



# Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

## LC-MS/MS Maintenance Log

Instrument: LCMS-2

Date	N <sub>2</sub> Tank Pressure	N <sub>2</sub> 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
12/14/2020	30 850	100	✓	✓	✓	✓	✓	✓	x	x		ra
12/15/2020	30 850	100	✓	✓	✓	✓	✓	✓	x	x		ra
<del>12/18/2020 JD</del>												

Signature:

Date Completed:

12/18/2020

# 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** 14 December 2020 12:37:44  
**Data Path** D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML  
**Ion Source** AJS ESI  
**Ionization Mode** AJS ESI  
**Tuned Resolution** All  
**Vacuum Pressure** 1.54E+0 [R] (Torr); 4.64E-5 [H] (Torr)

## Source Parameters

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

## Positive Results

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	0.70	0.70	0.00	Pass	755620
322.05	322.09	0.04	Pass	0.70	0.67	-0.03	Pass	243796
622.03	622.14	0.11	Pass	0.70	0.64	-0.06	Pass	318641
922.01	922.14	0.13	Pass	0.70	0.61	-0.09	Pass	355306
1521.97	1522.07	0.10	Pass	0.70	0.61	-0.09	Pass	170689
2121.93	2122.09	0.16	Pass	0.70	0.66	-0.04	Pass	150819

**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	528273
322.05	322.10	0.05	Pass	0.70	0.67	-0.03	Pass	214891
622.03	622.12	0.09	Pass	0.70	0.64	-0.06	Pass	249287
922.01	922.06	0.05	Pass	0.70	0.64	-0.06	Pass	209108
1521.97	1522.06	0.09	Pass	0.70	0.62	-0.08	Pass	117236
2121.93	2122.04	0.11	Pass	0.70	0.64	-0.06	Pass	159402

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.08	-0.01	Pass	1.20	1.18	-0.02	Pass	865403
322.05	322.08	0.03	Pass	1.20	1.40	0.20	Pass	404606
622.03	622.13	0.10	Pass	1.20	1.46	0.26	Pass	559073
922.01	922.15	0.14	Pass	1.20	1.32	0.12	Pass	655522
1521.97	1522.03	0.06	Pass	1.20	1.27	0.07	Pass	396451
2121.93	2122.07	0.14	Pass	1.20	1.15	-0.05	Pass	311287

**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	1.17	-0.03	Pass	674486
322.05	322.08	0.03	Pass	1.20	1.31	0.11	Pass	365584
622.03	622.08	0.05	Pass	1.20	1.17	-0.03	Pass	431696
922.01	922.05	0.04	Pass	1.20	1.03	-0.17	Pass	353783
1521.97	1522.02	0.05	Pass	1.20	0.89	-0.31	Pass	243666
2121.93	2121.97	0.04	Pass	1.20	0.95	-0.25	Pass	280303

**Analyzer: MS1 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	1067945
322.05	322.07	0.02	Pass	2.50	2.70	0.20	Pass	561682
622.03	622.10	0.07	Pass	2.50	2.85	0.35	Pass	780422
922.01	922.08	0.07	Pass	2.50	2.84	0.34	Pass	1012971
1521.97	1522.03	0.06	Pass	2.50	2.73	0.23	Pass	774952
2121.93	2122.05	0.12	Pass	2.50	2.50	0.00	Pass	786245

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Agilent

Trusted Answers

Analyzer: MS2 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.11	0.02	Pass	2.50	2.43	-0.07	Pass	985825
322.05	322.07	0.02	Pass	2.50	2.58	0.08	Pass	561508
622.03	622.06	0.03	Pass	2.50	2.54	0.04	Pass	734915
922.01	922.05	0.04	Pass	2.50	2.39	-0.11	Pass	849753
1521.97	1522.00	0.03	Pass	2.50	2.25	-0.25	Pass	910007
2121.93	2122.03	0.10	Pass	2.50	2.30	-0.20	Pass	1334949

## 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	0.63	-0.07	Pass	196803
302.00	302.09	0.09	Pass	0.70	0.65	-0.05	Pass	156790
601.98	602.08	0.10	Pass	0.70	0.61	-0.09	Pass	191952
1033.99	1034.14	0.15	Pass	0.70	0.59	-0.11	Pass	497755
1633.95	1633.98	0.03	Pass	0.70	0.68	-0.02	Pass	989705
2233.91	2234.00	0.09	Pass	0.70	0.66	-0.04	Pass	867395

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.00	0.01	Pass	0.70	0.69	-0.01	Pass	138628
302.00	302.00	0.00	Pass	0.70	0.70	0.00	Pass	138995
601.98	602.00	0.02	Pass	0.70	0.68	-0.02	Pass	183185
1033.99	1034.02	0.03	Pass	0.70	0.68	-0.02	Pass	561802
1633.95	1634.01	0.06	Pass	0.70	0.65	-0.05	Pass	1227854
2233.91	2234.01	0.10	Pass	0.70	0.67	-0.03	Pass	1008894

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.00	0.01	Pass	1.20	1.16	-0.04	Pass	252975
302.00	302.07	0.07	Pass	1.20	1.36	0.16	Pass	219624
601.98	602.09	0.11	Pass	1.20	1.42	0.22	Pass	328061
1033.99	1034.16	0.17	Pass	1.20	1.35	0.15	Pass	1054984
1633.95	1634.03	0.08	Pass	1.20	1.28	0.08	Pass	2220708
2233.91	2233.96	0.05	Pass	1.20	1.07	-0.13	Pass	2059572

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.00	0.01	Pass	1.20	1.18	-0.02	Pass	195829
302.00	302.00	0.00	Pass	1.20	1.29	0.09	Pass	206982
601.98	602.00	0.02	Pass	1.20	1.27	0.07	Pass	297680
1033.99	1034.01	0.02	Pass	1.20	1.15	-0.05	Pass	1057289
1633.95	1633.99	0.04	Pass	1.20	1.13	-0.07	Pass	2640616
2233.91	2234.00	0.09	Pass	1.20	1.10	-0.10	Pass	2247861

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	2.50	2.44	-0.06	Pass	303105
302.00	302.06	0.06	Pass	2.50	2.66	0.16	Pass	266876
601.98	602.09	0.11	Pass	2.50	2.74	0.24	Pass	455347
1033.99	1034.12	0.13	Pass	2.50	2.70	0.20	Pass	1902369
1633.95	1634.10	0.15	Pass	2.50	2.54	0.04	Pass	4637470
2233.91	2234.06	0.15	Pass	2.50	2.45	-0.05	Pass	5254401

**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	2.45	-0.05	Pass	267809
302.00	302.01	0.01	Pass	2.50	2.57	0.07	Pass	269911
601.98	602.02	0.04	Pass	2.50	2.55	0.05	Pass	433150
1033.99	1034.03	0.04	Pass	2.50	2.49	-0.01	Pass	1851973
1633.95	1634.00	0.05	Pass	2.50	2.46	-0.04	Pass	5700349
2233.91	2234.01	0.10	Pass	2.50	2.37	-0.13	Pass	6695146

# 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** 15 December 2020 12:59:51  
**Data Path** D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML  
**Ion Source** AJS ESI  
**Ionization Mode** AJS ESI  
**Tuned Resolution** All  
**Vacuum Pressure** 1.56E+0 [R] (Torr); 4.64E-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	735616
322.05	322.11	0.06	Pass	0.70	0.64	-0.06	Pass	231649
622.03	622.12	0.09	Pass	0.70	0.62	-0.08	Pass	265173
922.01	922.15	0.14	Pass	0.70	0.63	-0.07	Pass	242548
1521.97	1522.13	0.16	Pass	0.70	0.58	-0.12	Pass	93767
2121.93	2122.17	0.24	Pass	0.70	0.61	-0.09	Pass	75875

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.07	-0.02	Pass	0.70	0.73	0.03	Pass	517939
322.05	322.06	0.01	Pass	0.70	0.69	-0.01	Pass	221854
622.03	622.07	0.04	Pass	0.70	0.69	-0.01	Pass	242009
922.01	922.00	-0.01	Pass	0.70	0.69	-0.01	Pass	180689
1521.97	1521.99	0.02	Pass	0.70	0.68	-0.02	Pass	93069
2121.93	2121.90	-0.03	Pass	0.70	0.72	0.02	Pass	110316

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.10	0.01	Pass	1.20	1.18	-0.02	Pass	843106
322.05	322.14	0.09	Pass	1.20	1.37	0.17	Pass	364762
622.03	622.17	0.14	Pass	1.20	1.44	0.24	Pass	460470
922.01	922.15	0.14	Pass	1.20	1.35	0.15	Pass	463482
1521.97	1522.13	0.16	Pass	1.20	1.20	0.00	Pass	210945
2121.93	2122.14	0.21	Pass	1.20	1.09	-0.11	Pass	150863

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.10	0.01	Pass	1.20	1.18	-0.02	Pass	683309
322.05	322.03	-0.02	Pass	1.20	1.31	0.11	Pass	355596
622.03	622.02	-0.01	Pass	1.20	1.20	0.00	Pass	383951
922.01	921.99	-0.02	Pass	1.20	1.08	-0.12	Pass	294943
1521.97	1521.95	-0.02	Pass	1.20	0.97	-0.23	Pass	176604
2121.93	2121.89	-0.04	Pass	1.20	1.08	-0.12	Pass	195371

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.09	0.00	Pass	2.50	2.46	-0.04	Pass	1056867
322.05	322.11	0.06	Pass	2.50	2.68	0.18	Pass	504020
622.03	622.16	0.13	Pass	2.50	2.77	0.27	Pass	659815
922.01	922.17	0.16	Pass	2.50	2.70	0.20	Pass	753576
1521.97	1522.13	0.16	Pass	2.50	2.60	0.10	Pass	422090
2121.93	2122.12	0.19	Pass	2.50	2.42	-0.08	Pass	412194

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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	2.45	-0.05	Pass	956844
322.05	322.05	0.00	Pass	2.50	2.61	0.11	Pass	541386
622.03	622.02	-0.01	Pass	2.50	2.58	0.08	Pass	661899
922.01	922.01	0.00	Pass	2.50	2.44	-0.06	Pass	655665
1521.97	1521.95	-0.02	Pass	2.50	2.37	-0.13	Pass	563860
2121.93	2121.84	-0.09	Pass	2.50	2.37	-0.13	Pass	826880

## Negative Results

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.00	0.01	Pass	0.70	0.65	-0.05	Pass	197994
302.00	302.06	0.06	Pass	0.70	0.66	-0.04	Pass	146260
601.98	602.06	0.08	Pass	0.70	0.63	-0.07	Pass	195868
1033.99	1034.08	0.09	Pass	0.70	0.62	-0.08	Pass	428208
1633.95	1634.06	0.11	Pass	0.70	0.63	-0.07	Pass	855537
2233.91	2234.10	0.19	Pass	0.70	0.63	-0.07	Pass	635483

**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	0.71	0.01	Pass	136725
302.00	302.00	0.00	Pass	0.70	0.70	0.00	Pass	142073
601.98	601.98	0.00	Pass	0.70	0.69	-0.01	Pass	194717
1033.99	1034.00	0.01	Pass	0.70	0.70	0.00	Pass	642104
1633.95	1633.96	0.01	Pass	0.70	0.68	-0.02	Pass	1393036
2233.91	2233.92	0.01	Pass	0.70	0.71	0.01	Pass	1129336

**Analyzer: MS1 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	1.16	-0.04	Pass	243973
302.00	302.04	0.04	Pass	1.20	1.40	0.20	Pass	193163
601.98	602.06	0.08	Pass	1.20	1.45	0.25	Pass	333049
1033.99	1034.14	0.15	Pass	1.20	1.36	0.16	Pass	990272
1633.95	1634.09	0.14	Pass	1.20	1.19	-0.01	Pass	2012249
2233.91	2234.03	0.12	Pass	1.20	0.99	-0.21	Pass	1665662

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.97	-0.02	Pass	1.20	1.22	0.02	Pass	187939
302.00	301.99	-0.01	Pass	1.20	1.29	0.09	Pass	204450
601.98	601.98	0.00	Pass	1.20	1.30	0.10	Pass	305082
1033.99	1033.97	-0.02	Pass	1.20	1.20	0.00	Pass	1073547
1633.95	1633.96	0.01	Pass	1.20	1.14	-0.06	Pass	2781141
2233.91	2233.92	0.01	Pass	1.20	1.16	-0.04	Pass	2403110

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.98	-0.01	Pass	2.50	2.46	-0.04	Pass	293068
302.00	302.09	0.09	Pass	2.50	2.62	0.12	Pass	251845
601.98	602.13	0.15	Pass	2.50	2.73	0.23	Pass	453799
1033.99	1034.18	0.19	Pass	2.50	2.62	0.12	Pass	1791308
1633.95	1634.23	0.28	Pass	2.50	2.42	-0.08	Pass	4493838
2233.91	2234.15	0.24	Pass	2.50	2.37	-0.13	Pass	4654926

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.99	0.00	Pass	2.50	2.48	-0.02	Pass	284991
302.00	302.00	0.00	Pass	2.50	2.57	0.07	Pass	267153
601.98	602.04	0.06	Pass	2.50	2.59	0.09	Pass	411891
1033.99	1034.01	0.02	Pass	2.50	2.53	0.03	Pass	1817521
1633.95	1633.92	-0.03	Pass	2.50	2.45	-0.05	Pass	5893960
2233.91	2233.89	-0.02	Pass	2.50	2.38	-0.12	Pass	6647010