



Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LCMS-2

Date	N ₂ Tank Pressure	N ₂ Generator Pressure	Rough Pump Oil Level Checked	Waste Bottle Checked/Emptied	Prepared Mobile Phases	Wash Solvents Checked/Replaced	Spray Chamber Cleaned	Checktune	Autotune (Monthly)	Column Changed	Comments	Initials
5/2/22	30 1500	100	✓	✓	✓	✓	✓	✓	✓	✓ (THC)		EC
5/3/2022	30 1500	100	✓	✓	✓	✓	✓	✓	✗	✗		KMY
OR 05/10/22												

Signature:

Date Completed:

05/10/22

LAB-111

Issued By: Technical Supervisor - Toxicology

Issue Date: 2019-12-23 (2)

Instrument Name LCMS-2
MS Model G6470A
MS Instrument Serial SG1936G104
Software_Firmware Version 10.0.142, FW: A.00.08.100
Tune Date & Time 02 May 2022 08:53:55
Data Path D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.71E+0 [R] (Torr); 4.67E-5 [H] (Torr)

Source Parameters

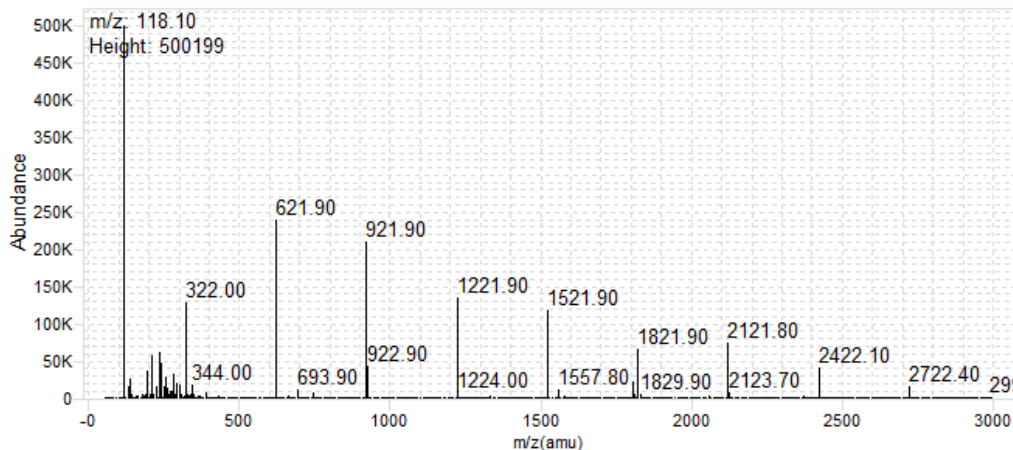
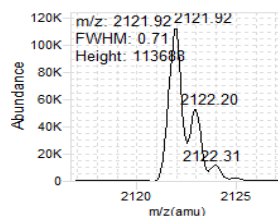
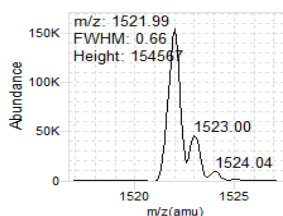
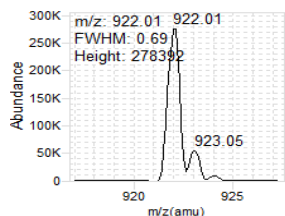
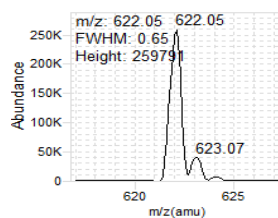
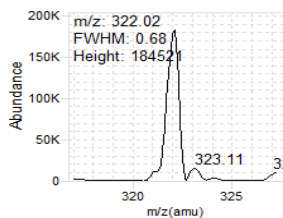
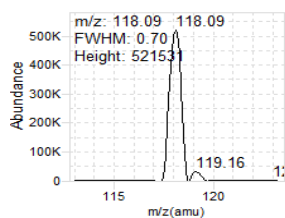
Parameter	Positive	Negative
Gas Temp (°C)	300	300
Gas Flow (l/min)	8	8
Nebulizer (psi)	15	15
Capillary (V)	4000	4000
Nozzle Voltage (V)	1500	1500
Sheath Gas Temp (°C)	250	250
Sheath Gas Flow (l/min)	7	7

Positive Results

Analyzer: MS1

Polarity: Positive

Width: Unit

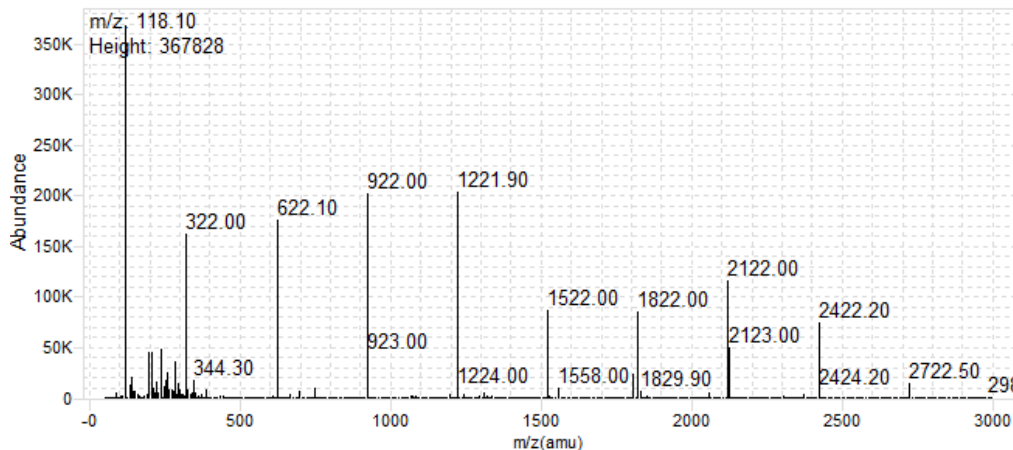
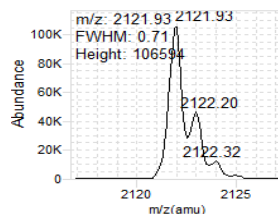
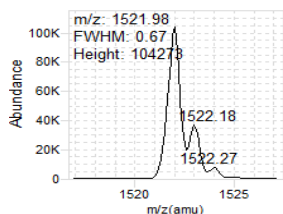
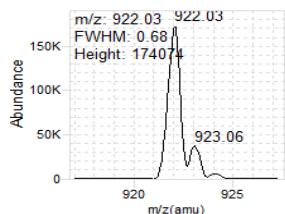
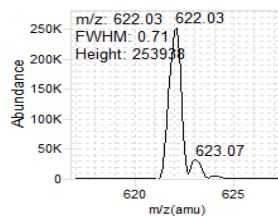
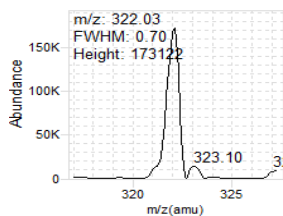
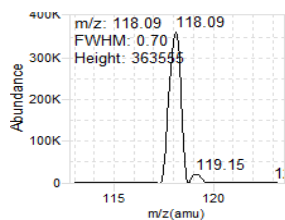


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.09	118.09	0.70	0.70	521531
322.02	322.05	0.68	0.70	184521
622.05	622.03	0.65	0.70	259791
922.01	922.01	0.69	0.70	278392
1521.99	1521.97	0.66	0.70	154567
2121.93	2121.93	0.71	0.70	113688

Analyzer: MS2

Polarity: Positive

Width: Unit

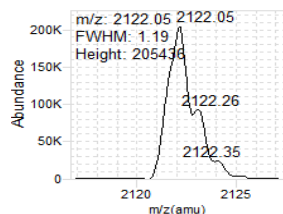
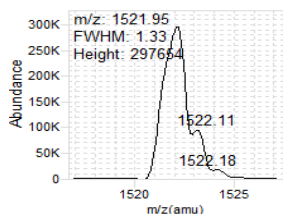
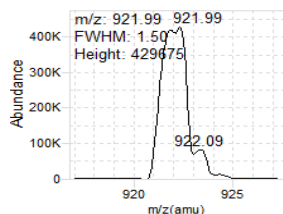
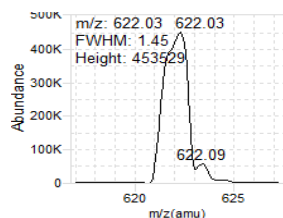
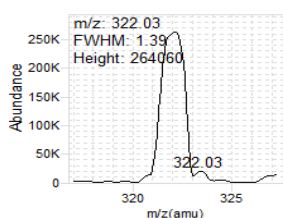
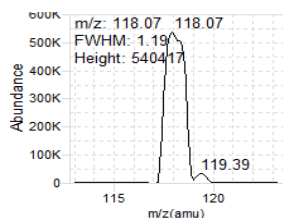


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.09	118.09	0.70	0.70	363555
322.03	322.05	0.70	0.70	173122
622.02	622.03	0.71	0.70	253938
922.02	922.01	0.68	0.70	174074
1521.98	1521.97	0.67	0.70	104273
2121.94	2121.93	0.71	0.70	106594

Analyzer: MS1

Polarity: Positive

Width: Wide

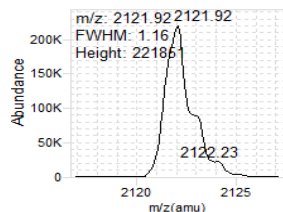
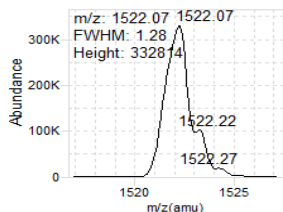
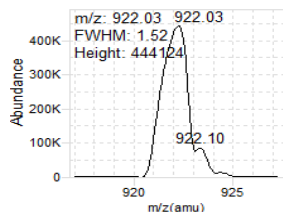
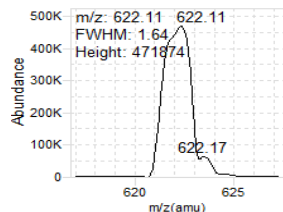
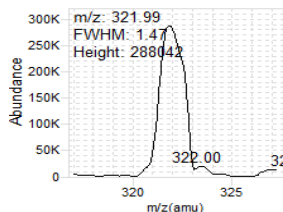
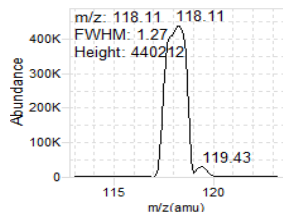


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.07	118.09	1.19	1.20	540417
322.03	322.05	1.39	1.20	264060
622.03	622.03	1.45	1.20	453529
921.99	922.01	1.50	1.20	429675
1521.94	1521.97	1.33	1.20	297654
2122.05	2121.93	1.19	1.20	205436

Analyzer: MS2

Polarity: Positive

Width: Wide

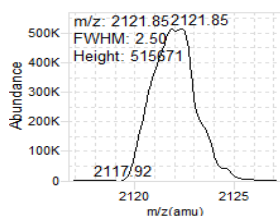
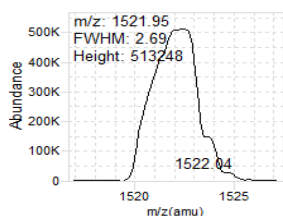
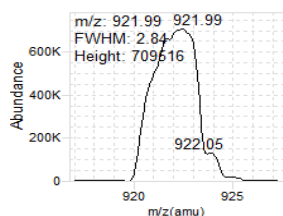
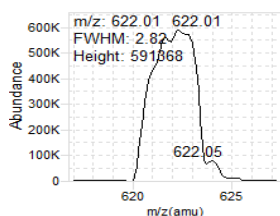
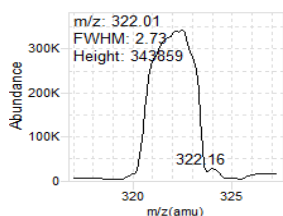
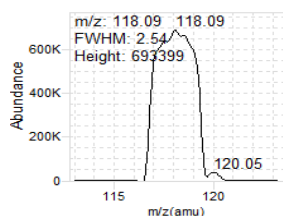


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.11	118.09	1.27	1.20	440212
321.99	322.05	1.47	1.20	288042
622.11	622.03	1.64	1.20	471874
922.03	922.01	1.52	1.20	444124
1522.07	1521.97	1.27	1.20	332814
2121.93	2121.93	1.16	1.20	221851

Analyzer: MS1

Polarity: Positive

Width: Widest

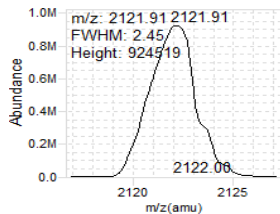
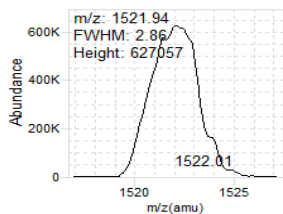
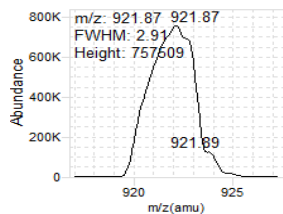
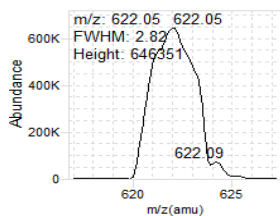
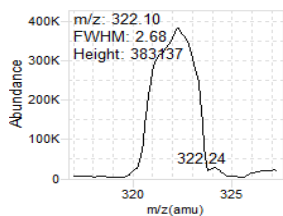
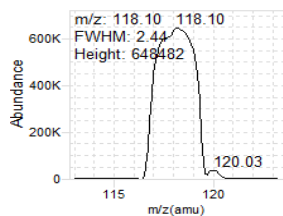


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.09	118.09	2.54	2.50	693399
322.01	322.05	2.73	2.50	343859
622.01	622.03	2.82	2.50	591368
921.98	922.01	2.84	2.50	709516
1521.95	1521.97	2.69	2.50	513248
2121.85	2121.93	2.50	2.50	515671

Analyzer: MS2

Polarity: Positive

Width: Widest



m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.10	118.09	2.44	2.50	648482
322.10	322.05	2.68	2.50	383137
622.05	622.03	2.82	2.50	646351
921.87	922.01	2.91	2.50	757509
1521.94	1521.97	2.86	2.50	627057
2121.91	2121.93	2.45	2.50	924519

Positive Results

Tune Parameters

Parameters	Setting
Fragmentor	135
Skimmer	15
Octopole DC	5
Octopole RF	600
Lens 1	3.50
MS1 PreFilter	-30
MS1 DC	3.00
MS1 PostFilter	2.00
MS1 Axis Offset	0.91
MS1 Axis Gain	8.75
MS1 Width Offset	0
MS1 Width Gain	3
MS1 Heater	100
MS2 DC	-10
MS2 PreFilter	-30
MS2 Axis Offset	0.78
MS2 Axis Gain	17.65
MS2 Width Offset	0
MS2 Width Gain	-8
MS2 Heater	100
Cell Entry	1
Hexapole DC	0.00
Hexapole RF	500
Hexapole Accel	5
Cell Exit	-7
Collision Gas	1
Iris	-150
HED	-10
EMV	1255
Collision Energy	0
Lens 1[MS2]	1.90
MS1 PreFilter[MS2]	1.80

Dynamic Ramp Tables

MS1 PreFilter

m/z	Setting
118.09	-10.6
322.05	-6.2
622.03	-9.2
922.01	-12.2
1521.97	-12.4
2121.93	-31.8

MS1 Axis Offset

m/z	Setting
118.09	0.914
322.05	1.077
622.03	1.186
922.01	1.17
1521.97	1.1
2121.93	0.914

MS1 Width Offset

m/z	Setting
118.09	0.1
322.05	-0.1
622.03	-0.15
922.01	-0.15
1521.97	-0.07
2121.93	0.1

MS2 PreFilter

m/z	Setting
58	-16.6
79	-21.4
117.97	-30
118	-13.4
154	-16.2
290	-31.2

MS2 Axis Offset

m/z	Setting
118.09	0.782
322.05	0.949
622.03	1.108
922.01	1.124
1521.97	0.962
2121.93	0.782

MS2 Width Offset

m/z	Setting
118.09	0.1
322.05	-0.13
622.03	-0.28
922.01	-0.27
1521.97	-0.14
2121.93	0.1

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	8.75	0.914	2.6	0.1
Wide	8.7	1.074	2.7	0.48
Widest	8.25	1.526	3.2	1.5

MS2 Calibrations

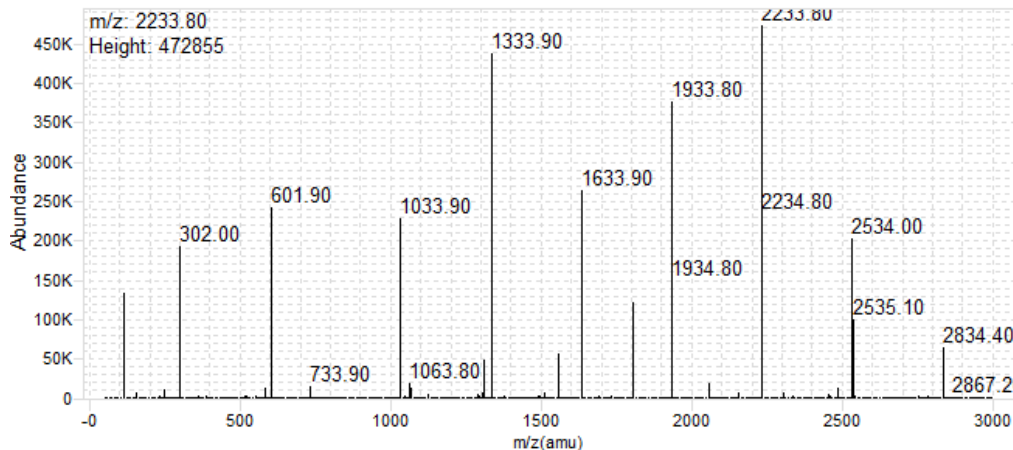
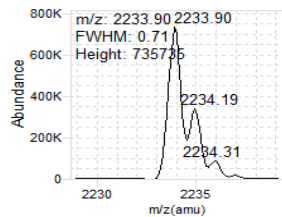
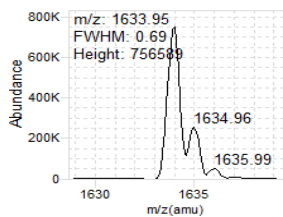
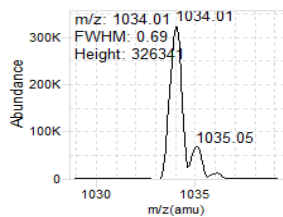
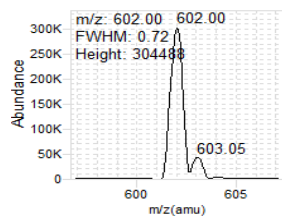
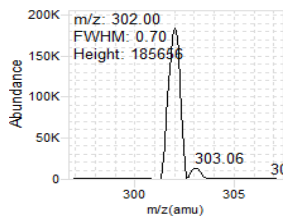
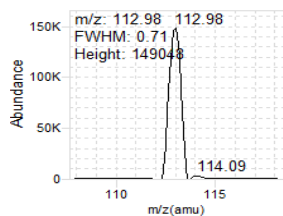
Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	17.65	0.782	-7.5	0.1
Wide	17.35	0.994	-7.5	0.55
Widest	17.1	1.394	-6.3	1.44

Negative Results

Analyzer: MS1

Polarity: Negative

Width: Unit

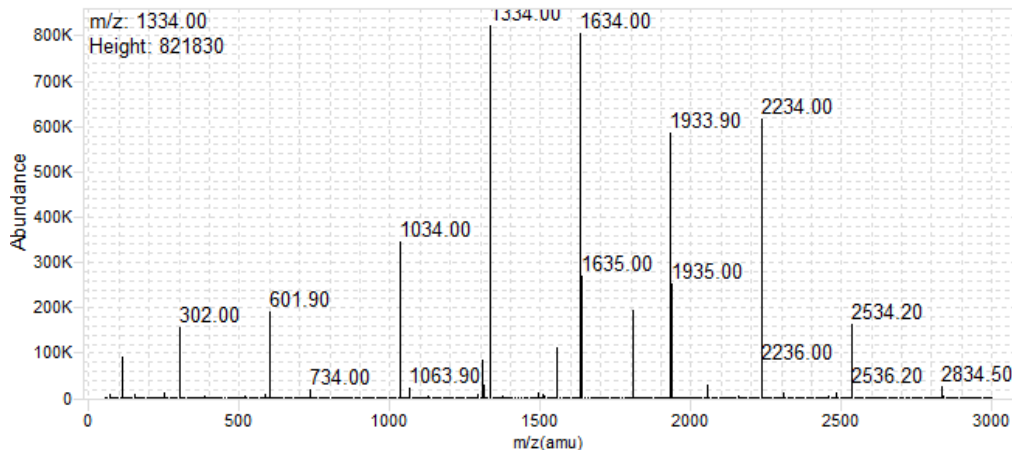
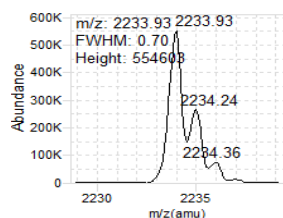
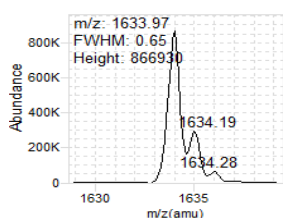
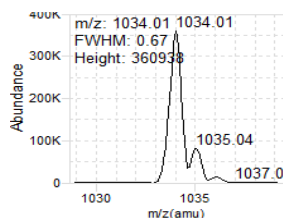
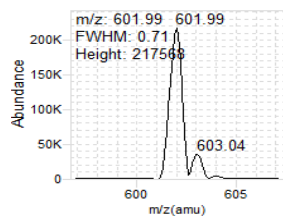
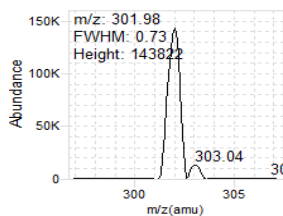
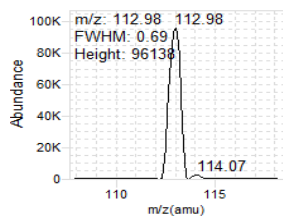


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.98	112.99	0.71	0.70	149048
302.00	302.00	0.70	0.70	185656
602.00	601.98	0.72	0.70	304488
1034.01	1033.99	0.69	0.70	326341
1633.95	1633.95	0.69	0.70	756589
2233.91	2233.91	0.71	0.70	735735

Analyzer: MS2

Polarity: Negative

Width: Unit

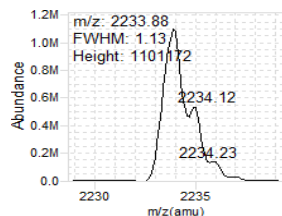
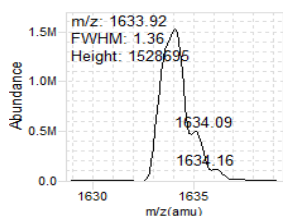
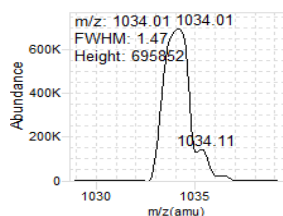
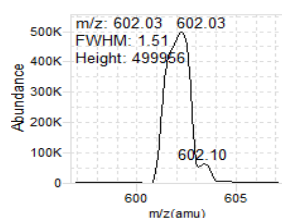
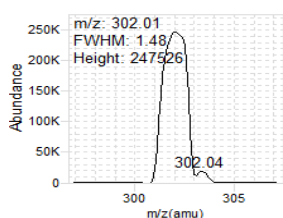
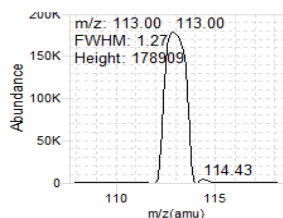


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.98	112.99	0.69	0.70	96138
301.98	302.00	0.73	0.70	143822
601.98	601.98	0.71	0.70	217568
1034.00	1033.99	0.67	0.70	360938
1633.96	1633.95	0.65	0.70	866930
2233.94	2233.91	0.70	0.70	554603

Analyzer: MS1

Polarity: Negative

Width: Wide

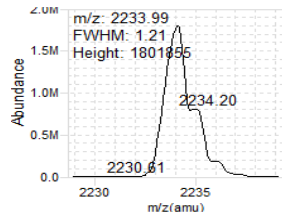
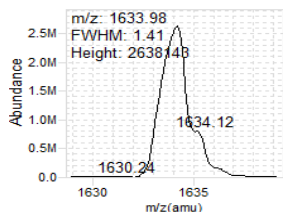
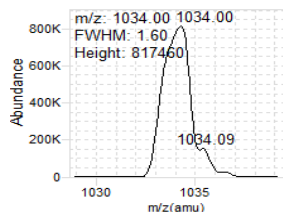
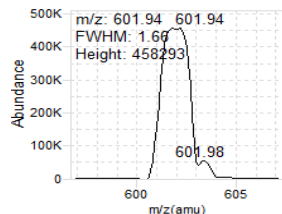
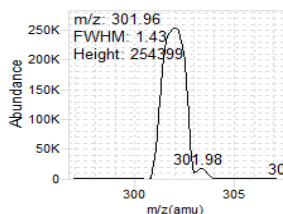
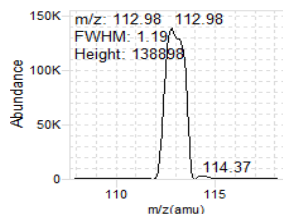


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.00	112.99	1.27	1.20	178909
302.01	302.00	1.48	1.20	247526
602.03	601.98	1.51	1.20	499956
1034.00	1033.99	1.47	1.20	695852
1633.91	1633.95	1.36	1.20	1528695
2233.89	2233.91	1.13	1.20	1101172

Analyzer: MS2

Polarity: Negative

Width: Wide

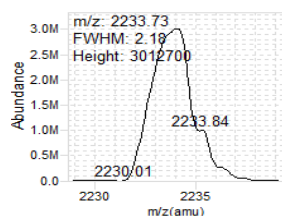
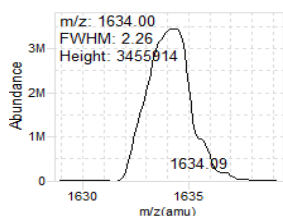
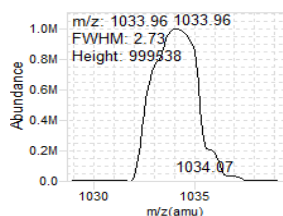
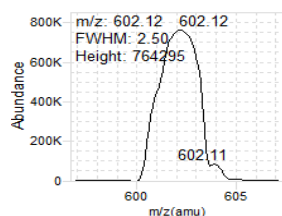
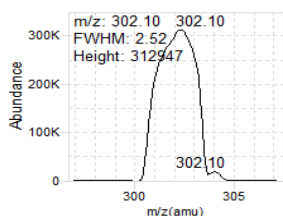
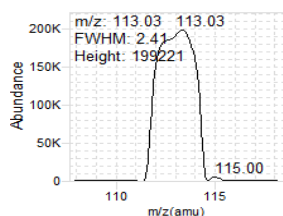


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.98	112.99	1.19	1.20	138898
301.96	302.00	1.43	1.20	254399
601.94	601.98	1.66	1.20	458293
1033.99	1033.99	1.60	1.20	817459
1633.98	1633.95	1.41	1.20	2638143
2233.99	2233.91	1.21	1.20	1801855

Analyzer: MS1

Polarity: Negative

Width: Widest

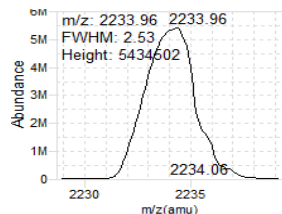
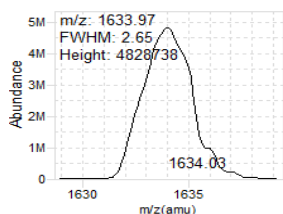
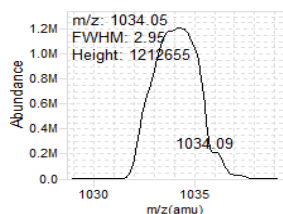
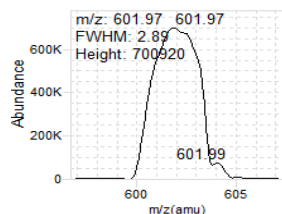
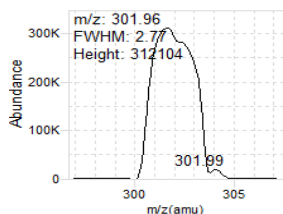
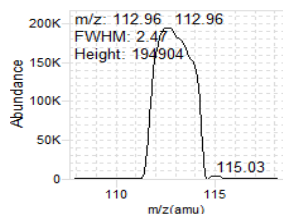


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.03	112.99	2.41	2.50	199221
302.10	302.00	2.52	2.50	312947
602.11	601.98	2.50	2.50	764295
1033.96	1033.99	2.73	2.50	999538
1634.00	1633.95	2.26	2.50	3455914
2233.74	2233.91	2.18	2.50	3012700

Analyzer: MS2

Polarity: Negative

Width: Widest



m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.96	112.99	2.47	2.50	194904
301.97	302.00	2.77	2.50	312104
601.97	601.98	2.89	2.50	700920
1034.05	1033.99	2.95	2.50	1212655
1633.97	1633.95	2.65	2.50	4828738
2233.97	2233.91	2.53	2.50	5434501

Negative Results

Tune Parameters

Parameters	Setting
Fragmentor	115
Skimmer	15
Octopole DC	5
Octopole RF	600
Lens 1	-3.90
MS1 PreFilter	17
MS1 DC	-3.00
MS1 PostFilter	-2.00
MS1 Axis Offset	0.92
MS1 Axis Gain	9
MS1 Width Offset	0.15
MS1 Width Gain	3
MS1 Heater	100
MS2 DC	10
MS2 PreFilter	30
MS2 Axis Offset	0.77
MS2 Axis Gain	18
MS2 Width Offset	0.07
MS2 Width Gain	-7
MS2 Heater	100
Cell Entry	1
Hexapole DC	0.00
Hexapole RF	500
Hexapole Accel	5
Cell Exit	7.00
Collision Gas	1
Iris	150
HED	18
EMV	1265
Collision Energy	0
Lens 1[MS2]	-3.80
MS1 PreFilter[MS2]	-2.80

Dynamic Ramp Tables

MS1 PreFilter

m/z	Setting
112.99	9.8
302	7.8
601.98	8
1033.99	19.9
1633.95	15.5
2233.91	13.7

MS1 Axis Offset

m/z	Setting
112.99	0.916
302	1.121
601.98	1.201
1033.99	1.217
1633.95	1.113
2233.91	0.916

MS1 Width Offset

m/z	Setting
112.99	0.15
302	-0.06
601.98	-0.15
1033.99	-0.15
1633.95	-0.07
2233.91	0.15

MS2 PreFilter

m/z	Setting
69	18.6
112.97	30
113	10
207	20.4
232	22.8
302	33.6

MS2 Axis Offset

m/z	Setting
112.99	0.772
302	0.952
601.98	1.122
1033.99	1.134
1633.95	0.994
2233.91	0.772

MS2 Width Offset

m/z	Setting
112.99	0.07
302	-0.08
601.98	-0.27
1033.99	-0.3
1633.95	-0.2
2233.91	0.07

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	8.6	0.916	2.5	0.15
Wide	8.25	1.154	2.3	0.62
Widest	7.9	1.554	2.7	1.53

MS2 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	17.6	0.772	-7.2	0.07
Wide	17.45	0.986	-7	0.52
Widest	17.2	1.432	-6.2	1.5

QQQ Check Tune Report

Instrument Name LCMS-2
MS Model G6470A
MS Instrument Serial SG1936G104
Software_Firmware Version 10.0.142, FW: A.00.08.100
Tune Date & Time 02 May 2022 08:53:55
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.71E+0 [R] (Torr); 4.67E-5 [H] (Torr)

Source Parameters

Parameter	Positive	Negative
Gas Temp (°C)	300	300
Gas Flow (l/min)	8	8
Nebulizer (psi)	15	15
Capillary (V)	4000	4000
Nozzle Voltage (V)	1500	1500
Sheath Gas Temp (°C)	250	250
Sheath Gas Flow (l/min)	7	7

Positive Results

Analyzer: MS1 Polarity: Positive Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	0.70	0.70	0.00	Pass	521531
322.05	322.02	-0.03	Pass	0.70	0.68	-0.02	Pass	184521
622.03	622.05	0.02	Pass	0.70	0.65	-0.05	Pass	259791
922.01	922.01	0.00	Pass	0.70	0.69	-0.01	Pass	278392
1521.97	1521.99	0.02	Pass	0.70	0.66	-0.04	Pass	154567
2121.93	2121.93	0.00	Pass	0.70	0.71	0.01	Pass	113688

Analyzer: MS2 Polarity: Positive Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	0.70	0.70	0.00	Pass	363555
322.05	322.03	-0.02	Pass	0.70	0.70	0.00	Pass	173122
622.03	622.02	-0.01	Pass	0.70	0.71	0.01	Pass	253938
922.01	922.02	0.01	Pass	0.70	0.68	-0.02	Pass	174074
1521.97	1521.98	0.01	Pass	0.70	0.67	-0.03	Pass	104273
2121.93	2121.94	0.01	Pass	0.70	0.71	0.01	Pass	106594

Analyzer: MS1 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.07	-0.02	Pass	1.20	1.19	-0.01	Pass	540417
322.05	322.03	-0.02	Pass	1.20	1.39	0.19	Pass	264060
622.03	622.03	0.00	Pass	1.20	1.45	0.25	Pass	453529
922.01	921.99	-0.02	Pass	1.20	1.50	0.30	Pass	429675
1521.97	1521.94	-0.03	Pass	1.20	1.33	0.13	Pass	297654
2121.93	2122.05	0.12	Pass	1.20	1.19	-0.01	Pass	205436

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.11	0.02	Pass	1.20	1.27	0.07	Pass	440212
322.05	321.99	-0.06	Pass	1.20	1.47	0.27	Pass	288042
622.03	622.11	0.08	Pass	1.20	1.64	0.44	Pass	471874
922.01	922.03	0.02	Pass	1.20	1.52	0.32	Pass	444124
1521.97	1522.07	0.10	Pass	1.20	1.27	0.07	Pass	332814
2121.93	2121.93	0.00	Pass	1.20	1.16	-0.04	Pass	221851

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	2.50	2.54	0.04	Pass	693399
322.05	322.01	-0.04	Pass	2.50	2.73	0.23	Pass	343859
622.03	622.01	-0.02	Pass	2.50	2.82	0.32	Pass	591368
922.01	921.98	-0.03	Pass	2.50	2.84	0.34	Pass	709516
1521.97	1521.95	-0.02	Pass	2.50	2.69	0.19	Pass	513248
2121.93	2121.85	-0.08	Pass	2.50	2.50	0.00	Pass	515671

QQQ Check Tune Report



Agilent

Trusted Answers

Analyzer: MS2 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.10	0.01	Pass	2.50	2.44	-0.06	Pass	648482
322.05	322.10	0.05	Pass	2.50	2.68	0.18	Pass	383137
622.03	622.05	0.02	Pass	2.50	2.82	0.32	Pass	646351
922.01	921.87	-0.14	Pass	2.50	2.91	0.41	Pass	757509
1521.97	1521.94	-0.03	Pass	2.50	2.86	0.36	Pass	627057
2121.93	2121.91	-0.02	Pass	2.50	2.45	-0.05	Pass	924519

Negative Results

Analyzer: MS1 Polarity: Negative Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	0.70	0.71	0.01	Pass	149048
302.00	302.00	0.00	Pass	0.70	0.70	0.00	Pass	185656
601.98	602.00	0.02	Pass	0.70	0.72	0.02	Pass	304488
1033.99	1034.01	0.02	Pass	0.70	0.69	-0.01	Pass	326341
1633.95	1633.95	0.00	Pass	0.70	0.69	-0.01	Pass	756589
2233.91	2233.91	0.00	Pass	0.70	0.71	0.01	Pass	735735

Analyzer: MS2 Polarity: Negative Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	0.70	0.69	-0.01	Pass	96138
302.00	301.98	-0.02	Pass	0.70	0.73	0.03	Pass	143822
601.98	601.98	0.00	Pass	0.70	0.71	0.01	Pass	217568
1033.99	1034.00	0.01	Pass	0.70	0.67	-0.03	Pass	360938
1633.95	1633.96	0.01	Pass	0.70	0.65	-0.05	Pass	866930
2233.91	2233.94	0.03	Pass	0.70	0.70	0.00	Pass	554603

Analyzer: MS1 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.00	0.01	Pass	1.20	1.27	0.07	Pass	178909
302.00	302.01	0.01	Pass	1.20	1.48	0.28	Pass	247526
601.98	602.03	0.05	Pass	1.20	1.51	0.31	Pass	499956
1033.99	1034.00	0.01	Pass	1.20	1.47	0.27	Pass	695852
1633.95	1633.91	-0.04	Pass	1.20	1.36	0.16	Pass	1528695
2233.91	2233.89	-0.02	Pass	1.20	1.13	-0.07	Pass	1101172

Analyzer: MS2 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	1.20	1.19	-0.01	Pass	138898
302.00	301.96	-0.04	Pass	1.20	1.43	0.23	Pass	254399
601.98	601.94	-0.04	Pass	1.20	1.66	0.46	Pass	458293
1033.99	1033.99	0.00	Pass	1.20	1.60	0.40	Pass	817459
1633.95	1633.98	0.03	Pass	1.20	1.41	0.21	Pass	2638143
2233.91	2233.99	0.08	Pass	1.20	1.21	0.01	Pass	1801855

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.03	0.04	Pass	2.50	2.41	-0.09	Pass	199221
302.00	302.10	0.10	Pass	2.50	2.52	0.02	Pass	312947
601.98	602.11	0.13	Pass	2.50	2.50	0.00	Pass	764295
1033.99	1033.96	-0.03	Pass	2.50	2.73	0.23	Pass	999538
1633.95	1634.00	0.05	Pass	2.50	2.26	-0.24	Pass	3455914
2233.91	2233.74	-0.17	Pass	2.50	2.18	-0.32	Pass	3012700

Analyzer: MS2 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.96	-0.03	Pass	2.50	2.47	-0.03	Pass	194904
302.00	301.97	-0.03	Pass	2.50	2.77	0.27	Pass	312104
601.98	601.97	-0.01	Pass	2.50	2.89	0.39	Pass	700920
1033.99	1034.05	0.06	Pass	2.50	2.95	0.45	Pass	1212655
1633.95	1633.97	0.02	Pass	2.50	2.65	0.15	Pass	4828738
2233.91	2233.97	0.06	Pass	2.50	2.53	0.03	Pass	5434501

QQQ Check Tune Report

Instrument Name LCMS-2
MS Model G6470A
MS Instrument Serial SG1936G104
Software_Firmware Version 10.0.142, FW: A.00.08.100
Tune Date & Time 03 May 2022 07:39:45
Data Path D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.63E+0 [R] (Torr); 4.56E-5 [H] (Torr)

Source Parameters

Parameter	Positive	Negative
Gas Temp (°C)	300	300
Gas Flow (l/min)	8	8
Nebulizer (psi)	15	15
Capillary (V)	4000	4000
Nozzle Voltage (V)	1500	1500
Sheath Gas Temp (°C)	250	250
Sheath Gas Flow (l/min)	7	7

Positive Results

Analyzer: MS1 Polarity: Positive Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.10	0.01	Pass	0.70	0.68	-0.02	Pass	544629
322.05	322.03	-0.02	Pass	0.70	0.68	-0.02	Pass	185514
622.03	622.03	0.00	Pass	0.70	0.68	-0.02	Pass	300880
922.01	922.04	0.03	Pass	0.70	0.65	-0.05	Pass	295802
1521.97	1521.99	0.02	Pass	0.70	0.66	-0.04	Pass	160323
2121.93	2121.93	0.00	Pass	0.70	0.68	-0.02	Pass	123461

Analyzer: MS2 Polarity: Positive Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	0.70	0.70	0.00	Pass	385203
322.05	322.01	-0.04	Pass	0.70	0.72	0.02	Pass	175085
622.03	622.02	-0.01	Pass	0.70	0.73	0.03	Pass	261201
922.01	922.02	0.01	Pass	0.70	0.70	0.00	Pass	200504
1521.97	1521.98	0.01	Pass	0.70	0.66	-0.04	Pass	125443
2121.93	2121.98	0.05	Pass	0.70	0.68	-0.02	Pass	122903

Analyzer: MS1 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.08	-0.01	Pass	1.20	1.20	0.00	Pass	593118
322.05	322.04	-0.01	Pass	1.20	1.41	0.21	Pass	270463
622.03	622.03	0.00	Pass	1.20	1.45	0.25	Pass	478516
922.01	922.03	0.02	Pass	1.20	1.41	0.21	Pass	512701
1521.97	1521.96	-0.01	Pass	1.20	1.30	0.10	Pass	322979
2121.93	2122.01	0.08	Pass	1.20	1.18	-0.02	Pass	226100

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.11	0.02	Pass	1.20	1.26	0.06	Pass	509533
322.05	322.01	-0.04	Pass	1.20	1.51	0.31	Pass	294278
622.03	622.11	0.08	Pass	1.20	1.64	0.44	Pass	502639
922.01	922.02	0.01	Pass	1.20	1.53	0.33	Pass	481795
1521.97	1522.08	0.11	Pass	1.20	1.26	0.06	Pass	352160
2121.93	2121.92	-0.01	Pass	1.20	1.16	-0.04	Pass	246147

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.10	0.01	Pass	2.50	2.54	0.04	Pass	704737
322.05	322.02	-0.03	Pass	2.50	2.72	0.22	Pass	353548
622.03	622.04	0.01	Pass	2.50	2.77	0.27	Pass	628492
922.01	921.99	-0.02	Pass	2.50	2.83	0.33	Pass	752426
1521.97	1521.95	-0.02	Pass	2.50	2.66	0.16	Pass	545601
2121.93	2121.86	-0.07	Pass	2.50	2.50	0.00	Pass	530530

QQQ Check Tune Report



Agilent

Trusted Answers

Analyzer: MS2 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.11	0.02	Pass	2.50	2.43	-0.07	Pass	668745
322.05	322.04	-0.01	Pass	2.50	2.73	0.23	Pass	388931
622.03	622.08	0.05	Pass	2.50	2.96	0.46	Pass	673797
922.01	921.87	-0.14	Pass	2.50	2.83	0.33	Pass	788229
1521.97	1521.99	0.02	Pass	2.50	2.62	0.12	Pass	770532
2121.93	2121.92	-0.01	Pass	2.50	2.43	-0.07	Pass	930386

Negative Results

Analyzer: MS1 Polarity: Negative Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	0.70	0.72	0.02	Pass	145410
302.00	302.02	0.02	Pass	0.70	0.68	-0.02	Pass	197532
601.98	602.06	0.08	Pass	0.70	0.65	-0.05	Pass	335363
1033.99	1034.01	0.02	Pass	0.70	0.69	-0.01	Pass	333576
1633.95	1633.97	0.02	Pass	0.70	0.70	0.00	Pass	766046
2233.91	2233.91	0.00	Pass	0.70	0.71	0.01	Pass	740886

Analyzer: MS2 Polarity: Negative Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	0.70	0.70	0.00	Pass	103349
302.00	301.96	-0.04	Pass	0.70	0.72	0.02	Pass	177712
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	292135
1033.99	1034.01	0.02	Pass	0.70	0.69	-0.01	Pass	315818
1633.95	1633.99	0.04	Pass	0.70	0.66	-0.04	Pass	862698
2233.91	2233.98	0.07	Pass	0.70	0.69	-0.01	Pass	617607

Analyzer: MS1 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.99	0.00	Pass	1.20	1.26	0.06	Pass	187913
302.00	301.94	-0.06	Pass	1.20	1.50	0.30	Pass	289826
601.98	602.00	0.02	Pass	1.20	1.53	0.33	Pass	654762
1033.99	1034.00	0.01	Pass	1.20	1.49	0.29	Pass	679681
1633.95	1633.92	-0.03	Pass	1.20	1.31	0.11	Pass	1738751
2233.91	2233.88	-0.03	Pass	1.20	1.12	-0.08	Pass	1231229

Analyzer: MS2 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	1.20	1.24	0.04	Pass	150571
302.00	301.96	-0.04	Pass	1.20	1.42	0.22	Pass	268832
601.98	601.97	-0.01	Pass	1.20	1.61	0.41	Pass	559240
1033.99	1034.04	0.05	Pass	1.20	1.65	0.45	Pass	747012
1633.95	1633.99	0.04	Pass	1.20	1.40	0.20	Pass	2637370
2233.91	2234.06	0.15	Pass	1.20	1.21	0.01	Pass	1703038

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	2.50	2.43	-0.07	Pass	210516
302.00	302.05	0.05	Pass	2.50	2.54	0.04	Pass	343068
601.98	601.98	0.00	Pass	2.50	2.64	0.14	Pass	894691
1033.99	1033.93	-0.06	Pass	2.50	2.71	0.21	Pass	1016259
1633.95	1633.95	0.00	Pass	2.50	2.35	-0.15	Pass	3566449
2233.91	2233.83	-0.08	Pass	2.50	2.14	-0.36	Pass	3109879

Analyzer: MS2 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.94	-0.05	Pass	2.50	2.49	-0.01	Pass	198395
302.00	302.00	0.00	Pass	2.50	2.70	0.20	Pass	333804
601.98	601.97	-0.01	Pass	2.50	2.93	0.43	Pass	779751
1033.99	1034.01	0.02	Pass	2.50	3.01	0.51	Pass	1209875
1633.95	1633.94	-0.01	Pass	2.50	2.86	0.36	Pass	4547992
2233.91	2233.97	0.06	Pass	2.50	2.52	0.02	Pass	5448878