Ritual revealed: psychotropic substances in a Ptolemaic Egyptian vase.

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SUPPLEMENTARY INFORMATION

aDNA Metabarcoding Consensus Sequences

Nitrariaceae:
ATCCTGTTTTACGAGAACAAACAAAGGTTCATAAAGCGAGAAAAAGT
Cleomaceae:
ATCCTGGTTTACGCGAACAAACAAGAGTTTAGAAAGCGAGAAAAAAGGG
Nymphaeaceae:
ATCCTGTTTACAGAAAACAAGGGTTCCTTTCCTAGAAAGCGAGAATCAAAAAAGAG

Figure S1. 3D model of the Bes-vase from the Tampa Museum of Art produced by the authors via structured light 3D scanning with an Artec Spider 3D scanner (https://skfb.ly/oFApP).

Table S1. Non-human proteins identified with coverage and unique peptides. The threshold of the unique peptides for the protein assignment was set at 3

Proteins	UniProt ID	Taxa	Score	Coverage (%)	Peptides	Unique peptides
Myosin heavy chain, muscle	P05661	*Drosophila melanogaster*	83,663	7,8	12	**12**
Arginine kinase	O61367	*Apis mellifera*	42,429	18,3	5	**4**
Heat shock protein SSC1, mitochondrial	P0CS90	*Saccharomyces cerevisiae* (strain ATCC 204508 / S288c)	40,478	8,4	5	**4**
Alpha-amylase/trypsin inhibitor	P17314	*Triticum aestivum*	115,1	38,7	4	**4**
Alpha-actinin, sarcomeric	P18091	*Drosophila melanogaster*	36,046	6	4	**4**
V-type proton ATPase subunit B	P31409	*Drosophila melanogaster*	24,728	10,8	4	**4**
11S globulin seed storage protein	Q9XHP0	*Sesamum indicum*	26,03	11,8	4	**4**
14-3-3 protein beta/alpha-A;14-3-3 protein eta;14-3-3-like protein 2;14-3-3-like protein 1;14-3-3 protein zeta	P29310	*Drosophila melanogaster*	28,56	19,8	4	**3**
Calmodulin	P62152	*Drosophila melanogaster*	18,205	29,5	3	**3**
Tropomyosin-2	P09491	*Drosophila melanogaster*	18,995	11,3	3	**3**
ADP-ribosylation factor 1	P36579	*Schizosaccharomyces pombe* (strain 972 / ATCC 24843)	20,419	21,7	3	**3**
Tropomyosin-1, isoforms 33/34	P49455	*Drosophila melanogaster*	35,855	15,1	4	**3**
Aconitate hydratase, mitochondrial	P19414	*Saccharomyces cerevisiae* (strain ATCC 204508 / S288c)	20,064	5,2	3	**3**

Table S2. Human proteins identified with coverage and unique peptides. The threshold of the unique peptides for the protein assignment was set at 3

Proteins	UniProt ID	Taxa	Score	Coverage (%)	Peptides	Unique peptides
Mucin-5B	Q9HC84	*Homo sapiens*	150,87	7	18	18
Lactotransferrin	P02788	*Homo sapiens*	123,89	20	19	**9**
Polymeric immunoglobulin receptor	P01833	*Homo sapiens*	60,595	14	9	**8**
Annexin A1	P04083	*Homo sapiens*	65,733	31,2	8	**8**
Arginase-1	P05089	*Homo sapiens*	77,198	35,4	10	**8**
Annexin A2	P07355	*Homo sapiens*	146,81	24,5	15	**8**
Prolactin-inducible protein	P12273	*Homo sapiens*	67,253	58,9	9	**7**
Serpin B12	Q96P63	*Homo sapiens*	117,89	24	11	**7**
IgGFc-binding protein	Q9Y6R7	*Homo sapiens*	46,66	3,4	7	**7**
Serpin B3	P29508	*Homo sapiens*	294,11	26,4	14	**6**
Ig kappa chain C region	P01834	*Homo sapiens*	80,7	80,4	6	**6**
Alpha-amylase 2B	P0DUB6	*Homo sapiens*	62,037	19	6	**6**
Ig alpha-1 chain C region	P01876	*Homo sapiens*	54,753	23,5	6	**5**
Alpha-2-macroglobulin-like protein 1	A8K2U0	*Homo sapiens*	45,368	4,2	7	**5**
BPI fold-containing family B member 1	Q8TDL5	*Homo sapiens*	30,776	15,5	5	**5**
Serum albumin	P02768	*Homo sapiens*	135,58	19,4	26	**4**
Cathepsin D	P07339	*Homo sapiens*	56,442	14,3	8	**4**

Zinc-alpha-2-glycoprotein	P25311	*Homo sapiens*	53,363	18,5	7	**4**
Calmodulin-like protein 3	P27482	*Homo sapiens*	38,298	35,6	4	**4**
Lysozyme C	P61626	*Homo sapiens*	67,759	40,5	5	**4**
Desmocollin-3	Q14574	*Homo sapiens*	42,15	6,8	6	**4**
Suprabasin	Q6UWP8	*Homo sapiens*	24,943	20,7	4	**4**
Zymogen granule protein 16 homolog B	Q96DA0	*Homo sapiens*	132,33	36,5	4	**4**
Protein S100-A14	Q9HCY8	*Homo sapiens*	35,287	54,8	4	**4**
Hemoglobin subunit beta	P68871	*Homo sapiens*	72,29	53,7	9	**3**
Cystatin-SN	P01037	*Homo sapiens*	46,359	56,7	5	**3**
Gamma-glutamylcyclotransferase	O75223	*Homo sapiens*	36,63	28,2	5	**3**
Immunoglobulin J chain	P01591	*Homo sapiens*	18,781	22,6	3	**3**
Myeloperoxidase;	P05164	*Homo sapiens*	17,718	4,6	3	**3**
Alpha-enolase	P06733	*Homo sapiens*	37,065	11,3	5	**3**
Protein S100-A7	P31151	*Homo sapiens*	30,075	22,8	5	**3**
Protein POF1B	Q8WVV4	*Homo sapiens*	28,17	6,1	4	**3**

Table S3. Identification of compounds undertaken bythe untarget/target HPLC-Exploris-Orbitrap®-MS procedure using the measured m/z values of parent feature in the resolved MS/MS mass spectra and the corresponding retention times (RT) accompanied by chromatographical peak area values.

Name	m/z	RT [min]	Area
Alkaloids			
Harmaline	215,1178	4,244	4,7E+09
Harmine	213,1022	4,272	3,7E+09
Tetrahydro-harmine	217,13356	3,943	1,2E+07
Harmol (demethylated harmaline)	199,0866	3,321	8,9E+06
Vasicine	189,10223	2,673	2,8E+08
Ruine (7-Methoxy-1-methyl-9H-beta-carbolin-8-yl beta-D-glucopyranoside)	391,15	3,082	1,8E+07
Probable degradation of indole alkaloid (1-(6-methoxy-1H-indol-2-yl)ethan-1-imine)	188,10696	3,943	7,5E+06
Cytisine	189,1023	4.85	1,7E+05
Probable degradation of isoquinoline alkaloid (1,5-isoquinolinediol or isomer)	162,055	1,059	3,1E+06
Nicotine	163,12299	1,287	7,3E+06
Sinapine	310,16473	3,46	2,3E+06
Nupharidine	250,18024	4,841	2,1E+06

Neferine	625,32721	14,54	1,7E+05 (traces)
Carbohydrates			
Cellobiose	377,08557	0,994	1,3E+08
Gluconic acid or isomer	195,05103	0,998	2,2E+07
Hexitol	181,07181	0,96	9,7E+06
Trisaccharide (tree hexose units)	503,16	0,998	3,3E+06
Xylitol or isomer	151,06126	1,008	2,6E+06
Chitobiose	407,24036	9,142	8,5E+05
Tannines			
Gallic acid	169,01431	1,712	1,6E+07
1,6-Bis-O-(3,4,5-trihydroxybenzoyl)hexopyranose	483,07806	3,059	2,4E+06
1,2,3,6-Tetra-O-galloyl-β-D-glucose	787,09961	3,624	7,7E+05
Fatty acid and derivates			
9,12,13-Trihydroxy-15-octadecenoic acid (9,12,13-TODEA)	329,23335	6,437	1,2E+08
Pinolenic acid	279,23193	11,437	1,5E+07

Suberic acid	173,08197	4,175	2,8E+07
12,13-Dihydroxy-9-octadecenoic acid (12,13-DIHOME)	313,23846	8,689	9,9E+06
9-Hydroxy-octadecadienoic acid (9-HODE)	295,22668	10,66	9,0E+06
O-Arachidonoyl ethanolamine	348,28955	9,118	1,0E+06
12-oxo Phytodienoic Acid	293,2111	9,989	4,3E+06
Heterocyclic compounds			
Uric acid	167,02112	1,055	8,8E+07
6-methoxyquinoline	160,07571	1,718	5,2E+06
Xanthine	151,02621	1,269	3,0E+06
Caffeine	195,0877	3,274	1,6E+06
Fraxetin	207,0299	3,805	1,4E+06
N1-[4-(1,3-Oxazol-5-yl)phenyl]cyclopropane-1-carboxamide	229,09724	3.58	2,1E+07
Amino acids and derivates			
N-Benzoyl-L-phenyalaninol	256,13321	6,093	4,8E+07
Arginine	175,11899	0,937	1,3E+07

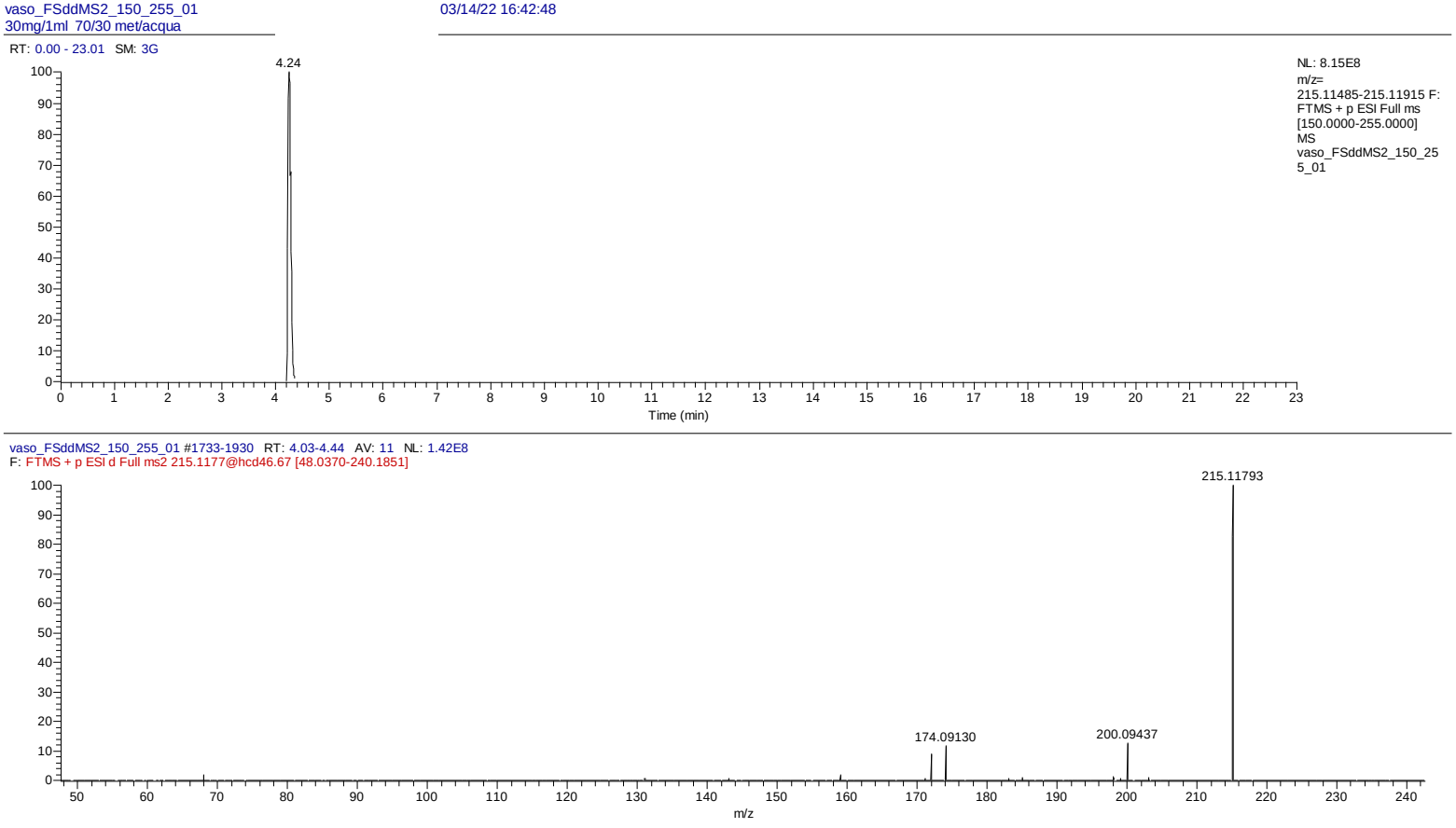
Tryptophan	188,0706	2,99	9,5E+06
Phenylalanine	166,08628	2,153	7,8E+06
Carnitine	162,11249	0,991	7,5E+06
N-Acetyl-glutamic acid	188,05644	1,308	7,0E+06
Tyrosine	182,08119	1,309	4,4E+06
Histidine	156,07681	0,951	2,4E+06
Organic acids and derivates			
Citric acid	191,01974	1,271	1,6E+07
P-coumaric acid	165,05467	1,307	3,3E+06
Gentisic acid (2,5-dihydroxybenzoic acid)	153,01938	2,833	1,7E+06
3-Anisic acid	151,0401	5,044	1,5E+06
4-Hydroxyphenylacetic acid	151,0401	6,717	1,0E+06
Ferulic acid	193.0506	4.62	1,2E+06
Isoferulic acid	193,0506	5,479	2,1E+06
Flavonoids			

Quercetin 3-O-acetyl-rhamnoside	489,10388	5,081	2,9E+07
Quercitrin	447,09311	4,477	2,4E+07
Myricitrin	463,08817	4,094	2,1E+07
Myricetin 3-O-galactopyranoside	479,08301	3,753	3,4E+06
7-Hydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-5-yl β-D-glucopyranoside (Salipurposide) o isomer Isosalipurposide	433,11395	4,99	1,1E+07
Isosalipurposide o isomer (salipurposide)	433,11393	4,10	0.87E+07
Kaempferol 3-(2''-acetylrhamnoside)	473,10896	5,493	8,3E+06
Naringenin	273,07575	4,97	4,4E+06
Afzelin (kaempferol 3-rhamnoside)	431,09833	4,819	6,9E+06
Triterpene			
18-β-Glycyrrhetinic acid	469,3323	9,785	1,2E+06
Various fungal metabolites			
Neovasipyridone E	308,22205	5,696	6,4E+06
Aspernigrin A	229,09724	4,69	2,1E+07
Libertellenone G	315,19537	9,835	1,2E+06

2-furoylglycine	168,0302	5,243	2,8E+06
Unknown			
Unknown I	252,10814	4,844	6,1E+06
Unknown II	403,17682	11,275	1,9E+06
Unknown III	201,1023	2,876	1,2E+07

TABLE S4. Extracted ion chromatogram from full MS and relative fragmentation pattern obtained in dd-MS2 acquisition mode for all compounds listed in Table 3

Harmaline

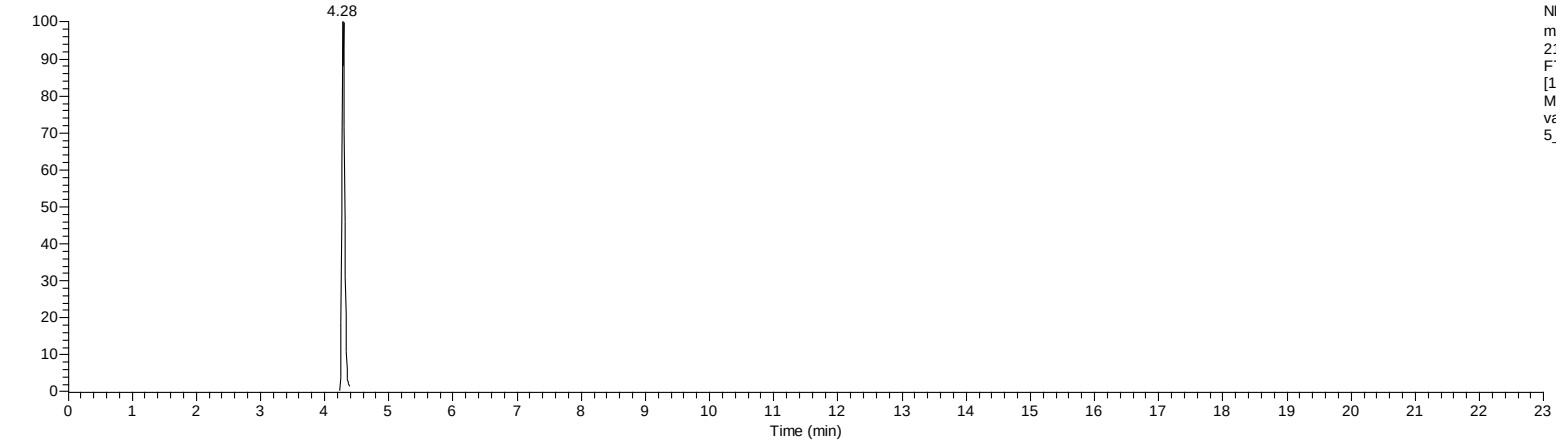


Harmine

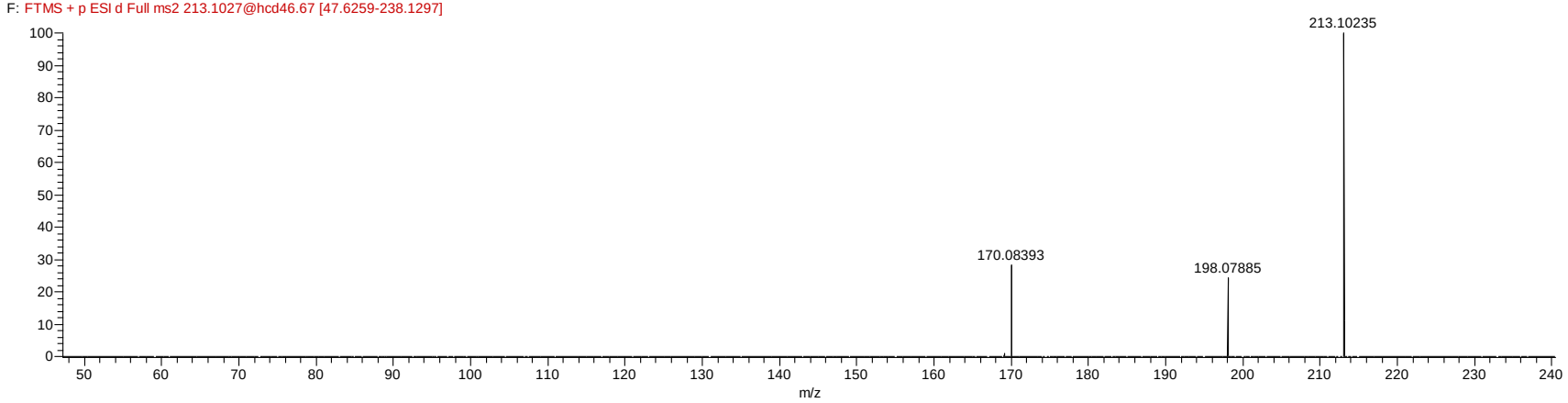
vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



vaso_FSddMS2_150_255_01 #1762-1903 RT: 4.16-4.39 AV: 5 NL: 8.20E7
F: FTMS + p ESI d Full ms2 213.1027@hcd46.67 [47.6259-238.1297]

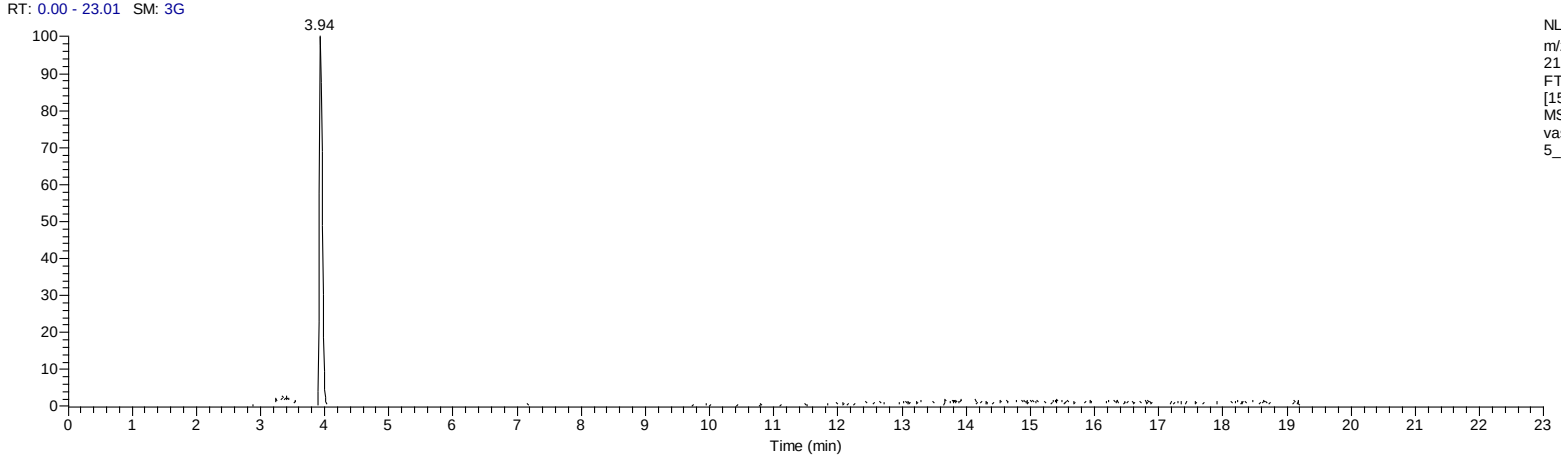


Tetrahydro-harmine

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

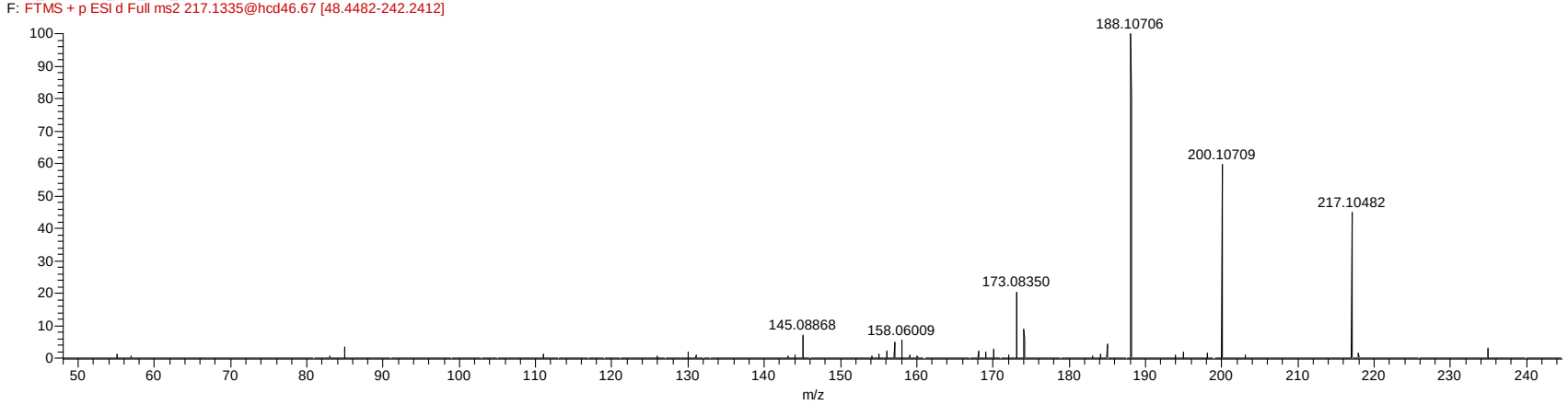
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



NL: 2.02E6
m/z=
217.13083-217.13517 F:
FTMS + p ESI Full ms
[150.0000-255.0000]
MS
vaso_FSddMS2_150_25
5_01

vaso_FSddMS2_150_255_01 #1661-1711 RT: 3.91-3.96 AV: 2 NL: 3.55E5
F: FTMS + p ESI d Full ms2 217.1335@hcd46.67 [48.4482-242.2412]

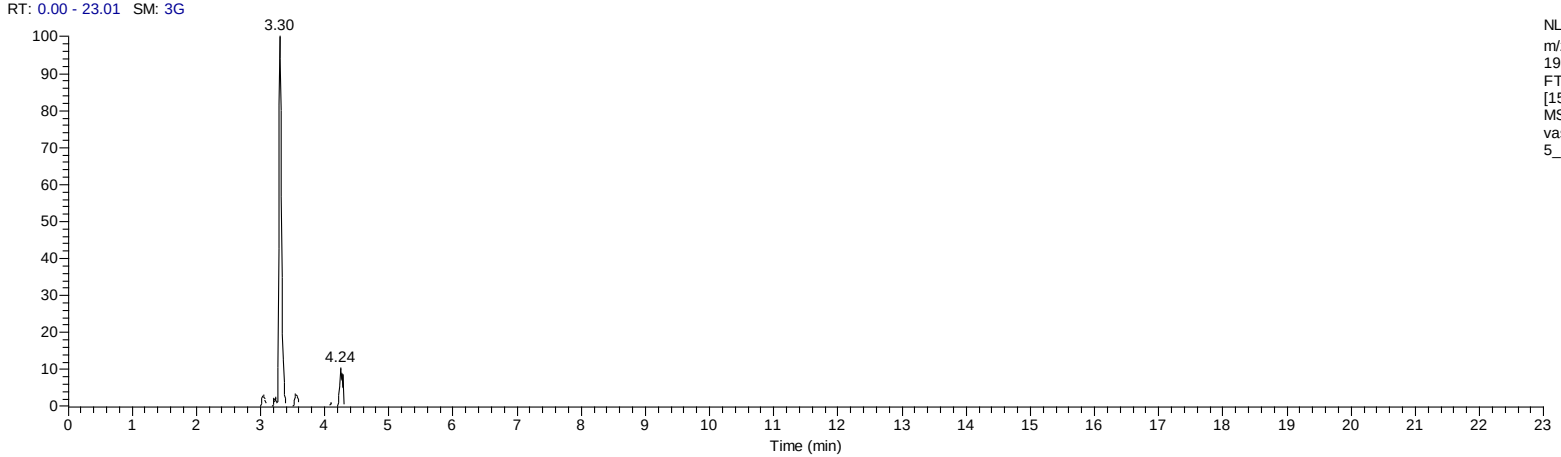


Harmol

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

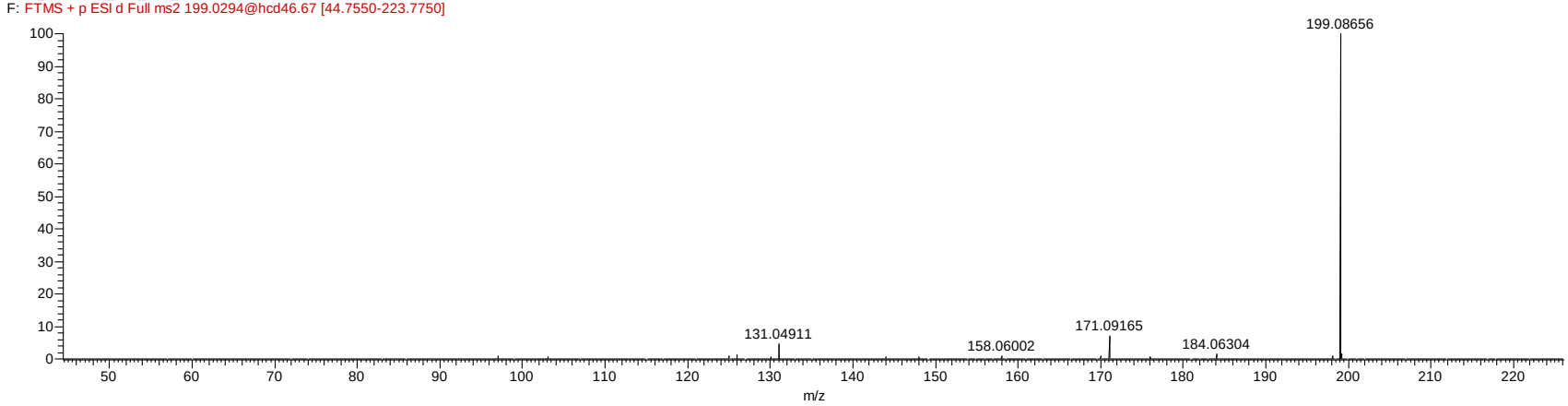
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



NL: 2.15E6
m/z=
199.08401-199.08799 F:
FTMS + p ESI Full ms
[150.0000-255.0000]
MS
vaso_FSddMS2_150_25
5_01

vaso_FSddMS2_150_255_01 #1365-1456 RT: 3.18-3.38 AV: 5 SB: 11 2.33-3.08 NL: 2.50E5
F: FTMS + p ESI d Full ms2 199.0294@hcd46.67 [44.7550-223.7750]

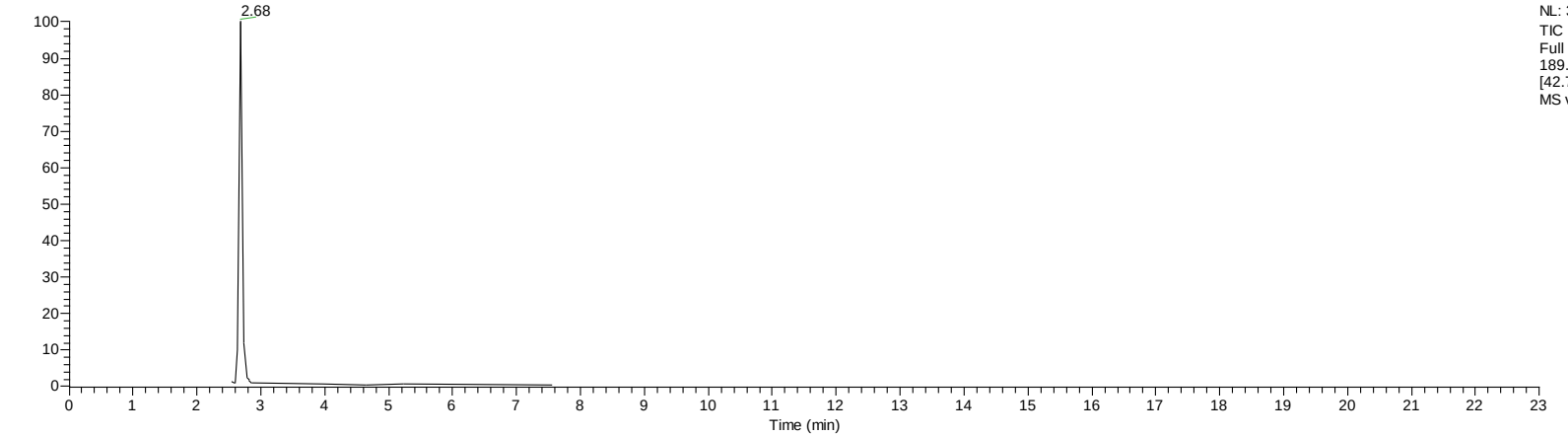


Vasicine

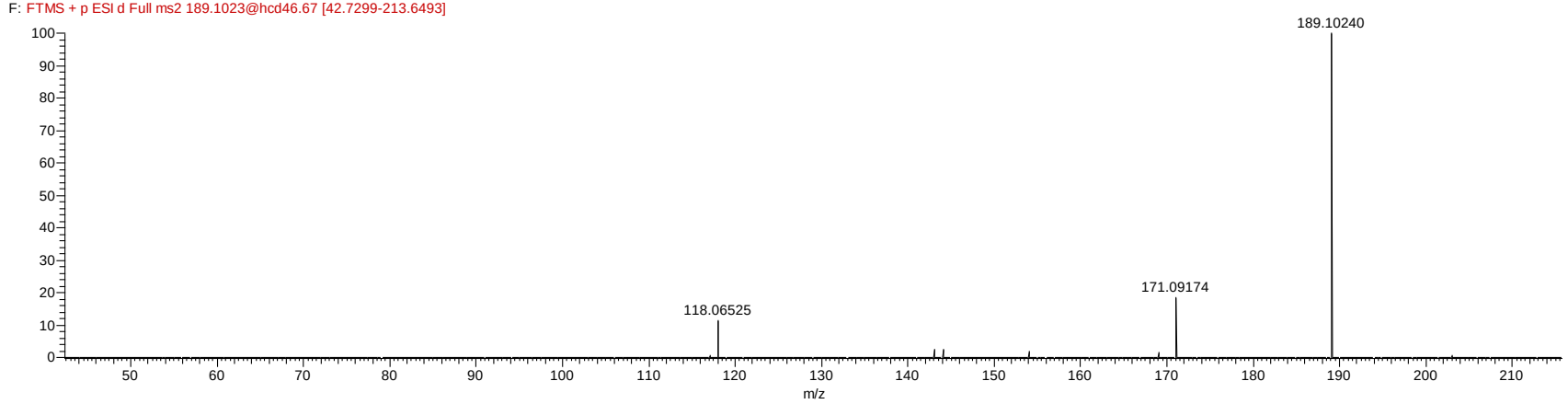
vaso_FSddMS2_01
30mg/1ml 70/30 met/acqua

03/14/22 16:18:45

RT: 0.00 - 23.00



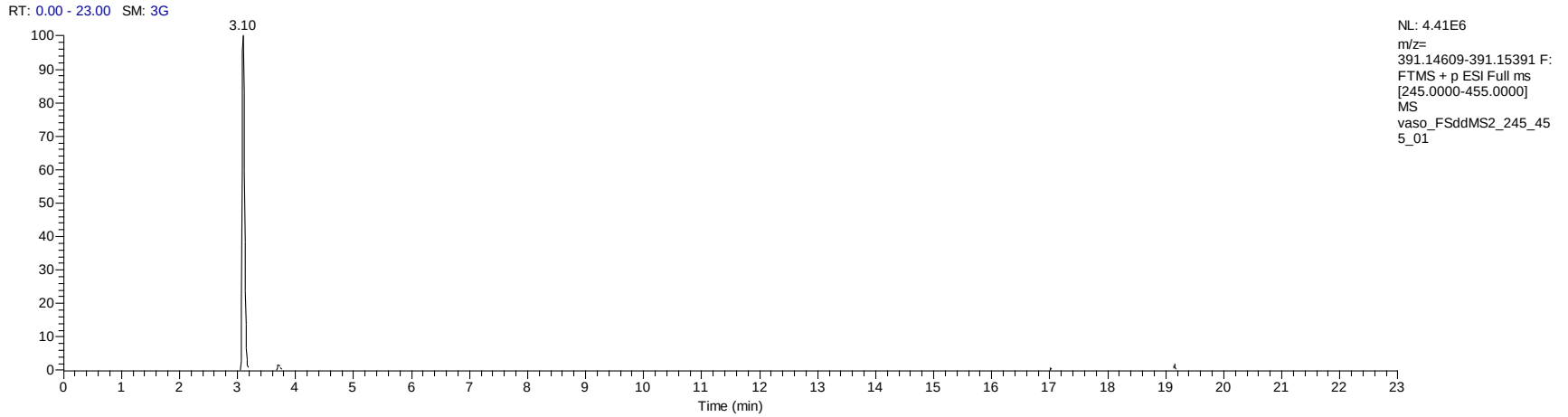
vaso_FSddMS2_01 #1106-1165 RT: 2.59-2.68 AV: 3 NL: 7.54E6
F: FTMS + p ESI d Full ms2 189.1023@hcd46.67 [42.7299-213.6493]



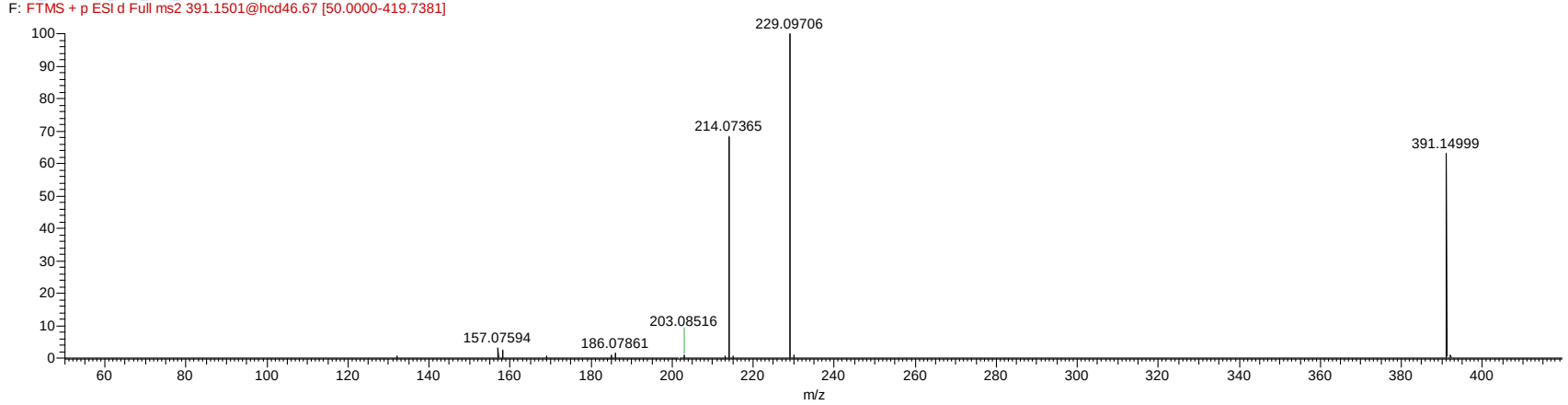
Ruine (7-Methoxy-1-methyl-9H-beta-carbolin-8-yl beta-D-glucopyranoside)

vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

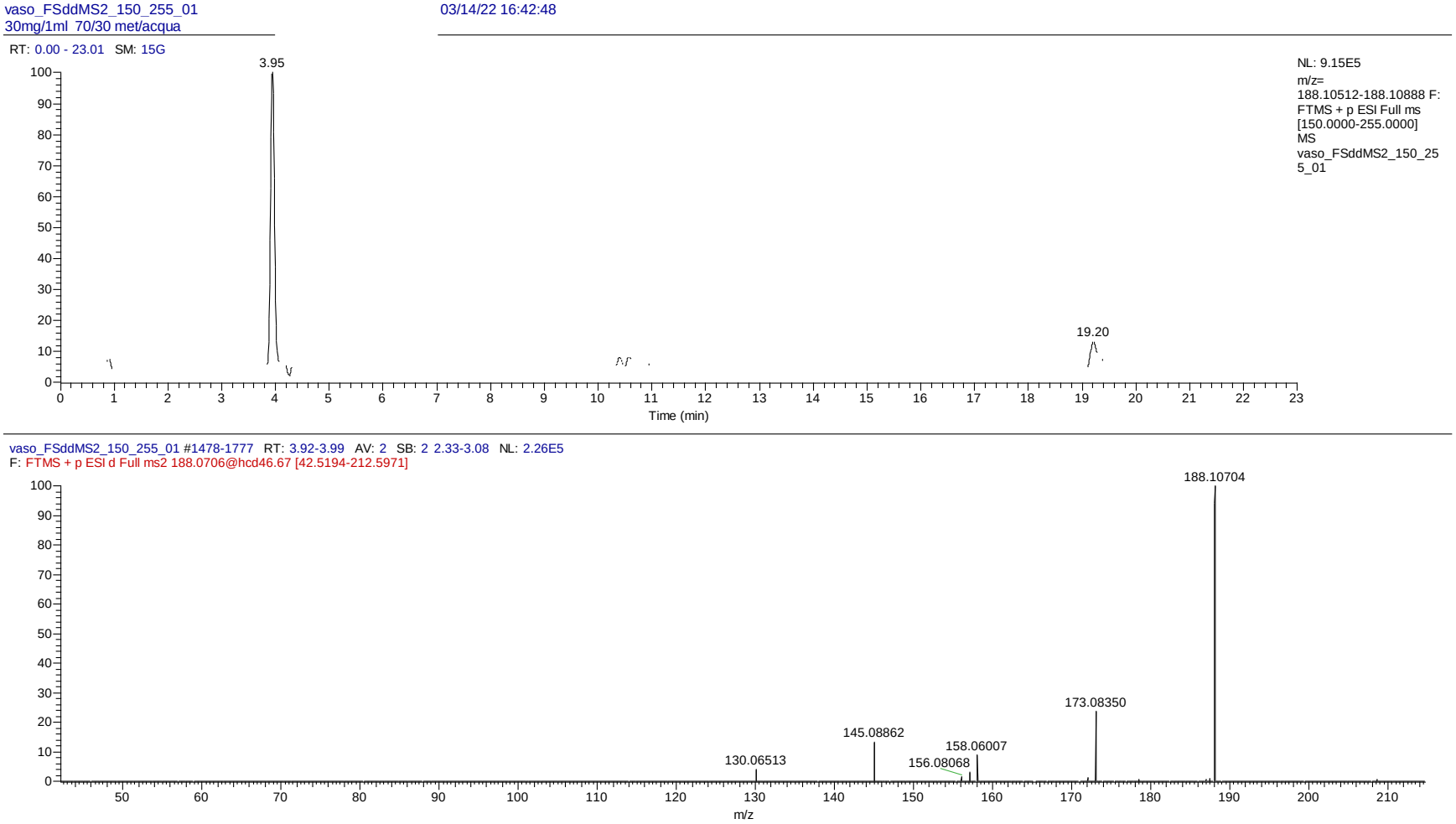
03/14/22 17:06:52



vaso_FSddMS2_245_455_01 #1232 RT: 3.12 AV: 1 NL: 9.35E5
F: FTMS + p ESI d Full ms2 391.1501@hcd46.67 [50.0000-419.7381]

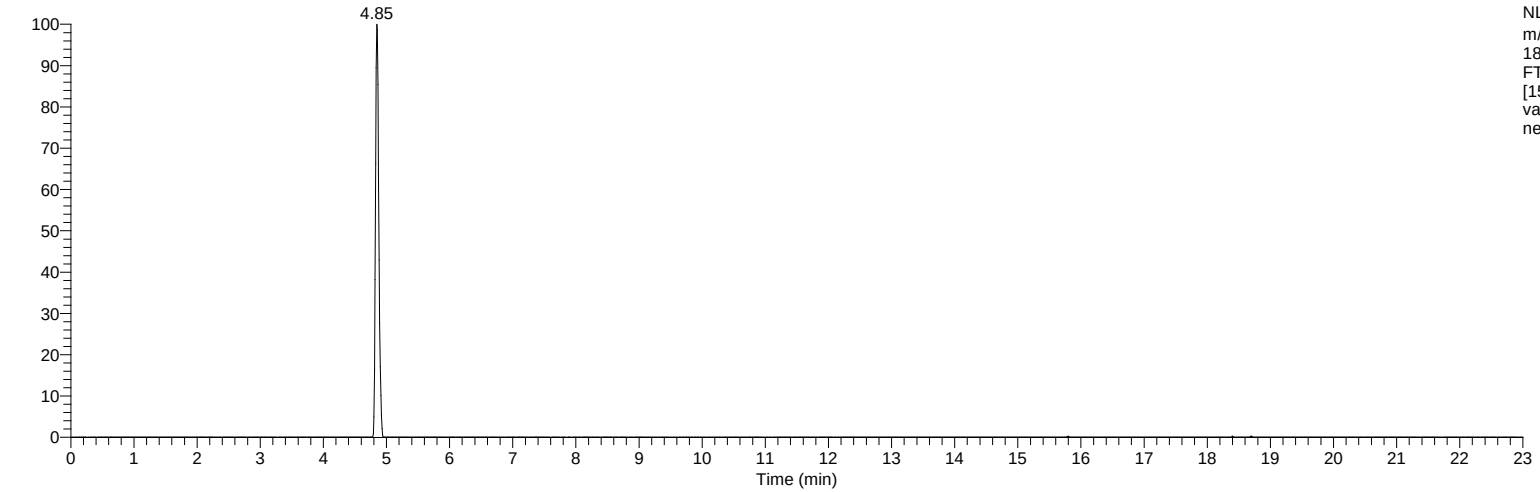


Probable degradation of indole alkaloid (1-(6-methoxy-1H-indol-2-yl)ethan-1-imine)

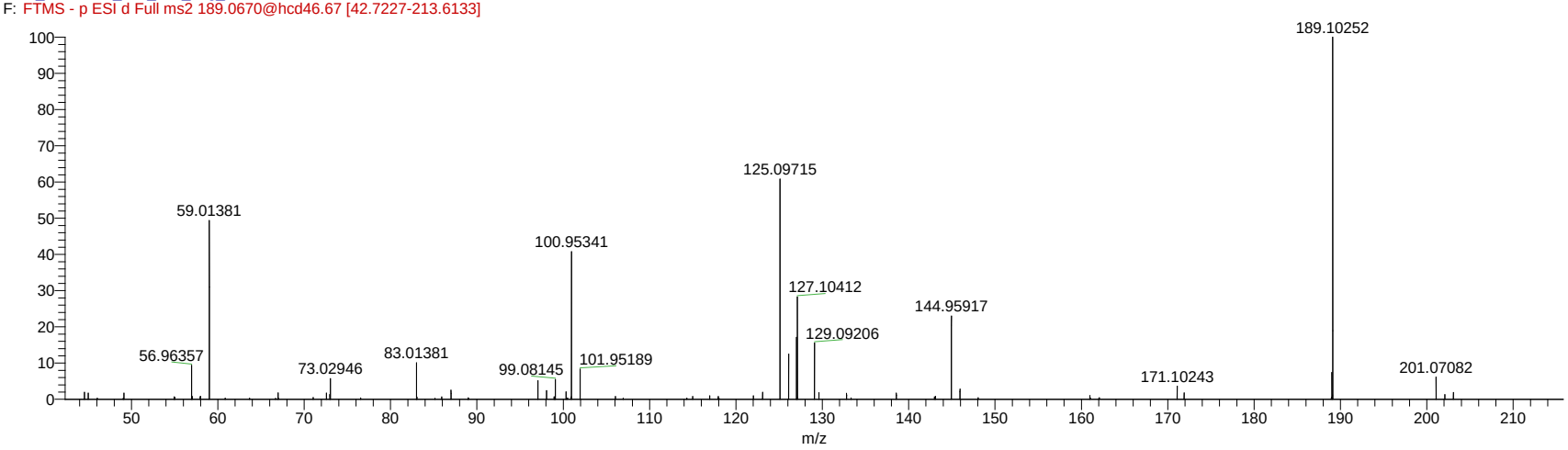


Cytisine

C:\Users\...\vaso_FSddMS2_150_255_neg_01 03/15/22 12:21:25
30mg/1ml 70/30 met/acqua
RT: 0.00 - 23.00 SM: 7G



vaso_FSddMS2_150_255_neg_01 #1836-1914 RT: 4.74-4.84 AV: 2 NL: 4.65E4
F: FTMS - p ESI d Full ms2 189.0670@hcd46.67 [42.7227-213.6133]

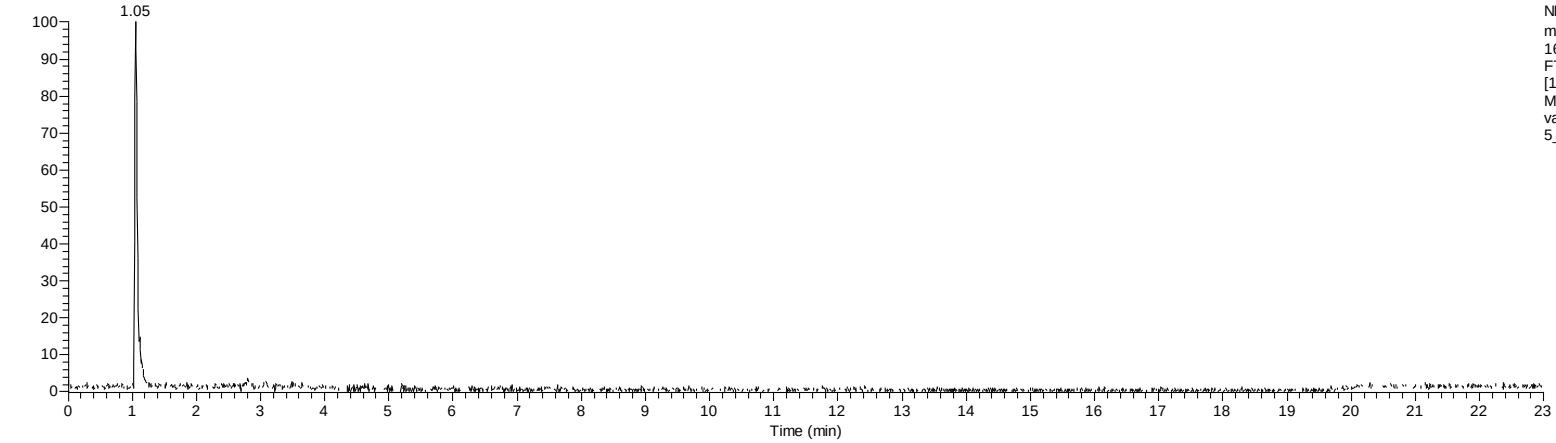


Probable degradation of isoquinoline alkaloid (1,5-isoquinolinediol or isomer)

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

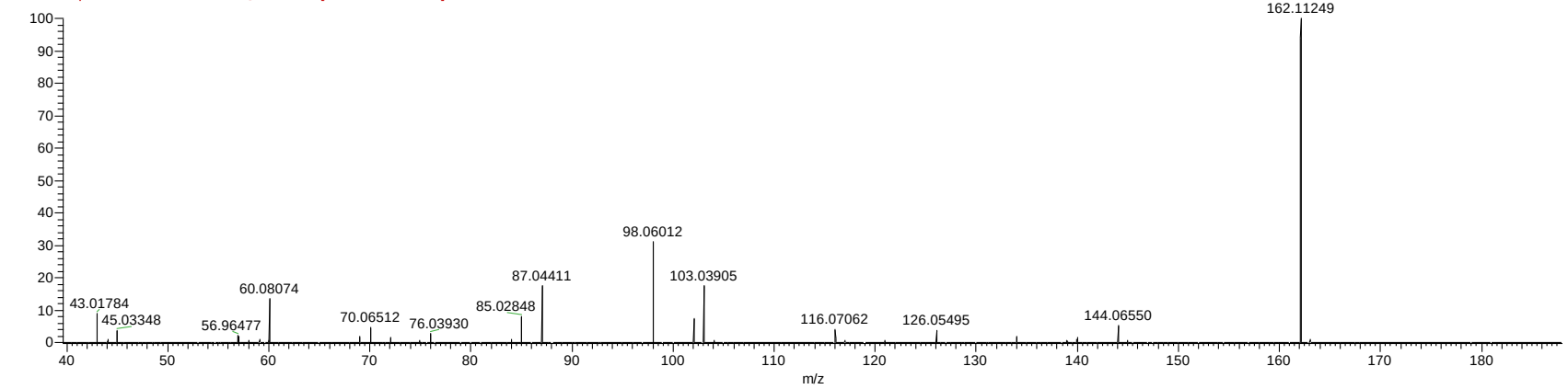
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



NL: 7.99E5
m/z=
162.05338-162.05662 F:
FTMS + p ESI Full ms
[150.0000-255.0000]
MS
vaso_FSddMS2_150_25
5_01

vaso_FSddMS2_150_255_01 #345-462 RT: 0.95-1.06 AV: 5 NL: 4.30E5
F: FTMS + p ESI d Full ms2 162.0762@hcd46.67 [40.0000-186.0827]

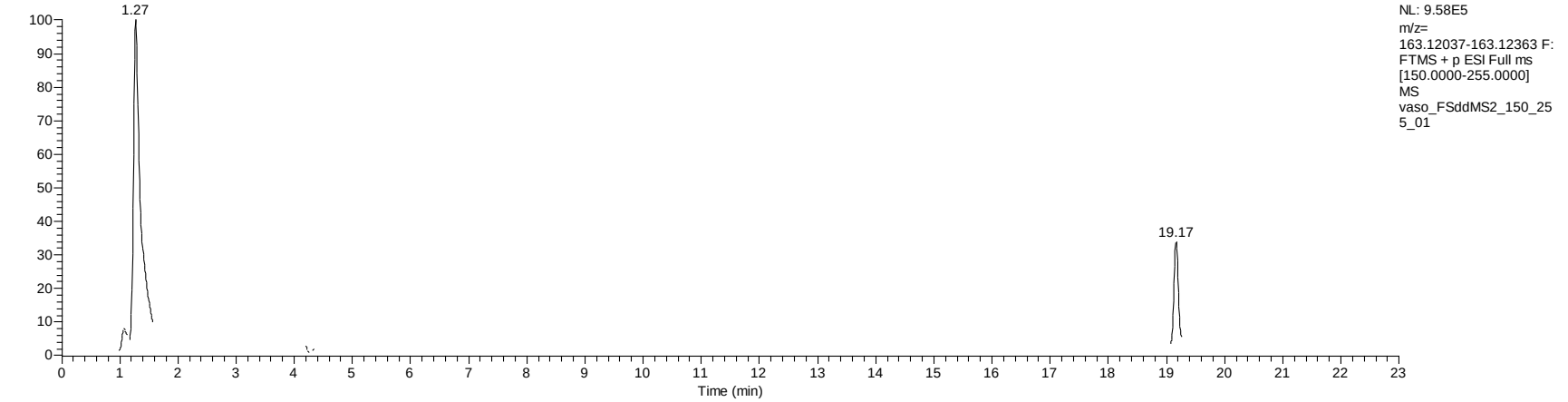


Nicotine

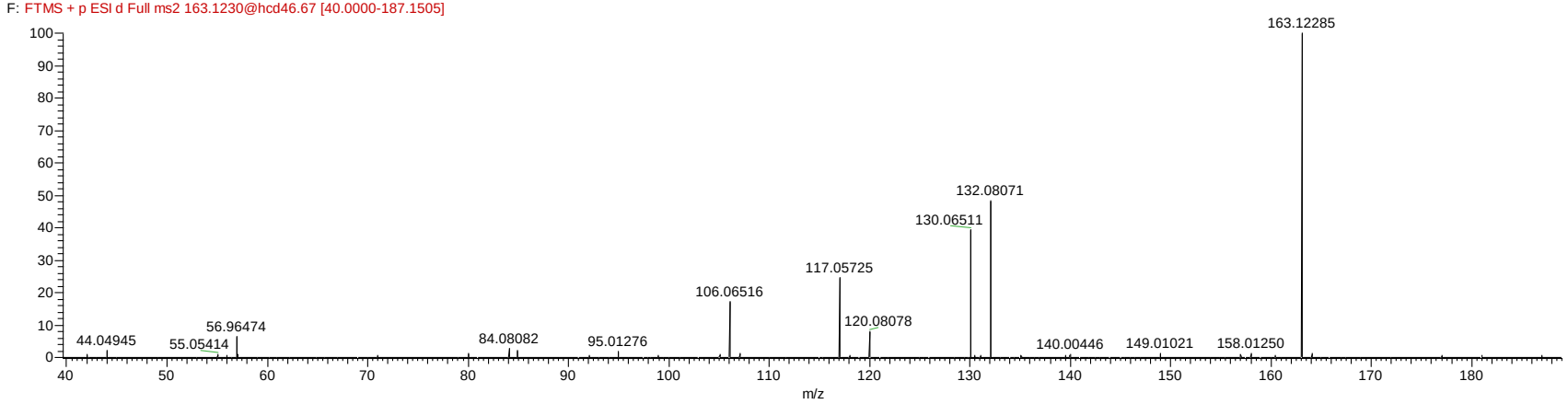
vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 15G



vaso_FSddMS2_150_255_01 #417-557 RT: 1.25-1.30 AV: 2 SB: 1 1.65-2.50 NL: 2.64E5
F: FTMS + p ESI d Full ms2 163.1230@hcd46.67 [40.0000-187.1505]

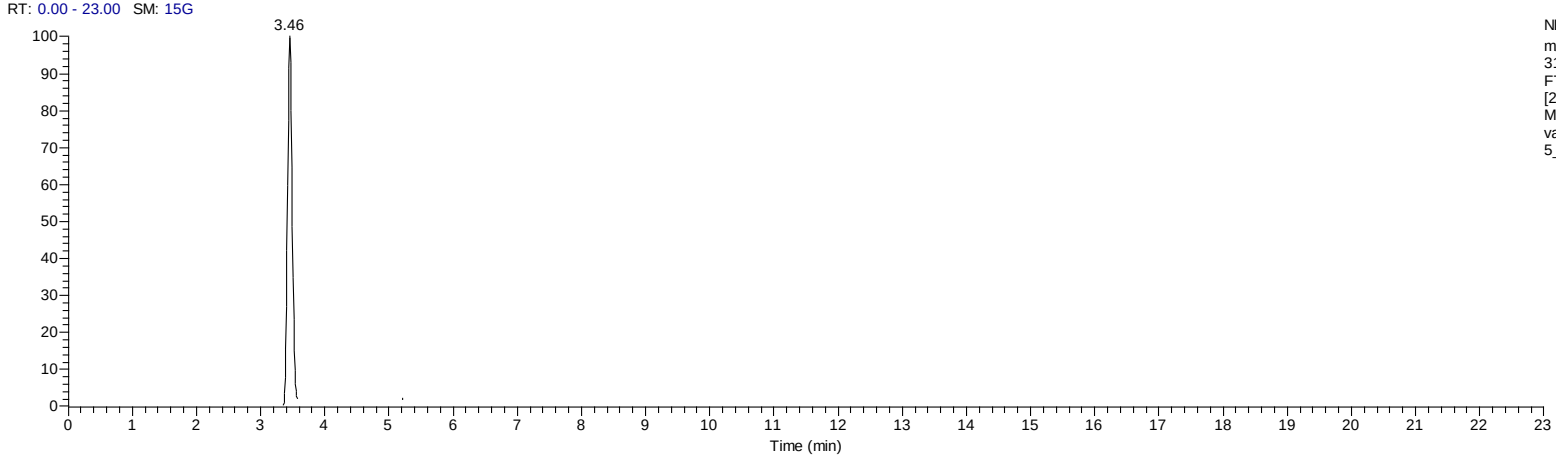


Sinapine

vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

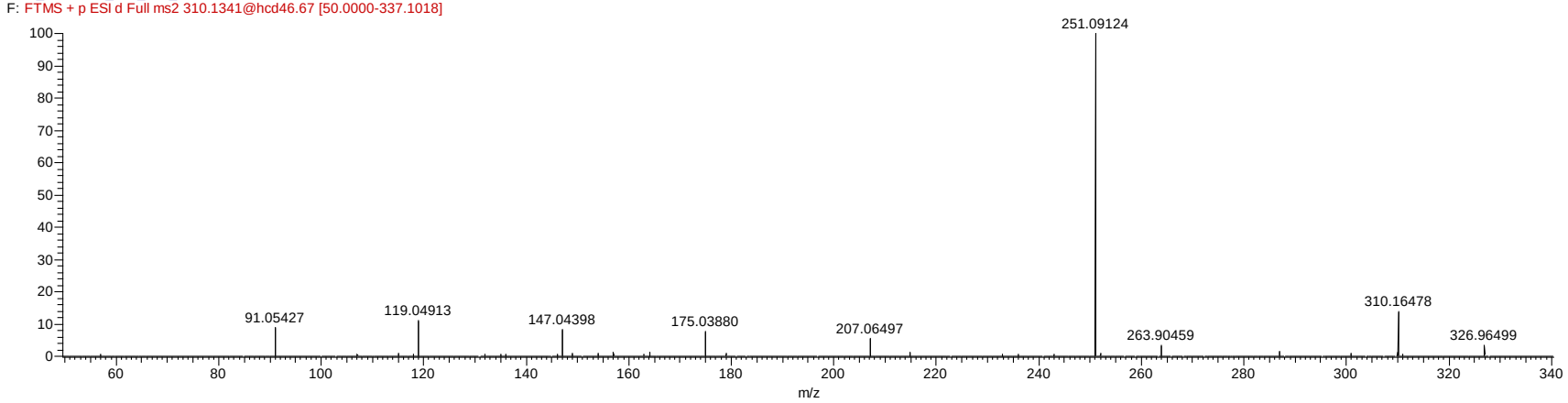
03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



NL: 3.19E5
m/z= 310.16245-310.16555 F: FTMS + p ESI Full ms [245.0000-455.0000] MS vaso_FSddMS2_245_455_01

vaso_FSddMS2_245_455_01 #1292-1390 RT: 3.45-3.48 AV: 2 SB: 4 5.55-8.24 , 1.27-3.73 NL: 9.67E4
F: FTMS + p ESI d Full ms2 310.1341@hcd46.67 [50.0000-337.1018]

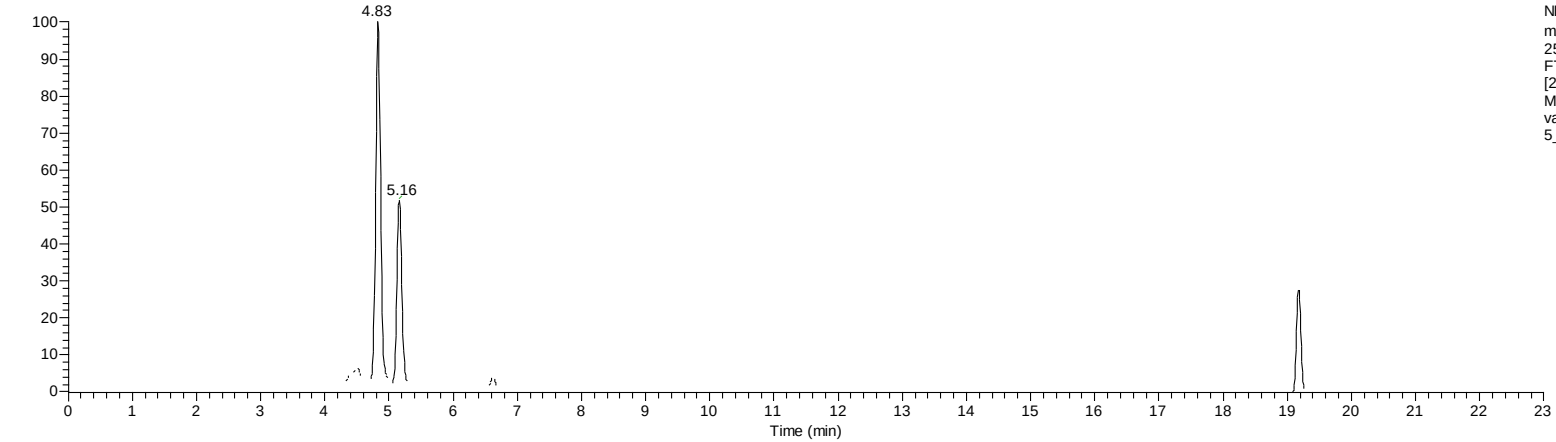


Nupharidine

vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

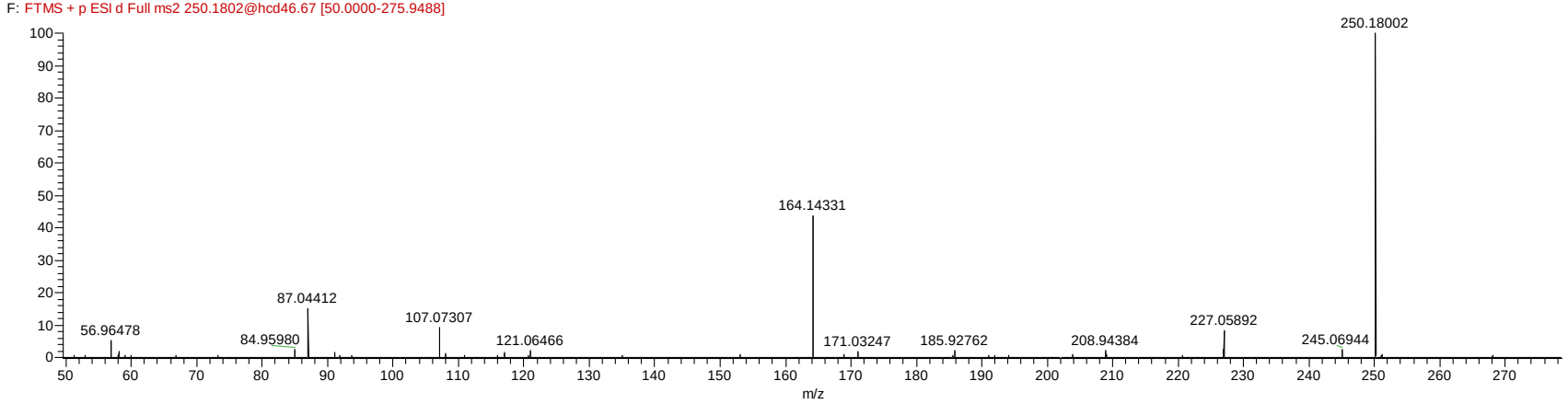
03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



NL: 2.99E5
m/z=
250.17899-250.18149 F:
FTMS + p ESI Full ms
[245.0000-455.0000]
MS
vaso_FSddMS2_245_45
5_01

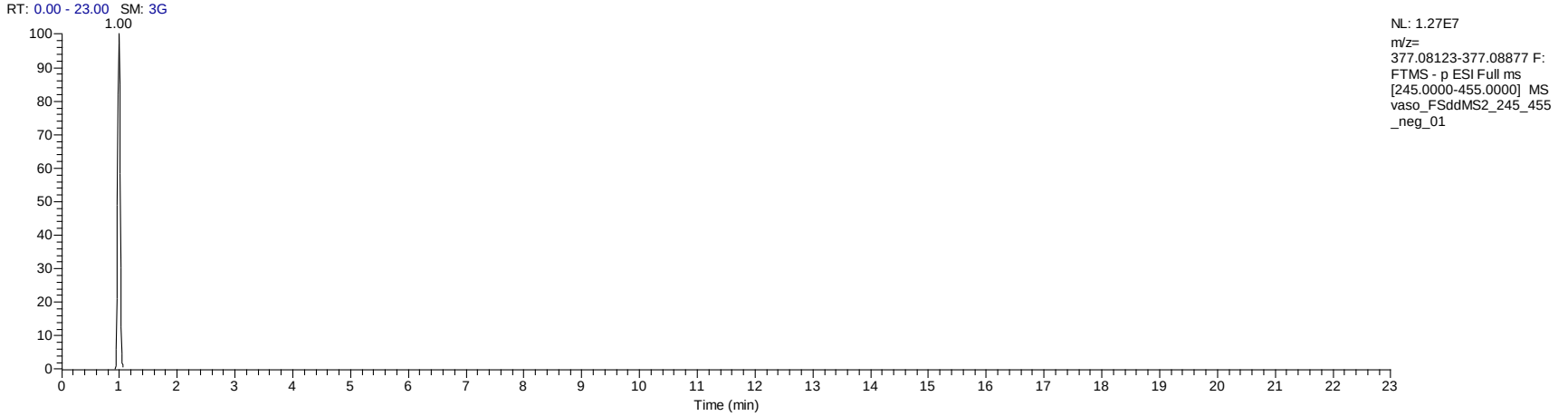
vaso_FSddMS2_245_455_01 #1883-1949 RT: 4.82-4.86 AV: 2 NL: 1.32E5
F: FTMS + p ESI d Full ms2 250.1802@hcd46.67 [50.0000-275.9488]



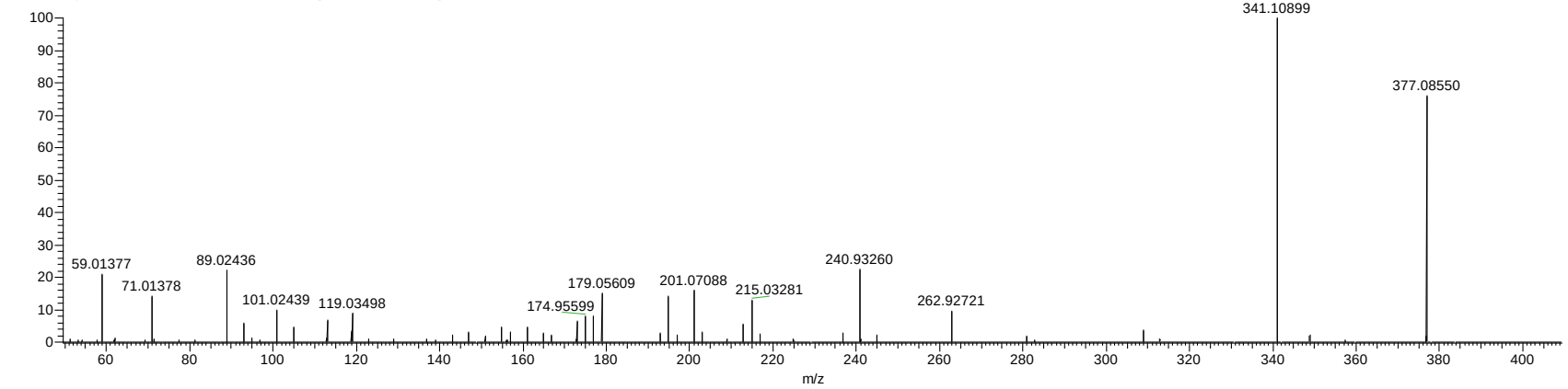
Cellobiose

vaso_FSddMS2_245_455_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:45:25



vaso_FSddMS2_245_455_neg_01 #333-549 RT: 0.83-1.02 AV: 4 NL: 1.02E5
F: FTMS - p ESI d Full ms2 377.0855@hcd46.67 [50.0000-405.3923]

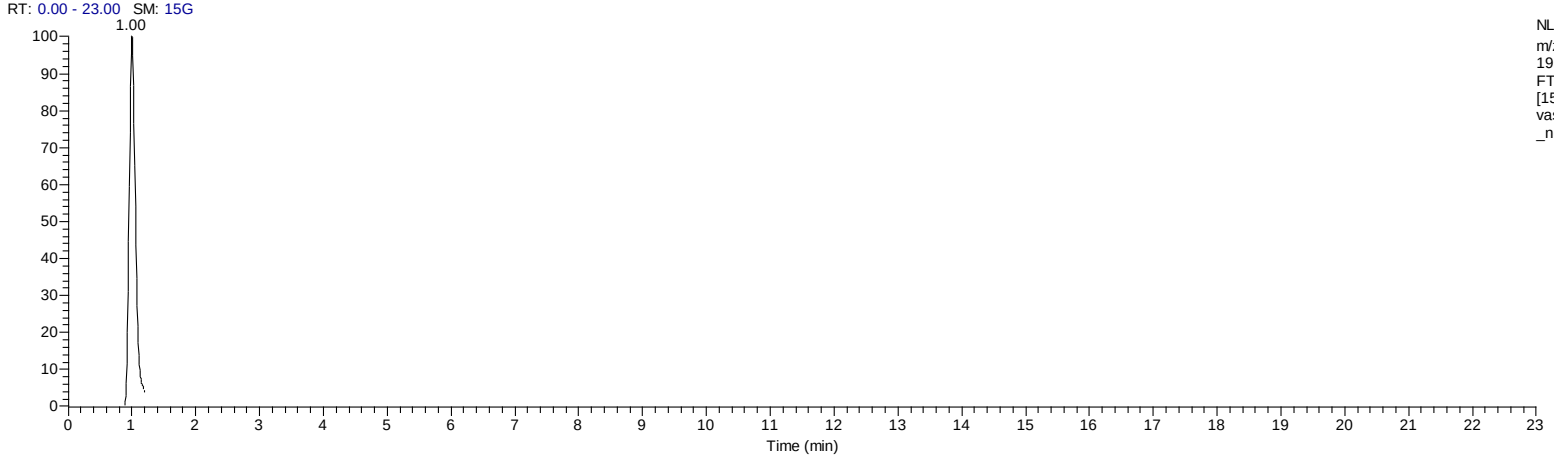


Gluconic acid or isomer

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

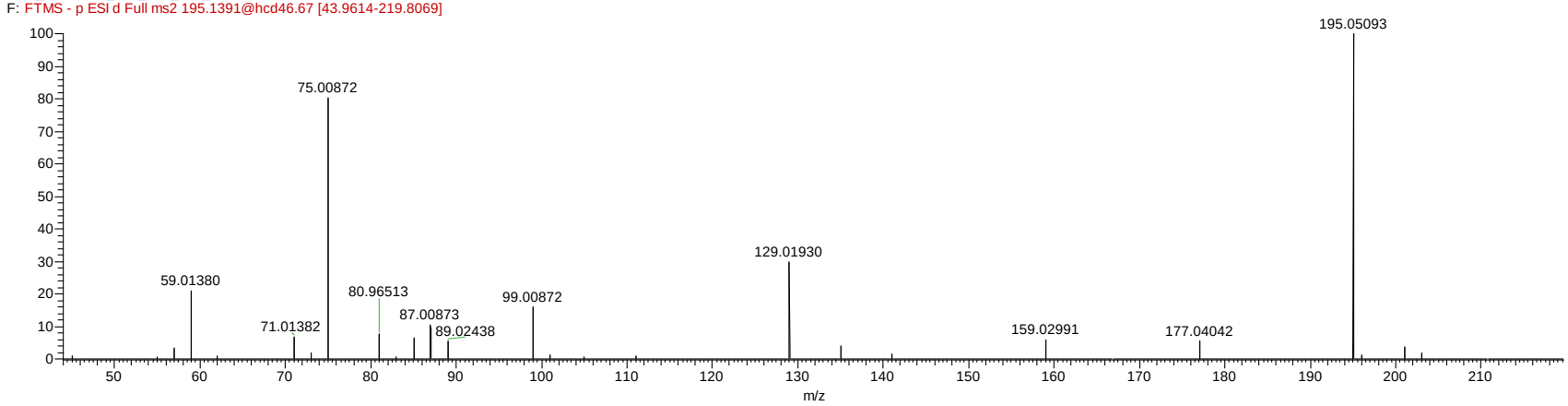
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



NL: 2.01E6
m/z=
195.04908-195.05298 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

vaso_FSddMS2_150_255_neg_01 #357 RT: 1.01 AV: 1 NL: 4.29E5
F: FTMS - p ESI d Full ms2 195.1391@hcd46.67 [43.9614-219.8069]

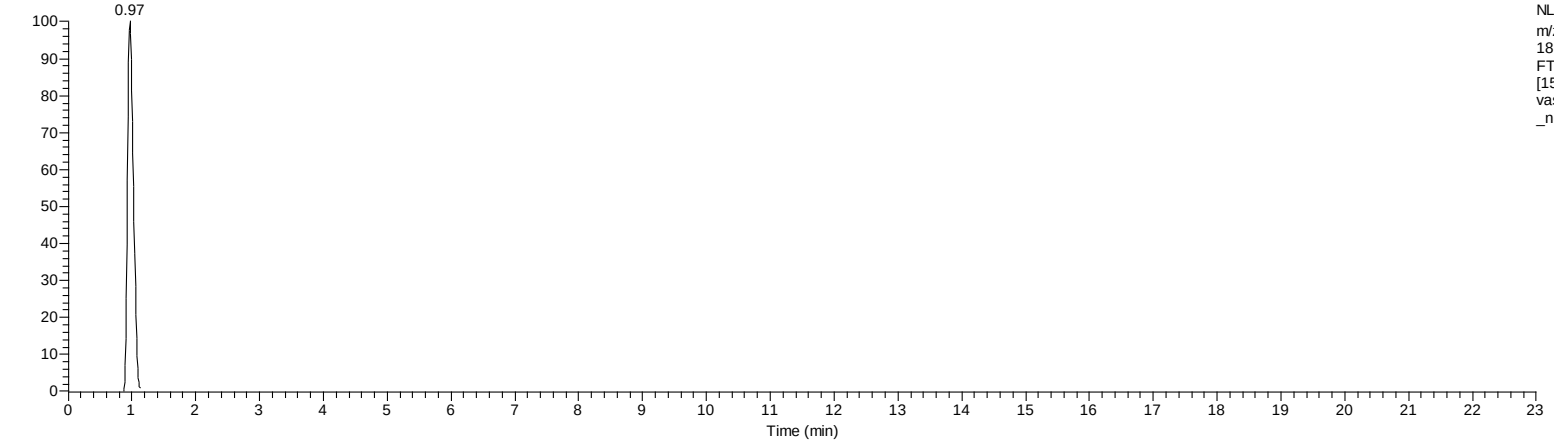


Hexitol

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

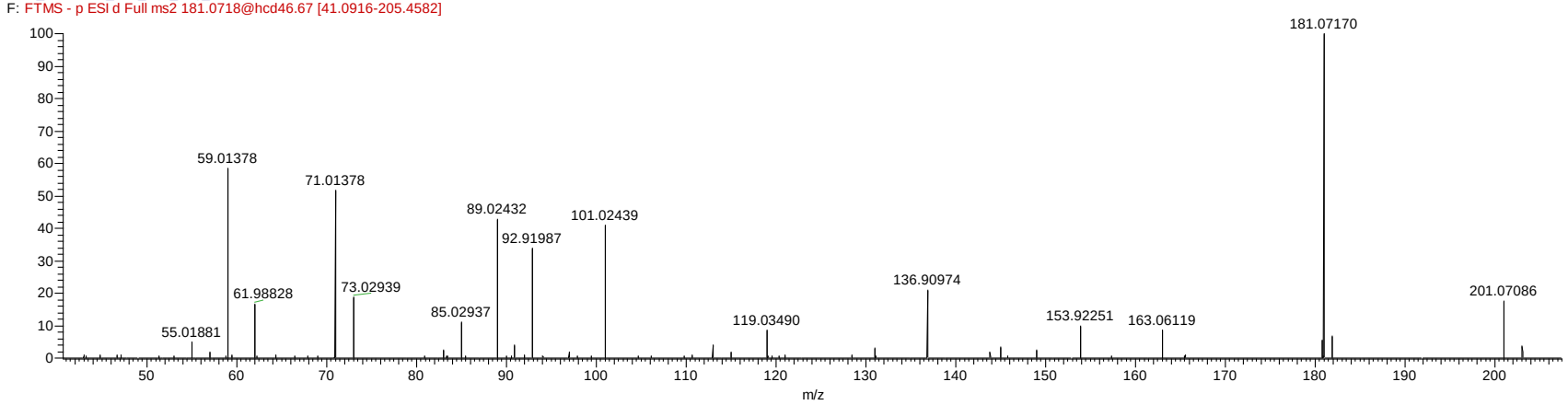
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



NL: 1.06E6
m/z=
181.06999-181.07361 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

vaso_FSddMS2_150_255_neg_01 #269-368 RT: 0.81-0.99 AV: 5 SB: 37 1.14-2.19 , 0.22-0.71 NL: 3.71E4
F: FTMS - p ESI d Full ms2 181.0718@hcd46.67 [41.0916-205.4582]

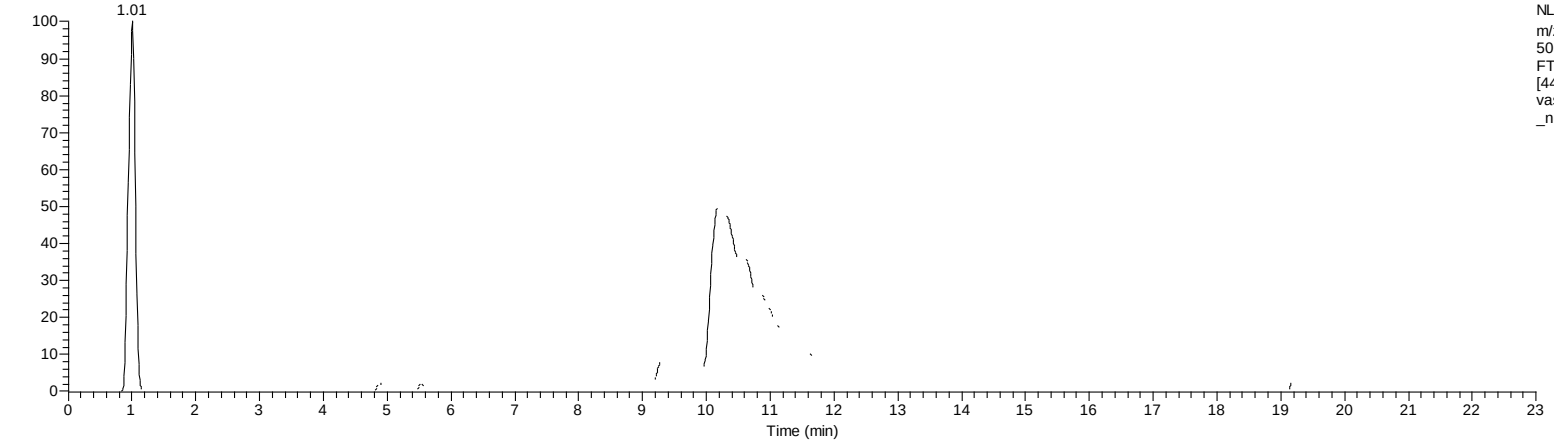


Trisaccharide (tree hexose units)

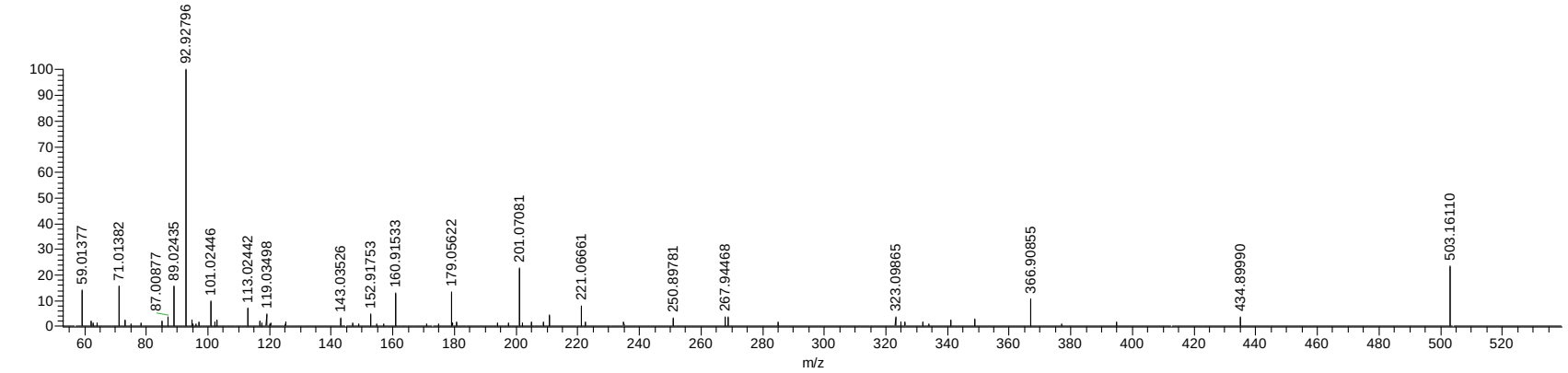
vaso_FSddMS2_445_850_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 13:09:26

RT: 0.00 - 23.00 SM: 15G



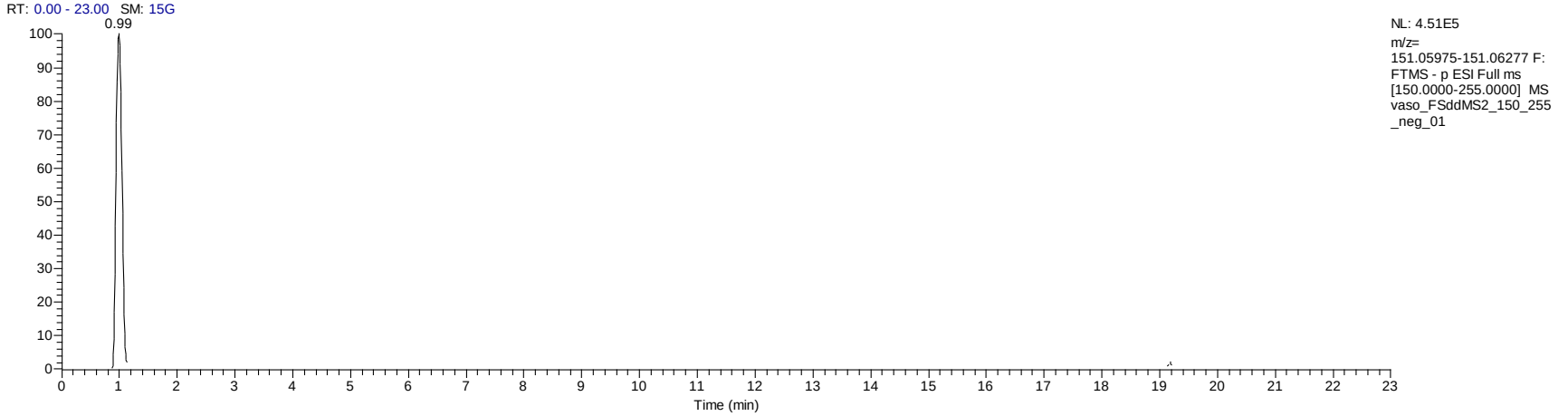
vaso_FSddMS2_445_850_neg_01 #337-448 RT: 1.00-1.04 AV: 2 SB: 19 0.32-0.54 , 1.34-13.23 NL: 5.60E4
F: FTMS - p ESI d Full ms2 503.1185@hcd46.67 [53.3946-533.9459]



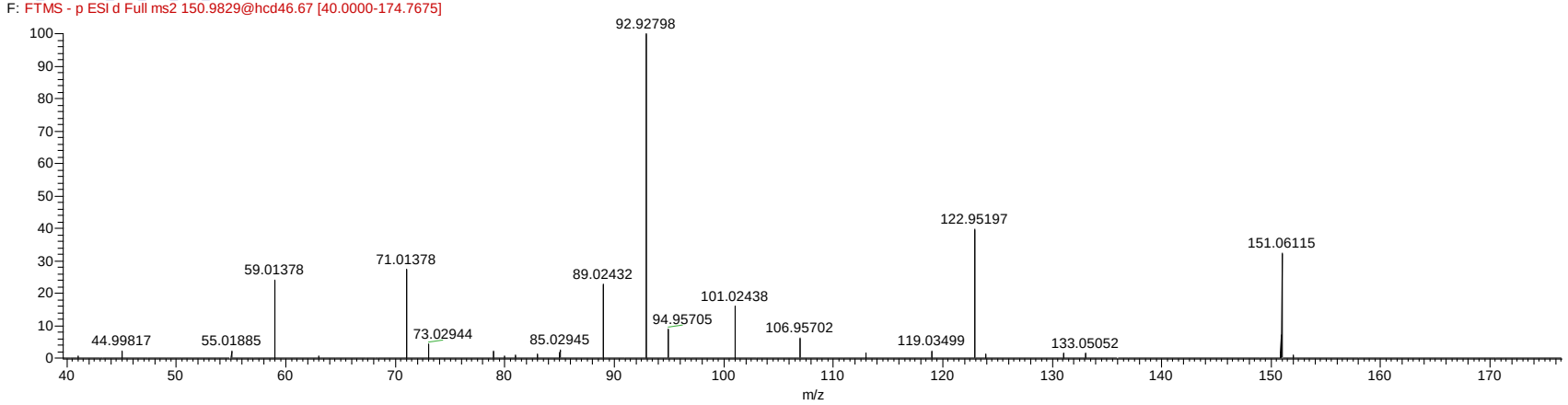
Xylitol

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:21:25



vaso_FSddMS2_150_255_neg_01 #281-390 RT: 0.96-1.02 AV: 3 NL: 1.65E5
F: FTMS - p ESI d Full ms2 150.9829@hcd46.67 [40.0000-174.7675]

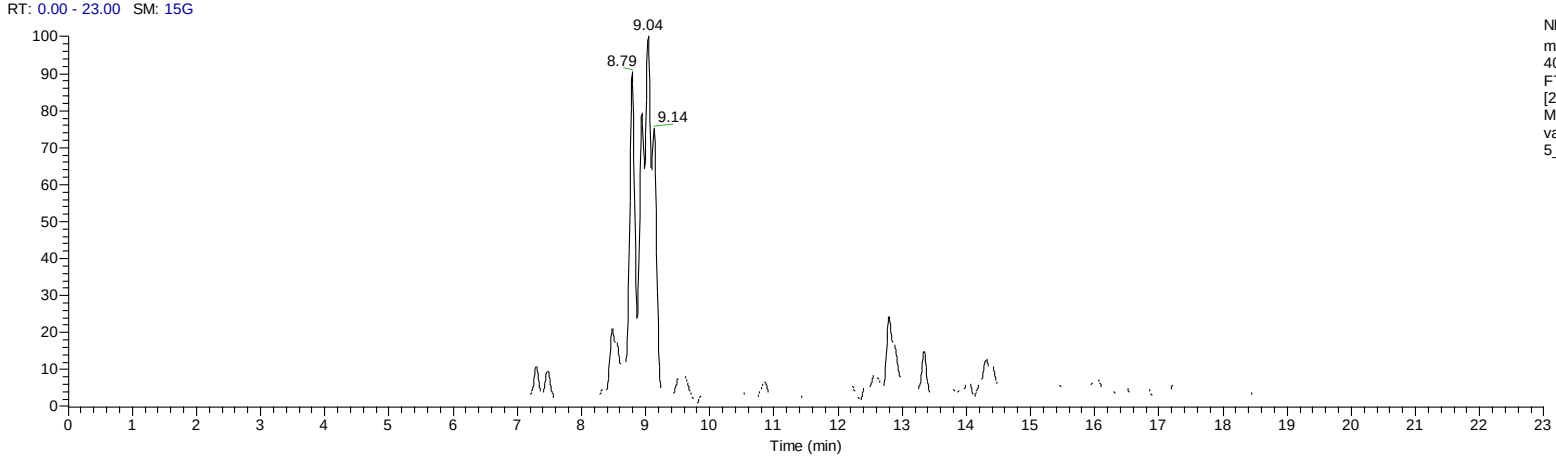


Chitobiose

vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

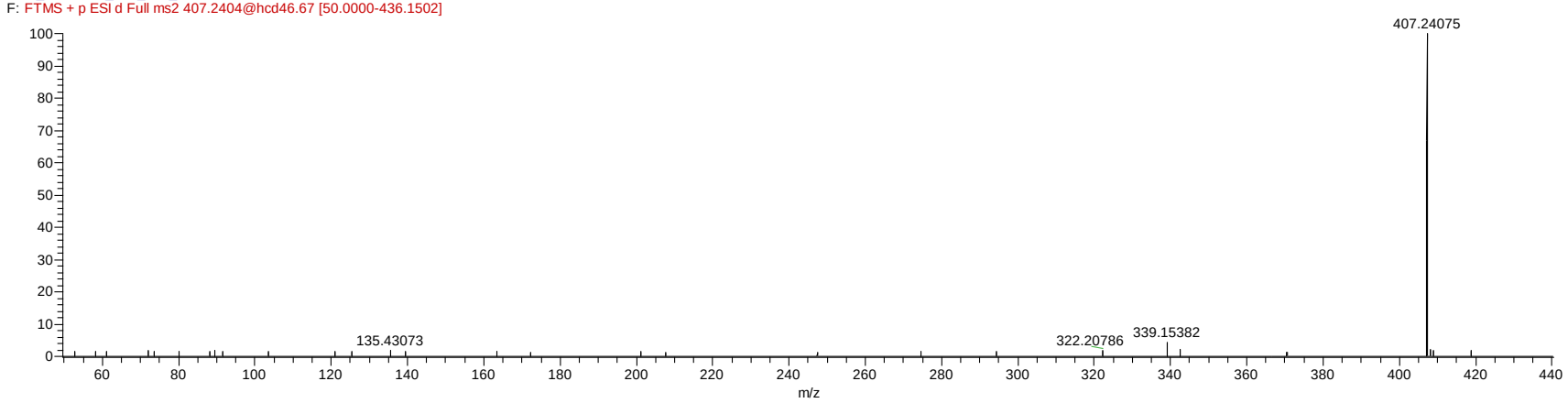
03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



NL: 1.76E5
m/z=
407.23796-407.24204 F:
FTMS + p ESI Full ms
[245.0000-455.0000]
MS
vaso_FSddMS2_245_45
5_01

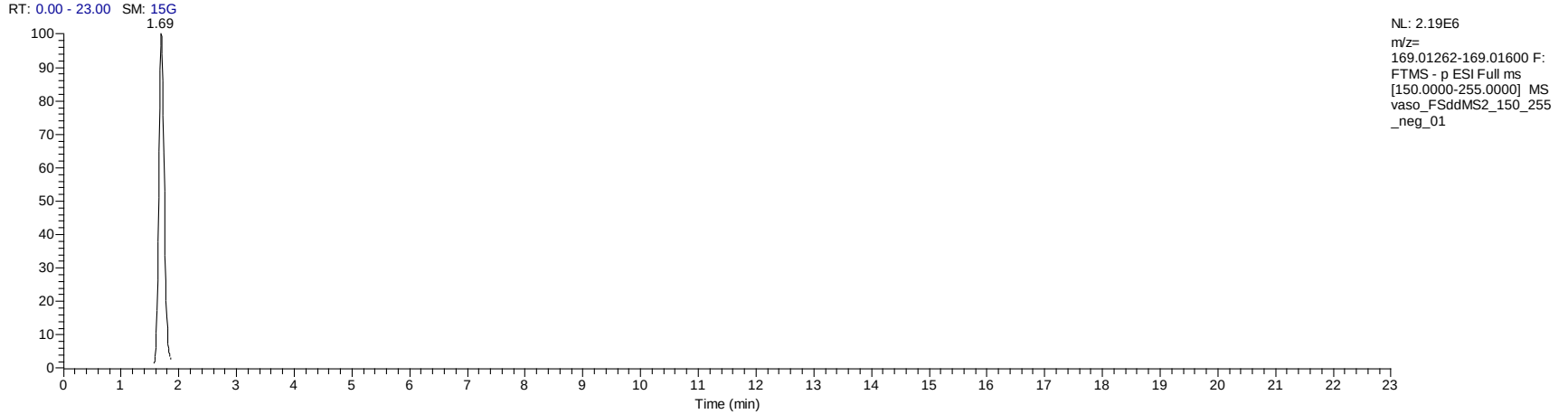
vaso_FSddMS2_245_455_01 #3560-3612 RT: 8.83-8.93 AV: 2 SB: 1 5.55-8.24 , 1.27-3.73 NL: 4.95E4
F: FTMS + p ESI d Full ms2 407.2404@hcd46.67 [50.0000-436.1502]



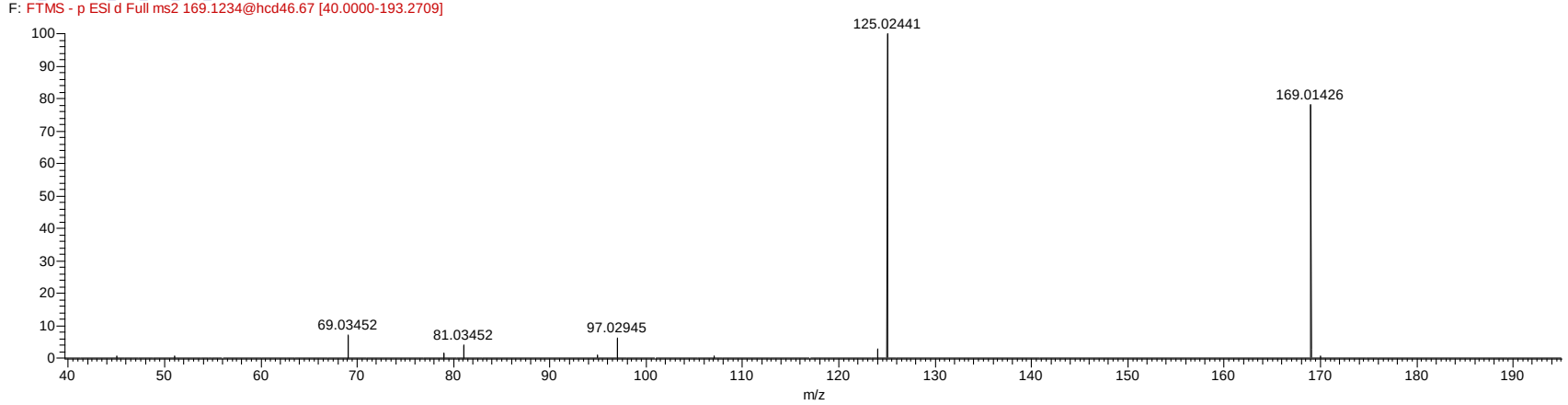
Gallic acid

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:21:25



vaso_FSddMS2_150_255_neg_01 #637-673 RT: 1.68-1.73 AV: 2 NL: 4.93E5
F: FTMS - p ESI d Full ms2 169.1234@hcd46.67 [40.0000-193.2709]

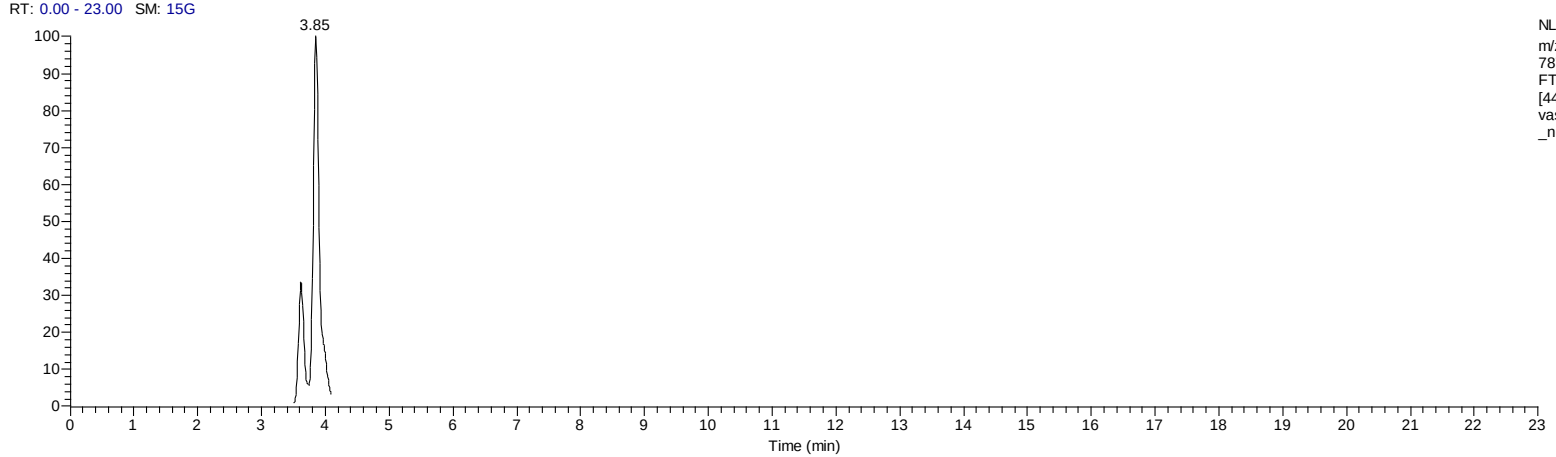


1,2,3,6-Tetra-O-galloyl-β-D-glucose

vaso_FSddMS2_445_850_neg_01
30mg/1ml 70/30 met/acqua

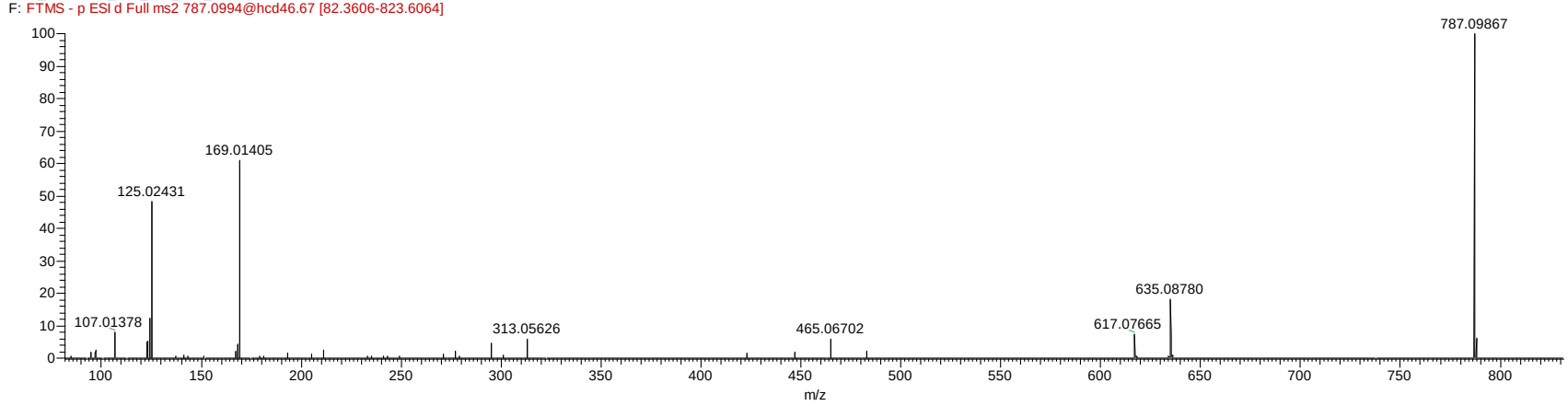
03/15/22 13:09:26

RT: 0.00 - 23.00 SM: 15G

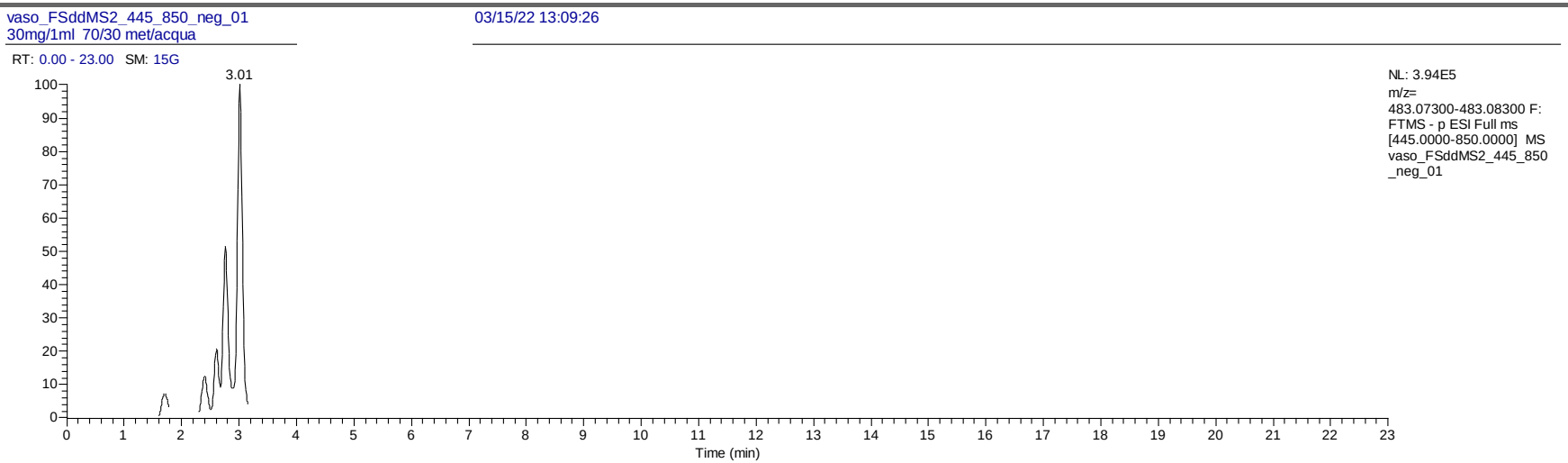


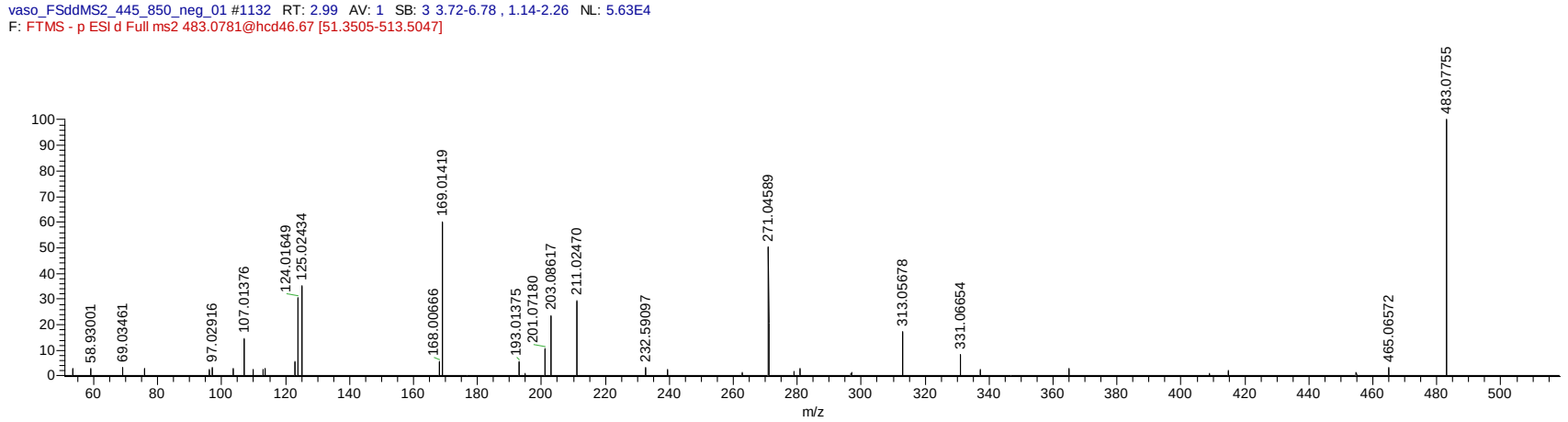
NL: 8.37E5
m/z=
787.09400-787.10400 F:
FTMS - p ESI Full ms
[445.0000-850.0000] MS
vaso_FSddMS2_445_850
_neg_01

vaso_FSddMS2_445_850_neg_01 #1492 RT: 3.83 AV: 1 SB: 6 3.72-6.78 , 1.14-2.26 NL: 1.31E5
F: FTMS - p ESI d Full ms2 787.0994@hcd46.67 [82.3606-823.6064]



1-O,6-O-digalloyl-β-D-glucose



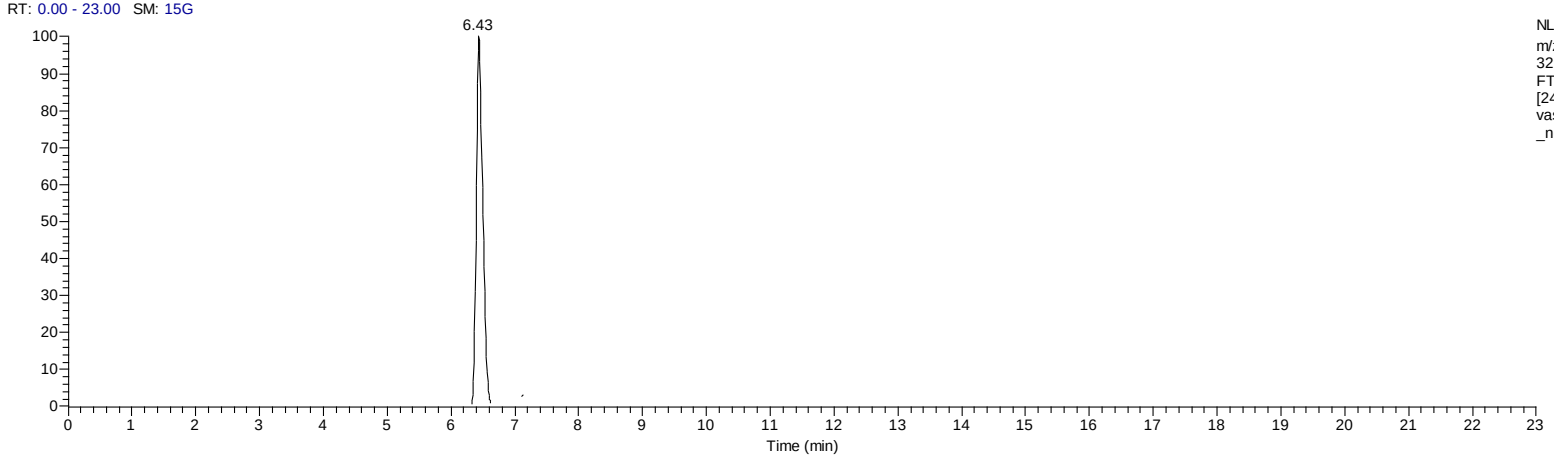


9,12,13-Trihydroxy-15-octadecenoic acid

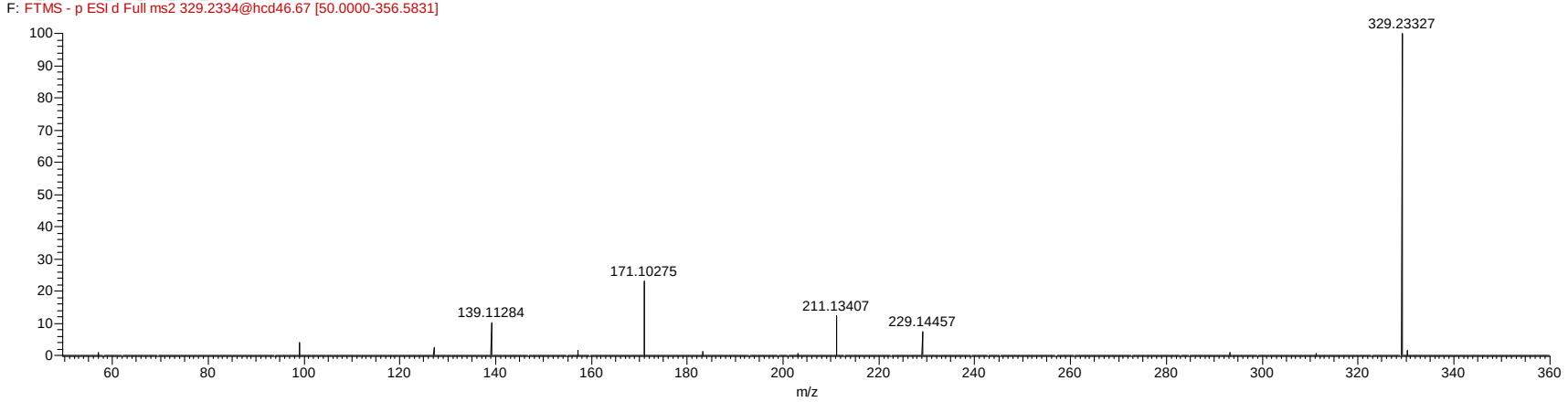
vaso_FSddMS2_245_455_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:45:25

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_245_455_neg_01 #2617-2762 RT: 6.36-6.52 AV: 4 NL: 2.50E6
F: FTMS - p ESI d Full ms2 329.2334@hcd46.67 [50.0000-356.5831]

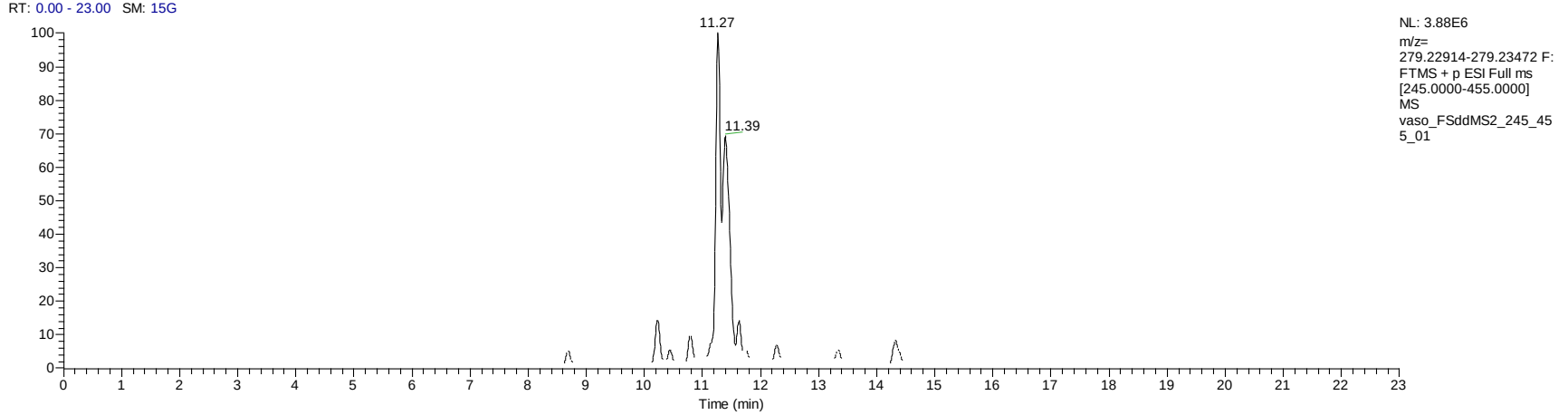


Pinolenic acid

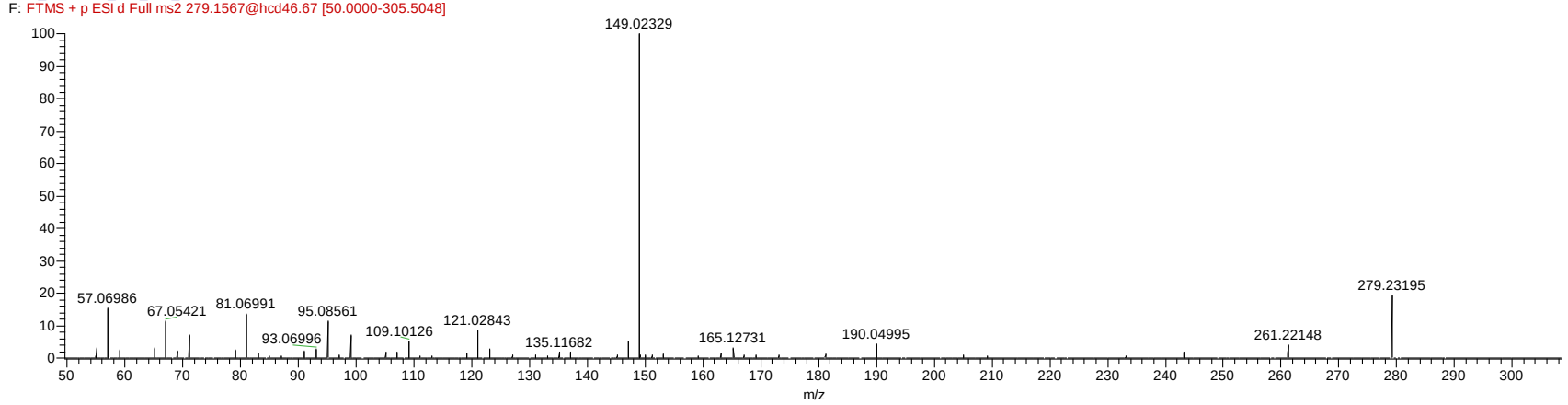
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_245_455_01 #4502-4661 RT: 11.06-11.40 AV: 12 NL: 4.79E5
F: FTMS + p ESI d Full ms2 279.1567@hcd46.67 [50.0000-305.5048]

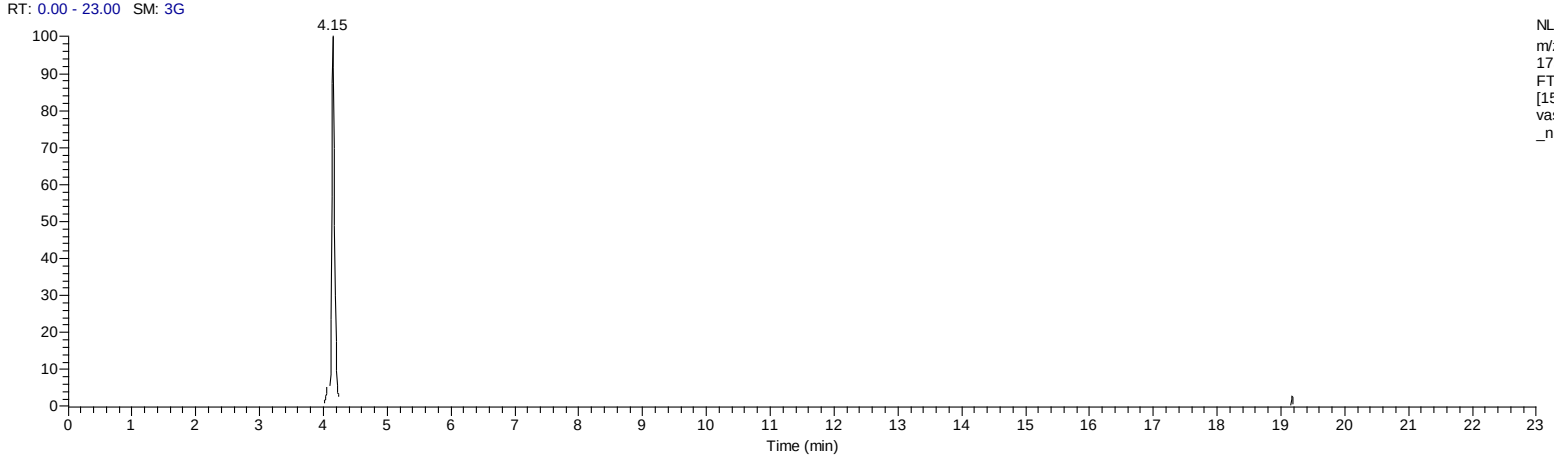


Suberic acid

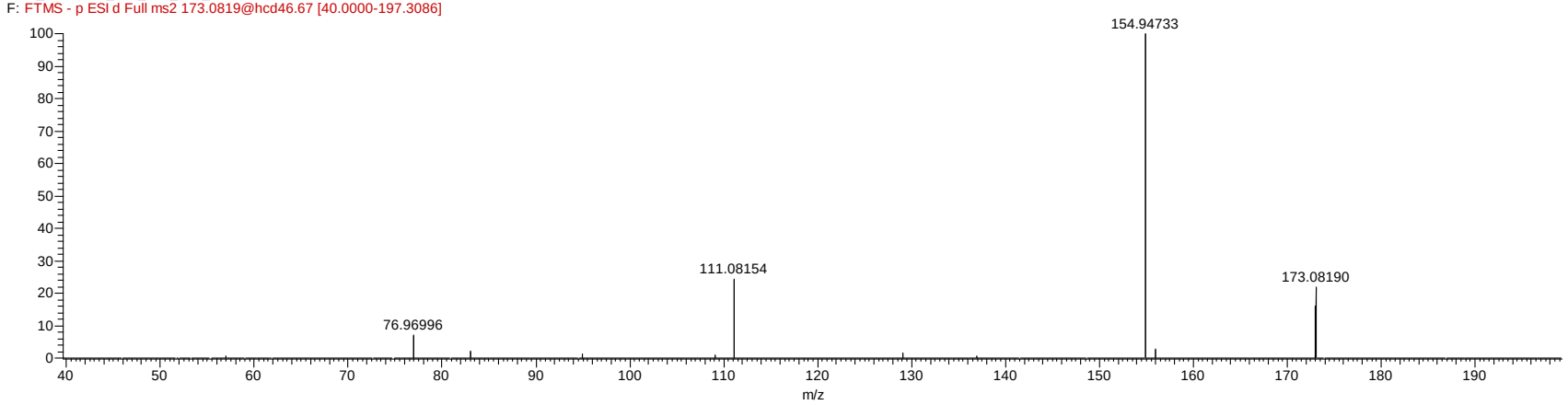
vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 3G



vaso_FSddMS2_150_255_neg_01 #1554-1632 RT: 4.03-4.20 AV: 6 NL: 1.44E6
F: FTMS - p ESI d Full ms2 173.0819@hcd46.67 [40.0000-197.3086]

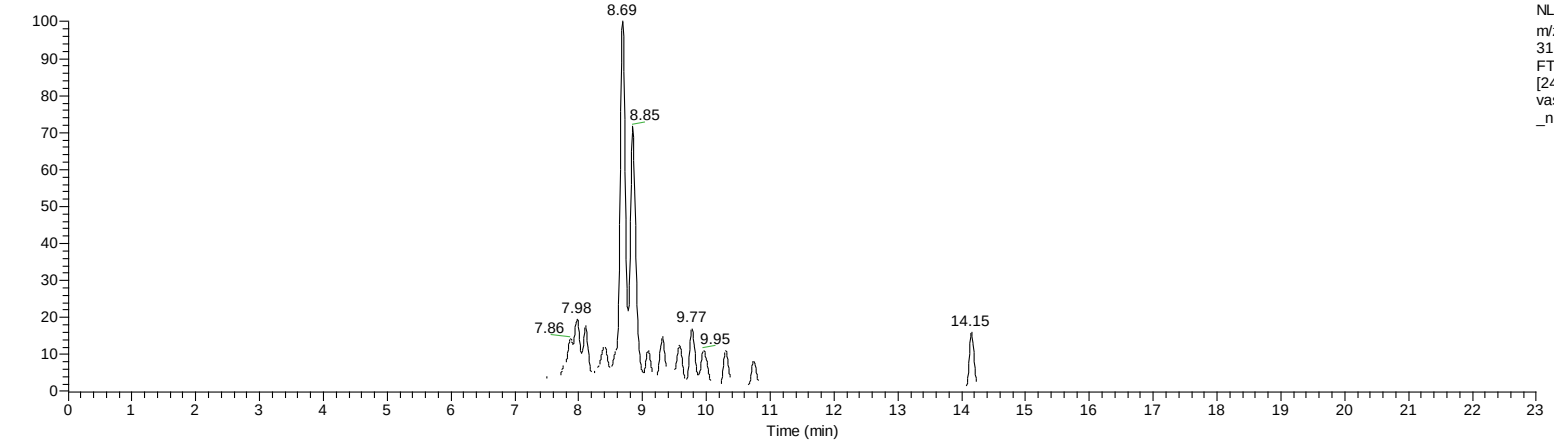


12,13-Dihydroxy-9-octadecenoic acid

vaso_FSddMS2_245_455_neg_01
30mg/1ml 70/30 met/acqua

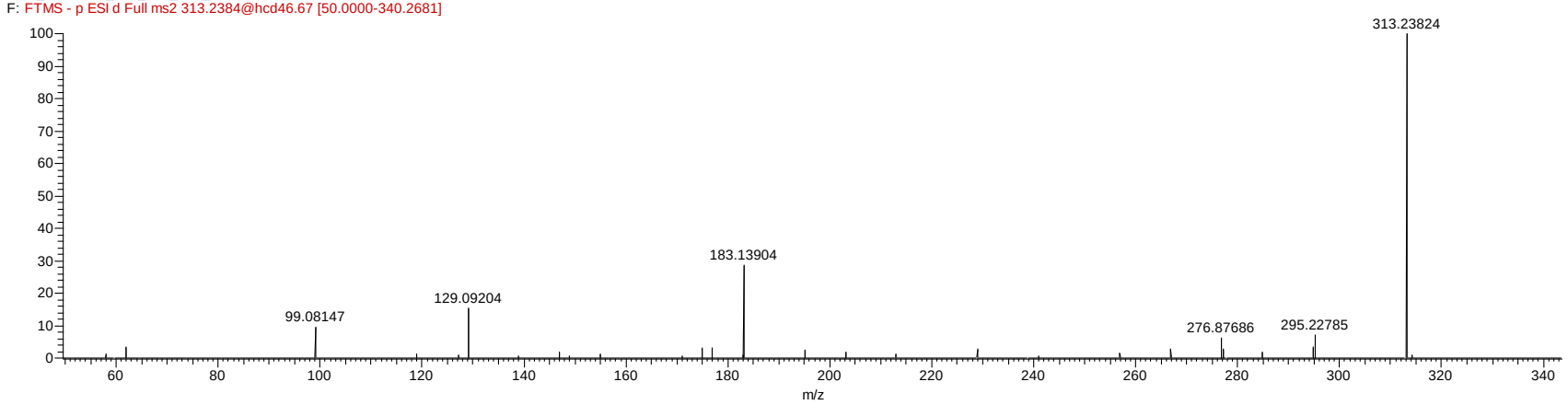
03/15/22 12:45:25

RT: 0.00 - 23.00 SM: 15G



NL: 1.40E6
m/z=
313.23527-313.24153 F:
FTMS - p ESI Full ms
[245.0000-455.0000] MS
vaso_FSddMS2_245_455
_neg_01

vaso_FSddMS2_245_455_neg_01 #3629-3709 RT: 8.69-8.74 AV: 2 NL: 3.49E5
F: FTMS - p ESI d Full ms2 313.2384@hcd46.67 [50.0000-340.2681]

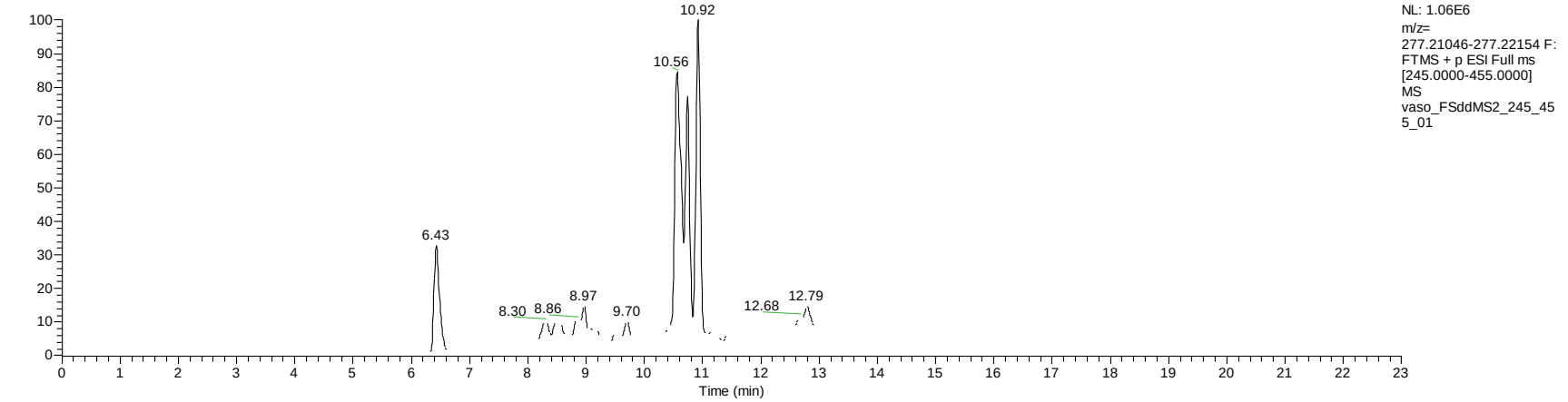


9-Hydroxy-octadecadienoic acid

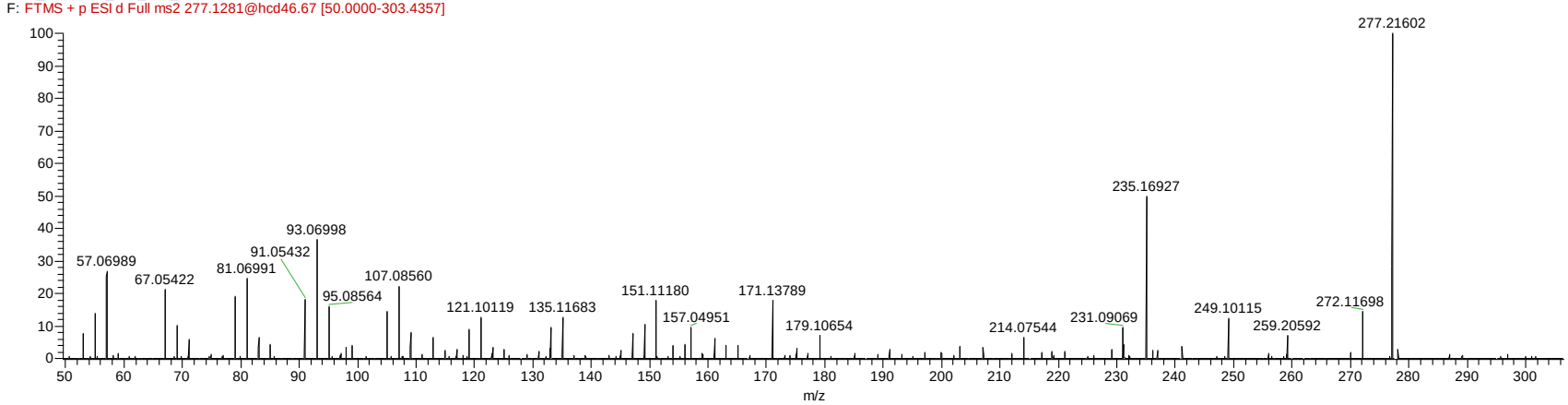
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_245_455_01 #4302-4431 RT: 10.61-10.87 AV: 8 NL: 2.99E4
F: FTMS + p ESI d Full ms2 277.1281@hcd46.67 [50.0000-303.4357]

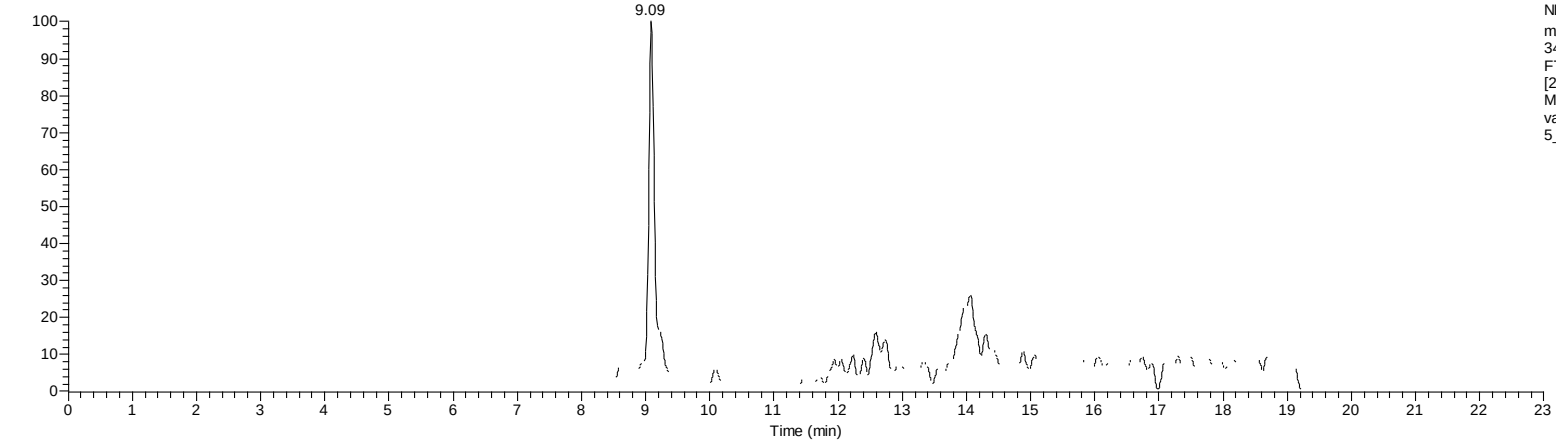


O-Arachidonoyl ethanolamine

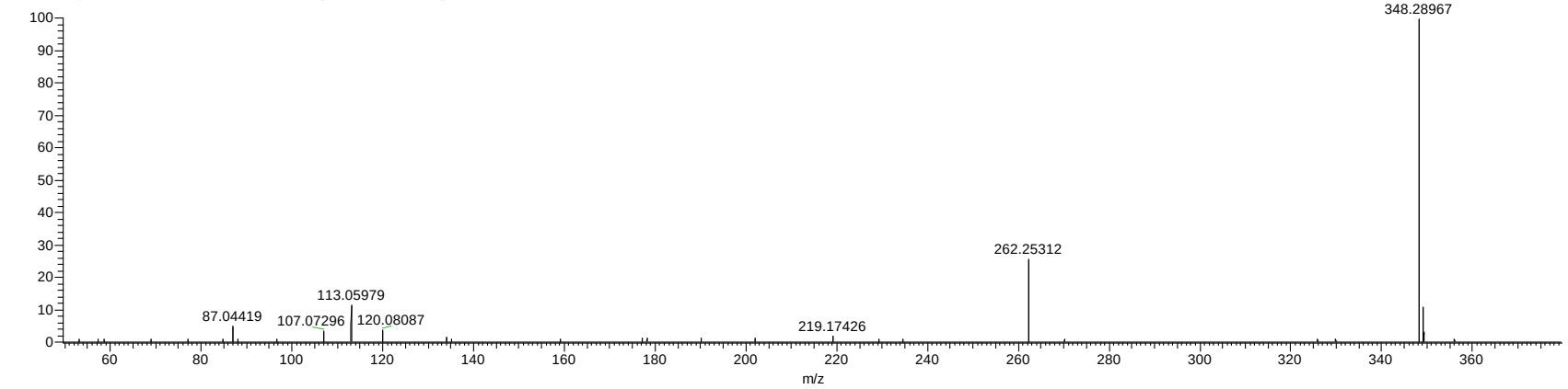
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_245_455_01 #3592-3740 RT: 9.09-9.13 AV: 2 SB: 6 5.55-8.24 , 1.27-3.73 NL: 7.97E4
F: FTMS + p ESI d Full ms2 348.2743@hcd46.67 [50.0000-376.0048]

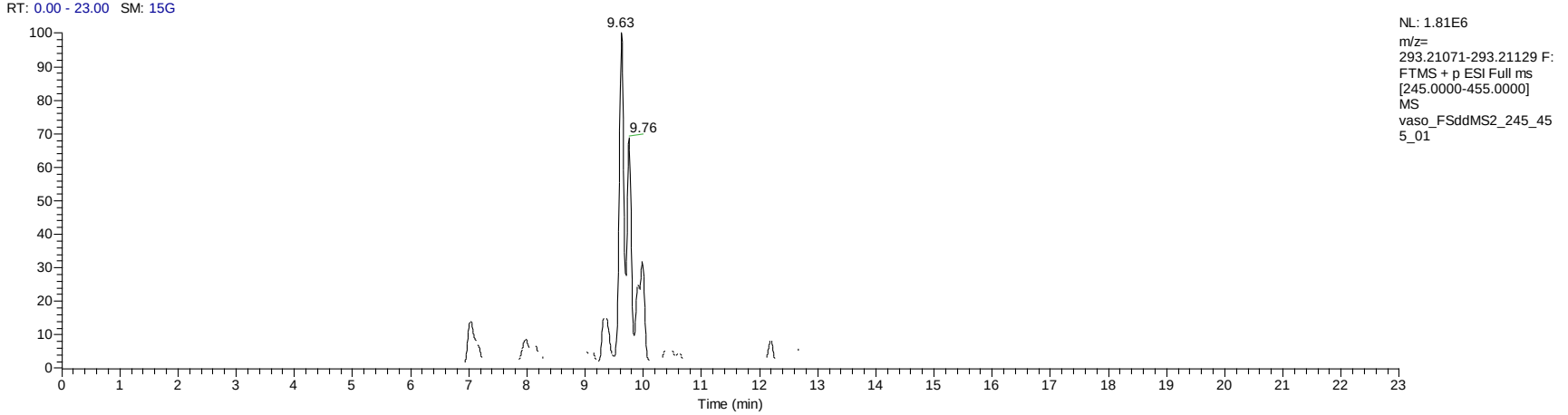


12-oxo Phytodienoic Acid

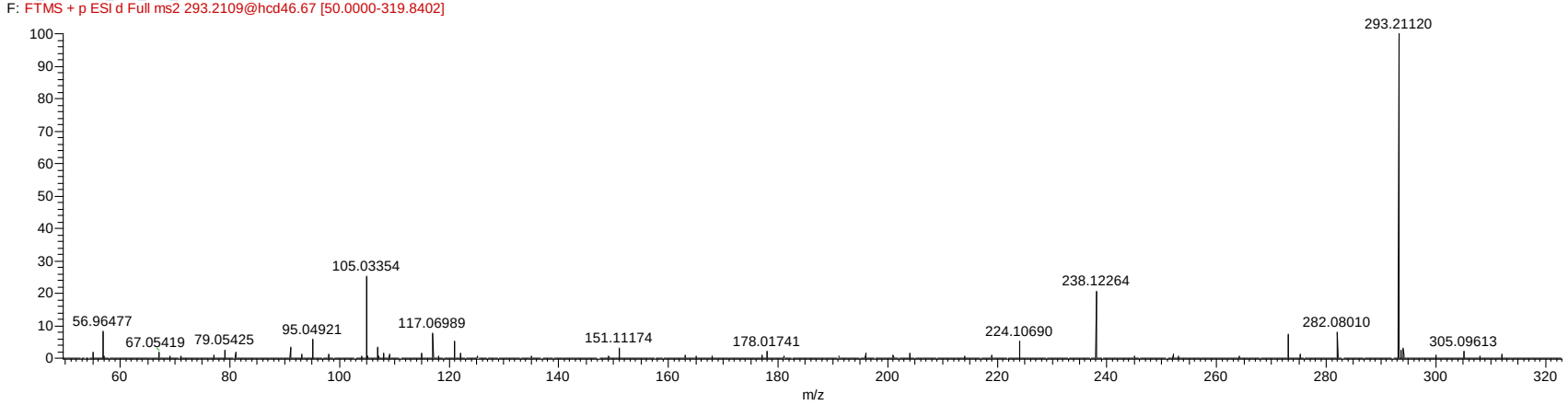
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



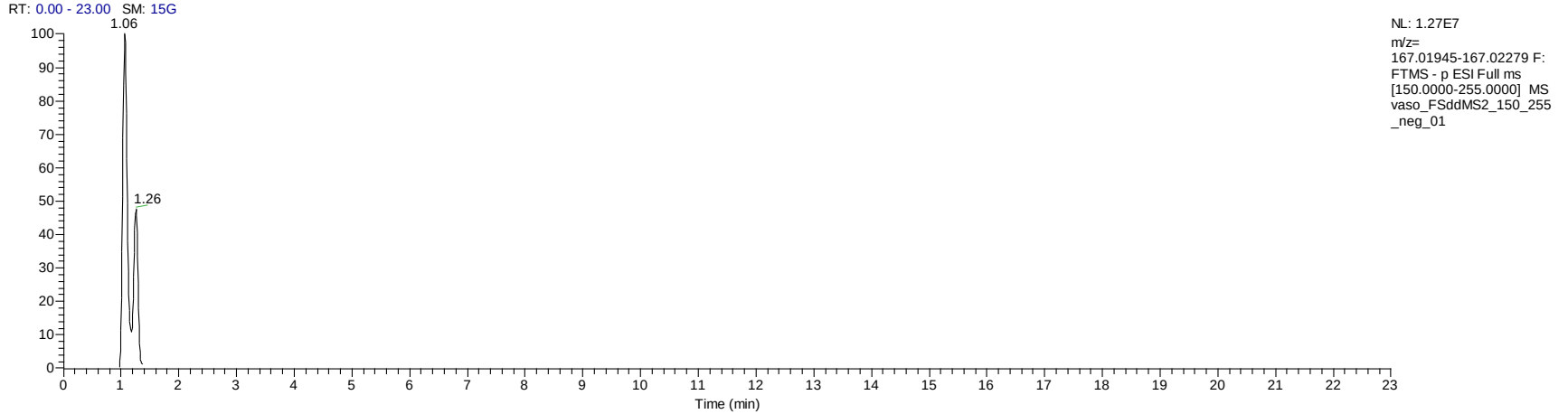
vaso_FSddMS2_245_455_01 #3832-4045 RT: 9.49-9.96 AV: 10 SB: 20 5.55-8.24 , 1.27-3.73 NL: 2.66E5
F: FTMS + p ESI d Full ms2 293.2109@hcd46.67 [50.0000-319.8402]



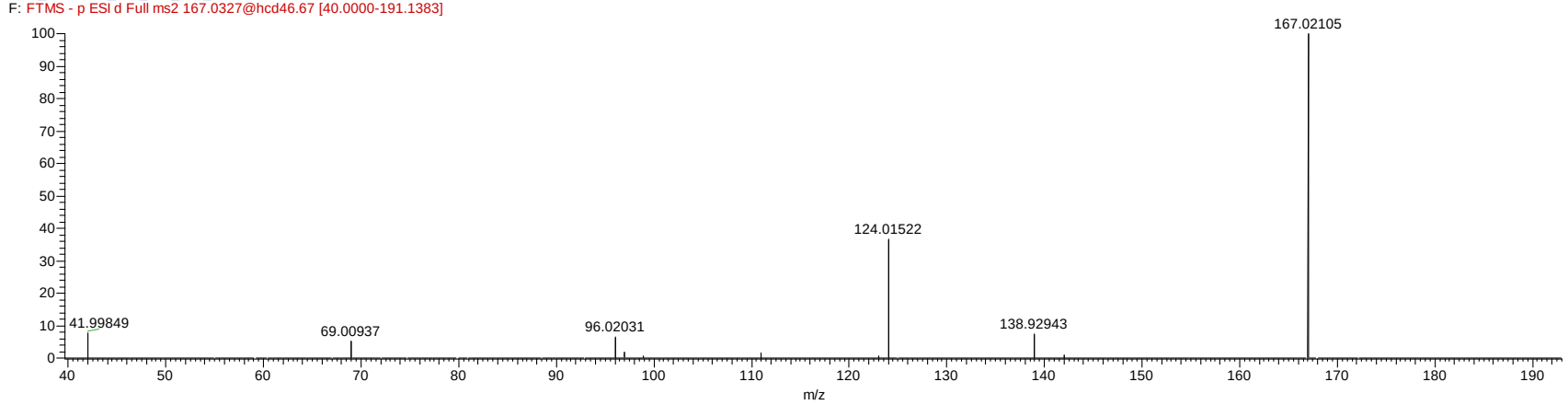
Uric acid

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:21:25



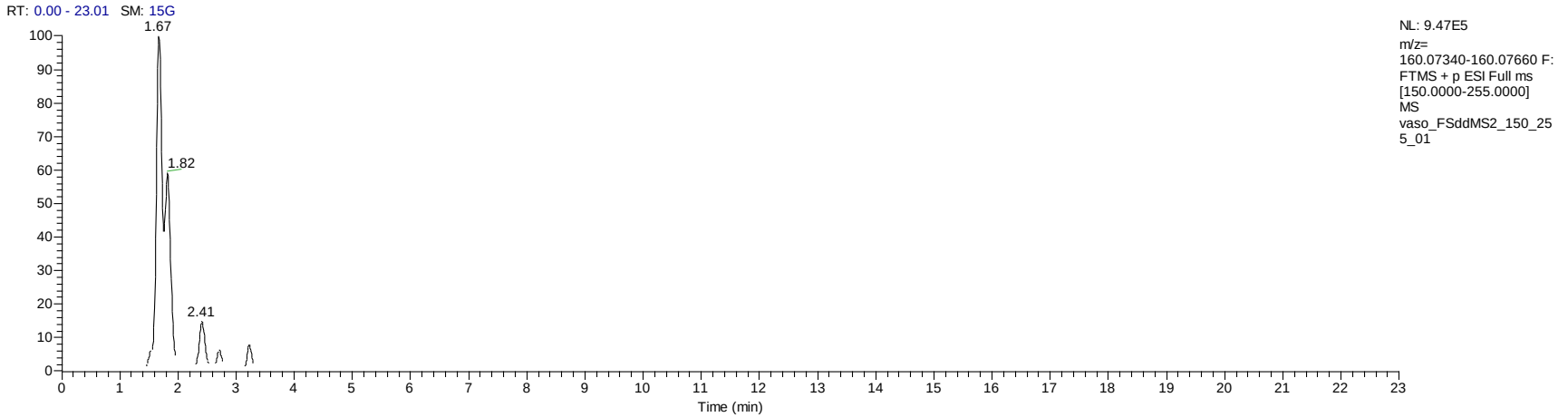
vaso_FSddMS2_150_255_neg_01 #304-427 RT: 0.92-1.14 AV: 6 NL: 9.38E5
F: FTMS - p ESI d Full ms2 167.0327@hcd46.67 [40.0000-191.1383]



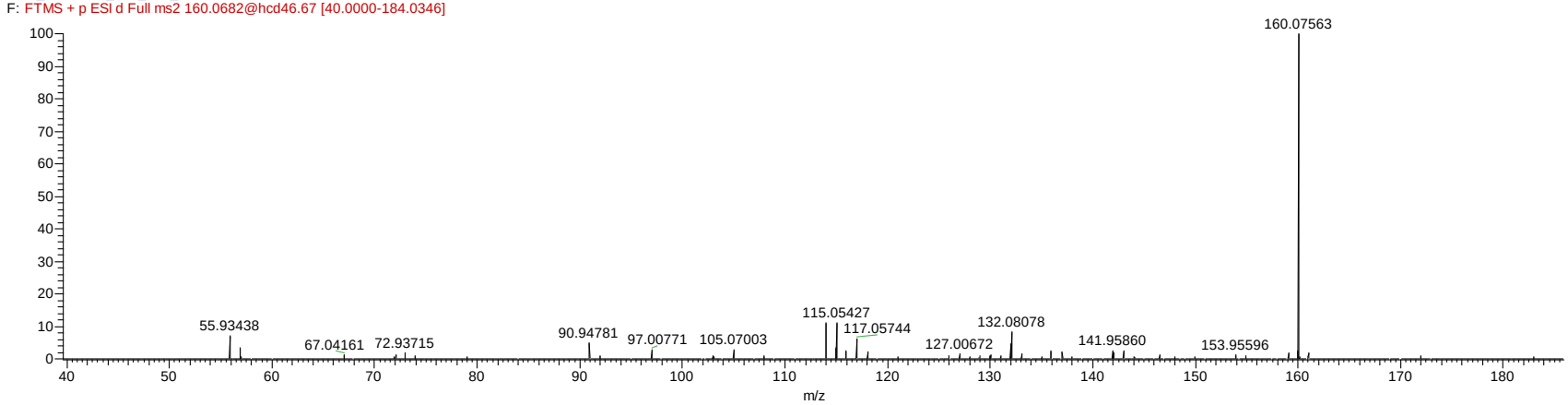
6-methoxyquinoline

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48



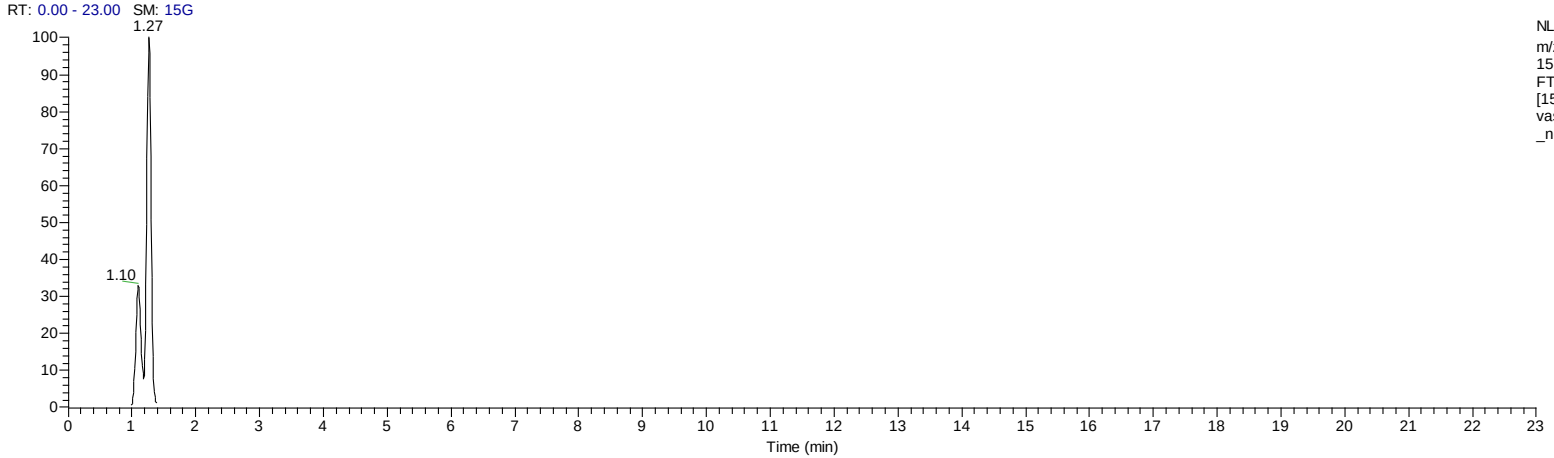
vaso_FSddMS2_150_255_01 #658-819 RT: 1.62-1.89 AV: 7 SB: 2 2.79-4.24 , 6.15-13.03 NL: 1.32E5
F: FTMS + p ESI d Full ms2 160.0682@hcd46.67 [40.0000-184.0346]



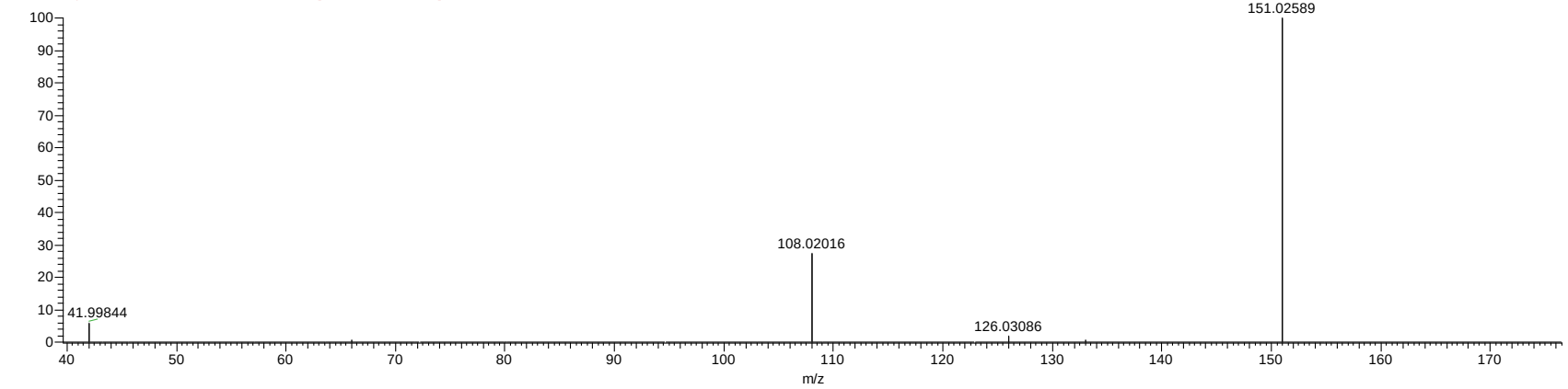
Xanthine

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:21:25



vaso_FSddMS2_150_255_neg_01 #460 RT: 1.26 AV: 1 SB: 2 1.14-2.19 , 0.22-0.71 NL: 2.18E5
F: FTMS - p ESI d Full ms2 150.9829@hcd46.67 [40.0000-174.7675]

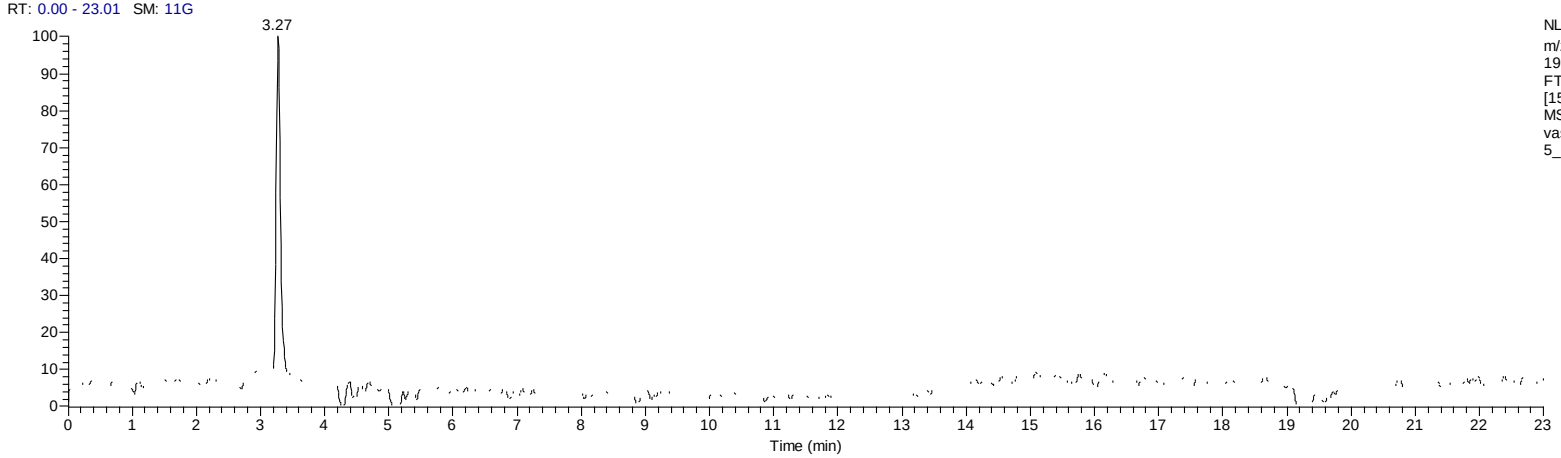


Caffeine

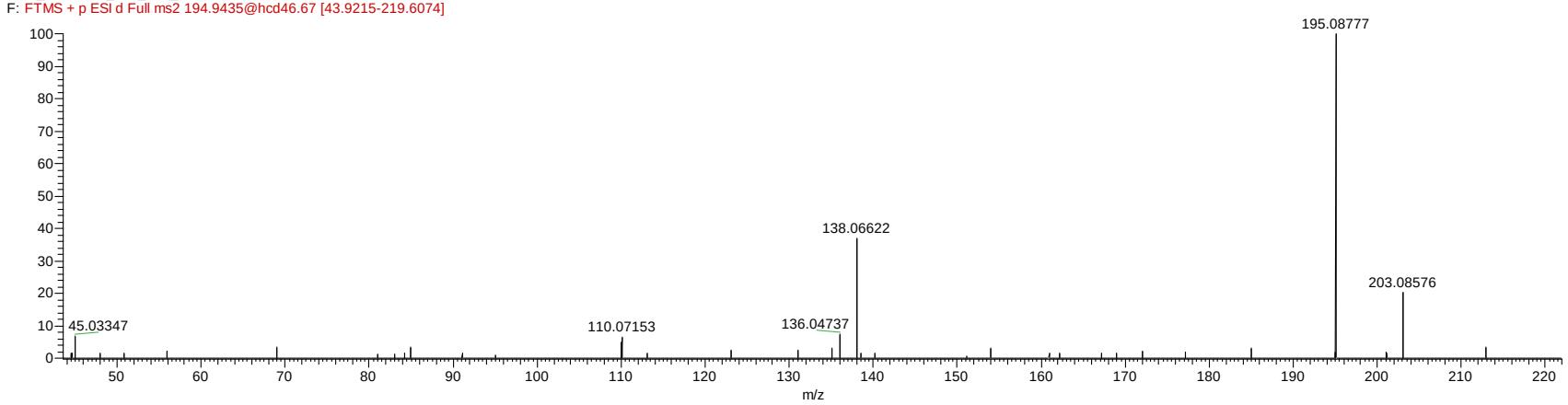
vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 11G



vaso_FSddMS2_150_255_01 #1330 RT: 3.27 AV: 1 SB: 44 9.46-13.43 , 8.65-9.13 NL: 9.57E4
F: FTMS + p ESI d Full ms2 194.9435@hcd46.67 [43.9215-219.6074]

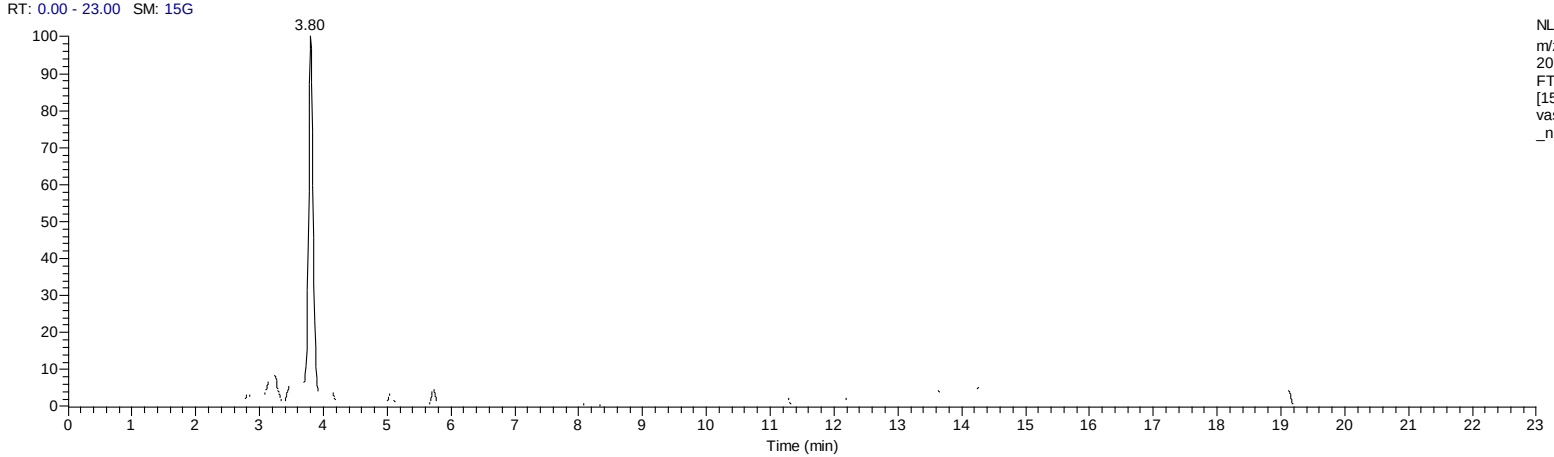


Fraxetin

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

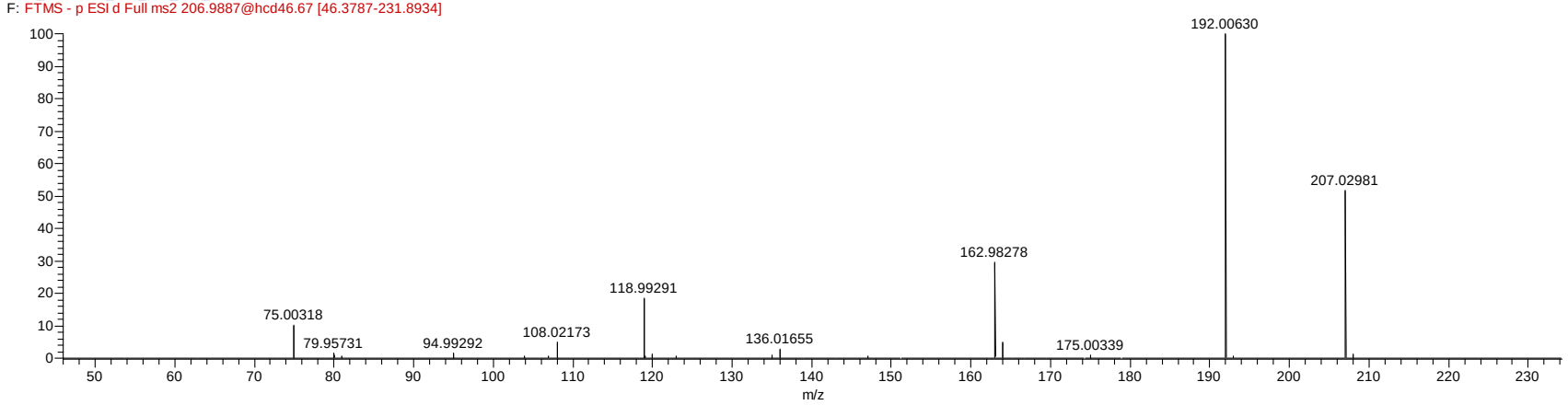
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



NL: 1.71E5
m/z=
207.02796-207.03004 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

vaso_FSddMS2_150_255_neg_01 #1456 RT: 3.80 AV: 1 SB: 4 5.84-7.14 , 0.26-4.50 NL: 5.26E4
F: FTMS - p ESI d Full ms2 206.9887@hcd46.67 [46.3787-231.8934]

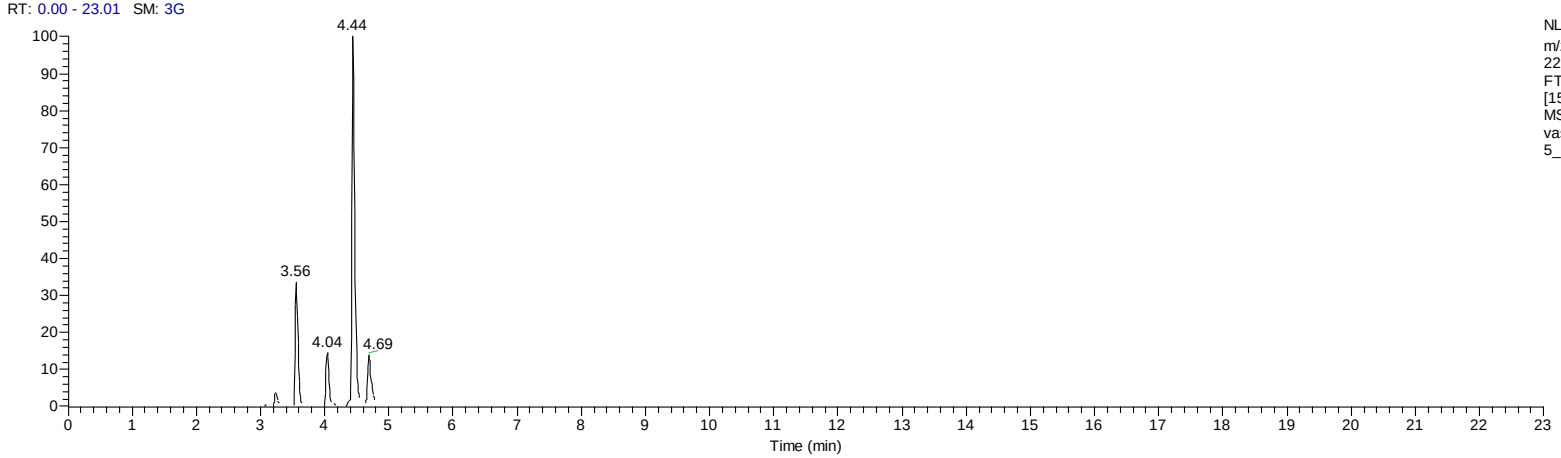


N1-[4-(1,3-Oxazol-5-yl)phenyl]cyclopropane-1-carboxamide

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

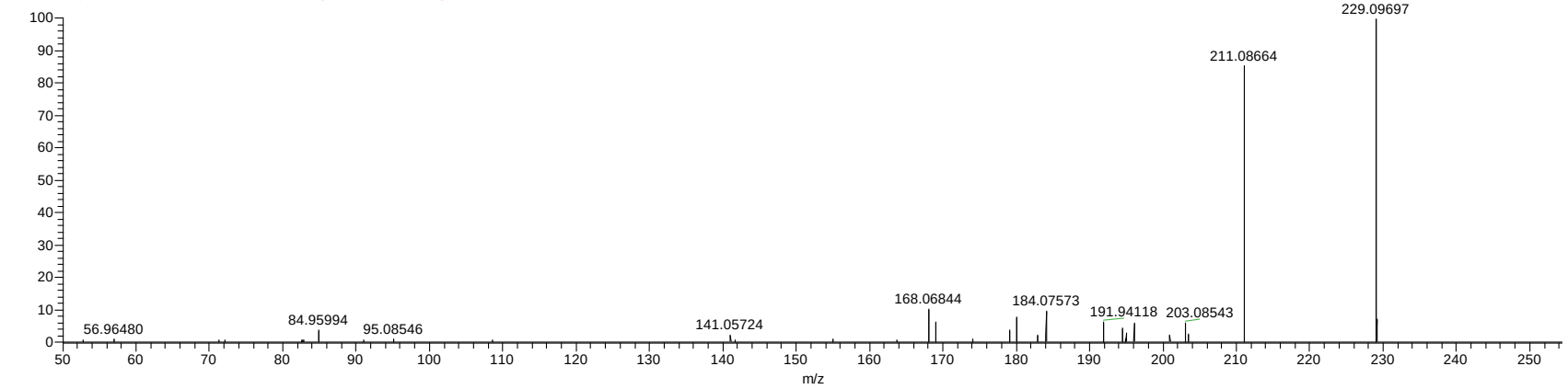
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



NL: 4.30E6
m/z=
229.09471-229.09929 F:
FTMS + p ESI Full ms
[150.0000-255.0000]
MS
vaso_FSddMS2_150_25
5_01

vaso_FSddMS2_150_255_01 #1735 RT: 4.03 AV: 1 NL: 2.05E5
F: FTMS + p ESI d Full ms2 229.0682@hcd46.67 [50.0000-254.4146]

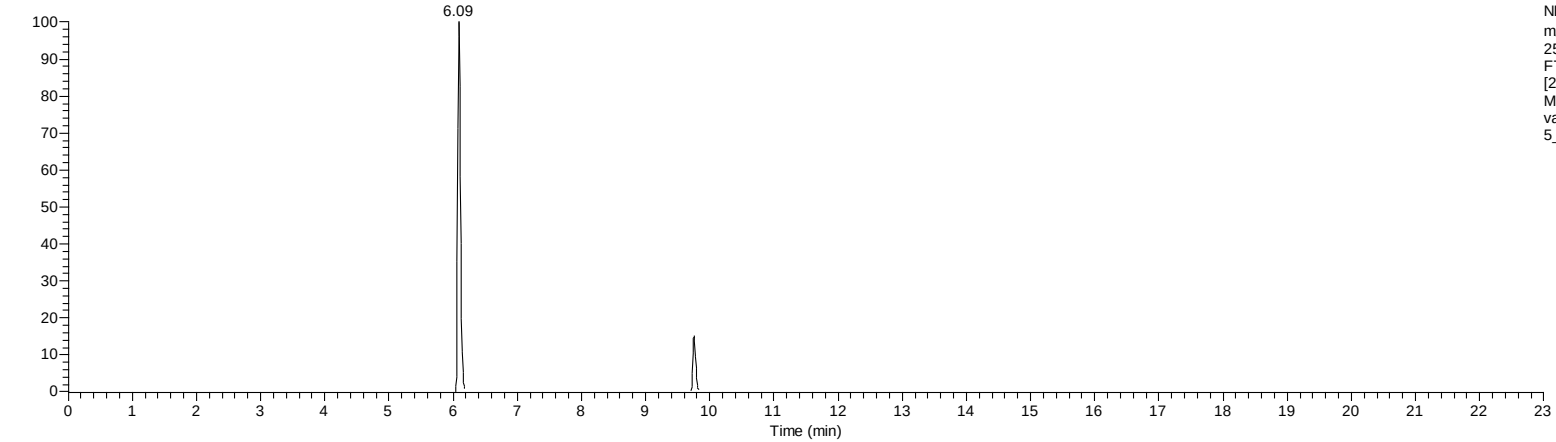


N-Benzoyl-L-phenyalaninol

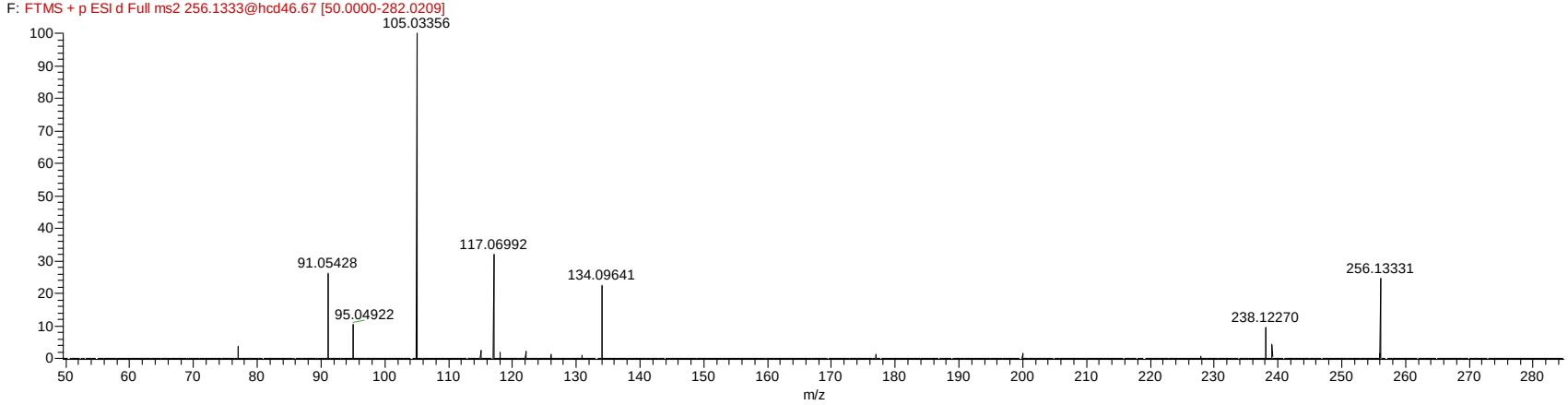
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 3G



vaso_FSddMS2_245_455_01 #2377-2461 RT: 5.99-6.15 AV: 6 SB: 8 6.34-6.81 , 5.39-5.82 NL: 9.61E5
F: FTMS + p ESI d Full ms2 256.1333@hcd46.67 [50.0000-282.0209]

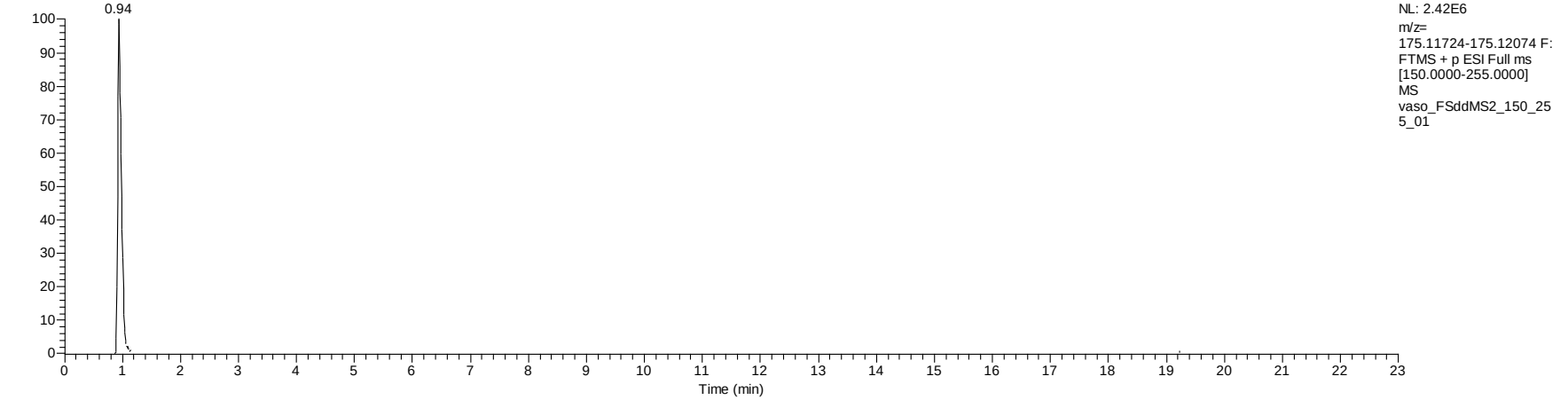


Arginine

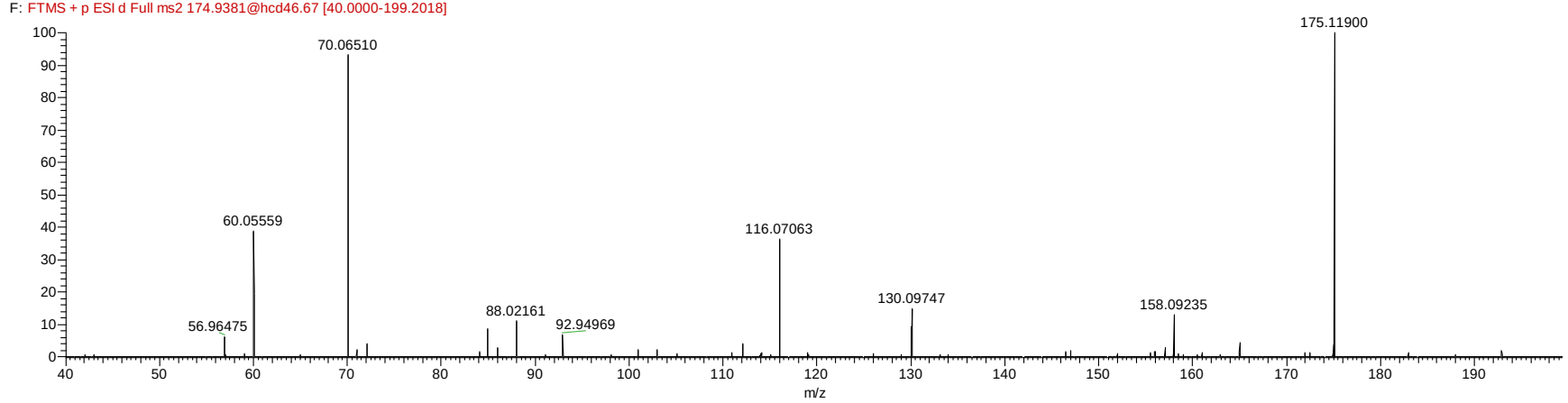
vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



vaso_FSddMS2_150_255_01 #390 RT: 0.92 AV: 1 NL: 2.40E5
F: FTMS + p ESI d Full ms2 174.9381@hcd46.67 [40.0000-199.2018]

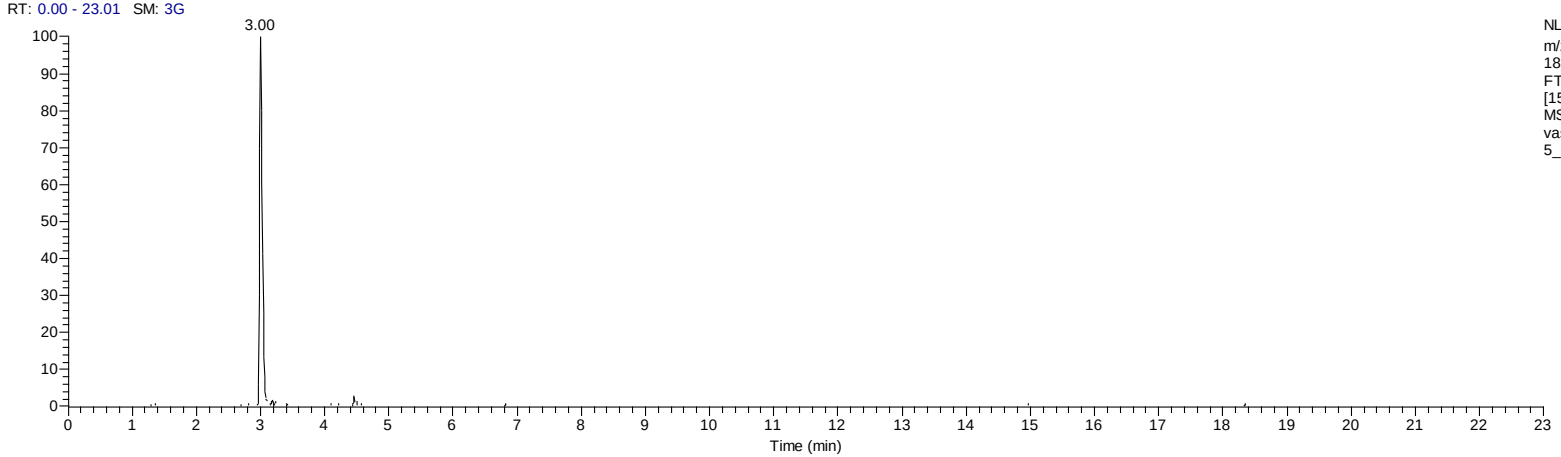


Tryptophan

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

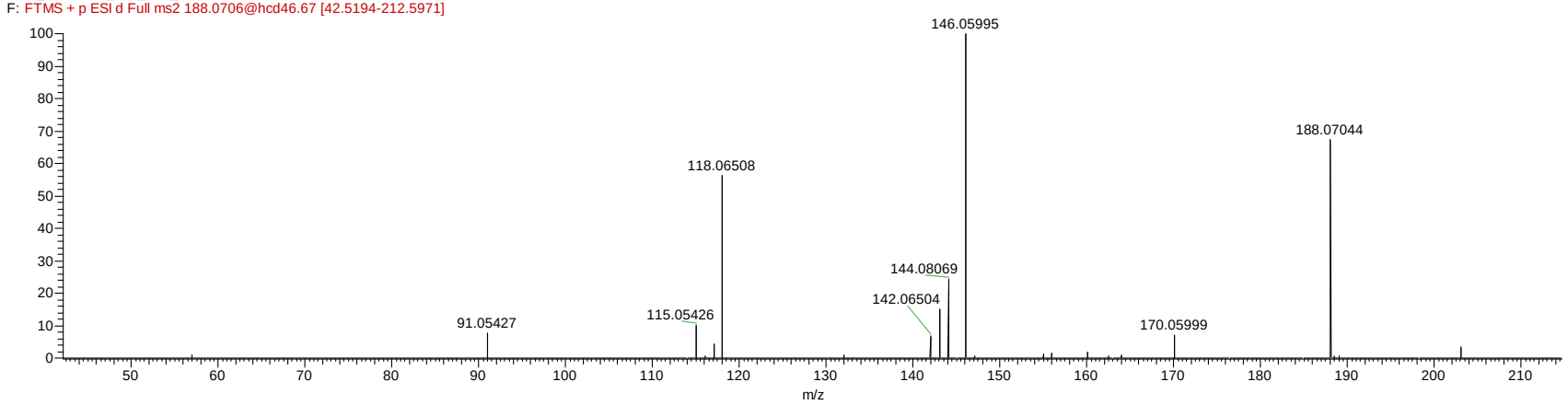
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



NL: 1.65E6
m/z=
188.06872-188.07248 F:
FTMS + p ESI Full ms
[150.0000-255.0000]
MS
vaso_FSddMS2_150_25
5_01

vaso_FSddMS2_150_255_01 #1286 RT: 2.99 AV: 1 SB: 2 2.33-3.08 NL: 8.77E4
F: FTMS + p ESI d Full ms2 188.0706@hcd46.67 [42.5194-212.5971]

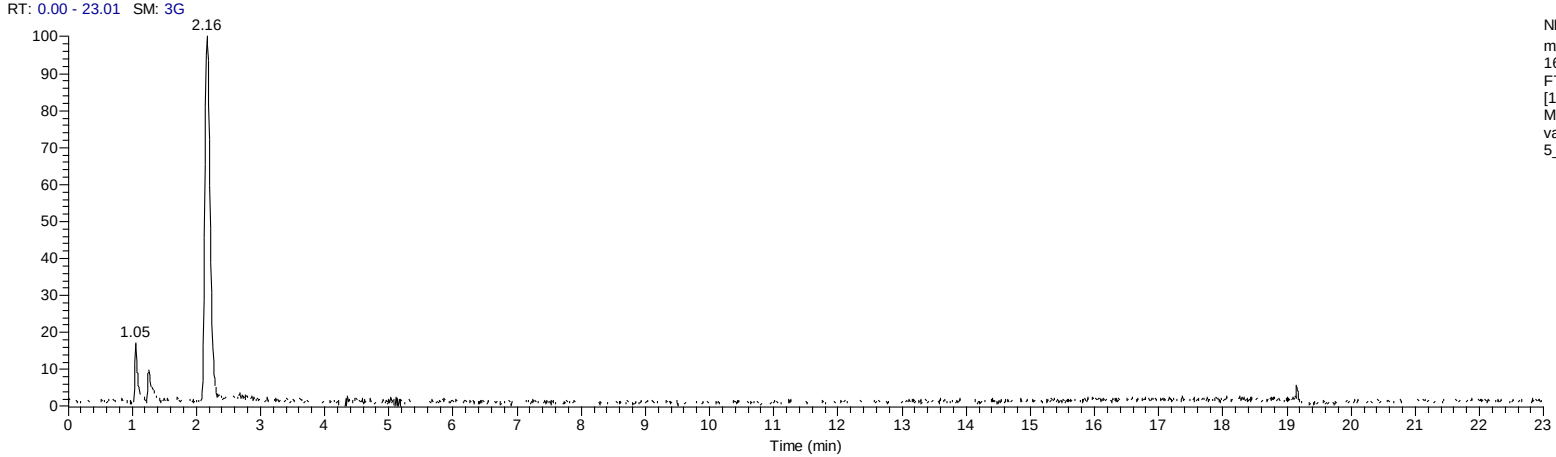


Phenylalanine

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

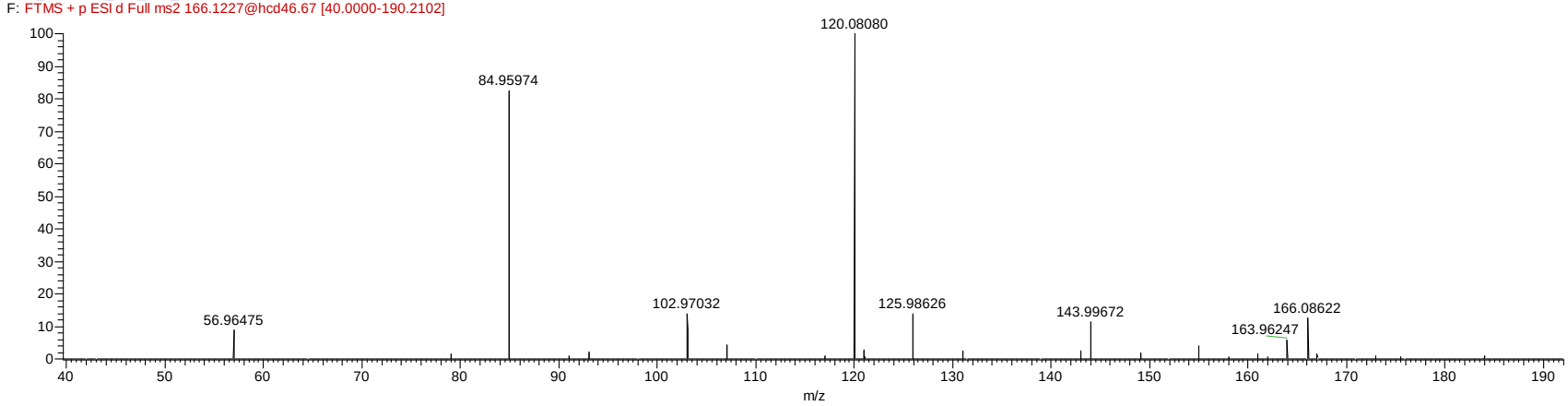
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



NL: 1.45E6
m/z= 166.08434-166.08766 F: FTMS + p ESI Full ms [150.0000-255.0000] MS vaso_FSddMS2_150_255_01

vaso_FSddMS2_150_255_01 #892-957 RT: 2.12-2.21 AV: 3 NL: 7.49E5
F: FTMS + p ESI d Full ms2 166.1227@hcd46.67 [40.0000-190.2102]

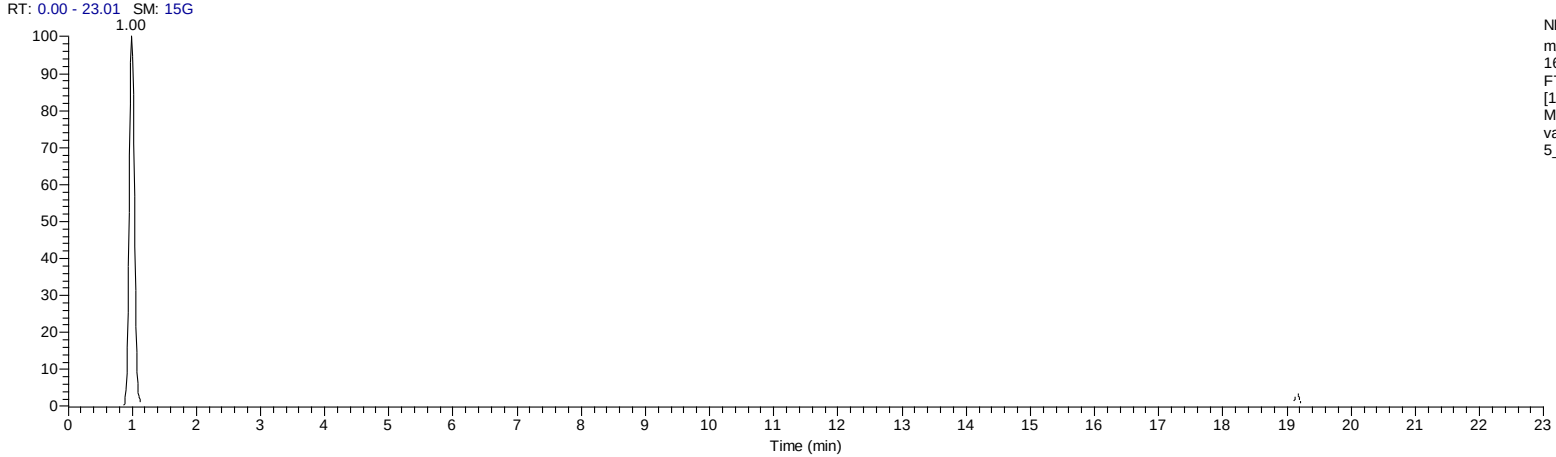


Carnitine

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

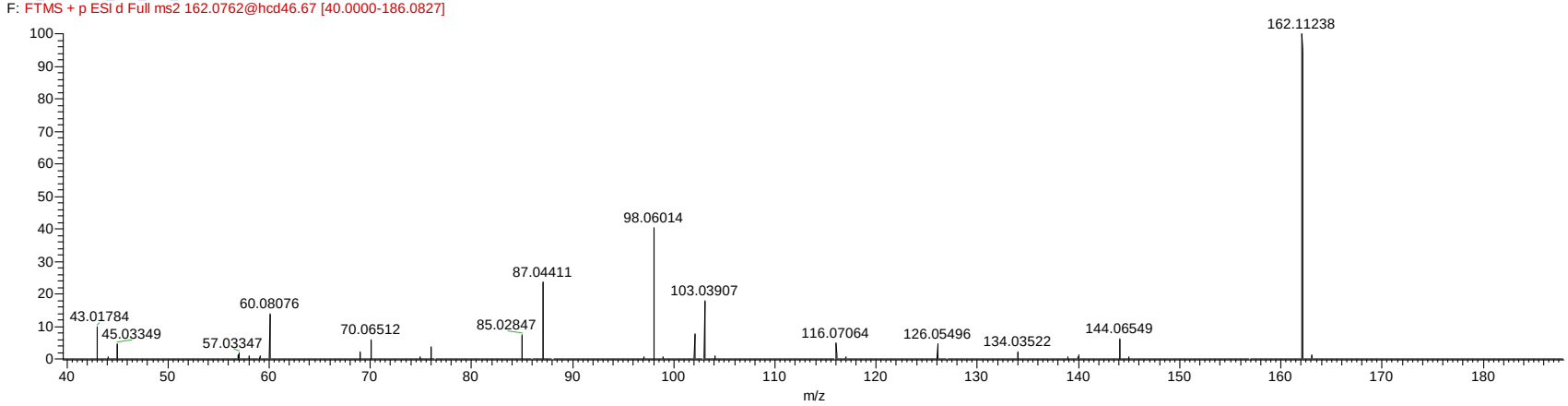
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 15G



NL: 1.71E6
m/z= 162.11038-162.11362 F: FTMS + p ESI Full ms [150.0000-255.0000] MS vaso_FSddMS2_150_255_01

vaso_FSddMS2_150_255_01 #414-433 RT: 1.00-1.01 AV: 2 NL: 7.60E5
F: FTMS + p ESI d Full ms2 162.0762@hcd46.67 [40.0000-186.0827]

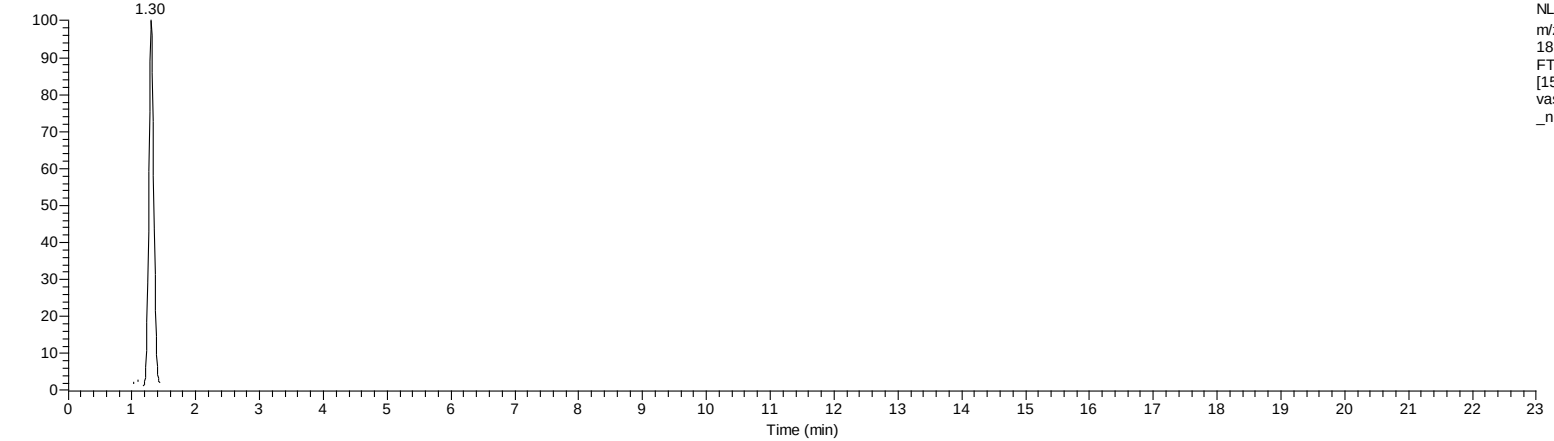


N-Acetyl-glutamic acid

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

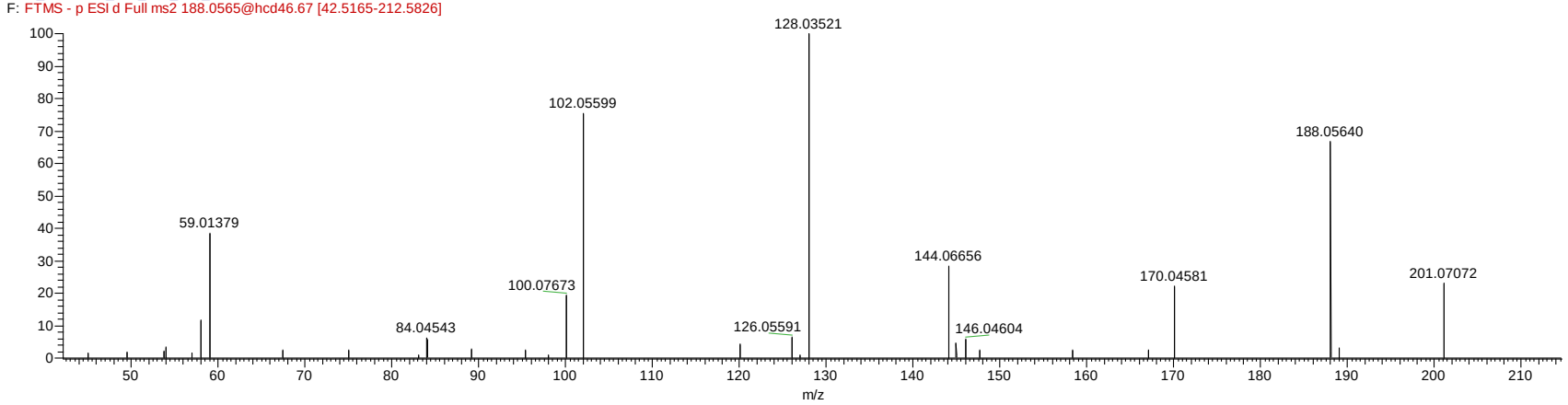
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



NL: 7.82E5
m/z=
188.05412-188.05788 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

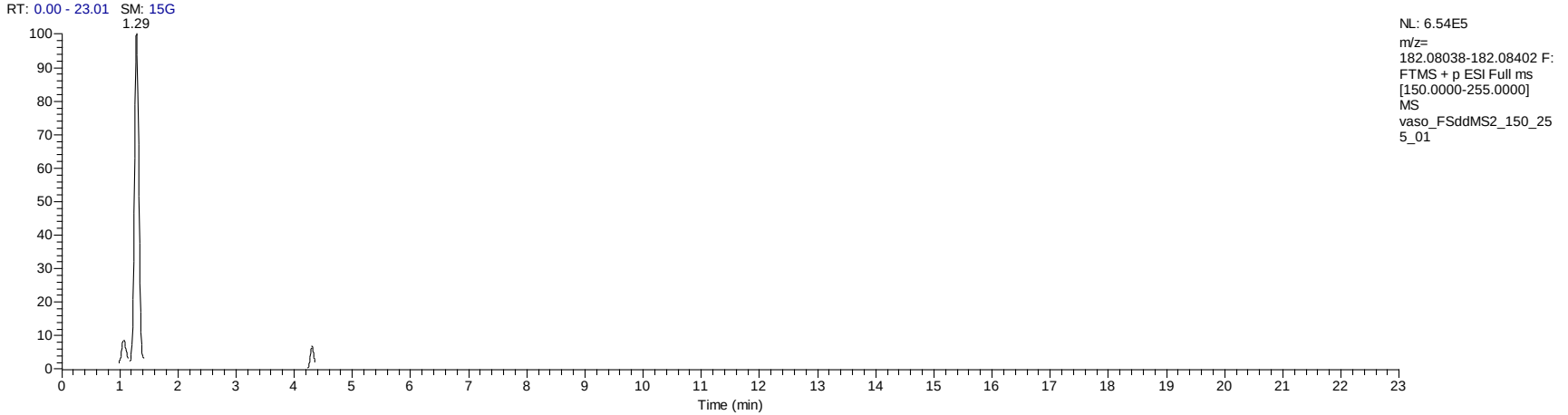
vaso_FSddMS2_150_255_neg_01 #475 RT: 1.28 AV: 1 SB: 3 1.14-2.19 , 0.22-0.71 NL: 4.88E4
F: FTMS - p ESI d Full ms2 188.0565@hcd46.67 [42.5165-212.5826]



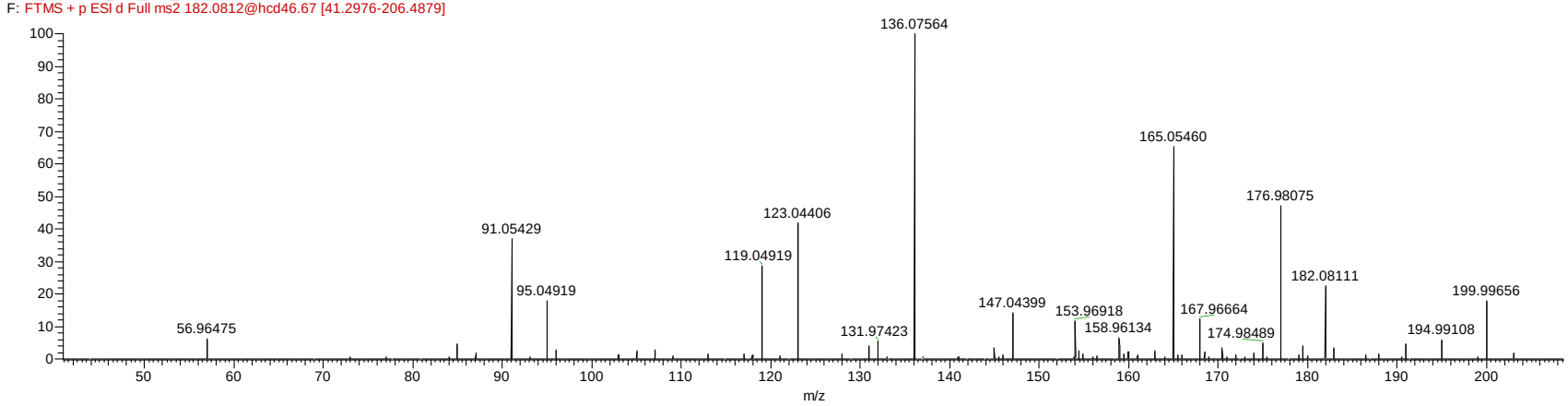
Tyrosine

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48



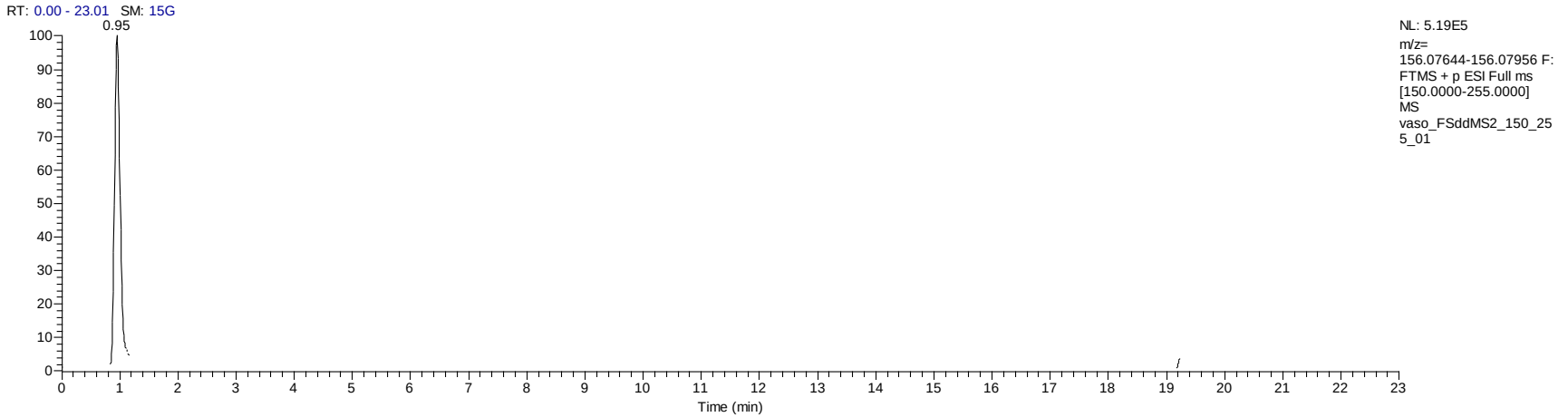
vaso_FSddMS2_150_255_01 #521-615 RT: 1.28-1.32 AV: 2 SB: 130 2.79-4.24 , 2.47-19.20 NL: 1.71E5
F: FTMS + p ESI d Full ms2 182.0812@hcd46.67 [41.2976-206.4879]



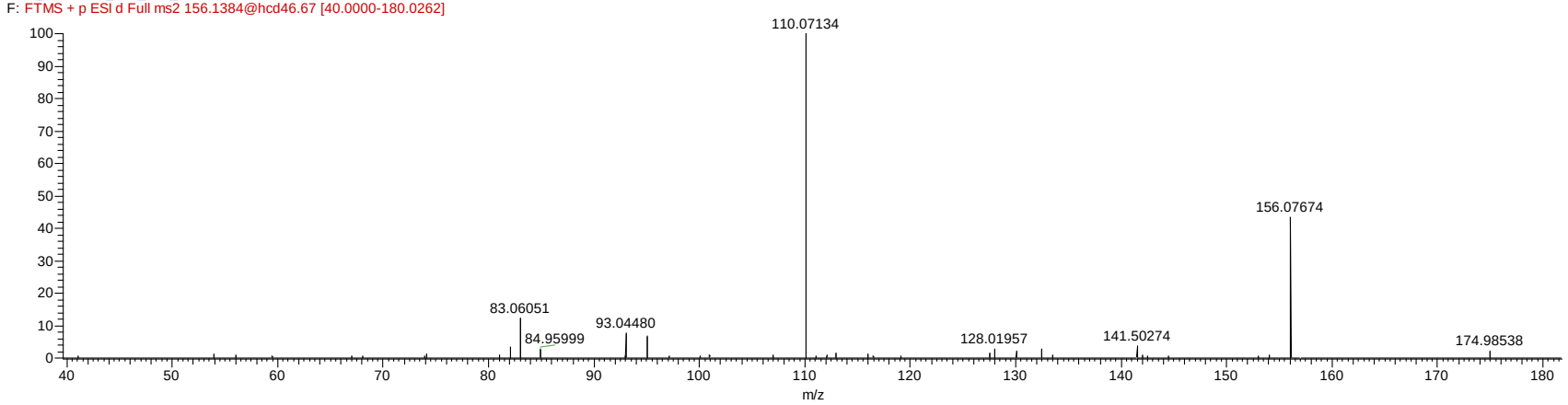
Histidine

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48



vaso_FSddMS2_150_255_01 #390 RT: 0.92 AV: 1 SB: 8 1.25-15.92 , 0.00-0.42 NL: 2.51E5
F: FTMS + p ESI d Full ms2 156.1384@hcd46.67 [40.0000-180.0262]

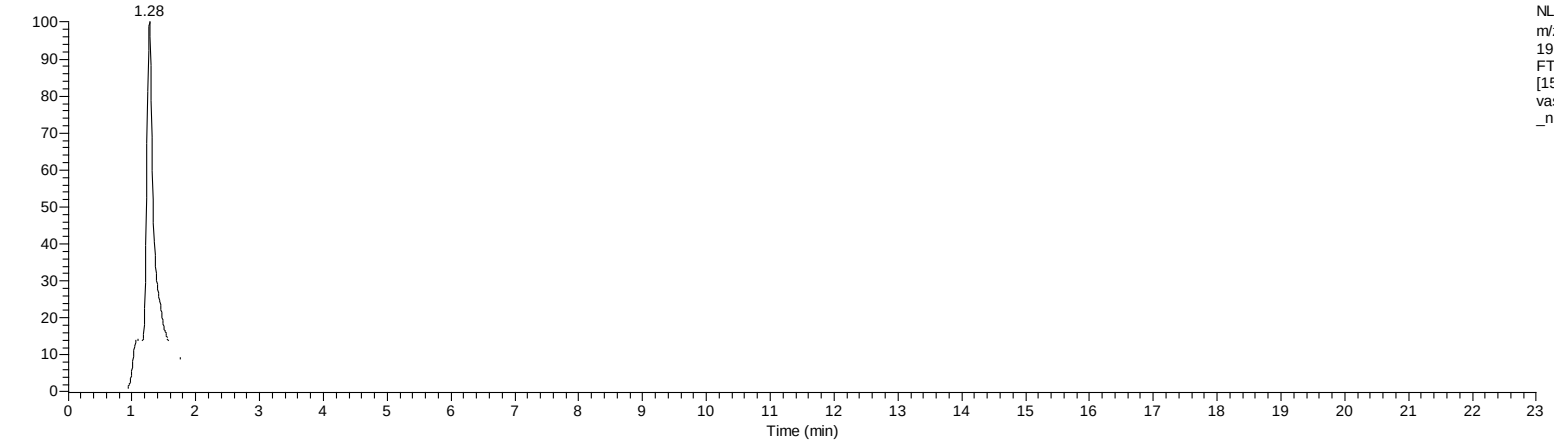


Citric acid

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

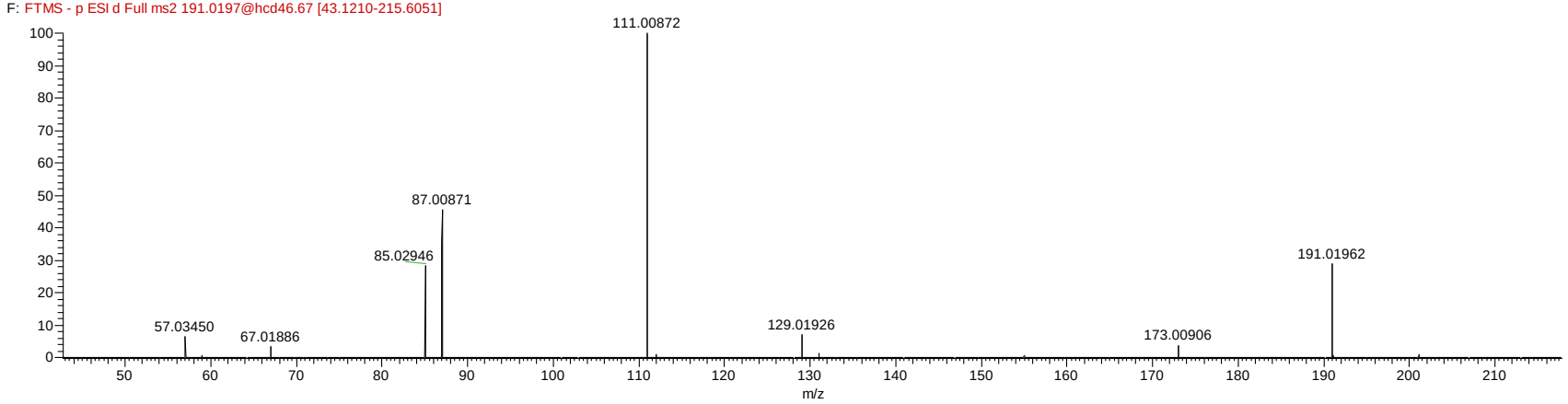
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



NL: 1.16E6
m/z=
191.01783-191.02165 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

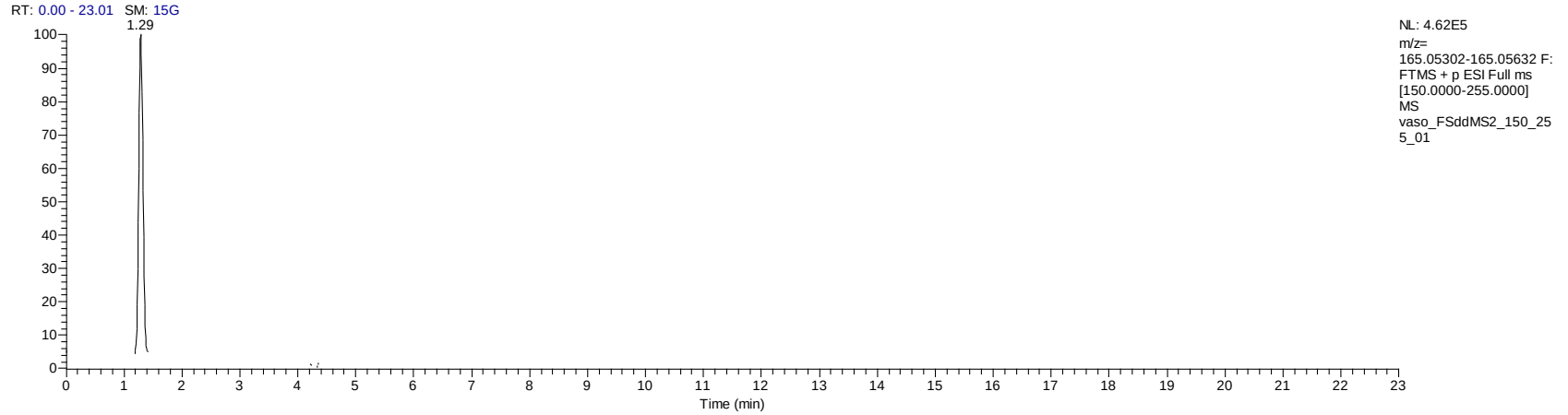
vaso_FSddMS2_150_255_neg_01 #434-507 RT: 1.25-1.33 AV: 3 SB: 18 1.92-3.04 , 0.29-0.83 NL: 2.47E5
F: FTMS - p ESI d Full ms2 191.0197@hcd46.67 [43.1210-215.6051]



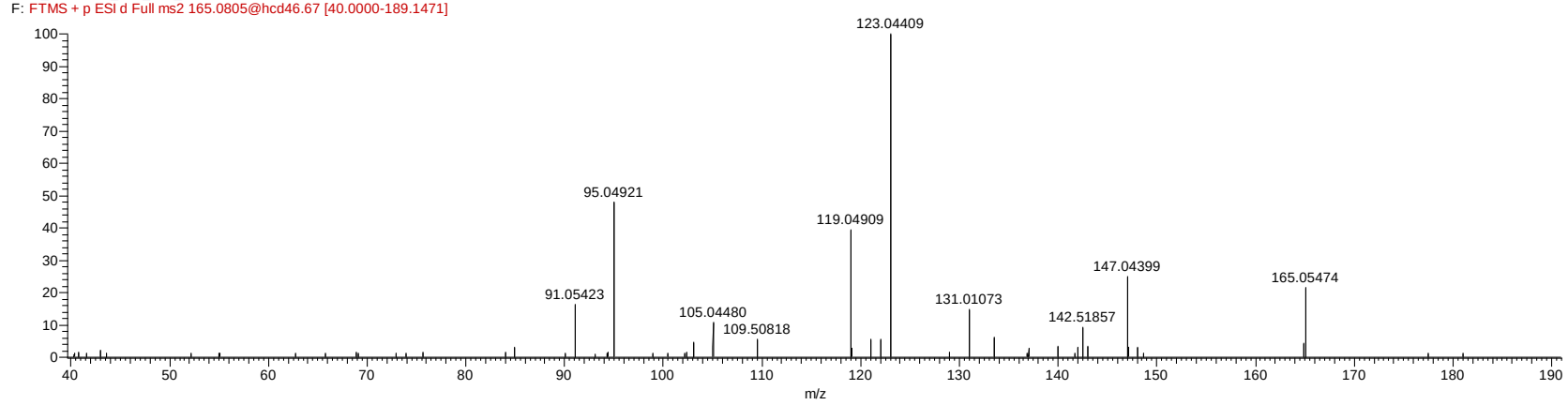
P-coumaric acid

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48



vaso_FSddMS2_150_255_01 #477-571 RT: 1.28-1.33 AV: 2 SB: 6 2.79-4.24 , 2.47-19.20 NL: 5.69E4
F: FTMS + p ESI d Full ms2 165.0805@hcd46.67 [40.0000-189.1471]

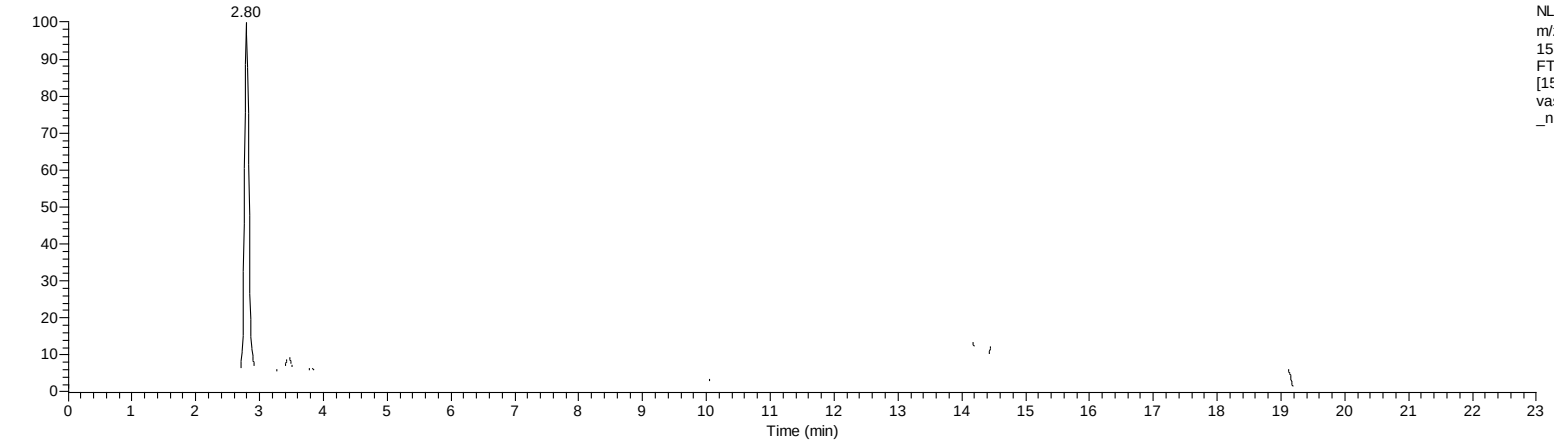


Gentisic acid

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

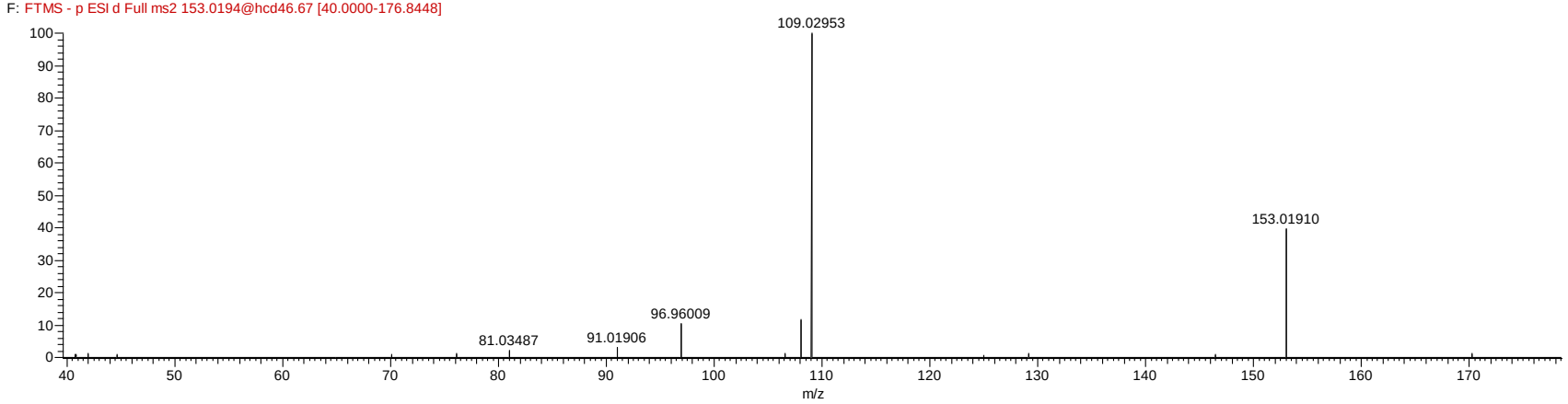
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



NL: 4.14E5
m/z=
153.01747-153.02053 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

vaso_FSddMS2_150_255_neg_01 #1054 RT: 2.79 AV: 1 SB: 4 1.34-4.93 , 0.25-0.56 NL: 1.03E5
F: FTMS - p ESI d Full ms2 153.0194@hcd46.67 [40.0000-176.8448]

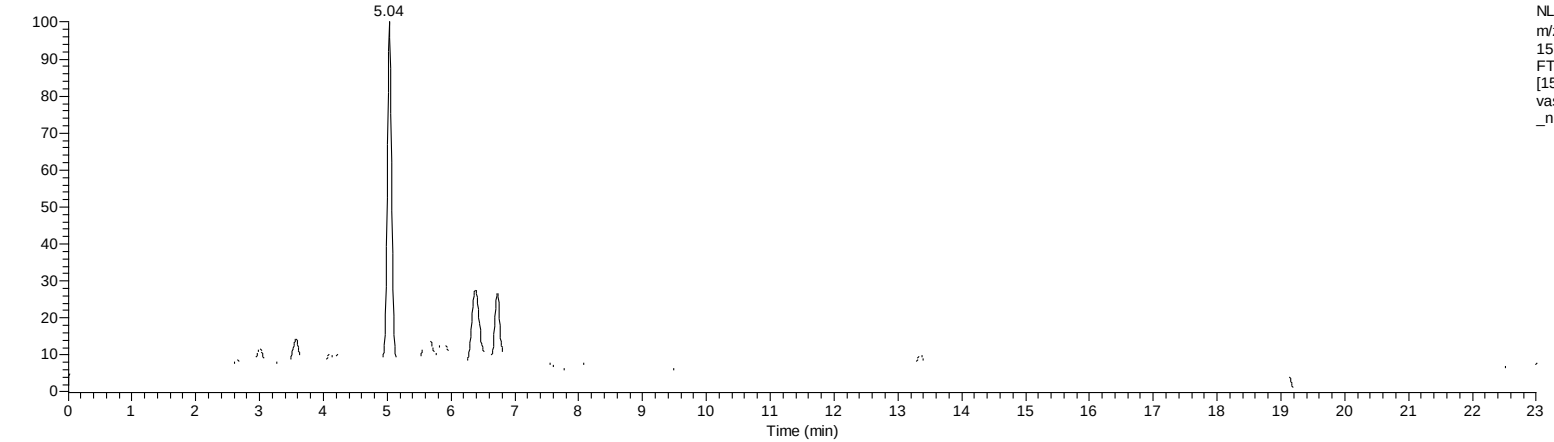


3-Anisic acid

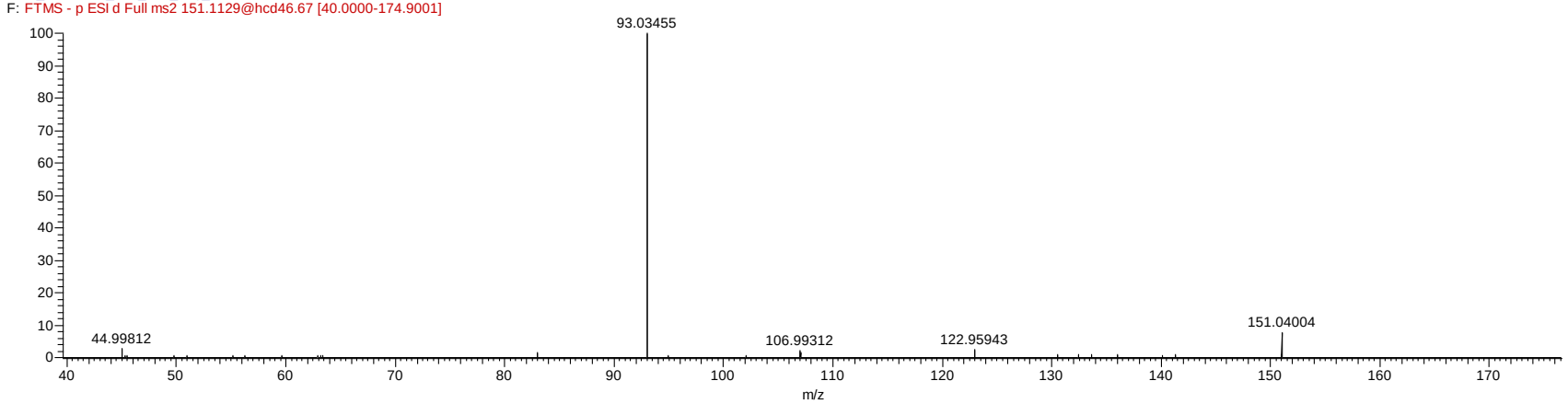
vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_150_255_neg_01 #1958 RT: 5.01 AV: 1 SB: 11 5.84-7.14 , 0.26-4.50 NL: 1.94E5
F: FTMS - p ESI d Full ms2 151.1129@hcd46.67 [40.0000-174.9001]

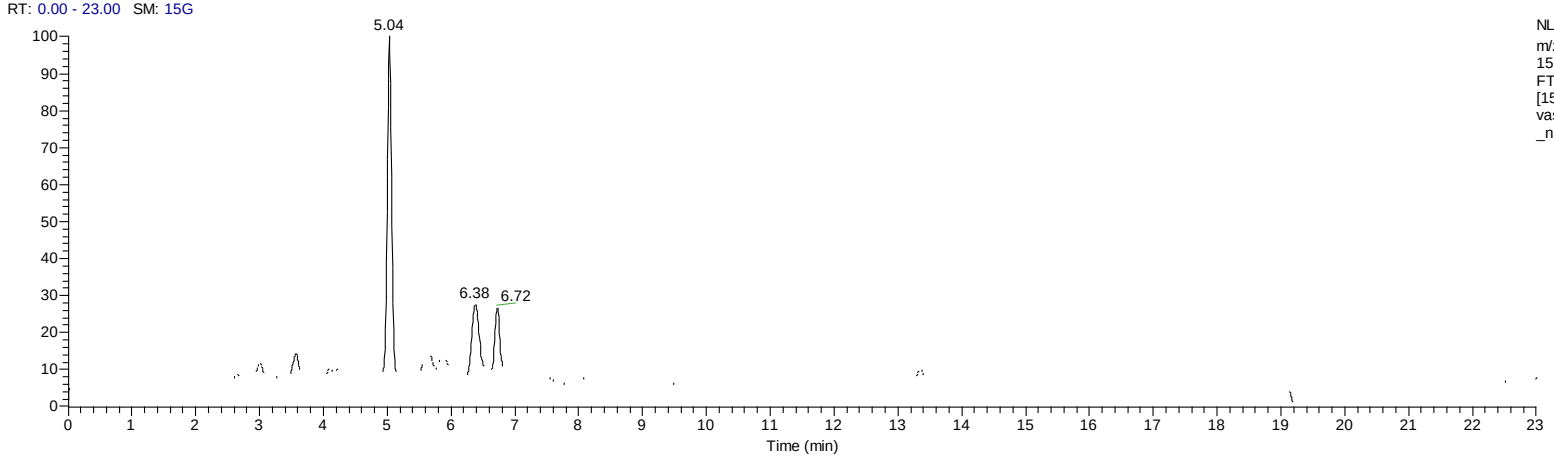


4-Hydroxyphenylacetic acid

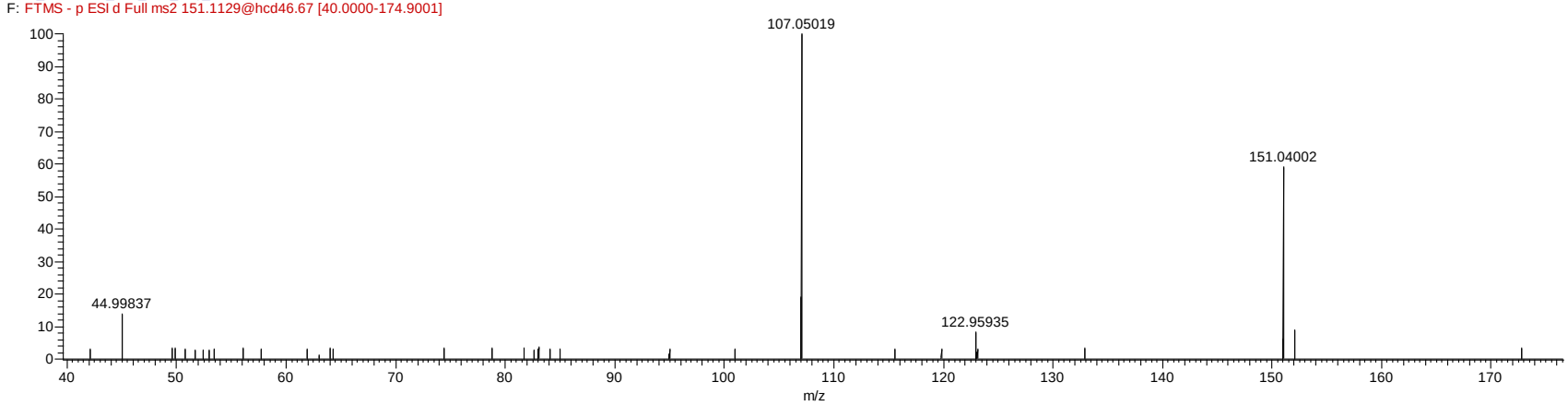
vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 12:21:25

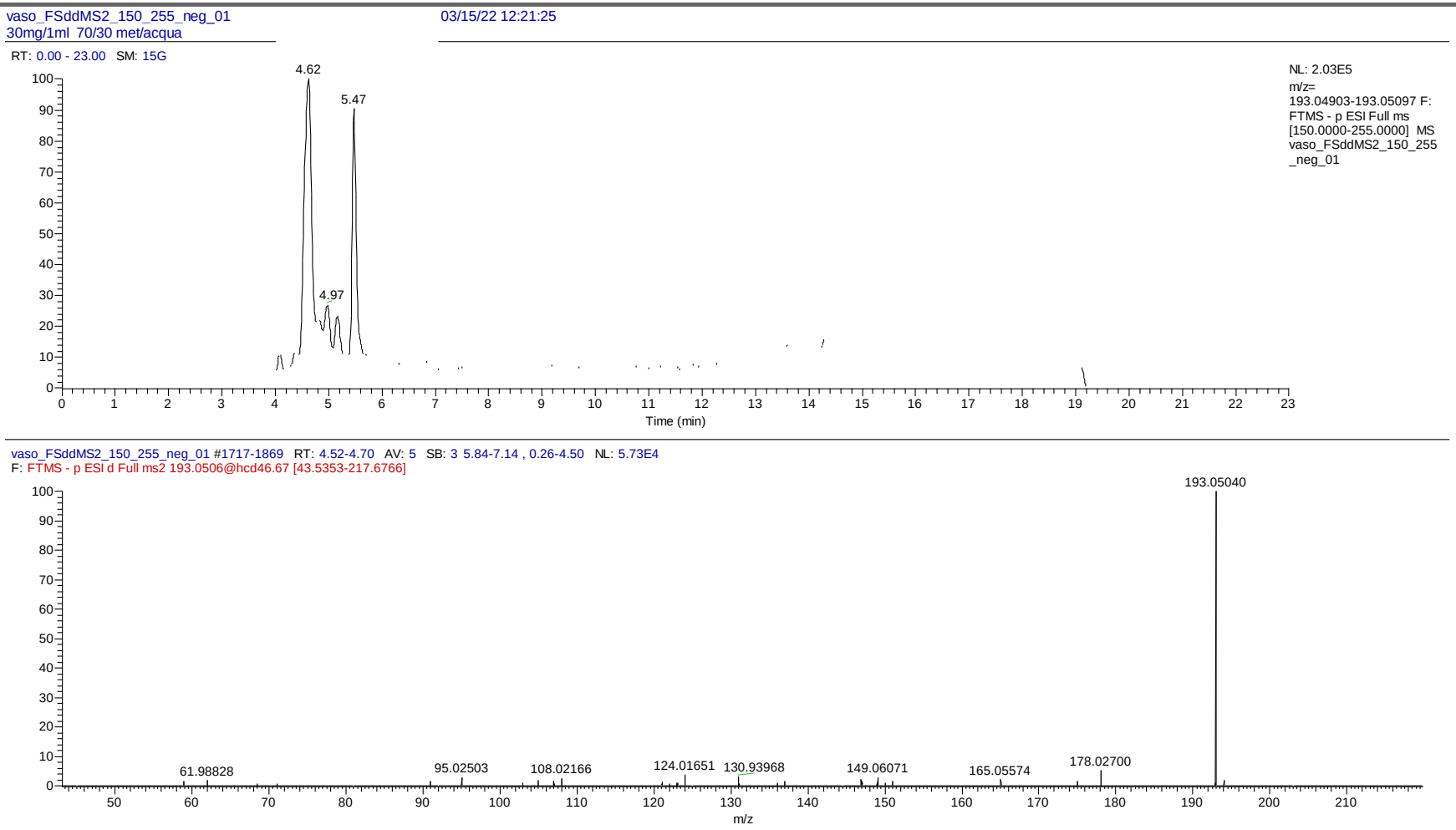
RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_150_255_neg_01 #2478-2515 RT: 6.36-6.41 AV: 2 SB: 11 5.84-7.14 , 0.26-4.50 NL: 1.96E4
F: FTMS - p ESI d Full ms2 151.1129@hcd46.67 [40.0000-174.9001]



Ferulic acid

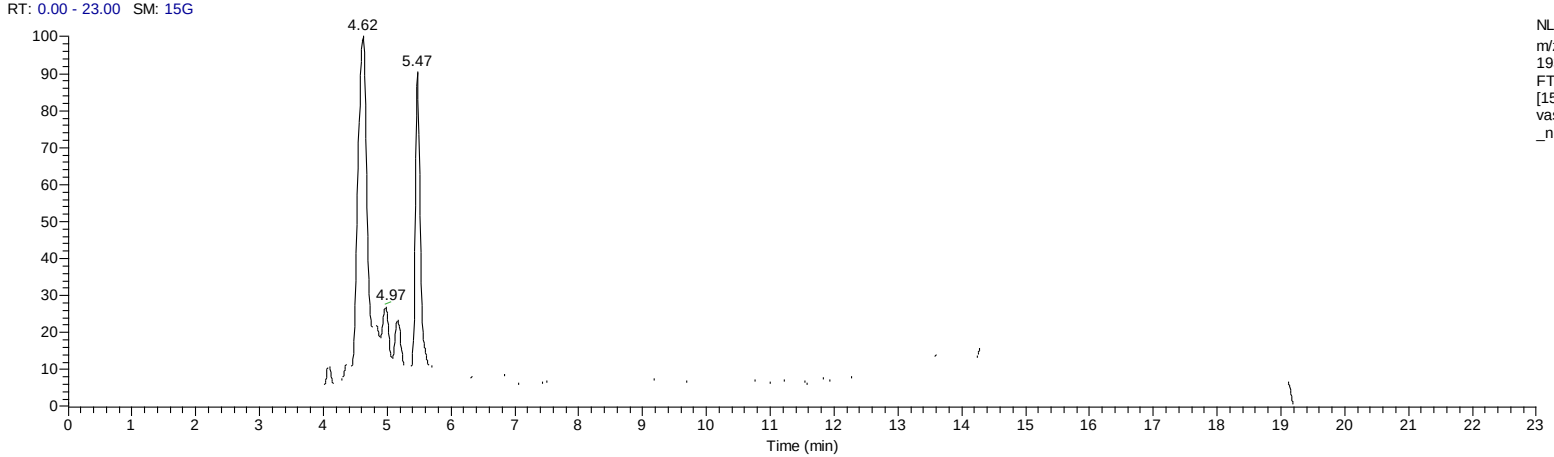


Isoferulic acid

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

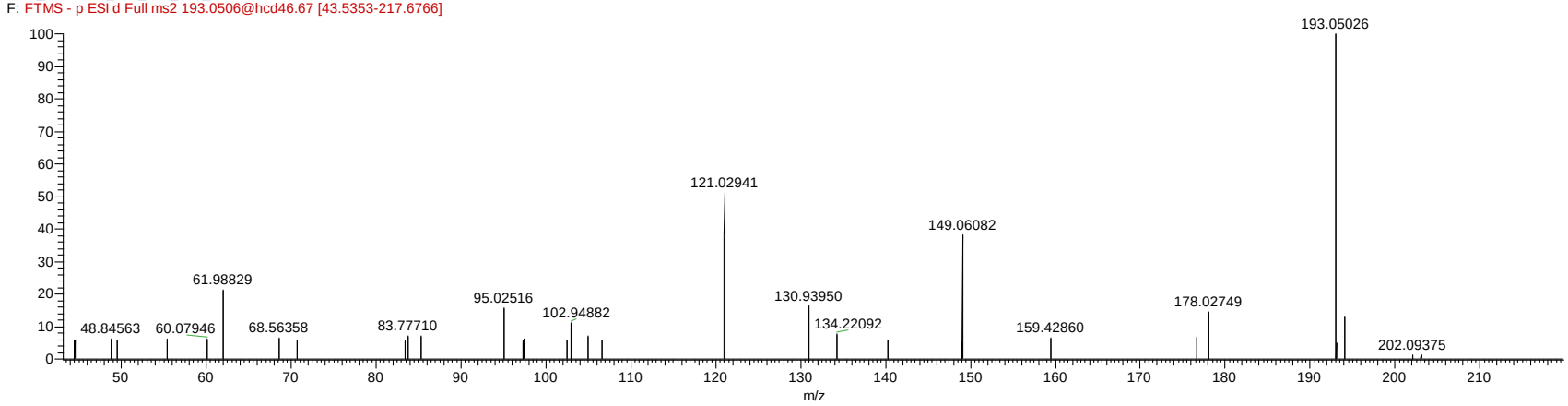
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G

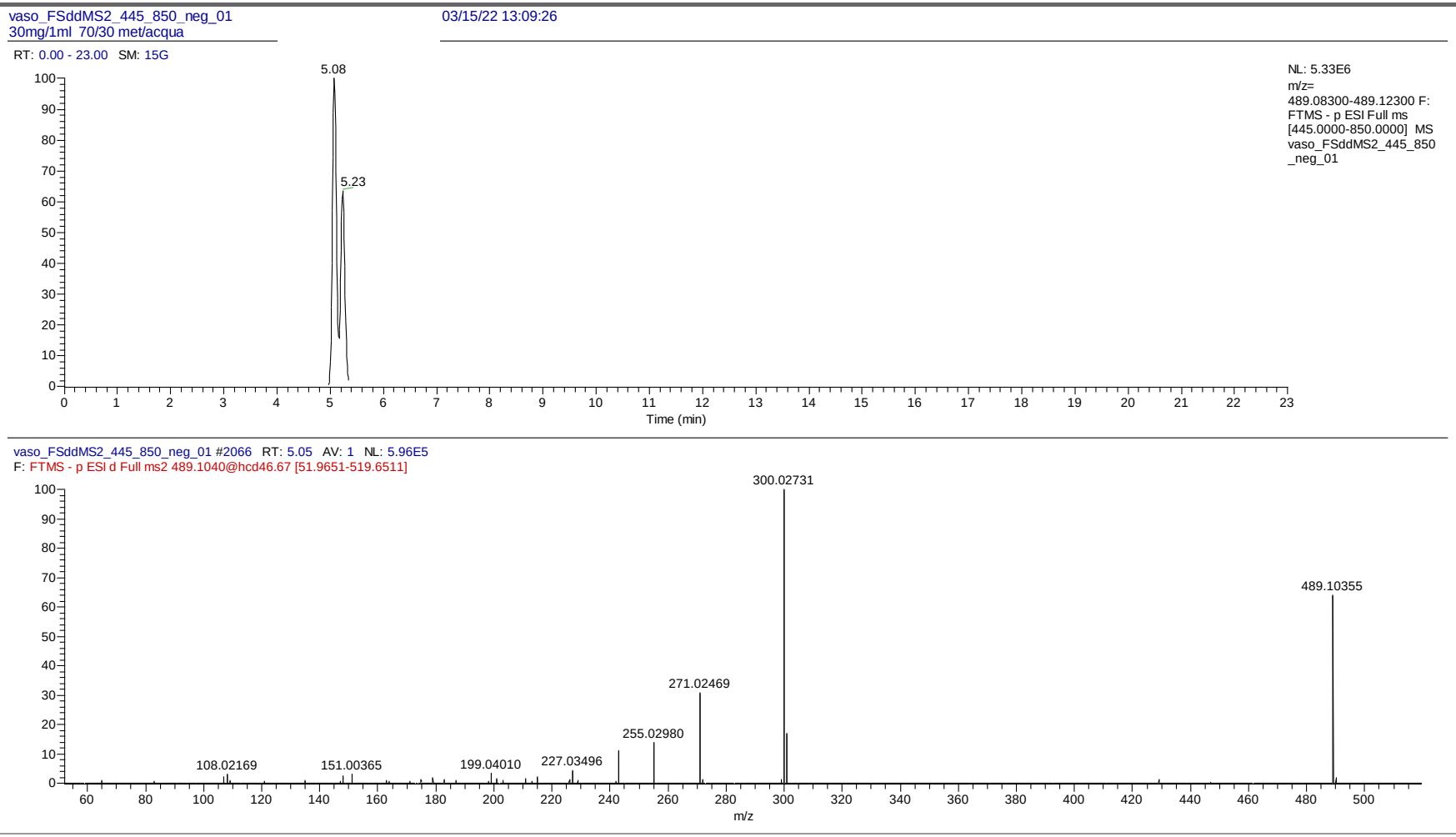


NL: 2.03E5
m/z=
193.04903-193.05097 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

vaso_FSddMS2_150_255_neg_01 #2098-2193 RT: 5.46-5.50 AV: 2 SB: 3 5.84-7.14 , 0.26-4.50 NL: 1.23E4
F: FTMS - p ESI d Full ms2 193.0506@hcd46.67 [43.5353-217.6766]



Quercetin 3-O-acetyl-rhamnoside

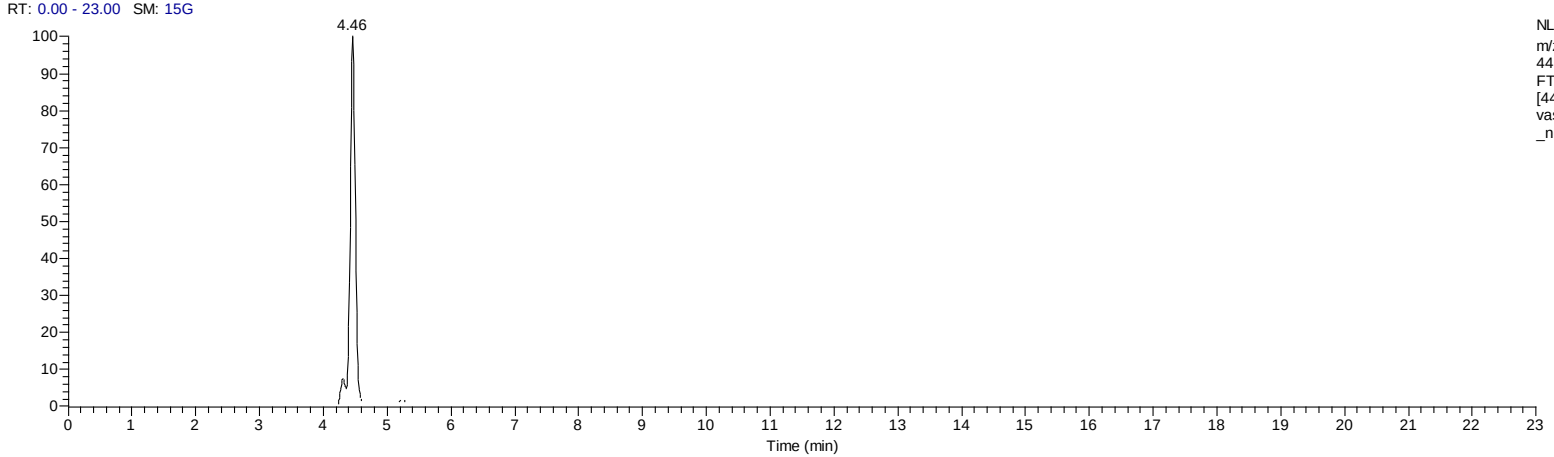


Quercitrin

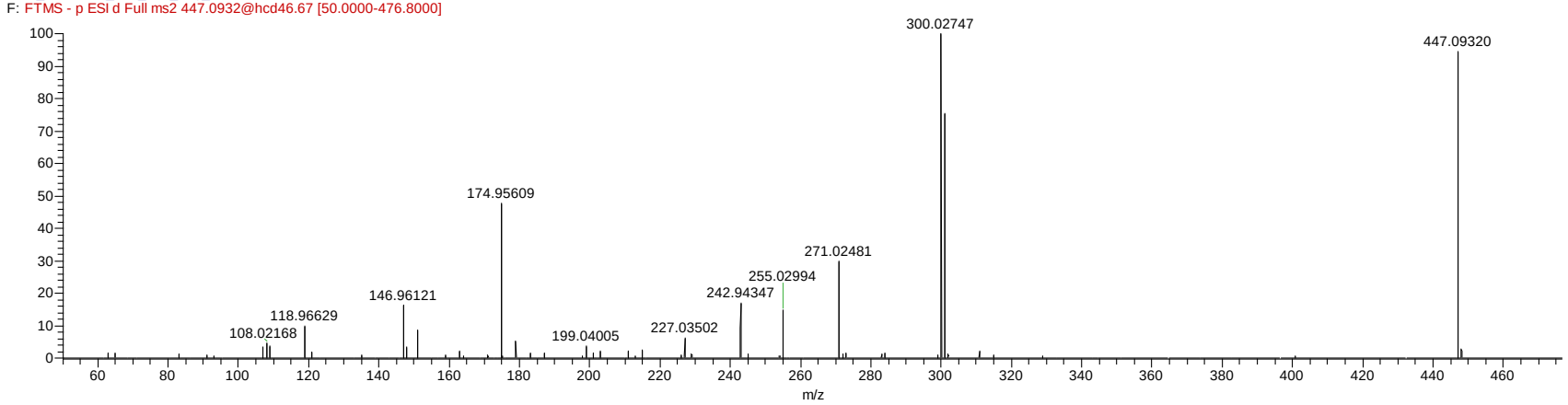
vaso_FSddMS2_445_850_neg_01
30mg/1ml 70/30 met/acqua

03/15/22 13:09:26

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_445_850_neg_01 #1814 RT: 4.44 AV: 1 NL: 9.60E5
F: FTMS - p ESI d Full ms2 447.0932@hcd46.67 [50.0000-476.8000]

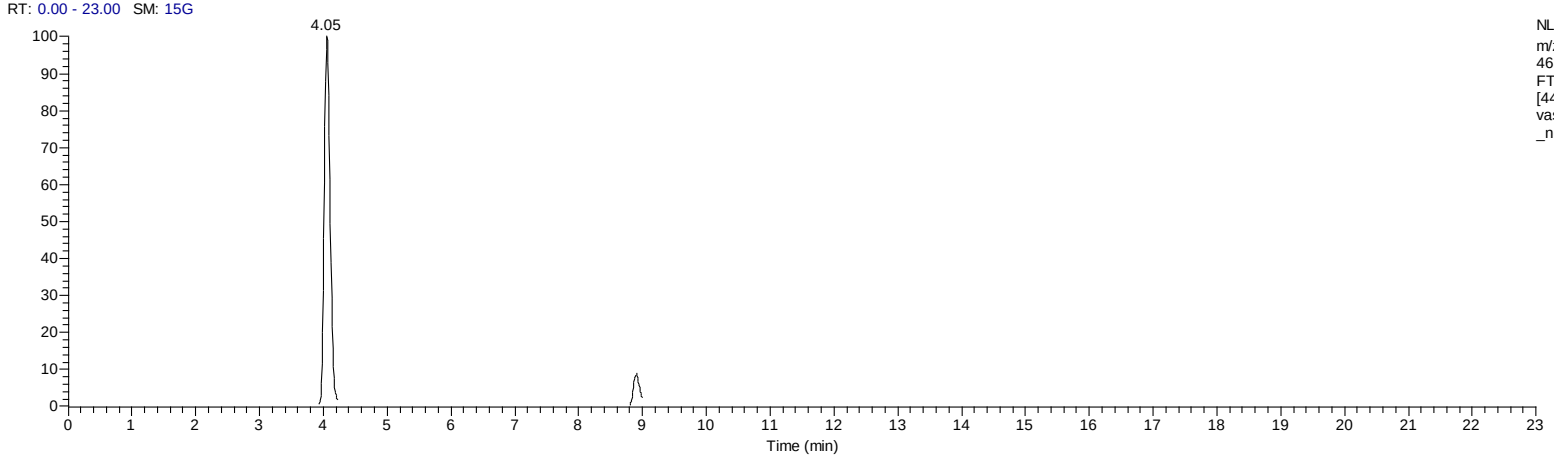


Myricitrin

vaso_FSddMS2_445_850_neg_01
30mg/1ml 70/30 met/acqua

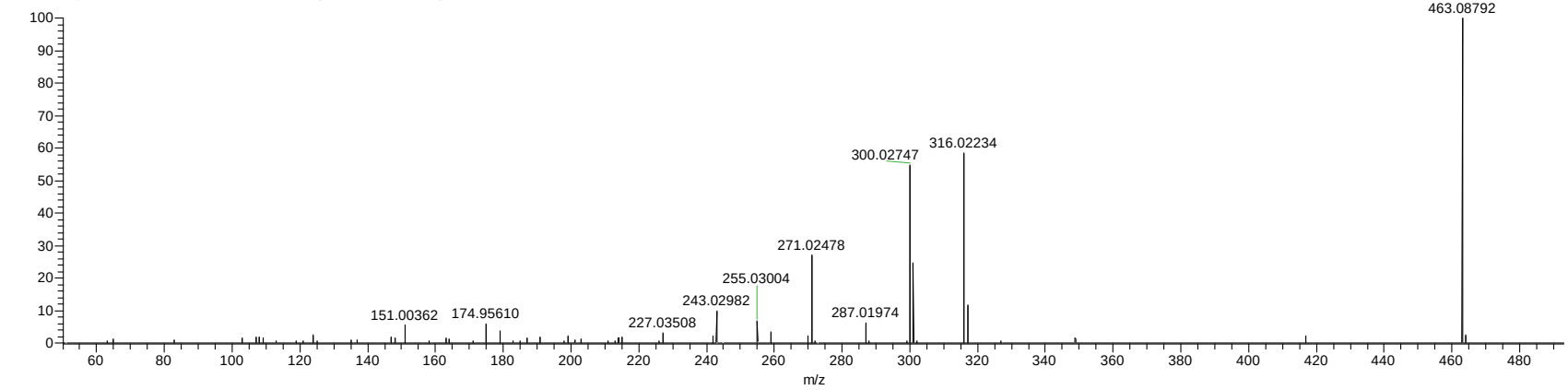
03/15/22 13:09:26

RT: 0.00 - 23.00 SM: 15G

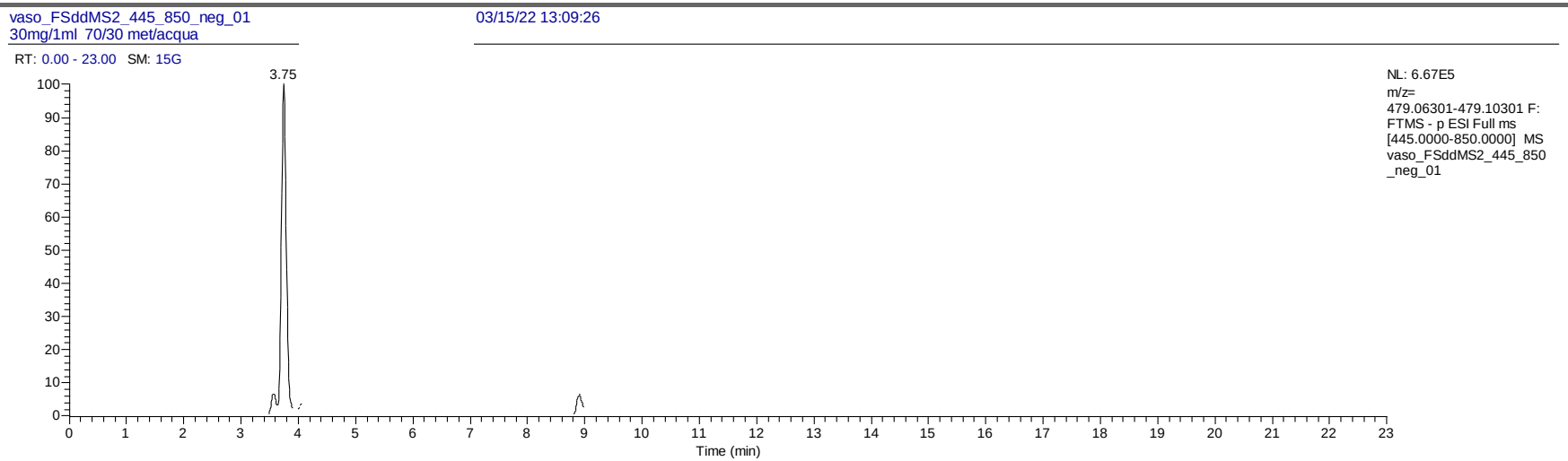


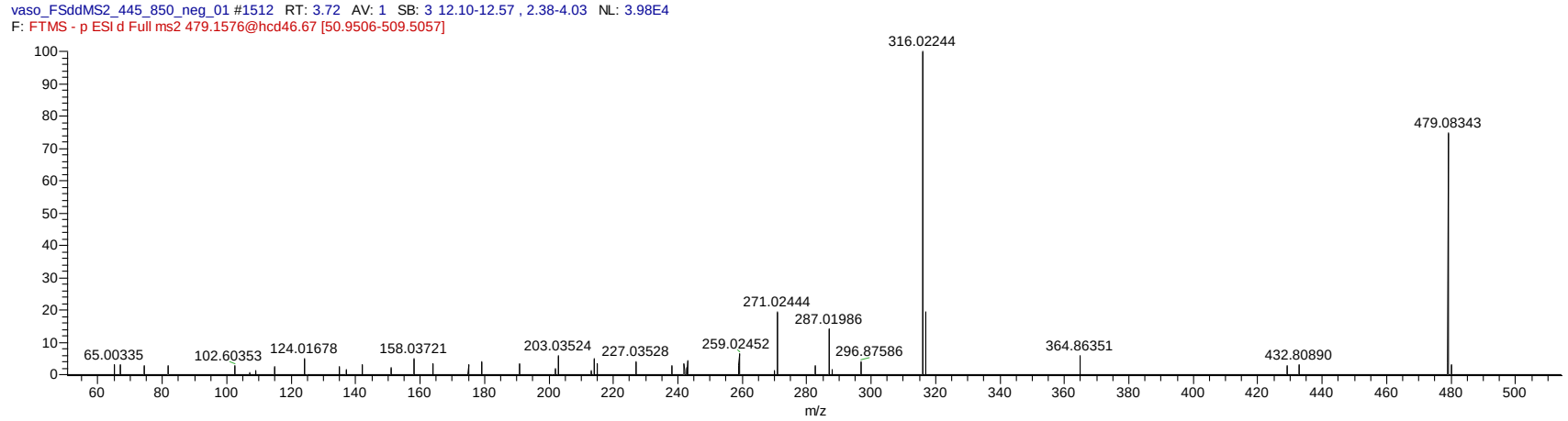
NL: 3.62E6
m/z=
463.06828-463.10828 F:
FTMS - p ESI Full ms
[445.0000-850.0000] MS
vaso_FSddMS2_445_850
_neg_01

vaso_FSddMS2_445_850_neg_01 #1654 RT: 4.06 AV: 1 NL: 8.47E5
F: FTMS - p ESI d Full ms2 463.0511@hcd46.67 [50.0000-493.0772]

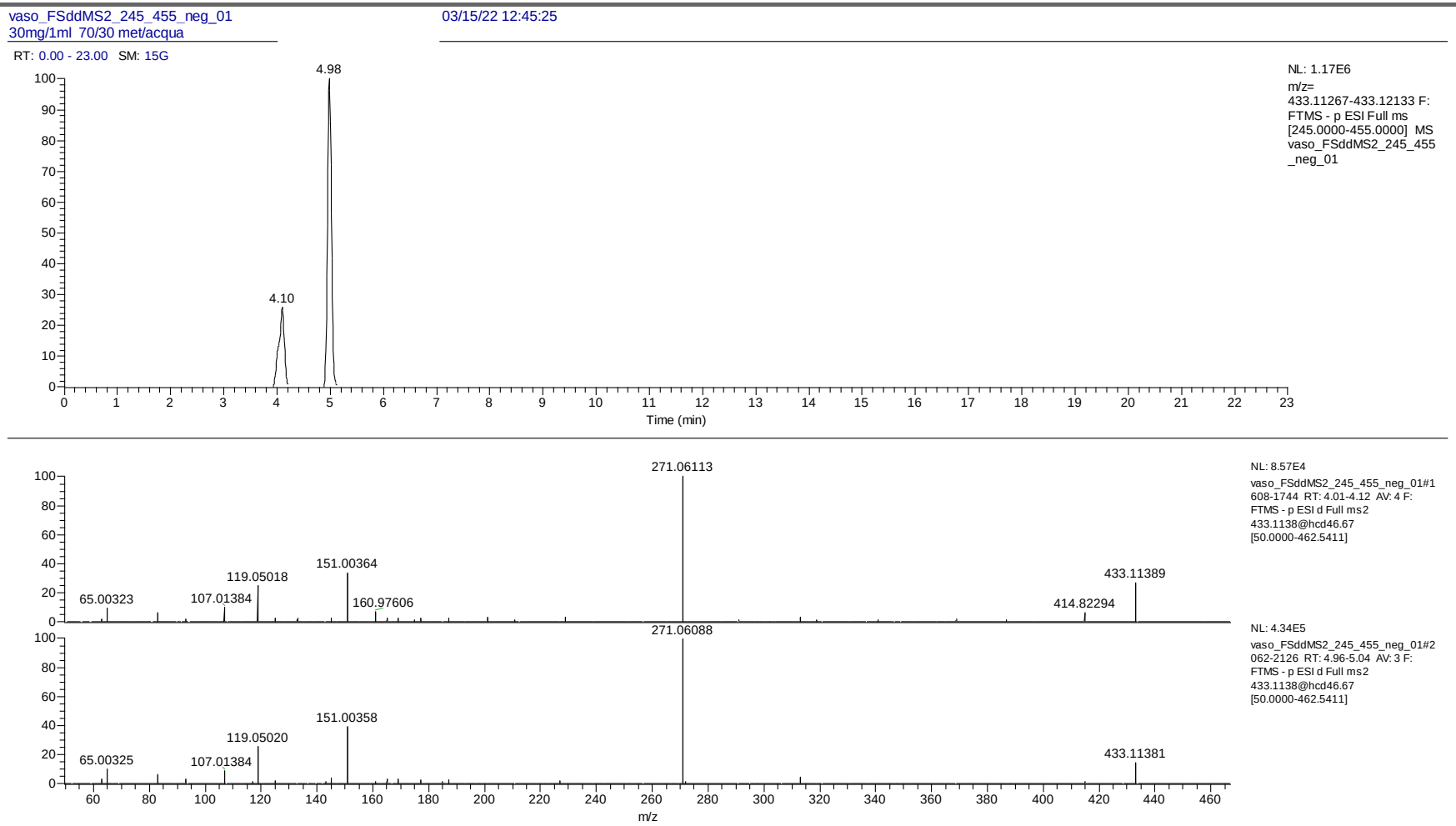


Myricetin 3-O-galactopyranoside





7-Hydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro-2H-chromen-5-yl β-D-glucopyranoside (Salipurposid) o isomero Isosalipurposide

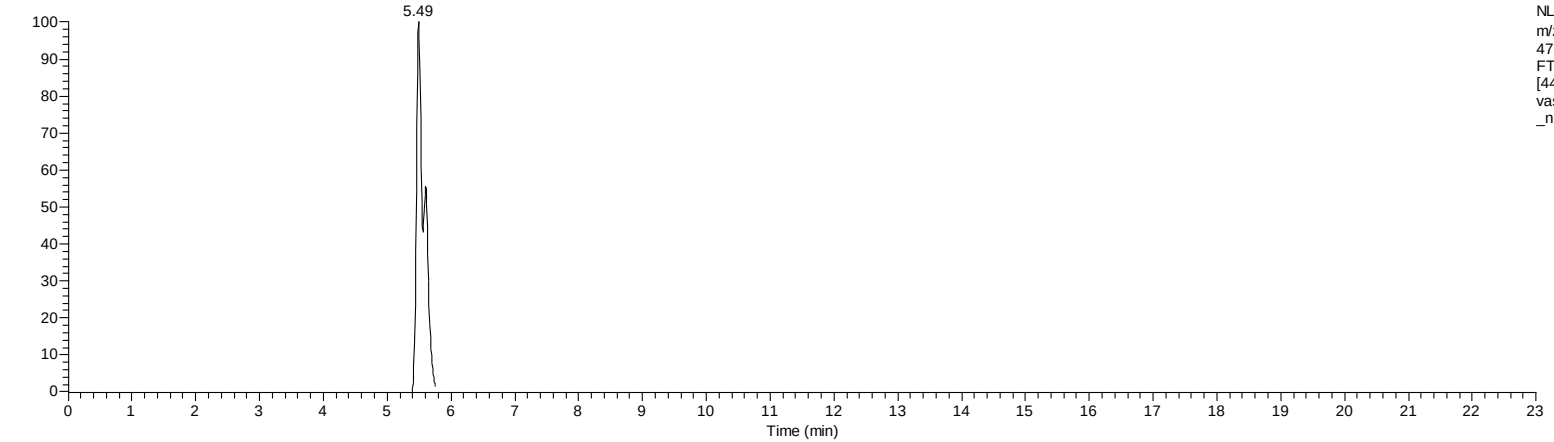


Kaempferol 3-(2''-acetylrhamnoside)

vaso_FSddMS2_445_850_neg_01
30mg/1ml 70/30 met/acqua

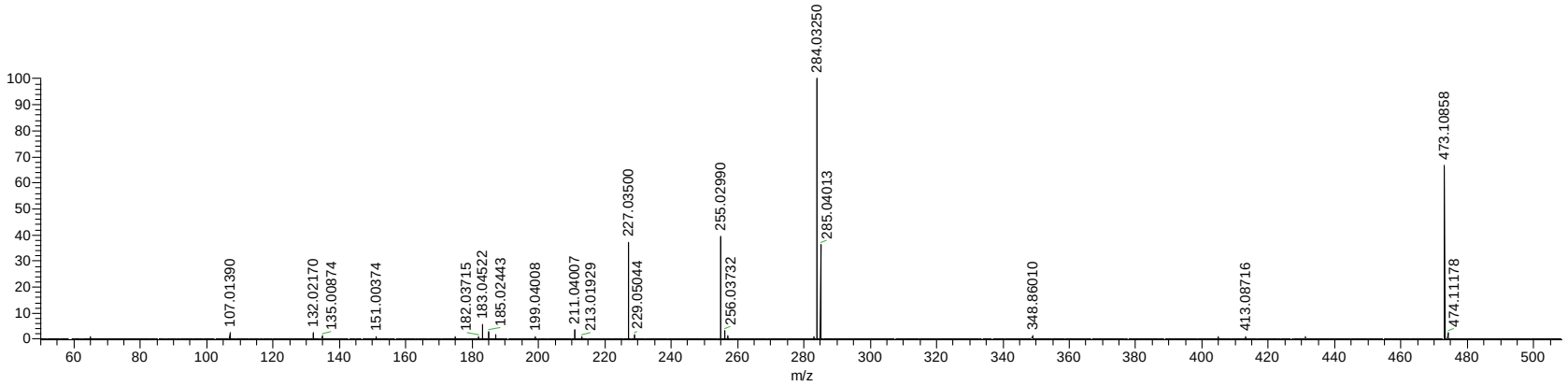
03/15/22 13:09:26

RT: 0.00 - 23.00 SM: 15G



NL: 1.58E6
m/z=
473.08896-473.12896 F:
FTMS - p ESI Full ms
[445.0000-850.0000] MS
vaso_FSddMS2_445_850
_neg_01

vaso_FSddMS2_445_850_neg_01 #2241-2276 RT: 5.47-5.55 AV: 3 SB: 3 12.10-12.57 , 2.38-4.03 NL: 2.41E5
F: FTMS - p ESI d Full ms2 473.1090@hcd46.67 [50.3336-503.3362]

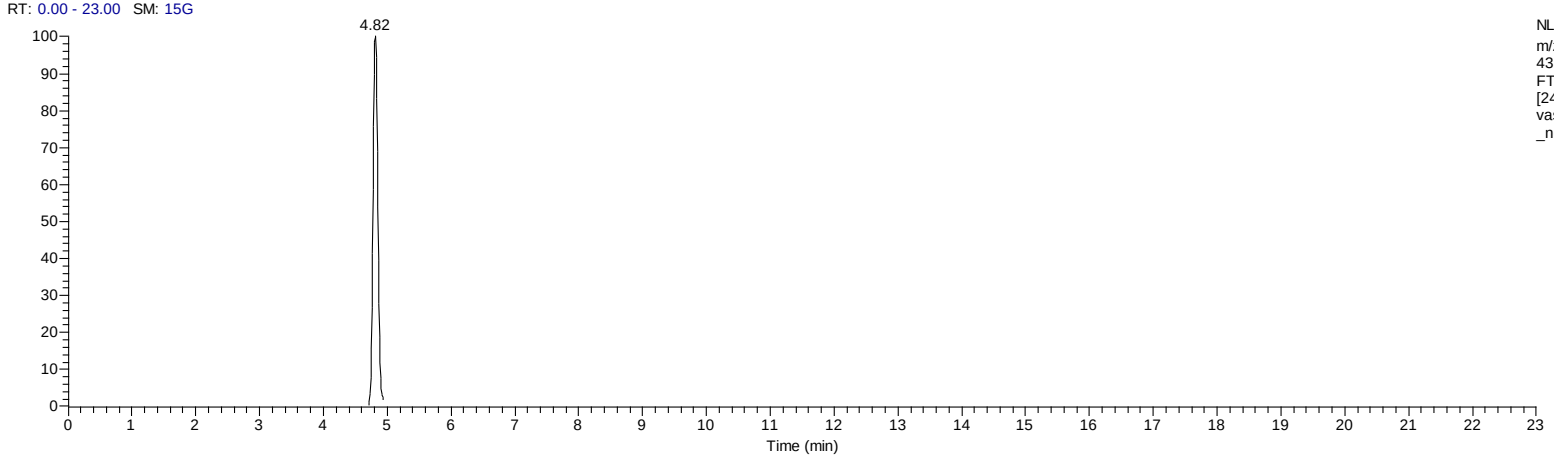


Afzelin (kaempferol 3-rhamnoside)

vaso_FSddMS2_245_455_neg_01
30mg/1ml 70/30 met/acqua

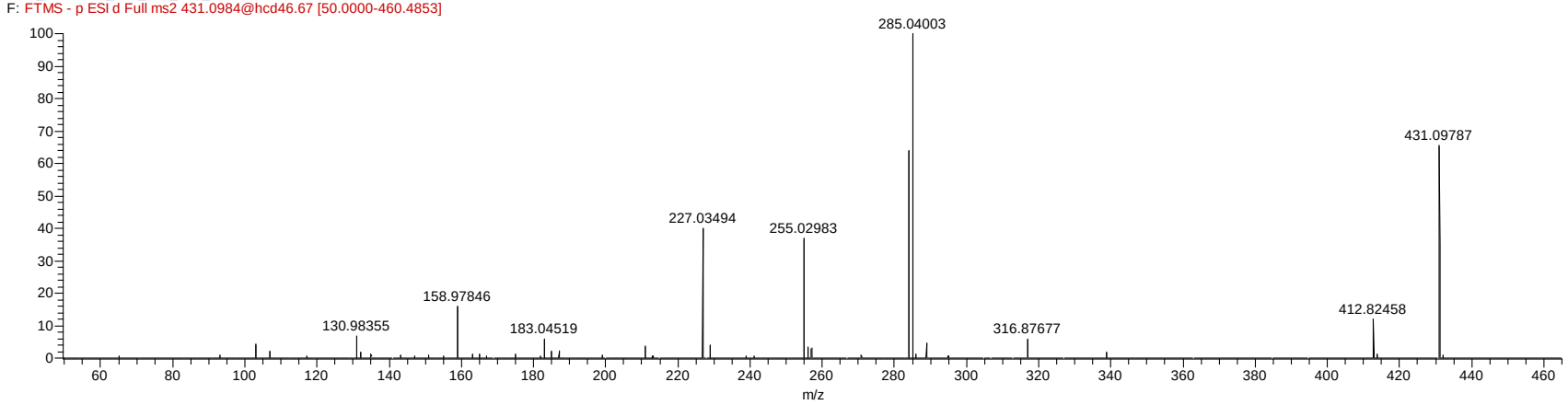
03/15/22 12:45:25

RT: 0.00 - 23.00 SM: 15G



NL: 7.88E5
m/z=
431.09369-431.10231 F:
FTMS - p ESI Full ms
[245.0000-455.0000] MS
vaso_FSddMS2_245_455
_neg_01

vaso_FSddMS2_245_455_neg_01 #1989-2093 RT: 4.79-4.83 AV: 2 NL: 2.36E5
F: FTMS - p ESI d Full ms2 431.0984@hcd46.67 [50.0000-460.4853]

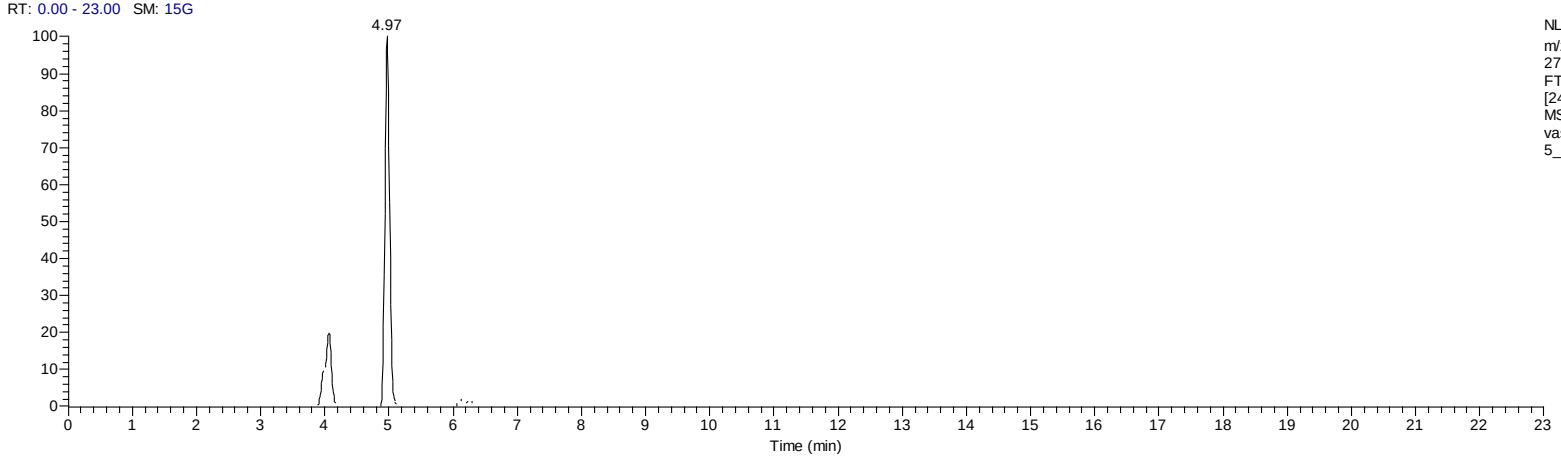


Naringenin

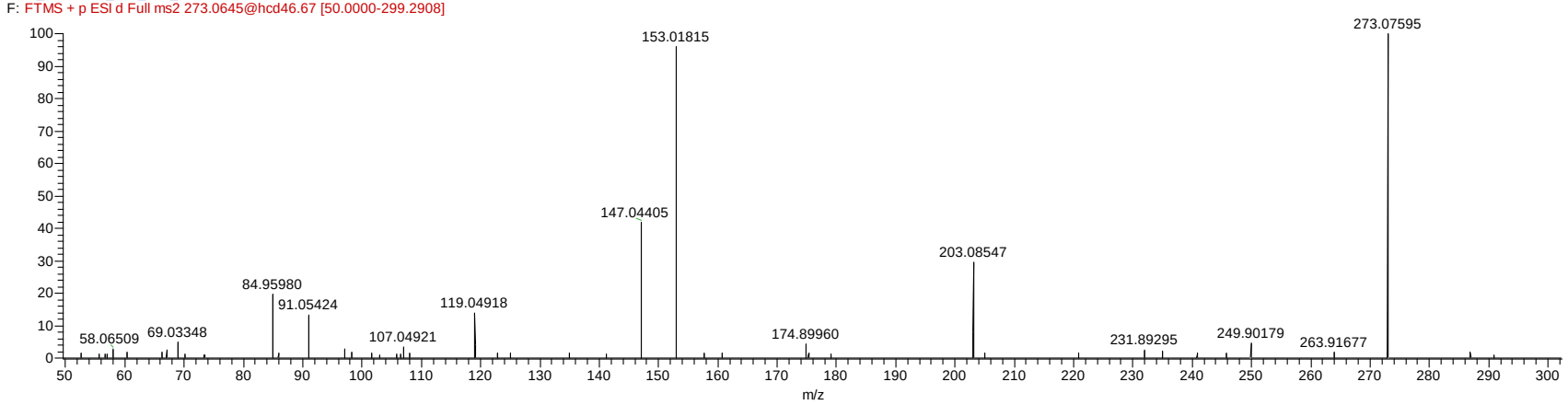
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

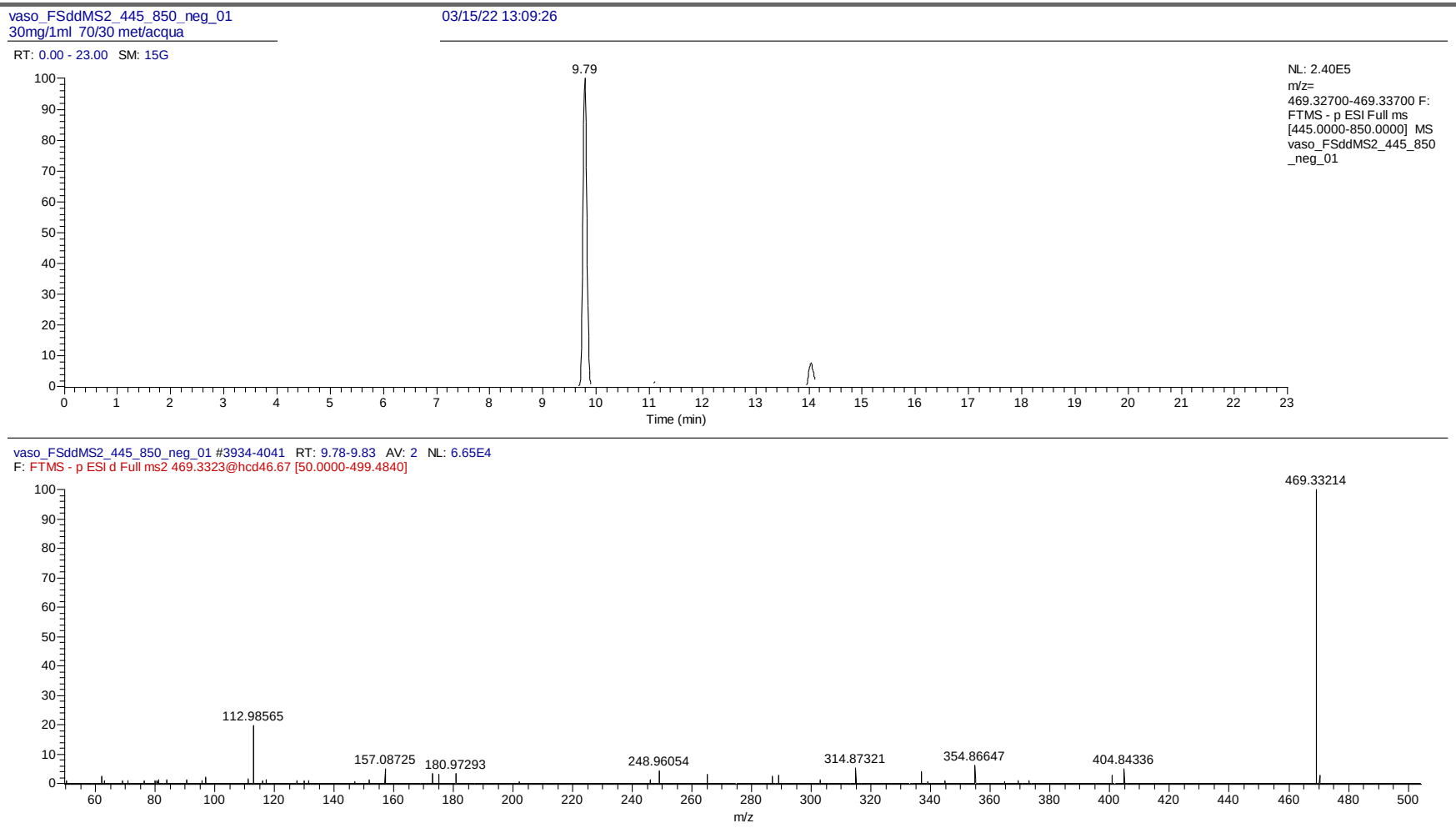
RT: 0.00 - 23.00 SM: 15G



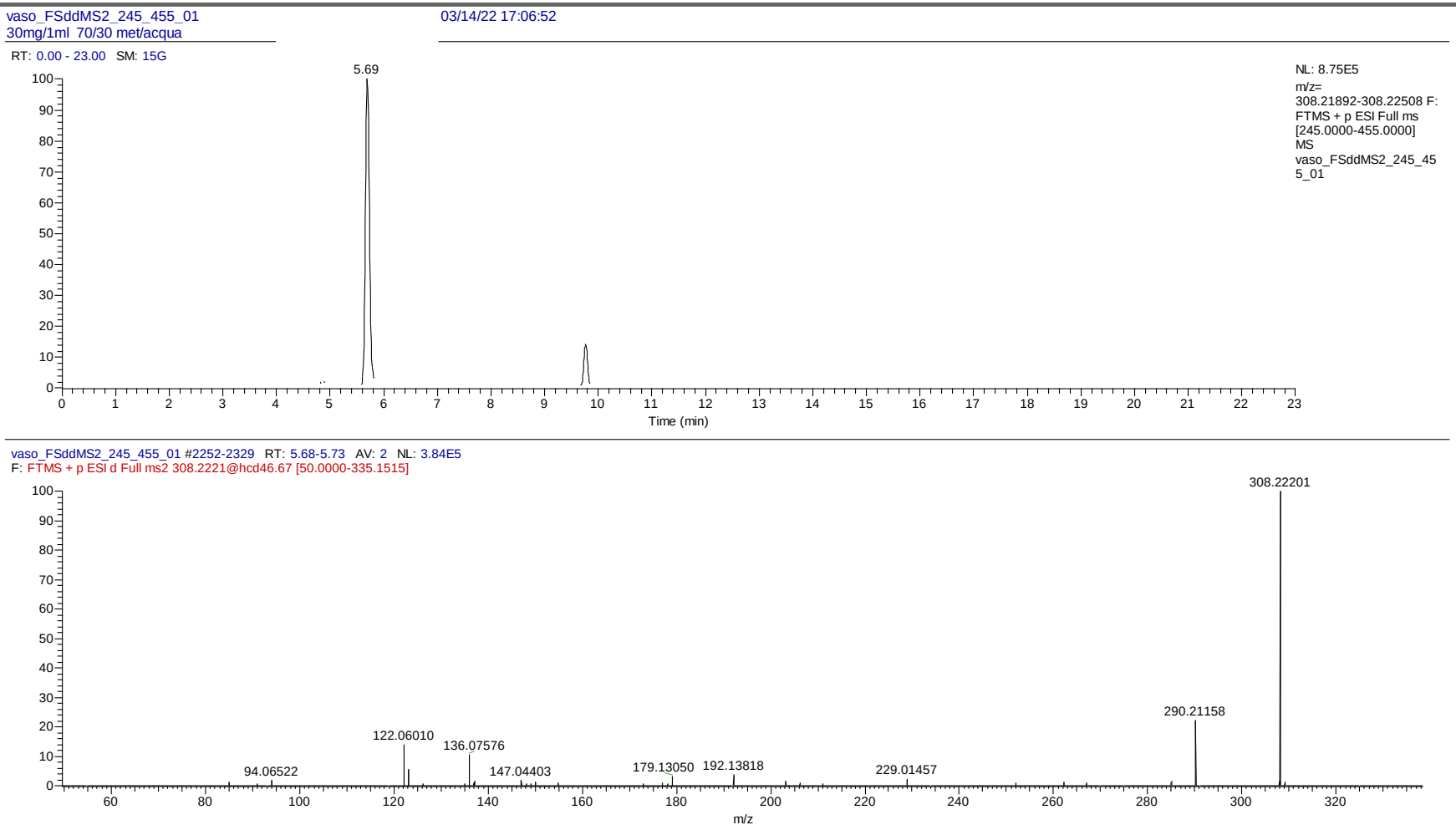
vaso_FSddMS2_245_455_01 #1905-2022 RT: 4.96-5.04 AV: 2 SB: 35 3.13-3.62 , 10.73-18.27 NL: 4.89E4
F: FTMS + p ESI d Full ms2 273.0645@hcd46.67 [50.0000-299.2908]



18-β-Glycyrrhetinic acid



Neovasipyridone E

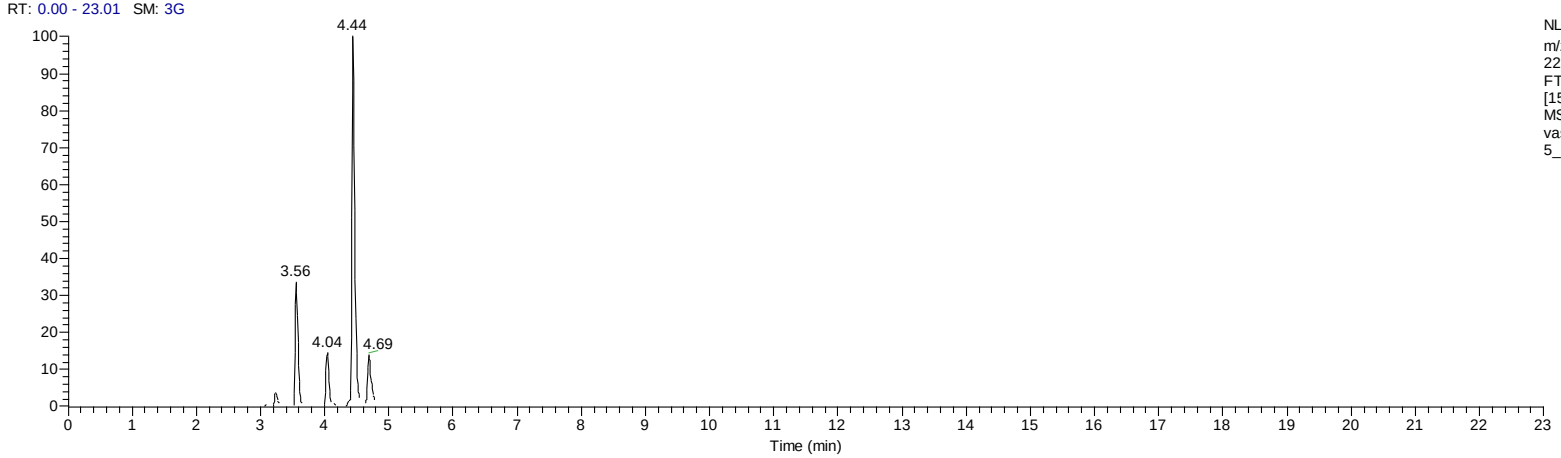


Aspernigrin A

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

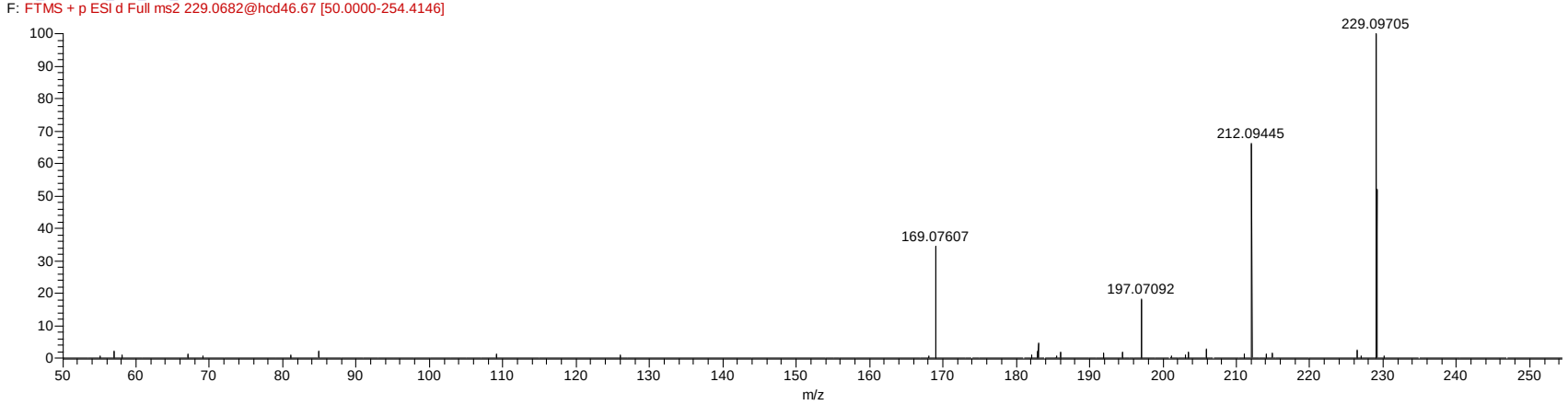
03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 3G



NL: 4.30E6
m/z=
229.09471-229.09929 F:
FTMS + p ESI Full ms
[150.0000-255.0000]
MS
vaso_FSddMS2_150_25
5_01

vaso_FSddMS2_150_255_01 #2018 RT: 4.67 AV: 1 NL: 1.60E5
F: FTMS + p ESI d Full ms2 229.0682@hcd46.67 [50.0000-254.4146]

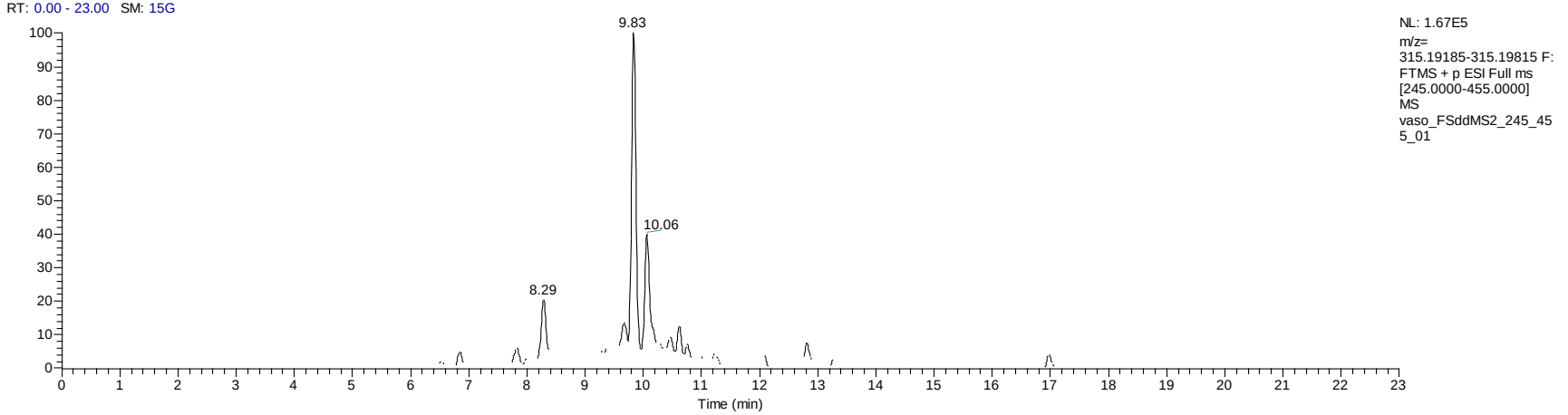


Libertellenone G

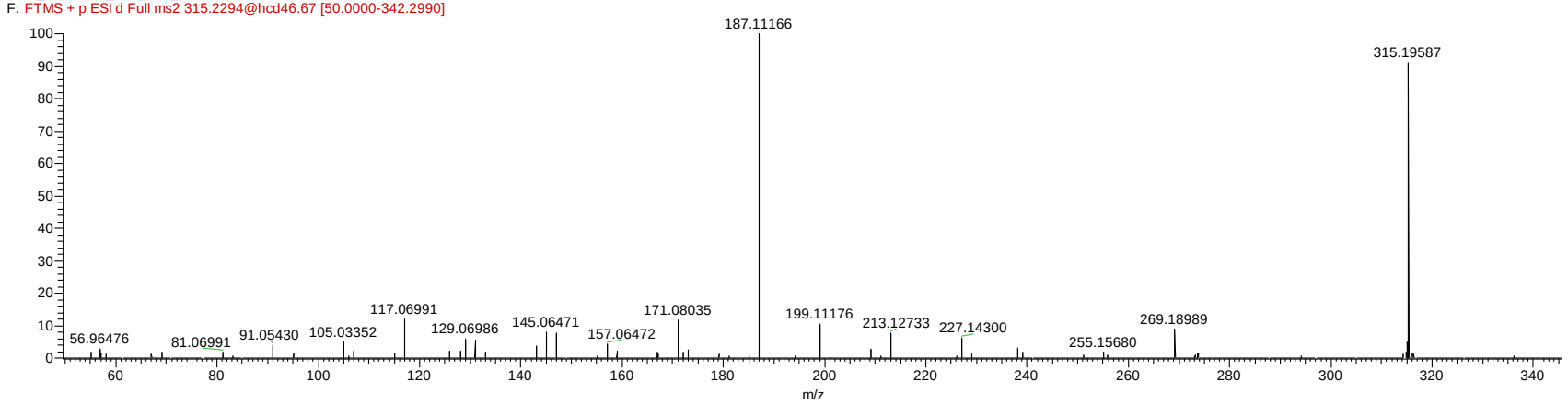
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_245_455_01 #3970-4008 RT: 9.83-9.87 AV: 2 SB: 2 5.55-8.24 , 1.27-3.73 NL: 4.42E4
F: FTMS + p ESI d Full ms2 315.2294@hcd46.67 [50.0000-342.2990]

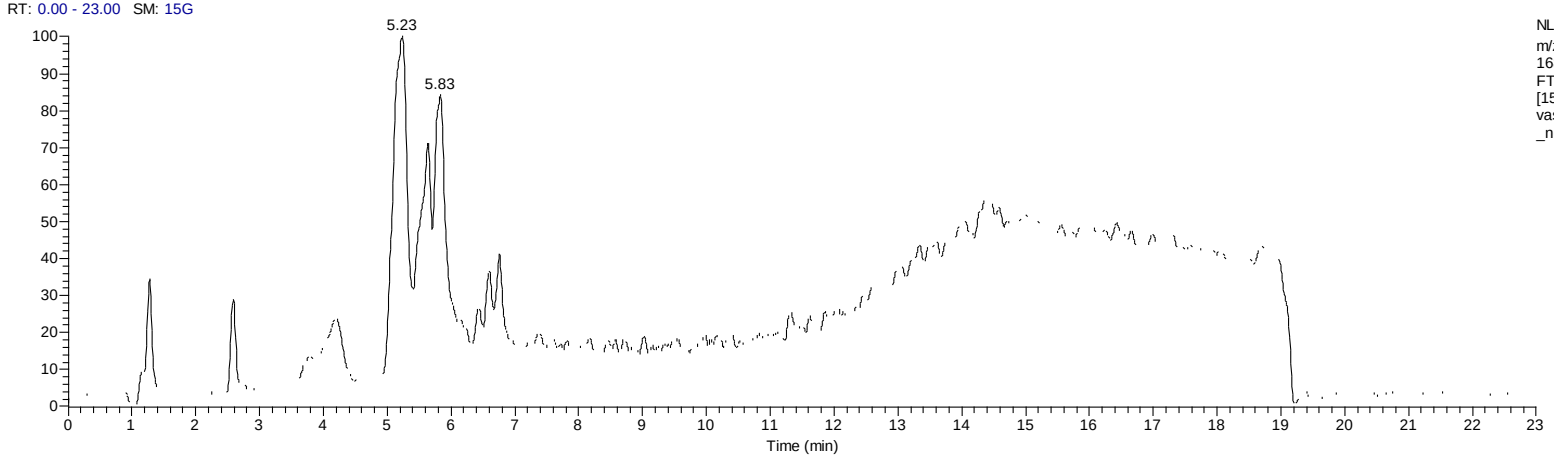


2-furoylglycine

vaso_FSddMS2_150_255_neg_01
30mg/1ml 70/30 met/acqua

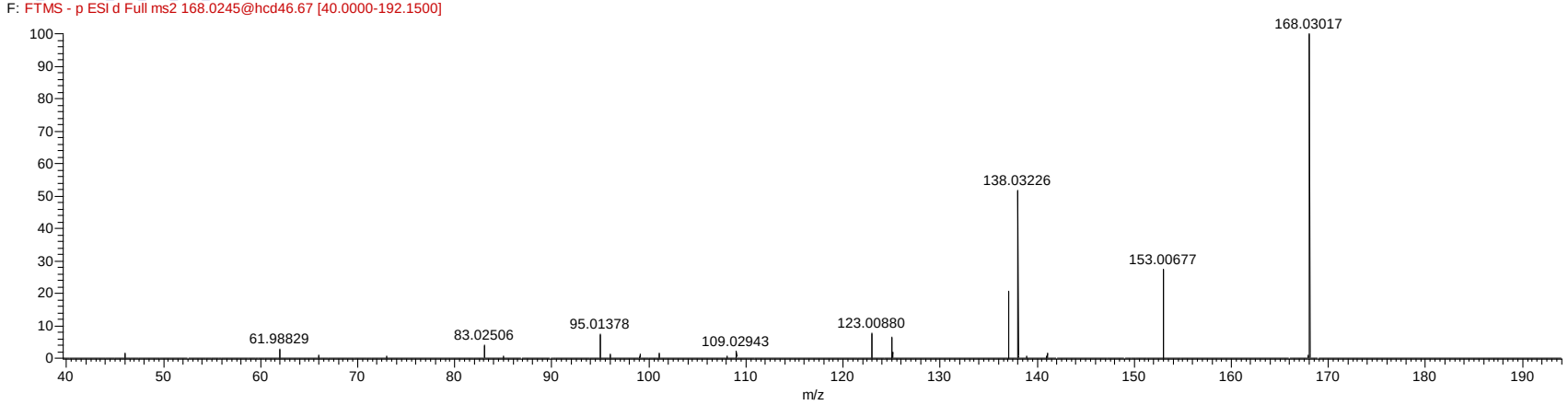
03/15/22 12:21:25

RT: 0.00 - 23.00 SM: 15G



NL: 1.14E5
m/z=
168.02936-168.03104 F:
FTMS - p ESI Full ms
[150.0000-255.0000] MS
vaso_FSddMS2_150_255
_neg_01

vaso_FSddMS2_150_255_neg_01 #1934-2071 RT: 5.12-5.26 AV: 4 SB: 2 1.34-4.93 , 0.25-0.56 NL: 2.18E4
F: FTMS - p ESI d Full ms2 168.0245@hcd46.67 [40.0000-192.1500]

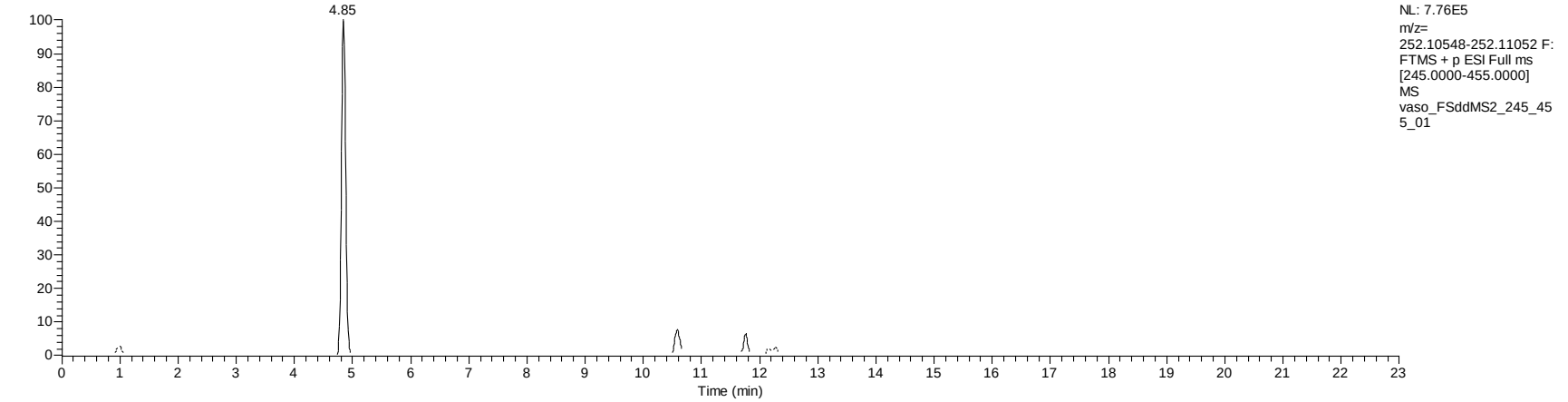


Unknown I

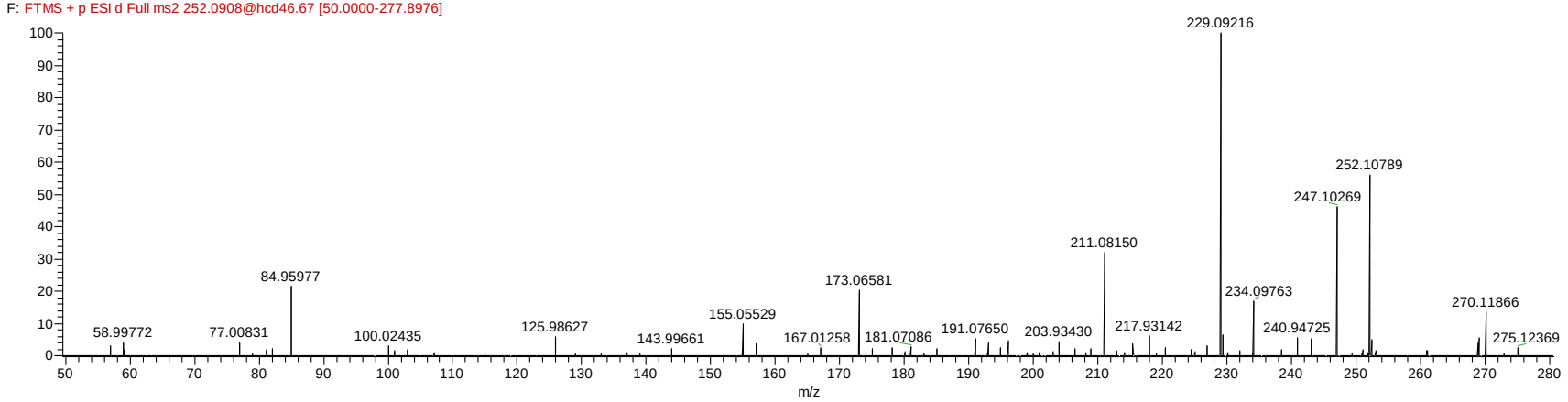
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_245_455_01 #1848-1985 RT: 4.83-4.88 AV: 2 NL: 1.53E5
F: FTMS + p ESI d Full ms2 252.0908@hcd46.67 [50.0000-277.8976]

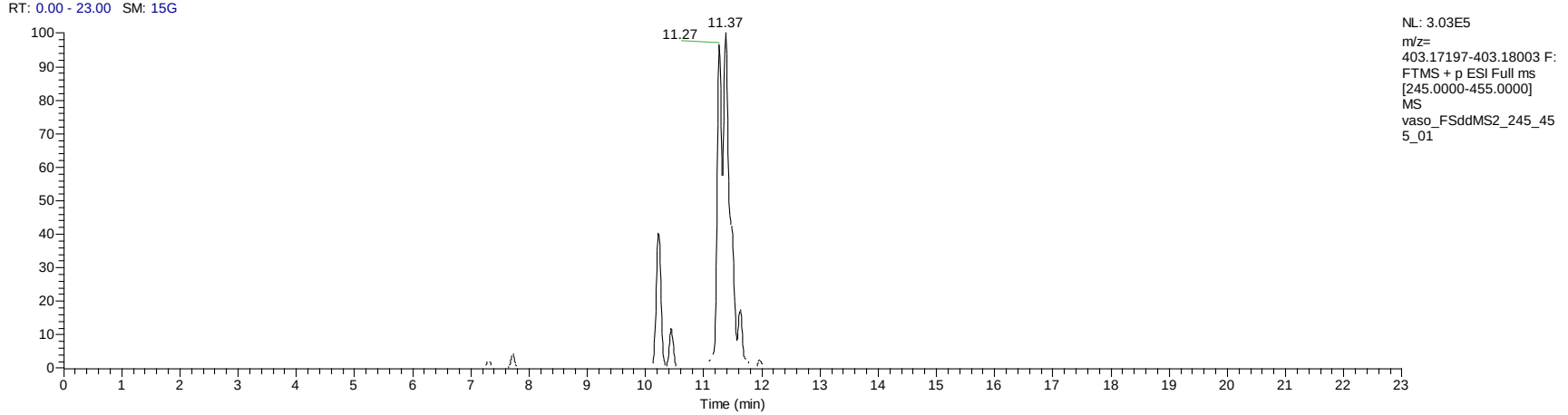


Unknown II

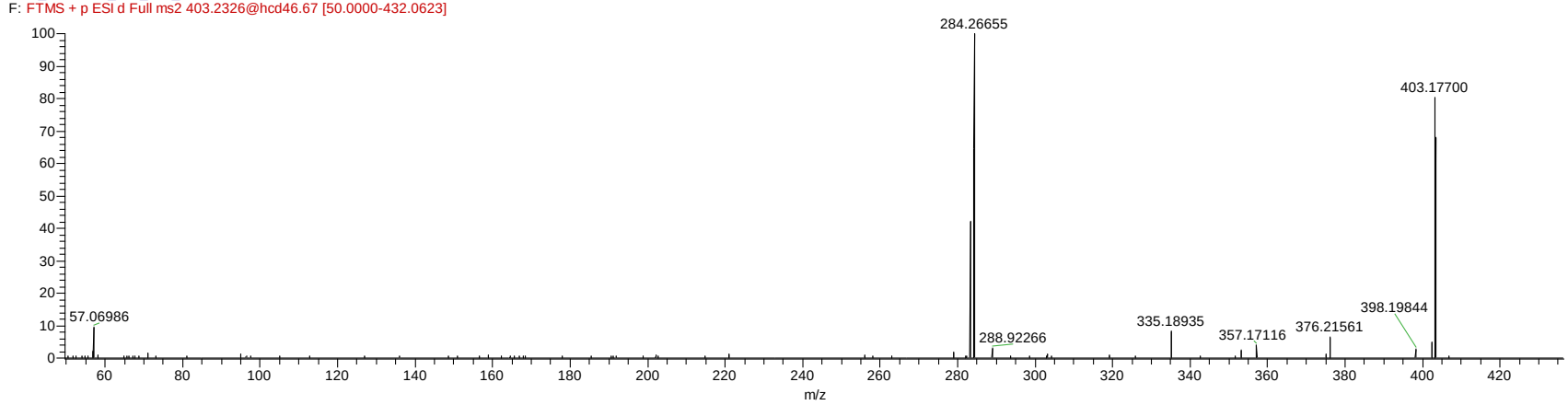
vaso_FSddMS2_245_455_01
30mg/1ml 70/30 met/acqua

03/14/22 17:06:52

RT: 0.00 - 23.00 SM: 15G



vaso_FSddMS2_245_455_01 #4588-4841 RT: 11.29-11.73 AV: 5 SB: 2 5.55-8.24 , 1.27-3.73 NL: 4.62E4
F: FTMS + p ESI d Full ms2 403.2326@hcd46.67 [50.0000-432.0623]

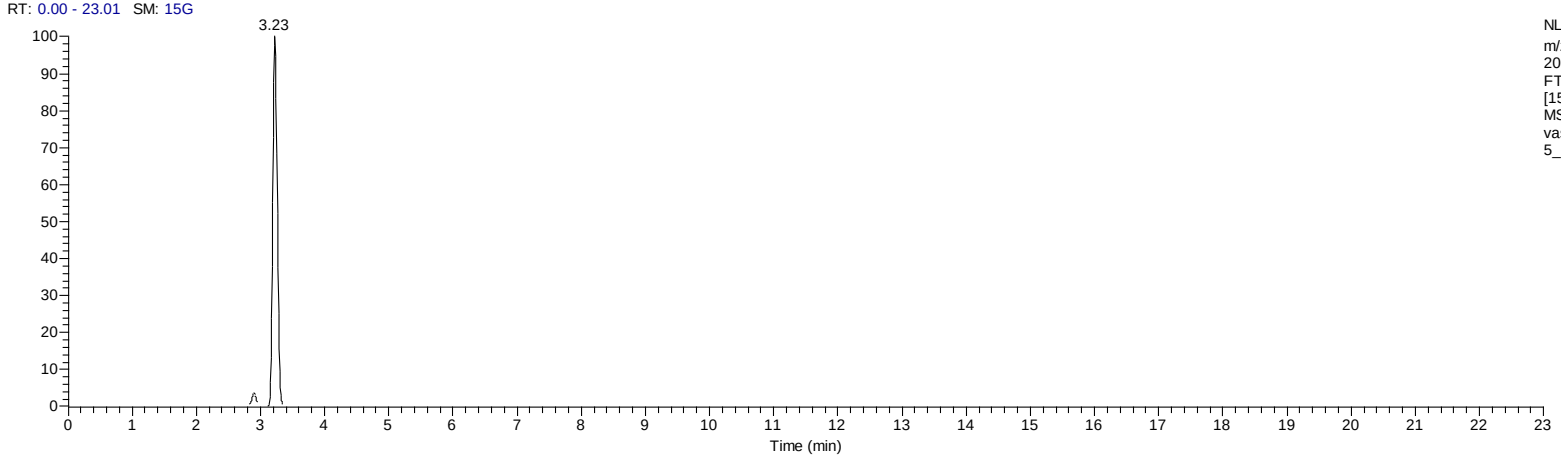


Unknown III

vaso_FSddMS2_150_255_01
30mg/1ml 70/30 met/acqua

03/14/22 16:42:48

RT: 0.00 - 23.01 SM: 15G



vaso_FSddMS2_150_255_01 #1257-1389 RT: 2.94-3.20 AV: 2 SB: 17 1.25-15.92 , 0.00-0.42 NL: 3.61E6
F: FTMS + p ESI d Full ms2 201.1361@hcd46.67 [45.1848-225.9238]