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
5/2/22	30 / 1700	100	✓	✓	✓	✓	✓	✓ (POS ONLY)	✓ (POS ONLY)	EC 5/13/22	Added THC column from LCMS-2 for troubleshooting	EC
5/3/2022	X	X	X	X	X	X	X	X	✓KMY 5/9/2022 (Neg only)	X	Replaced in-line filter	↓ KMY
						JE 05/10/22						

Signature: [signature] **Date Completed:** 05/10/22

QQQ Autotune Report

Agilent | Trusted Answers

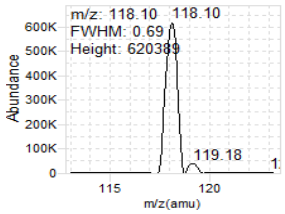
Instrument Name	LCMS-3
MS Model	G6470B
MS Instrument Serial	SG2050G211
Software_Firmware Version	10.1.67, FW: A.00.08.112
Tune Date & Time	02 May 2022 14:00:06
File Path	D:\MassHunter\Tune\QQQ\G6470B\atunes.TUNE.XML
Ion Source	AJS ESI
Ionization Mode	AJS ESI
Tuned Resolution	All
Vacuum Pressure	1.44E+0 [R] (Torr); 3.83E-5 [H] (Torr)

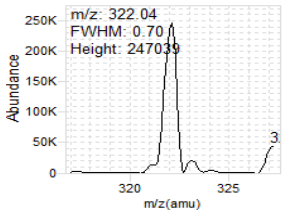
Source Parameters

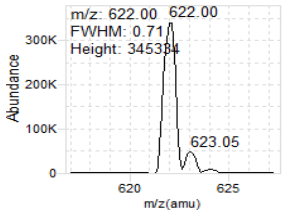
Parameter	Positive	Negative
Gas Temp (°C)	300	300
Gas Flow (l/min)	8	8
Nebulizer (psi)	15	15
Capillary (V)	4000	3500
Nozzle Voltage (V)	1500	1500
Sheath Gas Temp (°C)	250	250
Sheath Gas Flow (l/min)	7	7

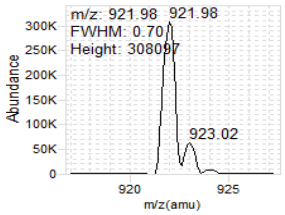
Positive Results

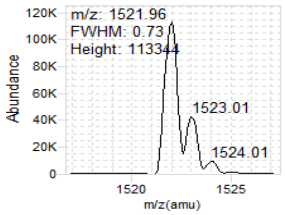
Analyzer: MS1 **Polarity: Positive** **Width: Unit**

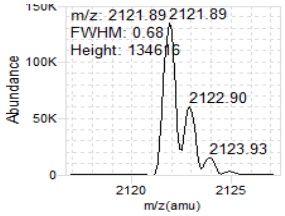


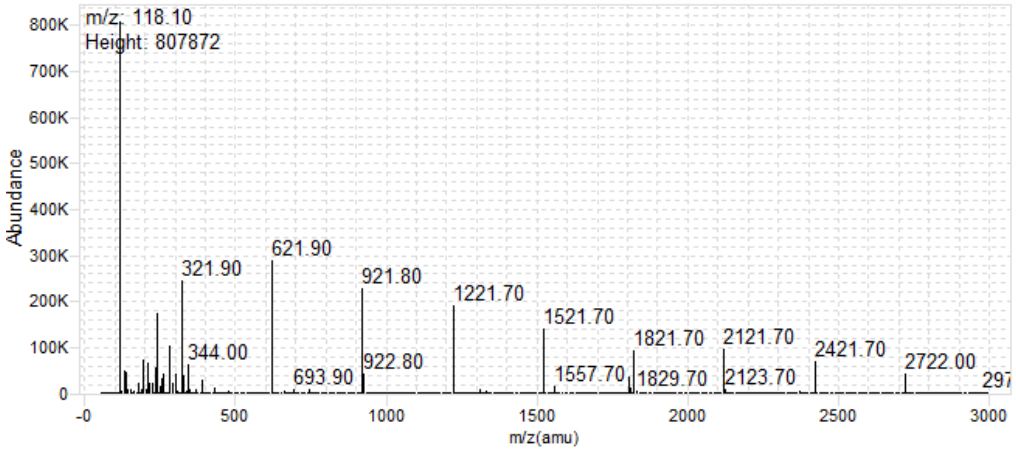






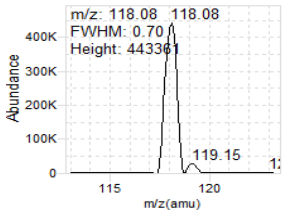


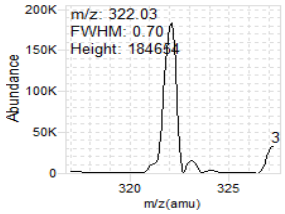


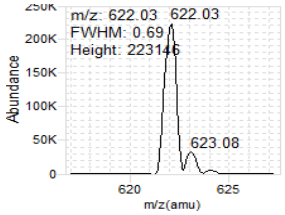


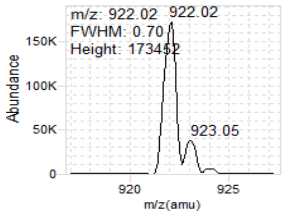
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.10	118.09	0.69	0.70	620389
322.04	322.05	0.70	0.70	247039
622.00	622.03	0.71	0.70	345334
921.98	922.01	0.70	0.70	308097
1521.96	1521.97	0.73	0.70	113344
2121.90	2121.93	0.68	0.70	134616

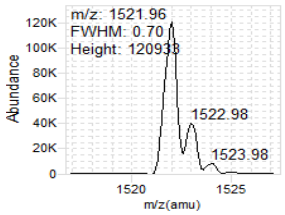
Analyzer: MS2 **Polarity: Positive** **Width: Unit**

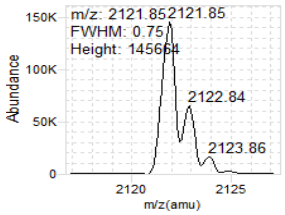


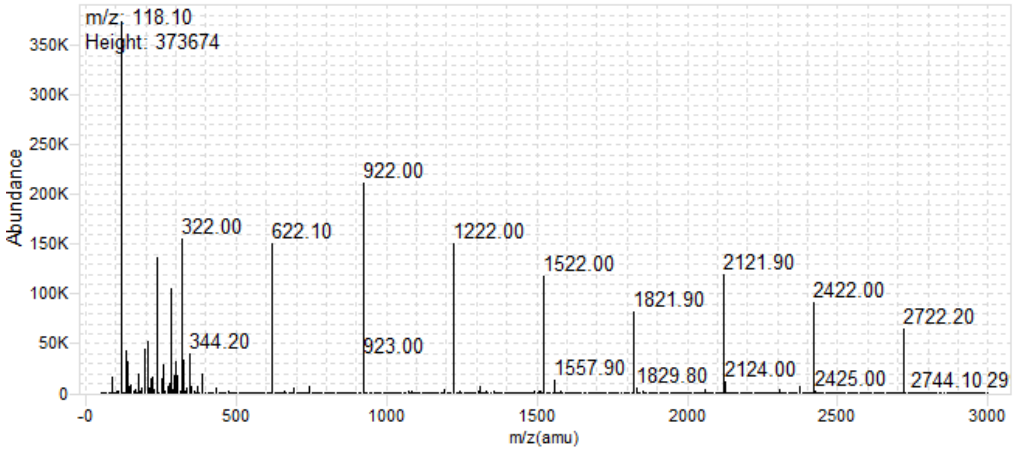






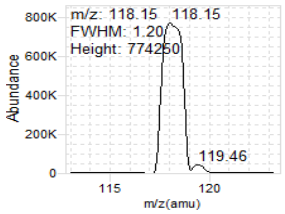


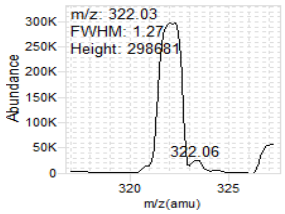


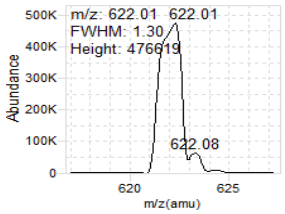


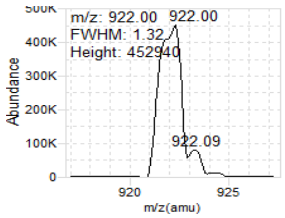
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.08	118.09	0.70	0.70	443361
322.03	322.05	0.70	0.70	184654
622.03	622.03	0.69	0.70	223146
922.02	922.01	0.70	0.70	173452
1521.96	1521.97	0.70	0.70	120933
2121.86	2121.93	0.75	0.70	145664

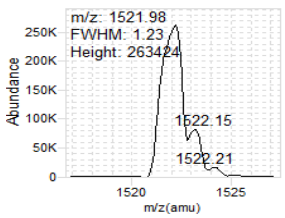
Analyzer: MS1 **Polarity: Positive** **Width: Wide**

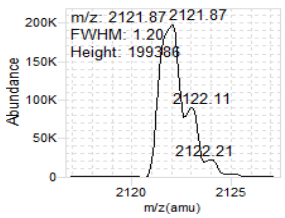






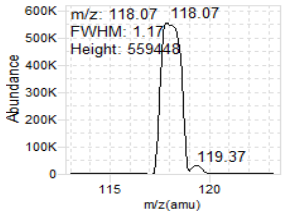


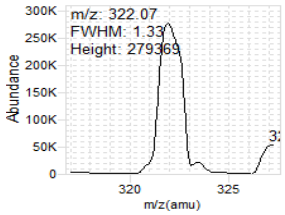


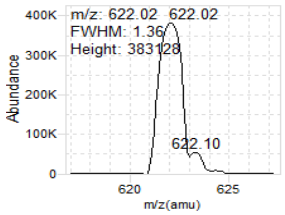


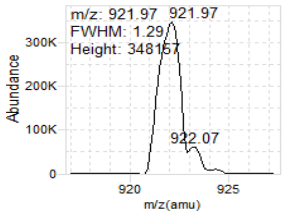
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.15	118.09	1.20	1.20	774250
322.03	322.05	1.27	1.20	298681
622.01	622.03	1.30	1.20	476619
922.00	922.01	1.32	1.20	452940
1521.98	1521.97	1.23	1.20	263424
2121.87	2121.93	1.21	1.20	199386

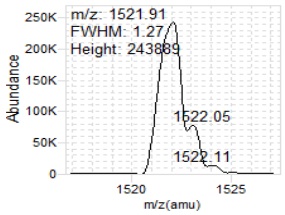
Analyzer: MS2 **Polarity: Positive** **Width: Wide**

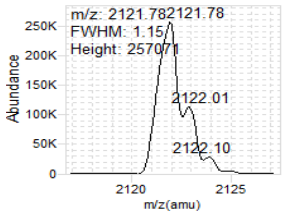






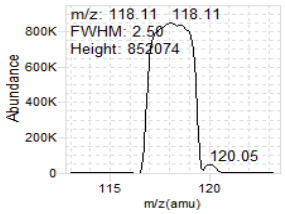


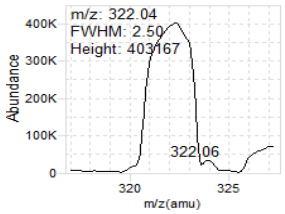


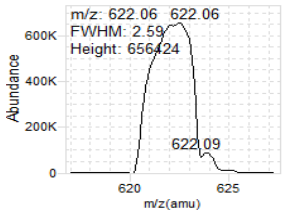


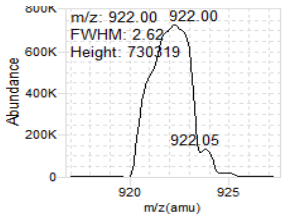
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.07	118.09	1.17	1.20	559448
322.07	322.05	1.33	1.20	279369
622.02	622.03	1.36	1.20	383129
921.97	922.01	1.29	1.20	348157
1521.91	1521.97	1.27	1.20	243889
2121.79	2121.93	1.15	1.20	257071

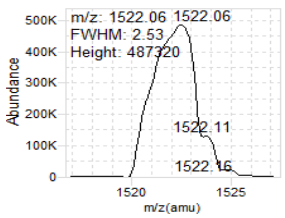
Analyzer: MS1 **Polarity: Positive** **Width: Widest**

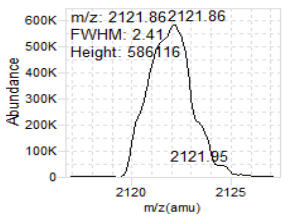






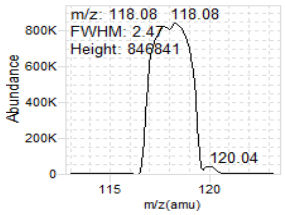


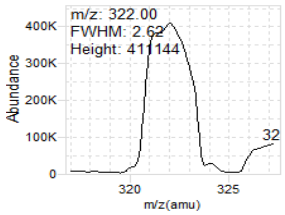


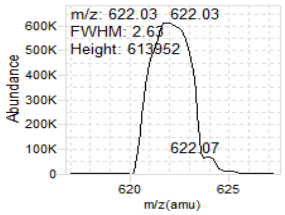


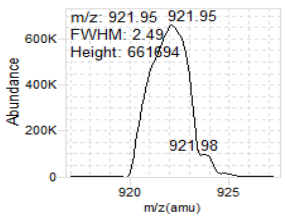
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.11	118.09	2.50	2.50	852074
322.04	322.05	2.51	2.50	403167
622.05	622.03	2.59	2.50	656424
922.00	922.01	2.62	2.50	730319
1522.06	1521.97	2.53	2.50	487320
2121.86	2121.93	2.41	2.50	586116

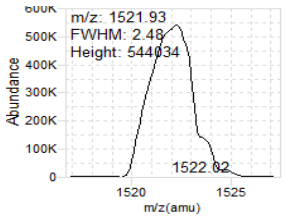
Analyzer: MS2 **Polarity: Positive** **Width: Widest**

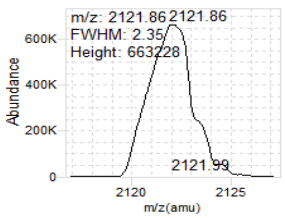












m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.08	118.09	2.47	2.50	846841
322.00	322.05	2.62	2.50	411144
622.03	622.03	2.63	2.50	613952
921.95	922.01	2.49	2.50	661694
1521.93	1521.97	2.48	2.50	544034
2121.87	2121.93	2.35	2.50	663228

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)	-16
MS1 DC (V)	3.00
MS1 PostFilter (V)	2.00
MS1 Axis Offset	0.87
MS1 Axis Gain	-7.85
MS1 Width Offset	0.12
MS1 Width Gain	-2
MS1 Heater (°C)	100
MS2 DC (V)	-10
MS2 PreFilter (V)	-14
MS2 Axis Offset	0.91
MS2 Axis Gain	19.55
MS2 Width Offset	-0.03
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)	1245
Collision Energy (eV)	0
Lens 1[MS2] (V)	2.70
MS1 PreFilter[MS2] (V)	3.00

Dynamic Ramp Tables

MS1 PreFilter (V)

m/z	Setting
118.09	-12.2
322.05	-5.4
622.03	-10
922.01	-13.8
1521.97	-12.6
2121.93	-15

MS1 Axis Offset

m/z	Setting
118.09	0.87
322.05	0.933
622.03	1.003
922.01	1.016
1521.97	1.033
2121.93	0.87

MS1 Width Offset

m/z	Setting
118.09	0.12
322.05	0.1
622.03	0.03
922.01	0.01
1521.97	0.06
2121.93	0.12

MS2 PreFilter (V)

m/z	Setting
58	-15.6
79	-20
117.97	-30
118	-11.8
154	-15.8
290	-33.4

MS2 Axis Offset

m/z	Setting
118.09	0.91
322.05	1.075
622.03	1.124
922.01	1.103
1521.97	1.059
2121.93	0.91

MS2 Width Offset

m/z	Setting
118.09	-0.03
322.05	-0.17
622.03	-0.21
922.01	-0.2
1521.97	-0.15
2121.93	-0.03

MS1 Calibrations

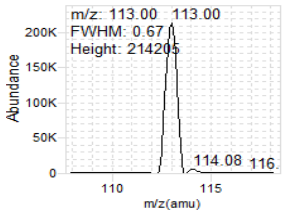
Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	-7.85	0.87	-1.5	0.12
Wide	-8.15	1.092	-1.6	0.54
Widest	-8.35	1.488	-0.9	1.5

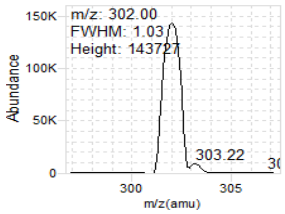
MS2 Calibrations

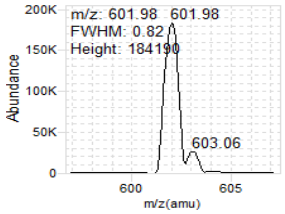
Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	19.55	0.91	-18.2	-0.03
Wide	19.25	1.098	-18.2	0.37
Widest	19.15	1.524	-17.8	1.41

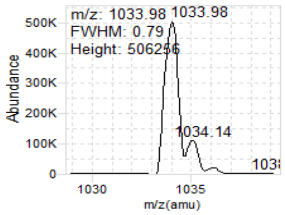
Negative Results

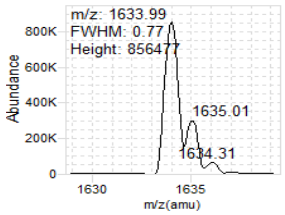
Analyzer: MS1 **Polarity: Negative** **Width: Unit**

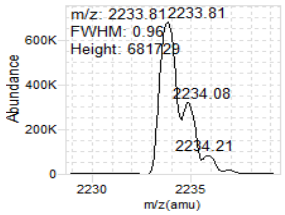


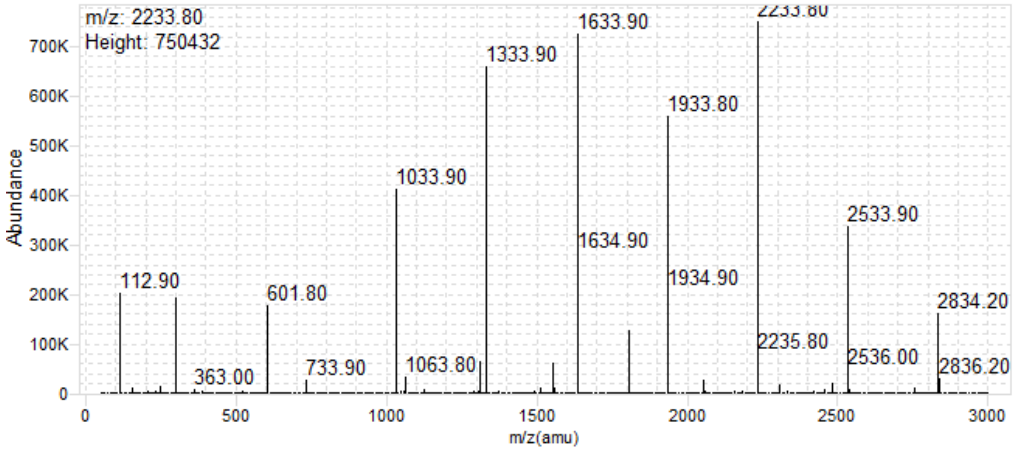






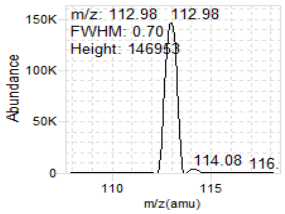


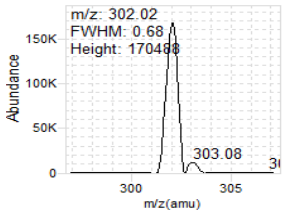


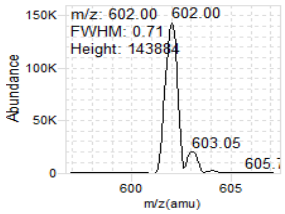


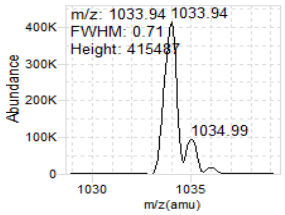
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.99	112.99	0.67	0.70	214205
302.00	302.00	1.03	0.70	143727
601.98	601.98	0.81	0.70	184190
1033.98	1033.99	0.79	0.70	506256
1633.99	1633.95	0.77	0.70	856477
2233.81	2233.91	0.96	0.70	681729

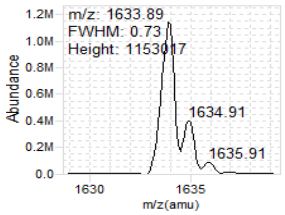
Analyzer: MS2 **Polarity: Negative** **Width: Unit**

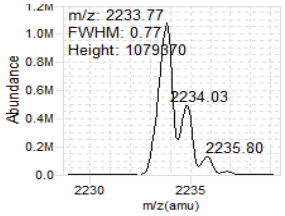


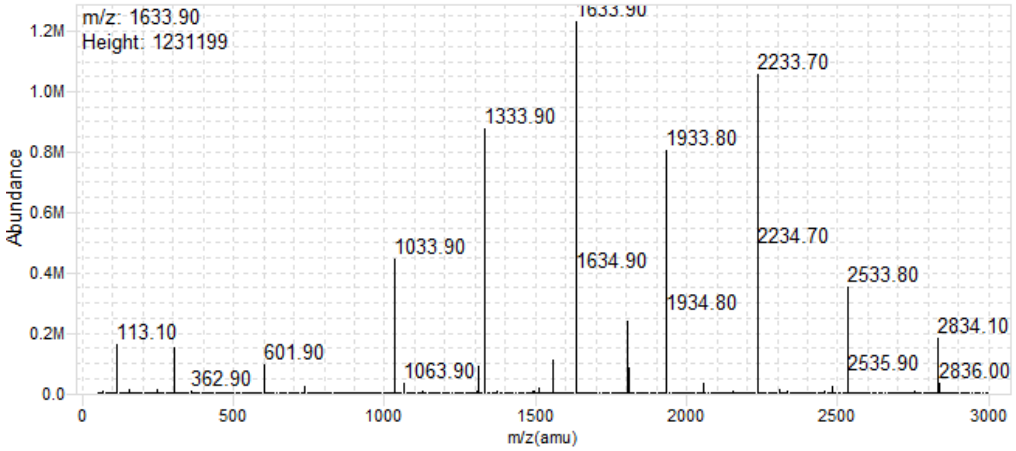






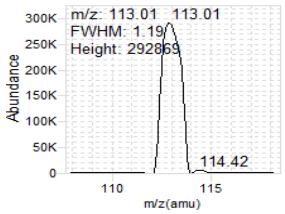


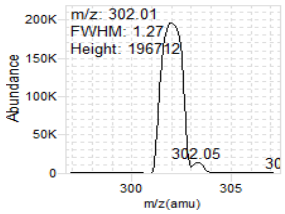


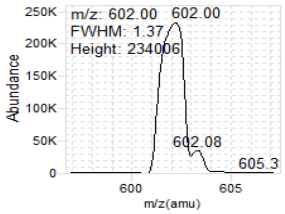


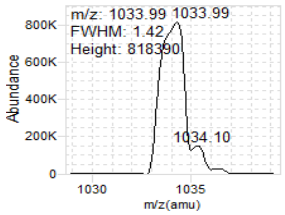
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.98	112.99	0.70	0.70	146953
302.02	302.00	0.68	0.70	170488
602.00	601.98	0.71	0.70	143884
1033.94	1033.99	0.71	0.70	415487
1633.89	1633.95	0.73	0.70	1153017
2233.77	2233.91	0.77	0.70	1079370

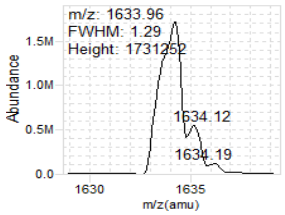
Analyzer: MS1 **Polarity: Negative** **Width: Wide**

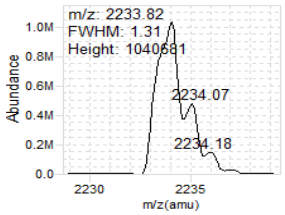






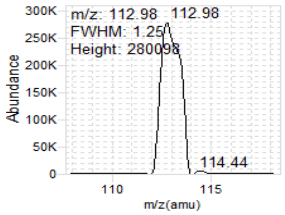


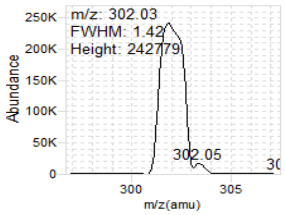


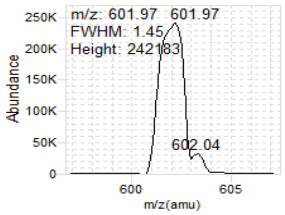


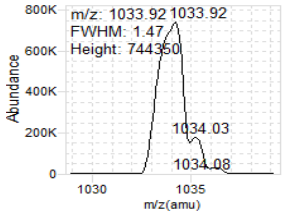
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.01	112.99	1.19	1.20	292869
302.01	302.00	1.27	1.20	196712
602.00	601.98	1.37	1.20	234006
1033.99	1033.99	1.42	1.20	818390
1633.96	1633.95	1.29	1.20	1731252
2233.83	2233.91	1.31	1.20	1040681

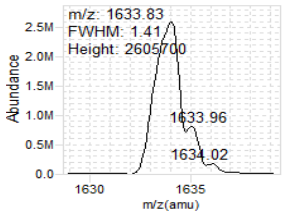
Analyzer: MS2 **Polarity: Negative** **Width: Wide**

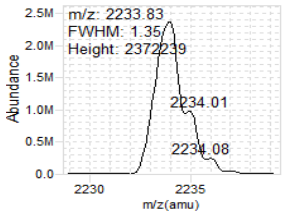






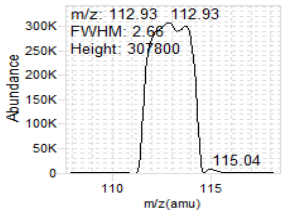


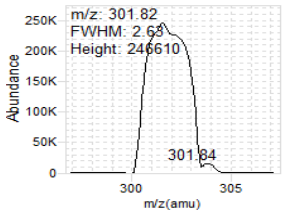


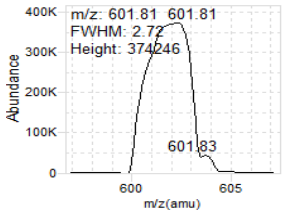


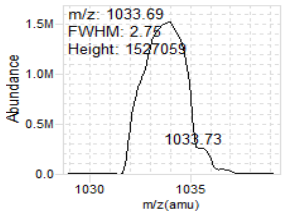
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.98	112.99	1.25	1.20	280098
302.03	302.00	1.42	1.20	242779
601.97	601.98	1.45	1.20	242183
1033.92	1033.99	1.47	1.20	744350
1633.82	1633.95	1.41	1.20	2605700
2233.83	2233.91	1.35	1.20	2372239

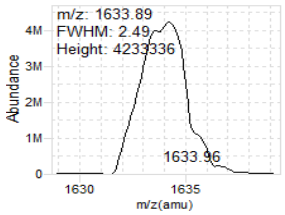
Analyzer: MS1 **Polarity: Negative** **Width: Widest**

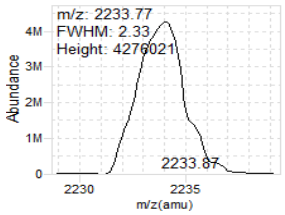






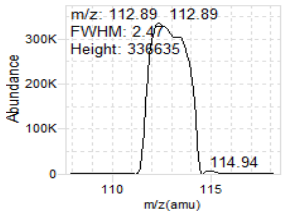


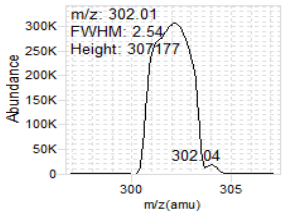


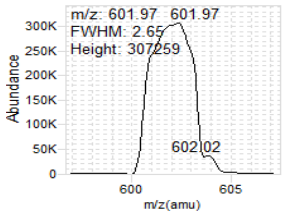


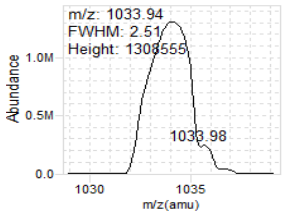
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.93	112.99	2.66	2.50	307800
301.82	302.00	2.63	2.50	246610
601.81	601.98	2.71	2.50	374246
1033.69	1033.99	2.75	2.50	1527059
1633.89	1633.95	2.49	2.50	4233336
2233.78	2233.91	2.33	2.50	4276021

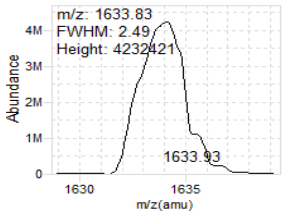
Analyzer: MS2 **Polarity: Negative** **Width: Widest**

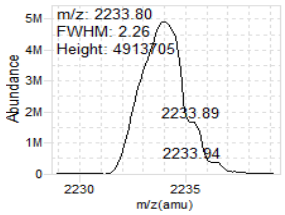












m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.89	112.99	2.47	2.50	336635
302.01	302.00	2.54	2.50	307177
601.97	601.98	2.65	2.50	307259
1033.94	1033.99	2.51	2.50	1308555
1633.83	1633.95	2.48	2.50	4232421
2233.81	2233.91	2.26	2.50	4913705

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	0.86
MS1 Axis Gain	-7.95
MS1 Width Offset	0.12
MS1 Width Gain	-1
MS1 Heater (°C)	100
MS2 DC (V)	10
MS2 PreFilter (V)	30
MS2 Axis Offset	0.92
MS2 Axis Gain	19.45
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)	-1.40

Dynamic Ramp Tables

MS1 PreFilter (V)

m/z	Setting
112.99	10.6
302	8.4
601.98	9.6
1033.99	21.3
1633.95	18.1
2233.91	14.7

MS1 Axis Offset

m/z	Setting
112.99	0.856
302	1.06
601.98	1.064
1033.99	1.114
1633.95	1.094
2233.91	0.856

MS1 Width Offset

m/z	Setting
112.99	0.12
302	0.38
601.98	0.06
1033.99	-0.03
1633.95	-0.02
2233.91	0.12

MS2 PreFilter (V)

m/z	Setting
69	15.8
112.97	30
113	10
207	20
232	23
302	35.8

MS2 Axis Offset

m/z	Setting
112.99	0.918
302	1.115
601.98	1.16
1033.99	1.127
1633.95	1.092
2233.91	0.918

MS2 Width Offset

m/z	Setting
112.99	-0.02
302	-0.12
601.98	-0.14
1033.99	-0.15
1633.95	-0.12
2233.91	-0.02

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	-7.95	0.856	-1.4	0.12
Wide	-8.2	1.072	-1.6	0.56
Widest	-8.55	1.506	-1.1	1.64

MS2 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	19.45	0.918	-18.1	-0.02
Wide	19.35	1.156	-18	0.49
Widest	19.2	1.48	-17.9	1.42

QQQ Check Tune Report

Agilent | Trusted Answers

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 May 2022 14:00:06
File Path	D:\MassHunter\Tune\QQQ\G6470B\atunes.TUNE.XML
Ion Source	AJS ESI
Ionization Mode	AJS ESI
Tuned Resolution	All
Vacuum Pressure	1.44E+0 [R] (Torr); 3.83E-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	0.69	-0.01	Pass	620389
322.05	322.04	-0.01	Pass	0.70	0.70	0.00	Pass	247039
622.03	622.00	-0.03	Pass	0.70	0.71	0.01	Pass	345334
922.01	921.98	-0.03	Pass	0.70	0.70	0.00	Pass	308097
1521.97	1521.96	-0.01	Pass	0.70	0.73	0.03	Pass	113344
2121.93	2121.90	-0.03	Pass	0.70	0.68	-0.02	Pass	134616

Analyzer: MS2 Polarity: Positive Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.08	-0.01	Pass	0.70	0.70	0.00	Pass	443361
322.05	322.03	-0.02	Pass	0.70	0.70	0.00	Pass	184654
622.03	622.03	0.00	Pass	0.70	0.69	-0.01	Pass	223146
922.01	922.02	0.01	Pass	0.70	0.70	0.00	Pass	173452
1521.97	1521.96	-0.01	Pass	0.70	0.70	0.00	Pass	120933
2121.93	2121.86	-0.07	Pass	0.70	0.75	0.05	Pass	145664

Analyzer: MS1 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.15	0.06	Pass	1.20	1.20	0.00	Pass	774250
322.05	322.03	-0.02	Pass	1.20	1.27	0.07	Pass	298681
622.03	622.01	-0.02	Pass	1.20	1.30	0.10	Pass	476619
922.01	922.00	-0.01	Pass	1.20	1.32	0.12	Pass	452940
1521.97	1521.98	0.01	Pass	1.20	1.23	0.03	Pass	263424
2121.93	2121.87	-0.06	Pass	1.20	1.21	0.01	Pass	199386

Analyzer: MS2 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	1.17	-0.03	Pass	559448
322.05	322.07	0.02	Pass	1.20	1.33	0.13	Pass	279369
622.03	622.02	-0.01	Pass	1.20	1.36	0.16	Pass	383129
922.01	921.97	-0.04	Pass	1.20	1.29	0.09	Pass	348157
1521.97	1521.91	-0.06	Pass	1.20	1.27	0.07	Pass	243889
2121.93	2121.79	-0.14	Pass	1.20	1.15	-0.05	Pass	257071

Analyzer: MS1 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	2.50	0.00	Pass	852074
322.05	322.04	-0.01	Pass	2.50	2.51	0.01	Pass	403167
622.03	622.05	0.02	Pass	2.50	2.59	0.09	Pass	656424
922.01	922.00	-0.01	Pass	2.50	2.62	0.12	Pass	730319
1521.97	1522.06	0.09	Pass	2.50	2.53	0.03	Pass	487320
2121.93	2121.86	-0.07	Pass	2.50	2.41	-0.09	Pass	586116

Analyzer: MS2 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.08	-0.01	Pass	2.50	2.47	-0.03	Pass	846841
322.05	322.00	-0.05	Pass	2.50	2.62	0.12	Pass	411144
622.03	622.03	0.00	Pass	2.50	2.63	0.13	Pass	613952
922.01	921.95	-0.06	Pass	2.50	2.49	-0.01	Pass	661694
1521.97	1521.93	-0.04	Pass	2.50	2.48	-0.02	Pass	544034
2121.93	2121.87	-0.06	Pass	2.50	2.35	-0.15	Pass	663228

QQQ Check Tune Report

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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	112.99	0.00	Pass	0.70	0.67	-0.03	Pass	214205
302.00	302.00	0.00	Pass	0.70	1.03	0.33	Adjust	143727
601.98	601.98	0.00	Pass	0.70	0.81	0.11	Pass	184190
1033.99	1033.98	-0.01	Pass	0.70	0.79	0.09	Pass	506256
1633.95	1633.99	0.04	Pass	0.70	0.77	0.07	Pass	856477
2233.91	2233.81	-0.10	Pass	0.70	0.96	0.26	Adjust	681729

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	146953
302.00	302.02	0.02	Pass	0.70	0.68	-0.02	Pass	170488
601.98	602.00	0.02	Pass	0.70	0.71	0.01	Pass	143884
1033.99	1033.94	-0.05	Pass	0.70	0.71	0.01	Pass	415487
1633.95	1633.89	-0.06	Pass	0.70	0.73	0.03	Pass	1153017
2233.91	2233.77	-0.14	Pass	0.70	0.77	0.07	Pass	1079370

Analyzer: MS1 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.01	0.02	Pass	1.20	1.19	-0.01	Pass	292869
302.00	302.01	0.01	Pass	1.20	1.27	0.07	Pass	196712
601.98	602.00	0.02	Pass	1.20	1.37	0.17	Pass	234006
1033.99	1033.99	0.00	Pass	1.20	1.42	0.22	Pass	818390
1633.95	1633.96	0.01	Pass	1.20	1.29	0.09	Pass	1731252
2233.91	2233.83	-0.08	Pass	1.20	1.31	0.11	Pass	1040681

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	1.25	0.05	Pass	280098
302.00	302.03	0.03	Pass	1.20	1.42	0.22	Pass	242779
601.98	601.97	-0.01	Pass	1.20	1.45	0.25	Pass	242183
1033.99	1033.92	-0.07	Pass	1.20	1.47	0.27	Pass	744350
1633.95	1633.82	-0.13	Pass	1.20	1.41	0.21	Pass	2605700
2233.91	2233.83	-0.08	Pass	1.20	1.35	0.15	Pass	2372239

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.93	-0.06	Pass	2.50	2.66	0.16	Pass	307800
302.00	301.82	-0.18	Pass	2.50	2.63	0.13	Pass	246610
601.98	601.81	-0.17	Pass	2.50	2.71	0.21	Pass	374246
1033.99	1033.69	-0.30	Pass	2.50	2.75	0.25	Pass	1527059
1633.95	1633.89	-0.06	Pass	2.50	2.49	-0.01	Pass	4233336
2233.91	2233.78	-0.13	Pass	2.50	2.33	-0.17	Pass	4276021

Analyzer: MS2 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.89	-0.10	Pass	2.50	2.47	-0.03	Pass	336635
302.00	302.01	0.01	Pass	2.50	2.54	0.04	Pass	307177
601.98	601.97	-0.01	Pass	2.50	2.65	0.15	Pass	307259
1033.99	1033.94	-0.05	Pass	2.50	2.51	0.01	Pass	1308555
1633.95	1633.83	-0.12	Pass	2.50	2.48	-0.02	Pass	4232421
2233.91	2233.81	-0.10	Pass	2.50	2.26	-0.24	Pass	4913705

QQQ Autotune Report

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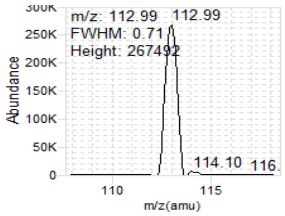
Instrument Name	LCMS-3
MS Model	G6470B
MS Instrument Serial	SG2050G211
Software_Firmware Version	10.1.67, FW: A.00.08.112
Tune Date & Time	03 May 2022 08:57:32
File Path	D:\MassHunter\Tune\QQQ\G6470B\atunes.TUNE.XML
Ion Source	AJS ESI
Ionization Mode	AJS ESI
Tuned Resolution	All
Vacuum Pressure	1.52E+0 [R] (Torr); 3.94E-5 [H] (Torr)

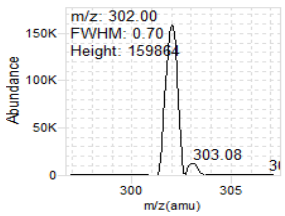
Source Parameters

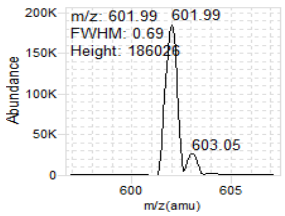
Parameter	**Negative**
Gas Temp (°C)	300
Gas Flow (l/min)	8
Nebulizer (psi)	15
Capillary (V)	3500
Nozzle Voltage (V)	1500
Sheath Gas Temp (°C)	250
Sheath Gas Flow (l/min)	7

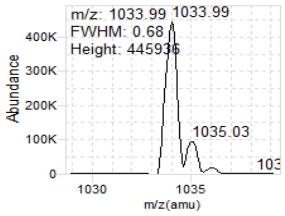
Negative Results

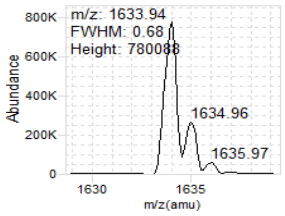
Analyzer: MS1 **Polarity: Negative** **Width: Unit**

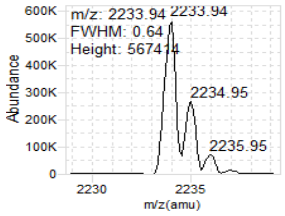


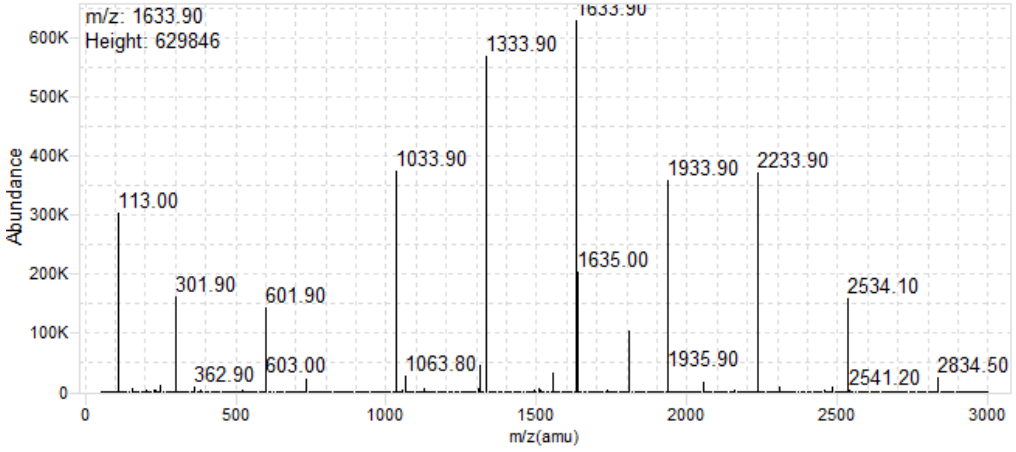






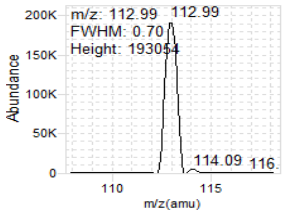


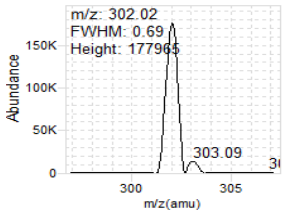


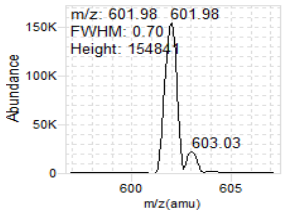


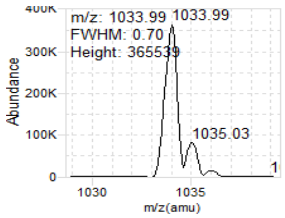
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.99	112.99	0.71	0.70	267492
302.00	302.00	0.70	0.70	159864
601.99	601.98	0.69	0.70	186026
1033.99	1033.99	0.68	0.70	445936
1633.94	1633.95	0.68	0.70	780088
2233.94	2233.91	0.64	0.70	567414

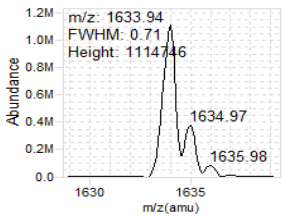
Analyzer: MS2 **Polarity: Negative** **Width: Unit**

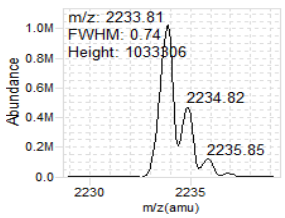


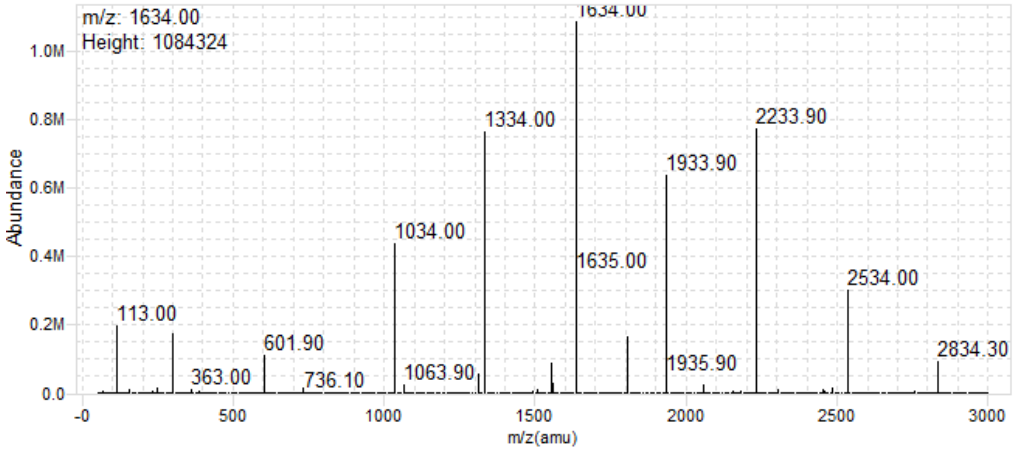






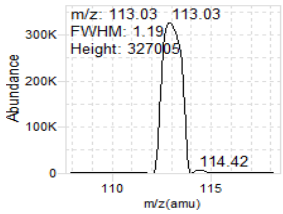


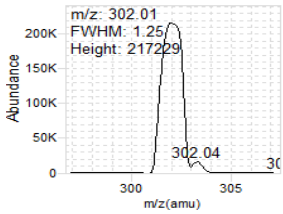


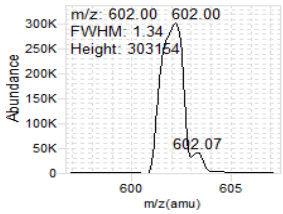


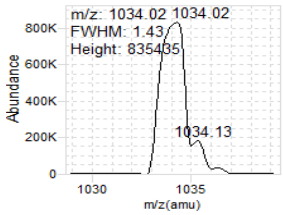
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.99	112.99	0.70	0.70	193054
302.02	302.00	0.69	0.70	177965
601.98	601.98	0.70	0.70	154841
1033.99	1033.99	0.70	0.70	365539
1633.94	1633.95	0.71	0.70	1114746
2233.82	2233.91	0.74	0.70	1033306

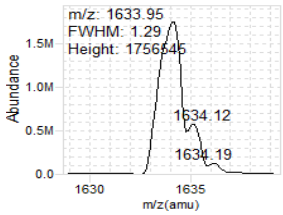
Analyzer: MS1 **Polarity: Negative** **Width: Wide**

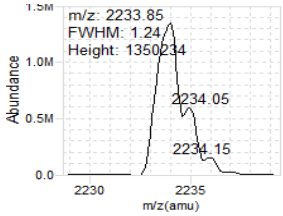






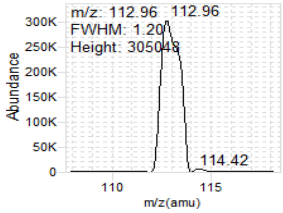


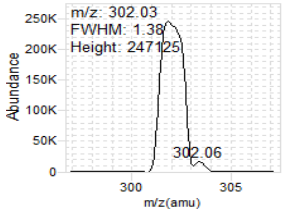


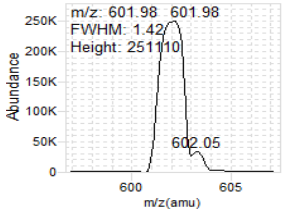


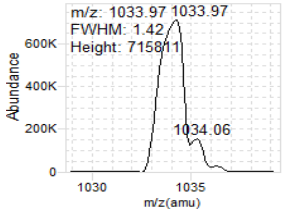
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.03	112.99	1.19	1.20	327005
302.01	302.00	1.25	1.20	217229
602.00	601.98	1.34	1.20	303154
1034.01	1033.99	1.43	1.20	835435
1633.95	1633.95	1.29	1.20	1756545
2233.85	2233.91	1.24	1.20	1350234

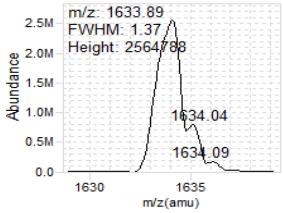
Analyzer: MS2 **Polarity: Negative** **Width: Wide**

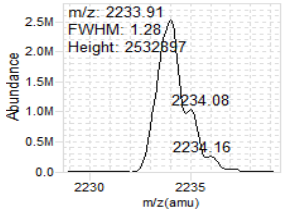






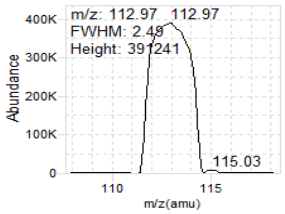


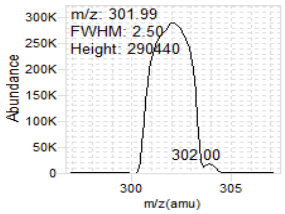


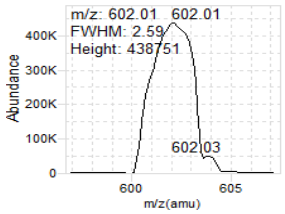


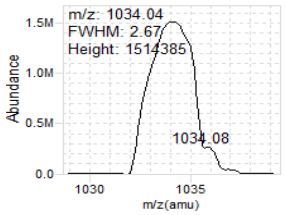
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.96	112.99	1.20	1.20	305048
302.03	302.00	1.38	1.20	247125
601.97	601.98	1.42	1.20	251110
1033.97	1033.99	1.42	1.20	715811
1633.89	1633.95	1.37	1.20	2564788
2233.91	2233.91	1.28	1.20	2532897

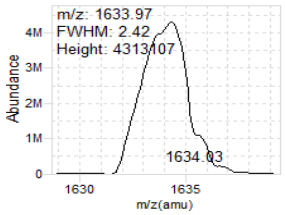
Analyzer: MS1 **Polarity: Negative** **Width: Widest**

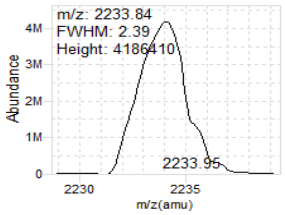






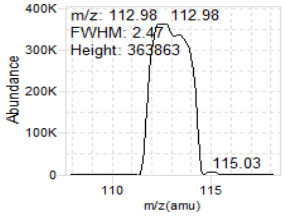


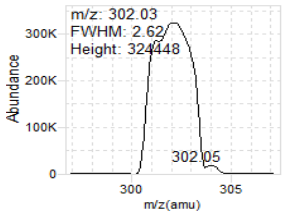


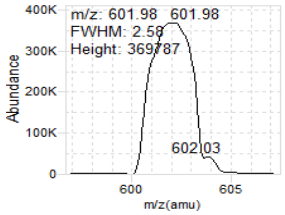


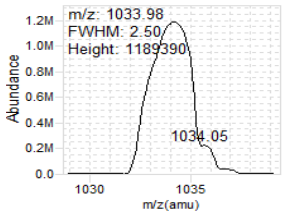
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.97	112.99	2.49	2.50	391241
301.99	302.00	2.50	2.50	290440
602.01	601.98	2.59	2.50	438751
1034.04	1033.99	2.67	2.50	1514385
1633.97	1633.95	2.42	2.50	4313106
2233.85	2233.91	2.39	2.50	4186410

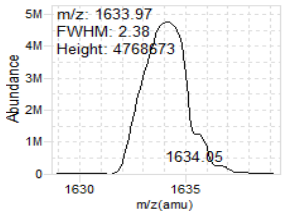
Analyzer: MS2 **Polarity: Negative** **Width: Widest**

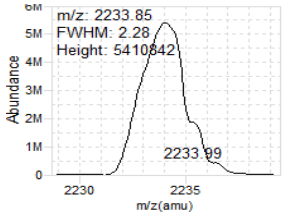












m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.98	112.99	2.47	2.50	363863
302.03	302.00	2.62	2.50	324448
601.98	601.98	2.58	2.50	369787
1033.98	1033.99	2.50	2.50	1189390
1633.97	1633.95	2.38	2.50	4768673
2233.86	2233.91	2.28	2.50	5410842

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	0.87
MS1 Axis Gain	-7.95
MS1 Width Offset	0.13
MS1 Width Gain	-2
MS1 Heater (°C)	100
MS2 DC (V)	10
MS2 PreFilter (V)	30
MS2 Axis Offset	0.92
MS2 Axis Gain	20
MS2 Width Offset	-0.01
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)	1230
Collision Energy (eV)	0
Lens 1[MS2] (V)	-4.00
MS1 PreFilter[MS2] (V)	-3.20

Dynamic Ramp Tables

MS1 PreFilter (V)

m/z	Setting
112.99	11
302	7.8
601.98	10
1033.99	21.5
1633.95	18.5
2233.91	14.7

MS1 Axis Offset

m/z	Setting
112.99	0.872
302	0.946
601.98	1.019
1033.99	1.059
1633.95	0.981
2233.91	0.872

MS1 Width Offset

m/z	Setting
112.99	0.13
302	0.08
601.98	-0.01
1033.99	-0.04
1633.95	0.06
2233.91	0.13

MS2 PreFilter (V)

m/z	Setting
69	16
112.97	30
113	10
207	18.8
232	22
302	36.2

MS2 Axis Offset

m/z	Setting
112.99	0.924
302	1.109
601.98	1.124
1033.99	1.13
1633.95	1.135
2233.91	0.924

MS2 Width Offset

m/z	Setting
112.99	-0.01
302	-0.1
601.98	-0.12
1033.99	-0.13
1633.95	-0.1
2233.91	-0.01

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	-7.95	0.872	-1.7	0.13
Wide	-8.3	1.104	-1.5	0.54
Widest	-8.5	1.52	-0.9	1.54

MS2 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	19.5	0.924	-18.2	-0.01
Wide	19.45	1.128	-18	0.46
Widest	19.15	1.558	-17.9	1.43

QQQ Check Tune Report

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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	03 May 2022 08:57:32
File Path	D:\MassHunter\Tune\QQQ\G6470B\atunes.TUNE.XML
Ion Source	AJS ESI
Ionization Mode	AJS ESI
Tuned Resolution	All
Vacuum Pressure	1.52E+0 [R] (Torr); 3.94E-5 [H] (Torr)

Source Parameters

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

QQQ Check Tune Report

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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	112.99	0.00	Pass	0.70	0.71	0.01	Pass	267492
302.00	302.00	0.00	Pass	0.70	0.70	0.00	Pass	159864
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	186026
1033.99	1033.99	0.00	Pass	0.70	0.68	-0.02	Pass	445936
1633.95	1633.94	-0.01	Pass	0.70	0.68	-0.02	Pass	780088
2233.91	2233.94	0.03	Pass	0.70	0.64	-0.06	Pass	567414

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	0.70	0.00	Pass	193054
302.00	302.02	0.02	Pass	0.70	0.69	-0.01	Pass	177965
601.98	601.98	0.00	Pass	0.70	0.70	0.00	Pass	154841
1033.99	1033.99	0.00	Pass	0.70	0.70	0.00	Pass	365539
1633.95	1633.94	-0.01	Pass	0.70	0.71	0.01	Pass	1114746
2233.91	2233.82	-0.09	Pass	0.70	0.74	0.04	Pass	1033306

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	1.19	-0.01	Pass	327005
302.00	302.01	0.01	Pass	1.20	1.25	0.05	Pass	217229
601.98	602.00	0.02	Pass	1.20	1.34	0.14	Pass	303154
1033.99	1034.01	0.02	Pass	1.20	1.43	0.23	Pass	835435
1633.95	1633.95	0.00	Pass	1.20	1.29	0.09	Pass	1756545
2233.91	2233.85	-0.06	Pass	1.20	1.24	0.04	Pass	1350234

Analyzer: MS2 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.96	-0.03	Pass	1.20	1.20	0.00	Pass	305048
302.00	302.03	0.03	Pass	1.20	1.38	0.18	Pass	247125
601.98	601.97	-0.01	Pass	1.20	1.42	0.22	Pass	251110
1033.99	1033.97	-0.02	Pass	1.20	1.42	0.22	Pass	715811
1633.95	1633.89	-0.06	Pass	1.20	1.37	0.17	Pass	2564788
2233.91	2233.91	0.00	Pass	1.20	1.28	0.08	Pass	2532897

Analyzer: MS1 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	2.49	-0.01	Pass	391241
302.00	301.99	-0.01	Pass	2.50	2.50	0.00	Pass	290440
601.98	602.01	0.03	Pass	2.50	2.59	0.09	Pass	438751
1033.99	1034.04	0.05	Pass	2.50	2.67	0.17	Pass	1514385
1633.95	1633.97	0.02	Pass	2.50	2.42	-0.08	Pass	4313106
2233.91	2233.85	-0.06	Pass	2.50	2.39	-0.11	Pass	4186410

Analyzer: MS2 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	2.47	-0.03	Pass	363863
302.00	302.03	0.03	Pass	2.50	2.62	0.12	Pass	324448
601.98	601.98	0.00	Pass	2.50	2.58	0.08	Pass	369787
1033.99	1033.98	-0.01	Pass	2.50	2.50	0.00	Pass	1189390
1633.95	1633.97	0.02	Pass	2.50	2.38	-0.12	Pass	4768673
2233.91	2233.86	-0.05	Pass	2.50	2.28	-0.22	Pass	5410842