

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 17 August 2020 08:49:32
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.60E+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	118.08	-0.01	Pass	0.70	0.69	-0.01	Pass	435390
322.05	322.03	-0.02	Pass	0.70	0.67	-0.03	Pass	231246
622.03	622.03	0.00	Pass	0.70	0.69	-0.01	Pass	159712
922.01	922.01	0.00	Pass	0.70	0.71	0.01	Pass	89676
1521.97	1521.99	0.02	Pass	0.70	0.70	0.00	Pass	33634
2121.93	2121.95	0.02	Pass	0.70	0.66	-0.04	Pass	32483

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	279682
322.05	322.07	0.02	Pass	0.70	0.67	-0.03	Pass	209739
622.03	622.01	-0.02	Pass	0.70	0.72	0.02	Pass	149761
922.01	922.00	-0.01	Pass	0.70	0.67	-0.03	Pass	75173
1521.97	1521.95	-0.02	Pass	0.70	0.69	-0.01	Pass	45219
2121.93	2121.94	0.01	Pass	0.70	0.62	-0.08	Pass	31917

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	1.22	0.02	Pass	454530
322.05	322.08	0.03	Pass	1.20	1.36	0.16	Pass	340301
622.03	622.03	0.00	Pass	1.20	1.51	0.31	Pass	251779
922.01	922.03	0.02	Pass	1.20	1.50	0.30	Pass	179848
1521.97	1522.01	0.04	Pass	1.20	1.27	0.07	Pass	100429
2121.93	2121.87	-0.06	Pass	1.20	1.21	0.01	Pass	78796

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	1.21	0.01	Pass	411753
322.05	322.05	0.00	Pass	1.20	1.28	0.08	Pass	311899
622.03	622.02	-0.01	Pass	1.20	1.25	0.05	Pass	242134
922.01	922.00	-0.01	Pass	1.20	1.05	-0.15	Pass	126686
1521.97	1521.96	-0.01	Pass	1.20	0.98	-0.22	Pass	75166
2121.93	2121.96	0.03	Pass	1.20	1.10	-0.10	Pass	60260

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	2.52	0.02	Pass	609869
322.05	322.05	0.00	Pass	2.50	2.67	0.17	Pass	434833
622.03	622.05	0.02	Pass	2.50	2.95	0.45	Pass	307898
922.01	922.03	0.02	Pass	2.50	2.81	0.31	Pass	257614
1521.97	1522.06	0.09	Pass	2.50	2.48	-0.02	Pass	180561
2121.93	2121.90	-0.03	Pass	2.50	2.43	-0.07	Pass	173553

QQQ Check Tune Report



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	118.13	0.04	Pass	2.50	2.58	0.08	Pass	571308
322.05	322.05	0.00	Pass	2.50	2.67	0.17	Pass	437770
622.03	622.01	-0.02	Pass	2.50	2.65	0.15	Pass	365469
922.01	922.13	0.12	Pass	2.50	2.42	-0.08	Pass	262520
1521.97	1521.97	0.00	Pass	2.50	2.32	-0.18	Pass	236731
2121.93	2121.88	-0.05	Pass	2.50	2.35	-0.15	Pass	289758

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	318723
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	79819
601.98	601.99	0.01	Pass	0.70	0.69	-0.01	Pass	119919
1033.99	1034.00	0.01	Pass	0.70	0.67	-0.03	Pass	709393
1633.95	1633.96	0.01	Pass	0.70	0.66	-0.04	Pass	1183605
2233.91	2233.97	0.06	Pass	0.70	0.65	-0.05	Pass	1050681

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	172228
302.00	301.96	-0.04	Pass	0.70	0.73	0.03	Pass	54956
601.98	601.98	0.00	Pass	0.70	0.70	0.00	Pass	94633
1033.99	1033.98	-0.01	Pass	0.70	0.69	-0.01	Pass	776314
1633.95	1633.92	-0.03	Pass	0.70	0.70	0.00	Pass	1638323
2233.91	2233.90	-0.01	Pass	0.70	0.68	-0.02	Pass	1026291

Analyzer: MS1 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	1.16	-0.04	Pass	399268
302.00	302.01	0.01	Pass	1.20	1.44	0.24	Pass	109127
601.98	602.01	0.03	Pass	1.20	1.52	0.32	Pass	202664
1033.99	1034.06	0.07	Pass	1.20	1.44	0.24	Pass	1567924
1633.95	1633.95	0.00	Pass	1.20	1.39	0.19	Pass	2788032
2233.91	2233.97	0.06	Pass	1.20	1.25	0.05	Pass	1993093

Analyzer: MS2 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	1.24	0.04	Pass	265599
302.00	301.99	-0.01	Pass	1.20	1.30	0.10	Pass	84366
601.98	601.93	-0.05	Pass	1.20	1.29	0.09	Pass	152205
1033.99	1034.02	0.03	Pass	1.20	1.03	-0.17	Pass	1173626
1633.95	1633.95	0.00	Pass	1.20	0.95	-0.25	Pass	2743273
2233.91	2234.11	0.20	Pass	1.20	0.84	-0.36	Pass	1540907

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	2.41	-0.09	Pass	497614
302.00	301.97	-0.03	Pass	2.50	2.63	0.13	Pass	150829
601.98	602.07	0.09	Pass	2.50	2.76	0.26	Pass	317949
1033.99	1034.02	0.03	Pass	2.50	2.75	0.25	Pass	2605171
1633.95	1633.99	0.04	Pass	2.50	2.71	0.21	Pass	6437468
2233.91	2233.96	0.05	Pass	2.50	2.55	0.05	Pass	5979312

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	2.55	0.05	Pass	398998
302.00	301.99	-0.01	Pass	2.50	2.61	0.11	Pass	120742
601.98	601.96	-0.02	Pass	2.50	2.52	0.02	Pass	236793
1033.99	1034.11	0.12	Pass	2.50	2.48	-0.02	Pass	2218499
1633.95	1633.96	0.01	Pass	2.50	2.44	-0.06	Pass	6197765
2233.91	2233.79	-0.12	Pass	2.50	2.20	-0.30	Pass	5844820

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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 18 August 2020 08:09:02
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.56E+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	118.11	0.02	Pass	0.70	0.69	-0.01	Pass	376853
322.05	322.12	0.07	Pass	0.70	0.63	-0.07	Pass	194052
622.03	622.06	0.03	Pass	0.70	0.68	-0.02	Pass	174843
922.01	922.01	0.00	Pass	0.70	0.69	-0.01	Pass	110568
1521.97	1522.00	0.03	Pass	0.70	0.62	-0.08	Pass	31143
2121.93	2121.96	0.03	Pass	0.70	0.68	-0.02	Pass	26951

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	269035
322.05	322.06	0.01	Pass	0.70	0.70	0.00	Pass	181062
622.03	622.02	-0.01	Pass	0.70	0.71	0.01	Pass	163233
922.01	921.97	-0.04	Pass	0.70	0.68	-0.02	Pass	88885
1521.97	1521.92	-0.05	Pass	0.70	0.73	0.03	Pass	42866
2121.93	2121.93	0.00	Pass	0.70	0.61	-0.09	Pass	32376

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	1.21	0.01	Pass	449882
322.05	322.08	0.03	Pass	1.20	1.34	0.14	Pass	324762
622.03	622.04	0.01	Pass	1.20	1.52	0.32	Pass	287509
922.01	922.03	0.02	Pass	1.20	1.49	0.29	Pass	207860
1521.97	1522.02	0.05	Pass	1.20	1.34	0.14	Pass	81024
2121.93	2121.87	-0.06	Pass	1.20	1.22	0.02	Pass	67991

Analyzer: MS2 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	1.19	-0.01	Pass	405126
322.05	322.07	0.02	Pass	1.20	1.28	0.08	Pass	293357
622.03	622.05	0.02	Pass	1.20	1.22	0.02	Pass	263667
922.01	921.96	-0.05	Pass	1.20	1.13	-0.07	Pass	130083
1521.97	1521.97	0.00	Pass	1.20	0.94	-0.26	Pass	72277
2121.93	2121.95	0.02	Pass	1.20	1.15	-0.05	Pass	60567

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	2.42	-0.08	Pass	601729
322.05	322.08	0.03	Pass	2.50	2.61	0.11	Pass	431152
622.03	622.07	0.04	Pass	2.50	2.86	0.36	Pass	372061
922.01	922.03	0.02	Pass	2.50	2.77	0.27	Pass	308086
1521.97	1522.04	0.07	Pass	2.50	2.59	0.09	Pass	152024
2121.93	2121.87	-0.06	Pass	2.50	2.46	-0.04	Pass	150284

QQQ Check Tune Report

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	575940
322.05	322.10	0.05	Pass	2.50	2.53	0.03	Pass	450413
622.03	622.01	-0.02	Pass	2.50	2.62	0.12	Pass	417412
922.01	922.14	0.13	Pass	2.50	2.35	-0.15	Pass	312852
1521.97	1521.97	0.00	Pass	2.50	2.36	-0.14	Pass	236591
2121.93	2121.81	-0.12	Pass	2.50	2.22	-0.28	Pass	287433

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	0.66	-0.04	Pass	274160
302.00	301.99	-0.01	Pass	0.70	0.70	0.00	Pass	69086
601.98	601.99	0.01	Pass	0.70	0.70	0.00	Pass	101050
1033.99	1034.01	0.02	Pass	0.70	0.66	-0.04	Pass	666526
1633.95	1633.97	0.02	Pass	0.70	0.63	-0.07	Pass	1097307
2233.91	2233.96	0.05	Pass	0.70	0.67	-0.03	Pass	968820

Analyzer: MS2 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	0.70	0.00	Pass	151393
302.00	301.97	-0.03	Pass	0.70	0.70	0.00	Pass	47843
601.98	601.95	-0.03	Pass	0.70	0.71	0.01	Pass	81463
1033.99	1033.97	-0.02	Pass	0.70	0.69	-0.01	Pass	755179
1633.95	1633.91	-0.04	Pass	0.70	0.70	0.00	Pass	1553652
2233.91	2233.86	-0.05	Pass	0.70	0.67	-0.03	Pass	1030906

Analyzer: MS1 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	1.18	-0.02	Pass	313723
302.00	301.99	-0.01	Pass	1.20	1.40	0.20	Pass	97007
601.98	602.00	0.02	Pass	1.20	1.52	0.32	Pass	180980
1033.99	1034.02	0.03	Pass	1.20	1.52	0.32	Pass	1370998
1633.95	1634.00	0.05	Pass	1.20	1.32	0.12	Pass	2829697
2233.91	2233.98	0.07	Pass	1.20	1.22	0.02	Pass	1978219

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	236931
302.00	301.94	-0.06	Pass	1.20	1.34	0.14	Pass	67227
601.98	601.92	-0.06	Pass	1.20	1.31	0.11	Pass	117784
1033.99	1033.95	-0.04	Pass	1.20	1.06	-0.14	Pass	1139838
1633.95	1633.94	-0.01	Pass	1.20	0.96	-0.24	Pass	2329531
2233.91	2234.06	0.15	Pass	1.20	0.86	-0.34	Pass	1497739

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	2.44	-0.06	Pass	435946
302.00	302.00	0.00	Pass	2.50	2.63	0.13	Pass	125677
601.98	602.02	0.04	Pass	2.50	2.81	0.31	Pass	248707
1033.99	1034.11	0.12	Pass	2.50	2.82	0.32	Pass	2422944
1633.95	1634.09	0.14	Pass	2.50	2.38	-0.12	Pass	5966515
2233.91	2233.92	0.01	Pass	2.50	2.60	0.10	Pass	5414581

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	2.52	0.02	Pass	363400
302.00	302.01	0.01	Pass	2.50	2.54	0.04	Pass	103515
601.98	601.92	-0.06	Pass	2.50	2.68	0.18	Pass	180791
1033.99	1034.10	0.11	Pass	2.50	2.49	-0.01	Pass	2066265
1633.95	1633.93	-0.02	Pass	2.50	2.53	0.03	Pass	5506134
2233.91	2233.81	-0.10	Pass	2.50	2.22	-0.28	Pass	5574254

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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 20 August 2020 07:54:29
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.53E+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	383441
322.05	322.05	0.00	Pass	0.70	0.68	-0.02	Pass	230299
622.03	622.03	0.00	Pass	0.70	0.72	0.02	Pass	128943
922.01	922.02	0.01	Pass	0.70	0.67	-0.03	Pass	127453
1521.97	1522.00	0.03	Pass	0.70	0.65	-0.05	Pass	39999
2121.93	2121.98	0.05	Pass	0.70	0.69	-0.01	Pass	31020

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	288355
322.05	322.08	0.03	Pass	0.70	0.69	-0.01	Pass	198053
622.03	622.03	0.00	Pass	0.70	0.71	0.01	Pass	166278
922.01	922.00	-0.01	Pass	0.70	0.67	-0.03	Pass	101349
1521.97	1521.95	-0.02	Pass	0.70	0.71	0.01	Pass	48118
2121.93	2121.94	0.01	Pass	0.70	0.62	-0.08	Pass	33787

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	445520
322.05	322.07	0.02	Pass	1.20	1.39	0.19	Pass	331890
622.03	622.07	0.04	Pass	1.20	1.53	0.33	Pass	305086
922.01	922.03	0.02	Pass	1.20	1.47	0.27	Pass	246990
1521.97	1522.01	0.04	Pass	1.20	1.35	0.15	Pass	100251
2121.93	2121.87	-0.06	Pass	1.20	1.20	0.00	Pass	80484

Analyzer: MS2 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	1.17	-0.03	Pass	382654
322.05	322.04	-0.01	Pass	1.20	1.29	0.09	Pass	304427
622.03	622.05	0.02	Pass	1.20	1.25	0.05	Pass	245296
922.01	922.00	-0.01	Pass	1.20	1.07	-0.13	Pass	153462
1521.97	1521.96	-0.01	Pass	1.20	0.98	-0.22	Pass	84345
2121.93	2121.96	0.03	Pass	1.20	1.12	-0.08	Pass	64748

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	557945
322.05	322.01	-0.04	Pass	2.50	2.61	0.11	Pass	435194
622.03	622.05	0.02	Pass	2.50	2.85	0.35	Pass	398986
922.01	922.09	0.08	Pass	2.50	2.71	0.21	Pass	355442
1521.97	1522.01	0.04	Pass	2.50	2.59	0.09	Pass	180303
2121.93	2121.87	-0.06	Pass	2.50	2.53	0.03	Pass	174280

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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	118.12	0.03	Pass	2.50	2.46	-0.04	Pass	544613
322.05	322.09	0.04	Pass	2.50	2.54	0.04	Pass	451805
622.03	621.99	-0.04	Pass	2.50	2.48	-0.02	Pass	426911
922.01	922.13	0.12	Pass	2.50	2.42	-0.08	Pass	323524
1521.97	1522.02	0.05	Pass	2.50	2.26	-0.24	Pass	251470
2121.93	2121.93	0.00	Pass	2.50	2.19	-0.31	Pass	310186

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	0.68	-0.02	Pass	273374
302.00	302.00	0.00	Pass	0.70	0.69	-0.01	Pass	62556
601.98	601.98	0.00	Pass	0.70	0.68	-0.02	Pass	84959
1033.99	1034.01	0.02	Pass	0.70	0.67	-0.03	Pass	630864
1633.95	1633.99	0.04	Pass	0.70	0.64	-0.06	Pass	979680
2233.91	2233.96	0.05	Pass	0.70	0.66	-0.04	Pass	885689

Analyzer: MS2 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	0.68	-0.02	Pass	147801
302.00	301.98	-0.02	Pass	0.70	0.71	0.01	Pass	43477
601.98	601.96	-0.02	Pass	0.70	0.73	0.03	Pass	68493
1033.99	1033.97	-0.02	Pass	0.70	0.71	0.01	Pass	727913
1633.95	1633.93	-0.02	Pass	0.70	0.72	0.02	Pass	1370359
2233.91	2233.89	-0.02	Pass	0.70	0.68	-0.02	Pass	981978

Analyzer: MS1 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	1.16	-0.04	Pass	321114
302.00	302.04	0.04	Pass	1.20	1.38	0.18	Pass	86903
601.98	602.00	0.02	Pass	1.20	1.51	0.31	Pass	143275
1033.99	1034.02	0.03	Pass	1.20	1.48	0.28	Pass	1369996
1633.95	1634.01	0.06	Pass	1.20	1.29	0.09	Pass	2607037
2233.91	2234.03	0.12	Pass	1.20	1.17	-0.03	Pass	1850596

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	226212
302.00	301.96	-0.04	Pass	1.20	1.32	0.12	Pass	64581
601.98	601.95	-0.03	Pass	1.20	1.27	0.07	Pass	111232
1033.99	1034.00	0.01	Pass	1.20	1.08	-0.12	Pass	1093254
1633.95	1633.95	0.00	Pass	1.20	0.95	-0.25	Pass	2486835
2233.91	2234.08	0.17	Pass	1.20	0.84	-0.36	Pass	1444056

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	2.44	-0.06	Pass	410609
302.00	301.99	-0.01	Pass	2.50	2.62	0.12	Pass	110255
601.98	602.02	0.04	Pass	2.50	2.95	0.45	Pass	197636
1033.99	1034.11	0.12	Pass	2.50	2.72	0.22	Pass	2465947
1633.95	1633.99	0.04	Pass	2.50	2.70	0.20	Pass	5585242
2233.91	2233.94	0.03	Pass	2.50	2.56	0.06	Pass	5340679

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	2.57	0.07	Pass	329848
302.00	301.99	-0.01	Pass	2.50	2.62	0.12	Pass	87205
601.98	601.97	-0.01	Pass	2.50	2.57	0.07	Pass	167769
1033.99	1034.07	0.08	Pass	2.50	2.38	-0.12	Pass	1994327
1633.95	1633.92	-0.03	Pass	2.50	2.41	-0.09	Pass	5962807
2233.91	2233.80	-0.11	Pass	2.50	2.44	-0.06	Pass	4667551