



Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LC-MS/MS 1

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
20200817	30/2000	100	✓	✓	X	checked	✓	✓	X	X		Rle
20200818	30/2000	100	✓	✓	X	checked	✓	✓	X	X		ra
20200820	30/1950	100	✓	✓	✓	checked	✓	✓	X	X		mh
8/27/2020												
 												
 												

Signature: _____

Date Completed: _____

8/27/2020

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 17 August 2020 09:09:59
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.47E+0 [R] (Torr); 4.49E-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	490296
322.05	322.04	-0.01	Pass	0.70	0.70	0.00	Pass	181461
622.03	622.05	0.02	Pass	0.70	0.66	-0.04	Pass	139652
922.01	922.02	0.01	Pass	0.70	0.69	-0.01	Pass	87224
1521.97	1521.99	0.02	Pass	0.70	0.65	-0.05	Pass	35102
2121.93	2121.92	-0.01	Pass	0.70	0.66	-0.04	Pass	21017

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	373894
322.05	322.03	-0.02	Pass	0.70	0.70	0.00	Pass	191785
622.03	622.02	-0.01	Pass	0.70	0.69	-0.01	Pass	170979
922.01	922.00	-0.01	Pass	0.70	0.67	-0.03	Pass	106530
1521.97	1521.98	0.01	Pass	0.70	0.68	-0.02	Pass	71698
2121.93	2121.91	-0.02	Pass	0.70	0.70	0.00	Pass	65511

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	542728
322.05	322.09	0.04	Pass	1.20	1.50	0.30	Pass	264162
622.03	622.06	0.03	Pass	1.20	1.58	0.38	Pass	238327
922.01	922.04	0.03	Pass	1.20	1.54	0.34	Pass	167541
1521.97	1521.99	0.02	Pass	1.20	1.41	0.21	Pass	77000
2121.93	2121.91	-0.02	Pass	1.20	1.16	-0.04	Pass	61100

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	467177
322.05	322.05	0.00	Pass	1.20	1.39	0.19	Pass	281223
622.03	622.03	0.00	Pass	1.20	1.53	0.33	Pass	265028
922.01	922.02	0.01	Pass	1.20	1.48	0.28	Pass	216823
1521.97	1521.96	-0.01	Pass	1.20	1.47	0.27	Pass	146742
2121.93	2121.84	-0.09	Pass	1.20	1.19	-0.01	Pass	127375

Analyzer: MS1 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	637413
322.05	322.04	-0.01	Pass	2.50	2.69	0.19	Pass	343962
622.03	622.05	0.02	Pass	2.50	2.85	0.35	Pass	284027
922.01	922.02	0.01	Pass	2.50	2.75	0.25	Pass	233678
1521.97	1522.01	0.04	Pass	2.50	2.61	0.11	Pass	136417
2121.93	2121.85	-0.08	Pass	2.50	2.30	-0.20	Pass	152152

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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	2.46	-0.04	Pass	661960
322.05	322.08	0.03	Pass	2.50	2.66	0.16	Pass	383257
622.03	622.07	0.04	Pass	2.50	2.81	0.31	Pass	355325
922.01	922.03	0.02	Pass	2.50	2.71	0.21	Pass	317624
1521.97	1521.99	0.02	Pass	2.50	2.67	0.17	Pass	251370
2121.93	2121.85	-0.08	Pass	2.50	2.35	-0.15	Pass	299598

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	156635
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	191783
601.98	601.98	0.00	Pass	0.70	0.67	-0.03	Pass	251755
1033.99	1034.00	0.01	Pass	0.70	0.66	-0.04	Pass	444596
1633.95	1633.95	0.00	Pass	0.70	0.68	-0.02	Pass	734921
2233.91	2233.92	0.01	Pass	0.70	0.63	-0.07	Pass	457122

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	97217
302.00	301.98	-0.02	Pass	0.70	0.71	0.01	Pass	146725
601.98	601.99	0.01	Pass	0.70	0.70	0.00	Pass	169333
1033.99	1033.99	0.00	Pass	0.70	0.70	0.00	Pass	347563
1633.95	1633.95	0.00	Pass	0.70	0.68	-0.02	Pass	1031015
2233.91	2233.92	0.01	Pass	0.70	0.70	0.00	Pass	570531

Analyzer: MS1 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	1.19	-0.01	Pass	186425
302.00	302.00	0.00	Pass	1.20	1.49	0.29	Pass	252059
601.98	602.00	0.02	Pass	1.20	1.62	0.42	Pass	432712
1033.99	1033.99	0.00	Pass	1.20	1.61	0.41	Pass	1005973
1633.95	1633.96	0.01	Pass	1.20	1.42	0.22	Pass	2127799
2233.91	2233.86	-0.05	Pass	1.20	1.21	0.01	Pass	1583047

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	1.20	0.00	Pass	143815
302.00	301.96	-0.04	Pass	1.20	1.41	0.21	Pass	210010
601.98	601.96	-0.02	Pass	1.20	1.57	0.37	Pass	301728
1033.99	1033.98	-0.01	Pass	1.20	1.54	0.34	Pass	817451
1633.95	1633.92	-0.03	Pass	1.20	1.46	0.26	Pass	2472283
2233.91	2233.83	-0.08	Pass	1.20	1.15	-0.05	Pass	1282912

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	2.51	0.01	Pass	229179
302.00	302.00	0.00	Pass	2.50	2.71	0.21	Pass	299340
601.98	602.00	0.02	Pass	2.50	2.92	0.42	Pass	543630
1033.99	1034.01	0.02	Pass	2.50	2.87	0.37	Pass	1624984
1633.95	1633.99	0.04	Pass	2.50	2.65	0.15	Pass	4429806
2233.91	2233.88	-0.03	Pass	2.50	2.39	-0.11	Pass	4269095

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	2.47	-0.03	Pass	200197
302.00	302.00	0.00	Pass	2.50	2.63	0.13	Pass	289989
601.98	601.98	0.00	Pass	2.50	2.81	0.31	Pass	448471
1033.99	1034.01	0.02	Pass	2.50	2.78	0.28	Pass	1354346
1633.95	1633.95	0.00	Pass	2.50	2.69	0.19	Pass	5000493
2233.91	2233.81	-0.10	Pass	2.50	2.38	-0.12	Pass	3639758

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 18 August 2020 08:17:55
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.45E+0 [R] (Torr); 4.46E-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	463170
322.05	322.03	-0.02	Pass	0.70	0.70	0.00	Pass	164743
622.03	622.05	0.02	Pass	0.70	0.67	-0.03	Pass	163216
922.01	922.01	0.00	Pass	0.70	0.68	-0.02	Pass	123127
1521.97	1521.95	-0.02	Pass	0.70	0.67	-0.03	Pass	43578
2121.93	2121.91	-0.02	Pass	0.70	0.67	-0.03	Pass	26050

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	357802
322.05	322.02	-0.03	Pass	0.70	0.71	0.01	Pass	175112
622.03	622.02	-0.01	Pass	0.70	0.69	-0.01	Pass	191722
922.01	922.01	0.00	Pass	0.70	0.68	-0.02	Pass	139654
1521.97	1521.98	0.01	Pass	0.70	0.68	-0.02	Pass	86900
2121.93	2121.93	0.00	Pass	0.70	0.68	-0.02	Pass	79391

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	1.24	0.04	Pass	517648
322.05	322.06	0.01	Pass	1.20	1.53	0.33	Pass	245177
622.03	622.05	0.02	Pass	1.20	1.63	0.43	Pass	270697
922.01	922.04	0.03	Pass	1.20	1.53	0.33	Pass	254228
1521.97	1521.99	0.02	Pass	1.20	1.40	0.20	Pass	94181
2121.93	2121.91	-0.02	Pass	1.20	1.15	-0.05	Pass	75954

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	446057
322.05	322.04	-0.01	Pass	1.20	1.38	0.18	Pass	266646
622.03	622.03	0.00	Pass	1.20	1.52	0.32	Pass	313318
922.01	922.03	0.02	Pass	1.20	1.49	0.29	Pass	285627
1521.97	1521.97	0.00	Pass	1.20	1.45	0.25	Pass	187897
2121.93	2121.84	-0.09	Pass	1.20	1.18	-0.02	Pass	154263

Analyzer: MS1 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	2.47	-0.03	Pass	613185
322.05	322.03	-0.02	Pass	2.50	2.68	0.18	Pass	326362
622.03	622.04	0.01	Pass	2.50	2.88	0.38	Pass	363143
922.01	922.01	0.00	Pass	2.50	2.78	0.28	Pass	363979
1521.97	1522.03	0.06	Pass	2.50	2.51	0.01	Pass	177079
2121.93	2121.81	-0.12	Pass	2.50	2.42	-0.08	Pass	175856

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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	2.49	-0.01	Pass	626595
322.05	322.07	0.02	Pass	2.50	2.65	0.15	Pass	360989
622.03	622.06	0.03	Pass	2.50	2.80	0.30	Pass	418282
922.01	922.04	0.03	Pass	2.50	2.68	0.18	Pass	442582
1521.97	1522.00	0.03	Pass	2.50	2.64	0.14	Pass	314475
2121.93	2121.85	-0.08	Pass	2.50	2.36	-0.14	Pass	362531

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	0.70	0.00	Pass	139624
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	168777
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	222494
1033.99	1034.00	0.01	Pass	0.70	0.67	-0.03	Pass	399076
1633.95	1633.93	-0.02	Pass	0.70	0.70	0.00	Pass	652962
2233.91	2233.92	0.01	Pass	0.70	0.64	-0.06	Pass	430015

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	85320
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	132911
601.98	601.99	0.01	Pass	0.70	0.70	0.00	Pass	151375
1033.99	1033.99	0.00	Pass	0.70	0.69	-0.01	Pass	316821
1633.95	1633.95	0.00	Pass	0.70	0.68	-0.02	Pass	936701
2233.91	2233.93	0.02	Pass	0.70	0.71	0.01	Pass	523319

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	162123
302.00	302.00	0.00	Pass	1.20	1.48	0.28	Pass	224709
601.98	601.98	0.00	Pass	1.20	1.61	0.41	Pass	390724
1033.99	1033.98	-0.01	Pass	1.20	1.60	0.40	Pass	923528
1633.95	1633.95	0.00	Pass	1.20	1.43	0.23	Pass	1916274
2233.91	2233.86	-0.05	Pass	1.20	1.20	0.00	Pass	1513056

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	1.20	0.00	Pass	126024
302.00	301.97	-0.03	Pass	1.20	1.41	0.21	Pass	187108
601.98	601.97	-0.01	Pass	1.20	1.56	0.36	Pass	272876
1033.99	1033.98	-0.01	Pass	1.20	1.54	0.34	Pass	738675
1633.95	1633.93	-0.02	Pass	1.20	1.45	0.25	Pass	2241273
2233.91	2233.85	-0.06	Pass	1.20	1.15	-0.05	Pass	1182012

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	2.48	-0.02	Pass	200748
302.00	301.99	-0.01	Pass	2.50	2.71	0.21	Pass	265989
601.98	601.99	0.01	Pass	2.50	2.93	0.43	Pass	476814
1033.99	1033.99	0.00	Pass	2.50	2.89	0.39	Pass	1474990
1633.95	1633.98	0.03	Pass	2.50	2.64	0.14	Pass	3947780
2233.91	2233.87	-0.04	Pass	2.50	2.40	-0.10	Pass	4003396

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	2.48	-0.02	Pass	178493
302.00	302.01	0.01	Pass	2.50	2.63	0.13	Pass	255232
601.98	601.97	-0.01	Pass	2.50	2.83	0.33	Pass	393189
1033.99	1034.03	0.04	Pass	2.50	2.76	0.26	Pass	1231179
1633.95	1633.96	0.01	Pass	2.50	2.67	0.17	Pass	4478997
2233.91	2233.81	-0.10	Pass	2.50	2.40	-0.10	Pass	3732907

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 20 August 2020 08:00:28
Data Path D:\MassHunter\Tune\QQQ\G6470A\atunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.45E+0 [R] (Torr); 4.46E-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	390975
322.05	322.05	0.00	Pass	0.70	0.69	-0.01	Pass	157607
622.03	622.05	0.02	Pass	0.70	0.67	-0.03	Pass	122878
922.01	922.02	0.01	Pass	0.70	0.69	-0.01	Pass	81009
1521.97	1521.98	0.01	Pass	0.70	0.68	-0.02	Pass	30533
2121.93	2121.92	-0.01	Pass	0.70	0.66	-0.04	Pass	19150

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	308207
322.05	322.03	-0.02	Pass	0.70	0.70	0.00	Pass	164547
622.03	622.02	-0.01	Pass	0.70	0.69	-0.01	Pass	153699
922.01	922.00	-0.01	Pass	0.70	0.68	-0.02	Pass	97682
1521.97	1521.98	0.01	Pass	0.70	0.67	-0.03	Pass	67318
2121.93	2121.92	-0.01	Pass	0.70	0.70	0.00	Pass	57728

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	433543
322.05	322.08	0.03	Pass	1.20	1.50	0.30	Pass	224405
622.03	622.07	0.04	Pass	1.20	1.60	0.40	Pass	208052
922.01	922.05	0.04	Pass	1.20	1.55	0.35	Pass	157372
1521.97	1522.02	0.05	Pass	1.20	1.37	0.17	Pass	69629
2121.93	2121.92	-0.01	Pass	1.20	1.14	-0.06	Pass	55166

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	382326
322.05	322.05	0.00	Pass	1.20	1.39	0.19	Pass	245350
622.03	622.03	0.00	Pass	1.20	1.54	0.34	Pass	238290
922.01	922.02	0.01	Pass	1.20	1.49	0.29	Pass	203532
1521.97	1521.96	-0.01	Pass	1.20	1.47	0.27	Pass	135803
2121.93	2121.83	-0.10	Pass	1.20	1.20	0.00	Pass	114380

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	500488
322.05	322.04	-0.01	Pass	2.50	2.70	0.20	Pass	288346
622.03	622.06	0.03	Pass	2.50	2.84	0.34	Pass	259801
922.01	922.01	0.00	Pass	2.50	2.79	0.29	Pass	218815
1521.97	1522.02	0.05	Pass	2.50	2.56	0.06	Pass	123541
2121.93	2121.85	-0.08	Pass	2.50	2.37	-0.13	Pass	129449

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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	2.46	-0.04	Pass	534251
322.05	322.08	0.03	Pass	2.50	2.65	0.15	Pass	333815
622.03	622.07	0.04	Pass	2.50	2.80	0.30	Pass	322337
922.01	922.03	0.02	Pass	2.50	2.69	0.19	Pass	297051
1521.97	1522.01	0.04	Pass	2.50	2.62	0.12	Pass	229406
2121.93	2121.83	-0.10	Pass	2.50	2.36	-0.14	Pass	270457

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	130024
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	167625
601.98	601.99	0.01	Pass	0.70	0.68	-0.02	Pass	239453
1033.99	1034.00	0.01	Pass	0.70	0.66	-0.04	Pass	392754
1633.95	1633.95	0.00	Pass	0.70	0.68	-0.02	Pass	659949
2233.91	2233.92	0.01	Pass	0.70	0.64	-0.06	Pass	411358

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	81904
302.00	301.99	-0.01	Pass	0.70	0.71	0.01	Pass	128164
601.98	601.99	0.01	Pass	0.70	0.70	0.00	Pass	153690
1033.99	1034.00	0.01	Pass	0.70	0.69	-0.01	Pass	314716
1633.95	1633.96	0.01	Pass	0.70	0.67	-0.03	Pass	930298
2233.91	2233.94	0.03	Pass	0.70	0.70	0.00	Pass	503170

Analyzer: MS1 **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	1.21	0.01	Pass	156531
302.00	302.00	0.00	Pass	1.20	1.48	0.28	Pass	227899
601.98	601.98	0.00	Pass	1.20	1.64	0.44	Pass	420142
1033.99	1033.99	0.00	Pass	1.20	1.61	0.41	Pass	908633
1633.95	1633.96	0.01	Pass	1.20	1.43	0.23	Pass	1896341
2233.91	2233.87	-0.04	Pass	1.20	1.20	0.00	Pass	1462058

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	122620
302.00	301.97	-0.03	Pass	1.20	1.41	0.21	Pass	185850
601.98	601.97	-0.01	Pass	1.20	1.56	0.36	Pass	283224
1033.99	1033.99	0.00	Pass	1.20	1.54	0.34	Pass	713691
1633.95	1633.93	-0.02	Pass	1.20	1.46	0.26	Pass	2188354
2233.91	2233.85	-0.06	Pass	1.20	1.17	-0.03	Pass	1125604

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	191152
302.00	302.00	0.00	Pass	2.50	2.73	0.23	Pass	281043
601.98	602.00	0.02	Pass	2.50	2.93	0.43	Pass	554136
1033.99	1034.00	0.01	Pass	2.50	2.87	0.37	Pass	1449309
1633.95	1633.99	0.04	Pass	2.50	2.63	0.13	Pass	3939523
2233.91	2233.88	-0.03	Pass	2.50	2.39	-0.11	Pass	3899284

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	2.49	-0.01	Pass	173014
302.00	302.01	0.01	Pass	2.50	2.64	0.14	Pass	253191
601.98	601.97	-0.01	Pass	2.50	2.82	0.32	Pass	422075
1033.99	1034.01	0.02	Pass	2.50	2.79	0.29	Pass	1185513
1633.95	1633.96	0.01	Pass	2.50	2.72	0.22	Pass	4357538
2233.91	2233.82	-0.09	Pass	2.50	2.39	-0.11	Pass	3612046