



MS Autotune Report - Ultivo

Instrument Information

Model	G6465B Ultivo	Autotune Date	2023-04-27T11:30:16-04:00
Serial Number	SG2018Q101	SW/FW Version	2.4.467/8.1.36
Autotune Version	4.10.268	Last Autotune Date	2023-04-27T11:30:16-04:00
Ion Source	AJS ESI	Overall Result	Passed

Positive Results

Components

Ion Source Settings

Gas Temperature(°C)	300	Gas Flow(l/min)	7.0
Nebulizer(psi)	15	Sheath Gas Temperature(°C)	200
Sheath Gas Flow(l/min)	11.0	Capillary Voltage(V)	4000
Nozzle Voltage(V)	1500		

Optics Settings

Fragmentor(V)	120	Skimmer(V)	10
Cyclone Outer DC(V)	3	Cyclone Accelerator(V)	0
Cyclone Exit DC(V)	3	Cyclone Exit Lens(V)	2
Cyclone Inner RF(V)	400	Cyclone Outer RF(V)	350

Quad 1 Settings

MS1 Entrance Lens(V)	-50
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MS1 Entrance Lens Dynamic Table

m/z	Setting
5.0	-24
50.0	-24
120.0	-24
320.0	-28
620.0	-34
920.0	-50
1220.0	-66
1400.0	-66

MS1 DC(V)	1	MS1 Heater(°C)	65
MS1 Exit Lens(V)	-50		

MS1 Exit Lens Dynamic Table

m/z	Setting
5.0	-61
50.0	-61
120.0	-61
320.0	-50
620.0	-35
920.0	-46
1220.0	-58
1400.0	-58

Collision Cell Settings

CC Entrance Lens(V)	0	CC Outer DC(V)	0
CAV(V)	7	CC Exit DC(V)	-7
CC Exit Lens(V)	-10	CC Inner RF(V)	400
CC Outer RF(V)	100		

Quad 2 Settings

MS2 Entrance Lens(V)	-100
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MS2 Entrance Lens Dynamic Table

m/z	Setting
5.0	-40
50.0	-40
120.0	-40
320.0	-54
620.0	-76
920.0	-78
1220.0	-80
1400.0	-80

MS2 DC(V)	-8	MS2 Heater(°C)	65
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Detector Settings

Iris(V)	-100	HED(kV)	-10
EMV(V)	964		

Gain

Minimum Gain Factor	0.1	Maximum Gain Factor	10.0
Measured Gain Factor	1.0	Result	Passed

Mass Calibration Results

MS1 Peak Width Unit, Scan Speed Normal

Calibration Information

Score	98	Result	Passed
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Calibration Parameters

MS1 Axis Gain	34.95	MS1 Axis Offset(amu)	1.620
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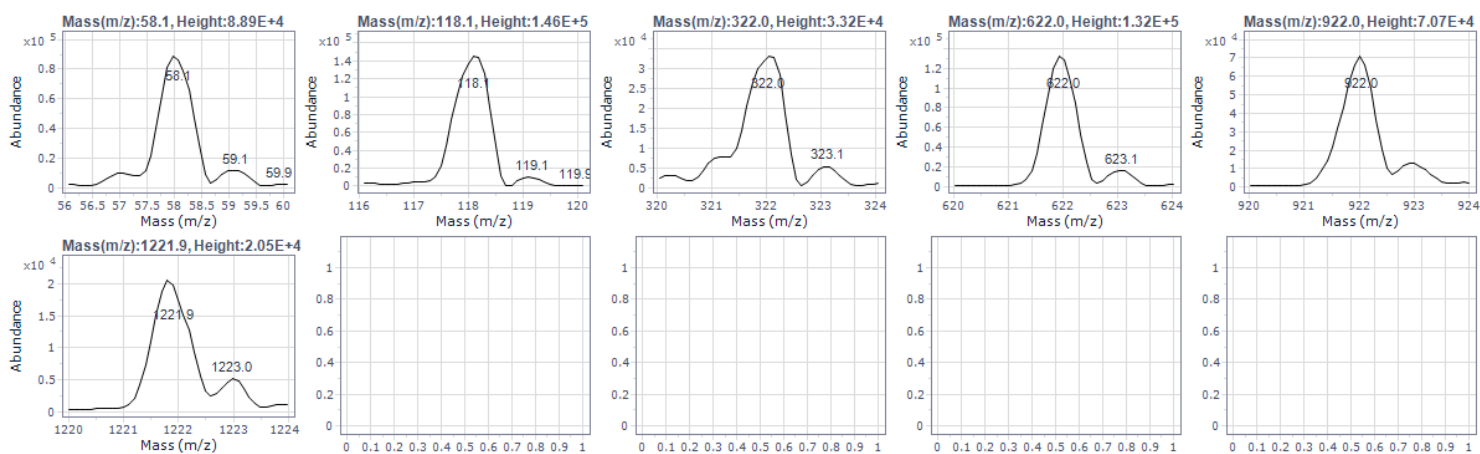
MS1 Axis Offset Dynamic Table

m/z	Setting
5.0	1.514
50.0	1.514
120.0	1.688
320.0	1.874
620.0	1.876
920.0	1.745
1220.0	1.498
1400.0	1.498

MS1 Width Gain(amu)	-11.3	MS1 Width Offset(amu)	0.42
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MS1 Width Offset Dynamic Table

m/z	Setting
5.0	0.53
50.0	0.53
120.0	0.32
320.0	0.14
620.0	0.16
920.0	0.32
1220.0	0.38
1400.0	0.38



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
58.07	0.00	-0.02	8.17E+4	98	Passed
118.09	0.00	0.00	1.52E+5	100	Passed
322.05	0.01	-0.02	4.23E+4	97	Passed
622.03	0.00	0.00	1.12E+5	100	Passed
922.01	-0.01	0.01	7.47E+4	97	Passed
1221.99	-0.02	0.00	3.10E+4	98	Passed

MS2 Peak Width Unit, Scan Speed Normal

Calibration Information

Score	98	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-17.78	MS2 Axis Offset(amu)	0.355
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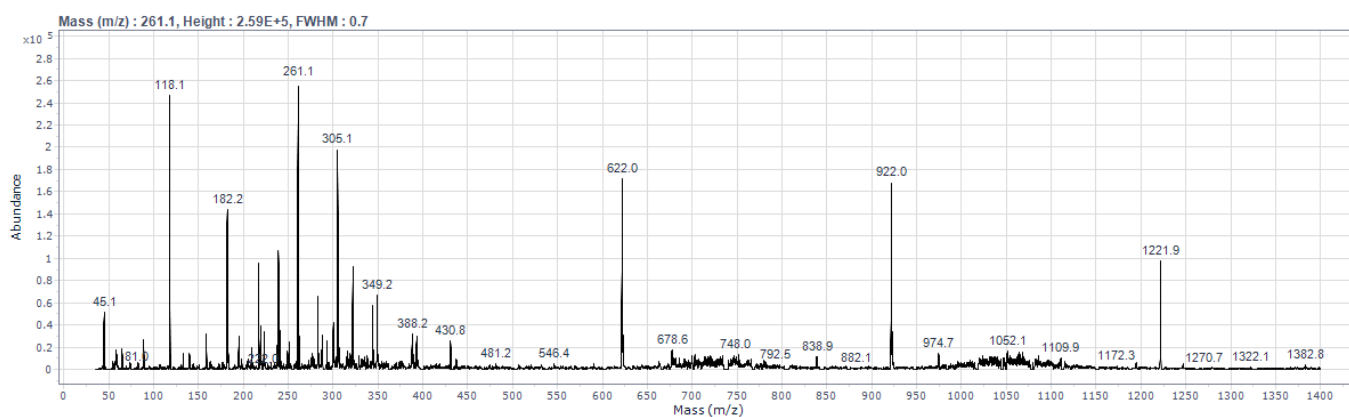
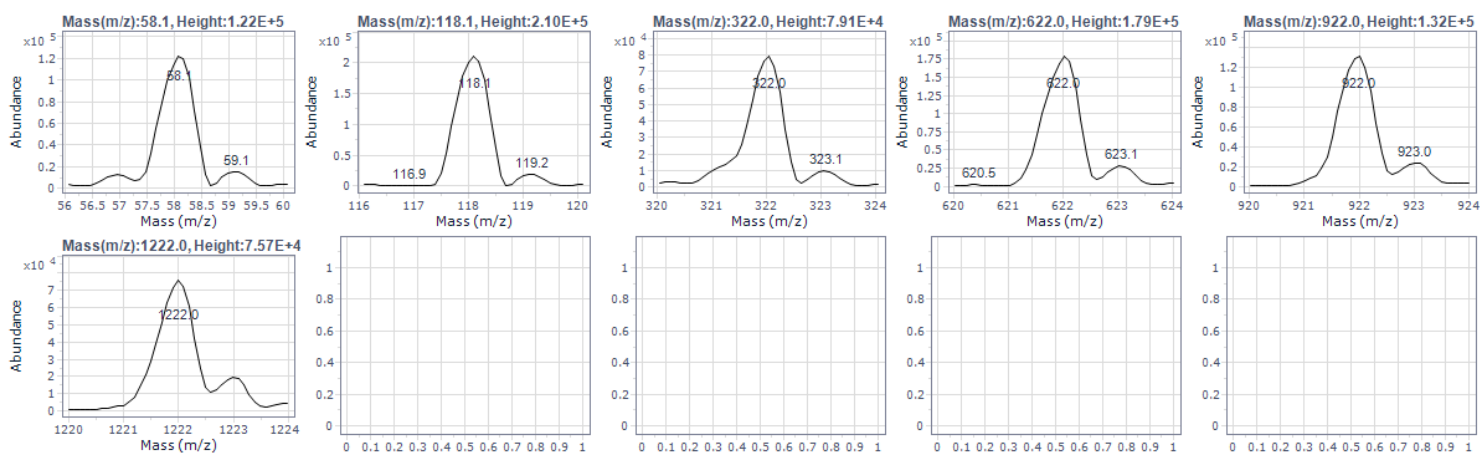
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	0.431
50.0	0.431
120.0	0.443
320.0	0.470
620.0	0.497
920.0	0.436
1220.0	0.342
1400.0	0.342

MS2 Width Gain(amu)	-15.4	MS2 Width Offset(amu)	-0.76
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	-0.69
50.0	-0.69
120.0	-0.77
320.0	-0.90
620.0	-0.97
920.0	-0.87
1220.0	-0.87
1400.0	-0.87



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
58.07	0.01	0.01	1.18E+5	98	Passed
118.09	0.01	0.00	2.28E+5	98	Passed
322.05	0.00	-0.02	7.73E+4	97	Passed
622.03	-0.01	-0.01	1.83E+5	98	Passed
922.01	0.00	0.01	1.35E+5	99	Passed
1221.99	-0.01	-0.01	6.76E+4	99	Passed

MS1 Peak Width Wide, Scan Speed Normal

Calibration Information

Score	100	Result	Passed
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Calibration Parameters

MS1 Axis Gain	34.63	MS1 Axis Offset(amu)	1.736
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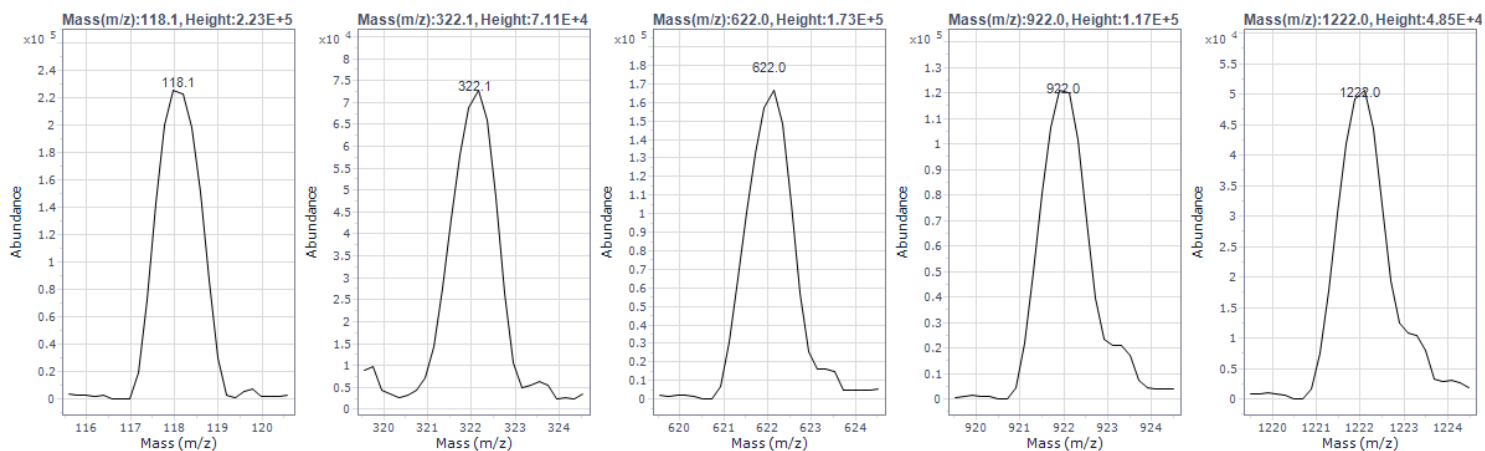
MS1 Axis Offset Dynamic Table

m/z	Setting
5.0	2.031
50.0	2.031
120.0	2.031
320.0	2.376
620.0	2.244
920.0	2.113
1220.0	1.907
1400.0	1.907

MS1 Width Gain(amu)	-11.2	MS1 Width Offset(amu)	1.42
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MS1 Width Offset Dynamic Table

m/z	Setting
5.0	1.25
50.0	1.25
120.0	1.25
320.0	1.10
620.0	1.09
920.0	1.20
1220.0	1.17
1400.0	1.17



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
118.09	0.01	0.01	2.23E+5	100	Passed
322.05	0.01	0.00	7.11E+4	100	Passed
622.03	0.00	-0.01	1.73E+5	100	Passed
922.01	-0.02	-0.01	1.17E+5	99	Passed
1221.99	0.01	-0.01	4.85E+4	100	Passed

MS2 Peak Width Wide, Scan Speed Normal

Calibration Information

Score	99	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-18.01	MS2 Axis Offset(amu)	0.376
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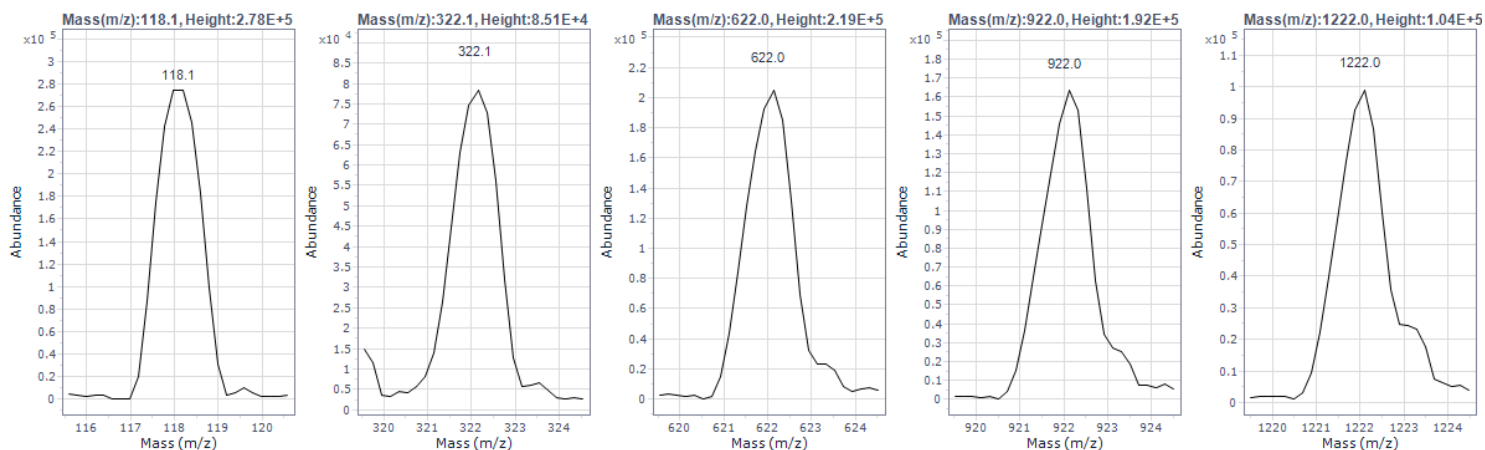
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	0.767
50.0	0.767
120.0	0.767
320.0	0.887
620.0	0.757
920.0	0.643
1220.0	0.694
1400.0	0.694

MS2 Width Gain(amu)	-15.5	MS2 Width Offset(amu)	-0.76
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	-0.03
50.0	-0.03
120.0	-0.03
320.0	-0.43
620.0	-0.11
920.0	-0.01
1220.0	0.03
1400.0	0.03



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
118.09	0.01	0.00	2.78E+5	100	Passed
322.05	0.02	0.00	8.51E+4	99	Passed
622.03	-0.03	0.01	2.19E+5	98	Passed
922.01	-0.01	0.00	1.92E+5	100	Passed
1221.99	0.00	-0.02	1.04E+5	100	Passed

MS1 Peak Width Widest, Scan Speed Normal

Calibration Information

Score	95	Result	Passed
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Calibration Parameters

MS1 Axis Gain	34.41	MS1 Axis Offset(amu)	2.082
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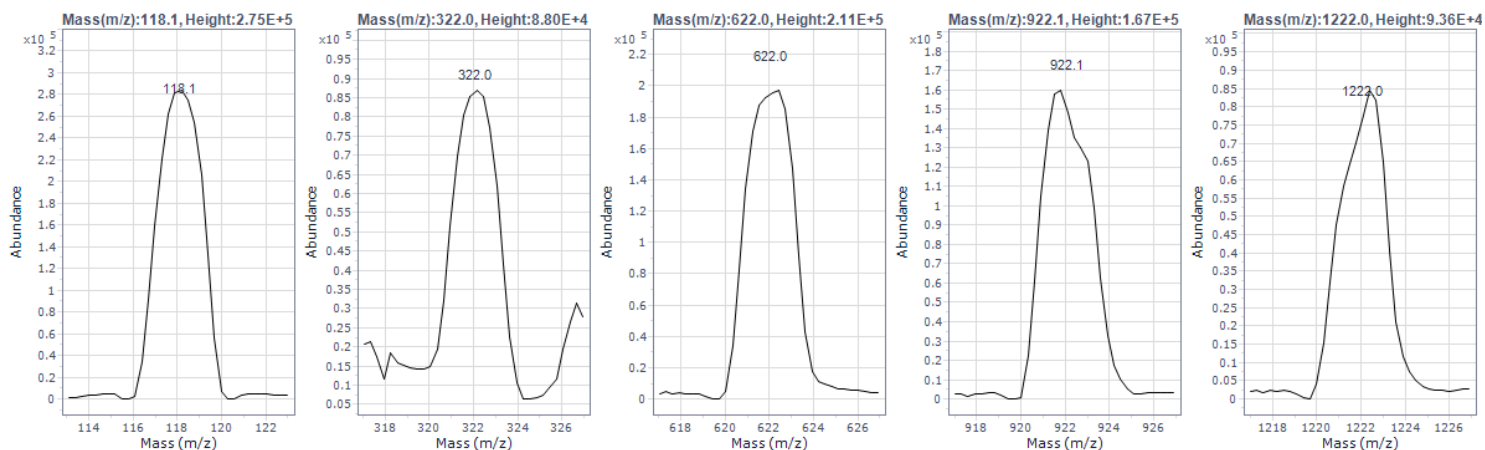
MS1 Axis Offset Dynamic Table

m/z	Setting
5.0	2.936
50.0	2.936
120.0	2.936
320.0	3.280
620.0	3.099
920.0	3.204
1220.0	2.796
1400.0	2.796

MS1 Width Gain(amu)	-11.4	MS1 Width Offset(amu)	2.86
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MS1 Width Offset Dynamic Table

m/z	Setting
5.0	3.56
50.0	3.56
120.0	3.56
320.0	3.09
620.0	3.30
920.0	3.62
1220.0	3.65
1400.0	3.65



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
118.09	0.01	-0.06	2.75E+5	99	Passed
322.05	-0.02	0.00	8.80E+4	100	Passed
622.03	0.02	0.07	2.11E+5	98	Passed
922.01	0.07	0.23	1.67E+5	81	Passed
1221.99	0.04	-0.01	9.36E+4	98	Passed

MS2 Peak Width Widest, Scan Speed Normal

Calibration Information

Score	93	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-18.01	MS2 Axis Offset(amu)	0.376
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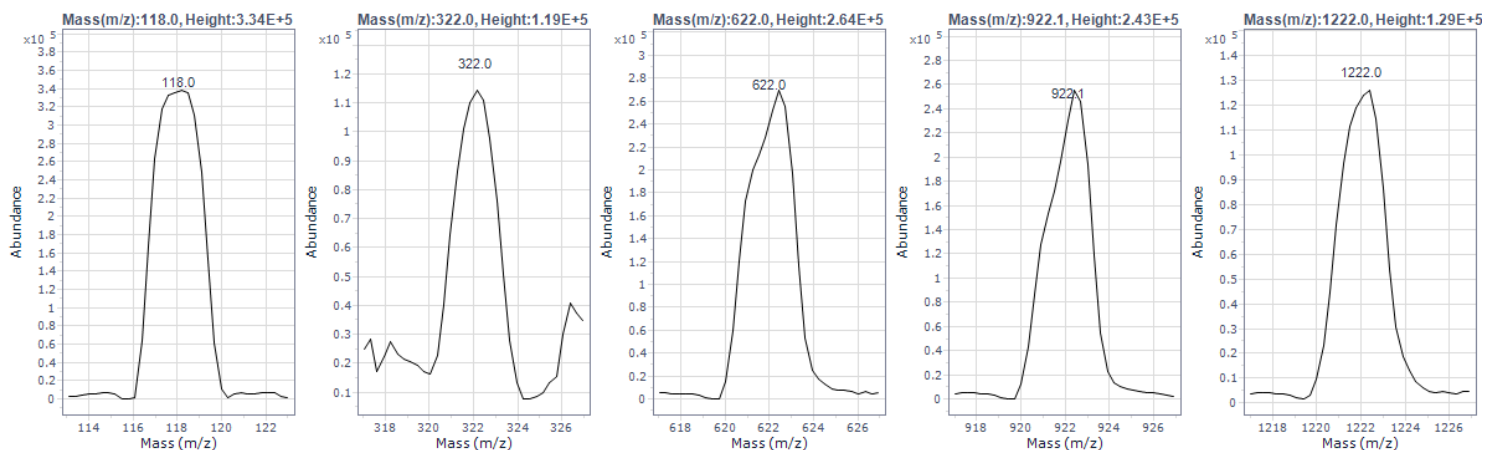
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	1.855
50.0	1.855
120.0	1.855
320.0	1.830
620.0	1.615
920.0	1.561
1220.0	1.294
1400.0	1.294

MS2 Width Gain(amu)	-15.5	MS2 Width Offset(amu)	-0.76
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	2.65
50.0	2.65
120.0	2.65
320.0	1.86
620.0	2.24
920.0	2.30
1220.0	2.06
1400.0	2.06



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
118.09	-0.06	0.14	3.34E+5	90	Passed
322.05	-0.02	-0.08	1.19E+5	97	Passed
622.03	-0.05	0.05	2.64E+5	96	Passed
922.01	0.12	-0.14	2.43E+5	82	Passed
1221.99	0.00	-0.08	1.29E+5	98	Passed

MS2 Scan Speed Fast

Calibration Information

Score	99	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-17.69	MS2 Axis Offset(amu)	1.392
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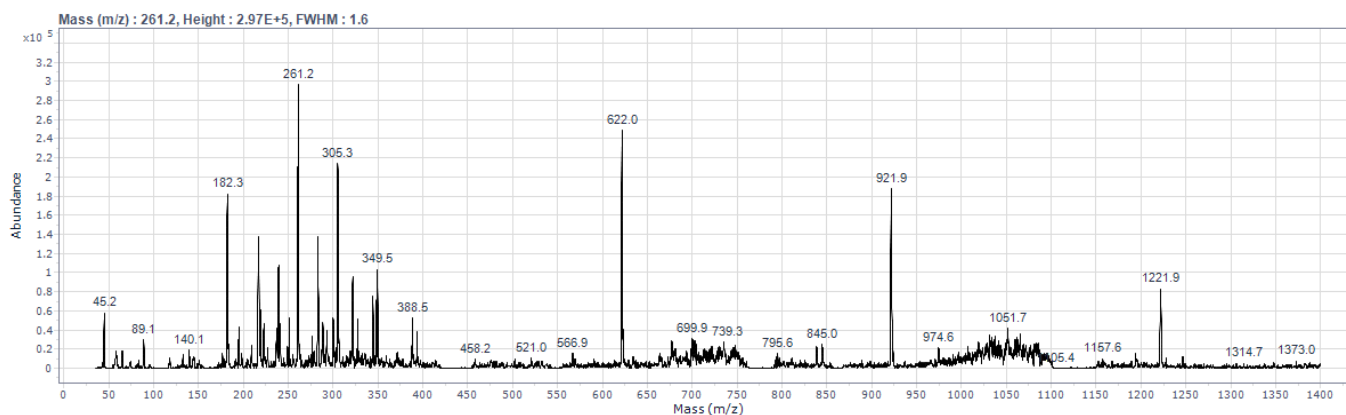
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	1.392
50.0	1.392
120.0	1.392
320.0	1.442
620.0	1.350
920.0	1.359
1220.0	1.328
1400.0	1.328

MS2 Width Gain(amu)	-17.4	MS2 Width Offset(amu)	0.66
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	0.66
50.0	0.66
120.0	0.66
320.0	0.24
620.0	0.33
920.0	0.61
1220.0	0.60
1400.0	0.60



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
118.09	0.02	0.00	2.50E+5	99	Passed
322.05	0.02	0.01	8.94E+4	99	Passed
622.03	0.02	-0.03	2.30E+5	98	Passed
922.01	0.01	-0.01	1.98E+5	100	Passed
1221.99	-0.01	0.02	1.05E+5	99	Passed

MS2 Scan Speed Ultra

Calibration Information

Score	99	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-17.17	MS2 Axis Offset(amu)	1.619
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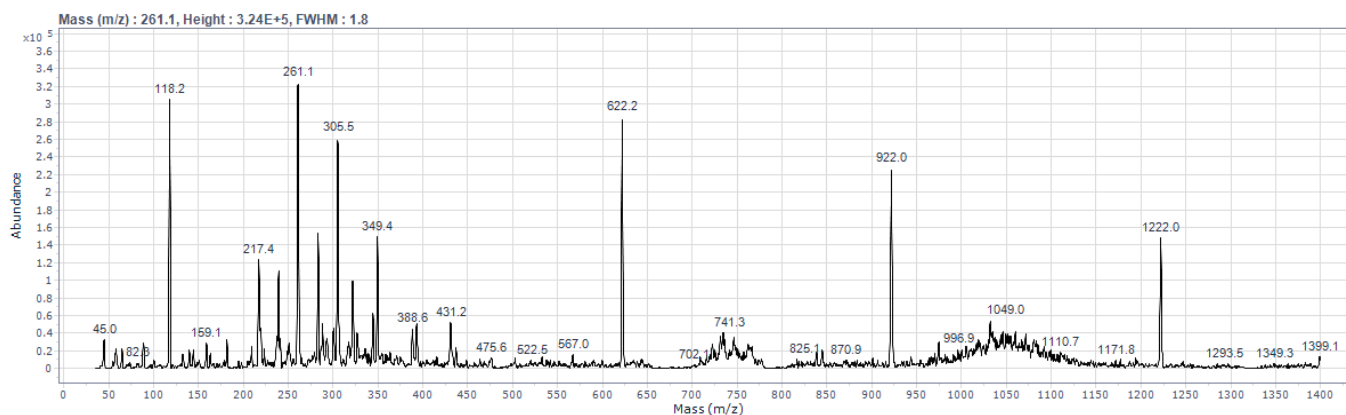
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	2.509
50.0	2.509
120.0	2.509
320.0	2.786
620.0	2.531
920.0	2.254
1220.0	2.014
1400.0	2.014

MS2 Width Gain(amu)	-18.5	MS2 Width Offset(amu)	2.14
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	3.05
50.0	3.05
120.0	3.05
320.0	2.74
620.0	2.68
920.0	2.92
1220.0	2.59
1400.0	2.59



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
118.09	-0.01	-0.02	2.19E+5	100	Passed
322.05	0.04	0.01	1.06E+5	99	Passed
622.03	0.03	-0.04	2.39E+5	99	Passed
922.01	0.01	-0.02	2.13E+5	100	Passed
1221.99	0.01	-0.01	1.01E+5	100	Passed

Negative Results

Components

Ion Source Settings

Gas Temperature(°C)	300	Gas Flow(l/min)	7.0
Nebulizer(psi)	15	Sheath Gas Temperature(°C)	200
Sheath Gas Flow(l/min)	11.0	Capillary Voltage(V)	4000
Nozzle Voltage(V)	1500		

Optics Settings

Fragmentor(V)	-90	Skimmer(V)	-10
Cyclone Outer DC(V)	-3	Cyclone Accelerator(V)	0
Cyclone Exit DC(V)	-3	Cyclone Exit Lens(V)	-2
Cyclone Inner RF(V)	400	Cyclone Outer RF(V)	350

Quad 1 Settings

MS1 Entrance Lens(V)	40
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MS1 Entrance Lens Dynamic Table

m/z	Setting
5.0	33
70.0	33
110.0	33
300.0	32
600.0	30
1030.0	82
1330.0	118
1400.0	118

MS1 DC(V)	-1	MS1 Heater(°C)	65
MS1 Exit Lens(V)	50		

MS1 Exit Lens Dynamic Table

m/z	Setting
5.0	29
70.0	29
110.0	29
300.0	39
600.0	56
1030.0	60
1330.0	63
1400.0	63

Collision Cell Settings

CC Entrance Lens(V)	0	CC Outer DC(V)	0
CAV(V)	-7	CC Exit DC(V)	7
CC Exit Lens(V)	10	CC Inner RF(V)	400
CC Outer RF(V)	100		

Quad 2 Settings

MS2 Entrance Lens(V)	100
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MS2 Entrance Lens Dynamic Table

m/z	Setting
5.0	49
70.0	49
110.0	49
300.0	61
600.0	80
1030.0	75
1330.0	72
1400.0	72

MS2 DC(V)	8	MS2 Heater(°C)	65
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Detector Settings

Iris(V)	100	HED(kV)	10
EMV(V)	980		

Gain

Minimum Gain Factor	0.1	Maximum Gain Factor	10.0
Measured Gain Factor	1.0	Result	Passed

Mass Calibration Results**MS1 Peak Width Unit, Scan Speed Normal****Calibration Information**

Score	99	Result	Passed
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Calibration Parameters

MS1 Axis Gain	34.52	MS1 Axis Offset(amu)	1.622
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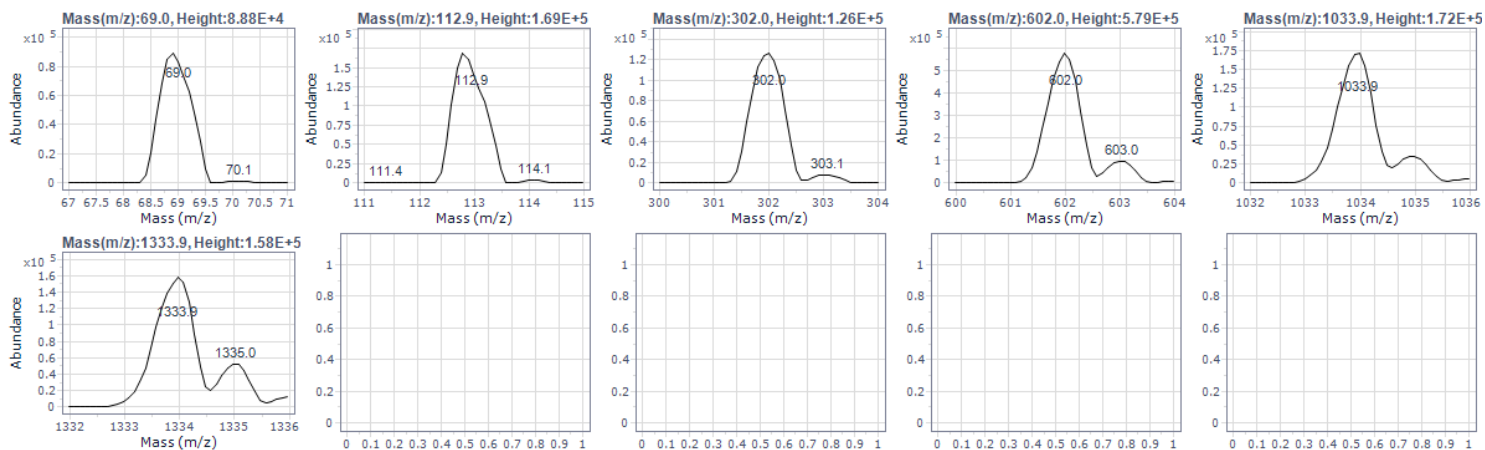
MS1 Axis Offset Dynamic Table

m/z	Setting
5.0	1.594
70.0	1.594
110.0	1.680
300.0	1.971
600.0	1.981
1030.0	1.916
1330.0	1.662
1400.0	1.662

MS1 Width Gain(amu)	-10.1	MS1 Width Offset(amu)	0.29
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MS1 Width Offset Dynamic Table

m/z	Setting
5.0	0.43
70.0	0.43
110.0	0.33
300.0	0.10
600.0	0.06
1030.0	0.22
1330.0	0.29
1400.0	0.29



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
69.00	0.01	0.02	1.05E+5	97	Passed
112.99	-0.01	0.00	1.82E+5	99	Passed
302.00	0.00	0.00	1.29E+5	100	Passed
601.98	0.01	0.01	5.93E+5	99	Passed
1033.99	-0.01	0.00	1.60E+5	99	Passed
1333.97	0.01	0.01	2.28E+5	99	Passed

MS2 Peak Width Unit, Scan Speed Normal

Calibration Information

Score	99	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-17.99	MS2 Axis Offset(amu)	0.415
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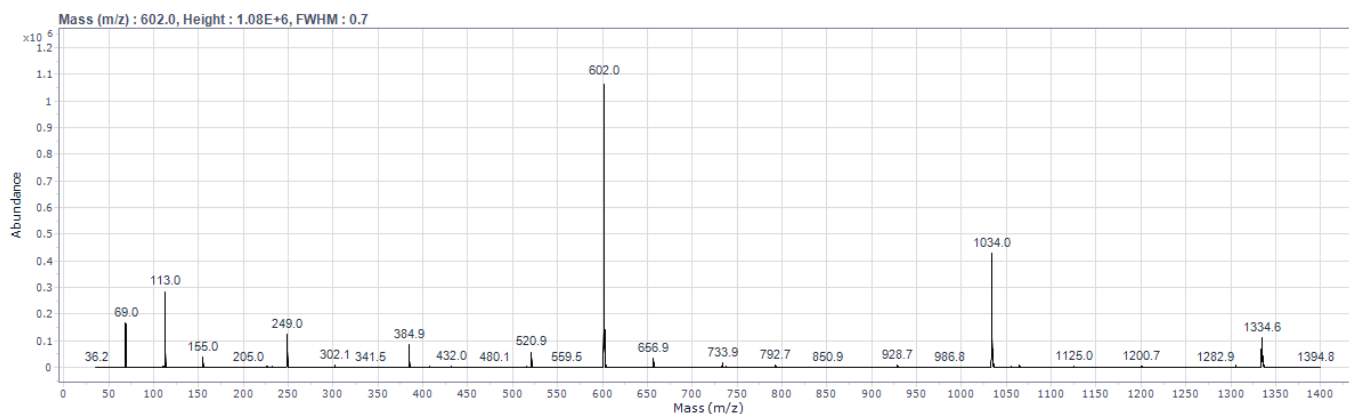
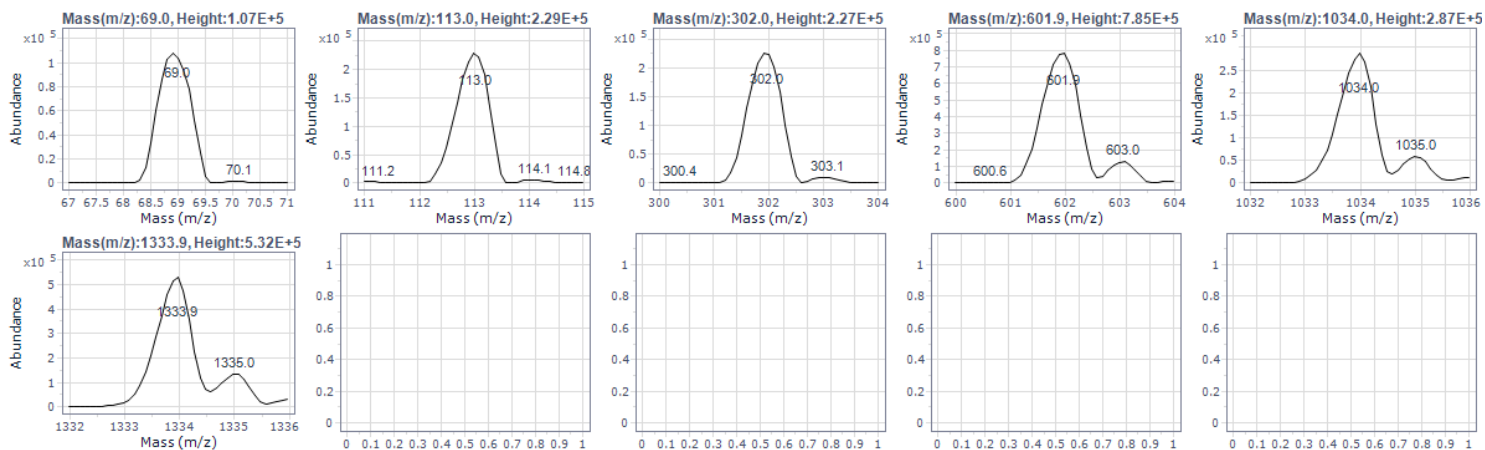
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	0.431
70.0	0.431
110.0	0.458
300.0	0.544
600.0	0.581
1030.0	0.570
1330.0	0.413
1400.0	0.413

MS2 Width Gain(amu)	-15.9	MS2 Width Offset(amu)	-0.81
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	-0.77
70.0	-0.77
110.0	-0.78
300.0	-0.85
600.0	-0.90
1030.0	-0.83
1330.0	-0.76
1400.0	-0.76



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
69.00	0.01	-0.01	1.10E+5	98	Passed
112.99	0.00	0.01	2.20E+5	100	Passed
302.00	-0.01	0.01	2.18E+5	97	Passed
601.98	0.00	0.01	8.73E+5	99	Passed
1033.99	-0.01	0.00	3.03E+5	99	Passed
1333.97	-0.02	0.00	5.97E+5	99	Passed

MS1 Peak Width Wide, Scan Speed Normal

Calibration Information

Score	99	Result	Passed
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Calibration Parameters

MS1 Axis Gain	34.41	MS1 Axis Offset(amu)	2.020
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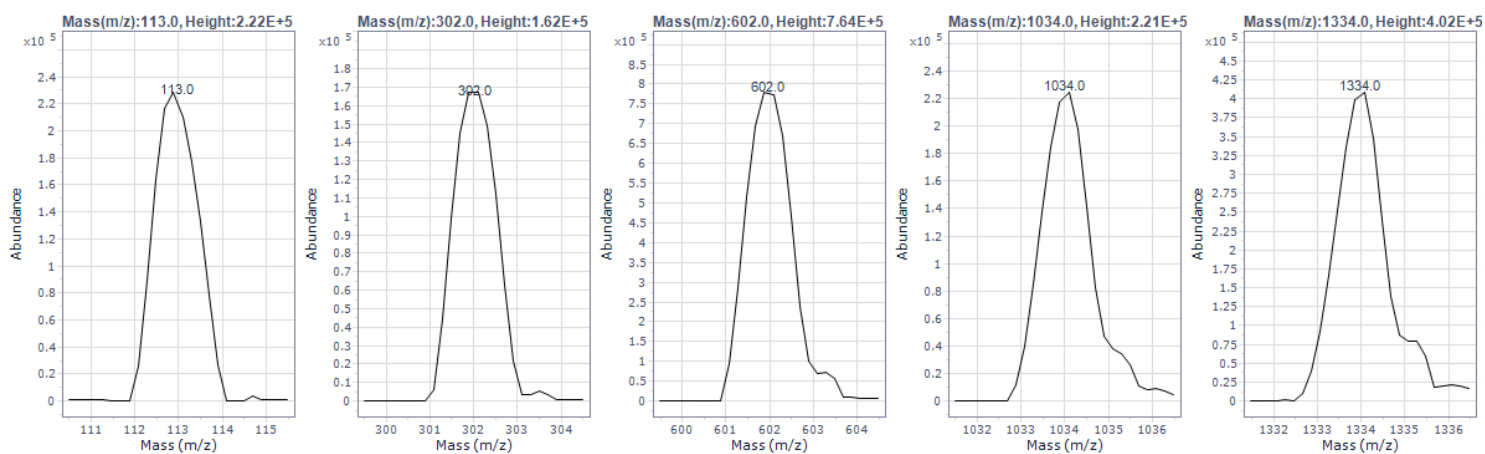
MS1 Axis Offset Dynamic Table

m/z	Setting
5.0	2.037
70.0	2.037
110.0	2.037
300.0	2.373
600.0	2.204
1030.0	2.096
1330.0	1.818
1400.0	1.818

MS1 Width Gain(amu)	-10.1	MS1 Width Offset(amu)	1.10
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MS1 Width Offset Dynamic Table

m/z	Setting
5.0	1.19
70.0	1.19
110.0	1.19
300.0	0.77
600.0	0.67
1030.0	0.85
1330.0	1.25
1400.0	1.25



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
112.99	-0.03	0.00	2.22E+5	98	Passed
302.00	0.02	-0.03	1.62E+5	98	Passed
601.98	-0.02	-0.02	7.64E+5	99	Passed
1033.99	0.00	0.00	2.21E+5	100	Passed
1333.97	-0.01	-0.02	4.02E+5	99	Passed

MS2 Peak Width Wide, Scan Speed Normal

Calibration Information

Score	98	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-18.39	MS2 Axis Offset(amu)	0.953
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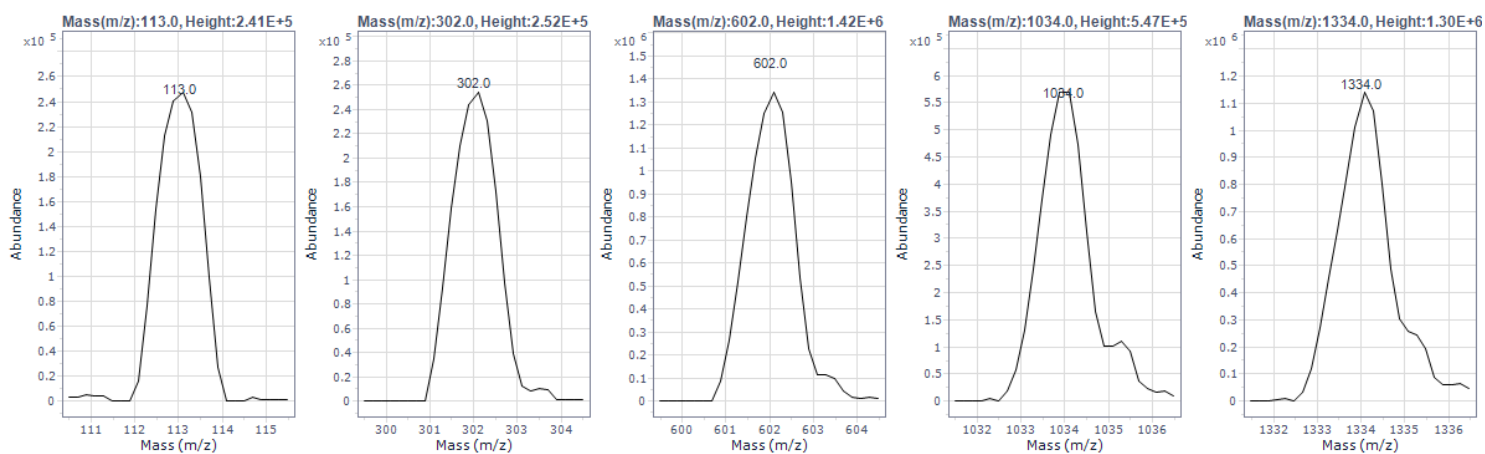
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	0.870
70.0	0.870
110.0	0.870
300.0	1.044
600.0	1.057
1030.0	1.116
1330.0	1.020
1400.0	1.020

MS2 Width Gain(amu)	-15.2	MS2 Width Offset(amu)	-0.08
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	-0.03
70.0	-0.03
110.0	-0.03
300.0	-0.18
600.0	-0.14
1030.0	0.01
1330.0	-0.11
1400.0	-0.11



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
112.99	0.02	0.02	2.41E+5	99	Passed
302.00	0.01	0.02	2.52E+5	99	Passed
601.98	0.02	0.03	1.42E+6	98	Passed
1033.99	-0.03	-0.03	5.47E+5	98	Passed
1333.97	0.03	0.02	1.30E+6	98	Passed

MS1 Peak Width Widest, Scan Speed Normal

Calibration Information

Score	97	Result	Passed
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Calibration Parameters

MS1 Axis Gain	34.41	MS1 Axis Offset(amu)	2.020
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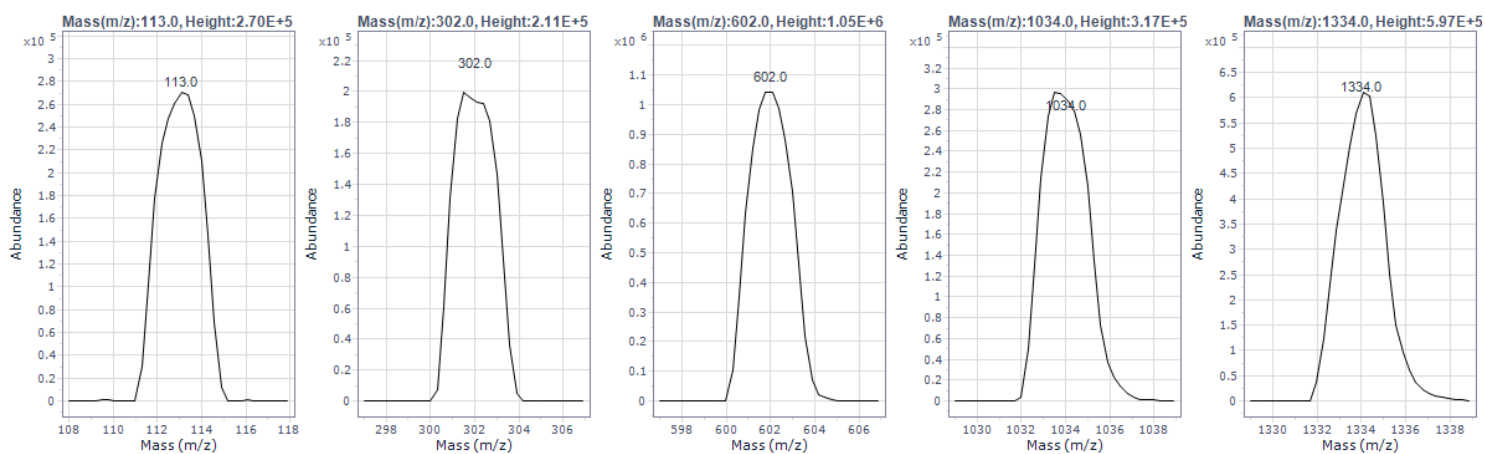
MS1 Axis Offset Dynamic Table

m/z	Setting
5.0	3.147
70.0	3.147
110.0	3.147
300.0	3.234
600.0	3.113
1030.0	2.924
1330.0	2.669
1400.0	2.669

MS1 Width Gain(amu)	-10.1	MS1 Width Offset(amu)	1.10
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MS1 Width Offset Dynamic Table

m/z	Setting
5.0	3.61
70.0	3.61
110.0	3.61
300.0	2.84
600.0	2.88
1030.0	3.03
1330.0	3.51
1400.0	3.51



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
112.99	0.06	0.11	2.70E+5	94	Passed
302.00	-0.02	-0.01	2.11E+5	100	Passed
601.98	0.02	-0.05	1.05E+6	99	Passed
1033.99	-0.01	0.08	3.17E+5	98	Passed
1333.97	0.00	-0.12	5.97E+5	95	Passed

MS2 Peak Width Widest, Scan Speed Normal

Calibration Information

Score	95	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-18.39	MS2 Axis Offset(amu)	0.953
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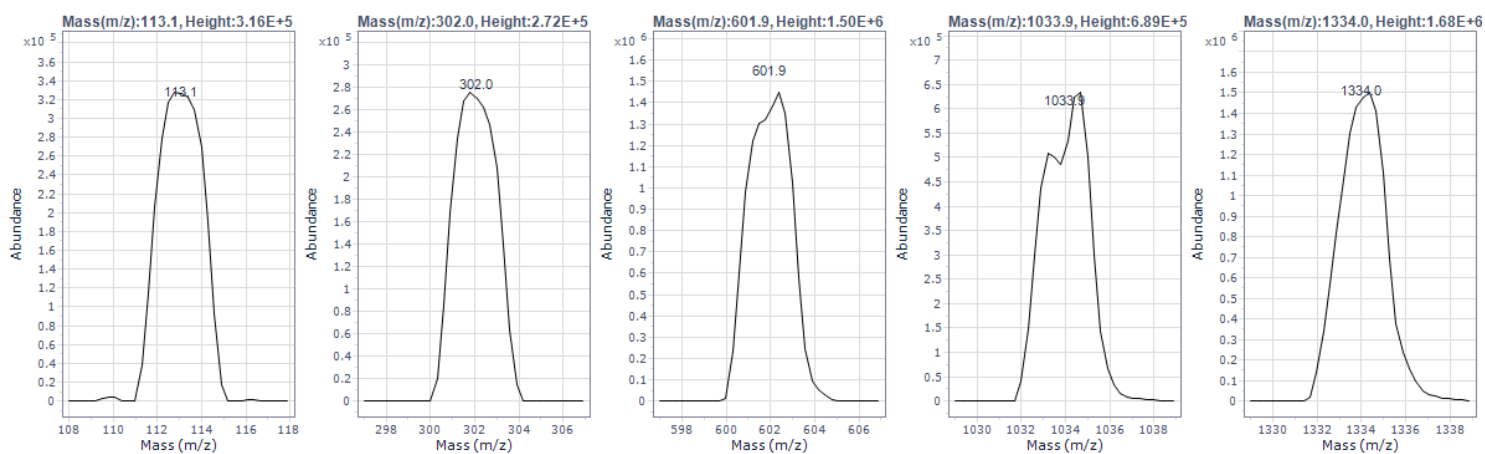
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	1.981
70.0	1.981
110.0	1.981
300.0	1.948
600.0	1.785
1030.0	1.674
1330.0	1.573
1400.0	1.573

MS2 Width Gain(amu)	-15.2	MS2 Width Offset(amu)	-0.08
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	2.66
70.0	2.66
110.0	2.66
300.0	1.94
600.0	1.93
1030.0	1.87
1330.0	2.03
1400.0	2.03



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
112.99	0.08	0.12	3.16E+5	90	Passed
302.00	0.05	0.02	2.72E+5	98	Passed
601.98	-0.03	0.01	1.50E+6	99	Passed
1033.99	-0.05	0.14	6.89E+5	92	Passed
1333.97	0.02	-0.06	1.68E+6	98	Passed

MS2 Scan Speed Fast

Calibration Information

Score	99	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-17.77	MS2 Axis Offset(amu)	1.337
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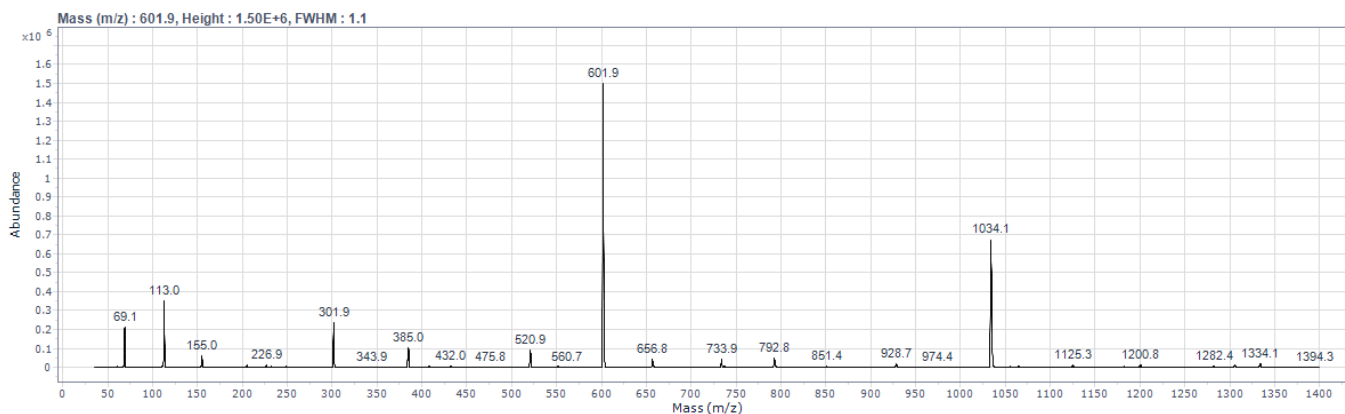
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	1.401
70.0	1.401
110.0	1.401
300.0	1.406
600.0	1.390
1030.0	1.538
1330.0	1.287
1400.0	1.287

MS2 Width Gain(amu)	-17.7	MS2 Width Offset(amu)	0.85
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	0.78
70.0	0.78
110.0	0.78
300.0	0.46
600.0	0.38
1030.0	0.63
1330.0	1.17
1400.0	1.17



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
112.99	0.00	0.02	3.08E+5	99	Passed
302.00	0.00	0.01	2.70E+5	100	Passed
601.98	-0.02	0.02	1.27E+6	99	Passed
1033.99	0.01	-0.02	4.58E+5	99	Passed
1333.97	0.01	0.03	1.15E+6	98	Passed

MS2 Scan Speed Ultra

Calibration Information

Score	99	Result	Passed
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Calibration Parameters

MS2 Axis Gain	-17.41	MS2 Axis Offset(amu)	1.736
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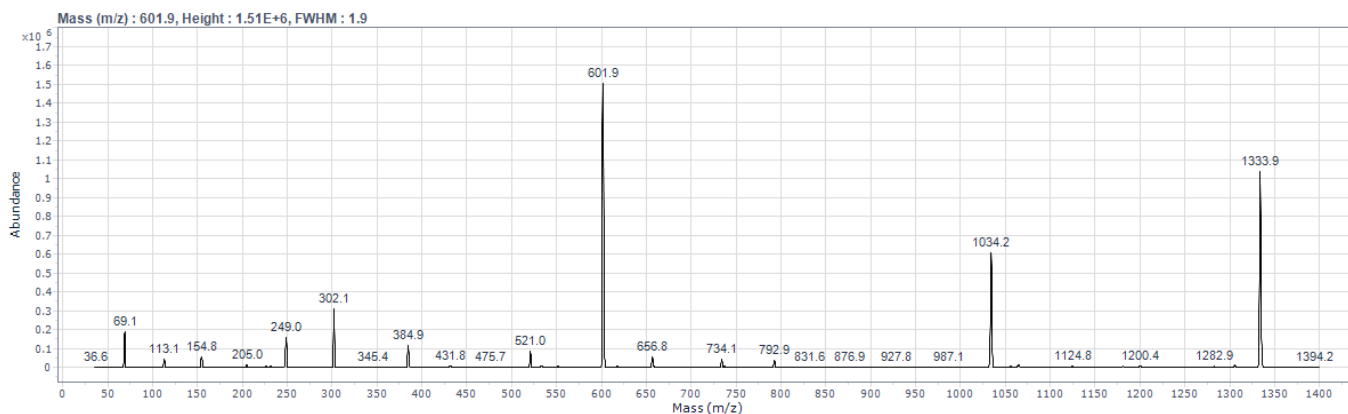
MS2 Axis Offset Dynamic Table

m/z	Setting
5.0	2.681
70.0	2.681
110.0	2.681
300.0	2.716
600.0	2.616
1030.0	2.449
1330.0	2.166
1400.0	2.166

MS2 Width Gain(amu)	-19.1	MS2 Width Offset(amu)	2.38
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MS2 Width Offset Dynamic Table

m/z	Setting
5.0	3.23
70.0	3.23
110.0	3.23
300.0	2.98
600.0	3.02
1030.0	2.92
1330.0	3.15
1400.0	3.15



Mass Calibration Results

Theoretical (m/z)	Mass Delta(m/z)	Width Delta(m/z)	Abundance	Score	Result
112.99	0.01	0.02	2.65E+5	100	Passed
302.00	0.02	-0.01	2.77E+5	100	Passed
601.98	0.00	-0.03	1.44E+6	100	Passed
1033.99	0.02	0.01	5.58E+5	100	Passed
1333.97	-0.06	0.02	9.06E+5	98	Passed

Vacuum And Temperature

Rough Vac(Torr) 1.58E+0
Turbo Speed(%) 100.0
MS2 Heater(°C) 65

High Vac(Torr) 2.46E-5
MS1 Heater(°C) 65