SpecLibMarineUnknown2018 Mass Spectral Library

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

Manuscript: Non-targeted analyses of multiple marine mammal species to enable proactive organic contaminant screening and selection of best 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

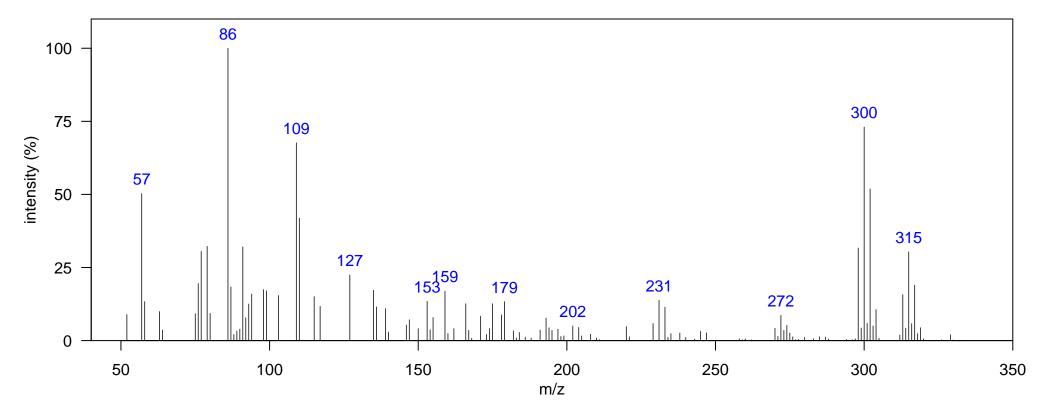
Prepared: 2018–03–21 14:24:03 SpecLibMarineUnknown2018 OrgMassSpecR version 0.5–3

R version 3.4.1 (2017–06–30)

Name: MMCP unknown 1 Class: MMCP unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

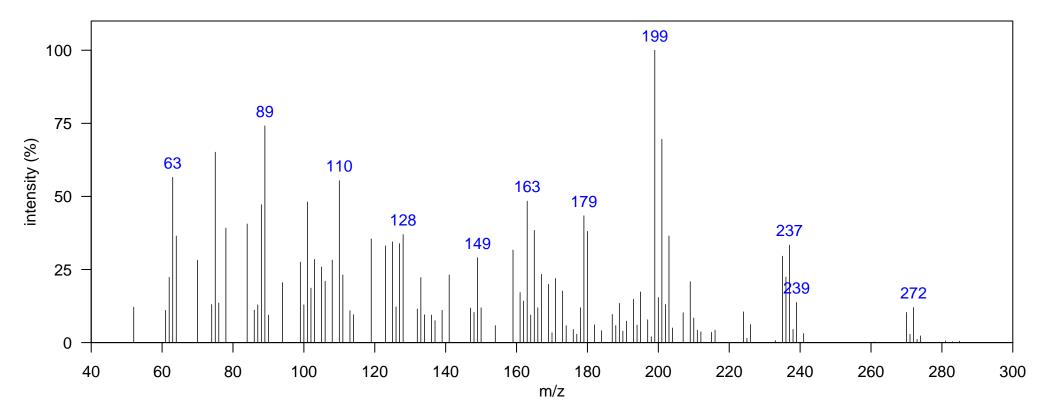
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1089.72, 0.931



Name: MMCP unknown 2 Class: MMCP unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

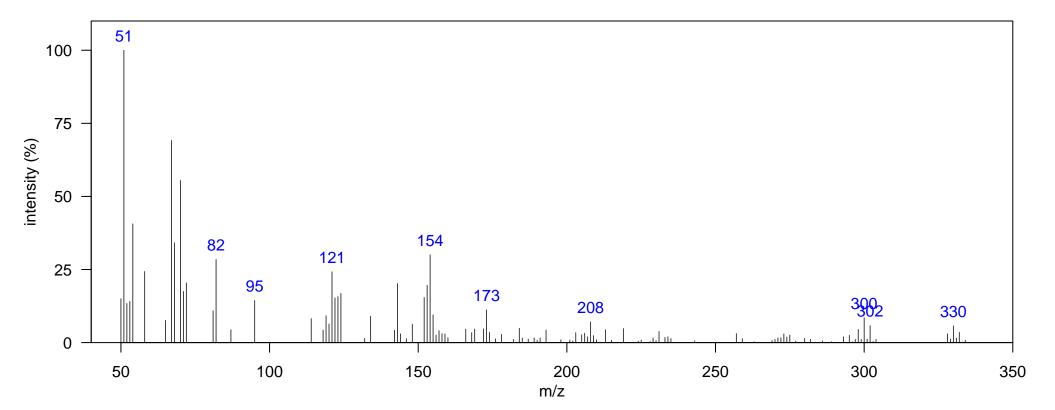
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1128.2, 0.898



Name: MMCP unknown 3 Class: MMCP unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

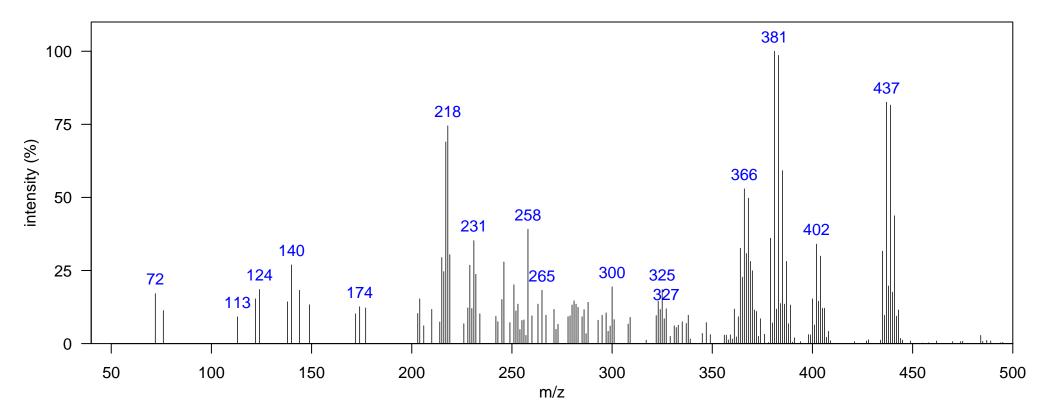
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1215.65, 1.016



Name: MMCP unknown 4 Class: MMCP unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

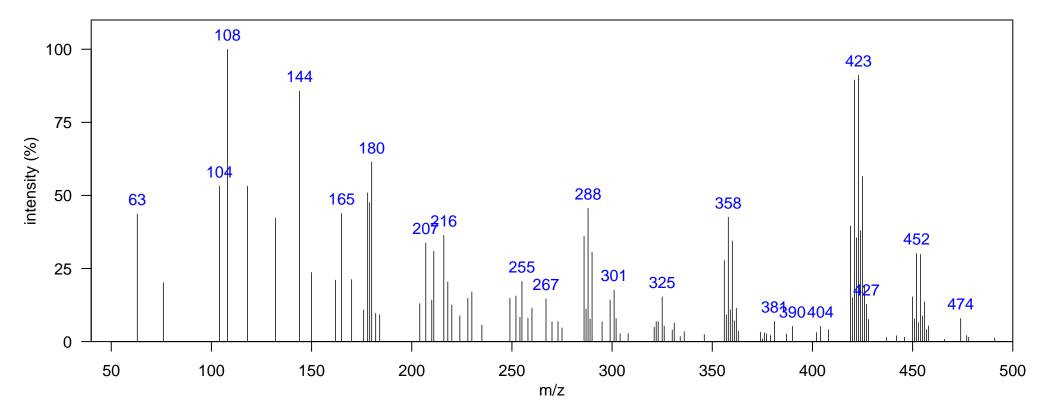
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1530.47, 1.168



Name: MMCP unknown 5 Class: MMCP unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

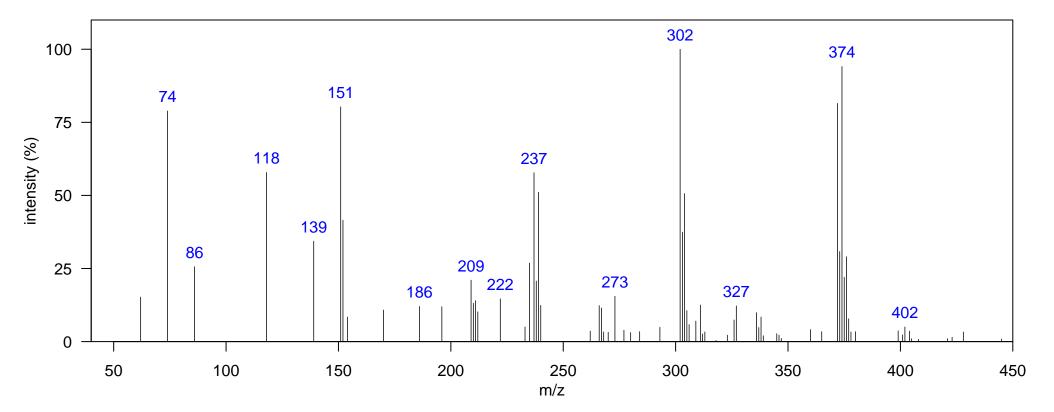
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1684.38, 1.459



Name: MMCP unknown 6 Class: MMCP unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

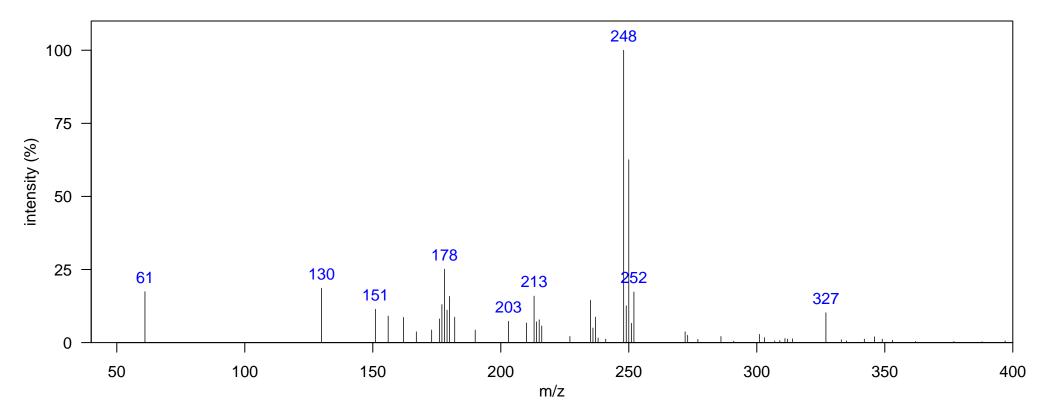
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1701.87, 1.525



Name: MMCP unknown 7 Class: MMCP unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

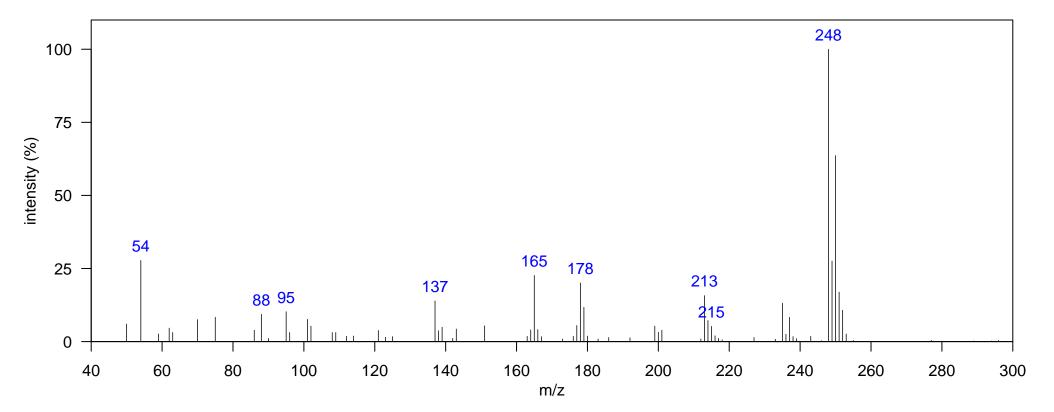
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 2023.69, 1.927



Name: MMCP unknown 8 Class: MMCP unknown

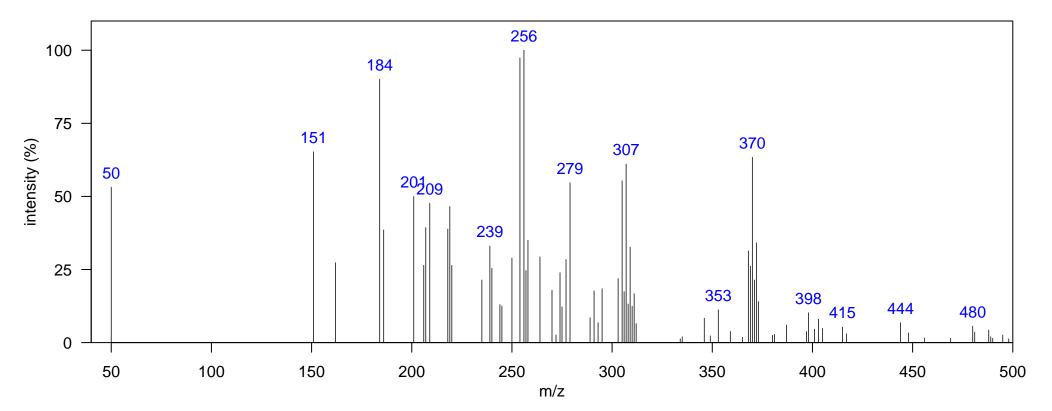
Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

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



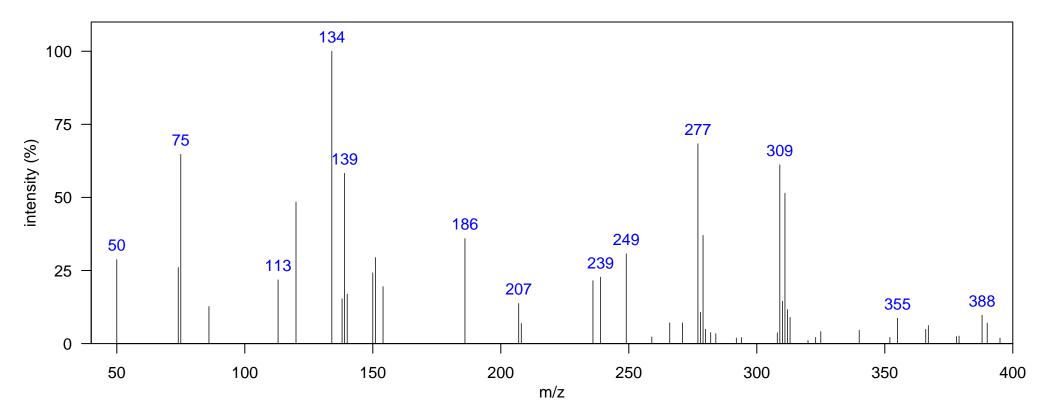
Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

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



Matrix: Marine Mammal Blubber In Bottlenose Dolphin: FALSE

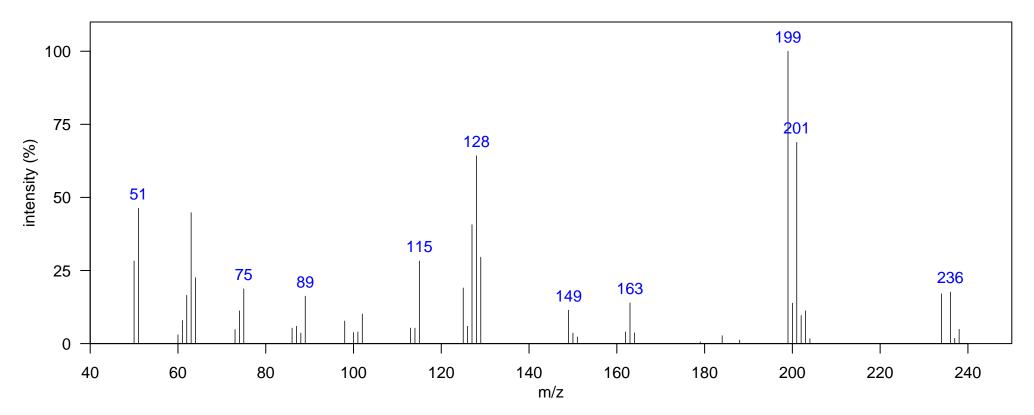
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1789.32, 1.610



Name: Unknown-11 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

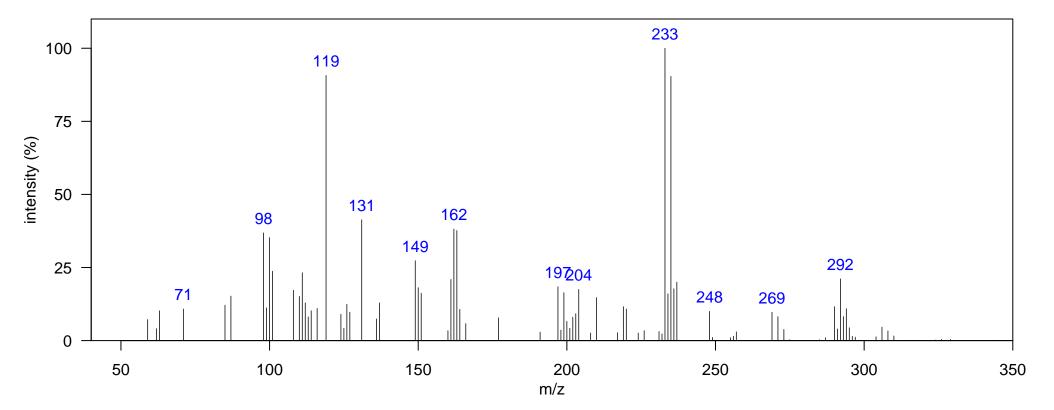
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1114.21, 0.904



Name: Unknown-14 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

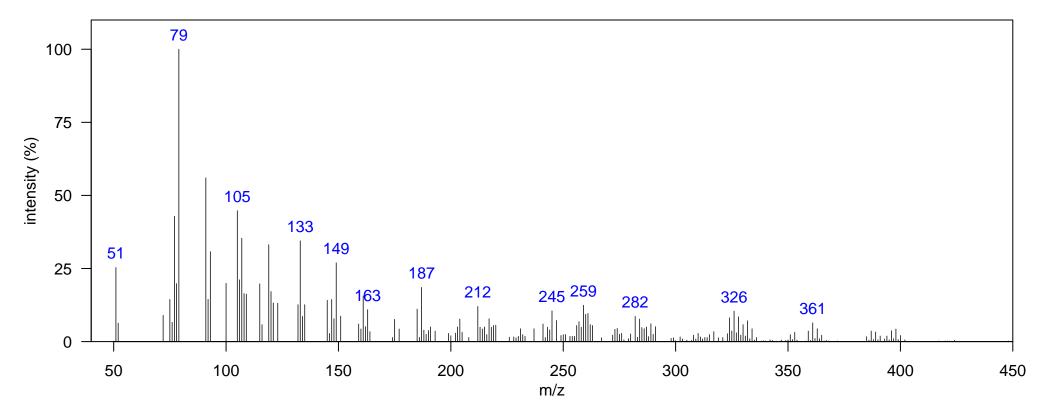
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1247.13, 0.970



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

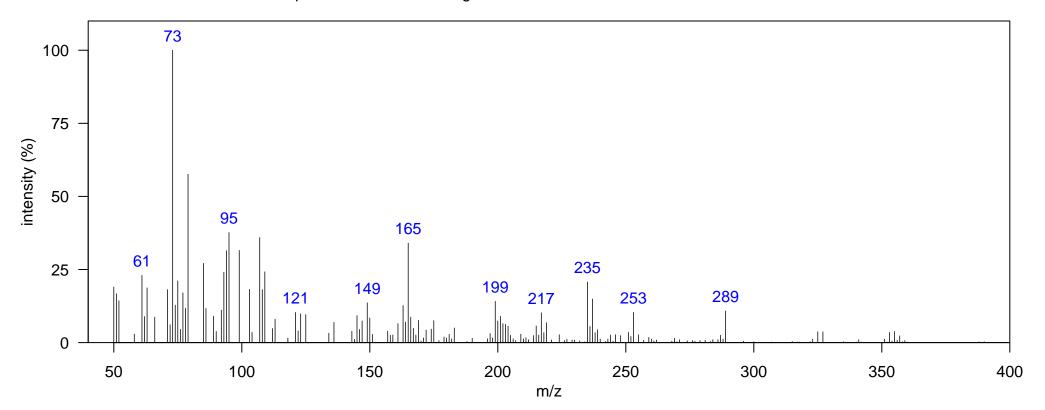


Name: Unknown-16 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

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

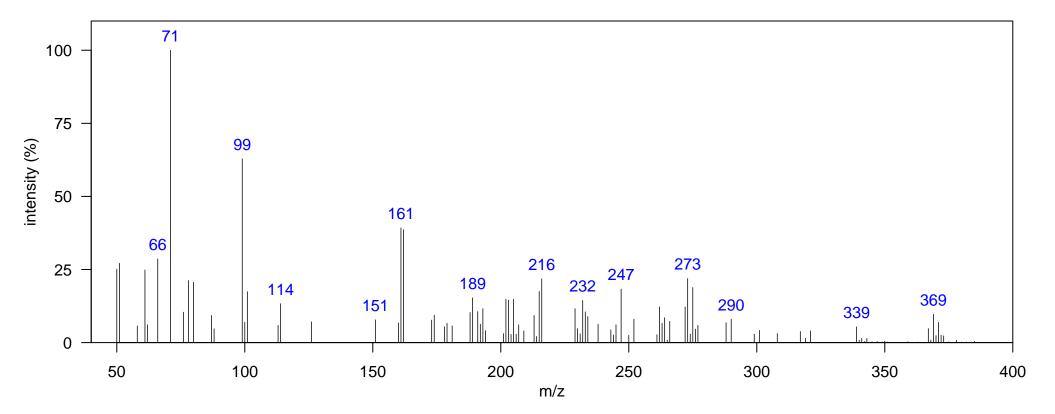
Comment: Interference with some compounds – ion 355 belongs to unknown–16



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

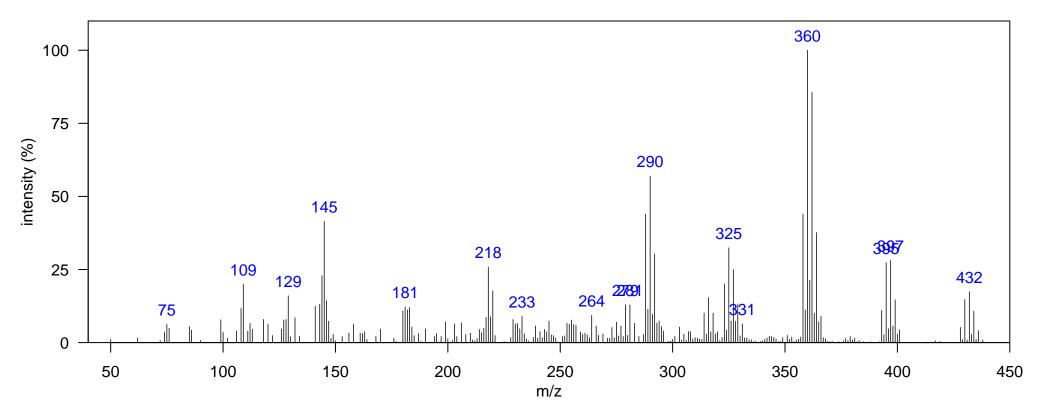


Name: Unknown-19 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

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

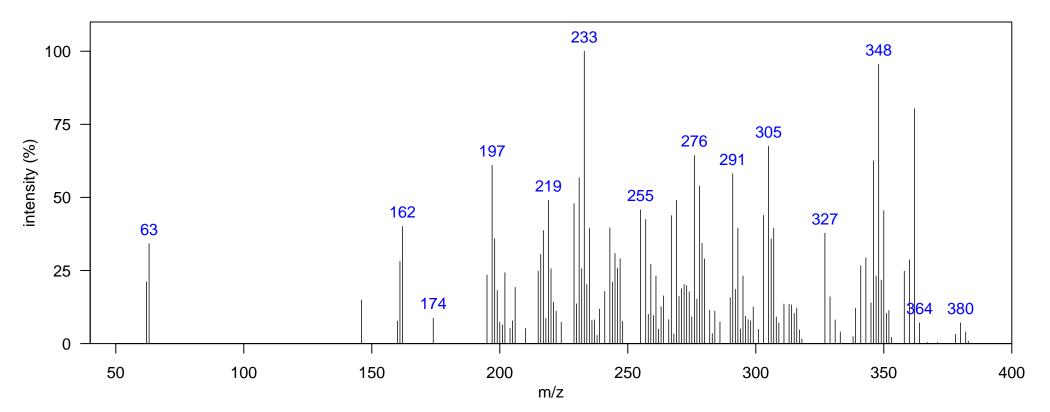
Comment: PCB interference



Name: Unknown–21 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

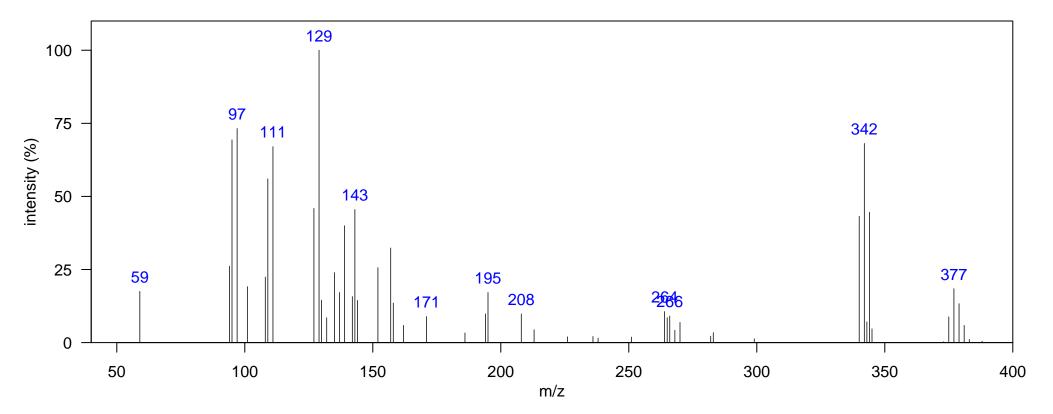
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1450.01, 1.069



Name: Unknown–22 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

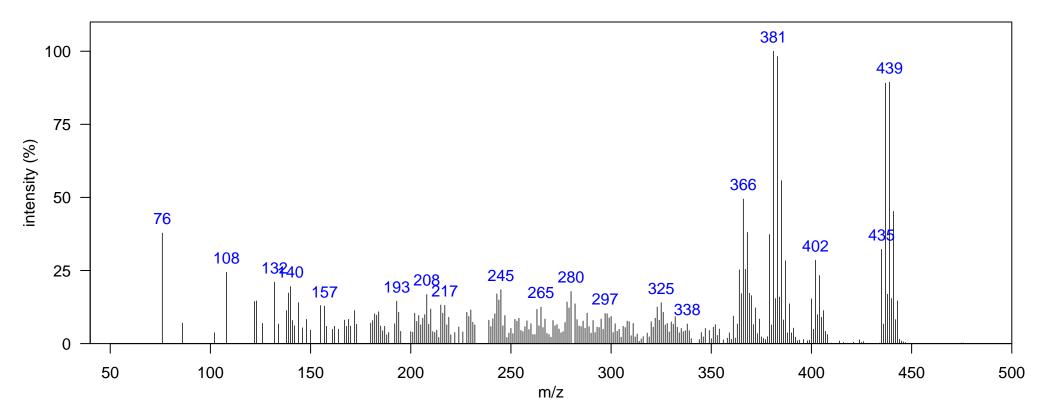
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1446.52, 1.063



Name: Unknown-34 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

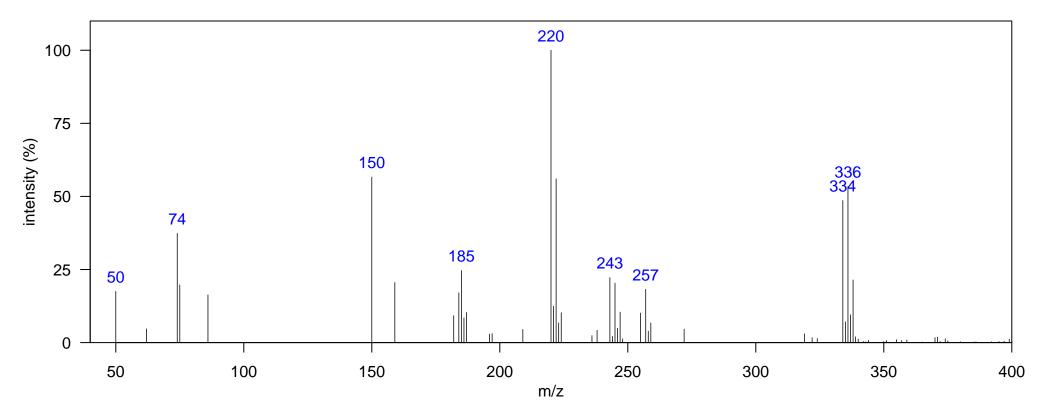
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1530.47, 1.195



Name: Unknown-36 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

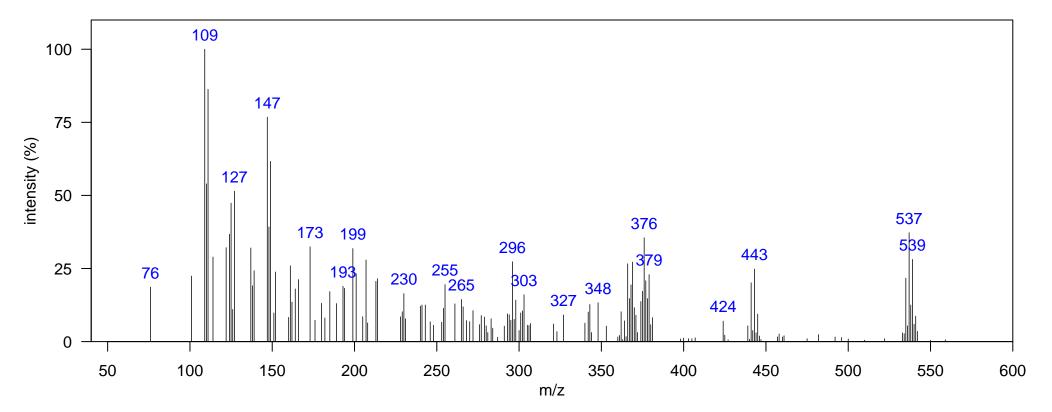
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1554.95, 1.300



Name: Unknown-38 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

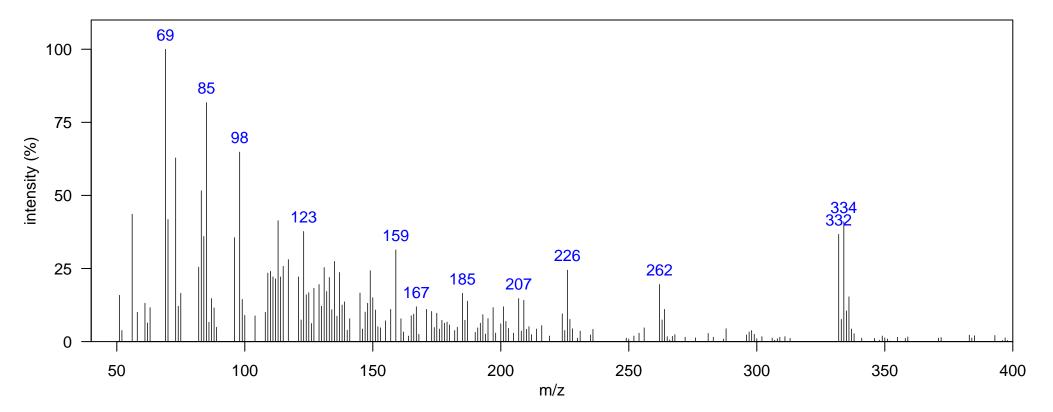
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1561.95, 1.274



Name: Unknown-39 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

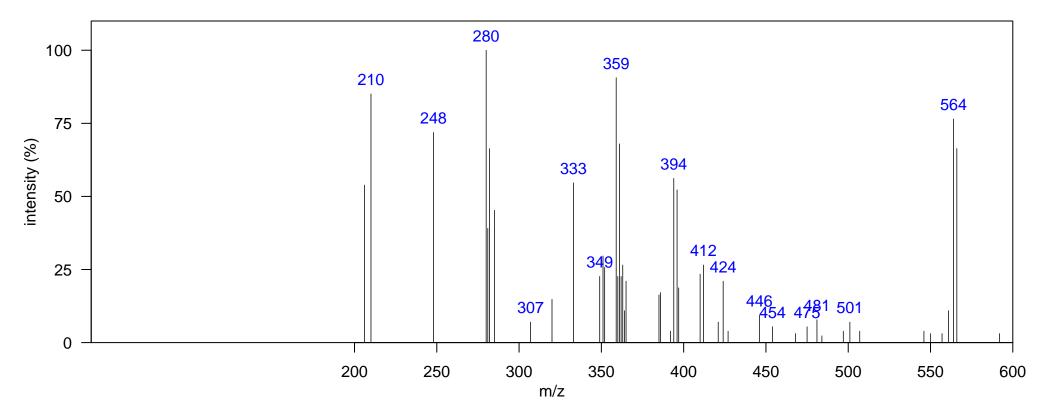
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1554.95, 1.267



Name: Unknown-44 Class: Unknown

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

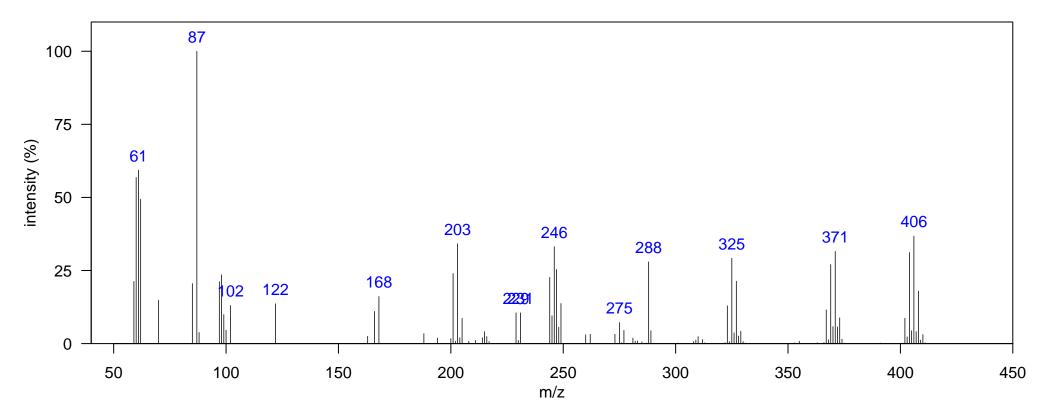
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1624.91, 1.518



Name: Unknown-3-1 Class: Unknown-3

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

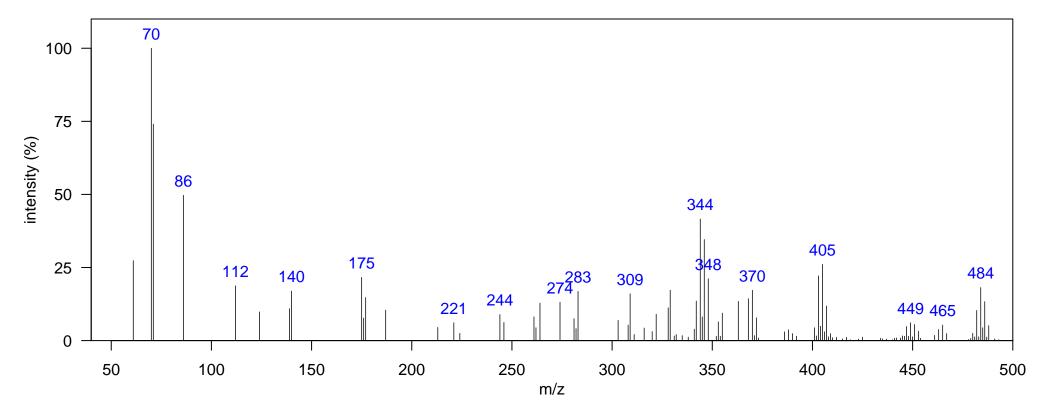
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1240.13, 1.010



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

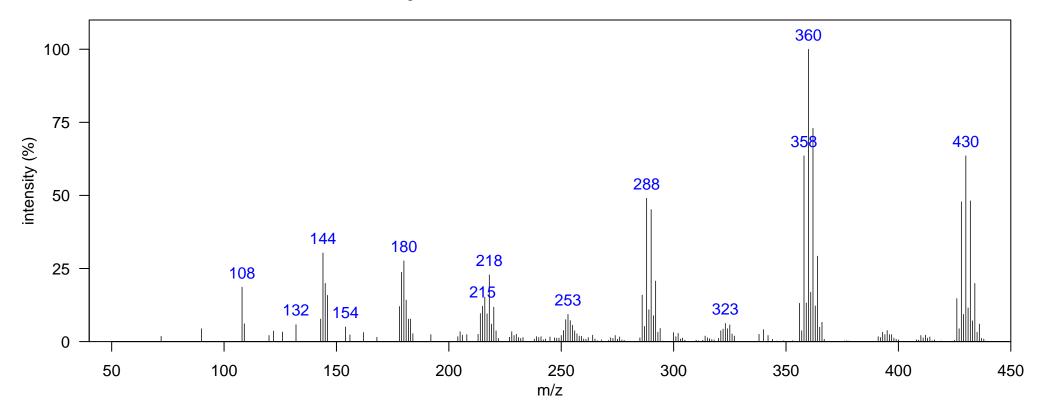


Name: Unknown-4-2 Class: Unknown-4

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

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

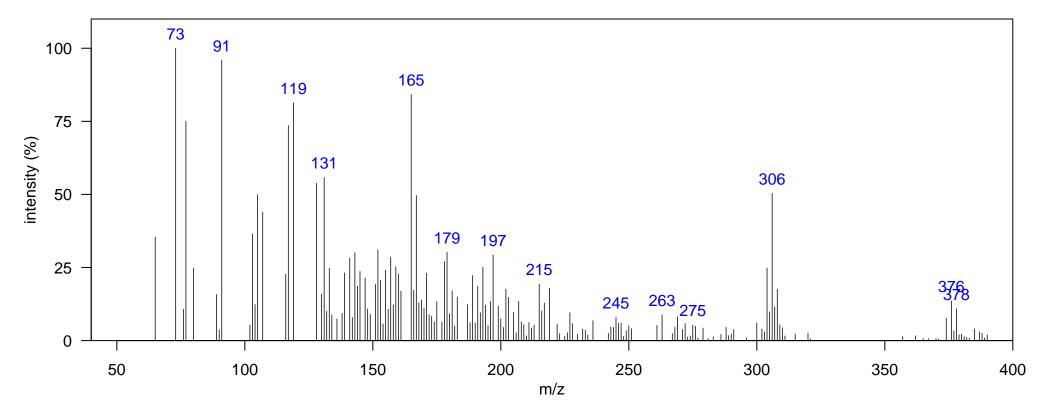
Comment: PCB interference – ions 412 and 340 belong to unknown–4–2



Name: Unknown-4-3 Class: Unknown-4

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

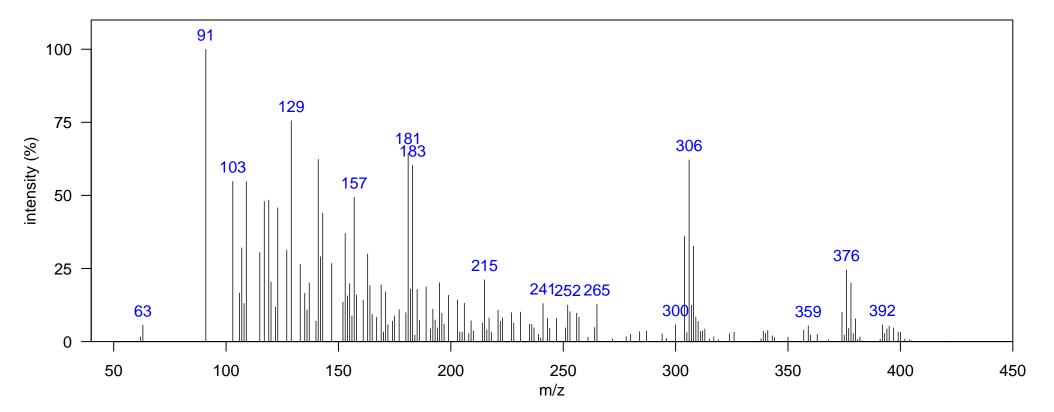
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1415.03, 0.997



Name: Unknown-4-5 Class: Unknown-4

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

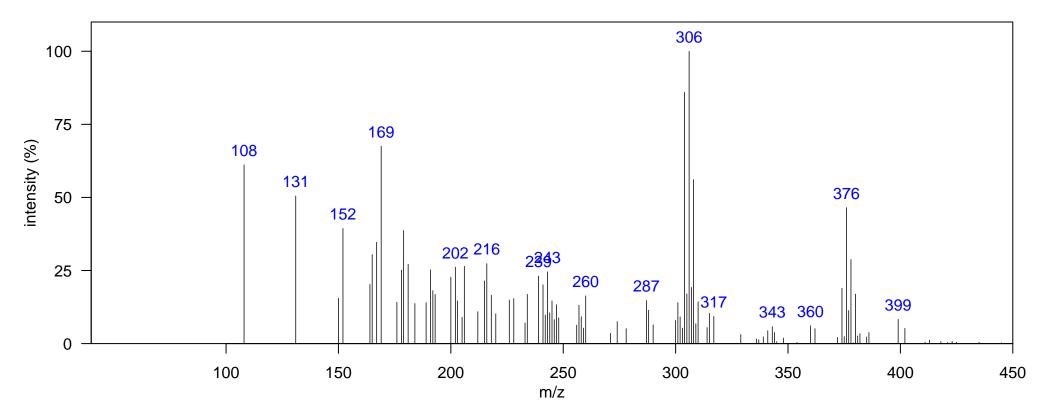
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1450.01, 1.069



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

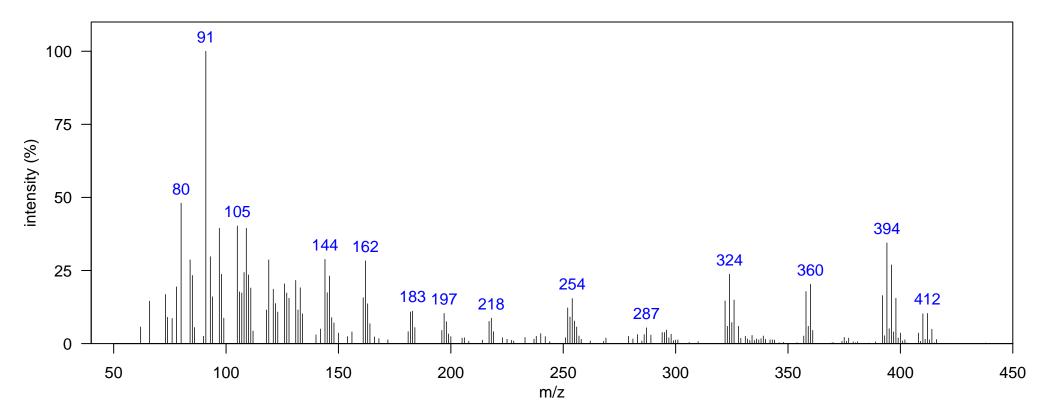


Name: Unknown-4-8 Class: Unknown-4

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

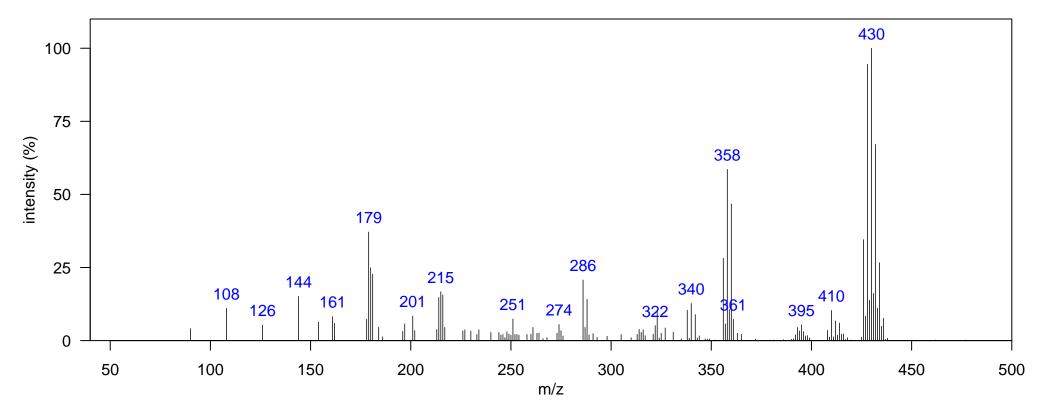


Name: Unknown-4-10 Class: Unknown-4

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

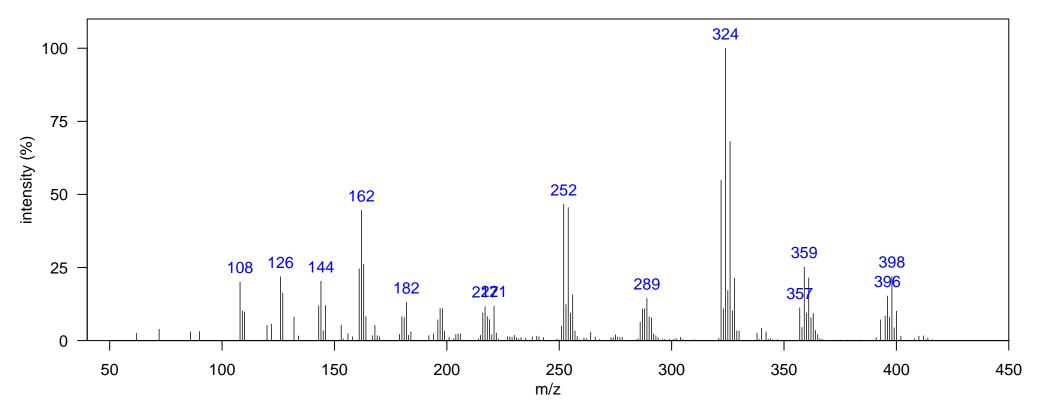


Name: Unknown-4-11 Class: Unknown-4

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

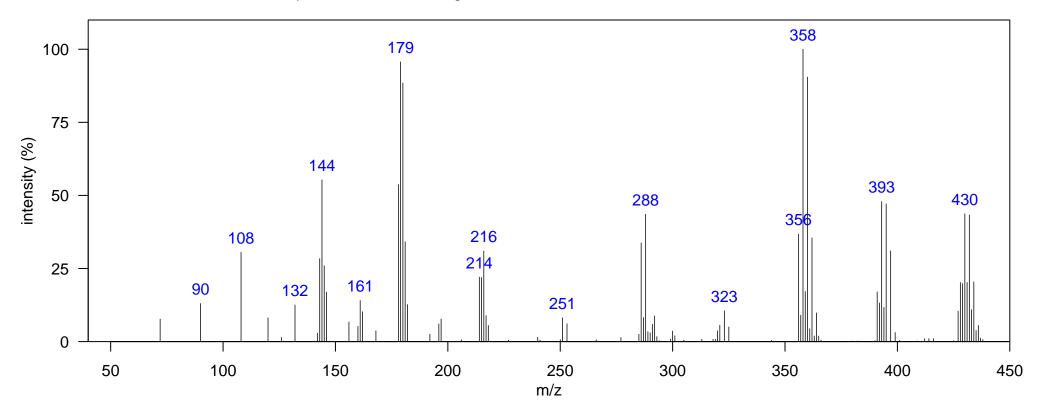


Name: Unknown-4-12 Class: Unknown-4

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

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

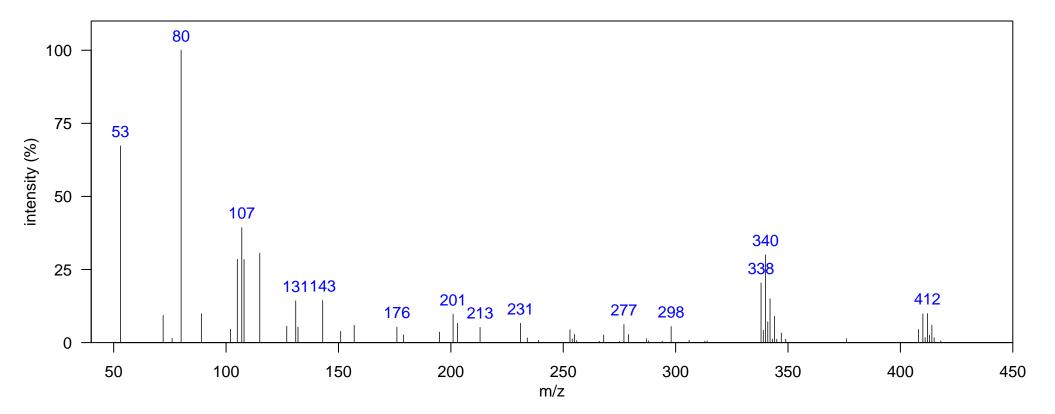
Comment: Interference from other compounds, ion 412 belongs to unknown-4-12



Name: Unknown-4-13 Class: Unknown-4

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

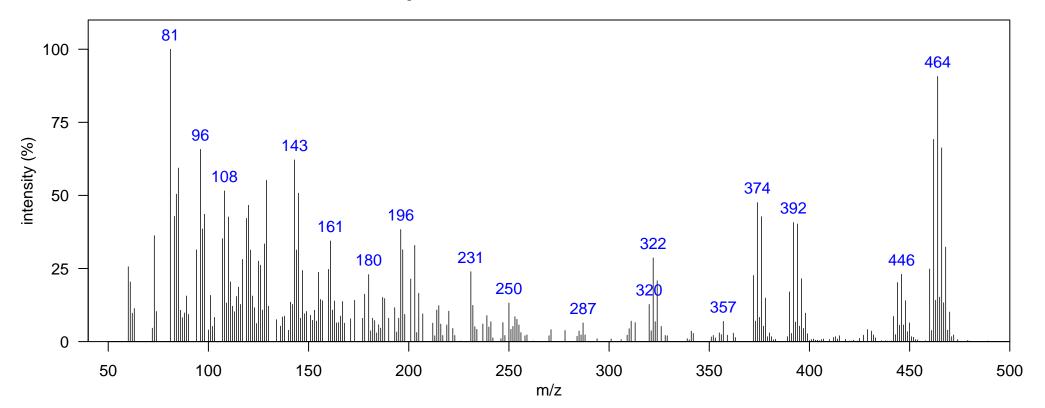
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1568.95, 1.228



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

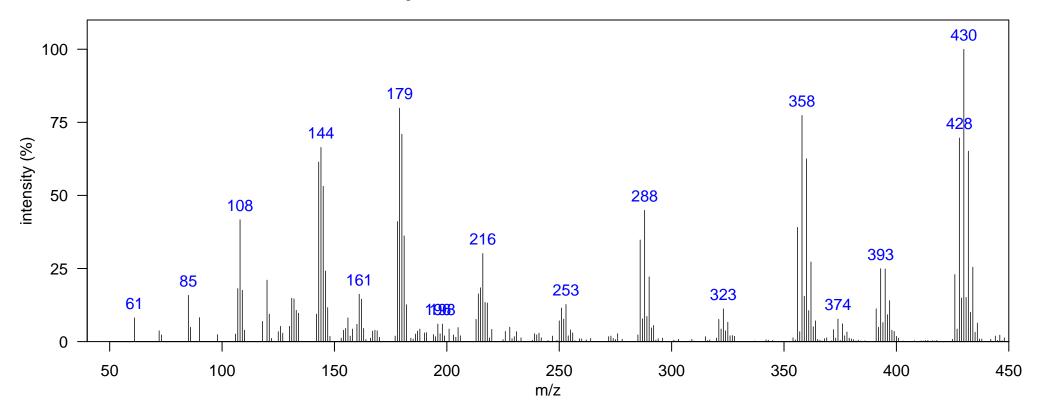


Name: Unknown-4-16 Class: Unknown-4

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

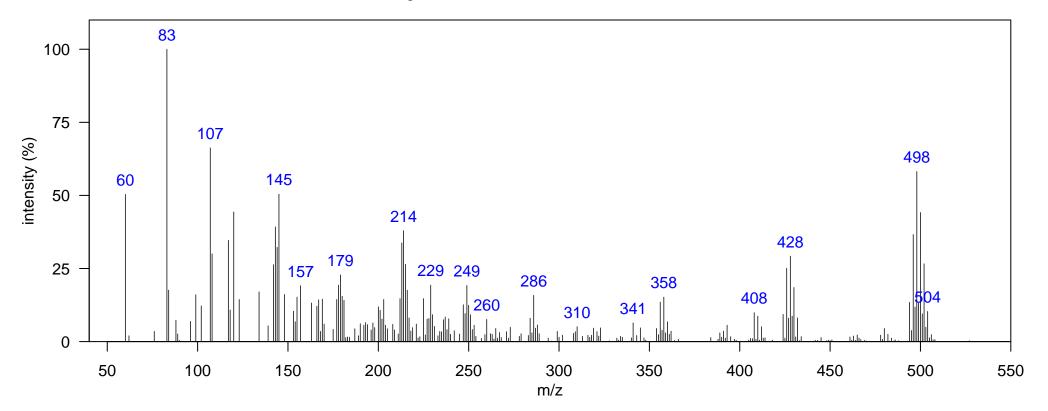


Name: Unknown-4-17 Class: Unknown-4

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

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

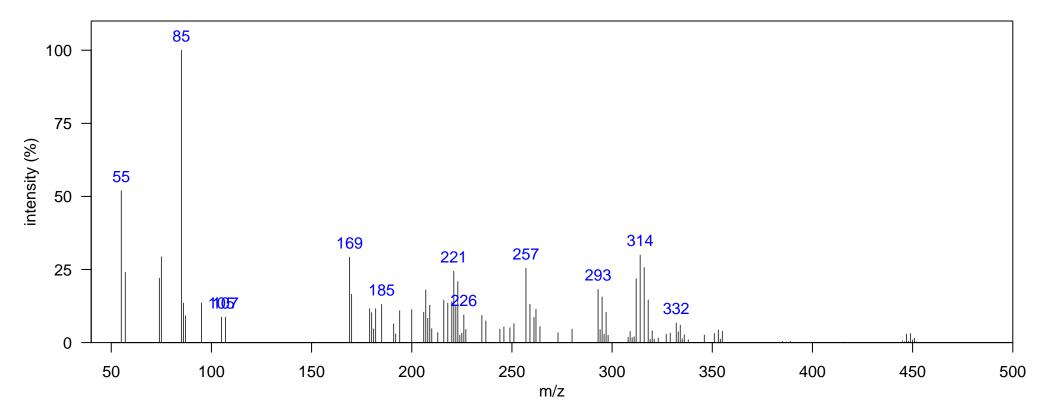
Comment: PCB interference - ions 408 and 480 belong to unknown-4-17



Name: Unknown-5-1 Class: Unknown-5

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

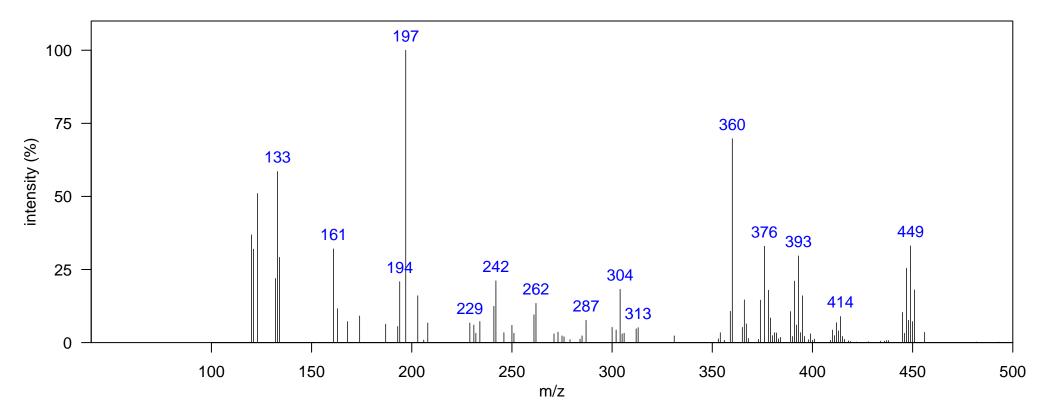
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1460.51, 1.089



Name: Unknown-5-2 Class: Unknown-5

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

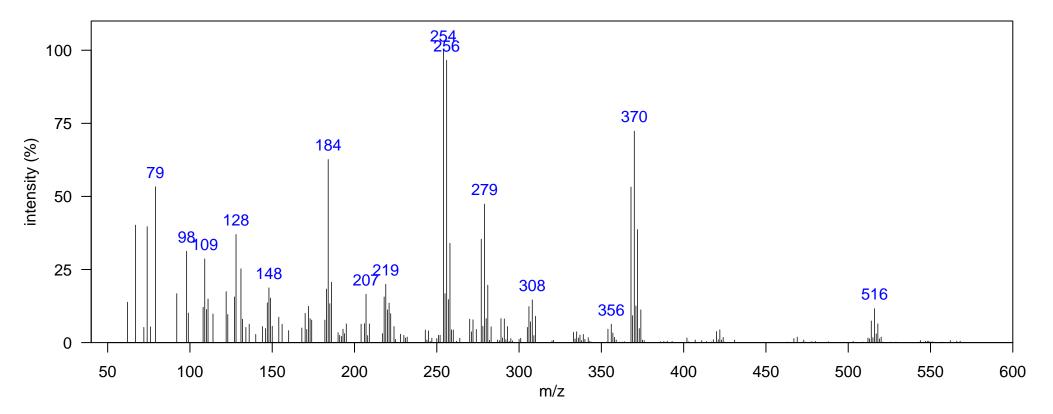
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1467.5 , 1.267



Name: Unknown-6-1 Class: Unknown-6

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

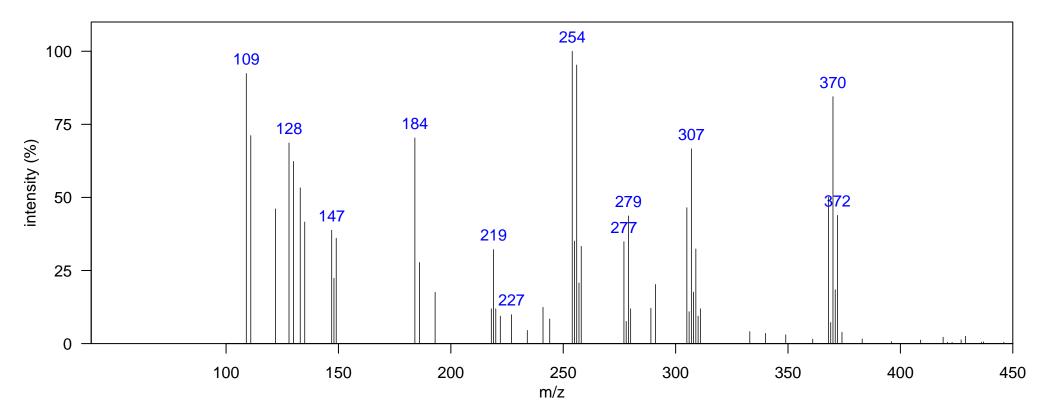
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1582.94, 1.373



Name: Unknown-6-2 Class: Unknown-6

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

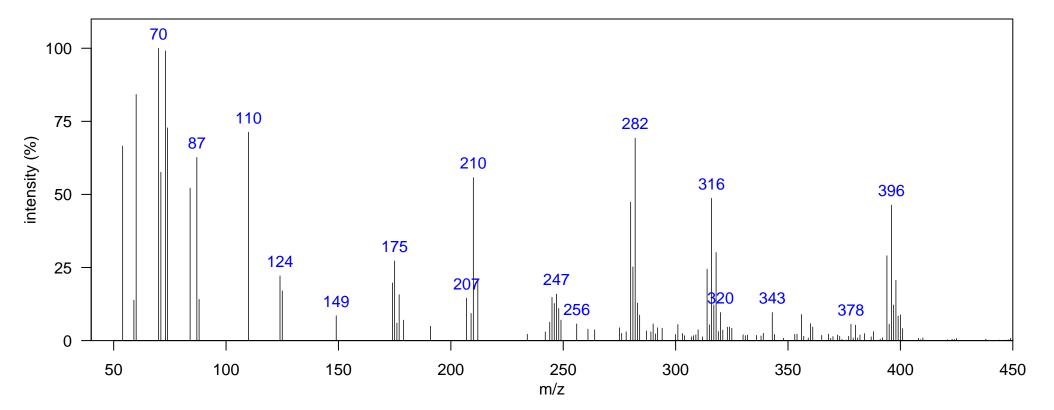
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1600.43, 1.445



Name: Unknown-7-1 Class: Unknown-7

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

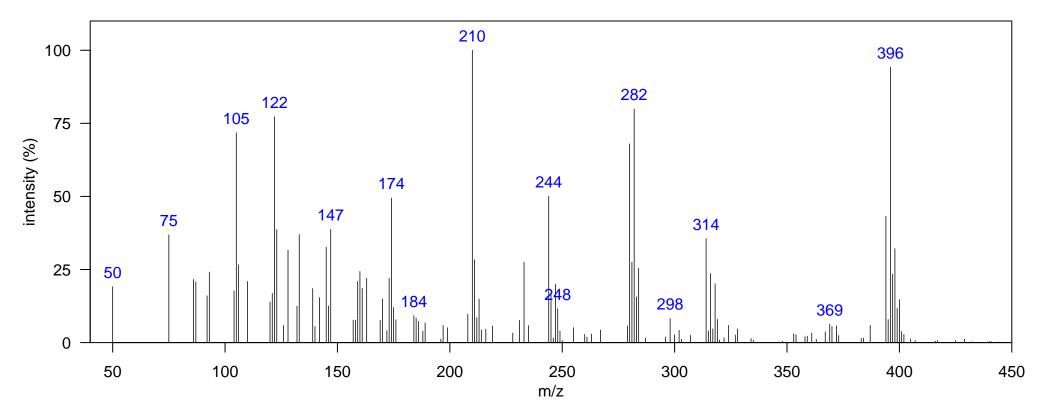
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1649.4 , 1.538



Name: Unknown-7-2 Class: Unknown-7

Matrix: Marine Mammal Blubber In Bottlenose Dolphin: TRUE

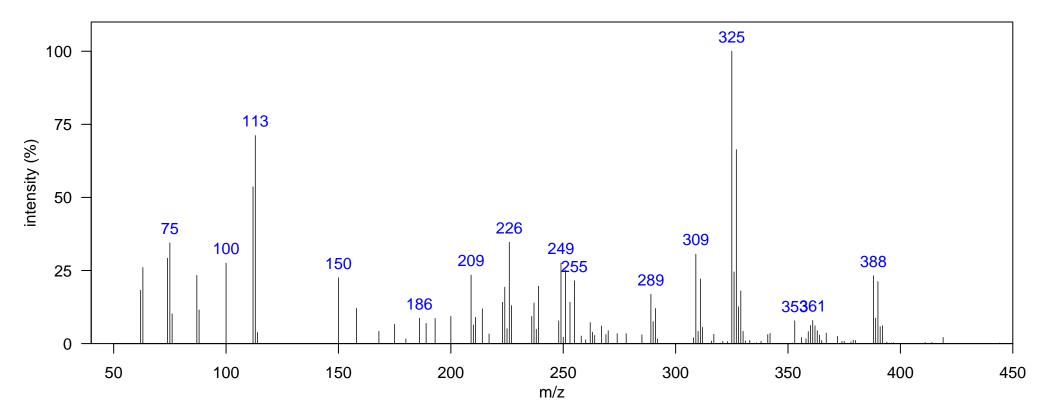
Instrument: GCxGC-TOF, EI Mode 1D RT, 2D RT (s): 1705.37, 1.690



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



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

