

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>

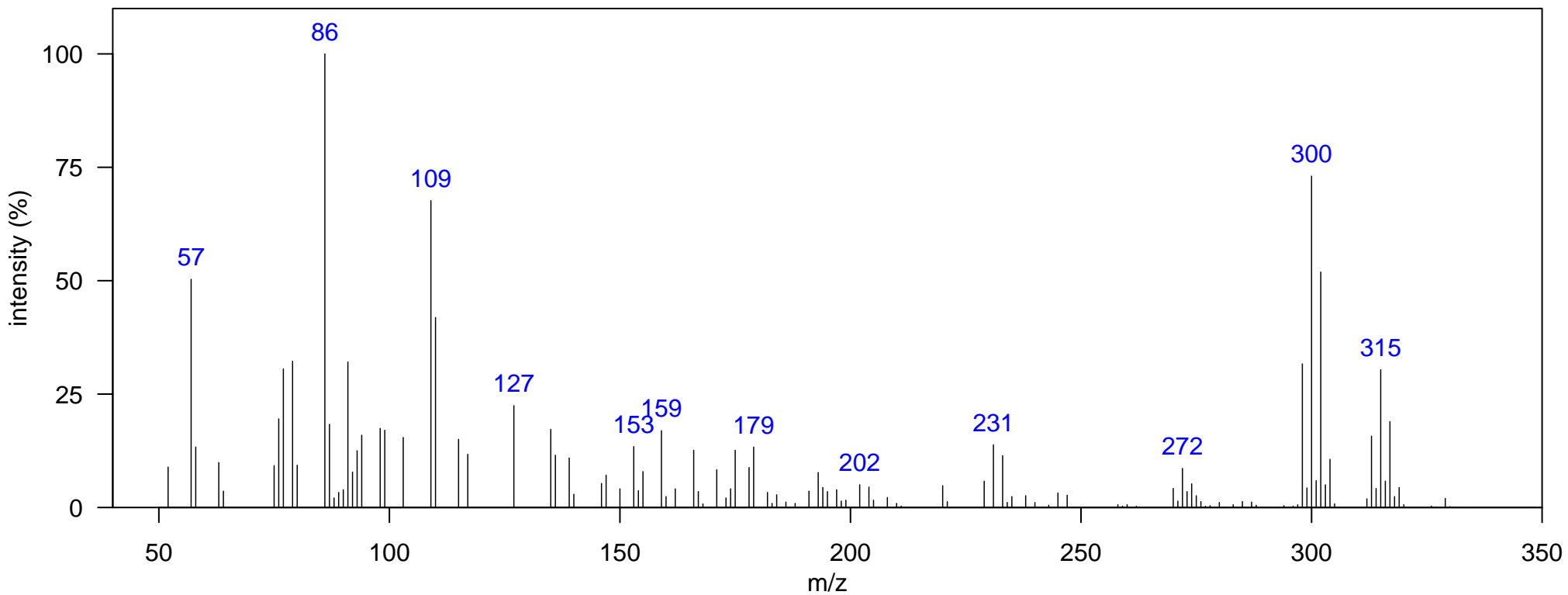
Prepared: 2018–05–09 11:44:52
SpecLibMarineUnknown2018
OrgMassSpecR version 0.5–3

R version 3.4.1 (2017–06–30)

Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

Comment:



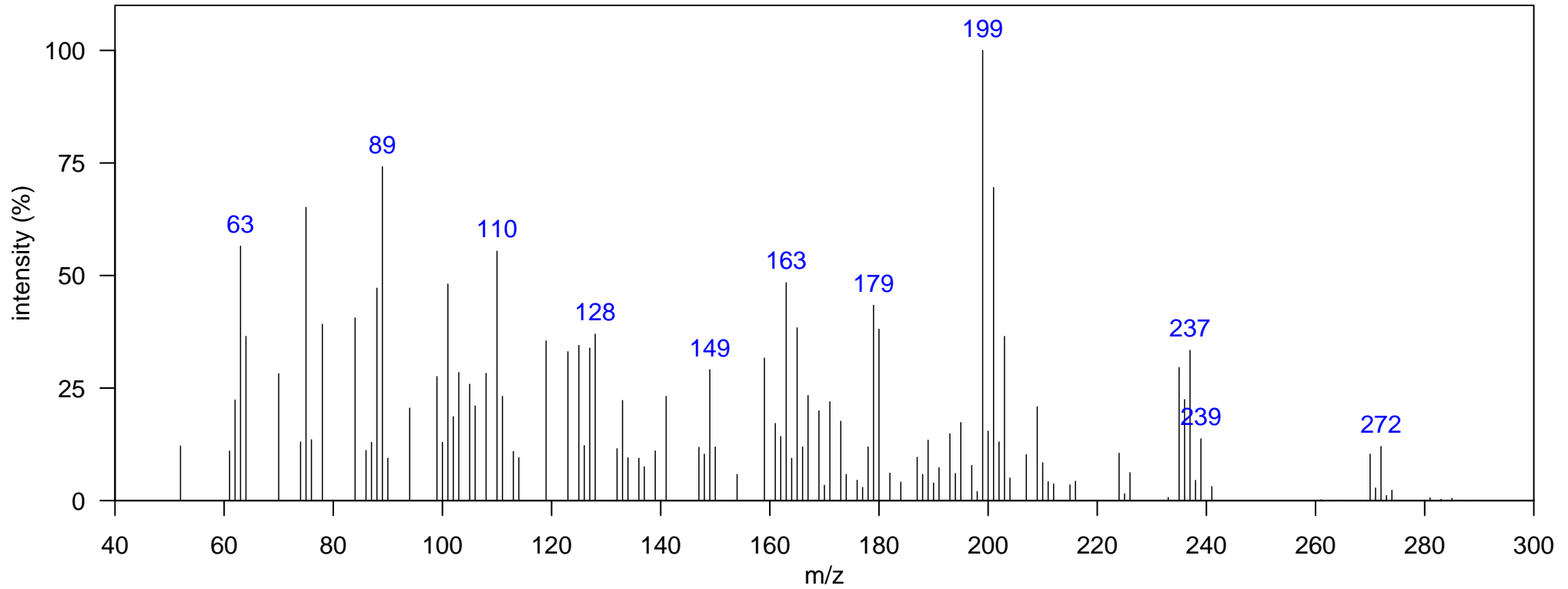
Name: MMCP unknown 2

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

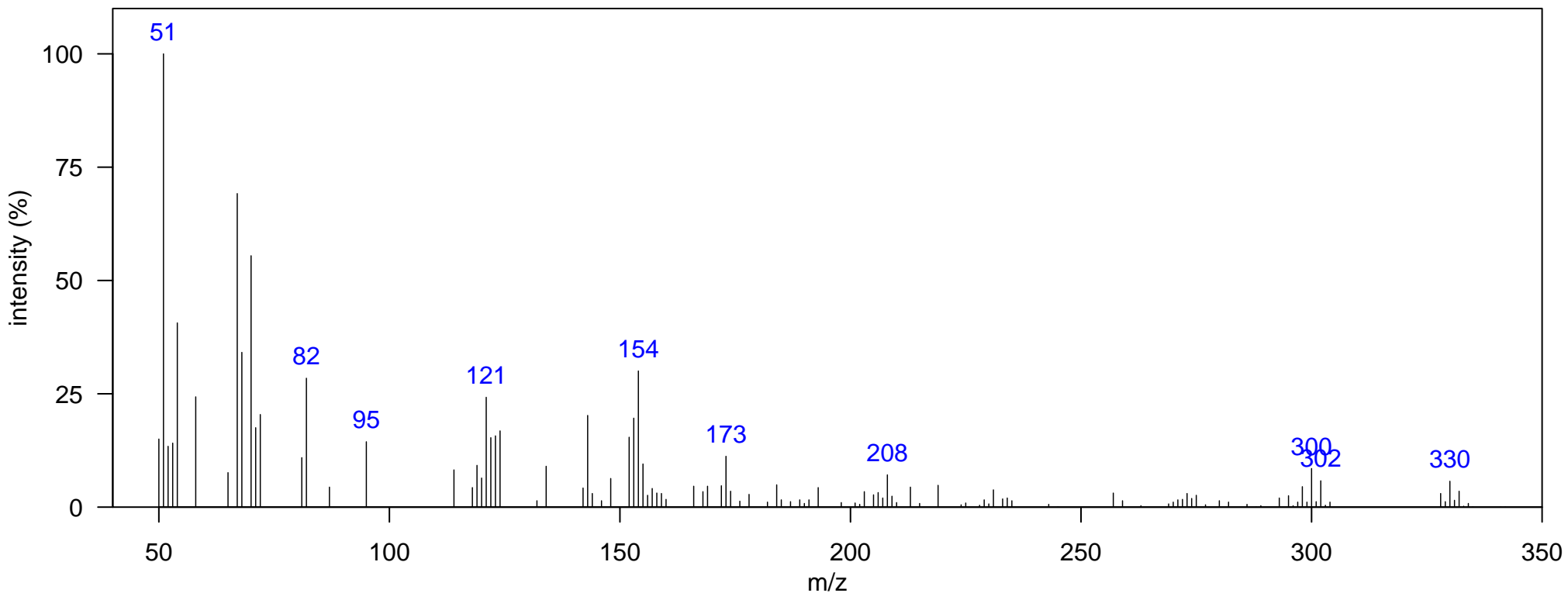
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

Comment:



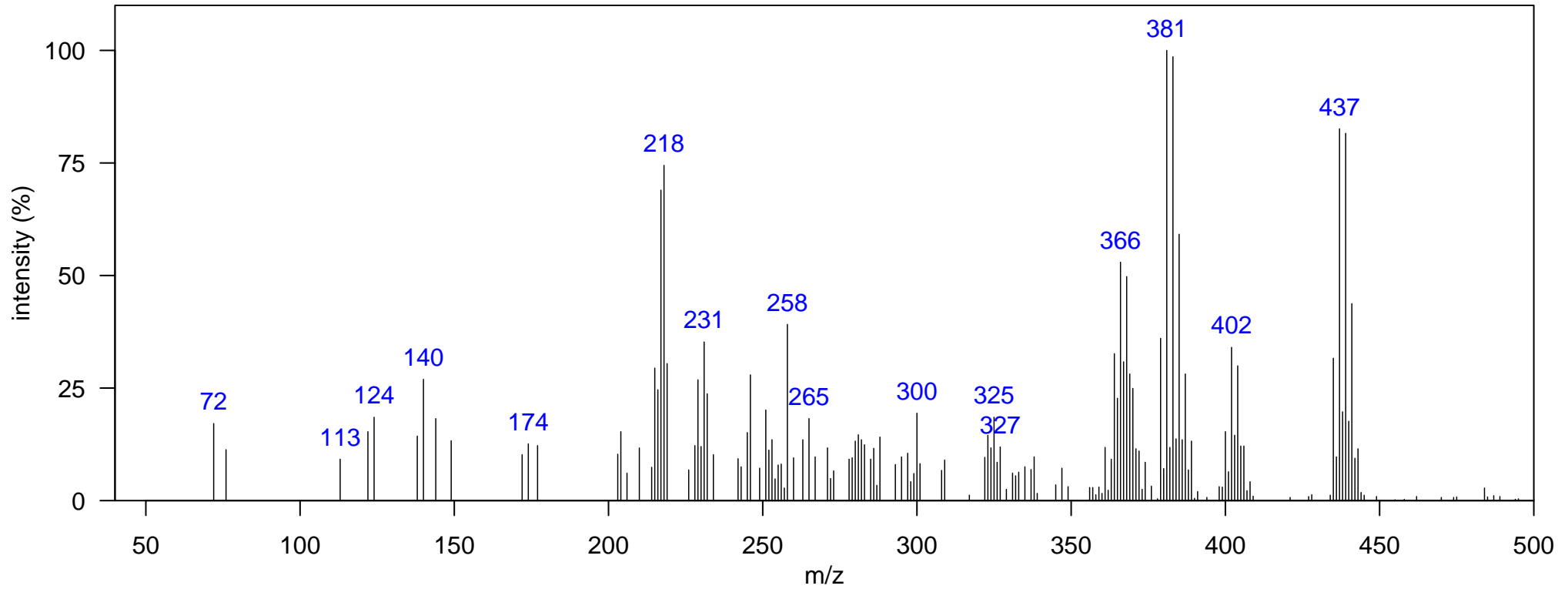
Name: MMCP unknown 4

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

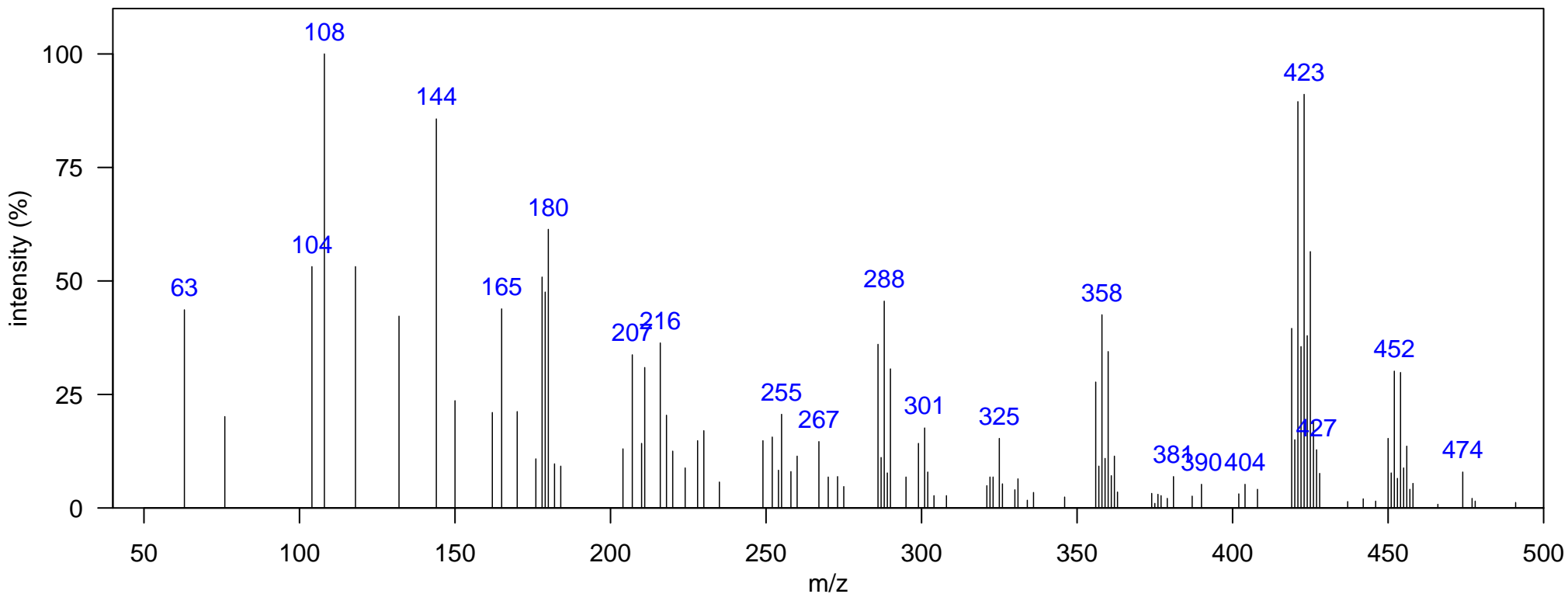
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

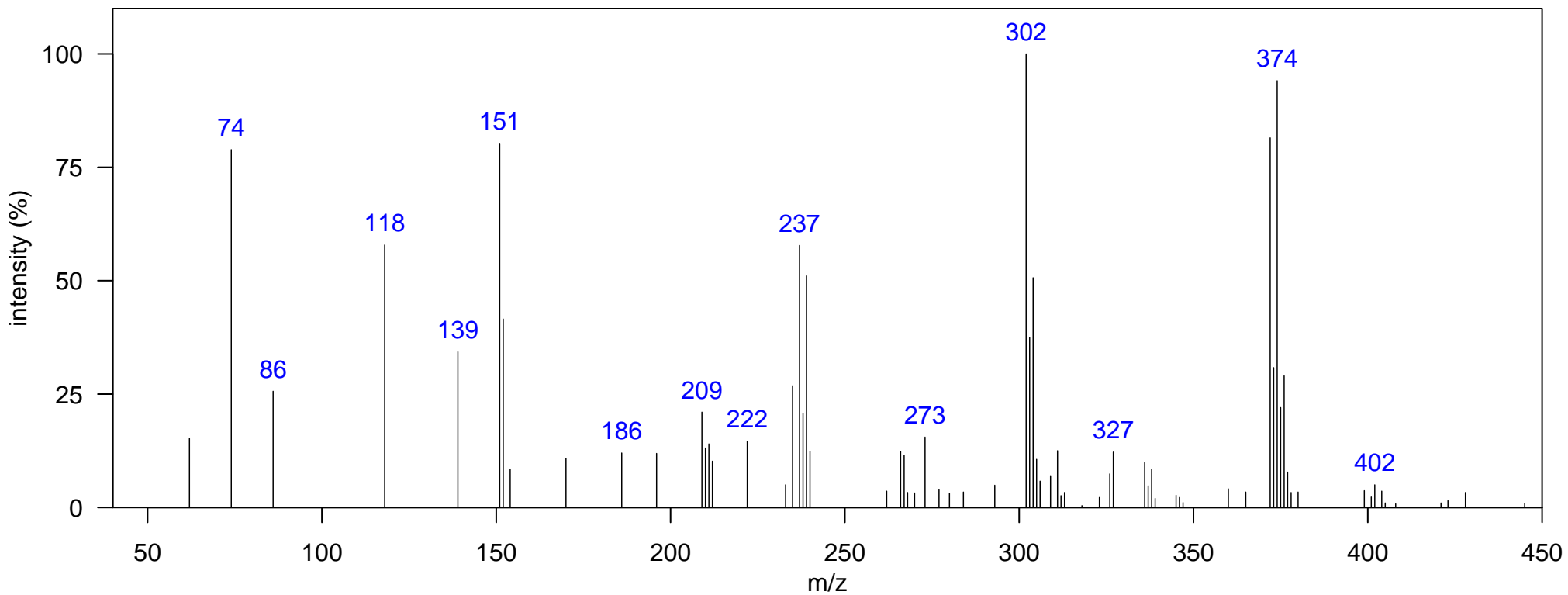
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

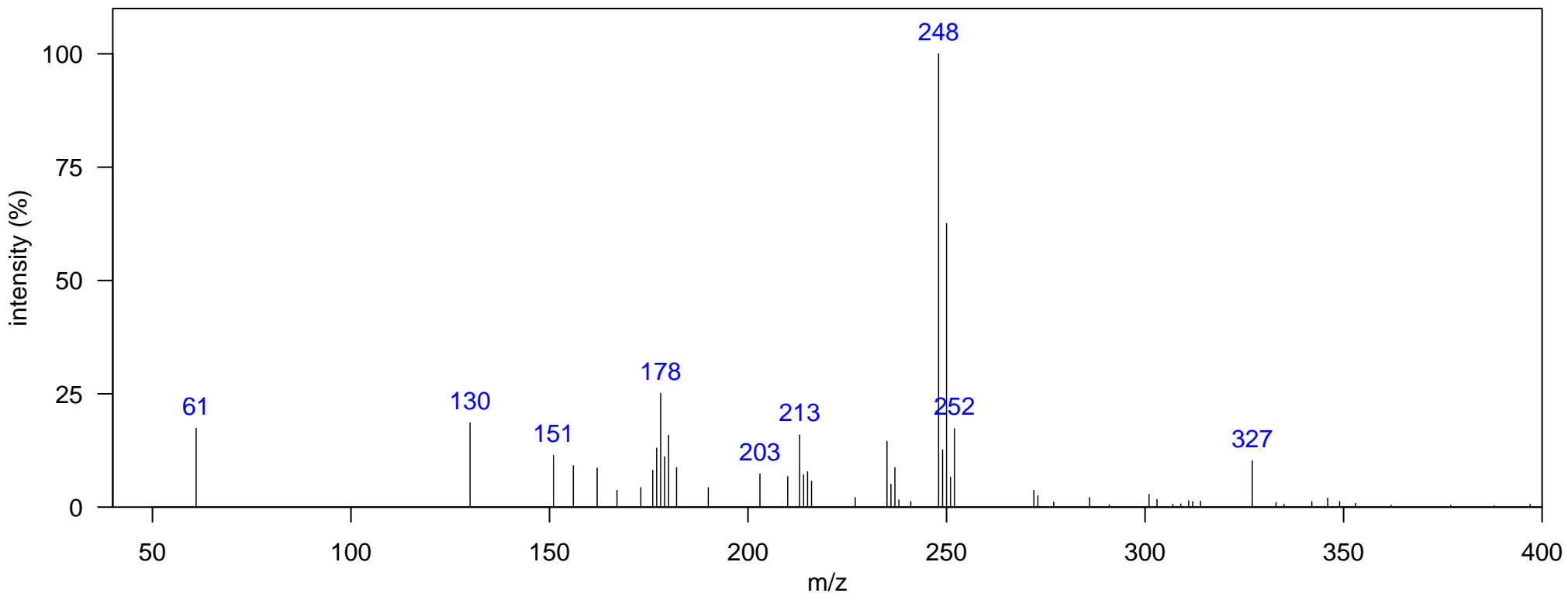
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

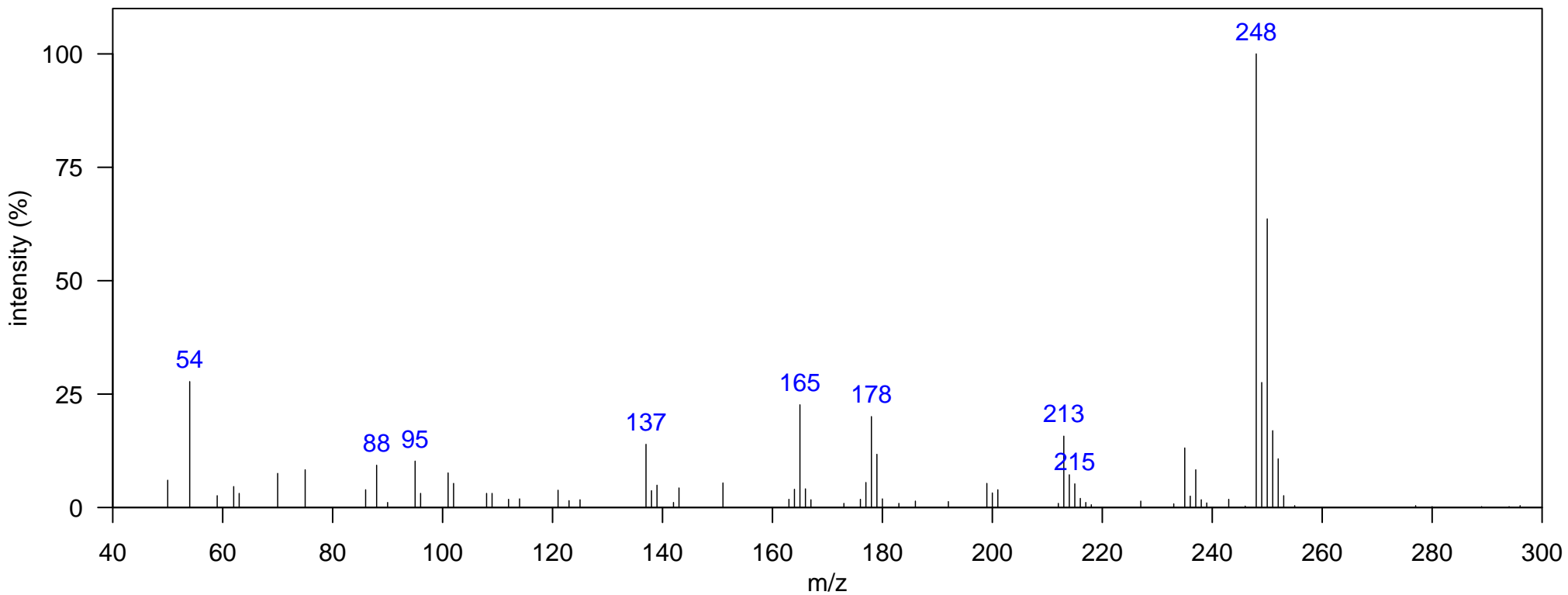
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

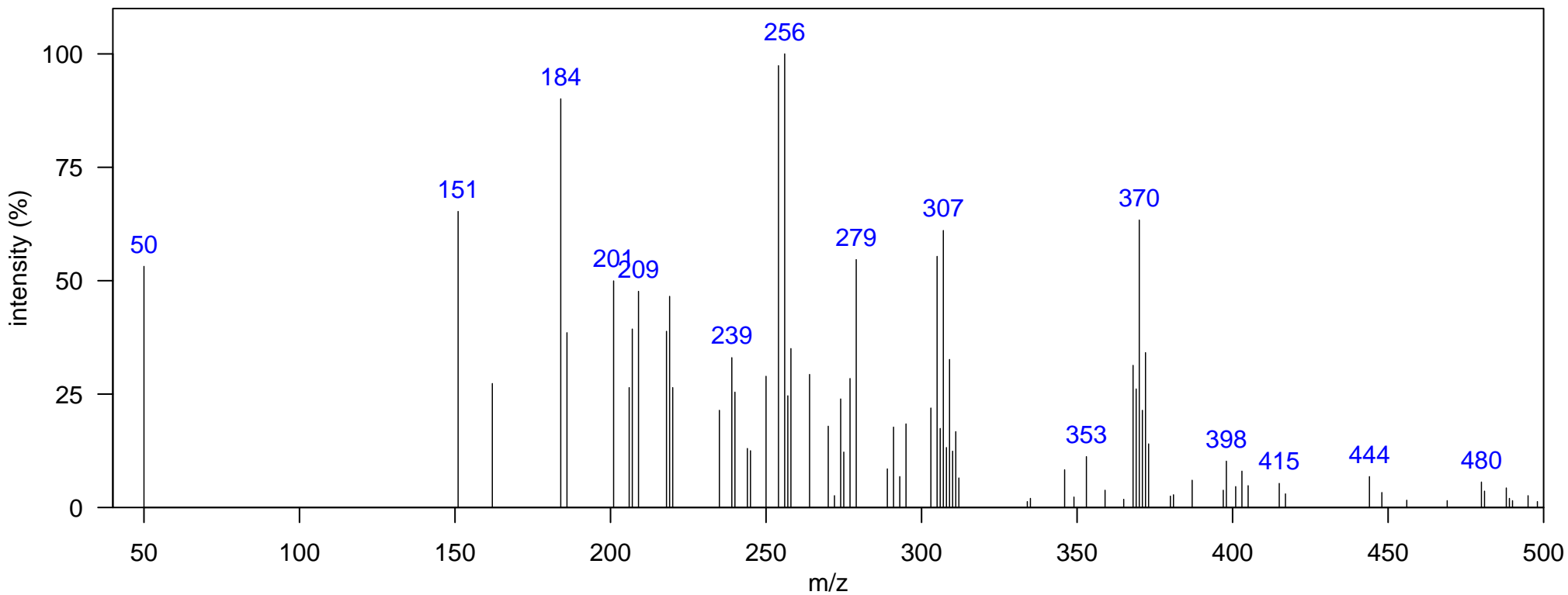
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

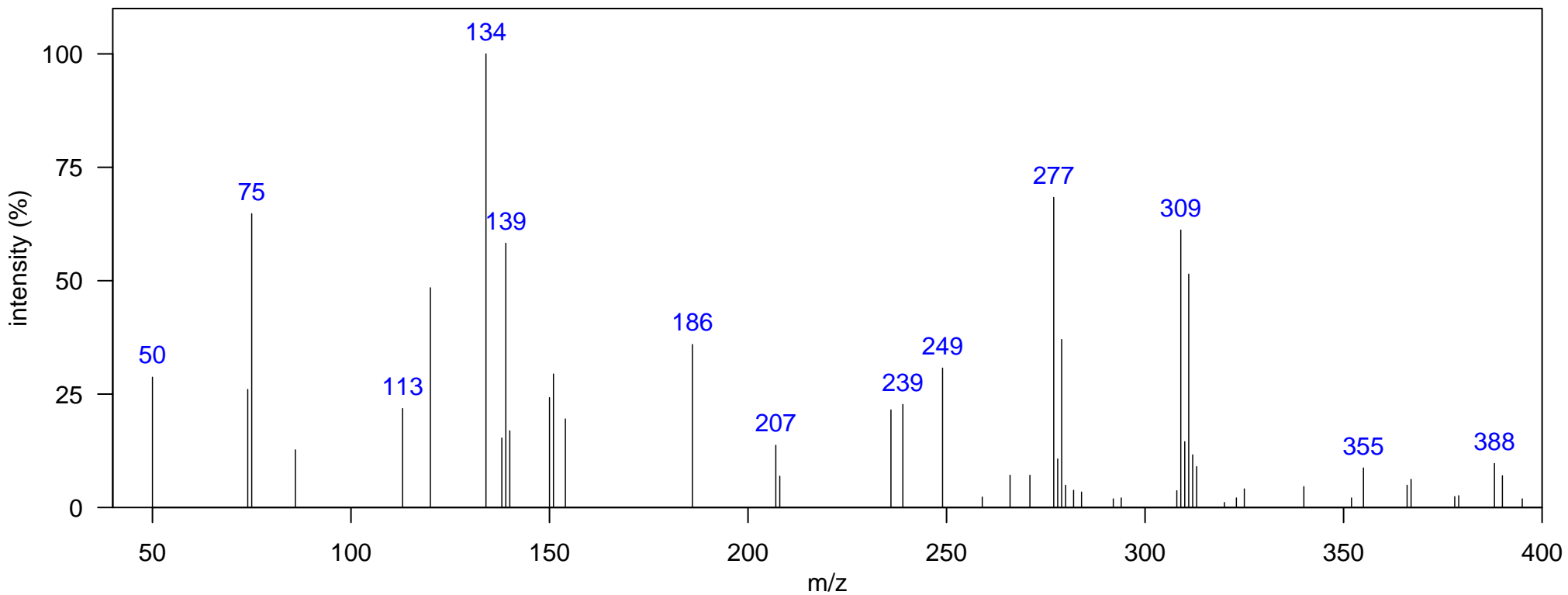
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: FALSE

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

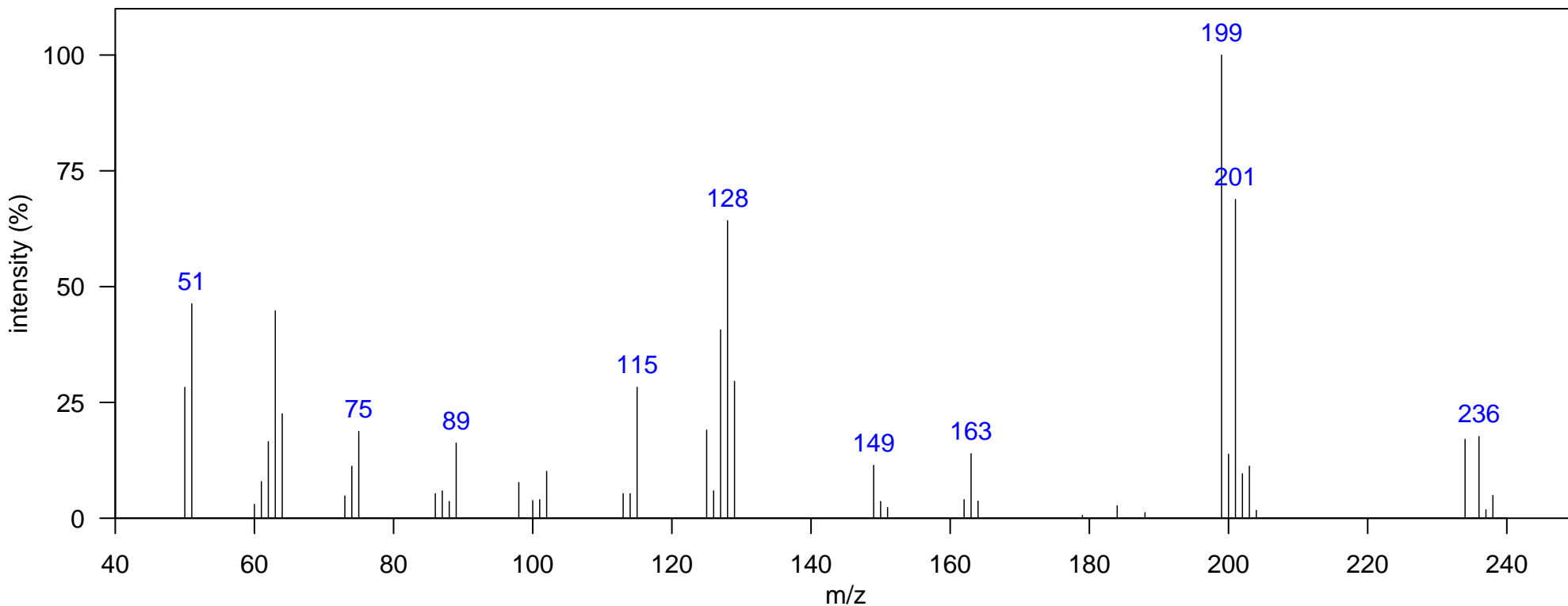
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

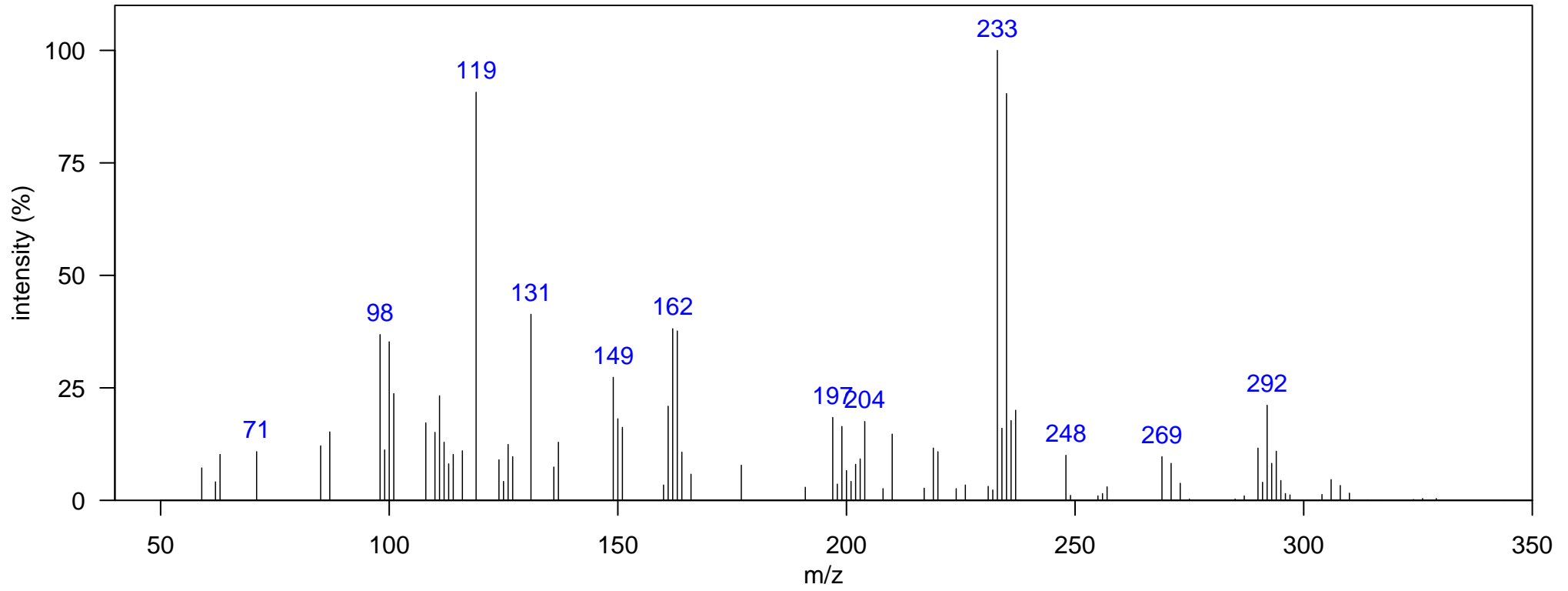
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

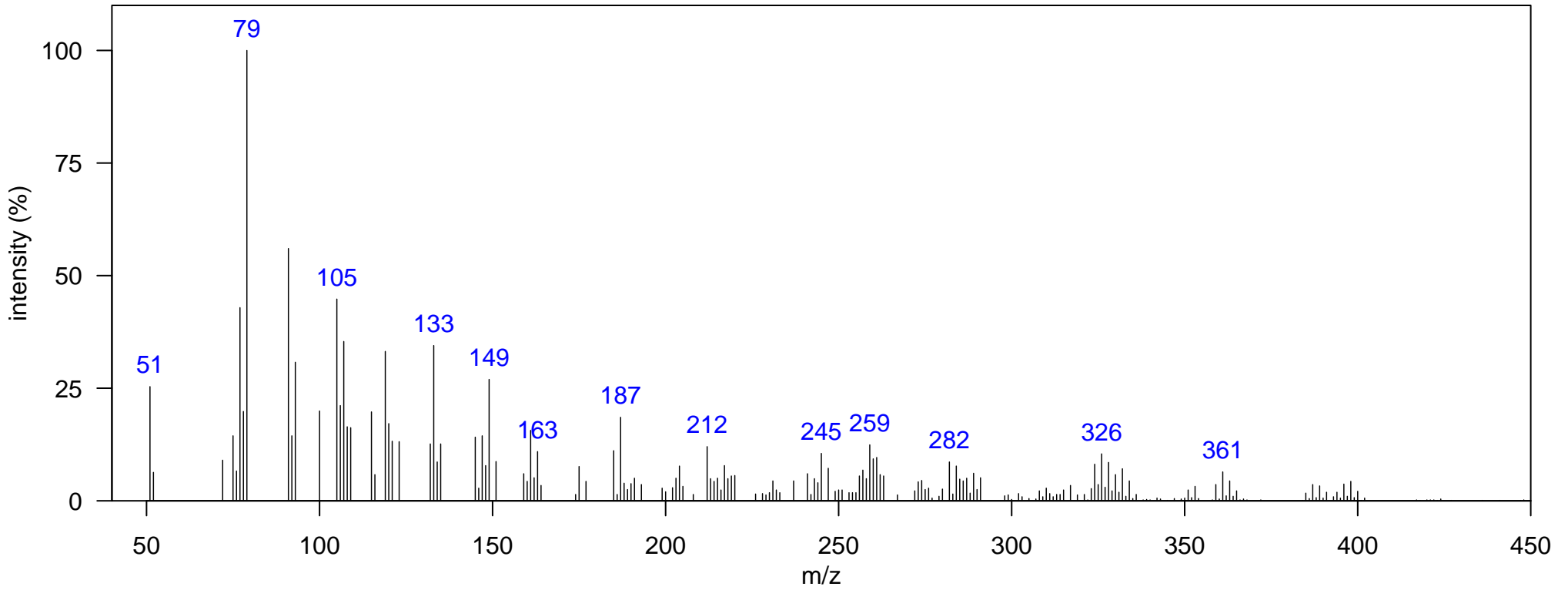
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

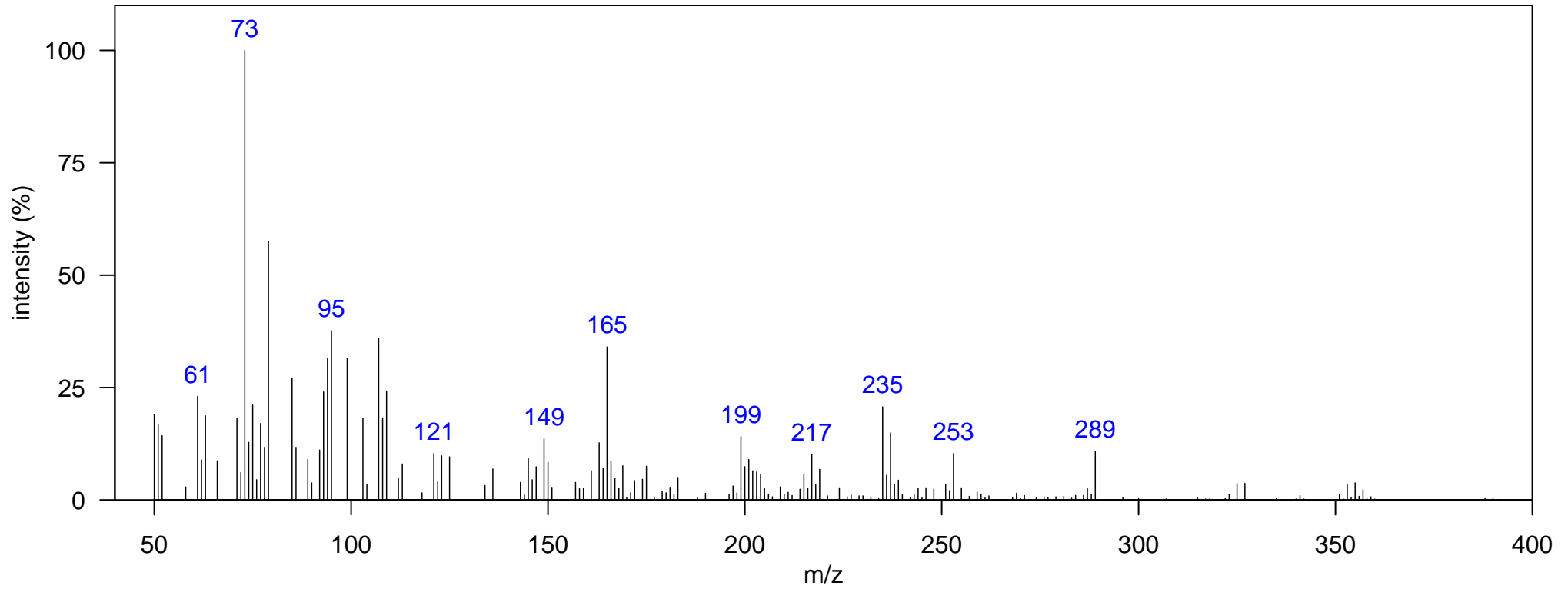
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

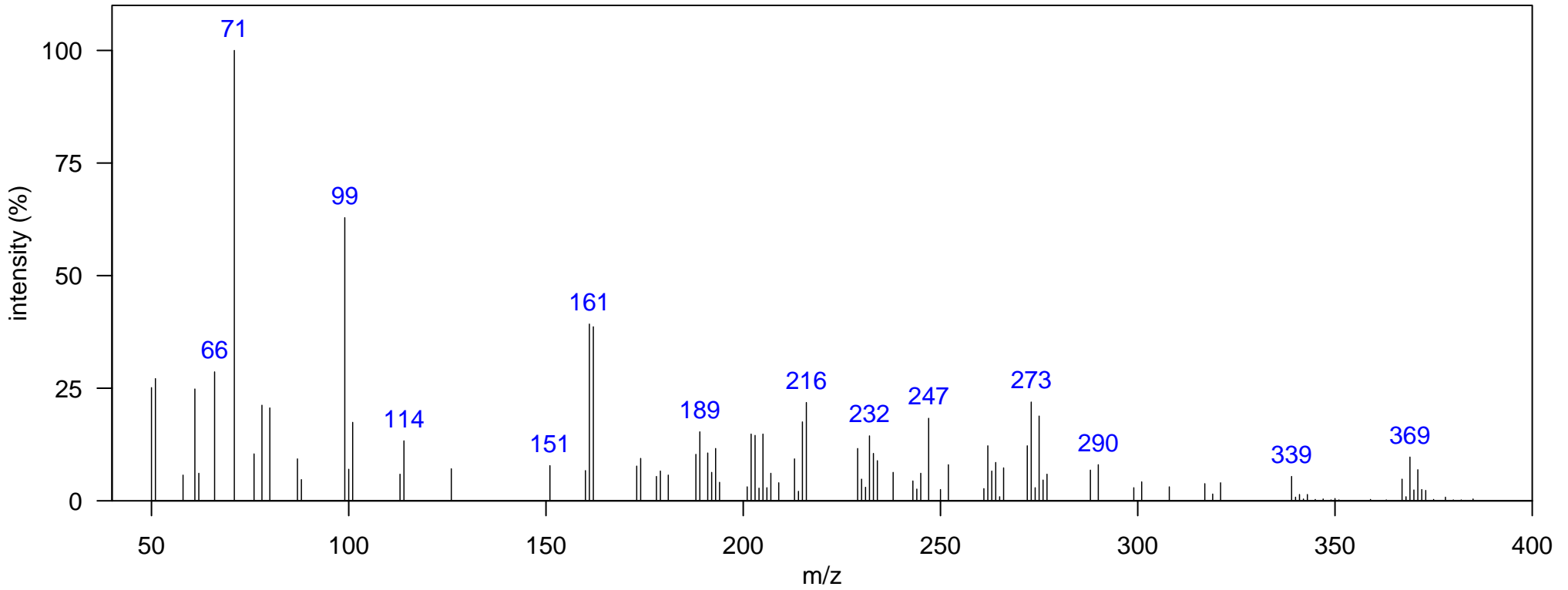
Comment: Interference with some compounds – ion 355 belongs to unknown-16



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

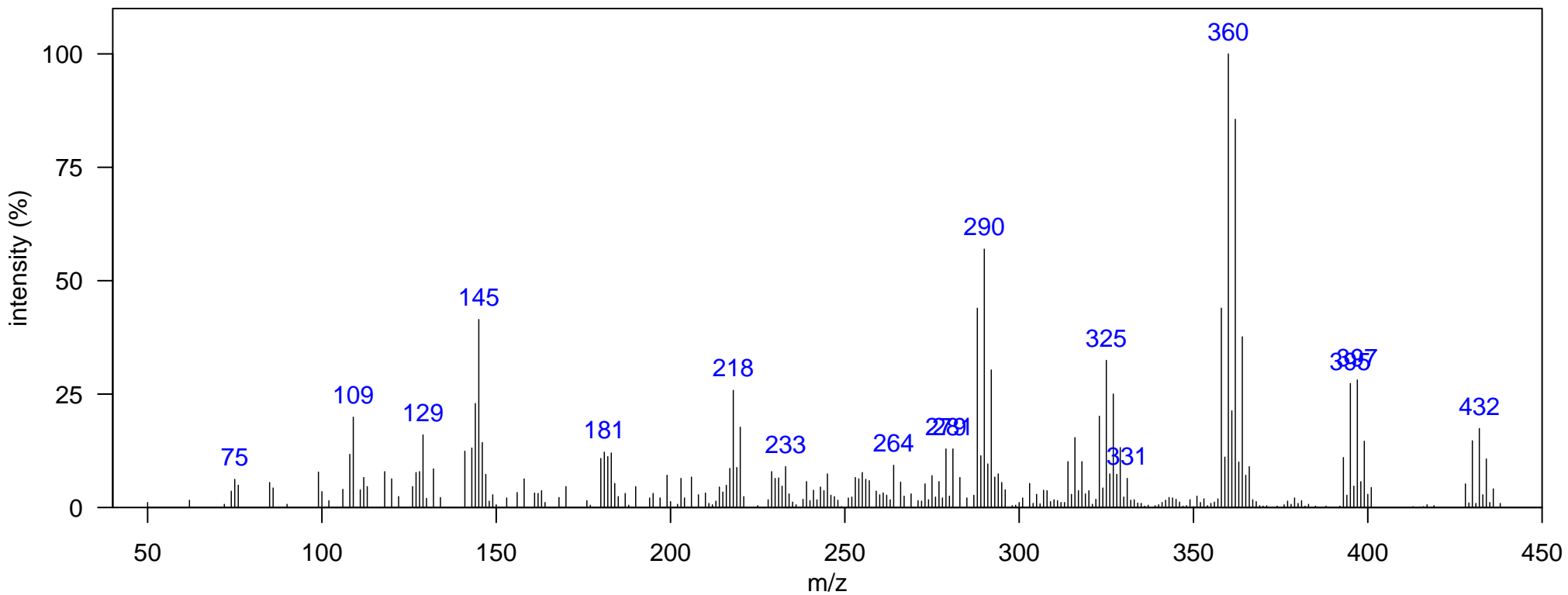
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

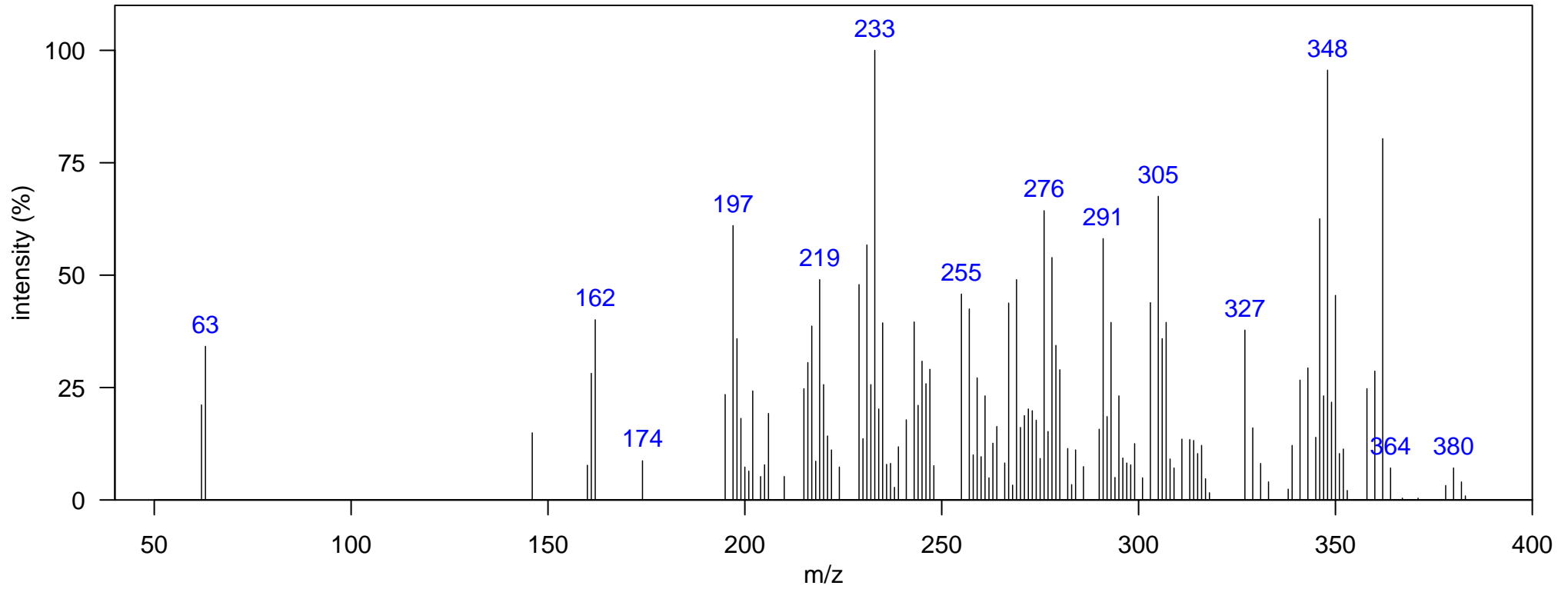
Comment: PCB interference



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

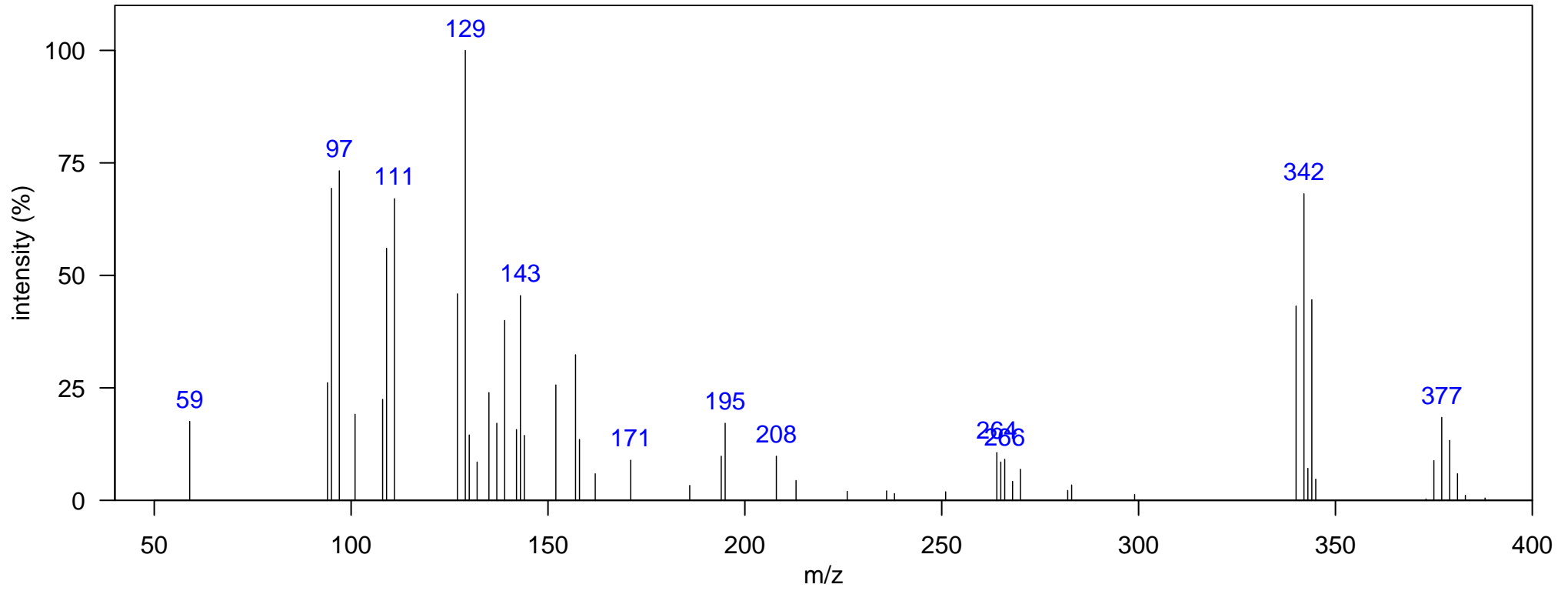
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

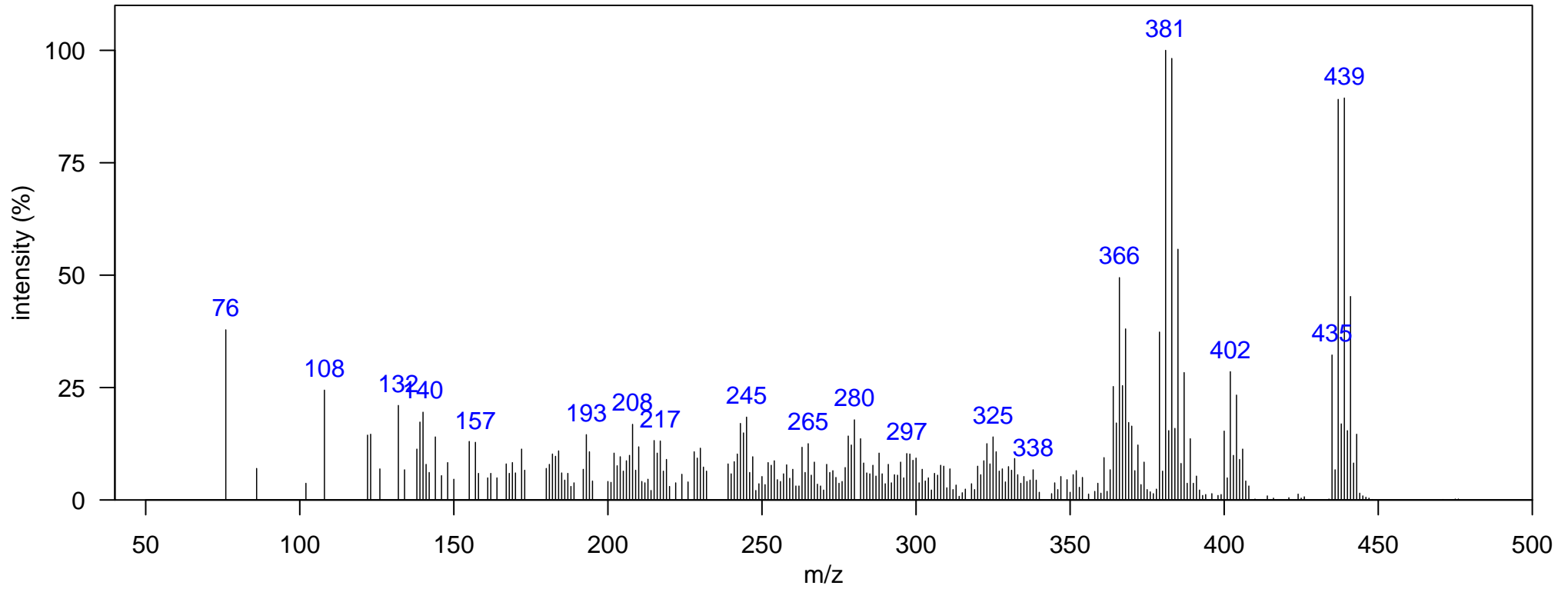
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

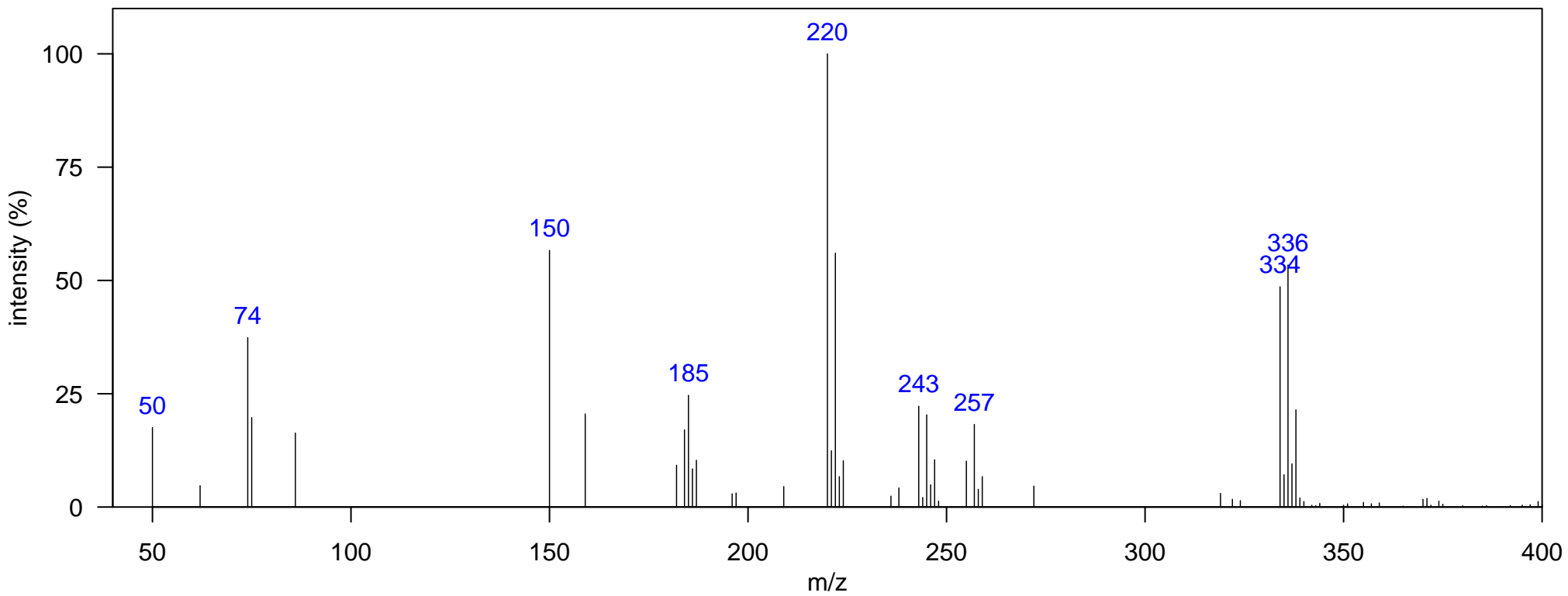
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

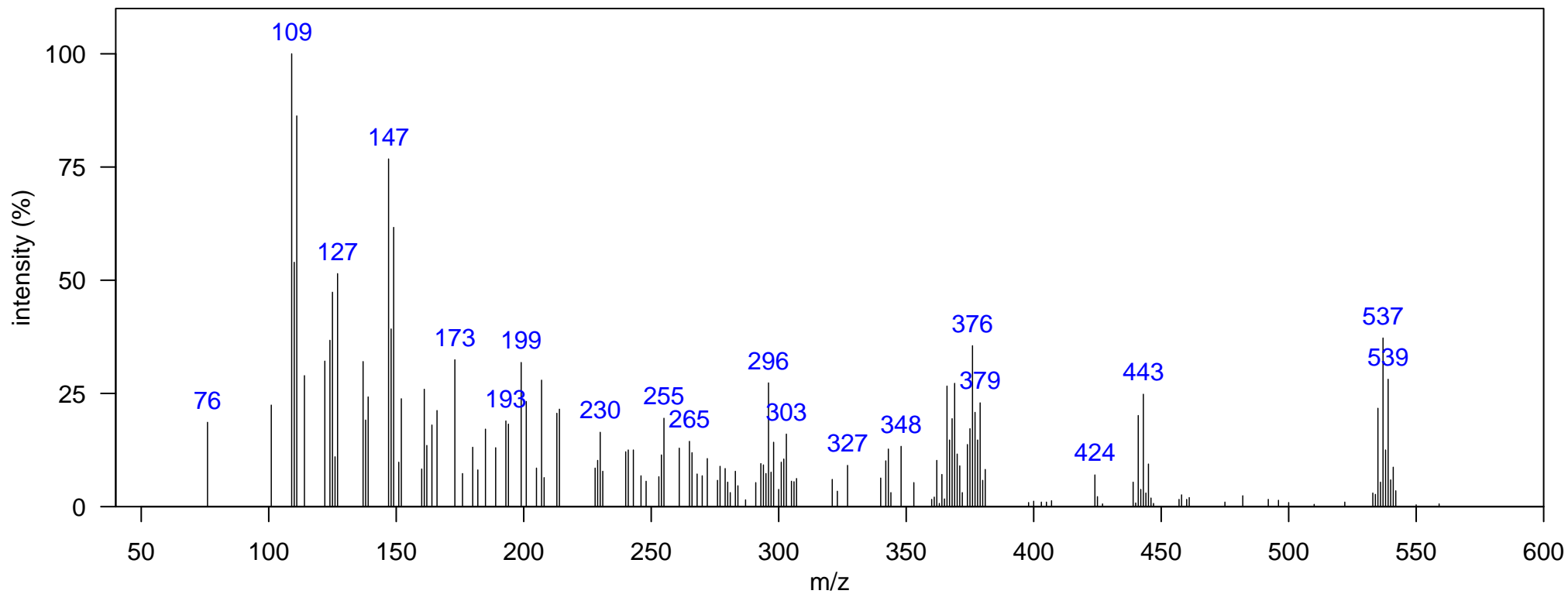
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

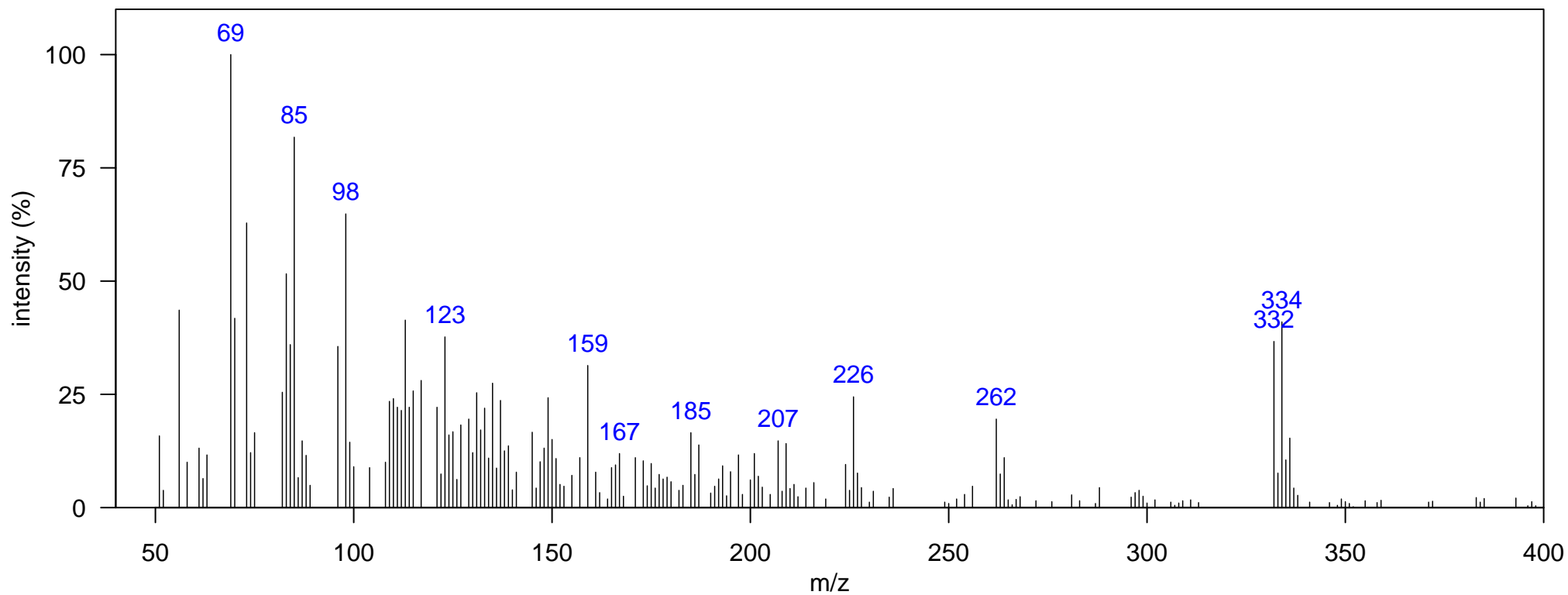
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

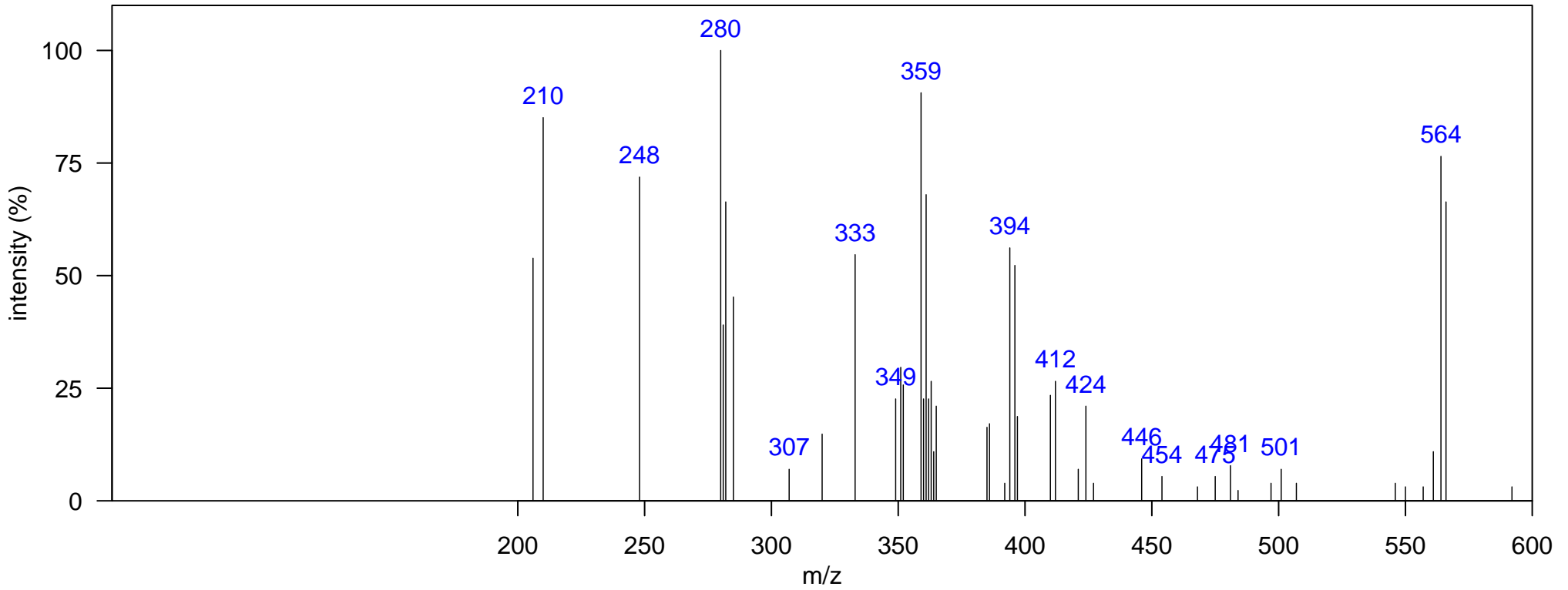
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

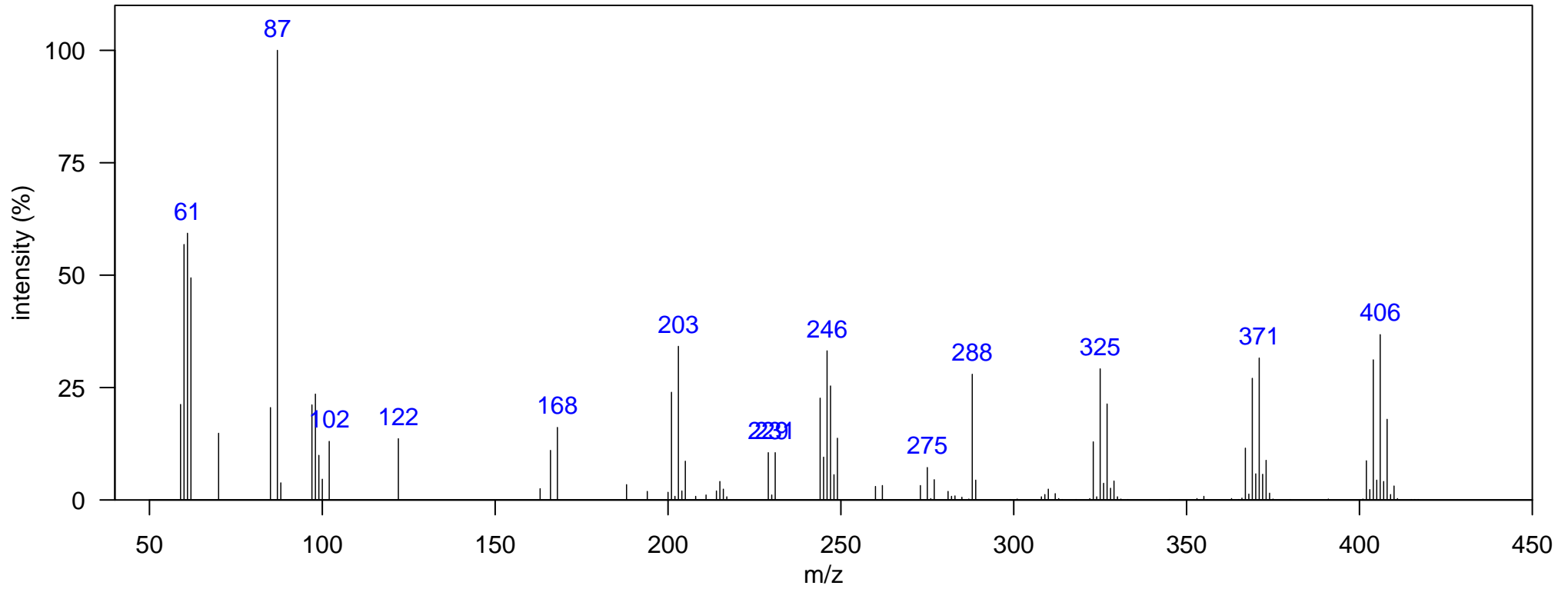
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

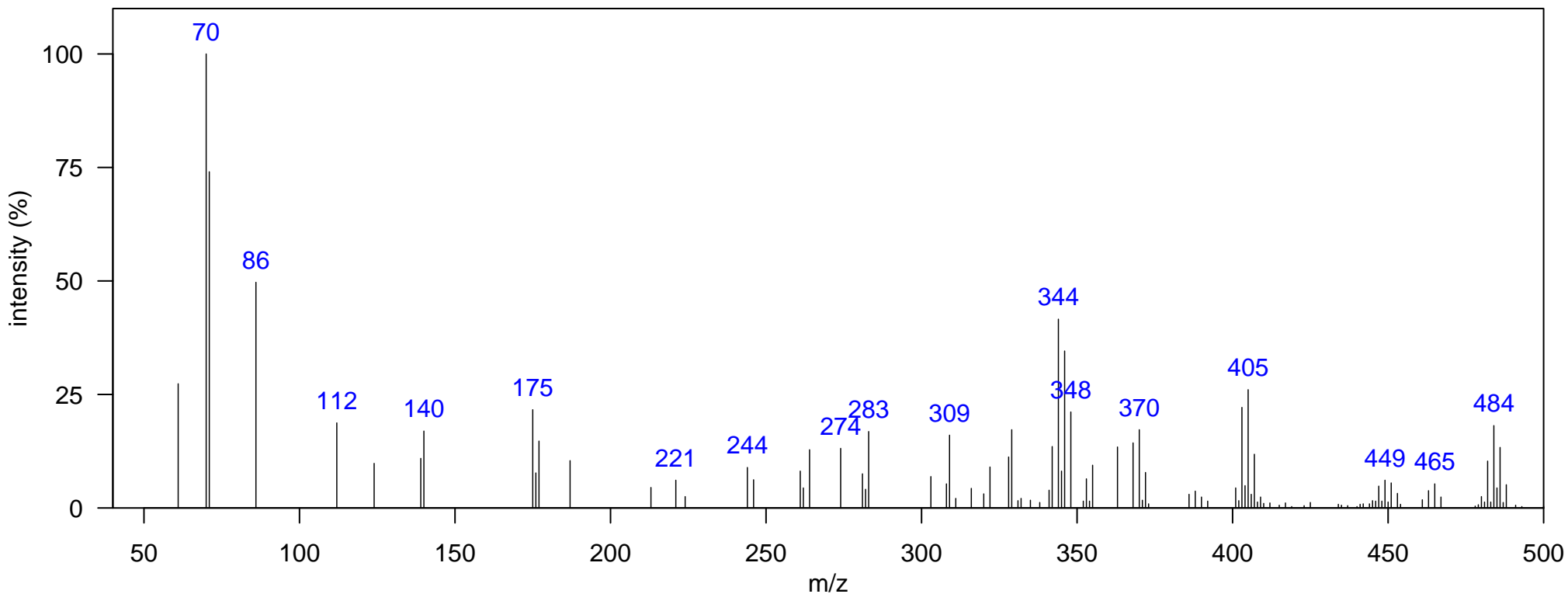
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

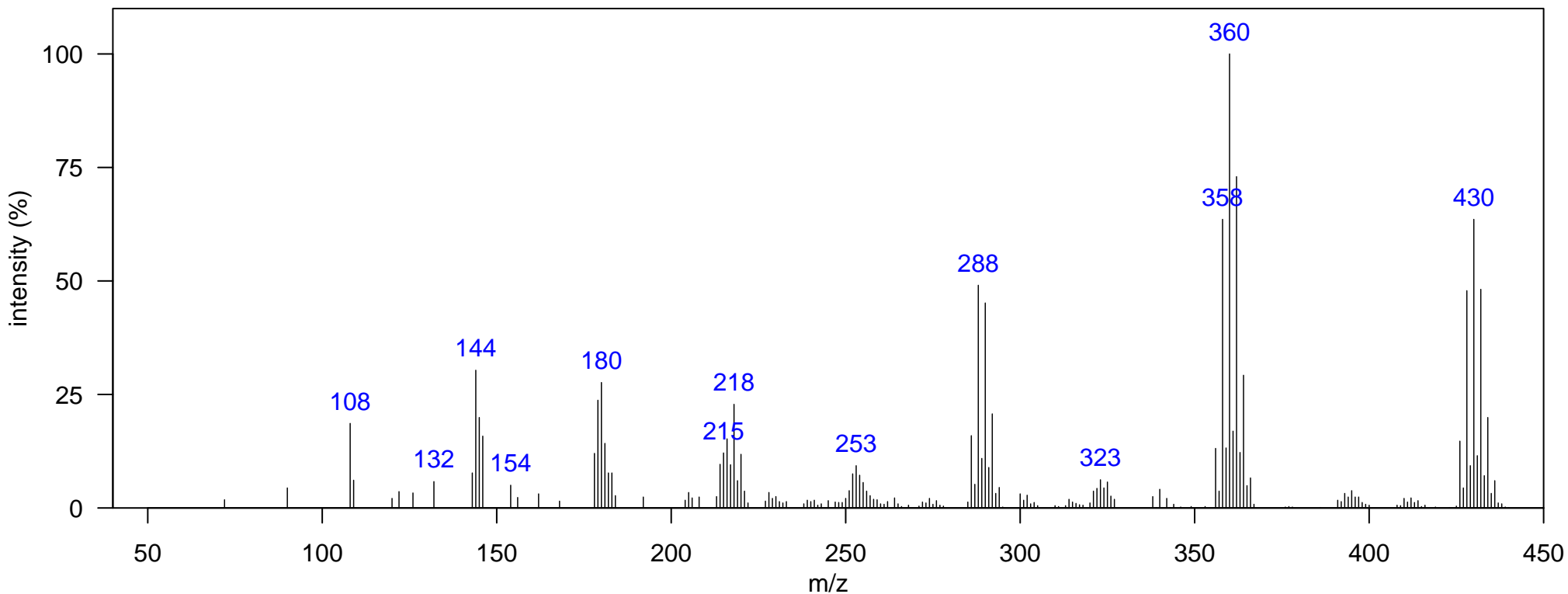
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

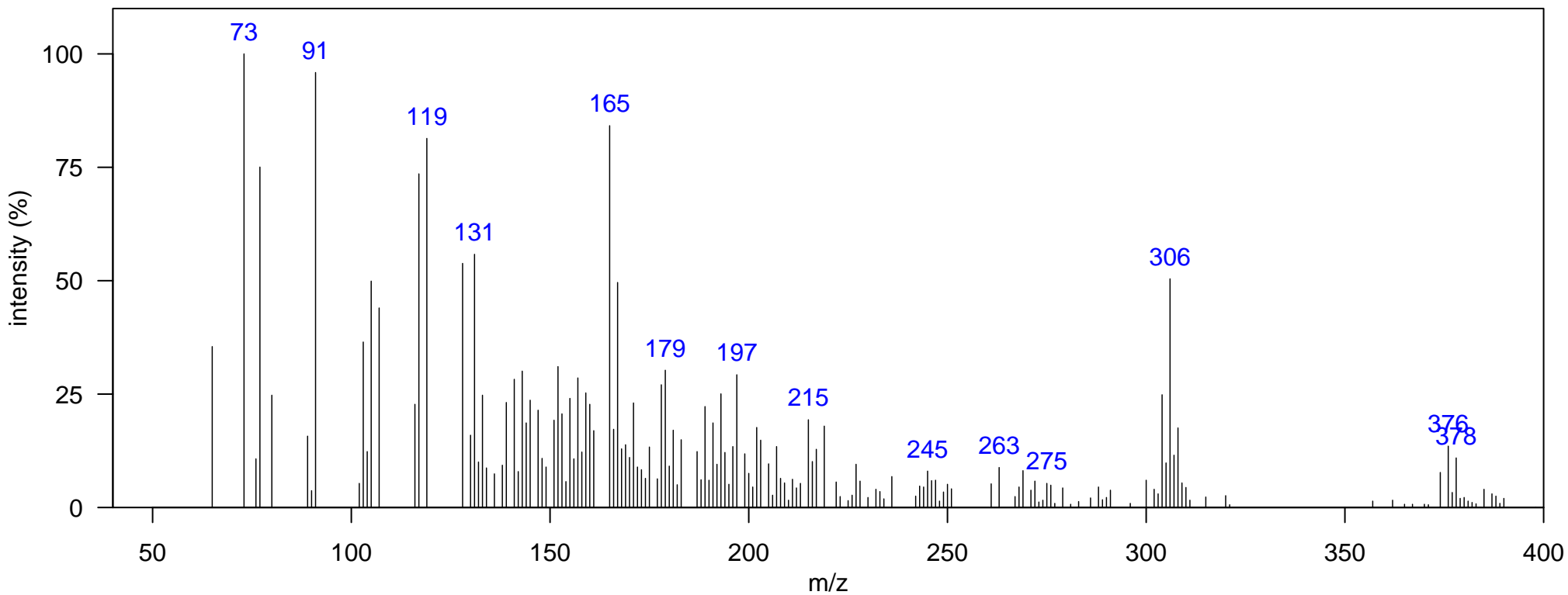
Comment: PCB interference – ions 412 and 340 belong to unknown-4-2



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

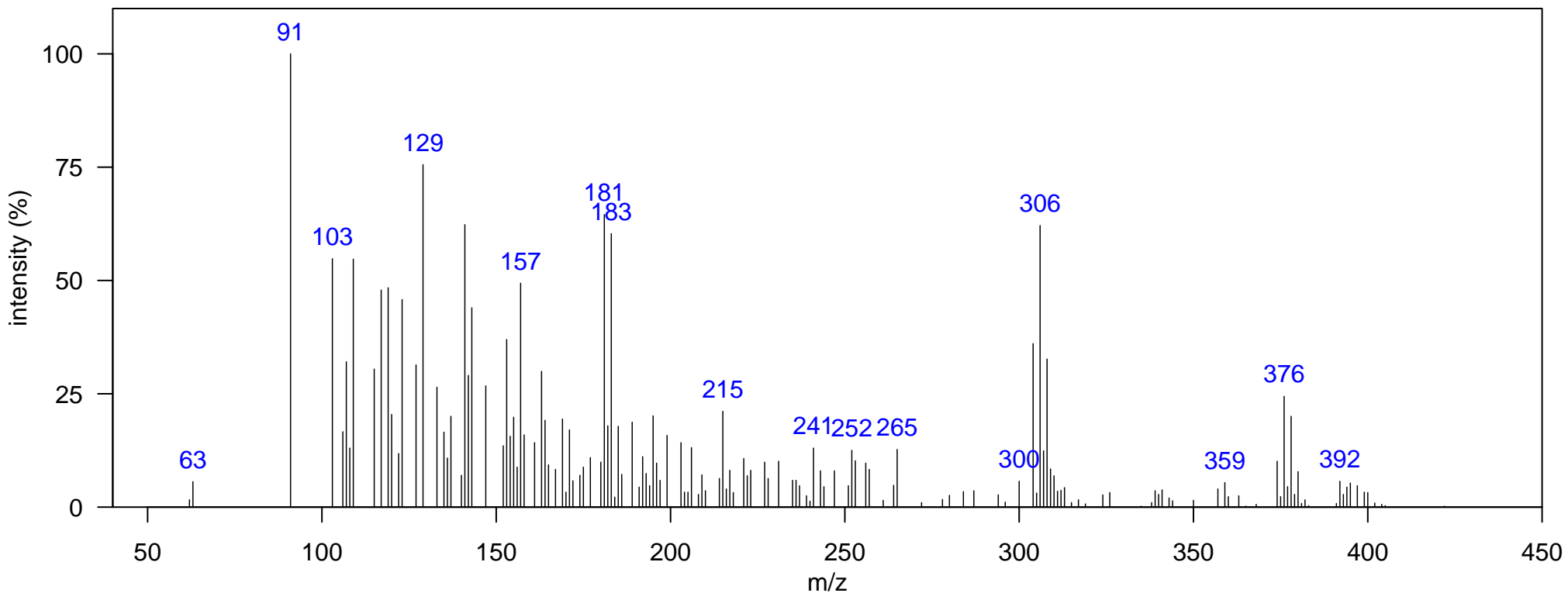
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

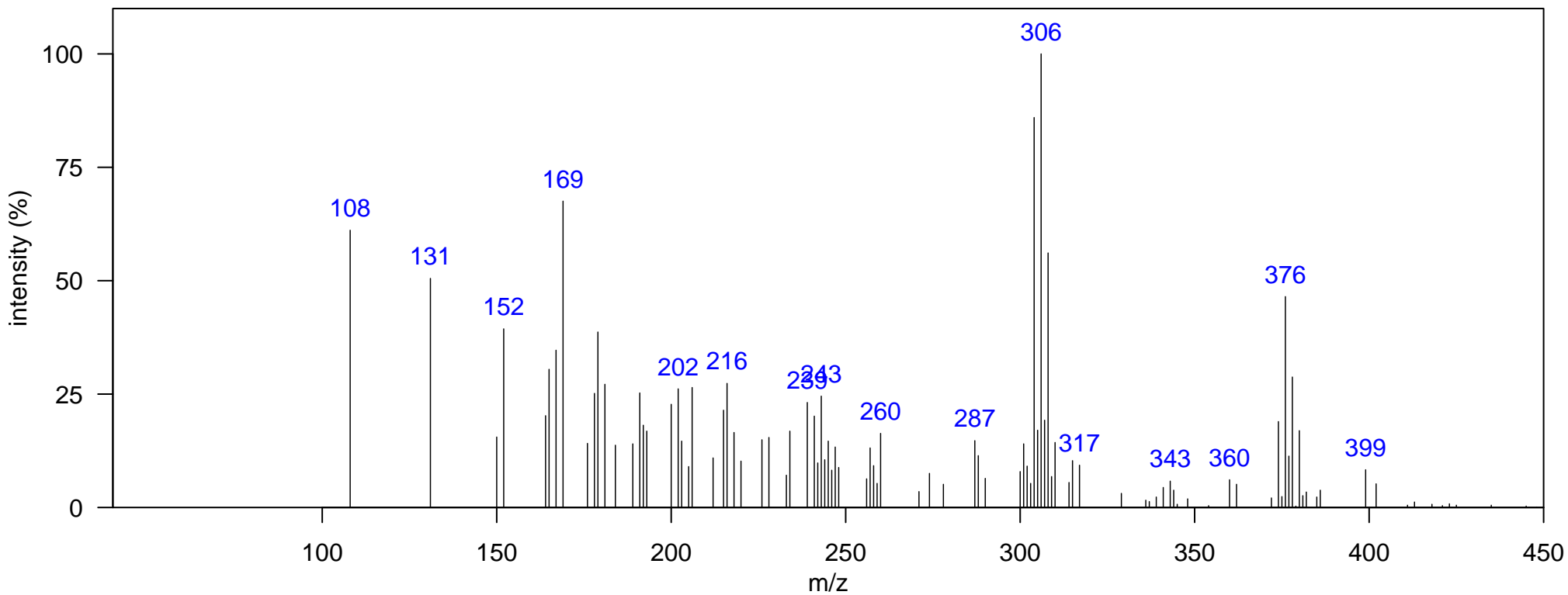
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

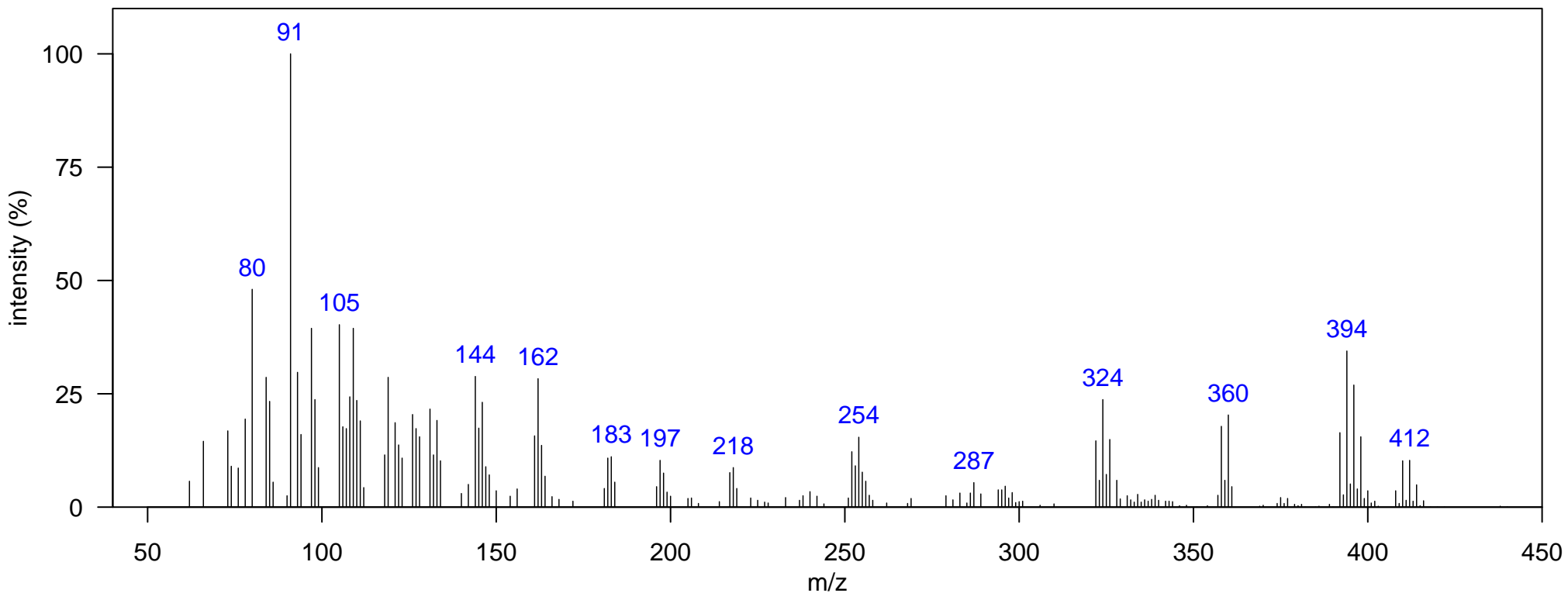
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

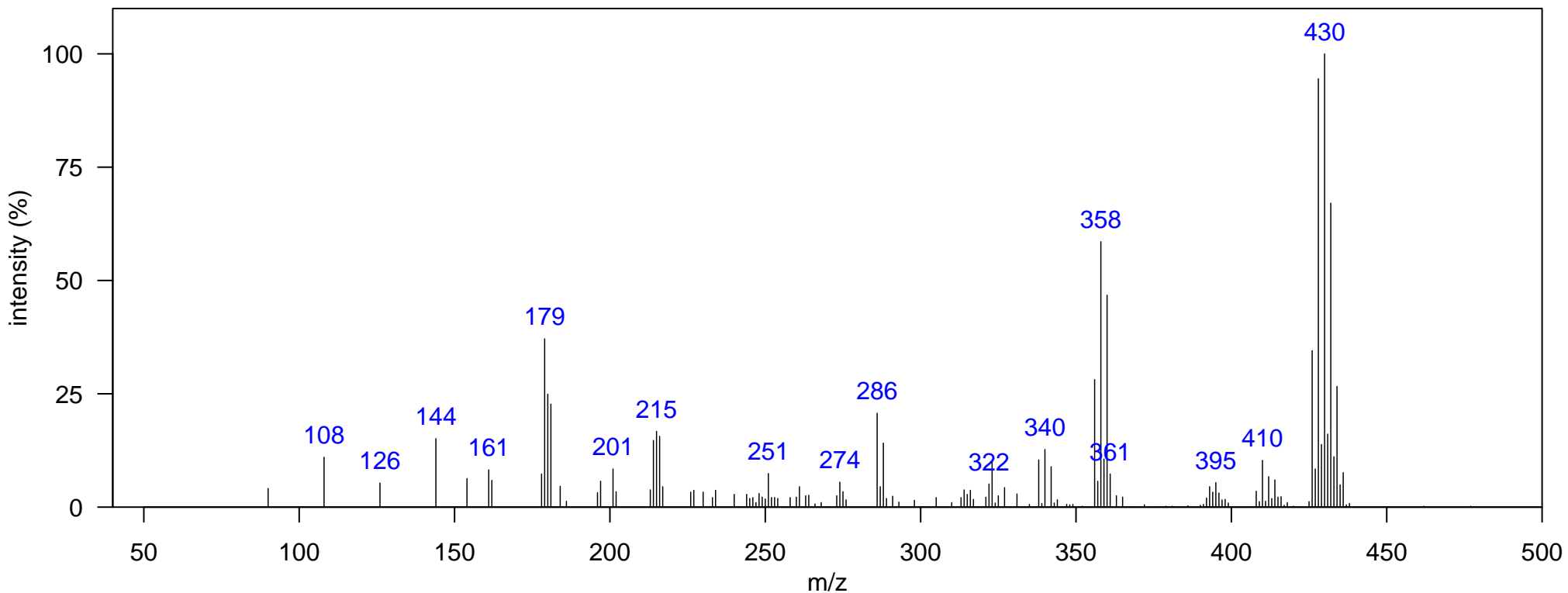
Comment: PCB interference



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

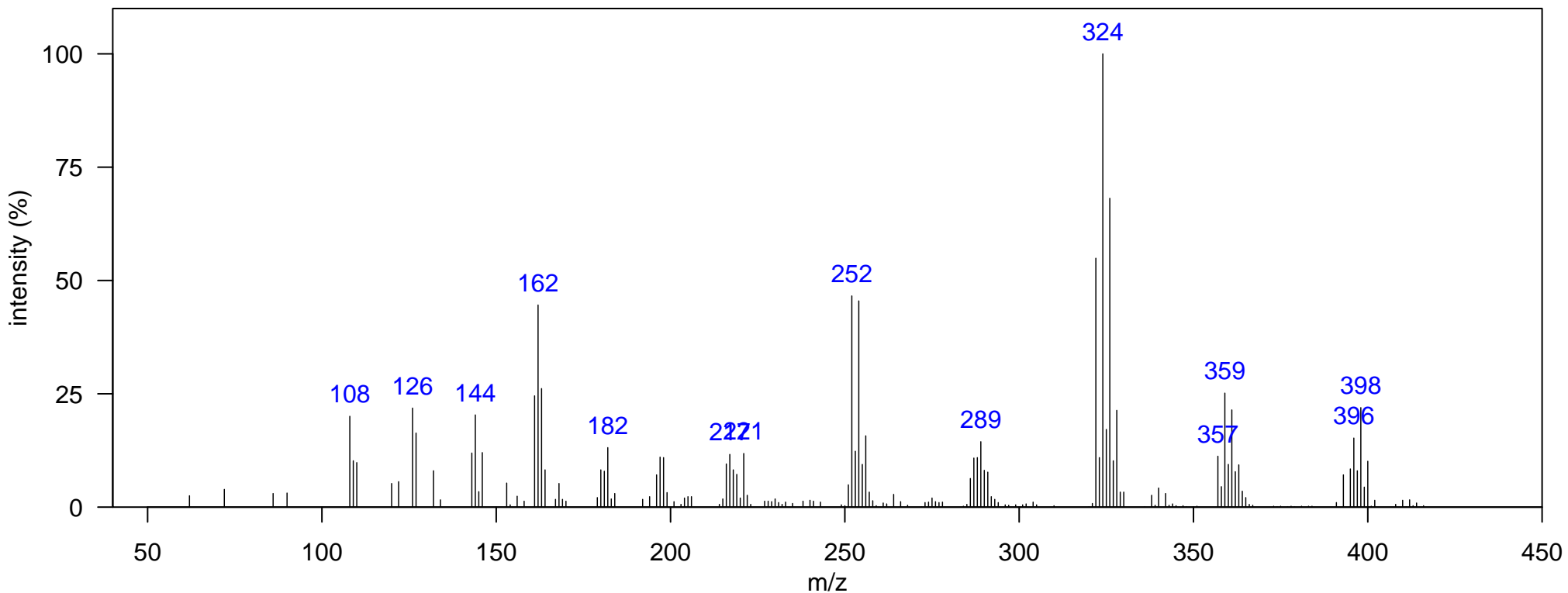
Comment: PCB interference – ions 410 and 340 belong to unknown-4-10



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

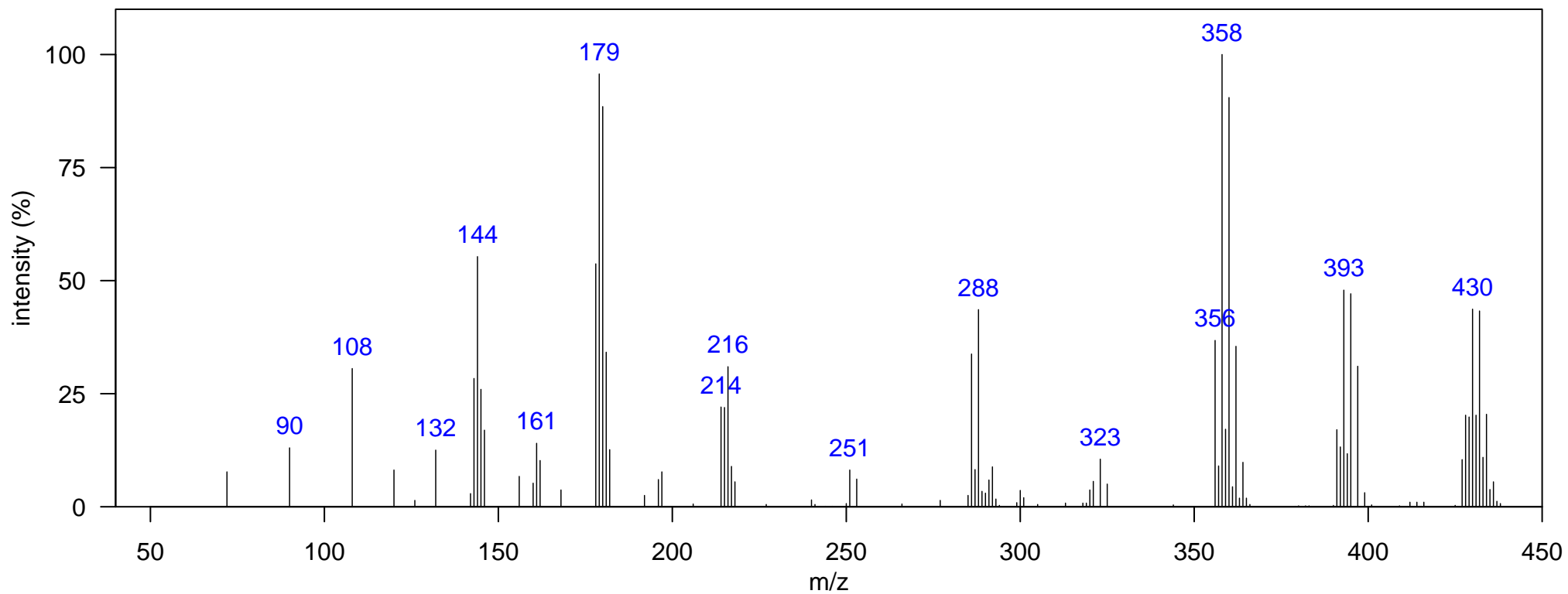
Comment: PCB interference – ions 412 and 340 belong to unknown-4-11



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

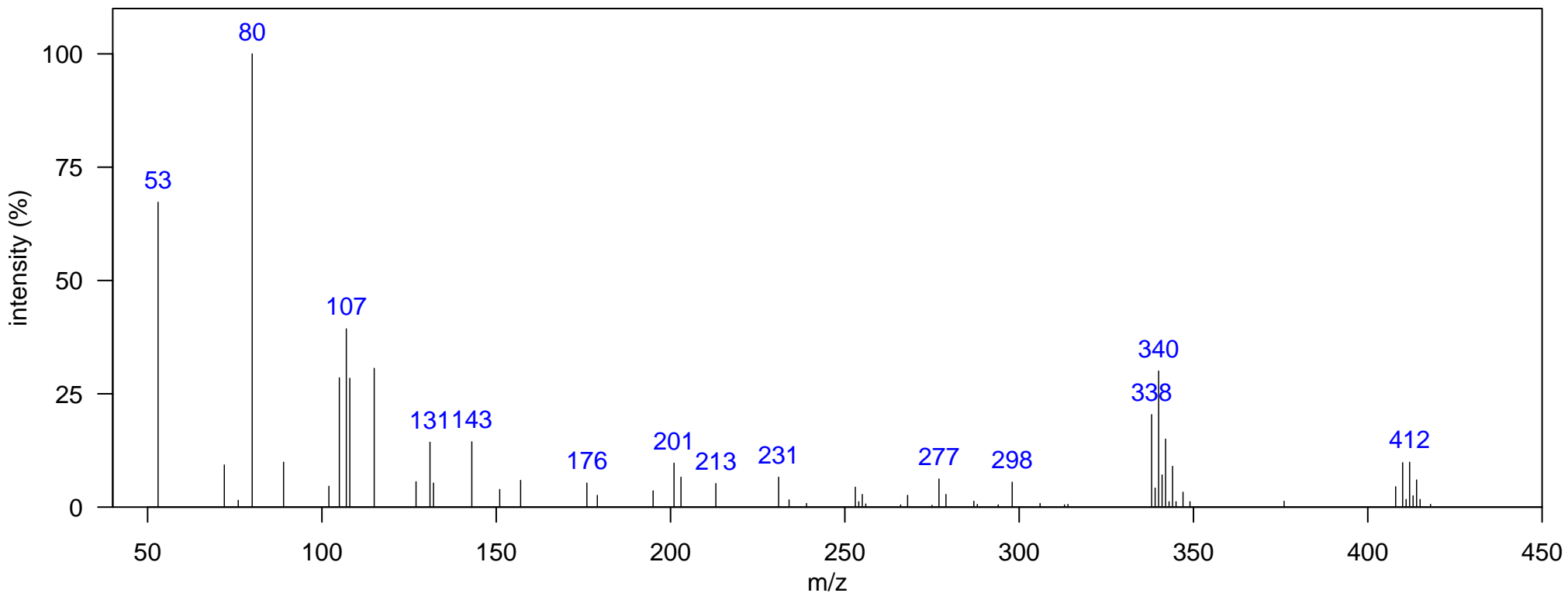
Comment: Interference from other compounds, ion 412 belongs to unknown-4-12



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

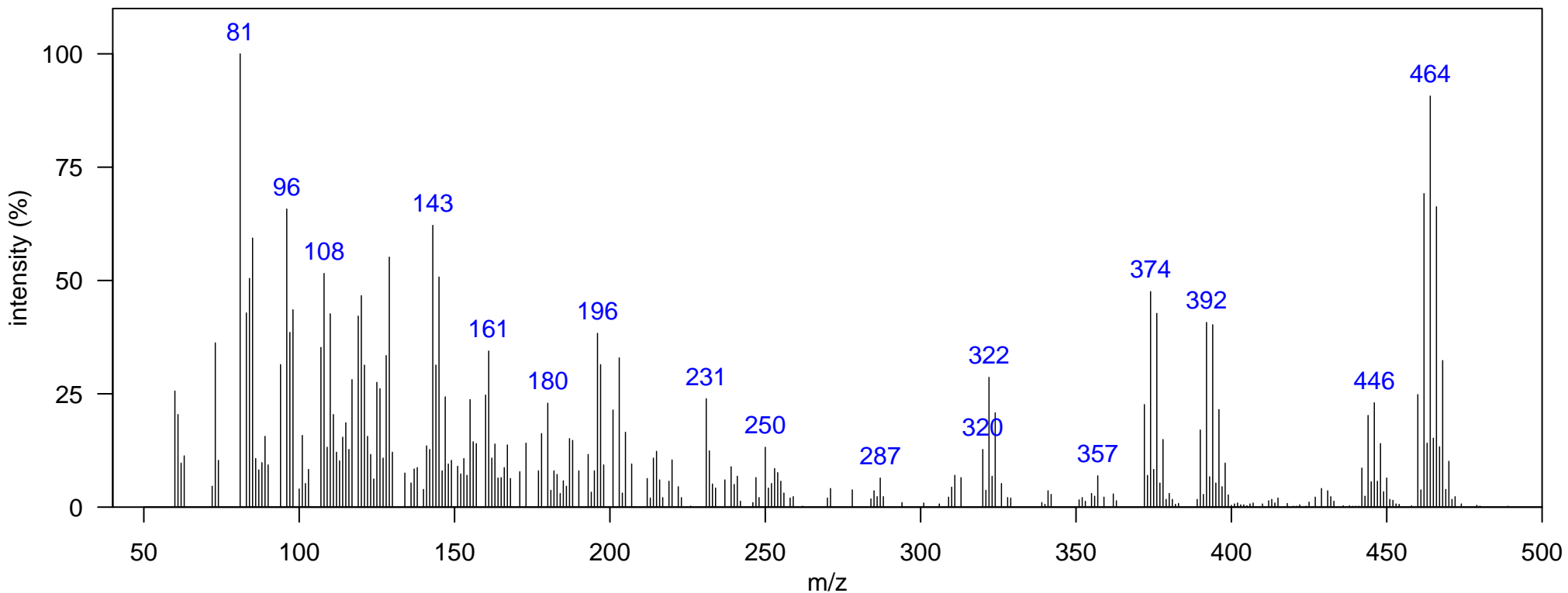
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

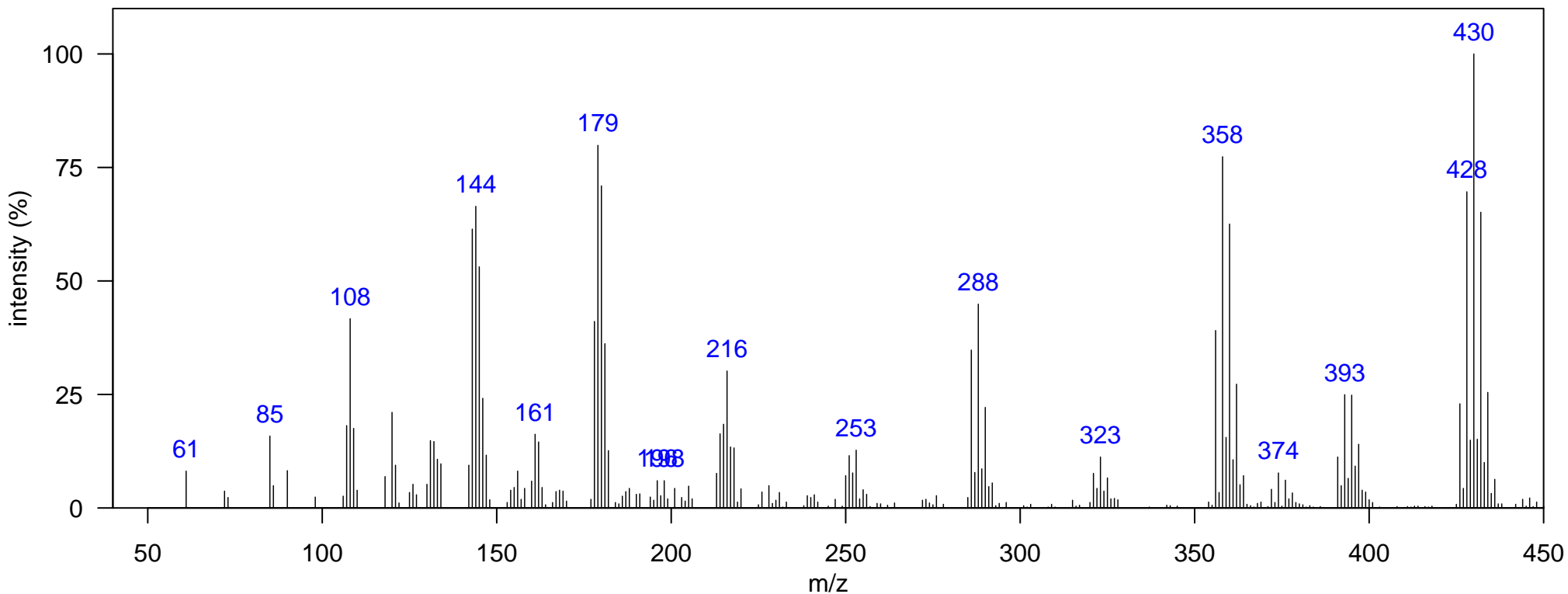
Comment: PCB interference – ions 446 and 374 belong to unknown-4-14



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

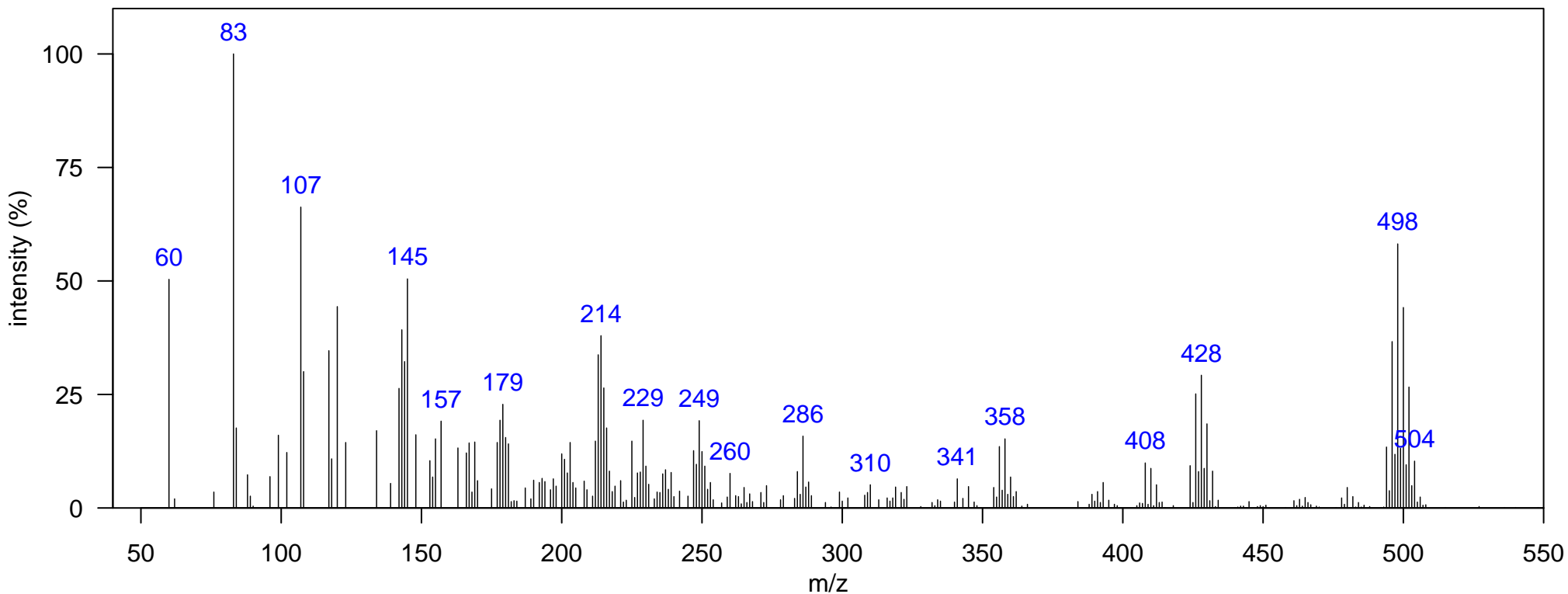
Comment: PCB interference – ions 446 and 374 belong to unknown-4-16



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

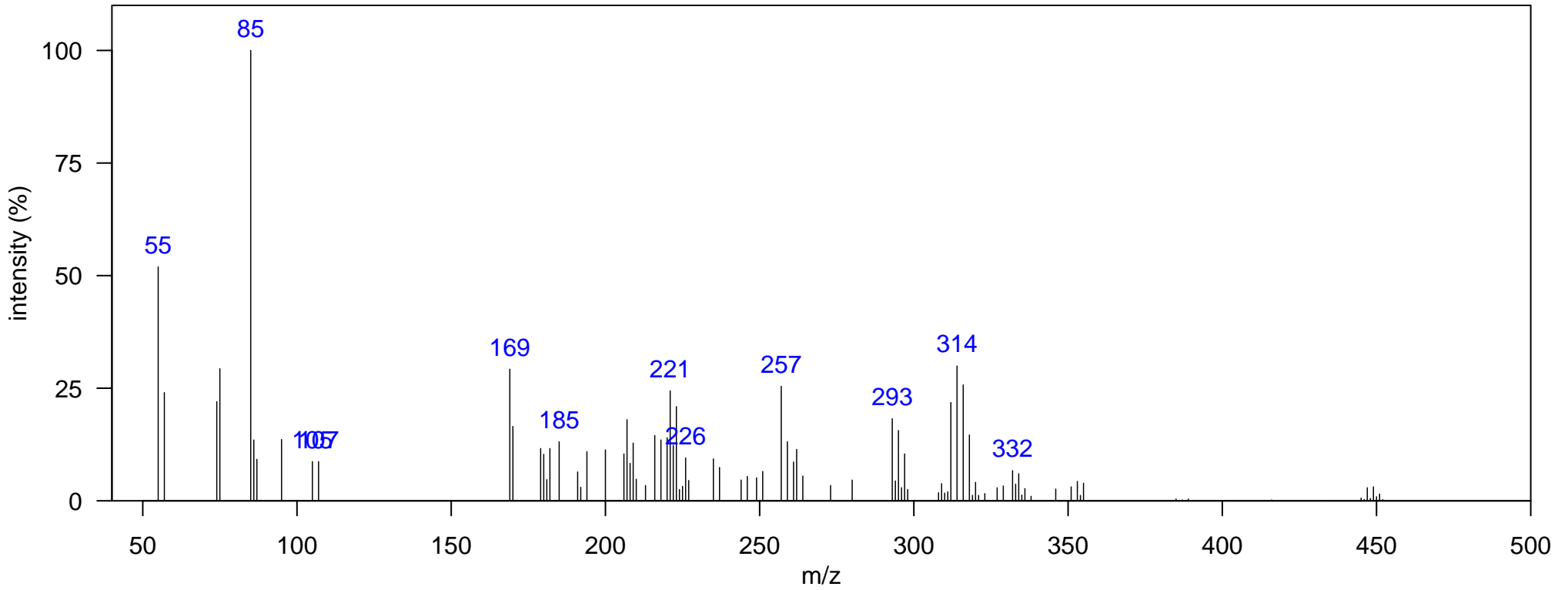
Comment: PCB interference – ions 408 and 480 belong to unknown-4-17



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

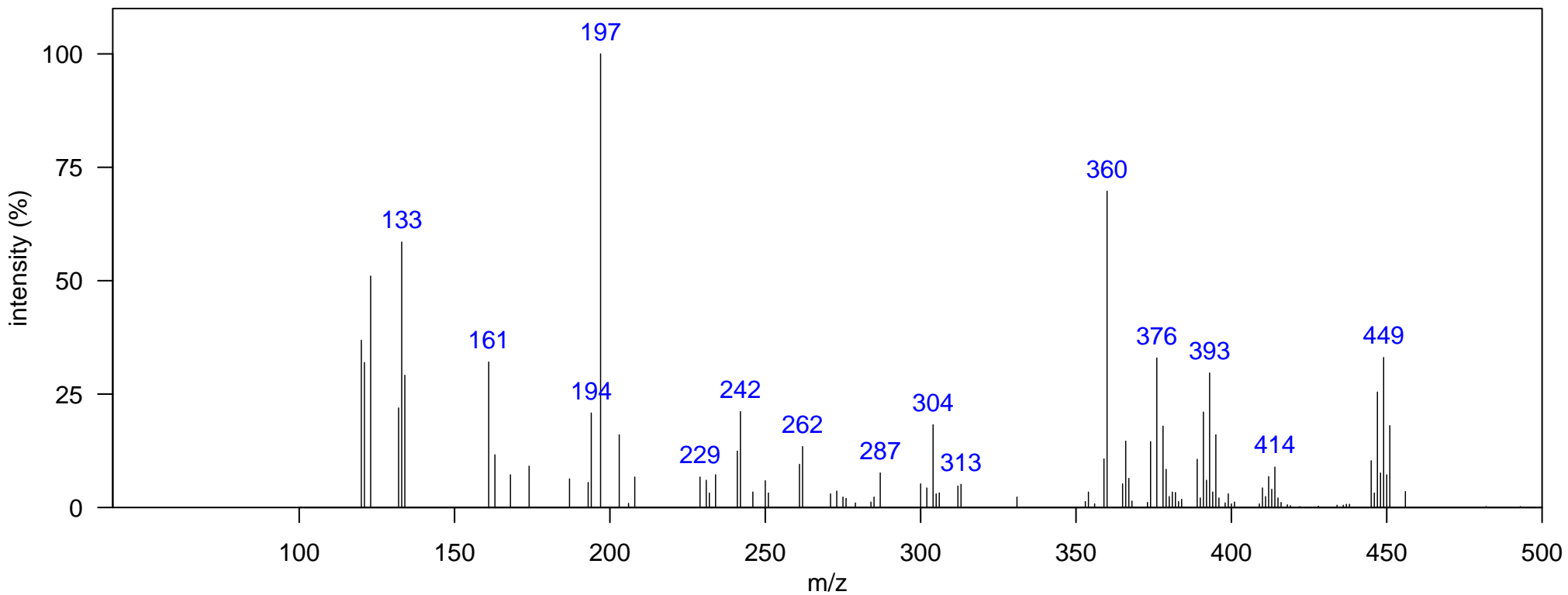
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

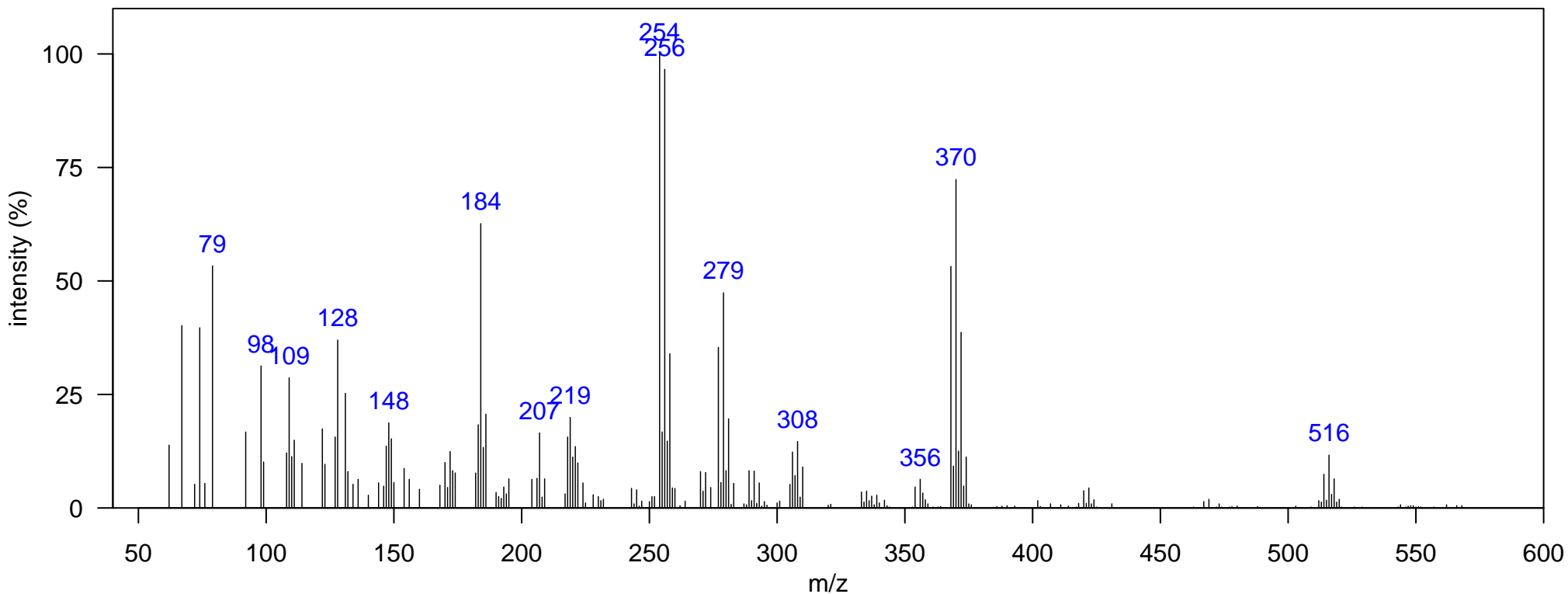
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

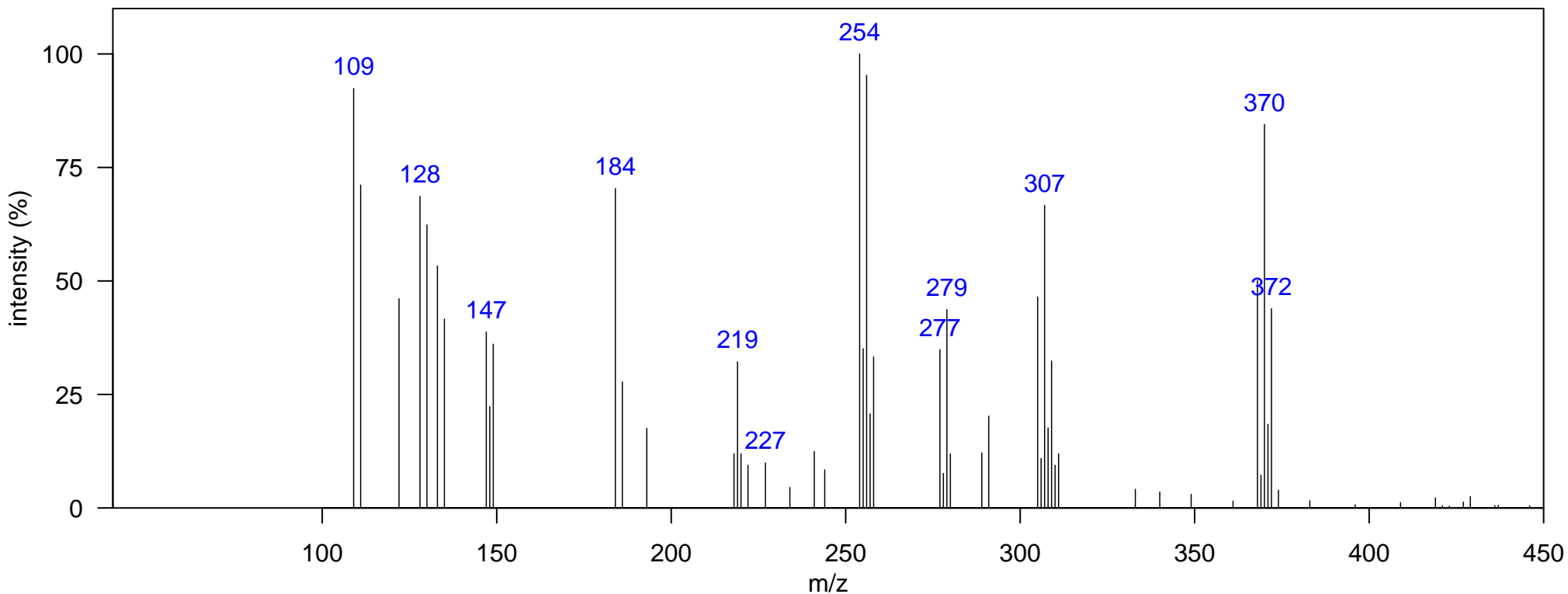
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

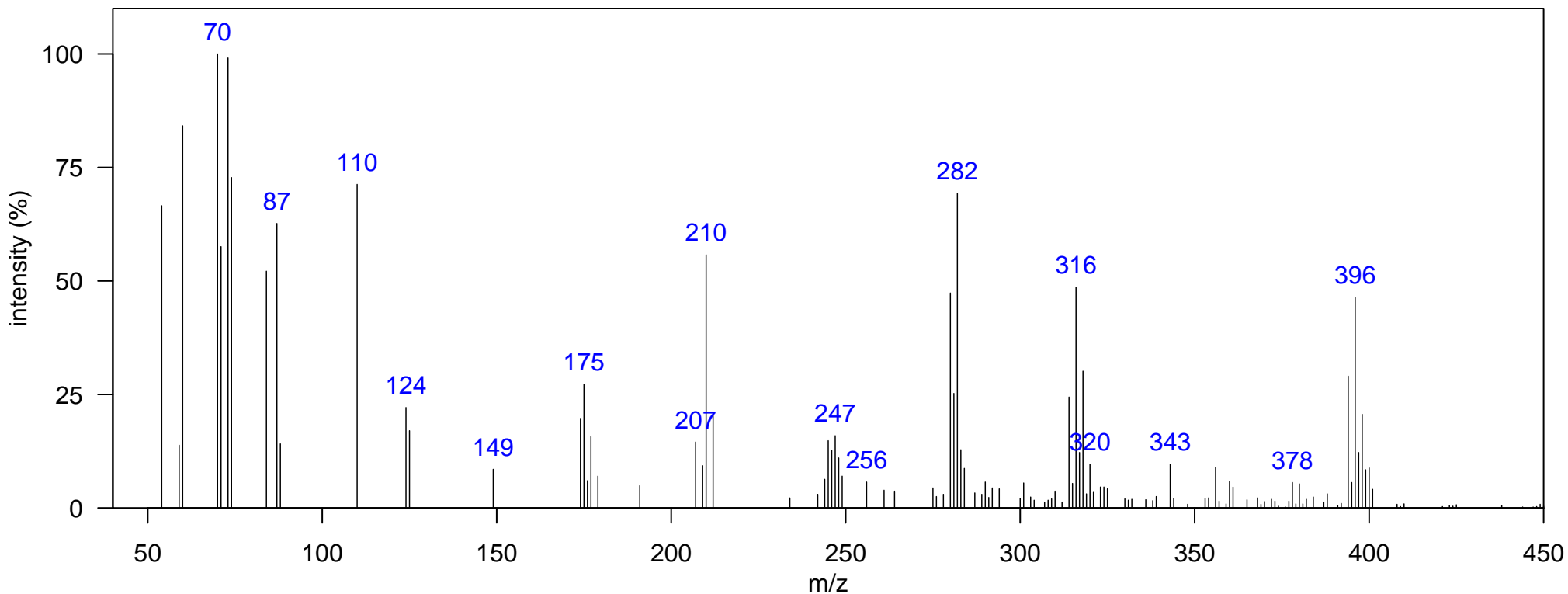
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

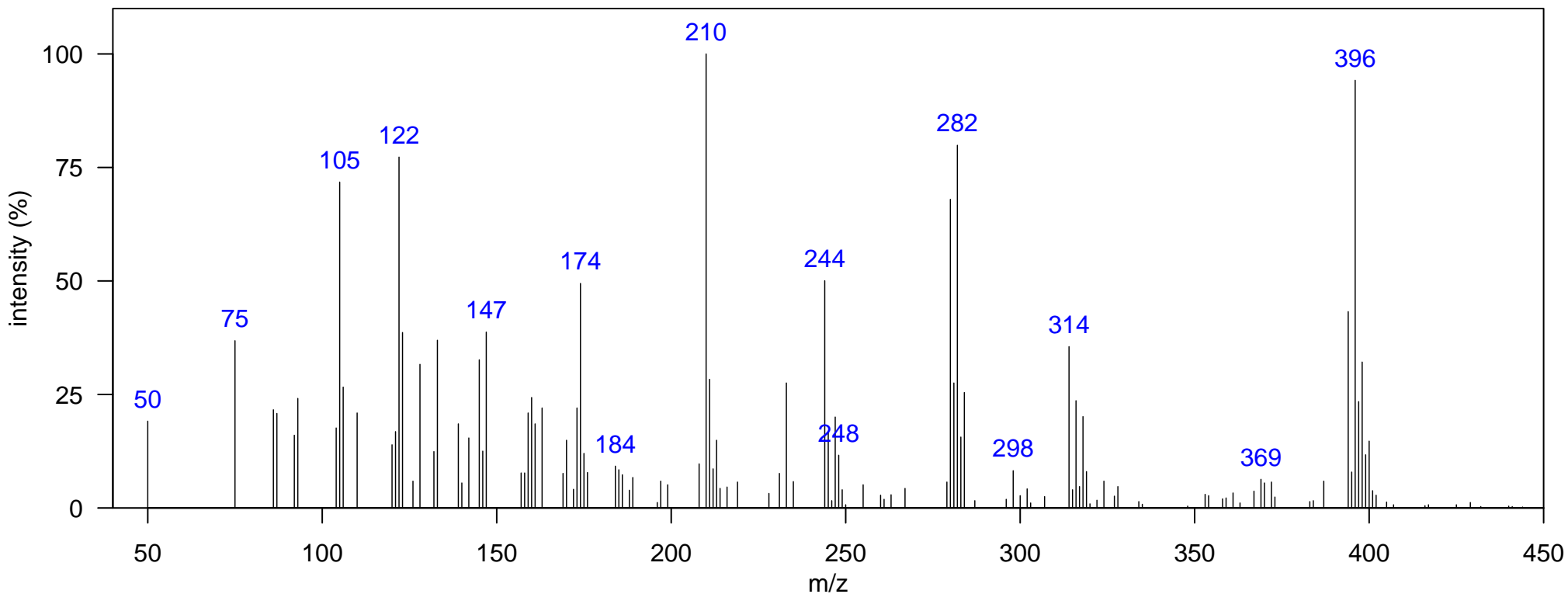
Comment:



Matrix: Marine Mammal Blubber
In Bottlenose Dolphin: TRUE

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

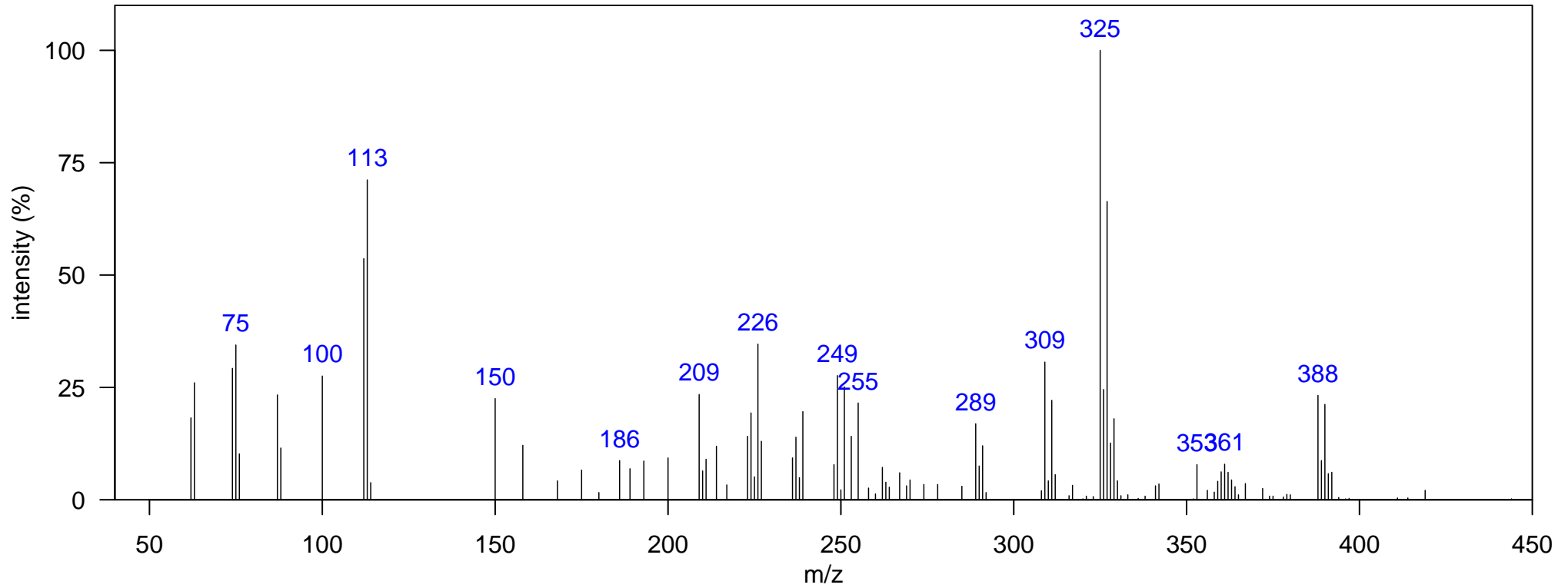
Comment:



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:

