L-cysteine sulfinate
Formula: C₃H₇NO₄S  Mass: 153.01  Std.RT: 930.2097108  Ion: NEG

- UL
- +1
- +2
- +3

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected
L-Aspartate
Formula: C₄H₇NO₄  Mass: 133.038  Std.RT: 963.9665046  Ion: NEG

% area under peak

Ratio

Trend of 1 C labelled isotopomer

Relative labelling pattern
Hydroxymethylphosphonate
Formula: CH₅O₄P  Mass: 111.993  Std.RT: 938.1511494  Ion: NEG

G1
N-Acetyl-L-glutamate
Formula: C7H11NO5  Mass: 189.064  Std.RT: 957.1572468  Ion: NEG

G1
N2–Succinyl–L–ornithine

Formula: C9H16N2O5  Mass: 232.106  Std.RT: 829.7585652  Ion: NEC

**G1**

![Graphical representation of N2–Succinyl–L–ornithine data]

- **Trend plot**
  - Ratio: % area under peak and mean peak area
- **Trend of 1 C labelled isotopomer**
  - Overlap: <Expected and >Expected
- **Relative labelling pattern**
  - % relative labelling
L-1-Pyrroline-3-hydroxy-5-carboxylate

Formula: C5H7NO3  Mass: 129.043  Std.RT: 628.0602492  Ion: NEG

UL  +1  +2  +3  +4  +5

G1

Ratio

% area under peak
0.0  0.2  0.4  0.6  0.8  1.0

mean peak area
0.0e+00  1.0e-07  3.0e-07

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

% relative labelling
0  1  2  3  4  5
Urea−1−carboxylate
Formula: C₂H₄N₂O₃ Mass: 104.022 Std.RT: 667.6412556 Ion: NEG

[Graphs showing mass spectra and trend plots]
L–Glutamate
Formula: C5H9NO4  Mass: 147.053  Std.RT: 952.8405024  Ion: NEG

![Graphs and charts showing data analysis results for L–Glutamate, including trend plots and relative labelling patterns.]

- **Ratio**: Graph showing the mean peak area and % area under peak.
- **Trend plot**: Graphs showing the trend of labelled isotopomers.
- **Trend of 1 C labelled isotopomer**: Graphs showing the overlap with expected values.
- **Relative labelling pattern**: Graph showing the % relative labelling.
Carbamoyl phosphate
Formula: CH$_4$NO$_5$P  Mass: 140.983  Std.RT: 2151.8066508  Ion: NEG

UL  +1

G1

% area under peak

Ratio

mean peak area

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Glycine
Formula: $\text{C}_2\text{H}_5\text{NO}_2$ Mass: 75.032 Std.RT: 1016.4774222 Ion: NEG

![Graphs and charts showing data analysis results for Glycine]
O–Acetyl–L–serine
Formula: C5H9NO4  Mass: 147.053  Std.RT: 667.6364976  Ion: NEG

G1

Trend of 1 C labelled isotopomer

Relative labelling pattern
(R)-2-Hydroxyglutarate
Formula: C5H8O5  Mass: 148.037  Std.RT: 964.0135038 Ion: NEG

![Graphs showing the analysis of (R)-2-Hydroxyglutarate](image)

**Ratio**
- % area under peak
- 0.0
- 0.2
- 0.4
- 0.6
- 0.8
- 1.0

**Trend plot**
- Mean peak area
- 0.0e+00
- 2b+07
- 4e+07
- 6e+07
- 8e+07

**Trend of 1C labelled isotopomer**
- Overlap
- <Expected
- >Expected

**Relative labelling pattern**
- 0
- 1
- 2
- 3
- 4
- 5

G1
2-Oxoglutaramate
Formula: C5H7NO4 Mass: 145.038 Std.RT: 641.5785042 Ion: NEG

UL 0+1 0+2 0+3 0+4 0+5

G1
N-Acetyl-D-glucosamine 6-phosphate

Formula: C8H16NO9P  Mass: 301.056  Std.RT: 986.2202934  Ion: NE/(ion)

UL  +1  +2  +3  +4  +5  +6  +7  +8

G1

Trend plot

Ratio

% area under peak

mean peak area

mean peak area

Trend of 1 C labelled isotopomer

Relative labelling pattern
D−Glucosamine 6−phosphate
Formula: C6H14NO8P  Mass: 259.046  Std.RT: 1003.4276148  Ion: NE

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

% area under peak

mean peak area

mean peak area

% relative labelling

Overlap
<Expected
>Expected
5-Oxoproline
Formula: C5H7NO3  Mass: 129.043  Std.RT: 806.964249 Ion: NEG
Ethanolamine phosphate
Formula: C2H8NO4P Mass: 141.019 Std.RT: 1049.5780902 Ion: NE⁻
(1−Ribosylimidazole)−4−acetate
Formula: C10H14N2O6  Mass: 258.085  Std.RT: 902.0539986  Ion: NE

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
4-Imidazolone-5-acetate
Formula: C5H6N2O3  Mass: 142.038  Std.RT: 804.5667546  Ion: NEG

G1

Trend plot

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected
N−Succinyl−LL−2,6−diaminoheptanedioate

Formula: C11H18N2O7  Mass: 290.111  Std.RT: 815.8988592  Ion: NE

UL +1 +2 +3 +4 +5 +6 +7 +8 +9 +10 +11

G1

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
5-Oxopentanoate
Formula: C5H8O3  Mass: 116.047  Std.RT: 358.27246092  Ion: NEG

UL  +1  +2  +3  +4  +5

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA oxo,methyl(4:0)] 2-oxo-4-methylthio-butanoic acid

Formula: C5H8O3S  Mass: 148.019  Std.RT: 270.13081002  Ion: NEG

G1

Trend plot

Ratio

Trend of 1 C labelled isotopomer

Relative labelling pattern
2-Hydroxy-2,4-pentadienoate

Formula: C5H6O3  Mass: 114.032  Std.RT: 958.032504  Ion: NEG

UL  +1  +2  +3  +4  +5

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Phenylpyruvate
Formula: C9H8O3  Mass: 164.047  Std.RT: 257.93895912  Ion: NEG

Trend plot

Overlap
<Expected
>Expected

Relative labelling pattern

Ratio

% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

mean peak area
0 e+00 1e+00 2e+00 3e+00 4e+00

mean peak area
0 50000 100000 150000

mean peak area
0 50000 100000 150000

mean peak area
0 50000 100000 150000

mean peak area
0 50000 100000 150000
Phenylpyruvate
Formula: C9H8O3  Mass: 164.047  Std.RT: 257.93895912  Ion: NEG
Quinate
Formula: C7H12O6  Mass: 192.063  Std.RT: 943.0802484  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7

G1
3-(4-Hydroxyphenyl)lactate

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA hydroxy(7:1/2:0)] 2,4–dihydroxy–2–heptenedioic acid

Formula: C7H10O6  Mass: 190.048  Std.RT: 666.1242474  Ion: NEG

**G1**

**Ratio**

**Trend plot**

**Trend of 1 C labelled isotopomer**

**Relative labelling pattern**
3-Methoxy-4-hydroxyphenylacetaldehyde

Formula: C9H10O3  Mass: 166.063  Std.RT: 268.59149928 Ion: NEG

Trend plot

Ratio

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected
3-(4-Hydroxyphenyl)pyruvate

Formula: C9H8O4  Mass: 180.042  Std.RT: 433.33956762  Ion: NEG

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
(S)–3–Methyl–2–oxopentanoic acid

Formula: C6H10O3  Mass: 130.063  Std.RT: 260.7654165  Ion: NEG

UL  +1  +2  +3  +4  +5  +6

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Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
3-Methyl-2-oxobutanoic acid
Formula: C5H8O3  Mass: 116.047  Std.RT: 275.44858548  Ion: NEG

UL  +1  +2  +3  +4  +5

Trend plot
Relative labelling pattern
L-Valine

Formula: C_5H_{11}NO_2  Mass: 117.079  Std.RT: 804.6172458  Ion: NEG

UL  +1  +2  +3  +4  +5

G1

Ratio  Trend plot  Trend of 1 C labelled isotopomer  Relative labelling pattern

% area under peak

mean peak area

mean peak area

% relative labelling
Erythrulose 1–phosphate
Formula: C4H9O7P Mass: 200.009 Std.RT: 798.507429 Ion: NEG

G1
Erythrulose 1-phosphate
Formula: C4H9O7P  Mass: 200.009  Std.RT: 798.507429  Ion: NEG

G2

Trend plot

Relative labelling pattern
Chitobiose
Formula: C16H28N2O11 Mass: 424.169 Std.RT: 1033.9099992 Ion: \_1

UL

\_1 +1 +2 +3 +4 +5 +6 +7 +8 +9 +10 +11 +12 +13

G1

0.0 0.2 0.4 0.6 0.8 1.0

\% area under peak

0 0.2 0.4 0.6 0.8 1.0

mean peak area

0 20000 40000 60000

Trend plot

0 2000 4000 6000 8000 10000

Trend of 1 C labelled isotopomer

Overlap <Expected >Expected

0 2 4 6 8 10 12

Relative labelling pattern

0 2 4 6 8 10 12

mean peak area

0 2000 4000 6000

Relative labelling pattern

0 2 4 6 8 10 12
UDP-N-acetyl-D-glucosamine
Formula: C17H27N3O17P2  Mass: 607.082  Std.RT: 980.7077112  Ion:

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
L–Arabinonate
Formula: C5H10O6  Mass: 166.048  Std.RT: 818.359749  Ion: NEG

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Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected
L–Arabinonate

Formula: C₅H₁₀O₆  Mass: 166.048  Std.RT: 818.359749  Ion: NEG

G2

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

% relative labelling

Overlap

<Expected

>Expected
D-Glucarate
Formula: C6H10O8  Mass: 210.038  Std.RT: 1088.947149 Ion: NEG

UL  +1  +2  +3  +4  +5  +6

G1

Trend plot

Relative labelling pattern
[FA trihydroxy(4:0)] 2,3,4−trihydroxy−butanoic acid

Formula: C₄H₈O₅  Mass: 136.037  Std.RT: 786.4229964  Ion: NEG

G1
[FA trihydroxy(4:0)] 2,3,4–trihydroxy–butanoic acid
Formula: C4H8O5  Mass: 136.037  Std.RT: 786.4229964  Ion: NEG

G2

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
(R)−3−((R)−3−Hydroxybutanoyloxy)butanoate
Formula: C8H14O5  Mass: 190.084  Std.RT: 813.8952486  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8

---

**Ratio**

**Trend plot**

**Trend of 1 C labelled isotopomer**

**Relative labelling pattern**
2–Acetolactate
Formula: C5H8O4  Mass: 132.042  Std.RT: 948.5175042 Ion: NEG

- UL
- +1
- +2
- +3
- +4
- +5

% area under peak

0.0 0.2 0.4 0.6 0.8 1.0

% relative labelling

0 2 4 6 8 10 12
4-Methylene-L-glutamate

Formula: C6H9NO4  Mass: 159.053  Std.RT: 824.7282462  Ion: NEG

![Graphs showing mass spectra and trend plots for different samples and isotopomers.]

**Ratio**

- % area under peak
- Mean peak area

**Trend plot**

- Trend of 1 C labelled isotopomer

- Overlap
- <Expected
- >Expected
2-Oxoglutarate
Formula: C5H6O5  Mass: 146.022  Std.RT: 991.6538418  Ion: NEG

UL  +1  +2  +3  +4  +5

Trend plot

Ratio

Overlap
<Expected
>Expected

Relative labelling pattern

% relative labelling
0  1  2  3  4  5

mean peak area
0.0e+00  1.0e+06  2.0e+06

mean peak area
0.0e+00  1.0e+06  2.0e+06
CoA

Formula: C21H36N7O16P3S  Mass: 767.115  Std.RT: 880.4337036  Ion

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

G1

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Oxaloacetate
Formula: C4H4O5  Mass: 132.006  Std.RT: 1024.5037512  Ion: NEG

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
Citrate
Formula: C6H8O7  Mass: 192.027  Std.RT: 1150.420008 Ion: NEG

G1

![Graphs and charts showing mass spectrometry data for Citrate, including trend plots, ratio of mean peak area, and relative labeling pattern.](image-url)
(S)−Malate
Formula: C4H6O5  Mass: 134.022  Std.RT: 1023.5170872  Ion: NEG

G2

[Graphs and charts showing data analysis for isotopomers, including mean peak area, % relative labelling, trend of 1 C labelled isotopomer, and relative labelling pattern.]
cis–Aconitate
Formula: C6H6O6  Mass: 174.016  Std.RT: 1136.7508392  Ion: NEG

G1

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Succinate
Formula: C4H6O4  Mass: 118.027  Std.RT: 967.3782504 Ion: NEG

G1

Trend plot

Relative labelling pattern

Ratio

% area under peak

0.0 0.2 0.4 0.6 0.8 1.0

0.0 0.2 0.4 0.6 0.8 1.0

0e+00 2e+07 4e+07 1e+08 4e+07 6e+07 8e+07

0e+00 1e+06 2e+06 3e+06 4e+06

0e+00 1e+06 2e+06 3e+06 4e+06

Overlap
<Expected
>Expected

% relative labelling

0 1 2 3 4

mean peak area

0e+00 2e+07 4e+07 1e+08 4e+07 6e+07 8e+07

Trend of 1 C labelled isotopomer

mean peak area

0e+00 1e+06 2e+06 3e+06 4e+06
Succinate
Formula: C4H6O4  Mass: 118.027  Std.RT: 967.3782504  Ion: NEG

G2

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
GDP–mannose
Formula: C16H25N5O16P2  Mass: 605.077  Std.RT: 1168.4676162 lor

UL
+1  +2  +3  +4  +5  +6  +7  +8  +9  +10 +11 +12 +13

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
D-Sorbitol
Formula: C6H14O6  Mass: 182.079  Std.RT: 902.0710836 Ion: NEG

G1

Mean peak area

Trend of 1 C labelled isotopomer

Relative labelling pattern
D–Fructose
Formula: C6H12O6  Mass: 180.063  Std.RT: 870.685257 Ion: NEG

UL  +1  +2  +3  +4  +5  +6

G1

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
D–Galactosamine
Formula: C6H13NO5  Mass: 179.079  Std.RT: 723.239751  Ion: NEG

![Graphs and charts showing the trend plots and relative labelling patterns for D–Galactosamine.](image-url)
Glycerol

Formula: C3H8O3  Mass: 92.047  Std.RT: 639.969498  Ion: NEG

UL
+1
+2
+3

G1

% area under peak

Ratio

mean peak area

Trend plot

mean peak area

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected

0.0 0.2 0.4 0.6 0.8 1.0
% area under peak

0.0 0.4 0.8 1.2e-07
mean peak area

0.0e+00 4.0e-06 8.0e-06 1.2e-07
mean peak area

0.0e+00 1.0e-05 3.0e-05 4.0e-05
mean peak area

0.0 0.5 1.0 1.5 2.0 2.5
% relative labelling
Sucrose

Ratio

% area under peak

0.0 0.2 0.4 0.6 0.8 1.0

mean peak area

0 200000 600000 1000000 1400000

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected

% relative labelling

0 2 4 6 8 10

mean peak area

0 20000 60000 100000 140000
D–Glycerate

Formula: C3H6O4  Mass: 106.027  Std.RT: 737.4837522  Ion: NEG

![Graphs showing the mass spectra and trend plots for D–Glycerate isotopomers.](image-url)
Maltotriose
Formula: C18H32O16  Mass: 504.169  Std.RT: 1097.4861828  Ion: NE

G1

Trend plot
Relative labelling pattern
Trend of 1 C labelled isotopomer

% relative labelling

Overlap
<Expected
>Expected

% area under peak

mean peak area

Ratio

mean peak area
Pyruvate


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Trend plot

Relative labelling pattern
Pyruvate
Formula: C3H4O3  Mass: 88.016  Std.RT: 435.8467089 Ion: NEG

UL  +1  +2  +3

Ratio
% area under peak
0.0  0.2  0.4  0.6  0.8  1.0

mean peak area
0.0e+00  5.0e-07  1.0e-08  1.5e-08

Trend plot

mean peak area
0.0e+00  1.0e-06  2.0e-06  3.0e-06  4.0e-06  5.0e-06

Trend of 1 C labelled isotopomer
Overlap
<Expected
>Expected

Relative labelling pattern

% relative labelling
0.0  0.5  1.0  1.5  2.0  2.5  3.0  3.5
Phosphoenolpyruvate

Formula: C3H5O6P  Mass: 167.982  Std.RT: 1117.66476  Ion: NEG

UL  +1  +2  +3

G1
3–Phospho–D–glycerate
Formula: C₃H₇O₇P  Mass: 185.993  Std.RT: 1084.4990532  Ion: NEG

UL  -1.0  0.0  1.0
UL+1  -1.0  -0.5  0.0  0.5  1.0
UL+2  -1.0  -0.5  0.0  0.5  1.0
UL+3  -1.0  -0.5  0.0  0.5  1.0

CMW  1060  1080  1100
L1H  0  50000  100000  150000  200000
L1M  0e+00  1e+05  2e+05  3e+05  4e+05
LM  0e+00  5e+05  1e+06

ULH  0e+00  1e+05  2e+05  3e+05  4e+05  5e+05  6e+05  7e+05
ULM  0e+00  5e+05  1e+06

0.0  0.2  0.4  0.6  0.8  1.0
% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected

0.0  0.5  1.0  1.5  2.0  2.5
% relative labelling
D−Glyceraldehyde 3−phosphate

Formula: C3H7O6P  Mass: 169.998  Std.RT: 995.5217172  Ion: NEG

UL  +1  +2  +3

0  200  400  600  800  1000  1200
970  990  1010  1030  1050  1070

ULM  +1  +2  +3

0  200  400  600  800  1000  1200
970  990  1010  1030  1050  1070

ULH  +1  +2  +3

0  200  400  600  800  1000  1200
970  990  1010  1030  1050  1070

QC  +1  +2  +3

0  200  400  600  800  1000  1200
970  990  1010  1030  1050  1070

LCM  +1  +2  +3

0  200  400  600  800  1000  1200
970  990  1010  1030  1050  1070

L1M  +1  +2  +3

0  200  400  600  800  1000  1200
970  990  1010  1030  1050  1070

L1H  +1  +2  +3

0  200  400  600  800  1000  1200
970  990  1010  1030  1050  1070

G1
D-Glyceraldehyde 3-phosphate
Formula: C3H7O6P  Mass: 169.998  Std.RT: 995.5217172  Ion: NEG

- UL
- +1
- +2
- +3

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
myo-Inositol
Formula: C6H12O6  Mass: 180.063  Std.RT: 1113.964167  Ion: NEG

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<td>LH</td>
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<td>QC</td>
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<td>ULH</td>
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<td>ULM</td>
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</tbody>
</table>

% area under peak

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap  <Expected  >Expected
1-O-Methyl-myo-inositol
Formula: C7H14O6  Mass: 194.079  Std.RT: 853.5622506  Ion: NEG

G1
D-Ribulose

Formula: C5H10O5  Mass: 150.053  Std.RT: 693.3349992  Ion: NEG

UL  +1  +2  +3  +4  +5

G1

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern

Overlap  <Expected  >Expected

% area under peak

Ratio

0.0  0.2  0.4  0.6  0.8  1.0

% area under peak

mean peak area

mean peak area

Relative labelling pattern

0.0  0.5  1.0  1.5  2.0  2.5  3.0  3.5

% relative labelling

0  5000  10000  15000  20000  25000  30000  35000

mean peak area

0  20000  40000  60000  80000  100000  120000  140000

mean peak area

0  5000  10000  15000  20000  25000  30000  35000

mean peak area

0  5000  10000  15000  20000  25000  30000  35000

mean peak area

0  5000  10000  15000  20000  25000  30000  35000

mean peak area

0  5000  10000  15000  20000  25000  30000  35000

mean peak area

0  5000  10000  15000  20000  25000  30000  35000

mean peak area

0  5000  10000  15000  20000  25000  30000  35000

mean peak area
D-Ribulose
Formula: C5H10O5  Mass: 150.053  Std.RT: 693.3349992  Ion: NEG
Xylitol
Formula: C5H12O5  Mass: 152.068  Std.RT: 832.1345412  Ion: NEG

![Trend plot and diagrams showing data analysis](image-url)
D-Glucuronate
Formula: C6H10O7 Mass: 194.043 Std.RT: 921.3669996 Ion: NEG

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
UDP-glucose
Formula: C15H24N2O17P2  Mass: 566.055  Std.RT: 1055.8433262

% area under peak

CMW1
CMW2
CMW3
L1H1
L1H2
L1H3
L1M1
L1M2
LH1
LH2
LH3
LM1
LM2
LM3
QC1
QC2
QC3
QC4
QC5
ULH1
ULH2
ULH3
ULM1
ULM2

Ratio
Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern

Mean peak area

0.0e+00 0.1e+07 1.0e+07 2.0e+07
0.0+00 5.0e+06 1.0e+07 1.5e+07 2.0e+07

% relative labelling

0 2 4 6 8 10 12 14
0 50000 100000 150000 200000 250000
0 50000 100000 150000 200000 250000
0 1040 1060

0 0.2 0.4 0.6 0.8 1.0
0 0.2 0.4 0.6 0.8 1.0

0.0e+00 0.1e+07 1.0e+07 2.0e+07
0.0e+00 5.0e+06 1.0e+07 1.5e+07 2.0e+07

G1
6-Phospho-D-gluconate

Formula: C6H13O10P  Mass: 276.025  Std.RT: 1130.2852488  Ion: NE

- UL  -1  -2  -3  -4  -5  -6
- +1  +2  +3  +4  +5  +6

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
D-Gluconic acid
Formula: C6H12O7  Mass: 196.058  Std.RT: 893.998497  Ion: NEG

UL  +1  +2  +3  +4  +5  +6

D-Gluconic acid molecule and its isotopomers are shown in the diagrams. The mass spectra indicate the presence of various isotopomers, and the ratio of their peak areas is shown in the graph. The mean peak area and the percent area under the peak for each isotopomer are also presented. The trend plot illustrates the trend of C-labeled isotopomers, and the relative labeling pattern is shown in the final graph.
D–Ribose
Formula: C5H10O5  Mass: 150.053  Std.RT: 717.3402456 Ion: NEG

UL  +1  +2  +3  +4  +5

G1

Trend plot

Overlap
<Expected
>Expected

Relative labelling pattern
D-Ribose
Formula: C5H10O5  Mass: 150.053  Std.RT: 717.3402456 Ion: NEG

G2

Trend of 1 C labelled isotopomer

Relative labelling pattern
2-Deoxy-D-ribose 5-phosphate

Formula: C5H11O7P  Mass: 214.024  Std.RT: 948.676569  Ion: NEG

UL  +1  +2  +3  +4  +5

G1

[Graphs and data tables related to MS/MS analysis of 2-Deoxy-D-ribose 5-phosphate, showing various peak areas and trend plots for different isotopomers.]
D–Sedoheptulose 7–phosphate
Formula: C7H15O10P  Mass: 290.04  Std.RT: 954.5970078  Ion: NEG

UL
+1 +2 +3 +4 +5 +6 +7

CMW
−1.0 0.0 1.0
−1.0 −0.5 0.0 0.5 1.0
−1.0 0.0 1.0

L1H
−1.0 0.0 1.0
−1.0 −0.5 0.0 0.5 1.0
−1.0 0.0 1.0

L1M
945 960 975
0 1000 2000 3000 4000

LH
950 960 970
0 500 1000 1500 2000 2500 3000

LM
950 960 970 0 500 1000 1500 2000 2500 3000 3500

QC
940 960 980
0 1000 2000 3000 4000 5000

ULH
940 960 980 0 2000 4000 6000 8000

ULM
940 960 980 0 2000 4000 6000 8000

% area under peak
CMW1 CMW2 CMW3 L1H1 L1H2 L1H3 L1M1 L1M2 L1M3 LH1 LH2 LH3 LM1 LM2 LM3 QC1 QC2 QC3 QC4 QC5 ULH1 ULH2 ULH3 ULM1 ULM2

Ratio

Trend plot

Trend of 1 C labelled isotopomer
Overlap <Expected >Expected
2-Dehydro-3-deoxy-D-gluconate
Formula: C6H10O6  Mass: 178.048  Std.RT: 660.3712488  Ion: NEG

UL  +1  +2  +3  +4  +5  +6

ULH  ULM  CMW  LH  LM  QC  L1H  L1M  L1H1  L1H2  L1H3  L1M1  L1M2  LM1  LM2  QC1  QC2  QC3  QC4  QC5

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap  <Expected  >Expected
D-Fructose 6-phosphate
Formula: C6H13O9P Mass: 260.03 Std.RT: 1037.8975068 Ion: NEG

UL
+1  +2  +3  +4  +5  +6

G1

CMW
L1H
L1M
LH
LM
QC
ULH
ULM

Ratio
% area under peak
mean peak area
Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
0.0  0.2  0.4  0.6  0.8  1.0
0e+00  2e+06  4e+06  6e+06  8e+06  1e+07
0e+00  2e+06  4e+06  6e+06  8e+06  1e+07
0e+00  2e+05  4e+05  6e+05  8e+05  1e+06
0  1  2  3  4
0  1  2  3  4
0e+00  2e+05  4e+05  6e+05  8e+05  1e+06

Overlap
Expected
>Expected

UL
+1  +2  +3  +4  +5  +6

mean peak area
0e+00  2e+06  4e+06  6e+06  8e+06  1e+07
0e+00  2e+06  4e+06  6e+06  8e+06  1e+07
0e+00  2e+05  4e+05  6e+05  8e+05  1e+06
0  1  2  3  4
0  1  2  3  4
0e+00  2e+05  4e+05  6e+05  8e+05  1e+06
**D–Fructose 6–phosphate**

Formula: C6H13O9P  Mass: 260.03  Std.RT: 1037.8975068  Ion: NEG

- UL
- +1
- +2
- +3
- +4
- +5
- +6

### Trend plot
- **Trend of 1 C labelled isotopomer**
  - Overlap
  - ≤Expected
  - >Expected

### Relative labelling pattern
- % relative labelling
  - 0
  - 1
  - 2
  - 3
  - 4
D–Ribose 5–phosphate

Formula: C5H11O8P  Mass: 230.019  Std.RT: 1013.046189  Ion: NEG

G1

Ratio  Trend plot  Trend of 1 C labelled isotopomer  Relative labelling pattern
2–Methylcitrate
Formula: C7H10O7  Mass: 206.043  Std.RT: 1109.390823  Ion: NEG

<table>
<thead>
<tr>
<th>Ul</th>
<th>+1</th>
<th>+2</th>
<th>+3</th>
<th>+4</th>
<th>+5</th>
<th>+6</th>
<th>+7</th>
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</tbody>
</table>

### Trend plot

Trend of 1 C labelled isotopomer

- Overlap
- <Expected
- >Expected
(R)-Lactate
Formula: C3H6O3  Mass: 90.032  Std.RT: 552.58095552  Ion: NEG

UL  +1  +2  +3

G1

Ratio
% area under peak
0.0  0.2  0.4  0.6  0.8  1.0
0.0e+00  0.2e+00  0.4e+00

Mean peak area
0.0e+00  1.0e-07  5.0e-06

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
% relative labelling
0.0  0.5  1.0  1.5  2.0  2.5  3.0

Glycogen
Formula: C24H42O21  Mass: 666.222  Std.RT: 1182.698556  Ion: NEG

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
D–Fructose 1,6–bisphosphate
Formula: C6H14O12P2  Mass: 339.996  Std.RT: 1156.223319  Ion: NE

| G1 |

UL  +1  +2  +3  +4  +5  +6

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

% area under peak

Mean peak area

Overlap

<Expected

>Expected

% relative labelling
ATP
Formula: C10H16N5O13P3  Mass: 506.996  Std.RT: 1062.654774  Ion:

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10

G1

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
ADP
Formula: C10H15N5O10P2 Mass: 427.029 Std.RT: 981.412287 Ion:

![Graphs showing trend and ratio analysis of isotopomers](image-url)

G1

Trend of 1 C labelled isotopomer

Relative labelling pattern
Glycodeoxycholate
Formula: C26H43NO5  Mass: 449.314  Std.RT: 250.0330956  Ion: NEC

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

Trend plot

Relative labelling pattern

Overlap
(Expected)
(Expected)
Taurine

Formula: C₂H₇NO₃S  Mass: 125.015  Std.RT: 950.2777188  Ion: NEG

UL  +1  +2

G1

Ratio

% area under peak

Trend plot

Trend of 1 C labelled isotopomer

<table>
<thead>
<tr>
<th>Overlap</th>
<th>&lt;Expected</th>
<th>&gt;Expected</th>
</tr>
</thead>
</table>

mean peak area

mean peak area
Icosadienoic acid

Formula: C20H36O2  Mass: 308.272  Std.RT: 211.79662002  Ion: NEG

UL
+1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

Trend plot

Relative labelling pattern

Ratio

% area under peak

0.0  0.2  0.4  0.6  0.8  1.0

mean peak area

0  20000  40000  60000  80000

Trend of 1 C labelled isotopomer

Overlap  <Expected  >Expected

% relative labelling

0  5  10  15

mean peak area

0  2000  4000  6000  8000  12000

Overlap  <Expected  >Expected

% relative labelling

0  5  10  15
Tetracosanoic acid
Formula: C24H48O2  Mass: 368.365  Std.RT: 209.76437442  Ion: NEG

UL
+1 +2 +3 +4 +5 +6 +7 +8 +9 +10 +11 +12 +13

Ratio
% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

Trend plot
mean peak area
0 20000 40000 60000

Trend of 1 C labelled isotopomer
mean peak area
0 20000 40000 60000

Relative labelling pattern
% relative labelling
0 5 10 15 20

Overlap
<Expected
>Expected
Docosanoic acid

---

Ratio
% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

mean peak area
0e-00 2e-04 4e-04 8e-04 1e-05

Trend plot
Trend of 1 C labelled isotopomer

Relative labelling pattern
% relative labelling
0 5 10 15

---

Overlap
Expected
>Expected

---

CMW  L1H  L1M  LH  LM  QC  ULH  ULM
Dodecanoic acid
Formula: C12H24O2  Mass: 200.178  Std.RT: 221.5577901  Ion: NEG

Ratio
% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

Trend plot
mean peak area
0 500000 1000000 1500000 2000000

Trend of 1 C labelled isotopomer
mean peak area
0 50000 100000 150000 200000

Relative labelling pattern
% relative labelling
0 2 4 6 8 10

Overlap
Expected
>Expected

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12
(9Z)–Hexadecenoic acid

Trend plot

Relative labelling pattern

Overlap
Expected
>Expected

Ratio

mean peak area

mean peak area

% area under peak

% relative labelling
Tetradecanoic acid

Formula: C14H28O2  Mass: 228.209  Std.RT: 217.23320898  Ion: NEG

UL
+1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

G1

% area under peak

CMW
L1H
L1M
LH
LM
QC
ULH
ULM

Ratio

Trend plot

Trend of C labelled isotopomer

Relative labelling pattern

% relative labelling

Overlap
<Expected
>Expected
Hexadecanoic acid

Formula: C16H32O2  Mass: 256.24  Std.RT: 214.69370778  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10 +11 +12 +13 +14 +15

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Tetradecanoyl-CoA

Formula: C35H62N7O17P3S  Mass: 977.314  Std.RT: 267.67452282

UL

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected
sn-Glycerol 3-phosphate
Formula: C3H9O6P  Mass: 172.014  Std.RT: 960.9317526  Ion: NEG

<table>
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<tr>
<th>UL</th>
<th>+1</th>
<th>+2</th>
<th>+3</th>
</tr>
</thead>
</table>

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
CDP–ethanolamine

Formula: C11H20N4O11P2  Mass: 446.06  Std.RT: 1062.9890538  Ion:

UL +1 +2 +3 +4 +5 +6 +7 +8 +9 +10 +11

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
12-OPDA

Formula: C18H28O3  Mass: 292.204  Std.RT: 230.68683312  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

CMW
L1H
L1M
LH
LM
QC
ULH
ULM

Ratio

% area under peak
0.0  0.2  0.4  0.6  0.8  1.0
0  0.2  0.4  0.6  0.8  1.0

mean peak area
0  1000  2000  3000  4000  5000
0  1000  2000  3000  4000

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern

Overlap
<Expected
>Expected

0  1  2  3  4  5  6  7
[FA (18:3)] 9Z,12Z,15Z–octadecatrienoic acid

Formula: C18H30O2  Mass: 278.225  Std.RT: 214.21220778  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

G1

% area under peak

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA (20:0)] 11Z-eicosenoic acid
Formula: C20H38O2  Mass: 310.287  Std.RT: 211.53029118  Ion: NEG

![Diagram of mass spectrometric analysis](image_url)
Docosahexaenoic acid

Formula: C22H32O2  Mass: 328.24  Std.RT: 211.1214759  Ion: NEG

UL
+1
+2
+3
+4
+5
+6
+7
+8
+9
+10
+11
+12
+13

ULH
ULM
G1

CMW
L1H
L1M
LH
LM
QC
ULH
ULM

Trend plot

Overlap
Expected
>Expected

Relative labelling pattern
[FA (20:5)] 5Z,8Z,11Z,14Z,17Z–eicosapentaenoic acid


UL

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA (22:5)] 7Z,10Z,13Z,16Z,19Z–docosapentaenoic acid

Formula: C22H34O2  Mass: 330.256  Std.RT: 211.11042858  Ion: NEG

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA (22:0)] 13Z–docosenoic acid

Formula: C$_{22}$H$_{42}$O$_2$  Mass: 338.318  Std.RT: 210.4329522  Ion: NEG

G1
Adipate
Formula: C6H10O4  Mass: 146.058  Std.RT: 890.7314964  Ion: NEG

![Graphs showing peak area and trend plots for different samples with labels UL, +1, +2, +3, +4, +5, +6.](image)

- **% area under peak**
- **Ratio**
- **Trend plot**
- **Trend of 1 C labelled isotopomer**
- **Relative labelling pattern**
[FA hydroxy, trihydroxy(3:0/2:0)] N-(1,3-dihydroxypropan−2−yl)−9S,11R,15S−trihydroxy−5Z,13E−prostadienoyl amine

Formula: C_{23}H_{41}NO_{6}  Mass: 427.293  Std.RT: 465.1741257  Ion: NEG

UL

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA (18:1)] 9Z–octadecenoic acid

Formula: C18H34O2  Mass: 282.256  Std.RT: 213.21608478  Ion: NEG

G1

![Trend plot](image)

![Relative labelling pattern](image)
[FA trihydroxy(4:0)] 2,2,4−trihydroxy−butanoic acid
Formula: C4H8O5  Mass: 136.037  Std.RT: 642.2094984  Ion: NEG

G1
[FA dimethyl(13:0)] 2,5–dimethyl–2E–tridecenoic acid

G1

Ratio

% area under peak

mean peak area

Trend plot

mean peak area

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected

% relative labelling

0 2 4 6 8 10
2S–Hydroxytetradecanoic acid

Formula: C_{14}H_{28}O_{3}  Mass: 244.204  Std.RT: 217.695003  Ion: NEG

UL
+1
+2
+3
+4
+5
+6
+7
+8
+9
+10
+11
+12
+13

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
12-Hydroxydodecanoic acid
Formula: C_{12}H_{24}O_{3}  Mass: 216.173  Std.RT: 224.5535844  Ion: NEG

G1

Trend plot

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected
(9Z)-Tetradecenoic acid
Formula: C14H26O2  Mass: 226.193  Std.RT: 218.3736738  Ion: NEG

UL
+1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

![Graphs showing distribution and trends of different isotopomers](image-url)

**Ratio**
- % area under peak
- Mean peak area

**Trend plot**
- Mean peak area

**Trend of 1 C labelled isotopomer**
- Overlap
- <Expected
- >Expected

**Relative labelling pattern**
- % relative labelling
13,16,19−Docsatrienoic acid


% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA hydroxy(17:2)] 7-hydroxy-10E,16-heptadecadien-
Formula: C_{17}H_{26}O_{3}  Mass: 278.188  Std.RT: 218.43391668  Ion: NEG

G1

Trend plot of 1 C labelled isotopemor
Relative labelling pattern
[FA (22:4)] 7Z,10Z,13Z,16Z–docosatetraenoic acid
Formula: C22H36O2  Mass: 332.272  Std.RT: 211.03933278 Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
[FA hydroxy(18:0)] 9,10–dihydroxy–octadecanoic acid

Formula: C18H36O4  Mass: 316.261  Std.RT: 223.9164168  Ion: NEG

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA (24:6)] \(6,9,12,15,18,21\)--Tetracosahexaynoic acid

Formula: \(C_{24}H_{24}O_2\)  Mass:  344.178  Std.RT:  235.8086664  Ion:  NEG

G1
omega-Cyclohexylundecanoic acid
Formula: C_{17}H_{32}O_{2}  Mass: 268.24  Std.RT: 214.33874958  Ion: NEG

- UL
- +1
- +2
- +3
- +4
- +5
- +6
- +7
- +8
- +9
- +10
- +11
- +12
- +13

Trend plot
Relative labelling pattern

Overlap
<Expected
>Expected

% relative labelling
0
2
4
6
8
10

mean peak area
0
5000
10000
15000
20000
25000

Ratio

% area under peak
0
0.2
0.4
0.6
0.8
1.0

mean peak area
0
25000
50000
75000
100000
125000
150000
200000
250000

[FA methyl(18:0)] 11R,12S–methylenoctadecanoic acid

Formula: C19H36O2  Mass: 296.272  Std.RT: 212.8600419  Ion: NEG

UL
+1
+2
+3
+4
+5
+6
+7
+8
+9
+10
+11
+12
+13

G1

Trend plot

Relative labelling pattern
[FA hydroxy(24:0)] 2-hydroxy-15-tetracosenoic acid
Formula: C24H46O3  Mass: 382.345  Std.RT: 207.98609202  Ion: NEG

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

% area under peak

mean peak area

mean peak area

% relative labelling

Overlap

<Expected

>Expected
[FA (17:0)] heptadecanoic acid
Formula: C17H34O2  Mass: 270.256  Std.RT: 213.8024991  Ion: NEG

G1
[FA hydroxy(18:0)] 2S−hydroxy−octadecanoic acid

Formula: C18H36O3  Mass: 300.266  Std.RT: 214.50229068  Ion: NEG

G1
[FA (20:3)] 8Z,11Z,14Z–eicosatrienoic acid
Formula: C20H34O2  Mass: 306.256  Std.RT: 212.31052578 Ion: NEG

G1

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern

% area under peak

Ratio

mean peak area

mean peak area

% relative labelling
[FA hydroxy(4:0/18:0)] 9,10,12,13–tetrahydroxy–octadecanoic acid
Formula: C18H36O6  Mass: 348.251  Std.RT: 253.342809  Ion: NEG

```
UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13
0.0  0.2  0.4  0.6  0.8  1.0
mean peak area

% area under peak
0.0  0.2  0.4  0.6  0.8  1.0
G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
```
Nonadecanoic acid
Formula: C₁₉H₃₈O₂  Mass: 298.287  Std.RT: 212.10966678  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA hydroxy(24:0)] 2-hydroxy-tetracosanoic acid


G1
[FA (20:4)] 5Z,8Z,11Z,14Z–eicosatetraenoic acid

Formula: C20H32O2  Mass: 304.24  Std.RT: 212.01971508  Ion: NEG

G1
[FA hydroxy(22:0)] 13−hydroxy−docosanoic acid

G1

Ratio

Trend plot

Trend of 1C labelled isotopomer

Relative labelling pattern

% area under peak

mean peak area

mean peak area

% relative labelling

Overlap

<Expected

>Expected
[FA (24:0/2:0)] Tetracosanedioic acid
Formula: C_{24}H_{46}O_{4}  Mass: 398.34  Std.RT: 208.45028322  Ion: NEG

- UL
- +1
- +2
- +3
- +4
- +5
- +6
- +7
- +8
- +9
- +10
- +11
- +12
- +13

G1
[FA hydroxy(6:0)] 4–hydroxy–hexanoic acid
Formula: C₆H₁₂O₃  Mass: 132.079  Std.RT: 269.84358468  Ion: NEG

G1

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[FA (18:2)] 9S–hydroperoxy–10E,12Z–octadecadienoic acid
Formula: C18H32O4  Mass: 312.23  Std.RT: 218.203083  Ion: NEG

G1
[FA trihydroxy(18:1)] 9S,12S,13S−trihydroxy−10E−octadecenoic acid

Formula: C18H34O5  Mass: 330.241  Std.RT: 233.33816778 Ion: NEG

G1

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected
[GP (18:0/18:0)] 1−octadecanoyl−2−(9Z−octadecenoyl)−sn−glycero−3−phosphothreonine

Formula: C43H82NO10P  Mass: 803.568  Std.RT: 232.946523  Ion: NE

Graphs and charts showing various parameters and trends related to the compound, including ratio, trend plot, and relative labelling pattern.
[GP (18:2/18:2)] 1,2-di-(9Z,12Z-octadecadienoyl)-sn-

Formula: C39H69O8P  Mass: 696.473  Std.RT: 207.5612379  Ion: NEC

G1
[GP (18:0/18:2)] 1-octadecanoyl-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphate


G1

Trend of 1 C labelled isotopomer

Relative labelling pattern
[PC (17:1)] 1−(1Z-heptadecenyl)−sn-glycero−3−phosphocholine

Formula: C25H52NO6P  Mass: 493.353  Std.RT: 245.2366662  Ion: \^*

UL
+1
+2
+3
+4
+5
+6
+7
+8
+9
+10
+11
+12
+13

G1

Ratio

Trend of 1 C labelled isotopomer

Relative labelling pattern
[PE (18:0/18:2)] 1-octadecanyl-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine
Formula: C₄₁H₇₈NO₈P Mass: 743.547 Std.RT: 223.14013068 Ion: N

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
LysoPE(0:0/22:4(7Z,10Z,13Z,16Z))
Formula: C27H48NO7P  Mass: 529.317  Std.RT: 246.60999918  Ion: \N

UL
+1  
+2  
+3  
+4  
+5  
+6  
+7  
+8  
+9  
+10  
+11  
+12  
+13  

Trend plot

Relative labelling pattern
LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

Formula: C27H44NO7P  Mass: 525.286  Std.RT: 248.7933807  Ion: NE

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
[PG (18:1/18:1)] 1,2-di-(9Z-octadecenoyl)-sn-glycerol

Formula: C42H79O10P  Mass: 774.541  Std.RT: 204.40899882  Ion: N

G1

% area under peak

mean peak area

Ratio

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected

Trend plot
PG(18:0/22:4(7Z,10Z,13Z,16Z))
Formula: C46H83O10P  Mass: 826.572  Std.RT: 204.57181002  Ion: N

-1.0  0.0  1.0  195  205  215  225

Overlap
<Expected
>Expected

-1.0  0.0  1.0  195  205  215  225

% area under peak
0.0  0.2  0.4  0.6  0.8  1.0

Ratio
% area under peak
0.0  0.2  0.4  0.6  0.8  1.0

Trend plot
mean peak area
0  50000  100000  150000

Trend of 1 C labelled isotopomer
mean peak area
0  10000  20000  30000

Relative labelling pattern
% relative labelling
0  5  10  15  20  25
**PG(18:0/22:5(4Z,7Z,10Z,13Z,16Z))**

Formula: C46H81O10P  Mass: 824.557  Std.RT: 203.90114898  Ion: N

- UL
- +1
- +2
- +3
- +4
- +5
- +6
- +7
- +8
- +9
- +10
- +11
- +12
- +13

**Trend plot**

**Trend of 1 C labelled isotopomer**

**Relative labelling pattern**
Formula: C46H75O10P Mass: 818.51 Std.RT: 204.18290352 Ion: NE

[Graphs showing various trends and distributions of peak areas and relative labelling patterns]
PIP(16:0/20:2(11Z,14Z))

Formula: C{45}H{84}O{16}P{2}  Mass: 942.523  Std.RT: 219.59257362  Ion: 1

UL

+1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

G1

Trend plot

Relative labelling pattern
[PI (18:0/18:0)] 1,2-di- (9Z-octadecenoyl)-sn-glycero-
Formula: C45H83O13P  Mass: 862.557  Std.RT: 211.03242858  Ion: N

G1
PI(16:0/20:3(5Z,8Z,11Z))
Formula: C45H81O13P  Mass: 860.541  Std.RT: 210.80304612  Ion: N

G1

Trend plot

Relative labelling pattern
Formula: C49H83O13P  Mass: 910.557  Std.RT: 210.3555225 Ion: NE

G1

![Graphs showing data for G1 with various plots of mean peak area, percentage area under peak, and relative labeling pattern.](image-url)
[SP (16:0)] N-(hexadecanoyl)-sphing-4-enine-1-phosphate
Formula: C34H68NO6P  Mass: 617.478  Std.RT: 243.92056932  Ion: N

G1

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
Cholesterolsulfate
Formula: C27H46O4S  Mass: 466.312  Std.RT: 205.347096  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

Trend plot
Relative labelling pattern

mean peak area
% area under peak

% relative labelling

Overlap
<Expected
>Expected

Trend of 1 C labelled isotopomer

Ratio

mean peak area
[ST hydrox] N-(3alpha,7alpha-dihydroxy-5beta-cholan-24-oxy)taurine

Formula: C26H45NO6S  Mass: 499.297  Std.RT: 234.46376178  Ion: N

UL

G1

Trend plot

Relative labelling pattern
Cholate

Formula: C24H40O5  Mass: 408.288  Std.RT: 267.42790728 Ion: NEG

G1
a Cysteine adduct

Formula: C6H9NO4S  Mass: 191.025  Std.RT: 961.7219994  Ion: NEG

G1

Ratio

Trend plot

Relative labelling pattern
2,3,6−Trihydroxypyridine
Formula: C5H5NO3 Mass: 127.027 Std.RT: 633.1613796 Ion: NEG

UL
+1
+2
+3
+4
+5

G1

2,3,6−Trihydroxypyridine
Formula: C5H5NO3 Mass: 127.027 Std.RT: 633.1613796 Ion: NEG

UL
+1
+2
+3
+4
+5

G1

2,3,6−Trihydroxypyridine
Formula: C5H5NO3 Mass: 127.027 Std.RT: 633.1613796 Ion: NEG

UL
+1
+2
+3
+4
+5

G1
Folate
Formula: C19H19N7O6  Mass: 441.14  Std.RT: 1070.5807152  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12  +13

G1

Ratio  Trend plot  Trend of 1 C labelled isotopomer  Relative labelling pattern

% area under peak

mean peak area

mean peak area

% relative labelling

Overlap

<Expected

>Expected
Allantoin
Formula: C4H6N4O3  Mass: 158.044  Std.RT: 879.030291  Ion: NEG

G1
Urate
Formula: C5H4N4O3 Mass: 168.028 Std.RT: 790.9528548 Ion: NEG

G1

![Graphs showing various distributions and trends related to the urate molecule.](chart.png)

Legend:
- [UL]  
- [+1]  
- [+2]  
- [+3]  
- [+4]  
- [+5]

Trend plot

Relative labelling pattern
N6-(1,2-Dicarboxyethyl)-AMP
Formula: C14H18N5O11P Mass: 463.074 Std.RT: 1158.1461942 Ion:

- UL
- +1
- +2
- +3
- +4
- +5
- +6
- +7
- +8
- +9
- +10
- +11
- +12
- +13

![Graphs and charts showing various trend plots and relative labelling patterns for N6-(1,2-Dicarboxyethyl)-AMP with overlapped peaks and trends labeled with different colors and markers.](image-url)
Xanthine

Formula: C₅H₄N₄O₂  Mass: 152.033  Std.RT: 714.4911384 Ion: NEG

UL  +1  +2  +3  +4  +5

G1
Glyoxylate
Formula: C2H2O3  Mass: 74  Std.RT: 1016.6023332  Ion: NEG

UL  +1  +2

C     L1H     L1M     LH     LM     QC     ULH     ULM

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected
GMP
Formula: C10H14N5O8P  Mass: 363.058  Std.RT: 1078.4147538 Ion:

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10

Trend plot
Trend of 1 C labelled isotopomer

Ratio
% area under peak

mean peak area
GTP
Formula: C10H16N5O14P3 Mass: 522.991 Std.RT: 1226.054757 Ion:

UL +1 +2 +3 +4 +5 +6 +7 +8 +9 +10

G1
UTP
Formula: C9H15N2O15P3  Mass: 483.969  Std.RT: 1142.1523902  Ion:

- U+1
- U+2
- U+3
- U+4
- U+5
- U+6
- U+7
- U+8
- U+9

Ratio
% area under peak

mean peak area

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected

% relative labelling

0 1 2 3 4 5 6
CTP

Formula: C9H16N3O14P3  Mass: 482.985  Std.RT: 1173.117153  Ion:

-UL  +1  +2  +3  +4  +5  +6  +7  +8  +9

Trend plot

Relative labelling pattern

Trend of 1 C labelled isotopomer
Deoxyuridine

Formula: C9H12N2O5  Mass: 228.075  Std.RT: 480.0595224  Ion: NEC

G1

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
(S)–Dihydroorotate
Formula: C5H6N2O4 Mass: 158.033 Std.RT: 684.5408616 Ion: NEG

G1

Ratio
Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern

- Mean peak area
- Relative labelling pattern

Overlap
<Expected
>Expected

% area under peak

0.0 0.2 0.4 0.6 0.8 1.0

0 200 000 60 000 1 00 000 40 00 0

0 200 000 60 000 1 00 000 40 00 0

0 0.5 1.0 1.5 2.0

0 0.5 1.0 1.5 2.0
Orotate
Formula: C5H4N2O4  Mass: 156.017  Std.RT: 604.2105246  Ion: NEG

Ratio

% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

mean peak area
0 50000 100000

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

0 20 40 60 80 100
Thymidine
Formula: C10H14N2O5  Mass: 242.09  Std.RT: 433.26193242  Ion: NE

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10

Trend plot

Ratio

% area under peak

0.0  0.2  0.4  0.6  0.8  1.0

mean peak area

1e-06  3e-06  5e-06  7e-06

Trend of 1 C labelled isotopomer

% relative labelling

0  2  4  6

Relative labelling pattern
Thymidine
Formula: C10H14N2O5  Mass: 242.09  Std.RT: 433.26193242  Ion: NE

G2

Trend plot

Overlap

<Expected

>Expected

Relative labelling pattern

Ratio

% area under peak

0.0 0.2 0.4 0.6 0.8 1.0

0e+00 1e+06 3e+06 4e+06

mean peak area

0 50000 100000 150000 200000 250000 300000 350000

mean peak area

0e+00 1e+06 3e+06 4e+06

% relative labelling

0 2 4 6
dTTP
Formula: C10H17N2O14P3 Mass: 481.989 Std.RT: 1033.464297 Ion: G1

% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

% relative labelling
0 2 4 6

Ratio

mean peak area

Trend plot

mean peak area

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected
5,6-Dihydouracil
Formula: C4H6N2O2  Mass: 114.043  Std.RT: 458.37375258  Ion: NEC

UL  +1  +2  +3  +4

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Uracil

Formula: C4H4N2O2  Mass: 112.027  Std.RT: 499.1936607  Ion: NEG

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
UMP

Formula: C9H13N2O9P  Mass: 324.036  Std.RT: 981.9428988  Ion: NE

G1

Trend plot

Trend of 1 C labelled isotopomer
UDP

Formula: C9H14N2O12P2  Mass: 404.002  Std.RT: 1060.66047  Ion: ~

1. Trend plot
2. Trend of 1 C labelled isotopomer
3. Relative labelling pattern

- **Ratio**
  - % area under peak
  - mean peak area

- **Trend plot**
  - % relative labelling

- **Relative labelling pattern**
  - Overlap
  - <Expected
  - >Expected
Aspartyl–L–proline

Trend plot of 1 C labelled isotopomer

- Overlap
- <Expected
- >Expected

Mean peak area and % area under peak

Ratio

Graphs showing mass spectrometry data with various isotopomers indicated.
Glu–Gly

Formula: C7H12N2O5  Mass: 204.075  Std.RT: 987.9877146  Ion: NEG

UL +1 +2 +3 +4 +5 +6 +7

UL

CMW

L1H

L1M

LH

LM

QC

ULH

ULM

% area under peak

Ratio

mean peak area

Overlap

Expected

>Expected

Trend plot

Trend of 1 C labelled isotopomer
Glu–Ser
Formula: C8H14N2O6 Mass: 234.085 Std.RT: 1005.663432 Ion: NEG

Ratio

<table>
<thead>
<tr>
<th>% area under peak</th>
<th>0.0</th>
<th>0.2</th>
<th>0.4</th>
<th>0.6</th>
<th>0.8</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>UL</td>
<td>1</td>
<td>+2</td>
<td>+3</td>
<td>+4</td>
<td>+5</td>
<td>+6</td>
</tr>
</tbody>
</table>

Trend plot

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected
Asp–Ser

Formula: C7H12N2O6  Mass: 220.07  Std.RT: 1014.3390468 Ion: NEC

<table>
<thead>
<tr>
<th>UL</th>
<th>+1</th>
<th>+2</th>
<th>+3</th>
<th>+4</th>
<th>+5</th>
<th>+6</th>
<th>+7</th>
</tr>
</thead>
</table>

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Glu–Met
Formula: C10H18N2O5S  Mass: 278.094  Std.RT: 798.9294318  Ion: \text{NEG}

G1

<table>
<thead>
<tr>
<th>UL</th>
<th>+1</th>
<th>+2</th>
<th>+3</th>
<th>+4</th>
<th>+5</th>
<th>+6</th>
<th>+7</th>
<th>+8</th>
<th>+9</th>
<th>+10</th>
</tr>
</thead>
</table>

Trend plot

Overlap

Relative labelling pattern
Glu−Val
Formula: C10H18N2O5  Mass: 246.122  Std.RT: 799.4142864  Ion: NE

G1

Trend of 1 C labelled isotopomer
Relative labelling pattern

Overlap <Expected >Expected

% relative labelling
0 2 4 6 8

mean peak area
0 10000 20000 30000 40000

mean peak area
0 10000 20000 30000 40000

% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

Ratio

mean peak area
0 1e+00 2e+05 3e+05 4e+05

Trend plot
Glu−Val
Formula: C10H18N2O5  Mass: 246.122  Std.RT: 799.4142864  Ion: NE

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10

G2

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Ala–Asn
Formula: C7H13N3O4  Mass: 203.091  Std.RT: 823.980858 Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7

<table>
<thead>
<tr>
<th>Mean peak area</th>
<th>% area under peak</th>
<th>Trend plot</th>
<th>Trend of 1 C labelled isotopomer</th>
<th>Relative labelling pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Overlap < Expected > Expected

Relative labelling pattern
Ala–Asn
Formula: C7H13N3O4  Mass: 203.091  Std.RT: 823.980858  Ion: NEG

G2

Trend plot

Relative labelling pattern
Thr–Ser
Formula: C7H14N2O5  Mass: 206.09  Std.RT: 793.0005786  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

% area under peak

mean peak area

mean peak area

% relative labelling

Overlap
<Expected
>Expected
Ser−Ser
Formula: C6H12N2O5  Mass: 192.075  Std.RT: 834.8697102  Ion: NEC

UL  +1  +2  +3  +4  +5  +6

CMW  L1H  L1M  LH  LM  QC  ULH  ULM

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Gly–Ser
Formula: C5H10N2O4  Mass: 162.064  Std.RT: 806.5217196  Ion: NEC

G1

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
Gly–Ser

Formula: C5H10N2O4  Mass: 162.064  Std.RT: 806.5217196  Ion: NEC

<table>
<thead>
<tr>
<th>UL</th>
<th>+1</th>
<th>+2</th>
<th>+3</th>
<th>+4</th>
<th>+5</th>
</tr>
</thead>
</table>

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected

% relative labelling

0.0 0.5 1.0 1.5 2.0 2.5
Asp–Met–Thr–Thr
Formula: C17H30N4O9S  Mass: 466.173  Std.RT: 482.18185122  Ion:

<p>| | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>UL</td>
<td>+1</td>
<td>+2</td>
<td>+3</td>
<td>+4</td>
<td>+5</td>
<td>+6</td>
<td>+7</td>
</tr>
<tr>
<td>+8</td>
<td>+9</td>
<td>+10</td>
<td>+11</td>
<td>+12</td>
<td>+13</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

G1
Ala–Gly–Ser

Formula: C8H15N3O5  Mass: 233.101  Std.RT: 806.8540008  Ion: NEC

 UL  +1  +2  +3  +4  +5  +6  +7  +8

G1

Trend plot

Relative labelling pattern
Parapyruvate
Formula: C6H8O6 Mass: 176.032 Std.RT: 966.0884982 Ion: NEG

UL  +1  +2  +3  +4  +5  +6

G1
2-Maleylacetate

Formula: C6H6O5  Mass: 158.022  Std.RT: 914.7904992  Ion: NEG

G1

Trend of 1 C labelled isotope

Relative labelling pattern
Phosphophosphinate
Formula: C6H15NO7P2 Mass: 275.032 Std.RT: 1021.1307612 Ion: N

Trend plot

Ratio
% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

mean peak area
0 50000 100000

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected
1–18:2–lysoosphatidylglycerol

Formula: C_{24}H_{45}O_{9}P  
Mass: 508.28  
Std.RT: 214.36029318  
Ion: NEC

![Graphs and charts showing data analysis results for 1–18:2–lysoosphatidylglycerol.]
octulose 8–phosphate
Formula: C8H17O11P  Mass: 320.051  Std.RT: 1079.8638042  Ion: NE

---

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
Glycerophosphoglycerol
Formula: C6H15O8P Mass: 246.05 Std.RT: 811.0402776 Ion: NEG
UL +1 +2 +3 +4 +5 +6
CMW 790 810 830 0 50000 100000 150000 200000 250000 300000
L1H 790 810 830 0e+00 1e+05 2e+05 3e+05 4e+05 5e+05 6e+05
L1M 790 810 830 0e+00 1e+05 2e+05 3e+05 4e+05 5e+05 6e+05 7e+05
LH 790 810 830 0 50000 100000 150000 200000 250000 300000 350000
LM 790 810 830 0e+00 1e+05 2e+05 3e+05 4e+05 5e+05 6e+05
QC 790 810 830 0e+00 2e+05 4e+05 6e+05 8e+05
ULH 790 810 830 0e+00 1e+05 2e+05 3e+05 4e+05 5e+05 6e+05 7e+05
ULM 790 810 830 0e+00 1e+05 2e+05 3e+05 4e+05 5e+05 6e+05 7e+05

% area under peak
Ratio
mean peak area
Trend plot
Trend of 1C labelled isotopomer
Relative labelling pattern

Overlap
<Expected
>Expected

G1
P-DPD

Formula: C5H9O7P  Mass: 212.009  Std.RT: 797.7542814  Ion: NEG

UL  +1  +2  +3  +4  +5

G1

Ratio

% area under peak

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap  <Expected  >Expected
Orotidine(fragment)
Formula: C9H12N2O6  Mass: 244.07  Std.RT: 764.687997  Ion: NEG

UL  +1  +2  +3  +4  +5  +7  +8  +9

CMW  L1H  L1M  LH  LM  QC  ULH  ULM

Ratio  Trend plot  Trend of 1 C labelled isotopomer  Relative labelling pattern
nocardicin G
Formula: C19H19N3O6  Mass: 385.127  Std.RT: 904.9671426  Ion: NE

G1

Trend of 1 C labelled isotopomer

Trend plot

Ratio

% area under peak

mean peak area

mean peak area

Overlap

<Expected

>Expected
1-18:0–2–18:3–phosphatidate

Formula: C39H71O8P  Mass: 698.489  Std.RT: 208.2654952  Ion: NE

G1
Muramic acid
Formula: C9H17NO7  Mass: 251.101  Std.RT: 795.5601372  Ion: NEG

G1
L-alpha-glutamyl-L-hydroxyproline
Formula: C10H16N2O6  Mass: 260.101  Std.RT: 819.7797156  Ion: NE

UL
UL +1 +2 +3 +4 +5 +6 +7 +8 +9 +10

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Overlap
(Expected
(Expected

% area under peak
0.0 0.2 0.4 0.6 0.8 1.0

mean peak area
0 10 20 30 40 50 60

mean peak area
0 1 2 3 4 5 6 7 8 9 10
N3–fumaramoyl–L–2,3–diaminopropanoate
Formula: C7H10N2O5  Mass: 202.059  Std.RT: 921.7731498  Ion: NEC

<table>
<thead>
<tr>
<th>UL</th>
<th>+1</th>
<th>+2</th>
<th>+3</th>
<th>+4</th>
<th>+5</th>
<th>+6</th>
<th>+7</th>
</tr>
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</tbody>
</table>

Trend plot
Trend of 1 C labelled isotopomer

Overlap
Expected
>Expected
2,7-Anhydro-alpha-N-acetylneuraminic acid

Formula: C11H17NO8  Mass: 291.095  Std.RT: 798.8148516  Ion: NEC

G1
sn-glycero-3-Phospho-1-inositol

G1

Trend of 1 C labelled isotopomer

Relative labelling pattern
sn-glycero-3-Phospho-1-inositol

G2

Ratio
% area under peak
0.0 0.2 0.4 0.6 0.8 1.0
0.0 0.2 0.4 0.6 0.8 1.0

mean peak area
0e+00 1e+06 2e+06 3e+06 4e+06 5e+06

Trend of 1 C labelled isotopomer
Overlap
<Expected
>Expected

Relative labelling pattern
0 1 2 3 4 5 6 7

Trend plot

mean peak area
0e+00 1e+05 2e+05 3e+05 4e+05 5e+05

% relative labelling
0 1 2 3 4 5 6 7

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9
L-thiazolidine-4-carboxylate
Formula: C₄H₇NO₂S  Mass: 133.02  Std.RT: 455.85323808  Ion: NEG

UL +1 +2 +3 +4

G1

% area under peak
CMW1 CMW2 CMW3 L1H1 L1H2 L1H3 L1H4 L1H5 L1M1 L1M2 L1M3 LH1 LH2 LH3 LM1 LM2 LM3 QC1 QC2 QC3 QC4 QC5 ULH1 ULH2 ULH3 ULM1 ULM2

Ratio
0.0 0.2 0.4 0.6 0.8 1.0

mean peak area
0e+00 2e+05 6e+05

mean peak area
0 5000 15000 25000

mean peak area
0 5000 15000 25000

Trend plot

Trend of 1 C labelled isotopomer

Overlap <Expected >Expected

Relative labelling pattern

% relative labelling
0.0 0.5 1.0 1.5 2.0

% area under peak
2-Dehydro-D-xylonate

Formula: C5H8O6  Mass: 164.032  Std.RT: 812.4240006  Ion: NEG

UL  +1  +2  +3  +4  +5

G1

Trend plot

Trend of 1 C labelled isotopomer

Overlap  <Expected  >Expected
sodium dodecyl sulfate
Formula: C12H26O4S Mass: 266.155 Std.RT: 208.0859559 Ion: NEC

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12

CMW
L1H
L1M
LH
LM
QC
ULH
ULM

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap
<Expected
>Expected
L–Glutamate methylester
Formula: C6H11NO4  Mass: 161.069  Std.RT: 564.2868729  Ion: NEG

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
3-sulfopropanoate
Formula: C₃H₆O₅S  Mass: 153.994  Std.RT: 1048.5345972  Ion: NEG

UL  1  2  3

G1

Trend plot

Overlap
<Expected
>Expected
Hydroxyacetone phosphate
Formula: C3H7O5P  Mass: 154.003  Std.RT: 709.812573  Ion: NEG

UL  +1  +2  +3

G1

Trend plot

Relative labelling pattern

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected
1-deoxynojirimycin

Formula: C6H13NO4  Mass: 163.084  Std.RT: 721.7427468  Ion: NEG

G1

---

**Ratio**

- % area under peak
  - 0.0
  - 0.2
  - 0.4
  - 0.6
  - 0.8
  - 1.0

**Trend plot**

- Trend plot of 1 C labelled isotopomer

**Relative labelling pattern**

- Overlap
- <Expected
- >Expected

---

**Mean peak area**

- Mean peak area
  - 0
  - 2000
  - 4000
  - 6000
  - 8000
  - 10000
  - 12000

---

**Graphs**

- Various graphs showing data related to 1-deoxynojirimycin.
Vinylacetylglycine
Formula: C6H9NO3  Mass: 143.058  Std.RT: 956.6002476 Ion: NEG

G1

Ratio
% area under peak

trend plot
Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected
4,4’−Sulfonyldiphenol
Formula: C12H10O4S  Mass: 250.03  Std.RT: 314.06238078  Ion: NEC

UL  +1  +2  +3  +4  +5  +6  +7  +8  +9  +10  +11  +12

% area under peak
0  0.2  0.4  0.6  0.8  1.0

mean peak area
50000 1000000 1500000 2000000

mean peak area
50000 100000 150000 200000

% relative labelling
0  2  4  6  8  10

Overlap  <Expected  >Expected

Relative labelling pattern
D-myo-Inositol 1,2-cyclic phosphate

Formula: C6H11O8P  Mass: 242.019  Std.RT: 1099.4171382  Ion: NEC

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
L–Azetidine 2–carboxylic acid
Formula: C4H7NO2  Mass: 101.048  Std.RT: 903.313497  Ion: NEG

UL  +1  +2  +3  +4
G1

CMW
L1H
L1M
LH
LM
QC
ULH
ULM

Trend plot

Ratio

Trend of 1 C labelled isotopomer

Relative labelling pattern
(S)–AMPA
Formula: C7H10N2O4  Mass: 186.064  Std.RT: 653.1720024  Ion: NEG

<table>
<thead>
<tr>
<th>630</th>
<th>650</th>
<th>660</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>100</td>
<td>200</td>
</tr>
<tr>
<td>300</td>
<td>400</td>
<td>500</td>
</tr>
</tbody>
</table>

UL
+1
+2
+3
+4
+5
+6
+7

G1

Ratio

% area under peak

0.0 0.2 0.4 0.6 0.8 1.0

Trend plot

mean peak area

0 20000 60000 100000

Trend of 1 C labelled isotopomer

mean peak area

0 2000 4000 6000 8000

Relative labelling pattern

% relative labelling

0.0 0.5 1.0 1.5 2.0 2.5 3.0

Overlap
<Expected
>Expected
DL–Methionine sulfone
Formula: C5H11NO4S  Mass: 181.041  Std.RT: 737.292267  Ion: NEG

- UL
- +1
- +2
- +3
- +4
- +5

Trend plot
- Trend of 1 C labelled isotopomer
  - Overlap
  - <Expected
  - >Expected

Relative labelling pattern
2-Aminobutan-4-olide

Formula: C4H7NO2  Mass: 101.048  Std.RT: 966.4559124  Ion: NEG

% area under peak

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
3–Sulfolactate
Formula: C3H6O6S  Mass: 169.989  Std.RT: 1102.3691562  Ion: NEG

UL  +1  +2  +3

Ratio

% area under peak
0.0  0.2  0.4  0.6  0.8  1.0
0  20  40  60  80  100

mean peak area
0  500000  1500000

Trend plot

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected

Relative labelling pattern

mean peak area
0  50000  150000

0  20  40  60  80  100

% relative labelling

0  100000  200000  300000  400000  500000
N−Glycosyl−L−asparagine

Formula: C10H18N2O8  Mass: 294.106  Std.RT: 945.832287  Ion: NEC

G1

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
N-formylmaleamate
Formula: C5H5NO4  Mass: 143.022  Std.RT: 810.5354994  Ion: NEG

<table>
<thead>
<tr>
<th>Ratio</th>
<th>Trend plot</th>
<th>Trend of 1 C labelled isotopomer</th>
</tr>
</thead>
<tbody>
<tr>
<td>% area under peak</td>
<td>mean peak area</td>
<td>mean peak area</td>
</tr>
<tr>
<td>0.0</td>
<td>0.2</td>
<td>0.4</td>
</tr>
<tr>
<td>0.6</td>
<td>0.8</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Overlap
<Expected
>Expected

UL  +1  +2  +3  +4  +5
Norepinephrine sulfate

Formula: C8H11NO6S  Mass: 249.031  Std.RT: 1197.13047  Ion: NEG

UL  +1  +2  +3  +4  +5  +6  +7  +8

G1

Ratio

% area under peak

mean peak area

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected

0  1  2  3  4  5  6

% relative labelling

0  5000  10000  15000  20000

mean peak area

0  5000  10000  15000  20000

mean peak area

0  5000  10000  15000  20000

mean peak area

0  5000  10000  15000  20000

mean peak area

0  5000  10000  15000  20000

mean peak area
(+/-)-6-Acetonyldihydrochelerythrine
Formula: C24H23NO5  Mass: 405.158  Std.RT: 216.88416738  Ion: NE

G1

Trend plot

Relative labelling pattern
1,4-Bis(2-ethylhexyl) sulfosuccinate

Formula: C20H38O7S  Mass: 422.234  Std.RT: 205.01136498  Ion: NE

% area under peak
0 0.2 0.4 0.6 0.8 1.0

mean peak area
0 150000 250000 350000

Overlap
Expected >Expected

% relative labelling
0 5 10 15

Trend of 1 C labelled isotopomer

Relative labelling pattern
4-hydroperoxyoctadeca-9-t-2-nonenal

Formula: C9H16O3  Mass: 172.11  Std.RT: 212.2257093  Ion: NEG

\[
\text{UL} +1 +2 +3 +4 +5 +6 +7 +8 +9
\]

G1

Ratio

% area under peak

0.0 0.2 0.4 0.6 0.8 1.0

mean peak area

0e+00 2e+04 4e+04 6e+04 8e+04 1e+05

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

Overlap

<Expected

>Expected

0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5

% relative labelling

0e+00 2e+04 4e+04 6e+04 8e+04 1e+05

mean peak area

2000 4000 6000 8000
4-hydroperoxyoctadeca-t-2-nonenal
Formula: C9H16O3  Mass: 172.11  Std.RT: 212.2257093  Ion: NEG

G2

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
N-Ethylglycocyamine
Formula: C8H17NO5  Mass: 207.111  Std.RT: 867.4571448  Ion: NEG

![Graphs showing trend plots and relative labelling patterns for different isotopomers.](image-url)
parabanate
Formula: C3H2N2O3  Mass: 114.007  Std.RT: 811.5734964  Ion: NEG

G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

% area under peak

mean peak area

mean peak area

% relative labelling

Overlap
<Expected
>Expected
5D−5−O−Methyl−2,3,5/4,6−pentahydroxycyclohexanone
Formula: C7H12O6  Mass: 192.063  Std.RT: 803.6734902  Ion: NEG

Trend plot
Trend of 1 C labelled isotopomer
Relative labelling pattern
Propane–1,2–diol 1–phosphate

Formula: C₃H₉O₅P  Mass: 156.019  Std.RT: 717.8616492  Ion: NEG

UL  +1  +2  +3
G1

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
2-oxobut-3-enanoate

Formula: C4H4O3  Mass: 100.016  Std.RT: 982.8730038  Ion: NEG

UL  +1  +2  +3  +4

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
2-oxobut-3-enanoate
Formula: C4H4O3 Mass: 100.016 Std.RT: 982.8730038 Ion: NEG

UL  +1  +2  +3  +4

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern
16-hydroxypalmitate
Formula: C16H32O3  Mass: 272.235  Std.RT: 213.50387568  Ion: NEG

% area under peak

Ratio

mean peak area

Trend plot

Trend of 1 C labelled isotopomer

Relative labelling pattern

- UL
- +1
- +2
- +3
- +4
- +5
- +6
- +7
- +8
- +9
- +10
- +11
- +12
- +13

G1
Acetone cyanohydrin
Formula: C4H7NO Mass: 85.053 Std.RT: 961.2041046 Ion: NEG

UL UL ±1 ±2 ±3 ±4

CMW1 CMW2 CMW3
L1H1 L1H2 L1H3
L1M1 L1M2 L1M3
LH1 LH2 LH3
LM1 LM2 LM3
QC1 QC2 QC3 QC4 QC5
ULH1 ULH2 ULH3
ULM1 ULM2 ULM3

Ratio

Trend plot

Trend of 1 C labelled isotopomer

Overlap
<Expected
>Expected