



Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LCMS-3

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
10/24/2022	30 1550	90	✓	✓	✓	✓	✓	✓	X	X		KMY
10/25/22	30 1550	90	✓	✓	✓	✓	✓	✓	X	X		EC
10/27/22	30 1550	90	✓	✓	✓	✓	✓	✓	X	X		
vc 11/3/2022												

Signature:

Date Completed: 11/1/2022

QQQ Check Tune Report

Instrument Name LCMS-3
MS Model G6470B
MS Instrument Serial SG2050G211
Software_Firmware Version 10.1.67, FW: A.00.08.112
Tune Date & Time 24 October 2022 08:44:33
File Path D:\MassHunter\Tune\QQQ\G6470B\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.26E+0 [R] (Torr); 3.83E-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	3500
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	614170
322.05	322.03	-0.02	Pass	0.70	0.68	-0.02	Pass	261745
622.03	622.01	-0.02	Pass	0.70	0.71	0.01	Pass	294015
922.01	922.01	0.00	Pass	0.70	0.71	0.01	Pass	255344
1521.97	1521.99	0.02	Pass	0.70	0.68	-0.02	Pass	128146
2121.93	2121.94	0.01	Pass	0.70	0.69	-0.01	Pass	86237

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	445870
322.05	322.01	-0.04	Pass	0.70	0.70	0.00	Pass	165491
622.03	622.05	0.02	Pass	0.70	0.70	0.00	Pass	190589
922.01	922.02	0.01	Pass	0.70	0.70	0.00	Pass	167054
1521.97	1522.00	0.03	Pass	0.70	0.70	0.00	Pass	91291
2121.93	2121.94	0.01	Pass	0.70	0.80	0.10	Pass	96186

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	744412
322.05	322.06	0.01	Pass	1.20	1.28	0.08	Pass	320582
622.03	622.03	0.00	Pass	1.20	1.32	0.12	Pass	407522
922.01	922.02	0.01	Pass	1.20	1.34	0.14	Pass	393409
1521.97	1522.00	0.03	Pass	1.20	1.28	0.08	Pass	212744
2121.93	2121.98	0.05	Pass	1.20	1.19	-0.01	Pass	146757

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	1.19	-0.01	Pass	597941
322.05	322.10	0.05	Pass	1.20	1.33	0.13	Pass	294417
622.03	622.05	0.02	Pass	1.20	1.36	0.16	Pass	327935
922.01	921.98	-0.03	Pass	1.20	1.35	0.15	Pass	306066
1521.97	1521.96	-0.01	Pass	1.20	1.34	0.14	Pass	187642
2121.93	2121.97	0.04	Pass	1.20	1.26	0.06	Pass	159077

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.04	-0.05	Pass	2.50	2.49	-0.01	Pass	900954
322.05	322.03	-0.02	Pass	2.50	2.53	0.03	Pass	431839
622.03	622.02	-0.01	Pass	2.50	2.64	0.14	Pass	563869
922.01	921.98	-0.03	Pass	2.50	2.66	0.16	Pass	596568
1521.97	1522.02	0.05	Pass	2.50	2.61	0.11	Pass	353325
2121.93	2121.82	-0.11	Pass	2.50	2.46	-0.04	Pass	344782

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	2.52	0.02	Pass	875963
322.05	322.07	0.02	Pass	2.50	2.63	0.13	Pass	445964
622.03	622.05	0.02	Pass	2.50	2.59	0.09	Pass	542858
922.01	921.99	-0.02	Pass	2.50	2.56	0.06	Pass	560447
1521.97	1521.96	-0.01	Pass	2.50	2.54	0.04	Pass	346874
2121.93	2121.93	0.00	Pass	2.50	2.32	-0.18	Pass	397840

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	234207
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	96059
601.98	601.98	0.00	Pass	0.70	0.68	-0.02	Pass	200276
1033.99	1034.01	0.02	Pass	0.70	0.69	-0.01	Pass	524016
1633.95	1633.96	0.01	Pass	0.70	0.72	0.02	Pass	891531
2233.91	2233.91	0.00	Pass	0.70	0.70	0.00	Pass	743270

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	139989
302.00	302.00	0.00	Pass	0.70	0.72	0.02	Pass	84746
601.98	601.98	0.00	Pass	0.70	0.69	-0.01	Pass	178950
1033.99	1033.91	-0.08	Pass	0.70	0.71	0.01	Pass	553624
1633.95	1633.96	0.01	Pass	0.70	0.68	-0.02	Pass	1193047
2233.91	2233.86	-0.05	Pass	0.70	0.68	-0.02	Pass	747617

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	1.21	0.01	Pass	268254
302.00	301.97	-0.03	Pass	1.20	1.26	0.06	Pass	143106
601.98	601.98	0.00	Pass	1.20	1.34	0.14	Pass	370137
1033.99	1034.01	0.02	Pass	1.20	1.45	0.25	Pass	1023990
1633.95	1633.94	-0.01	Pass	1.20	1.27	0.07	Pass	2154404
2233.91	2233.91	0.00	Pass	1.20	1.25	0.05	Pass	1702787

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	1.22	0.02	Pass	231010
302.00	302.00	0.00	Pass	1.20	1.47	0.27	Pass	119252
601.98	601.96	-0.02	Pass	1.20	1.42	0.22	Pass	312848
1033.99	1033.92	-0.07	Pass	1.20	1.44	0.24	Pass	996081
1633.95	1633.84	-0.11	Pass	1.20	1.31	0.11	Pass	2749896
2233.91	2233.80	-0.11	Pass	1.20	1.11	-0.09	Pass	1645665

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.95	-0.04	Pass	2.50	2.59	0.09	Pass	319380
302.00	302.04	0.04	Pass	2.50	2.55	0.05	Pass	179857
601.98	602.03	0.05	Pass	2.50	2.56	0.06	Pass	516626
1033.99	1034.03	0.04	Pass	2.50	2.73	0.23	Pass	1719839
1633.95	1634.00	0.05	Pass	2.50	2.36	-0.14	Pass	4697310
2233.91	2233.83	-0.08	Pass	2.50	2.38	-0.12	Pass	4222440

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	2.41	-0.09	Pass	293236
302.00	302.14	0.14	Pass	2.50	2.67	0.17	Pass	151557
601.98	602.06	0.08	Pass	2.50	2.64	0.14	Pass	434075
1033.99	1033.72	-0.27	Pass	2.50	2.79	0.29	Pass	1574372
1633.95	1633.99	0.04	Pass	2.50	2.62	0.12	Pass	5556557
2233.91	2233.92	0.01	Pass	2.50	2.25	-0.25	Pass	5357300

QQQ Check Tune Report

Instrument Name LCMS-3
MS Model G6470B
MS Instrument Serial SG2050G211
Software_Firmware Version 10.1.67, FW: A.00.08.112
Tune Date & Time 25 October 2022 08:41:00
File Path D:\MassHunter\Tune\QQQ\G6470B\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.29E+0 [R] (Torr); 3.88E-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	3500
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	0.69	-0.01	Pass	642816
322.05	322.04	-0.01	Pass	0.70	0.69	-0.01	Pass	235510
622.03	622.01	-0.02	Pass	0.70	0.71	0.01	Pass	229408
922.01	922.01	0.00	Pass	0.70	0.69	-0.01	Pass	166547
1521.97	1521.98	0.01	Pass	0.70	0.69	-0.01	Pass	85682
2121.93	2121.93	0.00	Pass	0.70	0.71	0.01	Pass	57367

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	0.71	0.01	Pass	448144
322.05	322.01	-0.04	Pass	0.70	0.70	0.00	Pass	176174
622.03	622.03	0.00	Pass	0.70	0.69	-0.01	Pass	159025
922.01	922.03	0.02	Pass	0.70	0.68	-0.02	Pass	128400
1521.97	1522.00	0.03	Pass	0.70	0.70	0.00	Pass	68019
2121.93	2121.93	0.00	Pass	0.70	0.79	0.09	Pass	72622

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	722766
322.05	322.06	0.01	Pass	1.20	1.27	0.07	Pass	295140
622.03	622.02	-0.01	Pass	1.20	1.31	0.11	Pass	311106
922.01	922.04	0.03	Pass	1.20	1.30	0.10	Pass	249868
1521.97	1521.96	-0.01	Pass	1.20	1.35	0.15	Pass	136870
2121.93	2121.94	0.01	Pass	1.20	1.27	0.07	Pass	93570

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	1.19	-0.01	Pass	584518
322.05	322.11	0.06	Pass	1.20	1.31	0.11	Pass	287257
622.03	622.05	0.02	Pass	1.20	1.37	0.17	Pass	277411
922.01	922.00	-0.01	Pass	1.20	1.35	0.15	Pass	228570
1521.97	1521.96	-0.01	Pass	1.20	1.33	0.13	Pass	135197
2121.93	2121.97	0.04	Pass	1.20	1.27	0.07	Pass	118456

Analyzer: MS1 Polarity: Positive Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
118.09	118.03	-0.06	Pass	2.50	2.47	-0.03	Pass	836380
322.05	322.04	-0.01	Pass	2.50	2.53	0.03	Pass	398100
622.03	622.02	-0.01	Pass	2.50	2.63	0.13	Pass	410813
922.01	922.02	0.01	Pass	2.50	2.61	0.11	Pass	382854
1521.97	1521.98	0.01	Pass	2.50	2.65	0.15	Pass	217422
2121.93	2121.81	-0.12	Pass	2.50	2.44	-0.06	Pass	220432

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	2.48	-0.02	Pass	841199
322.05	322.03	-0.02	Pass	2.50	2.59	0.09	Pass	422996
622.03	622.05	0.02	Pass	2.50	2.63	0.13	Pass	447692
922.01	921.94	-0.07	Pass	2.50	2.65	0.15	Pass	364664
1521.97	1522.04	0.07	Pass	2.50	2.37	-0.13	Pass	270737
2121.93	2121.90	-0.03	Pass	2.50	2.34	-0.16	Pass	280023

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	0.72	0.02	Pass	246460
302.00	301.99	-0.01	Pass	0.70	0.69	-0.01	Pass	108917
601.98	601.99	0.01	Pass	0.70	0.70	0.00	Pass	244080
1033.99	1034.01	0.02	Pass	0.70	0.70	0.00	Pass	513765
1633.95	1633.95	0.00	Pass	0.70	0.69	-0.01	Pass	877146
2233.91	2233.91	0.00	Pass	0.70	0.70	0.00	Pass	689742

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	162782
302.00	302.01	0.01	Pass	0.70	0.69	-0.01	Pass	98863
601.98	601.98	0.00	Pass	0.70	0.69	-0.01	Pass	199292
1033.99	1033.92	-0.07	Pass	0.70	0.69	-0.01	Pass	556610
1633.95	1633.92	-0.03	Pass	0.70	0.73	0.03	Pass	1141333
2233.91	2233.84	-0.07	Pass	0.70	0.71	0.01	Pass	703967

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	291173
302.00	301.96	-0.04	Pass	1.20	1.25	0.05	Pass	150760
601.98	601.98	0.00	Pass	1.20	1.34	0.14	Pass	408045
1033.99	1033.99	0.00	Pass	1.20	1.42	0.22	Pass	1022550
1633.95	1633.93	-0.02	Pass	1.20	1.26	0.06	Pass	2098198
2233.91	2233.95	0.04	Pass	1.20	1.23	0.03	Pass	1459031

Analyzer: MS2 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	1.29	0.09	Pass	262255
302.00	301.99	-0.01	Pass	1.20	1.35	0.15	Pass	146703
601.98	601.98	0.00	Pass	1.20	1.39	0.19	Pass	348098
1033.99	1033.92	-0.07	Pass	1.20	1.42	0.22	Pass	1001056
1633.95	1633.87	-0.08	Pass	1.20	1.34	0.14	Pass	2529894
2233.91	2233.82	-0.09	Pass	1.20	1.10	-0.10	Pass	1511563

Analyzer: MS1 Polarity: Negative Width: Widest

m/z Expected	m/z Measured	Delta	Result	FWHM Expected	FWHM Measured	Delta	Result	Abundance
112.99	112.95	-0.04	Pass	2.50	2.59	0.09	Pass	355990
302.00	301.97	-0.03	Pass	2.50	2.52	0.02	Pass	198647
601.98	602.01	0.03	Pass	2.50	2.63	0.13	Pass	581982
1033.99	1034.03	0.04	Pass	2.50	2.64	0.14	Pass	1812249
1633.95	1634.00	0.05	Pass	2.50	2.39	-0.11	Pass	4772119
2233.91	2233.78	-0.13	Pass	2.50	2.18	-0.32	Pass	4299483

Analyzer: MS2 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	2.34	-0.16	Pass	313361
302.00	302.14	0.14	Pass	2.50	2.62	0.12	Pass	182121
601.98	602.12	0.14	Pass	2.50	2.61	0.11	Pass	502641
1033.99	1033.76	-0.23	Pass	2.50	2.73	0.23	Pass	1605988
1633.95	1633.99	0.04	Pass	2.50	2.57	0.07	Pass	5656784
2233.91	2233.87	-0.04	Pass	2.50	2.33	-0.17	Pass	5252735

QQQ Check Tune Report



Trusted Answers

Instrument Name LCMS-3
MS Model G6470B
MS Instrument Serial SG2050G211
Software_Firmware Version 10.1.67, FW: A.00.08.112
Tune Date & Time 27 October 2022 11:56:48
File Path D:\MassHunter\Tune\QQQ\G6470B\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.31E+0 [R] (Torr); 3.88E-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	3500
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	0.68	-0.02	Pass	671712
322.05	322.04	-0.01	Pass	0.70	0.68	-0.02	Pass	242011
622.03	622.01	-0.02	Pass	0.70	0.69	-0.01	Pass	224705
922.01	922.01	0.00	Pass	0.70	0.70	0.00	Pass	159314
1521.97	1521.99	0.02	Pass	0.70	0.69	-0.01	Pass	79589
2121.93	2121.94	0.01	Pass	0.70	0.71	0.01	Pass	50743

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	0.71	0.01	Pass	452821
322.05	322.01	-0.04	Pass	0.70	0.69	-0.01	Pass	181062
622.03	622.03	0.00	Pass	0.70	0.70	0.00	Pass	162347
922.01	922.02	0.01	Pass	0.70	0.70	0.00	Pass	117533
1521.97	1521.99	0.02	Pass	0.70	0.71	0.01	Pass	65834
2121.93	2121.88	-0.05	Pass	0.70	0.80	0.10	Pass	70553

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	1.16	-0.04	Pass	733770
322.05	322.06	0.01	Pass	1.20	1.24	0.04	Pass	302154
622.03	622.03	0.00	Pass	1.20	1.31	0.11	Pass	301495
922.01	922.02	0.01	Pass	1.20	1.35	0.15	Pass	223082
1521.97	1521.96	-0.01	Pass	1.20	1.34	0.14	Pass	125348
2121.93	2121.97	0.04	Pass	1.20	1.21	0.01	Pass	89913

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	1.20	0.00	Pass	593033
322.05	322.11	0.06	Pass	1.20	1.32	0.12	Pass	290567
622.03	622.06	0.03	Pass	1.20	1.34	0.14	Pass	285416
922.01	921.97	-0.04	Pass	1.20	1.34	0.14	Pass	208721
1521.97	1521.95	-0.02	Pass	1.20	1.37	0.17	Pass	126207
2121.93	2121.94	0.01	Pass	1.20	1.28	0.08	Pass	113735

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	2.49	-0.01	Pass	830344
322.05	322.04	-0.01	Pass	2.50	2.48	-0.02	Pass	406945
622.03	622.04	0.01	Pass	2.50	2.58	0.08	Pass	392536
922.01	922.02	0.01	Pass	2.50	2.62	0.12	Pass	336827
1521.97	1522.01	0.04	Pass	2.50	2.64	0.14	Pass	200172
2121.93	2121.83	-0.10	Pass	2.50	2.40	-0.10	Pass	208599

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	2.52	0.02	Pass	860209
322.05	322.08	0.03	Pass	2.50	2.61	0.11	Pass	435994
622.03	622.05	0.02	Pass	2.50	2.63	0.13	Pass	439190
922.01	921.98	-0.03	Pass	2.50	2.56	0.06	Pass	375507
1521.97	1521.97	0.00	Pass	2.50	2.48	-0.02	Pass	256216
2121.93	2121.90	-0.03	Pass	2.50	2.33	-0.17	Pass	264234

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	0.72	0.02	Pass	248525
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	105614
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	242856
1033.99	1034.02	0.03	Pass	0.70	0.70	0.00	Pass	463900
1633.95	1633.98	0.03	Pass	0.70	0.69	-0.01	Pass	910564
2233.91	2233.91	0.00	Pass	0.70	0.70	0.00	Pass	718376

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	152477
302.00	302.01	0.01	Pass	0.70	0.71	0.01	Pass	99694
601.98	601.95	-0.03	Pass	0.70	0.69	-0.01	Pass	210679
1033.99	1033.90	-0.09	Pass	0.70	0.72	0.02	Pass	572278
1633.95	1633.93	-0.02	Pass	0.70	0.71	0.01	Pass	1312471
2233.91	2233.82	-0.09	Pass	0.70	0.75	0.05	Pass	779446

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	302964
302.00	301.99	-0.01	Pass	1.20	1.27	0.07	Pass	151181
601.98	601.98	0.00	Pass	1.20	1.36	0.16	Pass	400796
1033.99	1034.01	0.02	Pass	1.20	1.43	0.23	Pass	1032203
1633.95	1633.93	-0.02	Pass	1.20	1.31	0.11	Pass	2100139
2233.91	2233.89	-0.02	Pass	1.20	1.25	0.05	Pass	1643002

Analyzer: MS2 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	274347
302.00	302.02	0.02	Pass	1.20	1.38	0.18	Pass	139373
601.98	601.91	-0.07	Pass	1.20	1.46	0.26	Pass	289301
1033.99	1033.91	-0.08	Pass	1.20	1.44	0.24	Pass	1029250
1633.95	1633.84	-0.11	Pass	1.20	1.36	0.16	Pass	2899283
2233.91	2233.76	-0.15	Pass	1.20	1.15	-0.05	Pass	1807289

Analyzer: MS1 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	2.60	0.10	Pass	371343
302.00	302.02	0.02	Pass	2.50	2.56	0.06	Pass	194257
601.98	602.00	0.02	Pass	2.50	2.75	0.25	Pass	551204
1033.99	1034.06	0.07	Pass	2.50	2.63	0.13	Pass	1875372
1633.95	1634.05	0.10	Pass	2.50	2.18	-0.32	Pass	4900566
2233.91	2233.89	-0.02	Pass	2.50	2.21	-0.29	Pass	4507174

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	2.48	-0.02	Pass	326304
302.00	302.14	0.14	Pass	2.50	2.60	0.10	Pass	177630
601.98	602.10	0.12	Pass	2.50	2.62	0.12	Pass	493392
1033.99	1033.75	-0.24	Pass	2.50	2.73	0.23	Pass	1675573
1633.95	1633.96	0.01	Pass	2.50	2.63	0.13	Pass	5780714
2233.91	2233.82	-0.09	Pass	2.50	2.37	-0.13	Pass	5408070