-2,23-dihydroxy-28-oxoolean-12-en-28-yl)-.beta.-D-glucopyranose	
825.4	8.9	C42H66O16	1.		[M-H]-
286	1		1		
869.4	10.	C44H70O17	1.	Furostane base -1H2O -2H + 1O, O-Hex, O-Pen-dHex	[M-H]-
547	99		2		
				NCGC00380190-01!3,15,21-tris[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-	
873.4	10.	C40H74O20	18		[M-H]-
86	43		.2		

				(hydroxymethyl)oxan-2-yl]oxy]docosanoic acid	
891.236	4.54	C22H22O10	0.2	Trifolirhizin	[2M-H]-
909.486	11.67	C47H74O17	0.7	(3.beta.,5.Xi.,9.Xi.,18.Xi.,22.beta.)-22-Hydroxy-25-oxoolean-12-en-3-yl 6-deoxy-.alpha.-L-mannopyranosyl-(1->2)-.beta.-D-xylopyranosyl-(1->2)-.beta.-D-glucopyranosiduronic acid	[M-H]-
911.4652	12.62	C45H70O16	0.8	(1.beta.,3.beta.,8.xi.,9.xi.,14.xi.)-3-((6-Deoxy-.alpha.-L-mannopyranosyl)oxy)spiro[5,25(27)-dien-1-yl 6-deoxy-2-O-(6-deoxy-.alpha.-L-mannopyranosyl)-.beta.-D-galactopyranoside	[M+FA-H]-
911.5017	11.01	C47H76O17	0.6	NCGC00381308-01	[M-H]-
913.4799	12.26	C26H35NO6	6.4	2-(2',4-Dihydroxy-6-keto-1',1',4'a,6'-tetramethylspiro[3,8-dihydrofur[2,3-e]isoindole-2,5'-decalin]-7-yl)propionic acid	[2M-H]-
915.4964	11.47	C46H76O18	0.8	MCULE-8637503623	[M-H]-
939.4968	11.68	C48H76O18	0.9	(3.beta.,5.Xi.,9.Xi.,18.Xi.)-28-Hydroxy-28-oxoolean-12-en-3-yl 6-deoxy-.alpha.-L-mannopyranosyl-(1->3)-	[M-H]-

				[.beta.-D-glucopyranosyl-(1->2)]-.beta.-D-glucopyranosiduronic acid	
941.5 11	11. 01	C48H78O18	0. 6	MCULE-7407861812	[M-H]-
955.4 905	13. 43	C48H76O19	0. 6	Ginsenoside Ro	[M-H]-
955.4 916	10. 91	C48H76O19	2. 1	Soyasapogenol B base + O-HexA-HexA-dHex	[M-H]-
957.5 07	12. 7	C48H78O19	0. 7	Soyasaponin V	[M-H]-
971.4 865	8.7 5	C48H76O20	1	MCULE-1324860170	[M-H]-
985.5 021	11. 68	C48H76O18	1	4-O-(6-Deoxy-.alpha.-L-mannopyranosyl)-1-O-((3.beta.,5.Xi.,9.Xi.)-3-(.beta.-D-glucopyranuronosyloxy)-28-oxoolean-12-en-28-yl)-.beta.-D-glucopyranose	[M+FA-H]-

Table S2 Pathways enriched by different MPs

pathway	pval	padj	overlapping	size	MP_cluster
GOBP_NEGATIVE_REGULATION_OF_CELL_DEATH	3.09E-07	0.001789821	16	912	MP1
GOCC_SECRETORY_GRANULE	6.79E-07	0.001789821	15	848	MP1
GOBP_SECRETION	5.93E-06	0.005100002	14	884	MP1
GOBP_REGULATION_OF_CELL_DIFFERENTIATION	0.007431541	0.372409117	12	1425	MP1
GOBP_EPITHELIAL_CELL_PROLIFERATION	2.23E-06	0.002874675	10	389	MP1
GOBP_CELL_CYCLE	4.89E-61	7.56E-57	70	1650	MP2
GOBP_CELL_CYCLE_PROCESS	1.45E-54	4.49E-51	59	1132	MP2
GOBP_MITOTIC_CELL_CYCLE	2.42E-60	1.87E-56	58	848	MP2
GOBP_MITOTIC_CELL_CYCLE_PROCESS	4.90E-55	1.89E-51	52	703	MP2
GOBP_CELL_DIVISION	5.08E-57	2.62E-53	51	599	MP2
GOBP_DEFENSE_RESPONSE	3.31E-10	3.18E-06	25	1530	MP3
GOBP_IMMUNE_RESPONSE	7.33E-06	0.010049404	19	1597	MP3
GOBP_INFLAMMATORY_RESPONSE	5.26E-07	0.001626155	14	718	MP3
GOBP_BIOLOGICAL_PROCESS_INVOLVED_IN_INTERSPECIES_INTERACTION_BETWEEN_ORGANISMS	2.53E-08	9.79E-05	22	1478	MP3
GOBP_INNATE_IMMUNE_RESPONSE	4.56E-05	0.039198129	12	794	MP3
GOBP_LIPID_METABOLIC_PROCESS	6.36E-09	2.24E-05	19	1301	MP4

GOBP_ION_TRANSPORT	1.09E-06	7.70E-04	17	1457	MP4
GOBP_TRANSMEMBRANE_TRANSPORT	3.89E-06	0.002067904	16	1424	MP4
GOBP_SMALL_MOLECULE_METABOLIC_PROCESS	1.06E-08	2.74E-05	21	1659	MP4
GOBP_ANION_TRANSPORT	1.90E-10	2.94E-06	14	490	MP4
GOBP_G_PROTEIN_COUPLED_RECEPTOR_SIGNALING_PATHWAY	2.86E-06	0.022145074	4	734	MP5
GOCC_INTRINSIC_COMPONENT_OF_PLASMA_MEMBRANE	6.09E-05	0.065494332	4	1585	MP5
GOBP_RESPONSE_TO_ENDOGENOUS_STIMULUS	4.69E-05	0.065494332	4	1484	MP5
GOBP_POSITIVE_REGULATION_OF_SIGNALING	6.35E-05	0.065494332	4	1602	MP5
GOMF_G_PROTEIN_COUPLED_RECEPTOR_ACTIVITY	2.52E-05	0.054418412	3	364	MP5
GOBP_IMMUNE_RESPONSE	2.10E-08	8.13E-05	23	1597	MP6
GOBP_DEFENSE_RESPONSE	4.67E-08	9.14E-05	22	1530	MP6
GOBP_RESPONSE_TO_CYTOKINE	1.78E-09	9.65E-06	18	825	MP6
GOBP_ION_TRANSPORT	3.05E-05	0.015727065	17	1457	MP6
GOBP_INNATE_IMMUNE_RESPONSE	4.73E-08	9.14E-05	16	794	MP6
GOBP_REGULATION_OF_INTRACELLULAR_SIGNAL_TRANSDUCTION	5.10E-12	4.15E-09	28	1612	MP7
GOBP_IMMUNE_RESPONSE	4.28E-22	3.31E-18	39	1597	MP7
GOBP_LYMPHOCYTE_ACTIVATION	1.53E-22	2.37E-18	30	763	MP7
GOBP_CYTOKINE_PRODUCTION	6.05E-09	2.13E-06	16	685	MP7

GOBP_REGULATION_OF_IMMUNE_SYSTEM_PROCESS	1.20E -15	2.06E -12	30	13 53	MP7
GOBP_T_CELL_ACTIVATION	7.02E -16	1.55E -12	20	46 3	MP7
GOMF_RNA_BINDING	1.92E -70	2.70E -67	69	15 96	MP8
GOBP_CELLULAR_AMIDE_METABOLIC_PROCESS	8.96E -70	1.15E -66	62	10 34	MP8
GOBP_ORGANONITROGEN_COMPOUND_BIOSYNTHETIC_PROCESS	5.86E -59	6.05E -56	62	15 40	MP8
GOBP_PEPTIDE_BIOSYNTHETIC_PROCESS	8.40E -82	1.86E -78	61	62 1	MP8
GOBP_AMIDE_BIOSYNTHETIC_PROCESS	1.29E -76	2.22E -73	61	75 0	MP8
