Empower the Quantitation of Amino Acids and Acylcarnitine for Inborn Error of Metabolism Screening using Flow Injection – Orbitrap Mass Spectrometer

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Abstract

Purpose: Developed and validated a method to quantify 12 amino acids and 13 acylcarnitines in dried blood spots (DBS) in a commercial kit using a high-resolution Orbitrap[™] mass spectrometer.

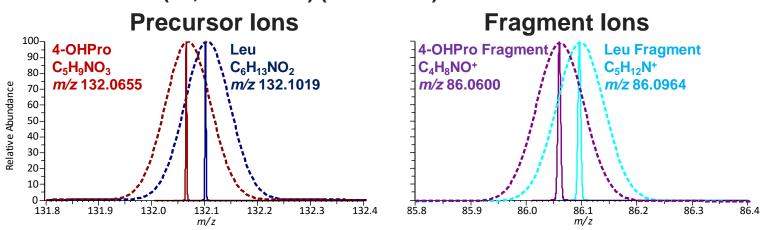
Methods: The analytes were quantified using a flow injection analysis, high-resolution accurate-mass, MS² mass spectrometric method (FIA-HRAM-MS/MS) on a Thermo Scientific[™] Vanguish Flex[™] UHPLC and Thermo Scientific[™] Orbitrap Exploris[™] 120 mass spectrometer.

Results: The method showed good accuracy and precision measurements that are comparable to those values

Introduction

The screening of newborns for inborn error of metabolism (IEM) is considered the largest and most successful disease prevention system in the United States. The quantitation of derivatized or non-derivatized amino acids and acylcarnitines from dried blood spots (DBS) via flow injection analysis – triple quadrupole tandem mass spectrometry (FIA-QqQ-MS/MS) serves as the main first-tier screening method. Although the QqQ-MS provides great robustness and sensitivity, the assay is incapable of separating nominal mass isobaric compounds with similar selected reaction monitoring (SRM) transitions in the absence of liquid chromatography separation (Figure 1). The hybrid high-resolution accurate mass spectrometers (HRAMS), such as Orbitrap Exploris MS, can detect ions with higher levels of confidence due to the low ppm mass accuracy to distinguish isobaric interferences from matrices, and good fragmentation spectra matching results against the spectra library.

Figure 1. Differentiation of the monoisotopic peaks of Leu and 4-OHPro precursor and their fragment ions simulated under nominal mass resolution employed by a QqQ MS (dash lines), and the resolution utilized by the Orbitrap Exploris 120 mass spectrometer for the full-MS (60,000 FWHM) and MS² scan events (15,000 FWHM) (solid lines).



Materials and methods

Sample Preparation

Analytes were extracted from the ClinChek[™] – Control Dried Blood Spot (DBS) Level I and II samples following the instruction of the ClinSpot LC-MS/MS Complete Kits, Amino Acids and Acylcarnitines in Dried Blood Spots (DBS) – non-derivatized (Figure 2). For the inter-day and intra-day precision measurements, each control level was prepared five times over three days.

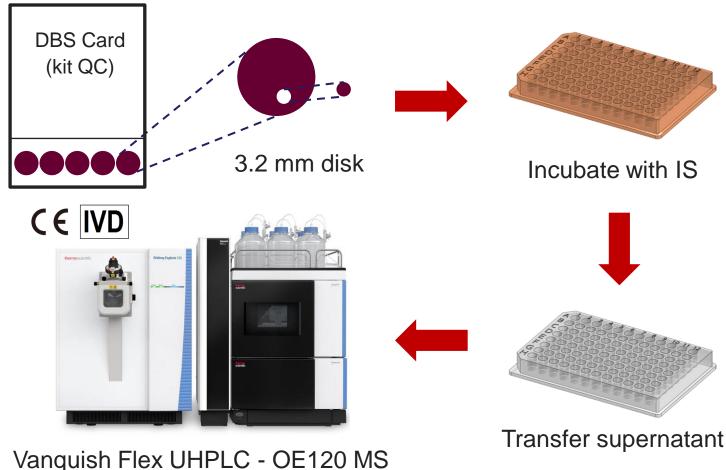
Liquid Chromatography

A Vanquish Flex UHPLC system was conditioned with the provided mobile phase. Each sample was injected twice at an injection volume of 5 µL. The flow rate and the rest of the LC gradient are specified in Table 1.

Data Analysis

Data were acquired and processed using Thermo Scientific[™] TraceFinder[™] software (ver 5.1 SP3 Clinical). The data processing parameters for the mzVault library matching, isotope pattern, and fragment matching are shown in Table 4. The mass tolerance for the analyte quantitation was set to 5 ppm.

Figure 2. Scheme for the DBS and FIA-HRAM-MS/MS workflow.



Materials and methods (cont')

Mass Spectrometry

The targeted-MS2 (tMS2) scan events were used for all analytes, except for Gly and 13C,15N-Gly, whose sole fragment ions had m/z values below the lowest m/z detection range (m/z 40) of the Orbitrap mass spectrometer (m/z 30.0338 for Gly and m/z32.0342 for ¹³C,¹⁵N-Gly). Thus, Gly was quantitated in the full-MS scan with the precursor ion. The mass spectrometer was equipped with a Thermo Scientific™ OptaMax[™] NG ion source with a heated electrospray ionization probe in the positive mode. The MS source parameters and scan event properties are listed in Tables 2 and 3. The precursor and fragment ions m/z values of the analytes and their internal standard (IS) are shown in Table 5.

Table 1. LC gradient

| Time | | Mahila Dhaqa (Daf | MS Sou | urce Parameters |
|-------|----------|-------------------|------------------------|-------------------------------------------|
| Time | | Mobile Phase (Ref | Ion Source Type | HESI (OptaMax [™] NG ion source) |
| (min) | (mL/min) | MS10010) (%) | HESI Probe Position | Center - 1.0 - L/M (x - y - z) |
| 0.00 | 0.05 | 100 | Spray Voltage | +3200 V |
| | | | Sheath Gas (Arb) | 50 |
| 0.70 | 0.05 | 100 | Aux Gas (Arb) | 5 |
| 0.71 | 0.50 | 100 | Sweep Gas (Arb) | 0 |
| | | | Ion Transfer Tube Temp | 325 °C |
| 0.89 | 0.50 | 100 | Vaporizer Temp | 75 °C |
| 0.90 | 0.10 | 100 | MS S | can Properties |
| 0.00 | 0.10 | 100 | Internal Calibrant | EASY-IC, run - start |
| 1.00 | 0.10 | 100 | Mild Trapping | On |

Table 3. OE120 scan event properties.

| | Scan I | Event 1 tMS ² |
|--------------------|--------------------|--------------------------|
| Resolution | | 15 |
| Isolation width (D | Da) | (|
| Targeted compoun | d list | See |
| RF lens | | 60 (precursor (m/z |
| Normalized CE | | |
| AGC | | 1 |
| Max injection time | (ms) | Sta |
| S | can E | vent 2 full-MS |
| Resolution | | 60 |
| m/z range | | 70 |
| RF lens | | |
| AGC | | 1 |
| Max injection time | (ms) | Sta |
| S | can E [,] | vent 3 full-MS |
| Resolution | | 60 |
| m/z range | | 200 |
| RF lens | | |
| AGC | | 1 |
| Max injection time | (ms) | Sta |
| | | |



Table 2. Global OE120 MS settings.

Table 4. TraceFinder data processing parameters.

| parameters. | |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| mzV | ault |
| Enabled | Checked |
| Search type | Highchem |
| Prefilter type | Precursor |
| Scan filter | MS ² |
| Precursor tolerance | 5 ppm |
| Score threshold | 10 |
| Passing value | 60 |
| Reverse Search | checked |
| Fragn | nents |
| Enabled | checked |
| Fragment tolerance | 5 ppm |
| Min # of fragments | 1 |
| Isotopes (for G | Bly and Gly-IS) |
| Enabled | checked |
| Fit threshold, % | 60 |
| Allowed mass | 5 |
| deviation (ppm) | Э |
| Allowed intensity | 20 |
| deviation (%) | 20 |
| | mzV Enabled Search type Prefilter type Scan filter Precursor tolerance Score threshold Passing value Reverse Search Fragment tolerance Min # of fragments Isotopes (for C Enabled Fit threshold, % Allowed mass deviation (ppm) Allowed intensity |

Table 5. The precursor and fragment ion *m*/*z* values of analytes and their internal standards.

| Analyte | Precursor (m/z) | Fragment ions (m/z) | IS | Precursor (m/z) | Fragment ions (m/z) |
|---------------------------------|--------------------|-------------------------------------------|----------------------------------------------------|--------------------|-------------------------------------------|
| Alanine (Ala) | 90.0550 | 44.0495* | ¹³ C ₃ , ¹⁵ N-Ala | 94.0621 | 47.0532* |
| Arginine (Arg) | 175.1190 | 770.0651*, 60.0556, 116.0706, 130.0975 | ¹³ C ₆ -Arg | 181.1391 | 74.0786*, 61.0590, 121.0873, 135.1143 |
| Aspartate (Asp) | 134.0448 | 88.0393*, 74.0237 | ¹³ C ₄ -Asp | 138.0582 | 76.0304*, 91.0494 |
| Citrulline (Cit) | 176.1035 | 159.0764*, 113.0709, 70.0651 | ² H ₇ -Cit | 183.1469 | 166.1204*, 120.1149, 77.1091 |
| Glutamate (Glu) | 148.0604 | 102.055*, 84.0444, 130.0499 | ¹³ C ₅ -Glu | 153.0772 | 106.0684*, 88.05781, 135.0666 |
| Glycine (Gly) | 76.0393* | | ¹³ C, ¹⁵ N-Gly | 78.0397* | |
| Leucine (Leu) | 132.1019 | 86.0964* | ² H ₃ -Leu | 135.1207 | 89.1153* |
| Methionine (Met) | 150.0583 | 104.0528*, 61.0106, 56.0495, 133.0318 | ² H ₃ -Met | 153.0772 | 107.0717*, 64.0295, 56.0495, 136.0506 |
| Ornithine (Orn) | 133.0972 | 116.0706*, 70.0651 | ² H ₆ -Orn | 139.1348 | 122.1083*, 76.1028 |
| Phenylalanine (Phe) | 166.0863 | 120.0808* | ¹³ C ₆ -Phe | 172.1064 | 126.1009* |
| Proline (Pro) | 116.0706 | 70.0651* | ¹³ C ₅ -Pro | 121.0874 | 74.0785* |
| Tyrosine (Tyr) | 182.0812 | 136.0757*, 91.0542, 123.0441, 165.0546 | ¹³ C ₆ −Tyr | 188.1013 | 142.0958*, 97.0744, 129.0642, 171.0748 |
| Valine (Val) | 118.0863 | 72.0808* | ² H ₈ -Val | 126.1365 | 80.1310* |
| Carnitine (C0) | 162.1125 | 85.0284*, 60.0808, 103.0390 | ² H ₉ -C0 | 171.1690 | 85.0284*, 69.1373, 103.0390 |
| Acetylcarnitine (C2) | 204.1230 | 85.0284*, 60.0808, 145.0495 | ² H ₃ -C2 | 207.1419 | 85.0284*, 63.0996, 145.0495 |
| Propionylcarnitine (C3) | 218.1387 | 85.0284*, 60.0808, 159.0652 | ² H ₃ -C3 | 221.1575 | 85.0284*, 63.0996, 159.0652 |
| Butyrylcarnintine (C4) | 232.1543 | 85.0284*, 60.0808, 173.0808 | ² H ₃ -C4 | 235.1732 | 85.0284*, 63.0996, 173.0808 |
| Isovalerylcarnitine (C5) | 246.1700 | 85.0284*, 60.0808, 187.0965 | ² H ₉ -C5 | 255.2265 | 85.0284*, 69.1373, 187.0965 |
| Glutarylcarnitine (C5DC) | 276.1442 | 85.0284*, 60.0808 | ² H ₉ -C5DC | 285.2007 | 85.0284*, 69.1373 |
| Hexanoylcarnitine (C6) | 260.1856 | 85.0284*, 60.0808, 201.1121 | ² H ₃ -C6 | 263.2045 | 85.0284*, 63.0996, 201.1121 |
| Octanoylcarnitine (C8) | 288.2169 | 85.0284*, 60.0808, 229.1434 | ² H ₃ -C8 | 291.2358 | 85.0284*, 63.0996, 229.1434 |
| Decanoylcarnitine (C10) | 316.2482 | 85.0284*, 60.0808, 257.1747 | ² H ₃ -C10 | 319.2671 | 85.0284*, 63.0996, 257.1747 |
| Dodecanoylcarnitine (C12) | 344.2795 | 85.0284*, 60.0808, 285.2060 | ² H ₃ -C12 | 347.2984 | 85.0284*, 63.0996, 285.2060 |
| Tetradecanoylcarnitine (C14) | 372.3108 | 85.0284*, 60.0808, 313.2373 | ² H ₃ -C14 | 375.3297 | 85.0284*, 63.0996, 313.2373 |
| Hexadecanoylcarnitine (C16) | 400.3421 | 85.0284*, 60.0808, 341.2686 | ² H ₃ -C16 | 403.3610 | 85.0284*, 63.0996, 341.2686 |
| Octadecanoylcarnitine (C18) | 428.3734 | 85.0284*, 60.0808, 369.3000 | ² H ₃ -C18 | 431.3923 | 85.0284*, 63.0996, 369.3000 |

: The ions used for analyte quantification are indicated with "", and the mass tolerance for the quantification was set to 5 ppm.

Results

Figure 3 shows the quantitation results for Met to demonstrate TraceFinder software data processing results. The extracted ion chromatograms (EIC) of the Met and its IS, ²H₃-Met, displayed as "stick," the library matching results, and the fragment matching results are also shown to highlight the confidence for the analyte detection. For Gly, which was quantified in the full-MS scan event, a similar plot was shown in Figure 4 to highlight the isotope pattern matching compared to the theoretical calculation.

The inter- and intra-day precision measurements from three different days with sample preparation performed five times are specified in Table 6. All the measured values were within the target range listed by the ClinChek – Control Dried Blood Spot (DBS) specification sheet, except Orn, which was slightly lower. This observation was consistent with the previous work on the verification of the same kit using a Vanquish MD HPLC and TSQ Quantis MD MS.¹ For all analyte quantitations, the %RSD was below 12%, and the %CV of the IS was below 9%, which supports the fact that the developed method was highly robust and reproducible.

Table 6. Inter-day and intra-day precision of the control level – I & II (acceptance criteria: %CV < 25), and the reproducibility of the IS (N = 30)

| | | | | C | ontrol L | evel l | | | | | |
|------------|--------|-----------------|--------|-------|----------|--------|--------|-------|--------|------|------|
| Analytes | Target | Range | Day | y-1 | Da | y-2 | Da | y-3 | Inter | -day | IS |
| | laiget | Range | Conc. | %RSD | Conc. | %RSD | Conc. | %RSD | Conc. | %RSD | %CV |
| Ala | 356.00 | 231.00 - 481.00 | 232.55 | 5.50 | 232.93 | 5.25 | 228.64 | 4.35 | 231.37 | 5.03 | 7.08 |
| Arg | 11.60 | 4.05 - 19.10 | 5.94 | 6.50 | 6.03 | 5.23 | 6.18 | 7.13 | 6.05 | 6.28 | 2.94 |
| Asp** | NA | NA | 17.69 | 2.67 | 17.79 | 5.10 | 19.37 | 4.46 | 18.28 | 4.08 | 3.58 |
| Cit | 19.70 | 9.85 - 29.50 | 11.50 | 10.46 | 11.19 | 4.23 | 11.39 | 5.02 | 11.36 | 6.57 | 3.84 |
| Glu | 274.00 | 178.00 - 370.00 | 332.24 | 4.72 | 327.35 | 4.29 | 336.59 | 5.60 | 332.06 | 4.87 | 4.10 |
| Gly | 313.00 | 188.00 - 439.00 | 222.47 | 4.43 | 224.98 | 4.83 | 222.88 | 5.85 | 223.44 | 5.04 | 3.37 |
| Leu | 225.00 | 146.00 - 304.00 | 176.74 | 3.17 | 173.69 | 3.57 | 173.95 | 4.25 | 174.79 | 3.66 | 6.95 |
| Met | 30.90 | 18.50 - 43.20 | 22.10 | 4.49 | 21.88 | 4.26 | 21.87 | 4.42 | 21.95 | 4.39 | 6.41 |
| Orn | 144.00 | 50.40 - 238.00 | 41.65* | 2.45 | 39.11* | 4.48 | 37.94* | 3.87 | 39.57* | 3.60 | 4.00 |
| Phe | 81.80 | 53.20 - 110.00 | 67.32 | 3.72 | 67.03 | 3.91 | 67.48 | 4.24 | 67.28 | 3.96 | 8.49 |
| Pro | 274.00 | 192.00 - 356.00 | 207.72 | 4.10 | 206.03 | 3.54 | 207.28 | 3.42 | 207.01 | 3.68 | 4.51 |
| Tyr | 61.10 | 36.70 - 85.50 | 53.88 | 3.24 | 54.58 | 2.91 | 54.41 | 3.16 | 54.29 | 3.10 | 7.64 |
| Val | 176.00 | 96.90 - 255.00 | 112.41 | 3.34 | 111.49 | 3.70 | 111.45 | 4.26 | 111.78 | 3.77 | 6.05 |
| C0 | 24.10 | 10.80 - 37.30 | 26.85 | 5.44 | 26.43 | 4.24 | 26.47 | 4.67 | 26.58 | 4.78 | 4.18 |
| C2 | 13.40 | 4.71 - 22.20 | 8.37 | 3.02 | 8.34 | 1.93 | 8.43 | 5.23 | 8.38 | 3.39 | 4.27 |
| C3 | 2.38 | 1.31 - 3.46 | 1.64 | 4.33 | 1.61 | 7.53 | 1.64 | 5.26 | 1.63 | 5.71 | 6.74 |
| C4 | 0.80 | 0.52 - 1.08 | 0.57 | 6.40 | 0.60 | 5.48 | 0.60 | 6.74 | 0.59 | 6.21 | 6.65 |
| C5 | 0.45 | 0.25 - 0.65 | 0.29 | 4.73 | 0.28 | 5.59 | 0.28 | 4.97 | 0.28 | 5.10 | 7.35 |
| C5DC | 1.01 | 0.35 - 1.66 | 0.90 | 5.76 | 0.88 | 8.27 | 0.89 | 5.34 | 0.89 | 6.46 | 6.84 |
| C 6 | 0.44 | 0.24 - 0.64 | 0.29 | 4.25 | 0.30 | 3.36 | 0.29 | 3.02 | 0.29 | 3.54 | 7.46 |
| C8 | 0.47 | 0.26 - 0.67 | 0.35 | 9.54 | 0.35 | 8.23 | 0.35 | 5.31 | 0.35 | 7.69 | 9.79 |
| C10 | 0.24 | 0.13 - 0.35 | 0.16 | 7.90 | 0.16 | 3.80 | 0.16 | 11.94 | 0.16 | 7.88 | 9.33 |
| C12 | 0.40 | 0.22 - 0.58 | 0.28 | 7.99 | 0.28 | 2.68 | 0.28 | 6.68 | 0.28 | 5.78 | 7.73 |
| C14 | 0.41 | 0.23 - 0.60 | 0.26 | 4.05 | 0.27 | 8.31 | 0.26 | 5.95 | 0.26 | 6.10 | 6.82 |
| C16 | 1.57 | 0.86 - 2.27 | 1.12 | 5.21 | 1.11 | 3.81 | 1.10 | 8.94 | 1.11 | 5.99 | 6.39 |
| C18 | 0.57 | 0.29 - 0.86 | 0.41 | 13.03 | 0.41 | 3.57 | 0.41 | 5.76 | 0.41 | 7.46 | 7.71 |

| | | | | C | ontrol L | evel II | | | | | |
|------------|---------------|------------------------------------|--------------|----------------------|--------------|---------|--------------|-------------|--------------|--------------|--------------|
| Analytes | Target | Range | Da | y-1 | Da | y-2 | Day | /- 3 | Inter | -day | IS |
| | Target | Kange | Conc. | %RSD | Conc. | %RSD | Conc. | %RSD | Conc. | %RSD | %CV |
| Ala | 1065.00 | 745.00 - 1384.00 | 678.81 | 3.97 | 659.91 | 5.51 | 690.84 | 5.43 | 676.52 | 4.97 | 6.62 |
| Arg | 102.00 | 40.80 - 163.00 | 53.24 | 4.67 | 53.46 | 5.30 | 54.77 | 3.47 | 53.82 | 4.48 | 2.50 |
| Asp** | NA | NA | 185.97 | 3.31 | 186.42 | 3.40 | 190.37 | 2.48 | 187.59 | 3.06 | 2.62 |
| Cit | 172.00 | 86.00 - 258.00 | 192.63 | 4.33 | 196.38 | 4.30 | 198.02 | 2.72 | 195.68 | 3.78 | 3.27 |
| Glu | 516.00 | 361.00 - 671.00 | 633.93 | 2.28 | 640.91 | 3.91 | 656.76 | 2.68 | 643.87 | 2.95 | 3.08 |
| Gly | 1216.00 | 730.00 - 1703.00 | 890.76 | 4.54 | 869.58 | 6.04 | 892.23 | 3.64 | 884.19 | 4.74 | 3.46 |
| Leu | 626.00 | 407.00 - 845.00 | 498.50 | 3.34 | 506.39 | 4.11 | 500.10 | 1.17 | 501.66 | 2.87 | 6.69 |
| Met | 355.00 | 231.00 - 480.00 | 250.59 | 3.90 | 249.85 | 4.91 | 247.24 | 1.47 | 249.23 | 3.42 | 6.13 |
| Orn | 441.00 | 242.00 - 639.00 | 179.11* | 4.36 | 171.99* | 5.42 | 171.07* | 4.19 | 174.06* | 4.66 | 2.63 |
| Phe | 664.00 | 431.00 - 896.00 | 606.61 | 3.40 | 611.44 | 3.56 | 615.30 | 1.54 | 611.12 | 2.83 | 8.56 |
| Pro | 497.00 | 323.00 - 671.00 | 389.99 | 3.59 | 390.16 | 3.41 | 394.21 | 0.90 | 391.45 | 2.64 | 4.80 |
| Tyr | 491.00 | 319.00 - 663.00 | 441.54 | 3.03 | 448.01 | 2.33 | 441.64 | 1.02 | 443.73 | 2.13 | 7.40 |
| Val | 550.00 | 330.00 - 770.00 | 354.23 | 4.00 | 351.05 | 4.52 | 356.26 | 2.37 | 353.85 | 3.63 | 5.56 |
| C0 | 97.80 | 48.90 - 147.00 | 102.23 | 5.74 | 102.33 | 2.78 | 102.38 | 2.78 | 102.31 | 3.77 | 4.68 |
| C2 | 102.00 | 41.00 - 164.00 | 65.30 | 3.76 | 65.55 | 3.32 | 65.50 | 2.82 | 65.45 | 3.30 | 4.69 |
| C3 | 15.20 | 9.86 - 20.50 | 10.35 | 2.40 | 10.16 | 4.27 | 10.54 | 2.07 | 10.35 | 2.91 | 5.66 |
| C4 | 8.52 | 5.96 - 11.10 | 6.10 | 3.33 | 6.09 | 6.33 | 6.22 | 3.56 | 6.14 | 4.41 | 6.14 |
| C5 | 1.97 | 1.18 - 2.76 | 1.44 | 6.93 | 1.44 | 3.51 | 1.48 | 4.64 | 1.45 | 5.02 | 7.68 |
| C5DC | 2.79 | 1.12 - 4.46 | 1.68 | 6.19 | 1.61 | 7.23 | 1.63 | 3.68 | 1.64 | 5.70 | 9.06 |
| C6 | 1.12 | 0.73 - 1.51 | 0.81 | 3.31 | 0.81 | 3.70 | 0.80 | 4.04 | 0.81 | 3.68 | 8.65 |
| C8 | 2.30 | 1.27 - 3.34 | 1.83 | 2.95 | 1.78 | 8.45 | 1.86 | 5.35 | 1.83 | 5.58 | 9.63 |
| C10 | 1.01 | 0.56 - 1.47 | 0.73 | 6.55 | 0.73 | 8.75 | 0.76 | 8.29 | 0.74 | 7.86 | 8.16 |
| C12 | 5.40 | 3.78 - 7.02 | 4.27 | 10.57 | 4.33 | 8.58 | 4.38 | 6.11 | 4.33 | 8.42 | 6.94 |
| C14 | 2.99 10.80 | <u>1.79 - 4.18</u> 5.96 - 15.70 | 2.13 | 4.32 | 2.24 | 4.88 | 2.12 | 5.86 | 2.16 | 5.02 | 7.00 |
| C16 C18 | 4.64 | 2.33 - 6.73 | 8.46 3.90 | <u>11.73</u> 4.32 | 8.42 3.88 | 4.44 | 8.46 3.86 | 4.36 | 8.45 3.88 | 6.84 4.02 | 9.47 4.99 |
| | 4.04 | 2.00 - 0.70 | 3.90 | 4.32 | J.00 | 4.12 | 5.00 | 5.05 | 5.00 | 4.02 | 4.33 |

*: The measured Orn level was slightly lower than the target range.

** Asp target value and ranges were not provided by the kit. NA, not available

Figure 3. TraceFinder interface showing the quantification results of Met in a tMS² scan with Calculated Amt, %RSD (of the Calculated Amt), and %CV (of the peak area), and Gly in full MS mode with isotope pattern matching.

Thermo Fisher

S C I E N T I F I C

| | | | | Sampl | e Results | | | | | | | | | | | 🚽 🕂 🗡 |
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| Compounds | | | → Ҭ × | Sampi | Results | | | | | | | | | | | * + ~ |
| Compound | RT | Туре | ^ | \$ [|] | Filename | ▲ ↓ Flag | gs 🕂 Stat | tus 👍 Area 🗄 | Calculat 👍 | Theoret 👍 | ISTD F ե | ISTD Amt | ⊣⊐ %RSD | -⊨ % CV | Active |
| <u>A</u> a 🔸 | <u>A</u> a | <u>A</u> a 👻 | | | <u>A</u> a | Aa | • | <u>A</u> a | | <u>A</u> a 🔻 | <u>A</u> a 🔻 | <u>A</u> a 🔻 | <u>A</u> a 🔻 | <u>A</u> a 🔻 | <u>A</u> a 🔻 | |
| 39 D7-Cit | 0.42 | Internal Standard | | ± 4 | ✓ | QC1_tMS2_Day- | 3_1-2 | • | 4461576 | 23.468 | 30.900 | 15323246 | 80.600 | 4.42 | 5.93 | ✓ |
| 40 D8-Val | 0.42 | Internal Standard | | ± 5 | \checkmark | QC1_tMS2_Day- | 3_2-1 | • | 902432 | 21.871 | 30.900 | 14381732 | 80.600 | 4.42 | 5.93 | \checkmark |
| 41 D9-C0 | 0.42 | Internal Standard | | ± e | \checkmark | QC1_tMS2_Day- | 3_2-2 | | 4029020 | 20.872 | 30.900 | 15558822 | 80.600 | 4.42 | 5.93 | ✓ |
| 42 D9-C5 | 0.42 | Internal Standard | | ± 7 | \checkmark | QC1_tMS2_Day- | 3_3-1 | • (| 4125693 | 22.102 | 30.900 | 15045446 | 80.600 | 4.42 | 5.93 | ✓ |
| 43 D9-C5DC | 0.42 | Internal Standard | | ±ε | \checkmark | QC1_tMS2_Day- | 3_3-2 | • (| 4241076 | 22.172 | 30.900 | 15417490 | 80.600 | 4.42 | 5.93 | ✓ |
| 44 Glu | 0.42 | Target Compound | ł | ÷g | ✓ | QC1_tMS2_Day- | 3_4-1 | | 4475419 | 20.561 | 30.900 | 17543647 | 80.600 | 4.42 | 5.93 | ✓ |
| 45 Gly | 0.42 | Target Compound | | ± 1 | | QC1_tMS2_Day- | | | 3966878 | 21.031 | 30.900 | 15202991 | 80.600 | 4.42 | 5.93 | ~ |
| 46 Leu | 0.42 | Target Compound | | ± 1 | | QC1_tMS2_Day- | | | 4087682 | 21.098 | 30.900 | 15615819 | 80.600 | 4.42 | 5.93 | ~ |
| 47 Met | 0.42 | Target Compound | | ± 1 | | QC1_tMS2_Day- | - | | 4375838 | 22.641 | 30.900 | 15577527 | | 4.42 | 5.93 | ✓ |
| 48 Orn | 0.42 | Target Compound | | ± 1 | | QC2_tMS2_Day- | | | 53579058 | | 355.000 | 17421349 | | 1.47 | 9.10 | ✓ |
| 49 Phe | 0.42 | Target Compound | | ± 1 | | QC2_tMS2_Day | | | 48052035 | | 355.000 | 15908324 | | 1.47 | 9.10 | Image: A start of the start of |
| 50 Pro | 0.42 | Target Compound | | ± 1 | | QC2_tMS2_Day- | | | 52223131 | | 355.000 | 16880695 | | 1.47 | 9.10 | Image: A start of the start of |
| 50 FIG | 0.42 | | | ± 1 | | QC2_tMS2_Day= | | | 42420344 | | 355.000 | 13970000 | | 1.47 | 9.10 | Image: A start of the start of |
| | | Target Compound | | ⊕_1 | _ | OC2 tMS2 Dav- | - | | 42420544 44335723 | | 355.000 | 14251193 | | 1.47 | 9.10 | Image: A state of the state of |
| 52 Val | 0.42 | Target Compound | ~ | < | ~ | OC2 TMS2 Dav- | 5 5-1 | | 44335773 | 250 748 | 1000 | 14/51193 | 80 600 | 147 | 9 10 | > |
| Compound Detail | s | | | | | | | | | | | | | | | → ₽ > |
| Quan Peak | \sim | | ▼ × | ISTD | | ~ | | × Libra | ry Match 🛛 🗸 | | - | × Fragm | nents | \sim | | • × |
| | | L | | _ | | | | | | H11NO26 | Score: 95 R | anki i | | Min | nimum # of frag | ments nee |
| QC1_tMS2_Day | y-3_5-1 N | let m/z: 104.0528 | | QC1_ | tMS2_Day-3 | 3_5-1 D3-Met m | /z: 107.071 | | #1: Met 95 | J #440 F:F | TMS + p ES | A | Il Fragments | | C1_tMS2_Day-3 | _5-1 #: |
| | RT: 0 | 38 | | | | RT: 0.38 | | M | S ² spec | tra | ···· | | 1: 56.0495 | F: I | FTMS + p ESI I | |
| | AA: 4 | 1087682 | | | | AA: 15615819 | | | o spee | 001 | | | 2: 61.0106 | | 4.0E5- *1 | *3 |
| 3.5E5- | AH: 3 | 353433 | | | | AH: 1350127 | | l n | natchin | G ental | | | | | - | *4 |
| | | | | | | | | | | | | | | | | |
| | | [↑] EIC, | | | 1.2E6- | . ∐ FI | C. | | | | | | 3: 104.0528 | | 3.0E5- | Ĺ |
| 3.0E5 | | † EIC, | MC | , | -1 | | IC, | | | 40 10 20 | | | 4: 133.0318 | | 2.0E5-*2 | Í |
| 3.0E5 | | | MS | , | 1.0E6 | | • | | | Experim 2011 | | • # | 4: 133.0318 | | 2.0E5- *2 1.0E5- | |
| 3.0E5 | . | † EIC, | MS | , | -1 | | • | et, tM | | Experim 20 1 1 1 1 0 | | • # | 4: 133.0318 | | 2.0E5- *2 1.0E5- | u |
| 3.0E5 | | † EIC, | MS | Intensity | 1.0E6 | | • | | | 0 ⁻ , | | • Fr | 4: 133.0318 agm | ent a | 2.0E5 1.0E5 | <u>∎</u> #3 |
| 3.0E5 2.5E5 2.0E5 1.5E5 | | † EIC, | MS | Intensity | 1.0E6 3.0E5 3.0E5 | | • | | | ₀ 크. #131 F: | =TMS + p ES | • Fr | 4: 133.0318 | ent a | 2.0E5- *2 1.0E5- | |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 | | † EIC, | MS | Intensity | 1.0E6- 3.0E5- 3.0E5- 4.0E5- | | • | | | 0 ⁻ , | =TMS + p ES | • Fr | 4: 133.0318 agm | ent a | 2.0E5 1.0E5 | <u>u</u> #3 #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 | | † EIC, | MS | Intensity | 1.0E6 3.0E5 3.0E5 | | • | | | 0 ¹ . #131 F: ¹⁰⁰ | TMS + p ES | • Fr | 4: 133.0318 agm | ent a | 2.0E5 1.0E5 0 4.0E5 4.0E5 2.0E5 2.0E5 | |
| 3.0E5 A:s 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 | | * EIC, Met, t | MS | Intensity | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 | 2 - | • | | | 0 ¹ . #131 F: ¹⁰⁰ | =TMS + p ES | • Fr | 4: 133.0318 agm | ent a | 2.0E5 1.0E5 0 4.0E5 2.0E5 #1 3.0E5 2.0E5 #2 #2 #1 | |
| 3.0E5 4:0 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 | | * EIC, Met, t | MS [;] | Intensity | 4.0E5- 2.0E5- | 2 - | • | | | 0 ⁻¹ . #131 F: 100-1 | TMS + p ES | • Fr | 4: 133.0318 agm | ent a | 2.0E5 1.0E5 0 4.0E5 4.0E5 2.0E5 2.0E5 | |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 | | * EIC, Met, t | + | Intensity | 1.0E6 3.0E5 4.0E5 2.0E5 0 0 0 0.0 | 2 - | • | | | 0 ¹ . #131 F: ¹⁰⁰ | =TMS + p ES | • Fr | 4: 133.0318 agm | ent a | 2.0E5 1.0E5 0 4.0E5 2.0E5 #1 3.0E5 2.0E5 #2 #2 #1 | |
| 3.0E5 A:s 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 | Left RT: | * EIC, Met, t | + | Intensity m/z: | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 | 2 - | • | et, tM | | 0 ¹ . #131 F: ¹⁰⁰ | TMS + p ES | • Fr | 4: 133.0318 agm | ent a | 2.0E5 1.0E5 4.0E5 2.0E5 2.0E5 1.0E5 #2 #1 3.0E5 #2 #1 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 | | * EIC, Met, t | + | Intensity m/z: | 1.0E6 3.0E5 4.0E5 2.0E5 0 0 0.0 | 2 | 1 ₃ -М(| et, tM | | 0 #131 F: 100 Internet Stars 0 | m/z | Fr m | agm atchi | ent ing | 2.0E5 1.0E5 2.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 | | * EIC, Met, t | - ↓ : 0.5 ~ | Intensity m/z: | 1.0E6 3.0E5 4.0E5 2.0E5 0 0 0.0 | 2 | i ₃ -Mt | et, tM | S ² | 0 #131 F: 100 Internet Stars 0 | | Fr m | agm atchi | ent ing | 2.0E5 1.0E5 2.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak | Left RT: | * EIC, Met, t 0.5 RT(min) | + : 0.5 ~ | m/z: Apex | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 0.0 107.0717 RT: 0.38 | 2 2 2 4 0.5 RT(min) Left RT: 0.13 | i ₃ -M€ | et, tM | S² | 0 #131 F: 100 Internet Stars 0 | m/z | Fr m patte | agm atchi | ent ing | 2.0E5 1.0E5 2.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak | Left RT: | * EIC, Met, t | + : 0.5 ~ | m/z: Apex | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 0.0 107.0717 RT: 0.38 | 2 2 2 - - - - - - - - - - - - - | i ₃ -M€ | et, tM | S ² | 4131 F: 100 100 100 100 100 100 100 10 | m/z tope Scan #; 2 Day-3 5-1 | • • • • • • • • • • • • • • • • • • • | 4: 133.0318 agm atchi ern r | ent ing ^{unun} | 2.0E5 1.0E5 2.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak | Left RT: | EIC, Met, t 0.5 RT(min) 0.12 Right RT | + : 0.5 ~ | m/z: Apex | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 0.0 107.0717 RT: 0.38 | 2 2 2 4 0.5 RT(min) Left RT: 0.13 | i ₃ -M€ | et, tM | S² | 4131 F: 100 100 100 100 100 100 100 10 | m/z tope | • • • • • • • • • • • • • • • • • • • | 4: 133.0318 agm atchi ern r | ent ing ^{unun} | 2.0E5 1.0E5 4.0E5 2.0E5 2.0E5 4.0E5 4.0E5 2.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak | Left RT: | EIC, Met, t Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 0.12 Right RT 0.12 Right RT | + : 0.5 ~ | m/z: Apex | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 0.0 107.0717 RT: 0.38 | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 | 13-M(Right RT: | et, tM | S2 ppe ~ All isotopes Multi-Isotopes | 4131 F: 100 100 100 100 100 100 100 10 | m/z tope Scan #, 2 Day-3 5-1 + p ESI Full n *1 | • • • • • • • • • • • • • • • • • • • | 4: 133.0318 agm atchi ern r | ent ing ^{unun} | 2.0E5 1.0E5 2.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1.0E5 1. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak | Left RT: | EIC, Met, t 0.5 RT(min) 0.12 Right RT 3.12 3.13 | + : 0.5 ~ | m/z: Apex ISTD | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 0.0 107.0717 RT: 0.38 | 2 | 13-M(Right RT: | et, tM | S2 ppe ~ All Isotopes Multi-Isotopes #1: 76.0393 | رم #131 F: 100 مدر الله CC1 the F: FTMS | m/z tope Scan #, 2 Day-3 5-1 + p ESI Full n *1 | • • • • • • • • • • • • • • • • • • • | 4: 133.0318 agm atchi ern r | ent ing ^{unun} | 2.0E5 1.0E5 4.0E5 2.0E5 2.0E5 4.0E5 4.0E5 2.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak | Left RT: | EIC, Met, t Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 0.12 Right RT 0.12 Right RT | + : 0.5 ~ | m/z: Apex ISTD | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0.0 107.0717 RT: 0.38 tMS2_Day- | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 | 13-M(Right RT: | et, tM | S2 ppe ~ All isotopes Multi-Isotopes | رم #131 F: 100 مدر الله CC1 the F: FTMS | m/z tope Scan #, 2 Day-3 5-1 + p ESI Full n *1 | • • • • • • • • • • • • • • • • • • • | 4: 133.0318 agm atchi ern r | ent ing ^{unun} | 2.0E5 1.0E5 4.0E5 2.0E5 2.0E5 4.0E5 4.0E5 2.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4. | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_1MS2_Day 4.0E6 | Left RT: | EIC, Met, t Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 0.12 Right RT 0.12 Right RT | + : 0.5 ~ | m/z: Apex QC1_ | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0,0 107.0717 RT: 0.38 tMS2_Day- 8.0E6 | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 | 13-M(Right RT: | et, tM | S2 ppe ~ All Isotopes Multi-Isotopes #1: 76.0393 | (1) (1) (1) (1) (1) (1) (1) (1) | m/z tope Scan #, 2 Day-3 5-1 + p ESI Full n *1 | • • • • • • • • • • • • • • • • • • • | 4: 133.0318 agm atchi atchi ern r RT: 0.24 - (200.0000] | ent suburn ing matc | 2.0E5 -2 1.0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 -4 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 .0E5 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_1MS2_Day 4.0E6 | Left RT: | <pre></pre> | | m/z: Apex QC1_ | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0.0 107.0717 RT: 0.38 tMS2_Day- | RT: 0.41 AA: 76971933 AH: 7980625 | 1 ₃ − M (Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 | () () () () () () () () () () | m/z tope Scan # 2_Day-3_5-1 • p ESI Full n *1 | patt 370-688 | 4: 133.0318 agm atchi ern r 200.0000j 78.5004 | ent Agent ing 0.75 AV: 7 | 2.0E5 1.0E5 0 4.0E5 1.0E5 1.0E5 1.0E5 0 m/z hing 80.9478 80.1310 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_1MS2_Day 4.0E6 | Left RT: | <pre></pre> | | m/z: Apex ISTD | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0,0 107.0717 RT: 0.38 4.0E2_Day-1 3.0E6 - - - - | RT: 0.41 AA: 76971933 AH: 7980625 | 13-M(Right RT: | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 | () () () () () () () () () () | m/z tope Scan # 2_Day-3_5-1 • p ESI Full n *1 | • • • • • • • • • • • • • • • • • • • | 4: 133.0318 agm atchi ern r 200.0000j 78.5004 | ent suburn ing matc | 2.0E5 1.0E5 0 4.0E5 1.0E5 1.0E5 1.0E5 0 m/z hing 80.9478 80.1310 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_tMS2_Day 4.0E6 2.5 0.0E4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0. | Left RT: | EIC, Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 0.12 Right RT 0.14 10407158 1552400 EIC | → : 0.5: → · × | Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intens | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0,0 107.0717 RT: 0.38 tMS2_Day- 8.0E6 | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 4 4 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 #4: 78.0436 | () () () () () () () () () () | m/z tope Scan # 2_Day-3_5-1 • p ESI Full n *1 | patt 370-688 | 4: 133.0318 agm atchi ern r 200.0000j 78.5004 | ent Agent ing 0.75 AV: 7 | 2.0E5 1.0E5 0 4.0E5 1.0E5 1.0E5 1.0E5 0 m/z hing 80.9478 80.1310 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_1MS2_Day 4.0E6 | Left RT: | <pre></pre> | → : 0.5: → · × | Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intensity Intens | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0,0 107.0717 RT: 0.38 4.0E2_Day-1 3.0E6 - - - - | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 4 4 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 | () () () () () () () () () () | m/z COPC Scan # 2 Day-3 5-1 P ESI Full n *1 | patt 370-688 | 4: 133.0318 agm atchi ern r 200.0000j 78.5004 | ent Agent ing 0.75 AV: 7 | 2.0E5 1.0E5 0 4.0E5 1.0E5 1.0E5 1.0E5 0 m/z hing 80.9478 80.1310 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_tMS2_Day 4.0E6 2.5 0.0E4 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0. | Left RT: | EIC, Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 0.12 Right RT 0.14 10407158 1552400 EIC | → : 0.5: → · × | m/z: Apex ISTD | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0,0 107.0717 RT: 0.38 4.0E2_Day-1 3.0E6 - - - - | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 4 4 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 #4: 78.0436 | 40 #131 F: 100 Keigin Viewight Soort MS F: FTMS 0 0 0 0 0 0 0 0 0 0 0 0 0 | m/z COPC Scan # 2 Day-3 5-1 P ESI Full n *1 | patt 370-688 | 4: 133.0318 agm atchi ern r 200.0000j 78.5004 | ent Agent ing 0.75 AV: 7 | 2.0E5 1.0E5 0 4.0E5 1.0E5 1.0E5 1.0E5 0 m/z hing 80.9478 80.1310 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_tMS2_Day 4.0E6 2.0E6 2.0E6 4.0E6 2.0E6 2.0E6 4.0E6 2.0E6 2.0E6 2.0E7 4.0E6 2.0E6 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2 | Left RT: | EIC, Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 0.12 Right RT 0.14 10407158 1552400 EIC | → : 0.5: → · × | m/z: Apex ISTD | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 107.0717 RT: 0.38 1082_Day-1 3.0E6 4.0E6 4.0E6 | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 4 4 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 #4: 78.0436 | () () () () () () () () () () | m/z COPC Scan # 2 Day-3 5-1 P ESI Full n *1 | patt 370-688 | 4: 133.0318 agm atchi ern r 200.0000j 78.5004 | ent Agent ing 0.75 AV: 7 | 2.0E5 1.0E5 0 4.0E5 1.0E5 1.0E5 1.0E5 0 m/z hing 80.9478 80.1310 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_tMS2_Day 4.0E6 2.0E6 2.0E6 4.0E6 2.0E6 2.0E6 4.0E6 2.0E6 2.0E6 2.0E7 4.0E6 2.0E6 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E6 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2.0E7 2 | Left RT: | EIC, Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 10407158 1552400 EIC Gly, | → : 0.5: → · × | m/z: Apex ISTD | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 107.0717 RT: 0.38 1082_Day-1 3.0E6 4.0E6 4.0E6 | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 ✓ 3_5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 1 1 1 1 1 1 1 1 1 1 1 1 1 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 #4: 78.0436 | 40 #131 F: 100 100 100 100 100 100 100 10 | m/z COPC Scan # 2 Day-3 5-1 P ESI Full n *1 | patt 370-688 | 4: 133.0318 agm atchi ern r 200.0000j 78.5004 | ent Agent ing 0.75 AV: 7 | 2.0E5 -2 1.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0E5 -4.0 | #4 |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_1MS2_Day 4.0E6 2.0E6 1.0E6 2.0E6 1.0E5 5.0E4 0.0 0.0 | Left RT: y-3_5-1 G AA: 4 AH: 4 | EIC, Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 0.12 Right RT 0.12 EIC Gly, 0.5 | → : 0.5: → · × | m/z: Apex ISTD | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 107.0717 RT: 0.38 1082_Day-1 3.0E6 4.0E6 4.0E6 | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 4 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 #4: 78.0436 | 40 #131 F: 100 Keigin Viewight Soort MS F: FTMS 0 0 0 0 0 0 0 0 0 0 0 0 0 | m/z COPC Scan # 2 Day-3 5-1 P ESI Full n *1 | Fr m patte 370-688 100000 2 77,5003 | 4: 133.0318 agm atchi atchi ern r RT: 0.24 - 0 200.0000] 78.5004 79. | ent ing natc 0.75 AV: 7 | 2.0E5 1.0E5 0 4.0E5 2.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 | #4 |
| 3.0E5 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_tMS2_Day 4.0E6 2.0E6 1.0E6 0.0 0.0 | Left RT: y-3_5-1 G AA: 4 AH: 4 | EIC, Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 10407158 1552400 EIC Gly, | | 2 Aistatu m/z: Apex ISTD QC1 | 1.0E6 3.0E5 4.0E5 2.0E5 0.0 107.0717 RT: 0.38 1MS2_Day-1 3.0E6 4.0E6 4.0E6 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0. | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 ✓ 3_5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 1 1 1 1 1 1 1 1 1 1 1 1 1 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 #4: 78.0436 | 40 4131 F: 100 100 100 100 100 100 100 10 | m/z tope Scan # 2 Day-3 5-1 5 ESI Full n 1 76.2821 #1 | #2 | 4: 133.0318 agm atchi atchi ern r RT: 0.24 - (200.0000) 78.5004 79. | ent ing natc 0.75 AV: 7 | 2.0E5 1.0E5 1.0E5 2.0E5 #2 1.0E5 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 1.0E5 #2 80.9478 80.9478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.0478 80.04788 80.0478 80.04788 80.04788 80.04788 80.04788 80.04788 | #4 • × |
| 3.0E5 2.5E5 2.0E5 1.5E5 1.0E5 5.0E4 0 0.0 m/z: 104.0528 Apex RT: 0.38 Quan Peak QC1_tMS2_Day 4.0E6 2.0E6 1.0E5 5.0E4 0,0 0,0 0,0 0,0 0,0 0,0 0,0 0, | Left RT: y-3_5-1 G AA: 4 AH: 4 | EIC, Met, t 0.5 RT(min) 0.12 Right RT 0.12 Right RT 6.12 Gly, 0.12 Gly, 0.5 0.5 | , • × • × • × | m/z: Apex ISTD QC1_ in/z: | 1.0E6 3.0E5 3.0E5 4.0E5 2.0E5 0,0 107.0717 RT: 0.38 tMS2_Day- 3.0E6 4.0E6 4.0E6 0,0 0,0 0,0 0,0 0,0 0,0 0,0 0, | 2 2 2 2 4 0.5 RT(min) Left RT: 0.13 3 3 5-1 15N,13C-C RT: 0.41 AA: 76971933 AH: 7980625 4 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 | H ₃ -M(Right RT: Sly m/z: 78 | et, tM | S2 All Isotopes Multi-Isotopes #1: 76.0393 #2: 77.0363 #3: 77.0427 #4: 78.0436 | #131 F: 100 #131 F: 100 for the second secon | m/z tope Scan #1 76_2821 #1 | #2 | 4: 133.0318 agm atchi atchi ern r RT: 0.24 - 0 200.0000] 78.5004 79. | ent ing natc 0.75 AV: 7 | 2.0E5 1.0E5 0 4.0E5 2.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 4.0E5 | #4 |

Conclusions

- 12 amino acids and 13 acylcarnitines were quantified from DBS in the ClinSpot LC-MS/MS Complete Kits, Amino Acids and Acylcarnitine, using a FIA-HRAM-MS/MS method.
- The method showed good accuracy and precision measurements that are comparable to those values quantified from the TSQ Quantis MD MS.
- Orbitrap MS provided high mass accuracy detection, full-MS spectra over the m/z ranges of common metabolites, and complete MS² spectra to increase the analyte identification confidence and improve the detection accuracy.

References

1. Guo, J., et. al. Thermo Fisher Scientific, 2023. TN001293

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