



Houston Forensic Science Center
Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LCMS-31 12/13/2015 SD

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
12/15/21	30 / 1500	100 ✓	✓	✓	✓	✓	✓	✓	X	X	AMP	SD
12/14/21	30 / 1500	100	✓	✓	✓	✓	✓	✓	X	X	BNZ	SD
12/16/21	30 / 1900	100	✓	✓	✓	✓	✓	✓	X	X	THC	CD
12/17/21	30 / 1750	100	✓	✓	✓	✓	✓	✓	X	X	CDC	EC
12/20/21 SD												

Signature:

Date Completed:

12/20/21

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 13 December 2021 09:45:58
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	0.71	0.01	Pass	116351
322.05	322.08	0.03	Pass	0.70	0.69	-0.01	Pass	58362
622.03	622.05	0.02	Pass	0.70	0.69	-0.01	Pass	59225
922.01	922.01	0.00	Pass	0.70	0.72	0.02	Pass	67749
1521.97	1521.98	0.01	Pass	0.70	0.68	-0.02	Pass	45449
2121.93	2121.92	-0.01	Pass	0.70	0.68	-0.02	Pass	31192

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	0.75	0.05	Pass	77599
322.05	322.03	-0.02	Pass	0.70	0.76	0.06	Pass	49300
622.03	622.03	0.00	Pass	0.70	0.66	-0.04	Pass	57187
922.01	922.02	0.01	Pass	0.70	0.67	-0.03	Pass	54820
1521.97	1521.98	0.01	Pass	0.70	0.67	-0.03	Pass	53090
2121.93	2121.96	0.03	Pass	0.70	0.67	-0.03	Pass	45602

Analyzer: MS1 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.13	0.04	Pass	1.20	1.16	-0.04	Pass	138123
322.05	322.08	0.03	Pass	1.20	1.44	0.24	Pass	81311
622.03	622.04	0.01	Pass	1.20	1.54	0.34	Pass	107264
922.01	922.01	0.00	Pass	1.20	1.57	0.37	Pass	131404
1521.97	1521.98	0.01	Pass	1.20	1.37	0.17	Pass	93734
2121.93	2121.92	-0.01	Pass	1.20	1.15	-0.05	Pass	83845

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.13	0.04	Pass	1.20	1.19	-0.01	Pass	106113
322.05	322.06	0.01	Pass	1.20	1.45	0.25	Pass	85583
622.03	622.03	0.00	Pass	1.20	1.49	0.29	Pass	98290
922.01	922.02	0.01	Pass	1.20	1.51	0.31	Pass	123602
1521.97	1521.93	-0.04	Pass	1.20	1.31	0.11	Pass	117858
2121.93	2121.97	0.04	Pass	1.20	1.21	0.01	Pass	81050

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.05	-0.04	Pass	2.50	2.55	0.05	Pass	153752
322.05	322.09	0.04	Pass	2.50	2.84	0.34	Pass	117233
622.03	622.15	0.12	Pass	2.50	2.94	0.44	Pass	143962
922.01	921.98	-0.03	Pass	2.50	2.86	0.36	Pass	203276
1521.97	1522.08	0.11	Pass	2.50	2.61	0.11	Pass	172161
2121.93	2121.71	-0.22	Pass	2.50	2.54	0.04	Pass	176525

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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	2.50	0.00	Pass	144965
322.05	321.84	-0.21	Pass	2.50	2.83	0.33	Pass	126152
622.03	622.06	0.03	Pass	2.50	2.73	0.23	Pass	140369
922.01	921.99	-0.02	Pass	2.50	2.86	0.36	Pass	191502
1521.97	1521.95	-0.02	Pass	2.50	2.82	0.32	Pass	217277
2121.93	2121.93	0.00	Pass	2.50	2.35	-0.15	Pass	242918

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	0.74	0.04	Pass	125361
302.00	302.01	0.01	Pass	0.70	0.67	-0.03	Pass	78975
601.98	601.99	0.01	Pass	0.70	0.70	0.00	Pass	153837
1033.99	1034.02	0.03	Pass	0.70	0.67	-0.03	Pass	137358
1633.95	1634.00	0.05	Pass	0.70	0.66	-0.04	Pass	232672
2233.91	2233.92	0.01	Pass	0.70	0.70	0.00	Pass	166634

Analyzer: MS2 Polarity: Negative Width: Unit

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.96	-0.03	Pass	0.70	0.72	0.02	Pass	99532
302.00	301.99	-0.01	Pass	0.70	0.71	0.01	Pass	66028
601.98	601.99	0.01	Pass	0.70	0.68	-0.02	Pass	130055
1033.99	1034.00	0.01	Pass	0.70	0.67	-0.03	Pass	131975
1633.95	1633.95	0.00	Pass	0.70	0.64	-0.06	Pass	317332
2233.91	2233.90	-0.01	Pass	0.70	0.74	0.04	Pass	204431

Analyzer: MS1 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	163769
302.00	302.02	0.02	Pass	1.20	1.44	0.24	Pass	122481
601.98	602.09	0.11	Pass	1.20	1.62	0.42	Pass	295306
1033.99	1034.03	0.04	Pass	1.20	1.70	0.50	Pass	321543
1633.95	1633.98	0.03	Pass	1.20	1.45	0.25	Pass	711032
2233.91	2233.92	0.01	Pass	1.20	1.25	0.05	Pass	518091

Analyzer: MS2 Polarity: Negative Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.99	0.00	Pass	1.20	1.25	0.05	Pass	119798
302.00	301.99	-0.01	Pass	1.20	1.34	0.14	Pass	87367
601.98	601.95	-0.03	Pass	1.20	1.59	0.39	Pass	192173
1033.99	1033.92	-0.07	Pass	1.20	1.57	0.37	Pass	279545
1633.95	1633.81	-0.14	Pass	1.20	1.50	0.30	Pass	750673
2233.91	2233.94	0.03	Pass	1.20	1.22	0.02	Pass	444208

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.01	0.02	Pass	2.50	2.38	-0.12	Pass	168341
302.00	302.02	0.02	Pass	2.50	2.74	0.24	Pass	133715
601.98	602.03	0.05	Pass	2.50	2.62	0.12	Pass	412792
1033.99	1034.05	0.06	Pass	2.50	2.79	0.29	Pass	482094
1633.95	1634.18	0.23	Pass	2.50	2.49	-0.01	Pass	1289373
2233.91	2233.91	0.00	Pass	2.50	2.30	-0.20	Pass	1367810

Analyzer: MS2 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.96	-0.03	Pass	2.50	2.54	0.04	Pass	186032
302.00	302.10	0.10	Pass	2.50	2.72	0.22	Pass	116052
601.98	601.91	-0.07	Pass	2.50	3.04	0.54	Pass	333958
1033.99	1034.12	0.13	Pass	2.50	3.07	0.57	Pass	487066
1633.95	1633.92	-0.03	Pass	2.50	2.92	0.42	Pass	1567396
2233.91	2233.83	-0.08	Pass	2.50	2.84	0.34	Pass	1728761

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 14 December 2021 07:27:58
Data Path D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.64E+0 [R] (Torr); 4.67E-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	152658
322.05	322.08	0.03	Pass	0.70	0.66	-0.04	Pass	78295
622.03	622.06	0.03	Pass	0.70	0.66	-0.04	Pass	68851
922.01	921.99	-0.02	Pass	0.70	0.71	0.01	Pass	65766
1521.97	1521.99	0.02	Pass	0.70	0.67	-0.03	Pass	32609
2121.93	2121.91	-0.02	Pass	0.70	0.71	0.01	Pass	21557

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	0.73	0.03	Pass	113671
322.05	322.03	-0.02	Pass	0.70	0.70	0.00	Pass	66497
622.03	622.03	0.00	Pass	0.70	0.67	-0.03	Pass	67477
922.01	922.02	0.01	Pass	0.70	0.66	-0.04	Pass	60500
1521.97	1521.96	-0.01	Pass	0.70	0.66	-0.04	Pass	42922
2121.93	2121.95	0.02	Pass	0.70	0.65	-0.05	Pass	40932

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	1.22	0.02	Pass	175880
322.05	322.07	0.02	Pass	1.20	1.48	0.28	Pass	101267
622.03	622.05	0.02	Pass	1.20	1.56	0.36	Pass	115308
922.01	922.04	0.03	Pass	1.20	1.60	0.40	Pass	120924
1521.97	1521.98	0.01	Pass	1.20	1.38	0.18	Pass	77042
2121.93	2121.88	-0.05	Pass	1.20	1.24	0.04	Pass	58578

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	1.22	0.02	Pass	136618
322.05	322.07	0.02	Pass	1.20	1.39	0.19	Pass	108244
622.03	622.06	0.03	Pass	1.20	1.55	0.35	Pass	113723
922.01	922.02	0.01	Pass	1.20	1.50	0.30	Pass	120200
1521.97	1521.95	-0.02	Pass	1.20	1.36	0.16	Pass	96160
2121.93	2121.95	0.02	Pass	1.20	1.20	0.00	Pass	65884

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.06	-0.03	Pass	2.50	2.58	0.08	Pass	203251
322.05	322.05	0.00	Pass	2.50	2.88	0.38	Pass	146531
622.03	622.12	0.09	Pass	2.50	2.93	0.43	Pass	156413
922.01	921.92	-0.09	Pass	2.50	3.19	0.69	Pass	185628
1521.97	1522.03	0.06	Pass	2.50	2.87	0.37	Pass	120723
2121.93	2121.73	-0.20	Pass	2.50	2.56	0.06	Pass	120318

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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	118.08	-0.01	Pass	2.50	2.51	0.01	Pass	198457
322.05	321.91	-0.14	Pass	2.50	2.71	0.21	Pass	140573
622.03	622.02	-0.01	Pass	2.50	2.86	0.36	Pass	157714
922.01	922.03	0.02	Pass	2.50	2.68	0.18	Pass	206093
1521.97	1521.94	-0.03	Pass	2.50	2.83	0.33	Pass	186542
2121.93	2121.90	-0.03	Pass	2.50	2.33	-0.17	Pass	201409

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	0.70	0.00	Pass	168998
302.00	302.03	0.03	Pass	0.70	0.64	-0.06	Pass	83902
601.98	602.00	0.02	Pass	0.70	0.70	0.00	Pass	190970
1033.99	1034.01	0.02	Pass	0.70	0.69	-0.01	Pass	149681
1633.95	1633.99	0.04	Pass	0.70	0.69	-0.01	Pass	264877
2233.91	2233.91	0.00	Pass	0.70	0.70	0.00	Pass	187184

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	128860
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	71729
601.98	601.99	0.01	Pass	0.70	0.68	-0.02	Pass	166371
1033.99	1033.99	0.00	Pass	0.70	0.68	-0.02	Pass	157400
1633.95	1633.95	0.00	Pass	0.70	0.72	0.02	Pass	433035
2233.91	2233.90	-0.01	Pass	0.70	0.72	0.02	Pass	294633

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	1.24	0.04	Pass	202956
302.00	302.02	0.02	Pass	1.20	1.57	0.37	Pass	127497
601.98	602.08	0.10	Pass	1.20	1.62	0.42	Pass	350117
1033.99	1034.03	0.04	Pass	1.20	1.67	0.47	Pass	343503
1633.95	1633.97	0.02	Pass	1.20	1.46	0.26	Pass	781104
2233.91	2233.94	0.03	Pass	1.20	1.17	-0.03	Pass	597656

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	1.21	0.01	Pass	182064
302.00	301.99	-0.01	Pass	1.20	1.52	0.32	Pass	115368
601.98	601.97	-0.01	Pass	1.20	1.56	0.36	Pass	291390
1033.99	1033.95	-0.04	Pass	1.20	1.59	0.39	Pass	375298
1633.95	1633.80	-0.15	Pass	1.20	1.48	0.28	Pass	1027951
2233.91	2233.96	0.05	Pass	1.20	1.27	0.07	Pass	596402

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	2.42	-0.08	Pass	239472
302.00	302.01	0.01	Pass	2.50	2.75	0.25	Pass	146091
601.98	602.01	0.03	Pass	2.50	2.74	0.24	Pass	463218
1033.99	1034.00	0.01	Pass	2.50	2.78	0.28	Pass	616247
1633.95	1634.20	0.25	Pass	2.50	2.43	-0.07	Pass	1547950
2233.91	2233.96	0.05	Pass	2.50	2.22	-0.28	Pass	1510959

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	2.54	0.04	Pass	216792
302.00	302.11	0.11	Pass	2.50	2.70	0.20	Pass	132646
601.98	601.91	-0.07	Pass	2.50	3.03	0.53	Pass	386416
1033.99	1034.09	0.10	Pass	2.50	3.00	0.50	Pass	519717
1633.95	1633.96	0.01	Pass	2.50	2.92	0.42	Pass	1850837
2233.91	2233.91	0.00	Pass	2.50	2.34	-0.16	Pass	1981840

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 16 December 2021 08:22:48
Data Path D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.61E+0 [R] (Torr); 4.61E-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	244551
322.05	322.05	0.00	Pass	0.70	0.69	-0.01	Pass	126388
622.03	622.06	0.03	Pass	0.70	0.66	-0.04	Pass	110805
922.01	922.01	0.00	Pass	0.70	0.70	0.00	Pass	111822
1521.97	1521.99	0.02	Pass	0.70	0.73	0.03	Pass	53196
2121.93	2121.92	-0.01	Pass	0.70	0.69	-0.01	Pass	37260

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	0.70	0.00	Pass	165900
322.05	322.03	-0.02	Pass	0.70	0.71	0.01	Pass	103722
622.03	622.02	-0.01	Pass	0.70	0.71	0.01	Pass	96259
922.01	922.01	0.00	Pass	0.70	0.70	0.00	Pass	85185
1521.97	1521.99	0.02	Pass	0.70	0.66	-0.04	Pass	62708
2121.93	2121.92	-0.01	Pass	0.70	0.70	0.00	Pass	52268

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	1.20	0.00	Pass	275923
322.05	322.09	0.04	Pass	1.20	1.49	0.29	Pass	180847
622.03	622.03	0.00	Pass	1.20	1.56	0.36	Pass	192765
922.01	922.03	0.02	Pass	1.20	1.52	0.32	Pass	214480
1521.97	1521.97	0.00	Pass	1.20	1.44	0.24	Pass	117210
2121.93	2121.92	-0.01	Pass	1.20	1.18	-0.02	Pass	95966

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.13	0.04	Pass	1.20	1.22	0.02	Pass	213061
322.05	322.07	0.02	Pass	1.20	1.39	0.19	Pass	169364
622.03	622.04	0.01	Pass	1.20	1.53	0.33	Pass	172774
922.01	922.02	0.01	Pass	1.20	1.48	0.28	Pass	199552
1521.97	1521.94	-0.03	Pass	1.20	1.38	0.18	Pass	148424
2121.93	2121.93	0.00	Pass	1.20	1.22	0.02	Pass	101654

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	2.54	0.04	Pass	321171
322.05	322.07	0.02	Pass	2.50	2.78	0.28	Pass	234758
622.03	622.11	0.08	Pass	2.50	2.95	0.45	Pass	241891
922.01	921.96	-0.05	Pass	2.50	2.96	0.46	Pass	291266
1521.97	1522.07	0.10	Pass	2.50	2.66	0.16	Pass	206416
2121.93	2121.73	-0.20	Pass	2.50	2.63	0.13	Pass	214328

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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	2.46	-0.04	Pass	288633
322.05	321.89	-0.16	Pass	2.50	2.66	0.16	Pass	227636
622.03	622.06	0.03	Pass	2.50	2.77	0.27	Pass	251186
922.01	922.01	0.00	Pass	2.50	2.84	0.34	Pass	316900
1521.97	1521.96	-0.01	Pass	2.50	2.72	0.22	Pass	263273
2121.93	2121.88	-0.05	Pass	2.50	2.47	-0.03	Pass	292904

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	0.72	0.02	Pass	173926
302.00	302.01	0.01	Pass	0.70	0.67	-0.03	Pass	131877
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	260621
1033.99	1034.02	0.03	Pass	0.70	0.66	-0.04	Pass	262472
1633.95	1633.98	0.03	Pass	0.70	0.70	0.00	Pass	400027
2233.91	2233.92	0.01	Pass	0.70	0.69	-0.01	Pass	284769

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	0.73	0.03	Pass	139126
302.00	301.99	-0.01	Pass	0.70	0.71	0.01	Pass	110024
601.98	601.99	0.01	Pass	0.70	0.67	-0.03	Pass	242554
1033.99	1033.99	0.00	Pass	0.70	0.69	-0.01	Pass	244847
1633.95	1633.95	0.00	Pass	0.70	0.71	0.01	Pass	686523
2233.91	2233.91	0.00	Pass	0.70	0.77	0.07	Pass	386603

Analyzer: MS1 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	1.23	0.03	Pass	215839
302.00	302.01	0.01	Pass	1.20	1.54	0.34	Pass	184954
601.98	602.07	0.09	Pass	1.20	1.66	0.46	Pass	507915
1033.99	1034.04	0.05	Pass	1.20	1.61	0.41	Pass	644379
1633.95	1633.97	0.02	Pass	1.20	1.46	0.26	Pass	1313887
2233.91	2233.93	0.02	Pass	1.20	1.18	-0.02	Pass	1020555

Analyzer: MS2 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	1.18	-0.02	Pass	191717
302.00	301.99	-0.01	Pass	1.20	1.42	0.22	Pass	155068
601.98	601.95	-0.03	Pass	1.20	1.60	0.40	Pass	381253
1033.99	1033.95	-0.04	Pass	1.20	1.66	0.46	Pass	561601
1633.95	1633.81	-0.14	Pass	1.20	1.51	0.31	Pass	1648865
2233.91	2233.95	0.04	Pass	1.20	1.18	-0.02	Pass	907226

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.02	0.03	Pass	2.50	2.42	-0.08	Pass	220162
302.00	302.02	0.02	Pass	2.50	2.67	0.17	Pass	210271
601.98	602.01	0.03	Pass	2.50	2.79	0.29	Pass	632739
1033.99	1034.01	0.02	Pass	2.50	2.81	0.31	Pass	915518
1633.95	1634.20	0.25	Pass	2.50	2.50	0.00	Pass	2282284
2233.91	2233.93	0.02	Pass	2.50	2.28	-0.22	Pass	2401404

Analyzer: MS2 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	2.51	0.01	Pass	223056
302.00	302.11	0.11	Pass	2.50	2.69	0.19	Pass	194259
601.98	601.90	-0.08	Pass	2.50	2.93	0.43	Pass	537847
1033.99	1034.14	0.15	Pass	2.50	2.88	0.38	Pass	881971
1633.95	1633.94	-0.01	Pass	2.50	2.93	0.43	Pass	2897244
2233.91	2233.81	-0.10	Pass	2.50	2.66	0.16	Pass	2804281

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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 17 December 2021 08:24:05
Data Path D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.61E+0 [R] (Torr); 4.61E-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	0.71	0.01	Pass	196030
322.05	322.06	0.01	Pass	0.70	0.65	-0.05	Pass	93384
622.03	622.08	0.05	Pass	0.70	0.71	0.01	Pass	67357
922.01	922.00	-0.01	Pass	0.70	0.70	0.00	Pass	84082
1521.97	1521.99	0.02	Pass	0.70	0.72	0.02	Pass	40723
2121.93	2121.93	0.00	Pass	0.70	0.68	-0.02	Pass	27221

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	0.70	0.00	Pass	111225
322.05	322.03	-0.02	Pass	0.70	0.72	0.02	Pass	61578
622.03	622.04	0.01	Pass	0.70	0.69	-0.01	Pass	68667
922.01	922.02	0.01	Pass	0.70	0.66	-0.04	Pass	67722
1521.97	1521.98	0.01	Pass	0.70	0.69	-0.01	Pass	45322
2121.93	2121.92	-0.01	Pass	0.70	0.69	-0.01	Pass	49436

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	1.22	0.02	Pass	168330
322.05	322.08	0.03	Pass	1.20	1.44	0.24	Pass	116747
622.03	622.04	0.01	Pass	1.20	1.52	0.32	Pass	162474
922.01	922.05	0.04	Pass	1.20	1.48	0.28	Pass	201068
1521.97	1521.98	0.01	Pass	1.20	1.45	0.25	Pass	88620
2121.93	2121.93	0.00	Pass	1.20	1.20	0.00	Pass	73402

Analyzer: MS2 Polarity: Positive Width: Wide

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.13	0.04	Pass	1.20	1.19	-0.01	Pass	155460
322.05	322.06	0.01	Pass	1.20	1.35	0.15	Pass	149756
622.03	622.01	-0.02	Pass	1.20	1.52	0.32	Pass	125738
922.01	922.01	0.00	Pass	1.20	1.53	0.33	Pass	134292
1521.97	1521.94	-0.03	Pass	1.20	1.41	0.21	Pass	111556
2121.93	2121.89	-0.04	Pass	1.20	1.04	-0.16	Pass	95904

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.06	-0.03	Pass	2.50	2.50	0.00	Pass	218054
322.05	322.05	0.00	Pass	2.50	2.83	0.33	Pass	155127
622.03	622.13	0.10	Pass	2.50	2.95	0.45	Pass	182338
922.01	921.96	-0.05	Pass	2.50	2.91	0.41	Pass	239809
1521.97	1522.05	0.08	Pass	2.50	2.80	0.30	Pass	177712
2121.93	2121.76	-0.17	Pass	2.50	2.49	-0.01	Pass	148730

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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	2.45	-0.05	Pass	264945
322.05	321.88	-0.17	Pass	2.50	2.68	0.18	Pass	236392
622.03	622.03	0.00	Pass	2.50	2.95	0.45	Pass	216333
922.01	922.05	0.04	Pass	2.50	2.64	0.14	Pass	284360
1521.97	1521.95	-0.02	Pass	2.50	2.79	0.29	Pass	225276
2121.93	2121.87	-0.06	Pass	2.50	2.42	-0.08	Pass	225600

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	0.69	-0.01	Pass	156809
302.00	302.03	0.03	Pass	0.70	0.67	-0.03	Pass	93515
601.98	601.98	0.00	Pass	0.70	0.68	-0.02	Pass	181237
1033.99	1034.02	0.03	Pass	0.70	0.65	-0.05	Pass	185960
1633.95	1633.99	0.04	Pass	0.70	0.68	-0.02	Pass	297645
2233.91	2233.92	0.01	Pass	0.70	0.72	0.02	Pass	179424

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	122564
302.00	301.98	-0.02	Pass	0.70	0.72	0.02	Pass	75069
601.98	601.99	0.01	Pass	0.70	0.71	0.01	Pass	136486
1033.99	1034.00	0.01	Pass	0.70	0.70	0.00	Pass	166277
1633.95	1633.95	0.00	Pass	0.70	0.66	-0.04	Pass	483794
2233.91	2233.89	-0.02	Pass	0.70	0.73	0.03	Pass	317801

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	1.25	0.05	Pass	179025
302.00	302.02	0.02	Pass	1.20	1.53	0.33	Pass	135010
601.98	602.09	0.11	Pass	1.20	1.66	0.46	Pass	335784
1033.99	1034.05	0.06	Pass	1.20	1.65	0.45	Pass	440880
1633.95	1634.00	0.05	Pass	1.20	1.47	0.27	Pass	884219
2233.91	2233.94	0.03	Pass	1.20	1.32	0.12	Pass	703749

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	1.22	0.02	Pass	160448
302.00	302.00	0.00	Pass	1.20	1.43	0.23	Pass	110518
601.98	601.95	-0.03	Pass	1.20	1.63	0.43	Pass	247041
1033.99	1033.96	-0.03	Pass	1.20	1.58	0.38	Pass	385695
1633.95	1633.80	-0.15	Pass	1.20	1.70	0.50	Pass	983512
2233.91	2233.93	0.02	Pass	1.20	1.09	-0.11	Pass	801340

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.01	0.02	Pass	2.50	2.47	-0.03	Pass	211418
302.00	302.04	0.04	Pass	2.50	2.75	0.25	Pass	154629
601.98	602.01	0.03	Pass	2.50	2.78	0.28	Pass	434617
1033.99	1034.00	0.01	Pass	2.50	2.75	0.25	Pass	652630
1633.95	1634.18	0.23	Pass	2.50	2.54	0.04	Pass	1678216
2233.91	2233.88	-0.03	Pass	2.50	2.33	-0.17	Pass	1736915

Analyzer: MS2 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	113.01	0.02	Pass	2.50	2.55	0.05	Pass	196713
302.00	302.12	0.12	Pass	2.50	2.73	0.23	Pass	131703
601.98	601.89	-0.09	Pass	2.50	2.95	0.45	Pass	407598
1033.99	1034.10	0.11	Pass	2.50	2.99	0.49	Pass	629304
1633.95	1633.98	0.03	Pass	2.50	2.94	0.44	Pass	2054547
2233.91	2233.81	-0.10	Pass	2.50	2.60	0.10	Pass	2105814