

## SUPPORTING INFORMATION

### Four-Dimensional Lipidomic Analysis Using Comprehensive Online UHPLC×UHPSFC/MS/MS

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Czech Republic*

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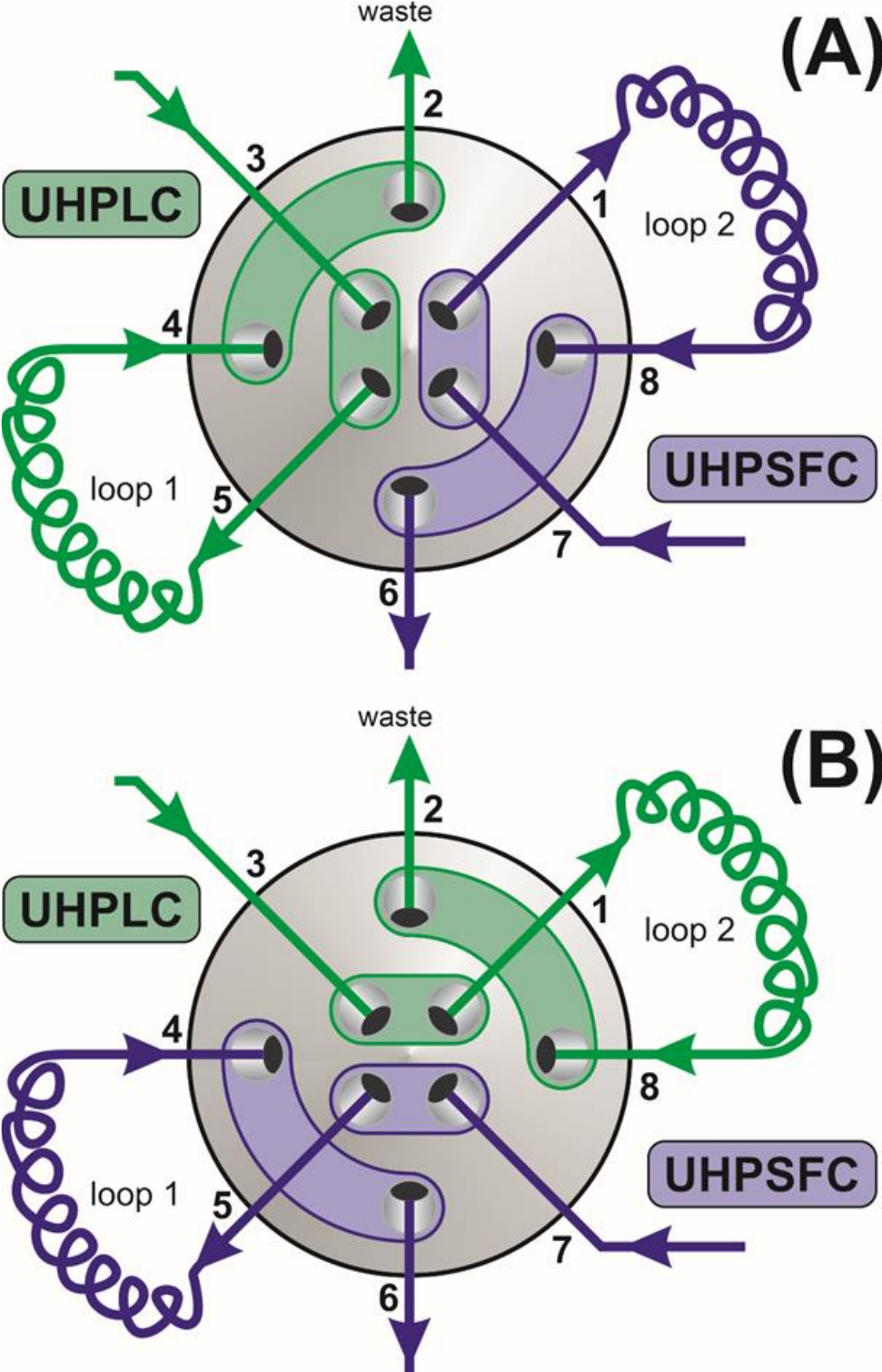
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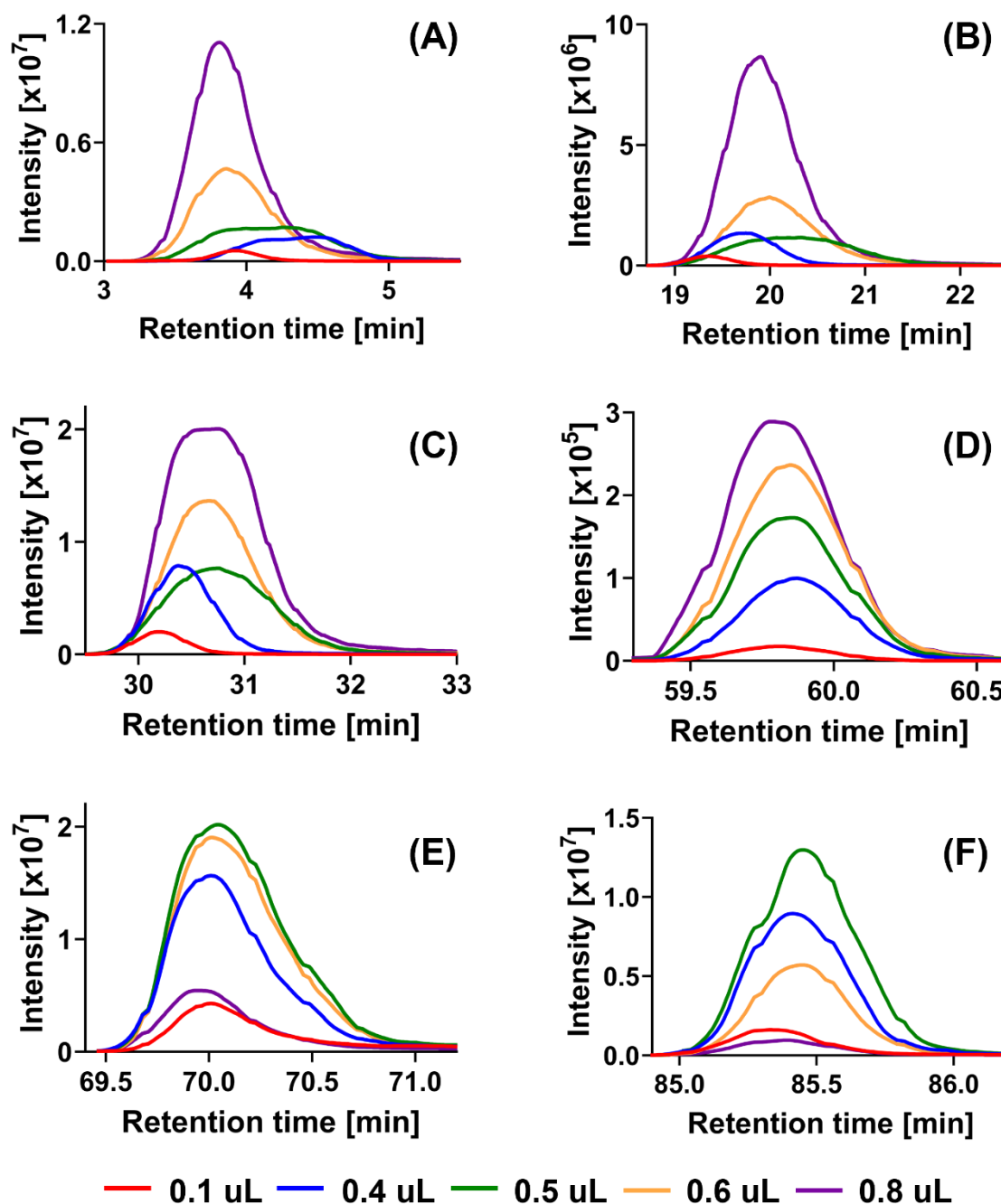
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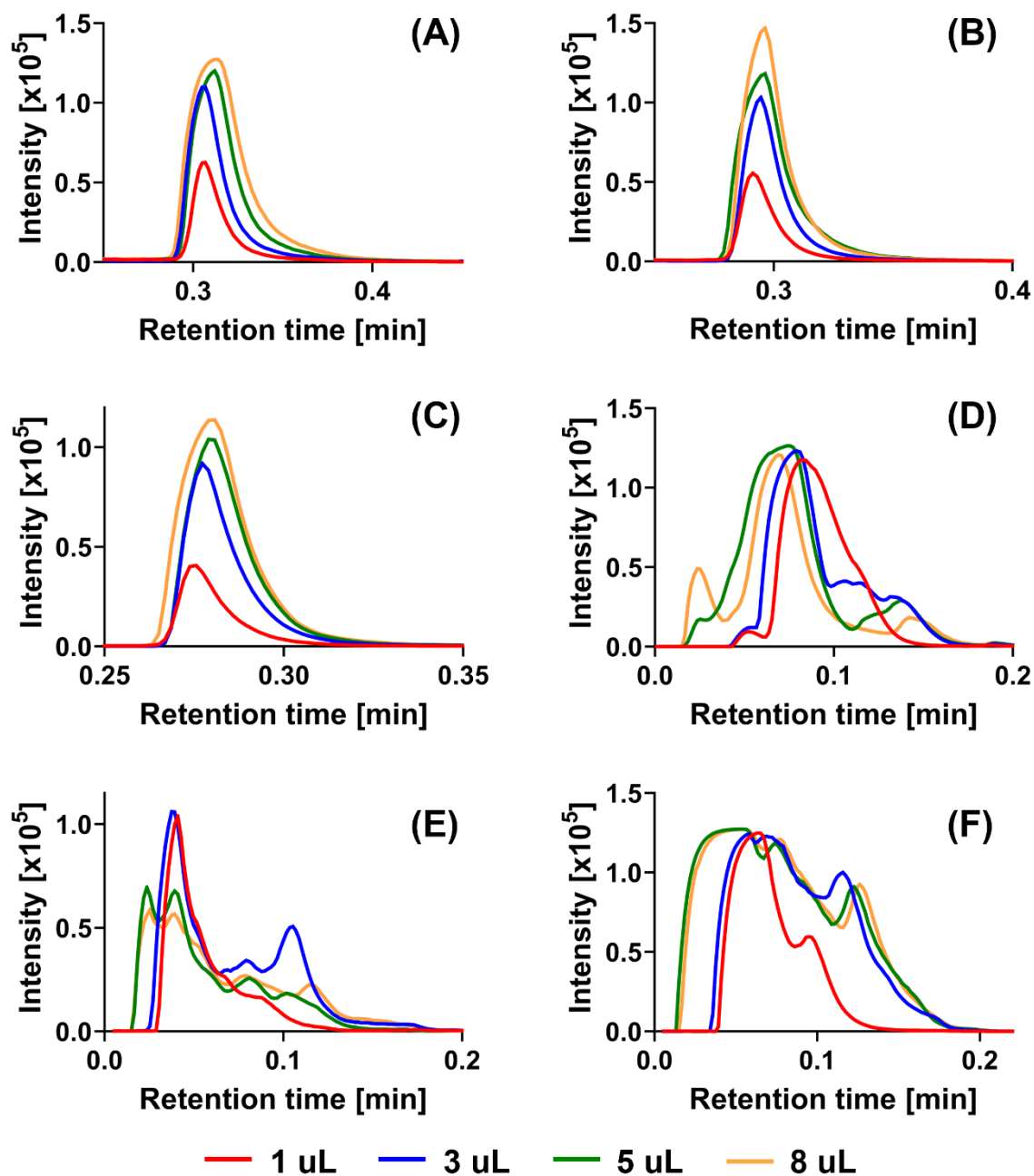
**Figure S1.** Two positions of the 2-position/4-port duo valve. (A) - position 1→7; (B) - position 1→3.



**Figure S2.** Effect of injection volume for RP-UHPLC method using YMC Triart C18 column (150×0.5 mm; 1.9 μm) for selected lipid standards: (A) LPC 13:0, (B) SM 18:1;O2/12:0, (C) PC 14:0/14:0, (D) DG 12:0/12:0, (E) CE 19:0, and (F) TG 19:1/19:1/19:1.

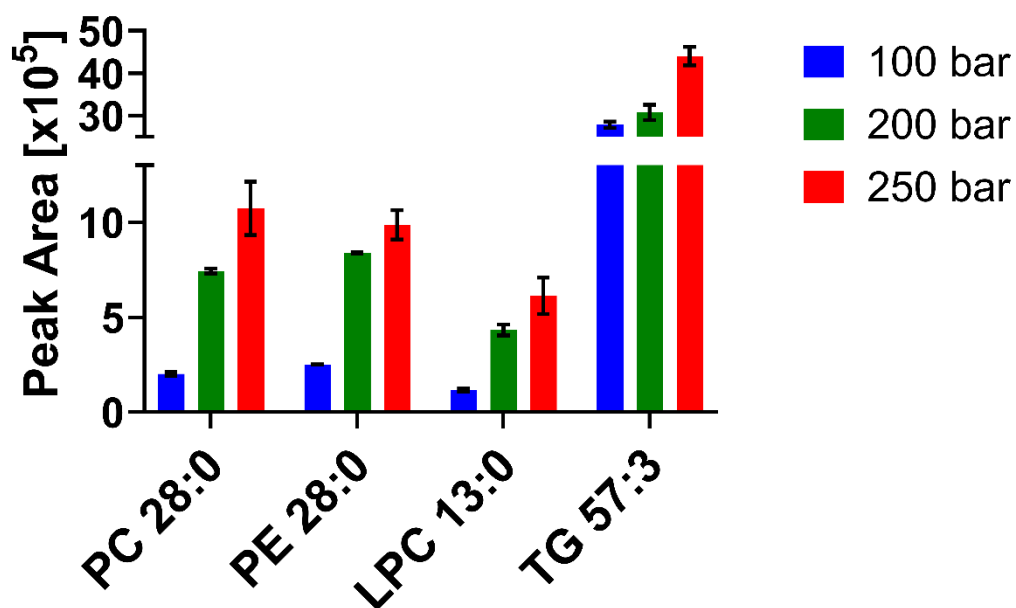


**Figure S3.** Effect of injection volume for UHPSFC method using Reprospher Si column (10×2.1 mm; 1.7 μm) for selected lipid standards: (A) LPC 13:0, (B) SM 18:1;O2/12:0, (C) PC 14:0/14:0, (D) DG 12:0/12:0, (E) CE 19:0, and (F) TG 19:1/19:1/19:1.

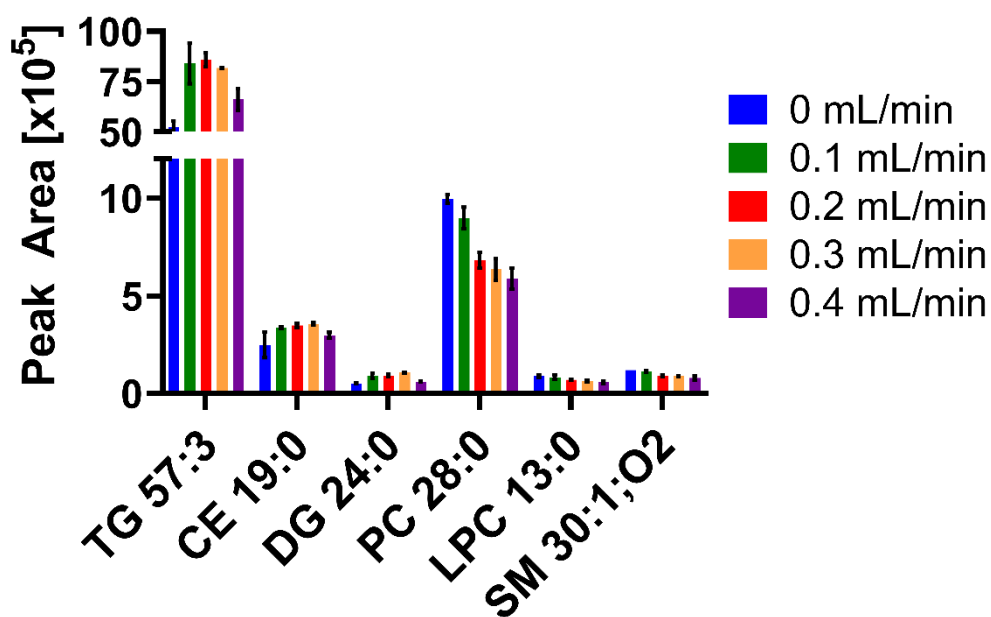


**Figure S4.** Optimization of UHPLC×UHPSFC/MS/MS conditions for selected lipid standards, whereas other standards follow the same trends: (A) UHPSFC back pressure, (B) make-up flow, and (C) ion source capillary voltage. Data are presented as the mean value  $\pm$  SD from three independent experiments.

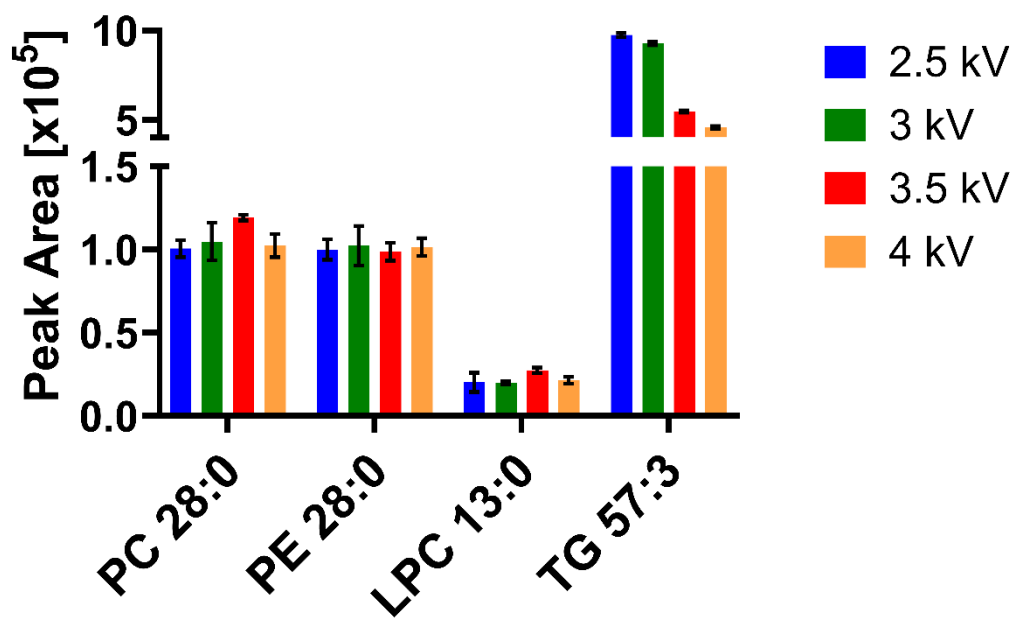
(A)



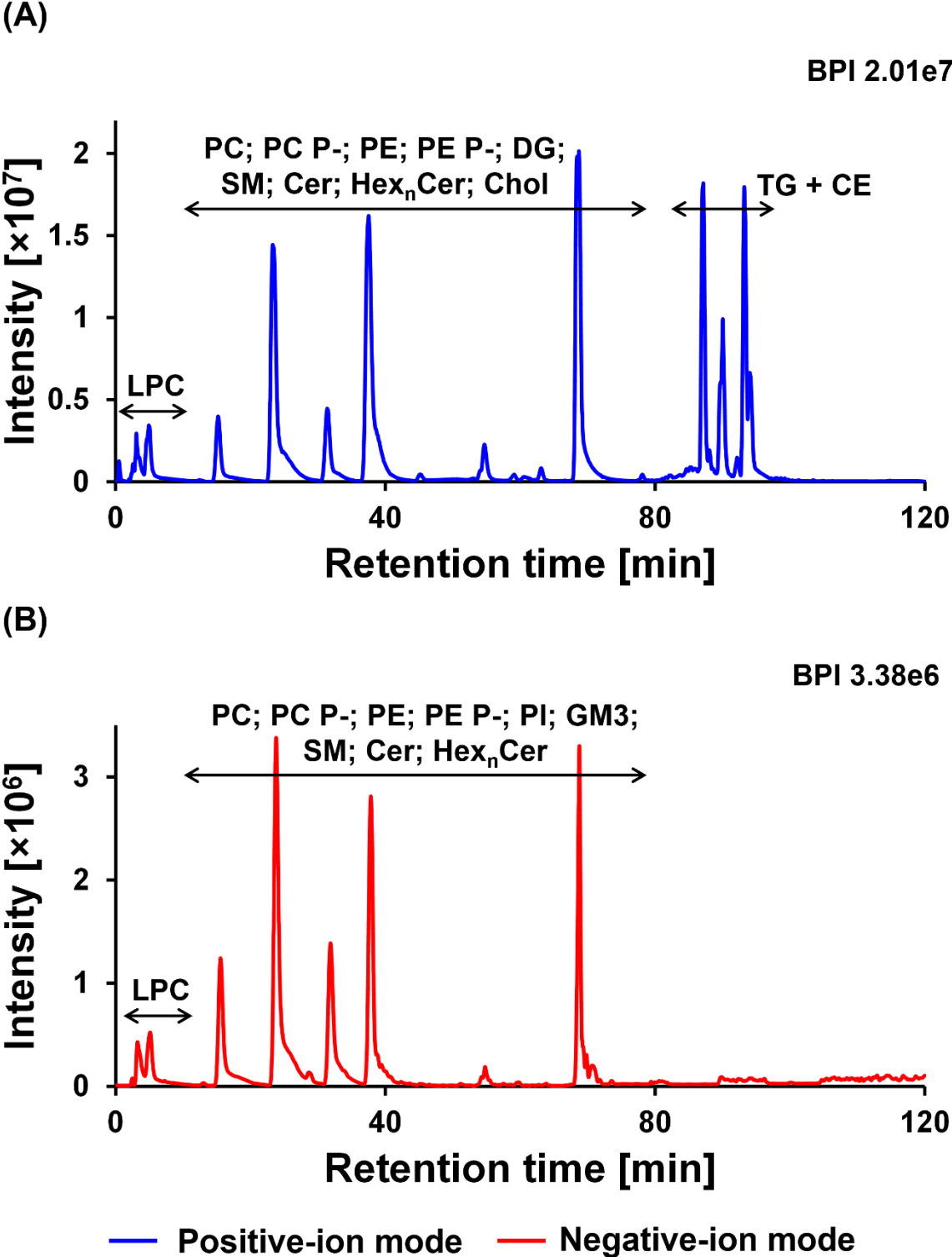
(B)



(C)

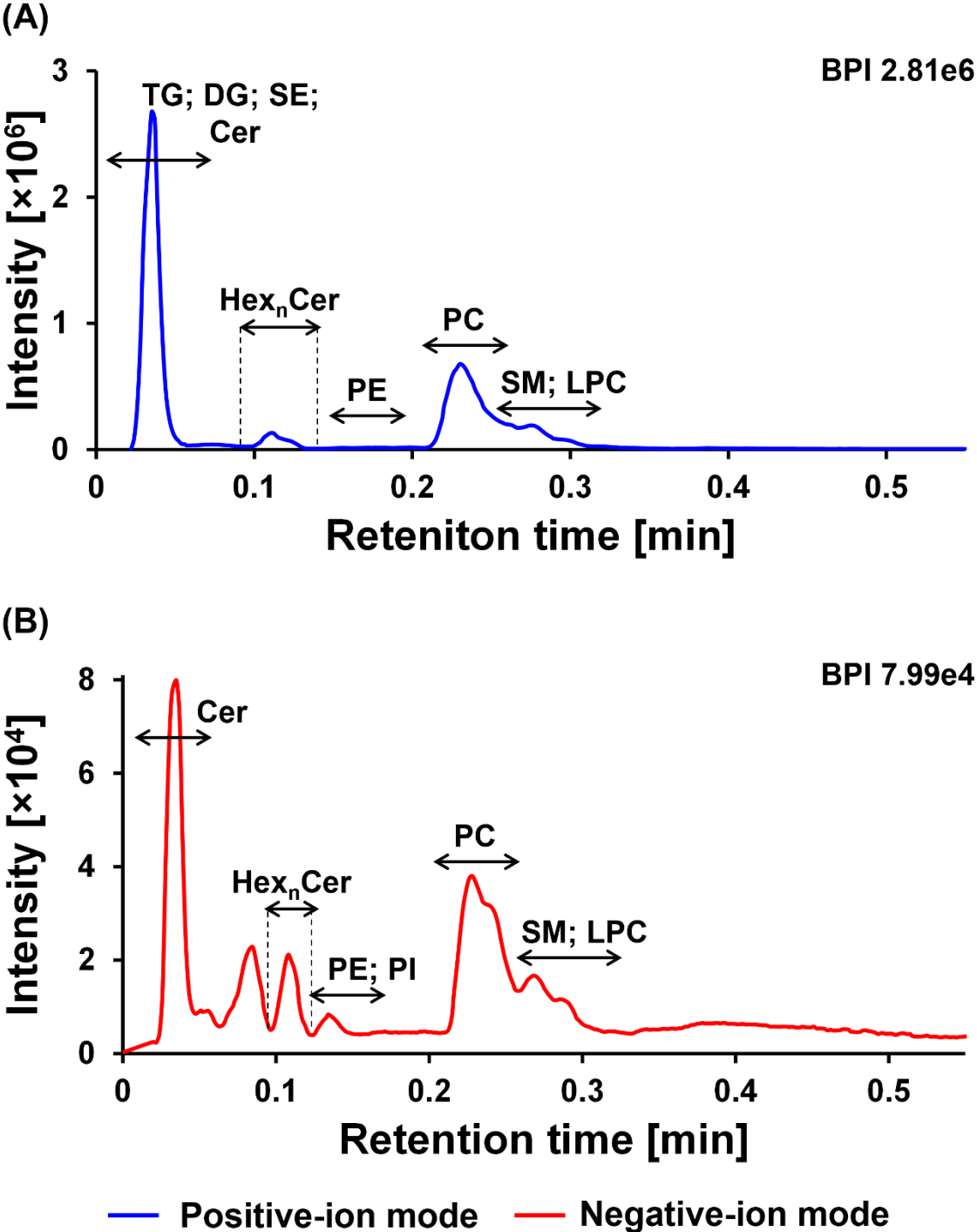


**Figure S5.** Base peak chromatograms of the lipid standard mixture measured by RP-UHPLC/MS in: (A) positive ion mode and (B) negative ion mode. The conditions of analysis are reported in Materials and methods.



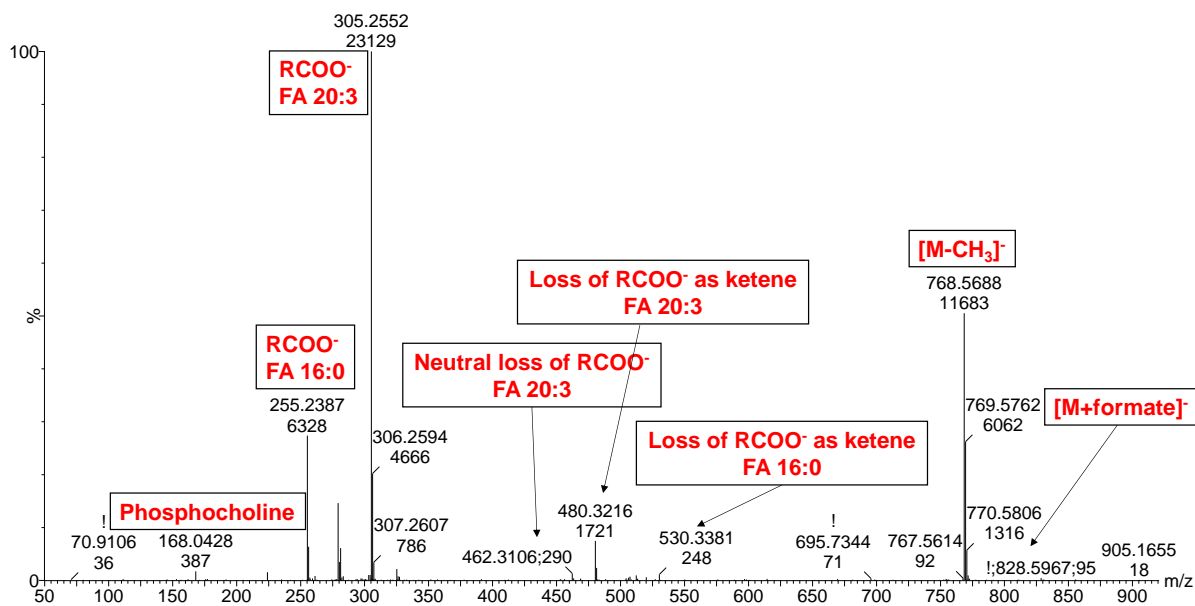


**Figure S6.** Base peak chromatograms of the lipid standard mixture measured by UHPSFC/MS in: (A) positive ion mode and (B) negative ion mode. The conditions of analysis are reported in Materials and methods.

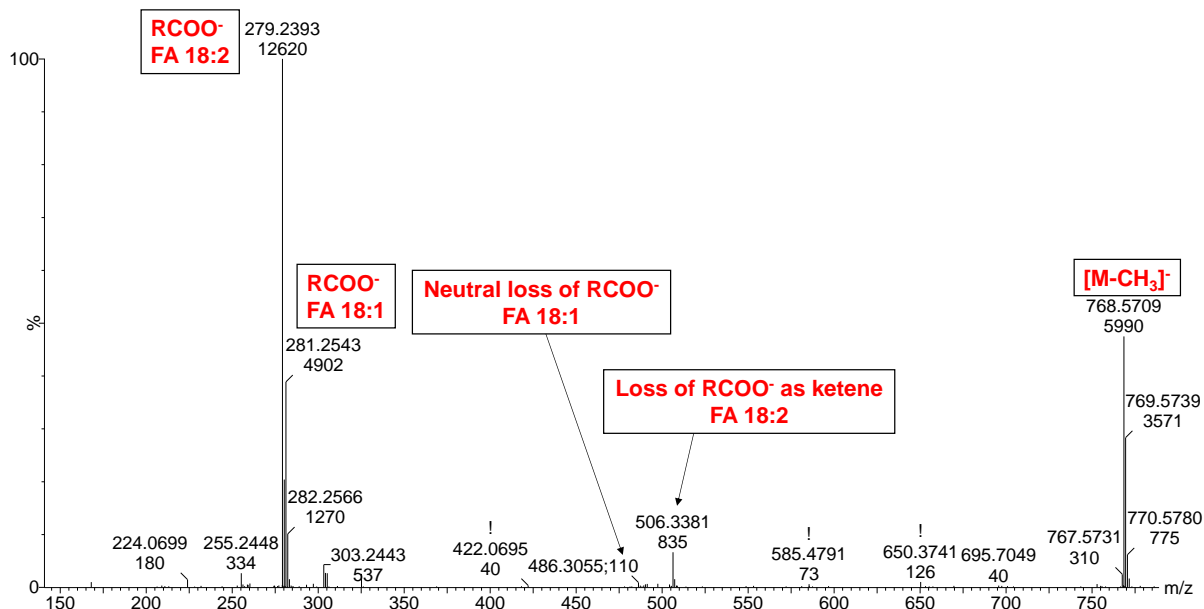


**Figure S7.** Raw annotated tandem mass spectra of selected isobaric molecules

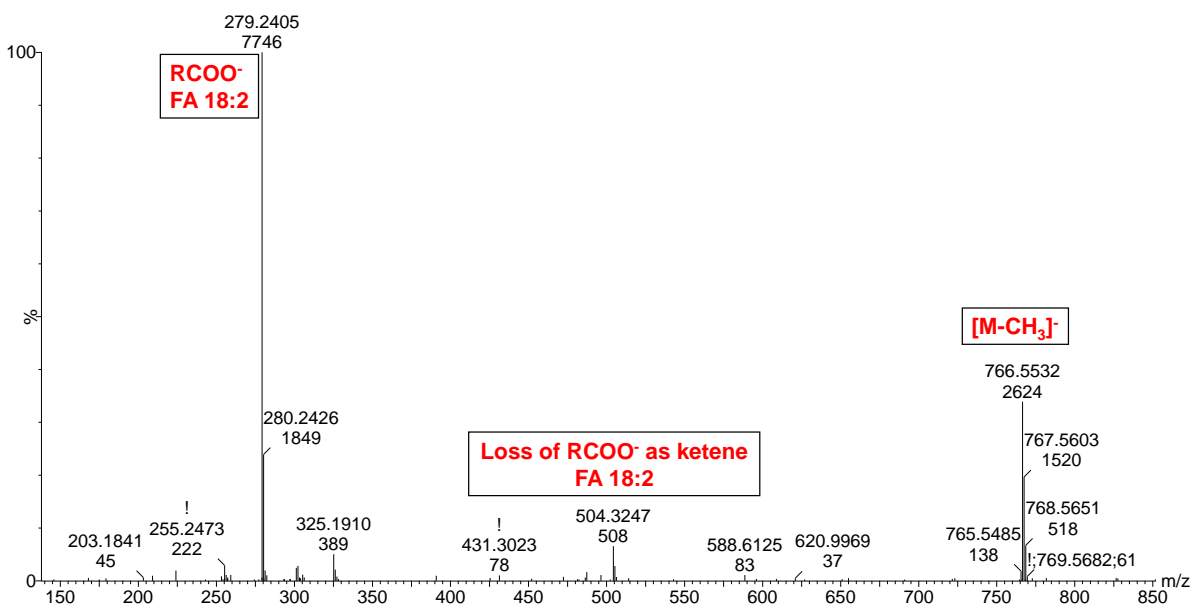
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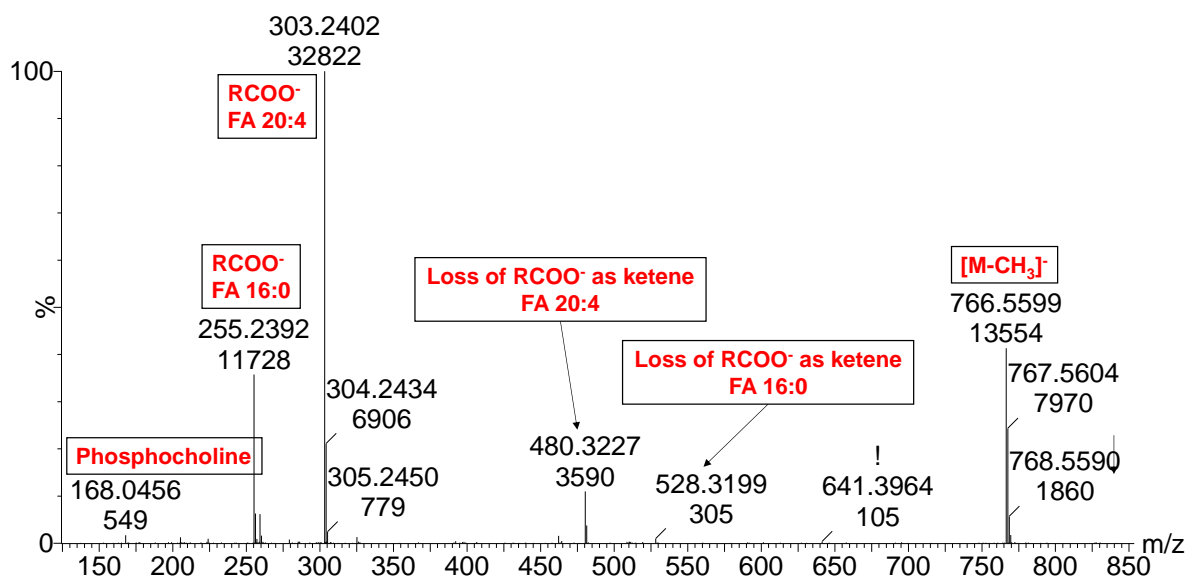
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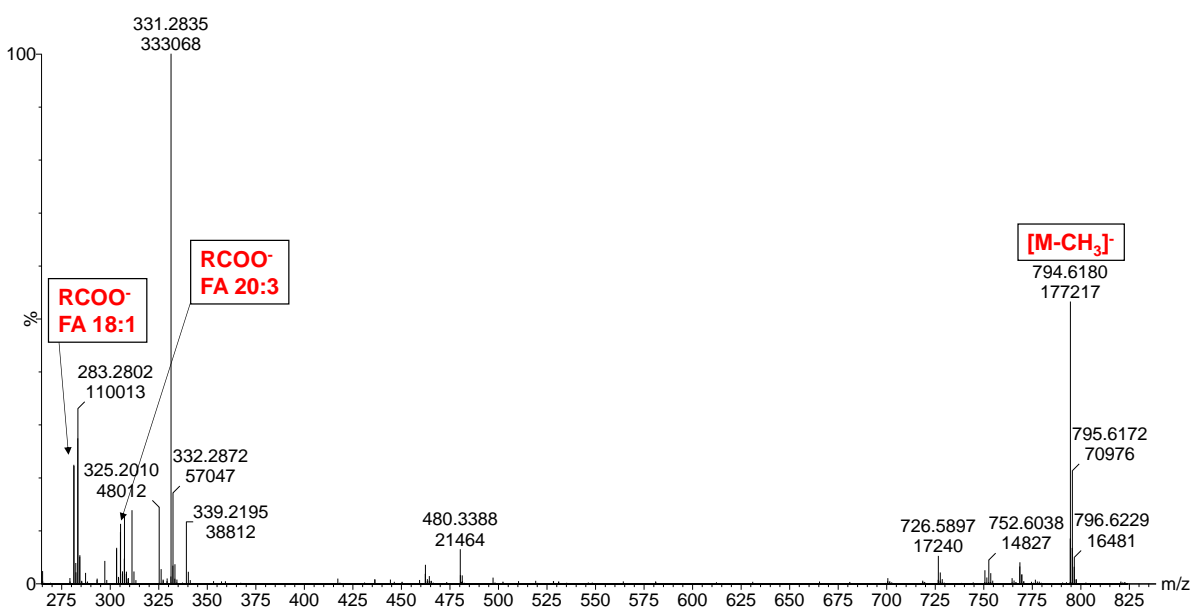
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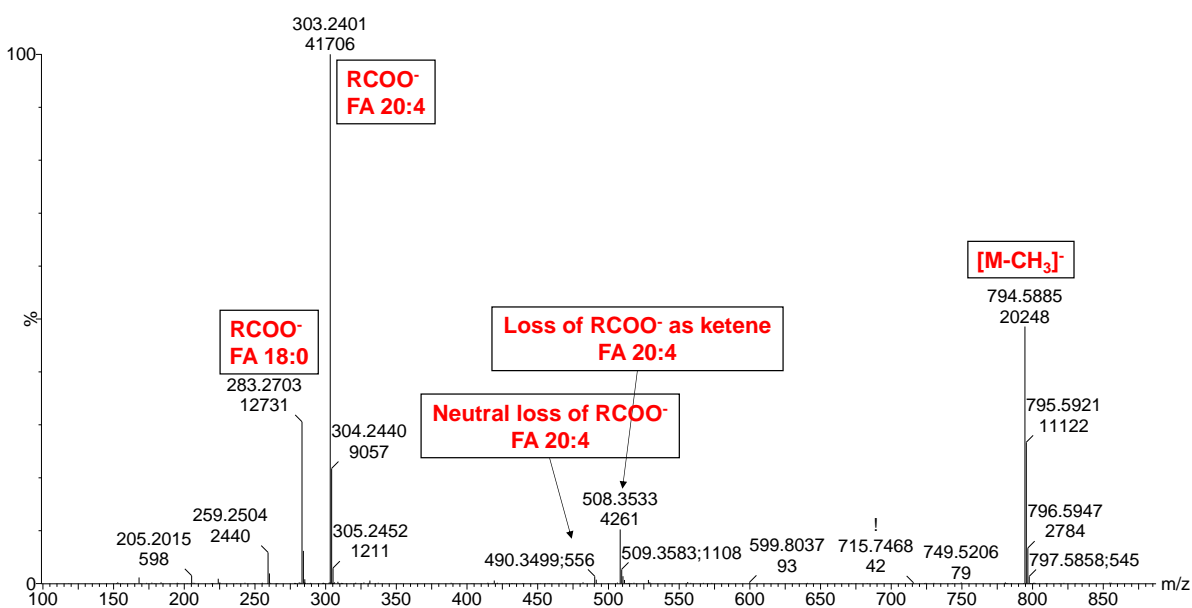
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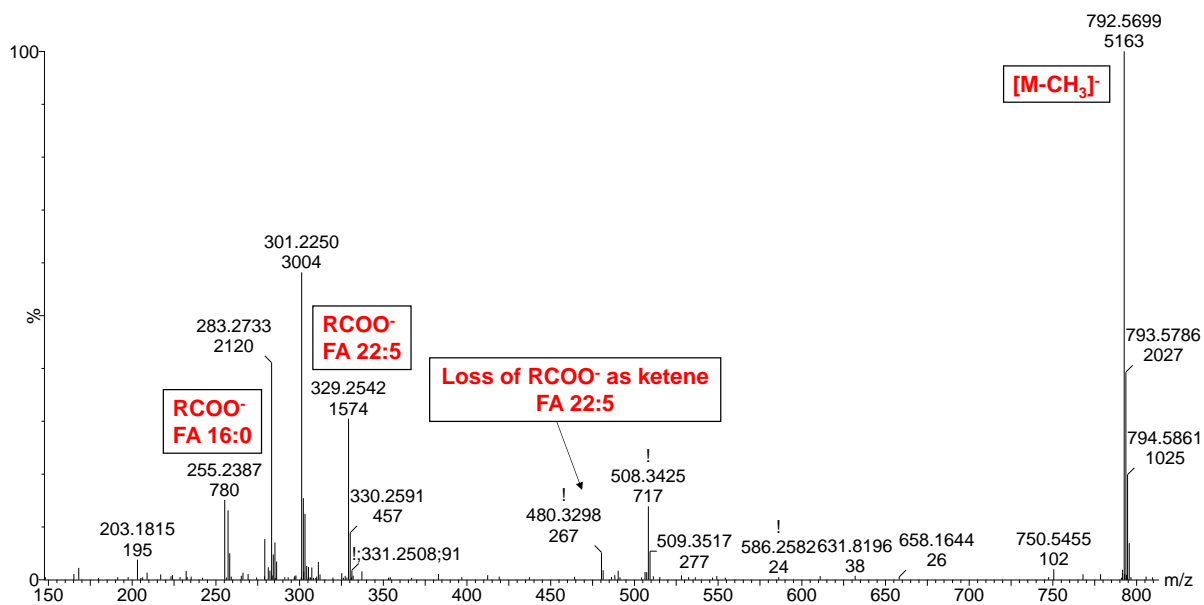
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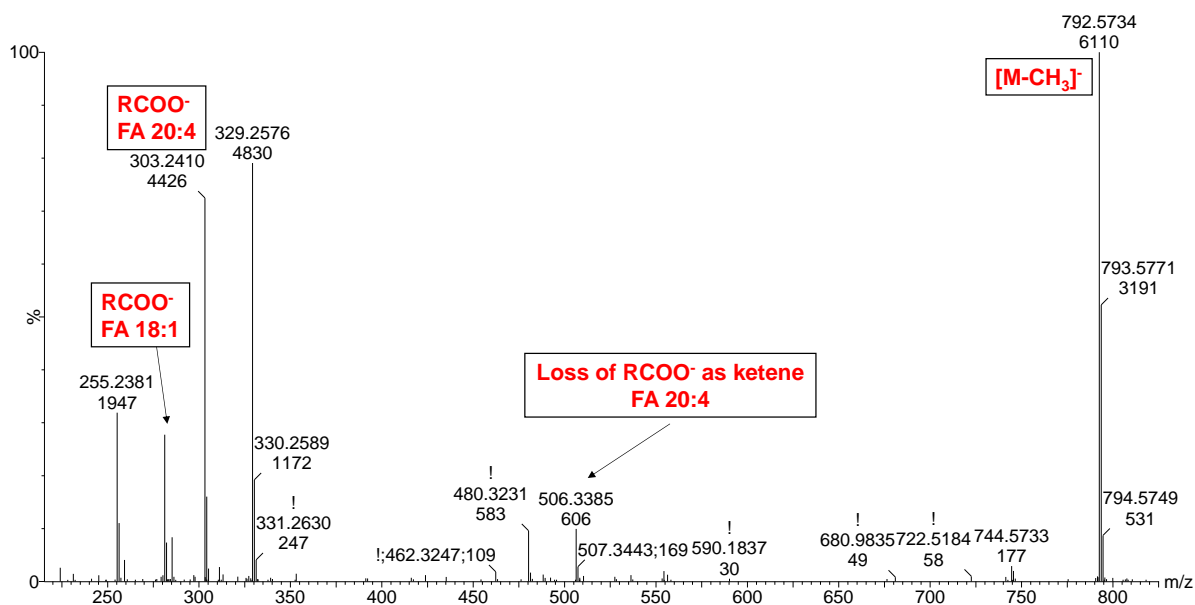
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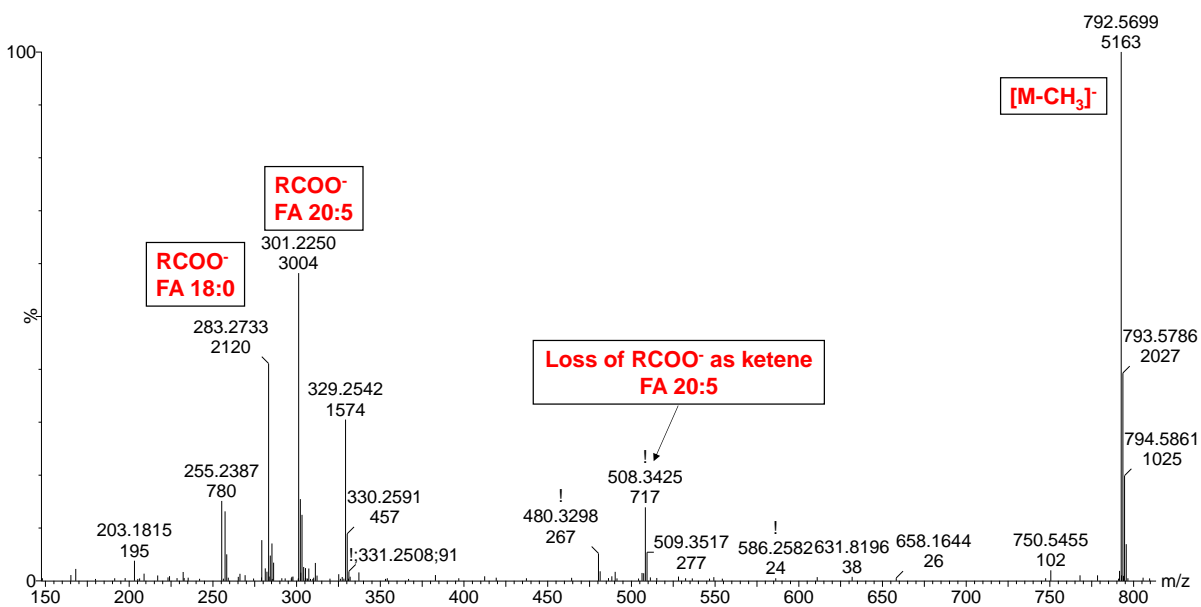
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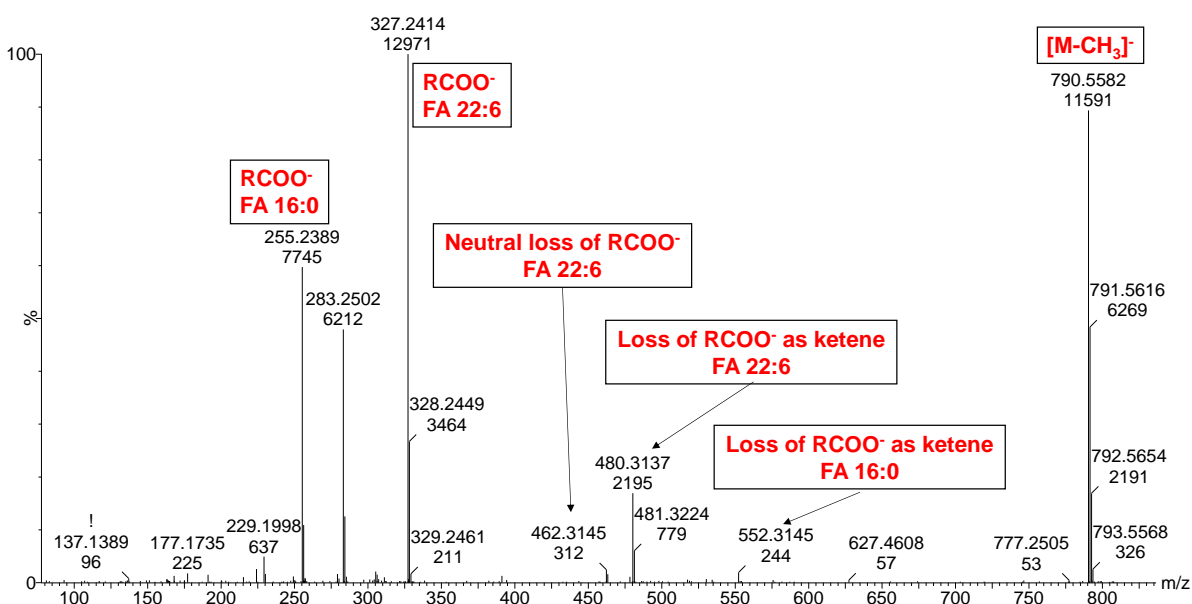
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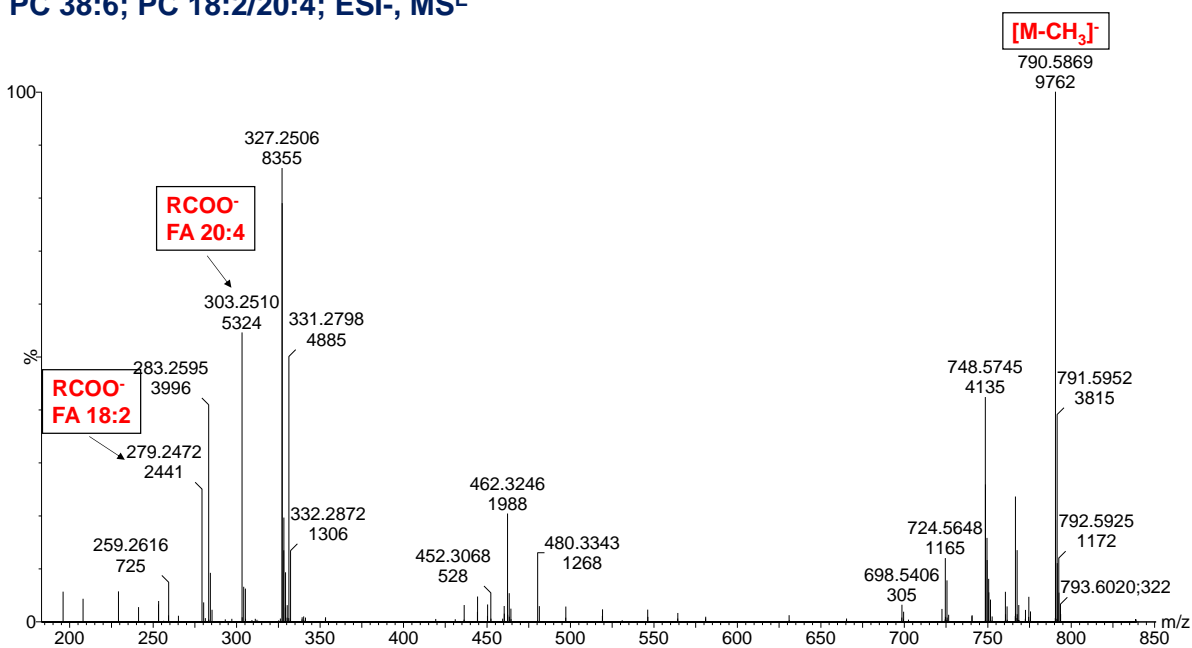
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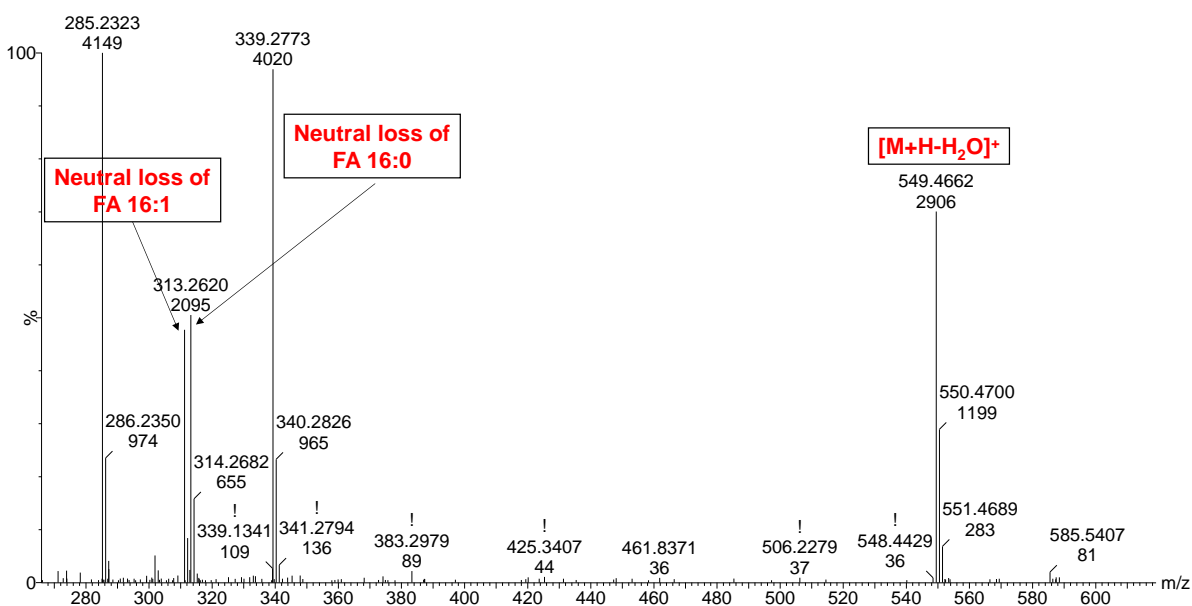
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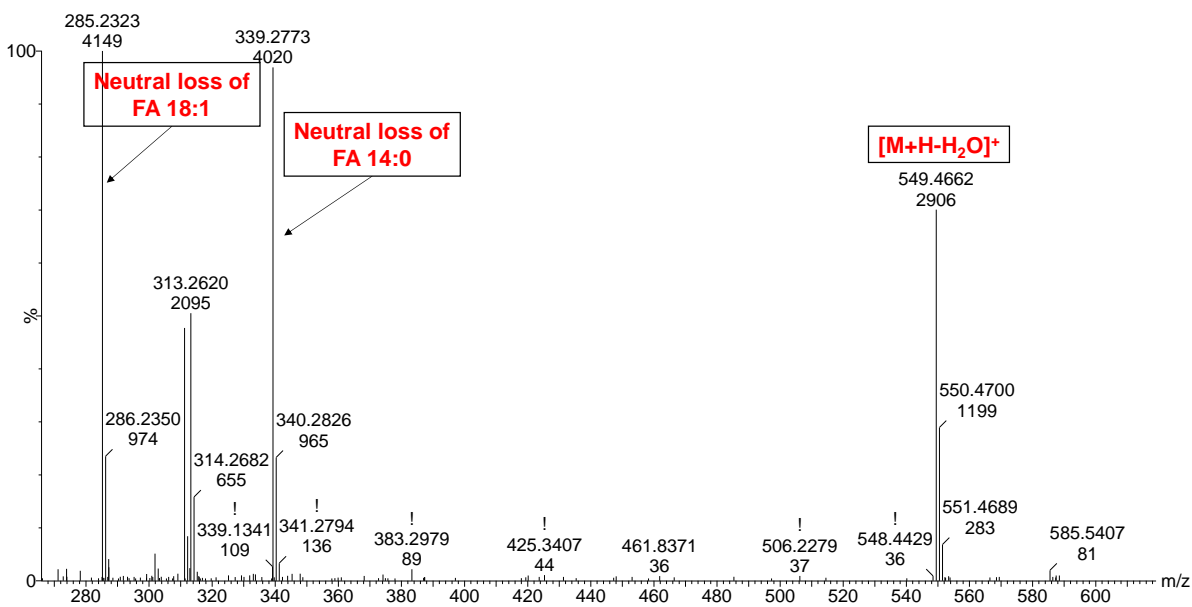
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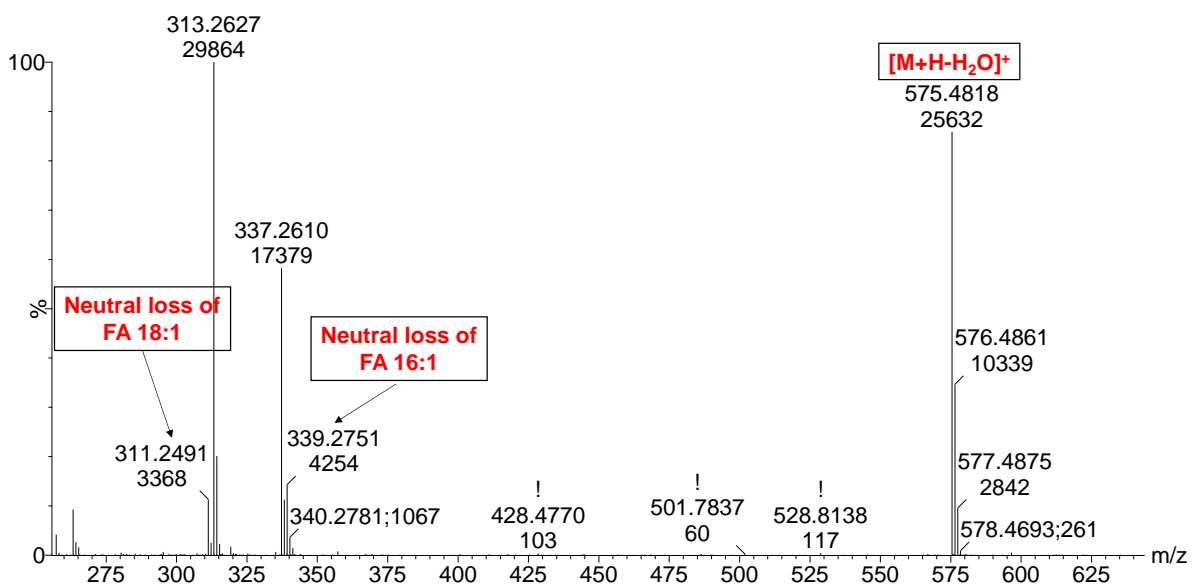
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DG 32:1; DG 18:1\_14:0; ESI+, fast DDA

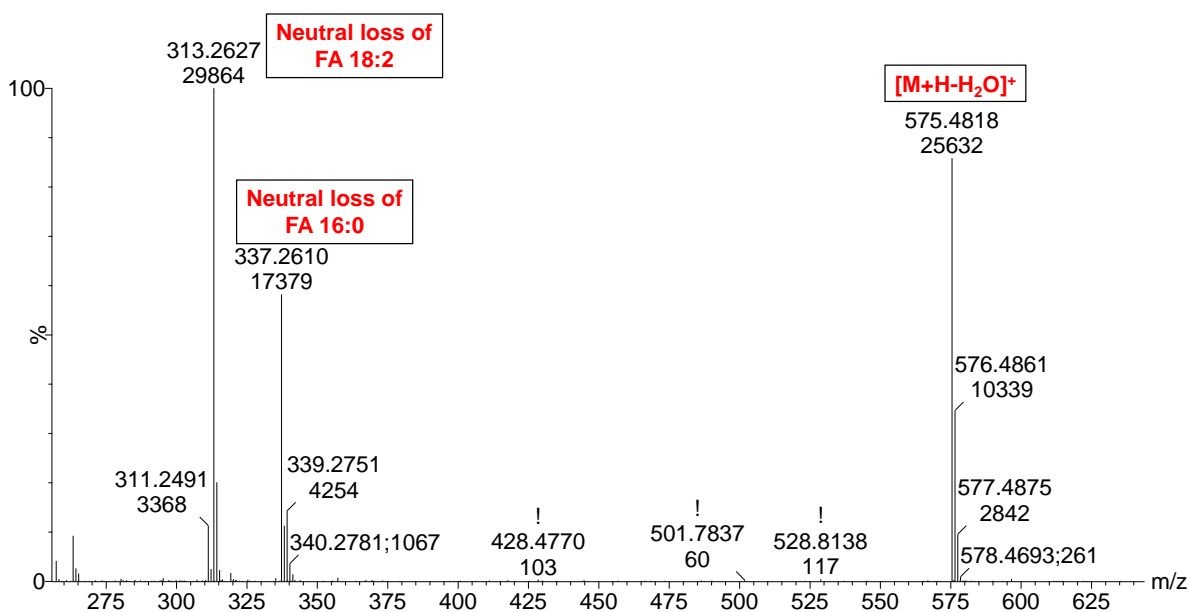


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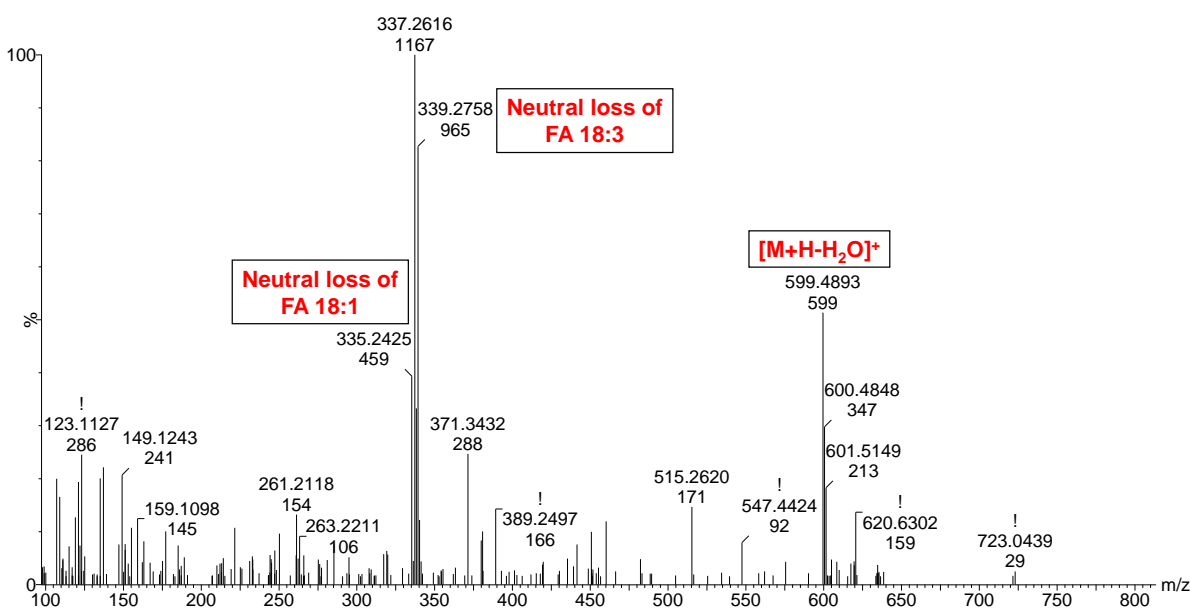




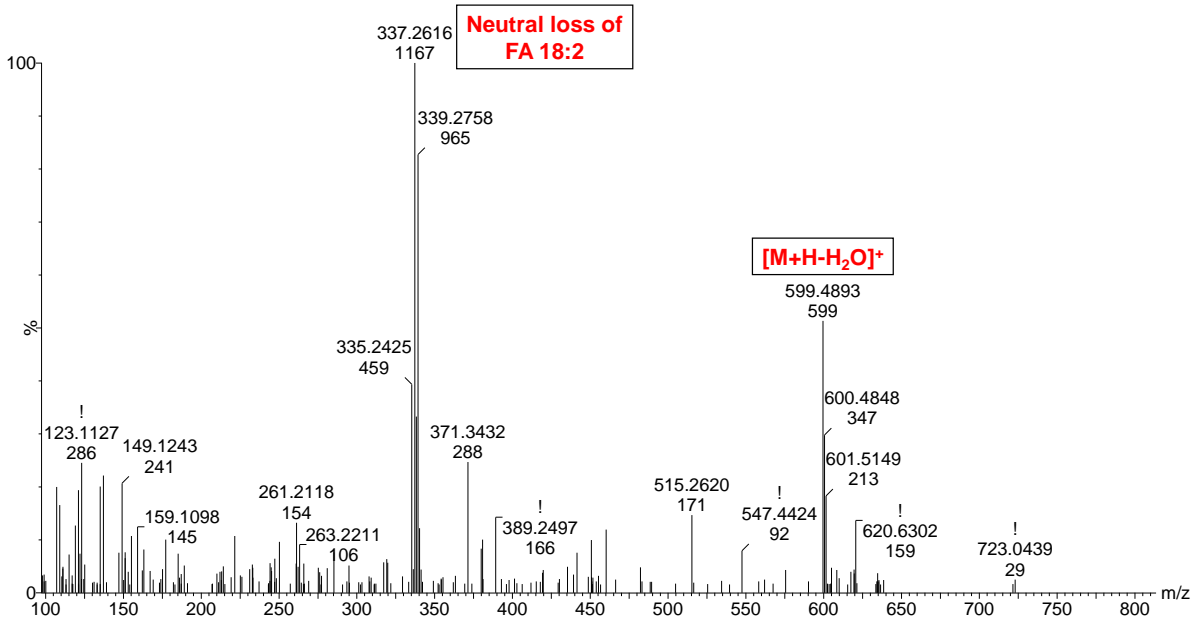
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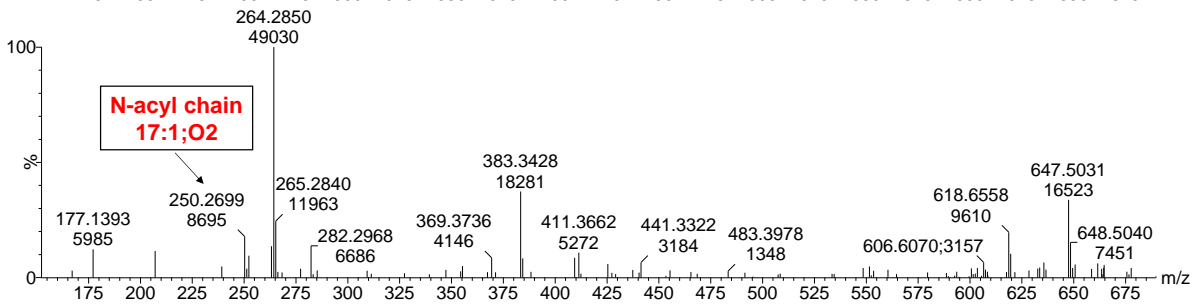
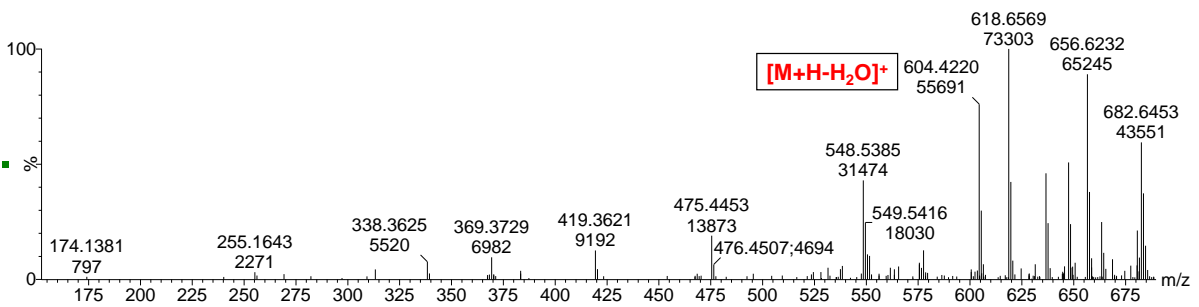
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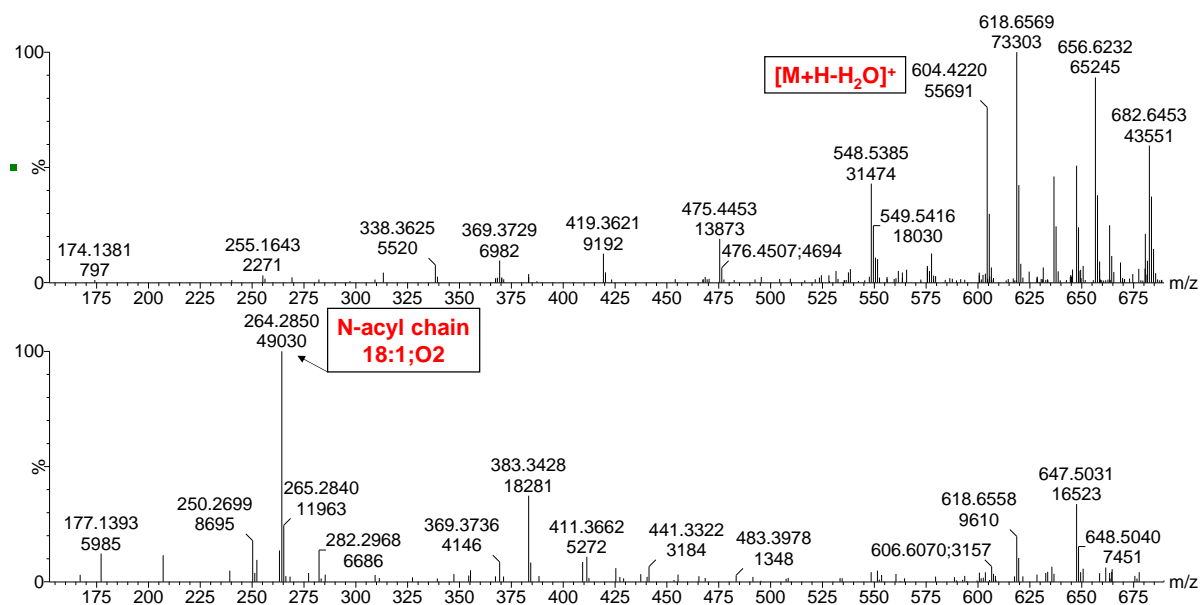
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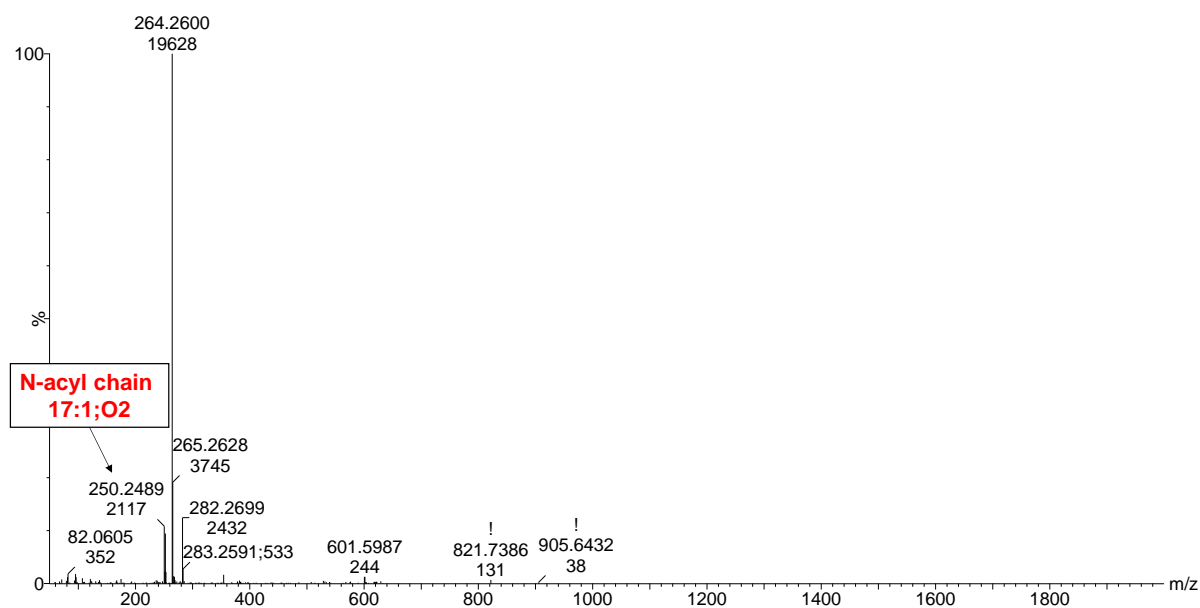
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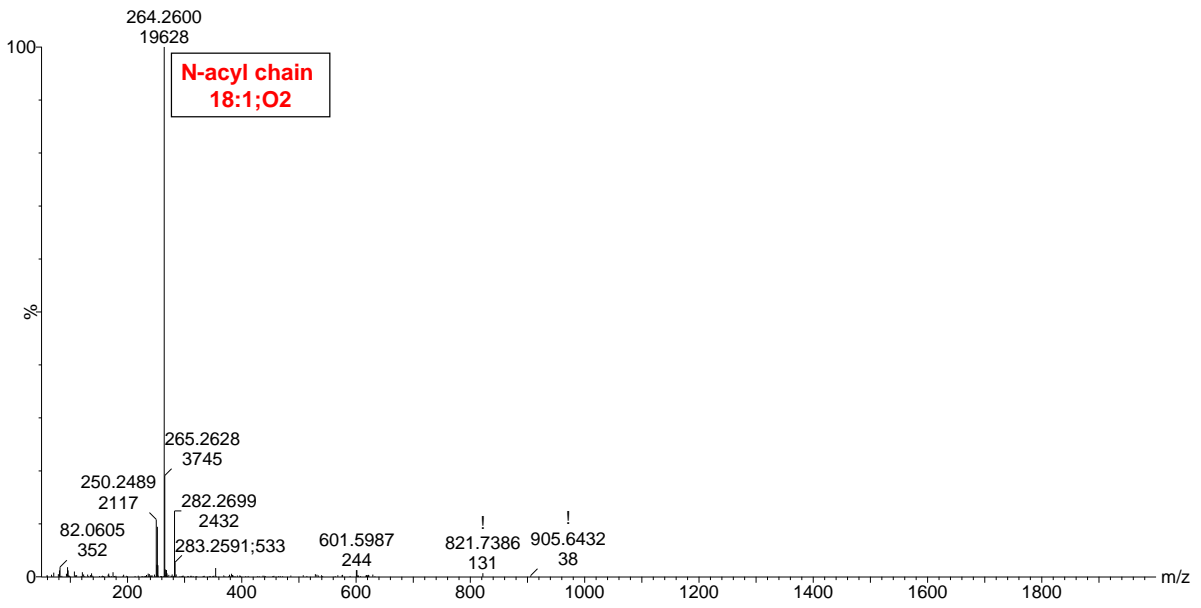
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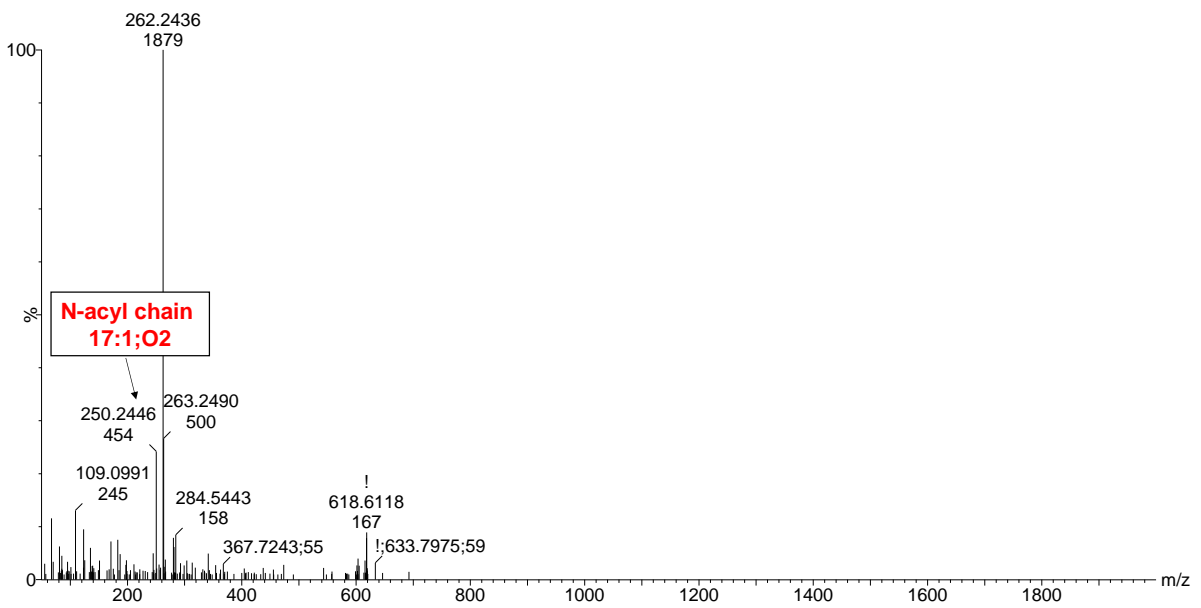
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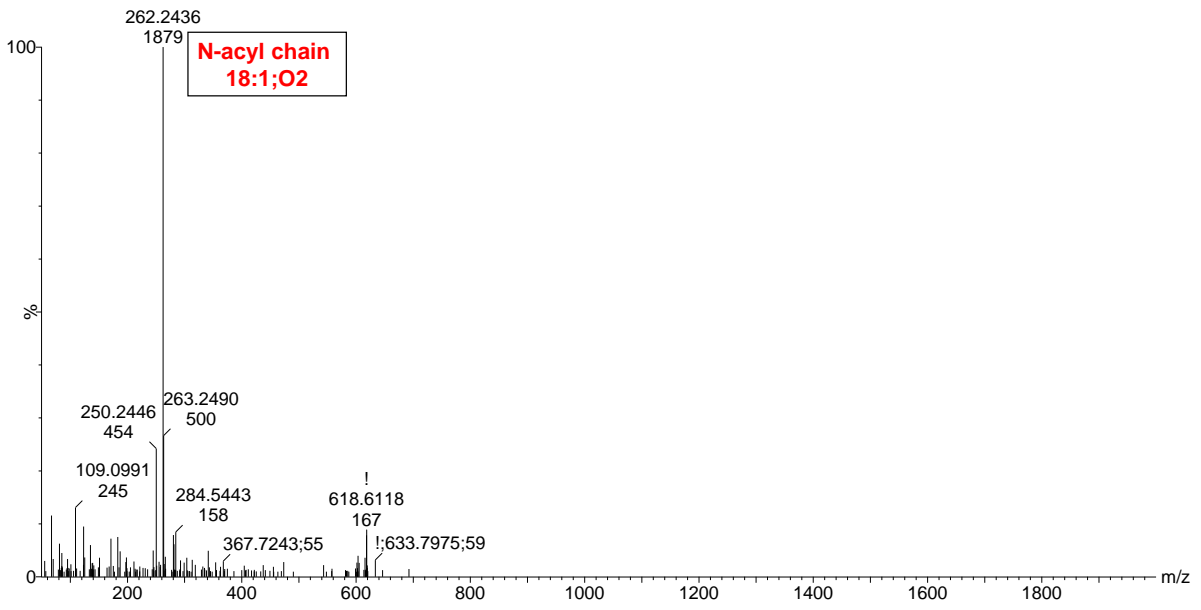
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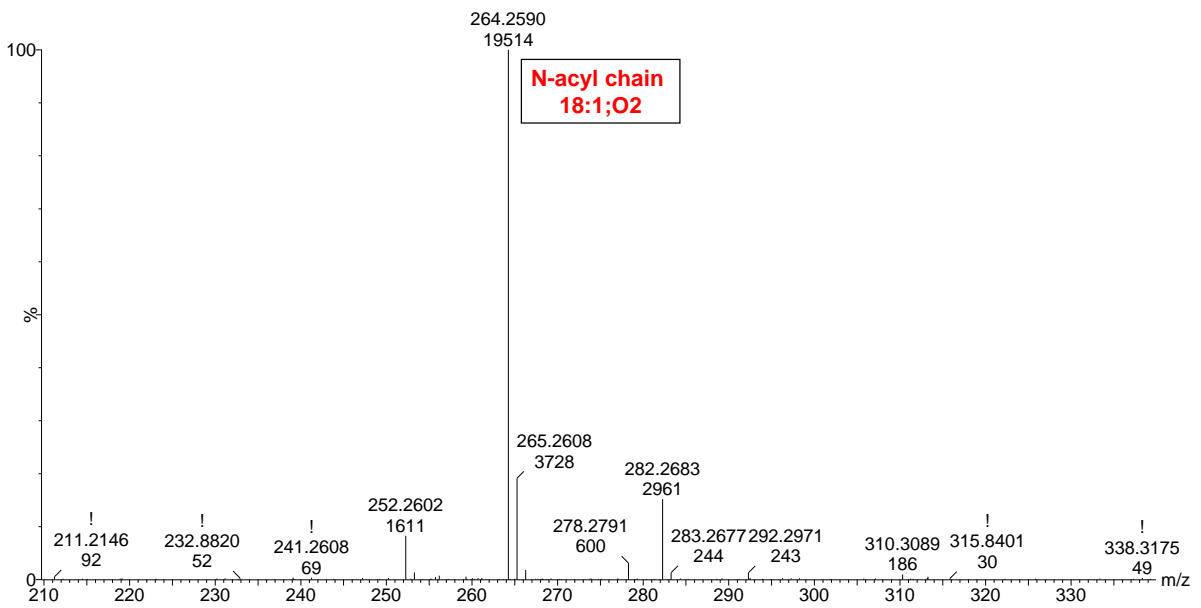
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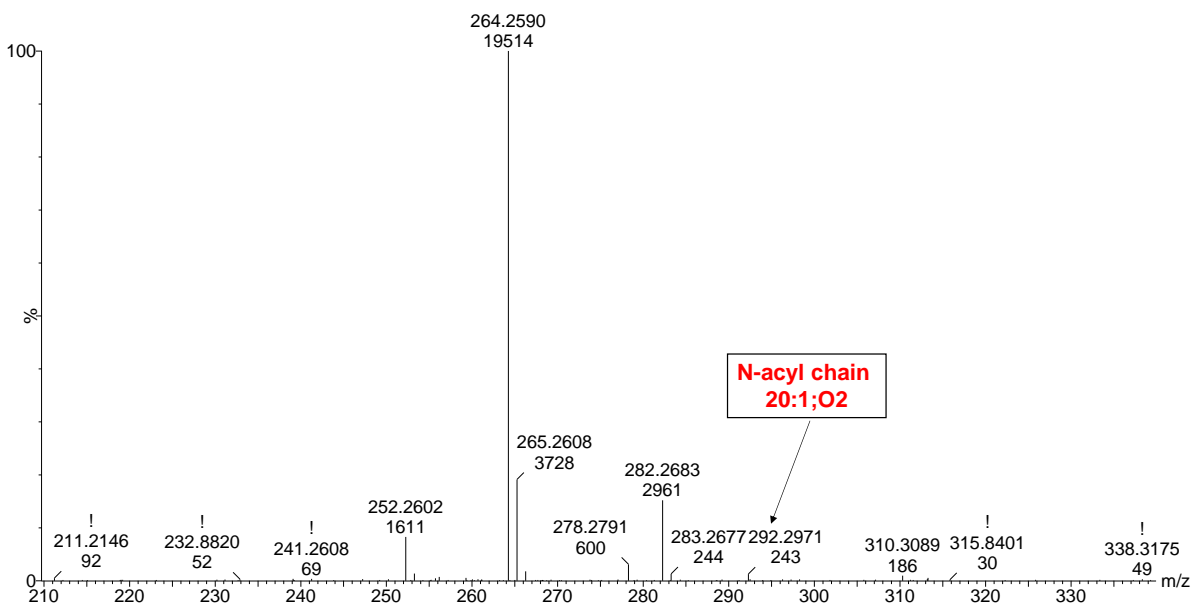
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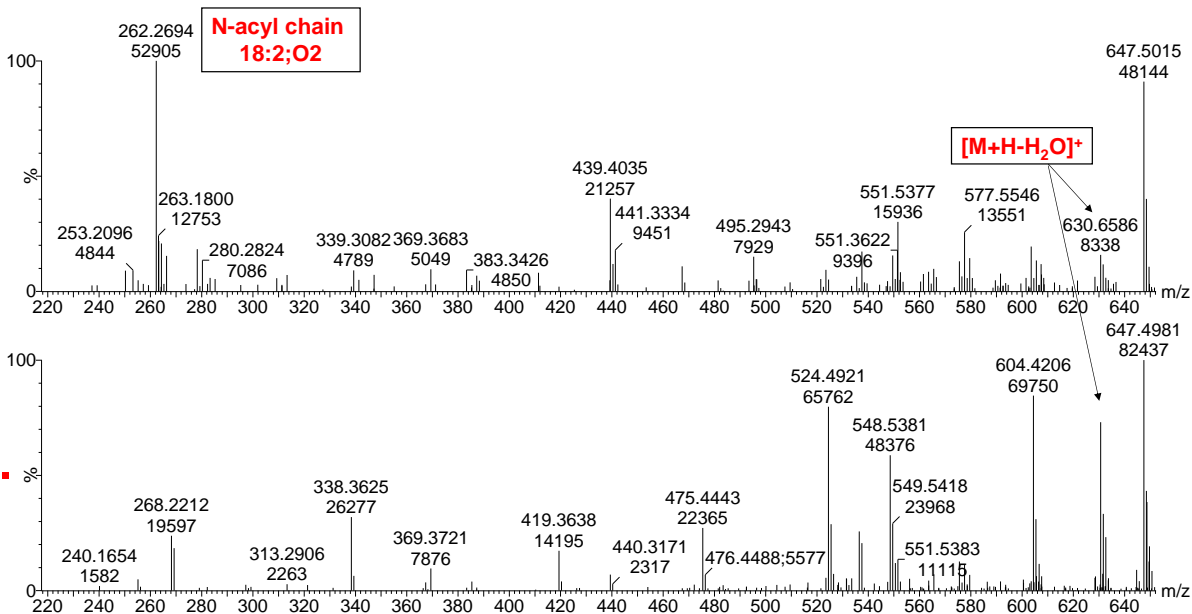
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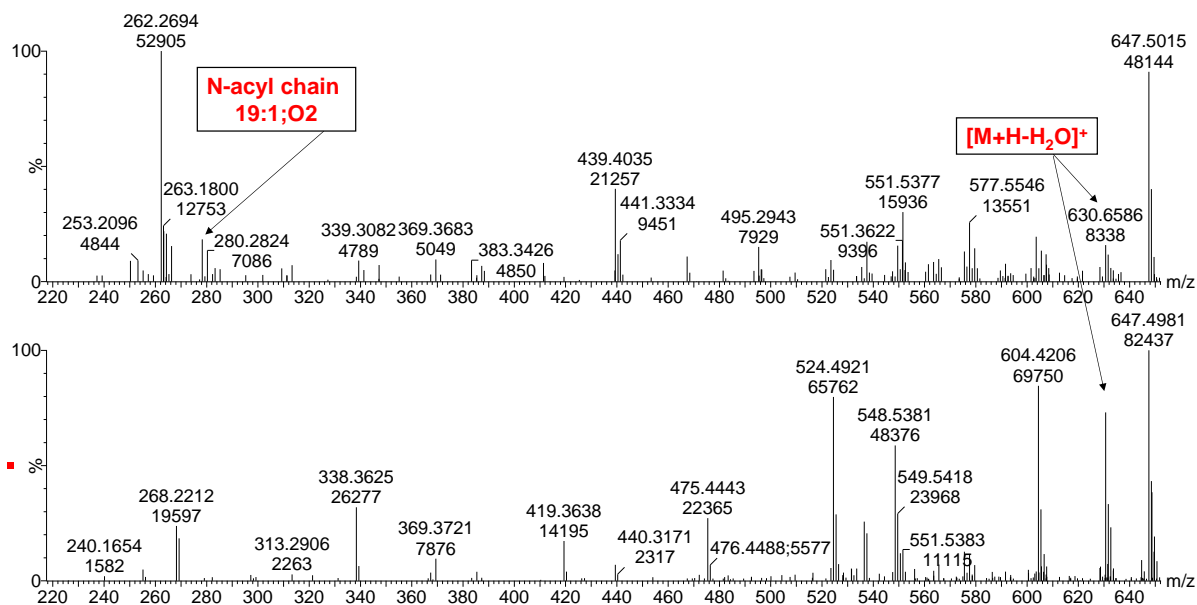
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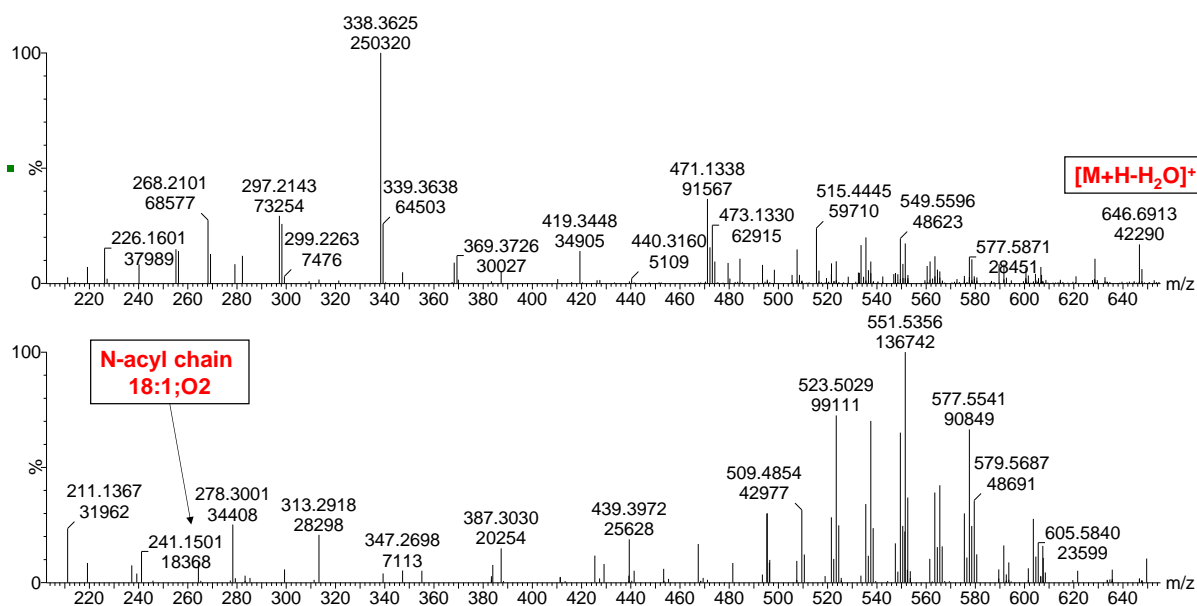
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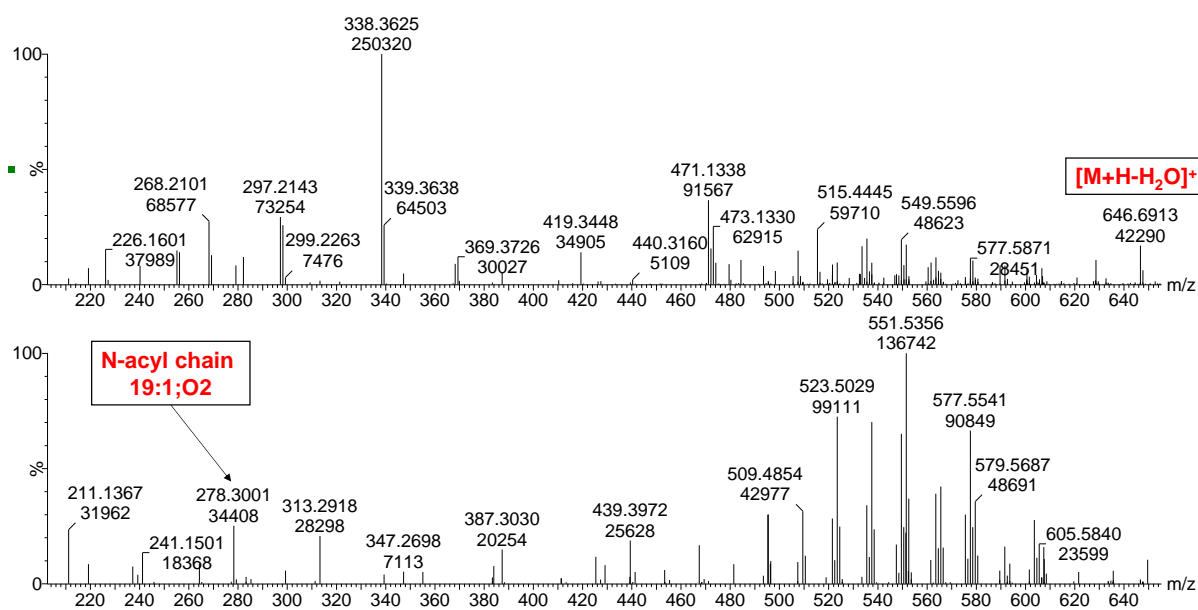
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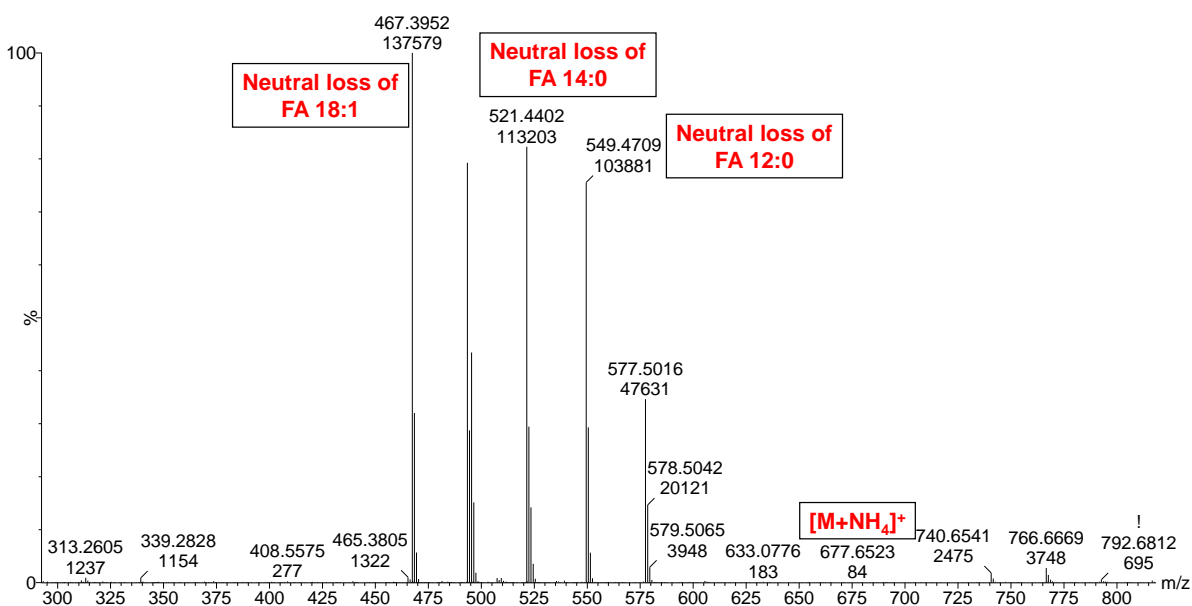
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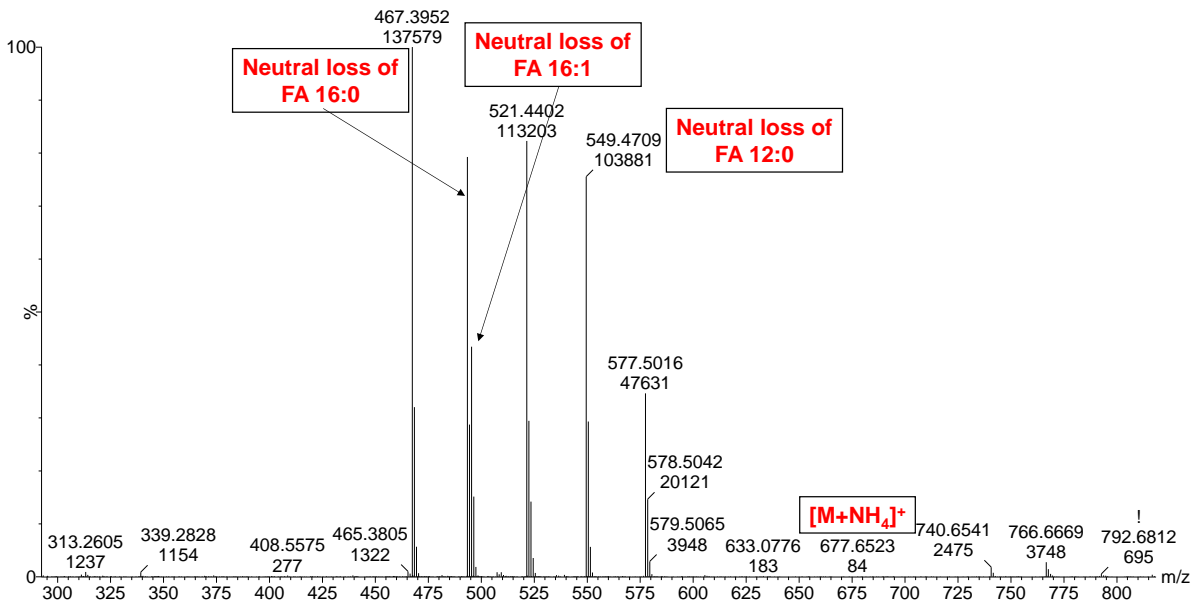


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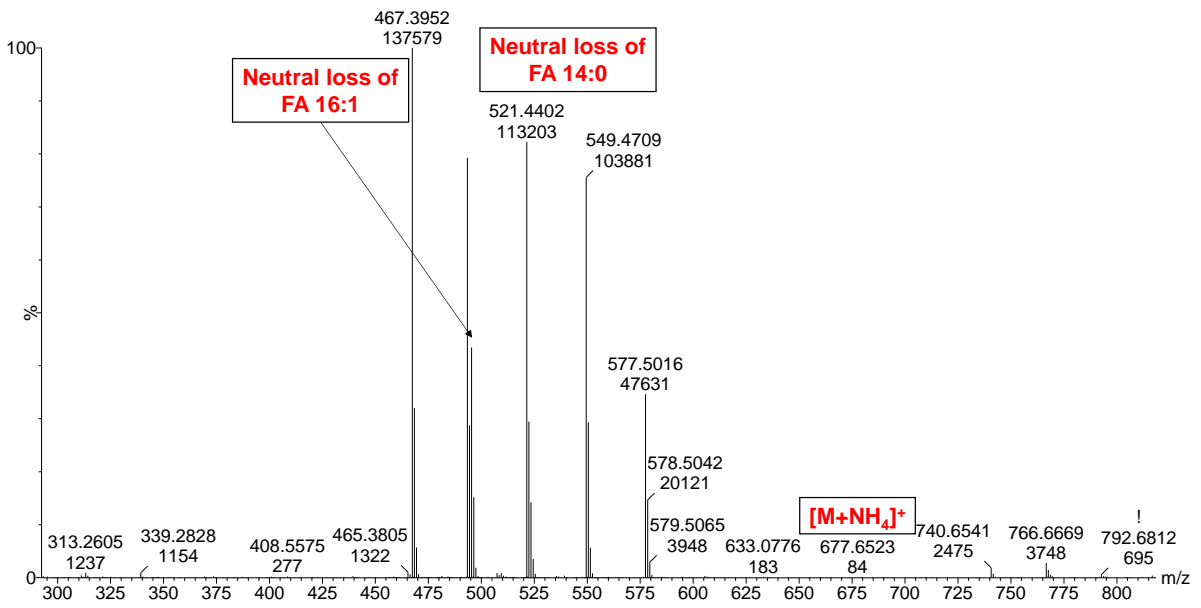




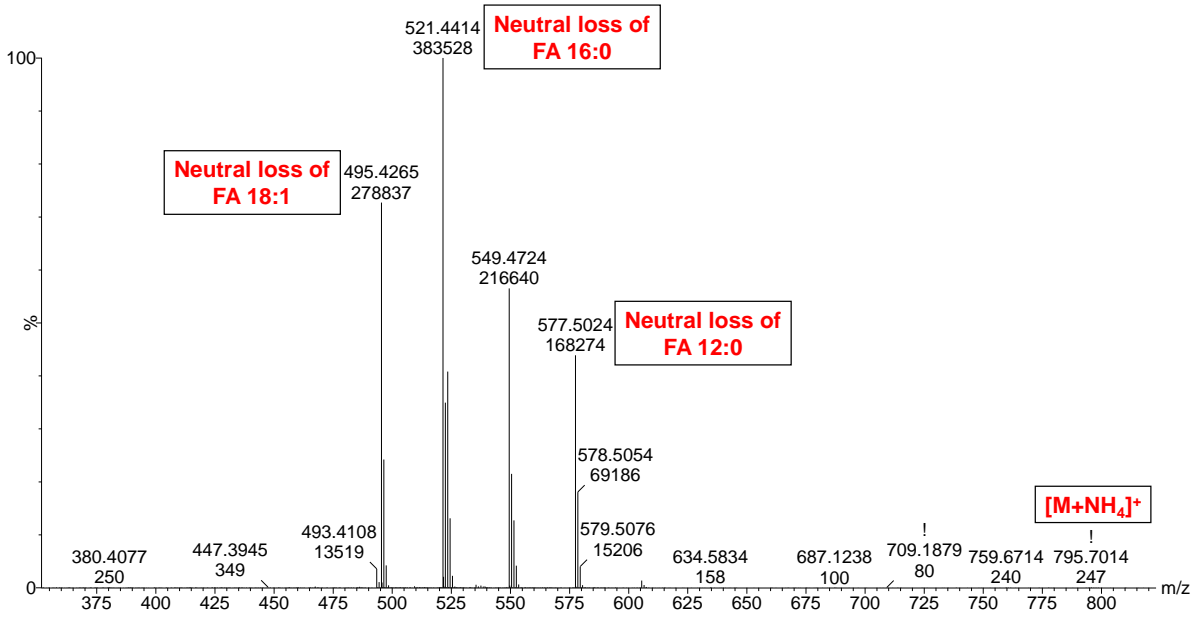
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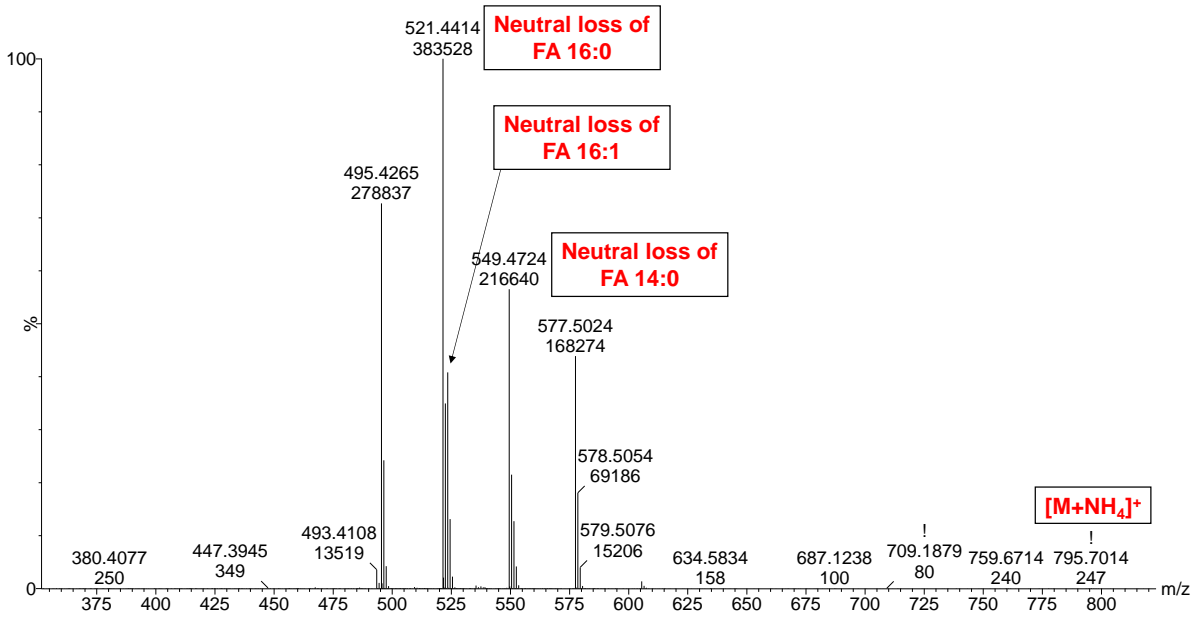
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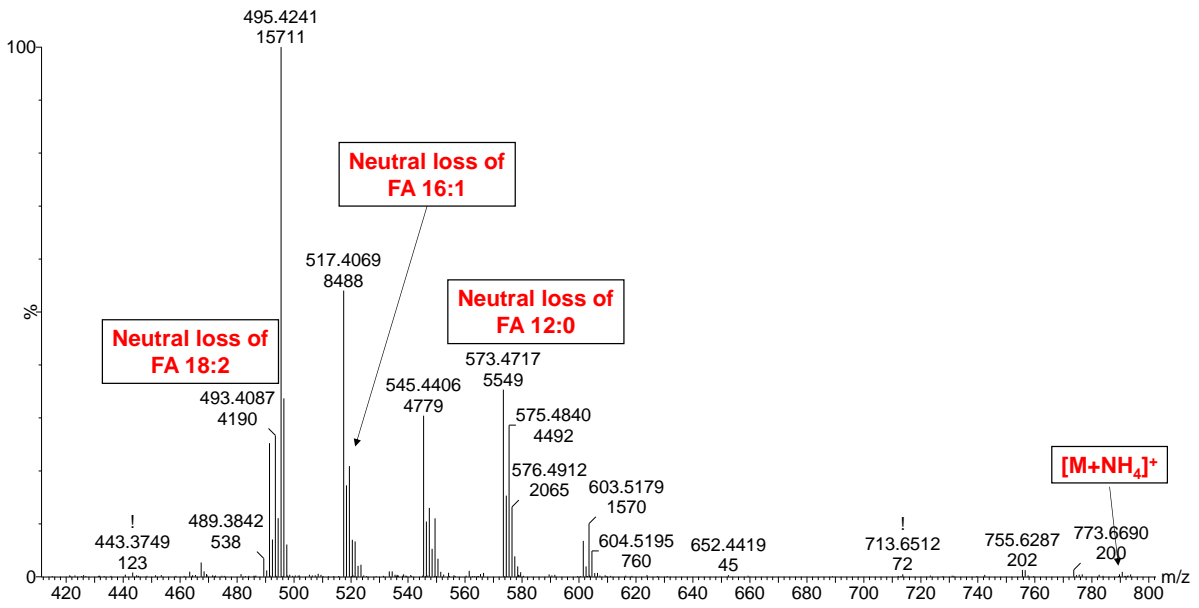
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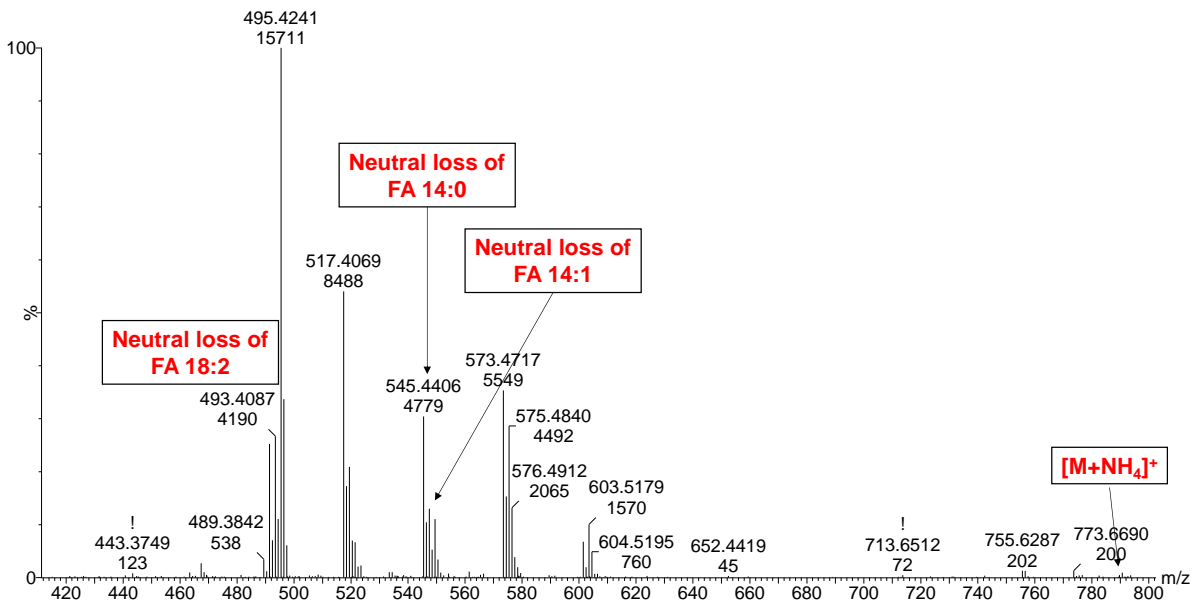
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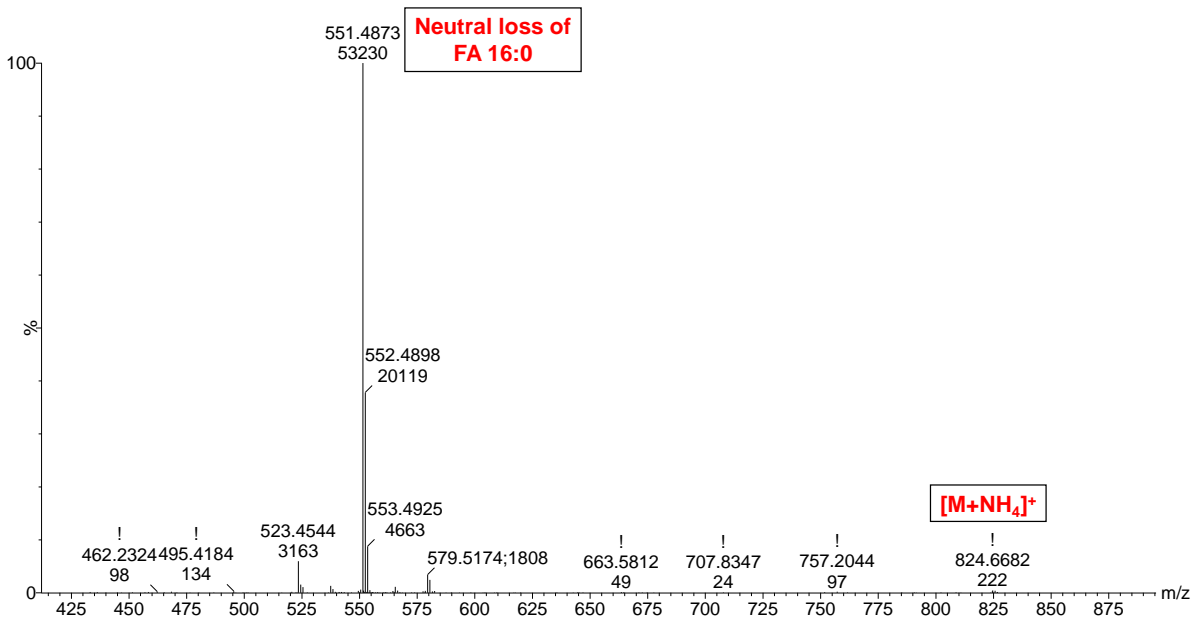
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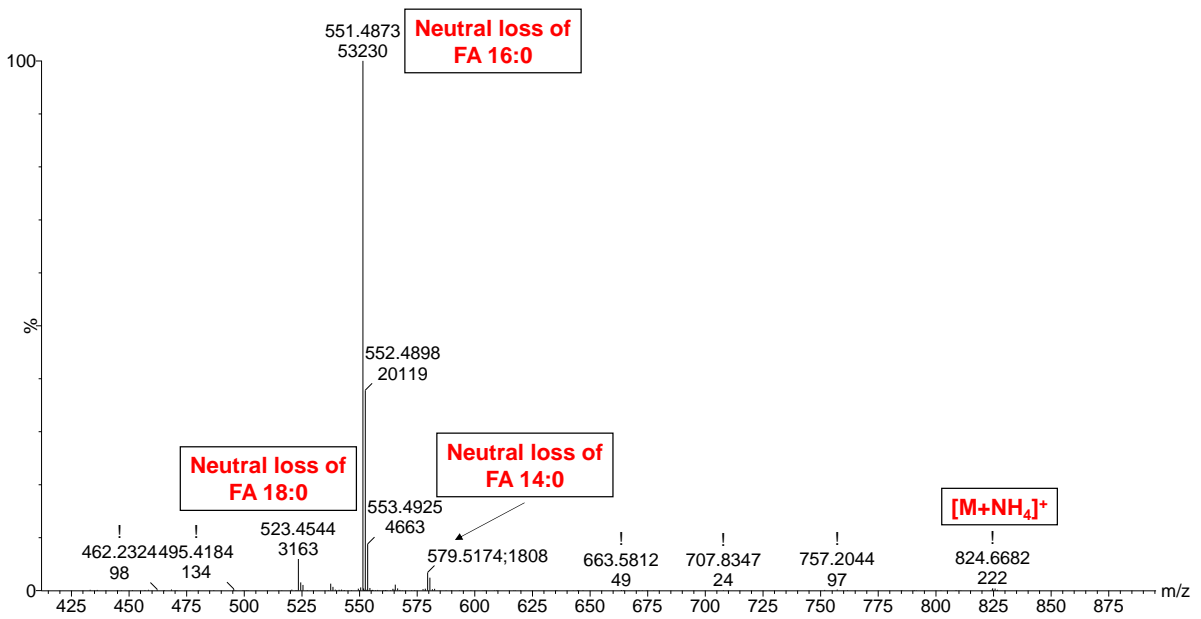
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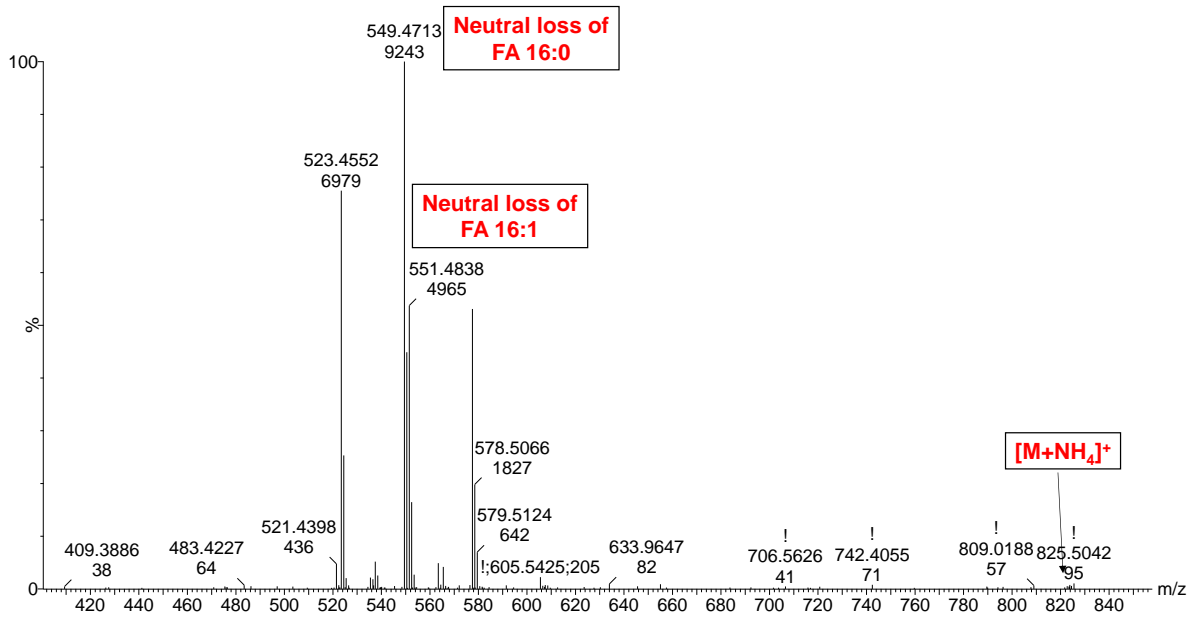
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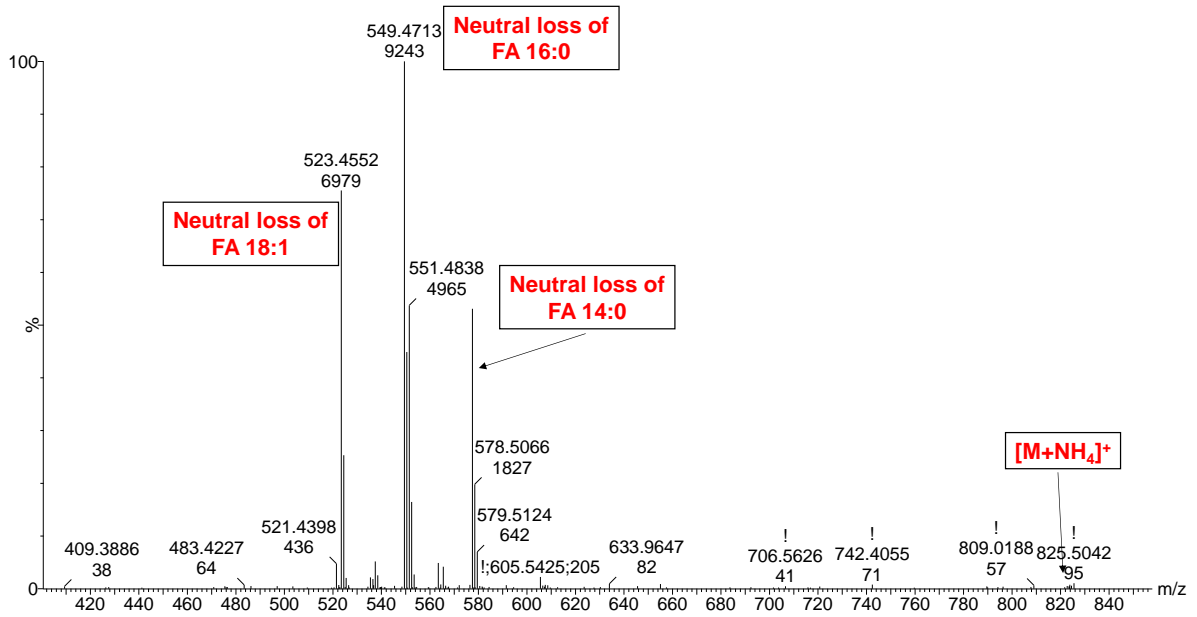
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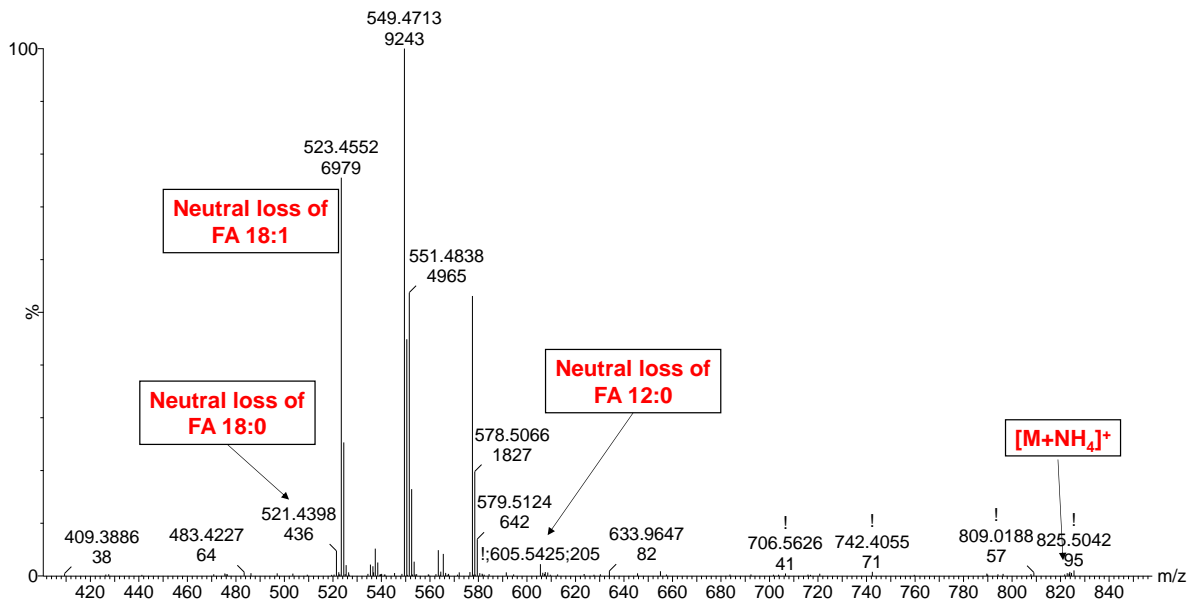
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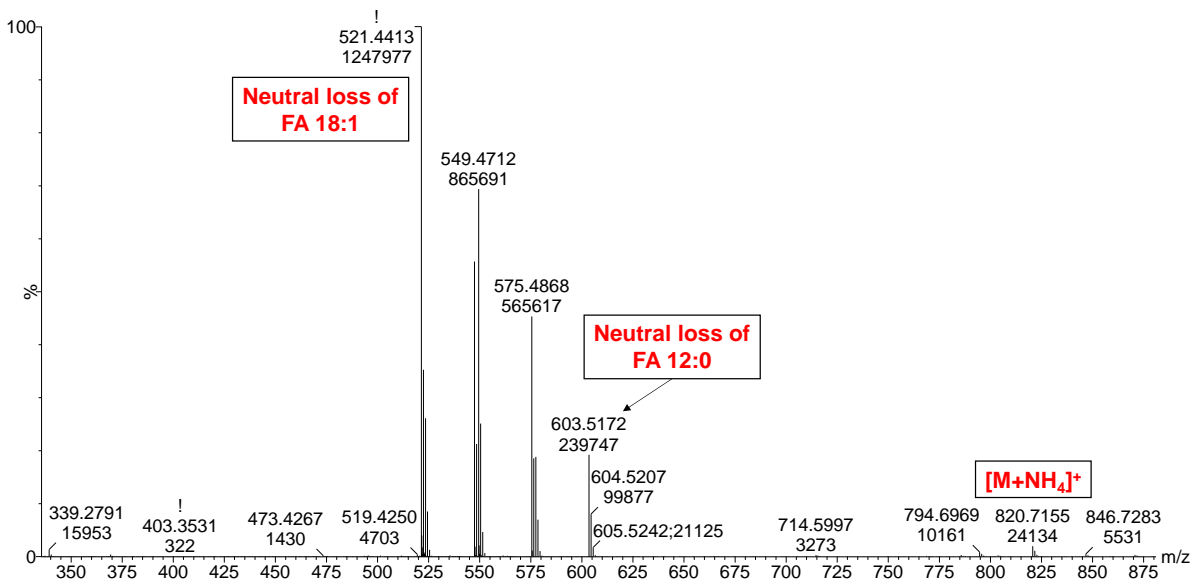
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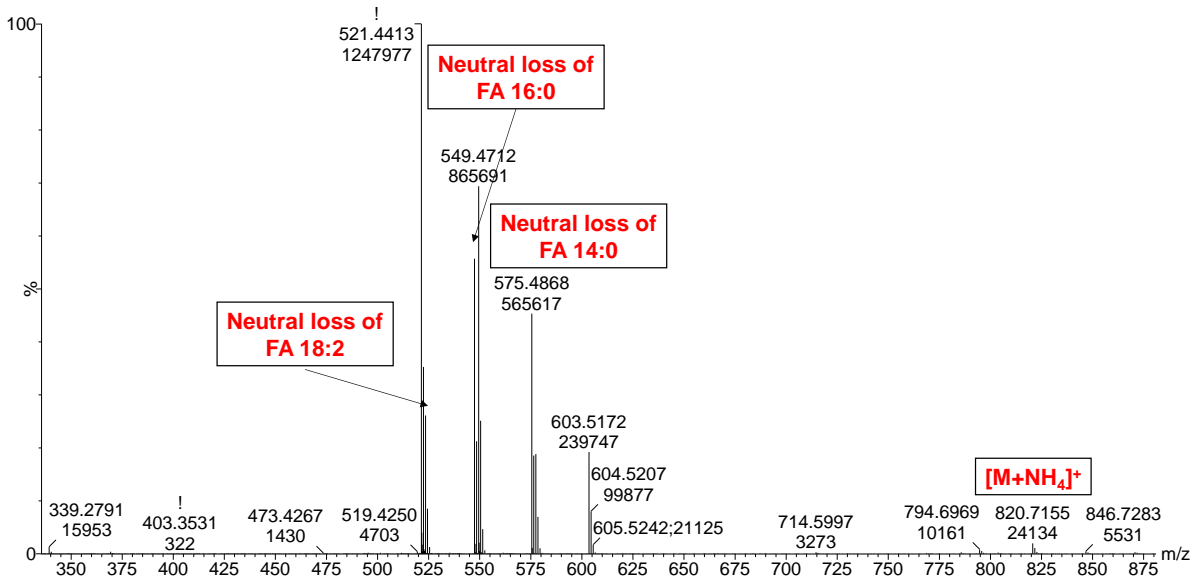
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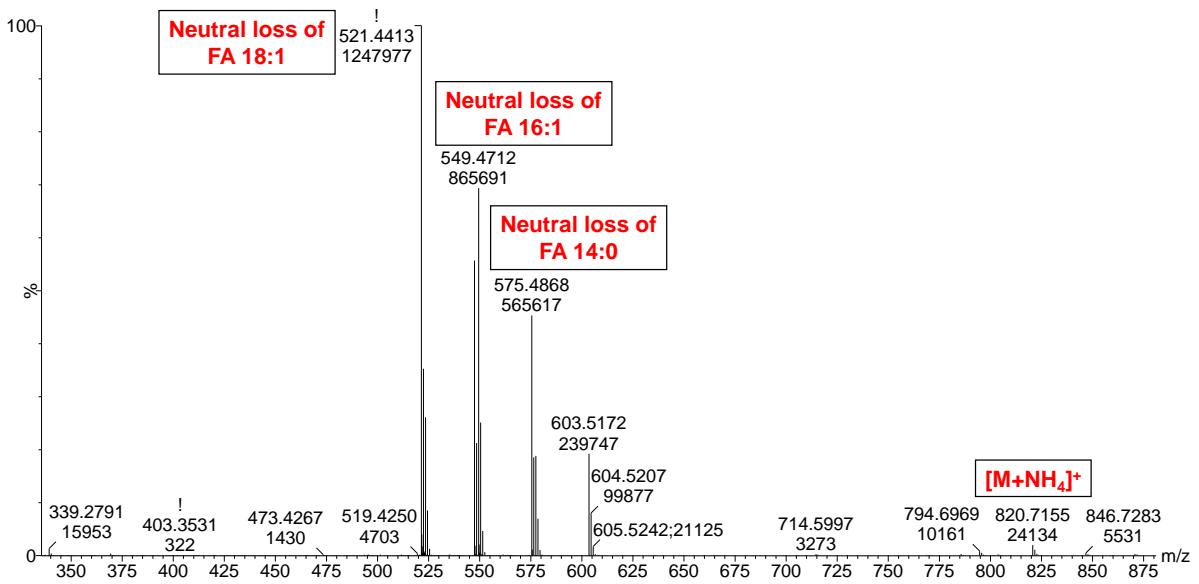
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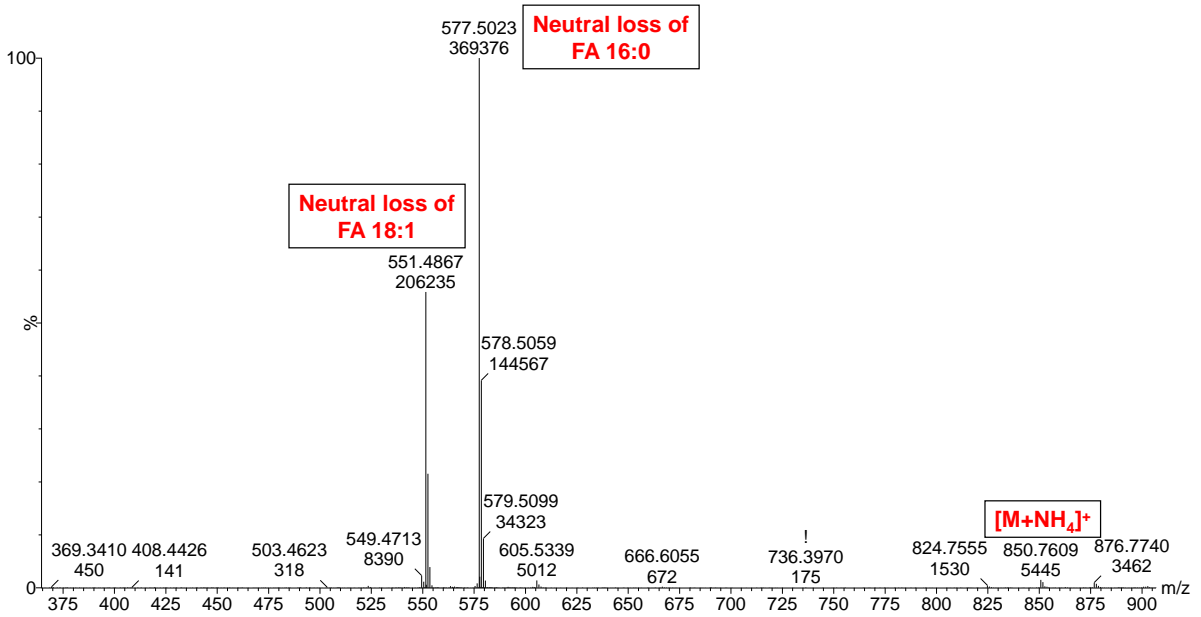
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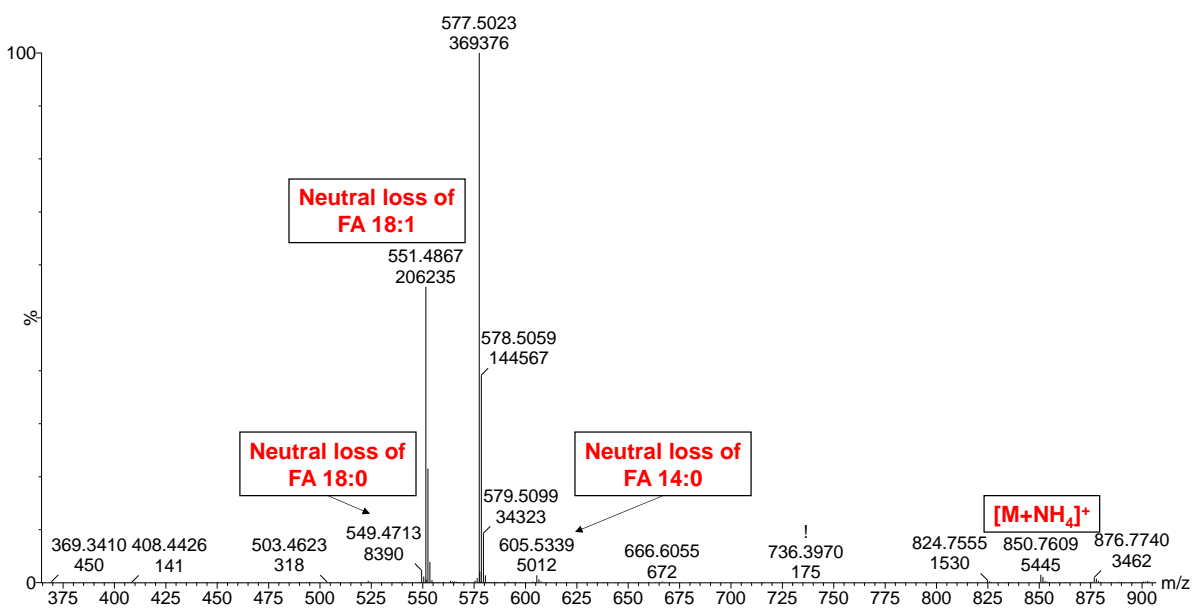
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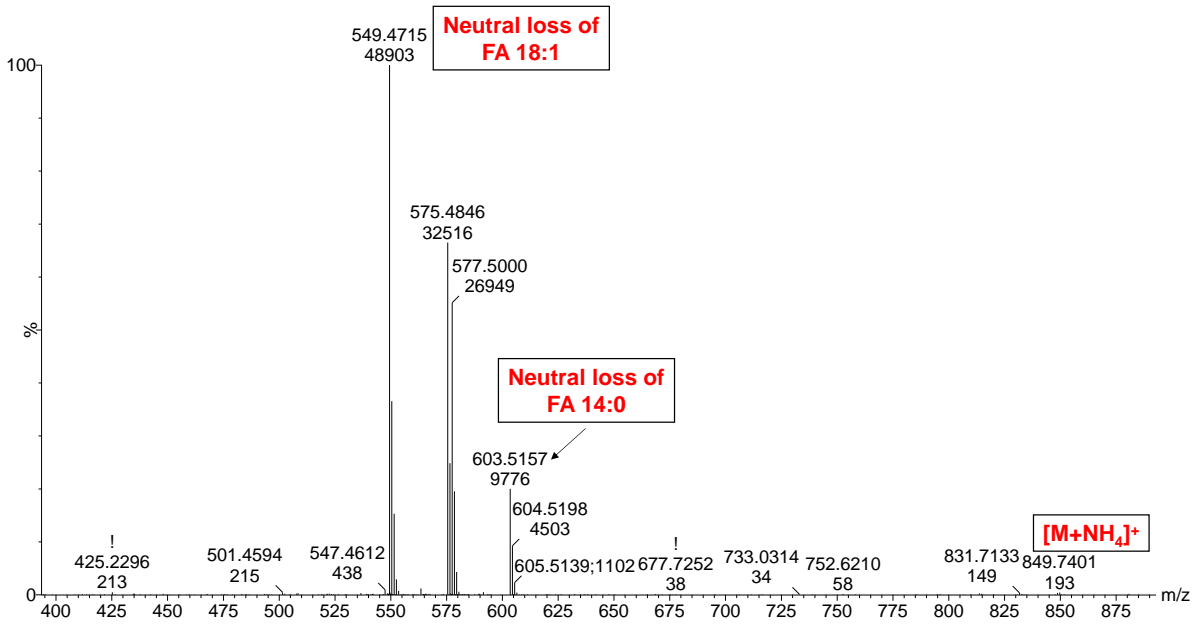


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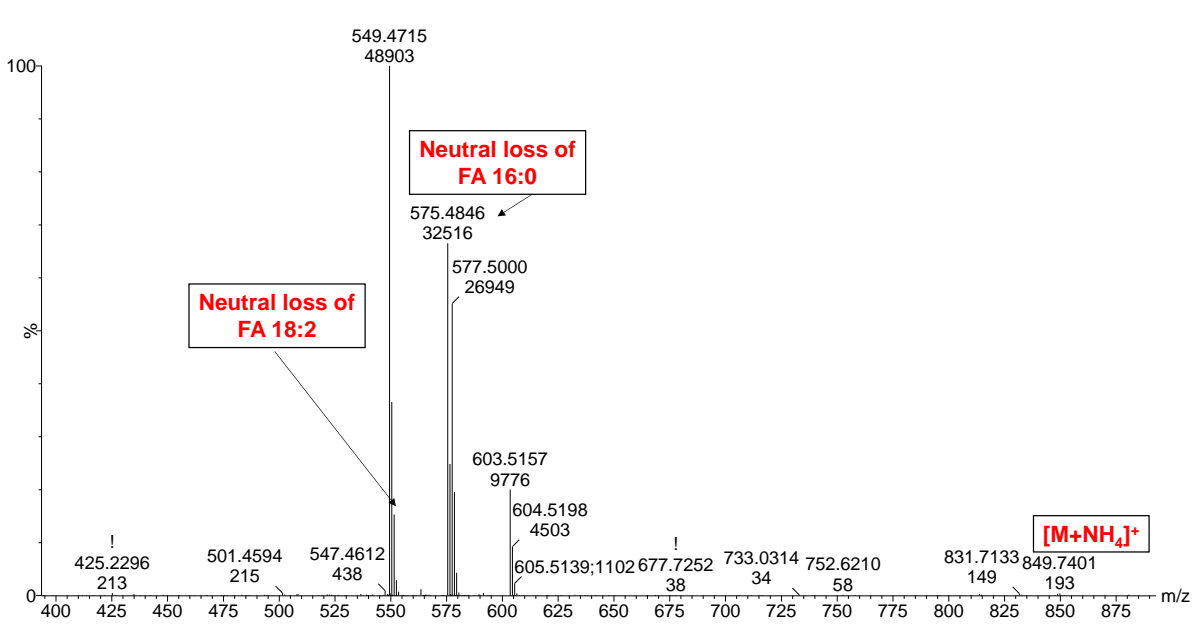




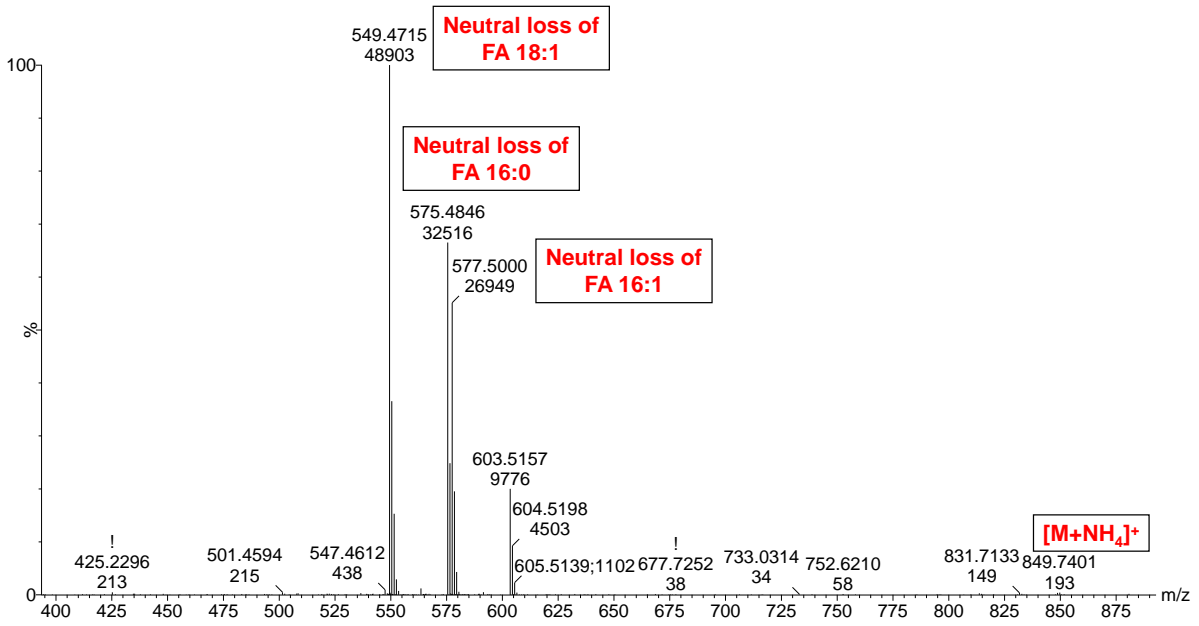
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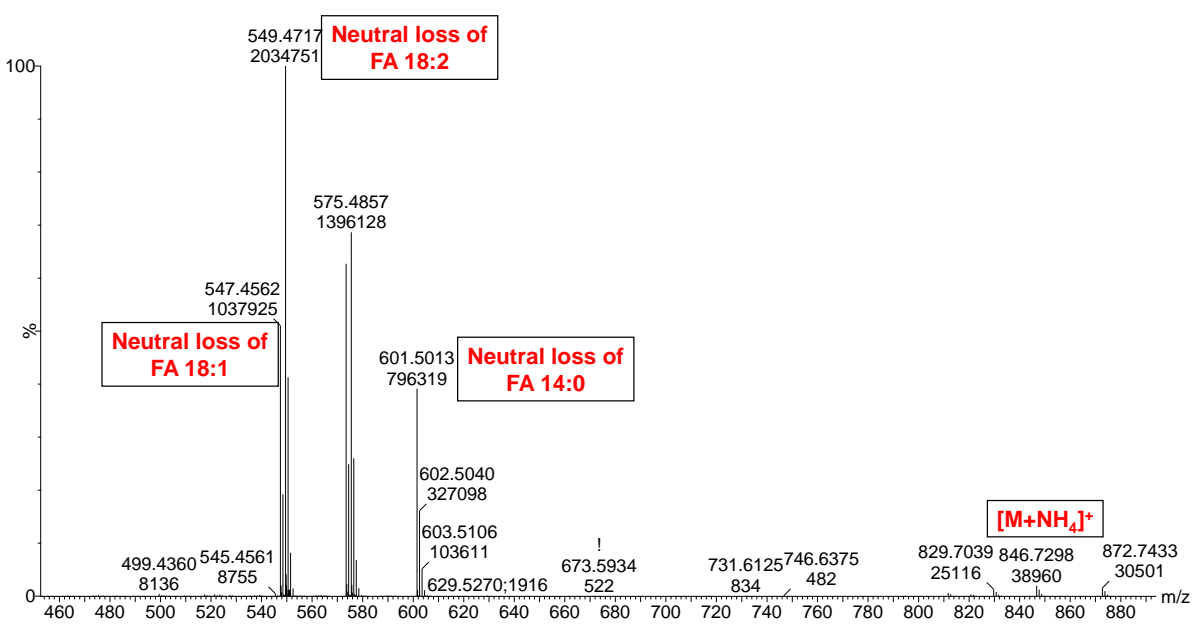
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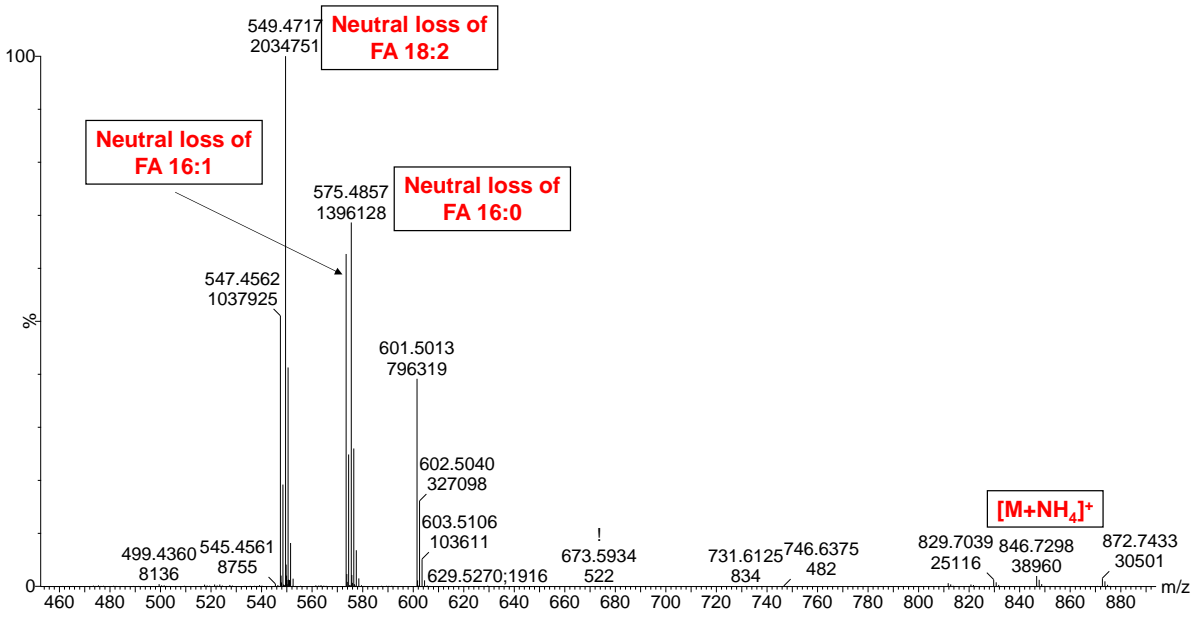
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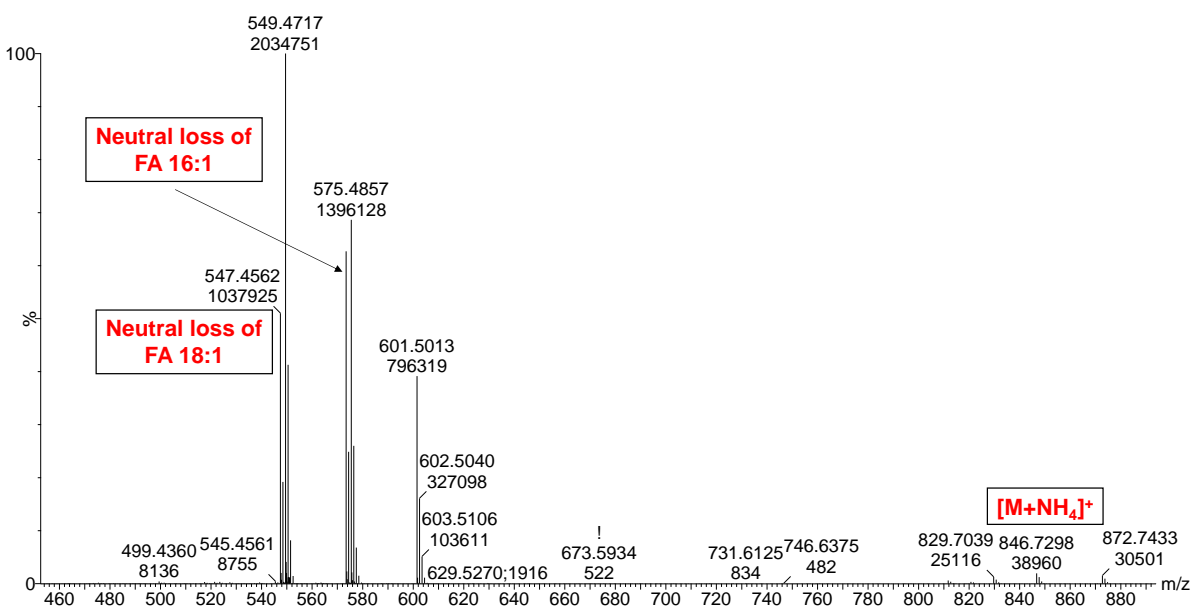
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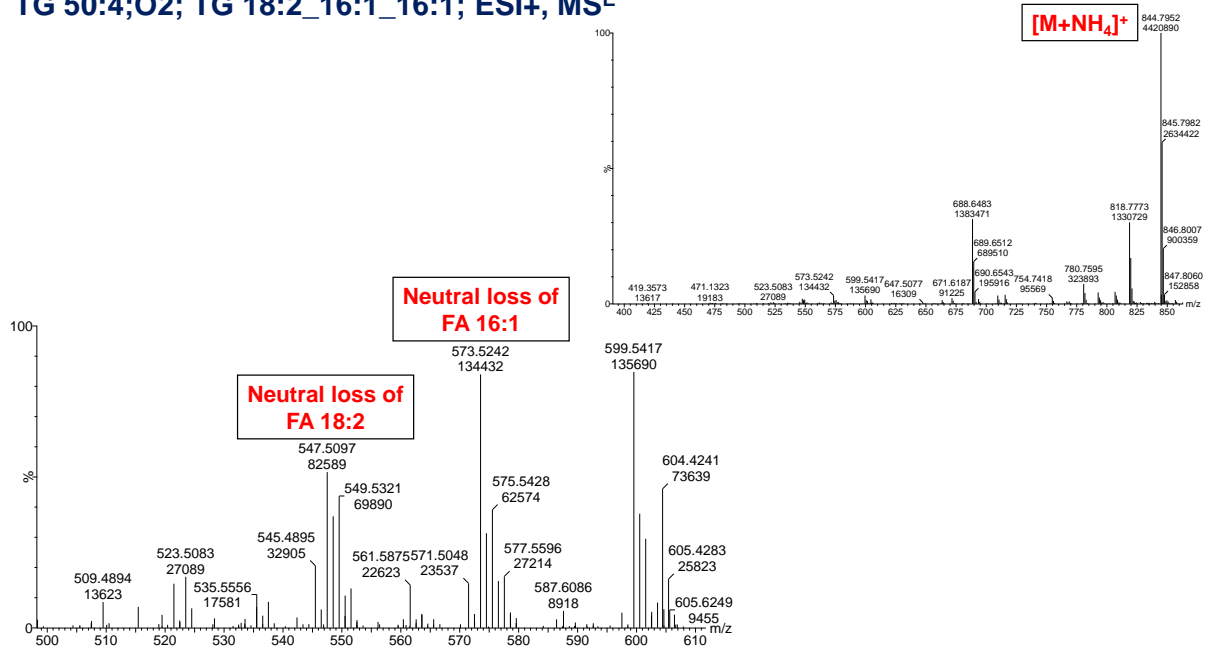
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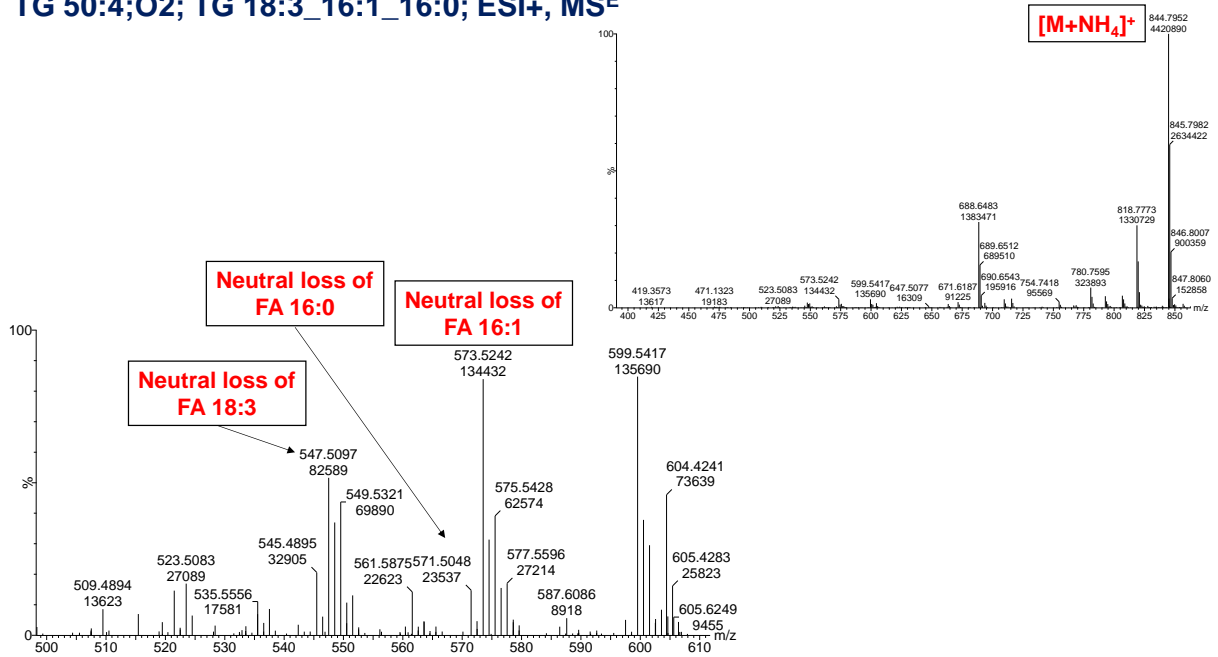
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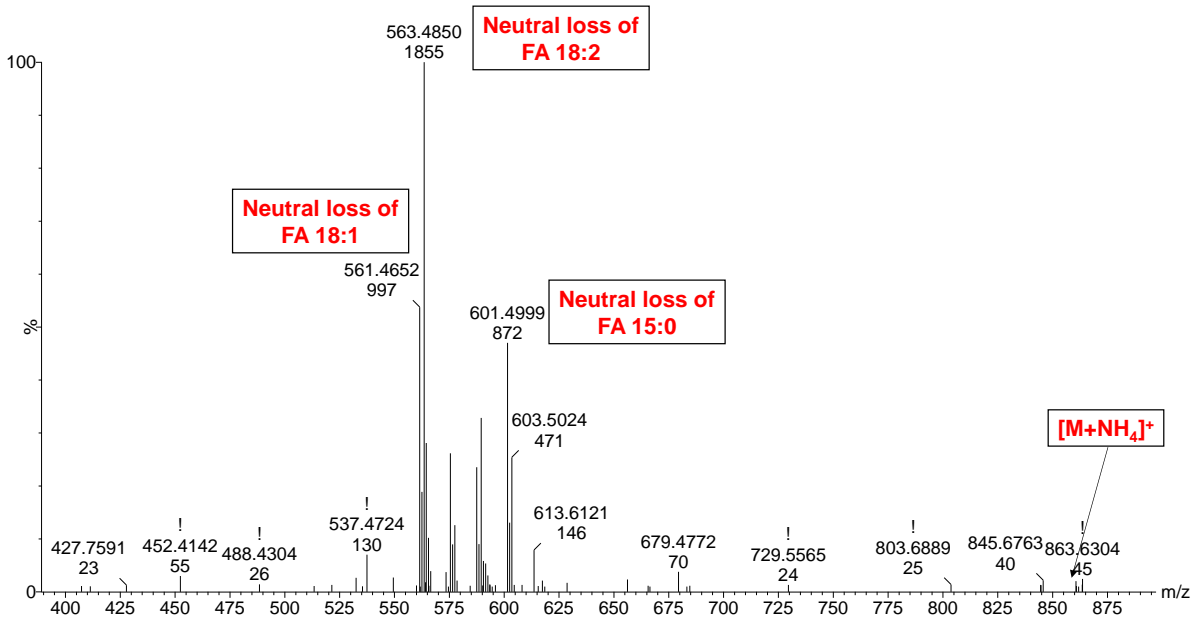
TG 50:4;O2; TG 18:2\_16:1\_16:1; ESI+, MS<sup>E</sup>



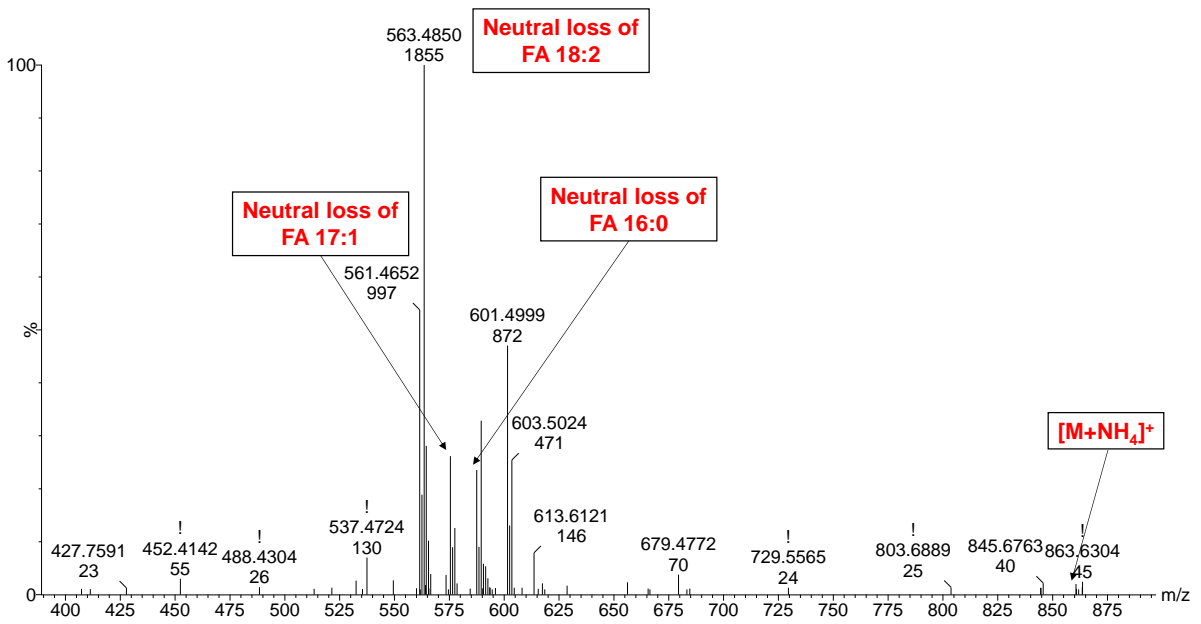
TG 50:4;O2; TG 18:3\_16:1\_16:0; ESI+, MS<sup>E</sup>



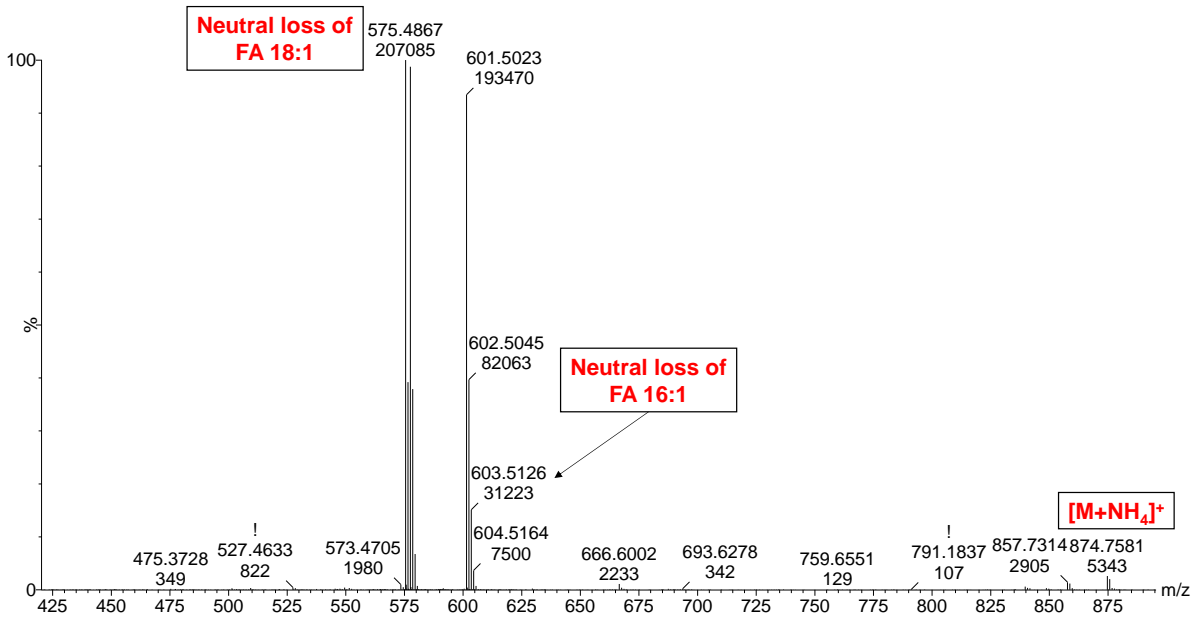
TG 51:3;O2; TG 18:2\_15:0\_18:1; ESI+, fast DDA



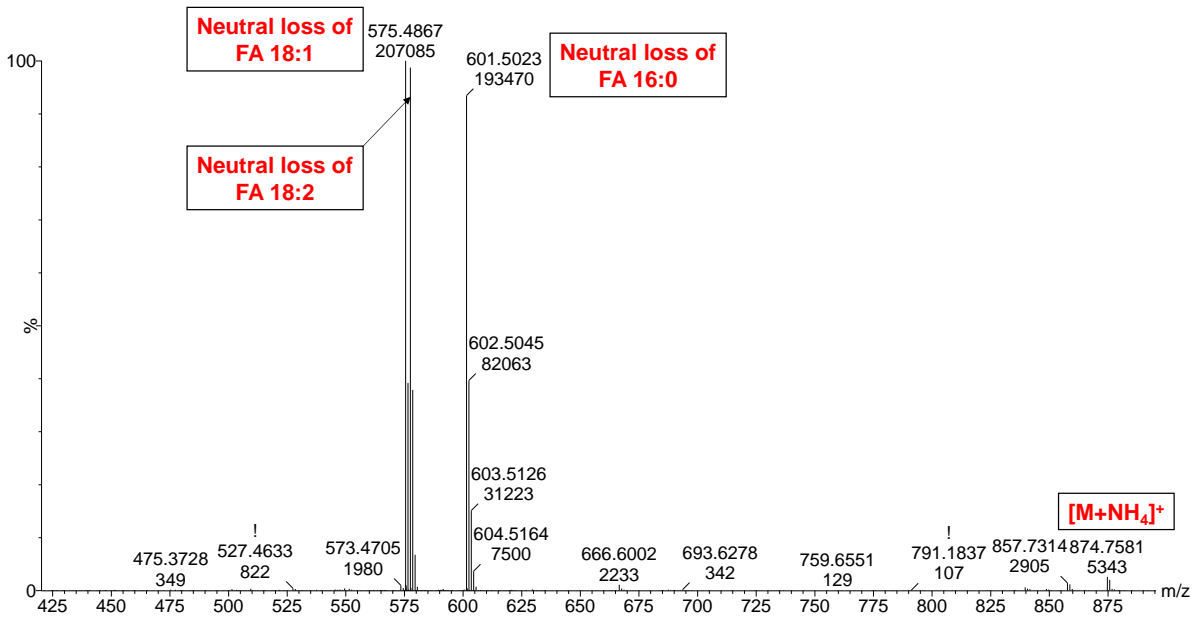
TG 51:3;O2; TG 17:1\_18:2\_16:0; ESI+, fast DDA



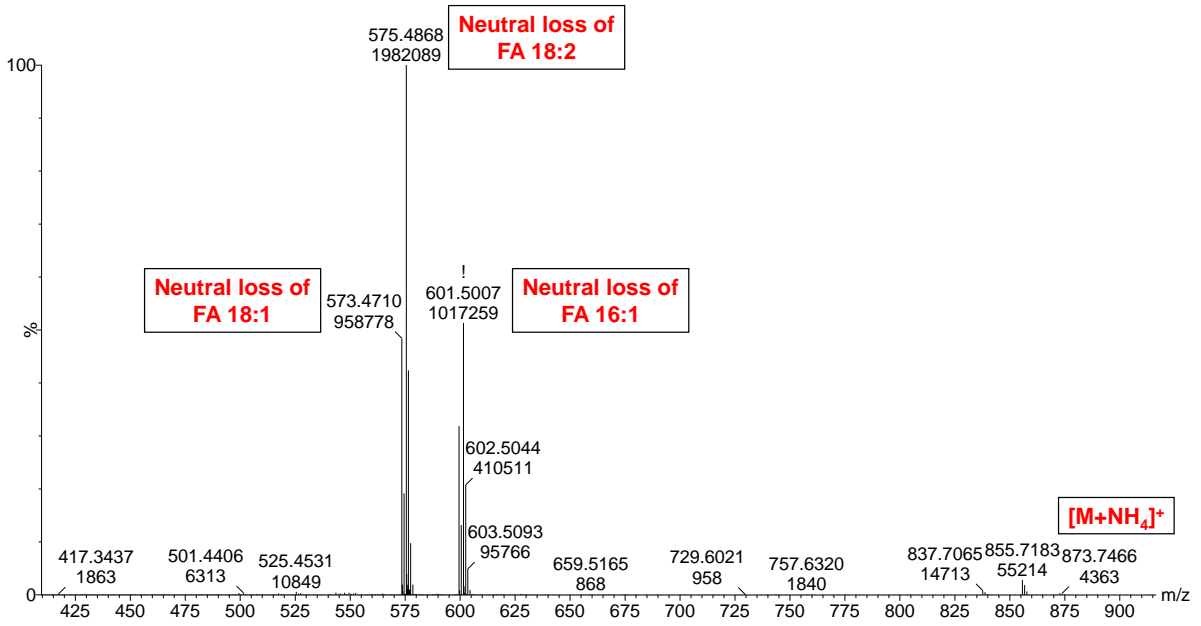
TG 52:3;O2; TG 18:1\_18:1\_16:1; ESI+, fast DDA



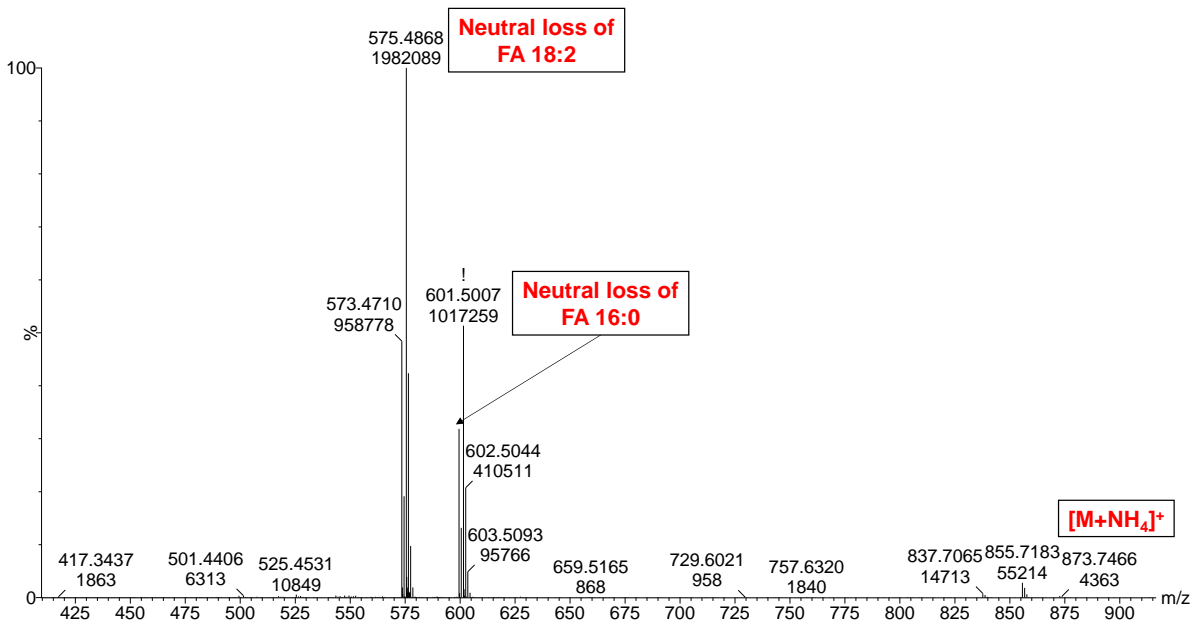
TG 52:3;O2; TG 18:1\_18:2\_16:0; ESI+, fast DDA



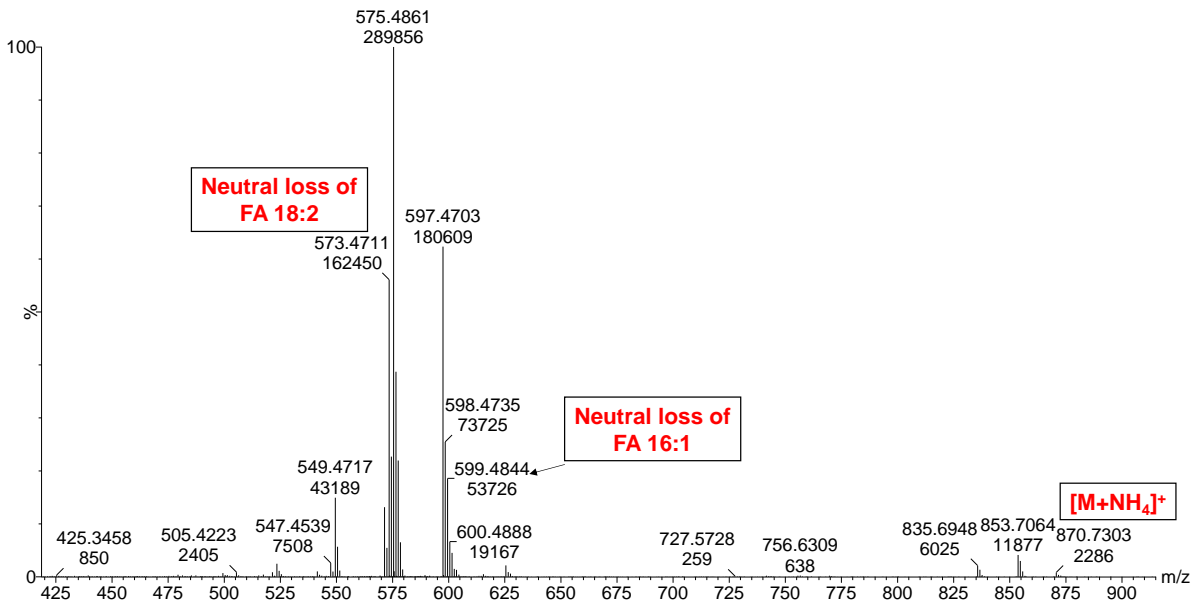
TG 52:4;O2; TG 18:1\_18:2\_16:1; ESI+, fast DDA



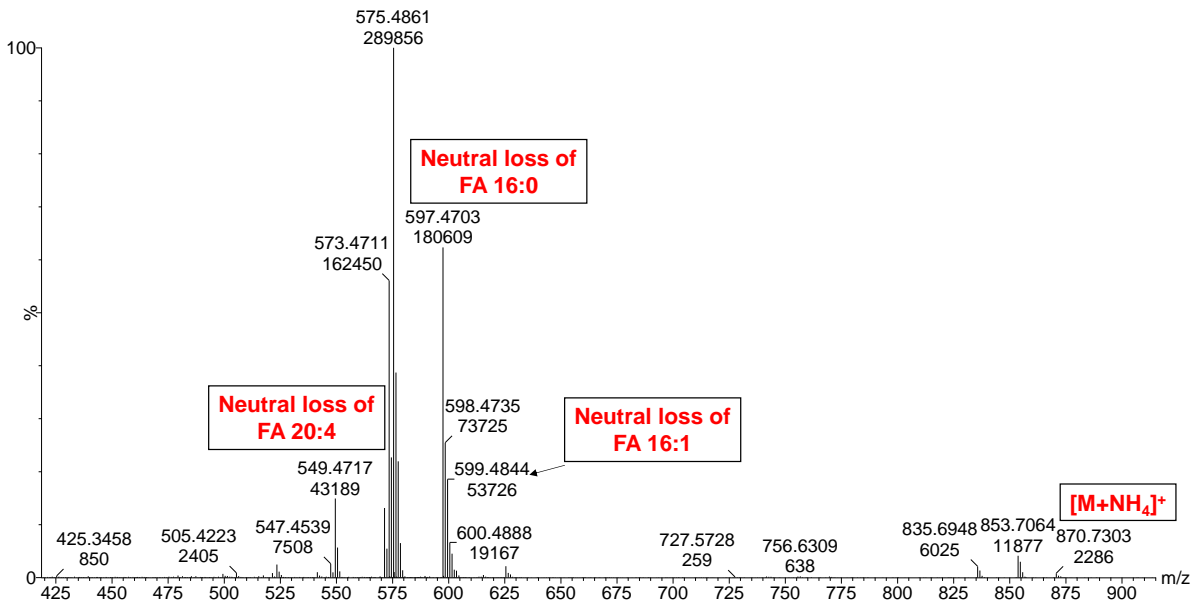
TG 52:4;O2; TG 18:2\_18:2\_16:0; ESI+, fast DDA



TG 52:5;O2; TG 18:2\_18:2\_16:1; ESI+, fast DDA

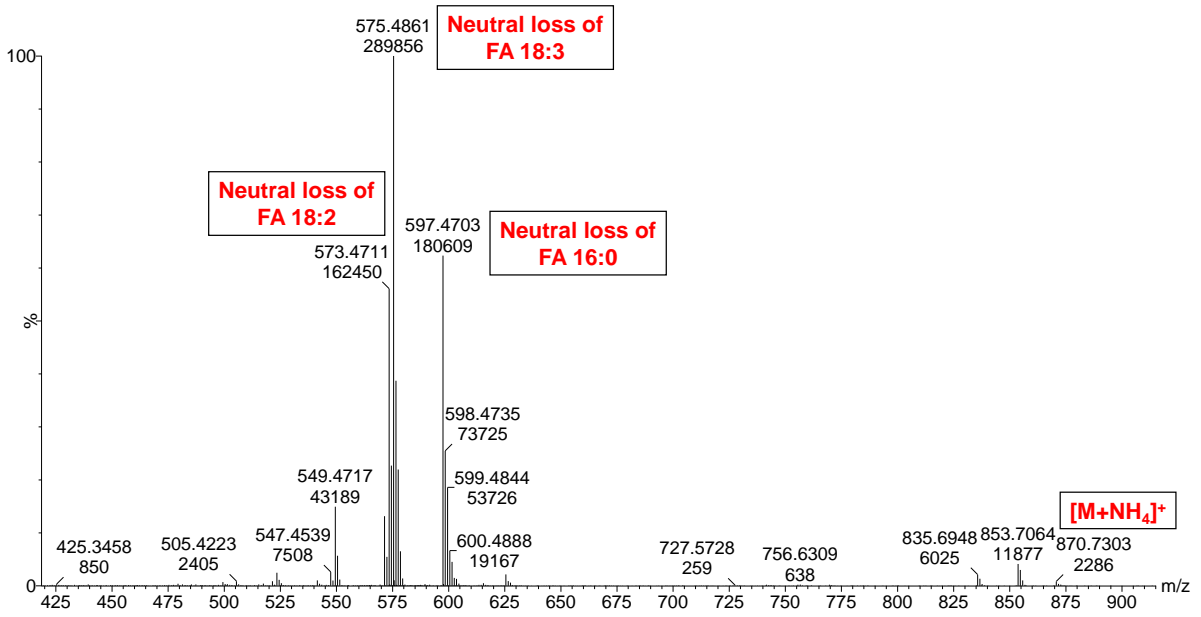


TG 52:5;O2; TG 16:0\_16:1\_20:4; ESI+, fast DDA

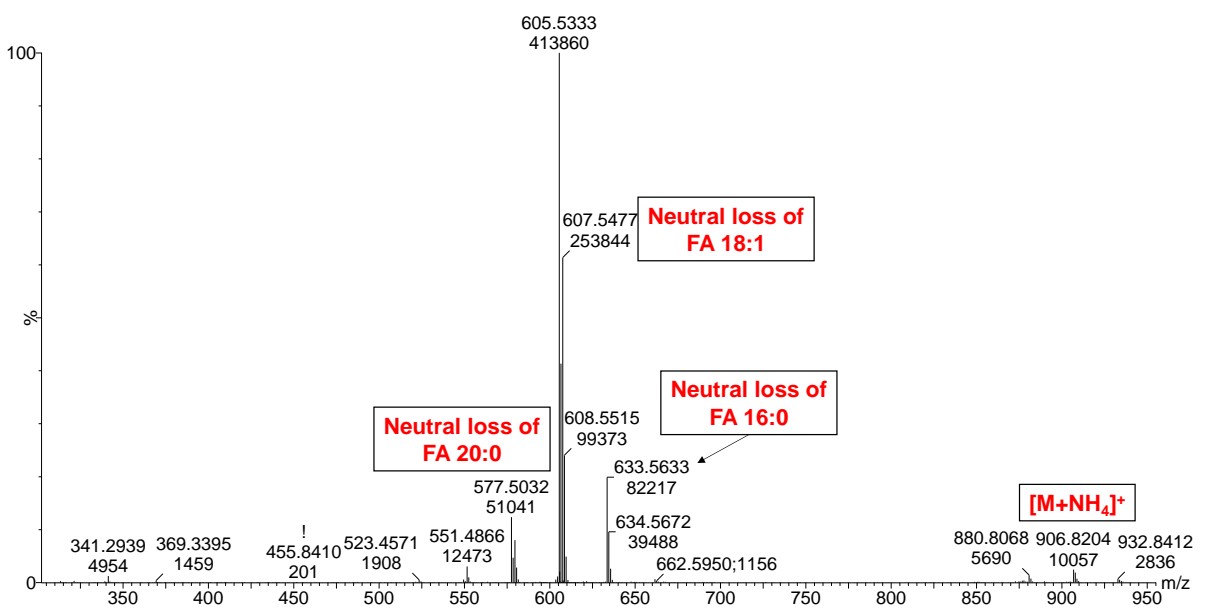




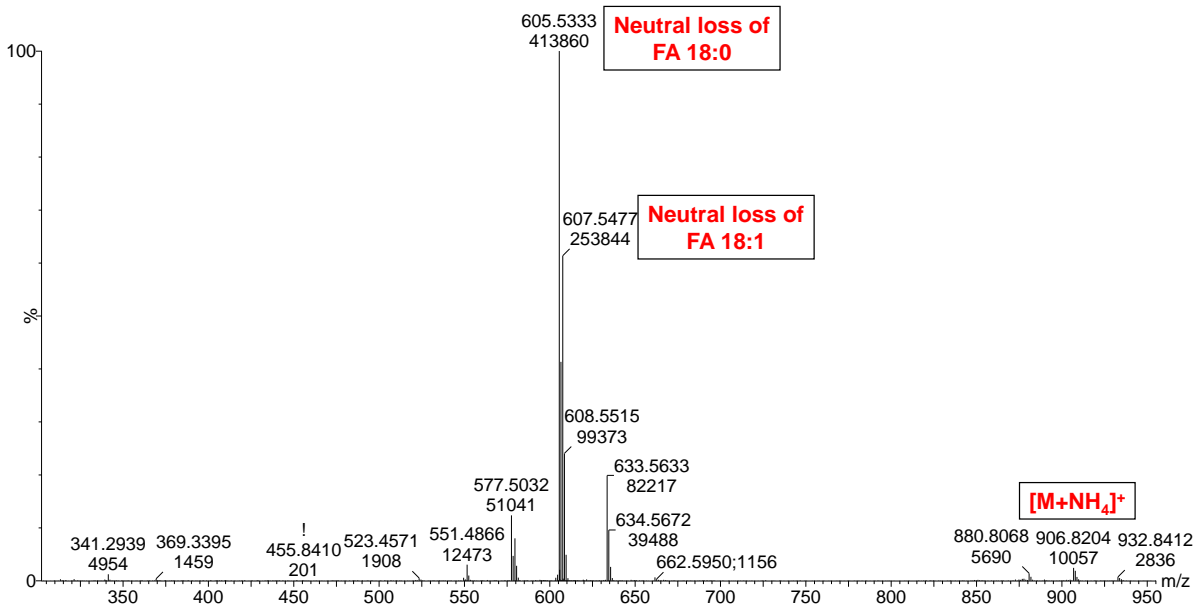
TG 52:5;O2; TG 18:3\_18:2\_16:0; ESI+, fast DDA



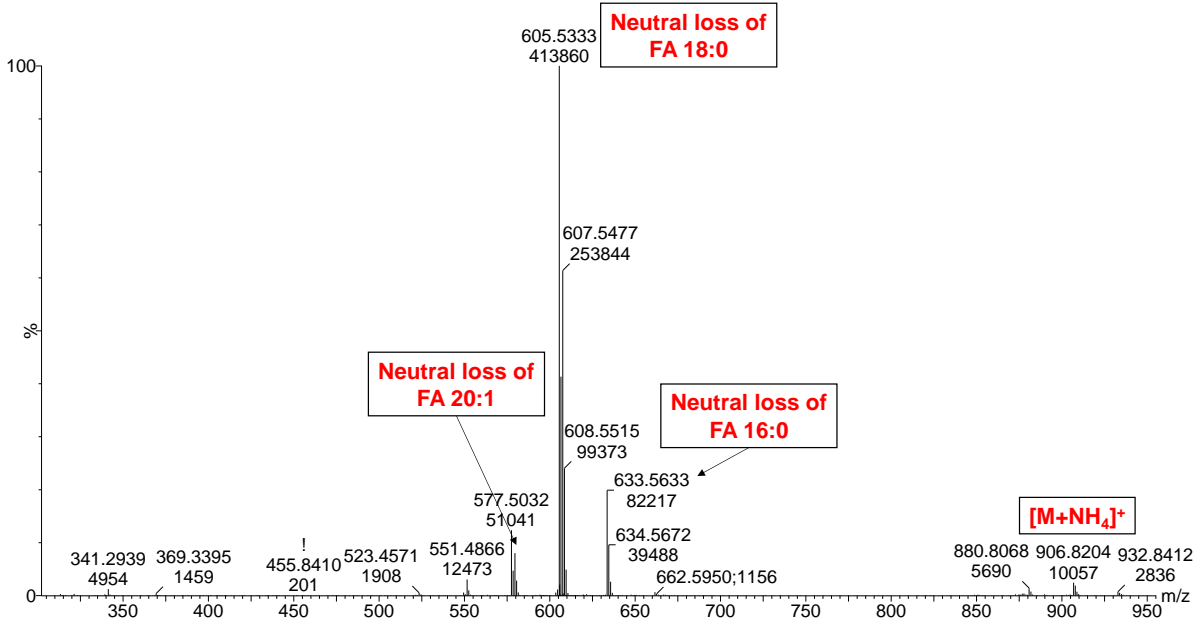
TG 54:1;O2; TG 20:0\_18:1\_16:0; ESI+, fast DDA



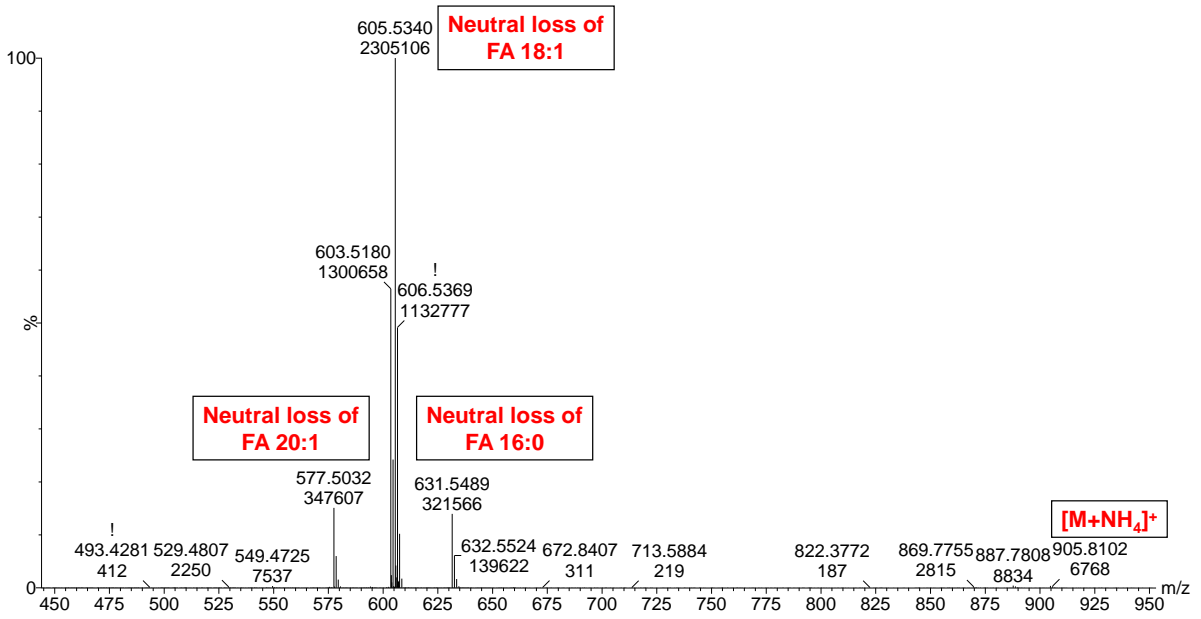
TG 54:1;O2; TG 18:1\_18:0\_18:0; ESI+, fast DDA



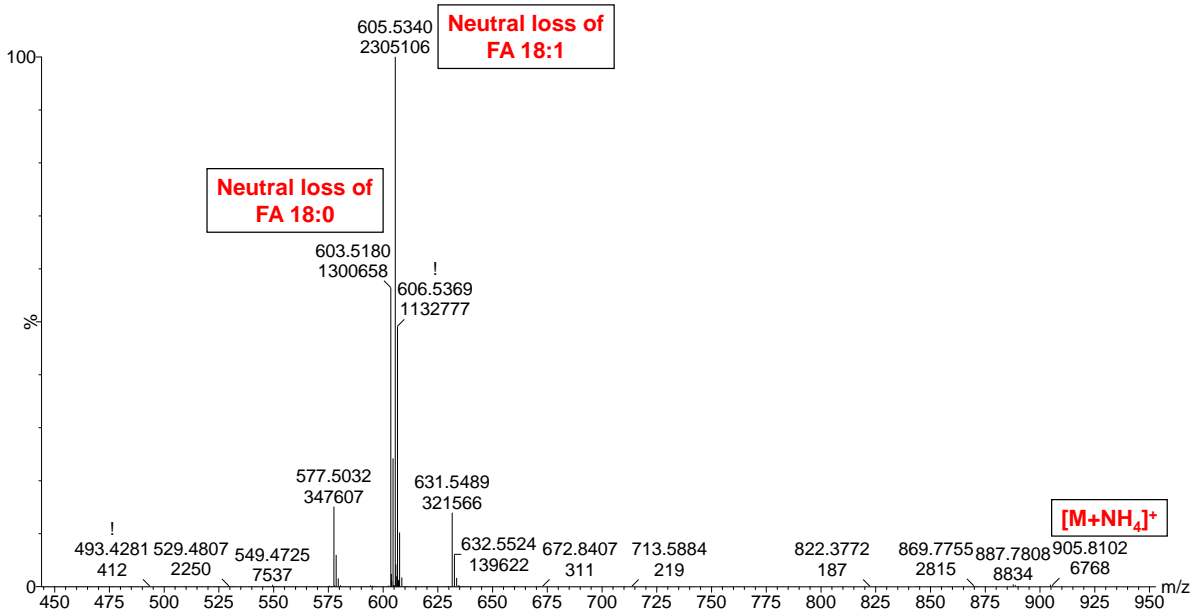
TG 54:1;O2; TG 18:0\_20:1\_16:0; ESI+, fast DDA



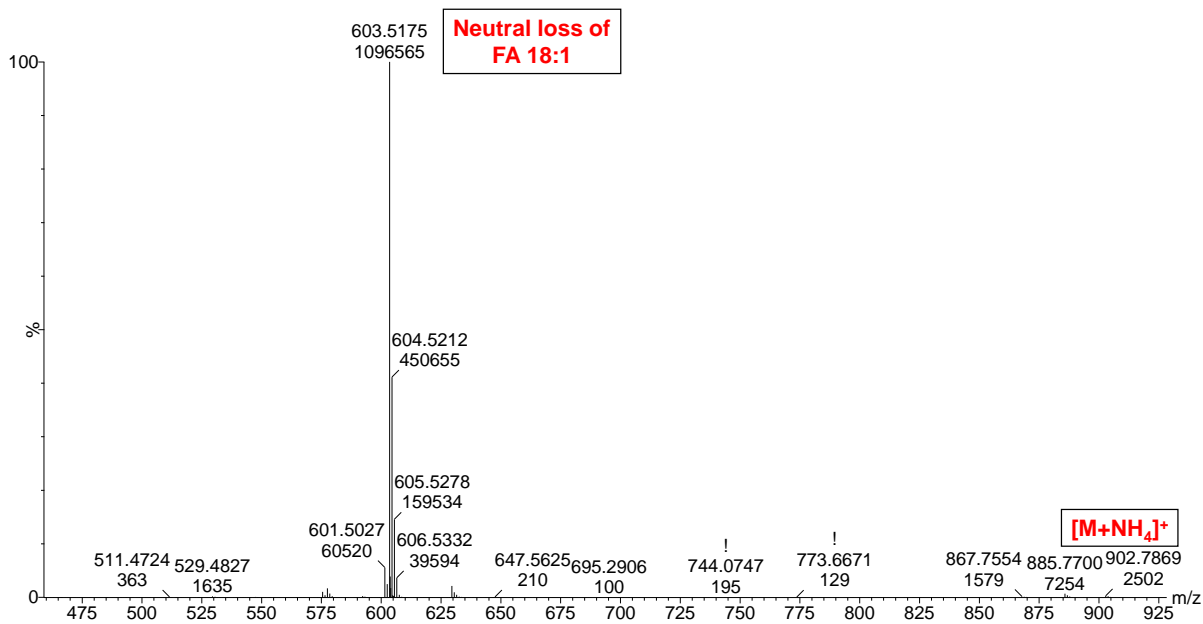
TG 54:2;O2; TG 20:1\_18:1\_16:0; ESI+, fast DDA



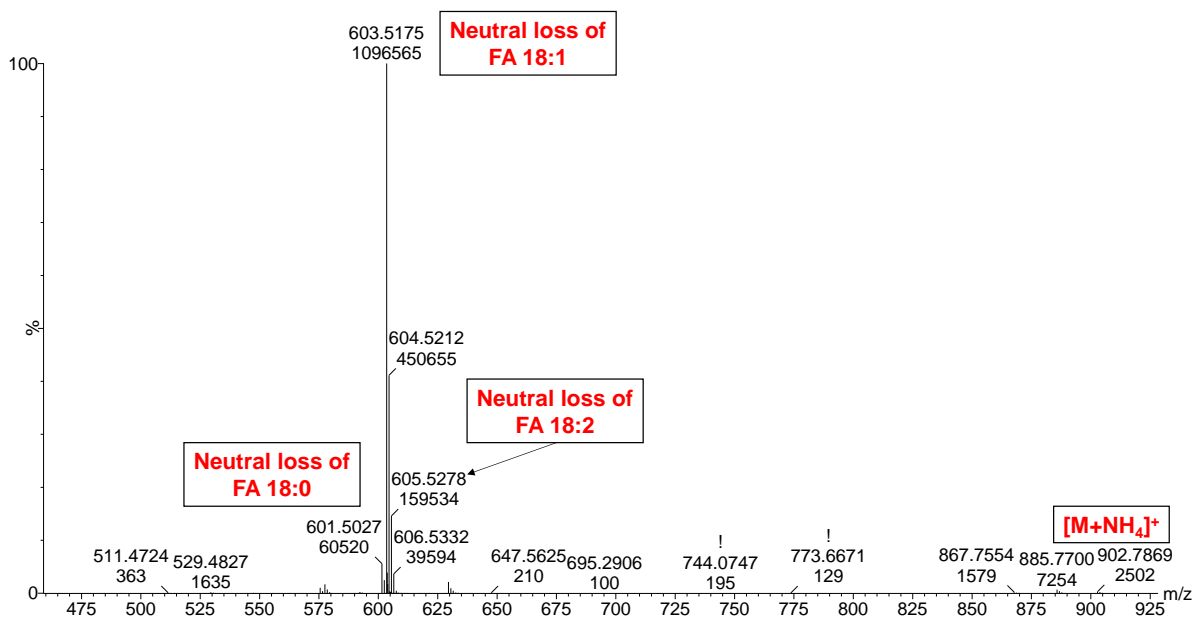
TG 54:2;O2; TG 18:0\_18:1\_18:1; ESI+, fast DDA



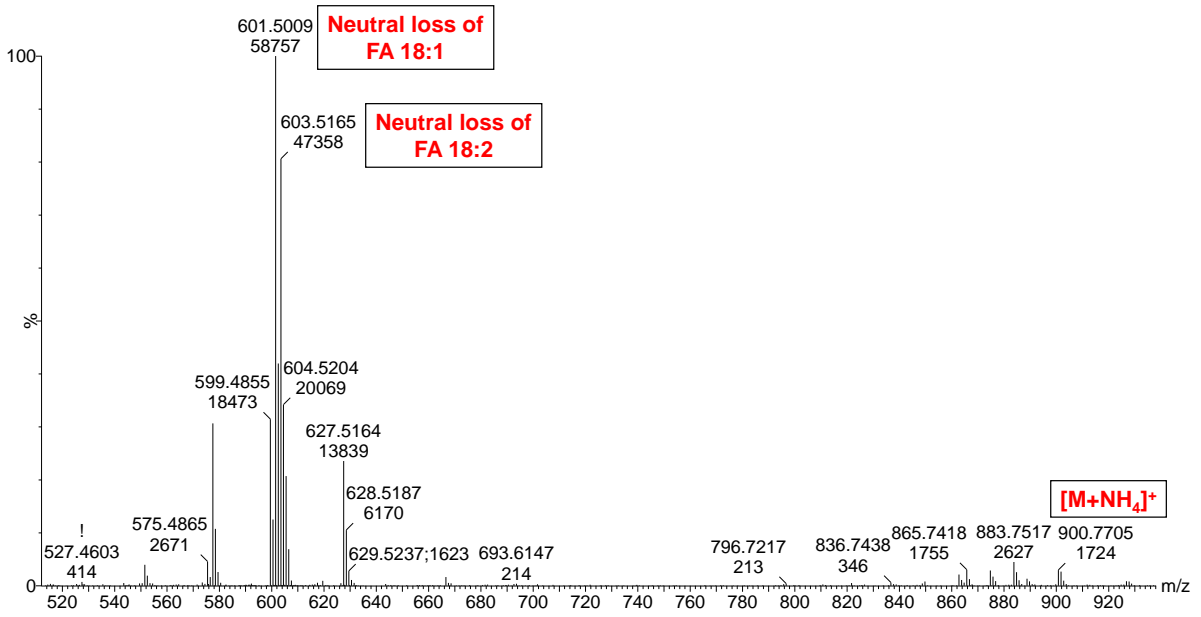
TG 54:3;O2; TG 18:1\_18:1\_18:1; ESI+, fast DDA



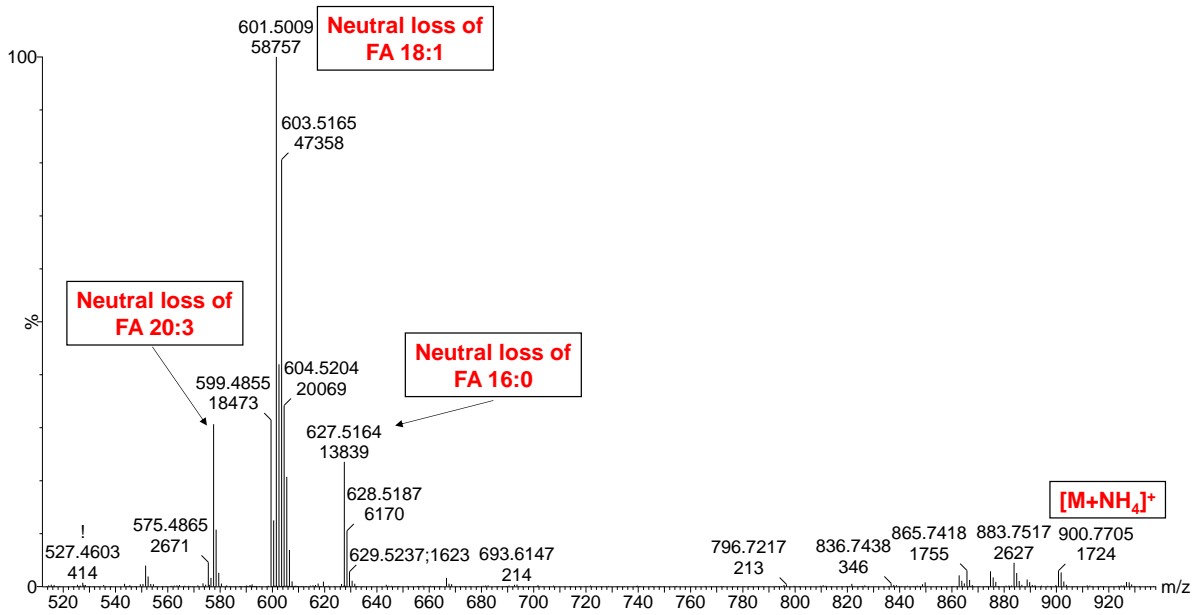
TG 54:3;O2; TG 18:0\_18:2\_18:1; ESI+, fast DDA



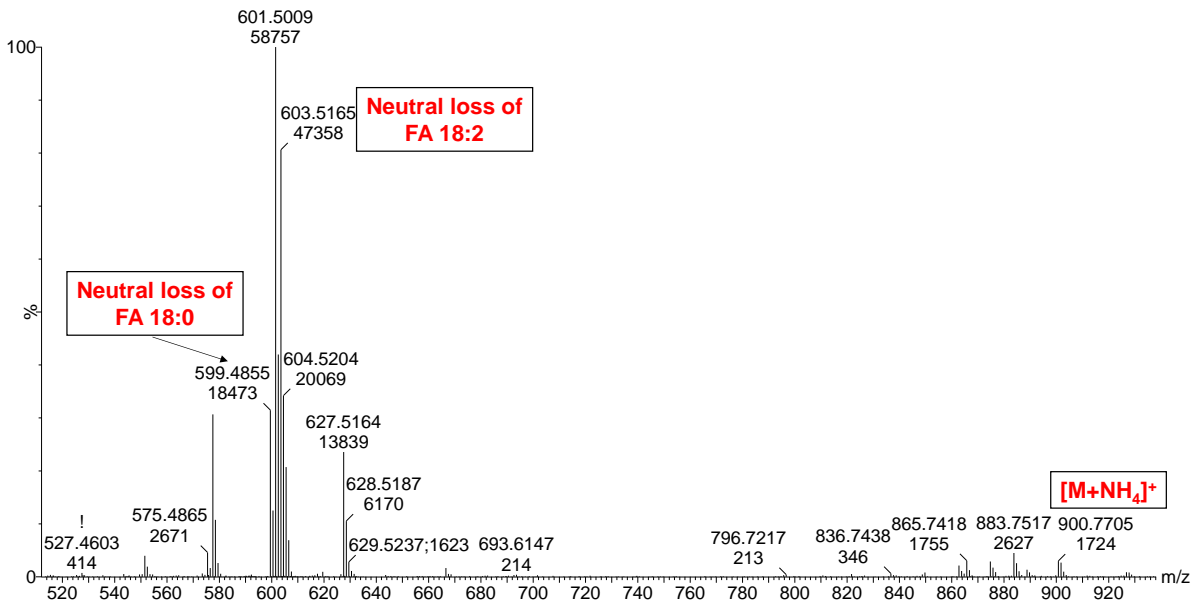
TG 54:4;O2; TG 18:1\_18:2\_18:1; ESI+, fast DDA



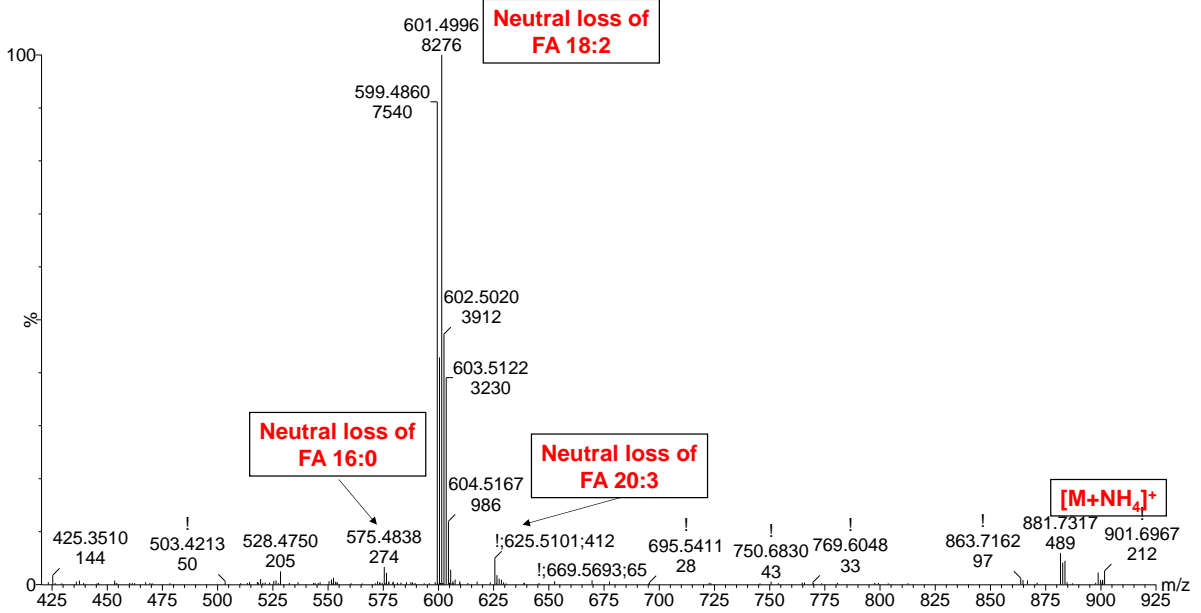
TG 54:4;O2; TG 16:0\_18:1\_20:3; ESI+, fast DDA



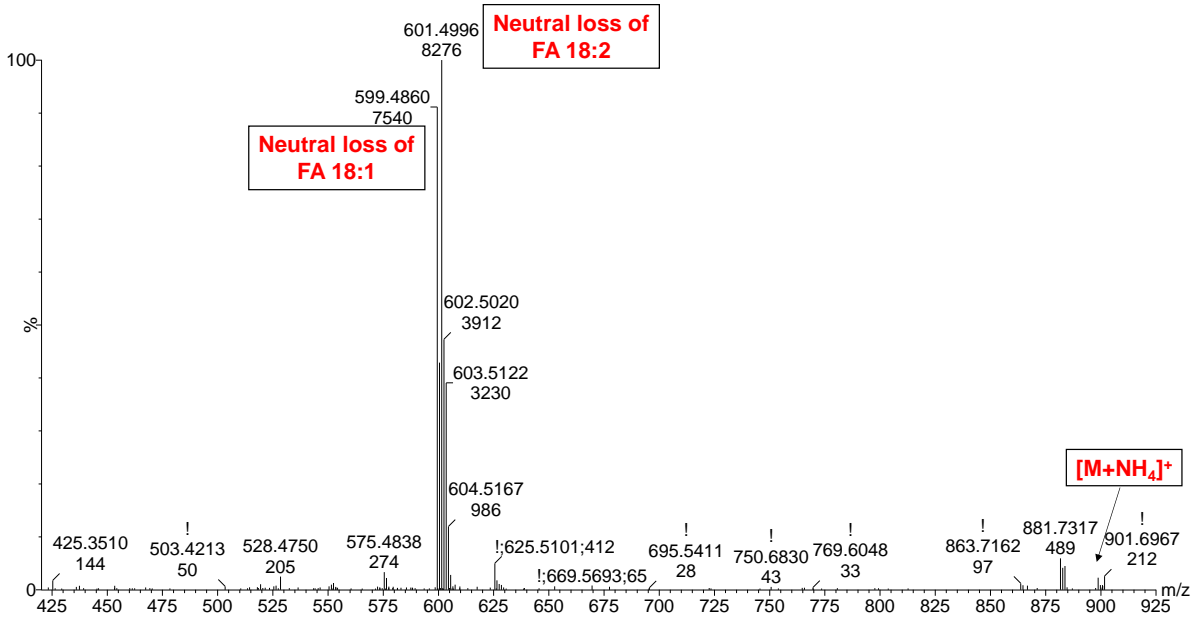
TG 54:4;O2; TG 18:0\_18:2\_18:2; ESI+, fast DDA



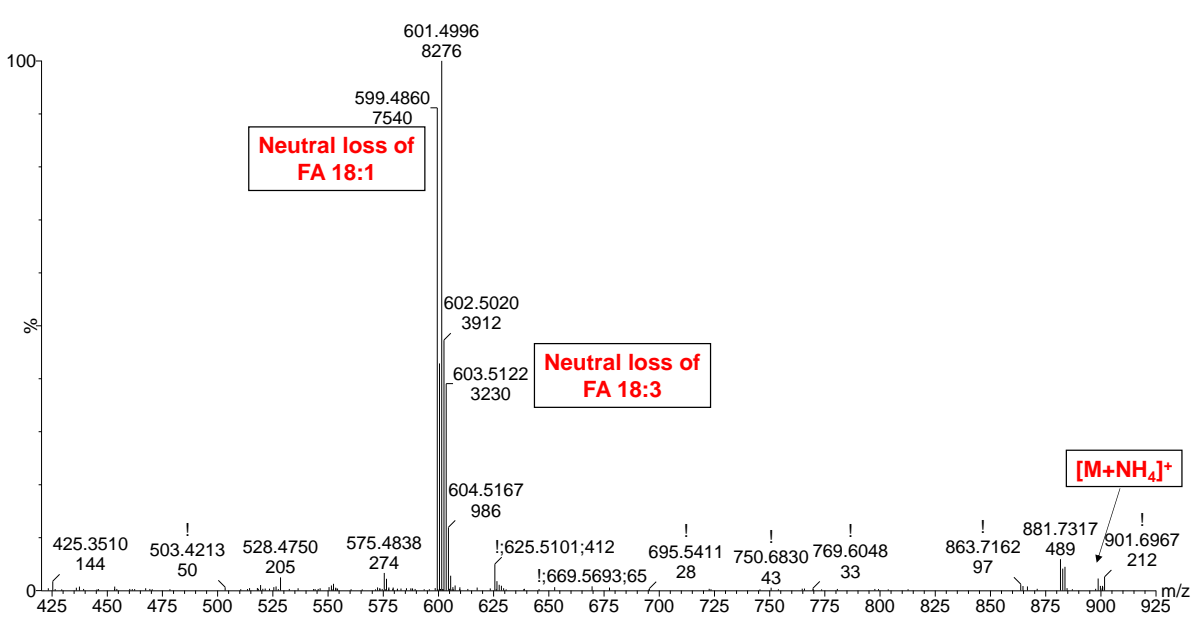
TG 54:5;O2; TG 16:0\_18:2\_20:3; ESI+, fast DDA



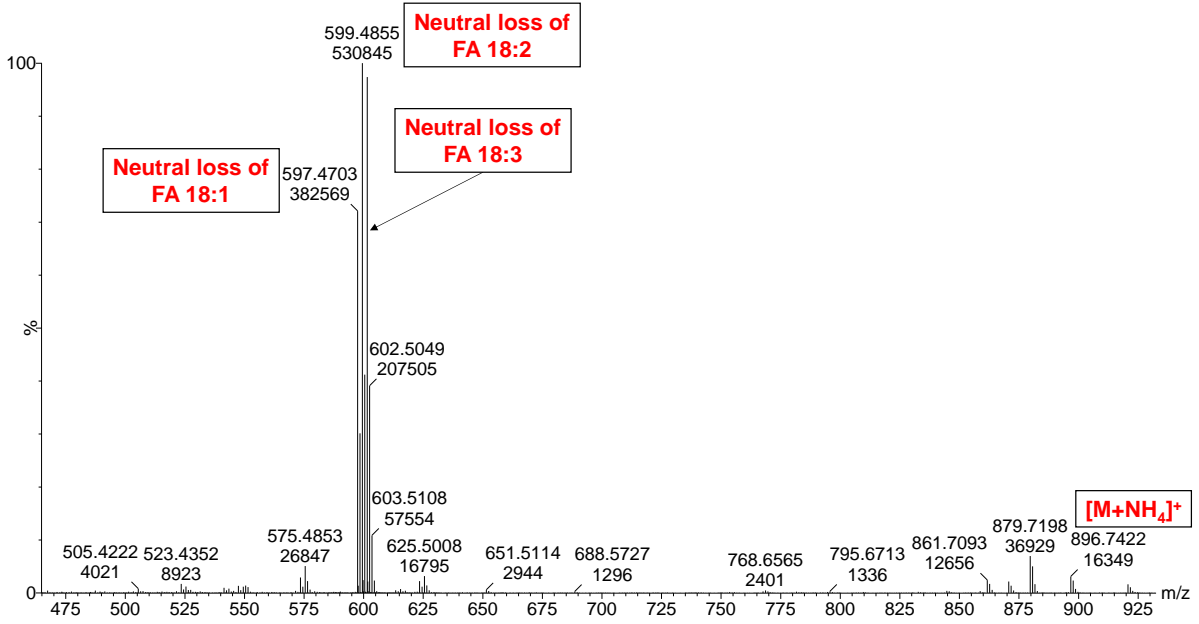
TG 54:5;O2; TG 18:1\_18:2\_18:2; ESI+, fast DDA



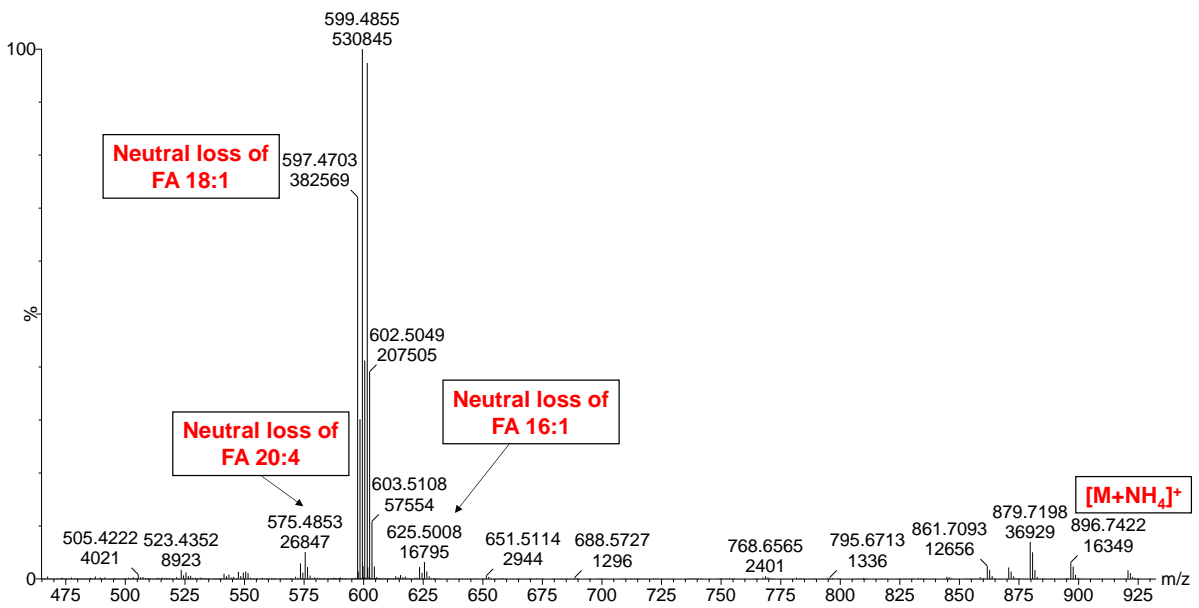
TG 54:5;O2; TG 18:1\_18:1\_18:3; ESI+, fast DDA



TG 54:6;O2; TG 18:1\_18:2\_18:3; ESI+, fast DDA

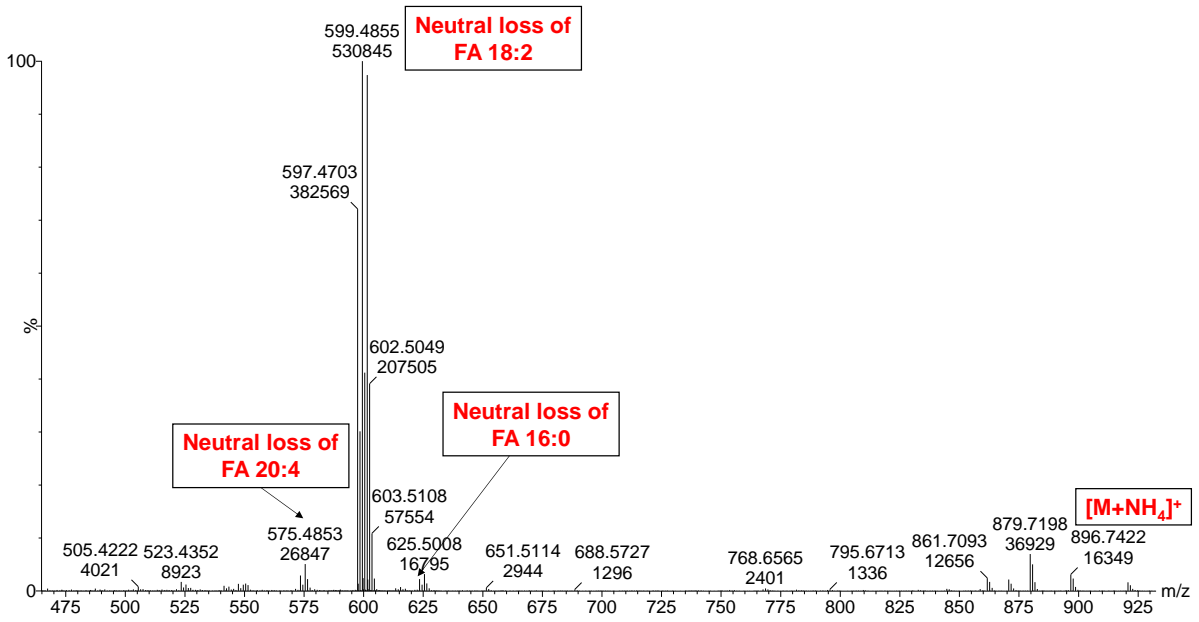


TG 54:6;O2; TG 20:4\_18:1\_16:1; ESI+, fast DDA

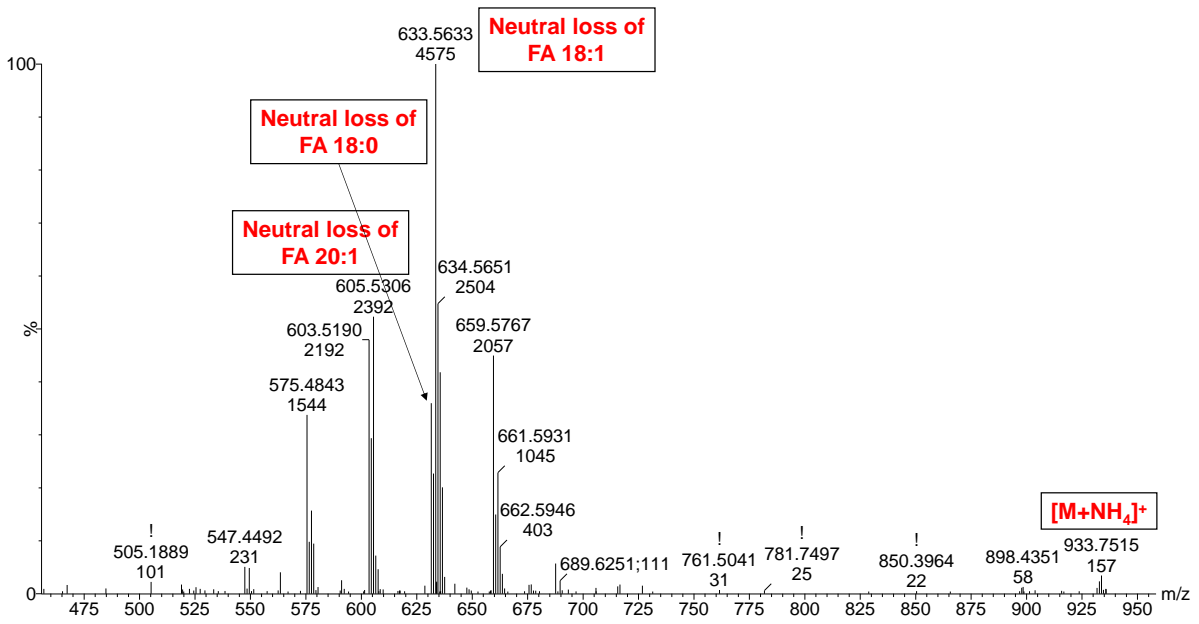




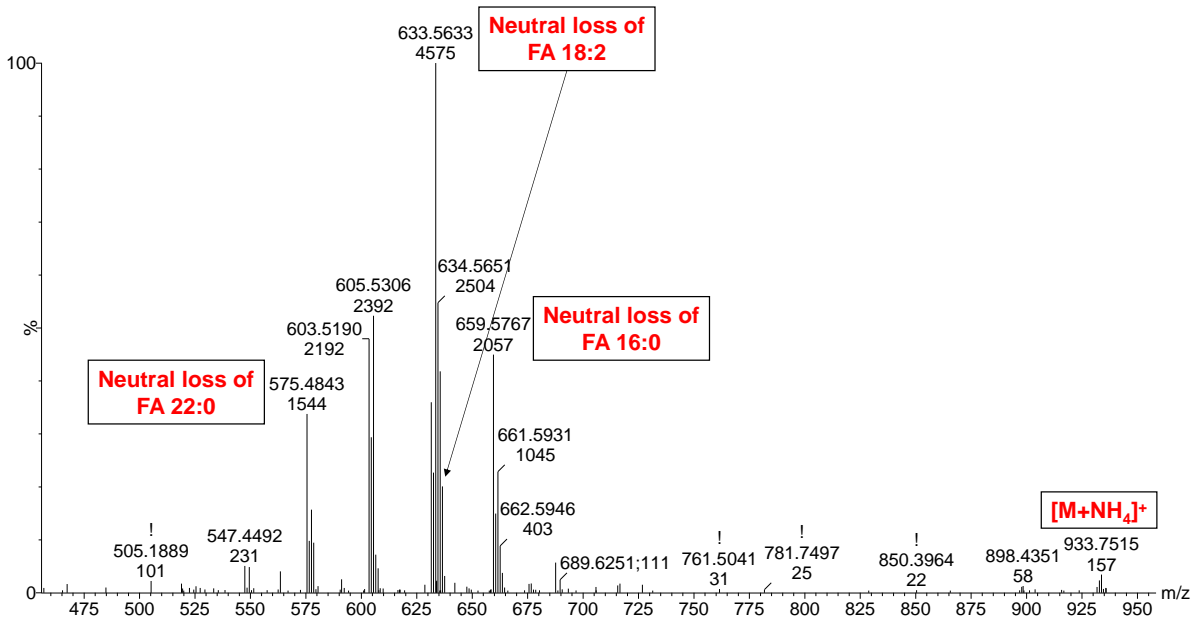
TG 54:6;O2; TG 20:4\_18:2\_16:0; ESI+, fast DDA



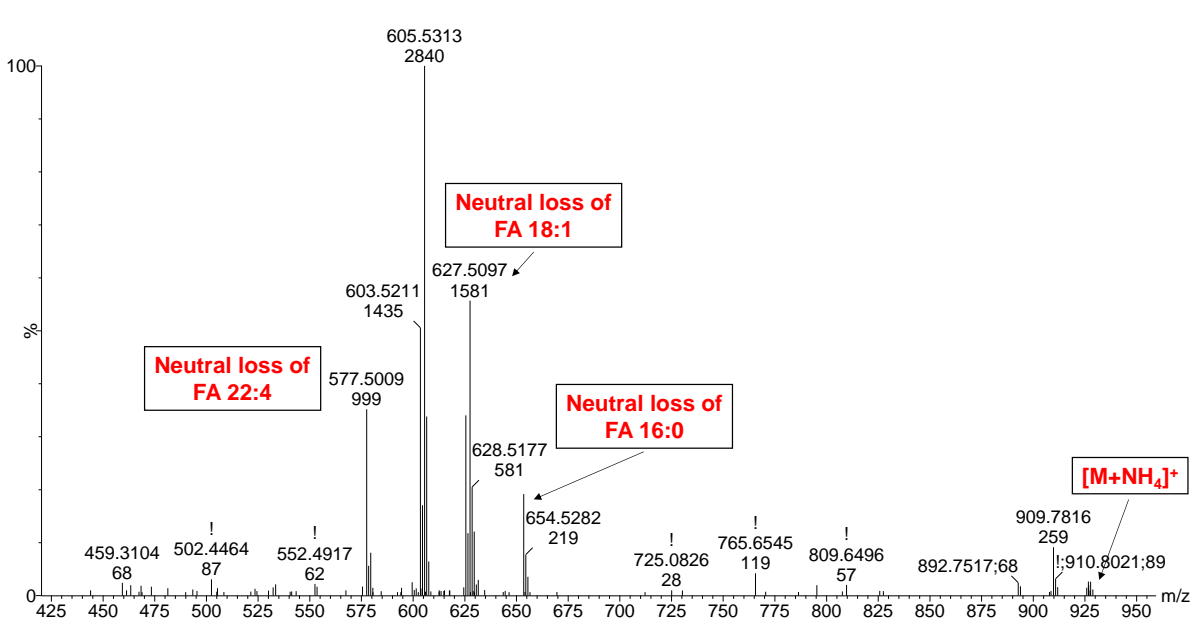
TG 56:2;O2; TG 20:1\_18:1\_18:0; ESI+, fast DDA



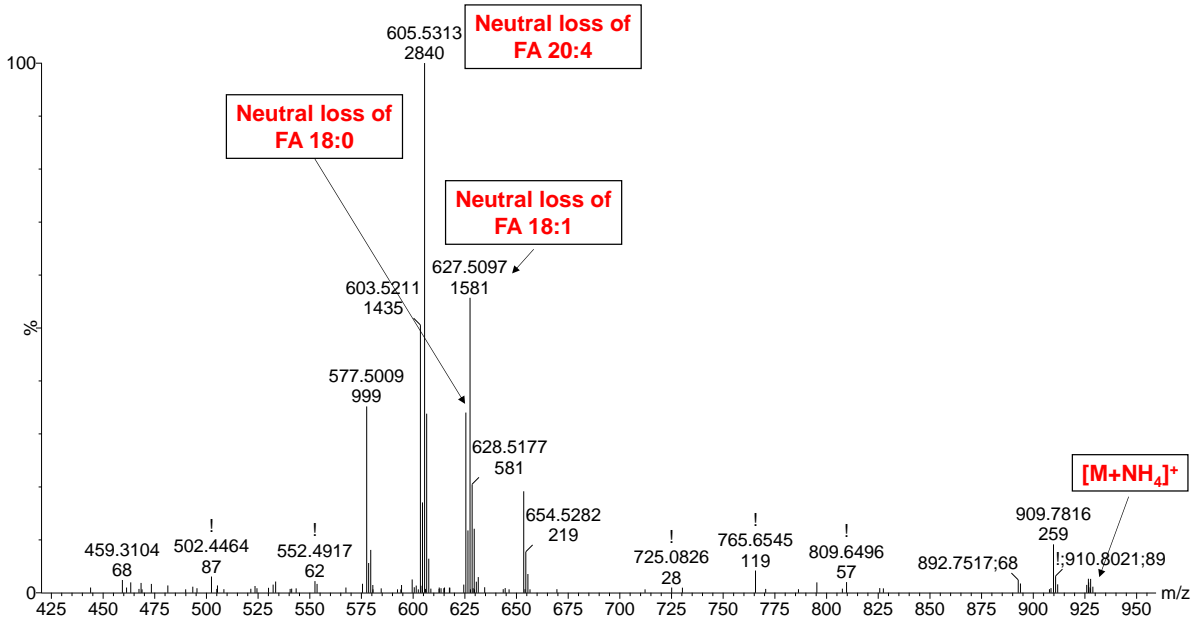
TG 56:2;O2; TG 22:0\_18:2\_16:0; ESI+, fast DDA



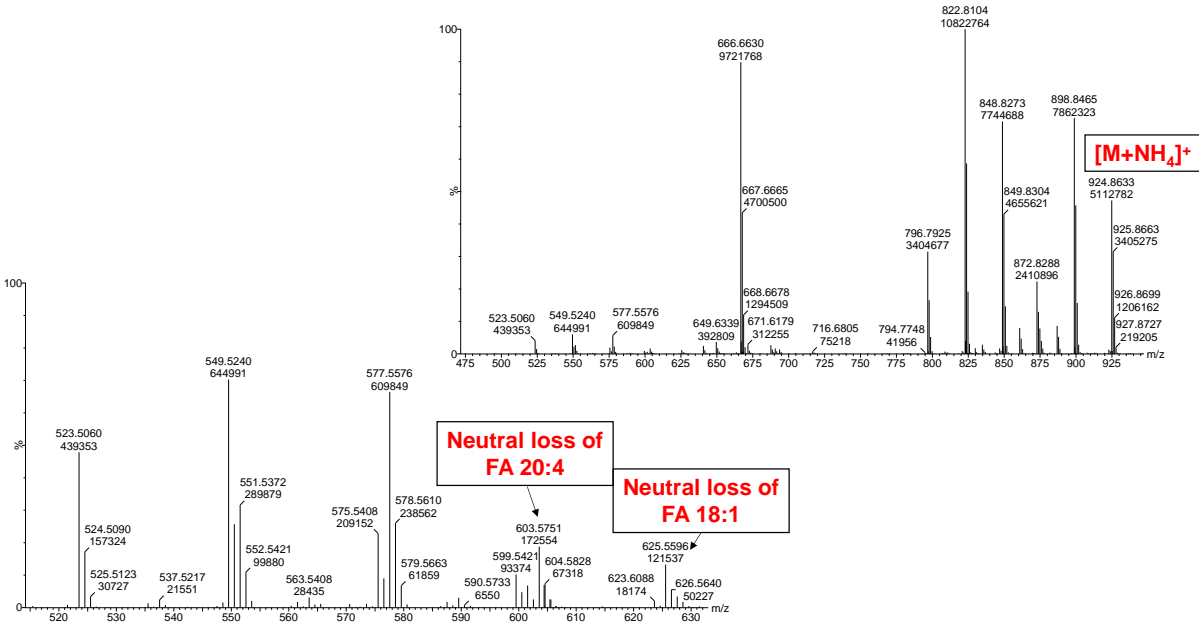
TG 56:5;O2; TG 22:4\_16:0\_18:1; ESI+, fast DDA



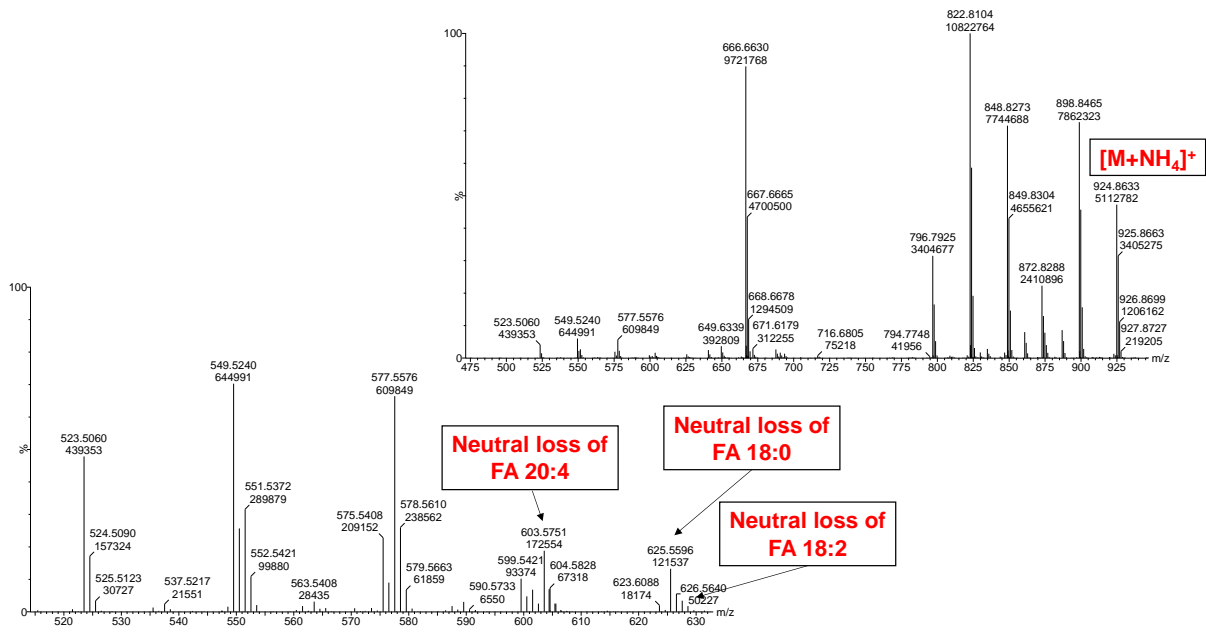
TG 56:5;O2; TG 20:4\_18:1\_18:0; ESI+, fast DDA



TG 56:6;O2; TG 18:1\_18:1\_20:4; ESI+, MS<sup>E</sup>



TG 56:6;O2; TG 18:0\_18:2\_20:4; ESI+, MS<sup>E</sup>



**Table S1.** Calculation of the lipid standard mix concentrations in body fluid.

| Lipid class  | Lipid species                  | Stock conc. [ $\mu\text{g}/\mu\text{L}$ ] | Volume [ $\mu\text{L}$ ] | StdMix [ $\mu\text{g}/\text{mL}$ ] | StdMix [ $\mu\text{g}/\text{mL}$ plasma] | StdMix [ $\text{nmol}/\text{mL}$ plasma] | Exact mass |
|--------------|--------------------------------|---|--------------------------|------------------------------------|--|--|------------|
| Cer          | Cer 18:1;O2/12:0               | 2   | 0.6                      | 1.2                                | 1.0                                      | 2.0                                      | 481.79     |
|              | Cer 18:1;O2-d7/18:0            | 1   | 1.4                      | 1.4                                | 1.1                                      | 2.0                                      | 572.59     |
| HexCer       | GlcCer 18:1;O2/12:0            | 2   | 0.4                      | 0.8                                | 0.6                                      | 1.0                                      | 643.94     |
|              | GlcCer 18:1;O2-d5/18:0         | 1   | 0.9                      | 0.9                                | 0.7                                      | 1.0                                      | 732.63     |
| Hex2Cer      | LacCer 18:1;O2/12:0            | 2   | 0.6                      | 1.2                                | 1  | 1.2                                      | 805.55     |
|              | LacCer 18:1;O2-d7/15:0         | 2   | 0.65                     | 1.3                                | 1  | 1.2                                      | 854.65     |
| GM3          | GM3 18:1;O2/16:0-d9            | 0.5                                       | 1.5                      | 0.8                                | 0.6                                      | 0.5                                      | 1179.50    |
|              | GM3 18:1;O2/18:0-d5            | 0.1                                       | 7                        | 0.7                                | 0.6                                      | 0.5                                      | 1202.80    |
| SM           | SM 18:1;O2/12:0                | 2   | 14                       | 28.0                               | 22                                       | 34.6                                     | 646.51     |
|              | SM 18:1;O2/18:1 d9             | 1   | 32                       | 32.0                               | 26                                       | 34.7                                     | 737.64     |
| PC           | PC 14:0/14:0                   | 4   | 15.9                     | 63.6                               | 51                                       | 75.1                                     | 677.50     |
|              | PC 15:0/18:1-d7                | 1   | 70.5                     | 70.5                               | 56                                       | 74.9                                     | 752.61     |
| PC P         | PC P-36:1 d9                   | 1   | 9.8                      | 9.8                                | 8  | 10.0                                     | 780.67     |
| LPC          | LPC 13:0                       | 2   | 10                       | 20.0                               | 16                                       | 35.3                                     | 453.55     |
|              | LPC 18:1 d7                    | 1   | 23                       | 23.0                               | 18                                       | 34.8                                     | 528.39     |
| PE           | PE 14:0/14:0                   | 2   | 2.4                      | 4.8                                | 4  | 6.0                                      | 635.45     |
|              | PE 15:0/18:1-d7                | 1   | 5.3                      | 5.3                                | 4  | 6.0                                      | 710.56     |
| PE P         | PE P-36:1 d9                   | 1   | 1.8                      | 1.8                                | 1  | 1.9                                      | 738.62     |
| PI           | PI 15:0/18:1                   | 1   | 6                        | 6.0                                | 5  | 5.7                                      | 839.55     |
|              | PI 15:0/18:1-d7                | 1   | 6                        | 6.0                                | 5  | 5.7                                      | 846.60     |
| CE           | CE 19:0                        | 6   | 55.5                     | 333.0                              | 266                                      | 400                                      | 666.63     |
|              | CE 16:0 d7                     | 6   | 45                       | 270.0                              | 216                                      | 342.0                                    | 631.63     |
| DG           | DG 18:1/18:1 d5                | 1   | 4.5                      | 4.5                                | 4  | 5.8                                      | 625.57     |
|              | DG 15:0/18:1-d7                | 1   | 4.2                      | 4.2                                | 3  | 5.7                                      | 587.55     |
| TG           | TG 19:1/19:1/19:1              | 4   | 16.5                     | 66.0                               | 53                                       | 57.0                                     | 926.83     |
|              | TG 15:0/18:1-d7/15:0           | 1   | 57.8                     | 57.8                               | 46                                       | 57.0                                     | 811.77     |
| Solvent      | CHCl <sub>3</sub> /MetOH (1/1) |   | 606.75                   |                                    |  |  |            |
| Total Volume |                                |   | 1000                     |                                    |  |  |            |

**Table S2.** Compositions of the solvents used for optimization of maximal injection volume in second-dimension.

| Solvent          | Composition [ $\mu\text{L}$ ] |        |        |
|------------------|-------------------------------|--------|--------|
|                  | 24 min                        | 58 min | 96 min |
| ACN              | 150                           | 112    | 56     |
| H <sub>2</sub> O | 88                            | 57.6   | 12.8   |
| IPA              | 162                           | 230.4  | 331.2  |
| StdMix           | 100                           | 100    | 100    |

**Table S3.** List of lipid species identified in pooled human plasma sample with their retention time, and observed ions in positive and negative ESI mode

| Lysophosphatidylcholines |                        |     |                                     |                                     |                          |          |                                |
|--------------------------|------------------------|-----|-------------------------------------|-------------------------------------|--------------------------|----------|--------------------------------|
| Lipid species level      | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) | m/z 184  | [M+formate] <sup>-</sup> (ppm) |
| LPC 16:0                 | LPC 16:0_0:0           | 16  | 4.97                                | 0.31                                | 496.3398 (0.7)           | 184.0733 | 540.3307 (-1.5)                |
| LPC 18:0                 | LPC 18:0_0:0           | 18  | 6.46                                | 0.31                                | 524.3711 (1.2)           | 184.0733 | 568.3620 (-1.2)                |
| LPC 18:1                 | LPC 18:1_0:0           | 16  | 5.02                                | 0.31                                | 522.3554 (1.7)           | 184.0733 | 566.3464 (-2.8)                |
| LPC 18:2                 | LPC 18:2_0:0           | 14  | 4.26                                | 0.31                                | 520.3398 (1.2)           | 184.0733 | 564.3307 (-2.1)                |
| LPC 18:3                 | LPC 18:3_0:0           | 12  | 3.47                                | 0.31                                | 518.3241 (1.7)           | 184.0733 | 562.3151 (-0.5)                |
| LPC 20:0                 | LPC 20:0_0:0           | 20  | 9.30                                | 0.31                                | 552.4024 (5.3)           | 184.0733 | 596.3933 (-2.7)                |
| LPC 20:1                 | LPC 20:1_0:0           | 18  | 6.70                                | 0.31                                | 550.3867 (-2.4)          | 184.0733 | 594.3777 (-4.0)                |
| LPC 20:2                 | LPC 20:2_0:0           | 16  | 5.37                                | 0.31                                | 548.3711 (-3.0)          | 184.0733 | 592.3620 (2.0)                 |
| LPC 20:3                 | LPC 20:3_0:0           | 14  | 4.50                                | 0.31                                | 546.3554 (-1.9)          | 184.0733 | 590.3464 (-3.0)                |
| LPC 20:4                 | LPC 20:4_0:0           | 12  | 4.18                                | 0.31                                | 544.3398 (0.1)           | 184.0733 | 588.3307 (4.8)                 |
| LPC 22:1                 | LPC 22:1_0:0           | 20  | 9.59                                | 0.31                                | 578.418 (-1.4)           | 184.0733 | 622.4089 (-3.9)                |
| LPC 22:4                 | LPC 22:4_0:0           | 14  | 4.93                                | 0.31                                | 572.3711 (3.8)           | 184.0733 | 616.3620 (2.1)                 |
| LPC 22:5                 | LPC 22:5_0:0           | 12  | 4.26                                | 0.31                                | 570.3554 (4.2)           | 184.0733 | 614.3464 (3.3)                 |
| LPC 22:6                 | LPC 22:6_0:0           | 10  | 4.00                                | 0.31                                | 568.3398 (1.1)           | 184.0733 | 612.3307 (2.4)                 |
| Fatty acids              |                        |     |                                     |                                     |                          |          |                                |
| Lipid species level      | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M-H] <sup>-</sup> (ppm) |          |                                |
| FA 14:0                  | FA 14:0                | 14  | 6.82                                | 0.03                                | 227.2017 (3.5)           |          |                                |
| FA 15:0                  | FA 15:0                | 15  | 9.20                                | 0.03                                | 241.2173 (3.3)           |          |                                |
| FA 16:0                  | FA 16:0                | 16  | 12.09                               | 0.03                                | 255.2330 (3.9)           |          |                                |
| FA 16:1                  | FA 16:1                | 14  | 8.73                                | 0.03                                | 253.2173 (1.6)           |          |                                |
| FA 17:0                  | FA 17:0                | 17  | 14.91                               | 0.03                                | 269.2486 (3.7)           |          |                                |
| FA 18:0                  | FA 18:0                | 18  | 18.07                               | 0.03                                | 283.2643 (-3.5)          |          |                                |

| FA 18:1             | FA 18:1                | 16  | 12.88                               | 0.03                                | 281.2486 (-3.6)                           |              |                                |
|---------------------|------------------------|-----|-------------------------------------|-------------------------------------|---|--------------|--------------------------------|
| FA 18:2             | FA 18:2                | 14  | 9.63                                | 0.03                                | 279.2330 (-2.9)                           |              |                                |
| FA 18:3             | FA 18:3                | 12  | 7.66                                | 0.03                                | 277.2173 (-1.4)                           |              |                                |
| FA 20:1             | FA 20:1                | 18  | 18.76                               | 0.03                                | 309.2799 (-4.8)                           |              |                                |
| FA 20:2             | FA 20:2                | 16  | 13.97                               | 0.03                                | 307.2643 (-1.3)                           |              |                                |
| FA 20:3             | FA 20:3                | 14  | 10.88                               | 0.03                                | 305.2486 (0.7)                            |              |                                |
| FA 20:4             | FA 20:4                | 12  | 9.05                                | 0.03                                | 303.2330 (-3.6)                           |              |                                |
| FA 20:5             | FA 20:5                | 10  | 7.25                                | 0.03                                | 301.2173 (1.3)                            |              |                                |
| FA 22:4             | FA 22:4                | 14  | 12.32                               | 0.03                                | 331.2643 (-3.0)                           |              |                                |
| FA 22:5             | FA 22:5                | 12  | 10.55                               | 0.03                                | 329.2486 (-1.2)                           |              |                                |
| FA 22:6             | FA 22:6                | 10  | 8.56                                | 0.03                                | 327.2330 (4.3)                            |              |                                |
| FA 24:0             | FA 24:0                | 24  | 50.74                               | 0.03                                | 367.3582 (4.9)                            |              |                                |
| <b>Ceramides</b>    |                        |     |                                     |                                     |   |              |                                |
| Lipid species level | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H-H <sub>2</sub> O] <sup>+</sup> (ppm) | N-acyl chain | [M+formate] <sup>-</sup> (ppm) |
| Cer 34:1;O2         | Cer 18:1;O2/16:0       | 32  | 42.62                               | 0.03                                | 520.5088 (-2.3)                           | 264.2686     | 582.5103 (0.5)                 |
| Cer 36:1;O2         | Cer 18:1;O2/18:0       | 34  | 50.63                               | 0.03                                | 548.5401 (-2.2)                           | 264.2686     | 610.5416 (-2.1)                |
| Cer 40:0;O2         | Cer 18:0;O2/22:0       | 40  | 64.15                               | 0.03                                | 606.6183 (1.3)                            | 266.2842     | 668.6188 (-2.1)                |
| Cer 40:1;O2         | Cer 17:1;O2/23:0       | 38  | 62.92                               | 0.03                                | 604.6027 (4.5)                            | 250.2529     | 666.6042 (4.7)                 |
|                     | Cer 18:1;O2/22:0       | 38  | 62.92                               | 0.03                                | 604.6027 (4.5)                            | 264.2686     | 666.6042 (4.7)                 |
| Cer 41:1;O2         | Cer 17:1;O2/24:0       | 39  | 65.39                               | 0.03                                | 618.6183 (-4.5)                           | 250.2529     | 680.6199 (-3.5)                |
|                     | Cer 18:1;O2/23:0       | 39  | 65.39                               | 0.03                                | 618.6183 (-4.5)                           | 264.2686     | 680.6199 (-3.5)                |
| Cer 41:2;O2         | Cer 17:1;O2/24:1       | 37  | 61.07                               | 0.03                                | 616.6027 (3.1)                            | 250.2529     | 678.6042 (-0.7)                |
|                     | Cer 18:2;O2/23:0       | 37  | 61.07                               | 0.03                                | 616.6027 (3.1)                            | 262.2529     | 678.6042 (-0.7)                |
| Cer 42:1;O2         | Cer 17:1;O2/25:0       | 40  | 67.26                               | 0.03                                | 632.6340 (-1.3)                           | 250.2529     | 694.6355 (-3.5)                |
|                     | Cer 18:1;O2/24:0       | 40  | 67.26                               | 0.03                                | 632.6340 (-1.3)                           | 264.2686     | 694.6355 (-3.5)                |
|                     | Cer 20:1;O2/22:0       | 40  | 67.26                               | 0.03                                | 632.6340 (-1.3)                           | 292.2999     | 694.6355 (-3.5)                |
| Cer 42:2;O2         | Cer 18:2;O2/24:0       | 38  | 62.36                               | 0.03                                | 630.6183 (0.5)                            | 262.2529     | 692.6199 (-5.0)                |
|                     | Cer 19:1;O2/23:1       | 38  | 62.36                               | 0.03                                | 630.6183 (0.5)                            | 278.2842     | 692.6199 (-5.0)                |
| Cer 42:3;O2         | Cer 18:2;O2/24:1       | 36  | 59.22                               | 0.03                                | 628.4724 (1.4)                            | 262.2529     | 690.6042 (-1.0)                |



| Cer 43:1;O2                 | Cer 18:1;O2/25:0       | 41  | 68.5                                | 0.03                                | 646.6496 (-3.2)          | 264.2686     | 708.6512 (-1.8)                |
|-----------------------------|------------------------|-----|-------------------------------------|-------------------------------------|--------------------------|--------------|--------------------------------|
|                             | Cer 19:1;O2/24:0       | 41  | 68.5                                | 0.03                                | 646.6496 (-3.2)          | 278.2842     | 708.6512 (-1.8)                |
| <b>Monohexosylceramides</b> |                        |     |                                     |                                     |                          |              |                                |
| Lipid species level         | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) | N-acyl chain | [M+formate] <sup>-</sup> (ppm) |
| HexCer 34:1;O2              | HexCer 18:1;O2/16:0    | 32  | 34.25                               | 0.10                                | 700.5722 (0.1)           | 264.2686     | 744.5632 (2.4)                 |
| HexCer 40:1;O2              | HexCer 18:1;O2/22:0    | 38  | 60.25                               | 0.10                                | 784.6661 (1.1)           | 264.2686     | 828.6569 (-1.9)                |
| HexCer 41:1;O2              | n.d.                   | 39  | 63.18                               | 0.10                                | 798.6818 (-1.6)          | -            | 842.6727 (4.9)                 |
| HexCer 42:1;O2              | n.d.                   | 40  | 66.03                               | 0.10                                | 812.6974 (4.7)           | -            | 856.6884 (2.5)                 |
| HexCer 42:2;O2              | n.d.                   | 38  | 60.12                               | 0.10                                | 810.6818 (4.7)           | -            | 854.6727 (2.5)                 |
| <b>Dihexosylceramised</b>   |                        |     |                                     |                                     |                          |              |                                |
| Lipid species level         | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) |              | [M+formate] <sup>-</sup> (ppm) |
| Hex2Cer 32:1;O2             | n.d.                   | 30  | 20.57                               | 0.13                                | 834.5937 (-3.0)          |              | 878.5847 (3.2)                 |
| Hex2Cer 34:1;O2             | n.d.                   | 32  | 27.99                               | 0.12                                | 862.6250 (1.2)           |              | 906.6159 (-1.2)                |
| Hex2Cer 40:1;O2             | n.d.                   | 38  | 53.35                               | 0.12                                | 946.7189 (-2.4)          |              | 990.7099 (1.0)                 |
| Hex2Cer 42:1;O2             | n.d.                   | 40  | 58.92                               | 0.12                                | 974.7502 (0.9)           |              | 1018.7412 (1.2)                |
| Hex2Cer 42:2;O2             | n.d.                   | 38  | 52.73                               | 0.12                                | 972.7346 (2.7)           |              | 1016.7255 (1.2)                |
| Hex2Cer 42:3;O2             | n.d.                   | 36  | 47.16                               | 0.12                                | 970.7233 (-0.8)          |              | 1014.7099 (2.3)                |
| <b>GM3 gangliosides</b>     |                        |     |                                     |                                     |                          |              |                                |
| Lipid species level         | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] |                          |              | [M-H] <sup>-</sup> (ppm)       |
| GM3 34:1;O2                 | n.d.                   | 32  | 20.01                               | 0.19                                |                          |              | 1151.7059 (-3.1)               |
| GM3 36:1;O2                 | n.d.                   | 34  | 26.82                               | 0.19                                |                          |              | 1179.7372 (-4.0)               |
| GM3 36:2;O2                 | n.d.                   | 32  | 20.64                               | 0.19                                |                          |              | 1177.7215 (-4.2)               |
| GM3 38:1;O2                 | n.d.                   | 36  | 35.48                               | 0.19                                |                          |              | 1207.7685 (-0.5)               |
| GM3 38:2;O2                 | n.d.                   | 34  | 31.51                               | 0.19                                |                          |              | 1205.7528 (-3.6)               |
| GM3 40:1;O2                 | n.d.                   | 38  | 43.51                               | 0.19                                |                          |              | 1235.7998 (-4.8)               |
| GM3 40:2;O2                 | n.d.                   | 36  | 37.33                               | 0.19                                |                          |              | 1233.7841 (-1.6)               |
| GM3 42:1;O2                 | n.d.                   | 40  | 50.94                               | 0.19                                |                          |              | 1263.8311 (-4.0)               |
| GM3 42:2;O2                 | n.d.                   | 38  | 43.51                               | 0.19                                |                          |              | 1261.8154 (-3.0)               |

| GM3 42:3;O2          |                        | n.d. |                                     | 36                                  | 36.71                    | 0.19     | 1259.7998 (-4.7)               |                             |
|----------------------|------------------------|------|-------------------------------------|-------------------------------------|--------------------------|----------|--------------------------------|-----------------------------|
| Sphingomyelins       |                        |      |                                     |                                     |                          |          |                                |                             |
| Lipid species level  | Lipid acyl/alkyl level | ECN  | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) | m/z 184  | [M+formate] <sup>-</sup> (ppm) |                             |
| SM 32:1;O2           | n.d.                   | 30   | 20.95                               | 0.28                                | 675.5436 (2.8)           | 184.0733 | 719.5346 (4.9)                 |                             |
| SM 33:1;O2           | n.d.                   | 31   | 24.71                               | 0.28                                | 689.5592 (0.9)           | 184.0733 | 733.5502 (-1.3)                |                             |
| SM 34:0;O2           | n.d.                   | 34   | 30.94                               | 0.28                                | 705.5905 (-0.4)          | 184.0733 | 749.5812 (-3.8)                |                             |
| SM 34:1;O2           | n.d.                   | 32   | 32.17                               | 0.28                                | 703.5749 (3.4)           | 184.0733 | 747.5659 (-3.7)                |                             |
| SM 34:2;O2           | n.d.                   | 30   | 28.86                               | 0.28                                | 701.5592 (1.3)           | 184.0733 | 745.5502 (-3.4)                |                             |
| SM 35:1;O2           | n.d.                   | 33   | 22.37                               | 0.28                                | 717.5905 (2.1)           | 184.0733 | 761.5815 (-0.7)                |                             |
| SM 36:1;O2           | n.d.                   | 34   | 38.32                               | 0.28                                | 731.6062 (1.6)           | 184.0733 | 775.5972 (3.5)                 |                             |
| SM 36:2;O2           | n.d.                   | 32   | 31.08                               | 0.28                                | 729.5905 (2.6)           | 184.0733 | 773.5815 (0.7)                 |                             |
| SM 38:1;O2           | n.d.                   | 36   | 48.20                               | 0.28                                | 759.6375 (-1.8)          | 184.0733 | 803.6285 (-2.9)                |                             |
| SM 38:2;O2           | n.d.                   | 34   | 40.44                               | 0.28                                | 757.6218 (0.3)           | 184.0733 | 801.6128 (-4.8)                |                             |
| SM 39:1;O2           | n.d.                   | 37   | 52.72                               | 0.28                                | 773.6531 (0.4)           | 184.0733 | 817.6441 (2.3)                 |                             |
| SM 40:1;O2           | n.d.                   | 38   | 56.15                               | 0.28                                | 787.6688 (3.0)           | 184.0733 | 831.6598 (3.2)                 |                             |
| SM 40:2;O2           | n.d.                   | 36   | 50.08                               | 0.28                                | 785.6531 (3.1)           | 184.0733 | 829.6441 (0.4)                 |                             |
| SM 41:1;O2           | n.d.                   | 39   | 59.75                               | 0.28                                | 801.6844 (3.4)           | 184.0733 | 845.6754 (-4.3)                |                             |
| SM 41:2;O2           | n.d.                   | 37   | 54.20                               | 0.28                                | 799.6688 (1.5)           | 184.0733 | 843.6598 (-3.9)                |                             |
| SM 42:1;O2           | n.d.                   | 40   | 62.76                               | 0.28                                | 815.7001 (3.2)           | 184.0733 | 859.6911 (4.2)                 |                             |
| SM 42:2;O2           | n.d.                   | 38   | 56.15                               | 0.28                                | 813.6844 (2.0)           | 184.0733 | 857.6754 (4.4)                 |                             |
| SM 42:3;O2           | n.d.                   | 36   | 49.91                               | 0.28                                | 811.6688 (0.1)           | 184.0733 | 855.6598 (2.2)                 |                             |
| SM 43:2;O2           | n.d.                   | 39   | 58.24                               | 0.28                                | 827.7001 (1.2)           | 184.0733 | 871.6911 (4.2)                 |                             |
| Phosphatidylcholines |                        |      |                                     |                                     |                          |          |                                |                             |
| Lipid species level  | Lipid acyl/alkyl level | ECN  | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) | m/z 184  | [M+formate] <sup>-</sup> (ppm) | sn-1/sn-2 RCOO <sup>-</sup> |
| PC 30:0              | PC 14:0/16:0           | 30   | 28.95                               | 0.22                                | 706.5381 (5.7)           | 184.0733 | 750.5291 (2.7)                 | 227.2017 / 255.233          |
| PC 32:0              | PC 16:0/16:0           | 32   | 39.78                               | 0.22                                | 734.5694 (2.0)           | 184.0733 | 778.5604 (3.9)                 | 255.2330                    |
| PC 32:1              | PC 16:0/16:1           | 30   | 32.17                               | 0.22                                | 732.5538 (3.0)           | 184.0733 | 776.5447 (-0.4)                | 255.2330 / 253.2173         |
| PC 32:2              | PC 14:0/18:2           | 28   | 25.83                               | 0.22                                | 730.5381 (0.8)           | 184.0733 | 774.5291 (-2.2)                | 227.2017 / 279.2330         |

|         |              |    |       |      |                |          |                 |                     |
|---------|--------------|----|-------|------|----------------|----------|-----------------|---------------------|
| PC 33:1 | PC 15:0/18:1 | 31 | 36.63 | 0.22 | 746.5694 (0.8) | 184.0733 | 790.5604 (2.8)  | 241.2173 / 281.2486 |
| PC 33:2 | PC 15:0/18:2 | 29 | 28.29 | 0.22 | 744.5538 (3.9) | 184.0733 | 788.5447 (-1.6) | 241.2173 / 279.2330 |
| PC 34:0 | PC 18:0/16:0 | 34 | 49.09 | 0.22 | 762.6007 (2.4) | 184.0733 | 806.5917 (4.8)  | 283.2643 / 255.2330 |
| PC 34:1 | PC 16:0/18:1 | 32 | 41.16 | 0.22 | 760.5851 (3.7) | 184.0733 | 804.5760 (-4.4) | 255.2330 / 281.2486 |
| PC 34:2 | PC 16:0/18:2 | 30 | 34.44 | 0.22 | 758.5694 (3.7) | 184.0733 | 802.5604 (-4.7) | 255.2330 / 279.2330 |
| PC 34:3 | PC 16:0/18:3 | 28 | 28.77 | 0.22 | 756.5538 (3.3) | 184.0733 | 800.5447 (4.5)  | 255.2330 / 277.2173 |
| PC 34:4 | PC 14:0/20:4 | 26 | 24.97 | 0.22 | 754.5381 (2.1) | 184.0733 | 798.5291 (2.5)  | 227.2017 / 303.2330 |
| PC 35:1 | PC 17:0/18:1 | 33 | 46.01 | 0.22 | 774.6007 (1.9) | 184.0733 | 818.5917 (2.3)  | 269.2486 / 281.2486 |
| PC 35:2 | PC 17:0/18:2 | 31 | 39.10 | 0.22 | 772.5851 (3.1) | 184.0733 | 816.5760 (2.7)  | 269.2486 / 279.2330 |
| PC 35:3 | PC 15:0/20:3 | 29 | 31.32 | 0.22 | 770.5694 (1.9) | 184.0733 | 814.5604 (4.3)  | 241.2173 / 305.2486 |
| PC 35:4 | PC 15:0/20:4 | 37 | 29.07 | 0.22 | 768.5538 (0.7) | 184.0733 | 812.5447 (0.1)  | 241.2173 / 303.2330 |
| PC 36:1 | PC 18:0/18:1 | 34 | 50.41 | 0.22 | 788.6164 (3.6) | 184.0733 | 832.6073 (0.4)  | 283.2643 / 281.2486 |
| PC 36:2 | PC 18:0/18:2 | 32 | 43.90 | 0.22 | 786.6007 (4.2) | 184.0733 | 830.5917 (-0.4) | 283.2643 / 279.2330 |
| PC 36:3 | PC 16:0/20:3 | 30 | 37.19 | 0.22 | 784.5851 (3.4) | 184.0733 | 828.5760 (-0.8) | 255.2330 / 305.2486 |
|         | PC 18:1/18:2 | 30 | 35.70 | 0.22 | 784.5851 (2.3) | 184.0733 | 828.5760 (-0.8) | 281.2486 / 279.2330 |
| PC 36:4 | PC 18:2/18:2 | 28 | 33.48 | 0.22 | 782.5694 (3.8) | 184.0733 | 826.5604 (-2.1) | 279.2330            |
|         | PC 16:0/20:4 | 28 | 33.48 | 0.22 | 782.5694 (3.8) | 184.0733 | 826.5604 (-2.1) | 255.2330 / 303.2330 |
| PC 36:5 | PC 16:0/20:5 | 26 | 28.06 | 0.22 | 780.5538 (2.8) | 184.0733 | 824.5447 (-2.1) | 255.2330 / 301.2173 |
| PC 37:3 | PC 17:0/20:3 | 31 | 41.16 | 0.22 | 798.6007 (3.1) | 184.0733 | 842.5917 (1.3)  | 269.2486 / 305.2486 |
| PC 37:4 | PC 17:0/20:4 | 29 | 34.44 | 0.22 | 796.5851 (1.4) | 184.0733 | 840.5760 (3.9)  | 269.2486 / 303.2330 |
| PC 38:2 | PC 18:1/20:1 | 34 | 51.70 | 0.22 | 814.6320 (3.2) | 184.0733 | 858.6230 (-3.6) | 281.2486 / 309.2799 |
|         | PC 18:0_20:2 | 34 | 51.70 | 0.22 | 814.6320 (3.2) | 184.0733 | 858.6230 (-3.6) | 283.2643 / 307.2643 |
| PC 38:3 | PC 18:0/20:3 | 32 | 46.49 | 0.22 | 812.6164 (2.3) | 184.0733 | 856.6073 (-4.4) | 283.2643 / 305.2486 |
| PC 38:4 | PC 18:1/20:3 | 30 | 42.76 | 0.22 | 810.6007 (3.6) | 184.0733 | 854.5917 (-4.6) | 281.2486 / 305.2486 |
|         | PC 18:0/20:4 | 30 | 42.76 | 0.22 | 810.6007 (3.6) | 184.0733 | 854.5917 (-4.6) | 283.2643 / 303.2330 |
| PC 38:5 | PC 16:0/22:5 | 28 | 34.44 | 0.22 | 808.5851 (1.5) | 184.0733 | 852.5760 (3.2)  | 255.2330 / 329.2486 |
|         | PC 18:1/20:4 | 28 | 34.44 | 0.22 | 808.5851 (1.5) | 184.0733 | 852.5760 (3.2)  | 281.2486 / 303.2330 |
|         | PC 18:0/20:5 | 28 | 37.19 | 0.22 | 808.5851 (3.0) | 184.0733 | 852.5760 (3.2)  | 283.2643 / 301.2173 |
| PC 38:6 | PC 16:0/22:6 | 26 | 31.52 | 0.22 | 806.5694 (3.3) | 184.0733 | 850.5604 (2.5)  | 255.2330 / 327.2330 |

|  | PC 18:2/20:4           | 26  | 31.52                               | 0.22                                | 806.5694 (3.3)           | 184.0733                 | 850.5604 (2.5)                 | 279.2330 / 303.2330    |
|--|------------------------|-----|-------------------------------------|-------------------------------------|--------------------------|--------------------------|--------------------------------|------------------------|
| PC 40:4                                    | PC 18:0/22:4           | 32  | 49.27                               | 0.22                                | 838.6320 (1.8)           | 184.0733                 | 882.6230 (2.0)                 | 283.2643 / 331.2643    |
| PC 40:5                                    | PC 18:0_22:5           | 30  | 43.53                               | 0.22                                | 836.6164 (2.3)           | 184.0733                 | 880.6073 (-3.3)                | 283.2643 / 329.2486    |
|  | PC 20:1_20:4           | 30  | 43.53                               | 0.22                                | 836.6164 (2.3)           | 184.0733                 | 880.6073 (-3.3)                | 309.2799 / 303.2330    |
| PC 40:6                                    | PC 18:0/22:6           | 28  | 40.83                               | 0.22                                | 834.6007 (3.5)           | 184.0733                 | 878.5917 (-2.8)                | 283.2643 / 327.2330    |
| PC 40:7                                    | PC 18:1/22:6           | 27  | 32.77                               | 0.22                                | 832.5851 (1.9)           | 184.0733                 | 876.5760 (-3.9)                | 281.2486 / 327.2330    |
| PC 40:8                                    | n.d.                   | 26  | 26.69                               | 0.22                                | 830.5695 (2.3)           | 184.0733                 | 874.5604 (-2.9)                | n.d.                   |
| <b>Phosphatidylcholines - plasmalogens</b> |                        |     |                                     |                                     |                          |                          |                                |                        |
| Lipid species level                        | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) | m/z 184                  | [M+formate] <sup>-</sup> (ppm) | sn-2 RCOO <sup>-</sup> |
| PC P-32:0                                  | PC P-16:0/16:0         | 32  | 44.03                               | 0.22                                | 718.5745 (-1.3)          | 184.0733                 | 762.5655 (4.7)                 | 255.2330               |
| PC P-34:1                                  | PC P-16:0/18:1         | 32  | 45.35                               | 0.22                                | 744.5902 (0.4)           | 184.0733                 | 788.5811 (-2.3)                | 281.2486               |
| PC P-34:2                                  | PC P-16:0/18:2         | 30  | 38.32                               | 0.22                                | 742.5745 (0.8)           | 184.0733                 | 786.5655 (-1.0)                | 279.2330               |
| PC P-36:2                                  | PC P-18:0/18:2         | 32  | 46.55                               | 0.22                                | 770.6058 (-0.4)          | 184.0733                 | 814.5968 (4.2)                 | 279.2330               |
| PC P-36:3                                  | PC P-18:1/18:2         | 30  | 38.68                               | 0.22                                | 768.5902 (2.7)           | 184.0733                 | 812.5811 (2.3)                 | 279.2330               |
| PC P-38:4                                  | PC P-18:0/20:4         | 30  | 39.60                               | 0.22                                | 794.6058 (2.6)           | 184.0733                 | 838.5968 (-3.5)                | 303.2330               |
| <b>Phosphatidylethanolamines</b>           |                        |     |                                     |                                     |                          |                          |                                |                        |
| Lipid species level                        | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) | [M-H] <sup>-</sup> (ppm) | sn-1/sn-2 RCOO <sup>-</sup>    |                        |
| PE 34:1                                    | PE 16:0/18:1           | 32  | 41.61                               | 0.14                                | 718.5381 (2.9)           | 716.5236 (-2.8)          | 255.2330 / 281.2486            |                        |
| PE 34:2                                    | PE 16:0/18:2           | 30  | 34.81                               | 0.14                                | 716.5225 (3.8)           | 714.5079 (-2.5)          | 255.2330 / 279.2330            |                        |
| PE 36:1                                    | PE 18:0/18:1           | 34  | 49.65                               | 0.14                                | 746.5694 (2.0)           | 744.5549 (1.9)           | 283.2643 / 281.2486            |                        |
| PE 36:2                                    | PE 18:0/18:2           | 32  | 44.08                               | 0.14                                | 744.5538 (2.6)           | 742.5392 (3.5)           | 283.2643 / 279.2330            |                        |
| PE 36:3                                    | PE 18:1/18:2           | 30  | 36.04                               | 0.14                                | 742.5381 (2.4)           | 740.5236 (2.8)           | 281.2486 / 279.2330            |                        |
| PE 36:4                                    | PE 16:0/20:4           | 28  | 33.57                               | 0.14                                | 740.5225 (4.9)           | 738.5079 (-1.8)          | 255.2330 / 303.2330            |                        |
| PE 38:3                                    | PE 18:0/20:3           | 32  | 45.93                               | 0.14                                | 770.5694 (2.9)           | 768.5549 (-3.3)          | 283.2643 / 305.2486            |                        |
| PE 38:4                                    | PE 18:0/20:4           | 30  | 42.84                               | 0.14                                | 768.5538 (4.6)           | 766.5392 (-4.2)          | 283.2643 / 303.2330            |                        |
| PE 38:5                                    | PE 18:1/20:4           | 28  | 37.28                               | 0.14                                | 766.5381 (2.5)           | 764.5236 (-1.0)          | 281.2486 / 303.2330            |                        |
| PE 38:6                                    | PE 16:0/22:6           | 26  | 31.72                               | 0.14                                | 764.5225 (3.5)           | 762.5079 (-3.5)          | 255.2330 / 327.2330            |                        |
| PE 40:4                                    | PE 18:0/22:4           | 32  | 48.42                               | 0.14                                | 796.5851 (4.0)           | 794.5705 (-2.8)          | 283.2643 / 331.2643            |                        |

| PE 40:5                                  | PE 18:0/22:5           | 30  | 43.46                               | 0.14                                | 794.5694 (3.1)           | 792.5549 (-4.5)   | 283.2643 / 329.2486      |                        |
|--|------------------------|-----|-------------------------------------|-------------------------------------|--------------------------|---|--------------------------|------------------------|
| PE 40:6                                  | PE 18:0/22:6           | 28  | 40.99                               | 0.14                                | 792.5538 (3.2)           | 790.5392 (-4.8)   | 283.2643 / 327.2330      |                        |
| PE 40:7                                  | PE 18:1/22:6           | 26  | 38.04                               | 0.14                                | 790.5381 (4.7)           | 788.5236 (-0.1)   | 281.2486 / 327.2330      |                        |
| Phosphatidylethanolamines - plasmalogens |                        |     |                                     |                                     |                          |   |                          |                        |
| Lipid species level                      | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+H] <sup>+</sup> (ppm) | [R <sub>2</sub> COO(C <sub>3</sub> H <sub>5</sub> )OH] <sup>+</sup> | [M-H] <sup>-</sup> (ppm) | sn-2 RCOO <sup>-</sup> |
| PE P-34:1                                | PE P-16:0/18:1         | 32  | 45.31                               | 0.14                                | 702.5432 (4.8)           | 339.2894  | 700.5287 (-4.6)          | 281.2486               |
| PE P-34:2                                | PE P-16:0/18:2         | 30  | 39.13                               | 0.14                                | 700.5276 (4.0)           | 337.2737  | 698.513 (-0.7)           | 279.2330               |
| PE P-36:1                                | PE P-18:0/18:1         | 34  | 56.57                               | 0.14                                | 730.5745 (-1.2)          | 339.2894  | 728.5600 (-0.7)          | 281.2486               |
| PE P-36:2                                | PE P-18:0/18:2         | 32  | 50.92                               | 0.14                                | 728.5589 (1.9)           | 339.2894  | 726.5443 (-1.5)          | 279.2330               |
| PE P-36:3                                | PE P-18:1/18:2         | 30  | 42.70                               | 0.14                                | 726.5432 (2.9)           | 337.2737  | 724.5287 (-1.2)          | 279.2330               |
| PE P-36:4                                | PE P-16:0/20:4         | 28  | 40.21                               | 0.14                                | 724.5276 (-0.7)          | 361.2737  | 722.513 (2.2)            | 303.2330               |
| PE P-36:5                                | PE P-16:0/20:5         | 26  | 34.39                               | 0.14                                | 722.5119 (2.1)           | 359.2581  | 720.4974 (-4.3)          | 301.2173               |
| PE P-38:2                                | PE P-20:0/18:2         | 34  | 54.6                                | 0.14                                | 756.5902 (4.5)           | 337.2737  | 754.5756 (3.8)           | 279.2330               |
| PE P-38:3                                | PE P-18:0/20:3         | 32  | 49.65                               | 0.14                                | 754.5745 (-2.4)          | 363.2894  | 752.5600 (-3.6)          | 305.2486               |
| PE P-38:4                                | PE P-18:0/20:4         | 30  | 49.71                               | 0.14                                | 752.5589 (4.7)           | 361.2737  | 750.5443 (-2.1)          | 303.2330               |
| PE P-38:5                                | PE P-18:1/20:4         | 28  | 41.38                               | 0.14                                | 750.5432 (-2.3)          | 361.2737  | 748.5287 (-2.4)          | 303.2330               |
| PE P-38:6                                | PE P-16:0/22:6         | 26  | 38.21                               | 0.14                                | 748.5276 (2.1)           | 385.2737  | 746.513 (-0.1)           | 327.2330               |
| PE P-40:4                                | PE P-20:0/20:4         | 32  | 51.51                               | 0.14                                | 780.5902 (1.8)           | 361.2737  | 778.5756 (4.8)           | 303.2330               |
| PE P-40:5                                | PE P-20:1/20:4         | 30  | 50.51                               | 0.14                                | 778.5745 (-2.2)          | 361.2737  | 776.5600 (2.7)           | 303.2330               |
| PE P-40:6                                | PE P-18:0/22:6         | 28  | 44.7                                | 0.14                                | 776.5589 (-1.0)          | 385.2737  | 774.5443 (1.9)           | 327.2330               |
| Phosphatidylinositols                    |                        |     |                                     |                                     |                          |   |                          |                        |
| Lipid species level                      | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M-H] <sup>-</sup> (ppm) | sn-1/sn-2 RCOO <sup>-</sup>   |                          |                        |
| PI 32:1                                  | PI 16:0_16:1           | 30  | 25.43                               | 0.16                                | 807.5029 (-1.2)          | 255.2330 / 253.2173   |                          |                        |
| PI 34:1                                  | PI 16:0_18:1           | 32  | 33.47                               | 0.16                                | 835.5342 (-2.9)          | 255.2330 / 281.2486   |                          |                        |
| PI 34:2                                  | PI 16:0_18:2           | 30  | 27.27                               | 0.16                                | 833.5186 (-4.1)          | 255.2330 / 279.2330   |                          |                        |
| PI 36:1                                  | PI 18:0_18:1           | 34  | 42.11                               | 0.16                                | 863.5655 (1.8)           | 283.2643 / 281.2486   |                          |                        |
| PI 36:2                                  | PI 18:0_18:2           | 32  | 35.8                                | 0.16                                | 861.5499 (0.3)           | 283.2643 / 279.2330   |                          |                        |
| PI 36:3                                  | PI 18:1_18:2           | 30  | 29.69                               | 0.16                                | 859.5342 (-2.3)          | 281.2486 / 279.2330   |                          |                        |

| PI 36:4             | PI 16:0_20:4           | 28  | 26.64                               | 0.16                                | 857.5186 (0.9)                          | 255.2330 / 303.2330                 |                                       |
|---------------------|------------------------|-----|-------------------------------------|-------------------------------------|---|-------------------------------------|---------------------------------------|
| PI 38:3             | PI 18:0_20:3           | 32  | 41.22                               | 0.16                                | 887.5655 (1.9)                          | 283.2643 / 305.2486                 |                                       |
| PI 38:4             | PI 18:0_20:4           | 30  | 35.05                               | 0.16                                | 885.5499 (3.7)                          | 283.2643 / 303.2330                 |                                       |
| PI 38:5             | PI 18:0_22:5           | 28  | 30.72                               | 0.16                                | 883.5342 (4.0)                          | 281.2486 / 303.2330                 |                                       |
| PI 38:6             | PI 16:0_22:6           | 26  | 25.09                               | 0.16                                | 881.5186 (-2.3)                         | 255.2330 / 327.2330                 |                                       |
| PI 40:4             | PI 18:0_22:4           | 32  | 41.24                               | 0.16                                | 913.5812 (-0.8)                         | 283.2643 / 331.2643                 |                                       |
| PI 40:5             | PI 18:0_22:5           | 30  | 35.63                               | 0.16                                | 911.5655 (-2.7)                         | 283.2643 / 329.2486                 |                                       |
| PI 40:6             | PI 18:0_22:6           | 28  | 33.21                               | 0.16                                | 909.5499 (3.3)                          | 283.2643 / 327.2330                 |                                       |
| Diacylglycerols     |                        |     |                                     |                                     |   |                                     |                                       |
| Lipid species level | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+NH <sub>4</sub> ] <sup>+</sup> (ppm) | [M+H-H <sub>2</sub> O] <sup>+</sup> | Neutral loss of <i>sn-1/sn-2/sn-3</i> |
| DG 30:0             | DG 14:0_16:0           | 30  | 49.51                               | 0.03                                | 558.5092 (4.3)                          | 523.4721                            | 313.2737 / 285.2424                   |
| DG 32:0             | DG 16:0/16:0           | 32  | 56.68                               | 0.03                                | 586.5405 (4.7)                          | 551.5034                            | 313.2737                              |
| DG 32:1             | DG 16:0_16:1           | 30  | 50.83                               | 0.03                                | 584.5248 (4.4)                          | 549.4877                            | 311.2581 / 313.2737                   |
|                     | DG 18:1_14:0           | 30  | 50.83                               | 0.03                                | 584.5248 (4.4)                          | 549.4877                            | 339.2894 / 285.2424                   |
| DG 32:2             | DG 18:1_14:0           | 28  | 44.29                               | 0.03                                | 582.5092 (4.9)                          | 547.4721                            | 337.2737 / 285.2424                   |
| DG 34:0             | DG 16:0_18:0           | 34  | 66.3                                | 0.03                                | 614.5718 (4.2)                          | 579.5347                            | 341.3050 / 313.2737                   |
| DG 34:1             | DG 16:0_18:1           | 32  | 61.18                               | 0.03                                | 612.5561 (1.6)                          | 577.5190                            | 339.2894 / 313.2737                   |
| DG 34:2             | DG 16:1_18:1           | 30  | 56.51                               | 0.03                                | 610.5405 (3.9)                          | 575.5034                            | 339.2894 / 311.2581                   |
|                     | DG 16:0_18:2           | 30  | 56.51                               | 0.03                                | 610.5405 (3.9)                          | 575.5034                            | 337.2737 / 313.2737                   |
| DG 34:3             | DG 18:2_16:1           | 28  | 46.26                               | 0.03                                | 608.5248 (4.6)                          | 573.4877                            | 337.2737 / 311.2581                   |
| DG 35:1             | DG 18:1_17:0           | 33  | 59.94                               | 0.03                                | 626.5718 (-2.9)                         | 591.5347                            | 339.2894 / 327.2894                   |
| DG 36:0             | DG 18:0/18:0           | 36  | 71.63                               | 0.03                                | 642.6031 (-1.4)                         | 607.5660                            | 341.3050                              |
| DG 36:1             | DG 18:0_18:1           | 34  | 66.95                               | 0.03                                | 640.5874 (1.4)                          | 605.5503                            | 339.2894 / 341.3050                   |
| DG 36:2             | DG 18:1/18:1           | 32  | 61.92                               | 0.03                                | 638.5718 (3.9)                          | 603.5347                            | 339.2894                              |
| DG 36:3             | DG 18:1_18:2           | 30  | 57.02                               | 0.03                                | 636.5561 (4.4)                          | 601.5190                            | 339.2894 / 337.2737                   |
| DG 36:4             | DG 18:1_18:3           | 28  | 51.92                               | 0.03                                | 634.5405 (4.3)                          | 599.5034                            | 335.2588 / 339.2894                   |
|                     | DG 18:2/18:2           | 26  | 51.92                               | 0.03                                | 634.5405 (4.3)                          | 599.5034                            | 337.2737                              |
| DG 38:4             | n.d.                   | 30  | 54.72                               | 0.03                                | 662.5718 (4.5)                          | 627.5347                            | n.d.                                  |

| DG 38:5                      | DG 18:1_20:4           | 28  | 51.47                               | 0.03                                | 660.5561 (4.8)                          | 625.519             | 361.2737 / 339.2894                                      |
|------------------------------|------------------------|-----|-------------------------------------|-------------------------------------|---|---------------------|--|
| DG 38:6                      | n.d.                   | 26  | 46.25                               | 0.03                                | 658.5405 (5.0)                          | 623.5034            | n.d.   |
| Cholesterol and sterolesters |                        |     |                                     |                                     |   |                     |  |
| Lipid species level          | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+NH <sub>4</sub> ] <sup>+</sup> (ppm) | m/z 369             |  |
| Chol                         | Chol                   | -   | 31.24                               | 0.03                                | -                                       | 369.3516            |  |
| SE 27:1/16:0                 | SE 27:1/16:0           | 16  | 89.69                               | 0.03                                | 642.6183 (-1.7)                         | 369.3516            |  |
| SE 27:1/16:1                 | SE 27:1/16:1           | 14  | 86.56                               | 0.03                                | 640.6027 (0.5)                          | 369.3516            |  |
| SE 27:1/18:0                 | SE 27:1/18:0           | 18  | 91.99                               | 0.03                                | 670.6496 (0.4)                          | 369.3516            |  |
| SE 27:1/18:1                 | SE 27:1/18:1           | 16  | 89.81                               | 0.03                                | 668.6340 (2.5)                          | 369.3516            |  |
| SE 27:1/18:2                 | SE 27:1/18:2           | 14  | 87.07                               | 0.03                                | 666.6183 (4.3)                          | 369.3516            |  |
| SE 27:1/18:3                 | SE 27:1/18:3           | 12  | 84.62                               | 0.03                                | 664.6027 (0.2)                          | 369.3516            |  |
| SE 27:1/20:1                 | SE 27:1/20:1           | 18  | 94.26                               | 0.03                                | 696.6653 (3.6)                          | 369.3516            |  |
| SE 27:1/20:2                 | SE 27:1/20:2           | 16  | 90.19                               | 0.03                                | 694.6496 (0.6)                          | 369.3516            |  |
| SE 27:1/20:3                 | SE 27:1/20:3           | 14  | 87.62                               | 0.03                                | 692.6340 (4.6)                          | 369.3516            |  |
| SE 27:1/20:4                 | SE 27:1/20:4           | 12  | 85.60                               | 0.03                                | 690.6183 (2.8)                          | 369.3516            |  |
| SE 27:1/20:5                 | SE 27:1/20:5           | 10  | 83.05                               | 0.03                                | 688.6027 (1.6)                          | 369.3516            |  |
| SE 27:1/22:1                 | SE 27:1/22:2           | 18  | 96.33                               | 0.03                                | 724.6966 (2.8)                          | 369.3516            |  |
| SE 27:1/22:4                 | SE 27:1/22:4           | 14  | 88.22                               | 0.03                                | 718.6496 (1.3)                          | 369.3516            |  |
| SE 27:1/22:5                 | SE 27:1/22:5           | 12  | 85.99                               | 0.03                                | 716.6340 (2.4)                          | 369.3516            |  |
| SE 27:1/22:6                 | SE 27:1/22:6           | 10  | 84.22                               | 0.03                                | 714.6183 (1.1)                          | 369.3516            |  |
| Triacylglycerols             |                        |     |                                     |                                     |   |                     |  |
| Lipid species level          | Lipid acyl/alkyl level | ECN | D <sup>1</sup> t <sub>R</sub> [min] | D <sup>2</sup> t <sub>R</sub> [min] | [M+NH <sub>4</sub> ] <sup>+</sup> (ppm) | [M+Na] <sup>+</sup> | Neutral loss of <i>sn</i> -1/ <i>sn</i> -2/ <i>sn</i> -3 |
| TG 42:0                      | TG 16:0_14:0_12:0      | 42  | 81.06                               | 0.03                                | 740.6763 (1.9)                          | 745.6317            | 523.4721 / 495.4408 / 467.4095                           |
| TG 42:1                      | TG 12:0_12:0_18:1      | 40  | 77.99                               | 0.03                                | 738.6606 (3.2)                          | 743.6160            | 521.4564 / 521.4564 / 439.3782                           |
| TG 42:2                      | TG 12:0_12:0_18:2      | 38  | 74.88                               | 0.03                                | 736.6450 (4.5)                          | 741.6004            | 519.4408 / 519.4408 / 439.3782                           |
| TG 44:0                      | TG 16:0_14:0_14:0      | 44  | 84.22                               | 0.03                                | 768.7076 (2.9)                          | 773.6630            | 495.4408 / 523.4721 / 523.4721                           |
| TG 44:1                      | TG 14:0_18:1_12:0      | 42  | 81.37                               | 0.03                                | 766.6919 (3.9)                          | 771.6473            | 521.4564 / 467.4095 / 549.4877                           |
|                              | TG 12:0_16:0_16:1      | 42  | 81.37                               | 0.03                                | 766.6919 (3.9)                          | 771.6473            | 549.4877 / 495.4408 / 493.4251                           |

|         |                   |    |       |      |                |          |                                |
|---------|-------------------|----|-------|------|----------------|----------|--------------------------------|
|         | TG 16:1_14:0_14:0 | 42 | 81.37 | 0.03 | 766.6919 (3.9) | 771.6473 | 495.4408 / 521.4564 / 521.4564 |
| TG 44:2 | TG 14:0_18:2_12:0 | 40 | 78.76 | 0.03 | 764.6763 (3.3) | 769.6317 | 519.4408 / 467.4095 / 547.4721 |
| TG 46:0 | TG 16:0_16:0_14:0 | 46 | 86.92 | 0.03 | 796.7389 (4.4) | 801.6943 | 523.4721 / 523.4721 / 551.5034 |
| TG 46:1 | TG 16:0_18:1_12:0 | 44 | 84.48 | 0.03 | 794.7232 (3.5) | 799.6786 | 521.4564 / 495.4408 / 577.5190 |
|         | TG 16:0_16:1_14:0 | 44 | 84.48 | 0.03 | 794.7232 (3.5) | 799.6786 | 521.4564 / 523.4721 / 549.4877 |
| TG 46:2 | TG 16:0_18:2_12:0 | 42 | 82.25 | 0.03 | 792.7076 (4.5) | 797.6630 | 519.4408 / 495.4408 / 575.5034 |
| TG 46:3 | TG 12:0_16:1_18:2 | 40 | 79.56 | 0.03 | 790.6919 (3.9) | 795.6473 | 573.4877 / 519.4408 / 493.4251 |
|         | TG 14:0_14:1_18:2 | 40 | 79.56 | 0.03 | 790.6919 (3.9) | 795.6473 | 547.4721 / 545.4564 / 493.4251 |
| TG 48:0 | TG 16:0_16:0_16:0 | 48 | 89.49 | 0.03 | 824.7702 (3.5) | 829.7256 | 551.5034 / 551.5034 / 551.5034 |
|         | TG 18:0_16:0_14:0 | 48 | 89.49 | 0.03 | 824.7702 (3.5) | 829.7256 | 523.4721 / 551.5034 / 579.5347 |
| TG 48:1 | TG 16:0_16:1_16:0 | 46 | 87.10 | 0.03 | 822.7545 (4.0) | 827.7099 | 549.4877 / 551.5034 / 549.4877 |
|         | TG 16:0_18:1_14:0 | 46 | 87.10 | 0.03 | 822.7545 (4.0) | 827.7099 | 549.4877 / 523.4721 / 577.5190 |
|         | TG 18:0_18:1_12:0 | 46 | 87.10 | 0.03 | 822.7545 (4.0) | 827.7099 | 521.4564 / 523.4721 / 605.5503 |
| TG 48:2 | TG 18:1_18:1_12:0 | 44 | 84.73 | 0.03 | 820.7389 (2.7) | 825.6943 | 521.4564 / 521.4564 / 603.5347 |
|         | TG 16:0_18:2_14:0 | 44 | 84.73 | 0.03 | 820.7389 (2.7) | 825.6943 | 547.4721 / 523.4721 / 575.5034 |
|         | TG 18:1_16:1_14:0 | 44 | 84.73 | 0.03 | 820.7389 (2.7) | 825.6943 | 521.4564 / 549.4877 / 575.5034 |
| TG 48:3 | TG 18:1_18:2_12:0 | 42 | 82.86 | 0.03 | 818.7232 (3.5) | 823.6786 | 519.4408 / 521.4564 / 601.5190 |
| TG 49:0 | TG 17:0_16:0_16:0 | 49 | 90.64 | 0.03 | 838.7858 (4.9) | 843.7412 | 551.5034 / 565.5190 / 565.5190 |
| TG 49:1 | TG 15:0_16:0_18:1 | 47 | 88.39 | 0.03 | 836.7702 (4.8) | 841.7256 | 577.5190 / 563.5034 / 537.4877 |
| TG 49:2 | TG 15:0_16:0_18:2 | 45 | 86.30 | 0.03 | 834.7545 (4.4) | 839.7099 | 575.5034 / 561.4877 / 537.4877 |
| TG 49:3 | TG 18:2_16:1_15:0 | 43 | 84.22 | 0.03 | 832.7389 (4.3) | 837.6943 | 535.4721 / 561.4877 / 573.4877 |
| TG 50:0 | TG 18:0_16:0_16:0 | 50 | 91.94 | 0.03 | 852.8015 (4.5) | 857.7569 | 551.5034 / 579.5347 / 579.5347 |
| TG 50:1 | TG 16:0_18:1_16:0 | 48 | 89.61 | 0.03 | 850.7858 (4.1) | 855.7412 | 577.5190 / 551.5034 / 577.5190 |
|         | TG 18:0_18:1_14:0 | 48 | 89.61 | 0.03 | 850.7858 (4.1) | 855.7412 | 549.4877 / 551.5034 / 605.5503 |
| TG 50:2 | TG 18:1_18:1_14:0 | 46 | 87.34 | 0.03 | 848.7702 (4.2) | 853.7256 | 549.4877 / 549.4877 / 603.5347 |
|         | TG 16:0_16:0_18:2 | 46 | 87.34 | 0.03 | 848.7702 (4.2) | 853.7256 | 575.5034 / 575.5034 / 551.5034 |
|         | TG 16:0_18:1_16:1 | 46 | 87.34 | 0.03 | 848.7702 (4.2) | 853.7256 | 575.5034 / 549.4877 / 577.5190 |
| TG 50:3 | TG 18:1_18:2_14:0 | 44 | 85.01 | 0.03 | 846.7545 (3.7) | 851.7099 | 547.4721 / 549.4877 / 601.5190 |
|         | TG 16:1_16:0_18:2 | 44 | 85.01 | 0.03 | 846.7545 (3.7) | 851.7099 | 575.5034 / 573.4877 / 549.4877 |



|         |                   |    |       |      |                |          |                                |
|---------|-------------------|----|-------|------|----------------|----------|--------------------------------|
|         | TG 16:1_16:1_18:1 | 44 | 85.01 | 0.03 | 846.7545 (3.7) | 851.7099 | 575.5034 / 575.5034 / 547.4721 |
| TG 50:4 | TG 18:2_16:1_16:1 | 42 | 82.86 | 0.03 | 844.7389 (2.8) | 849.6943 | 547.4721 / 573.4877 / 573.4877 |
|         | TG 18:3_16:1_16:0 | 42 | 82.86 | 0.03 | 844.7389 (2.8) | 849.6943 | 573.4877 / 571.4721 / 549.4877 |
| TG 51:1 | TG 17:0_18:1_16:0 | 49 | 90.85 | 0.03 | 864.8015 (4.5) | 869.7569 | 565.5190 / 577.5190 / 591.5347 |
| TG 51:2 | TG 17:1_18:1_16:0 | 47 | 88.59 | 0.03 | 862.7858 (4.2) | 867.7412 | 577.5195 / 563.5034 / 589.5190 |
| TG 51:3 | TG 18:2_15:0_18:1 | 45 | 86.47 | 0.03 | 860.7702 (4.3) | 865.7256 | 601.5190 / 563.5034 / 561.4877 |
|         | TG 17:1_18:2_16:0 | 45 | 86.47 | 0.03 | 860.7702 (4.3) | 865.7256 | 575.5034 / 563.5034 / 587.5034 |
| TG 51:4 | TG 18:2_18:2_15:0 | 43 | 84.22 | 0.03 | 858.7545 (4.1) | 863.7099 | 561.4877 / 561.4877 / 599.5034 |
| TG 52:0 | TG 18:0_18:0_16:0 | 52 | 94.12 | 0.03 | 880.8328 (4.9) | 885.7882 | 579.5347 / 579.5347 / 607.5660 |
| TG 52:1 | TG 18:0_18:1_16:0 | 50 | 91.99 | 0.03 | 878.8171 (4.4) | 883.7725 | 577.5190 / 579.5347 / 605.5503 |
| TG 52:2 | TG 18:1_18:1_16:0 | 48 | 89.78 | 0.03 | 876.8015 (3.4) | 881.7569 | 577.5190 / 577.5190 / 603.5347 |
| TG 52:3 | TG 18:1_18:1_16:1 | 46 | 87.70 | 0.03 | 874.7858 (4.8) | 879.7412 | 575.5034 / 575.5034 / 603.5347 |
|         | TG 18:1_18:2_16:0 | 46 | 87.70 | 0.03 | 874.7858 (4.8) | 879.7412 | 575.5034 / 577.5190 / 601.5190 |
| TG 52:4 | TG 18:1_18:2_16:1 | 44 | 85.53 | 0.03 | 872.7702 (2.7) | 877.7256 | 573.4877 / 575.5034 / 601.5190 |
|         | TG 18:2_18:2_16:0 | 44 | 85.53 | 0.03 | 872.7702 (2.7) | 877.7256 | 575.5034 / 575.5034 / 599.5034 |
| TG 52:5 | TG 18:2_18:2_16:1 | 42 | 83.44 | 0.03 | 870.7545 (3.0) | 875.7099 | 573.4877 / 573.4877 / 599.5034 |
|         | TG 16:0_16:1_20:4 | 42 | 83.44 | 0.03 | 870.7545 (3.0) | 875.7099 | 599.5034 / 597.4877 / 549.4877 |
|         | TG 18:3_18:2_16:0 | 42 | 83.44 | 0.03 | 870.7545 (3.0) | 875.7099 | 575.5034 / 573.4877 / 597.4877 |
| TG 53:1 | TG 18:0_18:1_17:0 | 51 | 93.16 | 0.03 | 892.8328 (3.5) | 897.7882 | 519.4408 / 521.4564 / 601.5190 |
| TG 53:2 | TG 18:1_18:1_17:0 | 49 | 90.99 | 0.03 | 892.8328 (3.5) | 895.7725 | 591.5347 / 591.5347 / 603.5347 |
| TG 53:3 | TG 18:1_18:2_17:0 | 47 | 88.91 | 0.03 | 888.8015 (4.1) | 893.7569 | 589.5190 / 591.5347 / 601.5190 |
| TG 54:1 | TG 20:0_18:1_16:0 | 52 | 94.26 | 0.03 | 906.8484 (3.0) | 911.8038 | 577.5190 / 607.5660 / 633.5816 |
|         | TG 18:1_18:0_18:0 | 52 | 94.26 | 0.03 | 906.8484 (3.0) | 911.8038 | 607.5660 / 605.5503 / 605.5503 |
|         | TG 18:0_20:1_16:0 | 52 | 94.26 | 0.03 | 906.8484 (3.0) | 911.8038 | 605.5503 / 579.5347 / 633.5816 |
| TG 54:2 | TG 20:1_18:1_16:0 | 50 | 92.10 | 0.03 | 904.8328 (4.1) | 909.7882 | 577.5190 / 605.5503 / 631.5660 |
|         | TG 18:0_18:1_18:1 | 50 | 92.10 | 0.03 | 904.8328 (4.1) | 909.7882 | 603.5347 / 605.5503 / 605.5503 |
| TG 54:3 | TG 18:1_18:1_18:1 | 48 | 90.03 | 0.03 | 902.8171 (4.5) | 907.7725 | 603.5347 / 603.5347 / 603.5347 |
|         | TG 18:0_18:2_18:1 | 48 | 90.03 | 0.03 | 902.8171 (4.5) | 907.7725 | 601.5190 / 605.5503 / 603.5347 |
| TG 54:4 | TG 18:1_18:2_18:1 | 46 | 87.88 | 0.03 | 900.8015 (4.2) | 905.7569 | 601.5190 / 603.5347 / 601.5190 |

|         |                   |    |       |      |                |          |                                |
|---------|-------------------|----|-------|------|----------------|----------|--------------------------------|
|         | TG 16:0_18:1_20:3 | 46 | 87.88 | 0.03 | 900.8015 (4.2) | 905.7569 | 627.5347 / 601.5190 / 577.5190 |
|         | TG 18:0_18:2_18:2 | 46 | 87.88 | 0.03 | 900.8015 (4.2) | 905.7569 | 599.5034 / 603.5347 / 603.5347 |
| TG 54:5 | TG 16:0_18:2_20:3 | 44 | 85.80 | 0.03 | 898.7858 (2.8) | 903.7412 | 625.5190 / 601.5190 / 575.5034 |
|         | TG 18:1_18:2_18:2 | 44 | 85.80 | 0.03 | 898.7858 (2.8) | 903.7412 | 599.5034 / 601.5190 / 601.5190 |
|         | TG 18:1_18:1_18:3 | 44 | 85.80 | 0.03 | 898.7858 (2.8) | 903.7412 | 599.5034 / 599.5034 / 603.5347 |
| TG 54:6 | TG 18:1_18:2_18:3 | 42 | 83.63 | 0.03 | 896.7702 (3.3) | 901.7256 | 597.4877 / 599.5034 / 601.5190 |
|         | TG 20:4_18:1_16:1 | 42 | 83.63 | 0.03 | 896.7702 (3.3) | 901.7256 | 575.5034 / 597.4877 / 625.5190 |
|         | TG 20:4_18:2_16:0 | 42 | 83.63 | 0.03 | 896.7702 (3.3) | 901.7256 | 575.5034 / 599.5034 / 623.5034 |
| TG 56:1 | TG 24:1_16:0_16:0 | 54 | 96.46 | 0.03 | 934.8797 (3.6) | 939.8351 | 551.5034 / 661.6129 / 661.6129 |
| TG 56:2 | TG 20:1_18:1_18:0 | 52 | 94.34 | 0.03 | 932.8641 (4.3) | 937.8195 | 605.5503 / 633.5816 / 631.5660 |
|         | TG 22:0_18:2_16:0 | 52 | 94.34 | 0.03 | 932.8641 (4.3) | 937.8195 | 575.5034 / 635.5973 / 659.5973 |
| TG 56:3 | TG 20:1_18:1_18:1 | 50 | 92.23 | 0.03 | 930.8484 (4.7) | 935.8038 | 603.5347 / 631.5660 / 631.5660 |
| TG 56:4 | TG 16:0_18:0_22:4 | 48 | 90.33 | 0.03 | 928.8328 (3.2) | 933.7882 | 655.5660 / 627.5347 / 579.5347 |
| TG 56:5 | TG 22:4_16:0_18:1 | 46 | 88.91 | 0.03 | 926.8171 (2.6) | 931.7725 | 577.5190 / 653.5503 / 627.5347 |
|         | TG 20:4_18:1_18:0 | 46 | 88.91 | 0.03 | 926.8171 (2.6) | 931.7725 | 605.5503 / 625.5190 / 627.5347 |
| TG 56:6 | TG 18:1_18:1_20:4 | 44 | 87.10 | 0.03 | 924.8015 (2.7) | 929.7569 | 625.5190 / 625.5190 / 603.5347 |
|         | TG 18:0_18:2_20:4 | 44 | 87.10 | 0.03 | 924.8015 (2.7) | 929.7569 | 627.5347 / 623.5034 / 603.5347 |
| TG 56:7 | TG 22:5_18:2_16:0 | 42 | 86.11 | 0.03 | 922.7858 (3.8) | 927.7412 | 649.5190 / 625.5190 / 649.5190 |
| TG 56:8 | TG 22:6_18:2_16:0 | 40 | 83.88 | 0.03 | 920.7702 (4.2) | 925.7256 | 575.5034 / 623.5034 / 647.5034 |
| TG 58:3 | TG 22:0_18:2_18:1 | 52 | 94.56 | 0.03 | 958.8797 (1.8) | 963.8351 | 601.5190 / 661.6129 / 659.5973 |

n.d. ... not detected

**Table S4.** Characteristic ions of individual lipid classes used for the identification of lipid species observed in positive and negative ESI mode.

| Lipid Class | Positive-ESI mode   | Negative-ESI mode   |
|-------------|---|---|
| Cer         | [M+H-H <sub>2</sub> O] <sup>+</sup> ; sphingoid base  | [M+formate] <sup>-</sup>  |
| HexCer      | [M+H] <sup>+</sup> ; sphingoid base   | [M+formate] <sup>-</sup>  |
| Hex2Cer     | [M+H] <sup>+</sup>  | [M+formate] <sup>-</sup>  |
| GM3         | n.d.  | [M-H] <sup>-</sup>  |
| SM          | [M+H] <sup>+</sup> ; <i>m/z</i> 184   | [M+formate] <sup>-</sup>  |
| PC          | [M+H] <sup>+</sup> ; <i>m/z</i> 184   | [M+formate] <sup>-</sup> ; <i>sn</i> -1/ <i>sn</i> -2 RCOO <sup>-</sup> |
| PC P        | [M+H] <sup>+</sup> ; <i>m/z</i> 184   | [M+formate] <sup>-</sup> ; <i>sn</i> -2 RCOO <sup>-</sup>               |
| LPC         | [M+H] <sup>+</sup> ; <i>m/z</i> 184   | [M+formate] <sup>-</sup>  |
| PE          | [M+H] <sup>+</sup> ; neutral loss of <i>m/z</i> 141   | [M-H] <sup>-</sup> ; <i>sn</i> -1/ <i>sn</i> -2 RCOO <sup>-</sup>       |
| PE P        | [M+H] <sup>+</sup> ; [R <sub>2</sub> COO(C <sub>3</sub> H <sub>5</sub> )OH] <sup>+</sup>  | [M-H] <sup>-</sup> ; <i>sn</i> -2 RCOO <sup>-</sup>                     |
| PI          | n.d.  | [M-H] <sup>-</sup> ; <i>sn</i> -1/ <i>sn</i> -2 RCOO <sup>-</sup>       |
| Chol        | [M+H-H <sub>2</sub> O] <sup>+</sup>   | n.d.  |
| CE          | [M+NH <sub>4</sub> ] <sup>+</sup> ; <i>m/z</i> 369  | n.d.  |
| DG          | [M+NH <sub>4</sub> ] <sup>+</sup> ; [M+H-H <sub>2</sub> O] <sup>+</sup> ; Neutral loss of <i>sn</i> -1/ <i>sn</i> -2/ <i>sn</i> -3 fatty acyl | n.d.  |
| TG          | [M+NH <sub>4</sub> ] <sup>+</sup> , [M+Na] <sup>+</sup> , neutral loss of <i>sn</i> -1/ <i>sn</i> -2/ <i>sn</i> -3 fatty acyl                 | n.d.  |
| FA          | n.d.  | [M-H] <sup>-</sup>  |

n.d. ... not detected