



Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LCMS-3

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
11/2/2022				KMY 11/2/2022				✓ pass KMY 11/8/2022	✓	✗		KMY

Signature:

Date Completed:

11/09/2022

Instrument Name LCMS-3
MS Model G6470B
MS Instrument Serial SG2050G211
Software_Firmware Version 10.1.67, FW: A.00.08.112
Tune Date & Time 02 November 2022 10:36:32
File Path D:\MassHunter\Tune\QQQ\G6470B\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.22E+0 [R] (Torr); 3.79E-5 [H] (Torr)

Source Parameters

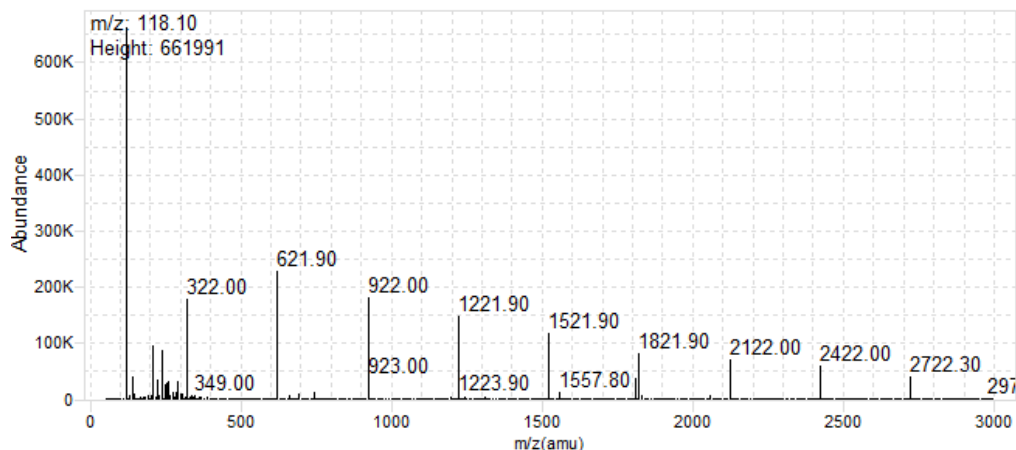
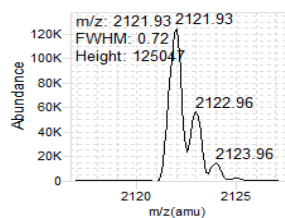
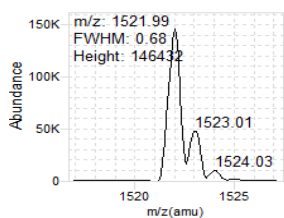
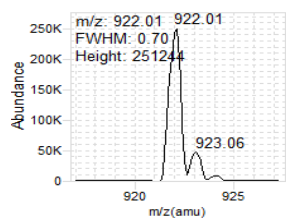
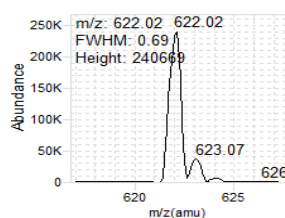
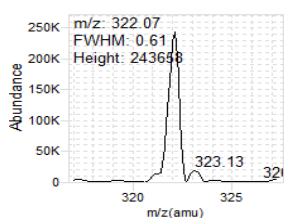
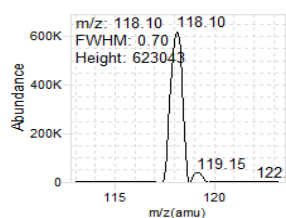
Parameter	Positive	Negative
Gas Temp (°C)	300	300
Gas Flow (l/min)	8	8
Nebulizer (psi)	15	15
Capillary (V)	4000	3500
Nozzle Voltage (V)	1500	1500
Sheath Gas Temp (°C)	250	250
Sheath Gas Flow (l/min)	7	7

Positive Results

Analyzer: MS1

Polarity: Positive

Width: Unit

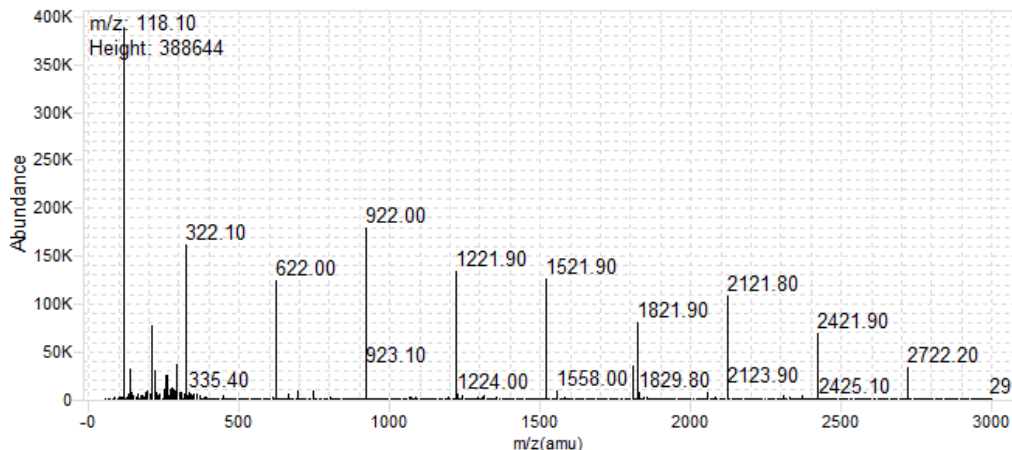
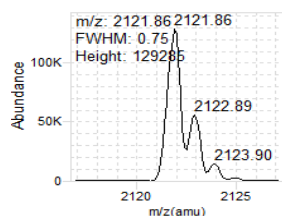
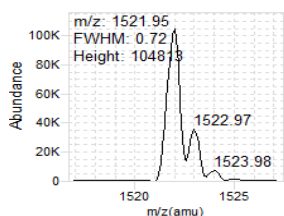
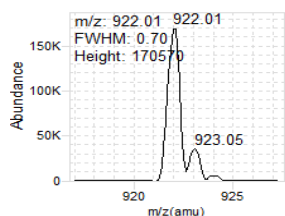
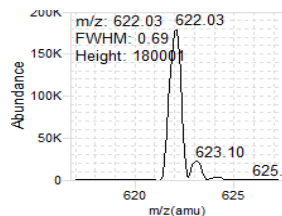
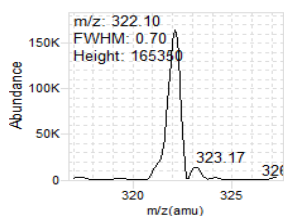
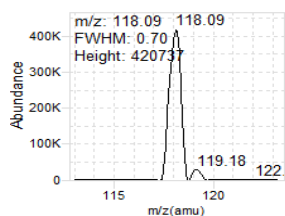


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.10	118.09	0.70	0.70	623043
322.07	322.05	0.61	0.70	243658
622.02	622.03	0.69	0.70	240669
922.01	922.01	0.70	0.70	251244
1521.99	1521.97	0.68	0.70	146432
2121.94	2121.93	0.72	0.70	125047

Analyzer: MS2

Polarity: Positive

Width: Unit

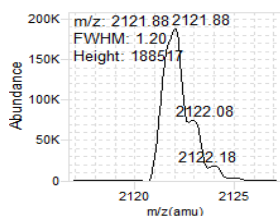
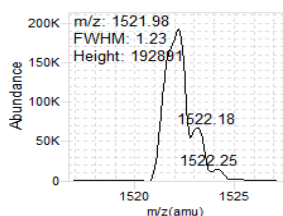
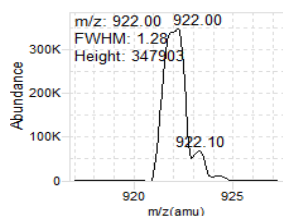
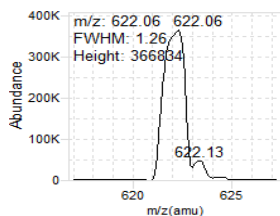
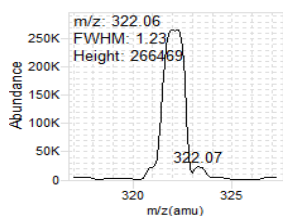
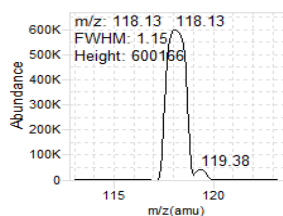


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.09	118.09	0.70	0.70	420737
322.10	322.05	0.70	0.70	165350
622.03	622.03	0.69	0.70	180001
922.01	922.01	0.70	0.70	170570
1521.95	1521.97	0.72	0.70	104813
2121.87	2121.93	0.75	0.70	129285

Analyzer: MS1

Polarity: Positive

Width: Wide

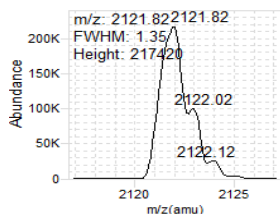
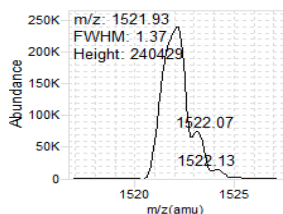
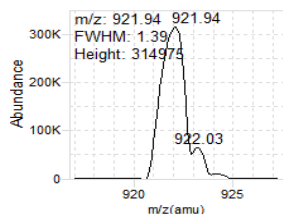
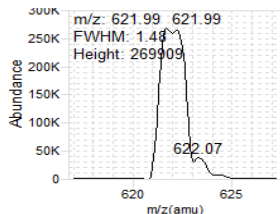
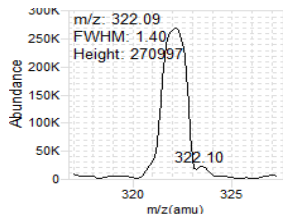
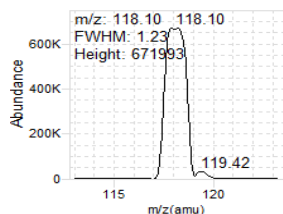


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.13	118.09	1.15	1.20	600166
322.06	322.05	1.23	1.20	266469
622.06	622.03	1.26	1.20	366834
922.00	922.01	1.28	1.20	347903
1521.98	1521.97	1.23	1.20	192891
2121.88	2121.93	1.20	1.20	188517

Analyzer: MS2

Polarity: Positive

Width: Wide

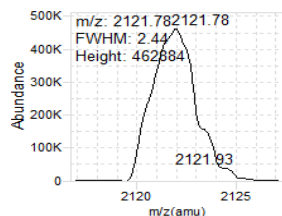
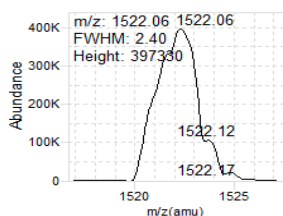
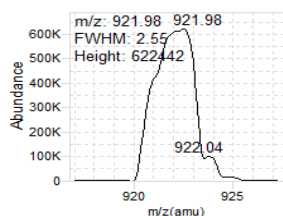
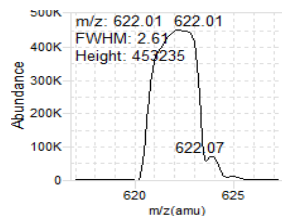
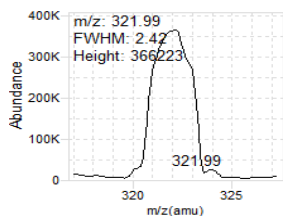
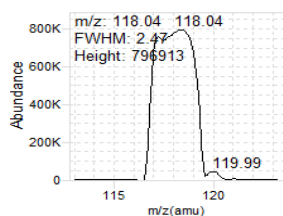


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.10	118.09	1.23	1.20	671993
322.09	322.05	1.40	1.20	270997
621.99	622.03	1.48	1.20	269909
921.94	922.01	1.39	1.20	314975
1521.92	1521.97	1.37	1.20	240429
2121.82	2121.93	1.35	1.20	217420

Analyzer: MS1

Polarity: Positive

Width: Widest

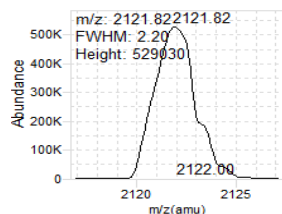
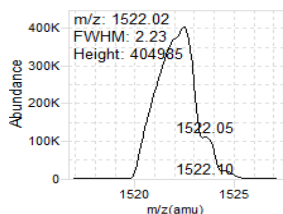
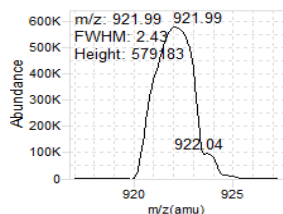
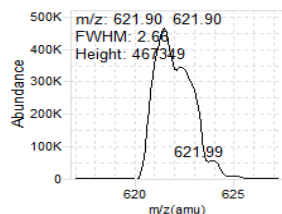
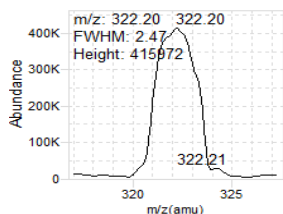
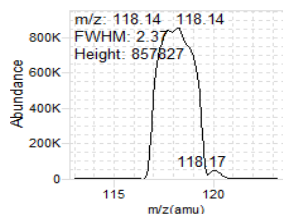


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.04	118.09	2.47	2.50	796913
321.99	322.05	2.42	2.50	366223
622.00	622.03	2.61	2.50	453235
921.98	922.01	2.55	2.50	622442
1522.06	1521.97	2.40	2.50	397330
2121.79	2121.93	2.45	2.50	462884

Analyzer: MS2

Polarity: Positive

Width: Widest



m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.14	118.09	2.37	2.50	857827
322.20	322.05	2.47	2.50	415972
621.90	622.03	2.66	2.50	467349
921.99	922.01	2.43	2.50	579183
1522.01	1521.97	2.23	2.50	404985
2121.82	2121.93	2.20	2.50	529030

Positive Results

Tune Parameters

Parameters	Setting
Fragmentor (V)	135
Skimmer (V)	15
Octopole DC (V)	5
Octopole RF (V)	600
Lens 1 DC[MS1] (V)	3.50
MS1 PreFilter (V)	-11
MS1 DC (V)	3.00
MS1 PostFilter (V)	2.00
MS1 Axis Offset	0.88
MS1 Axis Gain	-8
MS1 Width Offset	0
MS1 Width Gain	-1
MS1 Heater (°C)	100
MS2 DC (V)	-10
MS2 PreFilter (V)	-14
MS2 Axis Offset	0.90
MS2 Axis Gain	19.65
MS2 Width Offset	-0.02
MS2 Width Gain	-18
MS2 Heater (°C)	100
Cell Entry (V)	1
Hexapole DC (V)	0.00
Hexapole RF (V)	500
Hexapole Accel (V)	5
Cell Exit (V)	-7
Collision Gas	1
Iris (V)	-150
HED (kV)	-10
EMV (V)	1235
Collision Energy (eV)	0
Lens 1[MS2] (V)	1.40
MS1 PreFilter[MS2] (V)	1.80

Dynamic Ramp Tables

MS1 PreFilter (V)

m/z	Setting
118.09	-13.2
322.05	-5.4
622.03	-10.4
922.01	-16
1521.97	-13
2121.93	-14.6

MS1 Axis Offset

m/z	Setting
118.09	0.884
322.05	0.939
622.03	1.016
922.01	1.06
1521.97	1.015
2121.93	0.884

MS1 Width Offset

m/z	Setting
118.09	0.1
322.05	0.04
622.03	-0.02
922.01	-0.04
1521.97	0
2121.93	0.1

MS2 PreFilter (V)

m/z	Setting
58	-15.8
79	-20.6
117.97	-30
118	-14
154	-15.6
290	-34.2

MS2 Axis Offset

m/z	Setting
118.09	0.902
322.05	1.099
622.03	1.104
922.01	1.09
1521.97	1.052
2121.93	0.902

MS2 Width Offset

m/z	Setting
118.09	-0.02
322.05	-0.16
622.03	-0.19
922.01	-0.18
1521.97	-0.15
2121.93	-0.02

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	-7.9	0.884	-1.4	0.1
Wide	-8.2	1.066	-1.4	0.45
Widest	-8.45	1.476	-0.9	1.44

MS2 Calibrations

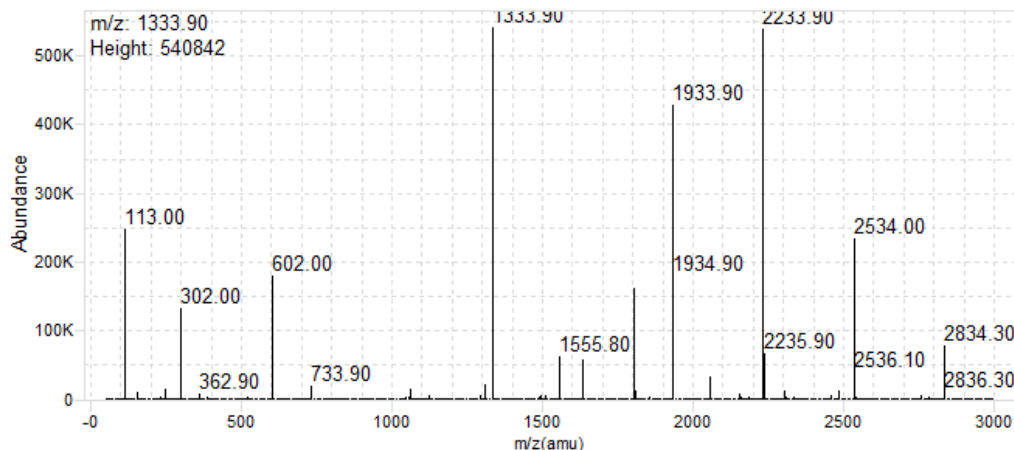
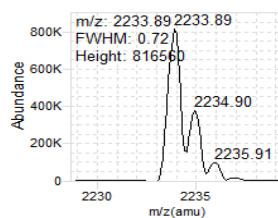
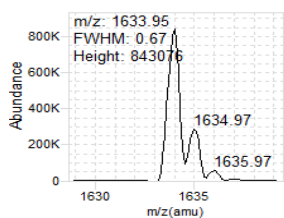
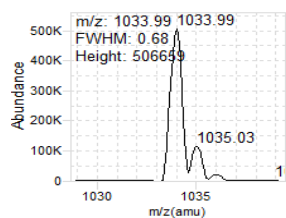
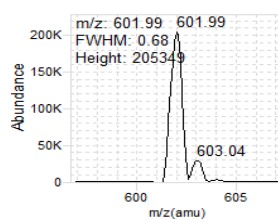
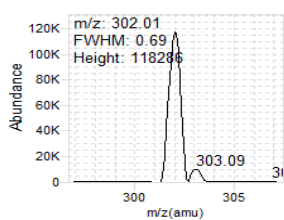
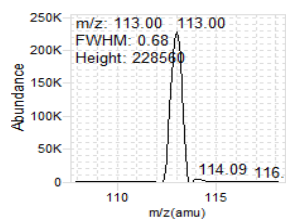
Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	19.65	0.902	-18.3	-0.02
Wide	19.35	1.118	-18.3	0.45
Widest	19.05	1.578	-18.2	1.38

Negative Results

Analyzer: MS1

Polarity: Negative

Width: Unit

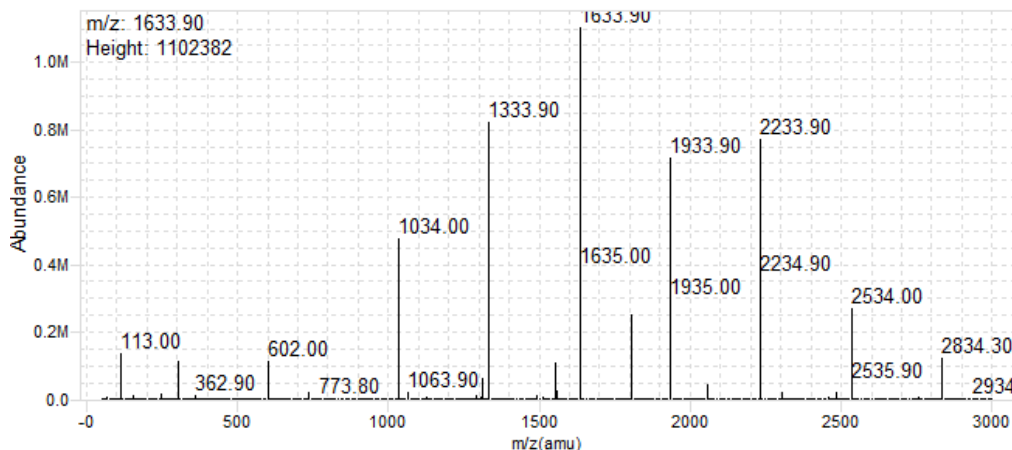
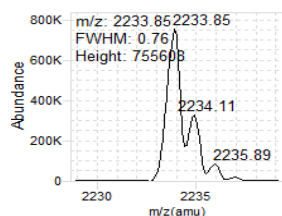
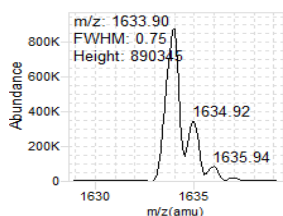
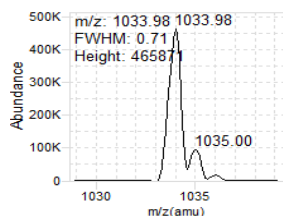
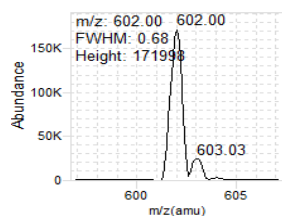
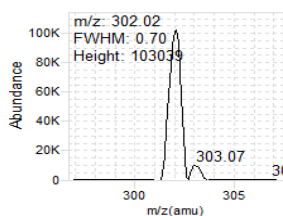
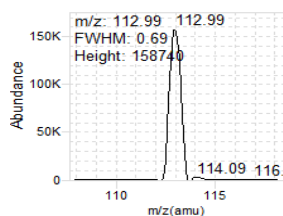


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.00	112.99	0.68	0.70	228560
302.01	302.00	0.69	0.70	118286
601.99	601.98	0.68	0.70	205349
1033.99	1033.99	0.68	0.70	506659
1633.95	1633.95	0.67	0.70	843076
2233.89	2233.91	0.72	0.70	816560

Analyzer: MS2

Polarity: Negative

Width: Unit

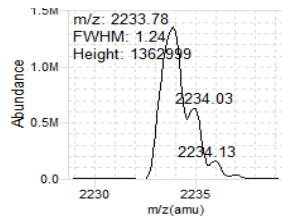
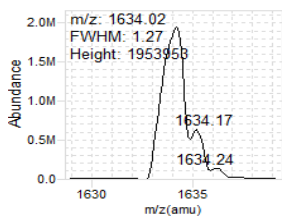
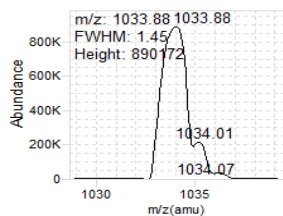
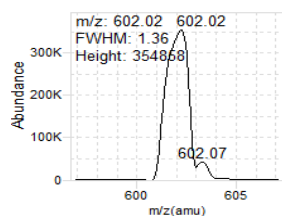
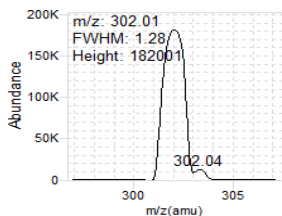
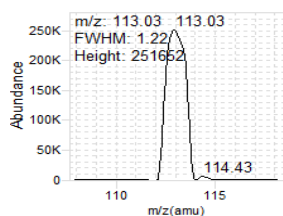


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.99	112.99	0.69	0.70	158740
302.02	302.00	0.70	0.70	103039
601.99	601.98	0.68	0.70	171998
1033.98	1033.99	0.71	0.70	465871
1633.90	1633.95	0.75	0.70	890345
2233.86	2233.91	0.76	0.70	755608

Analyzer: MS1

Polarity: Negative

Width: Wide

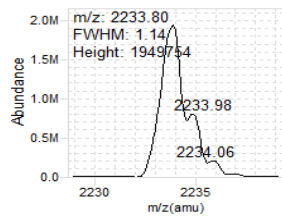
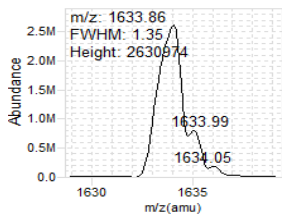
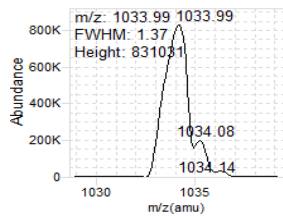
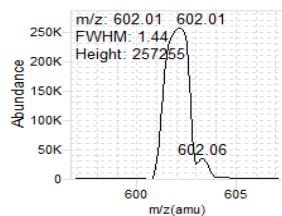
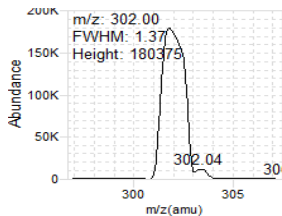
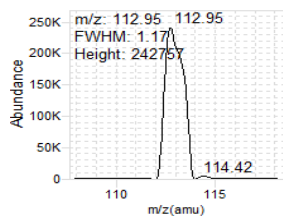


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.03	112.99	1.22	1.20	251652
302.01	302.00	1.28	1.20	182001
602.02	601.98	1.36	1.20	354858
1033.88	1033.99	1.45	1.20	890172
1634.02	1633.95	1.27	1.20	1953953
2233.79	2233.91	1.24	1.20	1362999

Analyzer: MS2

Polarity: Negative

Width: Wide

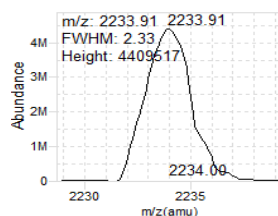
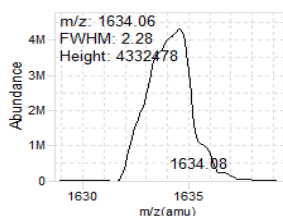
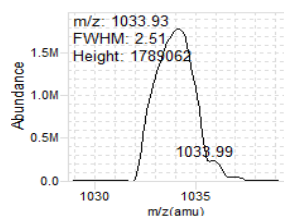
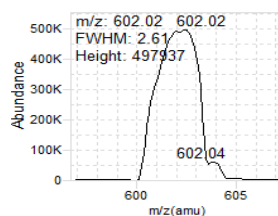
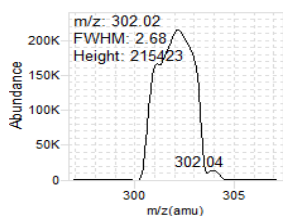
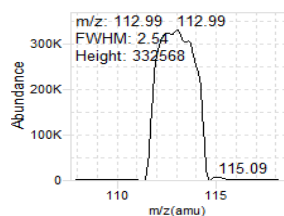


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.95	112.99	1.17	1.20	242757
302.00	302.00	1.37	1.20	180375
602.00	601.98	1.44	1.20	257255
1033.99	1033.99	1.36	1.20	831031
1633.86	1633.95	1.35	1.20	2630975
2233.80	2233.91	1.14	1.20	1949754

Analyzer: MS1

Polarity: Negative

Width: Widest

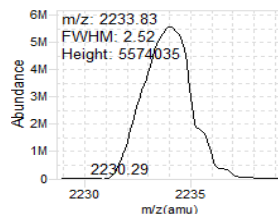
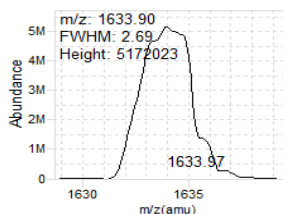
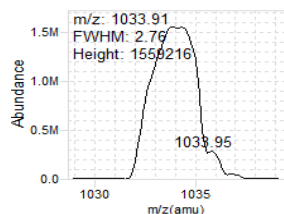
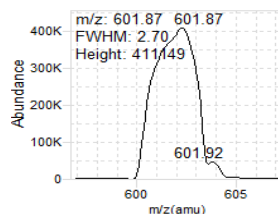
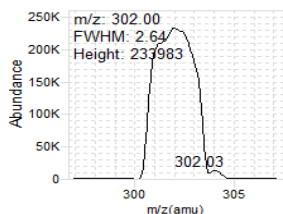
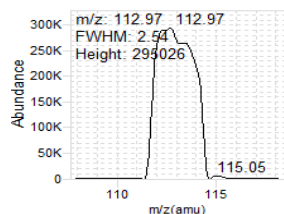


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.99	112.99	2.54	2.50	332568
302.02	302.00	2.68	2.50	215423
602.01	601.98	2.61	2.50	497937
1033.93	1033.99	2.51	2.50	1789062
1634.06	1633.95	2.28	2.50	4332478
2233.92	2233.91	2.34	2.50	4409517

Analyzer: MS2

Polarity: Negative

Width: Widest



m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.97	112.99	2.54	2.50	295026
302.00	302.00	2.64	2.50	233983
601.87	601.98	2.69	2.50	411149
1033.90	1033.99	2.76	2.50	1559217
1633.90	1633.95	2.69	2.50	5172023
2233.84	2233.91	2.53	2.50	5574035

Negative Results

Tune Parameters

Parameters	Setting
Fragmentor (V)	115
Skimmer (V)	15
Octopole DC (V)	5
Octopole RF (V)	600
Lens 1 DC[MS1] (V)	-3.50
MS1 PreFilter (V)	12
MS1 DC (V)	-3.00
MS1 PostFilter (V)	-2.00
MS1 Axis Offset	0.90
MS1 Axis Gain	-8.05
MS1 Width Offset	0.08
MS1 Width Gain	-2
MS1 Heater (°C)	100
MS2 DC (V)	10
MS2 PreFilter (V)	30
MS2 Axis Offset	0.93
MS2 Axis Gain	19.35
MS2 Width Offset	-0.02
MS2 Width Gain	-18
MS2 Heater (°C)	100
Cell Entry (V)	1
Hexapole DC (V)	0.00
Hexapole RF (V)	500
Hexapole Accel (V)	5
Cell Exit (V)	7.00
Collision Gas	1
Iris (V)	150
HED (kV)	18
EMV (V)	1240
Collision Energy (eV)	0
Lens 1[MS2] (V)	0.00
MS1 PreFilter[MS2] (V)	-1.80

Dynamic Ramp Tables

MS1 PreFilter (V)

m/z	Setting
112.99	11
302	8.6
601.98	10.2
1033.99	21.7
1633.95	18.5
2233.91	15.9

MS1 Axis Offset

m/z	Setting
112.99	0.902
302	0.985
601.98	1.047
1033.99	1.095
1633.95	1.038
2233.91	0.902

MS1 Width Offset

m/z	Setting
112.99	0.08
302	0.03
601.98	-0.08
1033.99	-0.12
1633.95	-0.06
2233.91	0.08

MS2 PreFilter (V)

m/z	Setting
69	16.4
112.97	30
113	10
207	21
232	23.4
302	33.6

MS2 Axis Offset

m/z	Setting
112.99	0.93
302	1.101
601.98	1.123
1033.99	1.123
1633.95	1.086
2233.91	0.93

MS2 Width Offset

m/z	Setting
112.99	-0.02
302	-0.11
601.98	-0.14
1033.99	-0.15
1633.95	-0.13
2233.91	-0.02

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	-8.05	0.902	-1.6	0.08
Wide	-8.4	1.134	-1.6	0.53
Widest	-8.5	1.59	-1.1	1.53

MS2 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	19.35	0.93	-18.3	-0.02
Wide	19.05	1.142	-18.2	0.46
Widest	18.95	1.584	-17.5	1.44

QQQ Check Tune Report

Instrument Name LCMS-3
MS Model G6470B
MS Instrument Serial SG2050G211
Software_Firmware Version 10.1.67, FW: A.00.08.112
Tune Date & Time 02 November 2022 10:36:32
File Path D:\MassHunter\Tune\QQQ\G6470B\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.22E+0 [R] (Torr); 3.79E-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	3500
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	0.70	0.00	Pass	623043
322.05	322.07	0.02	Pass	0.70	0.61	-0.09	Pass	243658
622.03	622.02	-0.01	Pass	0.70	0.69	-0.01	Pass	240669
922.01	922.01	0.00	Pass	0.70	0.70	0.00	Pass	251244
1521.97	1521.99	0.02	Pass	0.70	0.68	-0.02	Pass	146432
2121.93	2121.94	0.01	Pass	0.70	0.72	0.02	Pass	125047

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	420737
322.05	322.10	0.05	Pass	0.70	0.70	0.00	Pass	165350
622.03	622.03	0.00	Pass	0.70	0.69	-0.01	Pass	180001
922.01	922.01	0.00	Pass	0.70	0.70	0.00	Pass	170570
1521.97	1521.95	-0.02	Pass	0.70	0.72	0.02	Pass	104813
2121.93	2121.87	-0.06	Pass	0.70	0.75	0.05	Pass	129285

Analyzer: MS1 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.13	0.04	Pass	1.20	1.15	-0.05	Pass	600166
322.05	322.06	0.01	Pass	1.20	1.23	0.03	Pass	266469
622.03	622.06	0.03	Pass	1.20	1.26	0.06	Pass	366834
922.01	922.00	-0.01	Pass	1.20	1.28	0.08	Pass	347903
1521.97	1521.98	0.01	Pass	1.20	1.23	0.03	Pass	192891
2121.93	2121.88	-0.05	Pass	1.20	1.20	0.00	Pass	188517

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.10	0.01	Pass	1.20	1.23	0.03	Pass	671993
322.05	322.09	0.04	Pass	1.20	1.40	0.20	Pass	270997
622.03	621.99	-0.04	Pass	1.20	1.48	0.28	Pass	269909
922.01	921.94	-0.07	Pass	1.20	1.39	0.19	Pass	314975
1521.97	1521.92	-0.05	Pass	1.20	1.37	0.17	Pass	240429
2121.93	2121.82	-0.11	Pass	1.20	1.35	0.15	Pass	217420

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.04	-0.05	Pass	2.50	2.47	-0.03	Pass	796913
322.05	321.99	-0.06	Pass	2.50	2.42	-0.08	Pass	366223
622.03	622.00	-0.03	Pass	2.50	2.61	0.11	Pass	453235
922.01	921.98	-0.03	Pass	2.50	2.55	0.05	Pass	622442
1521.97	1522.06	0.09	Pass	2.50	2.40	-0.10	Pass	397330
2121.93	2121.79	-0.14	Pass	2.50	2.45	-0.05	Pass	462884

Analyzer: MS2 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.14	0.05	Pass	2.50	2.37	-0.13	Pass	857827
322.05	322.20	0.15	Pass	2.50	2.47	-0.03	Pass	415972
622.03	621.90	-0.13	Pass	2.50	2.66	0.16	Pass	467349
922.01	921.99	-0.02	Pass	2.50	2.43	-0.07	Pass	579183
1521.97	1522.01	0.04	Pass	2.50	2.23	-0.27	Pass	404985
2121.93	2121.82	-0.11	Pass	2.50	2.20	-0.30	Pass	529030

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	113.00	0.01	Pass	0.70	0.68	-0.02	Pass	228560
302.00	302.01	0.01	Pass	0.70	0.69	-0.01	Pass	118286
601.98	601.99	0.01	Pass	0.70	0.68	-0.02	Pass	205349
1033.99	1033.99	0.00	Pass	0.70	0.68	-0.02	Pass	506659
1633.95	1633.95	0.00	Pass	0.70	0.67	-0.03	Pass	843076
2233.91	2233.89	-0.02	Pass	0.70	0.72	0.02	Pass	816560

Analyzer: MS2 Polarity: Negative Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.99	0.00	Pass	0.70	0.69	-0.01	Pass	158740
302.00	302.02	0.02	Pass	0.70	0.70	0.00	Pass	103039
601.98	601.99	0.01	Pass	0.70	0.68	-0.02	Pass	171998
1033.99	1033.98	-0.01	Pass	0.70	0.71	0.01	Pass	465871
1633.95	1633.90	-0.05	Pass	0.70	0.75	0.05	Pass	890345
2233.91	2233.86	-0.05	Pass	0.70	0.76	0.06	Pass	755608

Analyzer: MS1 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.03	0.04	Pass	1.20	1.22	0.02	Pass	251652
302.00	302.01	0.01	Pass	1.20	1.28	0.08	Pass	182001
601.98	602.02	0.04	Pass	1.20	1.36	0.16	Pass	354858
1033.99	1033.88	-0.11	Pass	1.20	1.45	0.25	Pass	890172
1633.95	1634.02	0.07	Pass	1.20	1.27	0.07	Pass	1953953
2233.91	2233.79	-0.12	Pass	1.20	1.24	0.04	Pass	1362999

Analyzer: MS2 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.95	-0.04	Pass	1.20	1.17	-0.03	Pass	242757
302.00	302.00	0.00	Pass	1.20	1.37	0.17	Pass	180375
601.98	602.00	0.02	Pass	1.20	1.44	0.24	Pass	257255
1033.99	1033.99	0.00	Pass	1.20	1.36	0.16	Pass	831031
1633.95	1633.86	-0.09	Pass	1.20	1.35	0.15	Pass	2630975
2233.91	2233.80	-0.11	Pass	1.20	1.14	-0.06	Pass	1949754

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.99	0.00	Pass	2.50	2.54	0.04	Pass	332568
302.00	302.02	0.02	Pass	2.50	2.68	0.18	Pass	215423
601.98	602.01	0.03	Pass	2.50	2.61	0.11	Pass	497937
1033.99	1033.93	-0.06	Pass	2.50	2.51	0.01	Pass	1789062
1633.95	1634.06	0.11	Pass	2.50	2.28	-0.22	Pass	4332478
2233.91	2233.92	0.01	Pass	2.50	2.34	-0.16	Pass	4409517

Analyzer: MS2 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.97	-0.02	Pass	2.50	2.54	0.04	Pass	295026
302.00	302.00	0.00	Pass	2.50	2.64	0.14	Pass	233983
601.98	601.87	-0.11	Pass	2.50	2.69	0.19	Pass	411149
1033.99	1033.90	-0.09	Pass	2.50	2.76	0.26	Pass	1559217
1633.95	1633.90	-0.05	Pass	2.50	2.69	0.19	Pass	5172023
2233.91	2233.84	-0.07	Pass	2.50	2.53	0.03	Pass	5574035