



Houston Forensic Science Center

Comparative and Analytical Division - Toxicology

LC-MS/MS Maintenance Log

Instrument: LCMS-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 |
|--------------------|------------------------------|-----------------------------------|------------------------------|------------------------------|------------------------|--------------------------------|-----------------------|-----------|--------------------|----------------|------------------------|----------|
| 5/2/22 | 30 / 1700 | 100 | ✓ | | | EC 5/2/22 | ✓ | ✓ | ✓ | X | | EC |
| 5/5/22 | 30 / 1700 | 100 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | X | X | OP11 OP12 neat test | CD |
| <i>JE 05/10/22</i> | | | | | | | | | | | | |

Signature:

Date Completed:

05/10/22

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 02 May 2022 12:18:43
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); 4.56E-5 [H] (Torr)

Source Parameters

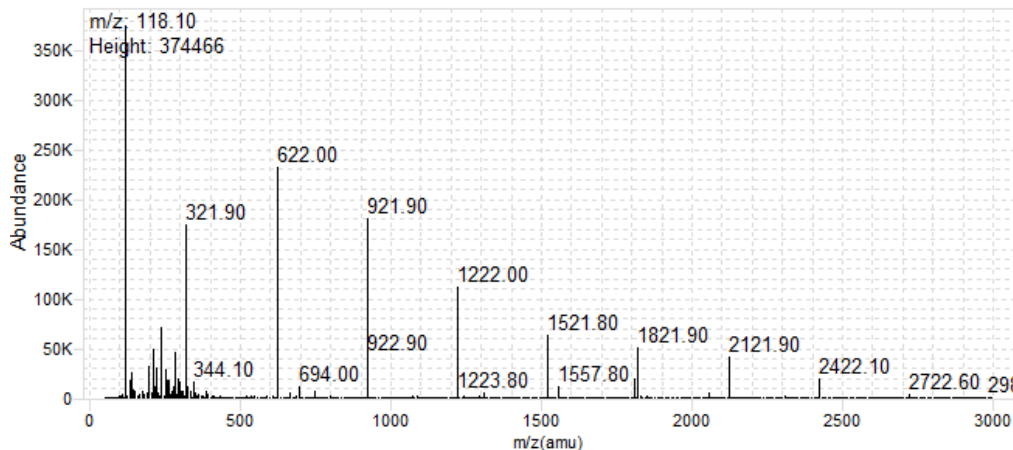
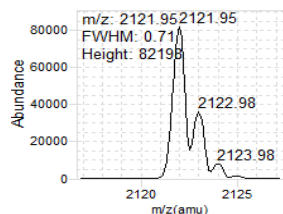
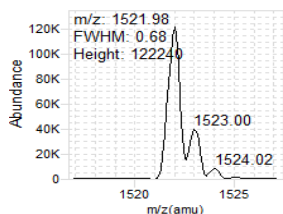
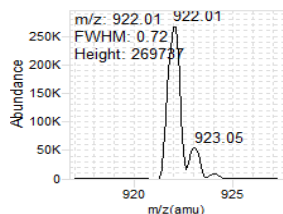
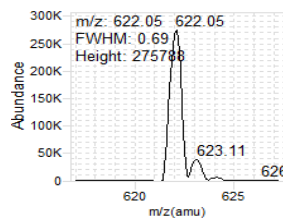
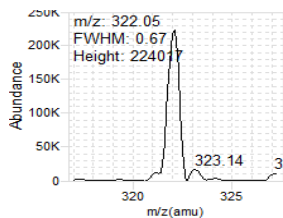
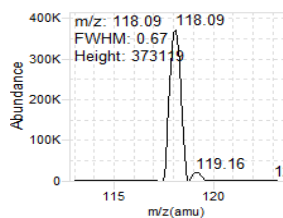
| Parameter | Positive | Negative |
|-------------------------|----------|----------|
| Gas Temp (°C) | 300 | 300 |
| Gas Flow (l/min) | 8 | 8 |
| Nebulizer (psi) | 15 | 15 |
| Capillary (V) | 4000 | 4000 |
| Nozzle Voltage (V) | 1500 | 1500 |
| Sheath Gas Temp (°C) | 250 | 250 |
| Sheath Gas Flow (l/min) | 7 | 7 |

Positive Results

Analyzer: MS1

Polarity: Positive

Width: Unit

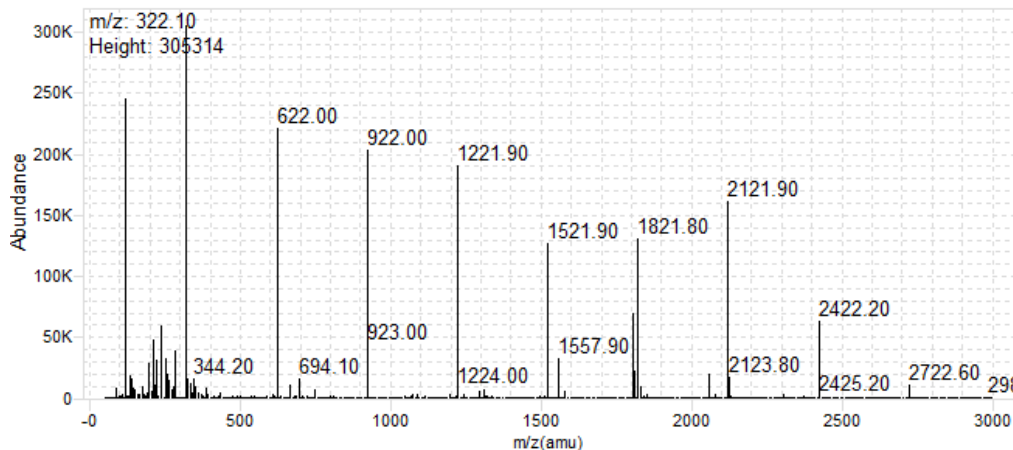
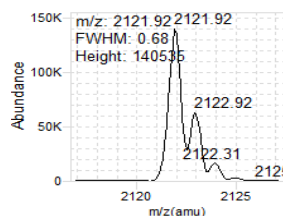
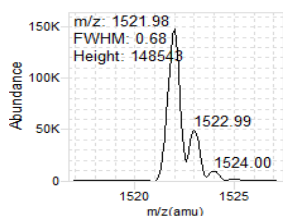
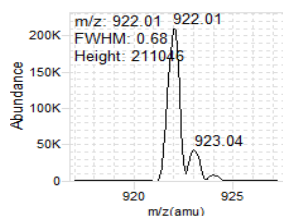
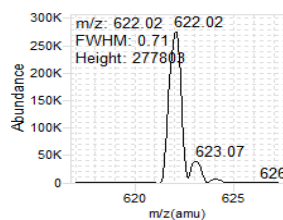
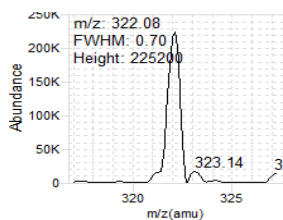
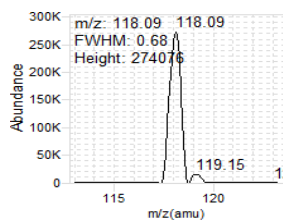


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 118.09 | 118.09 | 0.67 | 0.70 | 373119 |
| 322.05 | 322.05 | 0.67 | 0.70 | 224017 |
| 622.05 | 622.03 | 0.68 | 0.70 | 275788 |
| 922.01 | 922.01 | 0.72 | 0.70 | 269737 |
| 1521.98 | 1521.97 | 0.68 | 0.70 | 122240 |
| 2121.96 | 2121.93 | 0.71 | 0.70 | 82198 |

Analyzer: MS2

Polarity: Positive

Width: Unit

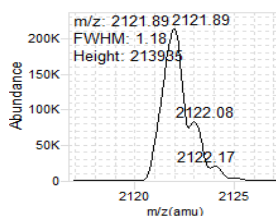
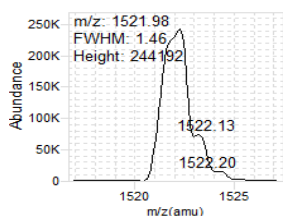
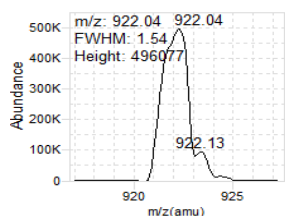
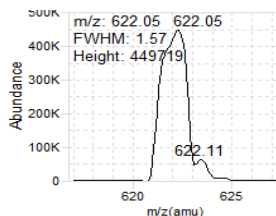
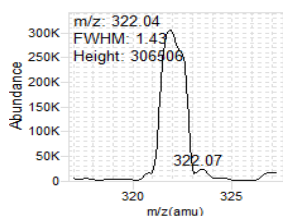
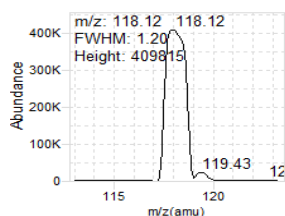


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 118.09 | 118.09 | 0.68 | 0.70 | 274076 |
| 322.08 | 322.05 | 0.70 | 0.70 | 225200 |
| 622.02 | 622.03 | 0.71 | 0.70 | 277803 |
| 922.01 | 922.01 | 0.68 | 0.70 | 211046 |
| 1521.98 | 1521.97 | 0.68 | 0.70 | 148543 |
| 2121.92 | 2121.93 | 0.68 | 0.70 | 140535 |

Analyzer: MS1

Polarity: Positive

Width: Wide

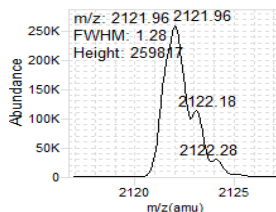
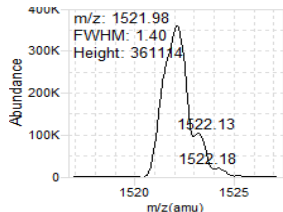
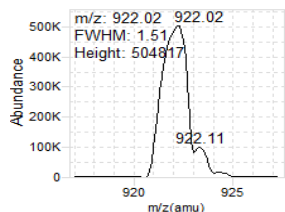
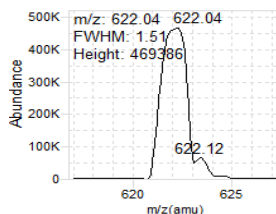
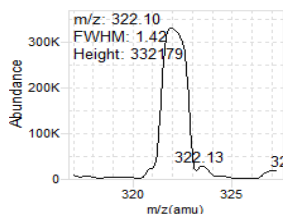
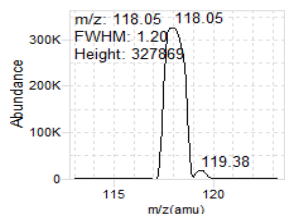


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 118.12 | 118.09 | 1.20 | 1.20 | 409815 |
| 322.04 | 322.05 | 1.43 | 1.20 | 306506 |
| 622.04 | 622.03 | 1.57 | 1.20 | 449719 |
| 922.04 | 922.01 | 1.54 | 1.20 | 496077 |
| 1521.98 | 1521.97 | 1.46 | 1.20 | 244192 |
| 2121.90 | 2121.93 | 1.18 | 1.20 | 213935 |

Analyzer: MS2

Polarity: Positive

Width: Wide

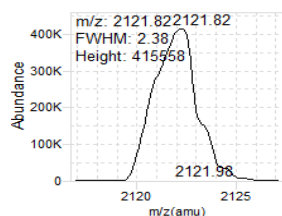
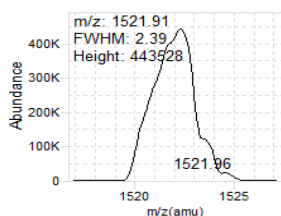
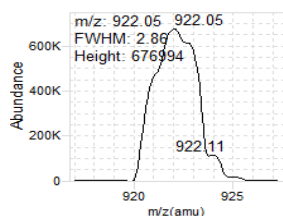
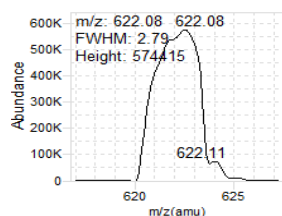
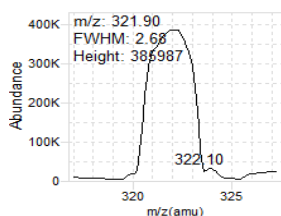
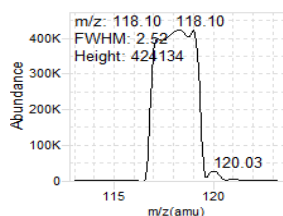


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 118.05 | 118.09 | 1.20 | 1.20 | 327869 |
| 322.10 | 322.05 | 1.42 | 1.20 | 332179 |
| 622.04 | 622.03 | 1.51 | 1.20 | 469386 |
| 922.02 | 922.01 | 1.51 | 1.20 | 504817 |
| 1521.98 | 1521.97 | 1.40 | 1.20 | 361114 |
| 2121.97 | 2121.93 | 1.28 | 1.20 | 259817 |

Analyzer: MS1

Polarity: Positive

Width: Widest

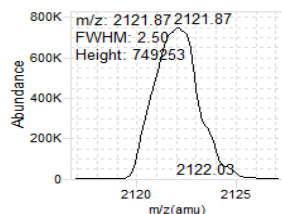
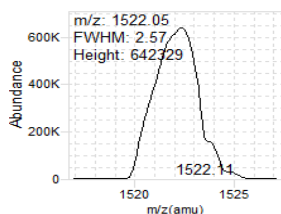
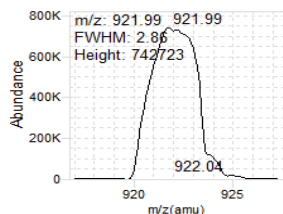
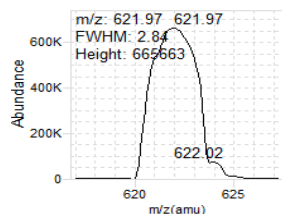
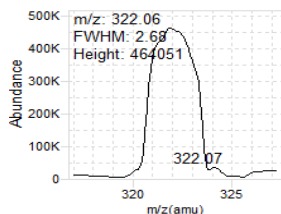
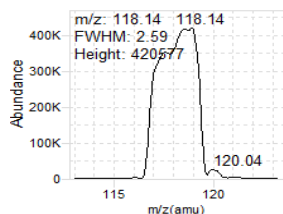


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 118.10 | 118.09 | 2.52 | 2.50 | 424134 |
| 321.90 | 322.05 | 2.68 | 2.50 | 385987 |
| 622.08 | 622.03 | 2.79 | 2.50 | 574415 |
| 922.04 | 922.01 | 2.86 | 2.50 | 676994 |
| 1521.91 | 1521.97 | 2.39 | 2.50 | 443528 |
| 2121.83 | 2121.93 | 2.38 | 2.50 | 415558 |

Analyzer: MS2

Polarity: Positive

Width: Widest



| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 118.14 | 118.09 | 2.59 | 2.50 | 420577 |
| 322.06 | 322.05 | 2.68 | 2.50 | 464051 |
| 621.97 | 622.03 | 2.83 | 2.50 | 665663 |
| 921.99 | 922.01 | 2.86 | 2.50 | 742723 |
| 1522.05 | 1521.97 | 2.57 | 2.50 | 642329 |
| 2121.88 | 2121.93 | 2.50 | 2.50 | 749253 |

Positive Results

Tune Parameters

| Parameters | Setting |
|--------------------|----------------|
| Fragmentor | 135 |
| Skimmer | 15 |
| Octopole DC | 5 |
| Octopole RF | 600 |
| Lens 1 | 3.50 |
| MS1 PreFilter | -10 |
| MS1 DC | 3.00 |
| MS1 PostFilter | 2.00 |
| MS1 Axis Offset | 0.92 |
| MS1 Axis Gain | 0.35 |
| MS1 Width Offset | 0.06 |
| MS1 Width Gain | -15 |
| MS1 Heater | 100 |
| MS2 DC | -10 |
| MS2 PreFilter | -30 |
| MS2 Axis Offset | 0.88 |
| MS2 Axis Gain | -11 |
| MS2 Width Offset | 0 |
| MS2 Width Gain | 1 |
| MS2 Heater | 100 |
| Cell Entry | 1 |
| Hexapole DC | 0.00 |
| Hexapole RF | 500 |
| Hexapole Accel | 5 |
| Cell Exit | -7 |
| Collision Gas | 1 |
| Iris | -150 |
| HED | -10 |
| EMV | 1035 |
| Collision Energy | 0 |
| Lens 1[MS2] | 1.40 |
| MS1 PreFilter[MS2] | 1.80 |

Dynamic Ramp Tables

MS1 PreFilter

| m/z | Setting |
|------------|----------------|
| 118.09 | -12 |
| 322.05 | -6.4 |
| 622.03 | -9 |
| 922.01 | -11.7 |
| 1521.97 | -13.2 |
| 2121.93 | -11.7 |

MS1 Axis Offset

| m/z | Setting |
|------------|----------------|
| 118.09 | 0.924 |
| 322.05 | 1.15 |
| 622.03 | 1.291 |
| 922.01 | 1.276 |
| 1521.97 | 1.134 |
| 2121.93 | 0.924 |

MS1 Width Offset

| m/z | Setting |
|------------|----------------|
| 118.09 | 0.06 |
| 322.05 | -0.16 |
| 622.03 | -0.27 |
| 922.01 | -0.24 |
| 1521.97 | -0.13 |
| 2121.93 | 0.06 |

MS2 PreFilter

| m/z | Setting |
|--------|---------|
| 58 | -16.6 |
| 79 | -22.6 |
| 117.97 | -30 |
| 118 | -12.8 |
| 154 | -17.2 |
| 290 | -33 |

MS2 Axis Offset

| m/z | Setting |
|---------|---------|
| 118.09 | 0.884 |
| 322.05 | 1.108 |
| 622.03 | 1.222 |
| 922.01 | 1.207 |
| 1521.97 | 1.151 |
| 2121.93 | 0.884 |

MS2 Width Offset

| m/z | Setting |
|---------|---------|
| 118.09 | 0 |
| 322.05 | -0.18 |
| 622.03 | -0.3 |
| 922.01 | -0.33 |
| 1521.97 | -0.24 |
| 2121.93 | 0 |

MS1 Calibrations

| Resolution | Mass Gain | Mass Offset | Width Gain | Width Offset |
|------------|-----------|-------------|------------|--------------|
| Unit | 0.35 | 0.924 | -14.9 | 0.06 |
| Wide | 0.15 | 1.092 | -14.5 | 0.42 |
| Widest | -0.25 | 1.496 | -14.2 | 1.4 |

MS2 Calibrations

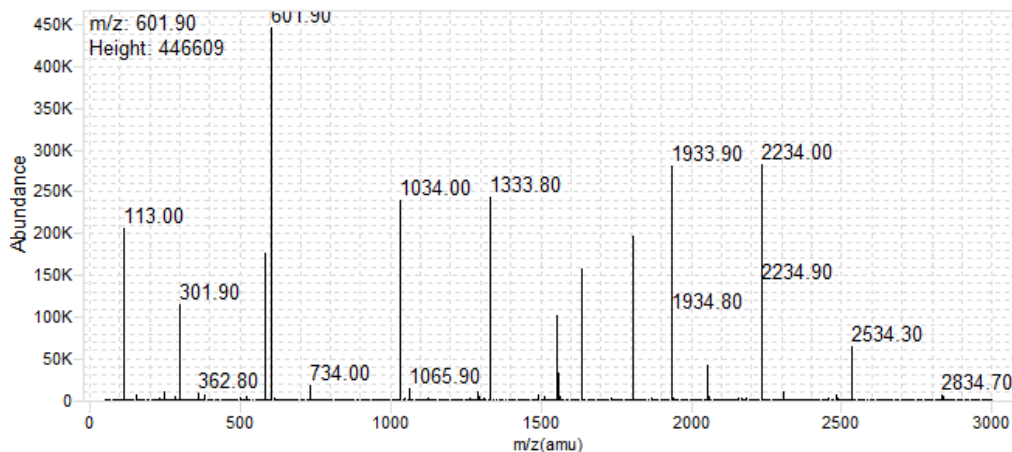
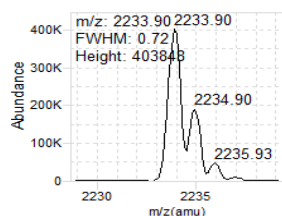
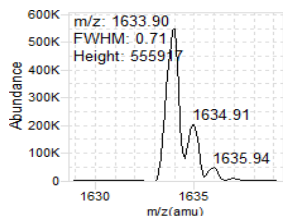
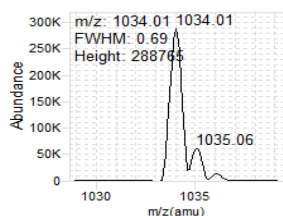
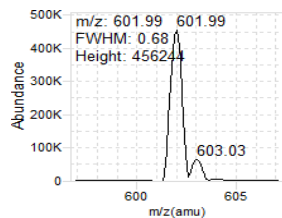
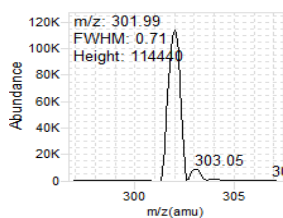
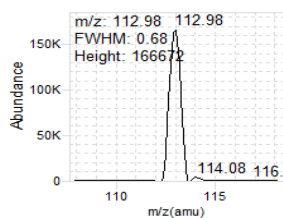
| Resolution | Mass Gain | Mass Offset | Width Gain | Width Offset |
|------------|-----------|-------------|------------|--------------|
| Unit | -10.9 | 0.884 | 0.6 | 0 |
| Wide | -10.95 | 1.044 | 0.7 | 0.4 |
| Widest | -11.3 | 1.498 | 1.2 | 1.41 |

Negative Results

Analyzer: MS1

Polarity: Negative

Width: Unit

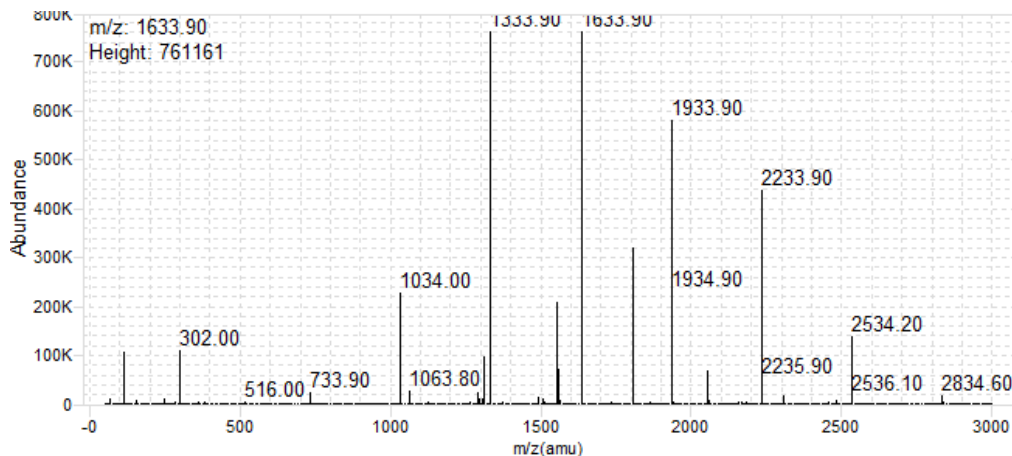
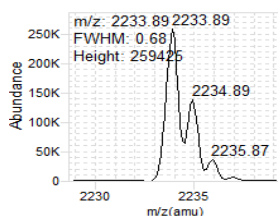
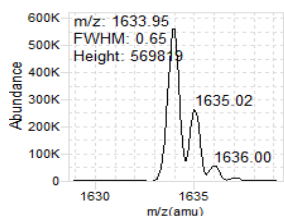
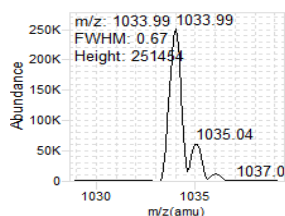
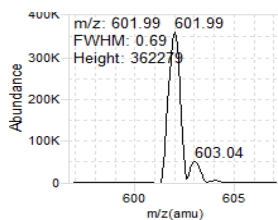
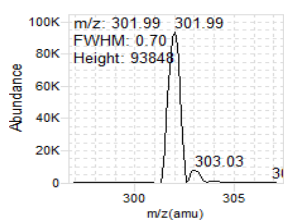
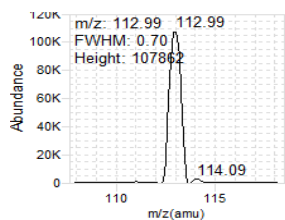


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 112.98 | 112.99 | 0.68 | 0.70 | 166672 |
| 301.99 | 302.00 | 0.71 | 0.70 | 114440 |
| 601.99 | 601.98 | 0.68 | 0.70 | 456244 |
| 1034.01 | 1033.99 | 0.69 | 0.70 | 288765 |
| 1633.90 | 1633.95 | 0.71 | 0.70 | 555917 |
| 2233.90 | 2233.91 | 0.72 | 0.70 | 403848 |

Analyzer: MS2

Polarity: Negative

Width: Unit

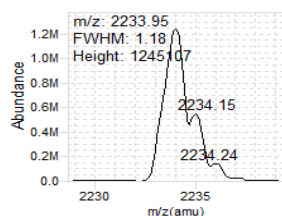
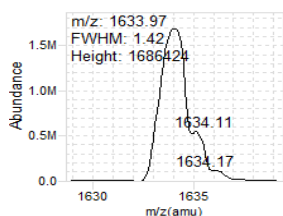
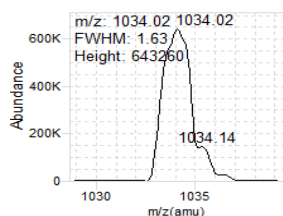
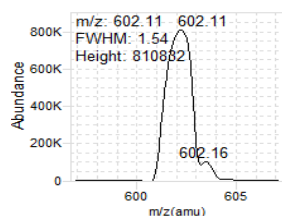
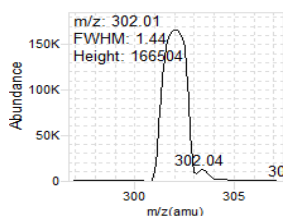
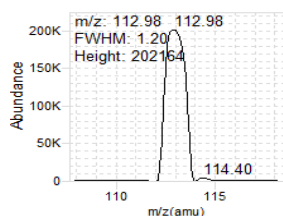


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 112.99 | 112.99 | 0.70 | 0.70 | 107862 |
| 301.99 | 302.00 | 0.70 | 0.70 | 93848 |
| 601.99 | 601.98 | 0.69 | 0.70 | 362279 |
| 1033.99 | 1033.99 | 0.67 | 0.70 | 251454 |
| 1633.95 | 1633.95 | 0.65 | 0.70 | 569819 |
| 2233.89 | 2233.91 | 0.68 | 0.70 | 259425 |

Analyzer: MS1

Polarity: Negative

Width: Wide

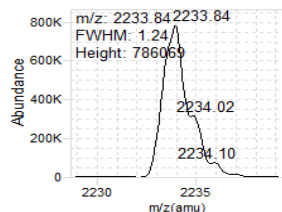
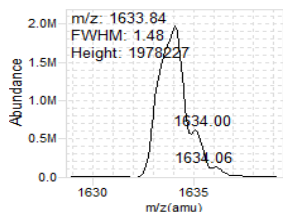
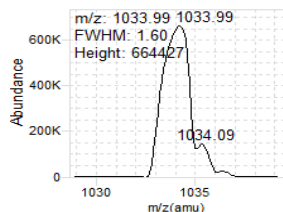
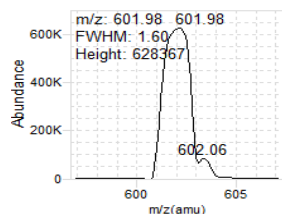
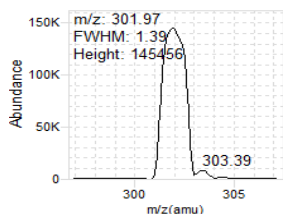
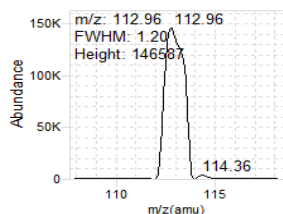


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 112.98 | 112.99 | 1.20 | 1.20 | 202164 |
| 302.01 | 302.00 | 1.44 | 1.20 | 166504 |
| 602.11 | 601.98 | 1.54 | 1.20 | 810832 |
| 1034.02 | 1033.99 | 1.63 | 1.20 | 643260 |
| 1633.96 | 1633.95 | 1.42 | 1.20 | 1686424 |
| 2233.96 | 2233.91 | 1.18 | 1.20 | 1245107 |

Analyzer: MS2

Polarity: Negative

Width: Wide

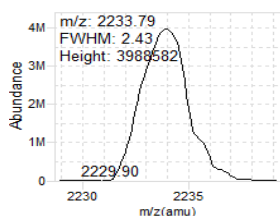
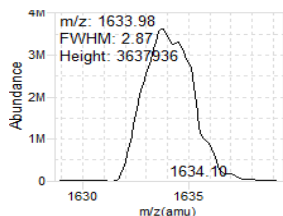
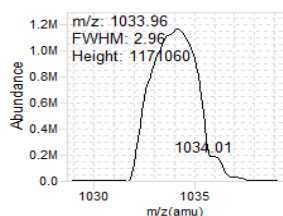
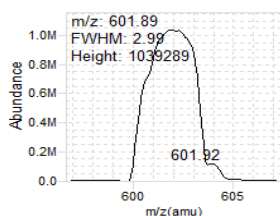
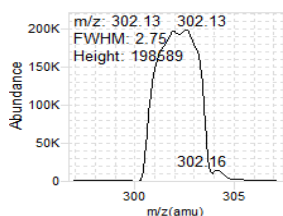
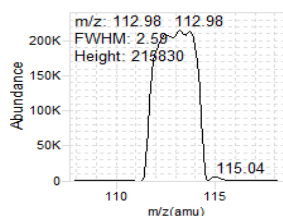


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 112.96 | 112.99 | 1.20 | 1.20 | 146587 |
| 301.97 | 302.00 | 1.39 | 1.20 | 145456 |
| 601.98 | 601.98 | 1.60 | 1.20 | 628367 |
| 1033.99 | 1033.99 | 1.60 | 1.20 | 664427 |
| 1633.84 | 1633.95 | 1.48 | 1.20 | 1978227 |
| 2233.85 | 2233.91 | 1.24 | 1.20 | 786069 |

Analyzer: MS1

Polarity: Negative

Width: Widest

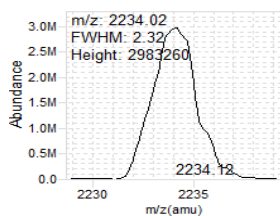
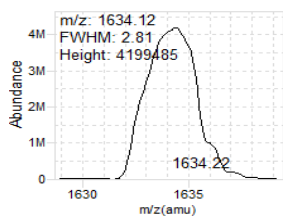
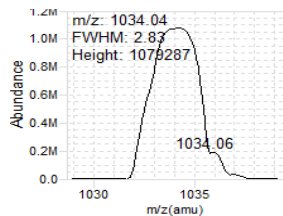
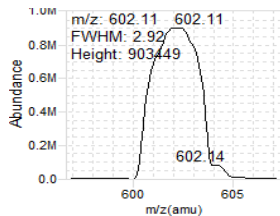
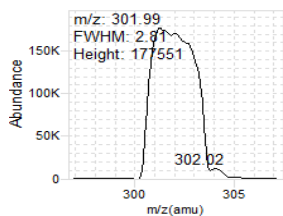
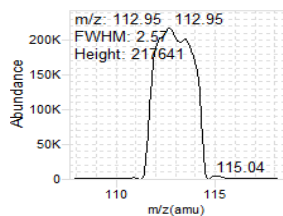


| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 112.98 | 112.99 | 2.59 | 2.50 | 215830 |
| 302.13 | 302.00 | 2.75 | 2.50 | 198589 |
| 601.89 | 601.98 | 2.99 | 2.50 | 1039289 |
| 1033.96 | 1033.99 | 2.96 | 2.50 | 1171060 |
| 1633.98 | 1633.95 | 2.87 | 2.50 | 3637936 |
| 2233.79 | 2233.91 | 2.43 | 2.50 | 3988582 |

Analyzer: MS2

Polarity: Negative

Width: Widest



| m/z | m/z Expected | FWHM | FWHM Expected | Abundance |
|---------|--------------|------|---------------|-----------|
| 112.95 | 112.99 | 2.57 | 2.50 | 217641 |
| 301.99 | 302.00 | 2.81 | 2.50 | 177551 |
| 602.11 | 601.98 | 2.92 | 2.50 | 903449 |
| 1034.04 | 1033.99 | 2.83 | 2.50 | 1079287 |
| 1634.11 | 1633.95 | 2.81 | 2.50 | 4199484 |
| 2234.03 | 2233.91 | 2.32 | 2.50 | 2983260 |

Negative Results

Tune Parameters

| Parameters | Setting |
|--------------------|---------|
| Fragmentor | 115 |
| Skimmer | 15 |
| Octopole DC | 5 |
| Octopole RF | 600 |
| Lens 1 | -3.50 |
| MS1 PreFilter | 16 |
| MS1 DC | -3.00 |
| MS1 PostFilter | -2.00 |
| MS1 Axis Offset | 0.91 |
| MS1 Axis Gain | 0.25 |
| MS1 Width Offset | 0 |
| MS1 Width Gain | -15 |
| MS1 Heater | 100 |
| MS2 DC | 10 |
| MS2 PreFilter | 30 |
| MS2 Axis Offset | 0.90 |
| MS2 Axis Gain | -11.05 |
| MS2 Width Offset | -0.06 |
| MS2 Width Gain | 1 |
| MS2 Heater | 100 |
| Cell Entry | 1 |
| Hexapole DC | 0.00 |
| Hexapole RF | 500 |
| Hexapole Accel | 5 |
| Cell Exit | 7.00 |
| Collision Gas | 1 |
| Iris | 150 |
| HED | 18 |
| EMV | 1060 |
| Collision Energy | 0 |
| Lens 1[MS2] | -3.80 |
| MS1 PreFilter[MS2] | -1.60 |

Dynamic Ramp Tables

MS1 PreFilter

| m/z | Setting |
|---------|---------|
| 112.99 | 9.2 |
| 302 | 9.4 |
| 601.98 | 8.6 |
| 1033.99 | 20.1 |
| 1633.95 | 16.3 |
| 2233.91 | 22.7 |

MS1 Axis Offset

| m/z | Setting |
|---------|---------|
| 112.99 | 0.912 |
| 302 | 1.129 |
| 601.98 | 1.3 |
| 1033.99 | 1.346 |
| 1633.95 | 1.117 |
| 2233.91 | 0.912 |

MS1 Width Offset

| m/z | Setting |
|---------|---------|
| 112.99 | 0.1 |
| 302 | -0.09 |
| 601.98 | -0.24 |
| 1033.99 | -0.24 |
| 1633.95 | -0.12 |
| 2233.91 | 0.1 |

MS2 PreFilter

| m/z | Setting |
|--------|---------|
| 69 | 18.8 |
| 112.97 | 30 |
| 113 | 10 |
| 207 | 22.4 |
| 232 | 26.2 |
| 302 | 35.6 |

MS2 Axis Offset

| m/z | Setting |
|---------|---------|
| 112.99 | 0.896 |
| 302 | 1.081 |
| 601.98 | 1.251 |
| 1033.99 | 1.28 |
| 1633.95 | 1.229 |
| 2233.91 | 0.896 |

MS2 Width Offset

| m/z | Setting |
|---------|---------|
| 112.99 | -0.06 |
| 302 | -0.19 |
| 601.98 | -0.35 |
| 1033.99 | -0.4 |
| 1633.95 | -0.29 |
| 2233.91 | -0.06 |

MS1 Calibrations

| Resolution | Mass Gain | Mass Offset | Width Gain | Width Offset |
|------------|-----------|-------------|------------|--------------|
| Unit | 0.25 | 0.912 | -15.1 | 0.1 |
| Wide | 0.1 | 1.116 | -14.9 | 0.53 |
| Widest | -0.2 | 1.552 | -14.3 | 1.58 |

MS2 Calibrations

| Resolution | Mass Gain | Mass Offset | Width Gain | Width Offset |
|------------|-----------|-------------|------------|--------------|
| Unit | -11.05 | 0.896 | 0.7 | -0.06 |
| Wide | -11.3 | 1.082 | 0.8 | 0.39 |
| Widest | -11.35 | 1.54 | 1.3 | 1.44 |

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 02 May 2022 12:18:43
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.61E+0 [R] (Torr); 4.56E-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 | 0.67 | -0.03 | Pass | 373119 |
| 322.05 | 322.05 | 0.00 | Pass | 0.70 | 0.67 | -0.03 | Pass | 224017 |
| 622.03 | 622.05 | 0.02 | Pass | 0.70 | 0.68 | -0.02 | Pass | 275788 |
| 922.01 | 922.01 | 0.00 | Pass | 0.70 | 0.72 | 0.02 | Pass | 269737 |
| 1521.97 | 1521.98 | 0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 122240 |
| 2121.93 | 2121.96 | 0.03 | Pass | 0.70 | 0.71 | 0.01 | Pass | 82198 |

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 | 0.68 | -0.02 | Pass | 274076 |
| 322.05 | 322.08 | 0.03 | Pass | 0.70 | 0.70 | 0.00 | Pass | 225200 |
| 622.03 | 622.02 | -0.01 | Pass | 0.70 | 0.71 | 0.01 | Pass | 277803 |
| 922.01 | 922.01 | 0.00 | Pass | 0.70 | 0.68 | -0.02 | Pass | 211046 |
| 1521.97 | 1521.98 | 0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 148543 |
| 2121.93 | 2121.92 | -0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 140535 |

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 | 409815 |
| 322.05 | 322.04 | -0.01 | Pass | 1.20 | 1.43 | 0.23 | Pass | 306506 |
| 622.03 | 622.04 | 0.01 | Pass | 1.20 | 1.57 | 0.37 | Pass | 449719 |
| 922.01 | 922.04 | 0.03 | Pass | 1.20 | 1.54 | 0.34 | Pass | 496077 |
| 1521.97 | 1521.98 | 0.01 | Pass | 1.20 | 1.46 | 0.26 | Pass | 244192 |
| 2121.93 | 2121.90 | -0.03 | Pass | 1.20 | 1.18 | -0.02 | Pass | 213935 |

Analyzer: MS2 Polarity: Positive Width: Wide

| m/z Expected | m/z Measured | Delta | Result | FWHM Expected | FWHM Measured | Delta | Result | Abundance |
|--------------|--------------|-------|--------|---------------|---------------|-------|--------|-----------|
| 118.09 | 118.05 | -0.04 | Pass | 1.20 | 1.20 | 0.00 | Pass | 327869 |
| 322.05 | 322.10 | 0.05 | Pass | 1.20 | 1.42 | 0.22 | Pass | 332179 |
| 622.03 | 622.04 | 0.01 | Pass | 1.20 | 1.51 | 0.31 | Pass | 469386 |
| 922.01 | 922.02 | 0.01 | Pass | 1.20 | 1.51 | 0.31 | Pass | 504817 |
| 1521.97 | 1521.98 | 0.01 | Pass | 1.20 | 1.40 | 0.20 | Pass | 361114 |
| 2121.93 | 2121.97 | 0.04 | Pass | 1.20 | 1.28 | 0.08 | Pass | 259817 |

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 | 2.52 | 0.02 | Pass | 424134 |
| 322.05 | 321.90 | -0.15 | Pass | 2.50 | 2.68 | 0.18 | Pass | 385987 |
| 622.03 | 622.08 | 0.05 | Pass | 2.50 | 2.79 | 0.29 | Pass | 574415 |
| 922.01 | 922.04 | 0.03 | Pass | 2.50 | 2.86 | 0.36 | Pass | 676994 |
| 1521.97 | 1521.91 | -0.06 | Pass | 2.50 | 2.39 | -0.11 | Pass | 443528 |
| 2121.93 | 2121.83 | -0.10 | Pass | 2.50 | 2.38 | -0.12 | Pass | 415558 |

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 | 118.14 | 0.05 | Pass | 2.50 | 2.59 | 0.09 | Pass | 420577 |
| 322.05 | 322.06 | 0.01 | Pass | 2.50 | 2.68 | 0.18 | Pass | 464051 |
| 622.03 | 621.97 | -0.06 | Pass | 2.50 | 2.83 | 0.33 | Pass | 665663 |
| 922.01 | 921.99 | -0.02 | Pass | 2.50 | 2.86 | 0.36 | Pass | 742723 |
| 1521.97 | 1522.05 | 0.08 | Pass | 2.50 | 2.57 | 0.07 | Pass | 642329 |
| 2121.93 | 2121.88 | -0.05 | Pass | 2.50 | 2.50 | 0.00 | Pass | 749253 |

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 | 0.68 | -0.02 | Pass | 166672 |
| 302.00 | 301.99 | -0.01 | Pass | 0.70 | 0.71 | 0.01 | Pass | 114440 |
| 601.98 | 601.99 | 0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 456244 |
| 1033.99 | 1034.01 | 0.02 | Pass | 0.70 | 0.69 | -0.01 | Pass | 288765 |
| 1633.95 | 1633.90 | -0.05 | Pass | 0.70 | 0.71 | 0.01 | Pass | 555917 |
| 2233.91 | 2233.90 | -0.01 | Pass | 0.70 | 0.72 | 0.02 | Pass | 403848 |

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 | 107862 |
| 302.00 | 301.99 | -0.01 | Pass | 0.70 | 0.70 | 0.00 | Pass | 93848 |
| 601.98 | 601.99 | 0.01 | Pass | 0.70 | 0.69 | -0.01 | Pass | 362279 |
| 1033.99 | 1033.99 | 0.00 | Pass | 0.70 | 0.67 | -0.03 | Pass | 251454 |
| 1633.95 | 1633.95 | 0.00 | Pass | 0.70 | 0.65 | -0.05 | Pass | 569819 |
| 2233.91 | 2233.89 | -0.02 | Pass | 0.70 | 0.68 | -0.02 | Pass | 259425 |

Analyzer: MS1 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 | 202164 |
| 302.00 | 302.01 | 0.01 | Pass | 1.20 | 1.44 | 0.24 | Pass | 166504 |
| 601.98 | 602.11 | 0.13 | Pass | 1.20 | 1.54 | 0.34 | Pass | 810832 |
| 1033.99 | 1034.02 | 0.03 | Pass | 1.20 | 1.63 | 0.43 | Pass | 643260 |
| 1633.95 | 1633.96 | 0.01 | Pass | 1.20 | 1.42 | 0.22 | Pass | 1686424 |
| 2233.91 | 2233.96 | 0.05 | Pass | 1.20 | 1.18 | -0.02 | Pass | 1245107 |

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 | 146587 |
| 302.00 | 301.97 | -0.03 | Pass | 1.20 | 1.39 | 0.19 | Pass | 145456 |
| 601.98 | 601.98 | 0.00 | Pass | 1.20 | 1.60 | 0.40 | Pass | 628367 |
| 1033.99 | 1033.99 | 0.00 | Pass | 1.20 | 1.60 | 0.40 | Pass | 664427 |
| 1633.95 | 1633.84 | -0.11 | Pass | 1.20 | 1.48 | 0.28 | Pass | 1978227 |
| 2233.91 | 2233.85 | -0.06 | Pass | 1.20 | 1.24 | 0.04 | Pass | 786069 |

Analyzer: MS1 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 | 2.59 | 0.09 | Pass | 215830 |
| 302.00 | 302.13 | 0.13 | Pass | 2.50 | 2.75 | 0.25 | Pass | 198589 |
| 601.98 | 601.89 | -0.09 | Pass | 2.50 | 2.99 | 0.49 | Pass | 1039289 |
| 1033.99 | 1033.96 | -0.03 | Pass | 2.50 | 2.96 | 0.46 | Pass | 1171060 |
| 1633.95 | 1633.98 | 0.03 | Pass | 2.50 | 2.87 | 0.37 | Pass | 3637936 |
| 2233.91 | 2233.79 | -0.12 | Pass | 2.50 | 2.43 | -0.07 | Pass | 3988582 |

Analyzer: MS2 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 | 2.57 | 0.07 | Pass | 217641 |
| 302.00 | 301.99 | -0.01 | Pass | 2.50 | 2.81 | 0.31 | Pass | 177551 |
| 601.98 | 602.11 | 0.13 | Pass | 2.50 | 2.92 | 0.42 | Pass | 903449 |
| 1033.99 | 1034.04 | 0.05 | Pass | 2.50 | 2.83 | 0.33 | Pass | 1079287 |
| 1633.95 | 1634.11 | 0.16 | Pass | 2.50 | 2.81 | 0.31 | Pass | 4199484 |
| 2233.91 | 2234.03 | 0.12 | Pass | 2.50 | 2.32 | -0.18 | Pass | 2983260 |

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 05 May 2022 08:49:14
Data Path D:\MassHunter\Tune\QQQ\G6470A\tunes.TUNE.XML
Ion Source AJS ESI
Ionization Mode AJS ESI
Tuned Resolution All
Vacuum Pressure 1.57E+0 [R] (Torr); 4.51E-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 | 0.69 | -0.01 | Pass | 430983 |
| 322.05 | 322.07 | 0.02 | Pass | 0.70 | 0.70 | 0.00 | Pass | 237960 |
| 622.03 | 622.06 | 0.03 | Pass | 0.70 | 0.67 | -0.03 | Pass | 274477 |
| 922.01 | 922.01 | 0.00 | Pass | 0.70 | 0.72 | 0.02 | Pass | 230159 |
| 1521.97 | 1521.99 | 0.02 | Pass | 0.70 | 0.69 | -0.01 | Pass | 78711 |
| 2121.93 | 2121.99 | 0.06 | Pass | 0.70 | 0.69 | -0.01 | Pass | 58556 |

Analyzer: MS2 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 | 315140 |
| 322.05 | 322.08 | 0.03 | Pass | 0.70 | 0.68 | -0.02 | Pass | 240479 |
| 622.03 | 622.02 | -0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 274583 |
| 922.01 | 922.00 | -0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 213016 |
| 1521.97 | 1521.98 | 0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 116475 |
| 2121.93 | 2121.93 | 0.00 | Pass | 0.70 | 0.67 | -0.03 | Pass | 112038 |

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 | 1.19 | -0.01 | Pass | 488412 |
| 322.05 | 322.07 | 0.02 | Pass | 1.20 | 1.45 | 0.25 | Pass | 333162 |
| 622.03 | 622.05 | 0.02 | Pass | 1.20 | 1.57 | 0.37 | Pass | 441662 |
| 922.01 | 922.04 | 0.03 | Pass | 1.20 | 1.54 | 0.34 | Pass | 455646 |
| 1521.97 | 1522.01 | 0.04 | Pass | 1.20 | 1.46 | 0.26 | Pass | 192563 |
| 2121.93 | 2121.95 | 0.02 | Pass | 1.20 | 1.16 | -0.04 | Pass | 166929 |

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 | 384627 |
| 322.05 | 322.11 | 0.06 | Pass | 1.20 | 1.38 | 0.18 | Pass | 381255 |
| 622.03 | 622.02 | -0.01 | Pass | 1.20 | 1.54 | 0.34 | Pass | 469269 |
| 922.01 | 922.02 | 0.01 | Pass | 1.20 | 1.51 | 0.31 | Pass | 447253 |
| 1521.97 | 1521.97 | 0.00 | Pass | 1.20 | 1.44 | 0.24 | Pass | 277281 |
| 2121.93 | 2122.00 | 0.07 | Pass | 1.20 | 1.25 | 0.05 | Pass | 223978 |

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 | 576912 |
| 322.05 | 321.91 | -0.14 | Pass | 2.50 | 2.68 | 0.18 | Pass | 427024 |
| 622.03 | 622.04 | 0.01 | Pass | 2.50 | 2.83 | 0.33 | Pass | 563015 |
| 922.01 | 922.12 | 0.11 | Pass | 2.50 | 2.73 | 0.23 | Pass | 637968 |
| 1521.97 | 1521.85 | -0.12 | Pass | 2.50 | 2.52 | 0.02 | Pass | 344318 |
| 2121.93 | 2121.82 | -0.11 | Pass | 2.50 | 2.35 | -0.15 | Pass | 327863 |

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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 | 2.49 | -0.01 | Pass | 534099 |
| 322.05 | 322.06 | 0.01 | Pass | 2.50 | 2.70 | 0.20 | Pass | 491412 |
| 622.03 | 622.00 | -0.03 | Pass | 2.50 | 2.82 | 0.32 | Pass | 657210 |
| 922.01 | 922.02 | 0.01 | Pass | 2.50 | 2.73 | 0.23 | Pass | 722876 |
| 1521.97 | 1521.97 | 0.00 | Pass | 2.50 | 2.73 | 0.23 | Pass | 501438 |
| 2121.93 | 2121.90 | -0.03 | Pass | 2.50 | 2.47 | -0.03 | Pass | 582191 |

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 | 0.69 | -0.01 | Pass | 206233 |
| 302.00 | 301.99 | -0.01 | Pass | 0.70 | 0.70 | 0.00 | Pass | 123107 |
| 601.98 | 601.99 | 0.01 | Pass | 0.70 | 0.68 | -0.02 | Pass | 486182 |
| 1033.99 | 1034.05 | 0.06 | Pass | 0.70 | 0.68 | -0.02 | Pass | 321579 |
| 1633.95 | 1633.91 | -0.04 | Pass | 0.70 | 0.69 | -0.01 | Pass | 645373 |
| 2233.91 | 2233.93 | 0.02 | Pass | 0.70 | 0.71 | 0.01 | Pass | 409772 |

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 | 0.68 | -0.02 | Pass | 134632 |
| 302.00 | 301.99 | -0.01 | Pass | 0.70 | 0.70 | 0.00 | Pass | 105135 |
| 601.98 | 601.99 | 0.01 | Pass | 0.70 | 0.69 | -0.01 | Pass | 393059 |
| 1033.99 | 1033.99 | 0.00 | Pass | 0.70 | 0.68 | -0.02 | Pass | 280178 |
| 1633.95 | 1633.95 | 0.00 | Pass | 0.70 | 0.67 | -0.03 | Pass | 767976 |
| 2233.91 | 2233.90 | -0.01 | Pass | 0.70 | 0.67 | -0.03 | Pass | 272219 |

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 | 1.21 | 0.01 | Pass | 248442 |
| 302.00 | 302.03 | 0.03 | Pass | 1.20 | 1.46 | 0.26 | Pass | 167931 |
| 601.98 | 602.09 | 0.11 | Pass | 1.20 | 1.58 | 0.38 | Pass | 900206 |
| 1033.99 | 1034.03 | 0.04 | Pass | 1.20 | 1.62 | 0.42 | Pass | 747603 |
| 1633.95 | 1633.98 | 0.03 | Pass | 1.20 | 1.38 | 0.18 | Pass | 1863848 |
| 2233.91 | 2233.98 | 0.07 | Pass | 1.20 | 1.14 | -0.06 | Pass | 1306862 |

Analyzer: MS2 Polarity: Negative Width: Wide

| m/z Expected | m/z Measured | Delta | Result | FWHM Expected | FWHM Measured | Delta | Result | Abundance |
|--------------|--------------|-------|--------|---------------|---------------|-------|--------|-----------|
| 112.99 | 112.94 | -0.05 | Pass | 1.20 | 1.17 | -0.03 | Pass | 200047 |
| 302.00 | 301.97 | -0.03 | Pass | 1.20 | 1.41 | 0.21 | Pass | 150666 |
| 601.98 | 602.01 | 0.03 | Pass | 1.20 | 1.53 | 0.33 | Pass | 713266 |
| 1033.99 | 1033.98 | -0.01 | Pass | 1.20 | 1.59 | 0.39 | Pass | 688786 |
| 1633.95 | 1633.82 | -0.13 | Pass | 1.20 | 1.47 | 0.27 | Pass | 1965815 |
| 2233.91 | 2233.84 | -0.07 | Pass | 1.20 | 1.23 | 0.03 | Pass | 736761 |

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 | 2.55 | 0.05 | Pass | 298008 |
| 302.00 | 302.13 | 0.13 | Pass | 2.50 | 2.72 | 0.22 | Pass | 221979 |
| 601.98 | 601.90 | -0.08 | Pass | 2.50 | 2.97 | 0.47 | Pass | 1206912 |
| 1033.99 | 1033.98 | -0.01 | Pass | 2.50 | 2.93 | 0.43 | Pass | 1292106 |
| 1633.95 | 1634.04 | 0.09 | Pass | 2.50 | 2.82 | 0.32 | Pass | 4118109 |
| 2233.91 | 2233.85 | -0.06 | Pass | 2.50 | 2.50 | 0.00 | Pass | 4216673 |

Analyzer: MS2 Polarity: Negative Width: Widest

| m/z Expected | m/z Measured | Delta | Result | FWHM Expected | FWHM Measured | Delta | Result | Abundance |
|--------------|--------------|-------|--------|---------------|---------------|-------|--------|-----------|
| 112.99 | 112.94 | -0.05 | Pass | 2.50 | 2.59 | 0.09 | Pass | 268944 |
| 302.00 | 301.97 | -0.03 | Pass | 2.50 | 2.70 | 0.20 | Pass | 197057 |
| 601.98 | 602.10 | 0.12 | Pass | 2.50 | 2.91 | 0.41 | Pass | 996688 |
| 1033.99 | 1033.99 | 0.00 | Pass | 2.50 | 3.02 | 0.52 | Pass | 1067280 |
| 1633.95 | 1634.13 | 0.18 | Pass | 2.50 | 2.83 | 0.33 | Pass | 4459839 |
| 2233.91 | 2234.00 | 0.09 | Pass | 2.50 | 2.35 | -0.15 | Pass | 2787970 |