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
5/12/22				JR 05/12/22				✓	✓	JR 5/12/22	Autotune after shutdown	JR
						KMY 5/16/2022						

Signature: Kayla M. Young **Date Completed:** 5/16/2022

QQQ Autotune Report

Agilent | Trusted Answers

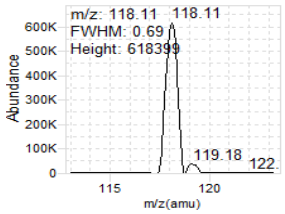
Instrument Name	LCMS-3
MS Model	G6470B
MS Instrument Serial	SG2050G211
Software_Firmware Version	10.1.67, FW: A.00.08.112
Tune Date & Time	12 May 2022 07:22:45
File Path	D:\MassHunter\Tune\QQQ\G6470B\atunes.TUNE.XML
Ion Source	AJS ESI
Ionization Mode	AJS ESI
Tuned Resolution	All
Vacuum Pressure	1.55E+0 [R] (Torr); 4.08E-5 [H] (Torr)

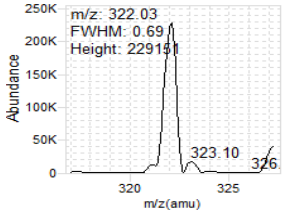
Source Parameters

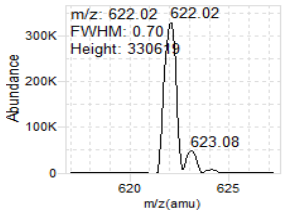
Parameter	Positive	Negative
Gas Temp (°C)	300	300
Gas Flow (l/min)	8	8
Nebulizer (psi)	15	15
Capillary (V)	4000	3500
Nozzle Voltage (V)	1500	1500
Sheath Gas Temp (°C)	250	250
Sheath Gas Flow (l/min)	7	7

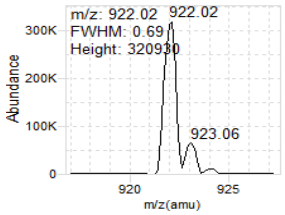
Positive Results

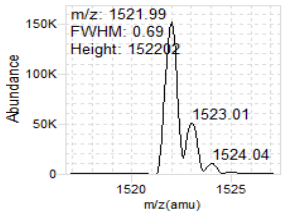
Analyzer: MS1 **Polarity: Positive** **Width: Unit**

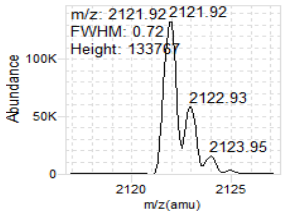


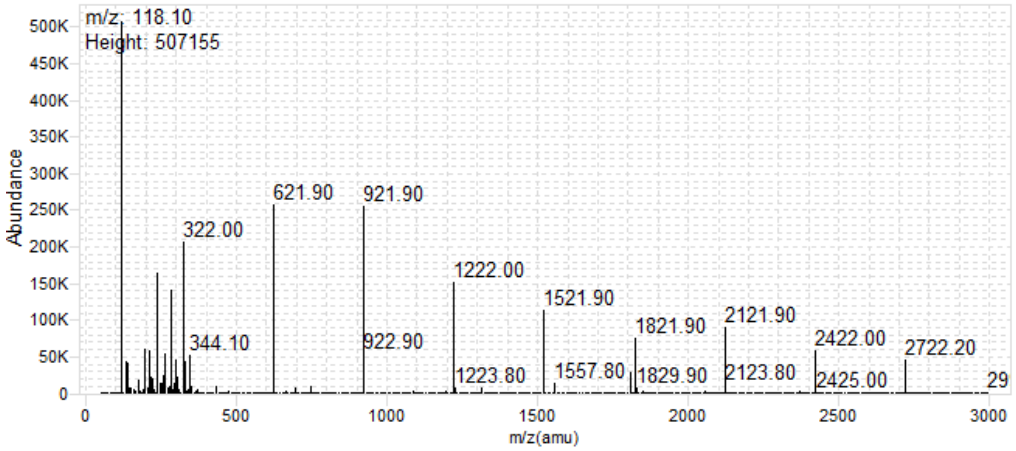






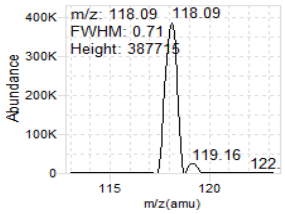


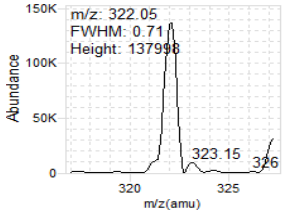


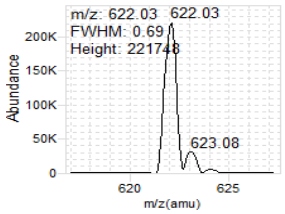


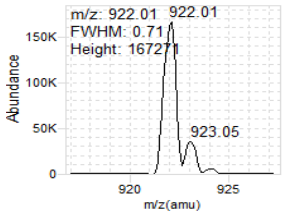
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.11	118.09	0.69	0.70	618399
322.03	322.05	0.69	0.70	229151
622.02	622.03	0.70	0.70	330619
922.02	922.01	0.69	0.70	320930
1521.99	1521.97	0.69	0.70	152202
2121.92	2121.93	0.72	0.70	133767

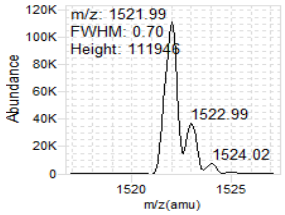
Analyzer: MS2 **Polarity: Positive** **Width: Unit**

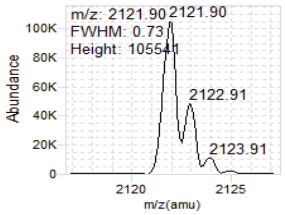


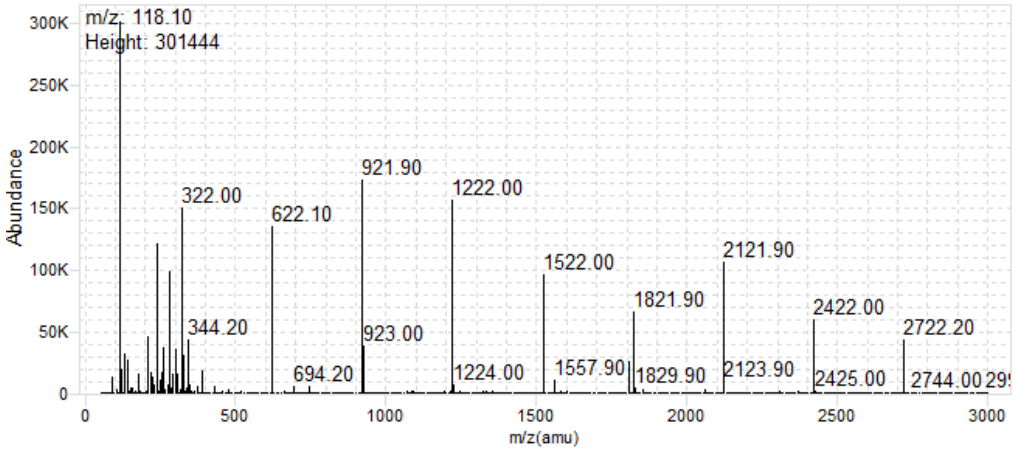






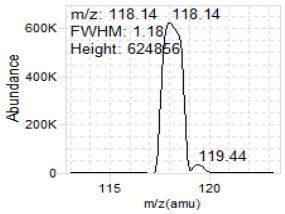


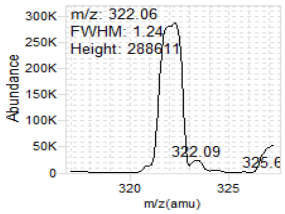


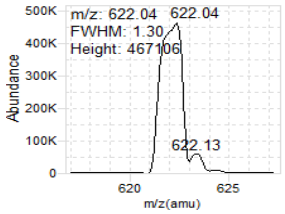


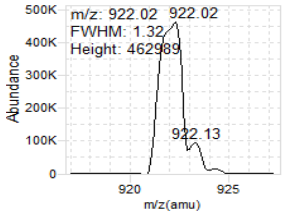
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.09	118.09	0.71	0.70	387715
322.05	322.05	0.71	0.70	137998
622.03	622.03	0.69	0.70	221748
922.01	922.01	0.71	0.70	167271
1521.98	1521.97	0.70	0.70	111946
2121.91	2121.93	0.73	0.70	105541

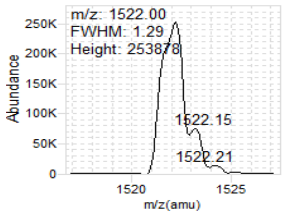
Analyzer: MS1 **Polarity: Positive** **Width: Wide**

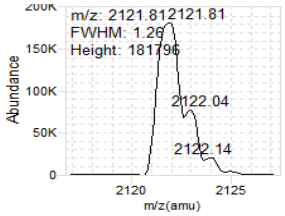






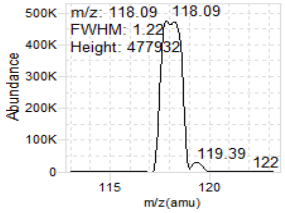


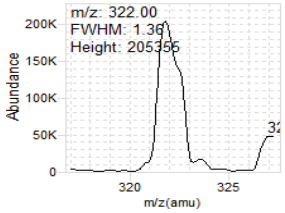


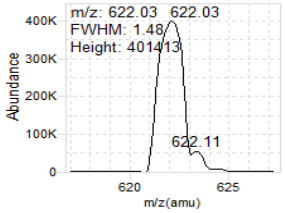


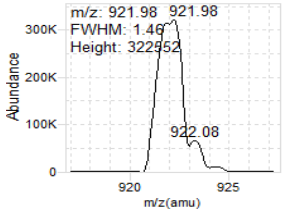
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.14	118.09	1.18	1.20	624856
322.06	322.05	1.24	1.20	288611
622.04	622.03	1.30	1.20	467106
922.02	922.01	1.32	1.20	462989
1522.00	1521.97	1.29	1.20	253878
2121.82	2121.93	1.26	1.20	181796

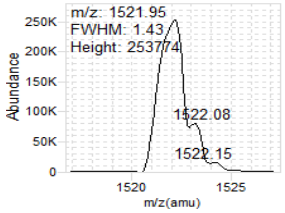
Analyzer: MS2 **Polarity: Positive** **Width: Wide**

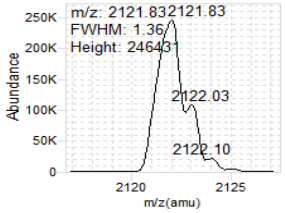






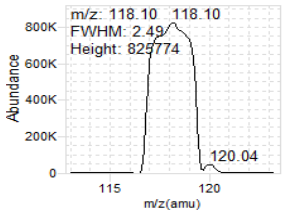


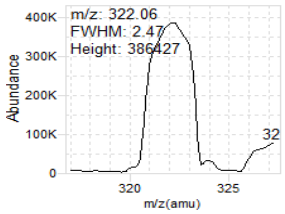


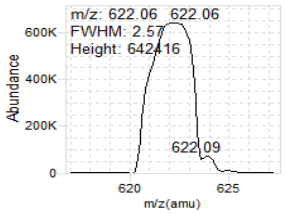


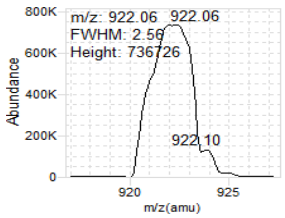
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.09	118.09	1.22	1.20	477932
322.00	322.05	1.36	1.20	205355
622.03	622.03	1.48	1.20	401413
921.97	922.01	1.46	1.20	322552
1521.95	1521.97	1.43	1.20	253774
2121.83	2121.93	1.36	1.20	246431

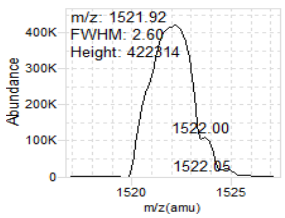
Analyzer: MS1 **Polarity: Positive** **Width: Widest**

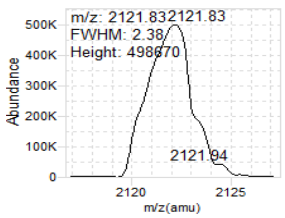






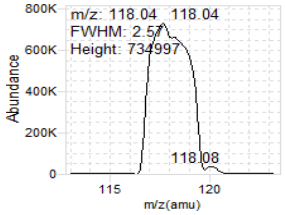


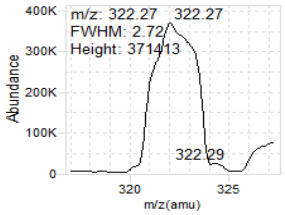


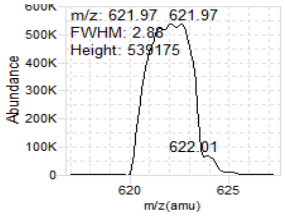


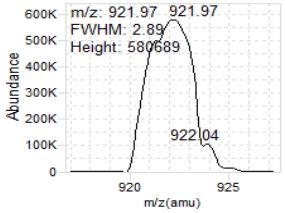
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.10	118.09	2.49	2.50	825774
322.06	322.05	2.47	2.50	386427
622.06	622.03	2.57	2.50	642416
922.06	922.01	2.56	2.50	736726
1521.92	1521.97	2.59	2.50	422314
2121.83	2121.93	2.38	2.50	498670

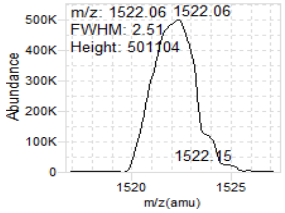
Analyzer: MS2 **Polarity: Positive** **Width: Widest**

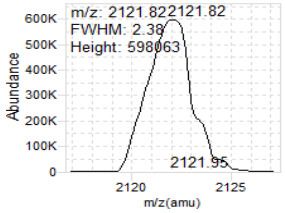












m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.04	118.09	2.57	2.50	734997
322.27	322.05	2.72	2.50	371413
621.97	622.03	2.87	2.50	539175
921.97	922.01	2.89	2.50	580689
1522.06	1521.97	2.51	2.50	501104
2121.83	2121.93	2.38	2.50	598063

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	0.90
MS1 Axis Gain	-8
MS1 Width Offset	0.13
MS1 Width Gain	-2
MS1 Heater (°C)	100
MS2 DC (V)	-10
MS2 PreFilter (V)	-14
MS2 Axis Offset	0.92
MS2 Axis Gain	19.25
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)	1195
Collision Energy (eV)	0
Lens 1[MS2] (V)	2.30
MS1 PreFilter[MS2] (V)	2.20

Dynamic Ramp Tables

MS1 PreFilter (V)

m/z	Setting
118.09	-12.8
322.05	-6.6
622.03	-10.8
922.01	-18
1521.97	-12
2121.93	-15.4

MS1 Axis Offset

m/z	Setting
118.09	0.896
322.05	0.938
622.03	1.047
922.01	1.079
1521.97	1.043
2121.93	0.896

MS1 Width Offset

m/z	Setting
118.09	0.13
322.05	0.07
622.03	-0.01
922.01	-0.03
1521.97	0
2121.93	0.13

MS2 PreFilter (V)

m/z	Setting
58	-16
79	-20.6
117.97	-30
118	-12.6
154	-15.6
290	-30.2

MS2 Axis Offset

m/z	Setting
118.09	0.924
322.05	1.151
622.03	1.17
922.01	1.123
1521.97	1.058
2121.93	0.924

MS2 Width Offset

m/z	Setting
118.09	-0.03
322.05	-0.22
622.03	-0.27
922.01	-0.22
1521.97	-0.16
2121.93	-0.03

MS1 Calibrations

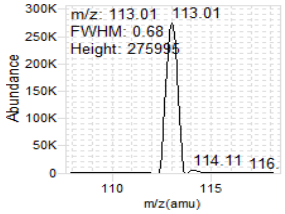
Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	-7.9	0.896	-1.5	0.13
Wide	-8.25	1.094	-1.5	0.5
Widest	-8.5	1.494	-0.9	1.46

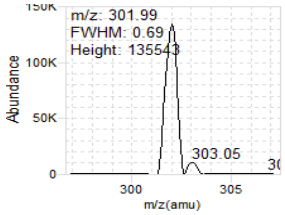
MS2 Calibrations

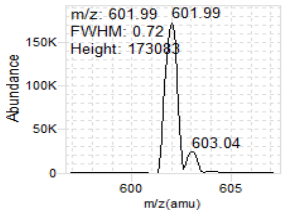
Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	19.25	0.924	-17.9	-0.03
Wide	19	1.102	-17.6	0.36
Widest	18.65	1.58	-17.4	1.47

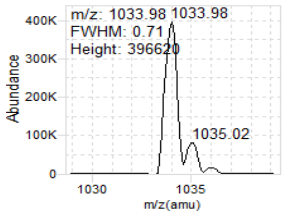
Negative Results

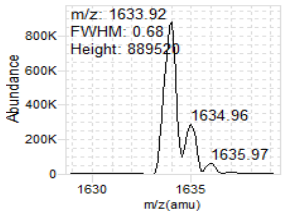
Analyzer: MS1 **Polarity: Negative** **Width: Unit**

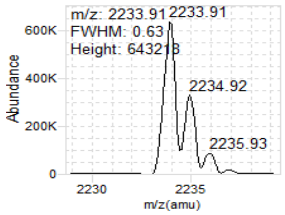


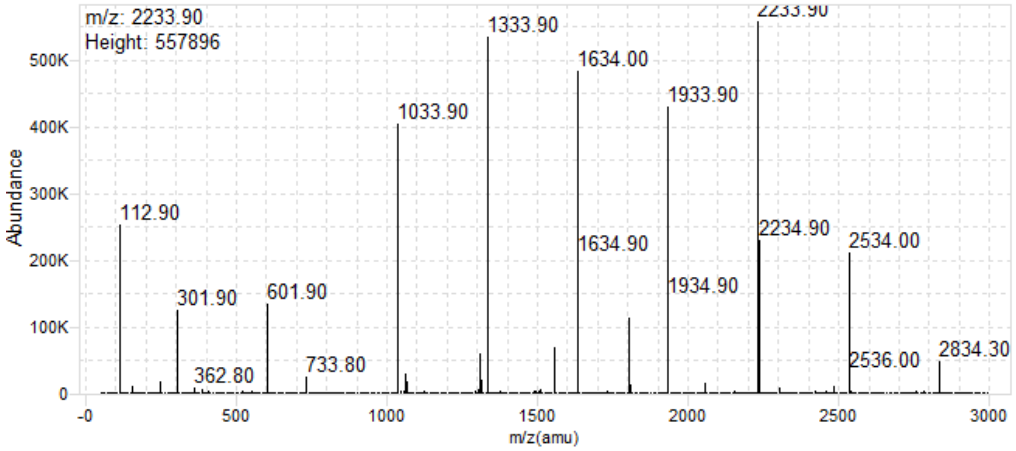






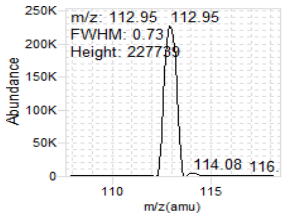


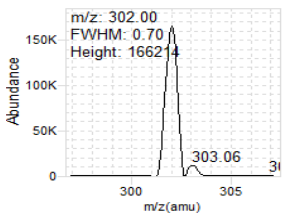


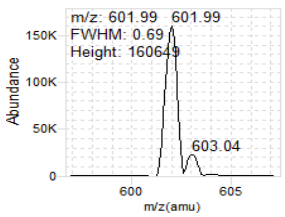


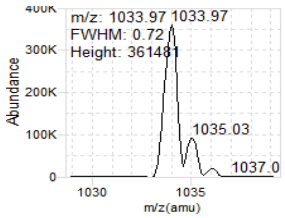
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.01	112.99	0.68	0.70	275995
301.99	302.00	0.69	0.70	135543
601.99	601.98	0.71	0.70	173083
1033.98	1033.99	0.71	0.70	396620
1633.92	1633.95	0.68	0.70	889521
2233.91	2233.91	0.63	0.70	643218

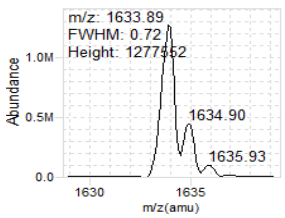
Analyzer: MS2 **Polarity: Negative** **Width: Unit**

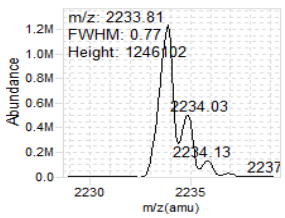


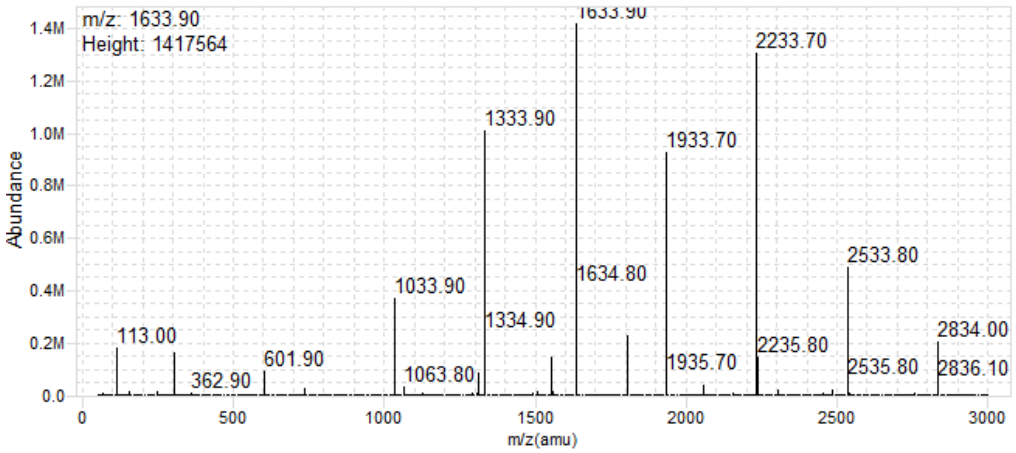






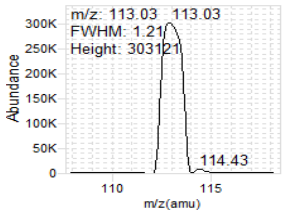


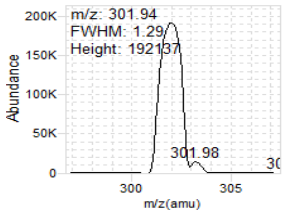


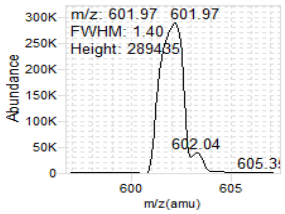


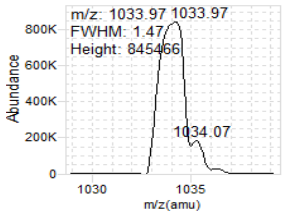
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.95	112.99	0.73	0.70	227739
302.00	302.00	0.70	0.70	166214
601.99	601.98	0.69	0.70	160649
1033.96	1033.99	0.72	0.70	361481
1633.89	1633.95	0.72	0.70	1277552
2233.81	2233.91	0.77	0.70	1246102

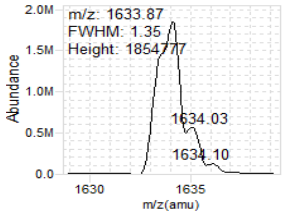
Analyzer: MS1 **Polarity: Negative** **Width: Wide**

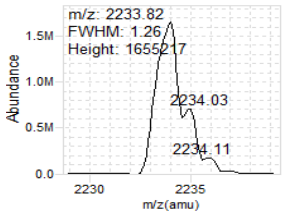






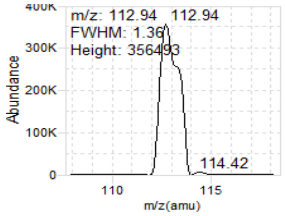


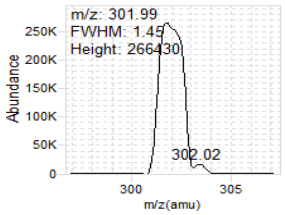


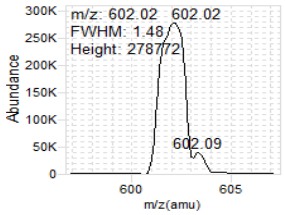


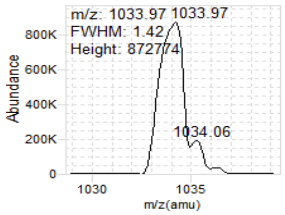
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.03	112.99	1.21	1.20	303121
301.94	302.00	1.29	1.20	192137
601.97	601.98	1.40	1.20	289435
1033.97	1033.99	1.47	1.20	845466
1633.87	1633.95	1.35	1.20	1854777
2233.82	2233.91	1.26	1.20	1655217

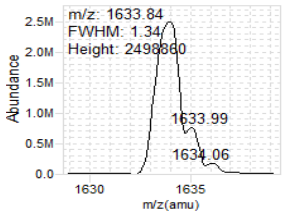
Analyzer: MS2 **Polarity: Negative** **Width: Wide**

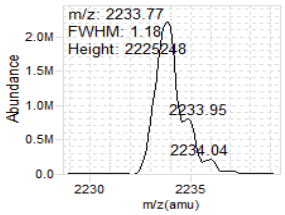






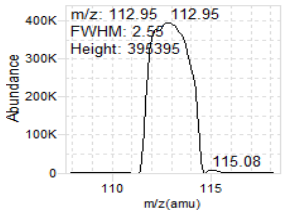


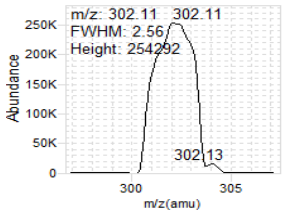


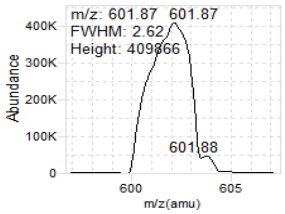


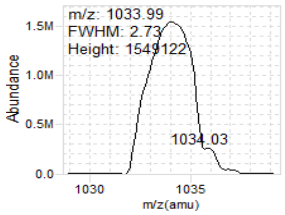
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.94	112.99	1.36	1.20	356493
301.99	302.00	1.45	1.20	266430
602.02	601.98	1.48	1.20	278772
1033.96	1033.99	1.41	1.20	872774
1633.83	1633.95	1.34	1.20	2498860
2233.78	2233.91	1.18	1.20	2225248

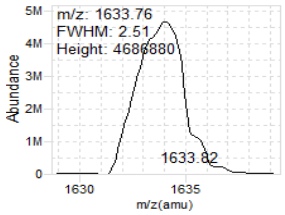
Analyzer: MS1 **Polarity: Negative** **Width: Widest**

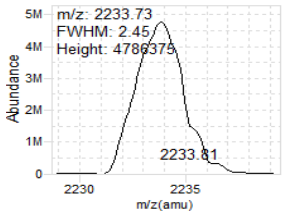






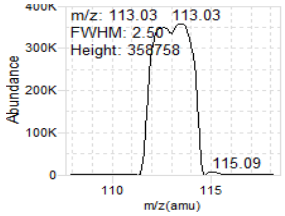


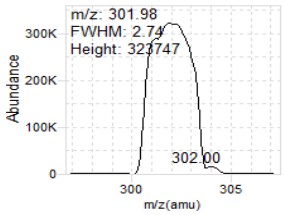


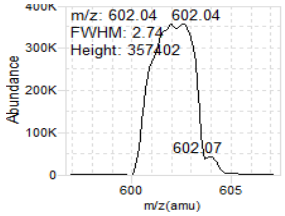


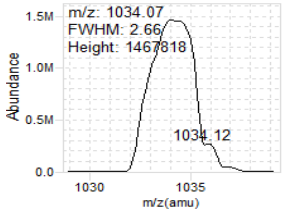
m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.95	112.99	2.55	2.50	395395
302.11	302.00	2.56	2.50	254292
601.87	601.98	2.62	2.50	409866
1033.99	1033.99	2.73	2.50	1549122
1633.76	1633.95	2.51	2.50	4686880
2233.74	2233.91	2.45	2.50	4786375

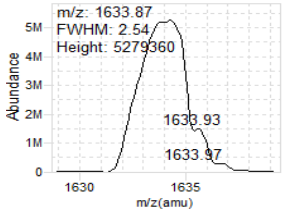
Analyzer: MS2 **Polarity: Negative** **Width: Widest**

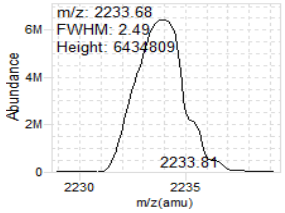












m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.03	112.99	2.50	2.50	358758
301.98	302.00	2.74	2.50	323747
602.04	601.98	2.73	2.50	357402
1034.07	1033.99	2.66	2.50	1467818
1633.87	1633.95	2.54	2.50	5279360
2233.68	2233.91	2.49	2.50	6434808

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)	15
MS1 DC (V)	-3.00
MS1 PostFilter (V)	-2.00
MS1 Axis Offset	0.93
MS1 Axis Gain	-8.05
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	19
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)	1175
Collision Energy (eV)	0
Lens 1[MS2] (V)	-0.40
MS1 PreFilter[MS2] (V)	-2.00

Dynamic Ramp Tables

MS1 PreFilter (V)

m/z	Setting
112.99	11.6
302	7.6
601.98	10.2
1033.99	20.9
1633.95	18.7
2233.91	14.9

MS1 Axis Offset

m/z	Setting
112.99	0.928
302	0.953
601.98	1.064
1033.99	1.12
1633.95	1.053
2233.91	0.928

MS1 Width Offset

m/z	Setting
112.99	0.13
302	0.05
601.98	-0.03
1033.99	-0.06
1633.95	0.03
2233.91	0.13

MS2 PreFilter (V)

m/z	Setting
69	17
112.97	30
113	10
207	20.6
232	23.6
302	34.4

MS2 Axis Offset

m/z	Setting
112.99	0.916
302	1.13
601.98	1.184
1033.99	1.148
1633.95	1.061
2233.91	0.916

MS2 Width Offset

m/z	Setting
112.99	0.01
302	-0.15
601.98	-0.2
1033.99	-0.17
1633.95	-0.11
2233.91	0.01

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	-8.05	0.928	-1.7	0.13
Wide	-8.35	1.138	-1.5	0.54
Widest	-8.6	1.568	-0.9	1.57

MS2 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	19.1	0.916	-17.8	0.01
Wide	18.9	1.144	-17.9	0.5
Widest	18.55	1.612	-17.3	1.45

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	12 May 2022 07:22:45
File Path	D:\MassHunter\Tune\QQQ\G6470B\atunes.TUNE.XML
Ion Source	AJS ESI
Ionization Mode	AJS ESI
Tuned Resolution	All
Vacuum Pressure	1.55E+0 [R] (Torr); 4.08E-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	118.11	0.02	Pass	0.70	0.69	-0.01	Pass	618399
322.05	322.03	-0.02	Pass	0.70	0.69	-0.01	Pass	229151
622.03	622.02	-0.01	Pass	0.70	0.70	0.00	Pass	330619
922.01	922.02	0.01	Pass	0.70	0.69	-0.01	Pass	320930
1521.97	1521.99	0.02	Pass	0.70	0.69	-0.01	Pass	152202
2121.93	2121.92	-0.01	Pass	0.70	0.72	0.02	Pass	133767

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	0.71	0.01	Pass	387715
322.05	322.05	0.00	Pass	0.70	0.71	0.01	Pass	137998
622.03	622.03	0.00	Pass	0.70	0.69	-0.01	Pass	221748
922.01	922.01	0.00	Pass	0.70	0.71	0.01	Pass	167271
1521.97	1521.98	0.01	Pass	0.70	0.70	0.00	Pass	111946
2121.93	2121.91	-0.02	Pass	0.70	0.73	0.03	Pass	105541

Analyzer: MS1 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.14	0.05	Pass	1.20	1.18	-0.02	Pass	624856
322.05	322.06	0.01	Pass	1.20	1.24	0.04	Pass	288611
622.03	622.04	0.01	Pass	1.20	1.30	0.10	Pass	467106
922.01	922.02	0.01	Pass	1.20	1.32	0.12	Pass	462989
1521.97	1522.00	0.03	Pass	1.20	1.29	0.09	Pass	253878
2121.93	2121.82	-0.11	Pass	1.20	1.26	0.06	Pass	181796

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	1.20	1.22	0.02	Pass	477932
322.05	322.00	-0.05	Pass	1.20	1.36	0.16	Pass	205355
622.03	622.03	0.00	Pass	1.20	1.48	0.28	Pass	401413
922.01	921.97	-0.04	Pass	1.20	1.46	0.26	Pass	322552
1521.97	1521.95	-0.02	Pass	1.20	1.43	0.23	Pass	253774
2121.93	2121.83	-0.10	Pass	1.20	1.36	0.16	Pass	246431

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	2.49	-0.01	Pass	825774
322.05	322.06	0.01	Pass	2.50	2.47	-0.03	Pass	386427
622.03	622.06	0.03	Pass	2.50	2.57	0.07	Pass	642416
922.01	922.06	0.05	Pass	2.50	2.56	0.06	Pass	736726
1521.97	1521.92	-0.05	Pass	2.50	2.59	0.09	Pass	422314
2121.93	2121.83	-0.10	Pass	2.50	2.38	-0.12	Pass	498670

Analyzer: MS2 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	2.57	0.07	Pass	734997
322.05	322.27	0.22	Pass	2.50	2.72	0.22	Pass	371413
622.03	621.97	-0.06	Pass	2.50	2.87	0.37	Pass	539175
922.01	921.97	-0.04	Pass	2.50	2.89	0.39	Pass	580689
1521.97	1522.06	0.09	Pass	2.50	2.51	0.01	Pass	501104
2121.93	2121.83	-0.10	Pass	2.50	2.38	-0.12	Pass	598063

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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	113.01	0.02	Pass	0.70	0.68	-0.02	Pass	275995
302.00	301.99	-0.01	Pass	0.70	0.69	-0.01	Pass	135543
601.98	601.99	0.01	Pass	0.70	0.71	0.01	Pass	173083
1033.99	1033.98	-0.01	Pass	0.70	0.71	0.01	Pass	396620
1633.95	1633.92	-0.03	Pass	0.70	0.68	-0.02	Pass	889521
2233.91	2233.91	0.00	Pass	0.70	0.63	-0.07	Pass	643218

Analyzer: MS2 Polarity: Negative Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.95	-0.04	Pass	0.70	0.73	0.03	Pass	227739
302.00	302.00	0.00	Pass	0.70	0.70	0.00	Pass	166214
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	160649
1033.99	1033.96	-0.03	Pass	0.70	0.72	0.02	Pass	361481
1633.95	1633.89	-0.06	Pass	0.70	0.72	0.02	Pass	1277552
2233.91	2233.81	-0.10	Pass	0.70	0.77	0.07	Pass	1246102

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	1.21	0.01	Pass	303121
302.00	301.94	-0.06	Pass	1.20	1.29	0.09	Pass	192137
601.98	601.97	-0.01	Pass	1.20	1.40	0.20	Pass	289435
1033.99	1033.97	-0.02	Pass	1.20	1.47	0.27	Pass	845466
1633.95	1633.87	-0.08	Pass	1.20	1.35	0.15	Pass	1854777
2233.91	2233.82	-0.09	Pass	1.20	1.26	0.06	Pass	1655217

Analyzer: MS2 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.94	-0.05	Pass	1.20	1.36	0.16	Pass	356493
302.00	301.99	-0.01	Pass	1.20	1.45	0.25	Pass	266430
601.98	602.02	0.04	Pass	1.20	1.48	0.28	Pass	278772
1033.99	1033.96	-0.03	Pass	1.20	1.41	0.21	Pass	872774
1633.95	1633.83	-0.12	Pass	1.20	1.34	0.14	Pass	2498860
2233.91	2233.78	-0.13	Pass	1.20	1.18	-0.02	Pass	2225248

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.95	-0.04	Pass	2.50	2.55	0.05	Pass	395395
302.00	302.11	0.11	Pass	2.50	2.56	0.06	Pass	254292
601.98	601.87	-0.11	Pass	2.50	2.62	0.12	Pass	409866
1033.99	1033.99	0.00	Pass	2.50	2.73	0.23	Pass	1549122
1633.95	1633.76	-0.19	Pass	2.50	2.51	0.01	Pass	4686880
2233.91	2233.74	-0.17	Pass	2.50	2.45	-0.05	Pass	4786375

Analyzer: MS2 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	2.50	0.00	Pass	358758
302.00	301.98	-0.02	Pass	2.50	2.74	0.24	Pass	323747
601.98	602.04	0.06	Pass	2.50	2.73	0.23	Pass	357402
1033.99	1034.07	0.08	Pass	2.50	2.66	0.16	Pass	1467818
1633.95	1633.87	-0.08	Pass	2.50	2.54	0.04	Pass	5279360
2233.91	2233.68	-0.23	Pass	2.50	2.49	-0.01	Pass	6434808