Supporting Information – Part 2 (SI-2)

SpecLibMarineUnknown2018 Mass Spectral Library

Halogenated Unknown Mass Spectra in Marine Mammal Blubber from the Southern California Bight.

Manuscript: Apex marine predators and ocean health: proactive screening of halogenated organic contaminants reveals ecosystem indicator species

Authors: Jennifer M. Cossaboon, Eunha Hoh, Susan J. Chivers, David W. Weller, Kerri Danil, Keith A. Maruya, and Nathan G. Dodder

Uses compound naming scheme from Environ. Sci. Technol. 2015, 49, 1328−1338.
(Compounds starting with MMCP are unique to this project.)

Web Reference: http://OrgMassSpec.github.io

Prepared: 2018−05−09 11:44:52
SpecLibMarineUnknown2018
OrgMassSpecR version 0.5−3

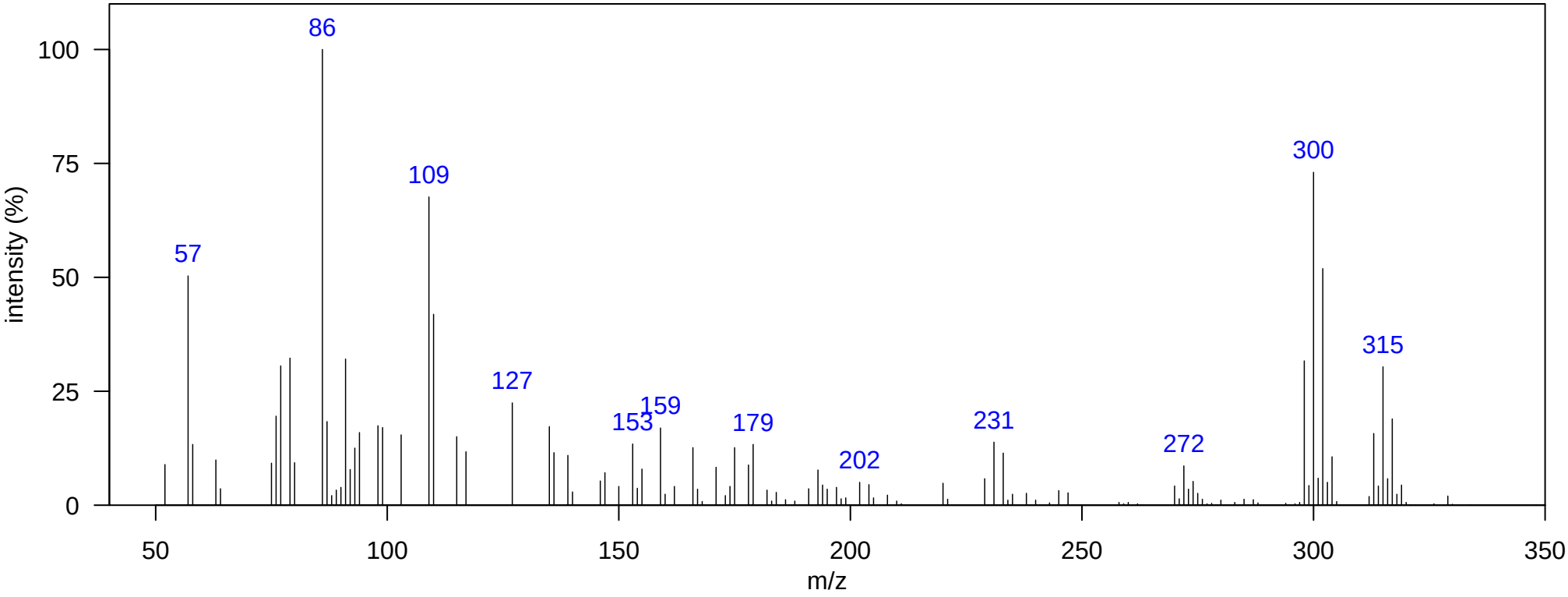
R version 3.4.1 (2017−06−30)

Name: MMCP unknown 1 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1089.72 , 0.931

Comment:

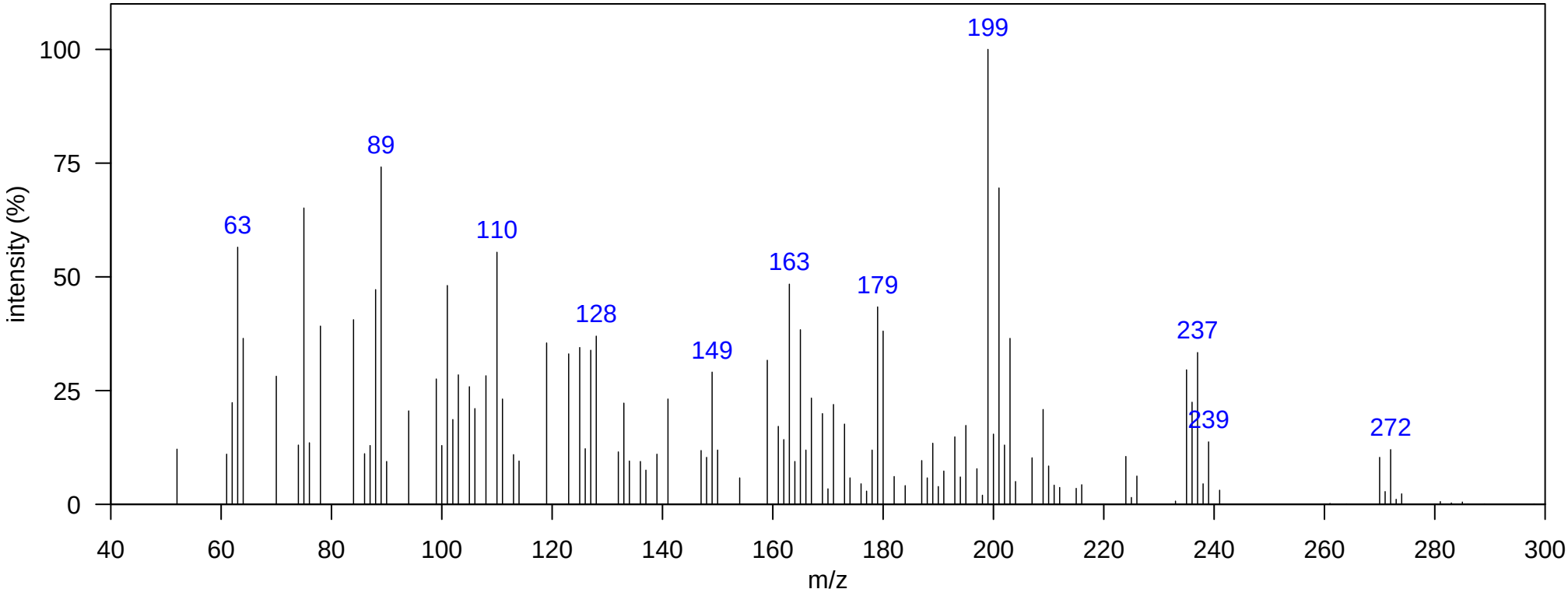


Name: MMCP unknown 2 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1128.2 , 0.898

Comment:

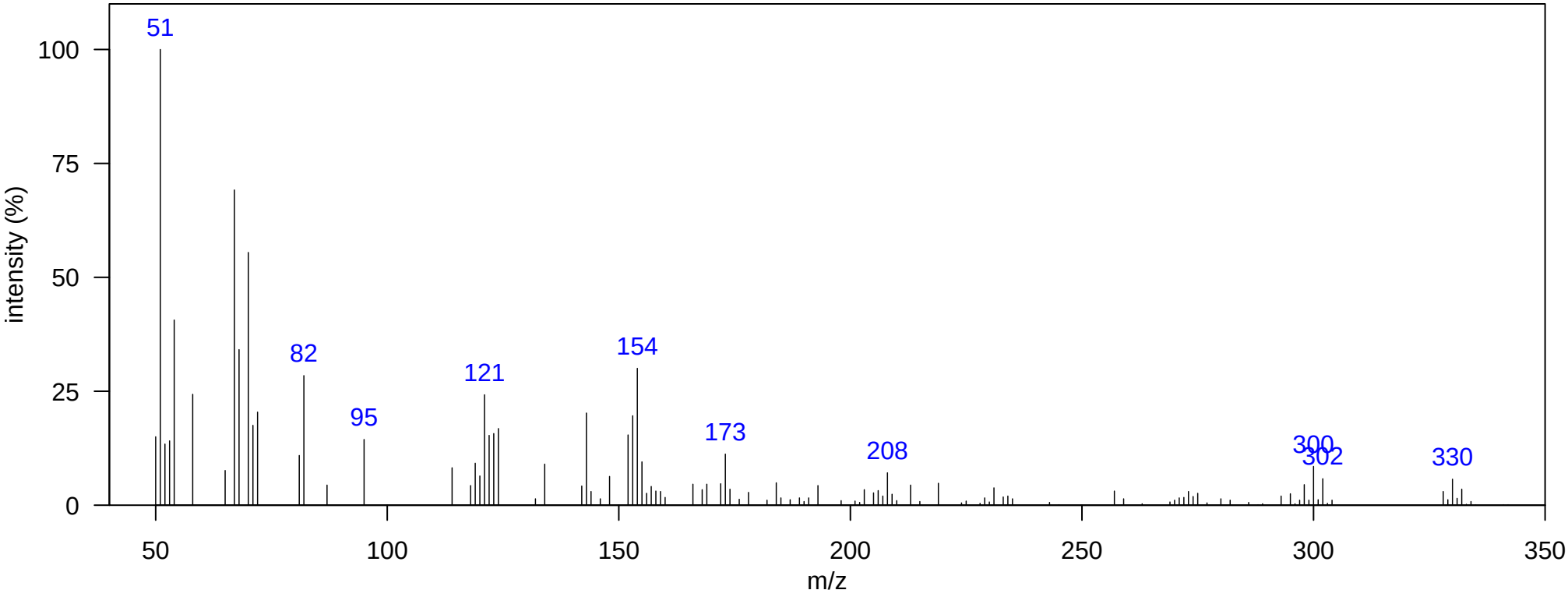


Name: MMCP unknown 3 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1215.65 , 1.016

Comment:

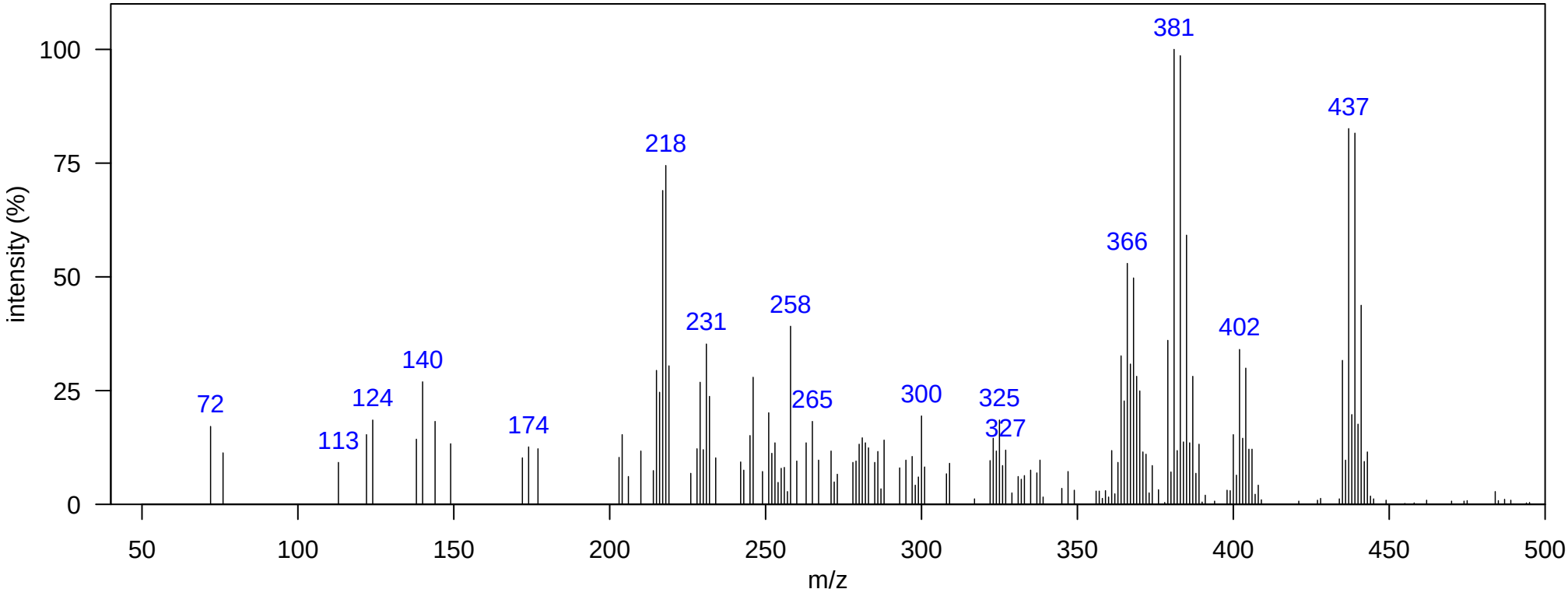


Name: MMCP unknown 4 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1530.47 , 1.168

Comment:

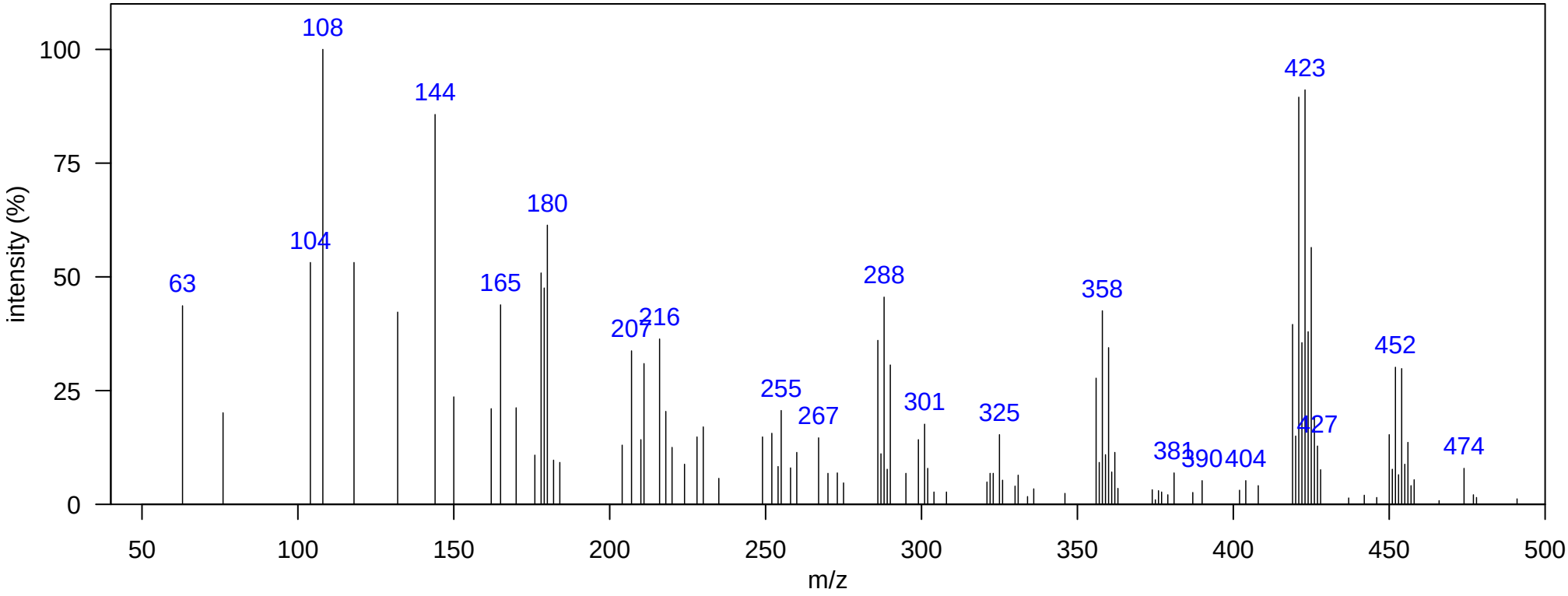


Name: MMCP unknown 5 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1684.38 , 1.459

Comment:

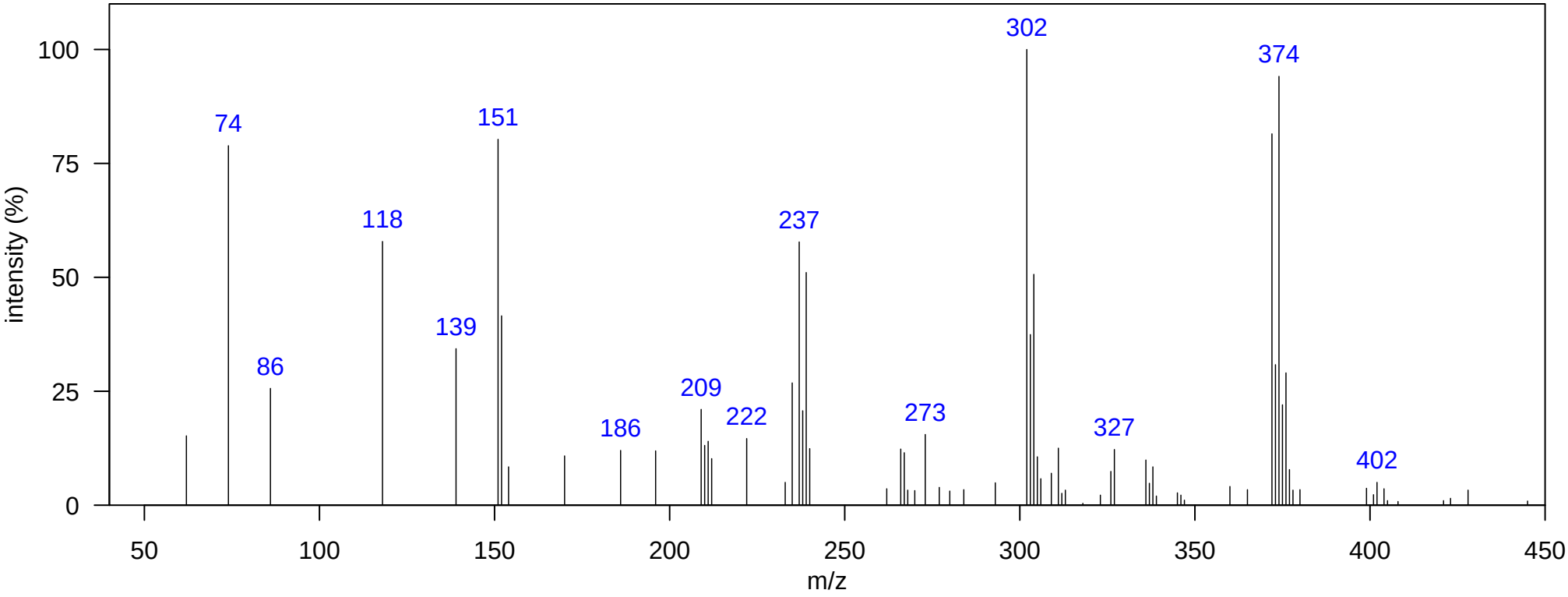


Name: MMCP unknown 6 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1701.87 , 1.525

Comment:

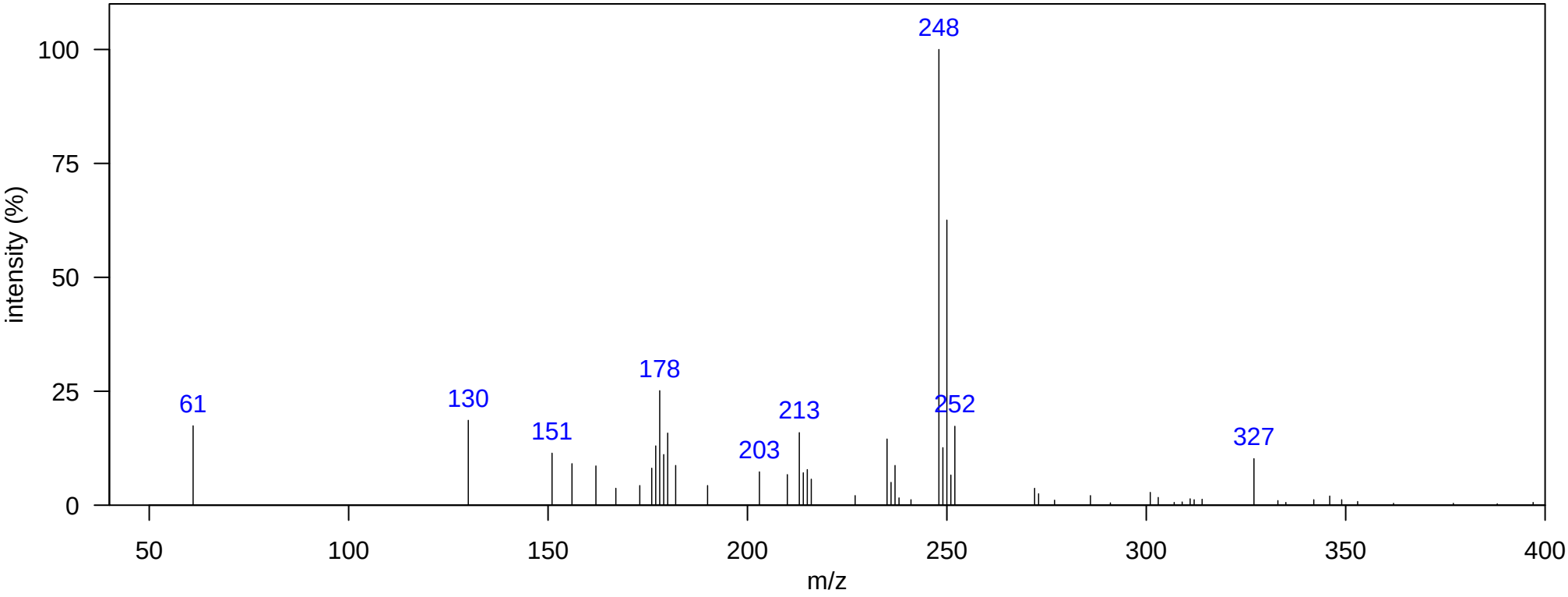


Name: MMCP unknown 7 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 2023.69 , 1.927

Comment:

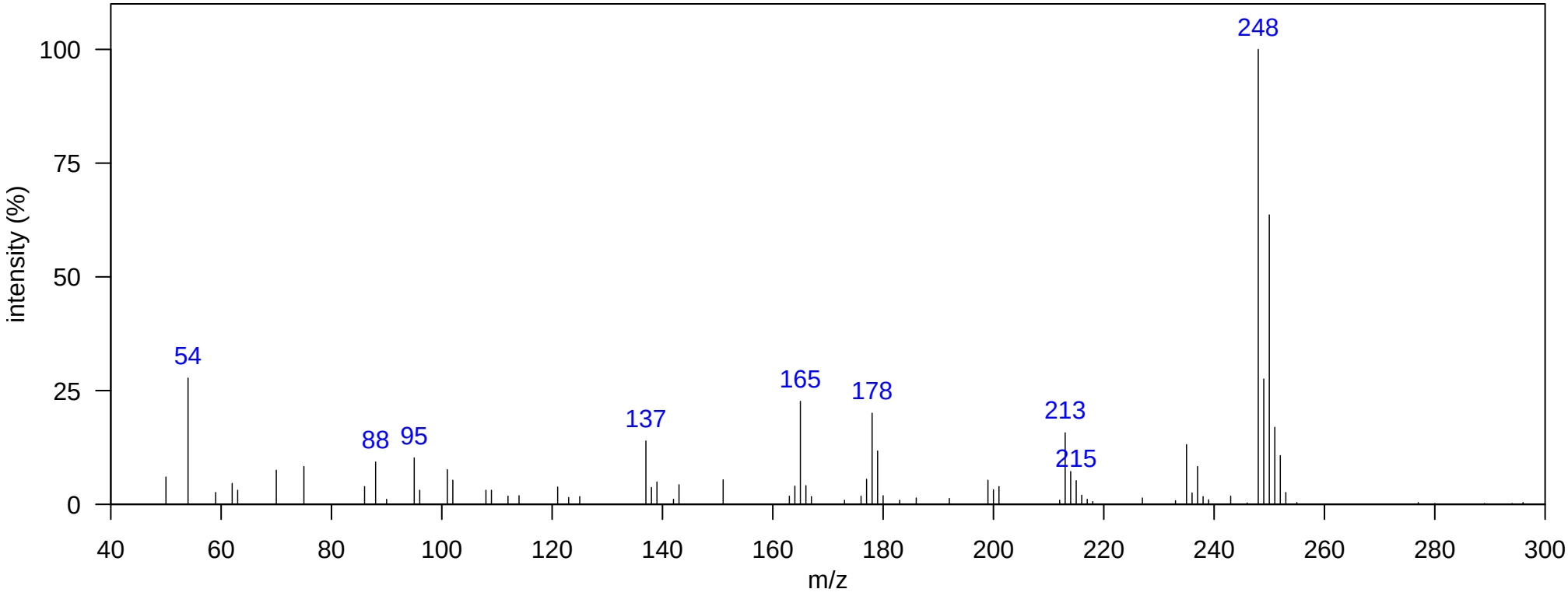


Name: MMCP unknown 8 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 2212.58 , 2.581

Comment:

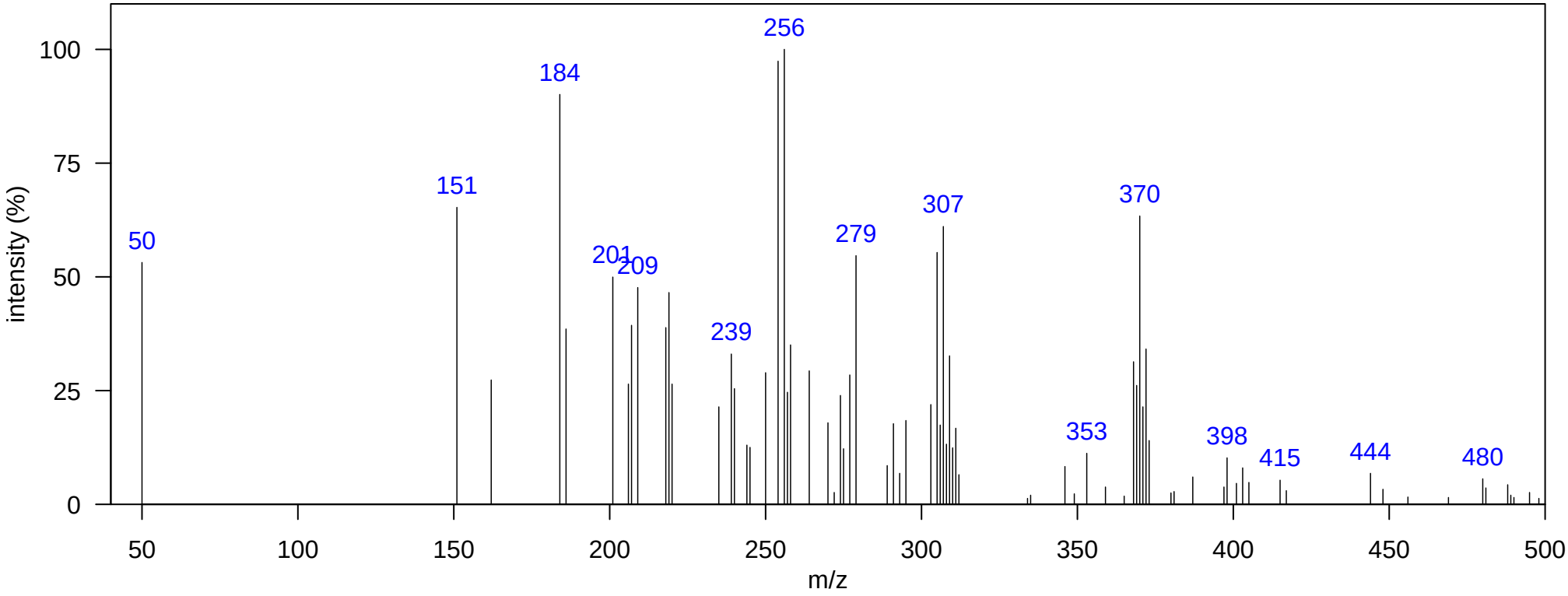


Name: MMCP unknown−6 related 1 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1596.93 , 1.452

Comment:

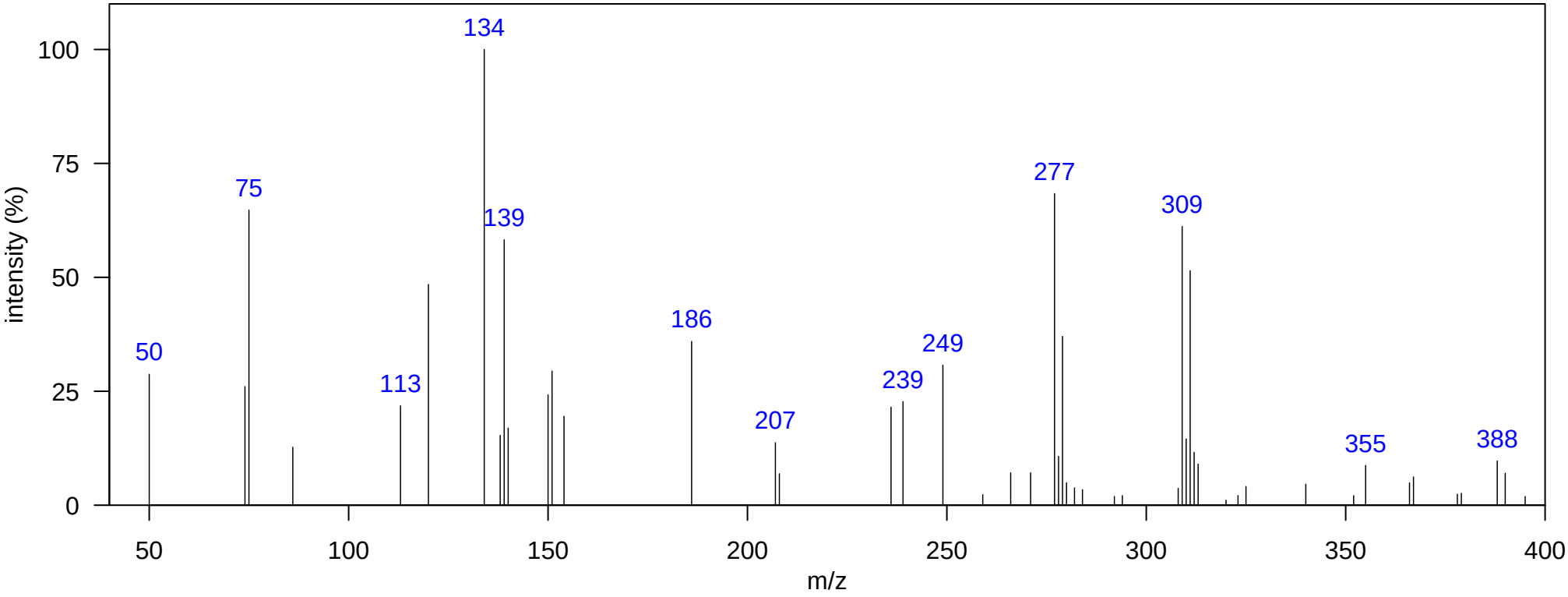


Name: MMCP unknown−52 related 1 Class: MMCP unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1789.32 , 1.610

Comment:

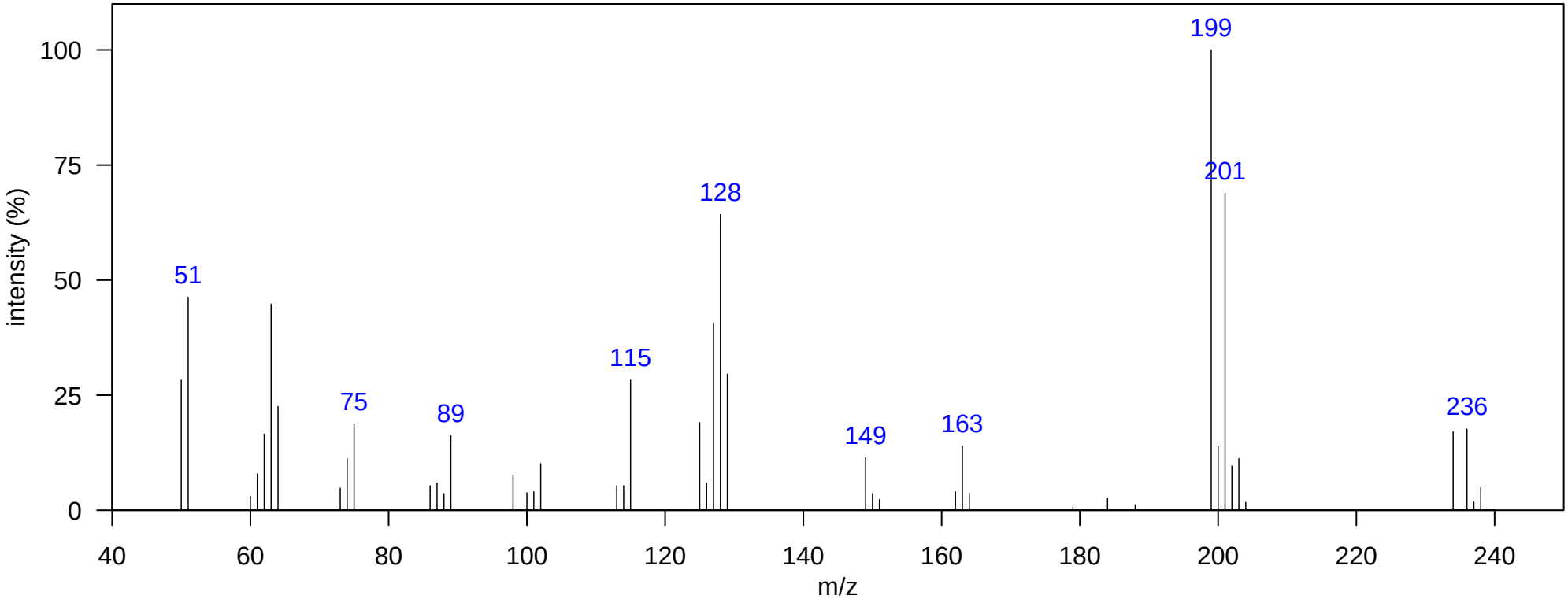


Name: Unknown−11 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1114.21 , 0.904

Comment:

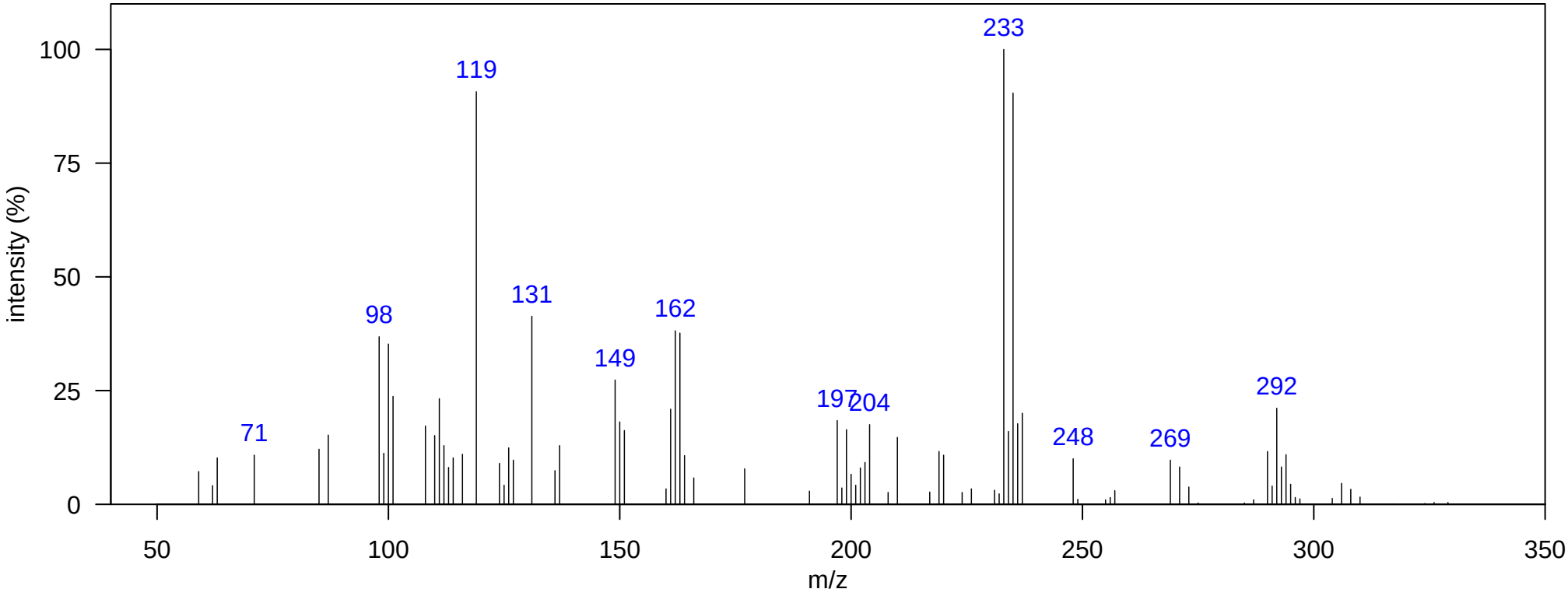


Name: Unknown−14 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1247.13 , 0.970

Comment:

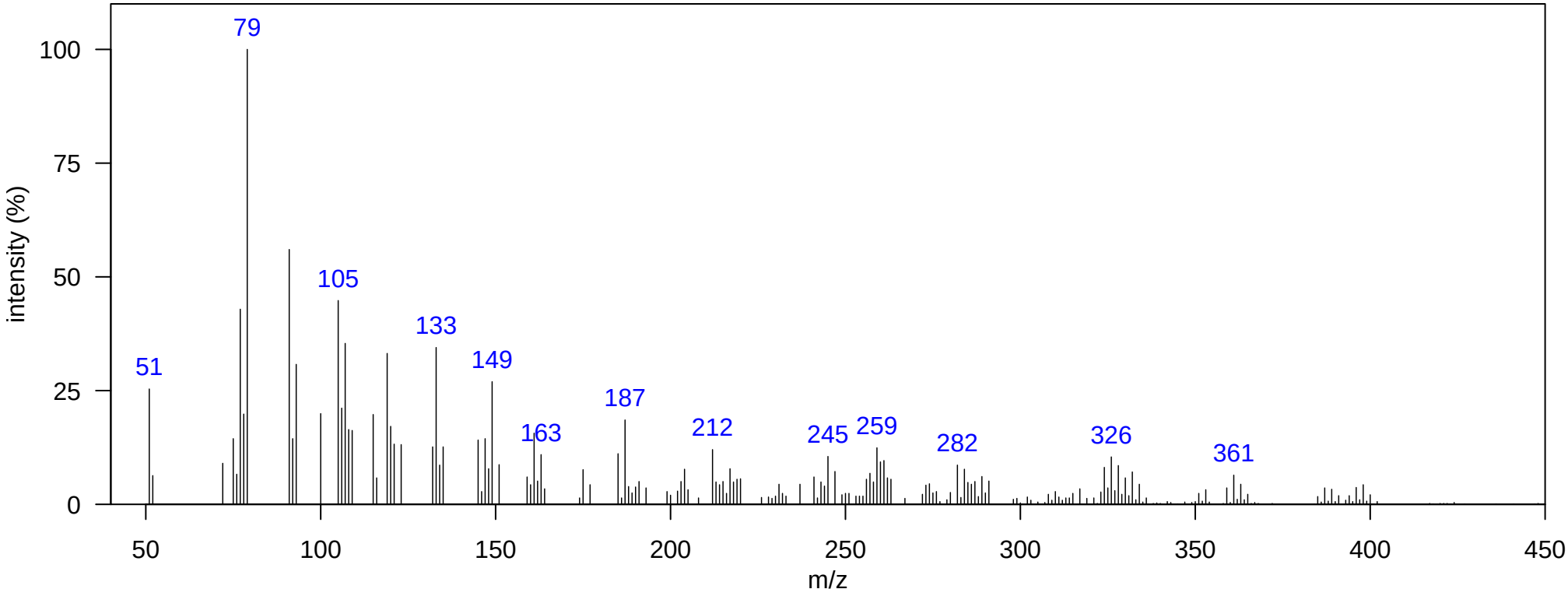


Name: Unknown−15 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1278.61 , 0.937

Comment:

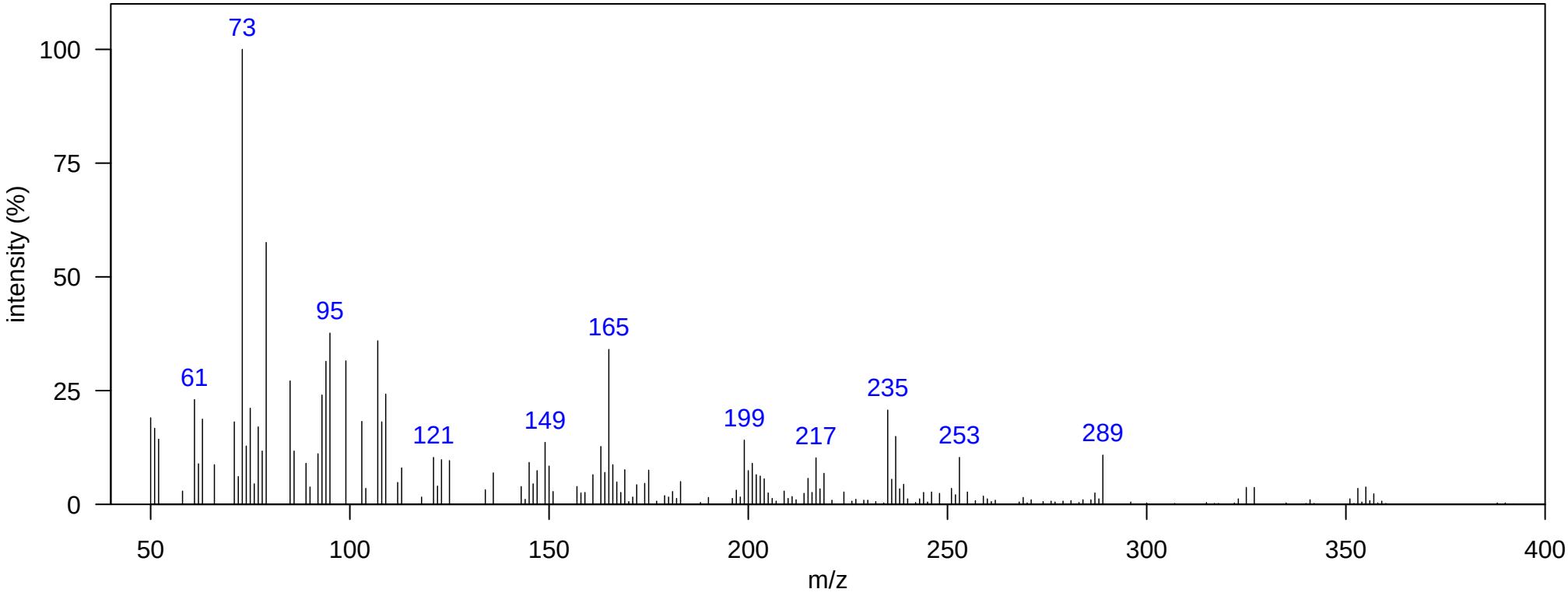


Name: Unknown−16 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1296.1 , 0.977

Comment: Interference with some compounds − ion 355 belongs to unknown−16

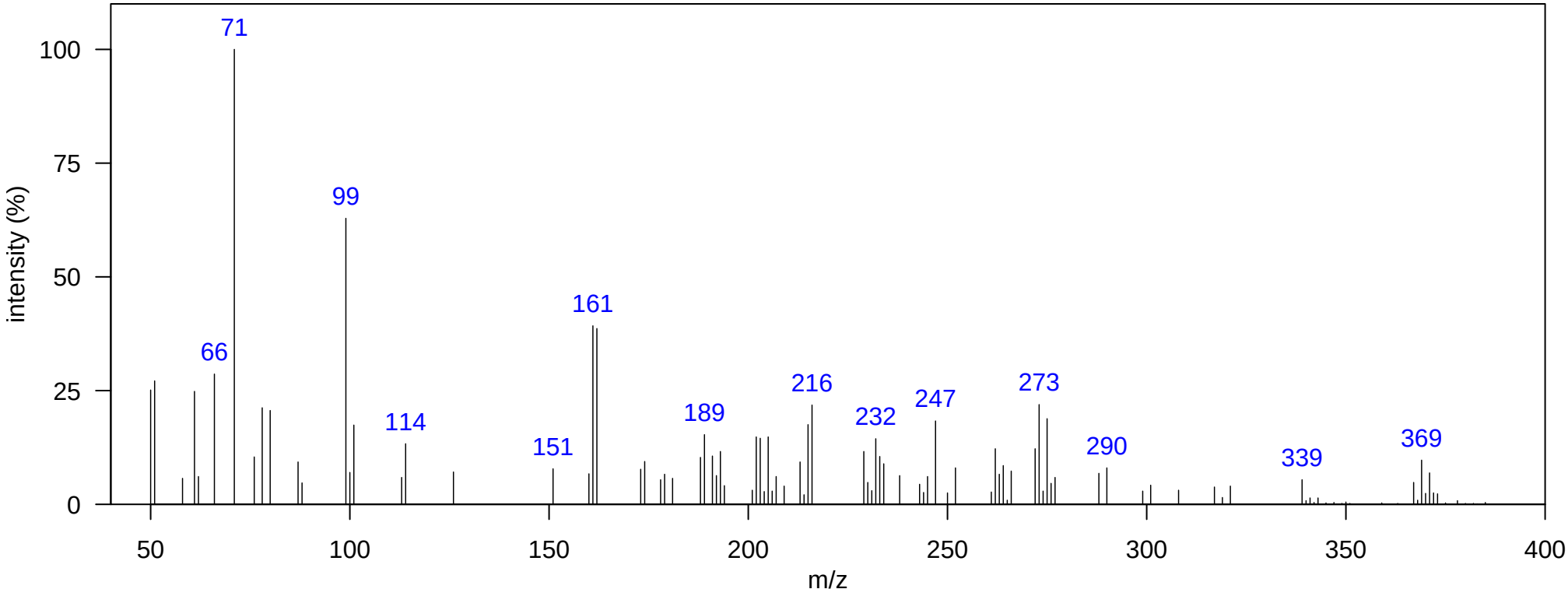


Name: Unknown−17 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1296.1 , 0.917

Comment:

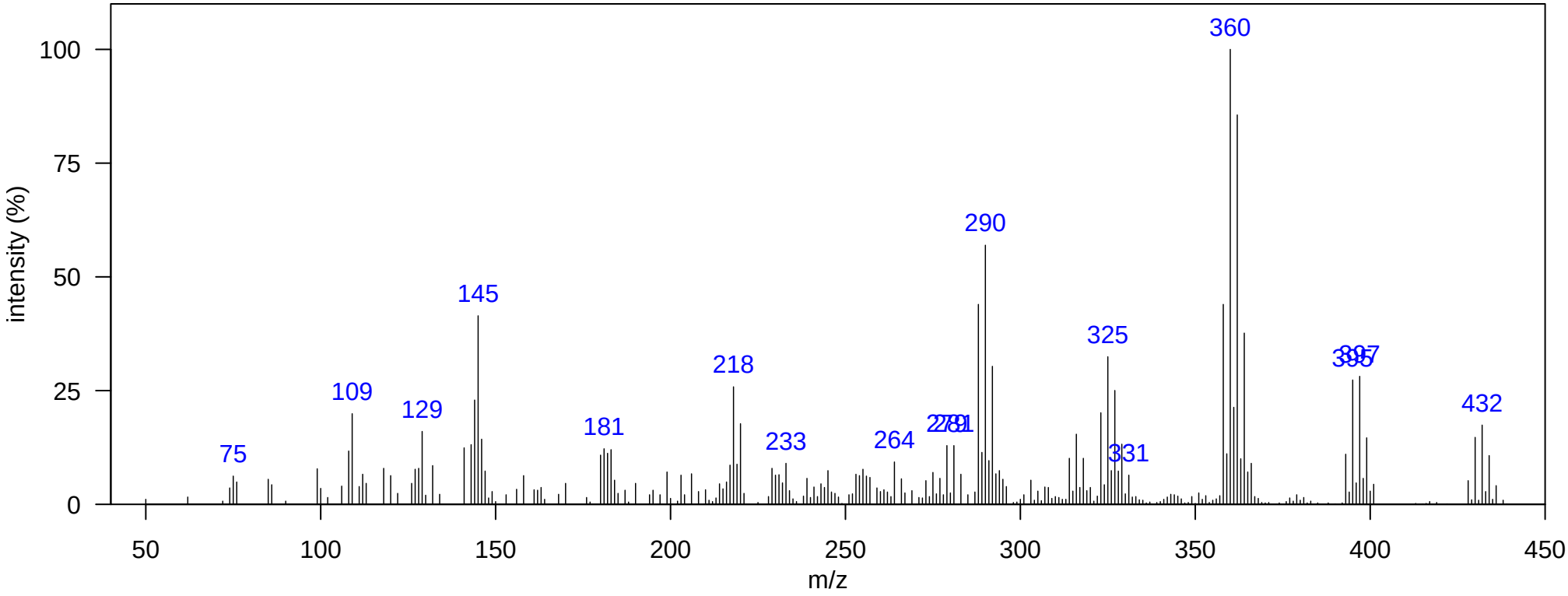


Name: Unknown−19 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1376.56 , 0.990

Comment: PCB interference

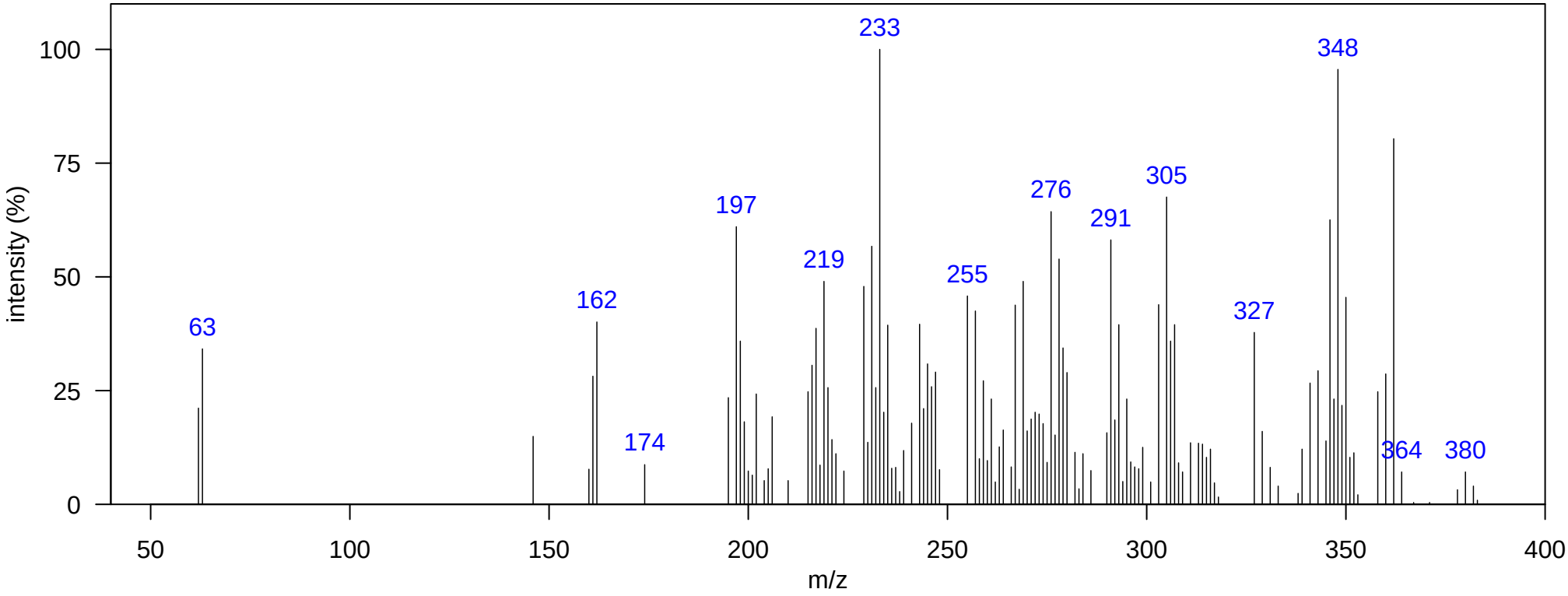


Name: Unknown−21 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1450.01 , 1.069

Comment:

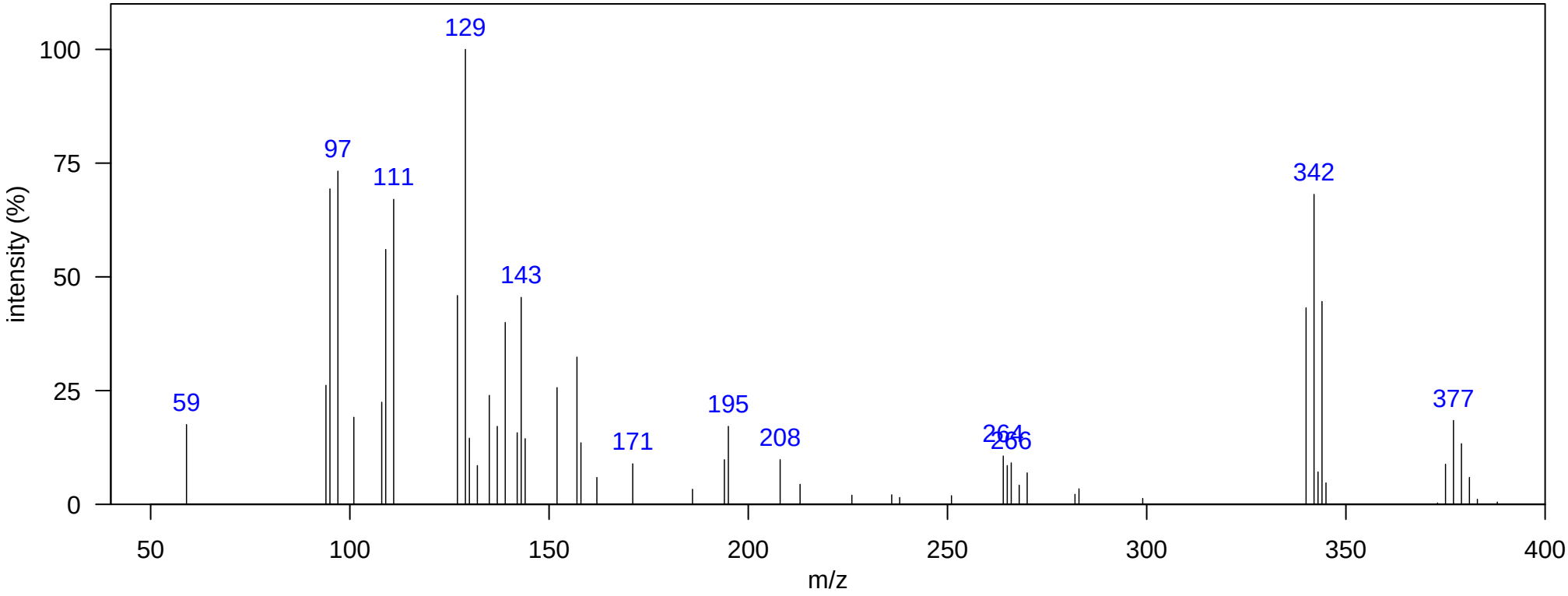


Name: Unknown−22 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1446.52 , 1.063

Comment:

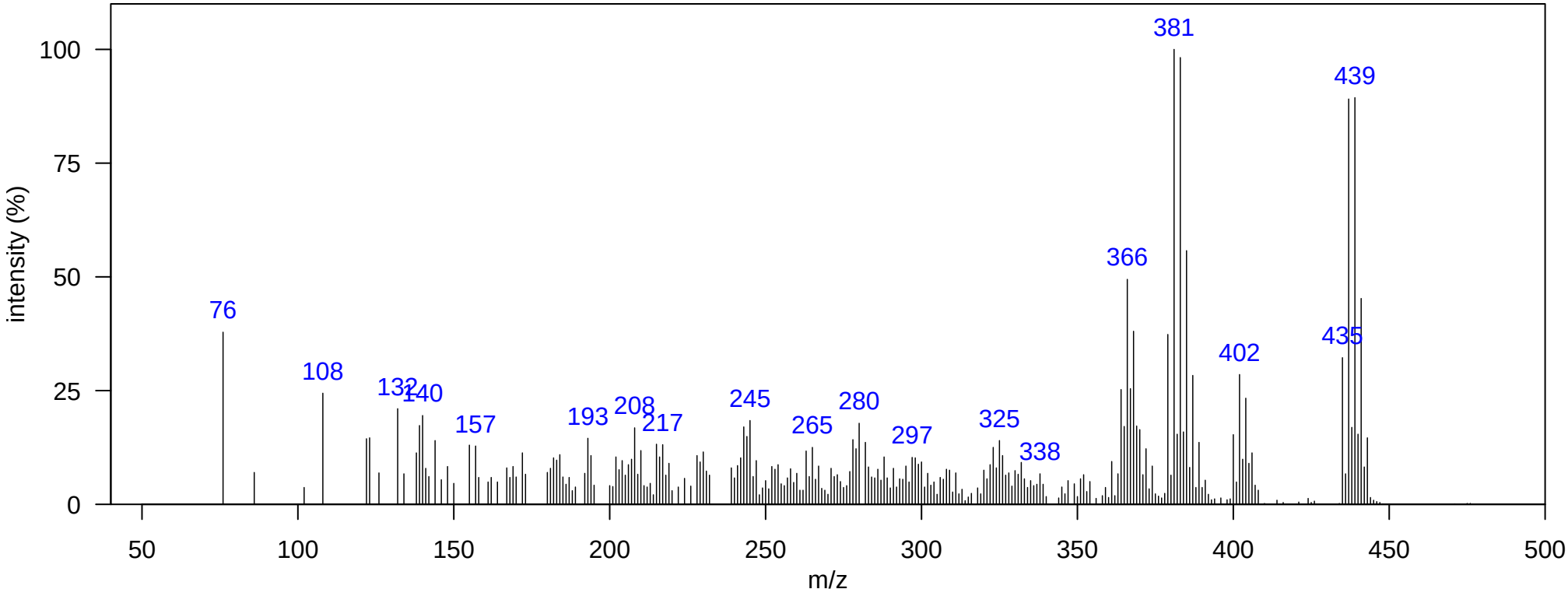


Name: Unknown−34 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1530.47 , 1.195

Comment:

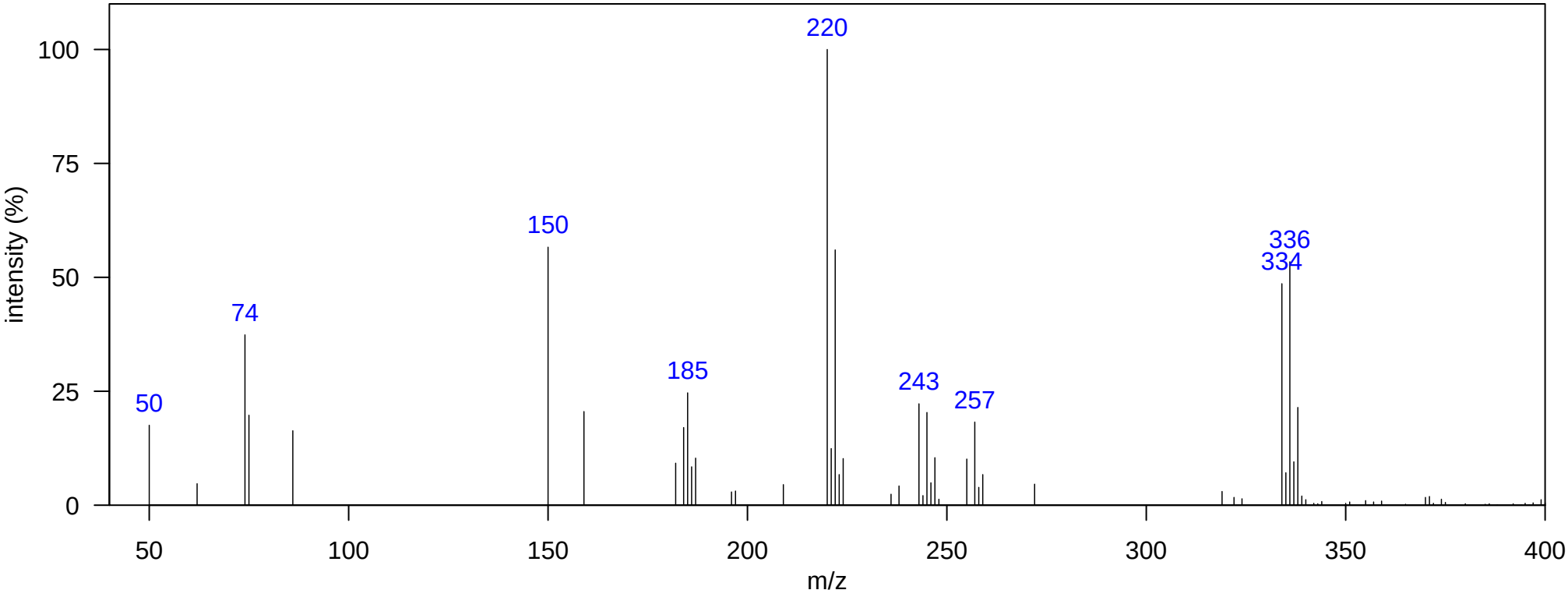


Name: Unknown−36 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1554.95 , 1.300

Comment:

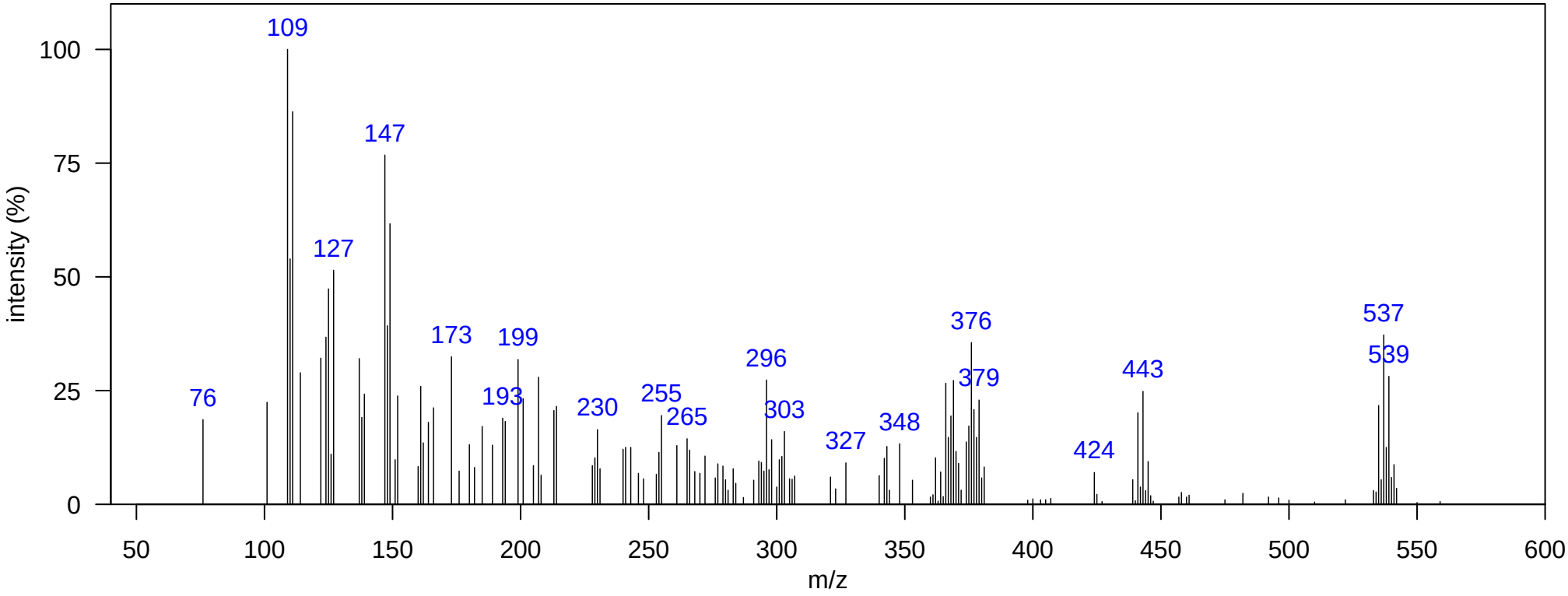


Name: Unknown−38 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1561.95 , 1.274

Comment:

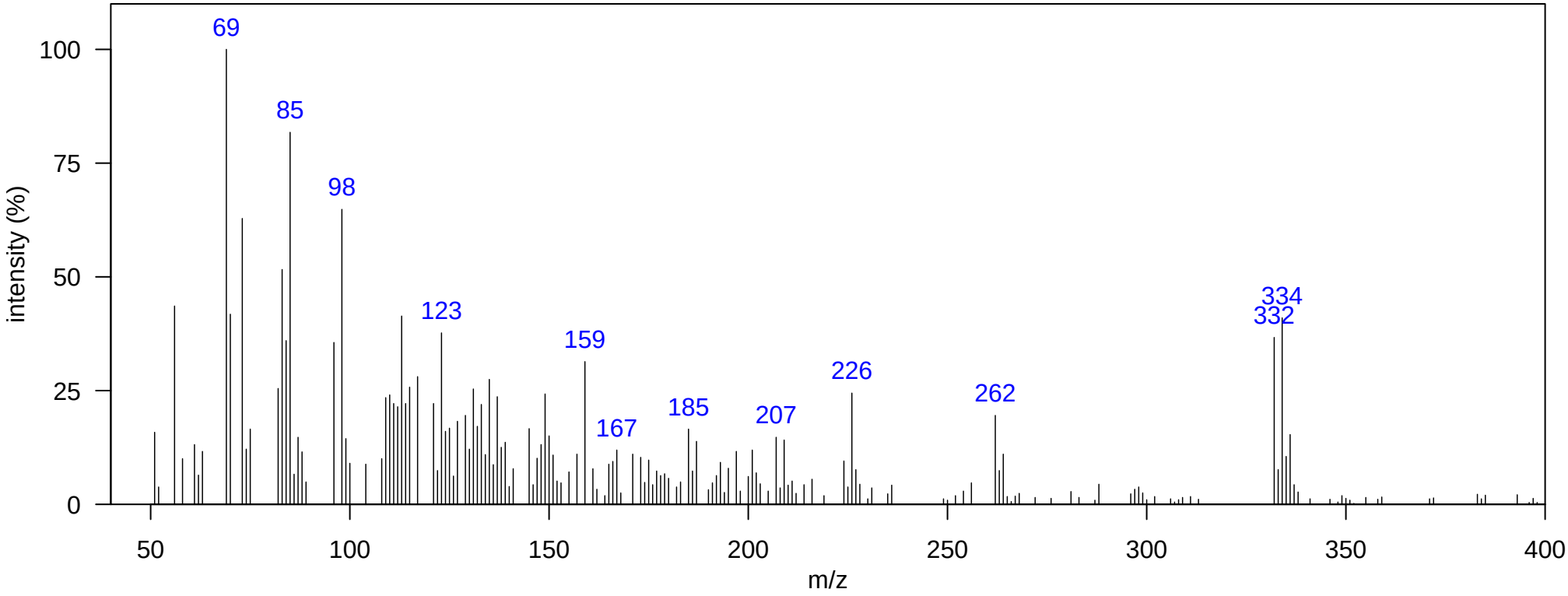


Name: Unknown−39 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1554.95 , 1.267

Comment:

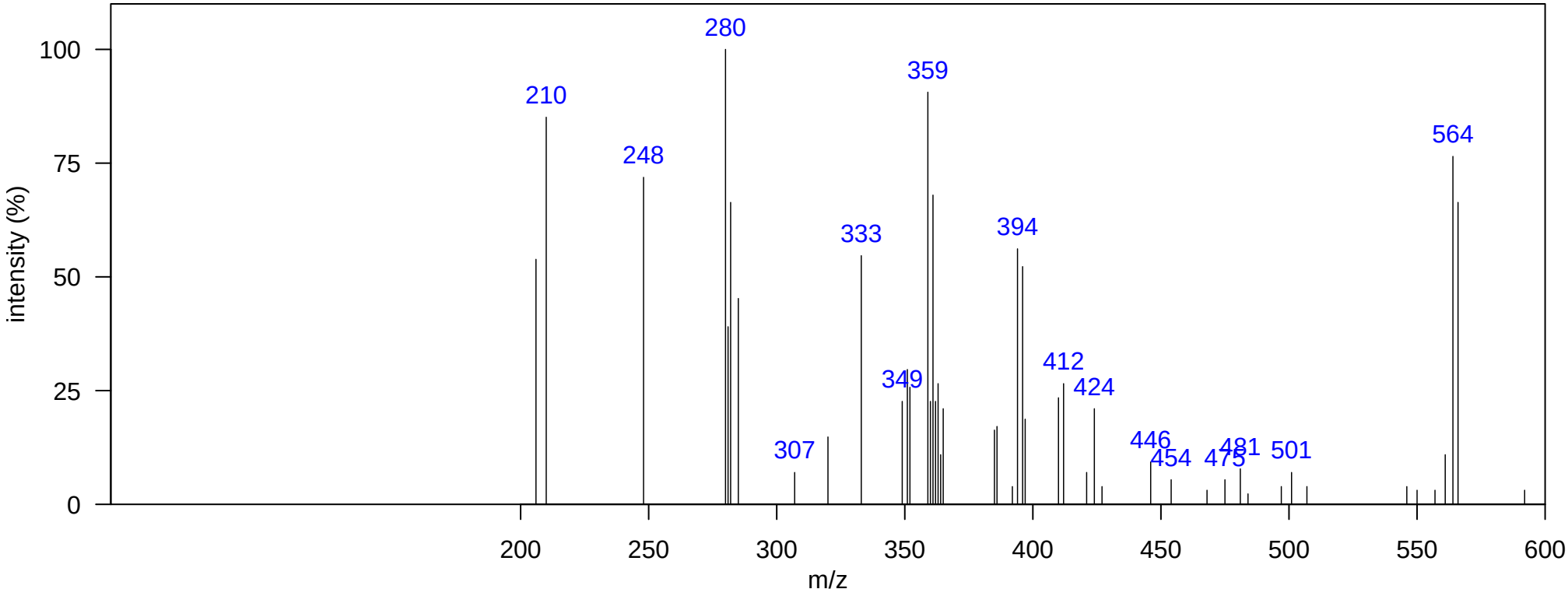


Name: Unknown−44 Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1624.91 , 1.518

Comment:

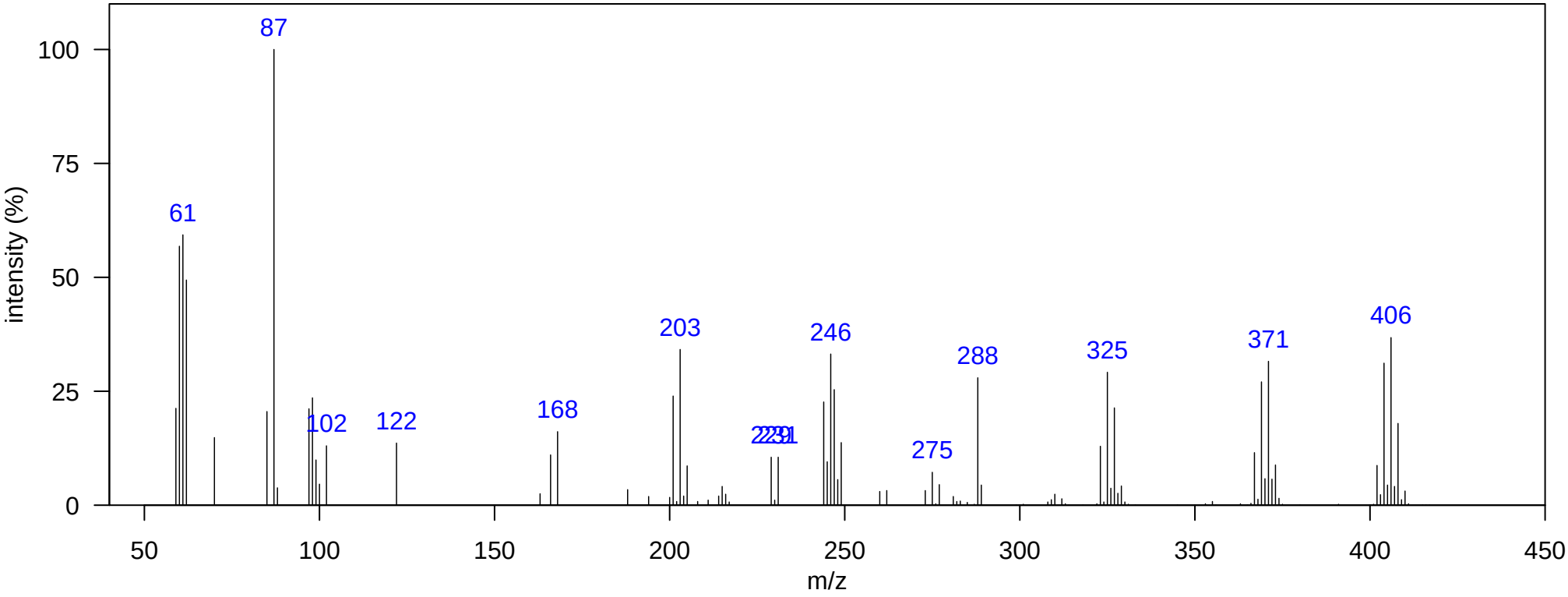


Name: Unknown−3−1 Class: Unknown−3

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1240.13 , 1.010

Comment:

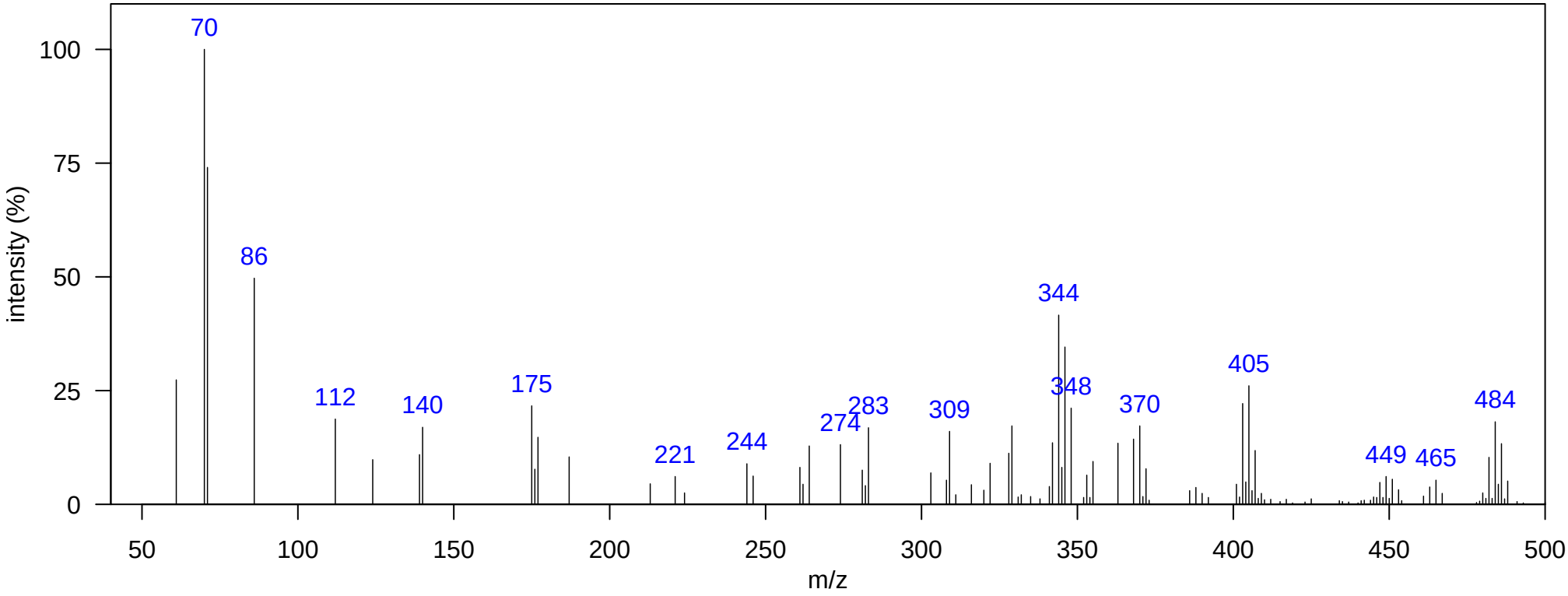


Name: Unknown−3−3 Class: Unknown−3

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1411.54 , 1.142

Comment:

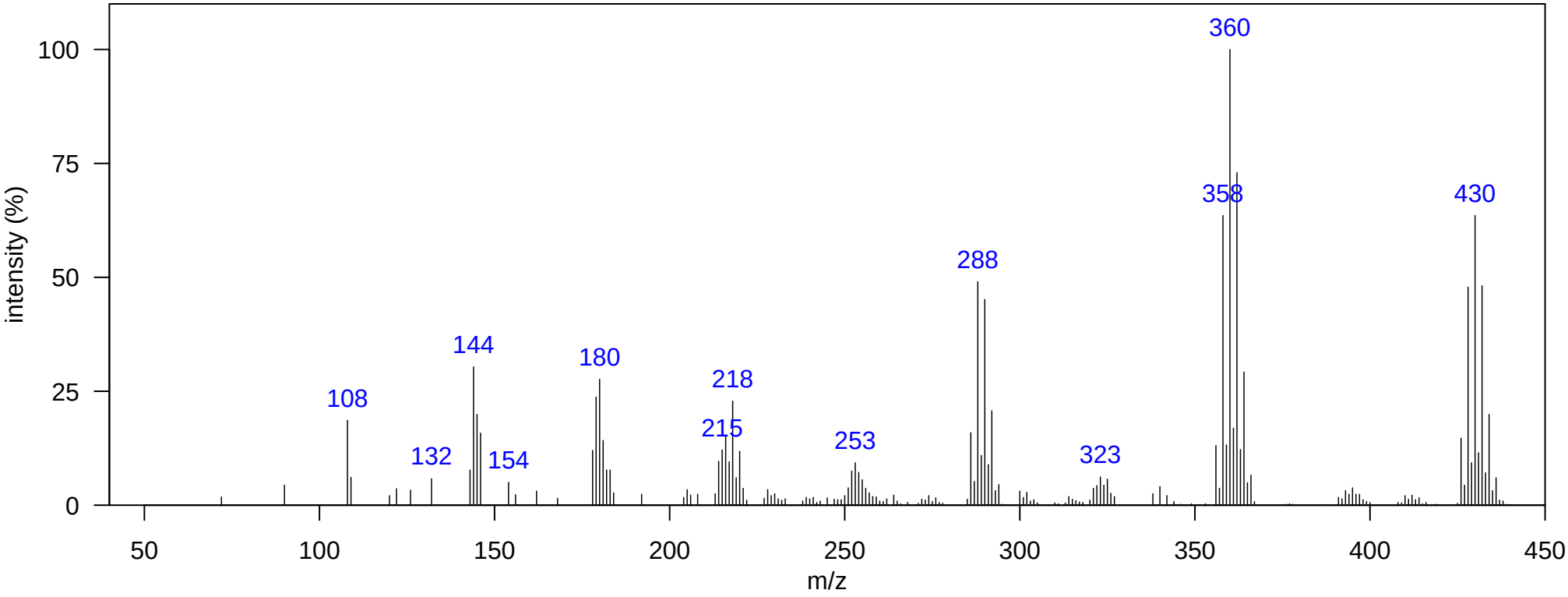


Name: Unknown−4−2 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1495.49 , 1.056

Comment: PCB interference − ions 412 and 340 belong to unknown−4−2

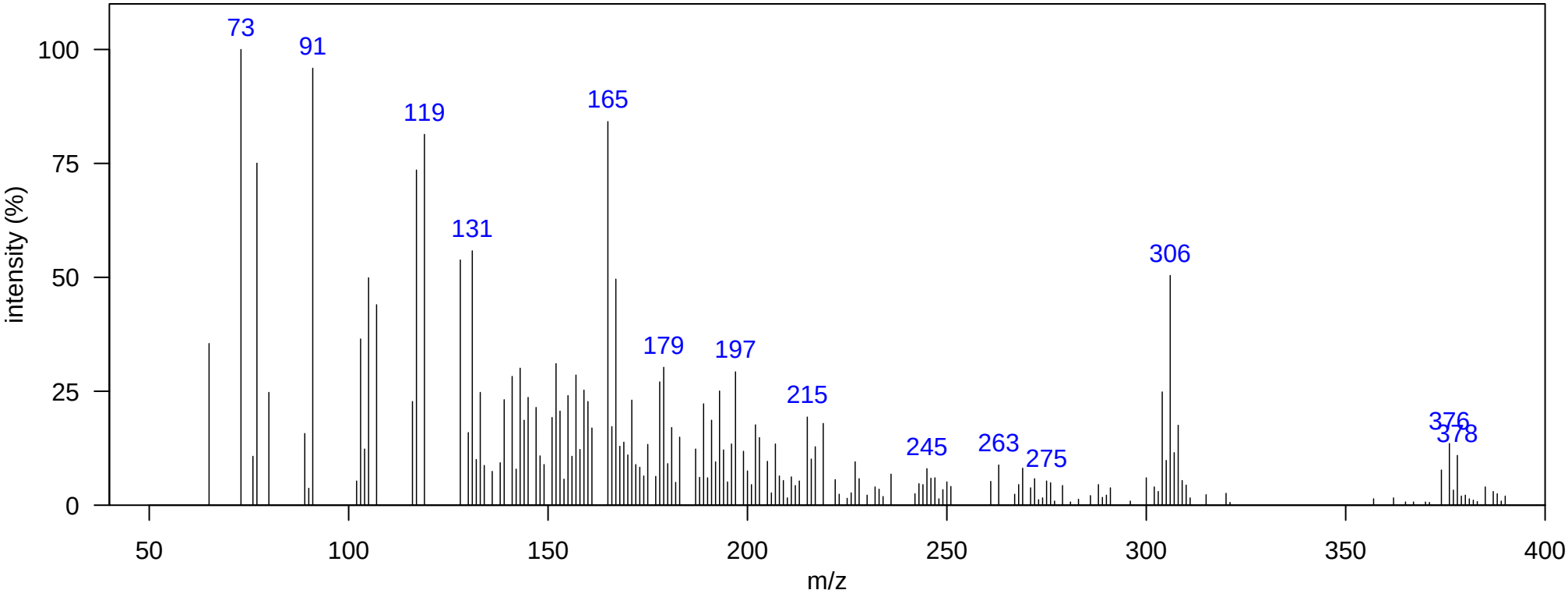


Name: Unknown−4−3 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1415.03 , 0.997

Comment:

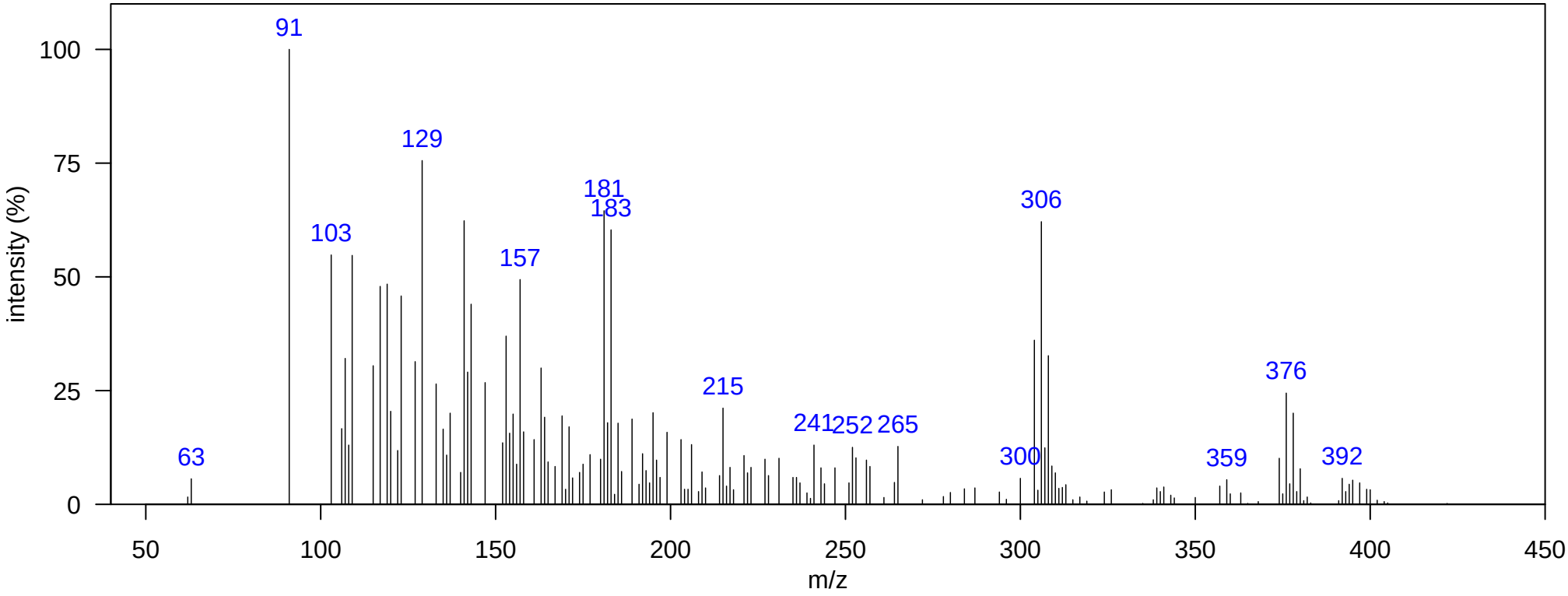


Name: Unknown−4−5 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1450.01 , 1.069

Comment:

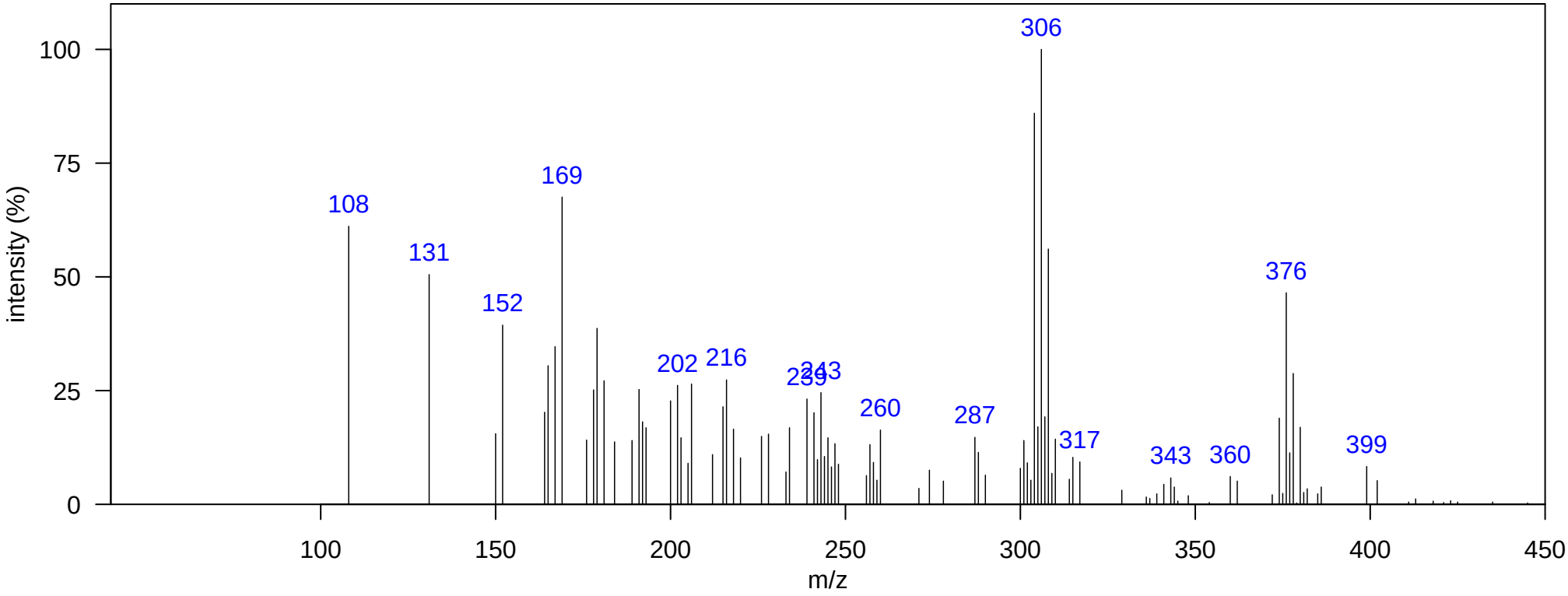


Name: Unknown−4−7 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1488.49 , 1.056

Comment:

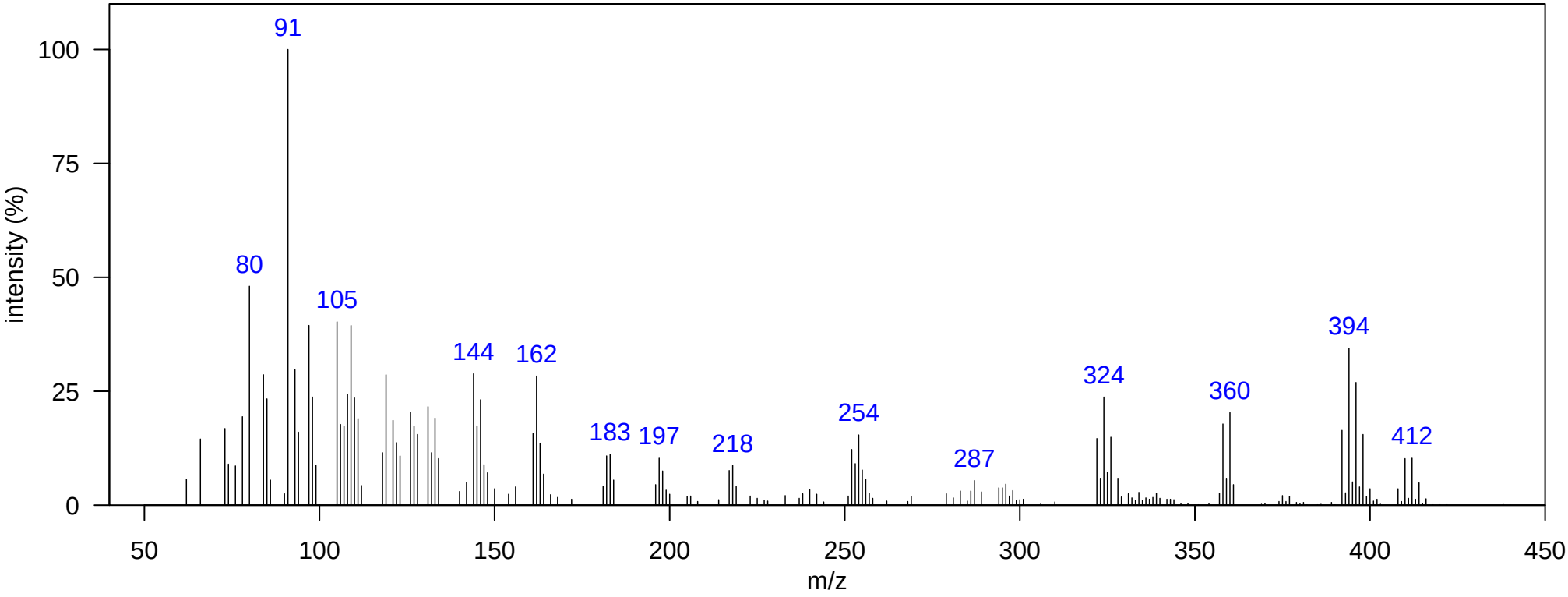


Name: Unknown−4−8 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1429.03 , 1.036

Comment: PCB interference

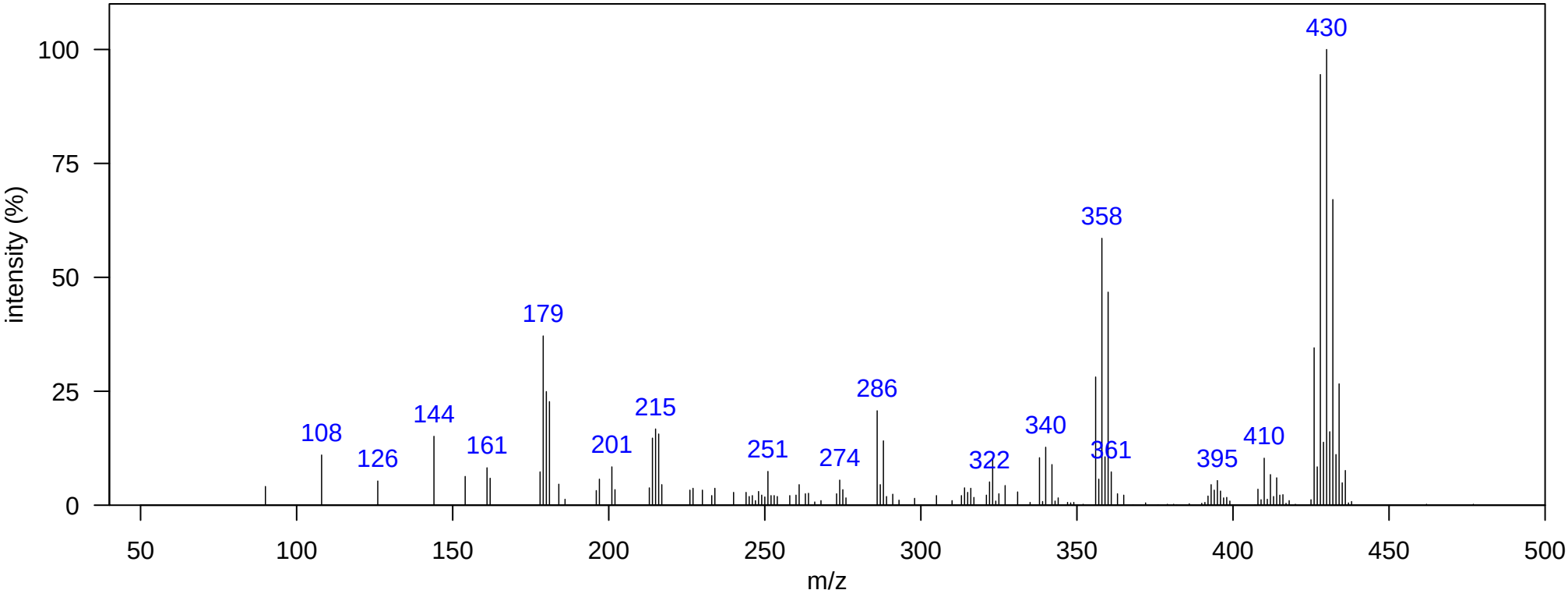


Name: Unknown−4−10 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1495.49 , 1.036

Comment: PCB interference − ions 410 and 340 belong to unknown−4−10

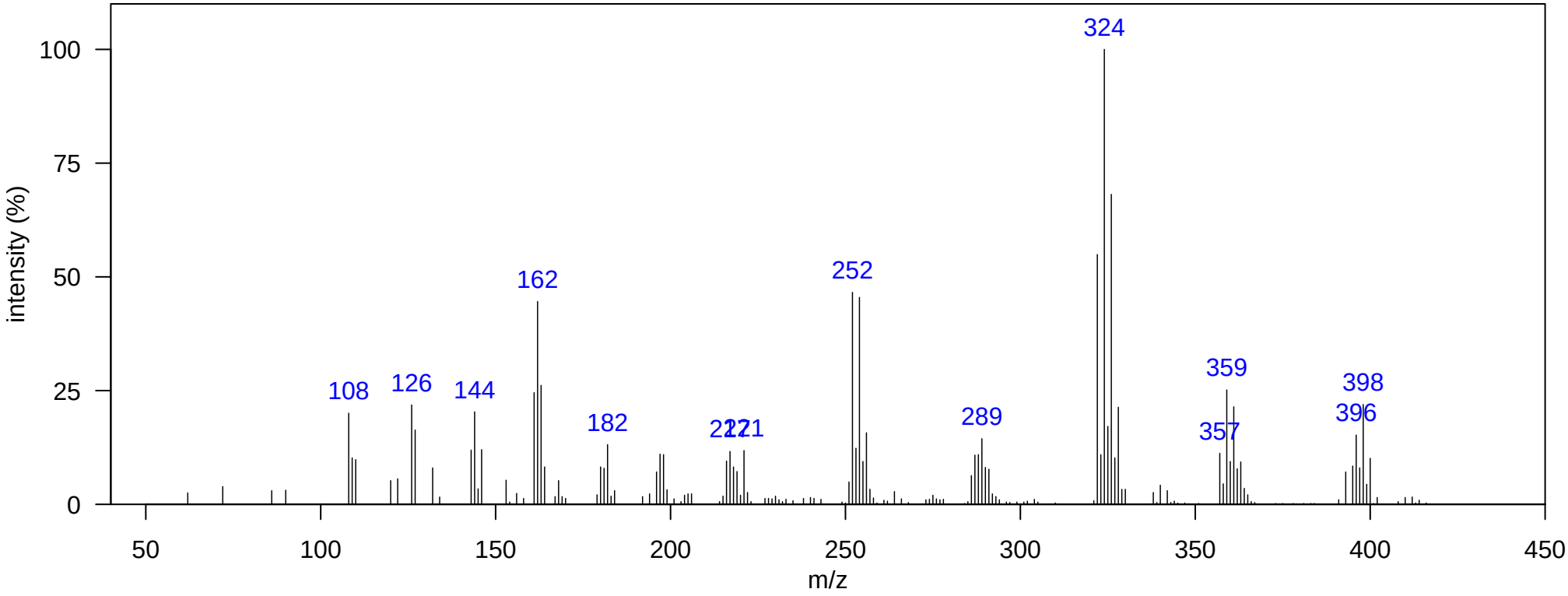


Name: Unknown−4−11 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1509.48 , 1.036

Comment: PCB interference − ions 412 and 340 belong to unknown−4−11

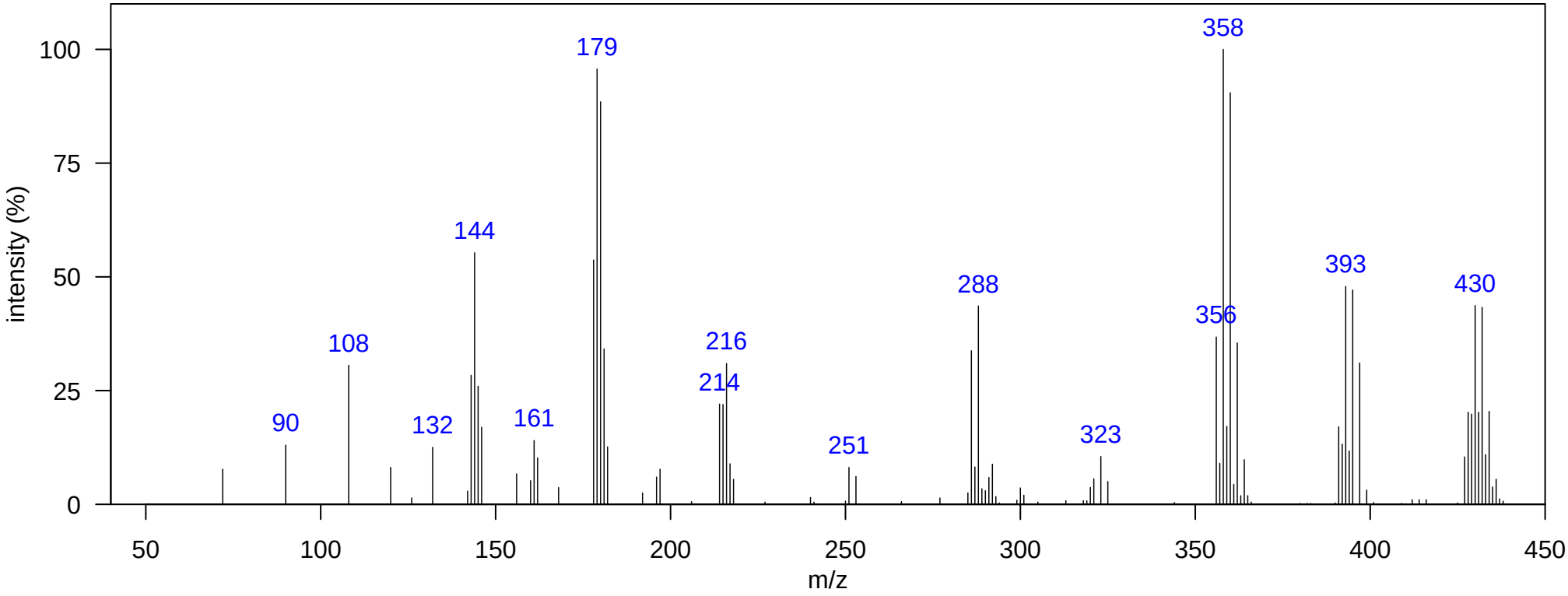


Name: Unknown−4−12 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1547.96 , 1.129

Comment: Interference from other compounds, ion 412 belongs to unknown−4−12

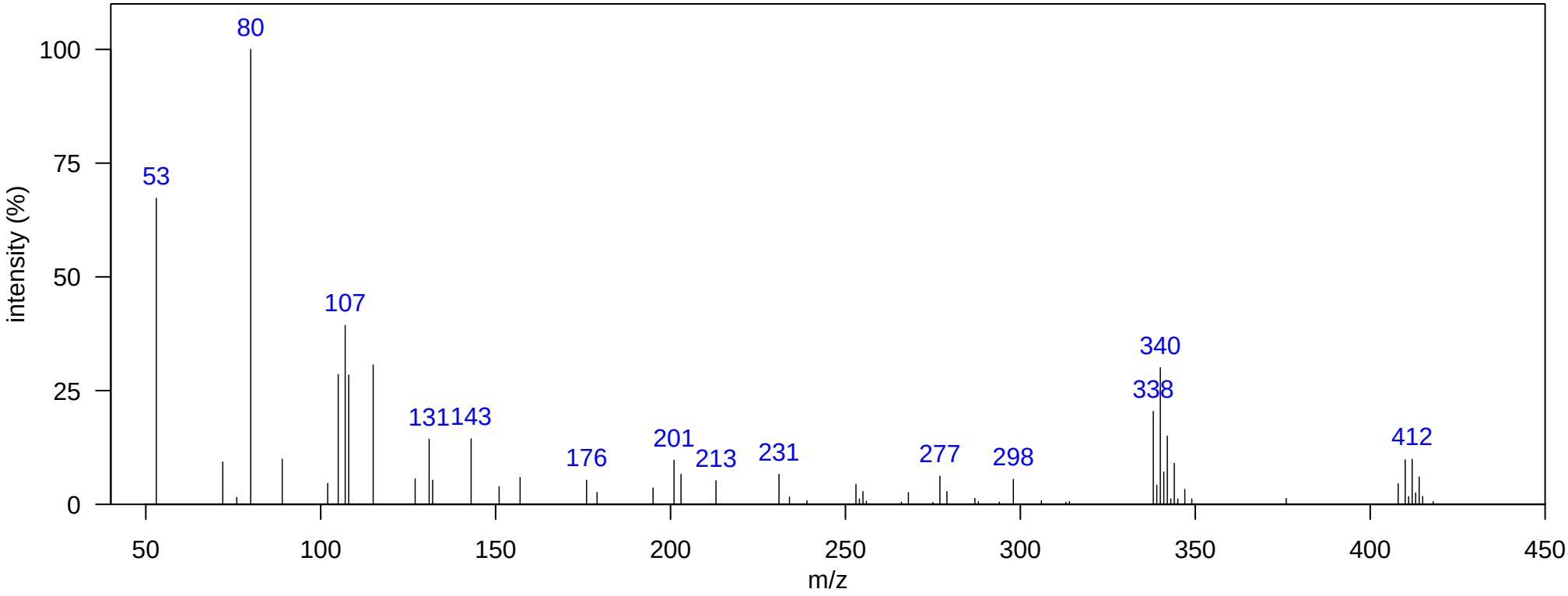


Name: Unknown−4−13 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1568.95 , 1.228

Comment:

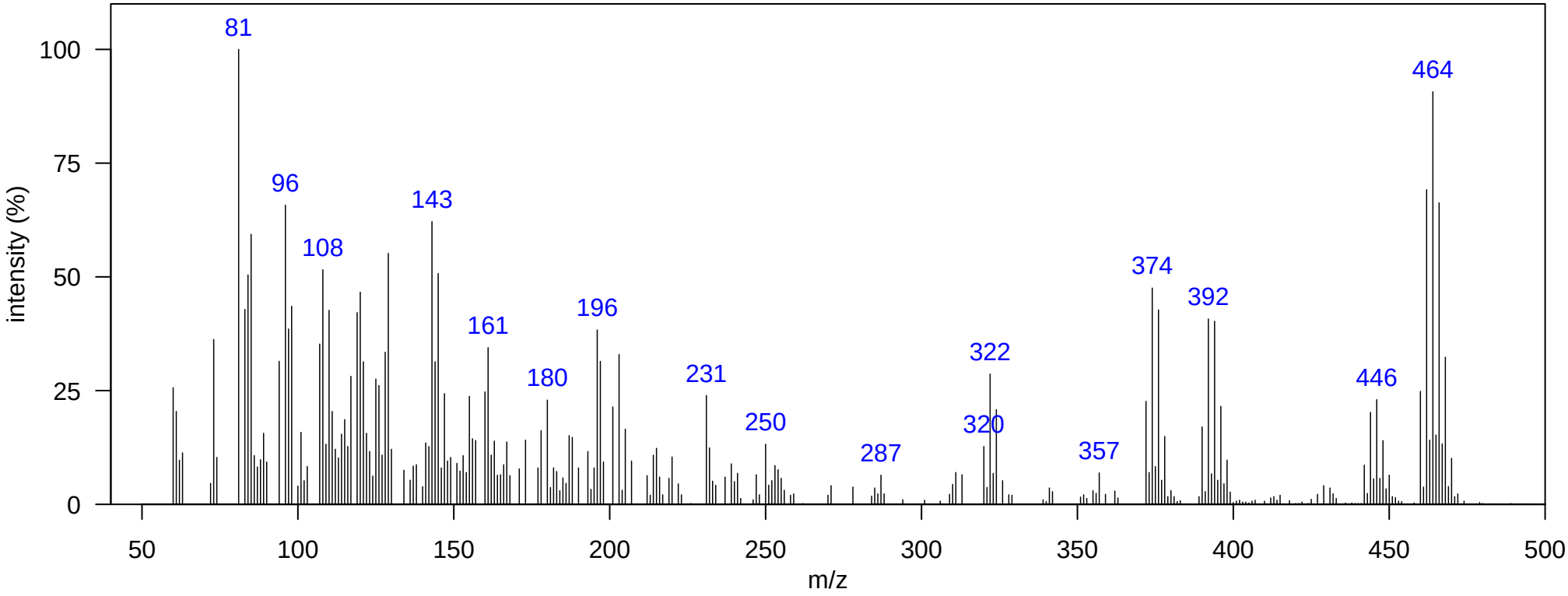


Name: Unknown−4−14 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1593.43 , 1.287

Comment: PCB interference − ions 446 and 374 belong to unknown−4−14

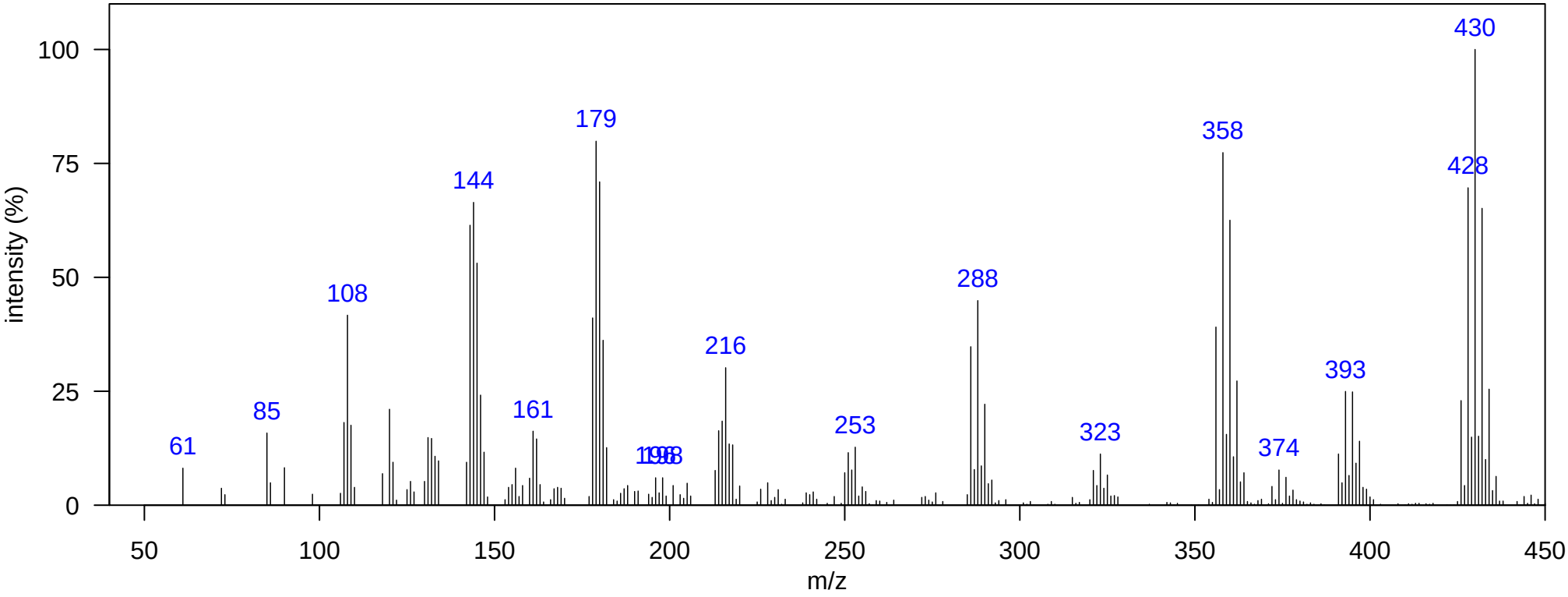


Name: Unknown−4−16 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1617.92 , 1.353

Comment: PCB interference − ions 446 and 374 belong to unknown−4−16

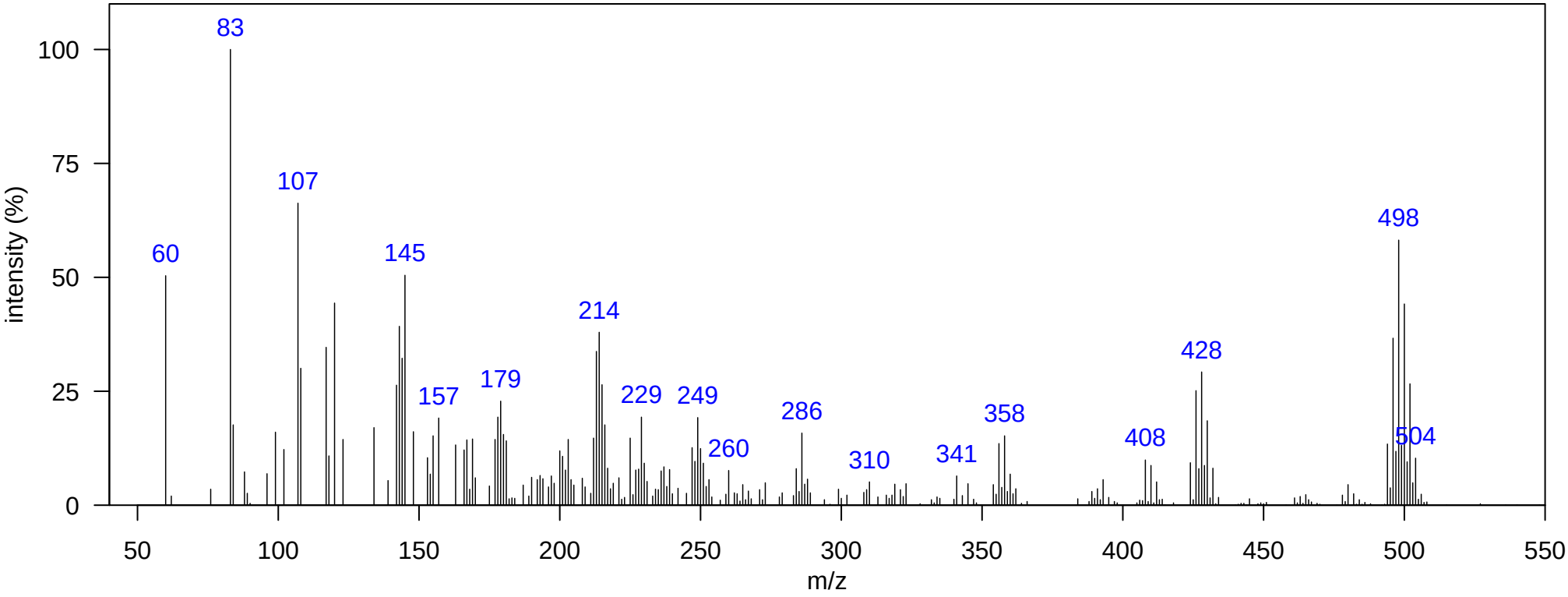


Name: Unknown−4−17 Class: Unknown−4

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1712.36 , 1.426

Comment: PCB interference − ions 408 and 480 belong to unknown−4−17

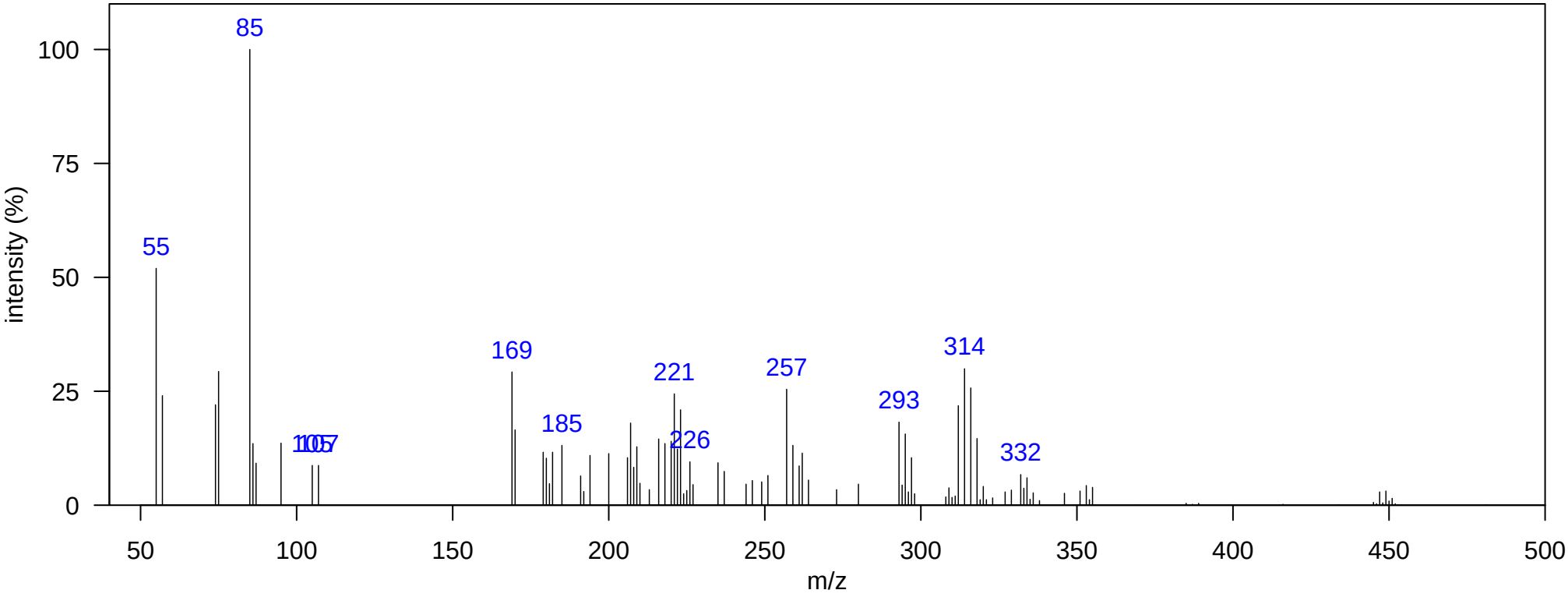


Name: Unknown−5−1 Class: Unknown−5

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1460.51 , 1.089

Comment:

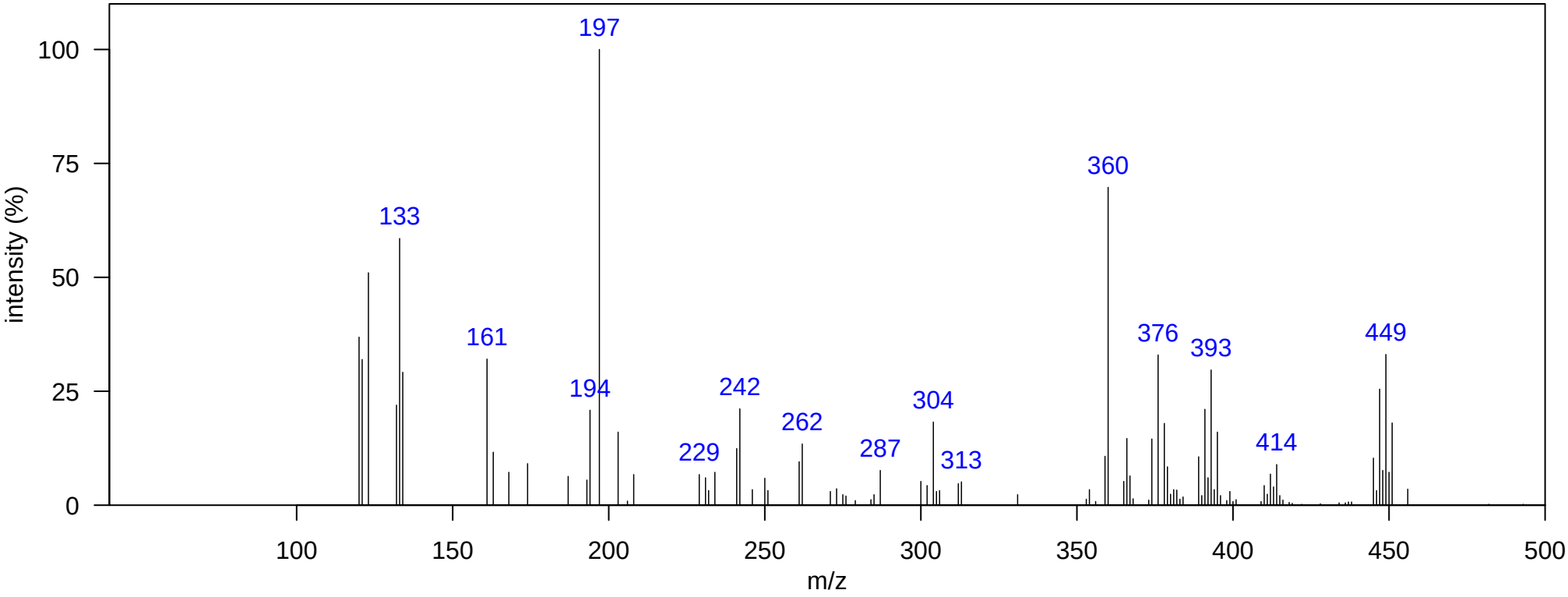


Name: Unknown−5−2 Class: Unknown−5

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1467.5 , 1.267

Comment:

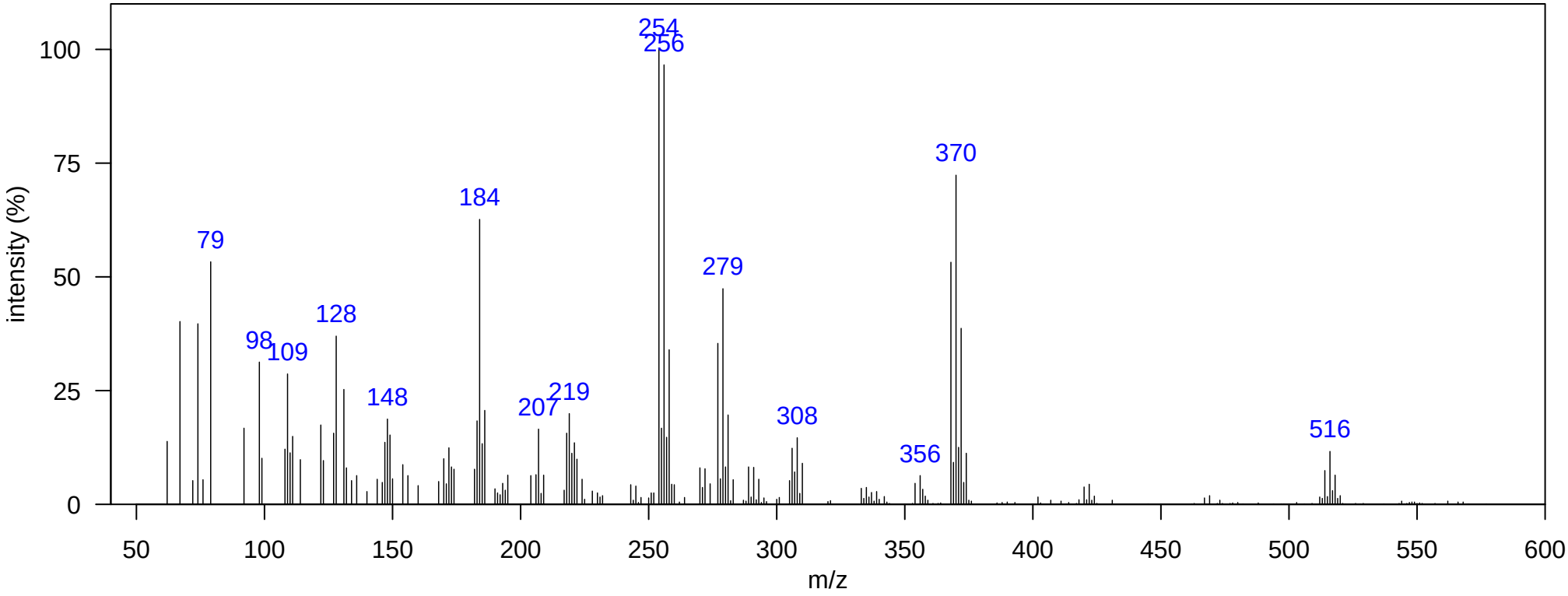


Name: Unknown−6−1 Class: Unknown−6

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1582.94 , 1.373

Comment:

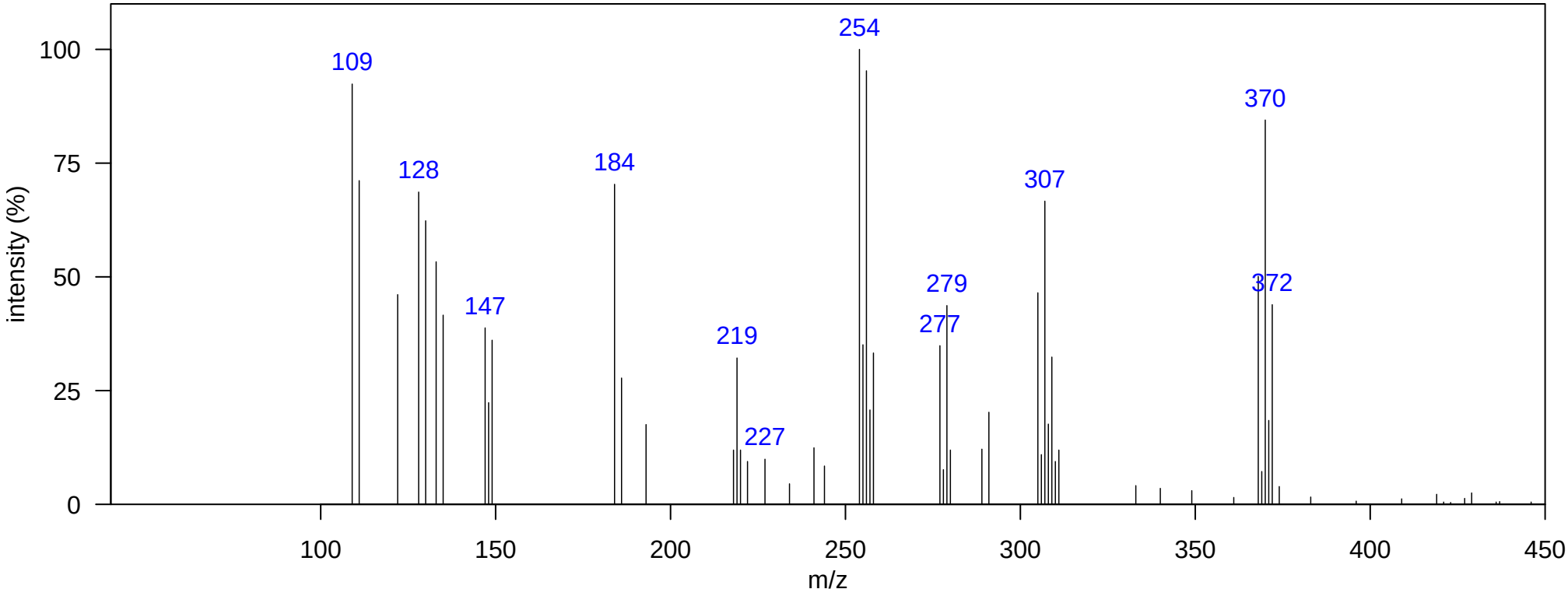


Name: Unknown−6−2 Class: Unknown−6

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1600.43 , 1.445

Comment:

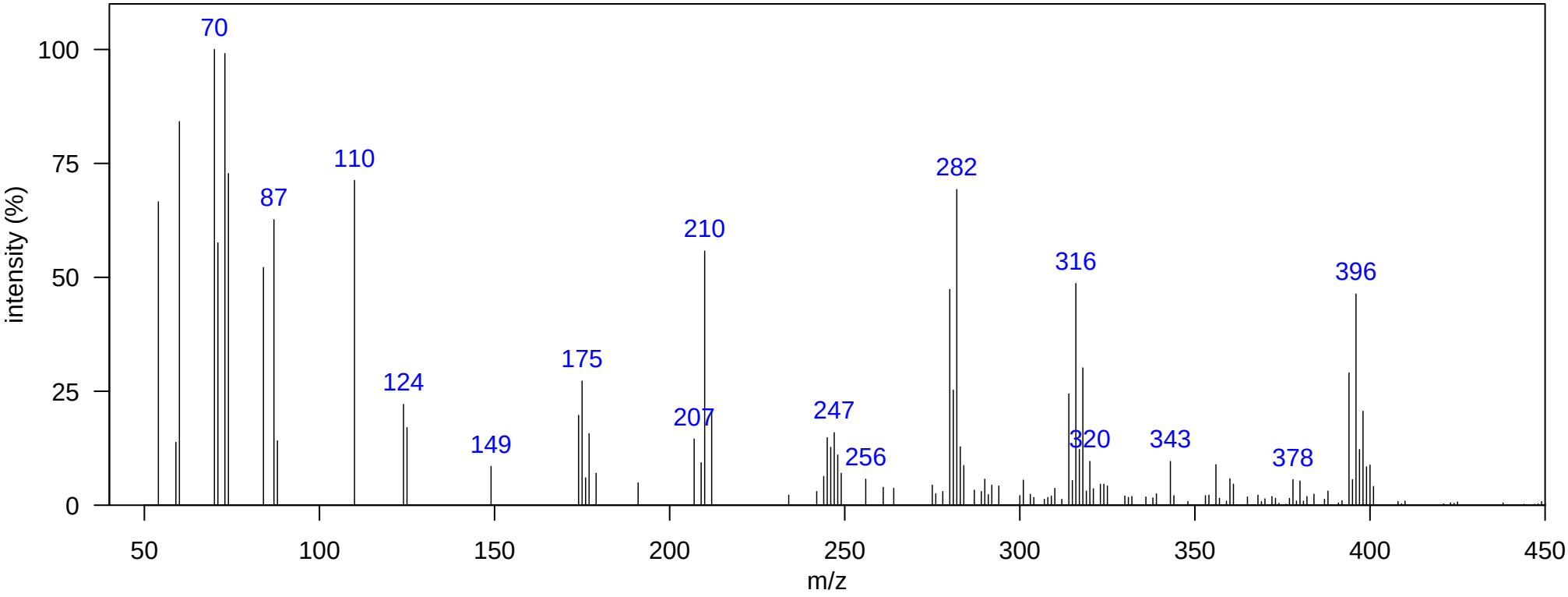


Name: Unknown−7−1 Class: Unknown−7

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1649.4 , 1.538

Comment:

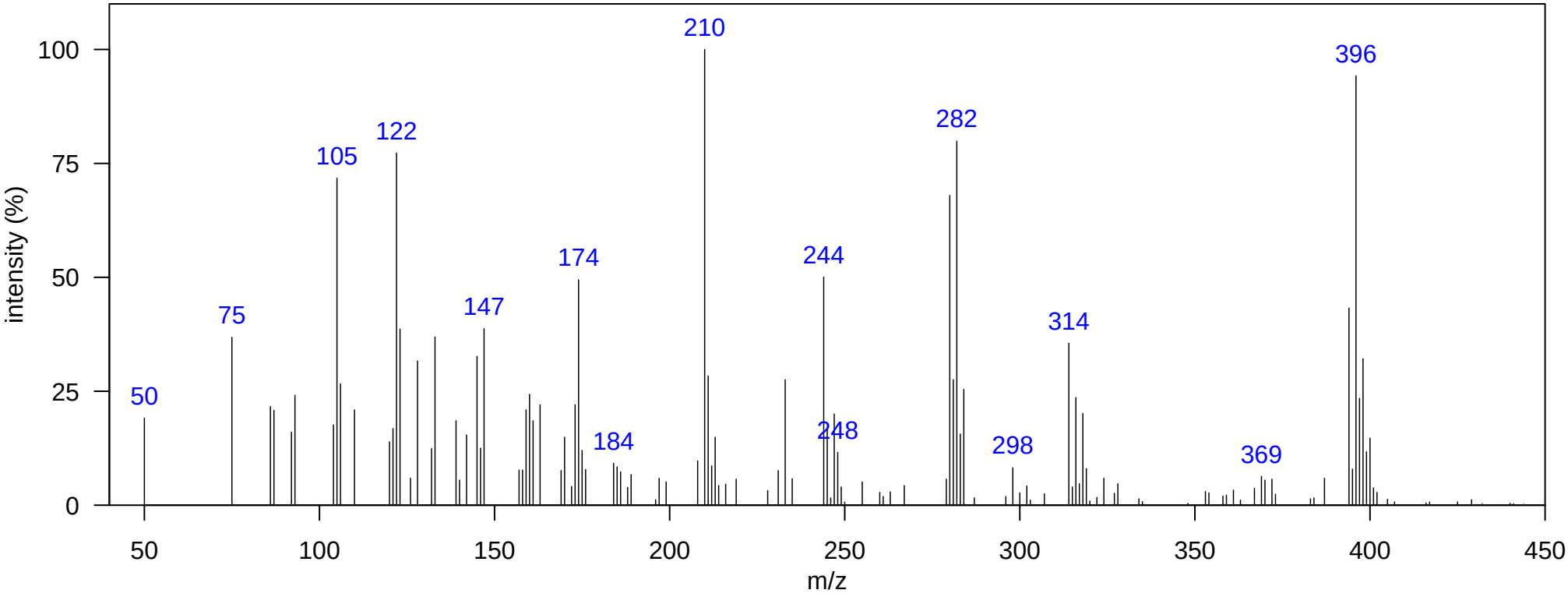


Name: Unknown−7−2 Class: Unknown−7

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1705.37 , 1.690

Comment:

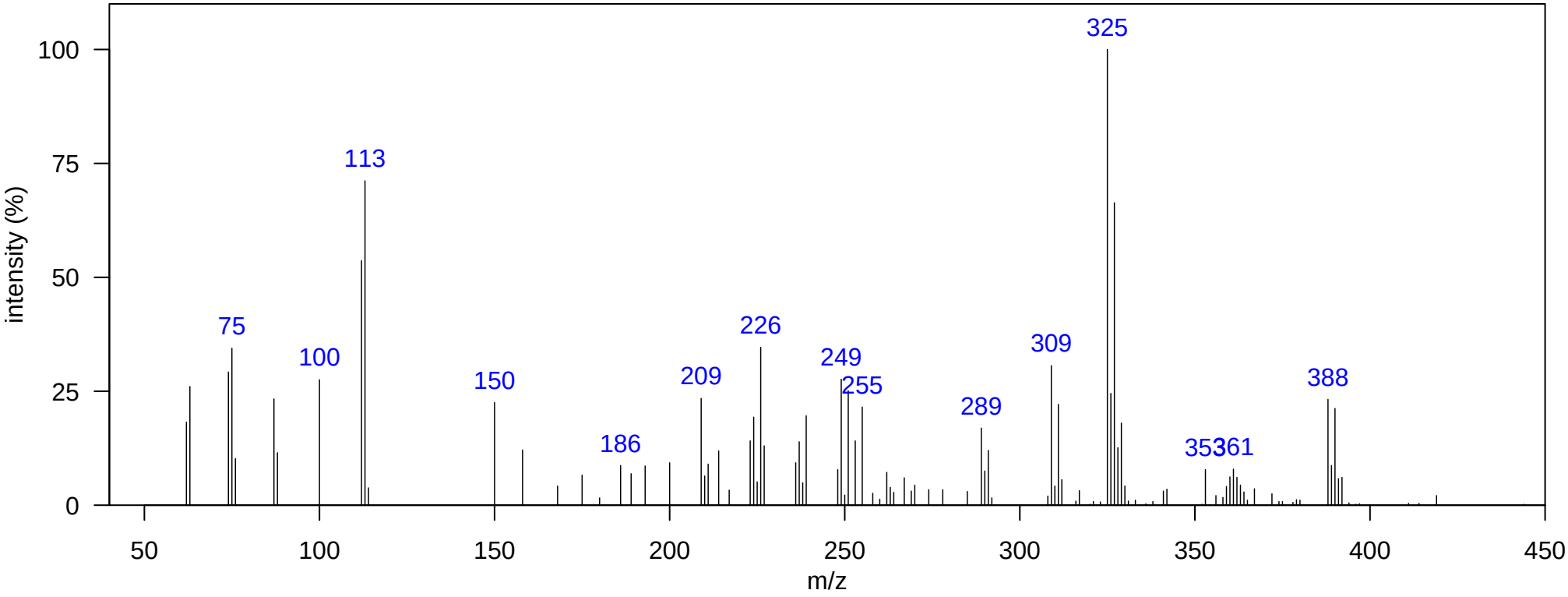


Name: Unknown−8−1 Class: Unknown−8

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1663.39 , 1.637

Comment:



Name: Unknown−8−2 Class: Unknown−8

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

Instrument: GCxGC−TOF, EI Mode
1D RT, 2D RT (s): 1691.38 , 1.591

Comment: