



Houston Forensic Science Center  
Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LCMS-1

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
10/26/2022	30 1600	100	✓	✓	✓	✓	✓	✓	X	X		KMP
10/27/2022	30 1600	100	✓	✓	✓	✓	✓	✓	<del>X</del>	<del>X</del>	Training 009/10/28/2022	009 009/10/28/2022

vc 11/3/2022

Signature:

*Valerie Cook*

Date Completed:

11/1/2022

# QQQ Check Tune Report

**Instrument Name** LCMS-1  
**MS Model** G6470A  
**MS Instrument Serial** SG1939G104  
**Software\_Firmware Version** 10.0.142, FW: A.00.08.100  
**Tune Date & Time** 26 October 2022 09:16:10  
**Data Path** D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML  
**Ion Source** AJS ESI  
**Ionization Mode** AJS ESI  
**Tuned Resolution** All  
**Vacuum Pressure** 1.59E+0 [R] (Torr); 4.59E-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	531611
322.05	322.07	0.02	Pass	0.70	0.69	-0.01	Pass	243653
622.03	622.03	0.00	Pass	0.70	0.67	-0.03	Pass	251808
922.01	922.02	0.01	Pass	0.70	0.70	0.00	Pass	201911
1521.97	1521.96	-0.01	Pass	0.70	0.68	-0.02	Pass	79739
2121.93	2122.00	0.07	Pass	0.70	0.68	-0.02	Pass	46526

**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	0.72	0.02	Pass	350535
322.05	322.03	-0.02	Pass	0.70	0.69	-0.01	Pass	245317
622.03	622.02	-0.01	Pass	0.70	0.70	0.00	Pass	262304
922.01	921.99	-0.02	Pass	0.70	0.68	-0.02	Pass	180593
1521.97	1521.95	-0.02	Pass	0.70	0.65	-0.05	Pass	106197
2121.93	2121.90	-0.03	Pass	0.70	0.70	0.00	Pass	111399

**Analyzer: MS1 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	1.25	0.05	Pass	587299
322.05	322.08	0.03	Pass	1.20	1.51	0.31	Pass	344656
622.03	622.06	0.03	Pass	1.20	1.61	0.41	Pass	428818
922.01	922.03	0.02	Pass	1.20	1.59	0.39	Pass	391613
1521.97	1521.97	0.00	Pass	1.20	1.45	0.25	Pass	175118
2121.93	2121.94	0.01	Pass	1.20	1.22	0.02	Pass	138593

**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	1.21	0.01	Pass	480010
322.05	322.04	-0.01	Pass	1.20	1.39	0.19	Pass	374401
622.03	622.03	0.00	Pass	1.20	1.52	0.32	Pass	447222
922.01	922.02	0.01	Pass	1.20	1.52	0.32	Pass	353097
1521.97	1521.97	0.00	Pass	1.20	1.36	0.16	Pass	233334
2121.93	2121.81	-0.12	Pass	1.20	1.09	-0.11	Pass	186930

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.07	-0.02	Pass	2.50	2.44	-0.06	Pass	700276
322.05	322.03	-0.02	Pass	2.50	2.66	0.16	Pass	447568
622.03	622.05	0.02	Pass	2.50	2.83	0.33	Pass	528826
922.01	922.05	0.04	Pass	2.50	2.69	0.19	Pass	539070
1521.97	1521.94	-0.03	Pass	2.50	2.58	0.08	Pass	301127
2121.93	2121.82	-0.11	Pass	2.50	2.36	-0.14	Pass	291487

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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	2.45	-0.05	Pass	680857
322.05	322.04	-0.01	Pass	2.50	2.68	0.18	Pass	509411
622.03	621.99	-0.04	Pass	2.50	2.79	0.29	Pass	625512
922.01	921.99	-0.02	Pass	2.50	2.77	0.27	Pass	614021
1521.97	1521.92	-0.05	Pass	2.50	2.66	0.16	Pass	454379
2121.93	2121.84	-0.09	Pass	2.50	2.45	-0.05	Pass	566523

## 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	112.98	-0.01	Pass	0.70	0.71	0.01	Pass	182017
302.00	302.00	0.00	Pass	0.70	0.70	0.00	Pass	83090
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	333786
1033.99	1033.99	0.00	Pass	0.70	0.66	-0.04	Pass	374062
1633.95	1633.94	-0.01	Pass	0.70	0.69	-0.01	Pass	734298
2233.91	2233.91	0.00	Pass	0.70	0.61	-0.09	Pass	342218

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.99	0.00	Pass	0.70	0.69	-0.01	Pass	123676
302.00	301.99	-0.01	Pass	0.70	0.71	0.01	Pass	74086
601.98	601.99	0.01	Pass	0.70	0.70	0.00	Pass	267645
1033.99	1034.00	0.01	Pass	0.70	0.68	-0.02	Pass	355181
1633.95	1633.95	0.00	Pass	0.70	0.69	-0.01	Pass	1143758
2233.91	2233.90	-0.01	Pass	0.70	0.67	-0.03	Pass	570895

**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	1.23	0.03	Pass	220296
302.00	302.00	0.00	Pass	1.20	1.44	0.24	Pass	121067
601.98	601.99	0.01	Pass	1.20	1.61	0.41	Pass	641456
1033.99	1034.04	0.05	Pass	1.20	1.59	0.39	Pass	912090
1633.95	1633.99	0.04	Pass	1.20	1.40	0.20	Pass	2216098
2233.91	2233.91	0.00	Pass	1.20	1.10	-0.10	Pass	1456076

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.95	-0.04	Pass	1.20	1.17	-0.03	Pass	187941
302.00	301.93	-0.07	Pass	1.20	1.42	0.22	Pass	104529
601.98	601.97	-0.01	Pass	1.20	1.59	0.39	Pass	492923
1033.99	1033.99	0.00	Pass	1.20	1.59	0.39	Pass	878623
1633.95	1633.94	-0.01	Pass	1.20	1.48	0.28	Pass	3064702
2233.91	2234.02	0.11	Pass	1.20	1.26	0.06	Pass	1543991

**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	271884
302.00	302.02	0.02	Pass	2.50	2.73	0.23	Pass	143644
601.98	601.79	-0.19	Pass	2.50	2.96	0.46	Pass	863745
1033.99	1034.04	0.05	Pass	2.50	2.94	0.44	Pass	1561159
1633.95	1633.99	0.04	Pass	2.50	2.74	0.24	Pass	4969142
2233.91	2233.97	0.06	Pass	2.50	2.59	0.09	Pass	4681350

**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	2.46	-0.04	Pass	241372
302.00	302.00	0.00	Pass	2.50	2.69	0.19	Pass	132701
601.98	601.96	-0.02	Pass	2.50	2.80	0.30	Pass	700679
1033.99	1034.00	0.01	Pass	2.50	2.82	0.32	Pass	1374817
1633.95	1634.00	0.05	Pass	2.50	2.67	0.17	Pass	5641627
2233.91	2233.83	-0.08	Pass	2.50	2.26	-0.24	Pass	4576459

# QQQ Check Tune Report

**Instrument Name** LCMS-1  
**MS Model** G6470A  
**MS Instrument Serial** SG1939G104  
**Software\_Firmware Version** 10.0.142, FW: A.00.08.100  
**Tune Date & Time** 27 October 2022 11:30:35  
**Data Path** D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML  
**Ion Source** AJS ESI  
**Ionization Mode** AJS ESI  
**Tuned Resolution** All  
**Vacuum Pressure** 1.62E+0 [R] (Torr); 4.94E-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	0.70	0.00	Pass	467171
322.05	322.07	0.02	Pass	0.70	0.69	-0.01	Pass	217358
622.03	622.03	0.00	Pass	0.70	0.67	-0.03	Pass	198541
922.01	922.02	0.01	Pass	0.70	0.71	0.01	Pass	145820
1521.97	1521.96	-0.01	Pass	0.70	0.69	-0.01	Pass	58516
2121.93	2122.00	0.07	Pass	0.70	0.68	-0.02	Pass	33898

**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	345275
322.05	322.03	-0.02	Pass	0.70	0.70	0.00	Pass	225877
622.03	622.02	-0.01	Pass	0.70	0.70	0.00	Pass	225583
922.01	922.00	-0.01	Pass	0.70	0.69	-0.01	Pass	143726
1521.97	1521.96	-0.01	Pass	0.70	0.67	-0.03	Pass	82879
2121.93	2121.90	-0.03	Pass	0.70	0.72	0.02	Pass	87126

**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	1.25	0.05	Pass	509832
322.05	322.08	0.03	Pass	1.20	1.52	0.32	Pass	302920
622.03	622.05	0.02	Pass	1.20	1.61	0.41	Pass	326978
922.01	922.05	0.04	Pass	1.20	1.57	0.37	Pass	261549
1521.97	1521.97	0.00	Pass	1.20	1.46	0.26	Pass	119972
2121.93	2121.95	0.02	Pass	1.20	1.20	0.00	Pass	101909

**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	1.21	0.01	Pass	434263
322.05	322.05	0.00	Pass	1.20	1.41	0.21	Pass	345056
622.03	622.03	0.00	Pass	1.20	1.53	0.33	Pass	368884
922.01	922.03	0.02	Pass	1.20	1.47	0.27	Pass	286145
1521.97	1521.97	0.00	Pass	1.20	1.36	0.16	Pass	173015
2121.93	2121.82	-0.11	Pass	1.20	1.10	-0.10	Pass	150884

**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	2.45	-0.05	Pass	580378
322.05	322.04	-0.01	Pass	2.50	2.67	0.17	Pass	382704
622.03	622.04	0.01	Pass	2.50	2.85	0.35	Pass	396997
922.01	922.03	0.02	Pass	2.50	2.73	0.23	Pass	362493
1521.97	1521.95	-0.02	Pass	2.50	2.60	0.10	Pass	204867
2121.93	2121.85	-0.08	Pass	2.50	2.32	-0.18	Pass	214545

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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	118.09	0.00	Pass	2.50	2.44	-0.06	Pass	600776
322.05	322.06	0.01	Pass	2.50	2.68	0.18	Pass	460540
622.03	621.97	-0.06	Pass	2.50	2.83	0.33	Pass	510054
922.01	922.01	0.00	Pass	2.50	2.74	0.24	Pass	453652
1521.97	1521.93	-0.04	Pass	2.50	2.65	0.15	Pass	336513
2121.93	2121.84	-0.09	Pass	2.50	2.45	-0.05	Pass	428666

## 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	112.98	-0.01	Pass	0.70	0.71	0.01	Pass	183087
302.00	302.00	0.00	Pass	0.70	0.71	0.01	Pass	73216
601.98	601.99	0.01	Pass	0.70	0.67	-0.03	Pass	307979
1033.99	1033.99	0.00	Pass	0.70	0.66	-0.04	Pass	344338
1633.95	1633.96	0.01	Pass	0.70	0.67	-0.03	Pass	686730
2233.91	2233.91	0.00	Pass	0.70	0.62	-0.08	Pass	317495

**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	125591
302.00	301.99	-0.01	Pass	0.70	0.71	0.01	Pass	65646
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	248225
1033.99	1034.00	0.01	Pass	0.70	0.68	-0.02	Pass	339476
1633.95	1633.96	0.01	Pass	0.70	0.67	-0.03	Pass	1125320
2233.91	2233.91	0.00	Pass	0.70	0.69	-0.01	Pass	536087

**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	1.21	0.01	Pass	229297
302.00	302.00	0.00	Pass	1.20	1.45	0.25	Pass	105108
601.98	602.00	0.02	Pass	1.20	1.60	0.40	Pass	589274
1033.99	1034.05	0.06	Pass	1.20	1.60	0.40	Pass	860943
1633.95	1634.01	0.06	Pass	1.20	1.41	0.21	Pass	1998298
2233.91	2233.89	-0.02	Pass	1.20	1.17	-0.03	Pass	1284426

**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	1.19	-0.01	Pass	189222
302.00	301.93	-0.07	Pass	1.20	1.41	0.21	Pass	93352
601.98	601.97	-0.01	Pass	1.20	1.58	0.38	Pass	447904
1033.99	1033.99	0.00	Pass	1.20	1.61	0.41	Pass	813670
1633.95	1633.96	0.01	Pass	1.20	1.50	0.30	Pass	2872557
2233.91	2234.03	0.12	Pass	1.20	1.25	0.05	Pass	1491365

**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	2.50	0.00	Pass	273435
302.00	302.02	0.02	Pass	2.50	2.72	0.22	Pass	126583
601.98	601.79	-0.19	Pass	2.50	2.98	0.48	Pass	767374
1033.99	1034.03	0.04	Pass	2.50	2.98	0.48	Pass	1429103
1633.95	1633.95	0.00	Pass	2.50	2.82	0.32	Pass	4472716
2233.91	2233.99	0.08	Pass	2.50	2.60	0.10	Pass	4111525

**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	247992
302.00	302.01	0.01	Pass	2.50	2.67	0.17	Pass	117910
601.98	602.01	0.03	Pass	2.50	2.85	0.35	Pass	640121
1033.99	1034.01	0.02	Pass	2.50	2.82	0.32	Pass	1287989
1633.95	1634.00	0.05	Pass	2.50	2.72	0.22	Pass	5319322
2233.91	2233.81	-0.10	Pass	2.50	2.35	-0.15	Pass	4315836