# Southern California Sea Lion Blubber (Example)

Authors: Nathan G. Dodder and Eunha Hoh

Web Reference:

http://OrgMassSpec.github.io

Prepared: 2013−11−23 09:06:00

SpecLibExample version 0.5−11

OrgMassSpecR version 0.4

png version 0.1−6

R version 3.0.2 (2013−09−25)

# Name: dichlorodiphenyltrichloroethane (DDT)

Elemental Formula: C14H9Cl5

Sample: southern CA sea lion blubber

Source: anthropogenic

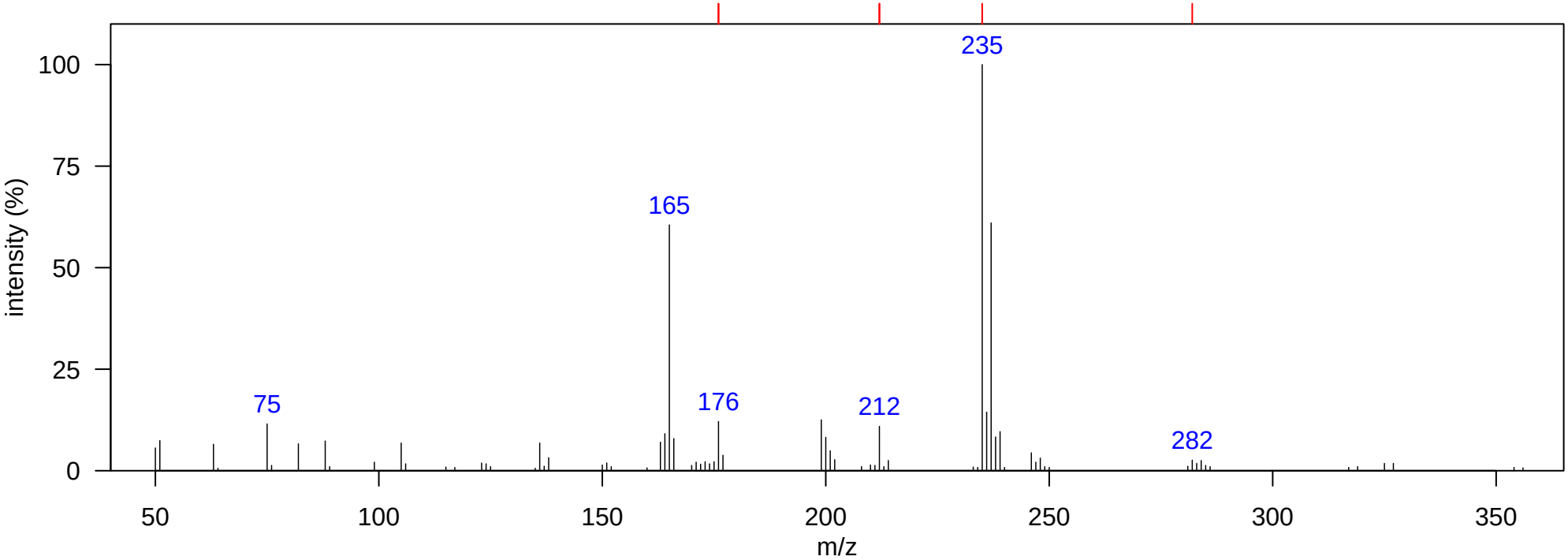
Instrument: GCxGC−TOF, electron impact, 70 eV

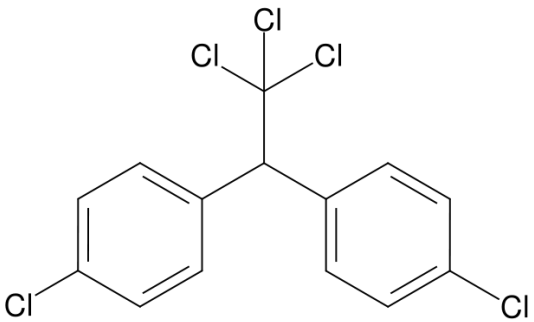
Class: DDT related

RT (s) (1D): 1452, RT (s) (2D): 0.92

Identification: match to NIST 2008 library

Comment: Isomer unknown.




Cl substitution p,p' (shown) or o,p'

| m/z | Identity |
|---|---|
| 176 | [M−H−5Cl]+ |
| 212 | [M−4Cl]+ |
| 235 | [M−CCl3]+ |
| 282 | [M−2Cl]+ |

Filename: ddt

# Name: dichlorodiphenyldichloroethylene (DDE)

Elemental Formula: C14H8Cl4

Sample: southern CA sea lion blubber

Source: anthropogenic

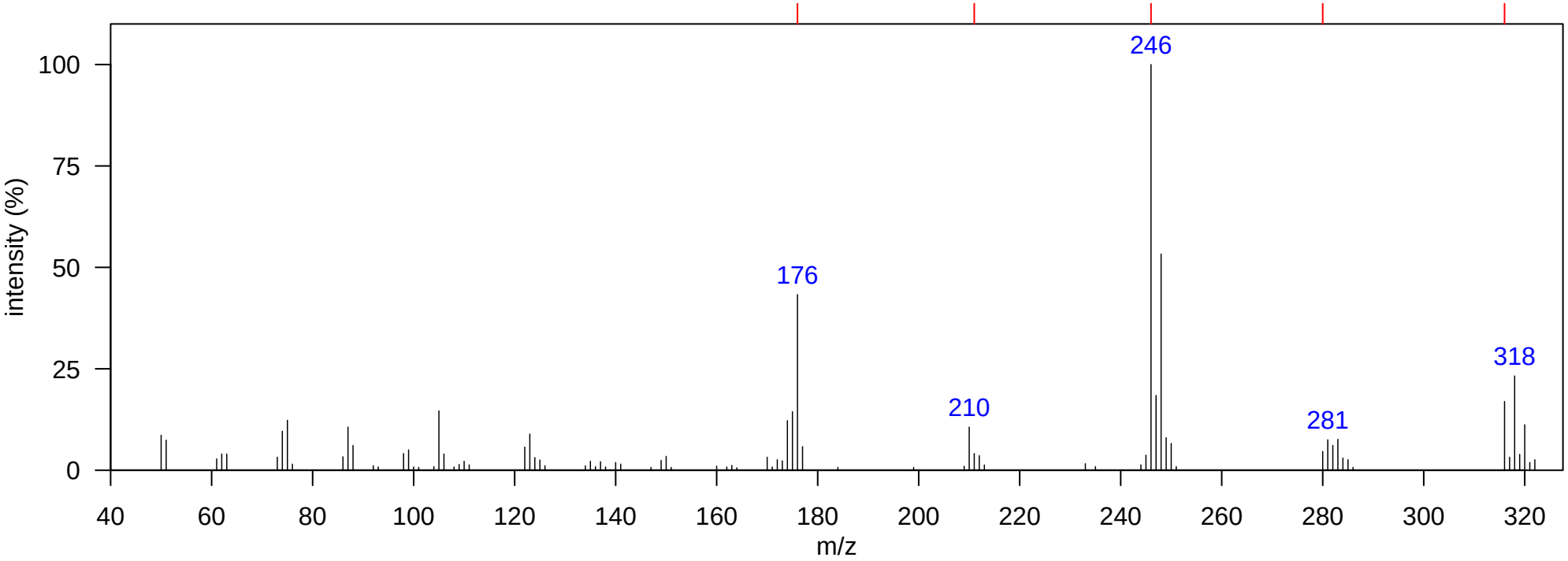
Instrument: GCxGC−TOF, electron impact, 70 eV

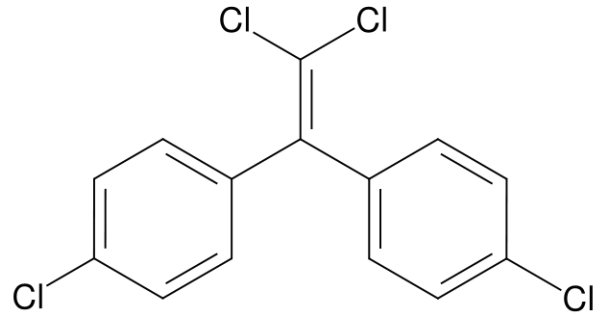
Class: DDT related

RT (s) (1D): 1386, RT (s) (2D): 0.87

Identification: match to NIST 2008 library

Comment: Possibly 3 isomers detected; one shown. There were problems deconvoluting the large DDE peak.




Cl substitution p,p' (shown), o,p', or other

| m/z | Identity |
|---|---|
| 176 | [M−4Cl]+ |
| 211 | [M−3Cl]+ |
| 246 | [M−2Cl]+ |
| 280 | [M−Cl]+ |
| 316 | M+ |

Filename: dde

# Name: dichlorodiphenyldichloroethane (DDD) isomer 1

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1410, RT (s) (2D): 0.91

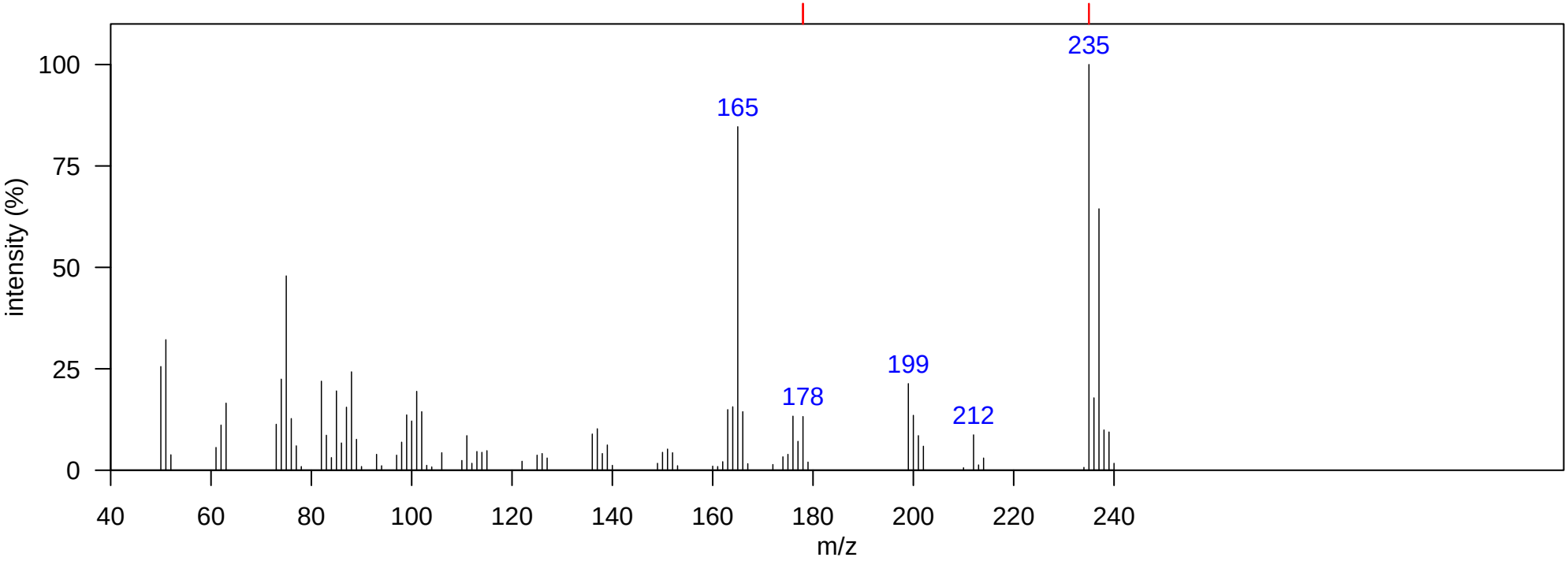
Comment: Isomer unknown.

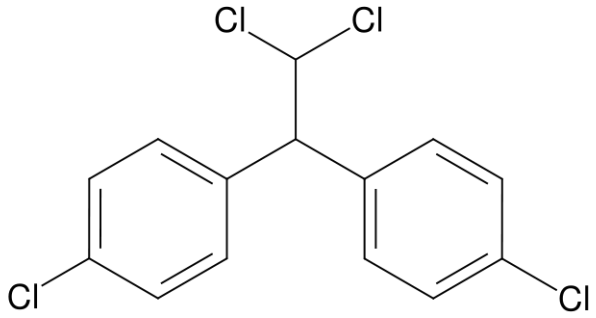
Elemental Formula: C14H10Cl4

Source: anthropogenic

Class: DDT related

Identification: match to NIST 2008 library




Cl substitution p,p' (shown) or o,p'

| m/z | Identity |
|---|---|
| 178 | [M−4Cl]+ |
| 235 | [M−CHCl2]+ |

Filename: ddd1

# Name: dichlorodiphenyldichloroethane (DDD) isomer 2

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1413, RT (s) (2D): 0.93

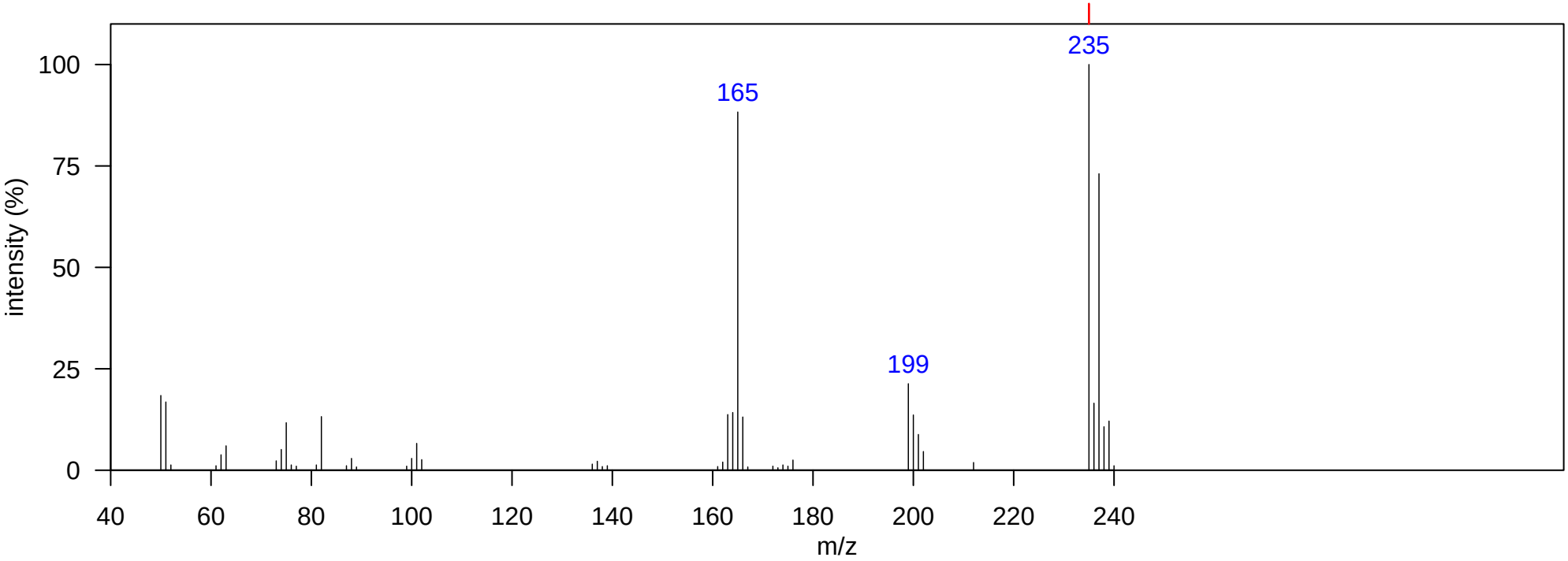
Comment: Isomer unknown.

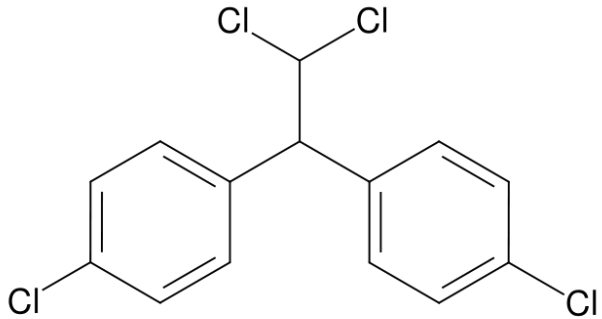
Elemental Formula: C14H10Cl4

Source: anthropogenic

Class: DDT related

Identification: match to NIST 2008 library




Cl substitution p,p' (shown) or o,p'

| m/z | Identity |
|---|---|
| 235 | [M−CHCl2]+ |

Filename: ddd2

Name: 1−chloro−2,2−bis(chlorophenyl)ethene (DDMU) isomer 1

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1257, RT (s) (2D): 0.86

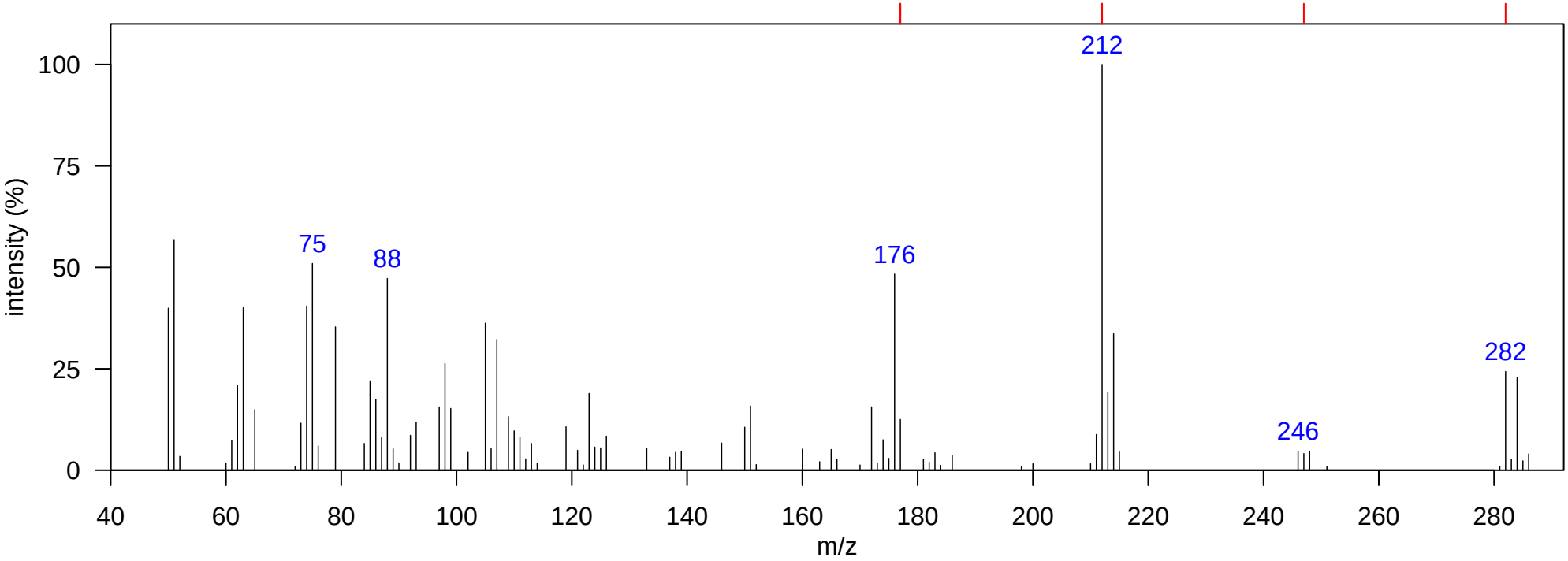
Comment: Isomer unknown.

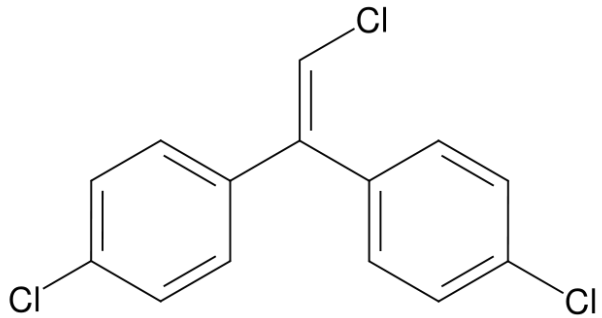
Elemental Formula: C14H9Cl3

Source: anthropogenic

Class: DDT related

Identification: match to NIST 2008 library




Cl substitution p,p' (shown) or o,p'

| m/z | Identity |
|---|---|
| 177 | [M−3Cl]+ |
| 212 | [M−2Cl]+ |
| 247 | [M−Cl]+ |
| 282 | M+ |

Filename: ddmu1

# Name: 1−chloro−2,2−bis(chlorophenyl)ethene (DDMU) isomer 2

Elemental Formula: C14H9Cl3

Sample: southern CA sea lion blubber

Source: anthropogenic

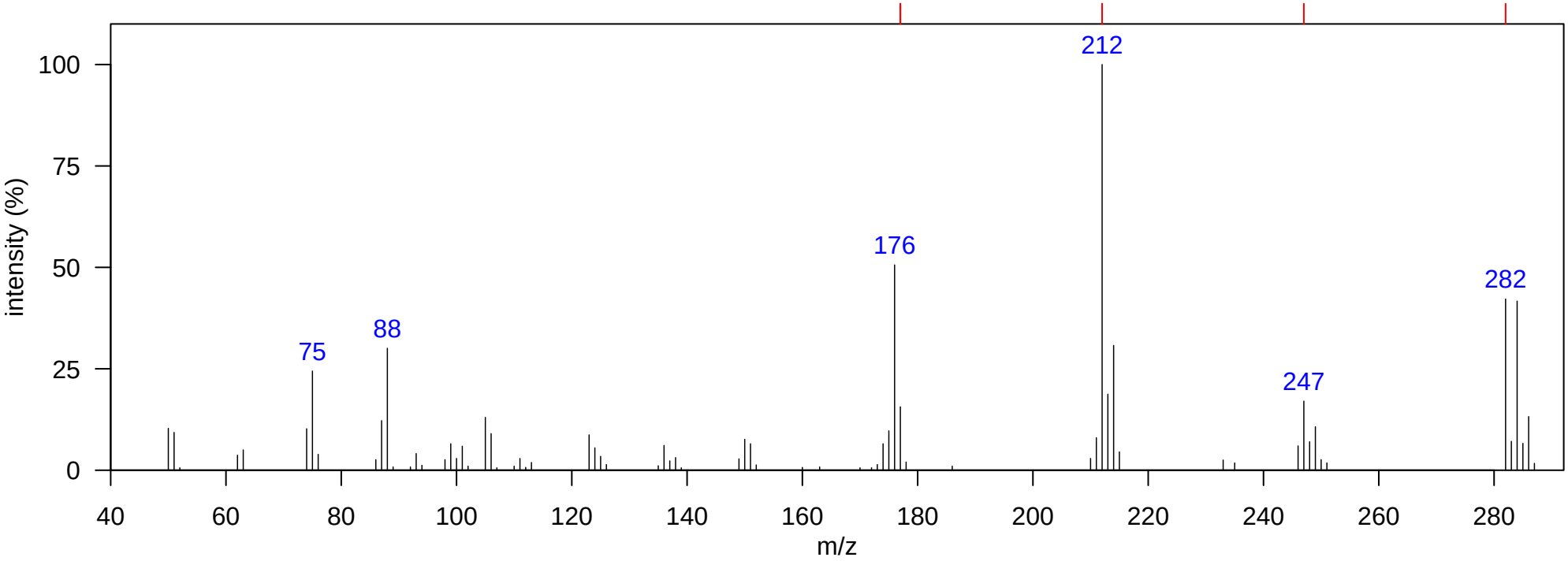
Instrument: GCxGC−TOF, electron impact, 70 eV

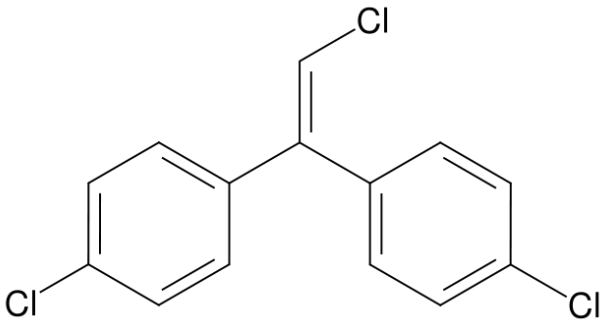
Class: DDT related

RT (s) (1D): 1326, RT (s) (2D): 0.88

Identification: match to NIST 2008 library

Comment: Isomer unknown.




Cl substitution p,p' (shown) or o,p'

| m/z | Identity |
|---|---|
| 177 | [M−3Cl]+ |
| 212 | [M−2Cl]+ |
| 247 | [M−Cl]+ |
| 282 | M+ |

Filename: ddmu2

Name: bis(chlorophenyl)ethane (DDEt)

Elemental Formula: C14H12Cl2

Sample: southern CA sea lion blubber

Source: anthropogenic

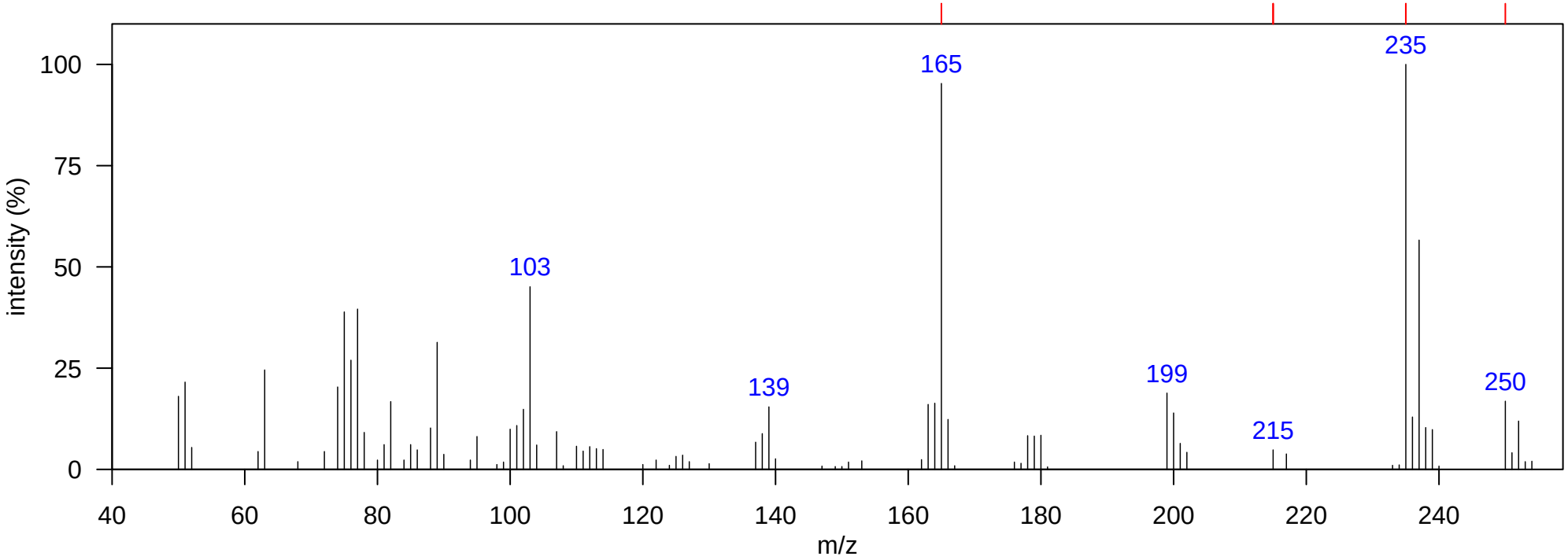
Instrument: GCxGC−TOF, electron impact, 70 eV

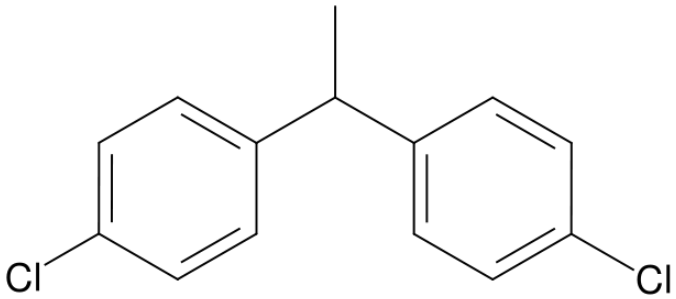
Class: DDT related

RT (s) (1D): 1218, RT (s) (2D): 0.83

Identification: match to NIST 2008 library

Comment: Isomer unknown. Reference: Environ. Sci. Technol., 2003, 37, 488−495, doi:10.1021/es0201451




Cl substitution p,p' (shown) or o,p'

| m/z | Identity |
|---|---|
| 165 | [M−CH3−2Cl]+ |
| 215 | [M−2Cl]+ |
| 235 | [M−CH3]+ |
| 250 | M+ |

Filename: ddet

# Name: dichlorobenzophenone (DBP)

Elemental Formula: C13H8Cl2O

Sample: southern CA sea lion blubber

Source: anthropogenic

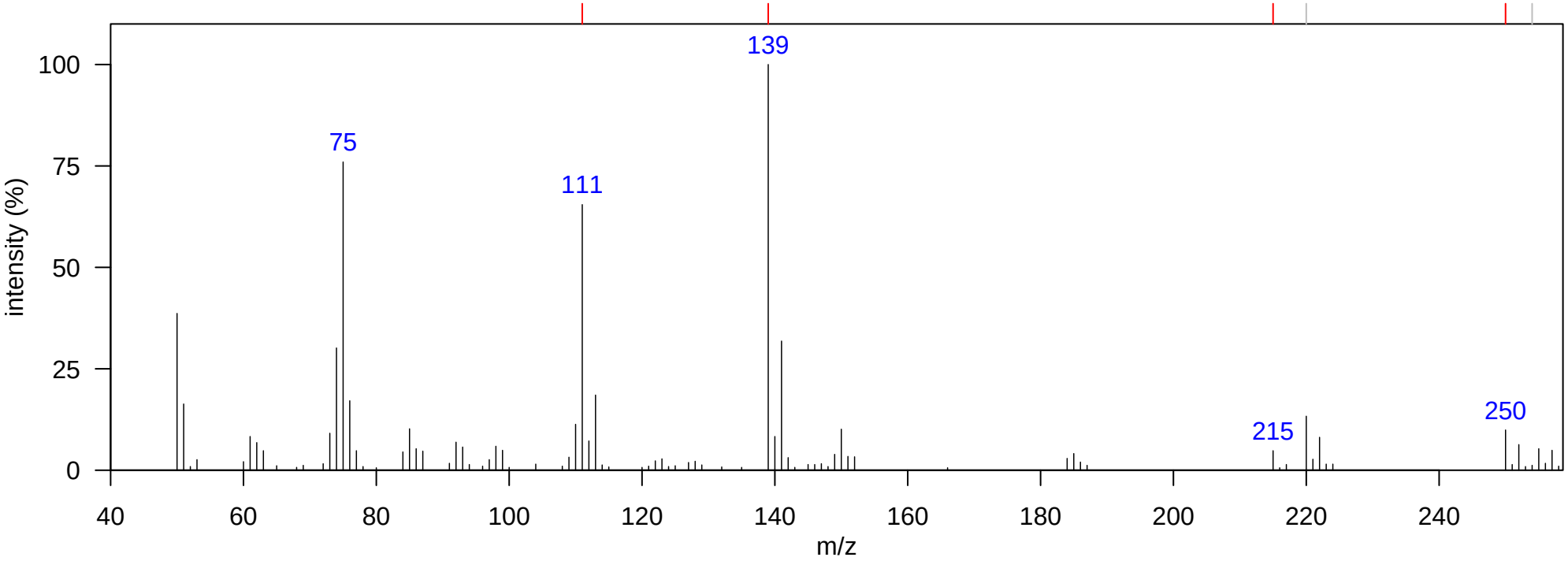
Instrument: GCxGC−TOF, electron impact, 70 eV

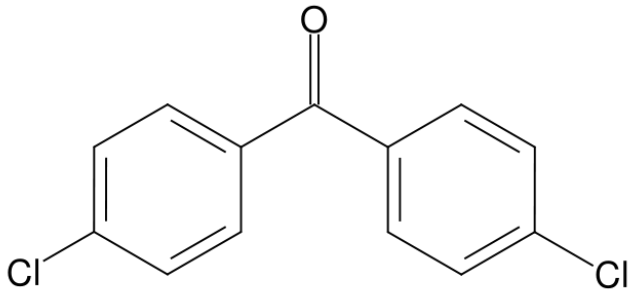
Class: DDT related

RT (s) (1D): 1266, RT (s) (2D): 0.88

Identification: match to NIST 2008 library

Comment: Isomer unknown. Reference: Environ. Sci. Technol., 2003, 37, 488−495, doi:10.1021/es0201451




Cl substitution p,p' (shown) or o,p'

| m/z | Identity |
|---|---|
| 111 | [C6H4Cl]+ |
| 139 | [M−C6H4ClO]+ |
| 215 | [M−Cl]+ |
| 220 | PCB interference |
| 250 | M+ |
| 254 | PCB interference |
| 290 | PCB interference |

Filename: dbp

# Name: tris(chlorophenyl)methane isomer 1

Elemental Formula: C19H13Cl3

Sample: southern CA sea lion blubber

Source: anthropogenic

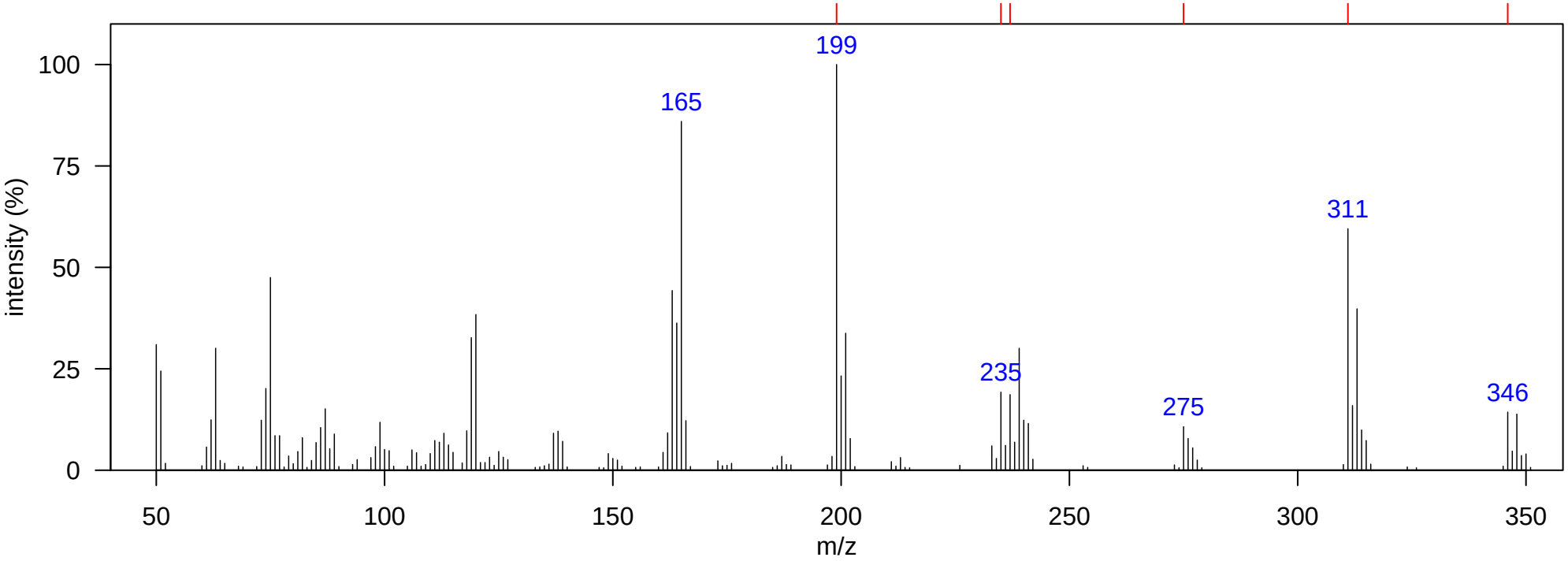
Instrument: GCxGC−TOF, electron impact, 70 eV

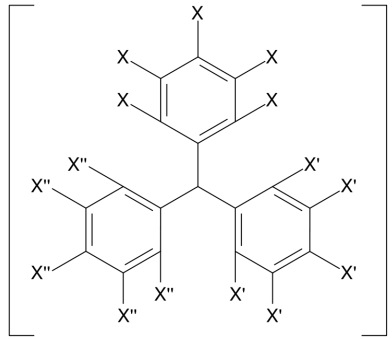
Class: DDT related

RT (s) (1D): 1557, RT (s) (2D): 0.96

Identification: manual identification

Comment: Reference: Environ. Sci. Technol. 1995, 29, 2133−2139. At least one 2−chloro ring based on 235/239 ratio.




X=Cl, 4H; X'=Cl, 4H; X''=Cl, 4H

At least one ortho-Cl present.

| m/z | Identity |
|---|---|
| 199 | [M−C6H4Cl−HCl]+ |
| 235 | [M−C6H4Cl]+ |
| 237 | [M−2Cl]+ |
| 275 | [M−Cl−HCl]+ |
| 311 | [M−Cl]+ |
| 346 | M+ |

Filename: tcpm1

# Name: tris(chlorophenyl)methane isomer 2

Elemental Formula: C19H13Cl3

Sample: southern CA sea lion blubber

Source: anthropogenic

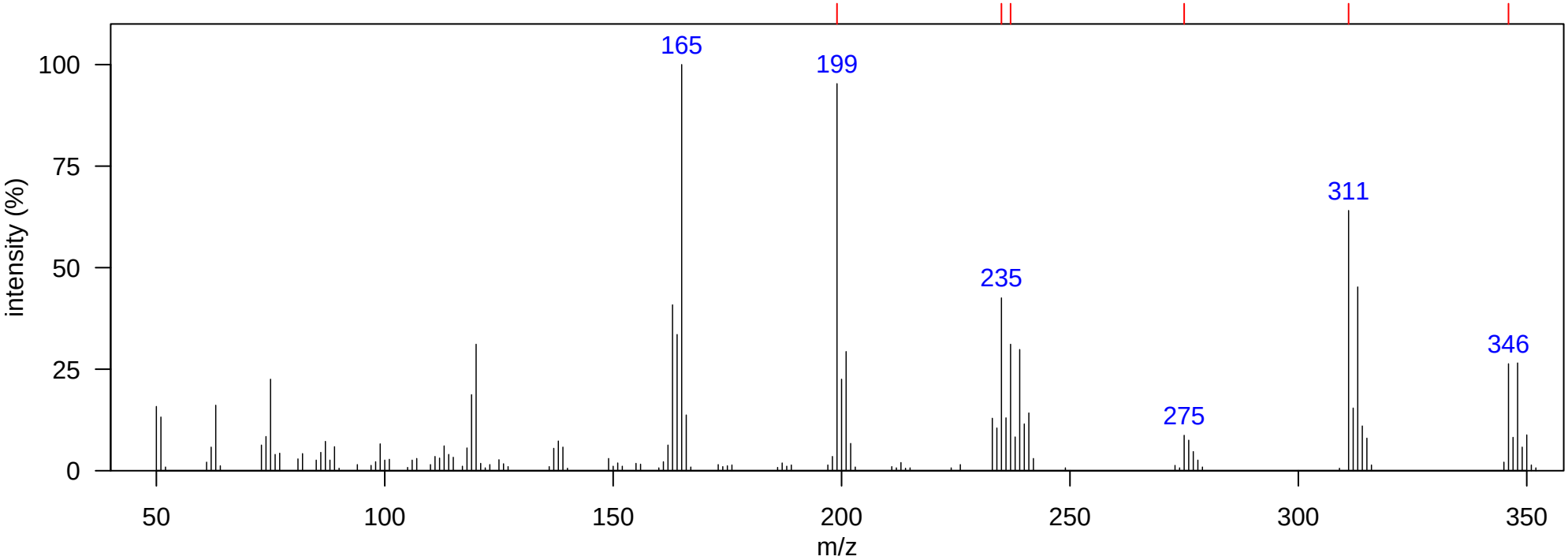
Instrument: GCxGC−TOF, electron impact, 70 eV

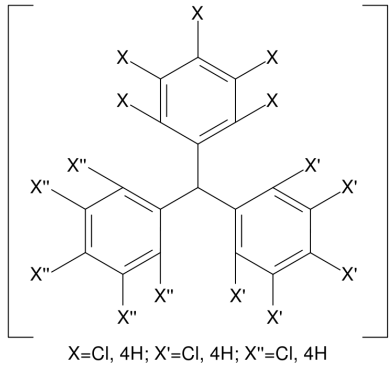
Class: DDT related

RT (s) (1D): 1596, RT (s) (2D): 1.03

Identification: manual identification

Comment: Reference: Environ. Sci. Technol. 1995, 29, 2133−2139. Only 3/4−chloro ring based on 235/239 ratio.




| m/z | Identity |
|---|---|
| 199 | [M−C6H4Cl−HCl]+ |
| 235 | [M−C6H4Cl]+ |
| 237 | [M−2Cl]+ |
| 275 | [M−Cl−HCl]+ |
| 311 | [M−Cl]+ |
| 346 | M+ |

Filename: tcpm2

Name: dichlorophenylacetylene (DCPA) (tentative)

Elemental Formula: C14H8Cl2

Sample: southern CA sea lion blubber

Source: anthropogenic

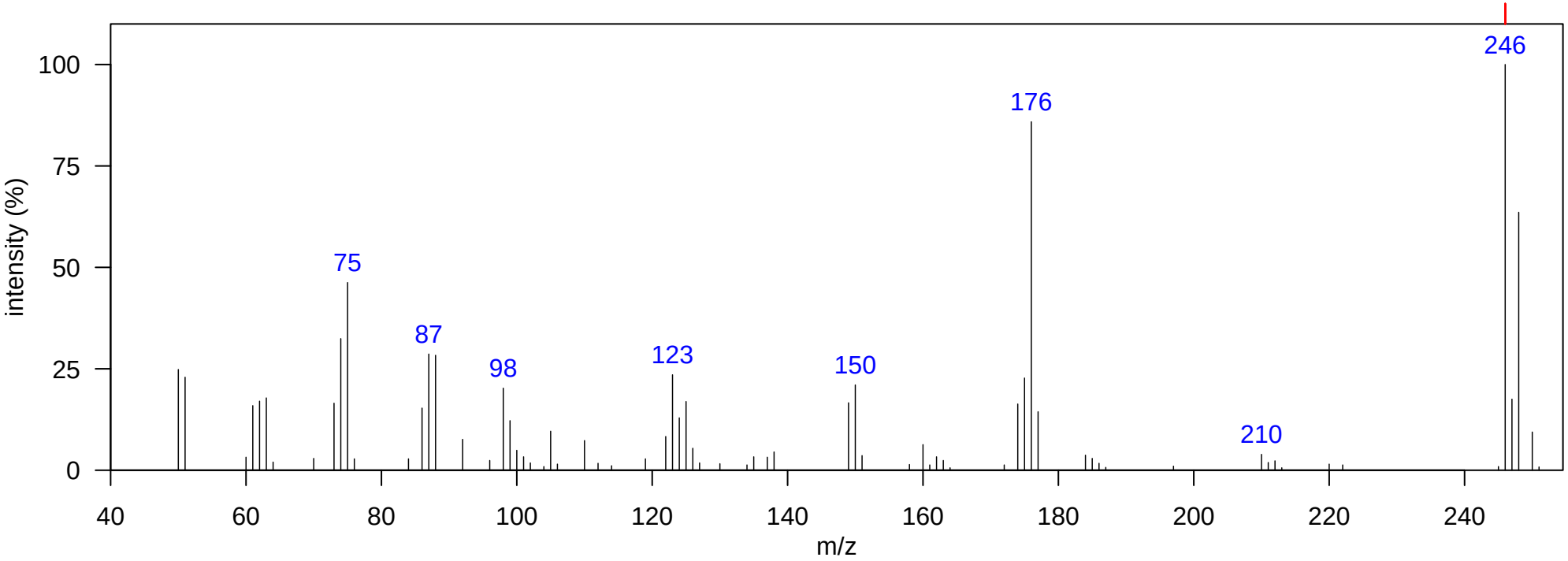
Instrument: GCxGC−TOF, electron impact, 70 eV

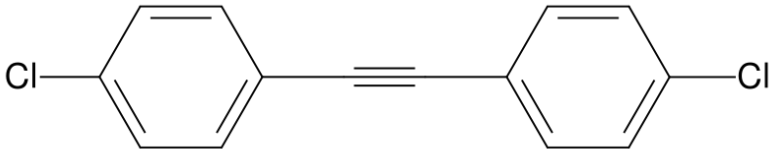
Class: DDT related

RT (s) (1D): 1296, RT (s) (2D): 0.86

Identification: match to NIST 2008 library

Comment: Likely ID based on: ES&T, 1996, 30, 3401−3407. Matches in NIST library: CAS 605−48−1, 76905−732, 835−17−6, 1820−42−4.




Possible structure; tentative.

| m/z | Identity |
|---|---|
| 246 | M+ |

Filename: dcpa

Name: hexachlorocyclohexane (HCH)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1125, RT (s) (2D): 0.88

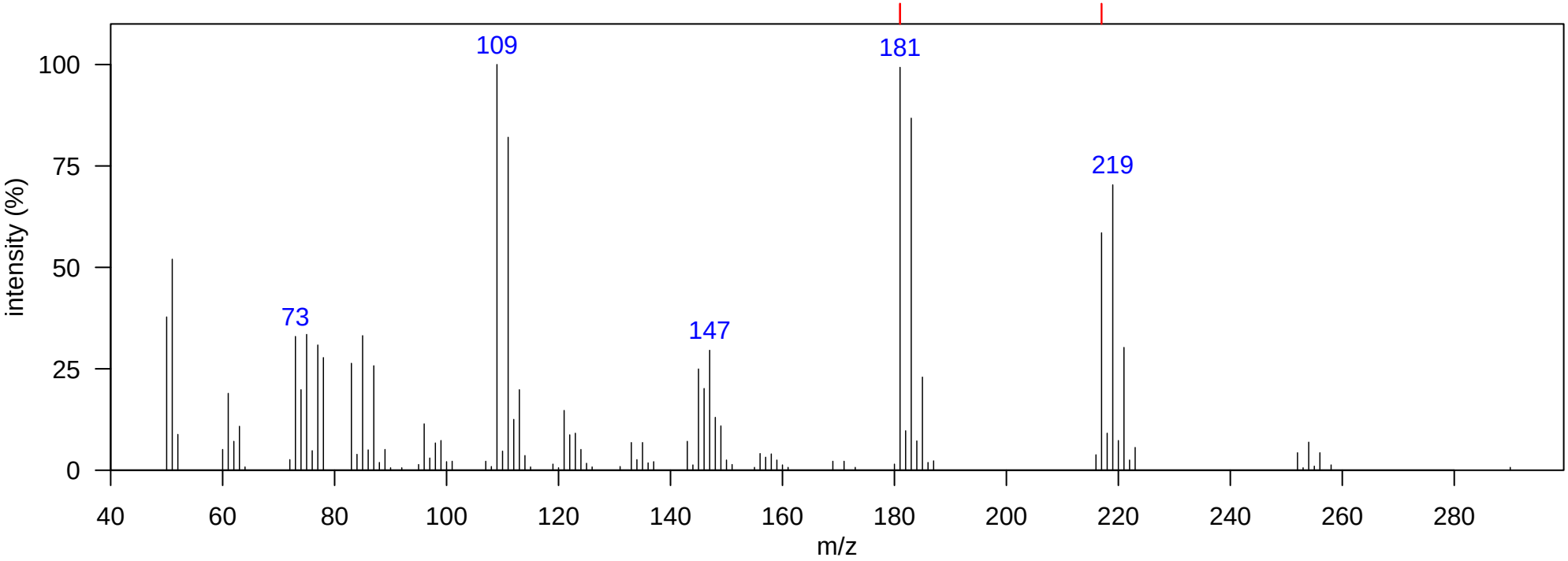
Comment: NA

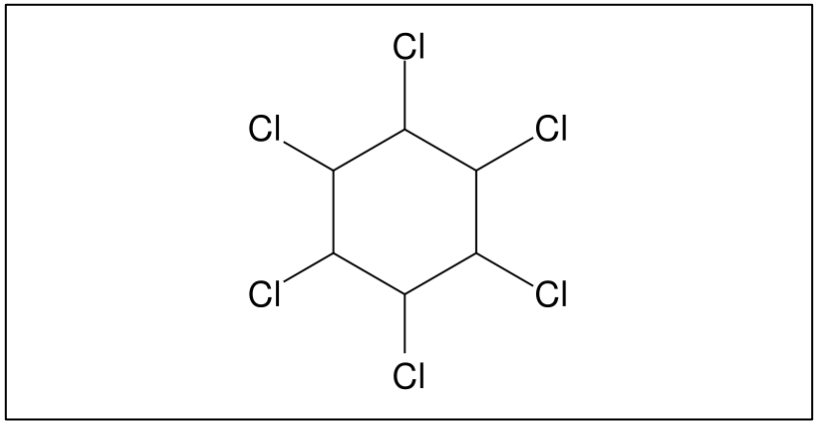
Elemental Formula: C6H6Cl6

Source: anthropogenic

Class: legacy pesticide

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 181 | [M−3Cl−2H]+ |
| 217 | [M−2Cl−H]+ |

Filename: hch

Name: heptachlor epoxide

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1305, RT (s) (2D): 0.87

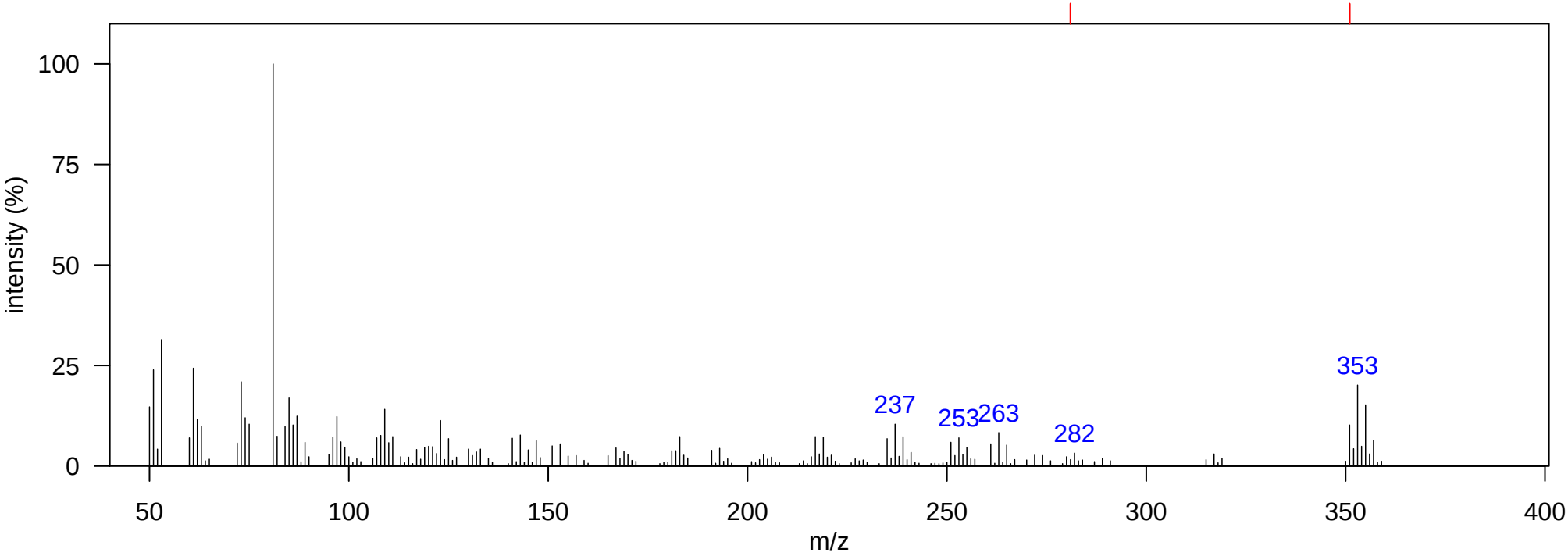
Comment: NA

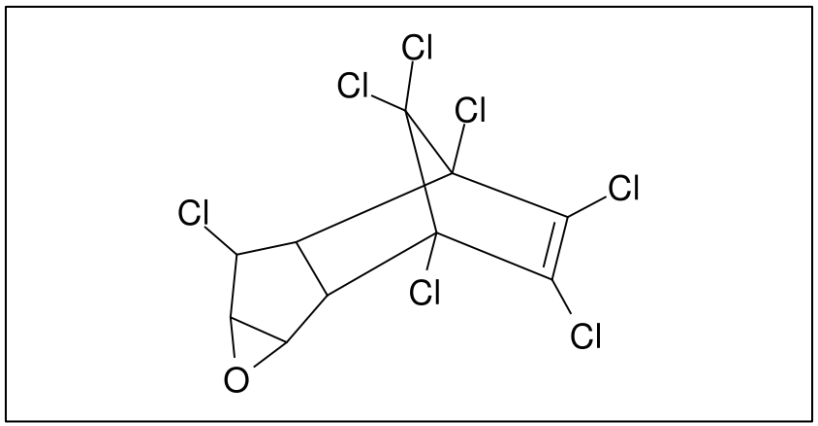
Elemental Formula: C10H5Cl7O

Source: anthropogenic

Class: legacy pesticide

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 281 | [M−3Cl]+ |
| 351 | [M−Cl]+ |

Filename: heptachlorepoxide

Name: nonachlor

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1347, RT (s) (2D): 0.84

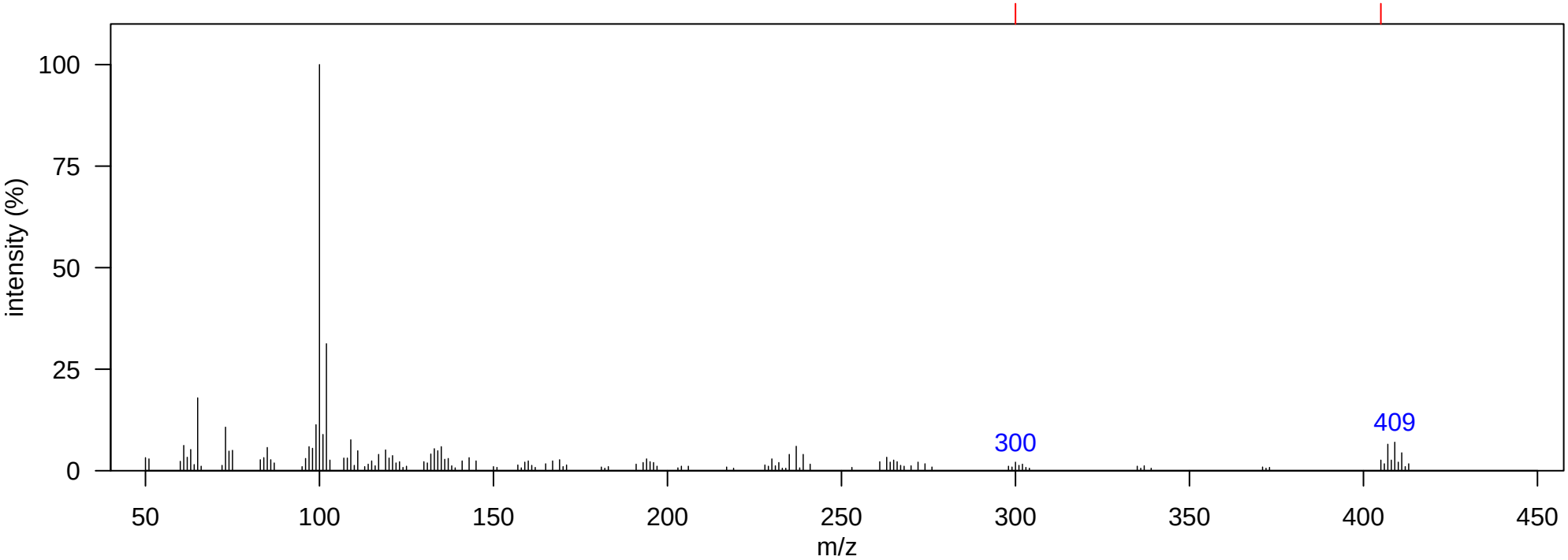
Comment: Isomer unknown.

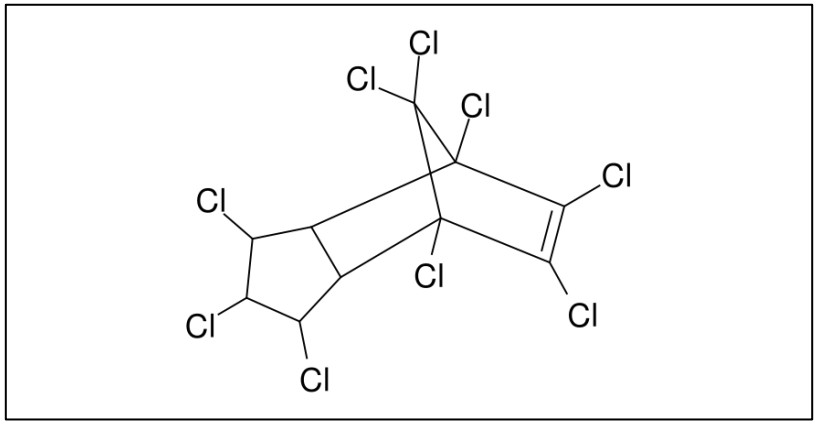
Elemental Formula: C10H5Cl9

Source: anthropogenic

Class: legacy pesticide

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 300 | [M−4Cl]+ |
| 405 | [M−Cl]+ |

Filename: nonachlor

Name: oxychlordane

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1308, RT (s) (2D): 0.84

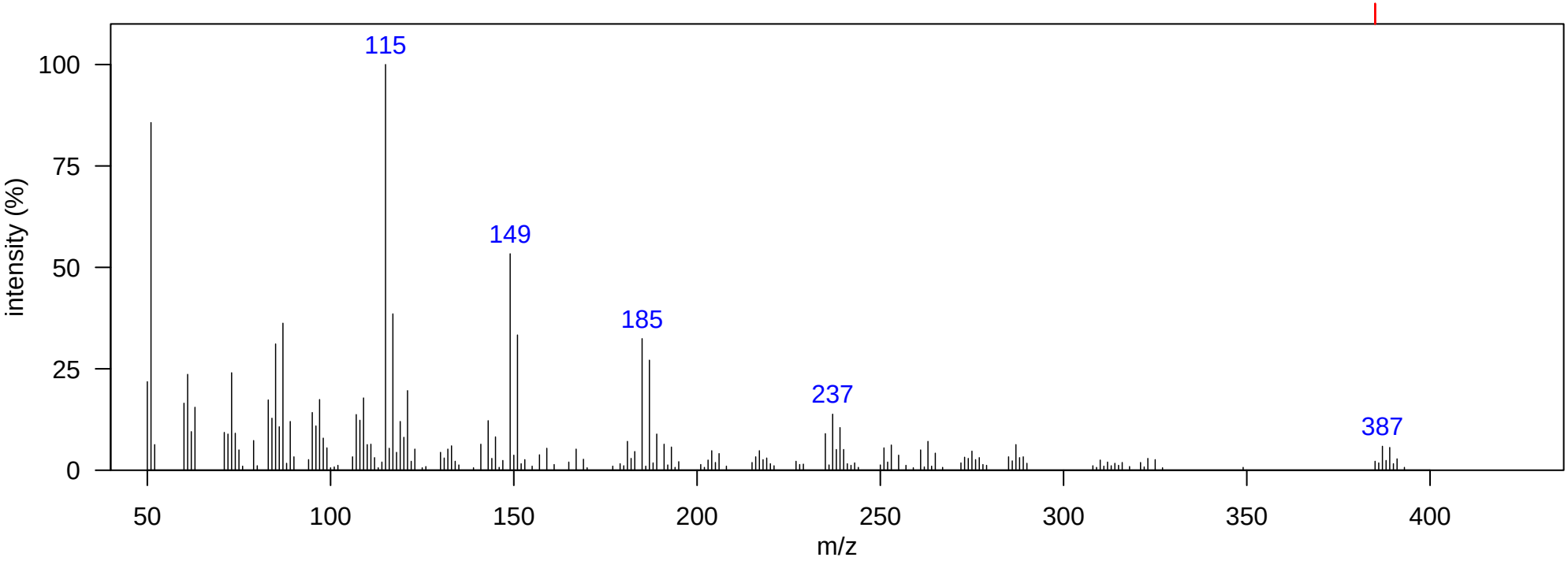
Comment: NA

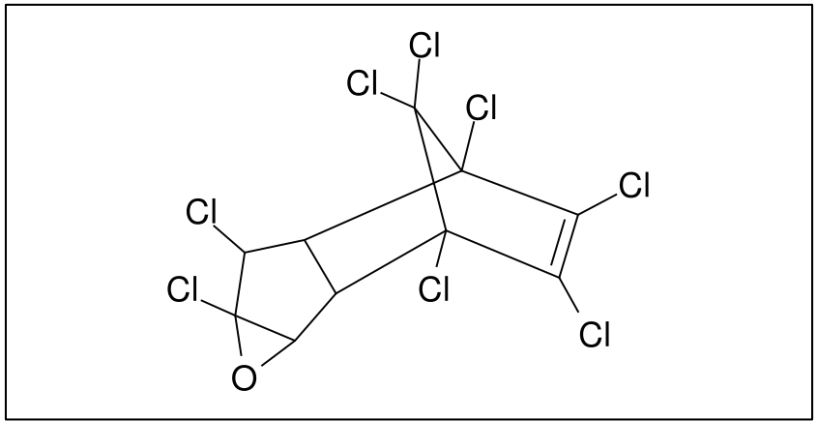
Elemental Formula: C10H4Cl8O

Source: anthropogenic

Class: legacy pesticide

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 385 | [M−Cl]+ |

Filename: oxychlordane

Name: mirex

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1569, RT (s) (2D): 0.99

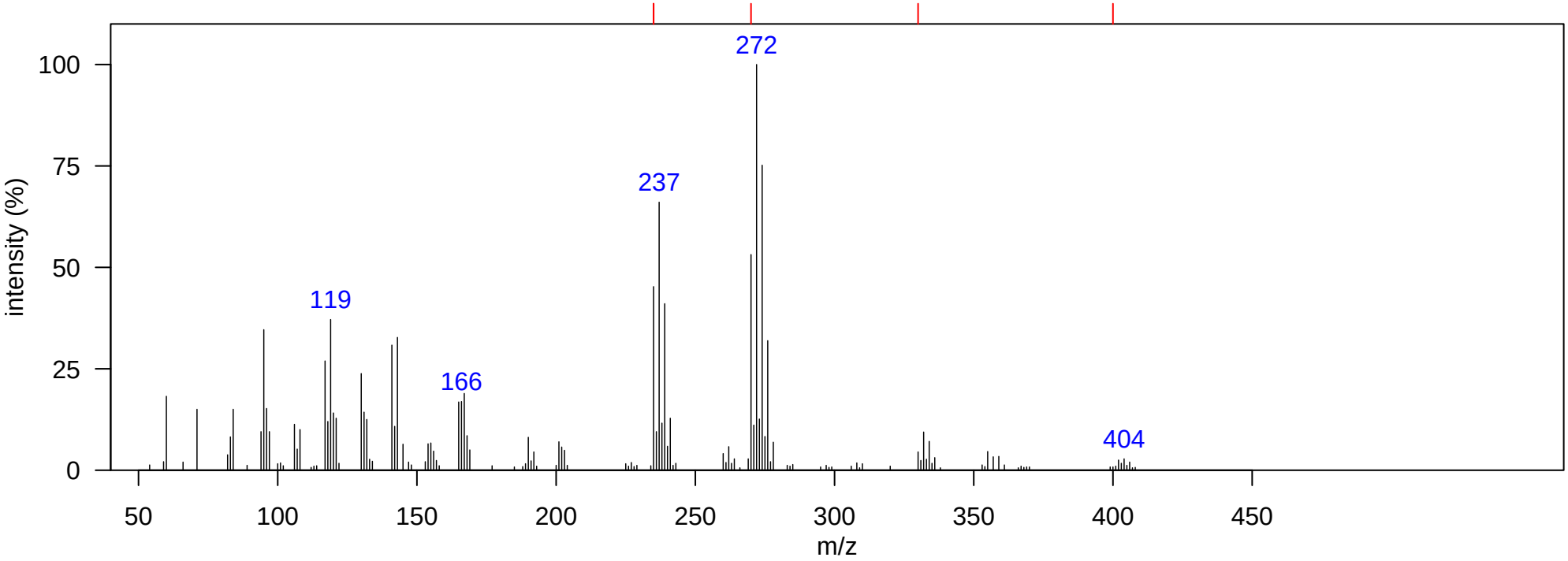
Comment: NA

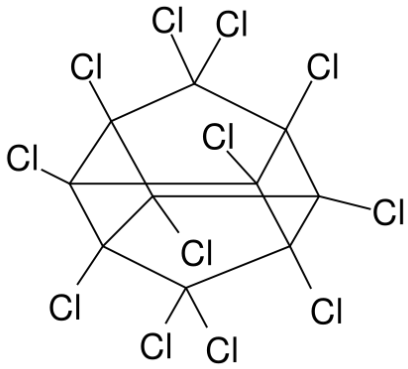
Elemental Formula: C10Cl12

Source: anthropogenic

Class: legacy pesticide

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 235 | [M−C5Cl7]+ |
| 270 | [M−C5Cl6]+ |
| 330 | [M−7Cl]+ |
| 400 | [M−4Cl]+ |

Filename: mirex

# Name: mirex (Cl11) (tentative)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1500, RT (s) (2D): 0.94

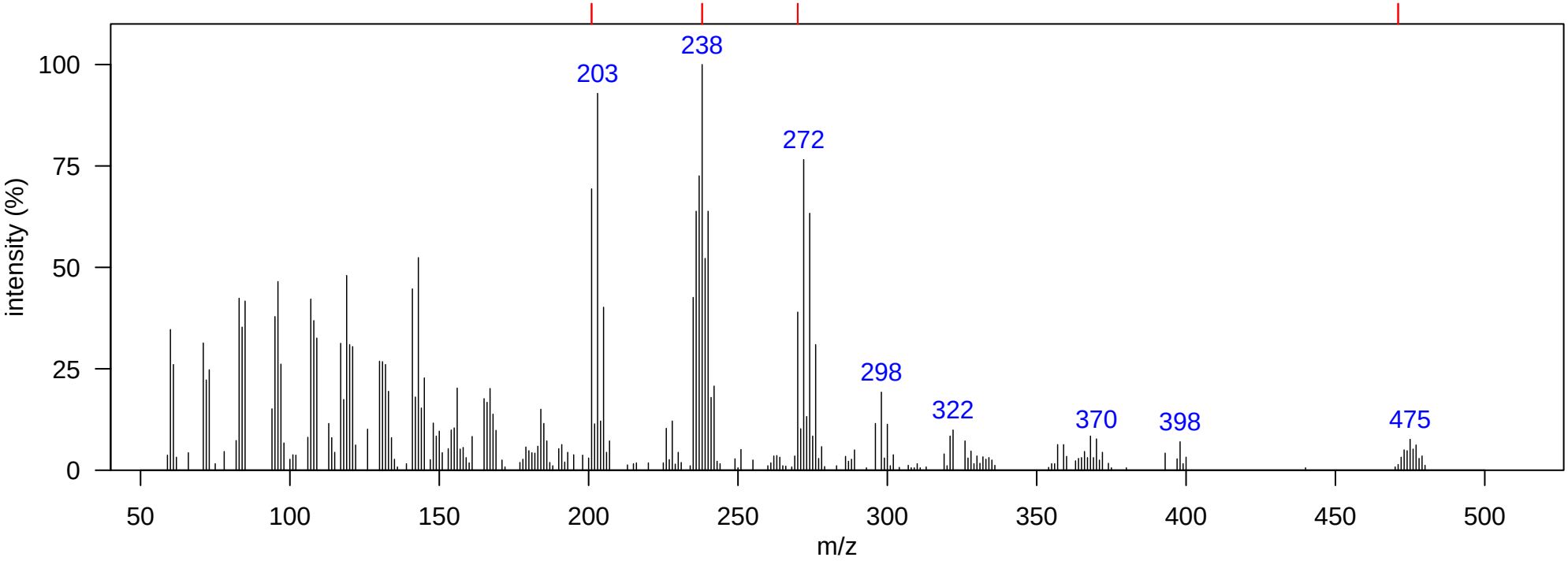
Comment: Degradation product or metabolite of mirex?

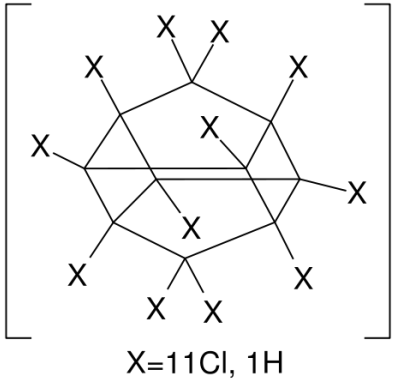
Elemental Formula: C10HCl11

Source: anthropogenic

Class: legacy pesticide

Identification: manual identification




| m/z | Identity |
|---|---|
| 201 | [M−C5Cl7]+ |
| 238 | overlap of [M−C5Cl6]+ and [M−C5HCl6]+ ? |
| 270 | [M−C5HCl5]+ |
| 471 | [M−Cl]+ |

Filename: mirexCl11

Name: unknown (possible dicofol)

Elemental Formula: C14H9Cl5O

Sample: southern CA sea lion blubber

Source: anthropogenic

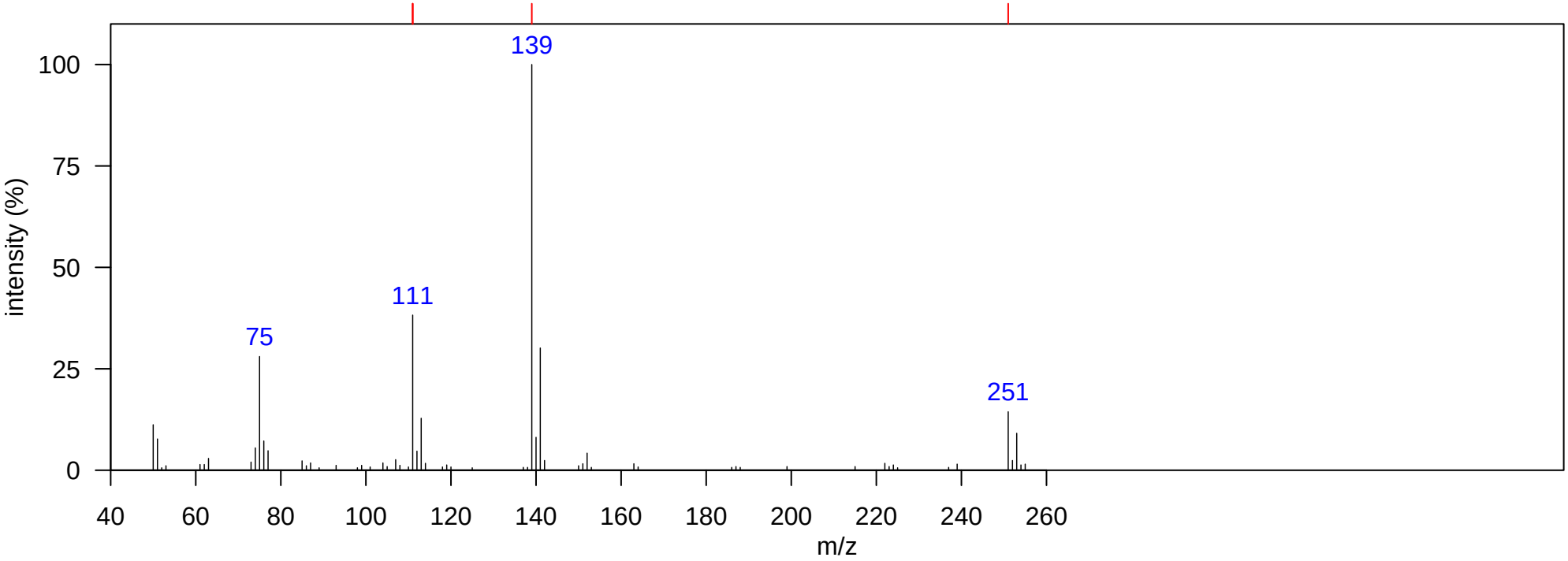
Instrument: GCxGC−TOF, electron impact, 70 eV

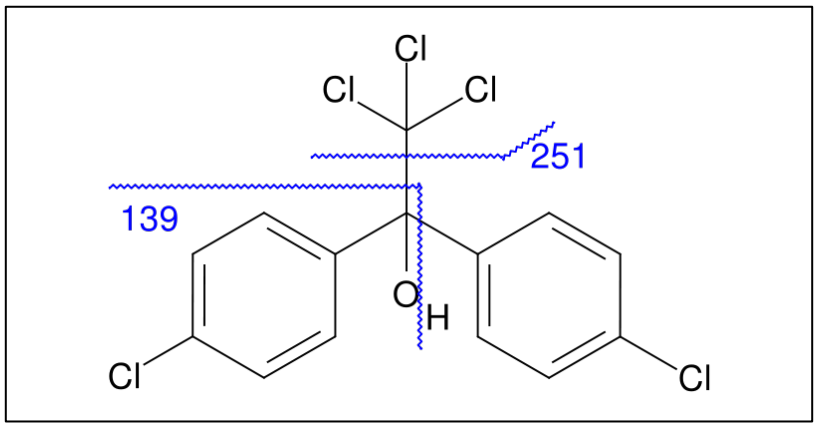
Class: unknown

RT (s) (1D): 1665, RT (s) (2D): 1.18

Identification: match to NIST 2008 library

Comment: Matches dicofol spectrum, but lack of molecular ion makes identification uncertain.




| m/z | Identity |
|---|---|
| 111 | [M−COH−CCl3−C6H4Cl]+ or [C6H4Cl]+ |
| 139 | [M−C6H4Cl−CCl3−H]+ |
| 251 | [M−CCl3]+ |

Filename: dicofol

Name: phenanthrene

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1149, RT (s) (2D): 0.89

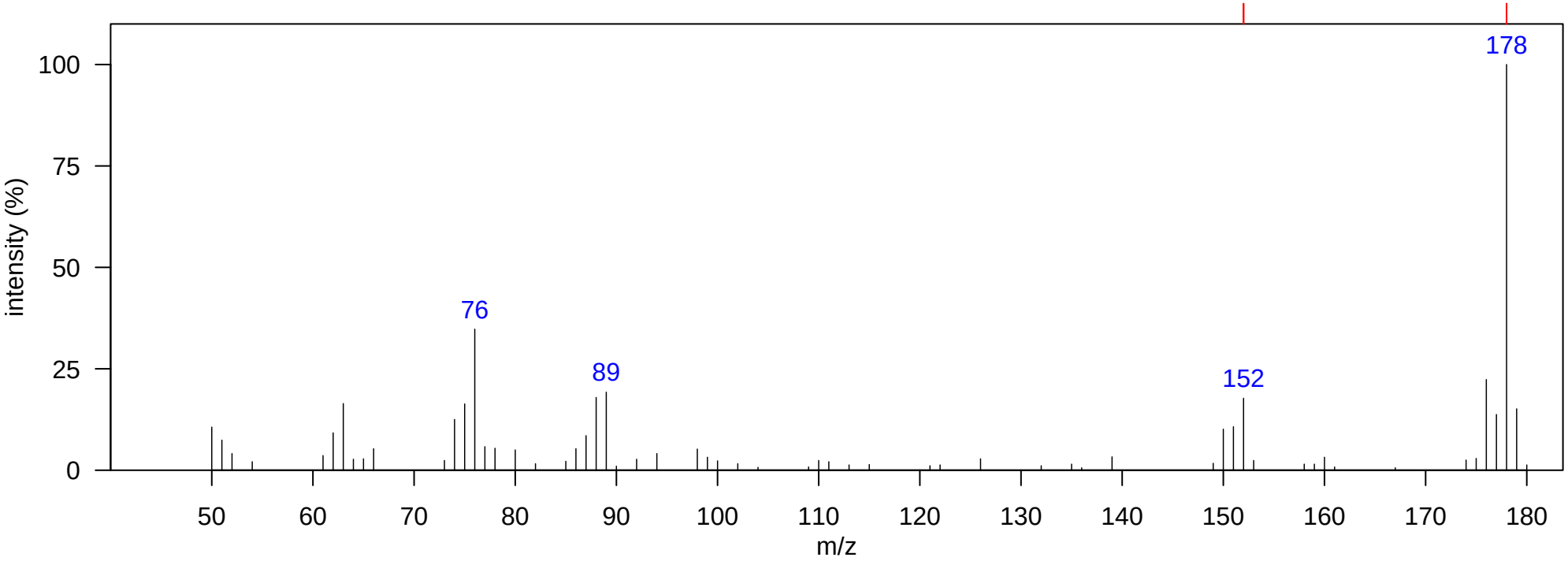
Comment: NA

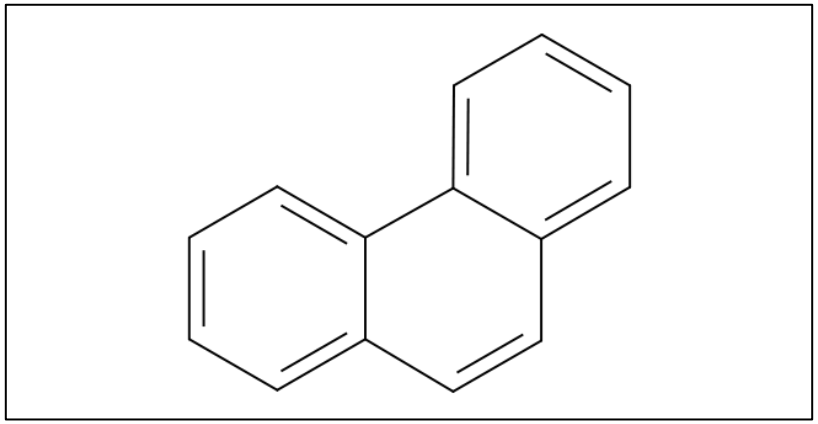
Elemental Formula: C14H10

Source: anthropogenic

Class: PAH

Identification: match to NIST 2008 library



| m/z | Identity |
|---|---|
| 152 | [M−C2H2]+ |
| 178 | M+ |
| 188 | interference |

Filename: phenanthrene

Name: pyrene

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1347, RT (s) (2D): 0.99

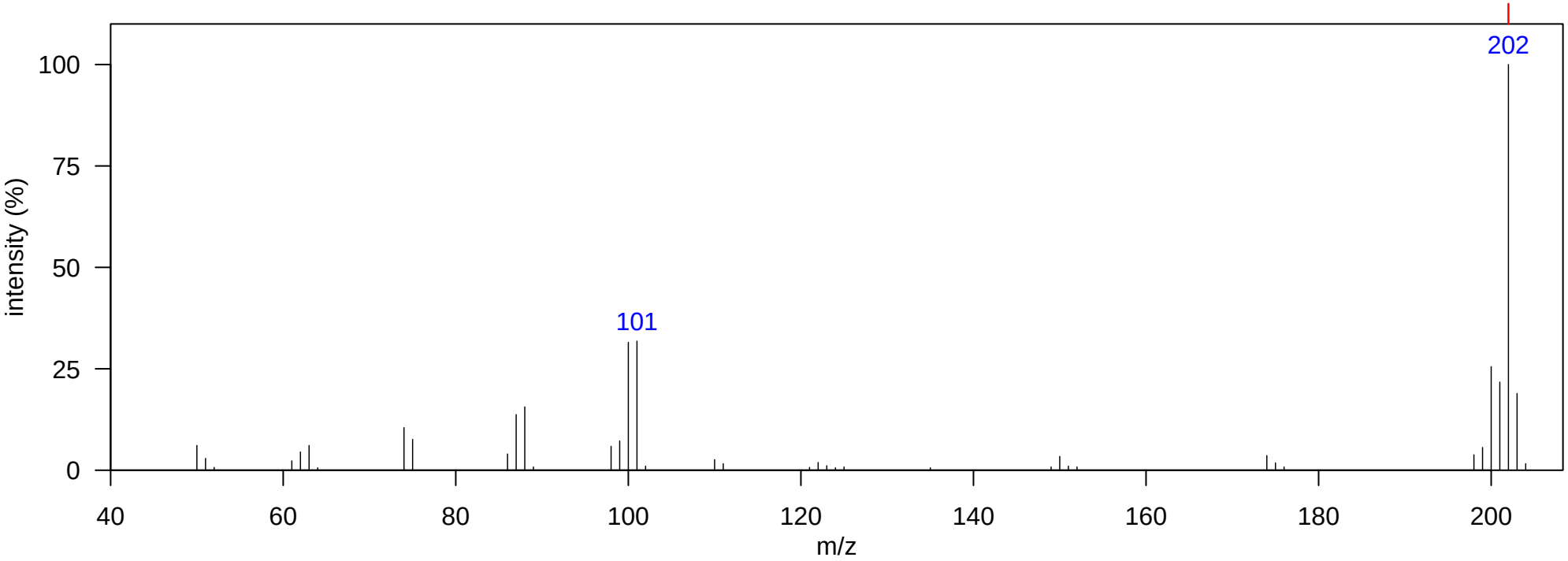
Comment: NA

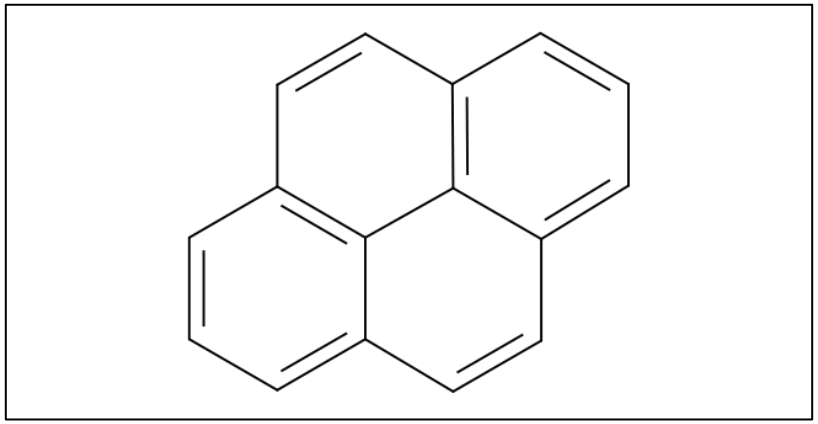
Elemental Formula: C16H10

Source: anthropogenic

Class: PAH

Identification: match to NIST 2008 library



| m/z | Identity |
|---|---|
| 202 | M+ |

Filename: pyrene

# Name: tetra brominated biphenyl (tetra−BB)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1455, RT (s) (2D): 0.97

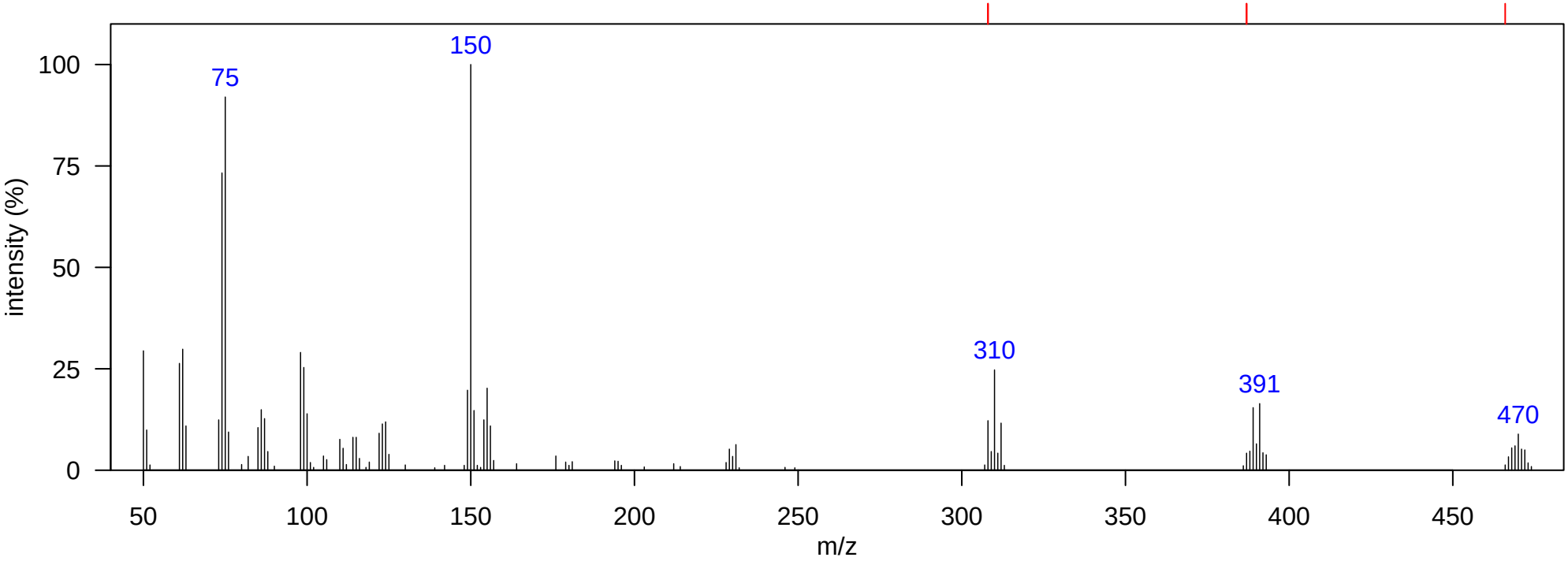
Comment: Isomer unknown.

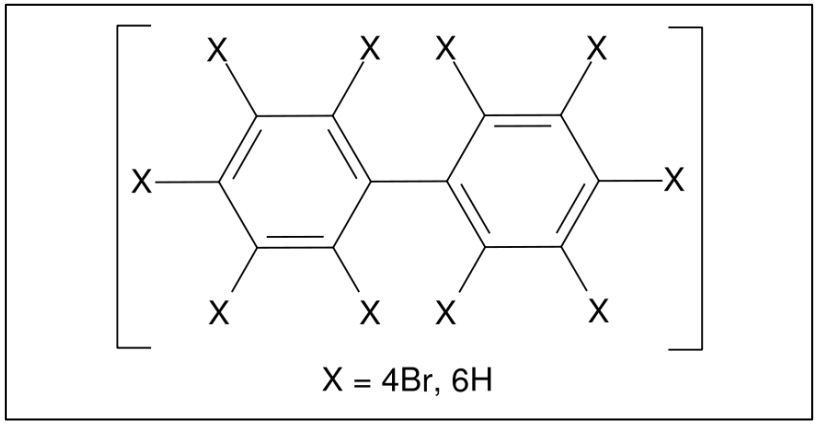
Elemental Formula: C12H6Br4

Source: anthropogenic

Class: BB

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 308 | [M−2Br]+ |
| 387 | [M−Br]+ |
| 466 | M+ |

Filename: tetraBB

# Name: tri brominated diphenyl ether (tri−BDE)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): NA, RT (s) (2D): NA

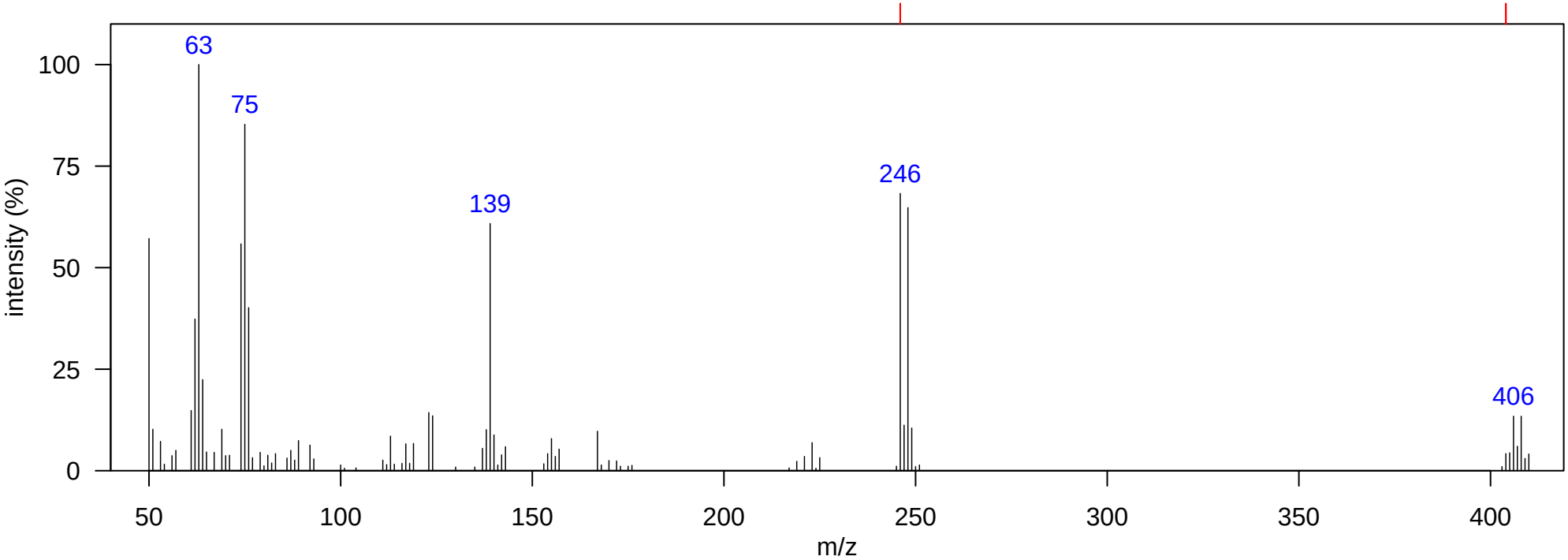
Comment: Two unknown isomers detected; one shown.

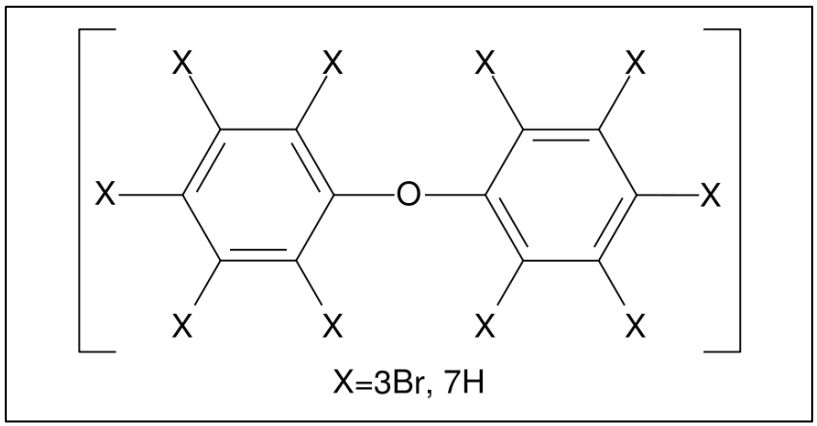
Elemental Formula: C12H7Br3O

Source: anthropogenic

Class: PBDE

Identification: manual identification




| m/z | Identity |
|---|---|
| 246 | [M−2Br]+ |
| 404 | M+ |

Filename: triBDE

Name: tetra brominated diphenyl ether (tetra−BDE)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1536, RT (s) (2D): 1.05

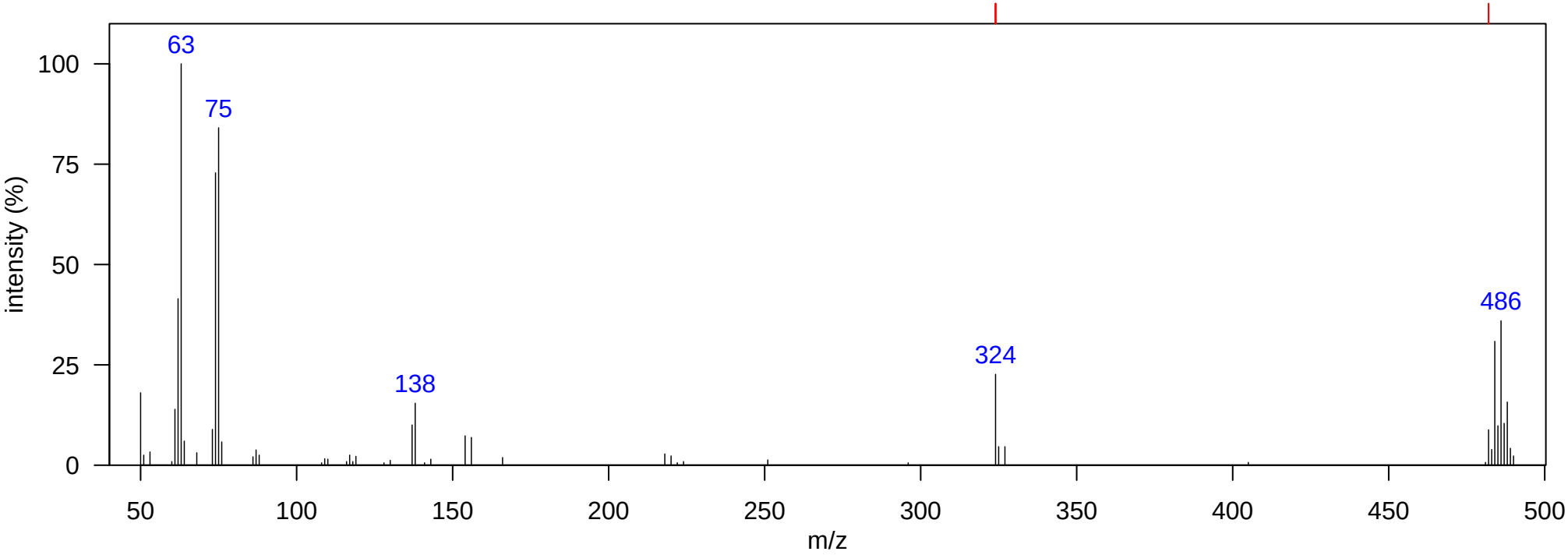
Comment: Isomer unknown.

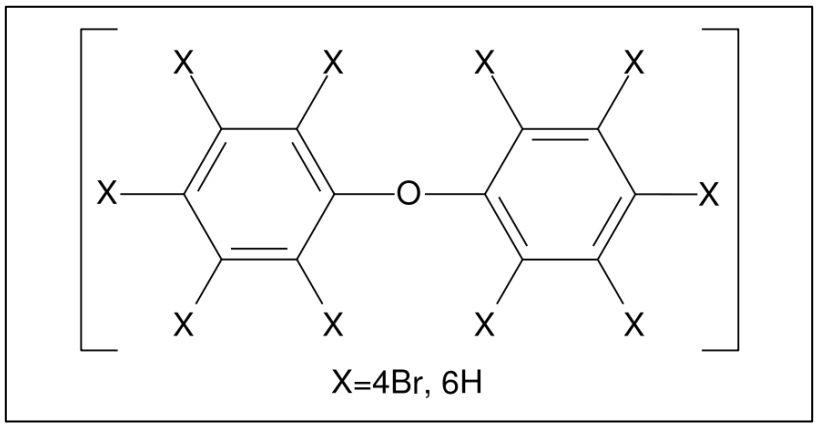
Elemental Formula: C12H6Br4O

Source: anthropogenic

Class: PBDE

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 324 | [M−2Br]+ |
| 482 | M+ |

Filename: tetraBDE

# Name: penta brominated diphenyl ether (penta−BDE) isomer 1

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1632, RT (s) (2D): 1.19

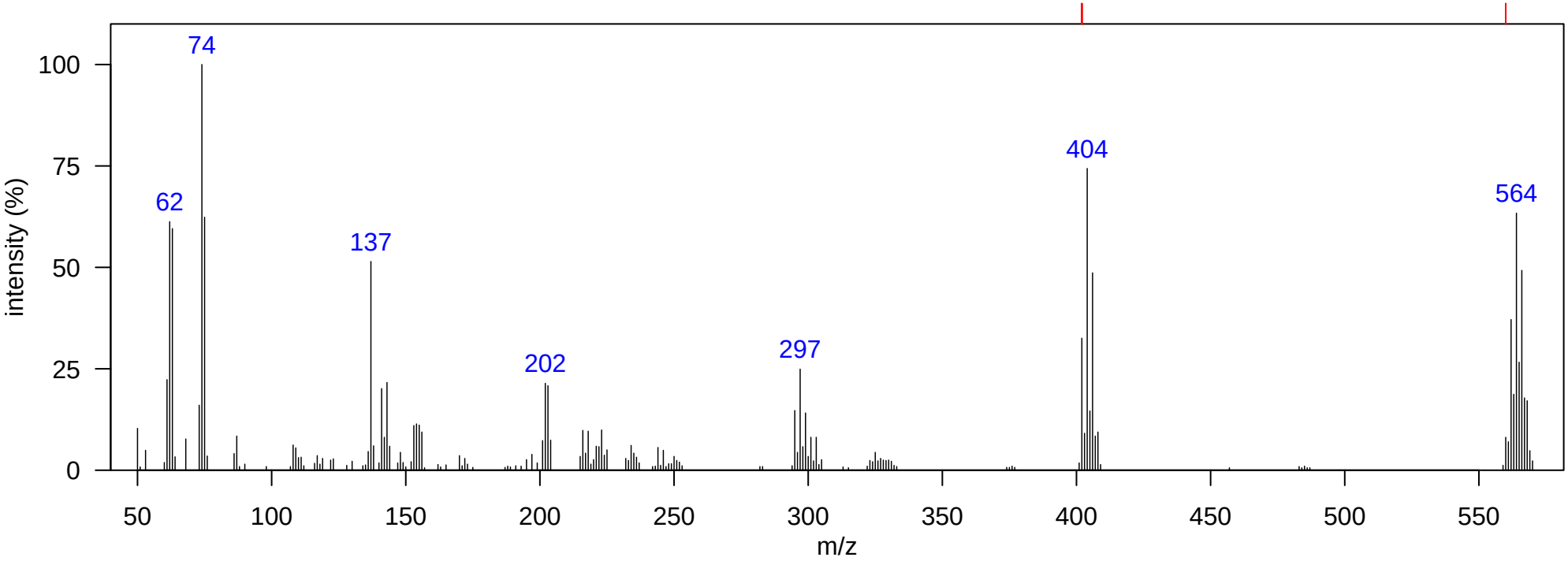
Comment: Isomer unknown; likely BDE−100.

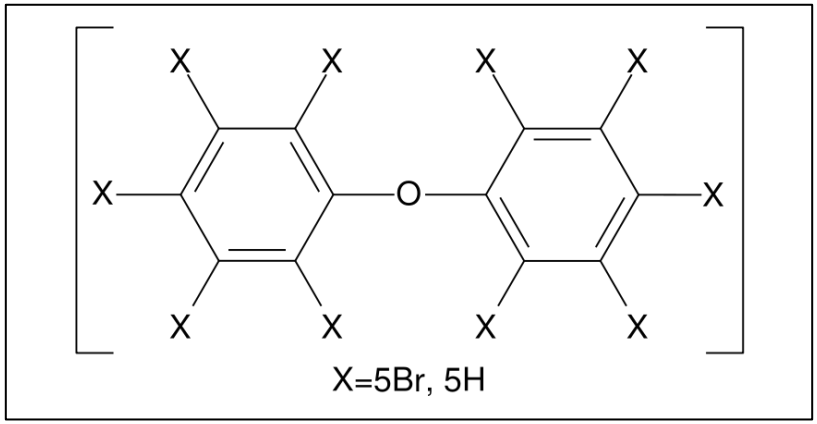
Elemental Formula: C12H5Br5O

Source: anthropogenic

Class: PBDE

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 402 | [M−2Br]+ |
| 560 | M+ |

Filename: pentaBDE1

# Name: penta brominated diphenyl ether (penta−BDE) isomer 2

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1659, RT (s) (2D): 1.23

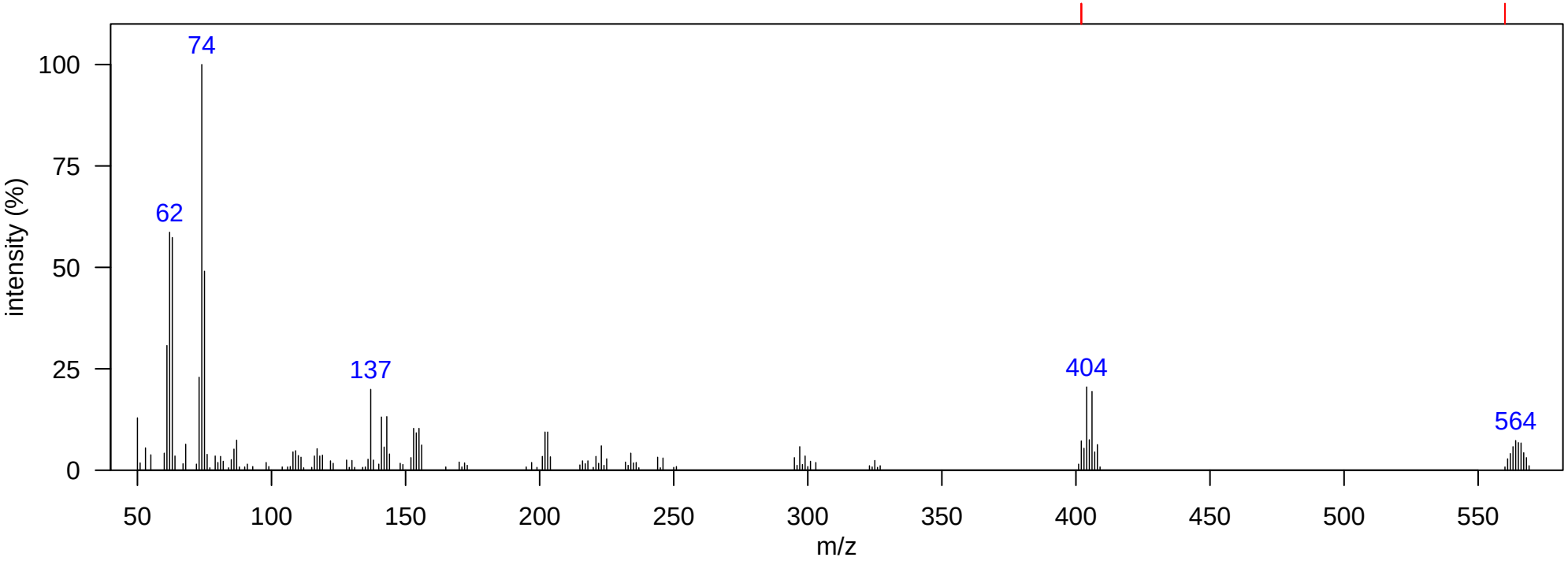
Comment: Isomer unknown; likely BDE−99.

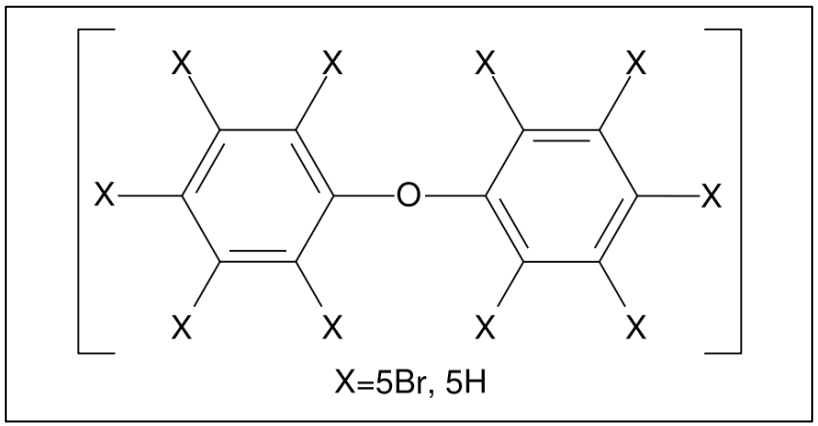
Elemental Formula: C12H5Br5O

Source: anthropogenic

Class: PBDE

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 402 | [M−2Br]+ |
| 560 | M+ |

Filename: pentaBDE2

# Name: hexa brominated diphenyl ether (hexa−BDE)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1761, RT (s) (2D): 1.52

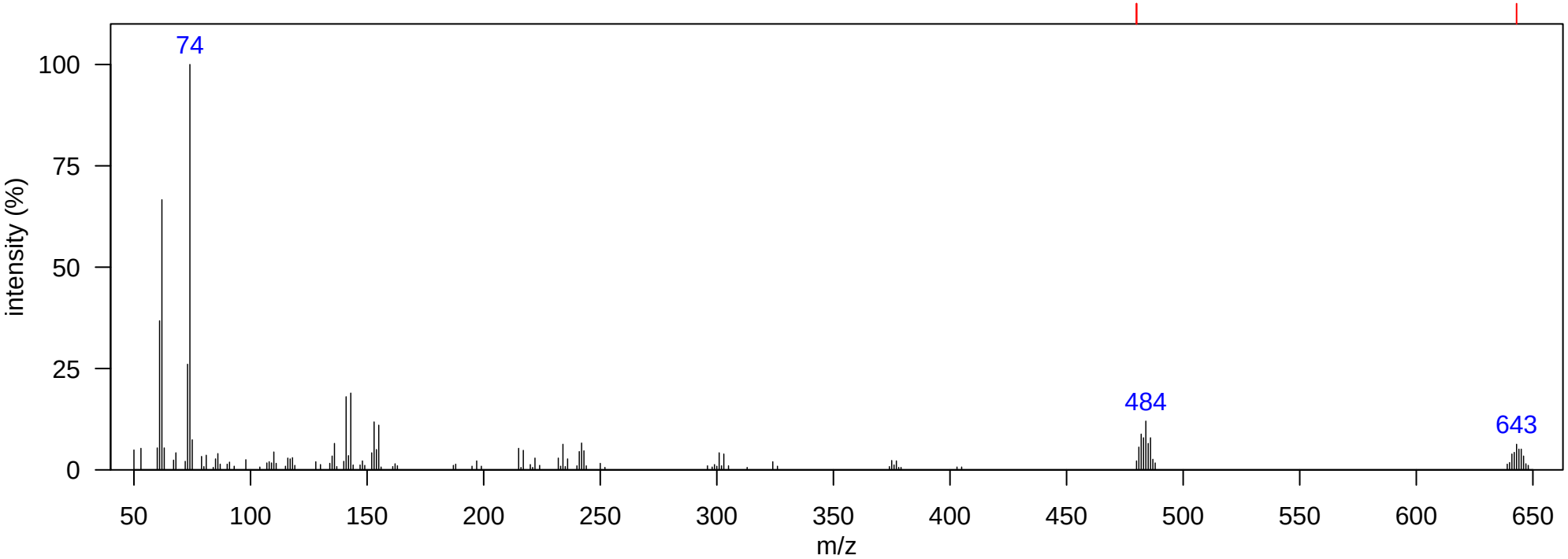
Comment: Isomer unknown.

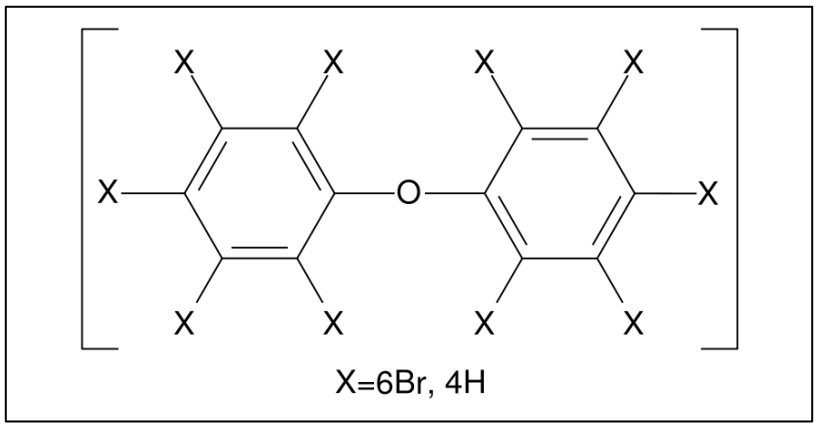
Elemental Formula: C12H4Br6O

Source: anthropogenic

Class: PBDE

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 480 | [M−2Br]+ |
| 643 | M+ (not monoisotopic) |

Filename: hexaBDE

Name: tri chlorinated biphenyl (tri−PCB)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1236, RT (s) (2D): 0.83

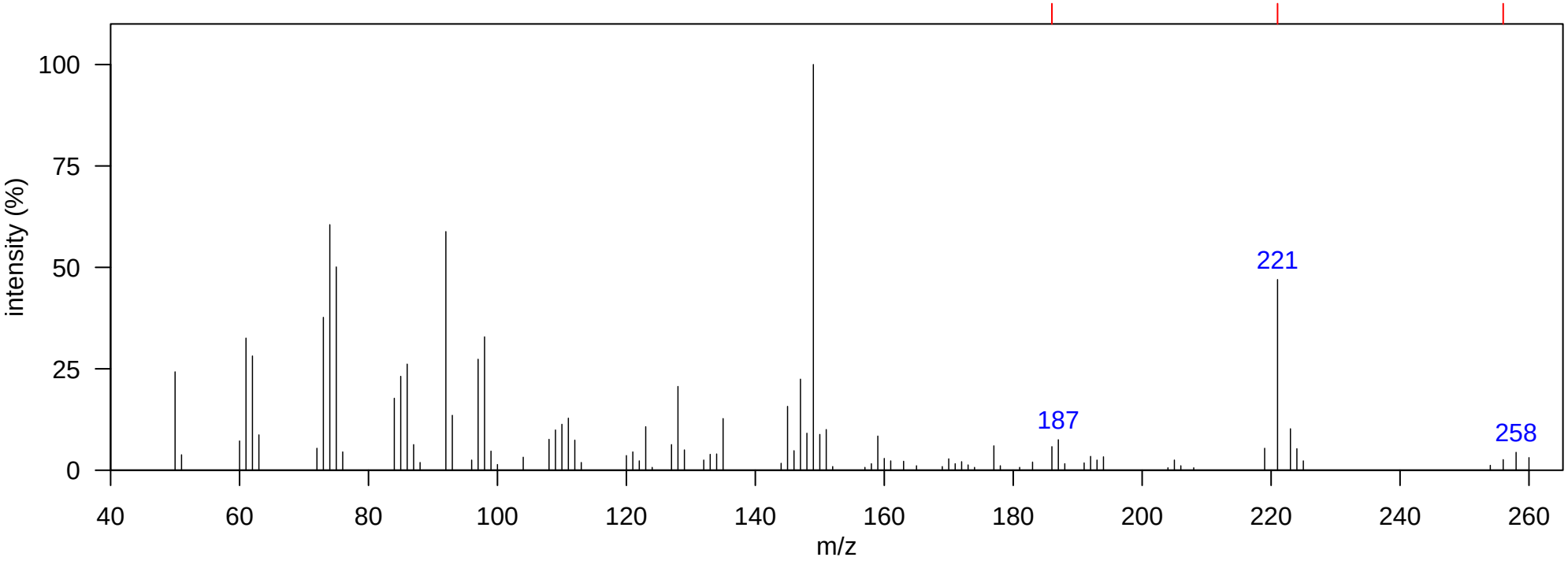
Comment: Isomer unknown.

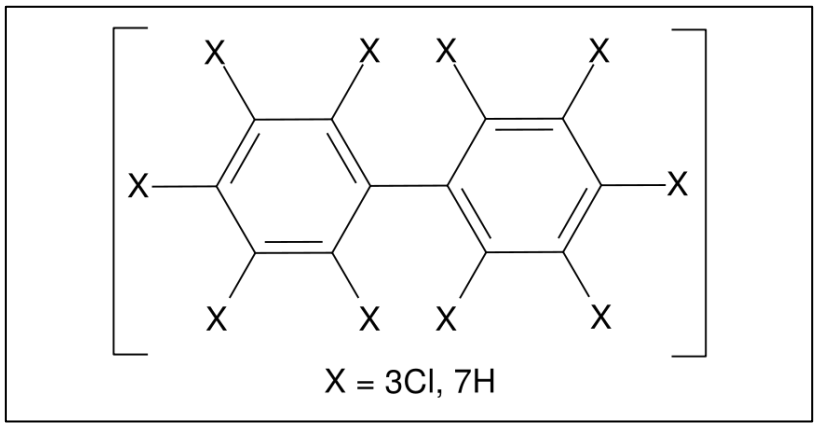
Elemental Formula: C12H7Cl3

Source: anthropogenic

Class: PCB

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 186 | [M−2Cl]+ |
| 221 | [M−Cl]+ |
| 256 | M+ |

Filename: triPCB

# Name: tetra chlorinated biphenyl (tetra−PCB)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): NA, RT (s) (2D): NA

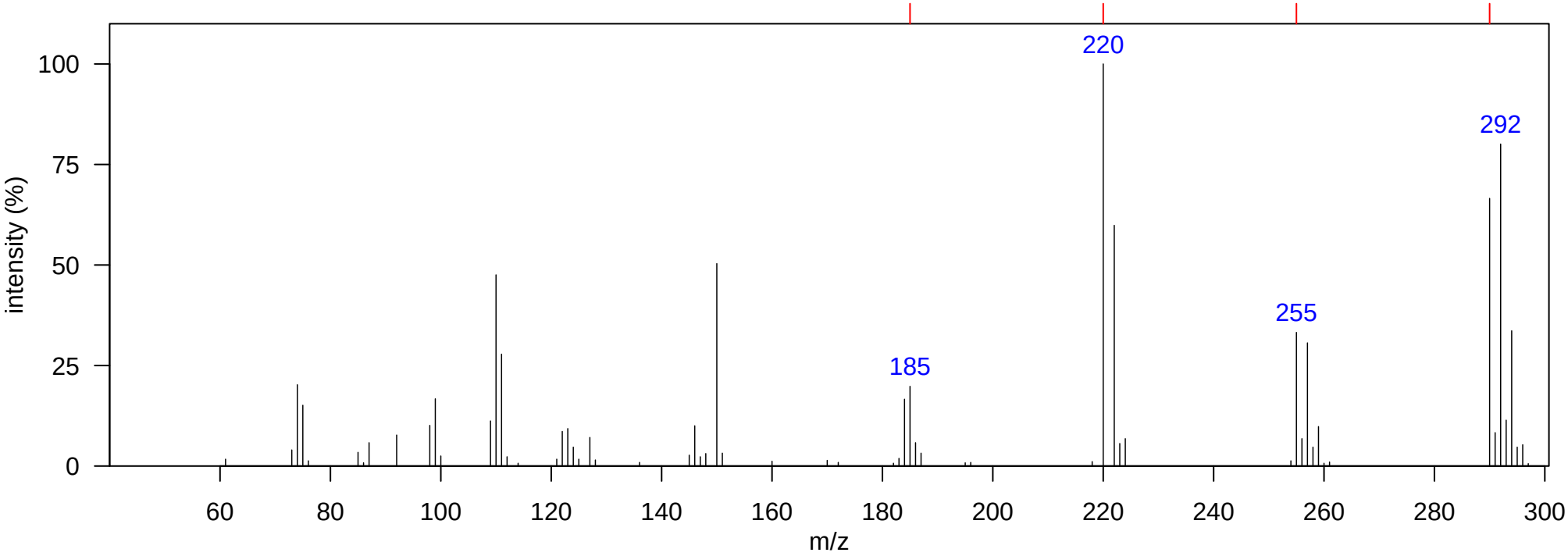
Comment: Seven unknown isomers detected; one shown.

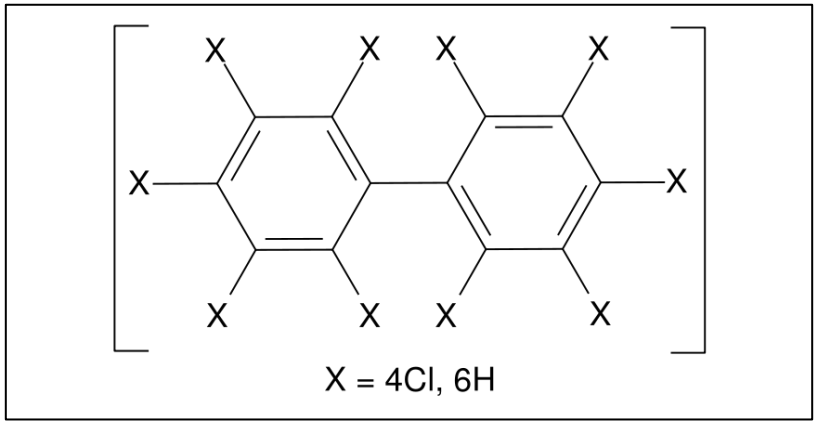
Elemental Formula: C12H6Cl4

Source: anthropogenic

Class: PCB

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 185 | [M−3Cl]+ |
| 220 | [M−2Cl]+ |
| 255 | [M−Cl]+ |
| 290 | M+ |

Filename: tetraPCB

# Name: penta chlorinated biphenyl (penta−PCB)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): NA, RT (s) (2D): NA

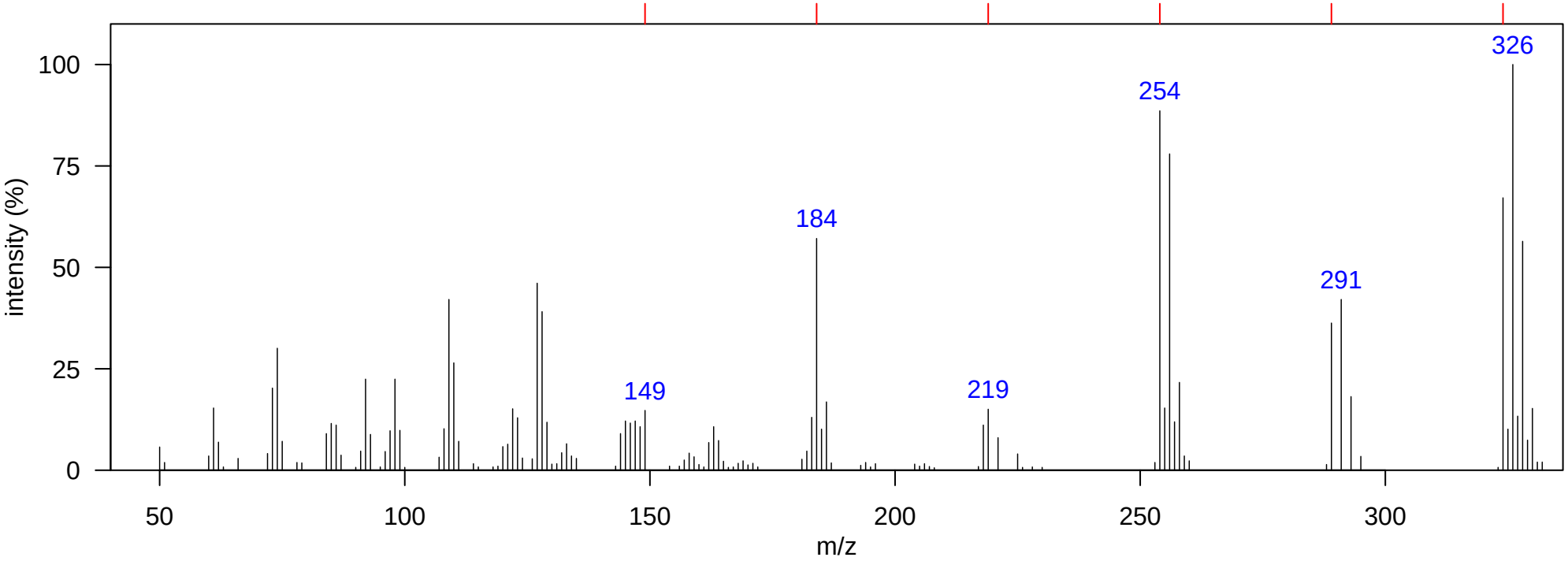
Comment: Nine unknown isomers detected; one shown.

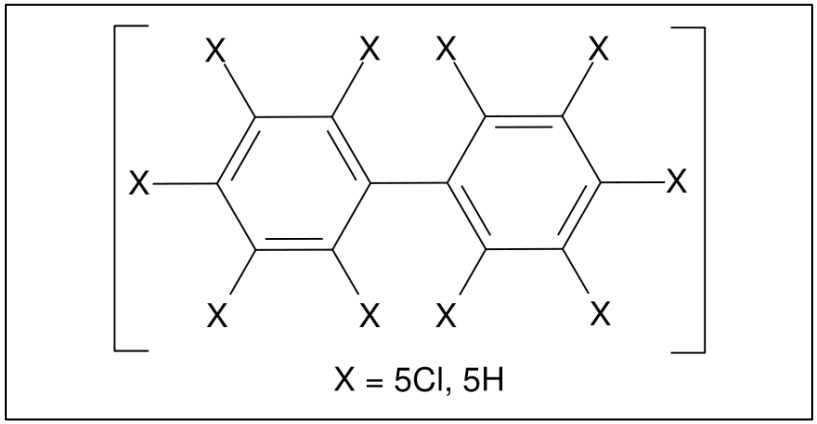
Elemental Formula: C12H5Cl5

Source: anthropogenic

Class: PCB

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 149 | [M−5Cl]+ |
| 184 | [M−4Cl]+ |
| 219 | [M−3Cl]+ |
| 254 | [M−2Cl]+ |
| 289 | [M−Cl]+ |
| 324 | M+ |

Filename: pentaPCB

# Name: hexa chlorinated biphenyl (hexa−PCB)

Elemental Formula: C12H4Cl6

Sample: southern CA sea lion blubber

Source: anthropogenic

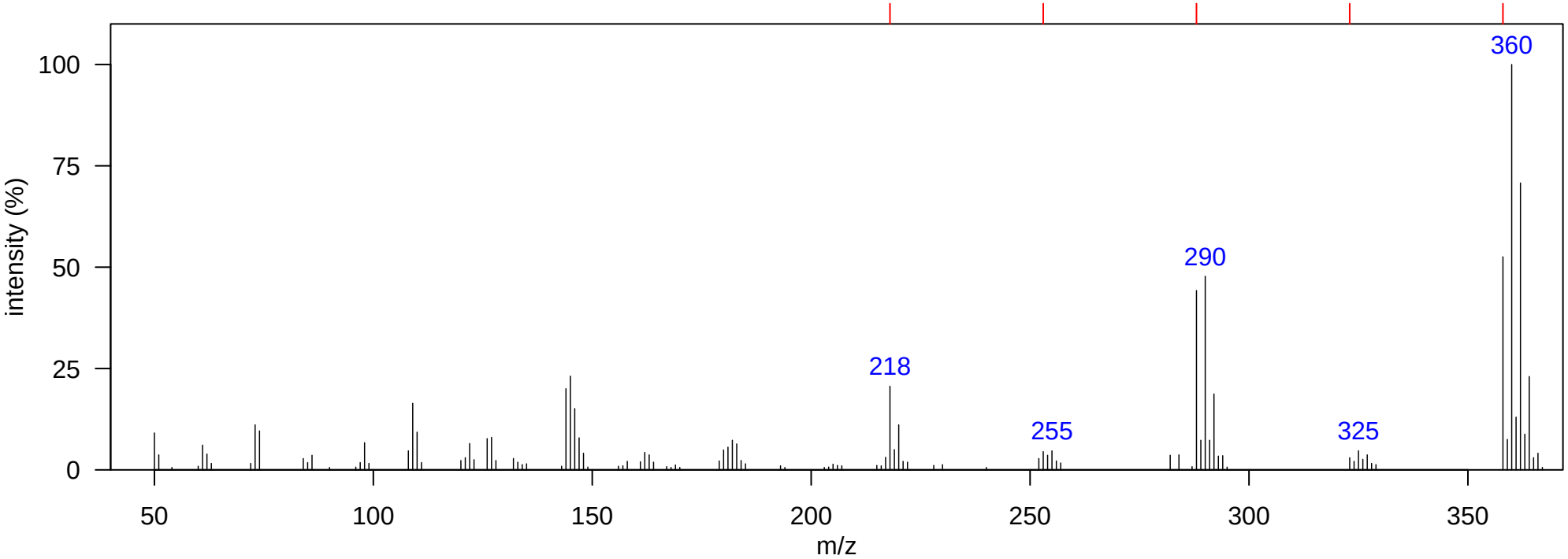
Instrument: GCxGC−TOF, electron impact, 70 eV

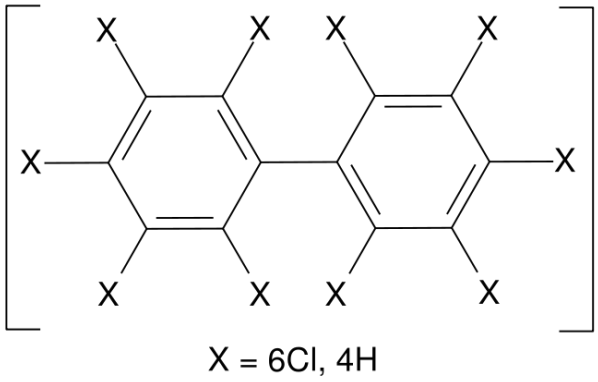
Class: PCB

RT (s) (1D): NA, RT (s) (2D): NA

Identification: match to NIST 2008 library

Comment: Nineteen unknown isomers detected; one shown.




| m/z | Identity |
|---|---|
| 218 | [M−4Cl]+ |
| 253 | [M−3Cl]+ |
| 288 | [M−2Cl]+ |
| 323 | [M−Cl]+ |
| 358 | M+ |

Filename: hexaPCB

# Name: hepta chlorinated biphenyl (hepta−PCB)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): NA, RT (s) (2D): NA

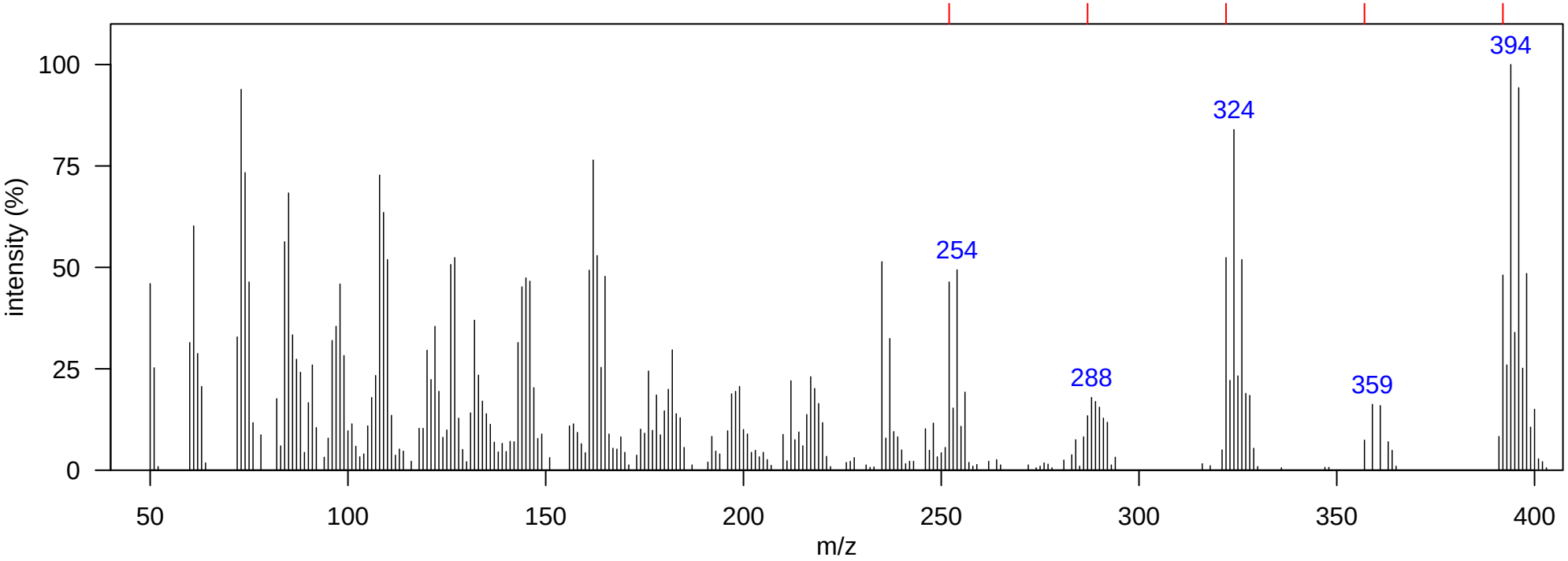
Comment: Nine unknown isomers detected; one shown.

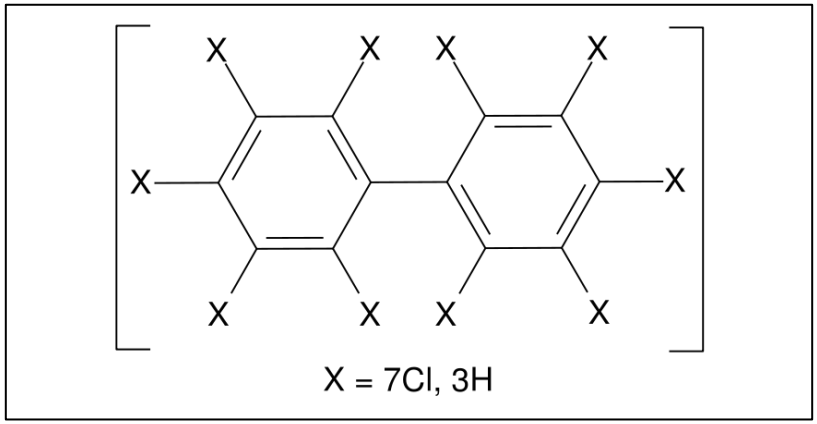
Elemental Formula: C12H3Cl7

Source: anthropogenic

Class: PCB

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 252 | [M−4Cl]+ |
| 287 | [M−3Cl]+ |
| 322 | [M−2Cl]+ |
| 357 | [M−Cl]+ |
| 392 | M+ |

Filename: heptaPCB

# Name: octa chlorinated biphenyl (octa−PCB)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): NA, RT (s) (2D): NA

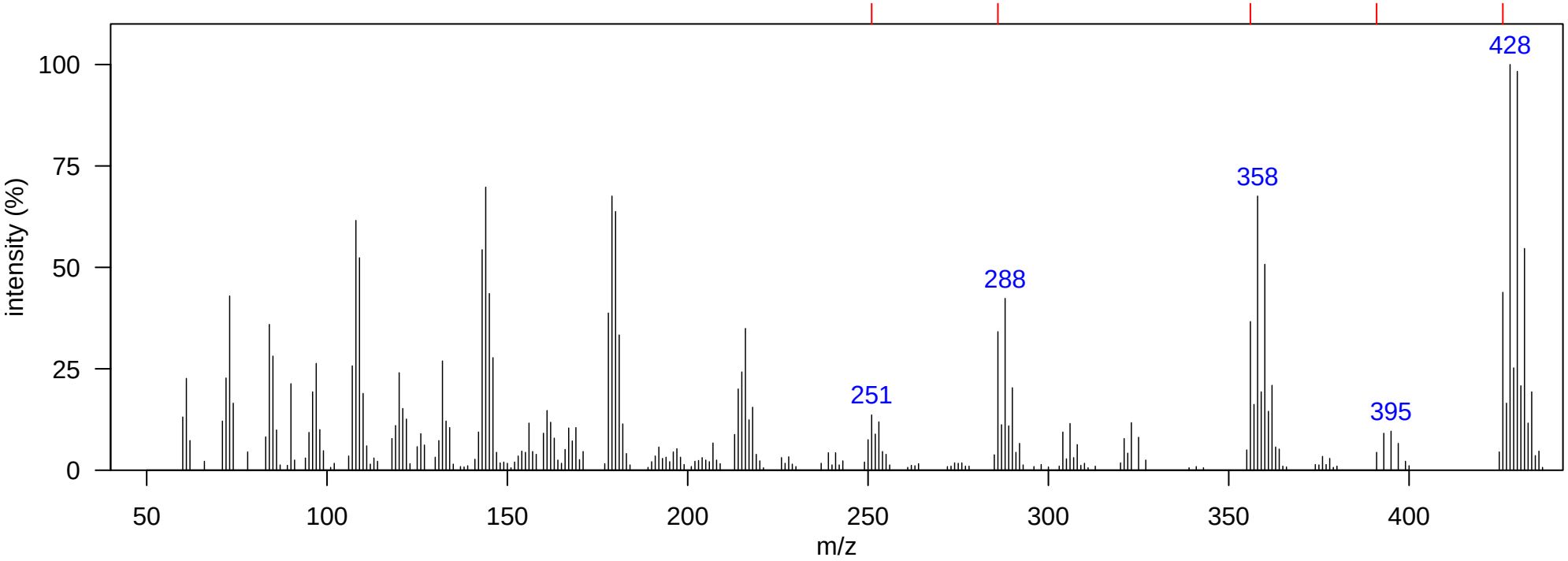
Comment: Seven unknown isomers detected; one shown.

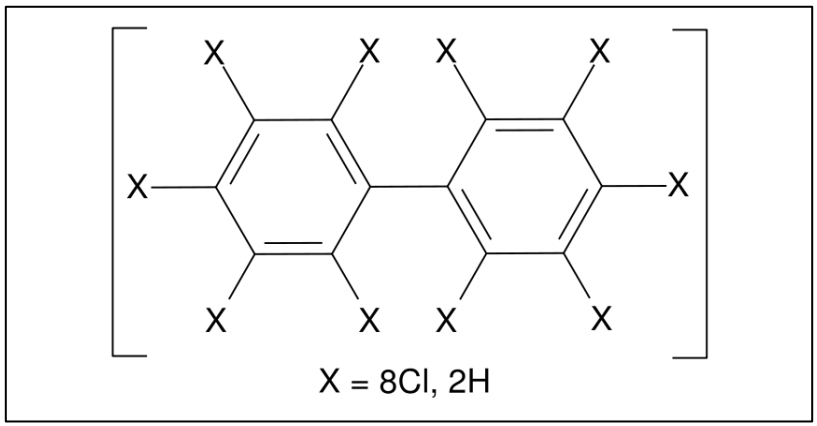
Elemental Formula: C12H2Cl8

Source: anthropogenic

Class: PCB

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 251 | [M−5Cl]+ |
| 286 | [M−4Cl]+ |
| 356 | [M−2Cl]+ |
| 391 | [M−Cl]+ |
| 426 | M+ |

Filename: octaPCB

# Name: hexa chlorinated diphenyl ether (hexa−CDE) isomer 1

Elemental Formula: C12H4Cl6O

Sample: southern CA sea lion blubber

Source: anthropogenic

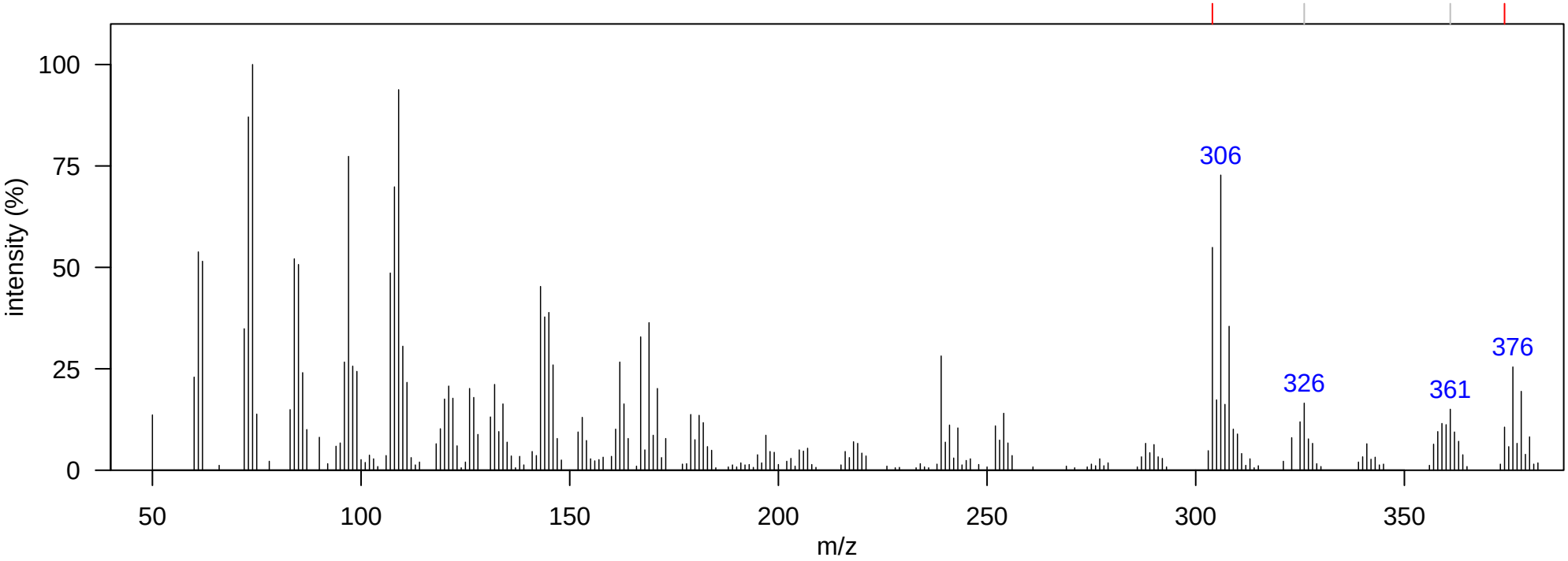
Instrument: GCxGC−TOF, electron impact, 70 eV

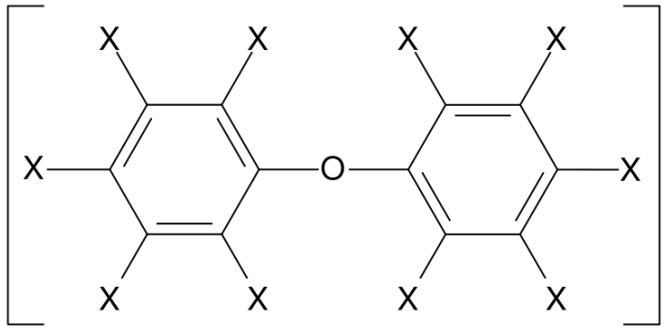
Class: PCDE

RT (s) (1D): 1467, RT (s) (2D): 0.87

Identification: manual identification

Comment: Isomer unknown. Reference: Environment International, 2006, 32, 121−127, doi:10.1016/j.envint.2005.05.021




| m/z | Identity |
|---|---|
| 304 | [M−2Cl]+ |
| 326 | hepta−PCB interference |
| 361 | hepta−PCB interference |
| 374 | M+ |
| 395 | hepta−PCB interference |

Filename: hexaCDE1

# Name: hexa chlorinated diphenyl ether (hexa−CDE) isomer 2

Elemental Formula: C12H4Cl6O

Sample: southern CA sea lion blubber

Source: anthropogenic

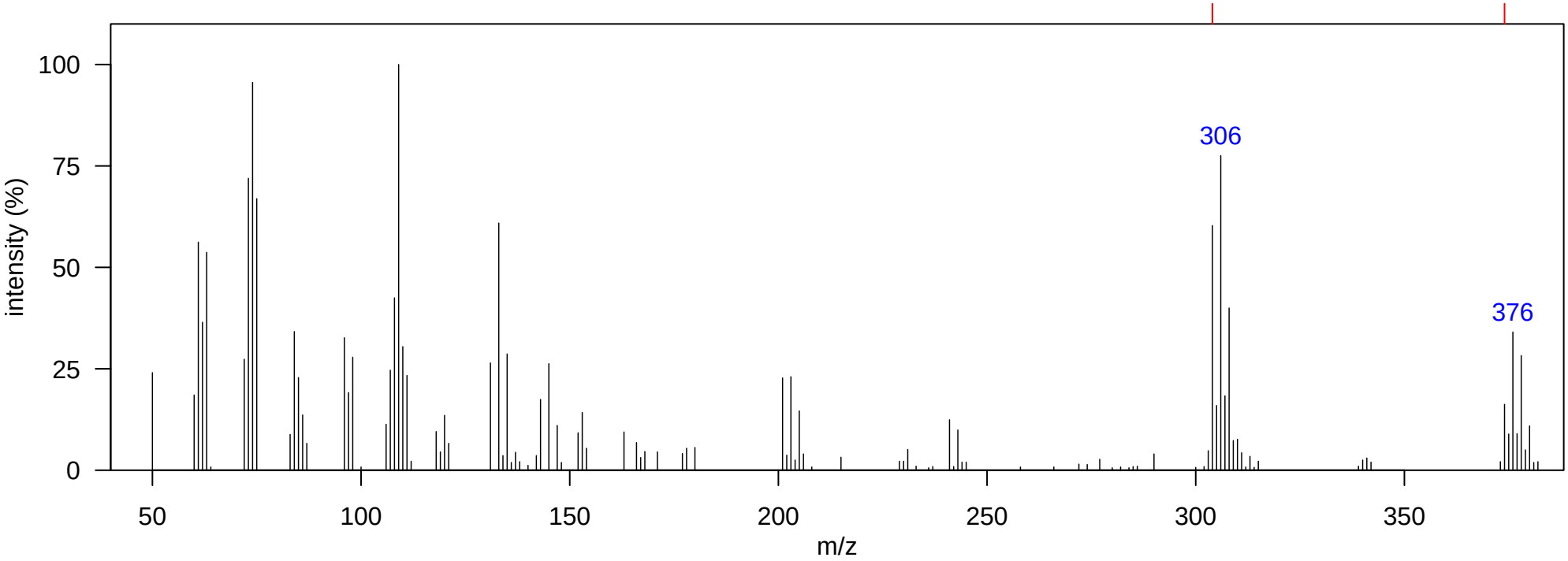
Instrument: GCxGC−TOF, electron impact, 70 eV

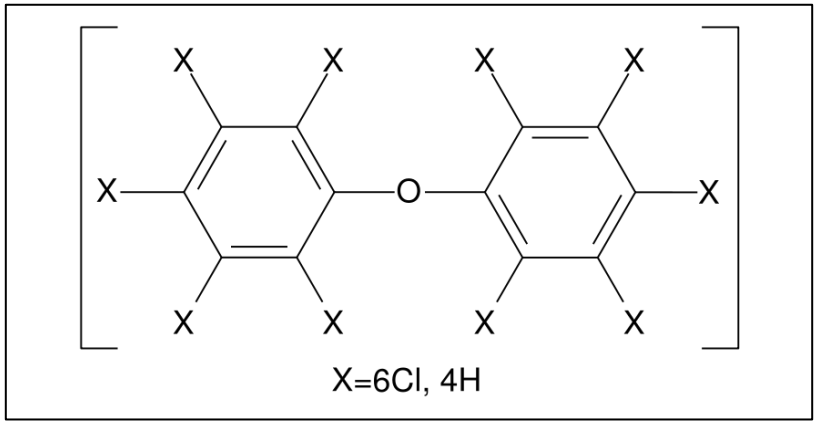
Class: PCDE

RT (s) (1D): 1473, RT (s) (2D): 0.9

Identification: manual identification

Comment: Isomer unknown. Reference: Environment International, 2006, 32, 121−127, doi:10.1016/j.envint.2005.05.021




| m/z | Identity |
|---|---|
| 304 | [M−2Cl]+ |
| 374 | M+ |

Filename: hexaCDE2

Name: bisphenol A

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1359, RT (s) (2D): 0.99

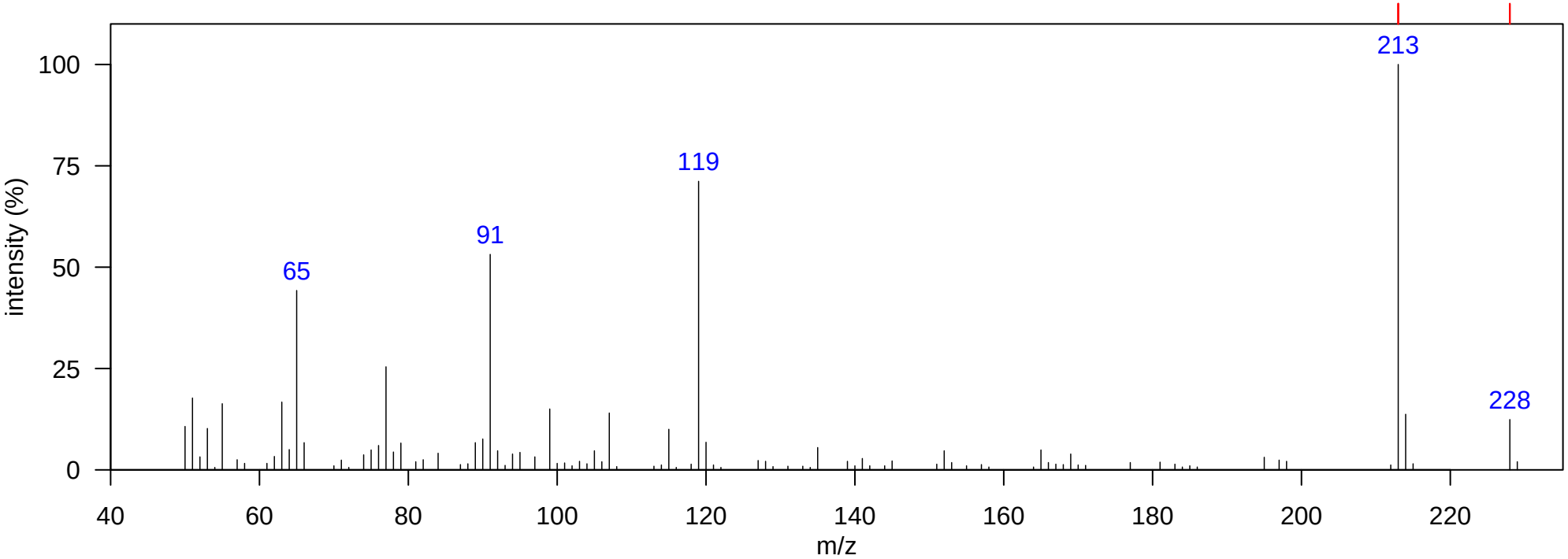
Comment: Found in hexane:DCM (1:1 v/v) SPE fraction.

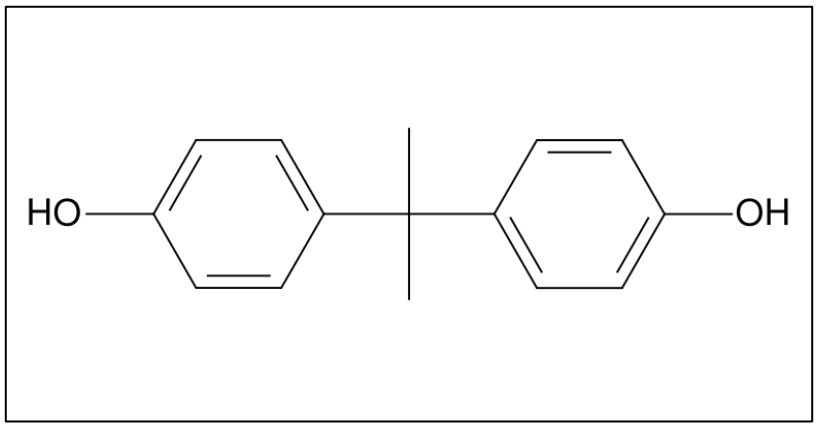
Elemental Formula: C15H16O2

Source: anthropogenic

Class: phenolic

Identification: match to NIST 2008 library




| m/z | Identity |
|---|---|
| 213 | [M−CH3]+ |
| 228 | M+ |

Filename: bisphenolA

Name: hepta chlorinated methyl bipyrrole (hepta−MBP)

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1350, RT (s) (2D): 0.87

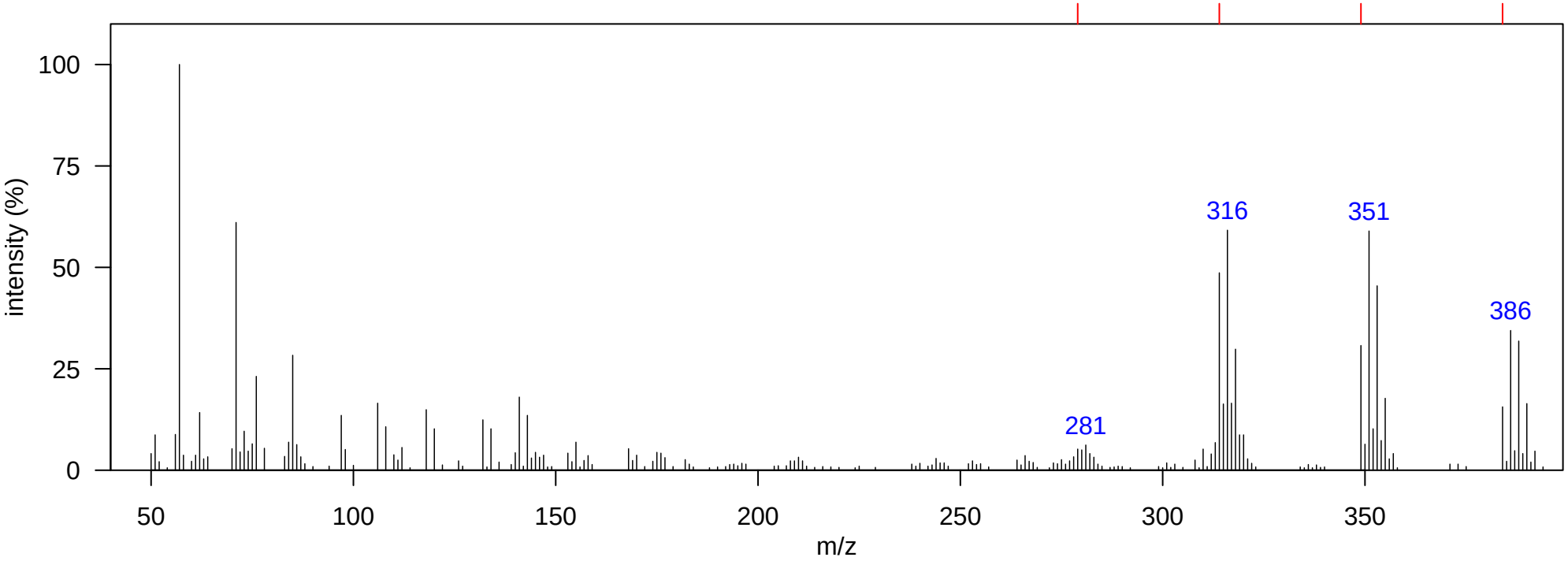
Comment: NA

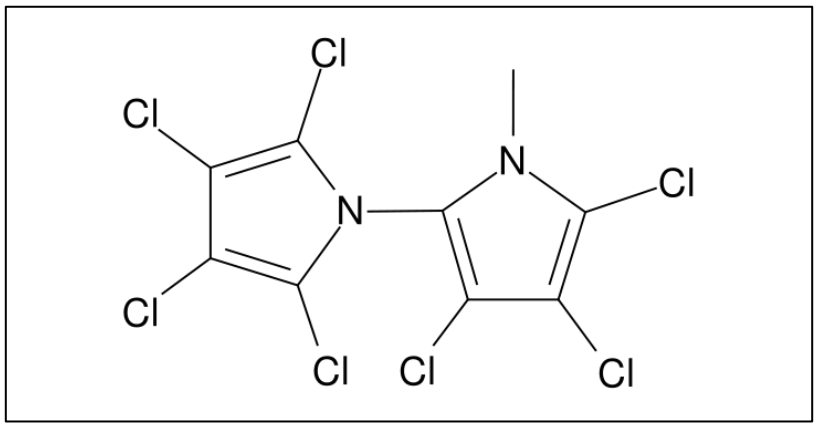
Elemental Formula: C9H3Cl7N2

Source: natural

Class: MBP

Identification: manual identification




| m/z | Identity |
|---|---|
| 279 | [M−3Cl]+ |
| 314 | [M−2Cl]+ |
| 349 | [M−Cl]+ |
| 384 | M+ |

Filename: heptaMBP

# Name: hexa chlorinated methyl bipyrrole (hexa−MBP) isomer 1

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1299, RT (s) (2D): 0.84

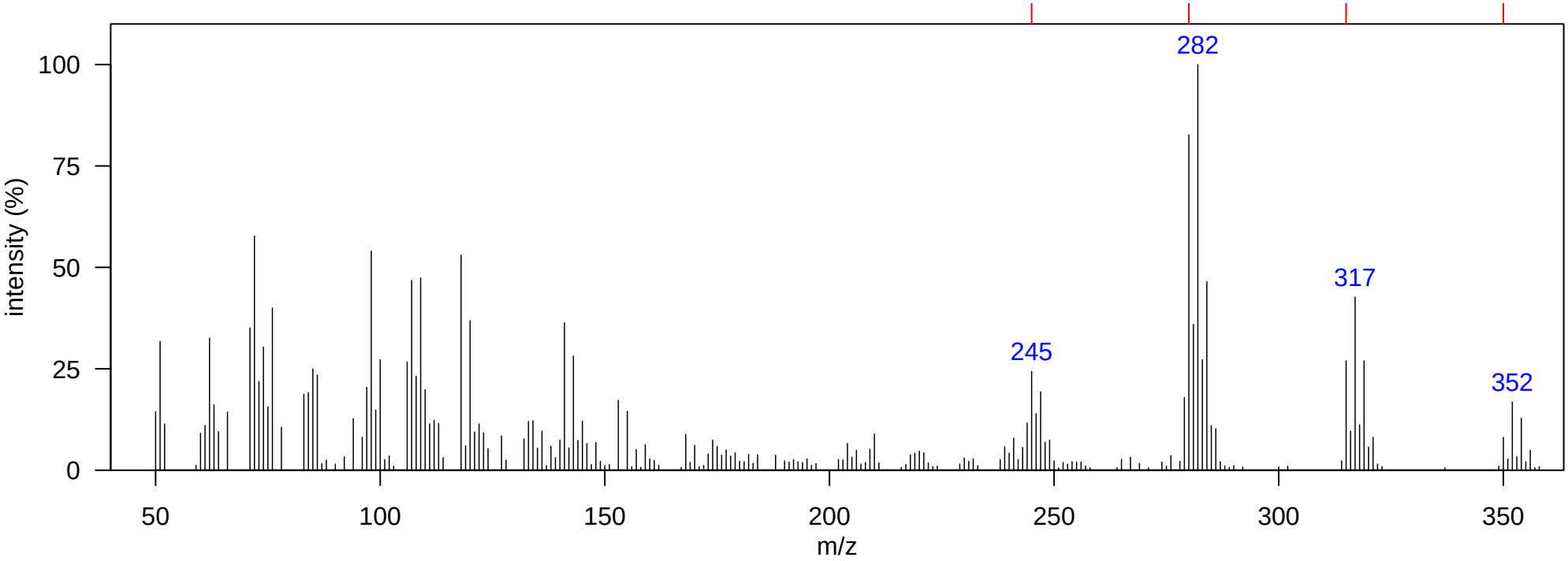
Comment: Isomer unknown.

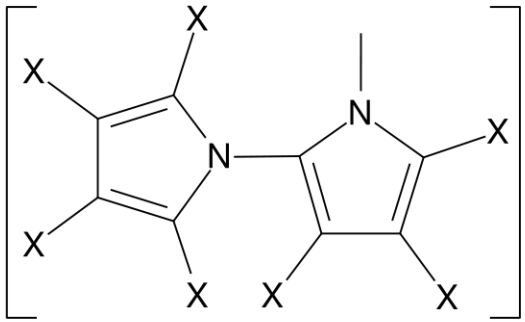
Elemental Formula: C9H4Cl6N2

Source: natural

Class: MBP

Identification: manual identification




| m/z | Identity |
|---|---|
| 245 | [M−3Cl]+ |
| 280 | [M−2Cl]+ |
| 315 | [M−Cl]+ |
| 350 | M+ |

Filename: hexaMBP1

# Name: hexa chlorinated methyl bipyrrole (hexa−MBP) isomer 2

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1455, RT (s) (2D): 0.89

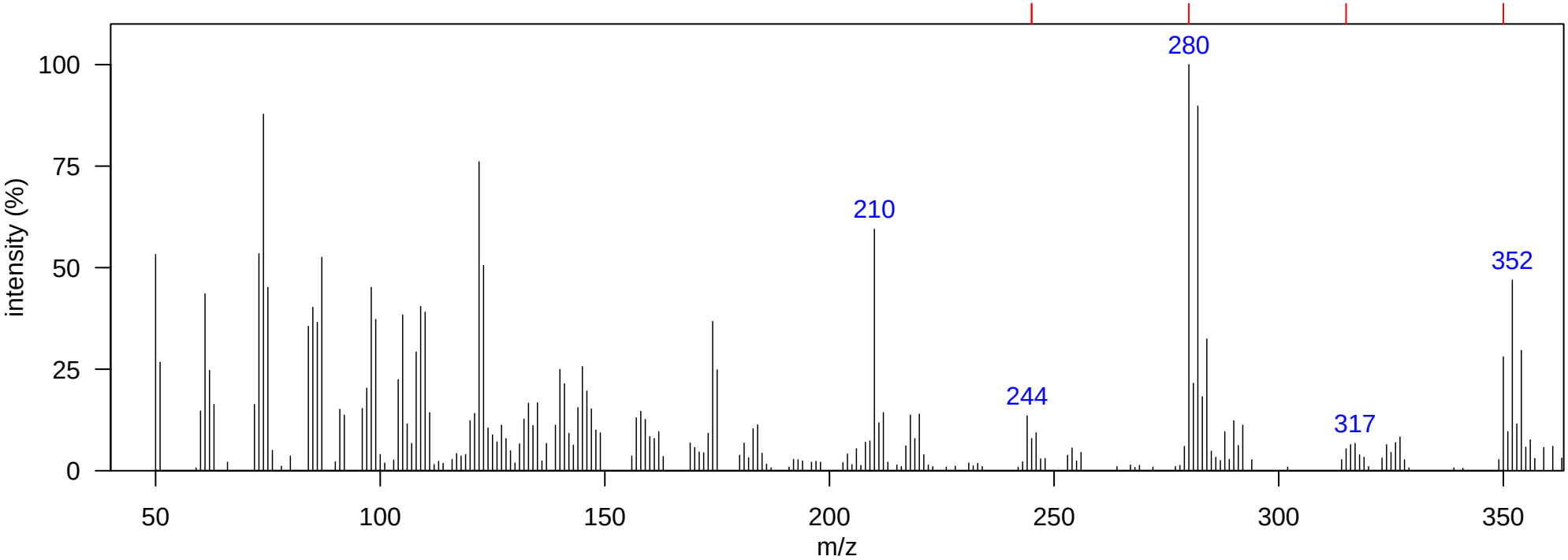
Comment: Isomer unknown.

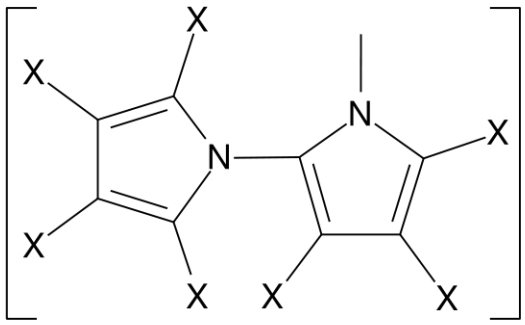
Elemental Formula: C9H4Cl6N2

Source: natural

Class: MBP

Identification: manual identification




| m/z | Identity |
|---|---|
| 245 | [M−3Cl]+ |
| 280 | [M−2Cl]+ |
| 315 | [M−Cl]+ |
| 350 | M+ |

Filename: hexaMBP2

Name: unknown

Sample: southern CA sea lion blubber

Instrument: GCxGC−TOF, electron impact, 70 eV

RT (s) (1D): 1491, RT (s) (2D): 0.95

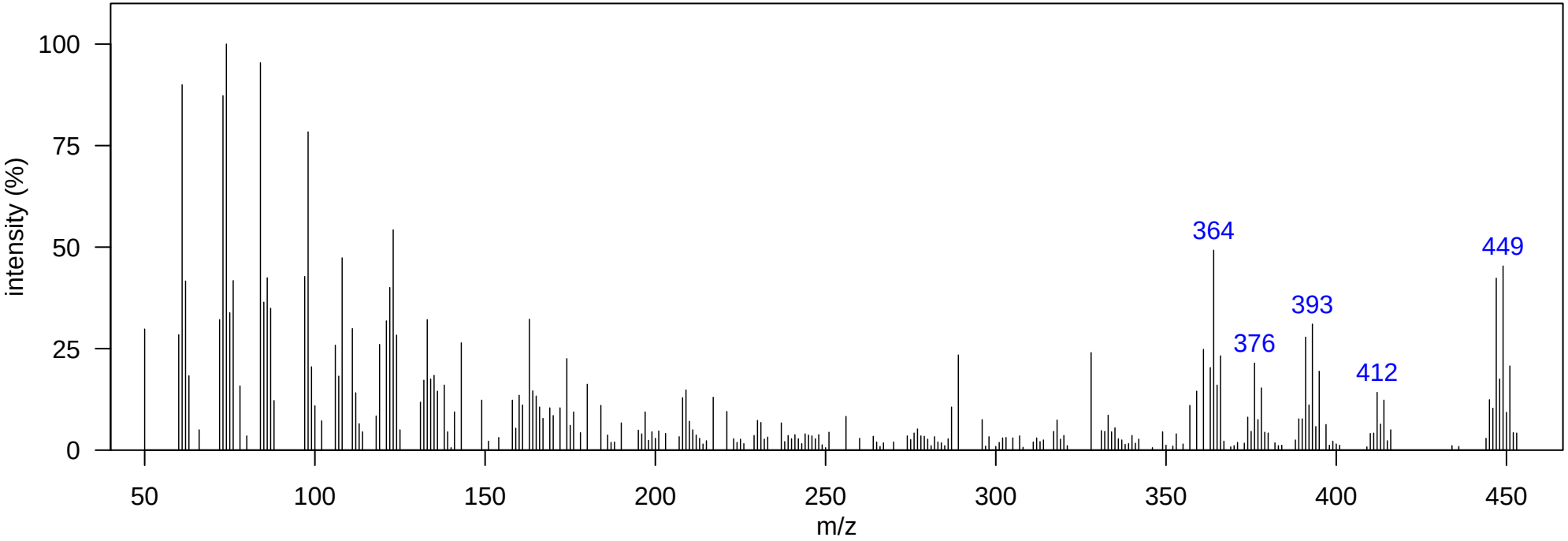
Comment: NA

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: NA




m/z Identity

Filename: unknown