

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 reveal ecosystem indicator species

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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: 2018–03–24 11:38:57
SpecLibMarineUnknown2018
OrgMassSpecR version 0.5–3

R version 3.4.1 (2017–06–30)

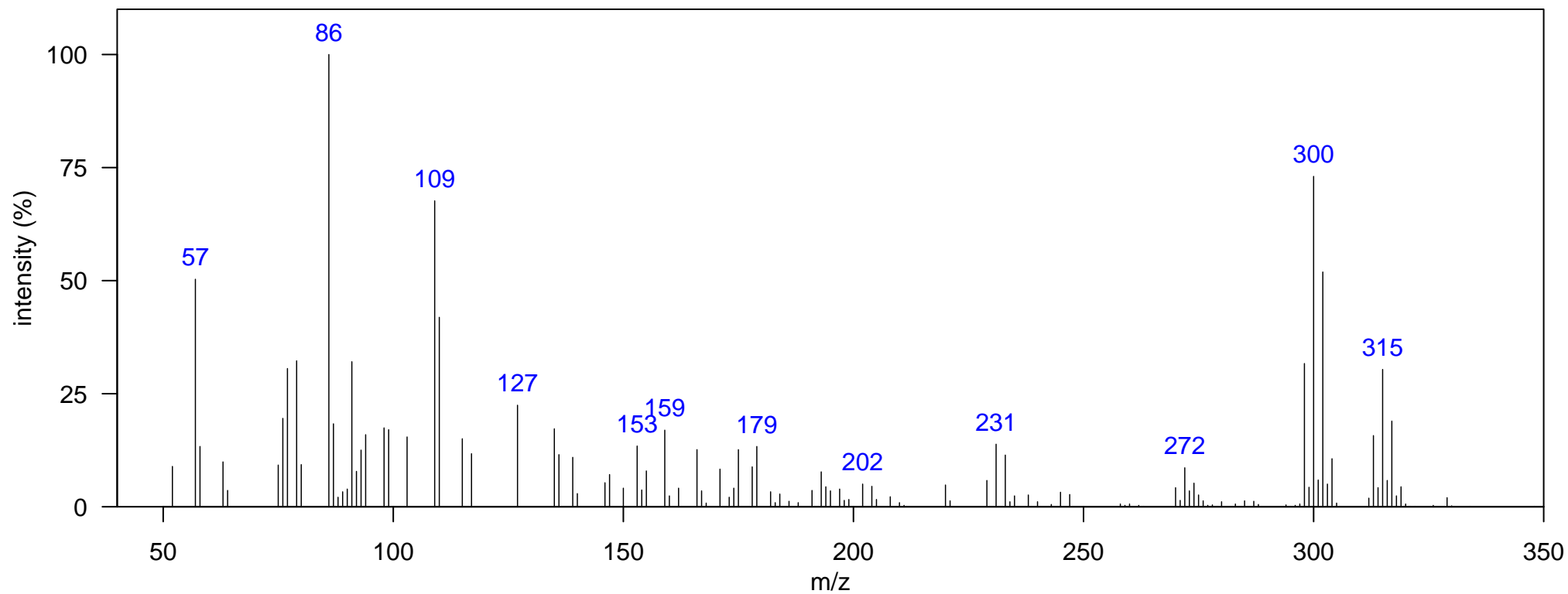
Name: MMCP unknown 1

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

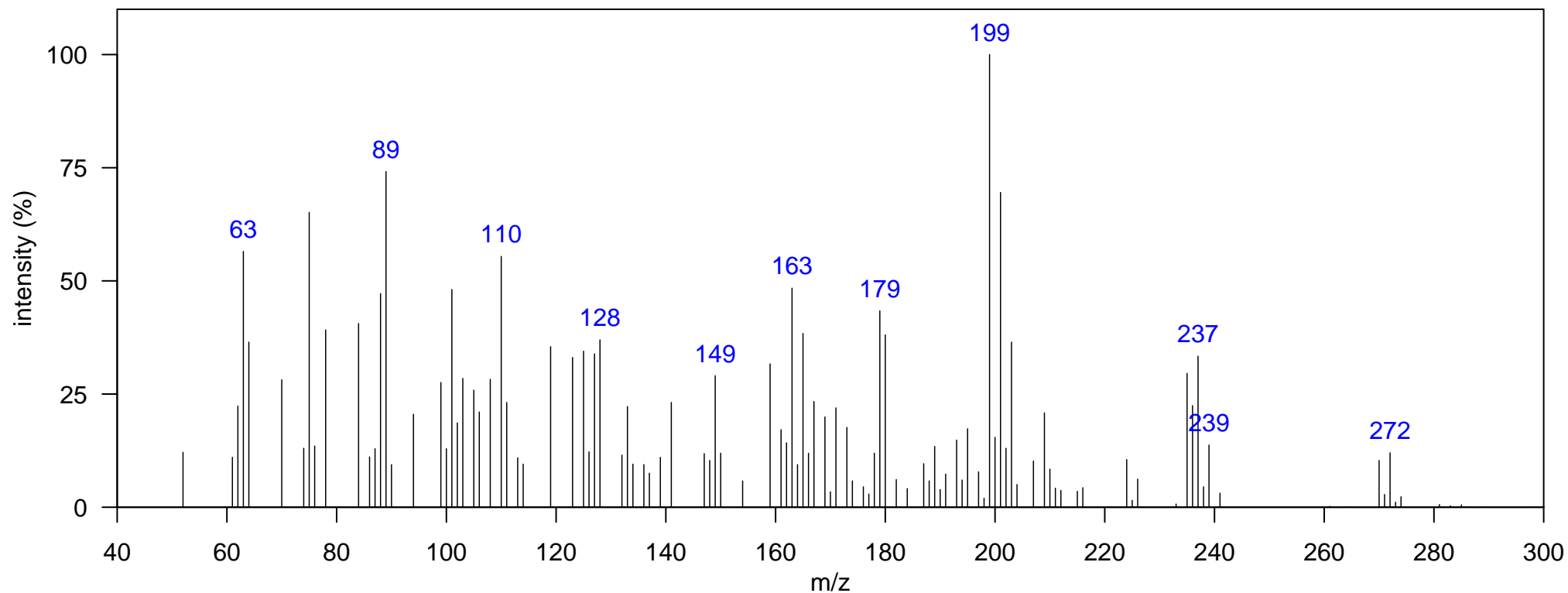
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

Comment:



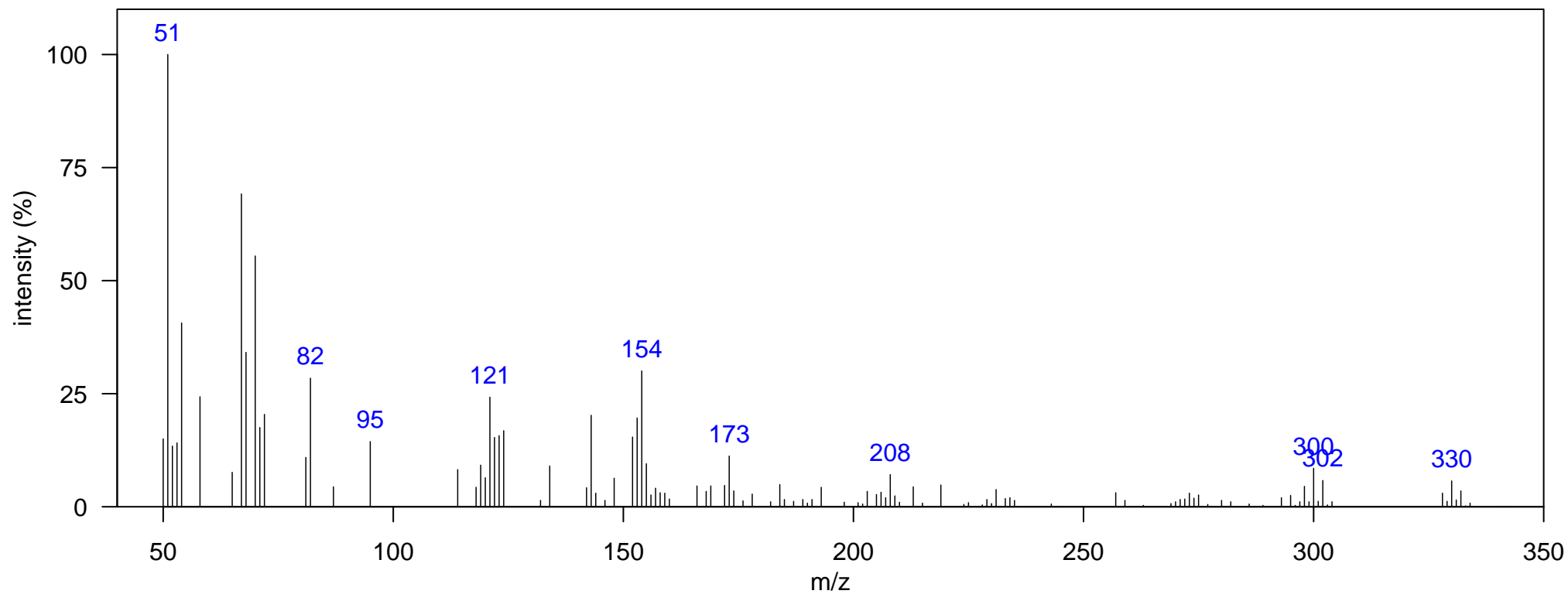
Name: MMCP unknown 3

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:



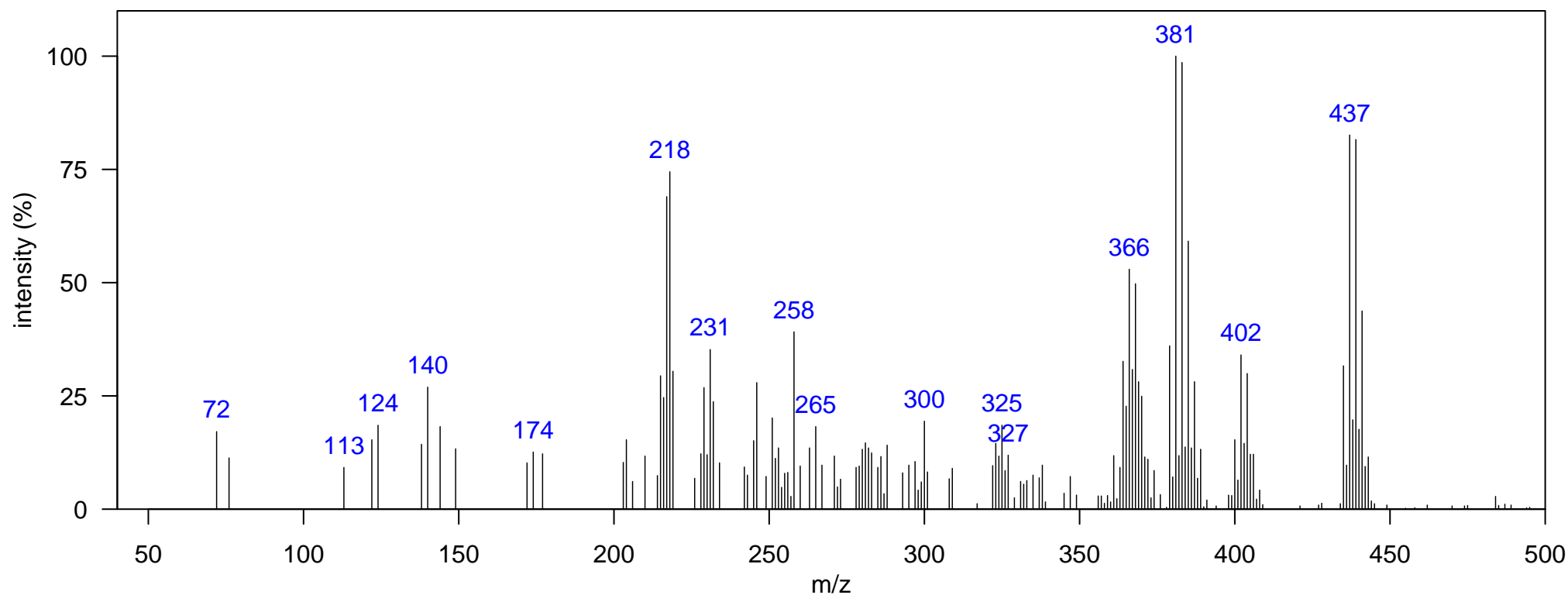
Name: MMCP unknown 4

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

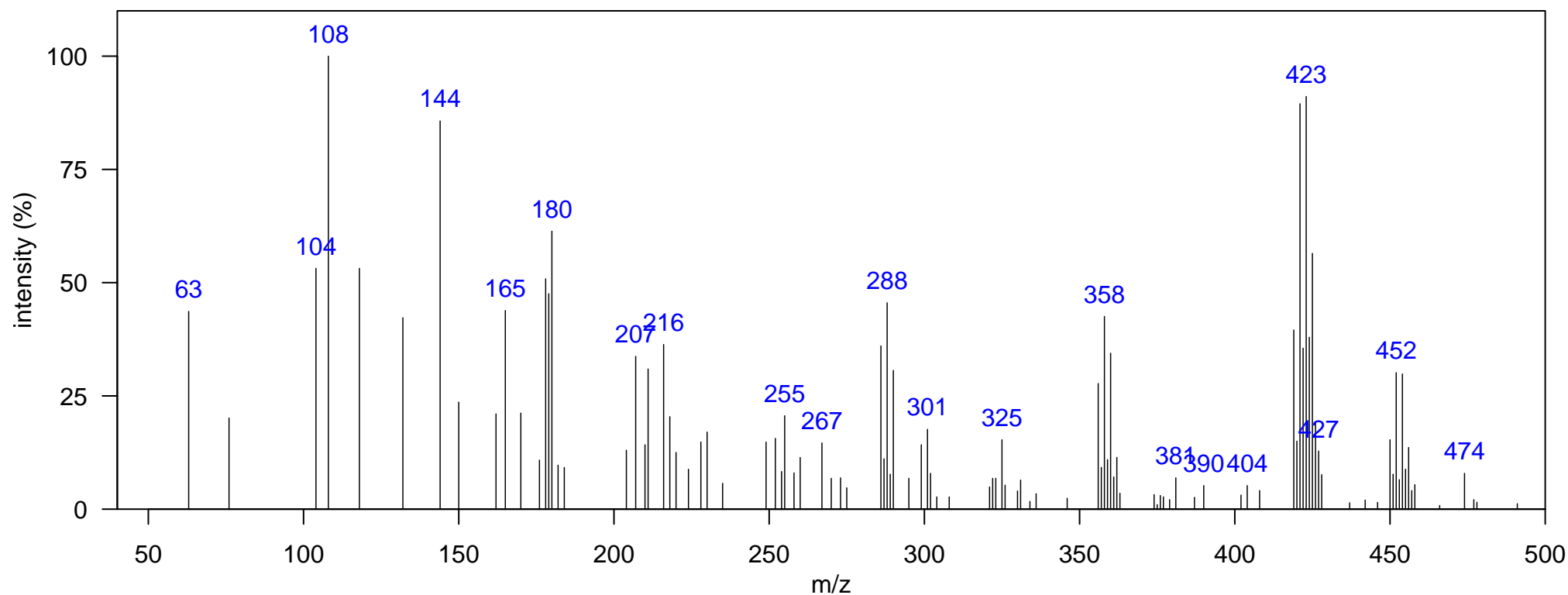
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

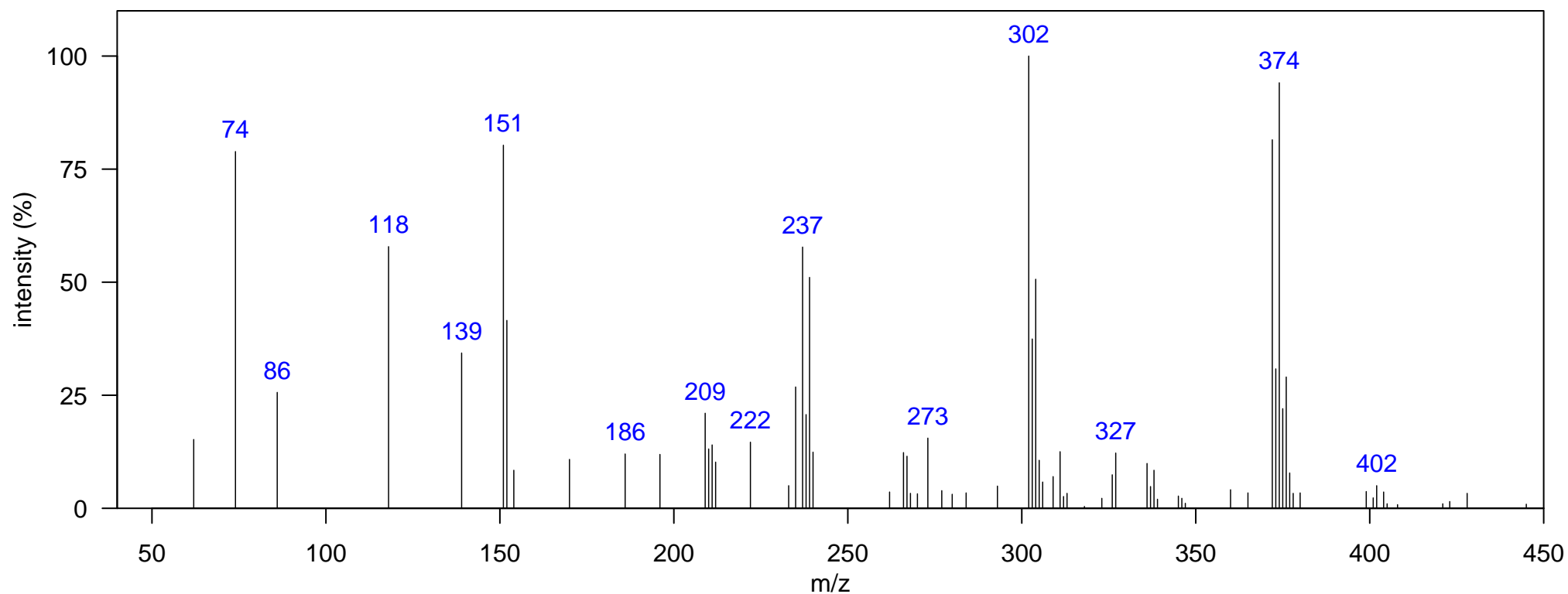
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

Comment:



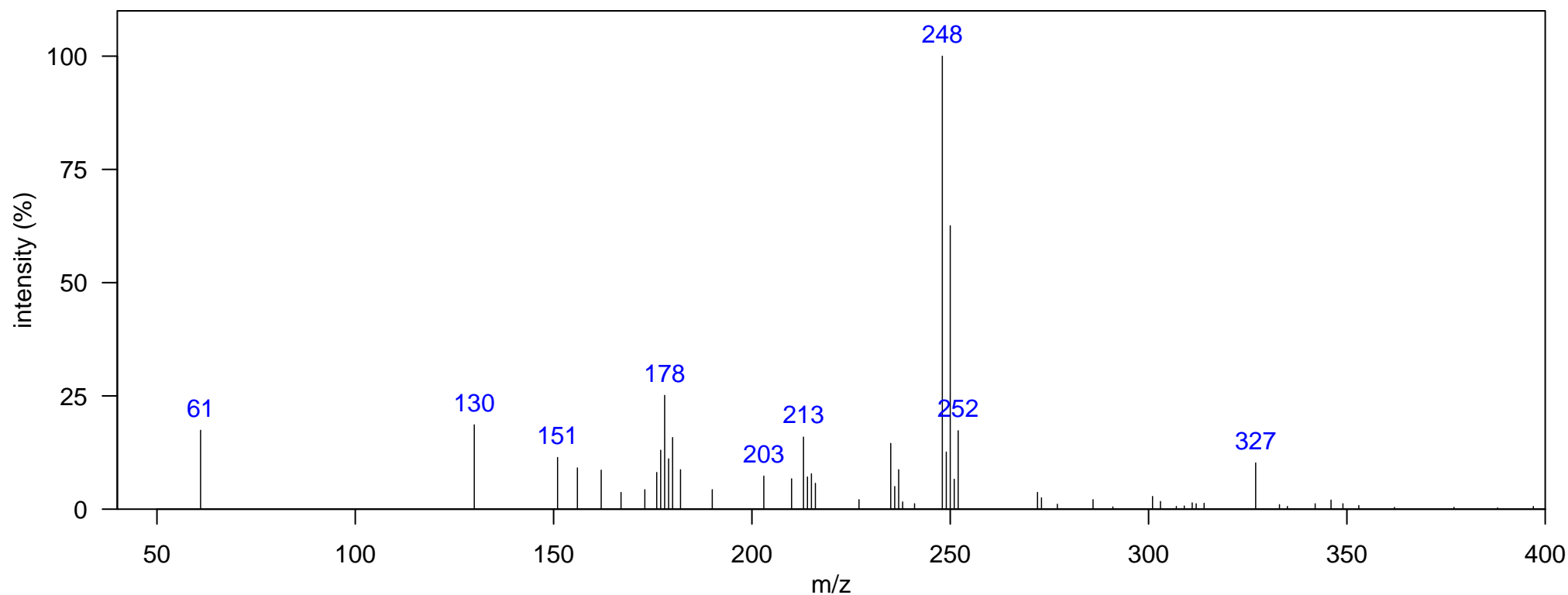
Name: MMCP unknown 7

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:



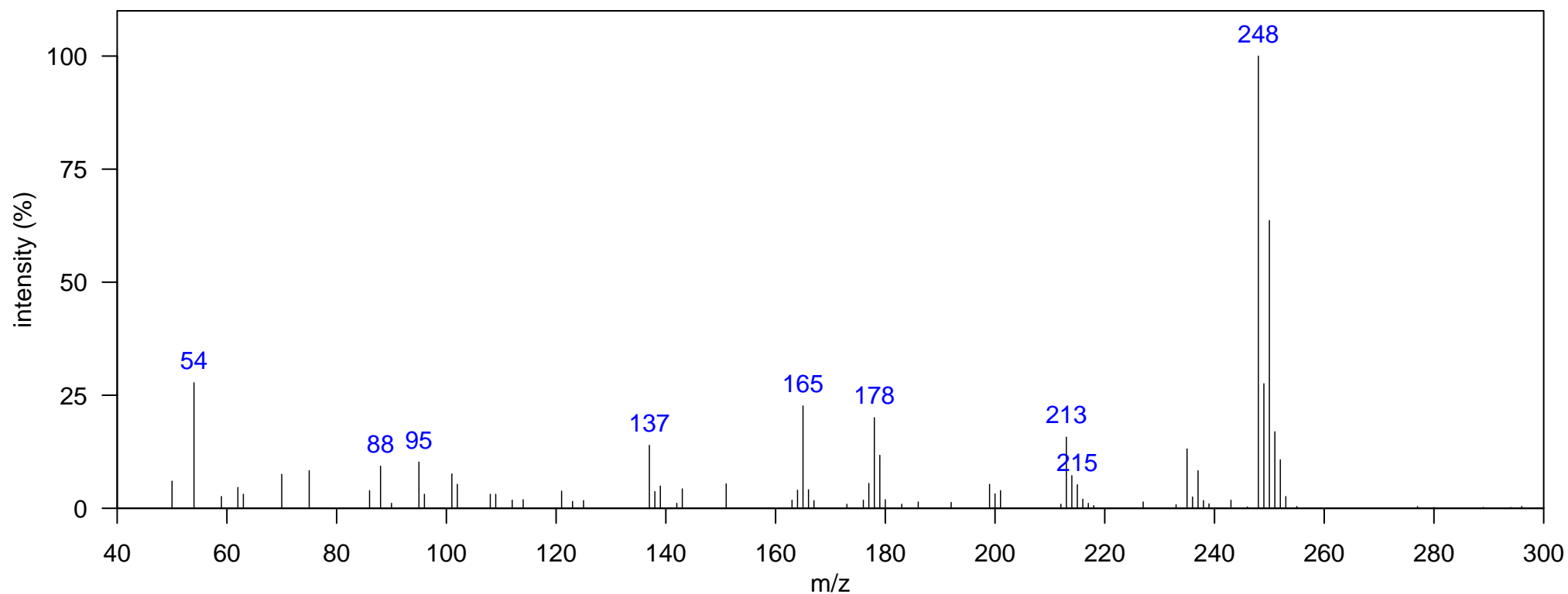
Name: MMCP unknown 8

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

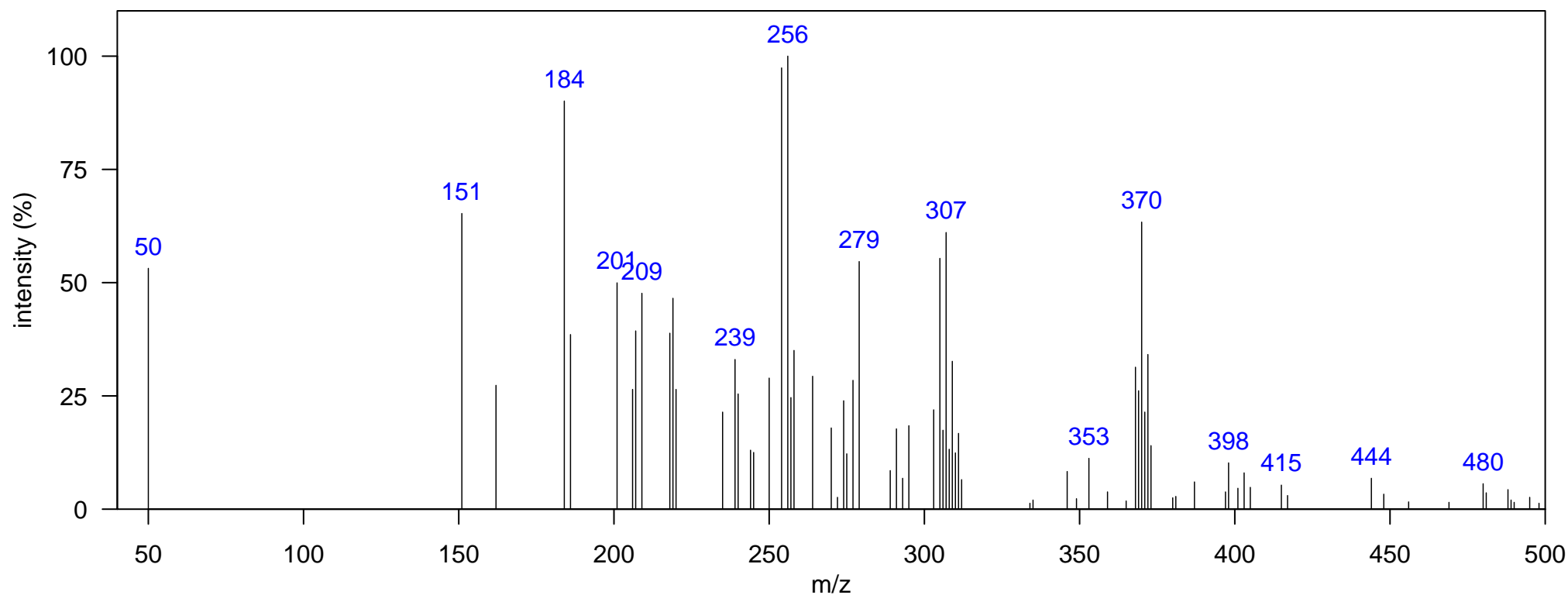
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

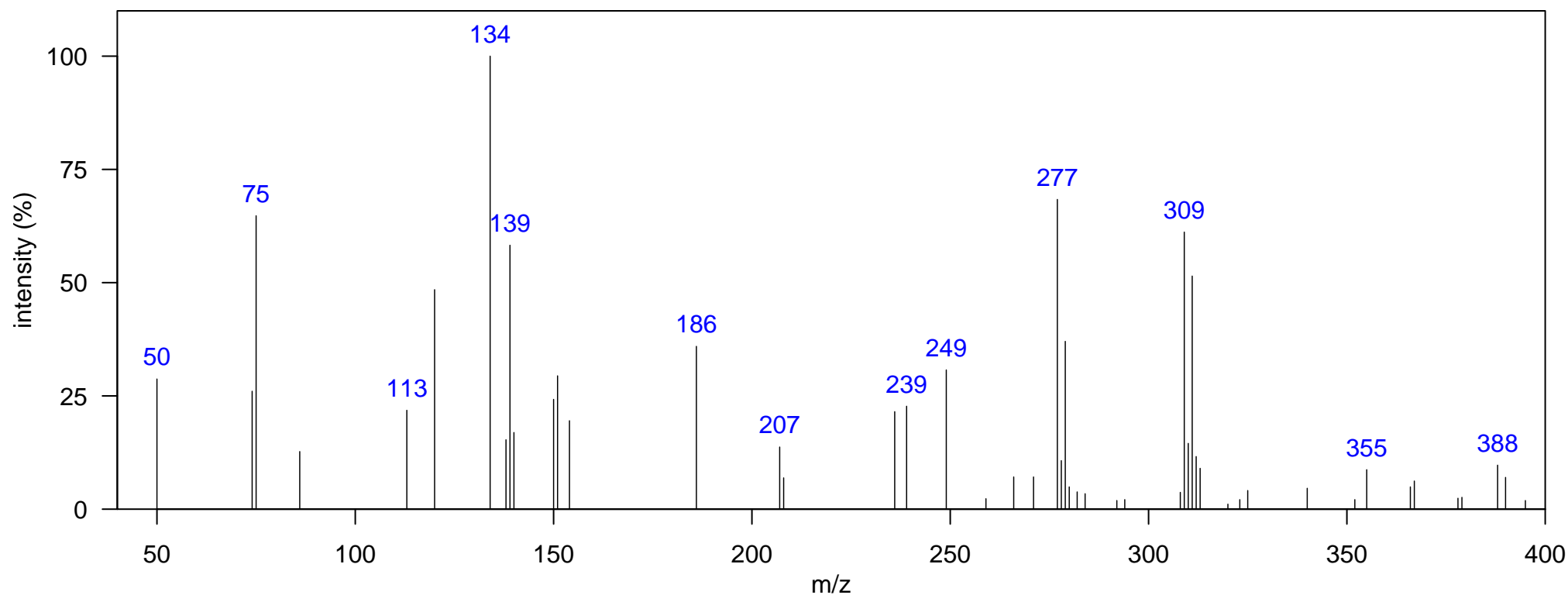
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

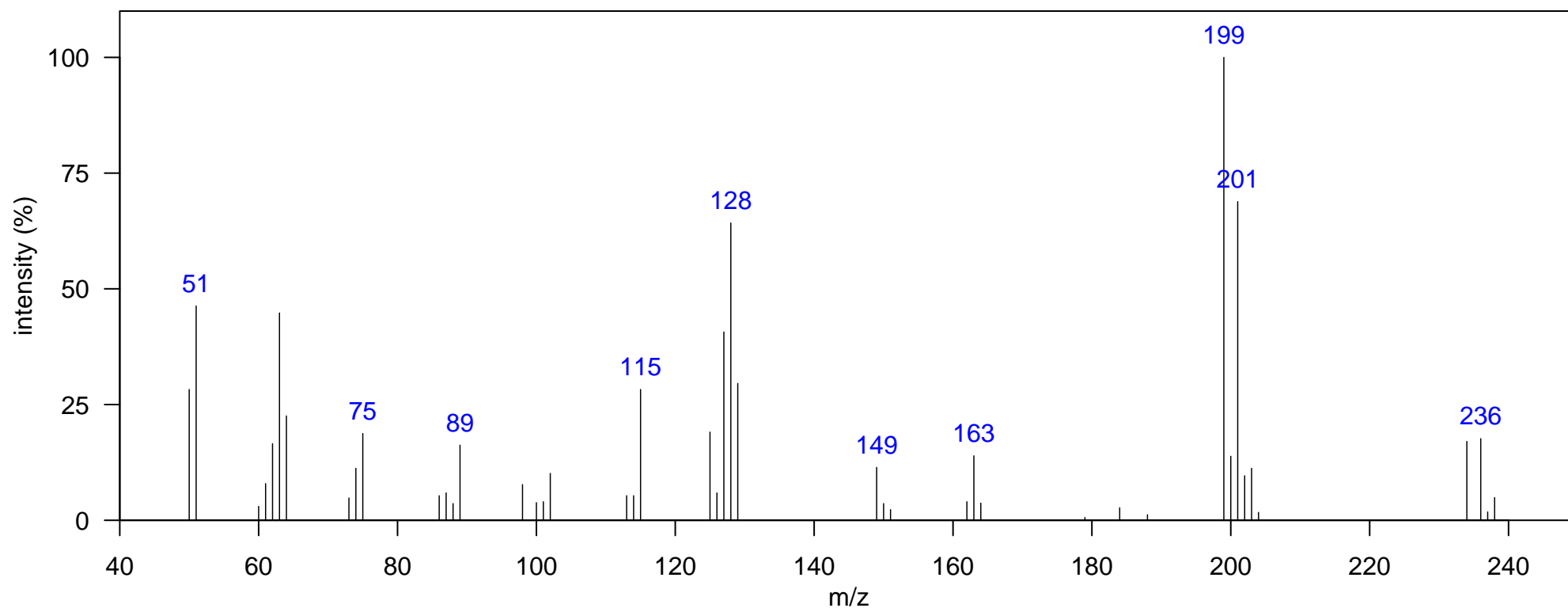
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

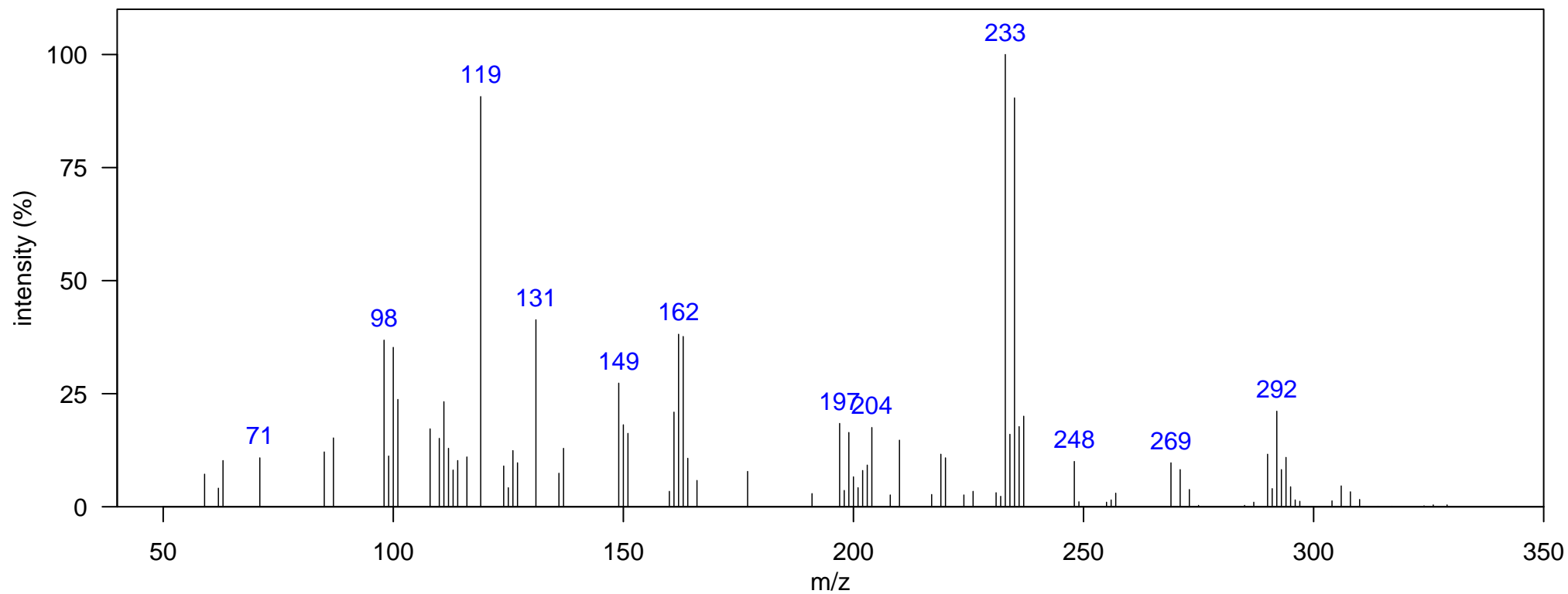
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

Comment:



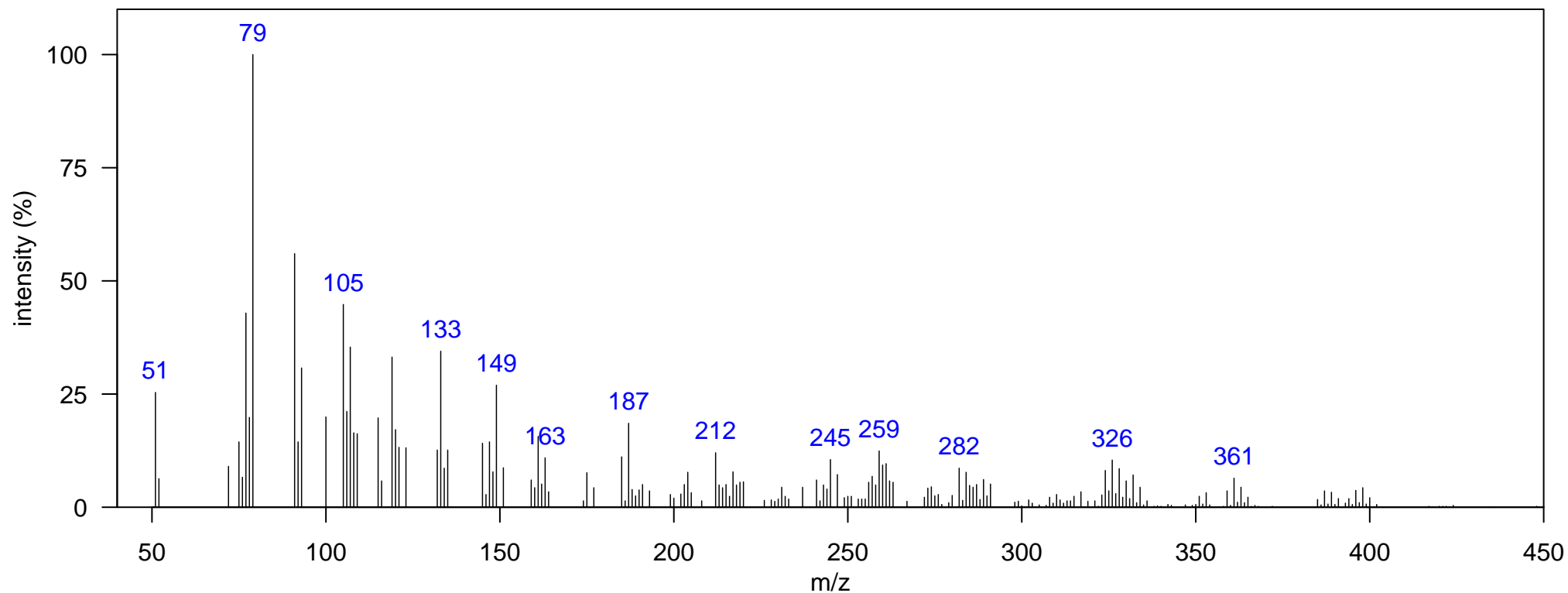
Name: Unknown-15

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:



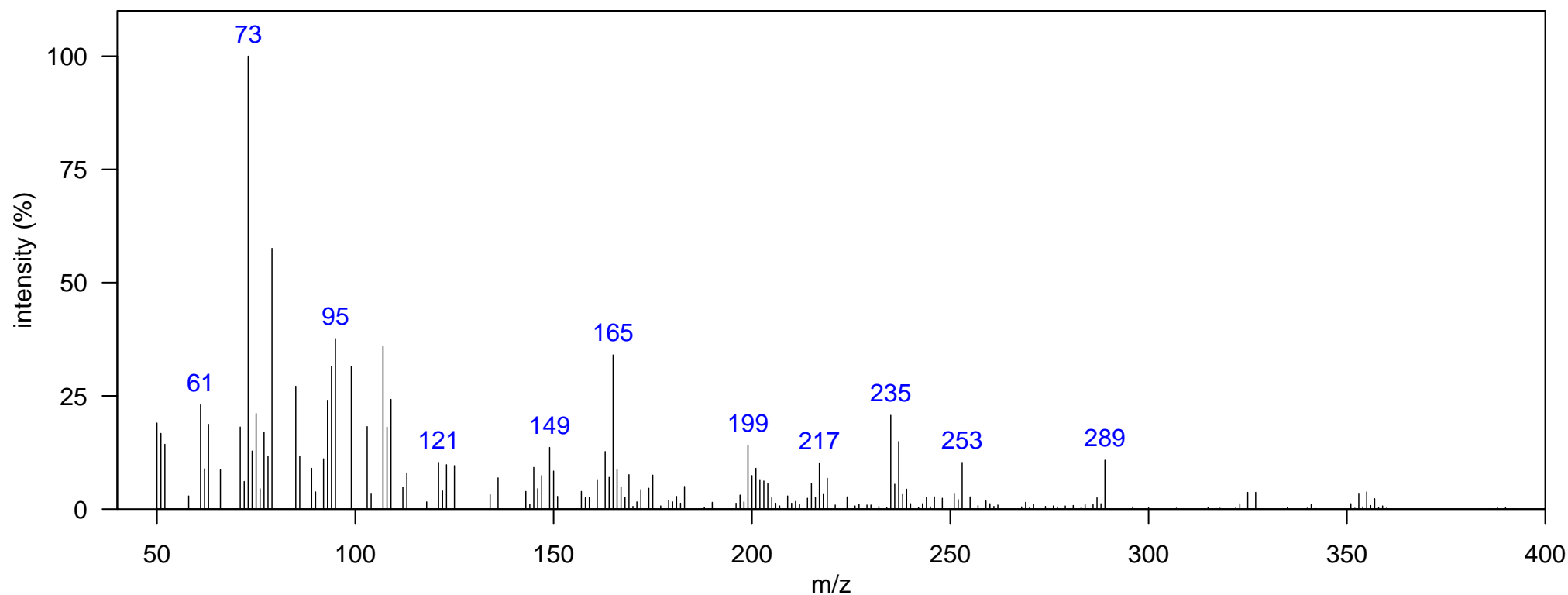
Name: Unknown-16

Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

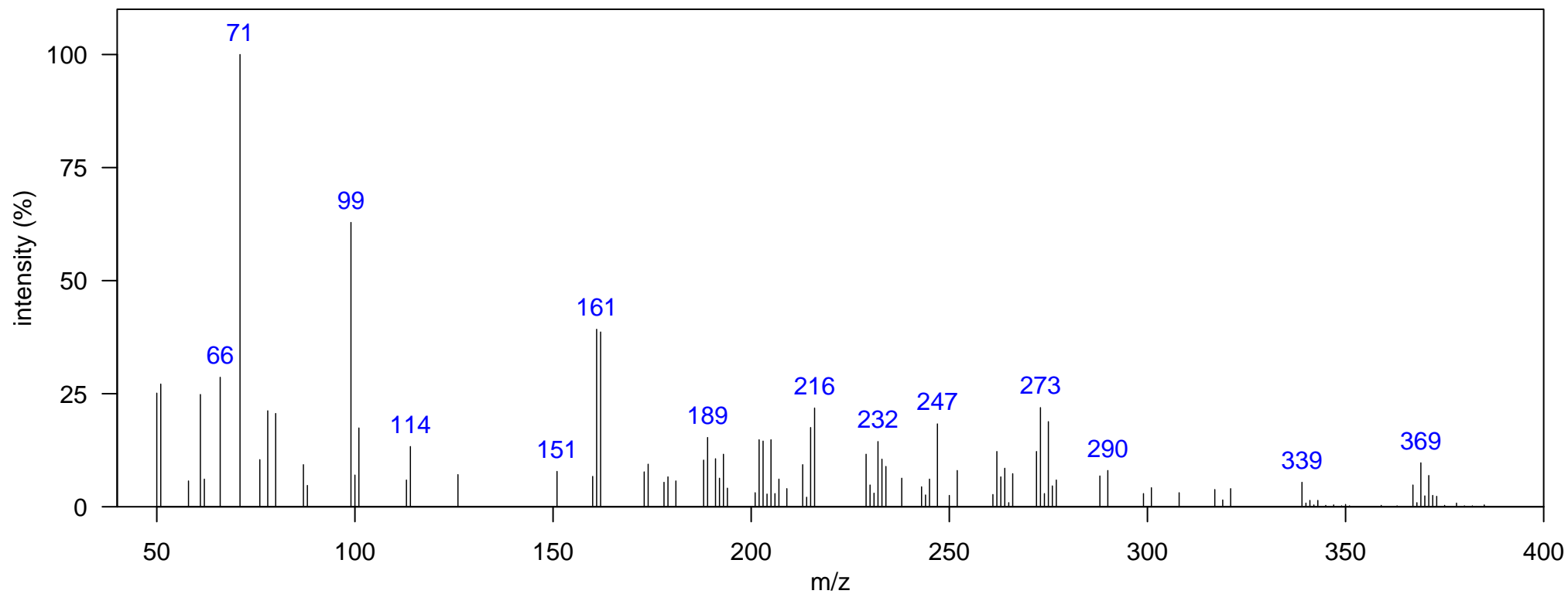
Comment: Interference with some compounds – ion 355 belongs to unknown-16



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

Comment:



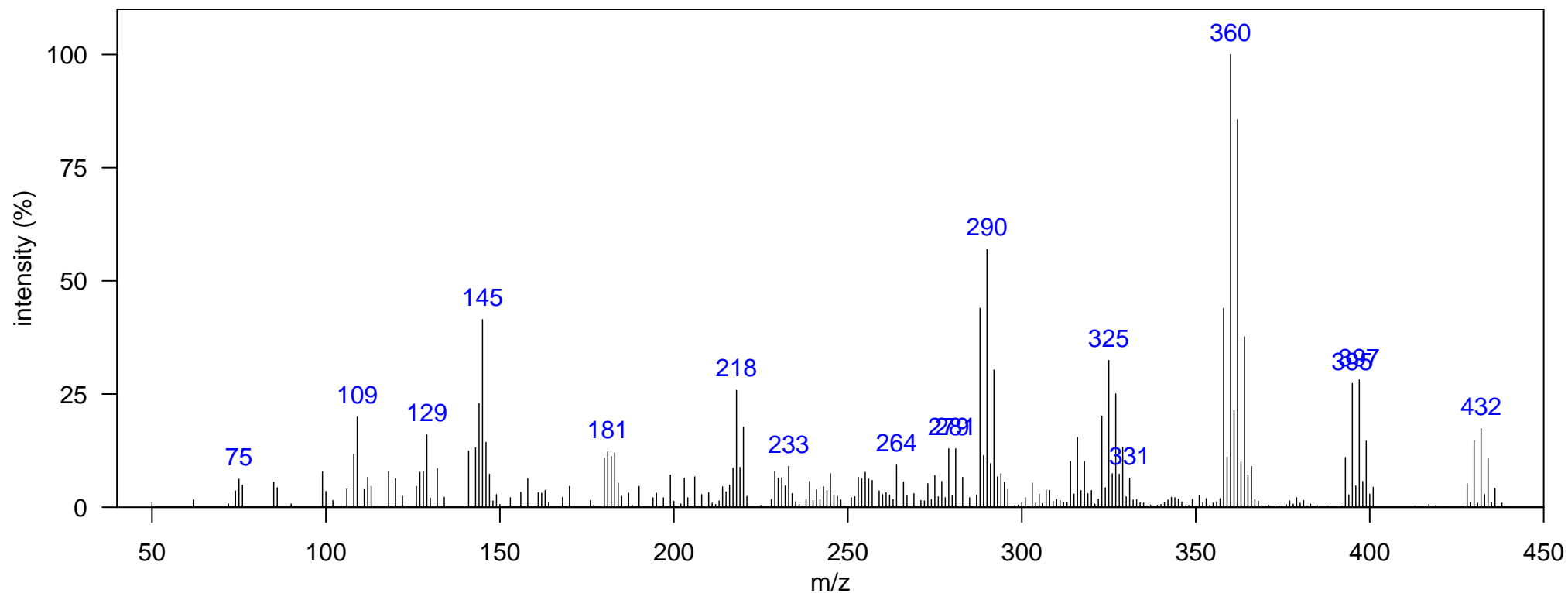
Name: Unknown-19

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



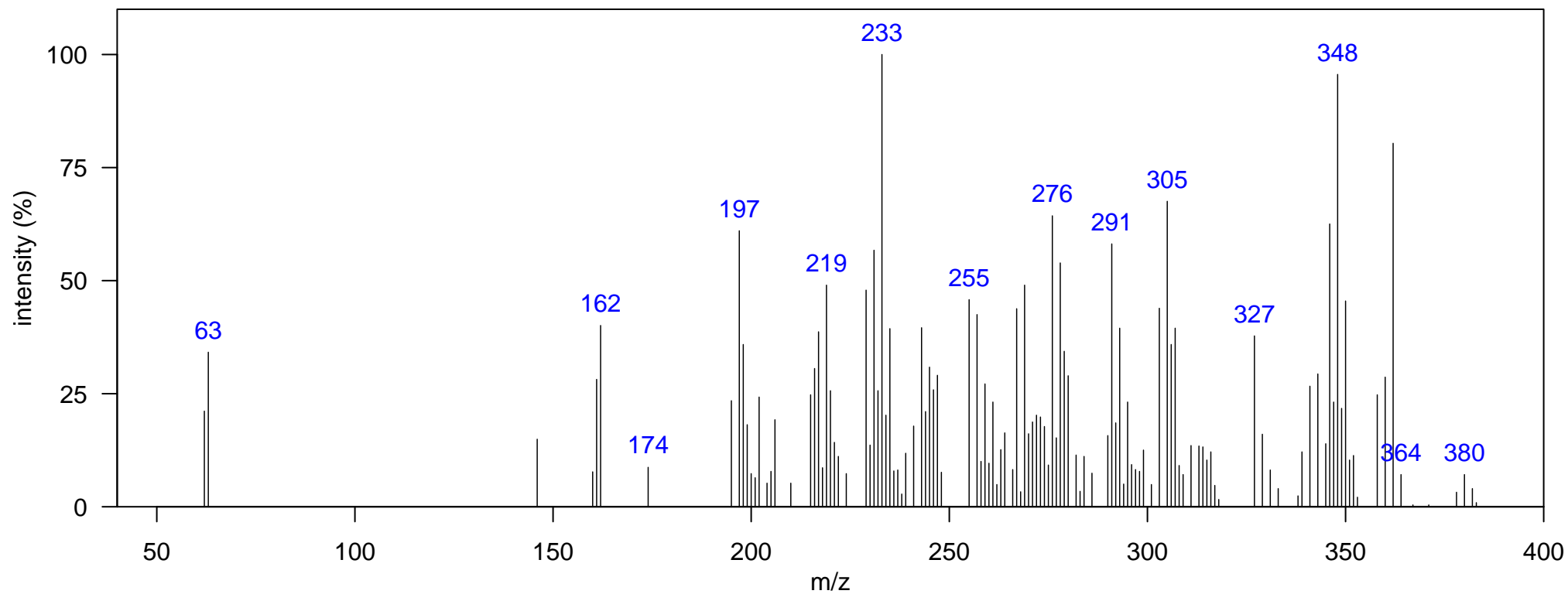
Name: Unknown-21

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:



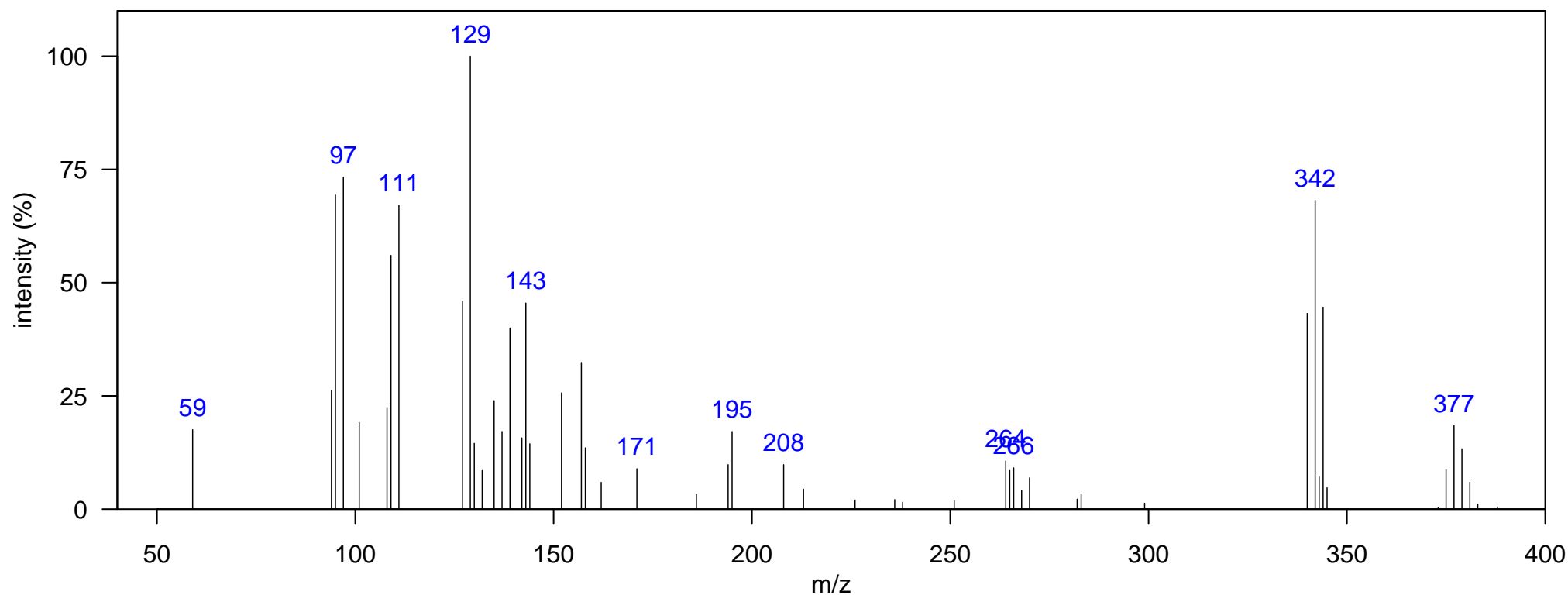
Name: Unknown-22

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:



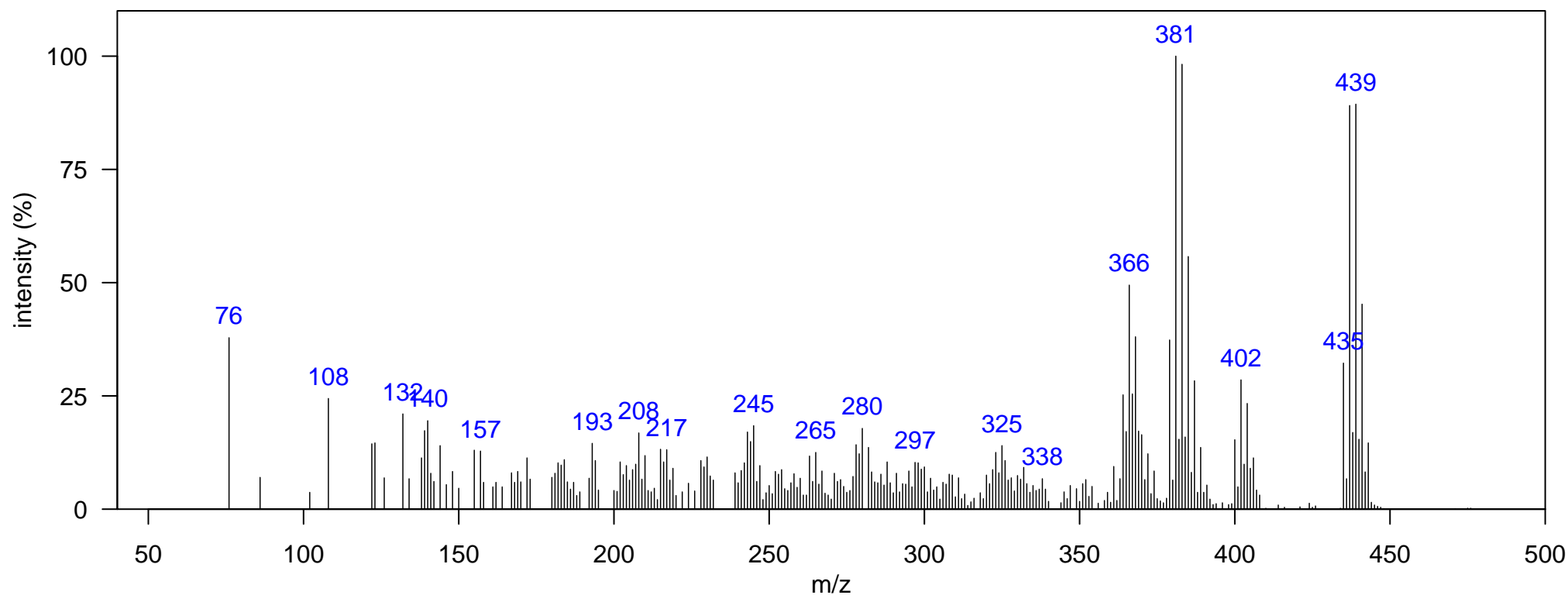
Name: Unknown-34

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:



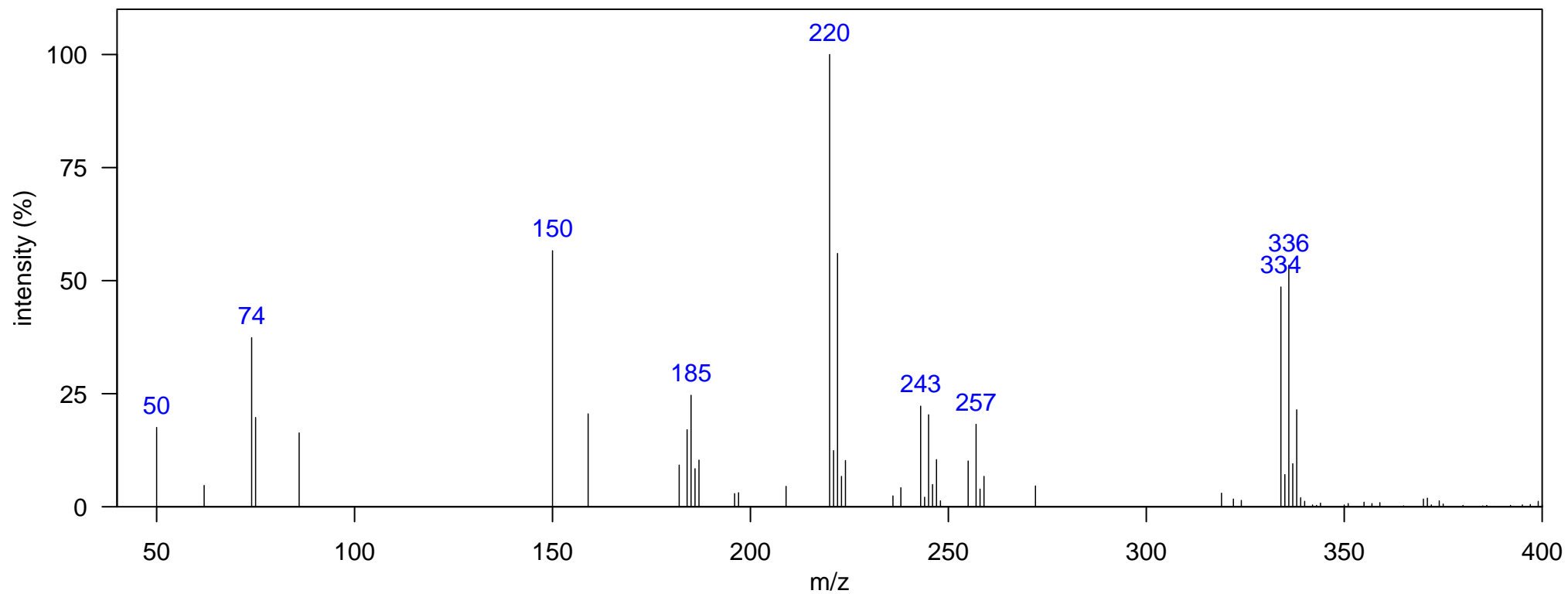
Name: Unknown-36

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:



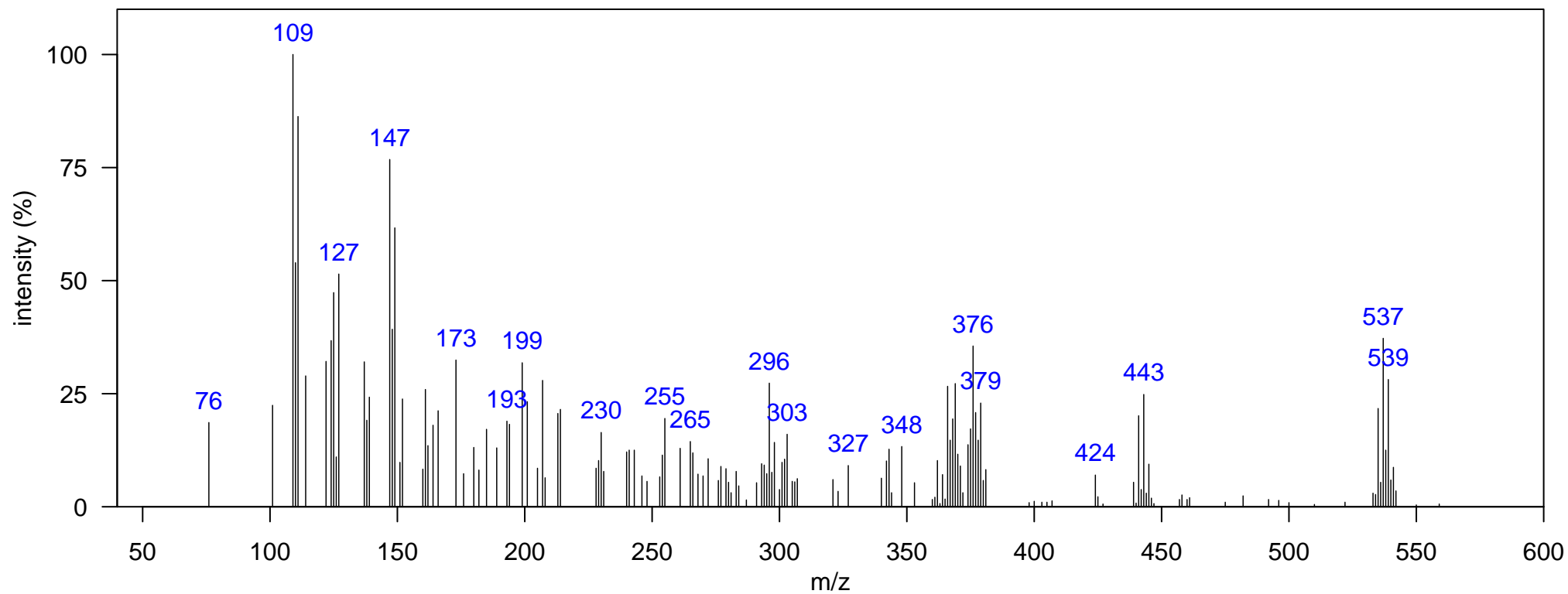
Name: Unknown-38

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:



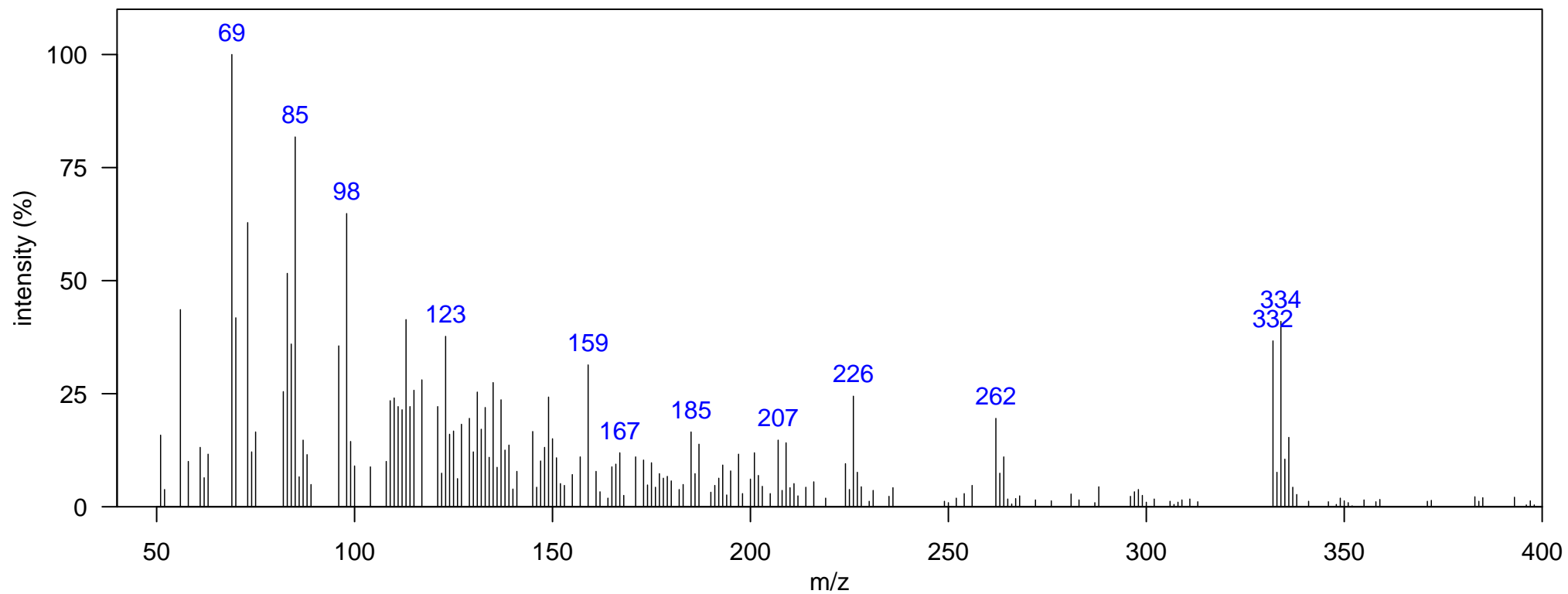
Name: Unknown-39

Class: Unknown

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

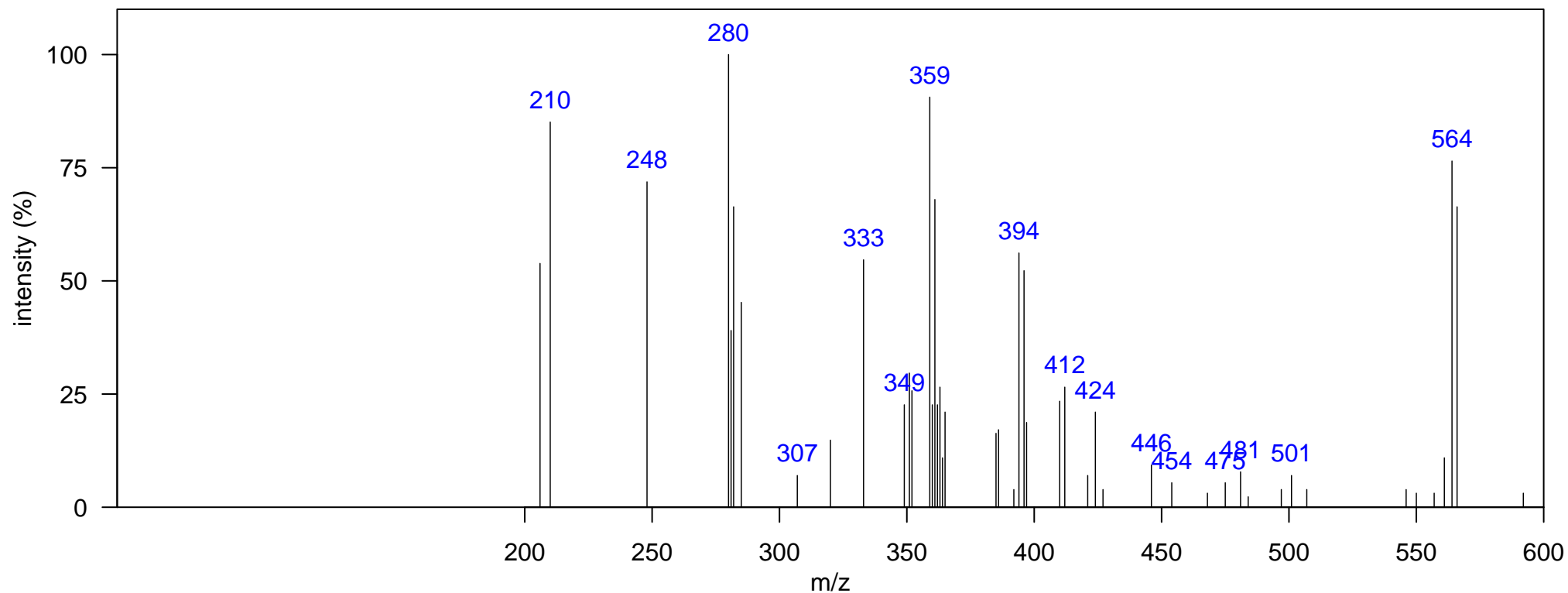
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

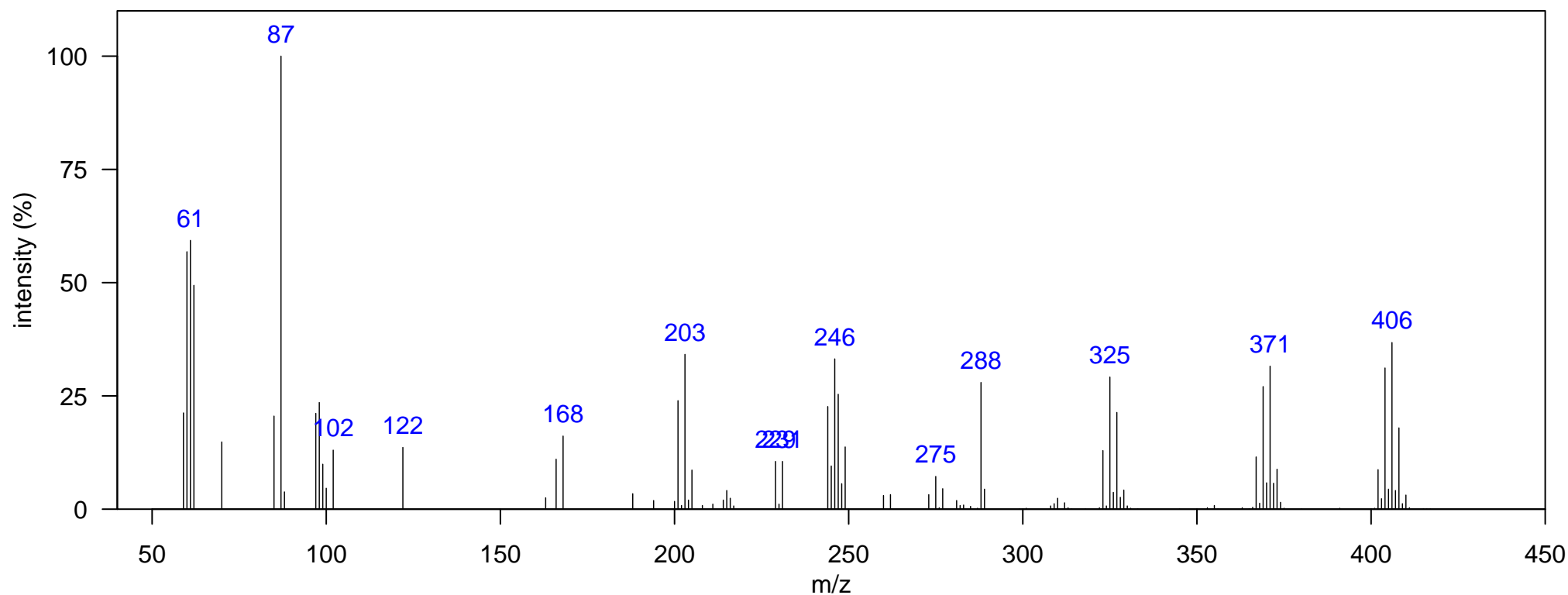
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

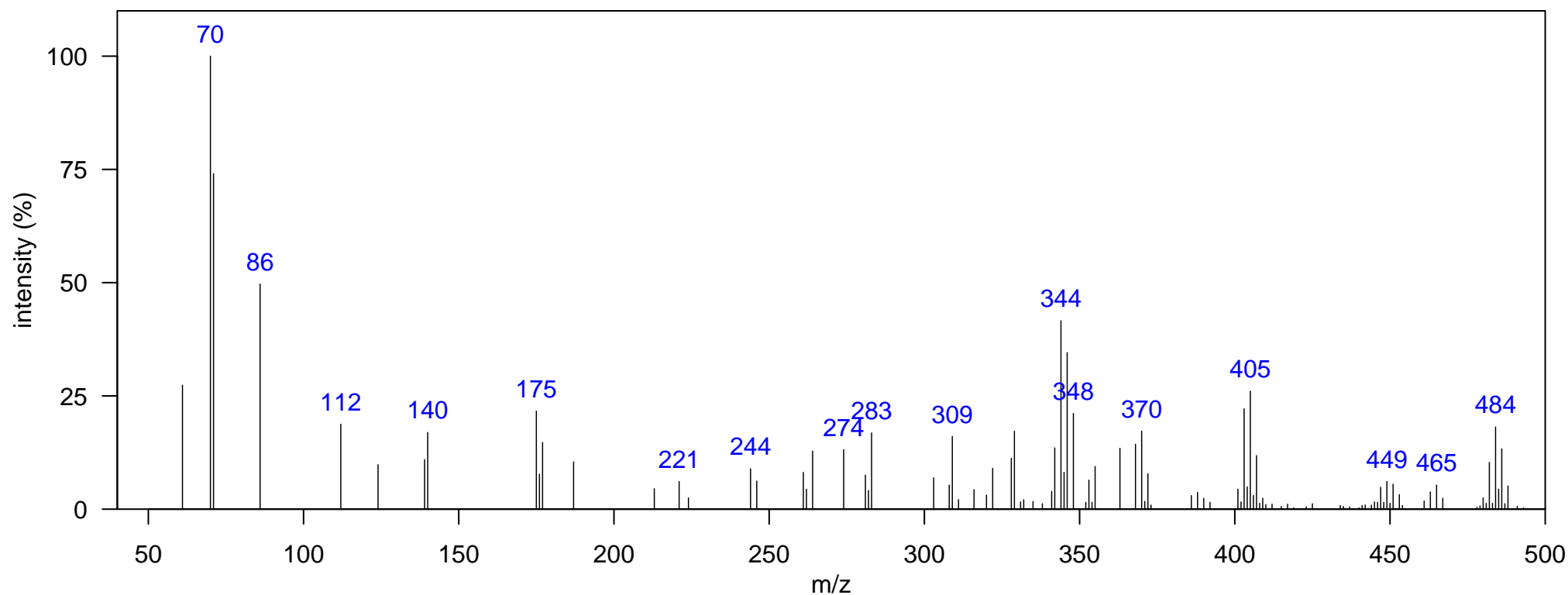
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

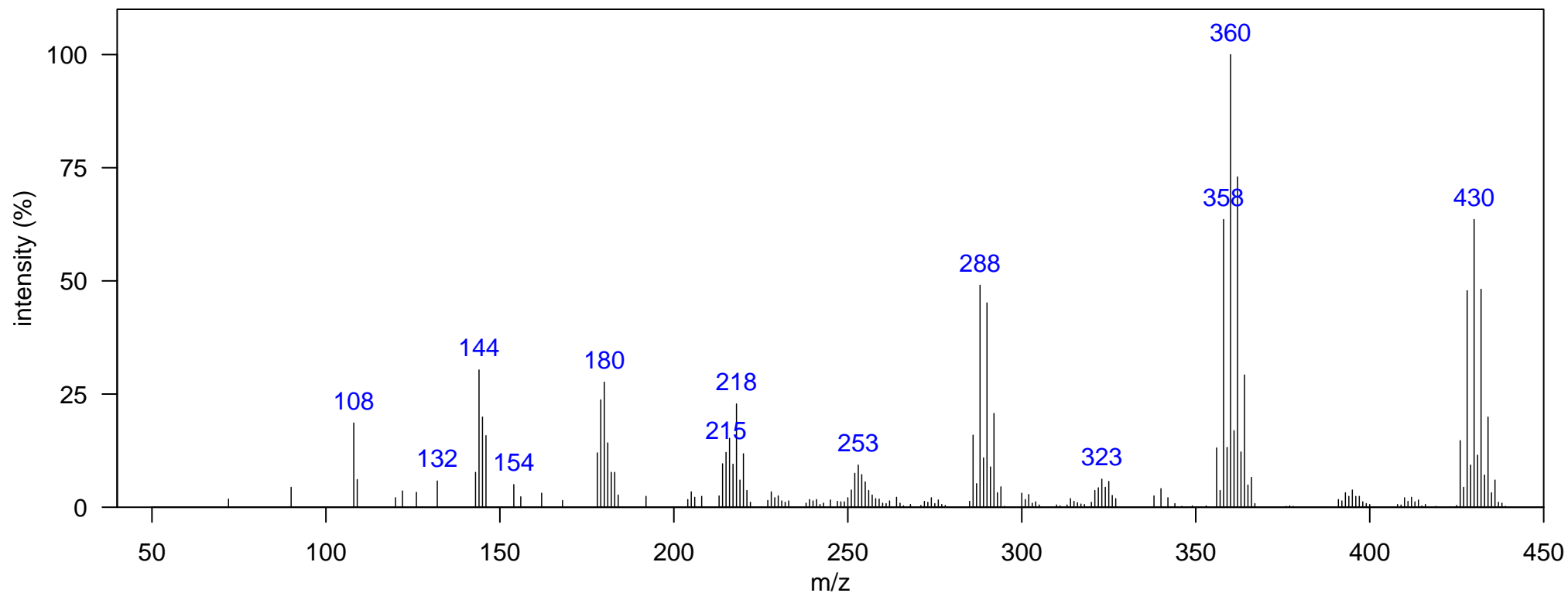
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

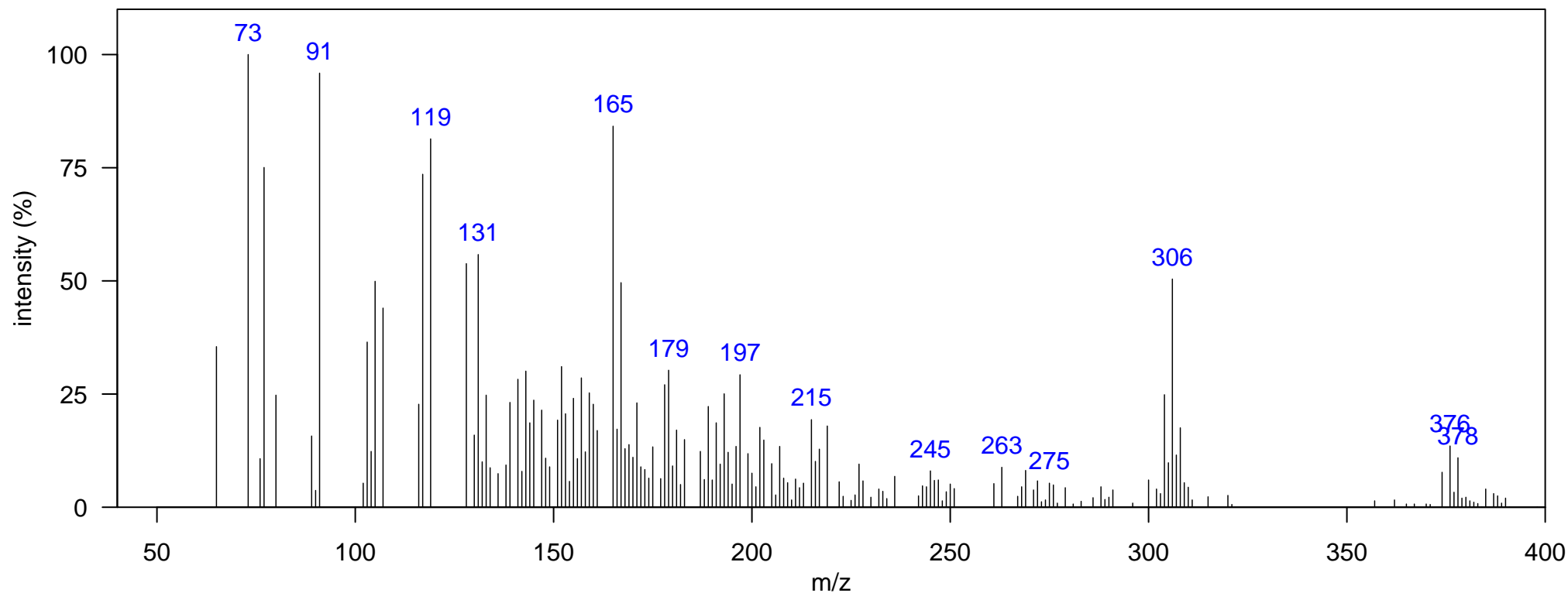
Comment: PCB interference – ions 412 and 340 belong to unknown-4-2



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

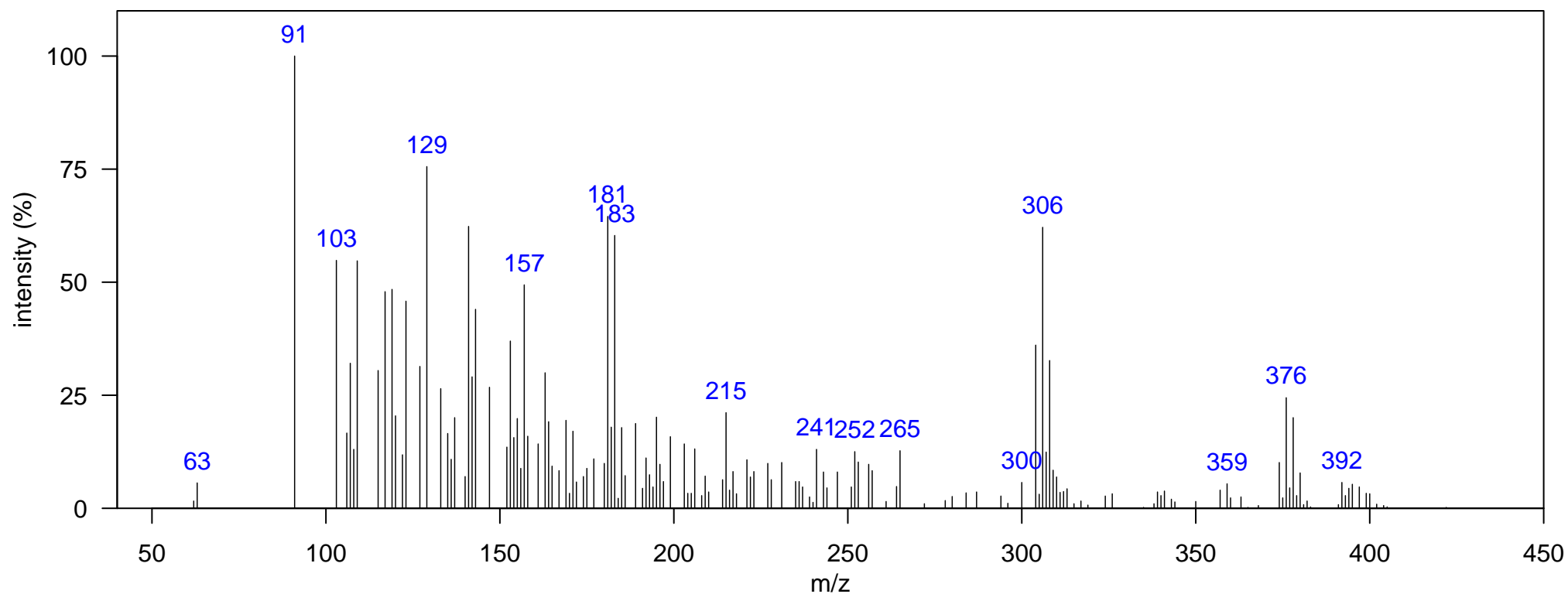
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

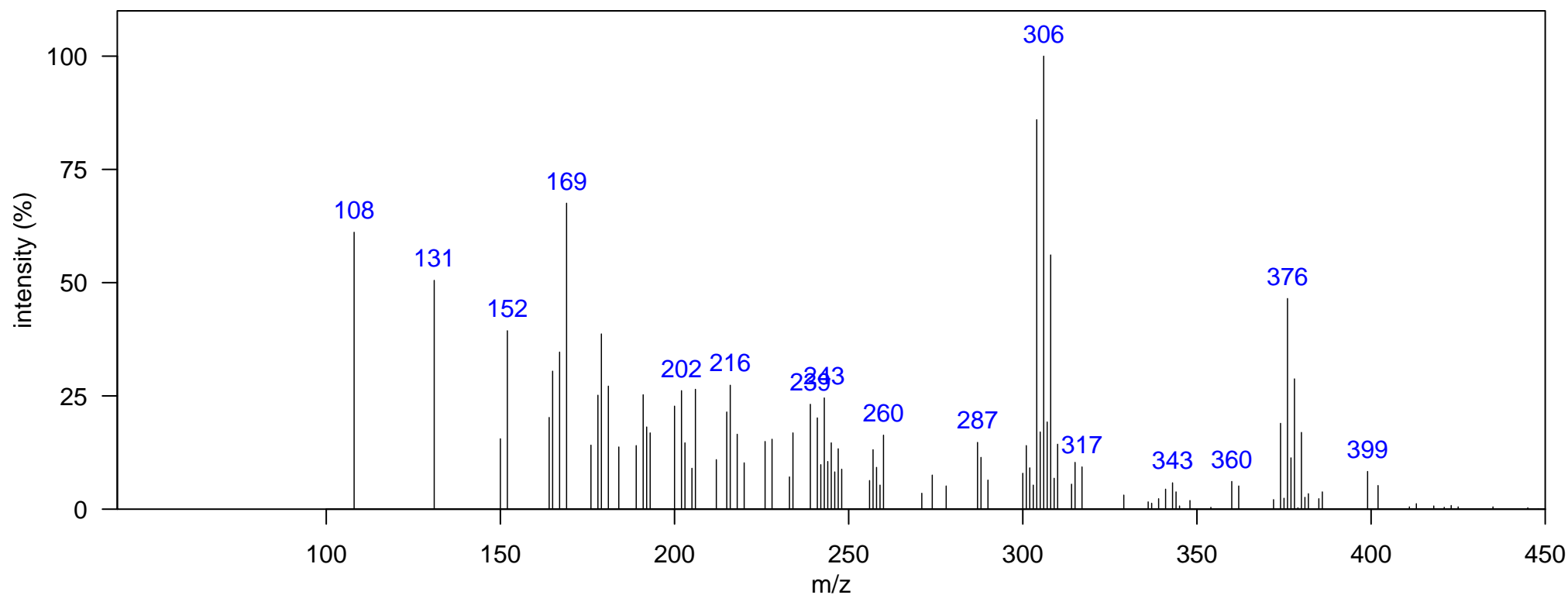
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

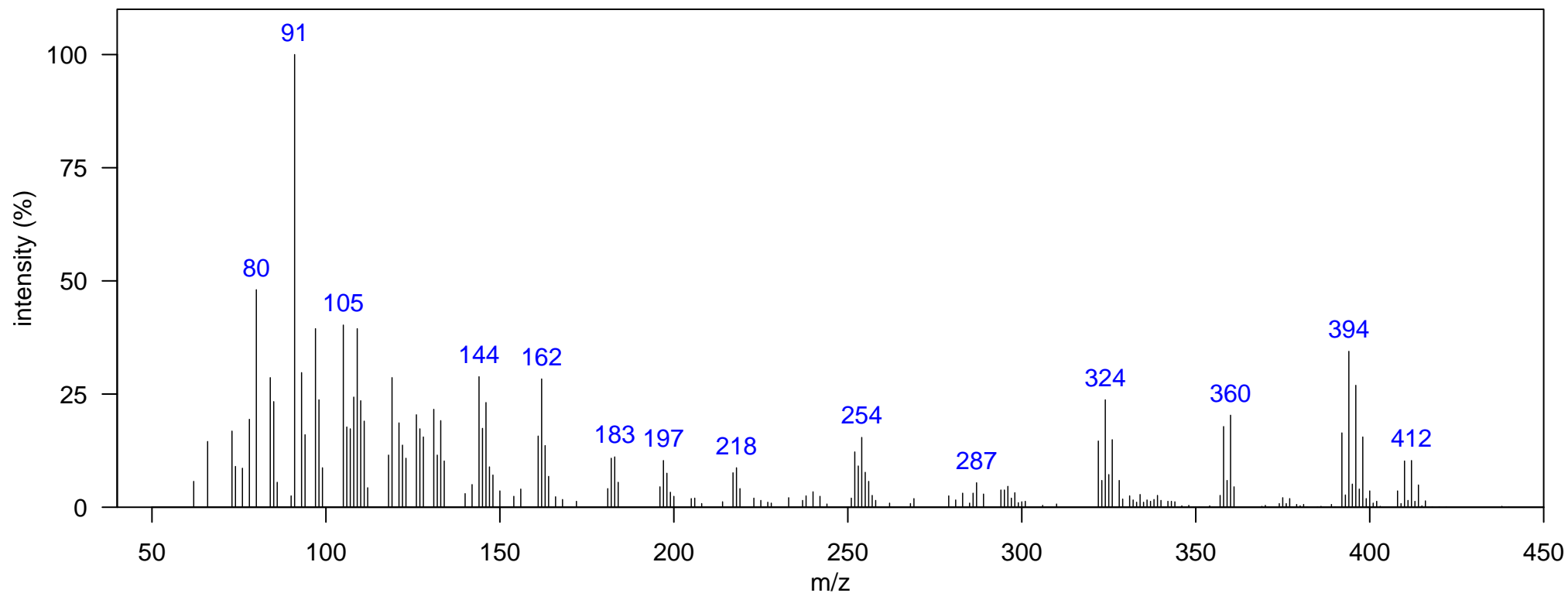
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

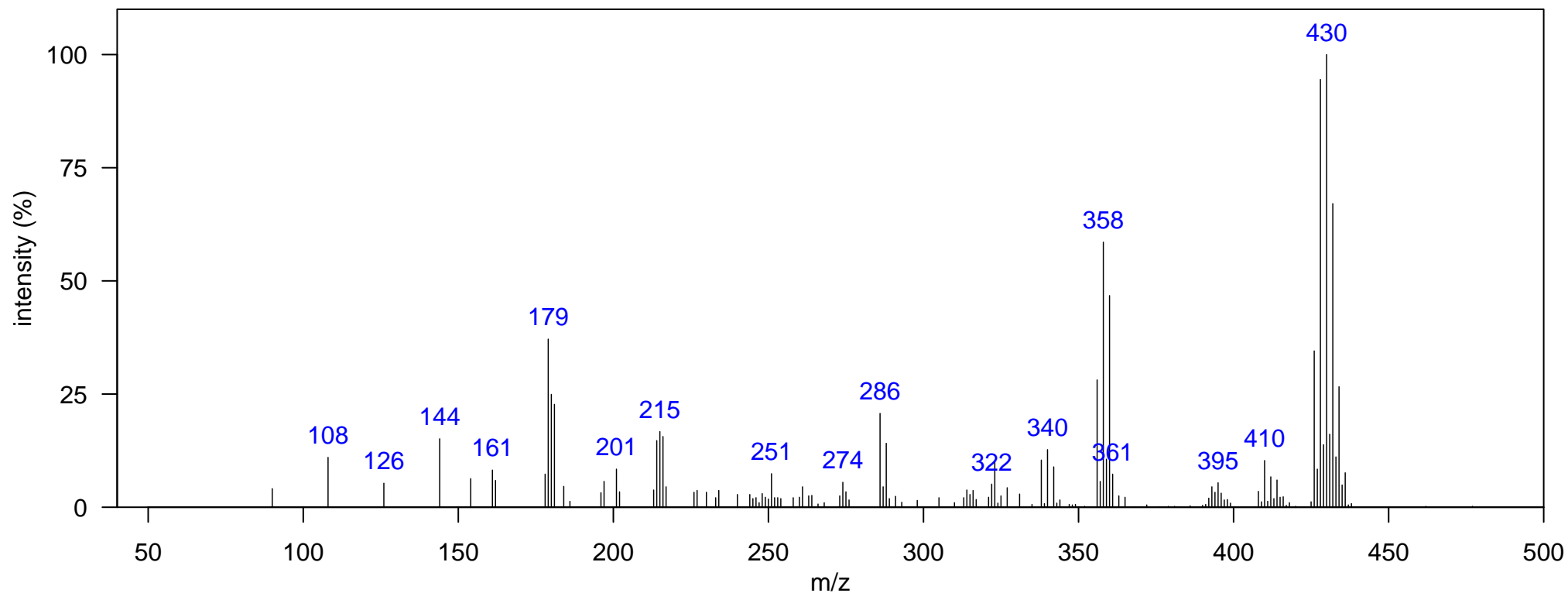
Comment: PCB interference



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

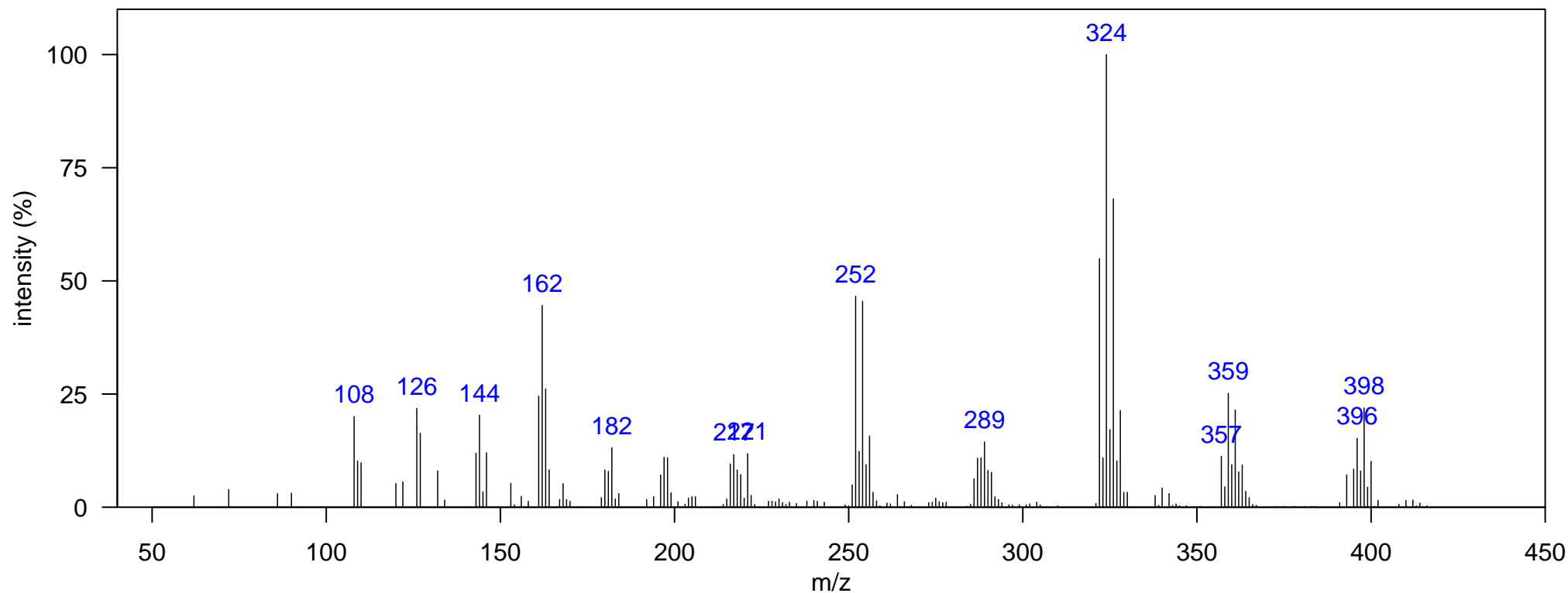
Comment: PCB interference – ions 410 and 340 belong to unknown-4-10



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

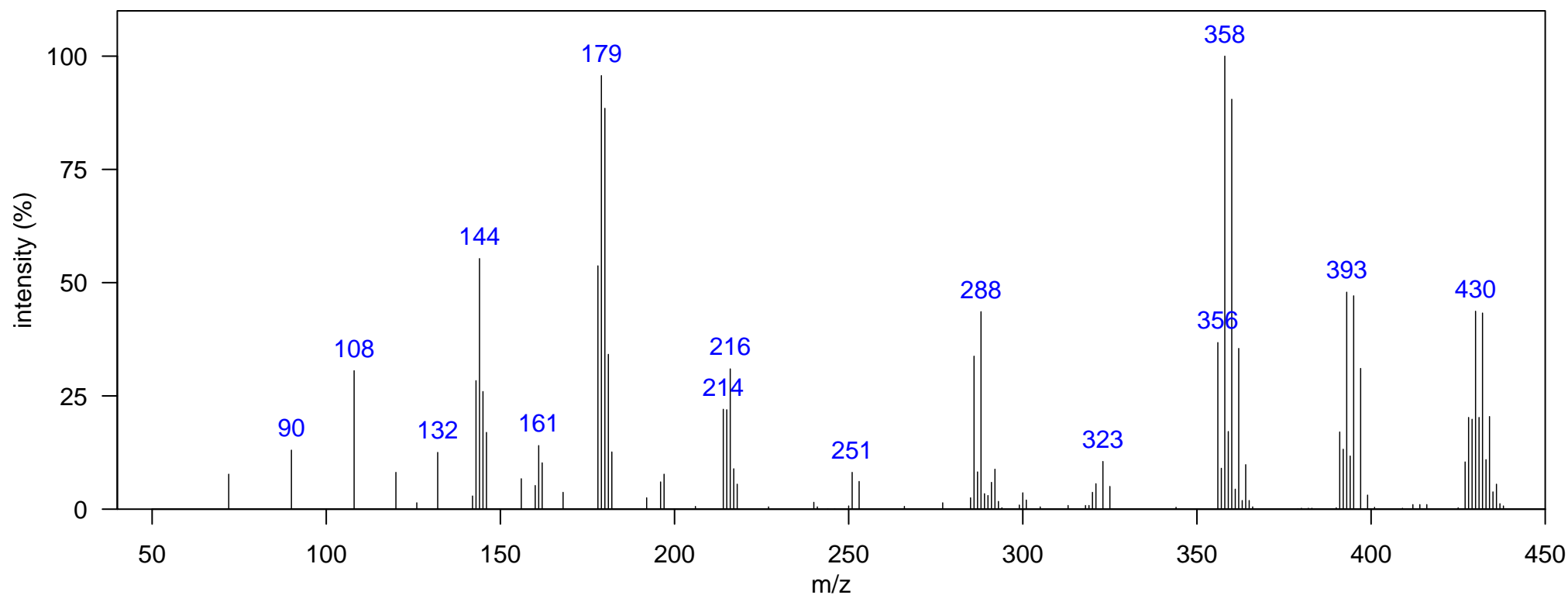
Comment: PCB interference – ions 412 and 340 belong to unknown-4-11



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

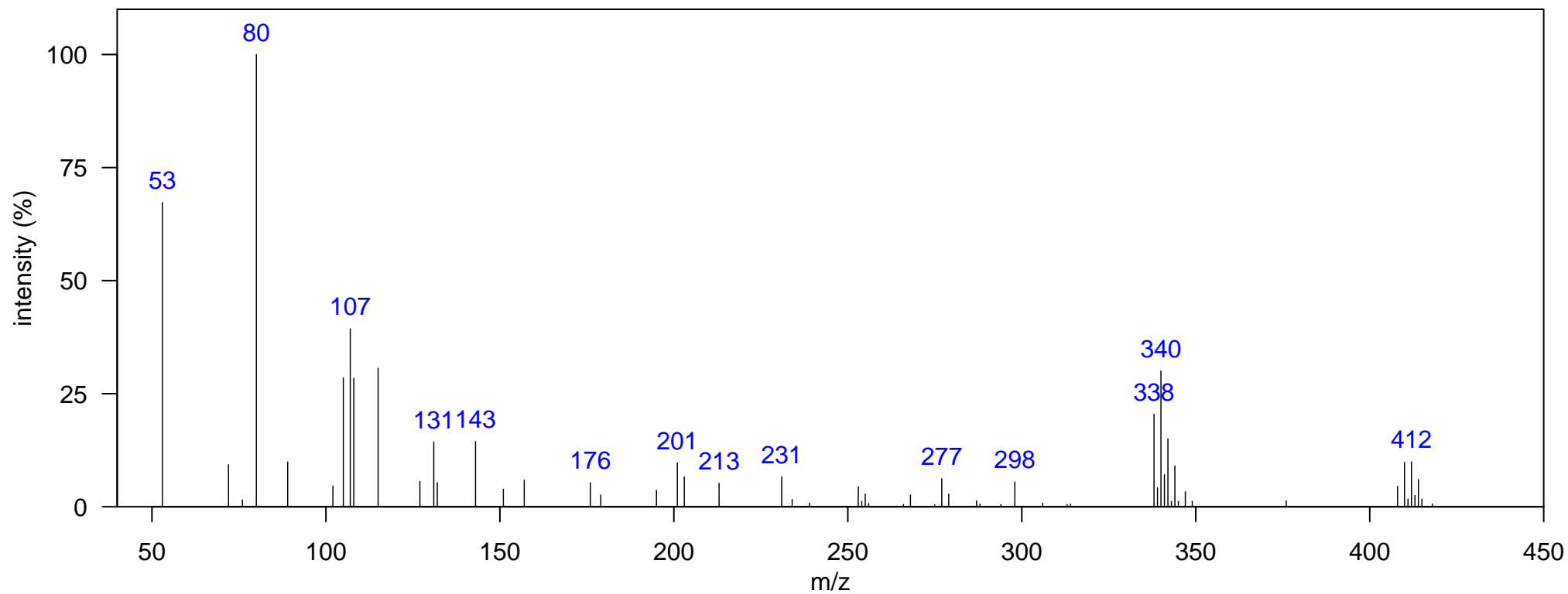
Comment: Interference from other compounds, ion 412 belongs to unknown-4-12



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

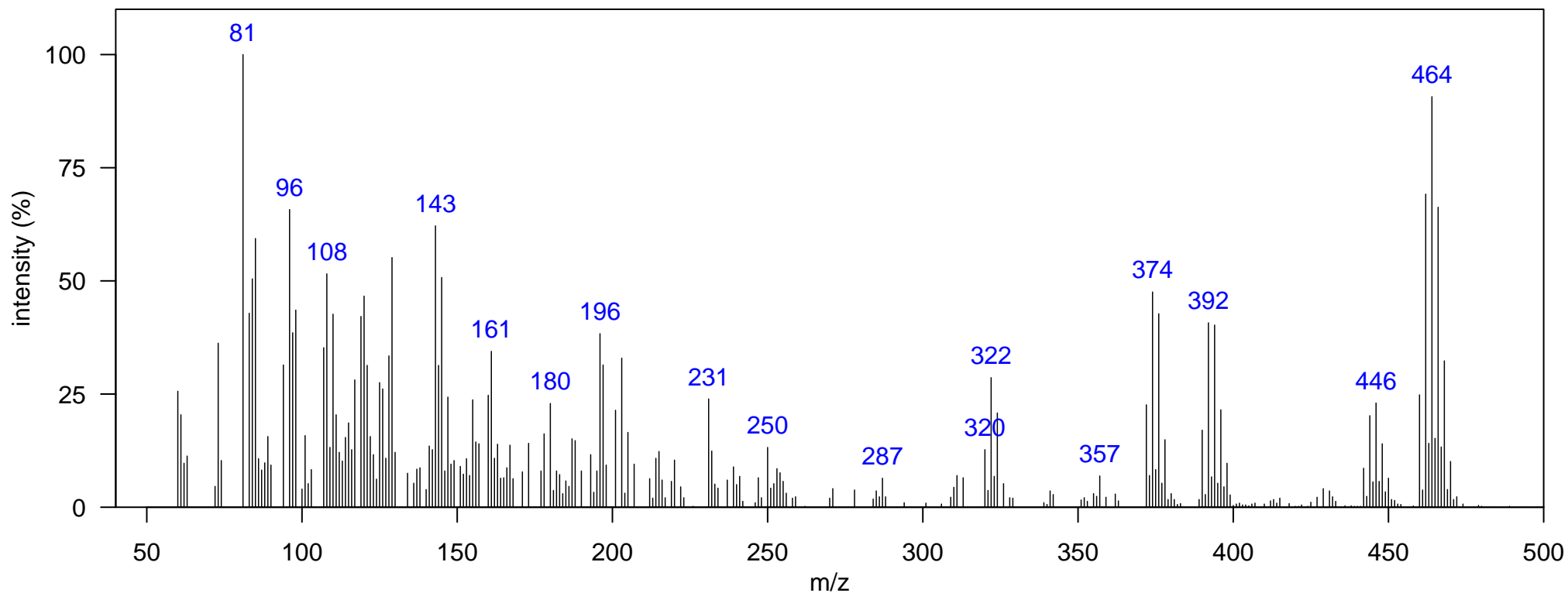
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

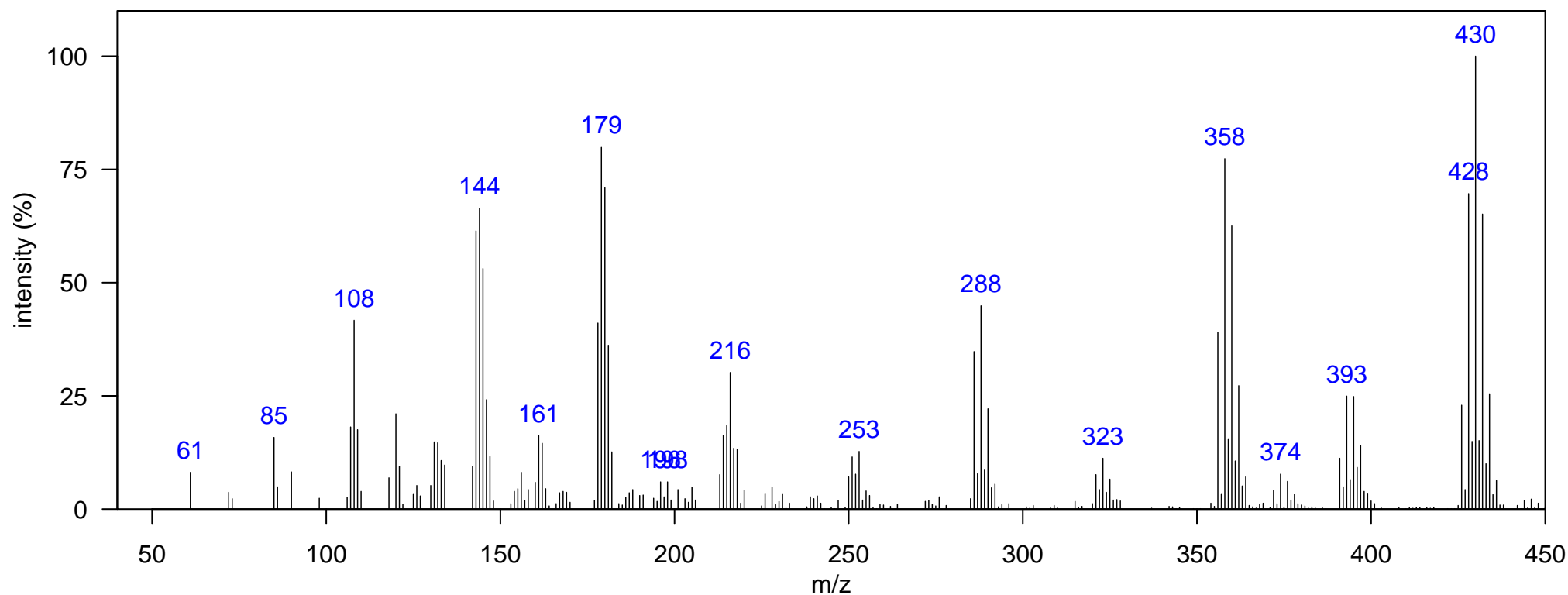
Comment: PCB interference – ions 446 and 374 belong to unknown-4-14



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

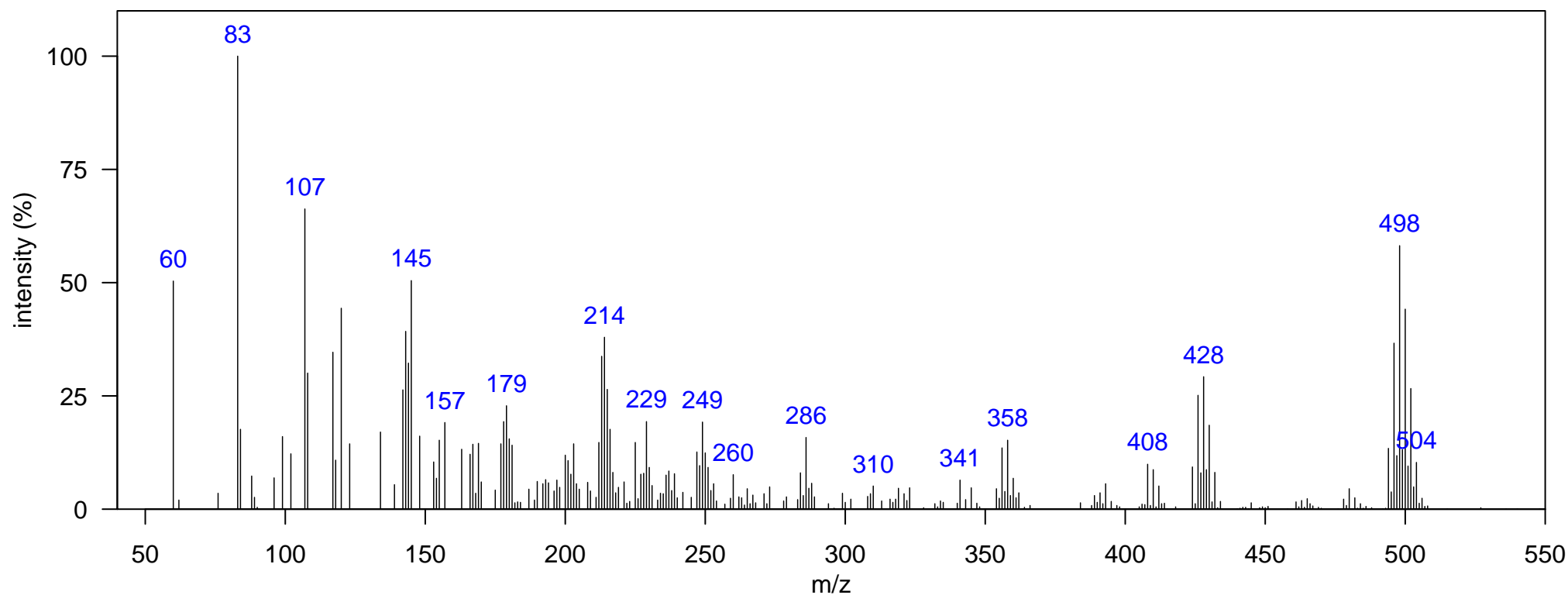
Comment: PCB interference – ions 446 and 374 belong to unknown-4-16



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

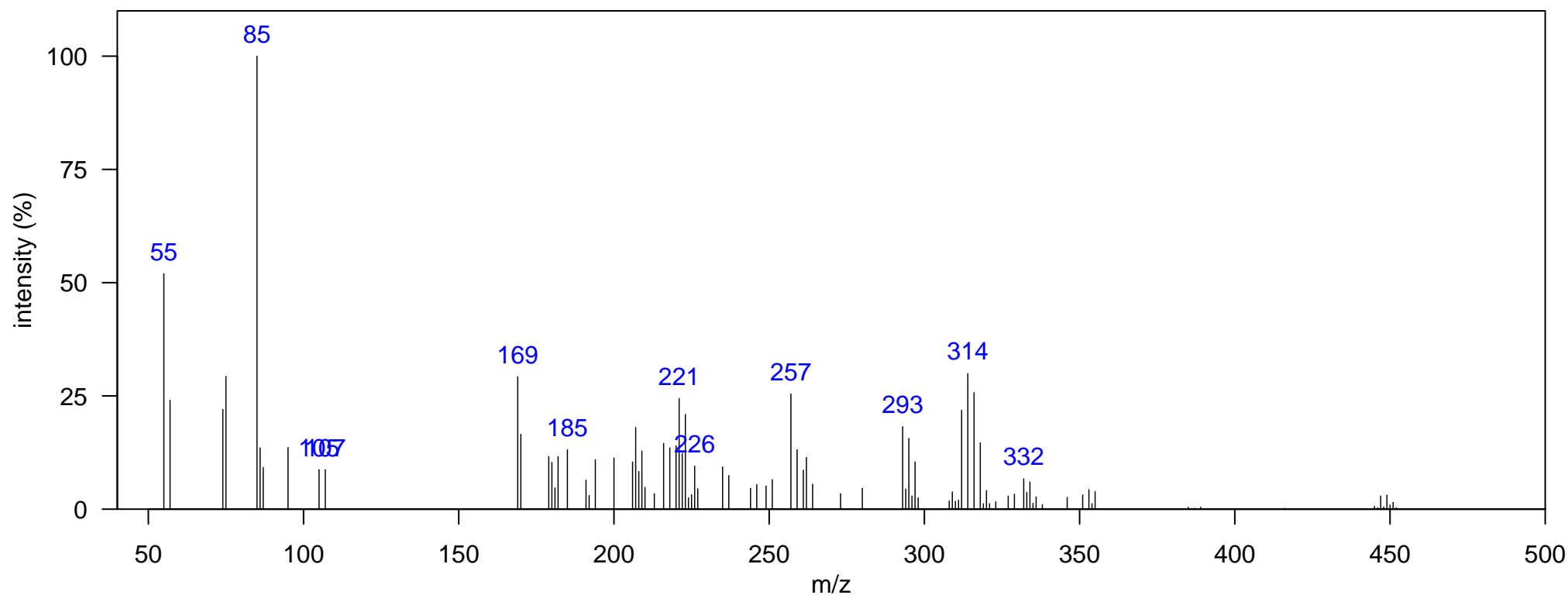
Comment: PCB interference – ions 408 and 480 belong to unknown-4-17



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

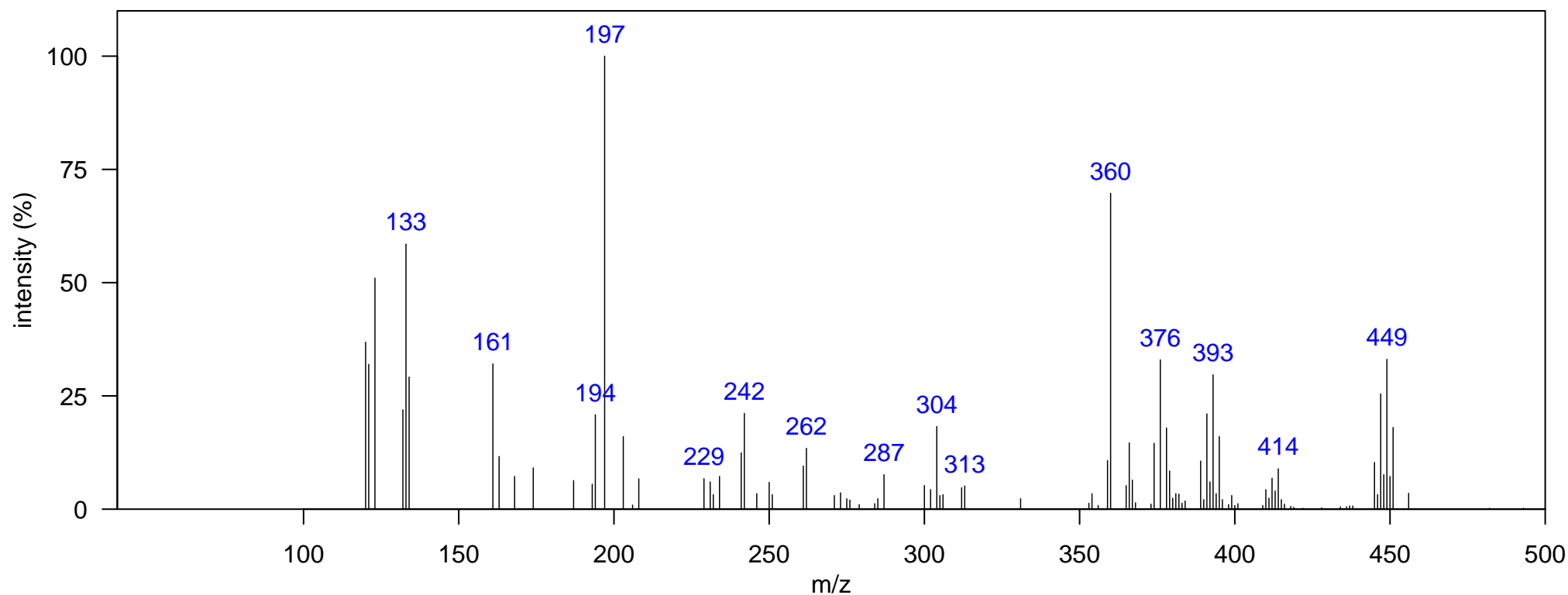
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

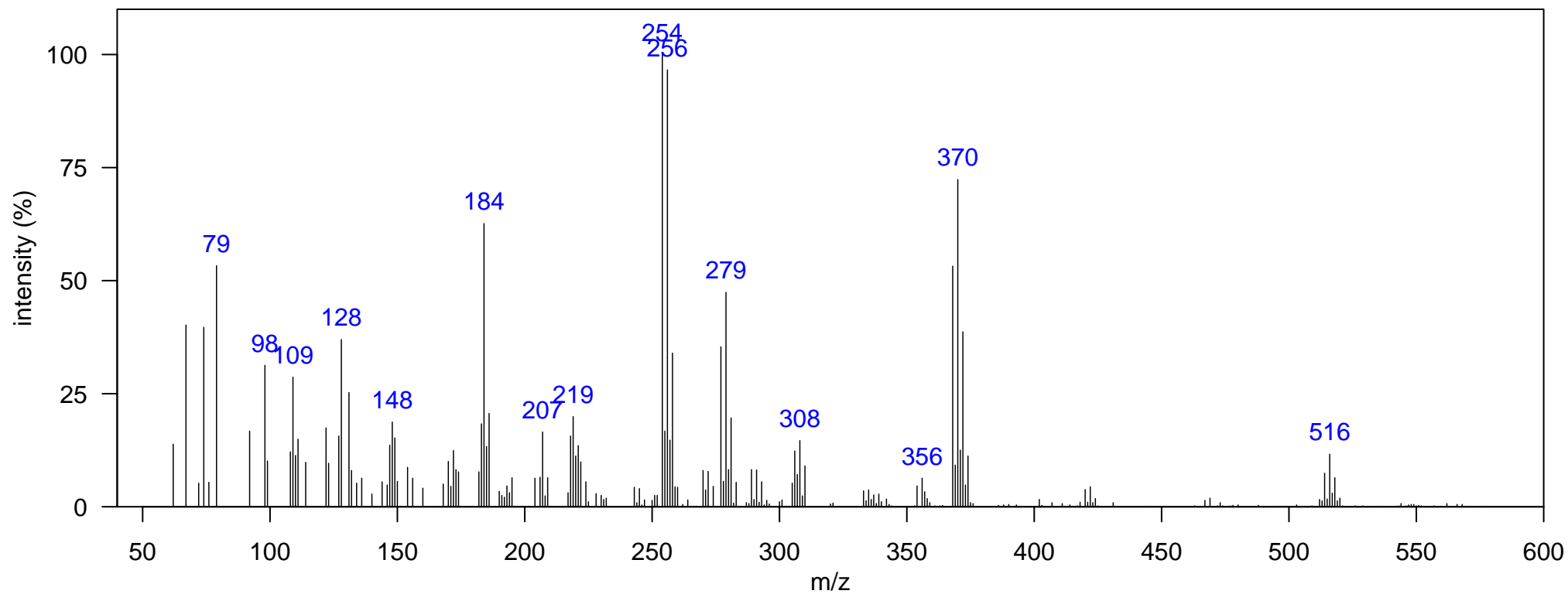
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

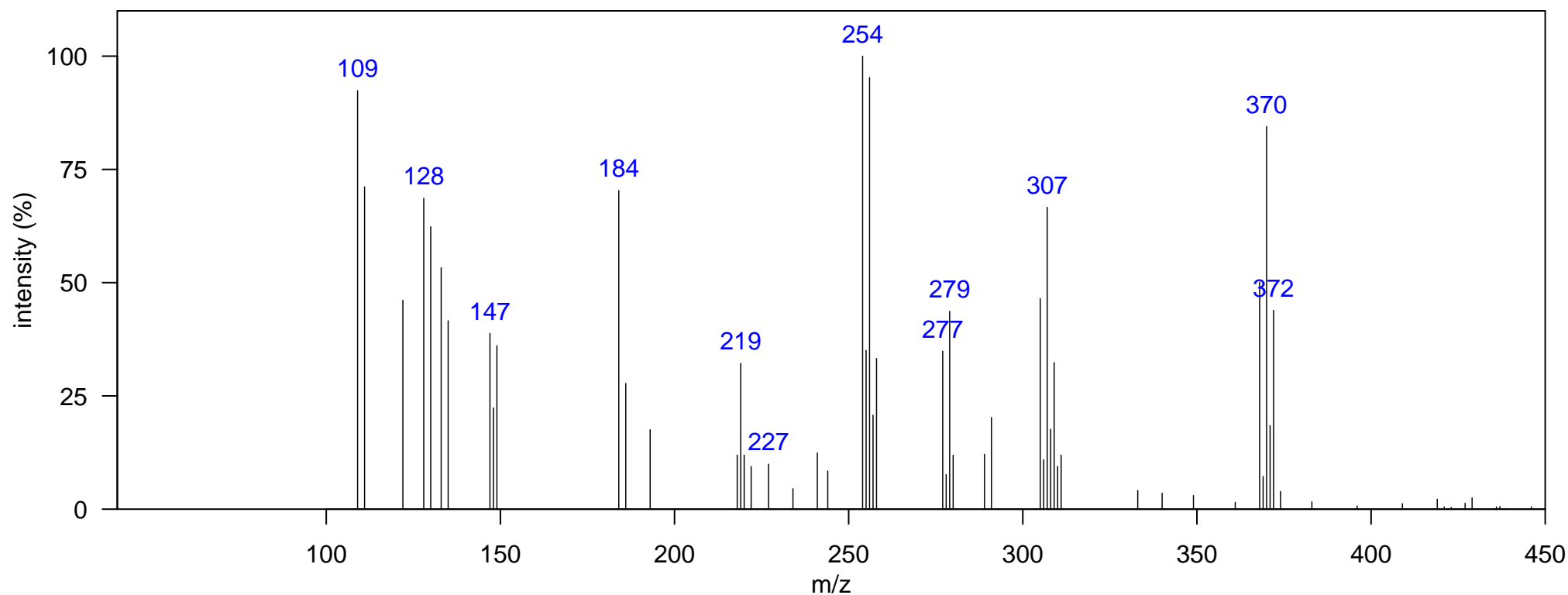
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

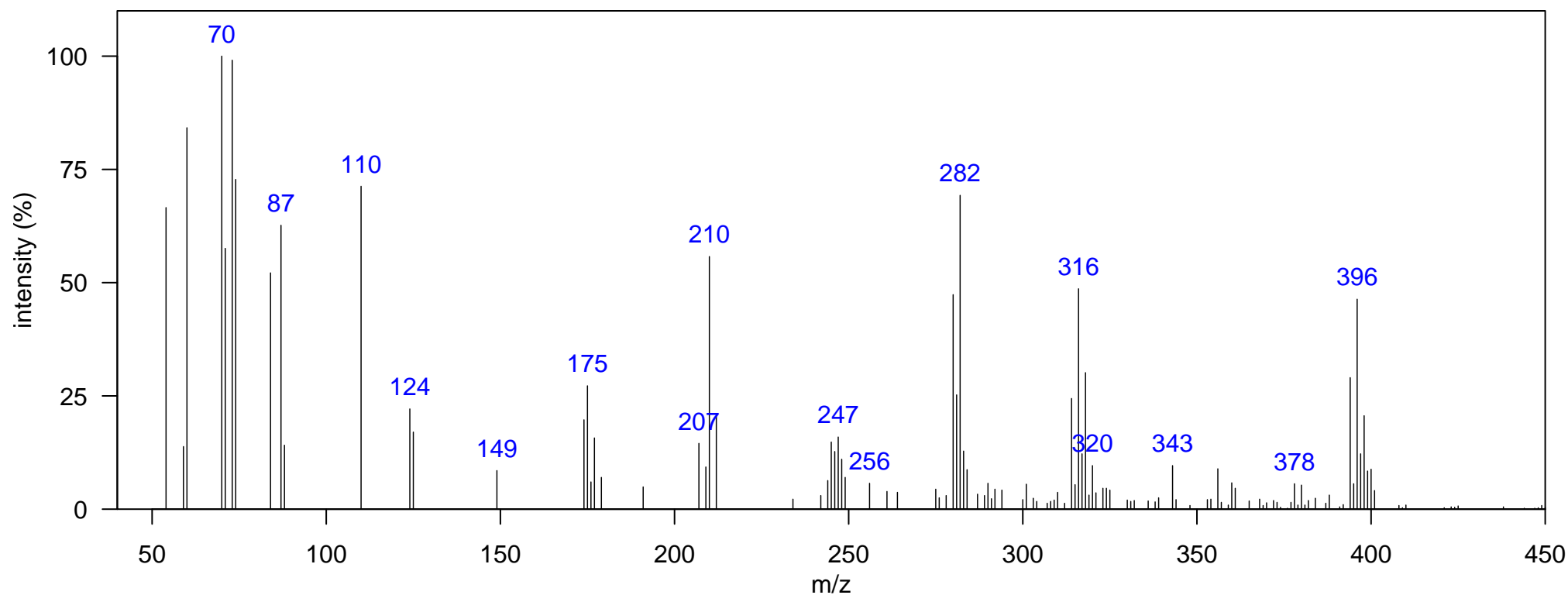
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

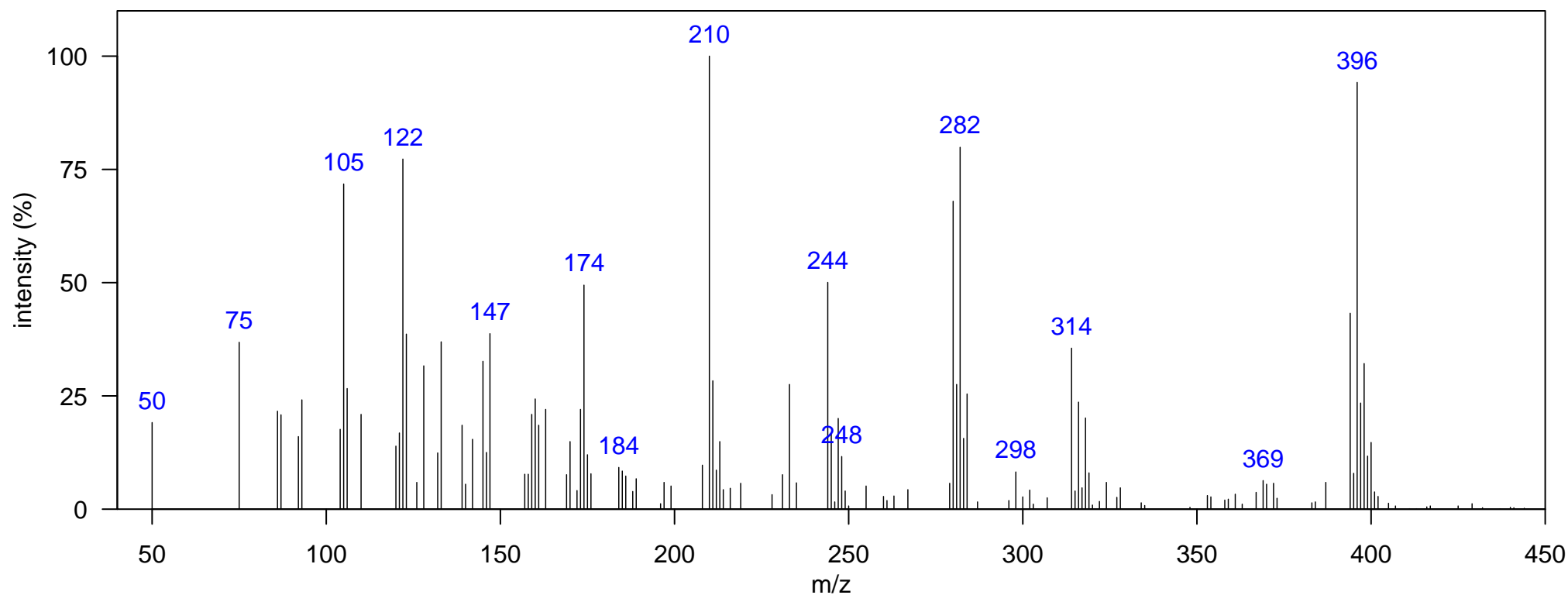
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

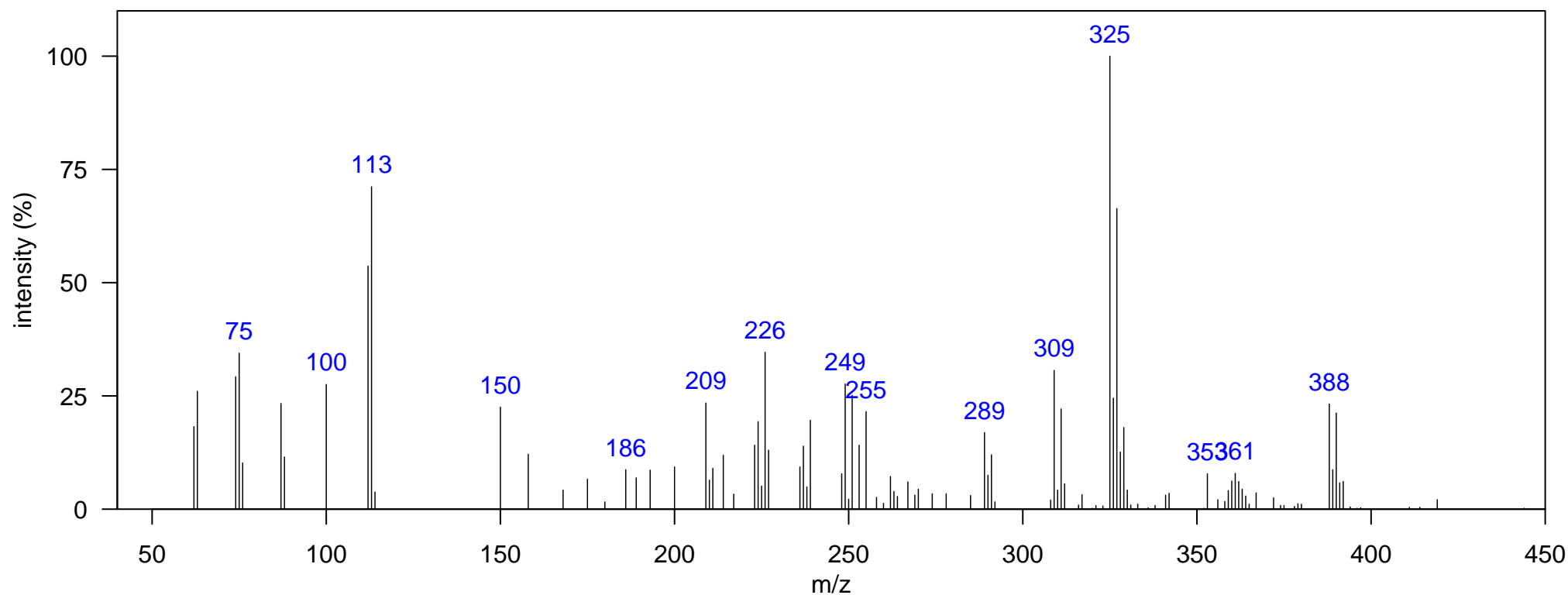
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

Comment:

