

Mass Spectrum List Report

Analysis Info

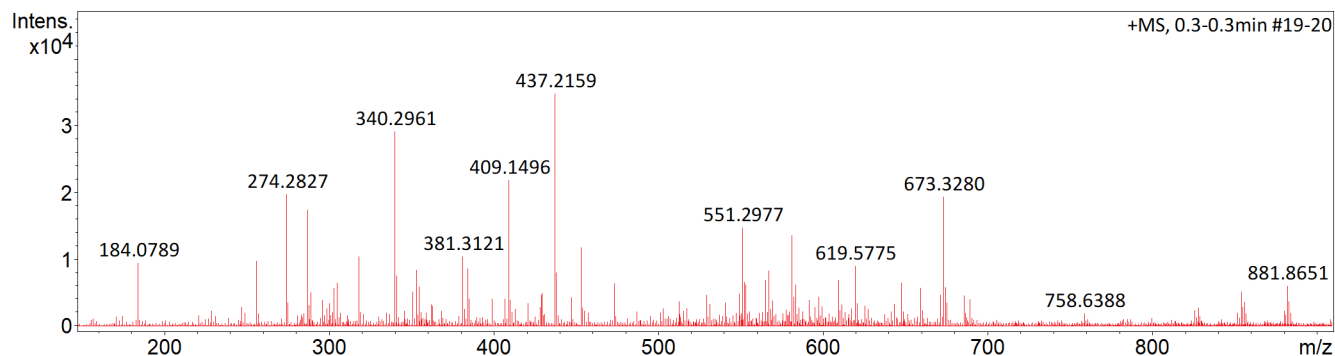
Analysis Name C:\Data\24-092015_P1-C-6_01_9464.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092015
 Comment GF-C9
 Sv: MeOH + HCOOH
 Manuela García

Acquisition Date 1/10/2024 16:23:29

Operator EB - MV
 Instrument / Ser# micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



#	m/z	I	I %
1	184.0789	9413	27.1
2	256.2716	9772	28.2
3	274.2827	19636	56.6
4	287.1339	17370	50.1
5	305.1446	6507	18.8
6	318.3113	10428	30.1
7	340.2961	29075	83.8
8	341.2928	7545	21.7
9	353.2794	8437	24.3
10	355.0857	5916	17.1
11	381.3121	10413	30.0
12	384.3254	8557	24.7
13	409.1496	21822	62.9
14	437.2159	34692	100.0
15	438.2172	8026	23.1
16	453.1832	11719	33.8
17	473.3731	6400	18.4
18	551.2977	14704	42.4
19	552.2903	6589	19.0
20	553.2935	6228	18.0
21	565.2849	6844	19.7
22	567.2956	8283	23.9
23	581.3099	13593	39.2
24	583.3143	6245	18.0
25	609.3177	6872	19.8
26	619.5775	8966	25.8
27	647.6186	6494	18.7
28	673.3280	19346	55.8
29	674.3277	5785	16.7
30	881.8651	6018	17.3

Qualitative Compound Report

Analysis Info

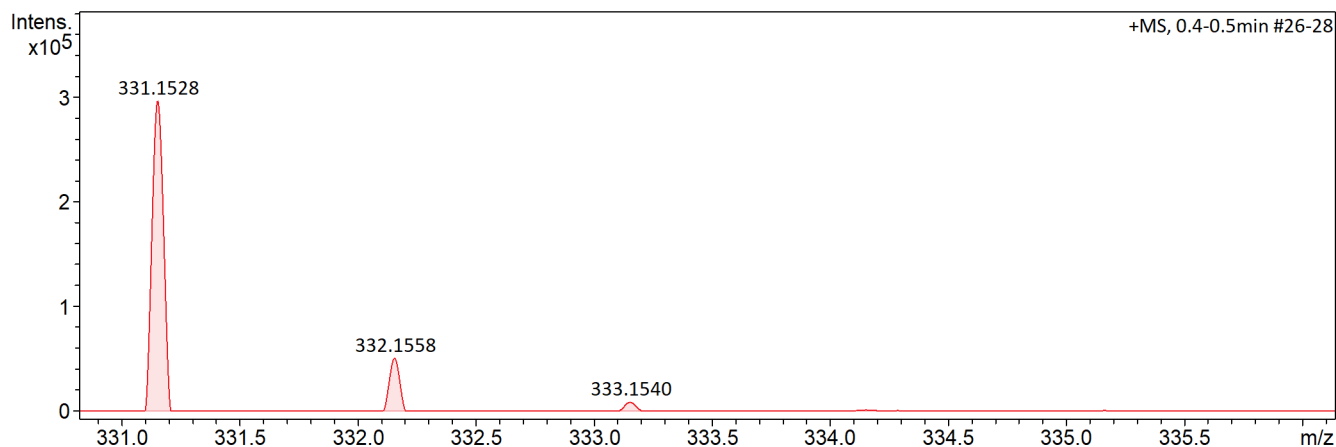
Analysis Name C:\Data\24-092016_P1-C-7_01_9465.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092016
 Comment 95C
 Sv: MeOH + HCOOH
 Manuela García

Acquisition Date 1/10/2024 16:28:36

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
331.1528	1	C17H24NaO5	331.1516	-3.7	9.9	2	76.24	5.5	even	ok

Qualitative Compound Report

Analysis Info

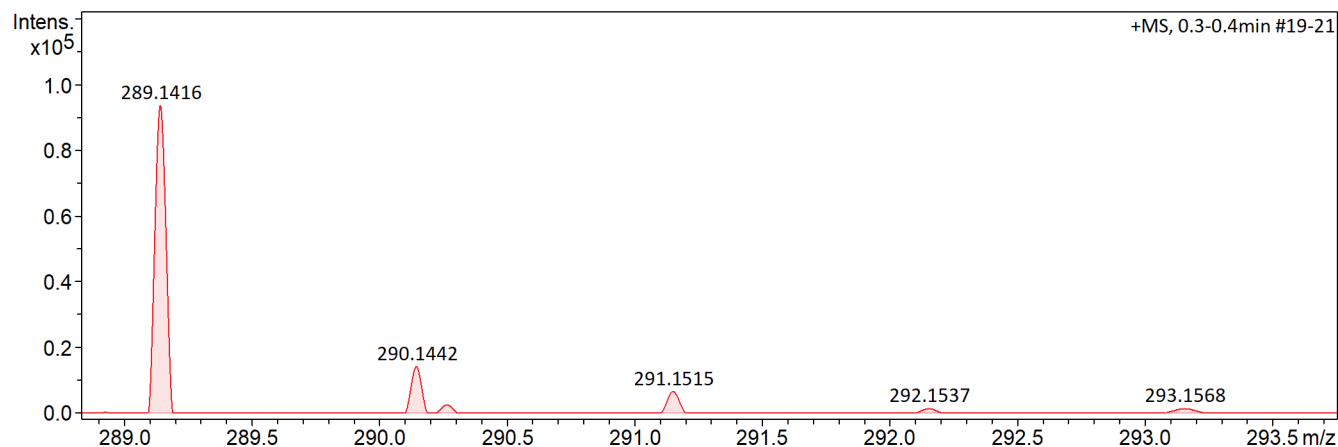
Analysis Name C:\Data\24-092017_P1-C-8_01_9466.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092017
 Comment 95TLC6
 Sv: MeOH + HCOOH
 Manuela García

Acquisition Date 1/10/2024 16:33:43

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
289.1416	1	C15H22NaO4	289.1410	-2.1	30.0	1	100.00	4.5	even	ok

Qualitative Compound Report

Analysis Info

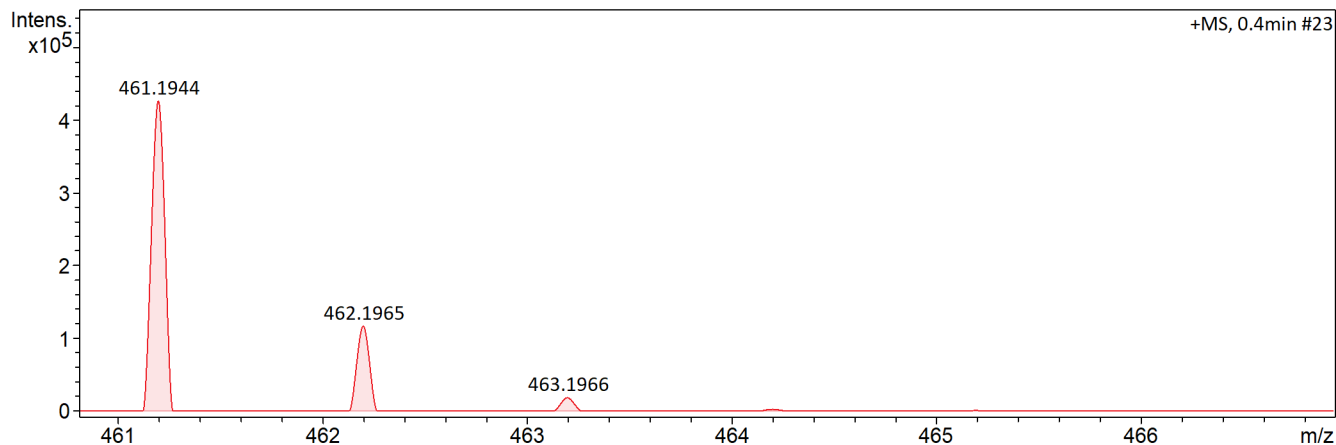
Analysis Name C:\Data\24-092018_P1-C-9_01_9467.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092018
 Comment AR47F3
 Sv: MeOH + HCOOH
 Manuela García

Acquisition Date 1/10/2024 16:38:52

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
461.1944	1	C26H30NaO6	461.1935	-2.0	7.4	1	100.00	11.5	even	ok

Qualitative Compound Report

Analysis Info

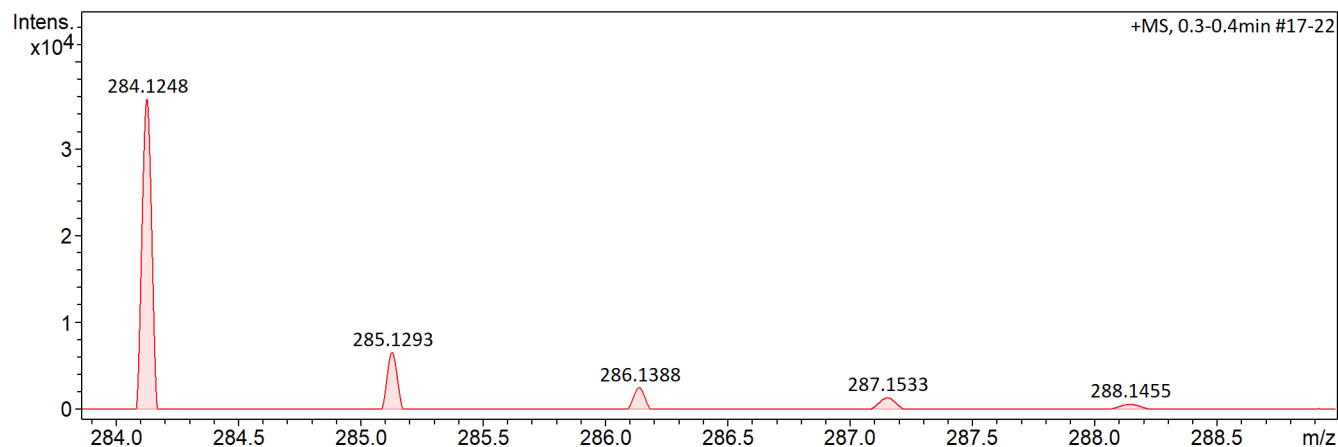
Analysis Name C:\Data\24-092019_P1-D-1_01_9468.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092019
 Comment AR48F2
 Sv: MeOH + HCOOH
 Manuela García

Acquisition Date 1/10/2024 16:43:59

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻ Conf	N-Rule
284.1248	1	C15H19NNaO3	284.1257	3.3	29.9	1	91.57	6.5	even	ok

Qualitative Compound Report

Analysis Info

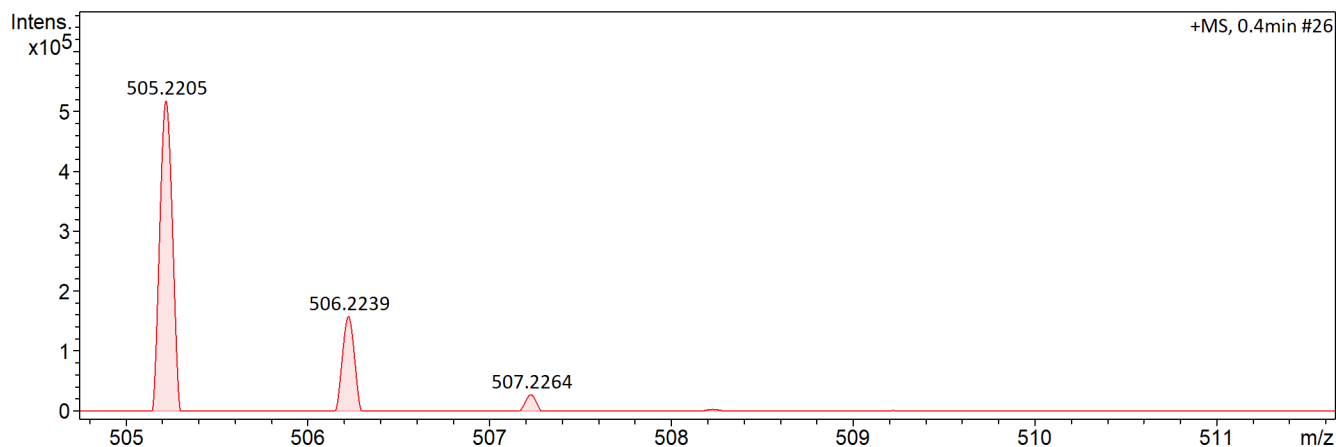
Analysis Name C:\Data\24-092020_P1-D-2_01_9469.d
 Method lc_ms directos tunelow300924.m
 Sample Name 24-092020
 Comment AR53F2
 Sv: MeOH + HCOOH
 Manuela García

Acquisition Date 1/10/2024 16:49:04

Operator EB - MV
 Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
505.2205	1	C28H34NaO7	505.2197	-1.5	4.3	1	100.00	11.5	even	ok