



Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LCMS-2

Date	N ₂ Tank Pressure	N ₂ Generator Pressure	Rough Pump Oil Level Checked	Waste Bottle Checked/Emptied	Prepared Mobile Phases	Wash Solvents Checked/Replaced	Spray Chamber Cleaned	Checktune	Autotune (Monthly)	Column Changed	Comments	Initials
11/9/2022				KMY 11/2/2022				✓ PASS -KMY 11/8/2022	✓	X		KMY

Signature:

Date Completed:

11/09/2022

Instrument Name LCMS-2
MS Model G6470A
MS Instrument Serial SG1936G104
Software_Firmware Version 10.0.142, FW: A.00.08.100
Tune Date & Time 02 November 2022 09:26:08
Data Path D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.70E+0 [R] (Torr); 4.69E-5 [H] (Torr)

Source Parameters

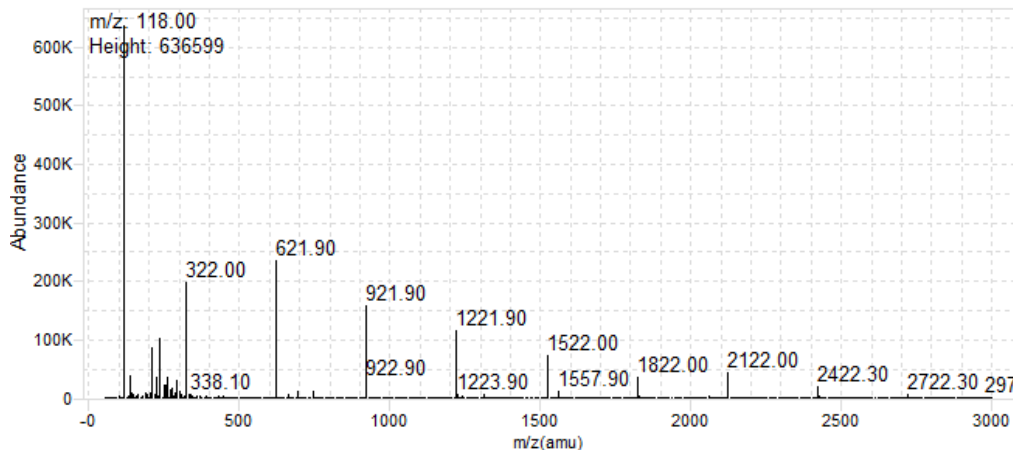
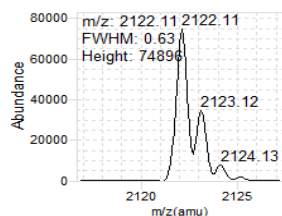
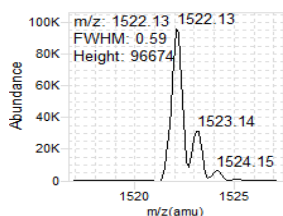
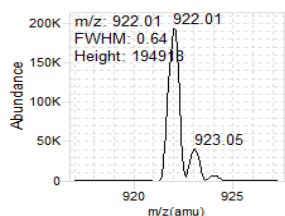
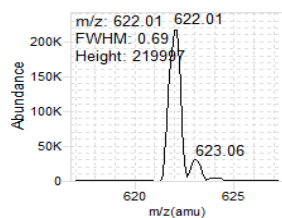
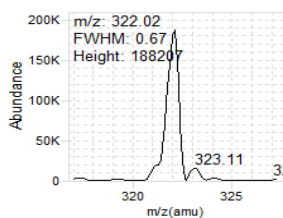
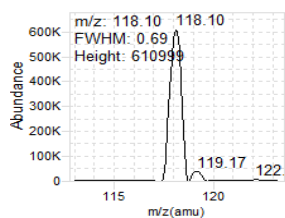
Parameter	Positive	Negative
Gas Temp (°C)	300	300
Gas Flow (l/min)	8	8
Nebulizer (psi)	15	15
Capillary (V)	4000	4000
Nozzle Voltage (V)	1500	1500
Sheath Gas Temp (°C)	250	250
Sheath Gas Flow (l/min)	7	7

Positive Results

Analyzer: MS1

Polarity: Positive

Width: Unit

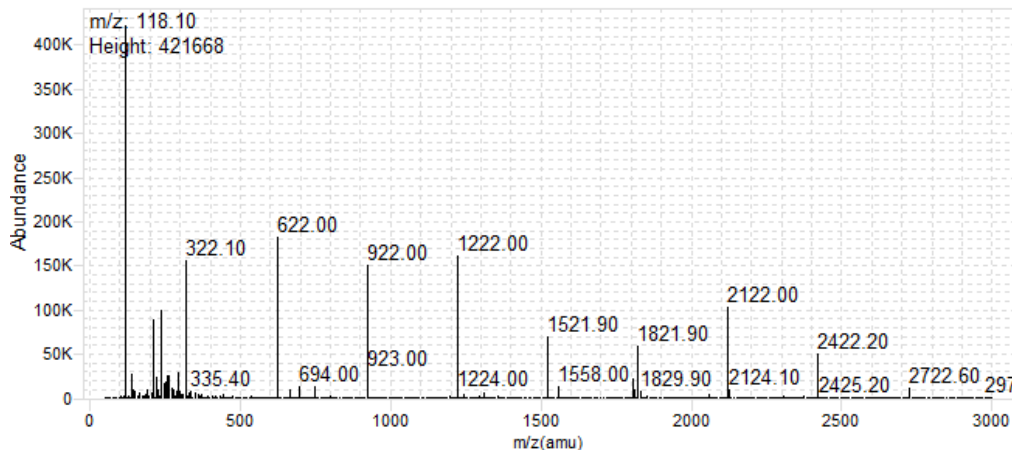
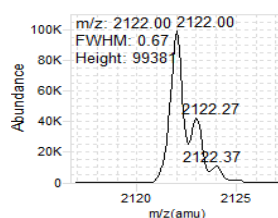
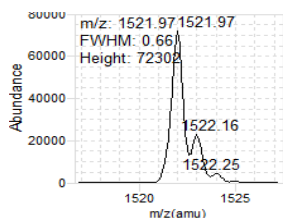
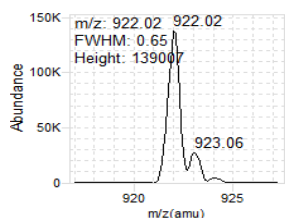
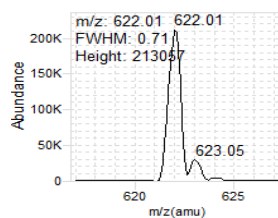
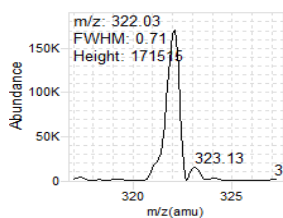
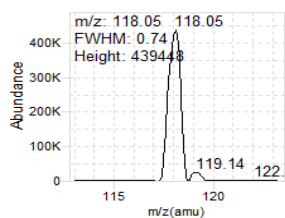


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.10	118.09	0.69	0.70	610999
322.02	322.05	0.68	0.70	188207
622.01	622.03	0.69	0.70	219997
922.01	922.01	0.64	0.70	194918
1522.13	1521.97	0.59	0.70	96674
2122.12	2121.93	0.63	0.70	74896

Analyzer: MS2

Polarity: Positive

Width: Unit

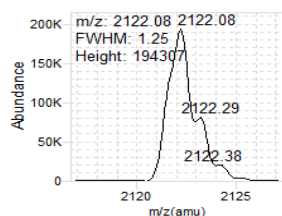
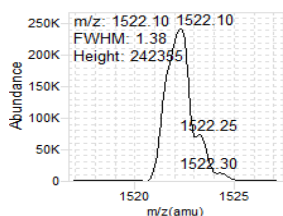
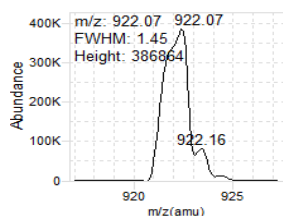
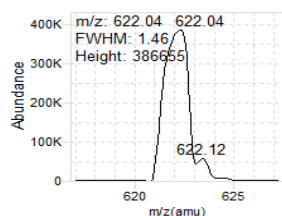
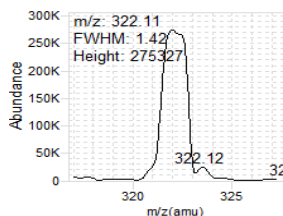
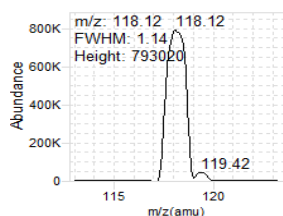


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.05	118.09	0.74	0.70	439448
322.03	322.05	0.71	0.70	171515
622.01	622.03	0.71	0.70	213057
922.01	922.01	0.65	0.70	139007
1521.96	1521.97	0.65	0.70	72302
2122.01	2121.93	0.67	0.70	99381

Analyzer: MS1

Polarity: Positive

Width: Wide

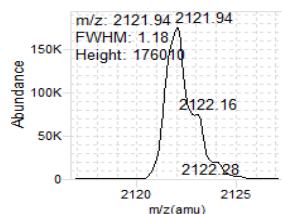
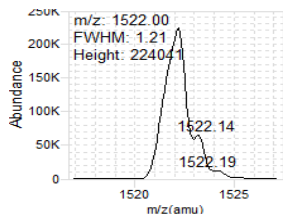
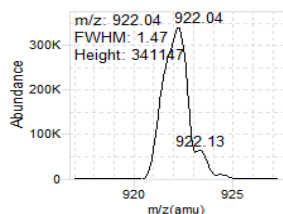
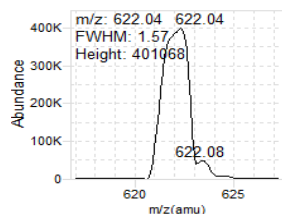
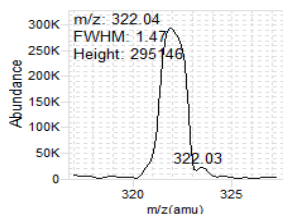
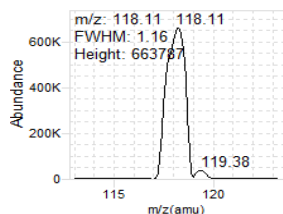


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.12	118.09	1.14	1.20	793020
322.11	322.05	1.42	1.20	275327
622.04	622.03	1.46	1.20	386655
922.07	922.01	1.45	1.20	386864
1522.10	1521.97	1.38	1.20	242355
2122.09	2121.93	1.25	1.20	194307

Analyzer: MS2

Polarity: Positive

Width: Wide

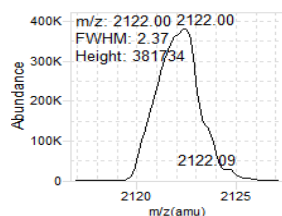
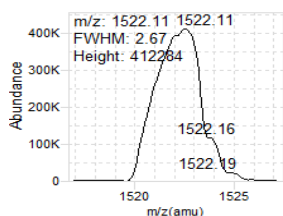
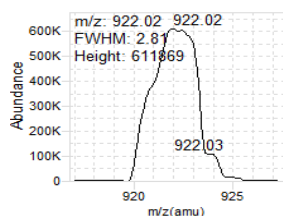
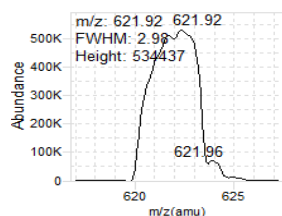
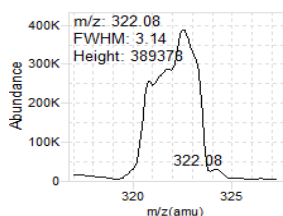
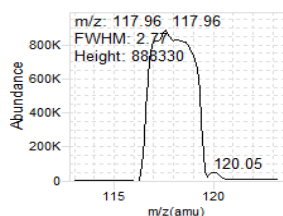


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.11	118.09	1.16	1.20	663787
322.04	322.05	1.47	1.20	295146
622.04	622.03	1.57	1.20	401068
922.04	922.01	1.47	1.20	341147
1522.00	1521.97	1.21	1.20	224041
2121.95	2121.93	1.18	1.20	176010

Analyzer: MS1

Polarity: Positive

Width: Widest

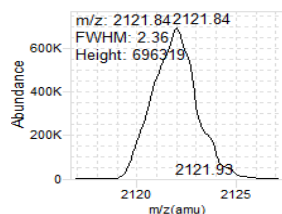
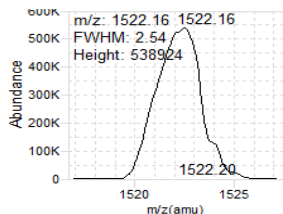
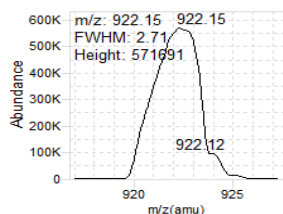
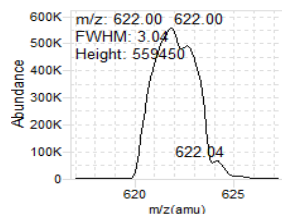
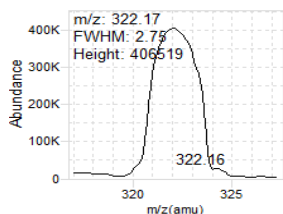
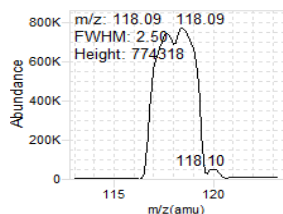


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
117.96	118.09	2.77	2.50	888330
322.08	322.05	3.14	2.50	389378
621.92	622.03	2.98	2.50	534437
922.01	922.01	2.81	2.50	611869
1522.11	1521.97	2.67	2.50	412284
2122.01	2121.93	2.37	2.50	381734

Analyzer: MS2

Polarity: Positive

Width: Widest



m/z	m/z Expected	FWHM	FWHM Expected	Abundance
118.09	118.09	2.50	2.50	774318
322.17	322.05	2.75	2.50	406519
622.00	622.03	3.04	2.50	559450
922.15	922.01	2.71	2.50	571691
1522.16	1521.97	2.54	2.50	538924
2121.84	2121.93	2.36	2.50	696319

Positive Results

Tune Parameters

Parameters	Setting
Fragmentor	135
Skimmer	15
Octopole DC	5
Octopole RF	600
Lens 1	3.50
MS1 PreFilter	-30
MS1 DC	3.00
MS1 PostFilter	2.00
MS1 Axis Offset	0.91
MS1 Axis Gain	9
MS1 Width Offset	0
MS1 Width Gain	3
MS1 Heater	100
MS2 DC	-10
MS2 PreFilter	-30
MS2 Axis Offset	0.77
MS2 Axis Gain	17.65
MS2 Width Offset	0.11
MS2 Width Gain	-8
MS2 Heater	100
Cell Entry	1
Hexapole DC	0.00
Hexapole RF	500
Hexapole Accel	5
Cell Exit	-7
Collision Gas	1
Iris	-150
HED	-10
EMV	1245
Collision Energy	0
Lens 1[MS2]	1.50
MS1 PreFilter[MS2]	3.20

Dynamic Ramp Tables

MS1 PreFilter

m/z	Setting
118.09	-11.8
322.05	-6
622.03	-8.2
922.01	-13.2
1521.97	-12.4
2121.93	-13

MS1 Axis Offset

m/z	Setting
118.09	0.906
322.05	1.033
622.03	1.079
922.01	1.046
1521.97	1.062
2121.93	0.906

MS1 Width Offset

m/z	Setting
118.09	0.1
322.05	-0.08
622.03	-0.12
922.01	-0.15
1521.97	-0.09
2121.93	0.1

MS2 PreFilter

m/z	Setting
58	-16.2
79	-20.6
117.97	-30
118	-12.4
154	-16.2
290	-33.2

MS2 Axis Offset

m/z	Setting
118.09	0.772
322.05	0.97
622.03	1.088
922.01	1.128
1521.97	0.941
2121.93	0.772

MS2 Width Offset

m/z	Setting
118.09	0.11
322.05	-0.15
622.03	-0.27
922.01	-0.27
1521.97	-0.16
2121.93	0.11

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	8.7	0.906	2.7	0.1
Wide	8.55	1.084	3.1	0.46
Widest	8.15	1.49	3.1	1.68

MS2 Calibrations

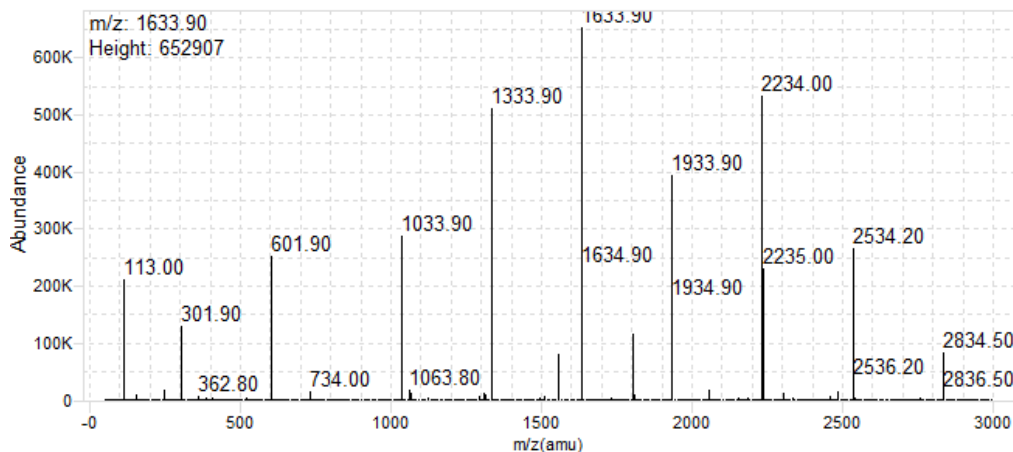
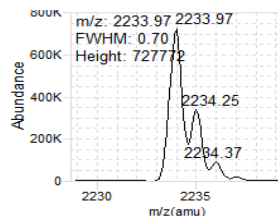
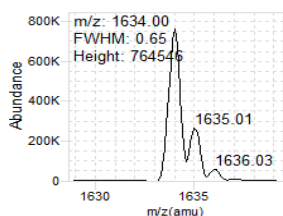
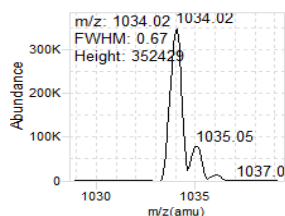
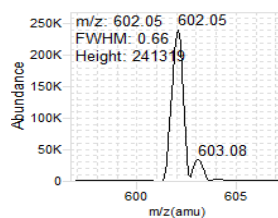
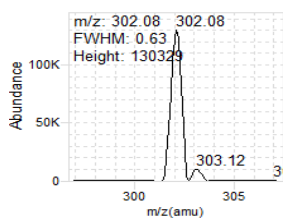
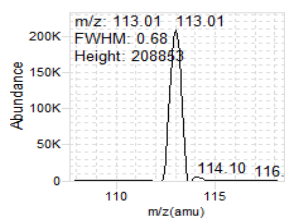
Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	17.65	0.772	-7.5	0.11
Wide	17.35	0.96	-7.5	0.5
Widest	17	1.404	-6.4	1.47

Negative Results

Analyzer: MS1

Polarity: Negative

Width: Unit

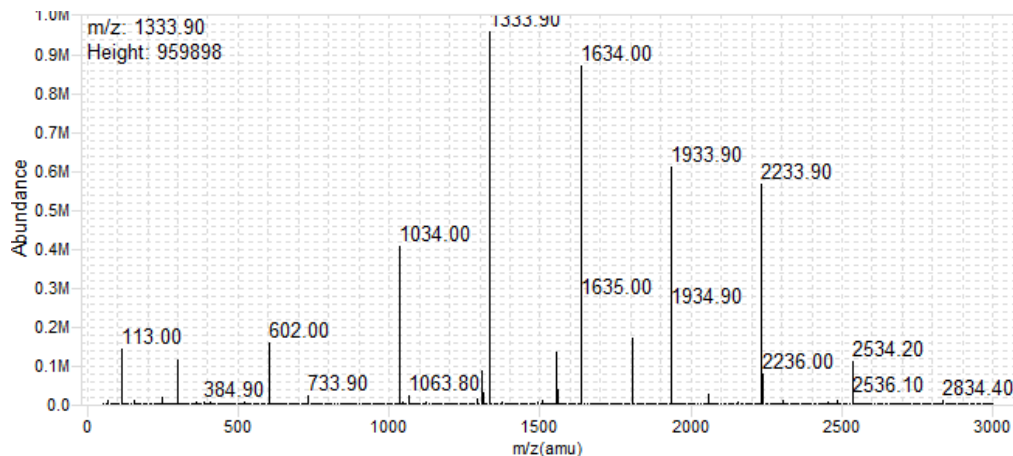
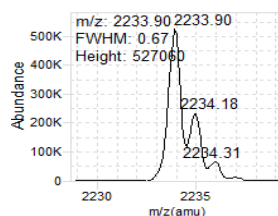
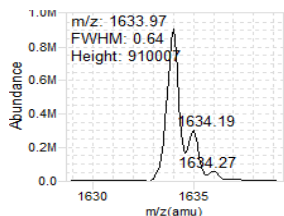
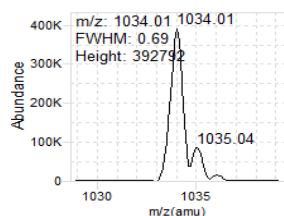
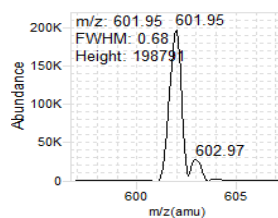
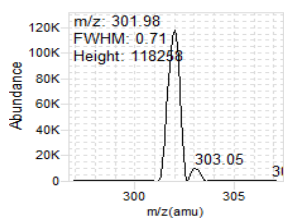
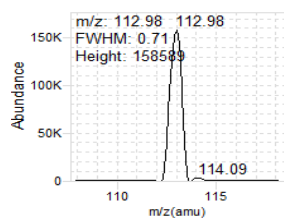


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.01	112.99	0.68	0.70	208853
302.08	302.00	0.63	0.70	130329
602.05	601.98	0.66	0.70	241319
1034.01	1033.99	0.67	0.70	352429
1634.00	1633.95	0.65	0.70	764546
2233.98	2233.91	0.70	0.70	727772

Analyzer: MS2

Polarity: Negative

Width: Unit

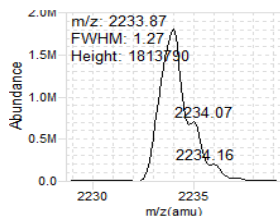
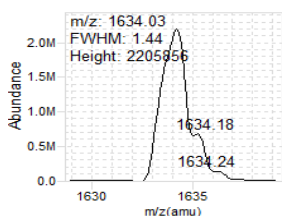
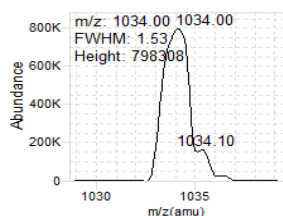
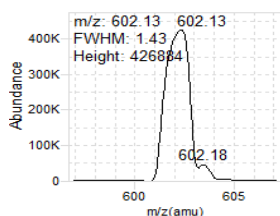
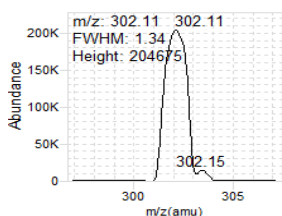
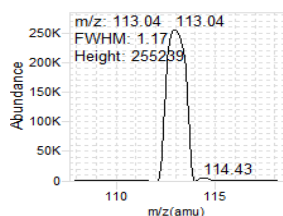


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.98	112.99	0.71	0.70	158589
301.98	302.00	0.71	0.70	118258
601.95	601.98	0.68	0.70	198791
1034.01	1033.99	0.69	0.70	392792
1633.97	1633.95	0.64	0.70	910007
2233.91	2233.91	0.68	0.70	527060

Analyzer: MS1

Polarity: Negative

Width: Wide

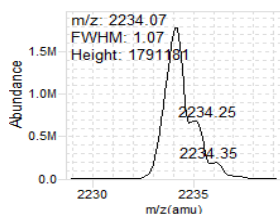
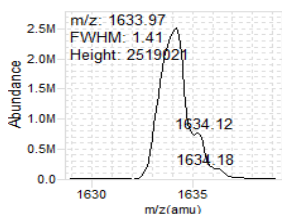
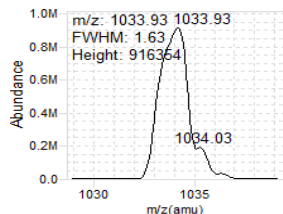
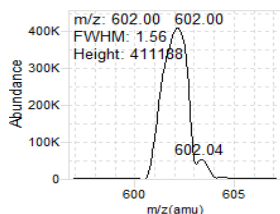
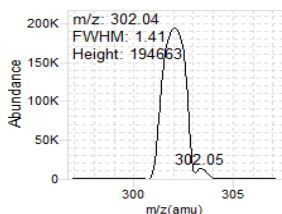
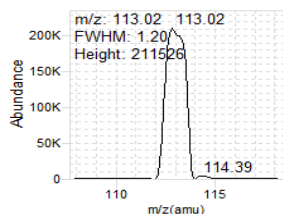


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.04	112.99	1.17	1.20	255239
302.11	302.00	1.34	1.20	204675
602.13	601.98	1.43	1.20	426884
1034.00	1033.99	1.53	1.20	798308
1634.03	1633.95	1.44	1.20	2205856
2233.88	2233.91	1.28	1.20	1813790

Analyzer: MS2

Polarity: Negative

Width: Wide

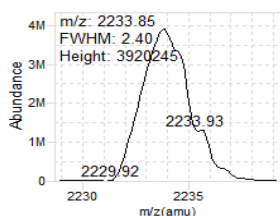
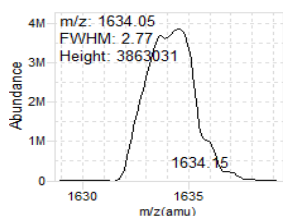
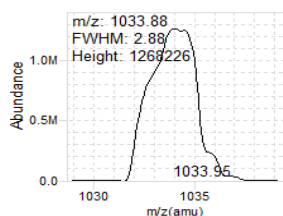
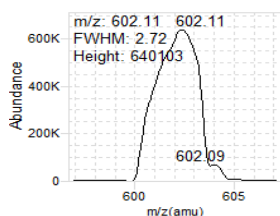
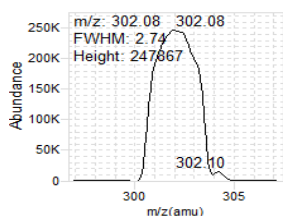
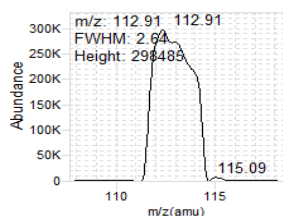


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
113.02	112.99	1.20	1.20	211526
302.04	302.00	1.41	1.20	194663
602.00	601.98	1.56	1.20	411188
1033.93	1033.99	1.63	1.20	916354
1633.97	1633.95	1.41	1.20	2519021
2234.07	2233.91	1.07	1.20	1791181

Analyzer: MS1

Polarity: Negative

Width: Widest

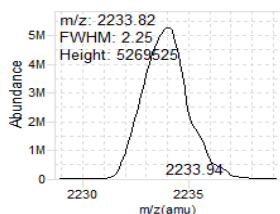
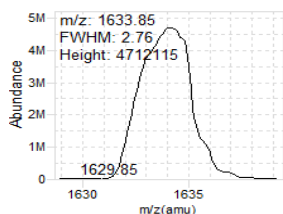
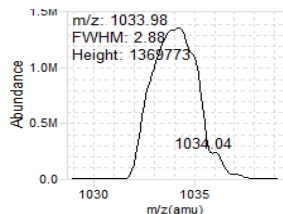
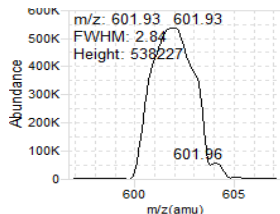
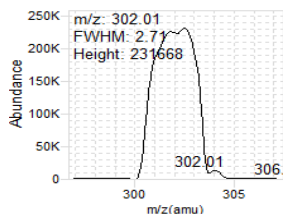
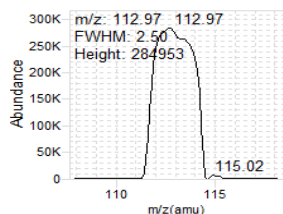


m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.91	112.99	2.64	2.50	298485
302.08	302.00	2.74	2.50	247867
602.10	601.98	2.72	2.50	640103
1033.88	1033.99	2.88	2.50	1268226
1634.05	1633.95	2.77	2.50	3863031
2233.85	2233.91	2.41	2.50	3920246

Analyzer: MS2

Polarity: Negative

Width: Widest



m/z	m/z Expected	FWHM	FWHM Expected	Abundance
112.97	112.99	2.50	2.50	284953
302.01	302.00	2.71	2.50	231668
601.92	601.98	2.84	2.50	538227
1033.98	1033.99	2.88	2.50	1369773
1633.85	1633.95	2.76	2.50	4712115
2233.82	2233.91	2.25	2.50	5269525

Negative Results

Tune Parameters

Parameters	Setting
Fragmentor	115
Skimmer	15
Octopole DC	5
Octopole RF	600
Lens 1	-3.90
MS1 PreFilter	16
MS1 DC	-3.00
MS1 PostFilter	-2.00
MS1 Axis Offset	0.91
MS1 Axis Gain	8
MS1 Width Offset	0.16
MS1 Width Gain	3
MS1 Heater	100
MS2 DC	10
MS2 PreFilter	30
MS2 Axis Offset	0.79
MS2 Axis Gain	18
MS2 Width Offset	0.11
MS2 Width Gain	-7
MS2 Heater	100
Cell Entry	1
Hexapole DC	0.00
Hexapole RF	500
Hexapole Accel	5
Cell Exit	7.00
Collision Gas	1
Iris	150
HED	18
EMV	1245
Collision Energy	0
Lens 1[MS2]	-0.70
MS1 PreFilter[MS2]	-1.80

Dynamic Ramp Tables

MS1 PreFilter

m/z	Setting
112.99	10.2
302	7.8
601.98	8.2
1033.99	20.7
1633.95	14.9
2233.91	17.3

MS1 Axis Offset

m/z	Setting
112.99	0.908
302	1.101
601.98	1.175
1033.99	1.138
1633.95	1.057
2233.91	0.908

MS1 Width Offset

m/z	Setting
112.99	0.16
302	-0.05
601.98	-0.13
1033.99	-0.12
1633.95	-0.06
2233.91	0.16

MS2 PreFilter

m/z	Setting
69	18.6
112.97	30
113	10
207	19.8
232	23.2
302	35

MS2 Axis Offset

m/z	Setting
112.99	0.79
302	0.98
601.98	1.111
1033.99	1.172
1633.95	1.041
2233.91	0.79

MS2 Width Offset

m/z	Setting
112.99	0.11
302	-0.08
601.98	-0.26
1033.99	-0.27
1633.95	-0.15
2233.91	0.11

MS1 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	8.4	0.908	2.8	0.16
Wide	8.1	1.126	3.1	0.56
Widest	7.9	1.57	3.4	1.65

MS2 Calibrations

Resolution	Mass Gain	Mass Offset	Width Gain	Width Offset
Unit	17.5	0.79	-7.3	0.11
Wide	17.45	1.014	-7	0.51
Widest	16.9	1.44	-6.5	1.51

QQQ Check Tune Report

Instrument Name LCMS-2
MS Model G6470A
MS Instrument Serial SG1936G104
Software_Firmware Version 10.0.142, FW: A.00.08.100
Tune Date & Time 02 November 2022 09:26:08
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.70E+0 [R] (Torr); 4.69E-5 [H] (Torr)

Source Parameters

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

Positive Results

Analyzer: MS1 Polarity: Positive Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.10	0.01	Pass	0.70	0.69	-0.01	Pass	610999
322.05	322.02	-0.03	Pass	0.70	0.68	-0.02	Pass	188207
622.03	622.01	-0.02	Pass	0.70	0.69	-0.01	Pass	219997
922.01	922.01	0.00	Pass	0.70	0.64	-0.06	Pass	194918
1521.97	1522.13	0.16	Pass	0.70	0.59	-0.11	Pass	96674
2121.93	2122.12	0.19	Pass	0.70	0.63	-0.07	Pass	74896

Analyzer: MS2 Polarity: Positive Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.05	-0.04	Pass	0.70	0.74	0.04	Pass	439448
322.05	322.03	-0.02	Pass	0.70	0.71	0.01	Pass	171515
622.03	622.01	-0.02	Pass	0.70	0.71	0.01	Pass	213057
922.01	922.01	0.00	Pass	0.70	0.65	-0.05	Pass	139007
1521.97	1521.96	-0.01	Pass	0.70	0.65	-0.05	Pass	72302
2121.93	2122.01	0.08	Pass	0.70	0.67	-0.03	Pass	99381

Analyzer: MS1 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.12	0.03	Pass	1.20	1.14	-0.06	Pass	793020
322.05	322.11	0.06	Pass	1.20	1.42	0.22	Pass	275327
622.03	622.04	0.01	Pass	1.20	1.46	0.26	Pass	386655
922.01	922.07	0.06	Pass	1.20	1.45	0.25	Pass	386864
1521.97	1522.10	0.13	Pass	1.20	1.38	0.18	Pass	242355
2121.93	2122.09	0.16	Pass	1.20	1.25	0.05	Pass	194307

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.11	0.02	Pass	1.20	1.16	-0.04	Pass	663787
322.05	322.04	-0.01	Pass	1.20	1.47	0.27	Pass	295146
622.03	622.04	0.01	Pass	1.20	1.57	0.37	Pass	401068
922.01	922.04	0.03	Pass	1.20	1.47	0.27	Pass	341147
1521.97	1522.00	0.03	Pass	1.20	1.21	0.01	Pass	224041
2121.93	2121.95	0.02	Pass	1.20	1.18	-0.02	Pass	176010

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	117.96	-0.13	Pass	2.50	2.77	0.27	Pass	888330
322.05	322.08	0.03	Pass	2.50	3.14	0.64	Pass	389378
622.03	621.92	-0.11	Pass	2.50	2.98	0.48	Pass	534437
922.01	922.01	0.00	Pass	2.50	2.81	0.31	Pass	611869
1521.97	1522.11	0.14	Pass	2.50	2.67	0.17	Pass	412284
2121.93	2122.01	0.08	Pass	2.50	2.37	-0.13	Pass	381734

QQQ Check Tune Report



Agilent

Trusted Answers

Analyzer: MS2 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	2.50	2.50	0.00	Pass	774318
322.05	322.17	0.12	Pass	2.50	2.75	0.25	Pass	406519
622.03	622.00	-0.03	Pass	2.50	3.04	0.54	Pass	559450
922.01	922.15	0.14	Pass	2.50	2.71	0.21	Pass	571691
1521.97	1522.16	0.19	Pass	2.50	2.54	0.04	Pass	538924
2121.93	2121.84	-0.09	Pass	2.50	2.36	-0.14	Pass	696319

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	208853
302.00	302.08	0.08	Pass	0.70	0.63	-0.07	Pass	130329
601.98	602.05	0.07	Pass	0.70	0.66	-0.04	Pass	241319
1033.99	1034.01	0.02	Pass	0.70	0.67	-0.03	Pass	352429
1633.95	1634.00	0.05	Pass	0.70	0.65	-0.05	Pass	764546
2233.91	2233.98	0.07	Pass	0.70	0.70	0.00	Pass	727772

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	0.71	0.01	Pass	158589
302.00	301.98	-0.02	Pass	0.70	0.71	0.01	Pass	118258
601.98	601.95	-0.03	Pass	0.70	0.68	-0.02	Pass	198791
1033.99	1034.01	0.02	Pass	0.70	0.69	-0.01	Pass	392792
1633.95	1633.97	0.02	Pass	0.70	0.64	-0.06	Pass	910007
2233.91	2233.91	0.00	Pass	0.70	0.68	-0.02	Pass	527060

Analyzer: MS1 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.04	0.05	Pass	1.20	1.17	-0.03	Pass	255239
302.00	302.11	0.11	Pass	1.20	1.34	0.14	Pass	204675
601.98	602.13	0.15	Pass	1.20	1.43	0.23	Pass	426884
1033.99	1034.00	0.01	Pass	1.20	1.53	0.33	Pass	798308
1633.95	1634.03	0.08	Pass	1.20	1.44	0.24	Pass	2205856
2233.91	2233.88	-0.03	Pass	1.20	1.28	0.08	Pass	1813790

Analyzer: MS2 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.02	0.03	Pass	1.20	1.20	0.00	Pass	211526
302.00	302.04	0.04	Pass	1.20	1.41	0.21	Pass	194663
601.98	602.00	0.02	Pass	1.20	1.56	0.36	Pass	411188
1033.99	1033.93	-0.06	Pass	1.20	1.63	0.43	Pass	916354
1633.95	1633.97	0.02	Pass	1.20	1.41	0.21	Pass	2519021
2233.91	2234.07	0.16	Pass	1.20	1.07	-0.13	Pass	1791181

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.91	-0.08	Pass	2.50	2.64	0.14	Pass	298485
302.00	302.08	0.08	Pass	2.50	2.74	0.24	Pass	247867
601.98	602.10	0.12	Pass	2.50	2.72	0.22	Pass	640103
1033.99	1033.88	-0.11	Pass	2.50	2.88	0.38	Pass	1268226
1633.95	1634.05	0.10	Pass	2.50	2.77	0.27	Pass	3863031
2233.91	2233.85	-0.06	Pass	2.50	2.41	-0.09	Pass	3920246

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	2.50	0.00	Pass	284953
302.00	302.01	0.01	Pass	2.50	2.71	0.21	Pass	231668
601.98	601.92	-0.06	Pass	2.50	2.84	0.34	Pass	538227
1033.99	1033.98	-0.01	Pass	2.50	2.88	0.38	Pass	1369773
1633.95	1633.85	-0.10	Pass	2.50	2.76	0.26	Pass	4712115
2233.91	2233.82	-0.09	Pass	2.50	2.25	-0.25	Pass	5269525