



# 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
12/14/21	30 1400	100	✓	✓	✓	✓	✓	✓	X	X	OPI	CD
12/16/21	30 1400	100	✓	✓	✓	✓	✓	✓	X	X	OPI	SD
12/17/21	30 1400	100	✓	✓	✓	✓	✓	✓	X	X	AMP	SD

12/20/21 SD

Signature:

Date Completed:

12/20/21

# 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 2021 11:58:01  
**Data Path** D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML  
**Ion Source** AJS ESI  
**Ionization Mode** AJS ESI  
**Tuned Resolution** All  
**Vacuum Pressure** 1.74E+0 [R] (Torr); 4.72E-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	625712
322.05	322.02	-0.03	Pass	0.70	0.68	-0.02	Pass	353492
622.03	622.06	0.03	Pass	0.70	0.68	-0.02	Pass	251224
922.01	921.99	-0.02	Pass	0.70	0.68	-0.02	Pass	208971
1521.97	1521.91	-0.06	Pass	0.70	0.69	-0.01	Pass	91892
2121.93	2121.85	-0.08	Pass	0.70	0.80	0.10	Pass	80114

**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	0.75	0.05	Pass	402999
322.05	322.02	-0.03	Pass	0.70	0.70	0.00	Pass	317553
622.03	622.01	-0.02	Pass	0.70	0.69	-0.01	Pass	224724
922.01	921.99	-0.02	Pass	0.70	0.67	-0.03	Pass	150698
1521.97	1521.95	-0.02	Pass	0.70	0.69	-0.01	Pass	74130
2121.93	2121.96	0.03	Pass	0.70	0.66	-0.04	Pass	55311

**Analyzer: MS1 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	1.18	-0.02	Pass	694710
322.05	322.07	0.02	Pass	1.20	1.38	0.18	Pass	516998
622.03	622.10	0.07	Pass	1.20	1.44	0.24	Pass	395130
922.01	922.00	-0.01	Pass	1.20	1.39	0.19	Pass	363719
1521.97	1521.91	-0.06	Pass	1.20	1.33	0.13	Pass	177486
2121.93	2121.89	-0.04	Pass	1.20	1.19	-0.01	Pass	129053

**Analyzer: MS2 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	1.19	-0.01	Pass	568551
322.05	321.95	-0.10	Pass	1.20	1.45	0.25	Pass	531236
622.03	622.03	0.00	Pass	1.20	1.59	0.39	Pass	429454
922.01	922.01	0.00	Pass	1.20	1.49	0.29	Pass	350672
1521.97	1521.87	-0.10	Pass	1.20	1.26	0.06	Pass	189531
2121.93	2121.91	-0.02	Pass	1.20	1.17	-0.03	Pass	106281

**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	2.39	-0.11	Pass	812142
322.05	322.08	0.03	Pass	2.50	2.57	0.07	Pass	631982
622.03	622.02	-0.01	Pass	2.50	2.77	0.27	Pass	537730
922.01	922.01	0.00	Pass	2.50	2.81	0.31	Pass	558623
1521.97	1521.97	0.00	Pass	2.50	2.76	0.26	Pass	317692
2121.93	2121.89	-0.04	Pass	2.50	2.93	0.43	Pass	303536

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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	2.46	-0.04	Pass	748106
322.05	322.08	0.03	Pass	2.50	2.73	0.23	Pass	691720
622.03	621.90	-0.13	Pass	2.50	3.01	0.51	Pass	558571
922.01	922.01	0.00	Pass	2.50	2.79	0.29	Pass	580508
1521.97	1521.96	-0.01	Pass	2.50	2.66	0.16	Pass	398540
2121.93	2121.84	-0.09	Pass	2.50	2.39	-0.11	Pass	416861

## 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	112.97	-0.02	Pass	0.70	0.71	0.01	Pass	208118
302.00	302.00	0.00	Pass	0.70	0.71	0.01	Pass	97318
601.98	601.98	0.00	Pass	0.70	0.68	-0.02	Pass	167008
1033.99	1033.98	-0.01	Pass	0.70	0.68	-0.02	Pass	385096
1633.95	1633.91	-0.04	Pass	0.70	0.68	-0.02	Pass	873938
2233.91	2233.85	-0.06	Pass	0.70	0.75	0.05	Pass	736963

**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	0.69	-0.01	Pass	144503
302.00	301.98	-0.02	Pass	0.70	0.73	0.03	Pass	89238
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	162495
1033.99	1034.00	0.01	Pass	0.70	0.67	-0.03	Pass	483505
1633.95	1633.94	-0.01	Pass	0.70	0.66	-0.04	Pass	1056621
2233.91	2233.95	0.04	Pass	0.70	0.65	-0.05	Pass	702231

**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	1.20	0.00	Pass	226032
302.00	301.98	-0.02	Pass	1.20	1.41	0.21	Pass	146130
601.98	601.97	-0.01	Pass	1.20	1.44	0.24	Pass	303340
1033.99	1033.94	-0.05	Pass	1.20	1.48	0.28	Pass	710858
1633.95	1633.91	-0.04	Pass	1.20	1.28	0.08	Pass	1886460
2233.91	2233.79	-0.12	Pass	1.20	1.07	-0.13	Pass	1145535

**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	1.20	0.00	Pass	211930
302.00	301.91	-0.09	Pass	1.20	1.42	0.22	Pass	133043
601.98	601.96	-0.02	Pass	1.20	1.59	0.39	Pass	298117
1033.99	1034.01	0.02	Pass	1.20	1.56	0.36	Pass	994922
1633.95	1634.01	0.06	Pass	1.20	1.29	0.09	Pass	2792934
2233.91	2233.87	-0.04	Pass	1.20	1.06	-0.14	Pass	1650199

**Analyzer: MS1 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	2.53	0.03	Pass	312777
302.00	302.07	0.07	Pass	2.50	2.75	0.25	Pass	179926
601.98	601.99	0.01	Pass	2.50	2.78	0.28	Pass	430549
1033.99	1033.98	-0.01	Pass	2.50	2.71	0.21	Pass	1433834
1633.95	1633.77	-0.18	Pass	2.50	2.50	0.00	Pass	4164123
2233.91	2233.99	0.08	Pass	2.50	2.23	-0.27	Pass	3676848

**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	2.57	0.07	Pass	281474
302.00	301.99	-0.01	Pass	2.50	2.76	0.26	Pass	167984
601.98	601.97	-0.01	Pass	2.50	2.97	0.47	Pass	386566
1033.99	1034.00	0.01	Pass	2.50	2.96	0.46	Pass	1443958
1633.95	1633.98	0.03	Pass	2.50	2.63	0.13	Pass	5248496
2233.91	2233.82	-0.09	Pass	2.50	2.22	-0.28	Pass	5318691

# 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** 16 December 2021 12:16:52  
**Data Path** D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML  
**Ion Source** AJS ESI  
**Ionization Mode** AJS ESI  
**Tuned Resolution** All  
**Vacuum Pressure** 1.61E+0 [R] (Torr); 4.51E-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	587843
322.05	322.03	-0.02	Pass	0.70	0.69	-0.01	Pass	358209
622.03	622.05	0.02	Pass	0.70	0.70	0.00	Pass	266624
922.01	922.01	0.00	Pass	0.70	0.68	-0.02	Pass	331727
1521.97	1521.96	-0.01	Pass	0.70	0.66	-0.04	Pass	196642
2121.93	2121.90	-0.03	Pass	0.70	0.75	0.05	Pass	209411

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.06	-0.03	Pass	0.70	0.73	0.03	Pass	386713
322.05	322.02	-0.03	Pass	0.70	0.69	-0.01	Pass	302187
622.03	622.02	-0.01	Pass	0.70	0.68	-0.02	Pass	256878
922.01	922.01	0.00	Pass	0.70	0.67	-0.03	Pass	214610
1521.97	1521.97	0.00	Pass	0.70	0.69	-0.01	Pass	151253
2121.93	2121.96	0.03	Pass	0.70	0.66	-0.04	Pass	126233

**Analyzer: MS1 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	1.17	-0.03	Pass	676878
322.05	322.06	0.01	Pass	1.20	1.42	0.22	Pass	530567
622.03	622.14	0.11	Pass	1.20	1.40	0.20	Pass	507400
922.01	922.01	0.00	Pass	1.20	1.44	0.24	Pass	589736
1521.97	1521.94	-0.03	Pass	1.20	1.33	0.13	Pass	413684
2121.93	2121.95	0.02	Pass	1.20	1.19	-0.01	Pass	342530

**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	1.19	-0.01	Pass	494856
322.05	321.96	-0.09	Pass	1.20	1.45	0.25	Pass	505457
622.03	622.04	0.01	Pass	1.20	1.61	0.41	Pass	464707
922.01	922.02	0.01	Pass	1.20	1.50	0.30	Pass	499699
1521.97	1521.88	-0.09	Pass	1.20	1.25	0.05	Pass	407640
2121.93	2121.88	-0.05	Pass	1.20	1.23	0.03	Pass	220604

**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	2.43	-0.07	Pass	771686
322.05	322.03	-0.02	Pass	2.50	2.64	0.14	Pass	627975
622.03	622.01	-0.02	Pass	2.50	2.75	0.25	Pass	652981
922.01	922.02	0.01	Pass	2.50	2.85	0.35	Pass	914557
1521.97	1521.98	0.01	Pass	2.50	2.85	0.35	Pass	743771
2121.93	2121.96	0.03	Pass	2.50	2.70	0.20	Pass	843643

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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	118.07	-0.02	Pass	2.50	2.47	-0.03	Pass	691950
322.05	322.04	-0.01	Pass	2.50	2.73	0.23	Pass	694226
622.03	621.87	-0.16	Pass	2.50	3.02	0.52	Pass	642566
922.01	922.01	0.00	Pass	2.50	2.86	0.36	Pass	845065
1521.97	1521.98	0.01	Pass	2.50	2.62	0.12	Pass	871959
2121.93	2121.89	-0.04	Pass	2.50	2.41	-0.09	Pass	990778

## 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	0.70	0.00	Pass	149214
302.00	302.00	0.00	Pass	0.70	0.69	-0.01	Pass	82113
601.98	602.00	0.02	Pass	0.70	0.68	-0.02	Pass	147201
1033.99	1034.01	0.02	Pass	0.70	0.66	-0.04	Pass	357749
1633.95	1633.95	0.00	Pass	0.70	0.69	-0.01	Pass	721744
2233.91	2233.90	-0.01	Pass	0.70	0.74	0.04	Pass	785945

**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	102283
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	75685
601.98	602.00	0.02	Pass	0.70	0.70	0.00	Pass	121803
1033.99	1034.01	0.02	Pass	0.70	0.68	-0.02	Pass	383870
1633.95	1633.95	0.00	Pass	0.70	0.66	-0.04	Pass	922979
2233.91	2233.95	0.04	Pass	0.70	0.65	-0.05	Pass	716247

**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	1.16	-0.04	Pass	186712
302.00	302.01	0.01	Pass	1.20	1.38	0.18	Pass	126343
601.98	601.99	0.01	Pass	1.20	1.45	0.25	Pass	260665
1033.99	1033.98	-0.01	Pass	1.20	1.43	0.23	Pass	692507
1633.95	1633.96	0.01	Pass	1.20	1.27	0.07	Pass	1568802
2233.91	2233.82	-0.09	Pass	1.20	1.07	-0.13	Pass	1229989

**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	1.20	0.00	Pass	146680
302.00	301.94	-0.06	Pass	1.20	1.42	0.22	Pass	110127
601.98	601.97	-0.01	Pass	1.20	1.60	0.40	Pass	245485
1033.99	1034.02	0.03	Pass	1.20	1.55	0.35	Pass	864485
1633.95	1634.01	0.06	Pass	1.20	1.32	0.12	Pass	2341355
2233.91	2233.88	-0.03	Pass	1.20	1.05	-0.15	Pass	1677500

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.04	0.05	Pass	2.50	2.57	0.07	Pass	201074
302.00	302.08	0.08	Pass	2.50	2.77	0.27	Pass	149524
601.98	601.98	0.00	Pass	2.50	2.73	0.23	Pass	365056
1033.99	1034.05	0.06	Pass	2.50	2.63	0.13	Pass	1256714
1633.95	1633.81	-0.14	Pass	2.50	2.43	-0.07	Pass	3643938
2233.91	2234.10	0.19	Pass	2.50	2.07	-0.43	Pass	3736043

**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	2.58	0.08	Pass	203022
302.00	302.00	0.00	Pass	2.50	2.76	0.26	Pass	137936
601.98	602.01	0.03	Pass	2.50	2.90	0.40	Pass	326891
1033.99	1034.01	0.02	Pass	2.50	2.97	0.47	Pass	1238753
1633.95	1633.98	0.03	Pass	2.50	2.61	0.11	Pass	4422094
2233.91	2233.86	-0.05	Pass	2.50	2.31	-0.19	Pass	5094722

# QQQ Check Tune Report



Agilent

Trusted Answers

**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** 17 December 2021 12:06:03  
**Data Path** D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML  
**Ion Source** AJS ESI  
**Ionization Mode** AJS ESI  
**Tuned Resolution** All  
**Vacuum Pressure** 1.60E+0 [R] (Torr); 4.51E-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	0.73	0.03	Pass	434269
322.05	322.03	-0.02	Pass	0.70	0.69	-0.01	Pass	347795
622.03	622.08	0.05	Pass	0.70	0.67	-0.03	Pass	267789
922.01	922.00	-0.01	Pass	0.70	0.69	-0.01	Pass	326519
1521.97	1521.95	-0.02	Pass	0.70	0.66	-0.04	Pass	218966
2121.93	2121.88	-0.05	Pass	0.70	0.78	0.08	Pass	191722

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

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.06	-0.03	Pass	0.70	0.74	0.04	Pass	374261
322.05	322.02	-0.03	Pass	0.70	0.71	0.01	Pass	300788
622.03	622.02	-0.01	Pass	0.70	0.69	-0.01	Pass	250135
922.01	922.00	-0.01	Pass	0.70	0.68	-0.02	Pass	212162
1521.97	1521.95	-0.02	Pass	0.70	0.67	-0.03	Pass	161317
2121.93	2121.96	0.03	Pass	0.70	0.67	-0.03	Pass	128943

**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	608999
322.05	322.06	0.01	Pass	1.20	1.42	0.22	Pass	530916
622.03	622.11	0.08	Pass	1.20	1.43	0.23	Pass	472608
922.01	922.00	-0.01	Pass	1.20	1.42	0.22	Pass	585596
1521.97	1521.93	-0.04	Pass	1.20	1.32	0.12	Pass	426379
2121.93	2121.95	0.02	Pass	1.20	1.18	-0.02	Pass	347948

**Analyzer: MS2 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	1.17	-0.03	Pass	488423
322.05	321.95	-0.10	Pass	1.20	1.46	0.26	Pass	456616
622.03	622.05	0.02	Pass	1.20	1.57	0.37	Pass	473153
922.01	922.01	0.00	Pass	1.20	1.46	0.26	Pass	515183
1521.97	1521.88	-0.09	Pass	1.20	1.25	0.05	Pass	419519
2121.93	2121.91	-0.02	Pass	1.20	1.19	-0.01	Pass	259406

**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	2.39	-0.11	Pass	711356
322.05	322.05	0.00	Pass	2.50	2.62	0.12	Pass	675159
622.03	622.02	-0.01	Pass	2.50	2.82	0.32	Pass	634598
922.01	922.00	-0.01	Pass	2.50	2.85	0.35	Pass	893929
1521.97	1522.01	0.04	Pass	2.50	2.67	0.17	Pass	811757
2121.93	2121.91	-0.02	Pass	2.50	2.71	0.21	Pass	845529



# QQQ Check Tune Report



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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	118.10	0.01	Pass	2.50	2.44	-0.06	Pass	658014
322.05	322.03	-0.02	Pass	2.50	2.72	0.22	Pass	703880
622.03	621.96	-0.07	Pass	2.50	2.92	0.42	Pass	642546
922.01	922.10	0.09	Pass	2.50	2.67	0.17	Pass	876168
1521.97	1522.03	0.06	Pass	2.50	2.61	0.11	Pass	857163
2121.93	2121.89	-0.04	Pass	2.50	2.43	-0.07	Pass	1065798

## 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	0.69	-0.01	Pass	127621
302.00	302.01	0.01	Pass	0.70	0.69	-0.01	Pass	82378
601.98	601.99	0.01	Pass	0.70	0.68	-0.02	Pass	171344
1033.99	1034.00	0.01	Pass	0.70	0.68	-0.02	Pass	315949
1633.95	1633.95	0.00	Pass	0.70	0.67	-0.03	Pass	692933
2233.91	2233.89	-0.02	Pass	0.70	0.72	0.02	Pass	763737

**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	90516
302.00	301.99	-0.01	Pass	0.70	0.71	0.01	Pass	79939
601.98	601.98	0.00	Pass	0.70	0.70	0.00	Pass	148879
1033.99	1034.00	0.01	Pass	0.70	0.68	-0.02	Pass	404387
1633.95	1633.93	-0.02	Pass	0.70	0.67	-0.03	Pass	869798
2233.91	2233.92	0.01	Pass	0.70	0.66	-0.04	Pass	626995

**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	1.18	-0.02	Pass	168056
302.00	302.02	0.02	Pass	1.20	1.40	0.20	Pass	130083
601.98	601.99	0.01	Pass	1.20	1.46	0.26	Pass	312884
1033.99	1033.98	-0.01	Pass	1.20	1.43	0.23	Pass	638245
1633.95	1633.96	0.01	Pass	1.20	1.27	0.07	Pass	1484843
2233.91	2233.81	-0.10	Pass	1.20	1.04	-0.16	Pass	1175130

**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	1.18	-0.02	Pass	148028
302.00	301.93	-0.07	Pass	1.20	1.42	0.22	Pass	106860
601.98	601.97	-0.01	Pass	1.20	1.60	0.40	Pass	299087
1033.99	1034.00	0.01	Pass	1.20	1.59	0.39	Pass	804656
1633.95	1634.00	0.05	Pass	1.20	1.30	0.10	Pass	2319988
2233.91	2233.87	-0.04	Pass	1.20	1.03	-0.17	Pass	1625591

**Analyzer: MS1 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	2.55	0.05	Pass	200429
302.00	302.13	0.13	Pass	2.50	2.73	0.23	Pass	159558
601.98	601.96	-0.02	Pass	2.50	2.83	0.33	Pass	416266
1033.99	1033.99	0.00	Pass	2.50	2.75	0.25	Pass	1133962
1633.95	1633.82	-0.13	Pass	2.50	2.56	0.06	Pass	3074672
2233.91	2233.98	0.07	Pass	2.50	2.18	-0.32	Pass	3389847

**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	2.59	0.09	Pass	191014
302.00	301.99	-0.01	Pass	2.50	2.77	0.27	Pass	149221
601.98	601.97	-0.01	Pass	2.50	2.95	0.45	Pass	397978
1033.99	1034.00	0.01	Pass	2.50	3.00	0.50	Pass	1150878
1633.95	1633.98	0.03	Pass	2.50	2.56	0.06	Pass	4303165
2233.91	2233.86	-0.05	Pass	2.50	2.26	-0.24	Pass	5040701