Massachusetts Common Dolphin (Delphinus delphis) Blubber

Literature Reference:

Eunha Hoh, Nathan G. Dodder, Steven J. Lehotay, Kristin C. Pangallo, Christopher M. Reddy, and Keith A. Maruya
"Nontargeted Comprehensive Two−Dimensional Gas Chromatography/Time−of−Flight Mass Spectrometry Method and Software for Inventorying Persistent and Bioaccumulative Contaminants in Marine Environments",
Environmental Science and Technology, 2012, 46 (15), 8001−8008. DOI: 10.1021/es301139q.

Web Reference:

http://orgmassspecr.r−forge.r−project.org/

Prepared: 2012−08−22 12:24:23

SpecLibDolphin2011 version 0.5

OrgMassSpecR version 0.3−13

png version 0.1−4

R version 2.15.1 (2012−06−22)

Name: chlordane related 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1315, RT (s) (2D): 0.969

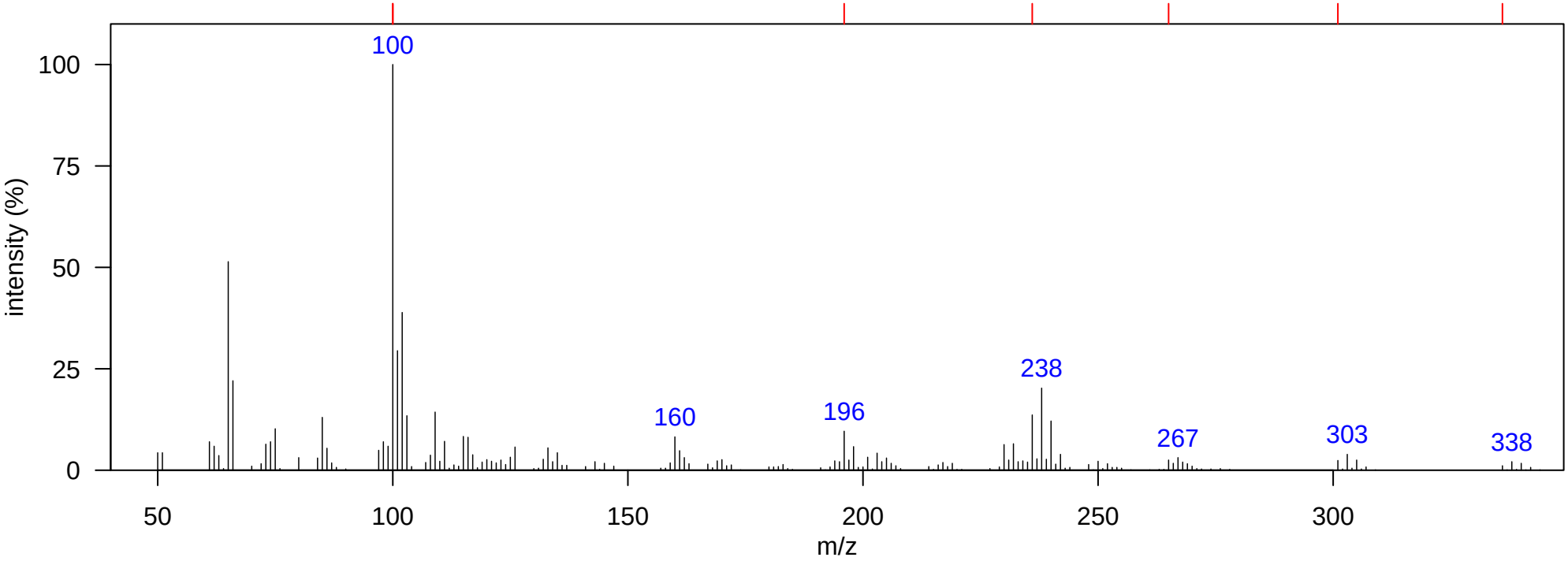
Comment:

Elemental Formula: C10H6Cl6

Source: anthropogenic

Class: chlordane related

Identification: Manual



m/z	Identity
100	[C5H5Cl]+
196	[M−4Cl]+
236	[C5HCl5]+
265	[M−HCl2]+
301	[M−Cl]+
336	M+

Name: chlordane related 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1360.5, RT (s) (2D): 0.952

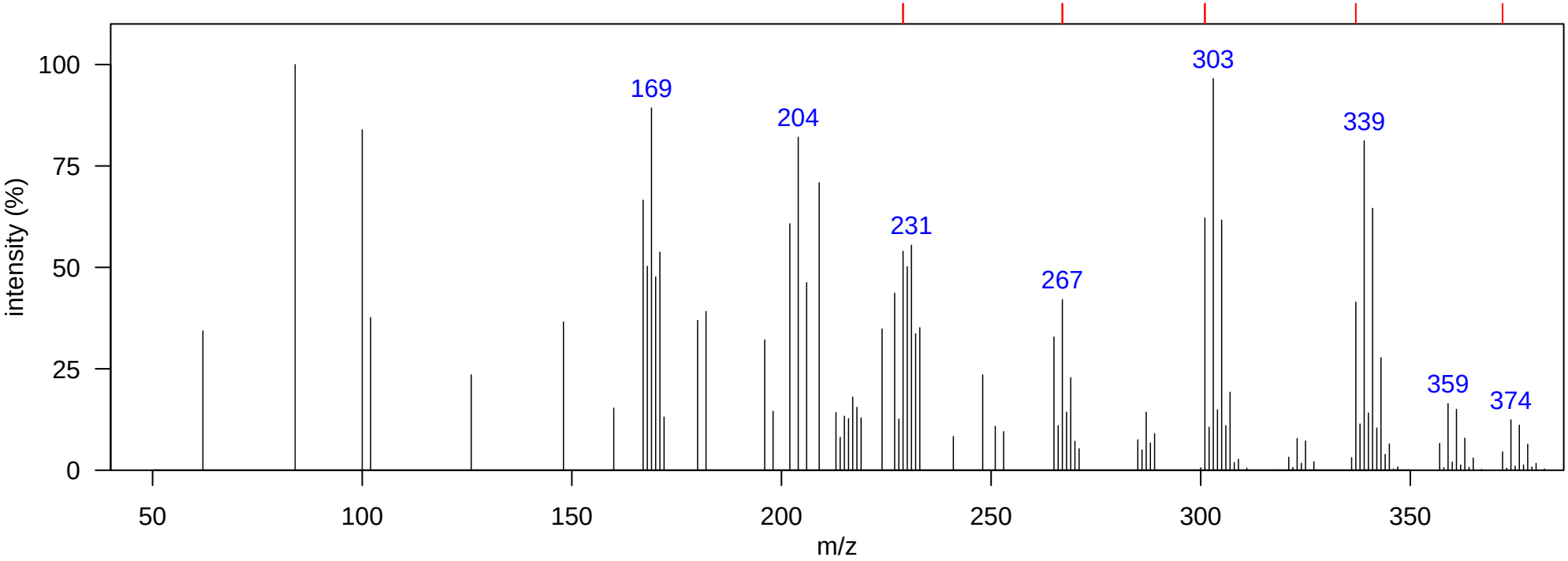
Comment:

Elemental Formula: C10H7Cl7

Source: anthropogenic

Class: chlordane related

Identification: Manual



m/z	Identity
229	[M−H3Cl4]+
267	[M−H2Cl3]+
301	[M−HCl2]+
337	[M−Cl]+
372	M+

Name: gamma−chlordene

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1378, RT (s) (2D): 1.395

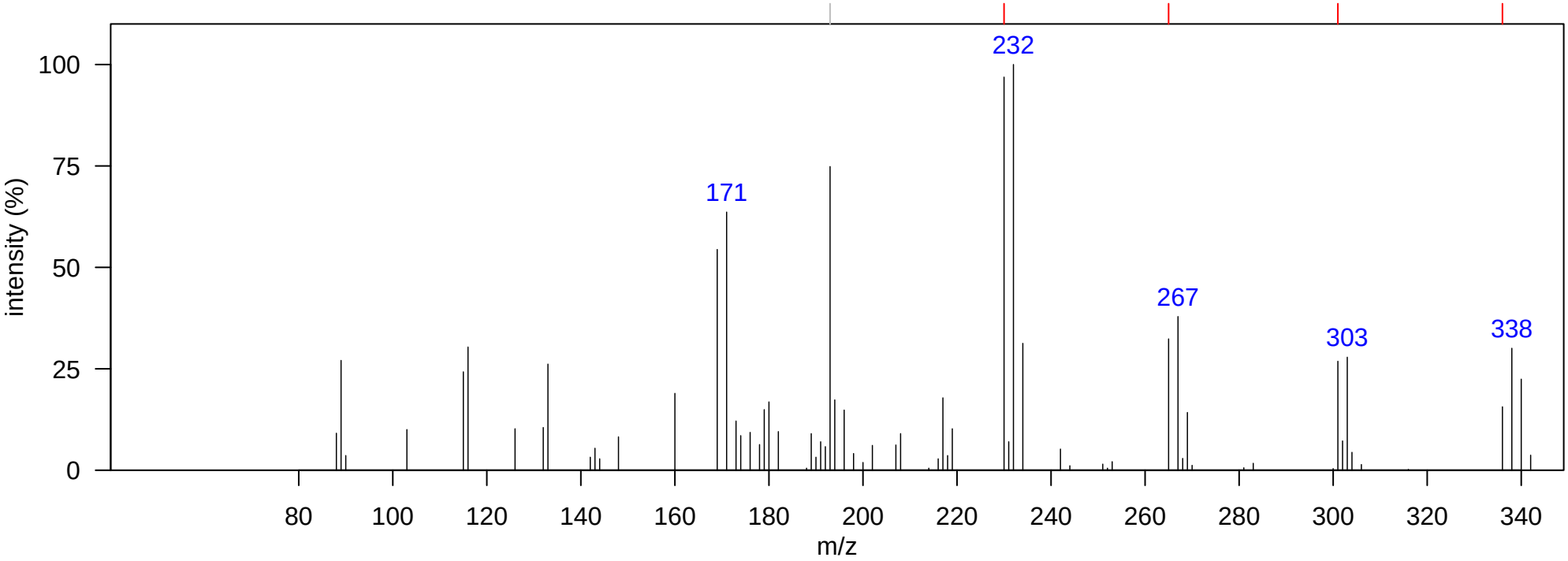
Comment:

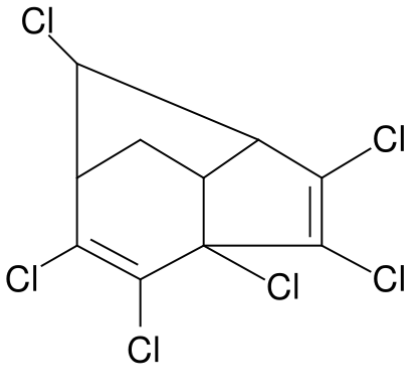
Elemental Formula: C10H6Cl6

Source: anthropogenic

Class: chlordane related

Identification: Reference Database MS





m/z	Identity
193	interference
230	[M−HCl3]+
265	[M−HCl2]+
301	[M−Cl]+
336	M+

Filename: gamma_chlordene

Name: chlordane related 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1381.5, RT (s) (2D): 1.431

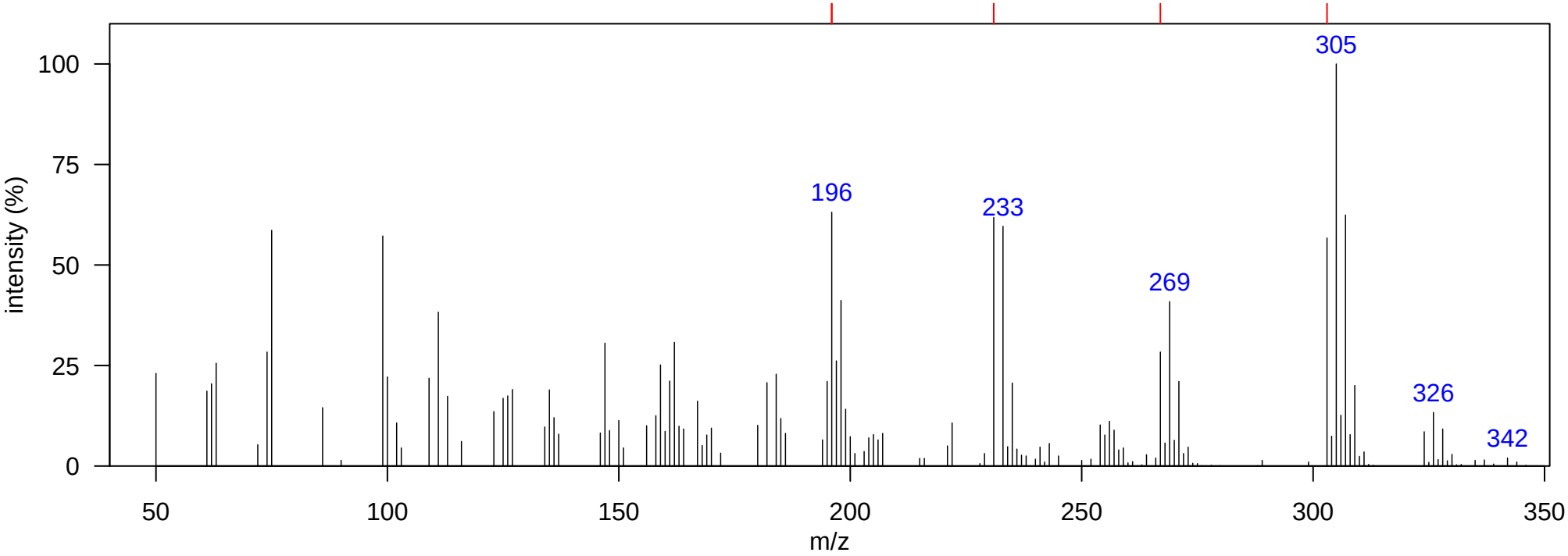
Comment: Suggested elemental formula is C10H8Cl6.

Elemental Formula: C10H8Cl6

Source: anthropogenic

Class: chlordane related

Identification: Manual



m/z	Identity
196	[Frag−H2Cl3]+
231	[Frag−H2Cl2]+
267	[Frag−HCl]+
303	[Frag]+ contains 5Cl

Name: chlordane related 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1385, RT (s) (2D): 1.143

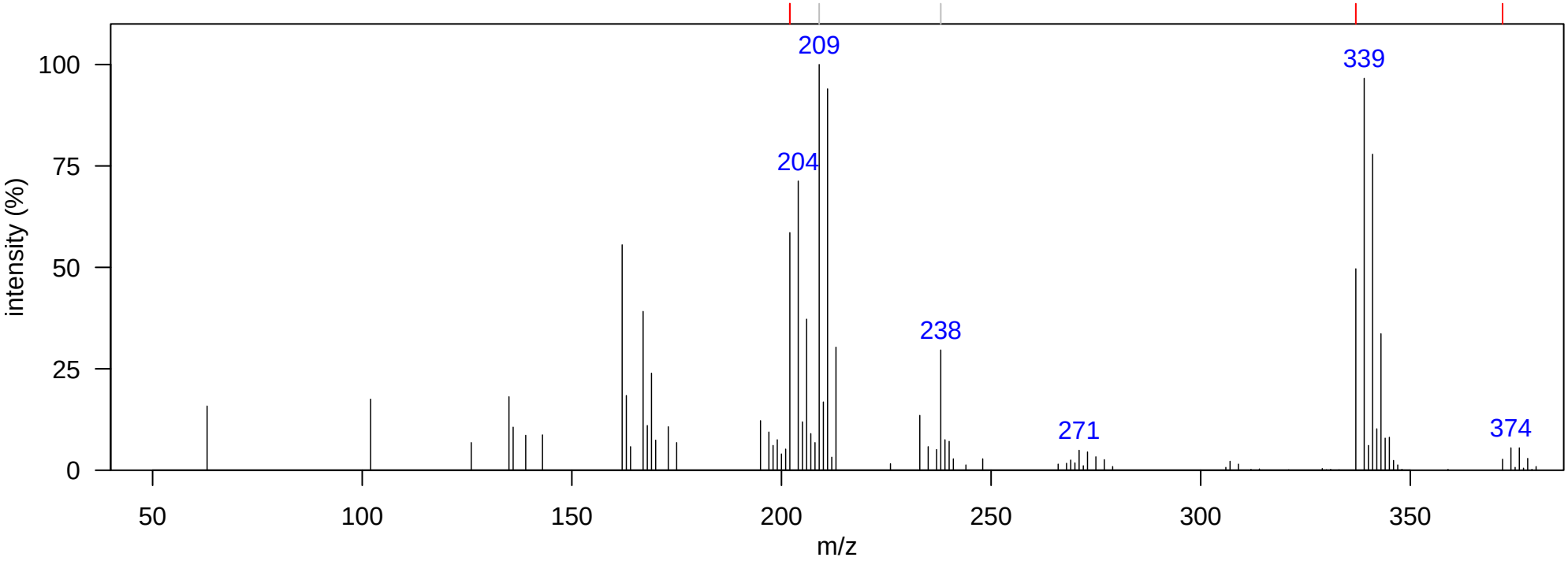
Comment:

Elemental Formula: C10H7Cl7

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group



m/z	Identity
202	[C5H2Cl4]+
209	interference
238	interference
337	[M−Cl]+
372	M+

Name: chlordane related 5

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1395.5, RT (s) (2D): 0.806

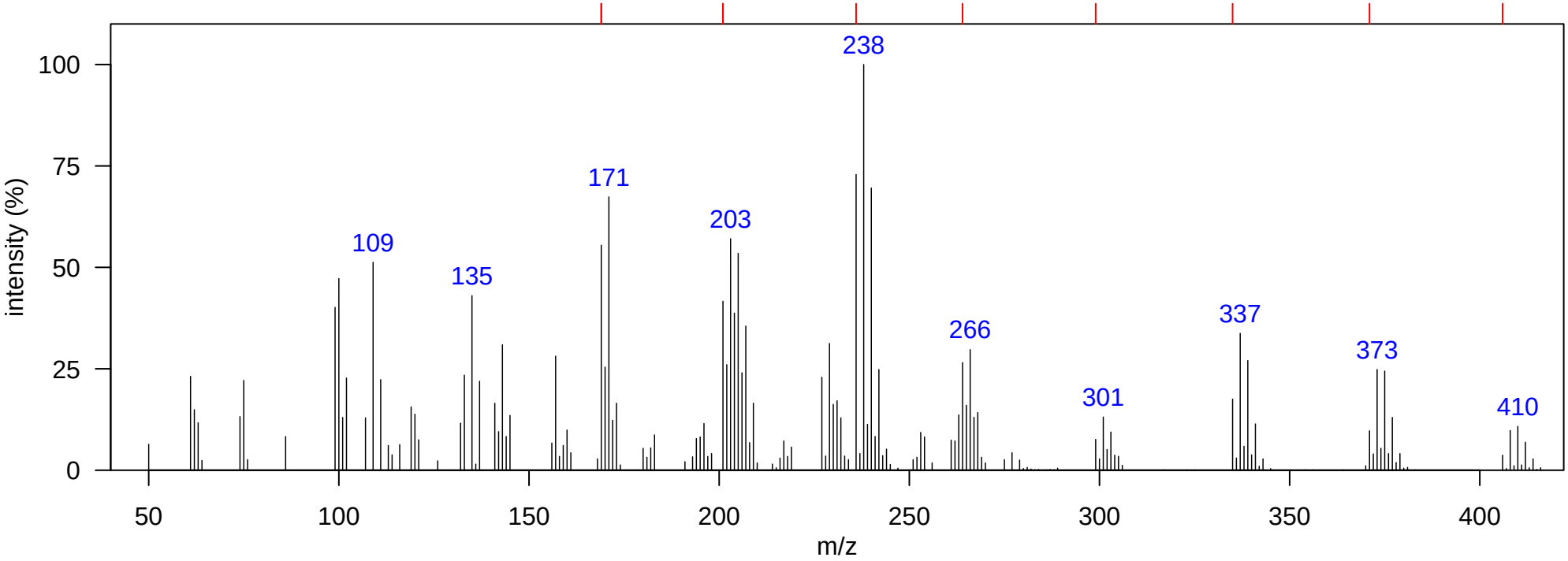
Comment: Similar to chlordane, but different fragment ion intensities,

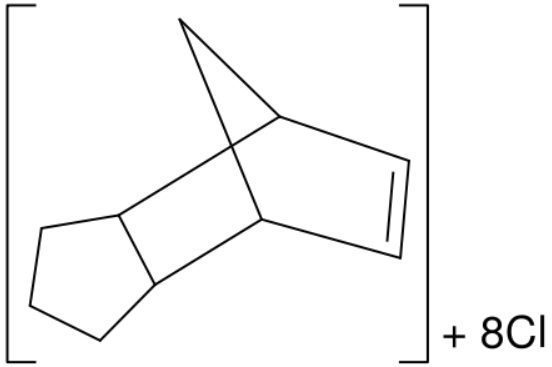
Elemental Formula: C10H6Cl8

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
169	[C5H4Cl3]+
201	[C5HCl4]+
236	[C5HCl5]+
264	[M−H2Cl4]+
299	[M−HCl3]+
335	[M−HCl2]+
371	[M−Cl]+
406	[M]+

Filename: chlordane_related_5

Name: chlordane related 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1413, RT (s) (2D): 0.945

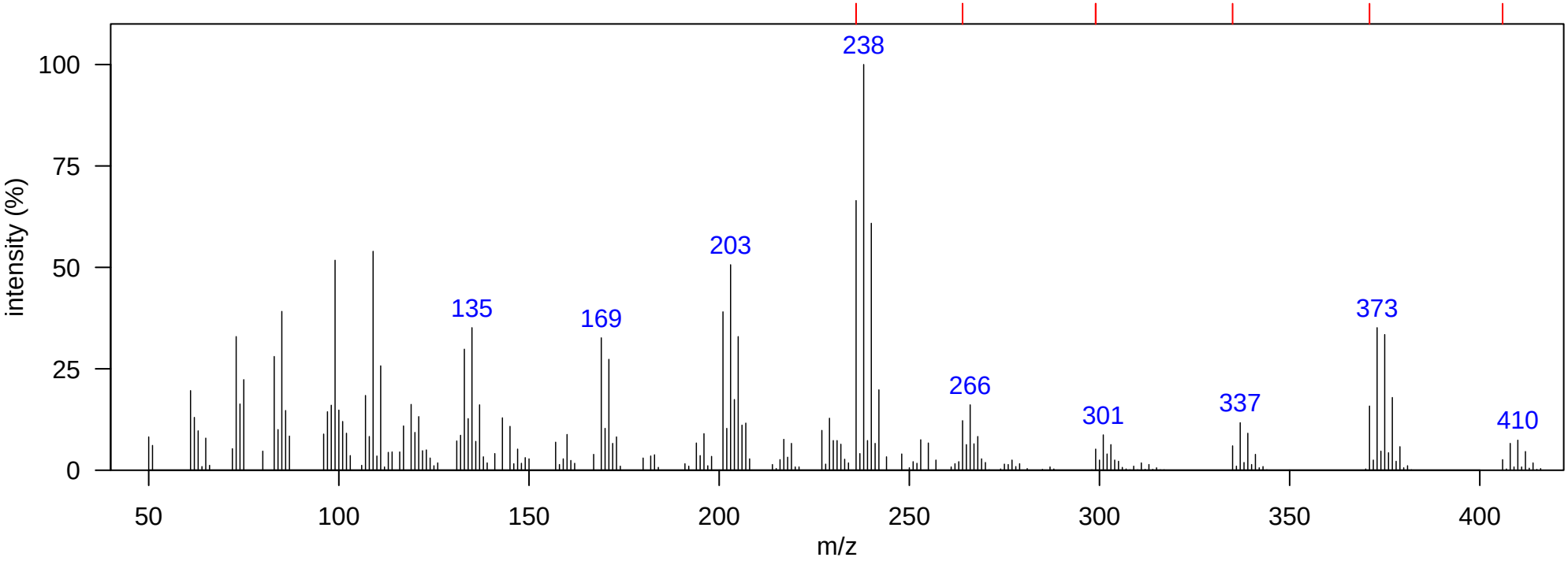
Comment: Similar to chlordane, but ion cluster at m/z 272 is not present.

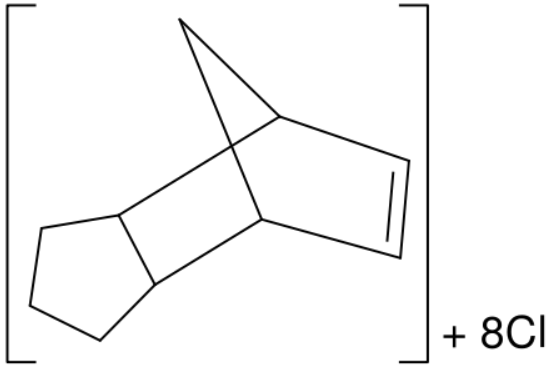
Elemental Formula: C10H6Cl8

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
236	[C5HCl5]+
264	[M−H2Cl3]+
299	[M−H2Cl3]+
335	[M−HCl2]+
371	[M−Cl]+
406	M+

Filename: chlordane_related_6

Name: oxychlordane

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1427, RT (s) (2D): 1.169

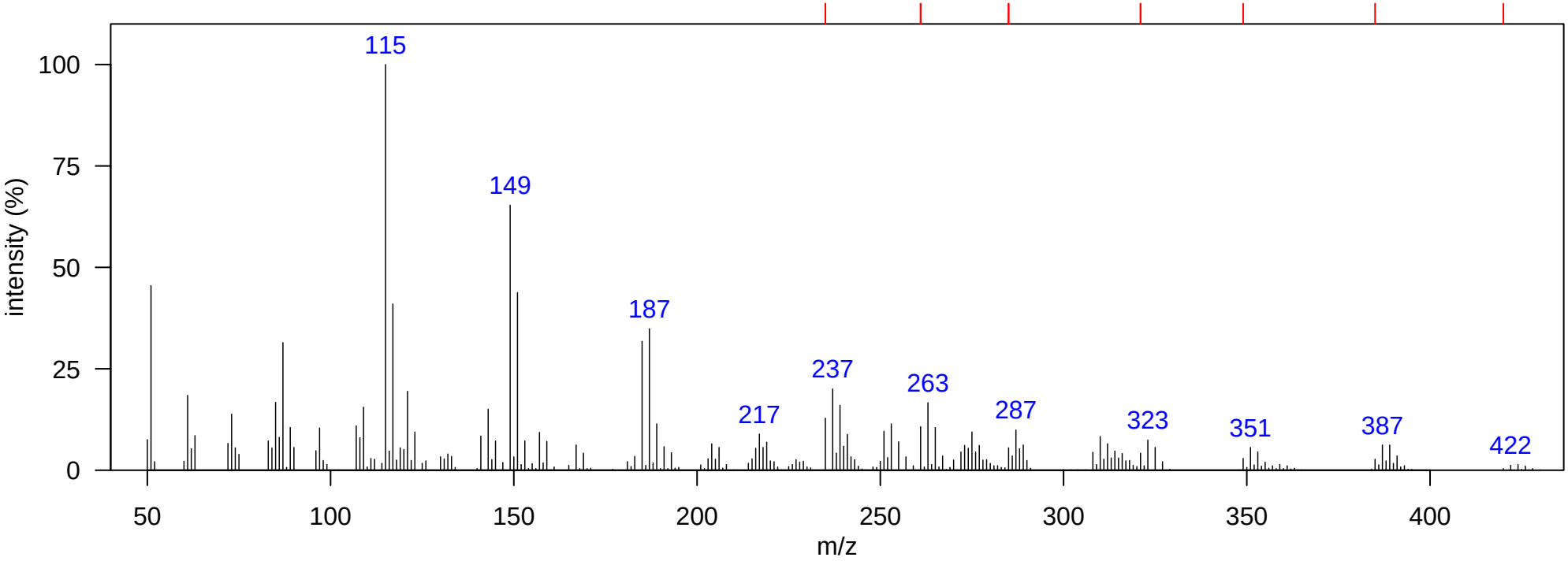
Comment:

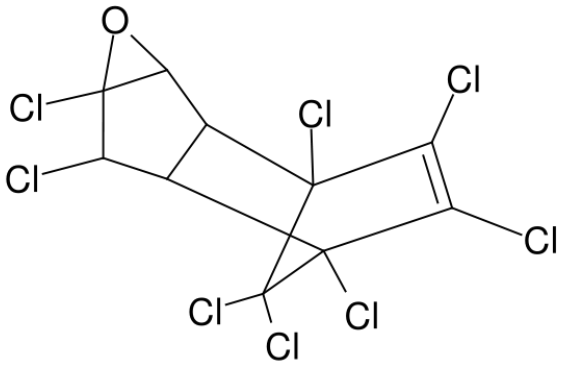
Elemental Formula: C10H4Cl8O

Source: anthropogenic

Class: chlordane related

Identification: Reference Database MS





m/z	Identity
235	[C5Cl5]+
261	[C7H2Cl5]+
285	[M−H2Cl3−CO]+
321	[M−HCl2−CO]+
349	[M−HCl2]+
385	[M−Cl]+
420	[M]+

Filename: oxychlordane

Name: chlordane related 7

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1434, RT (s) (2D): 1.525

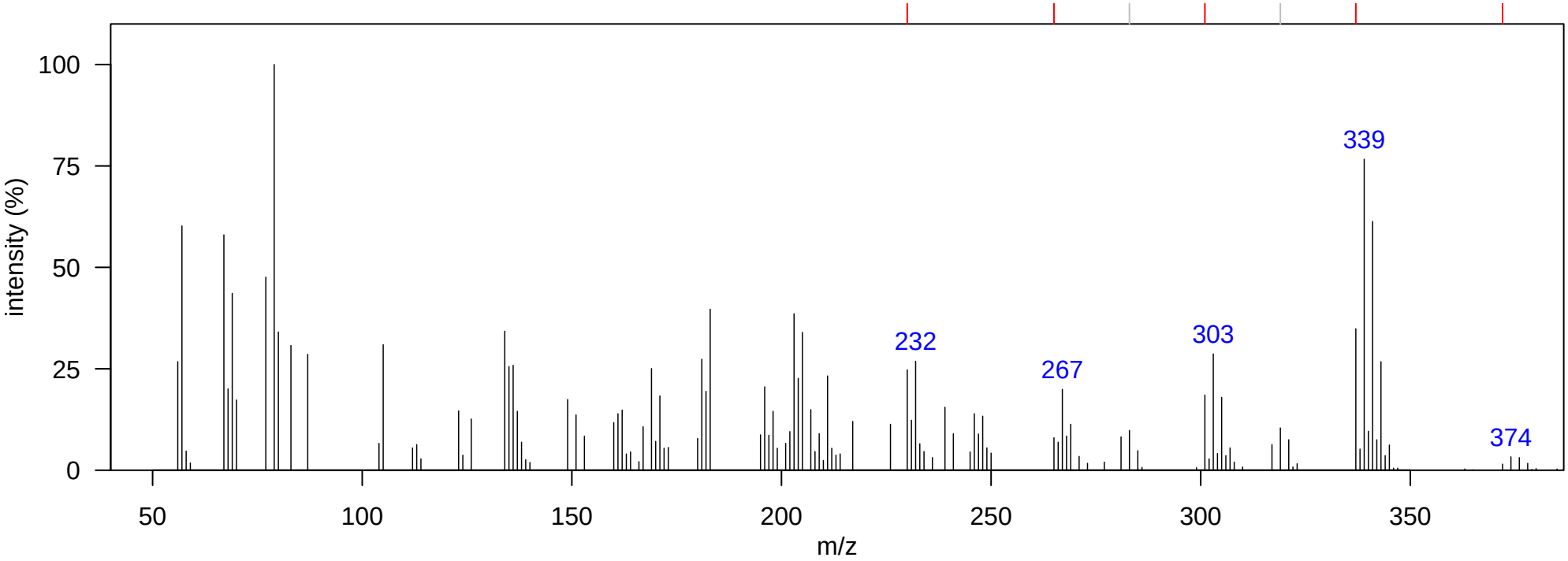
Comment: Similar to heptachlor, but ion cluster at m/z 272 is not present.

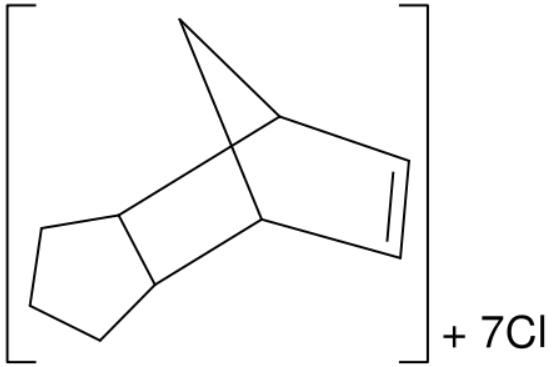
Elemental Formula: C10H7Cl7

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
230	[M−H2Cl4]+
265	[M−H2Cl3]+
283	interference
301	[M−HCl2]+
319	interference
337	[M−Cl]+
372	M+

Filename: chlordane_related_7

Name: chlordane related 8

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1444.5, RT (s) (2D): 1.091

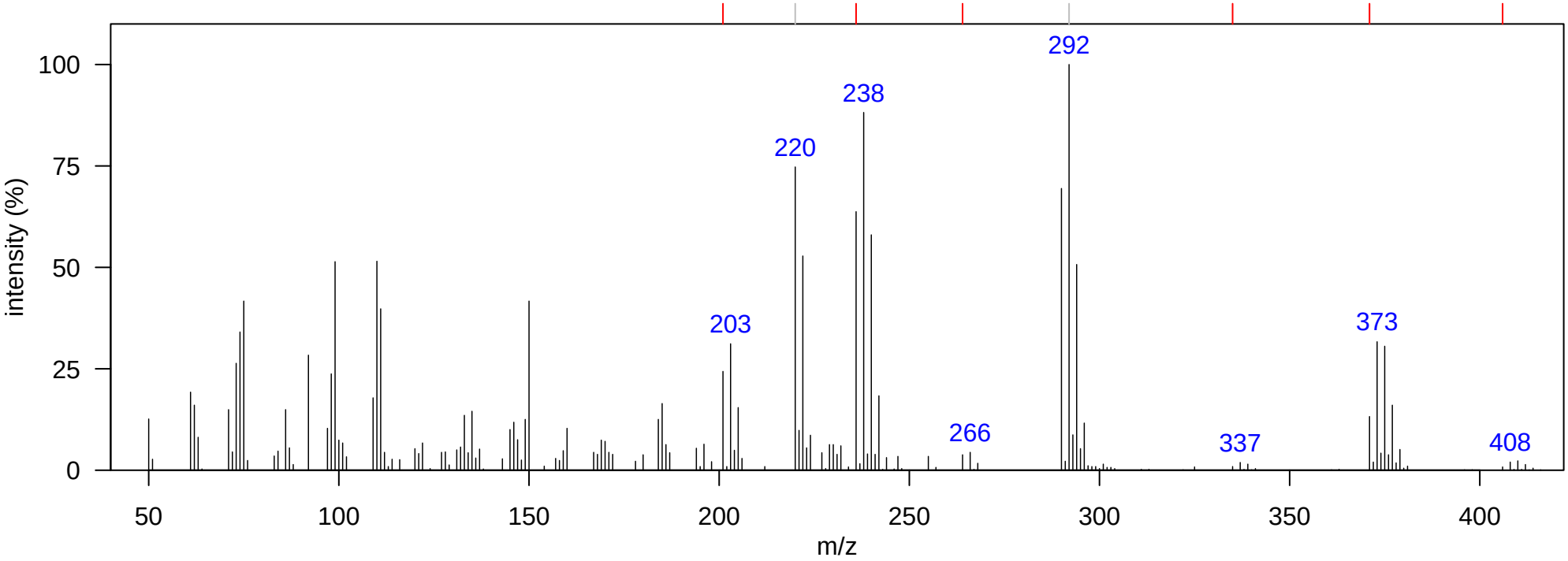
Comment: Similar to chlordane.

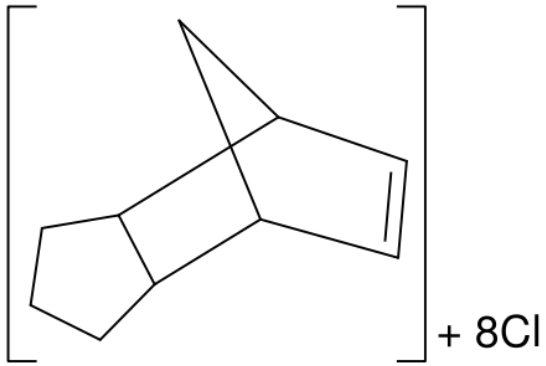
Elemental Formula: C10H6Cl8

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
201	[C5HCl4]+
220	PCB interference
236	[C5HCl5]+
264	[M−H2Cl4]+
292	PCB interference
335	[M−HCl2]+
371	[M−Cl]+
406	M+

Filename: chlordane_related_8

Name: chlordane related 9

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1451.5, RT (s) (2D): 1.243

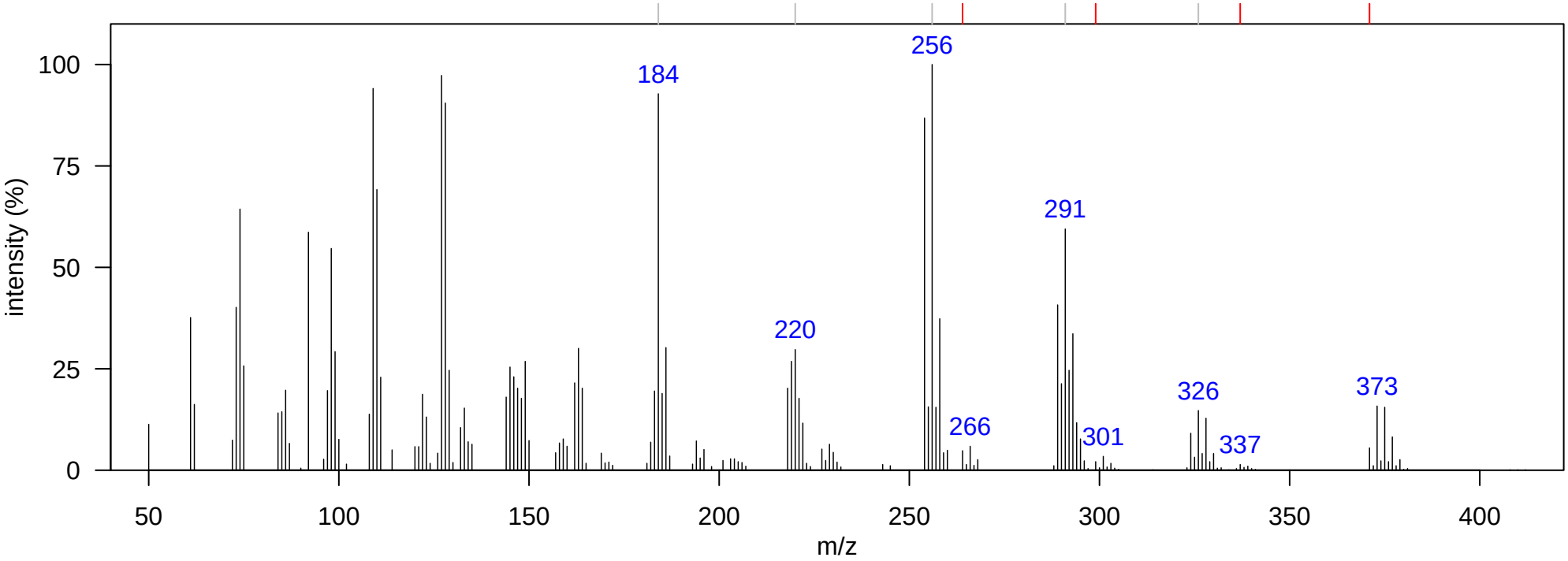
Comment: Ion cluster at m/z 373 related to chlordane. M+ not detected.

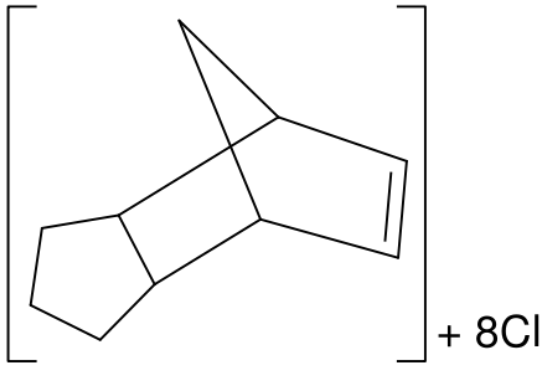
Elemental Formula: C10H6Cl8

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
184	PCB interference
220	PCB interference
256	PCB interference
264	[M−H2Cl4]+
291	PCB interference
299	[M−H2Cl3]+
326	PCB interference
337	[M−HCl2]+ (not monoisotopic)
371	[M−Cl]+

Filename: chlordane_related_9

Name: chlordane related 10

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1451.5, RT (s) (2D): 1.844

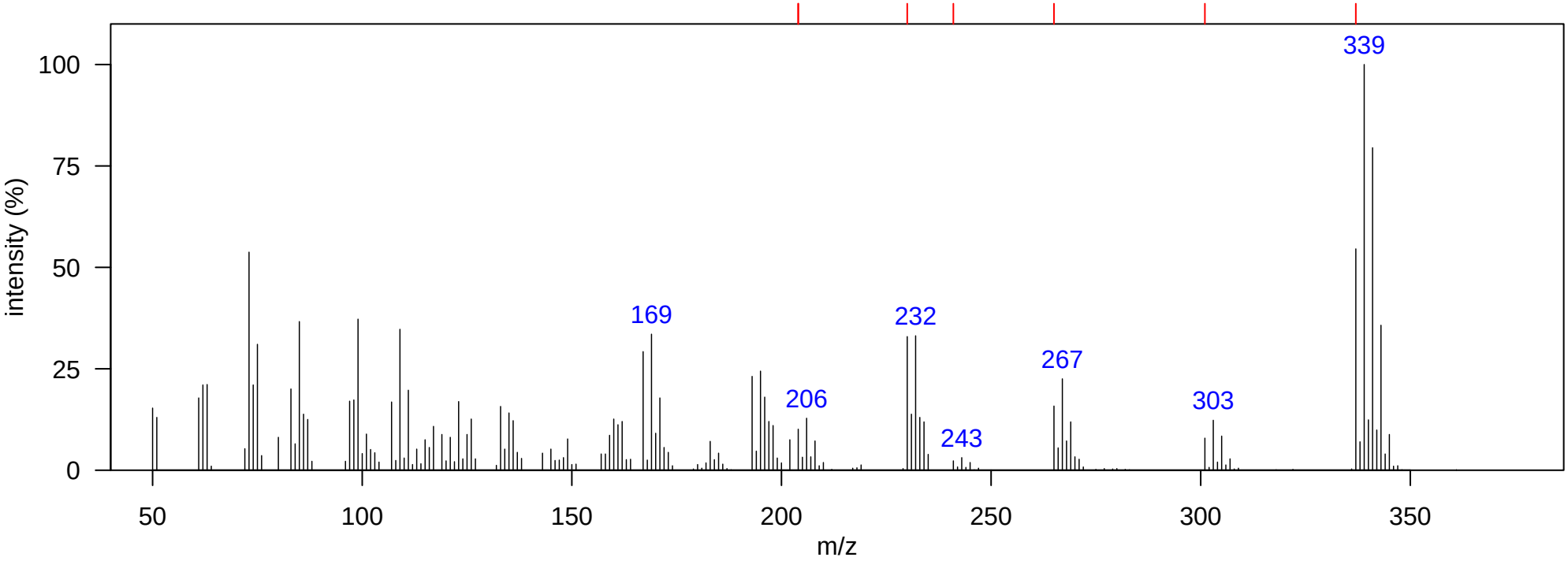
Comment: Ion cluster at m/z 339 suggests C10H6Cl6. M+ not detected.

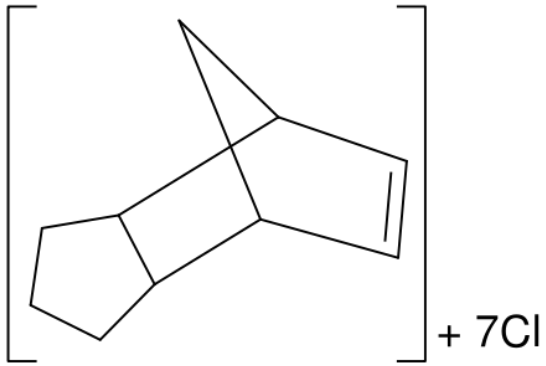
Elemental Formula: C10H7Cl7

Source: anthropogenic

Class: chlordane related

Identification: Manual





m/z	Identity
204	[C5H4Cl4]+
230	[M−H2Cl4]+
241	[C5H6Cl5]+
265	[M−H2Cl3]+
301	[M−HCl2]+
337	[M−Cl]+

Filename: chlordane_related_10

Name: gamma−chlordane

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1458.5, RT (s) (2D): 1.431

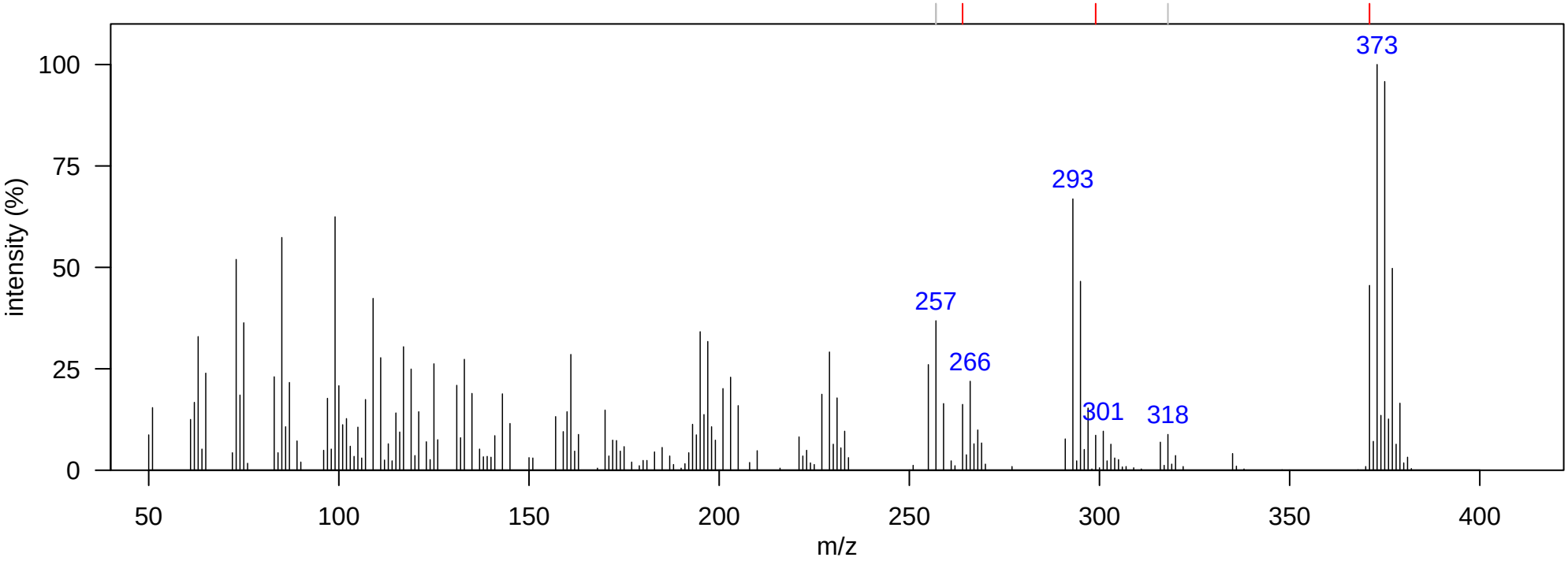
Elemental Formula: C10H6Cl8

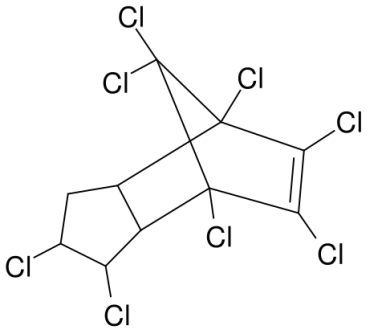
Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT

Comment: M+ not present in the "peak true" mass spectrum, but is present in the caliper mass spectrum.





(stereochemistry not shown)

m/z	Identity
257	interference
264	[M−H2Cl4]+
299	[M−H2Cl3]+
318	DDE interference
371	[M−Cl]+

Filename: gamma_chlordane

Name: alpha−chlordane

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1469, RT (s) (2D): 1.482

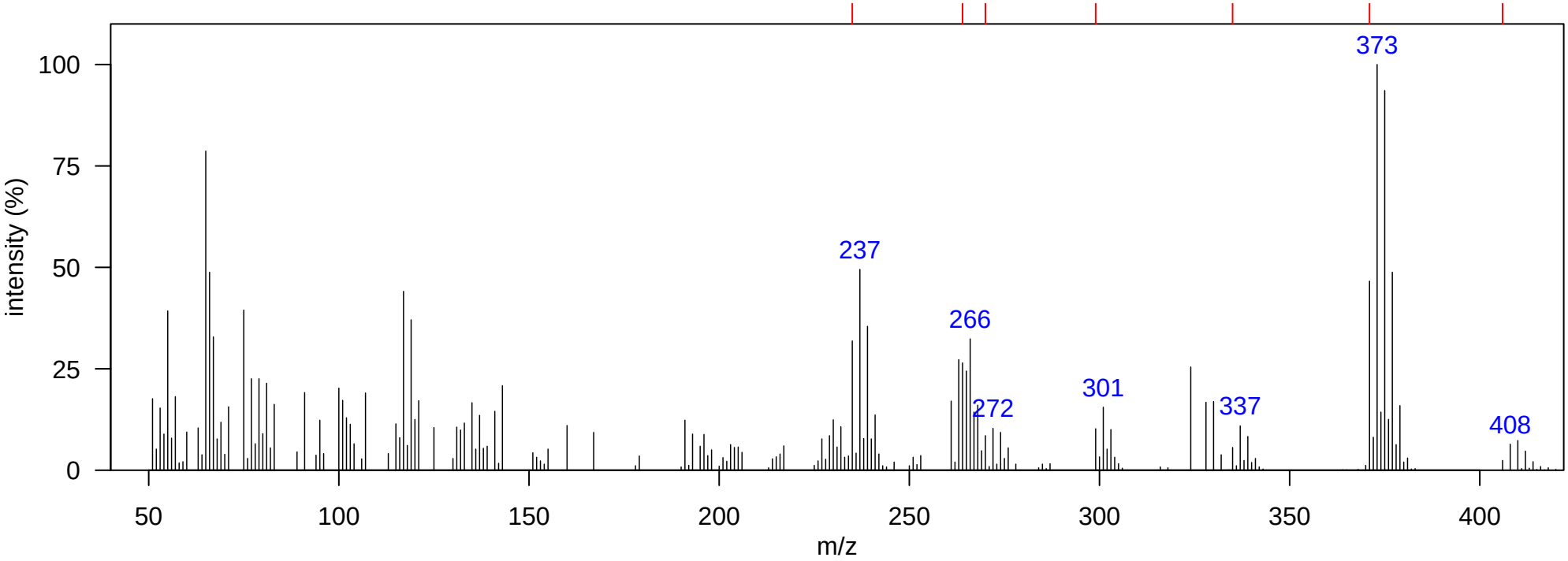
Comment:

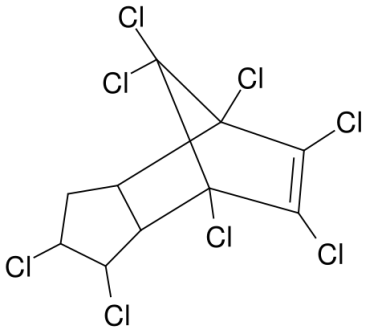
Elemental Formula: C10H6Cl8

Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT





(stereochemistry not shown)

m/z	Identity
235	[C5Cl5]+
264	[M−H2Cl4]+
270	[C5Cl6]+
299	[M−H2Cl3]+
335	[M−HCl2]+
371	[M−Cl]+
406	M+

Filename: alpha_chlordane

Name: trans−nonachlor

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1479.5, RT (s) (2D): 1.06

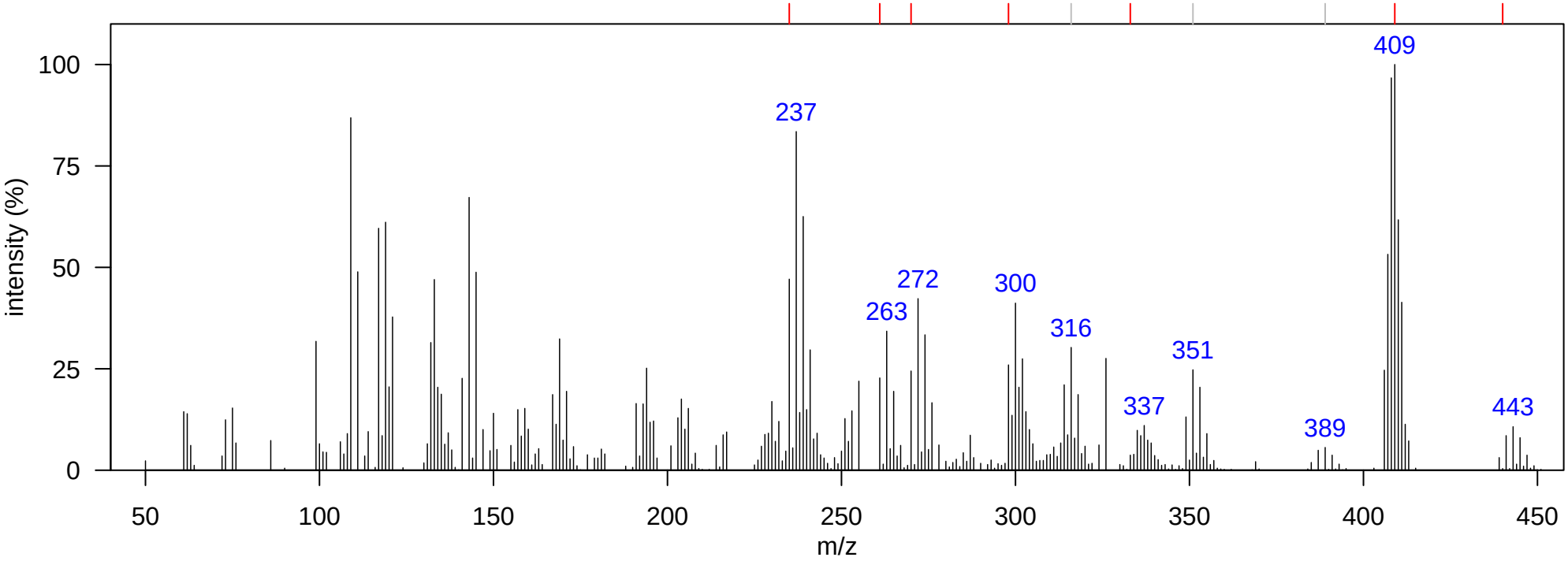
Comment: Chromatographic peak is saturated.

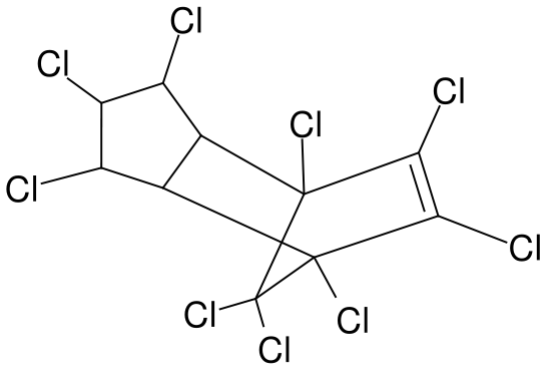
Elemental Formula: C10H5Cl9

Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT





m/z	Identity
235	[C5Cl5]+
261	[M−H4Cl5]+
270	[C5Cl6]+
298	[M−H2Cl4]+
316	interference MBP(7Cl)
333	[M−H2Cl3]+
351	interference MBP(7Cl)
389	interference MBP(7Cl)
409	[M−Cl]+ (not monoisotopic)
440	M+

Filename: trans_nonachlor

Name: chlordane related 11

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1514.5, RT (s) (2D): 1.73

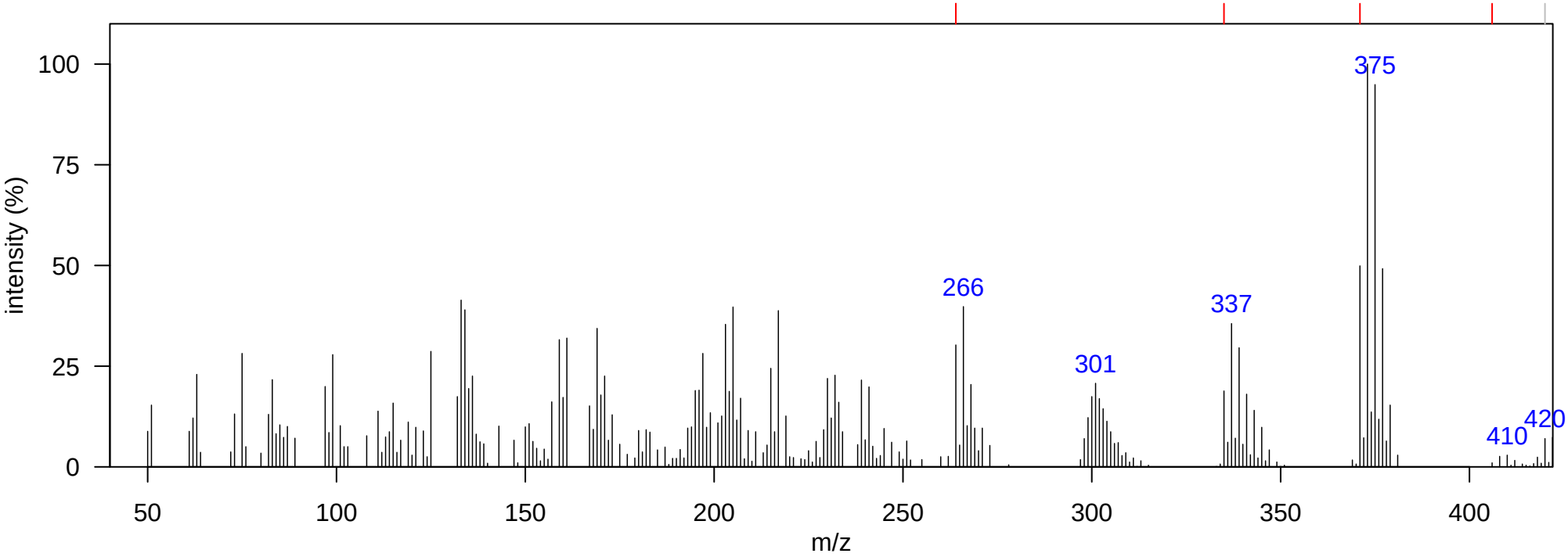
Comment: Chlordane isomer.

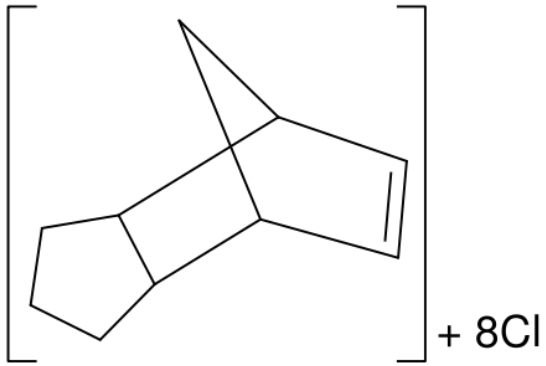
Elemental Formula: C10H6Cl8

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
264	[M−H2Cl4]+
335	[M−HCl2]+
371	[M−Cl]+
406	M+
420	interference
452	interference

Filename: chlordane_related_11

Name: chlordane related 12

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1532, RT (s) (2D): 1.081

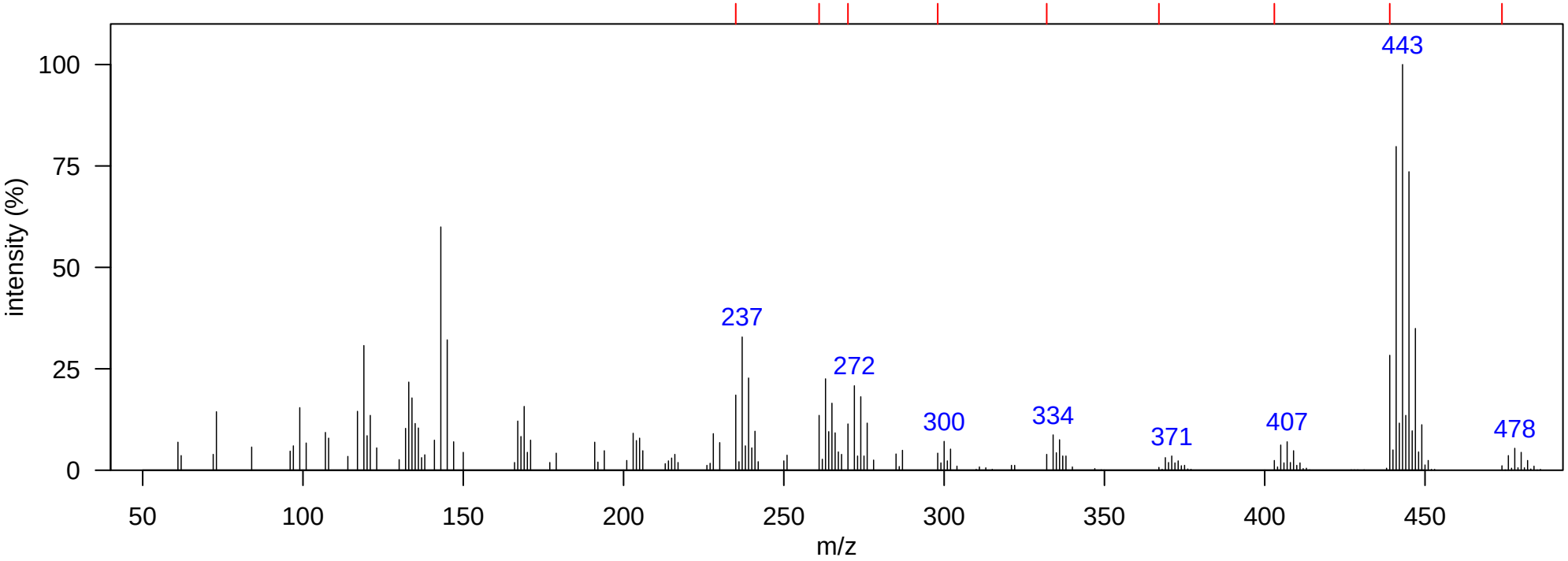
Comment:

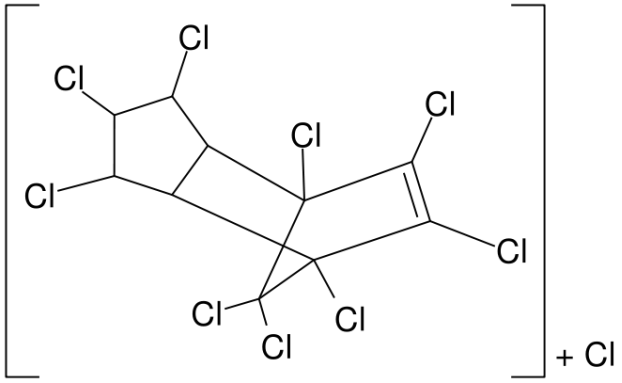
Elemental Formula: C10H4Cl10

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
235	[C5Cl5]+
261	[C7H2Cl5]+
270	[C5Cl6]+
298	[M−HCl5]+
332	[M−H2Cl4]+
367	[M−H2Cl3]+
403	[M−HCl2]+
439	[M−Cl]+
474	M+

Name: cis−nonachlor

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1553, RT (s) (2D): 1.529

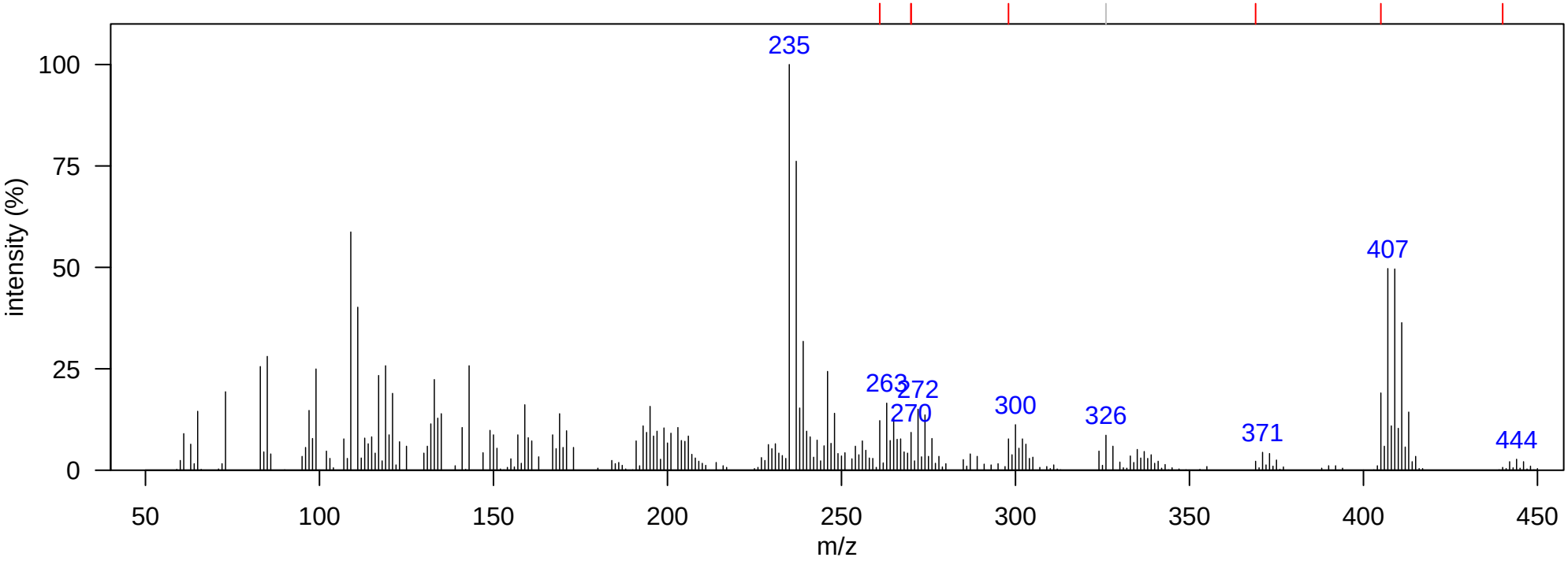
Comment:

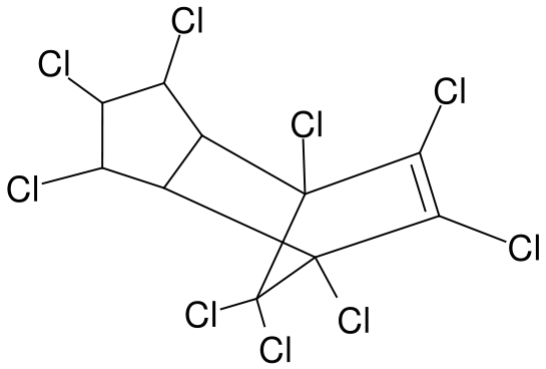
Elemental Formula: C10H5Cl9

Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT





m/z	Identity
261	[M−H4Cl5]+
270	[C5Cl6]+
298	[M−H2Cl4]+
326	PCB interference
369	[M−HCl2]+
405	[M−Cl]+
440	M+

Filename: cis_nonachlor

Name: chlordane related 13

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1574, RT (s) (2D): 2.269

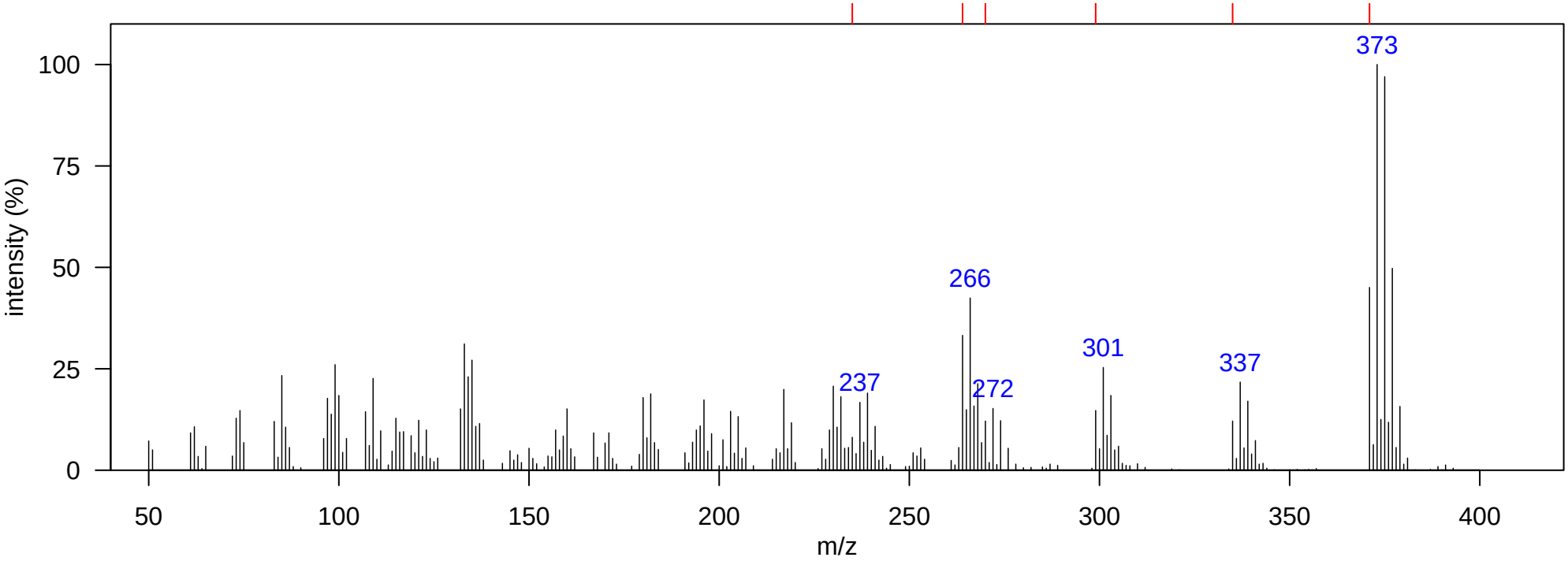
Comment: Chlordane isomer. M+ is not detected.

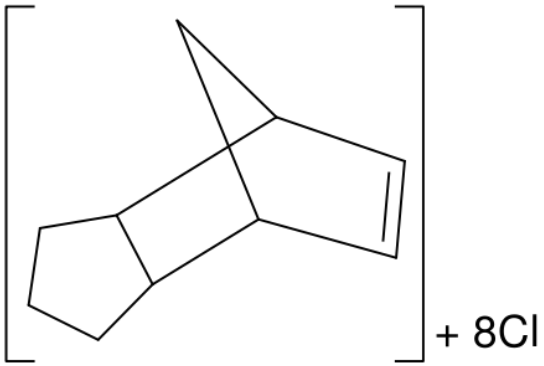
Elemental Formula: C10H6Cl8

Source: anthropogenic

Class: chlordane related

Identification: Manual − Congener Group





m/z	Identity
235	[C5Cl5]+
264	[M−H2Cl4]+
270	[C5Cl6]+
299	[M−H2Cl3]+
335	[M−HCl2]+
371	[M−Cl]+

Filename: chlordane_related_13

Name: chlordane related 14

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1581, RT (s) (2D): 1.295

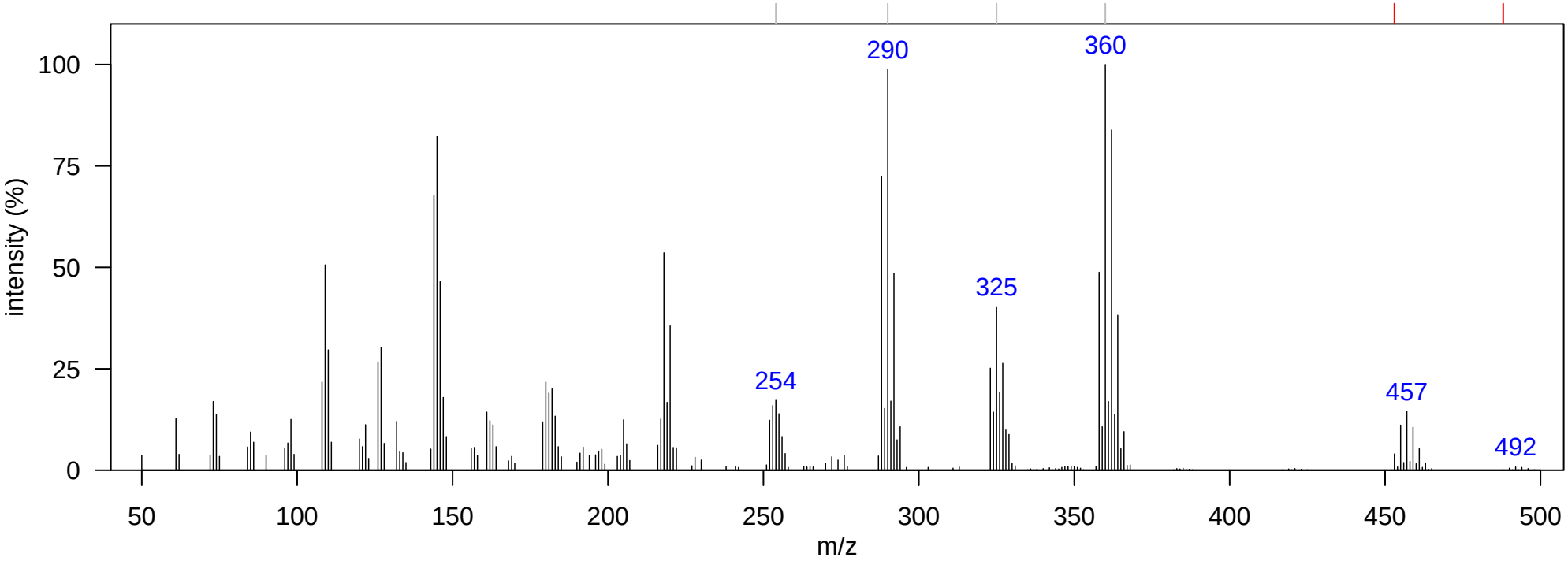
Comment: Ref: ES&T. 1991, 25, 245−254.

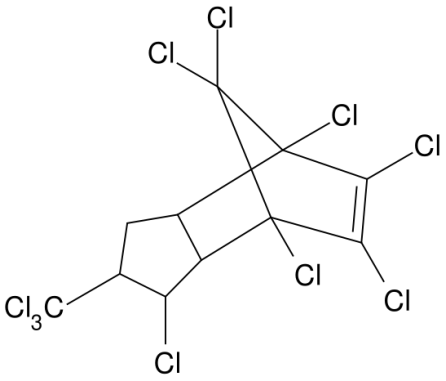
Elemental Formula: C11H6Cl10

Source: anthropogenic

Class: chlordane related

Identification: Literature MS





m/z	Identity
254	PCB interference
290	PCB interference
325	PCB interference
360	PCB interference
453	[M−Cl]+
488	M+

Filename: chlordane_related_14

Name: 2 co−eluting: 1−hydroxychlordene (A) and CAS# 69653−75−4 (B)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1318.5, RT (s) (2D): 1.08

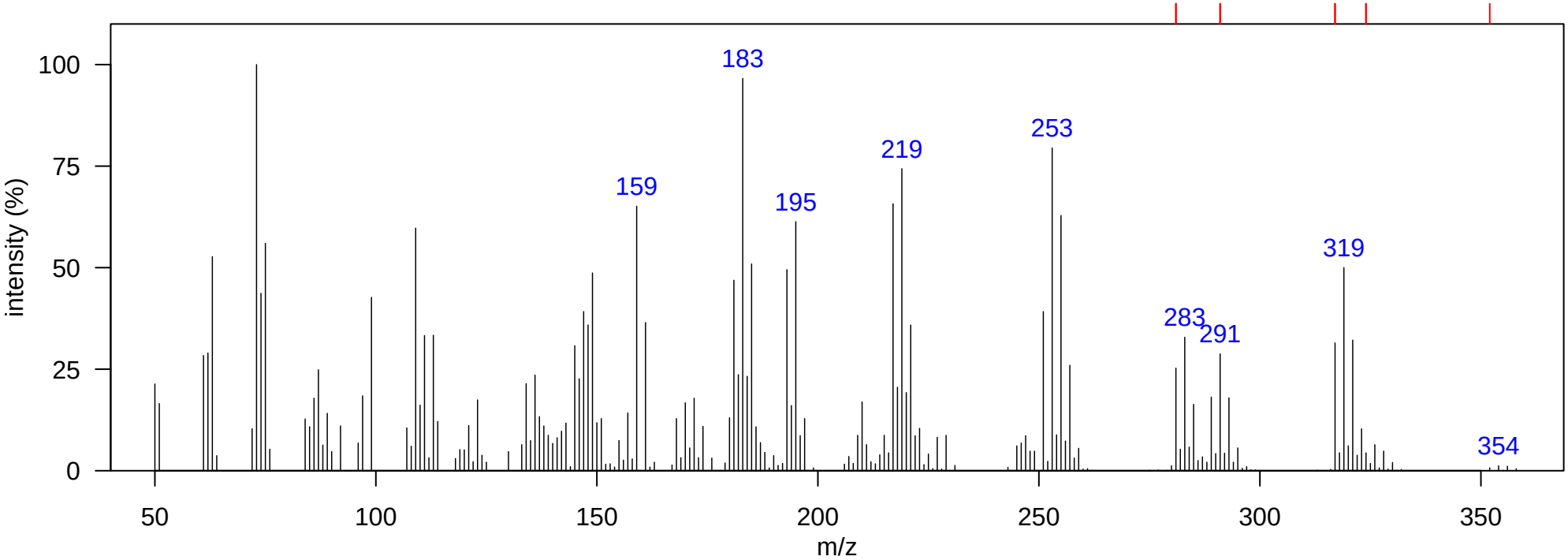
Comment: C10H6Cl6O (A); C10H6Cl6O (B)

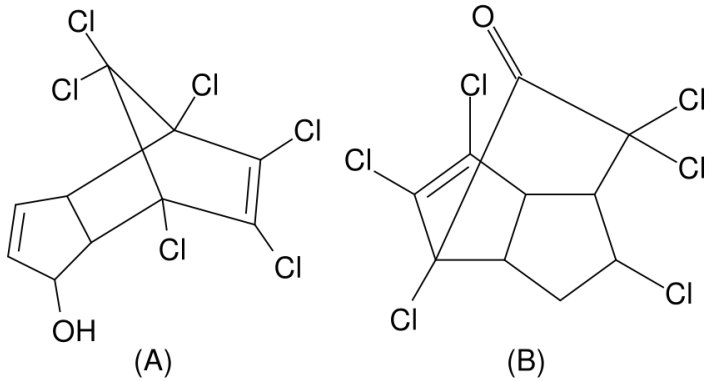
Elemental Formula: NA

Source: anthropogenic

Class: heptachlor related

Identification: Reference Database MS





m/z	Identity
281	[M−HCl2]+ (compound A)
291	[M−CO−Cl]+ (compound B)
317	[M−Cl]+ (compound A)
324	[M−CO]+ (compound B)
352	M+ (compound B)

Filename: 2_coeluting_hydroxychlordene_69653754

Name: heptachlor

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1339.5, RT (s) (2D): 0.968

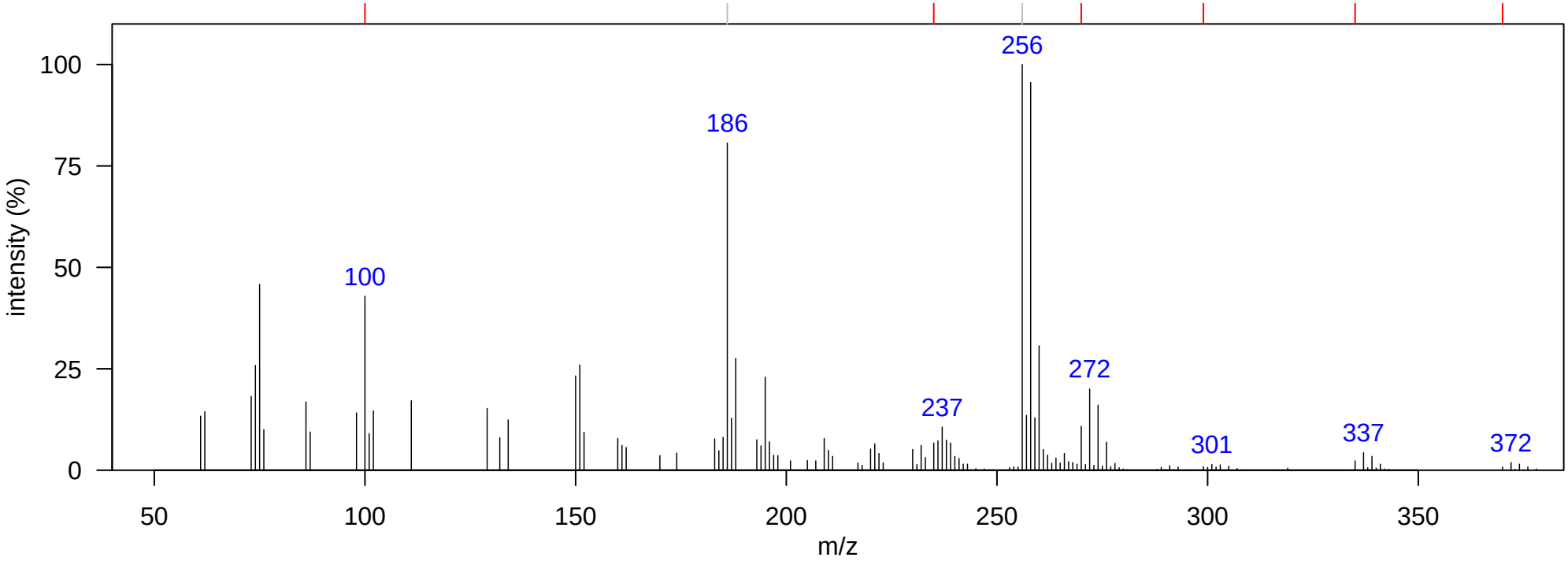
Comment: Low intensity, but visible in raw data. Interference from trichlorobiphenyl.

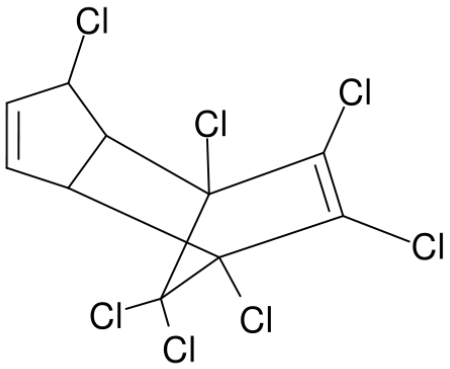
Elemental Formula: C10H5Cl7

Source: anthropogenic

Class: heptachlor related

Identification: Authentic MS RT





m/z	Identity
100	[C5H5Cl]+
186	interference PCB
235	[C5Cl5]+
256	interference PCB
270	[C5Cl6]+
299	[M−HCl2]+
335	[M−Cl]+
370	M+

Filename: heptachlor

Name: heptachlor related 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1402.5, RT (s) (2D): 1.122

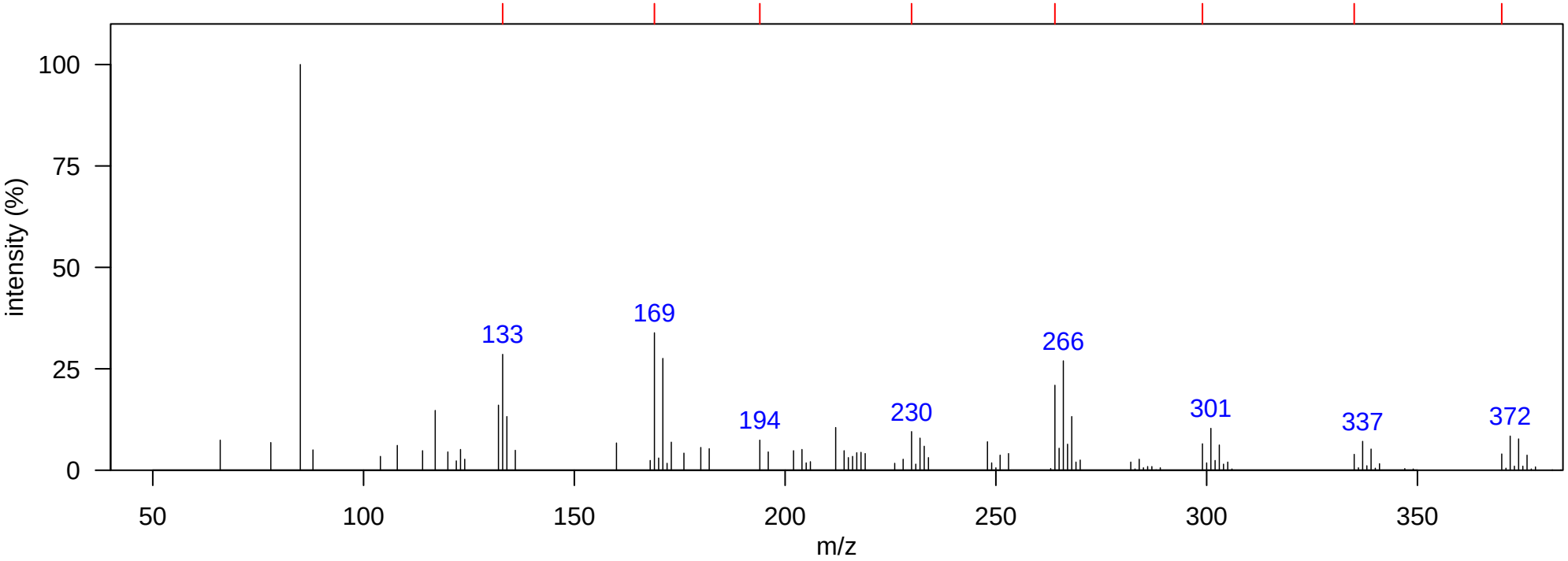
Comment: Similar to heptachlor, but ion cluster at m/z 272 is not present.

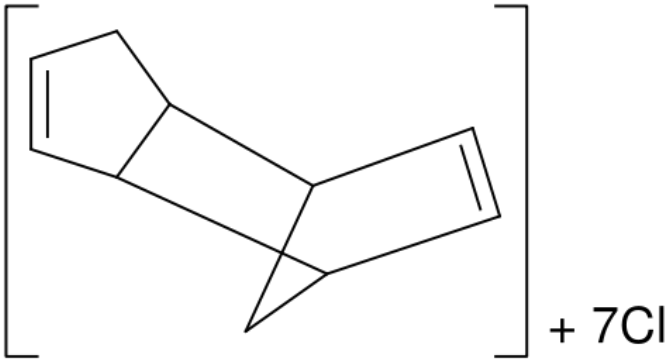
Elemental Formula: C10H5Cl7

Source: anthropogenic

Class: heptachlor related

Identification: Manual − Congener Group





m/z	Identity
133	[M−HCl3]2+
169	[C8H3Cl2]+
194	[M−HCl5]+
230	[M−4Cl]+
264	[M−HCl3]+
299	[M−HCl2]+
335	[M−Cl]+
370	[M]+

Filename: heptachlor_related_1

Name: heptachlor related 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1409.5, RT (s) (2D): 1.569

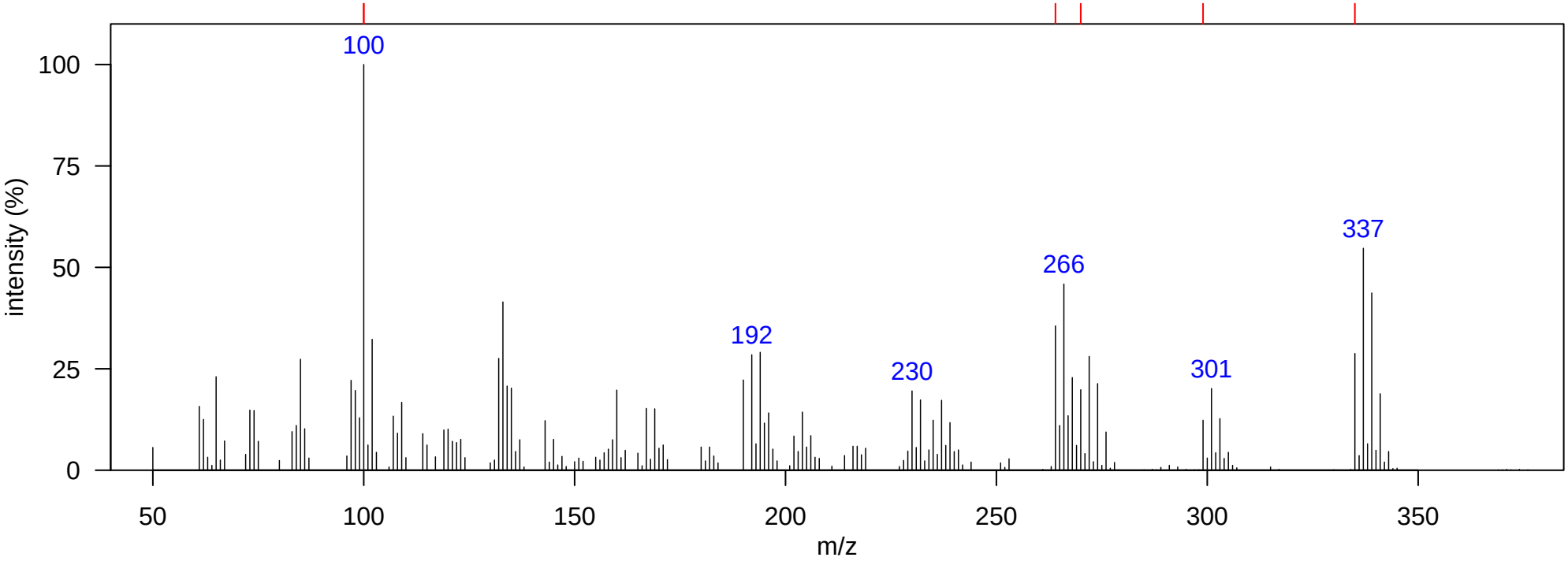
Comment:

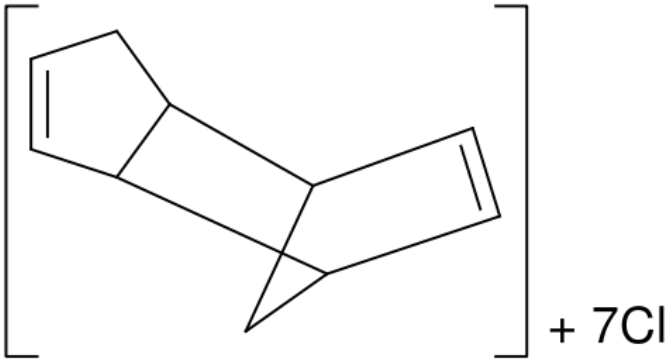
Elemental Formula: C10H5Cl7

Source: anthropogenic

Class: heptachlor related

Identification: Manual − Congener Group





m/z	Identity
100	[C5H5Cl]+
264	[M−HCl3]+
270	[C5Cl6]+
299	[M−HCl2]+
335	[M−Cl]+

Filename: heptachlor_related_2

Name: heptachlor epoxide

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1430.5, RT (s) (2D): 1.431

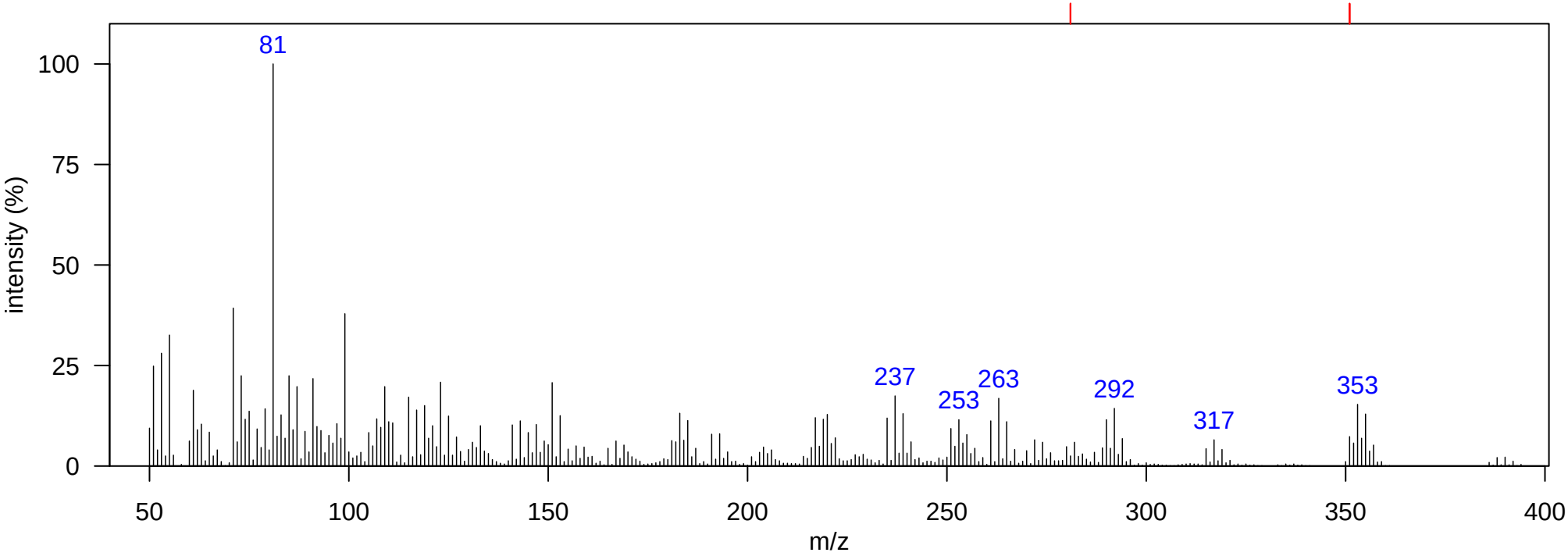
Comment:

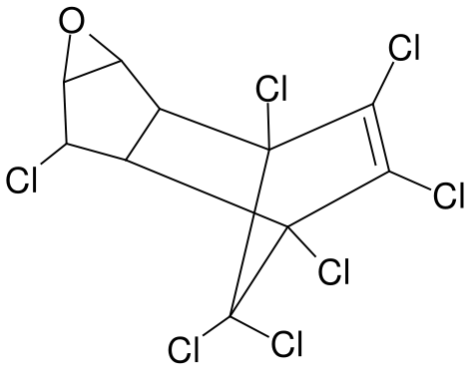
Elemental Formula: C10H5Cl7O

Source: anthropogenic

Class: heptachlor related

Identification: Authentic MS RT





m/z	Identity
281	[M−3Cl]+
351	[M−Cl]+

Filename: heptachlor_epoxide

Name: heptachlor related 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1462, RT (s) (2D): 1.689

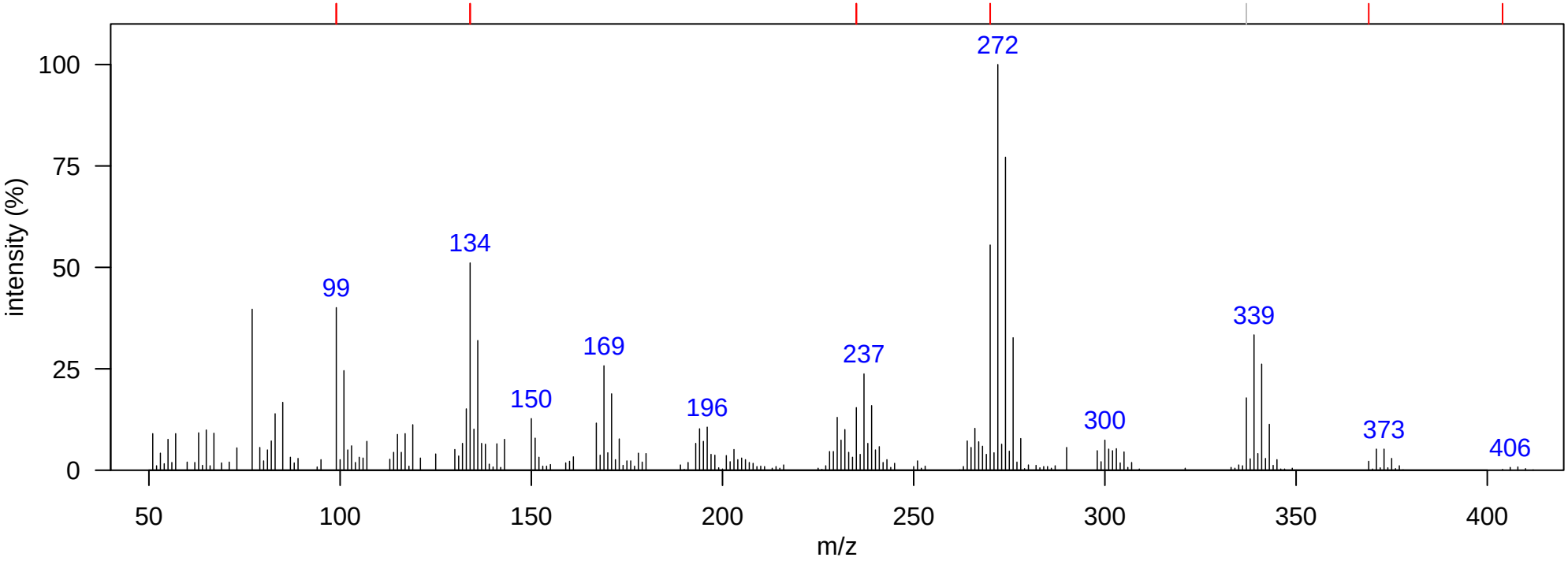
Comment:

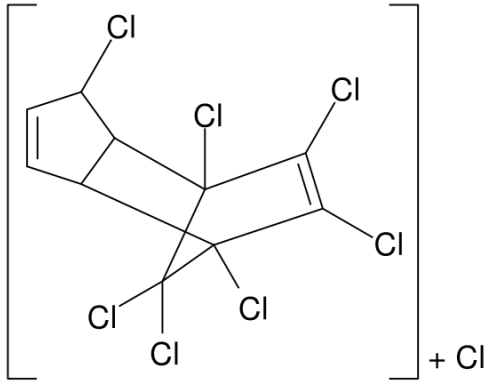
Elemental Formula: C10H4Cl8

Source: anthropogenic

Class: heptachlor related

Identification: Manual − Congener Group





m/z	Identity
99	[C5H4Cl]+
134	[C5H4Cl2]+
235	[C5Cl5]+
270	[C5Cl6]+
337	interference
369	[M−Cl]+
404	M+

Filename: heptachlor_related_3

Name: heptachlor related 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1574, RT (s) (2D): 2.192

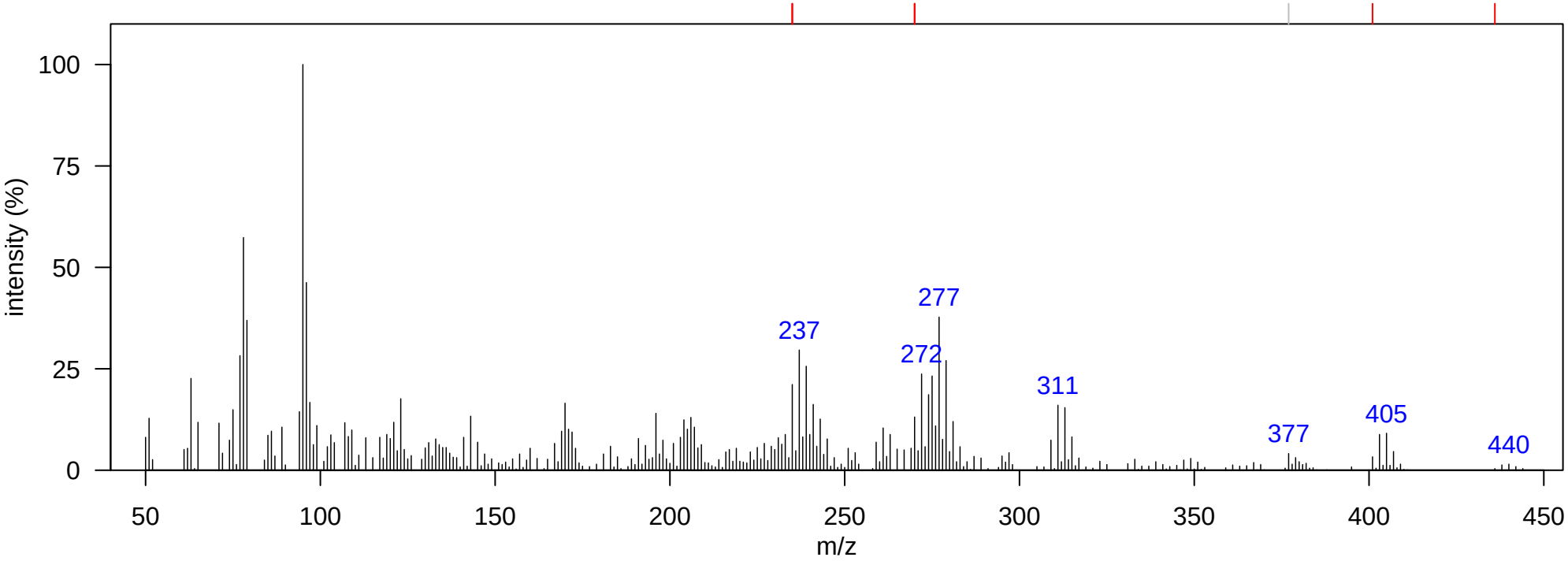
Comment: PM = Possible Molecular Ion

Elemental Formula: C10H3Cl9

Source: anthropogenic

Class: heptachlor related

Identification: Manual − Congener Group



m/z	Identity
235	[C5Cl5]+
270	[C5Cl6]+
377	interference
401	[PM−Cl]+ contains 8Cl
436	[PM]+ contains 9Cl

Name: 1,1'−bis(chlorophenyl)−ethane (DDEt)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1350, RT (s) (2D): 1.019

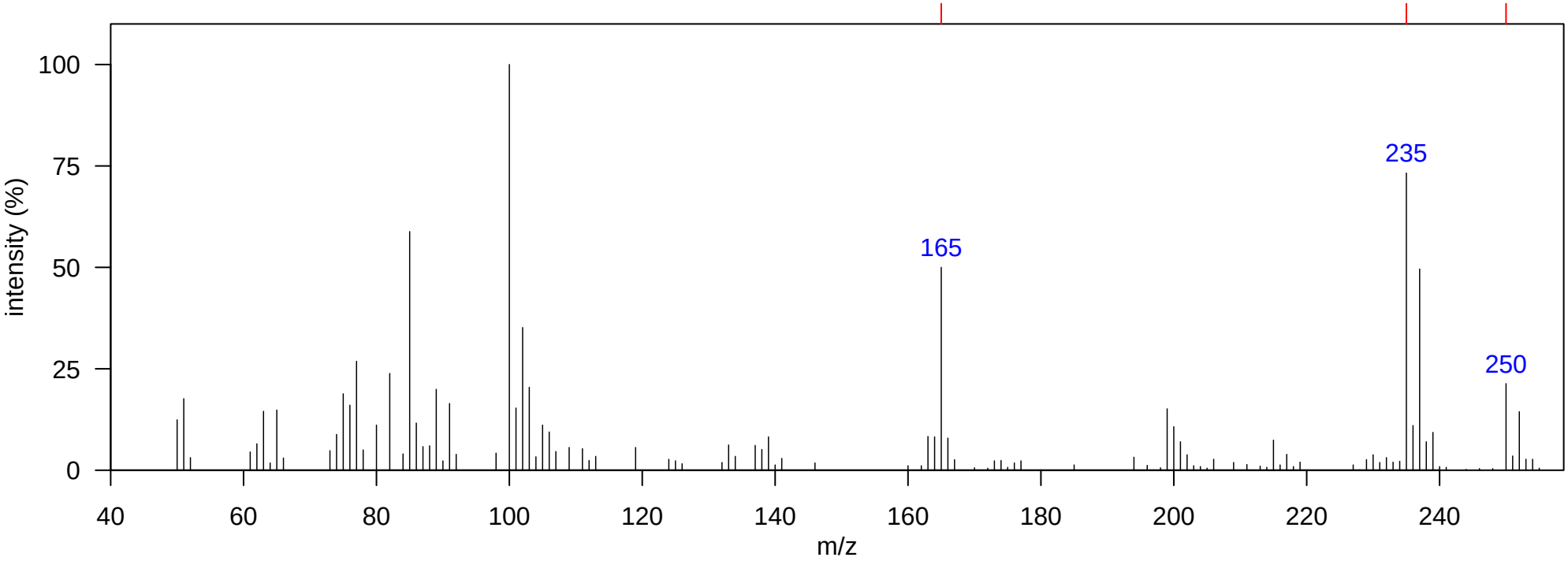
Comment:

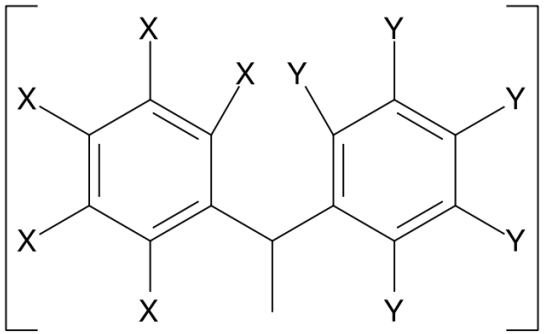
Elemental Formula: C14H12Cl2

Source: anthropogenic

Class: DDT related

Identification: Reference Database MS





X=Cl, 4H; Y=Cl, 4H

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

Filename: DDEt

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

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1462, RT (s) (2D): 1.341

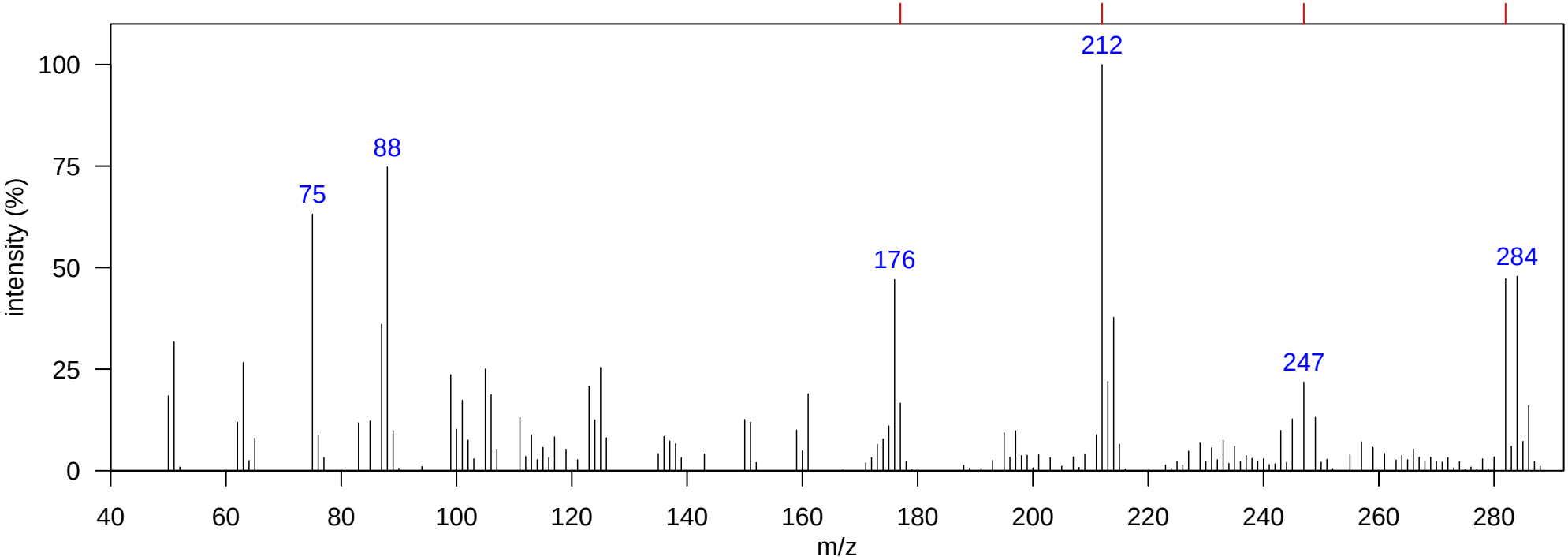
Comment:

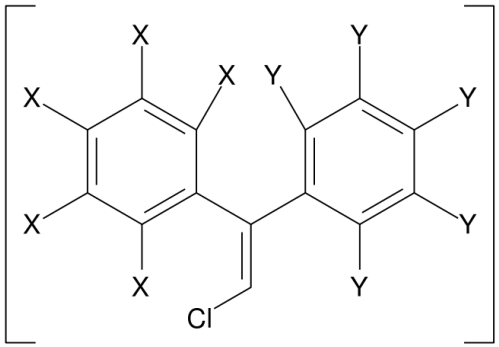
Elemental Formula: C14H9Cl3

Source: anthropogenic

Class: DDT related

Identification: Reference Database MS





X=Cl, 4H; Y=Cl, 4H

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

Filename: DDMU

Name: dichlorodiphenyldichloroethylene (DDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1462, RT (s) (2D): 1.437

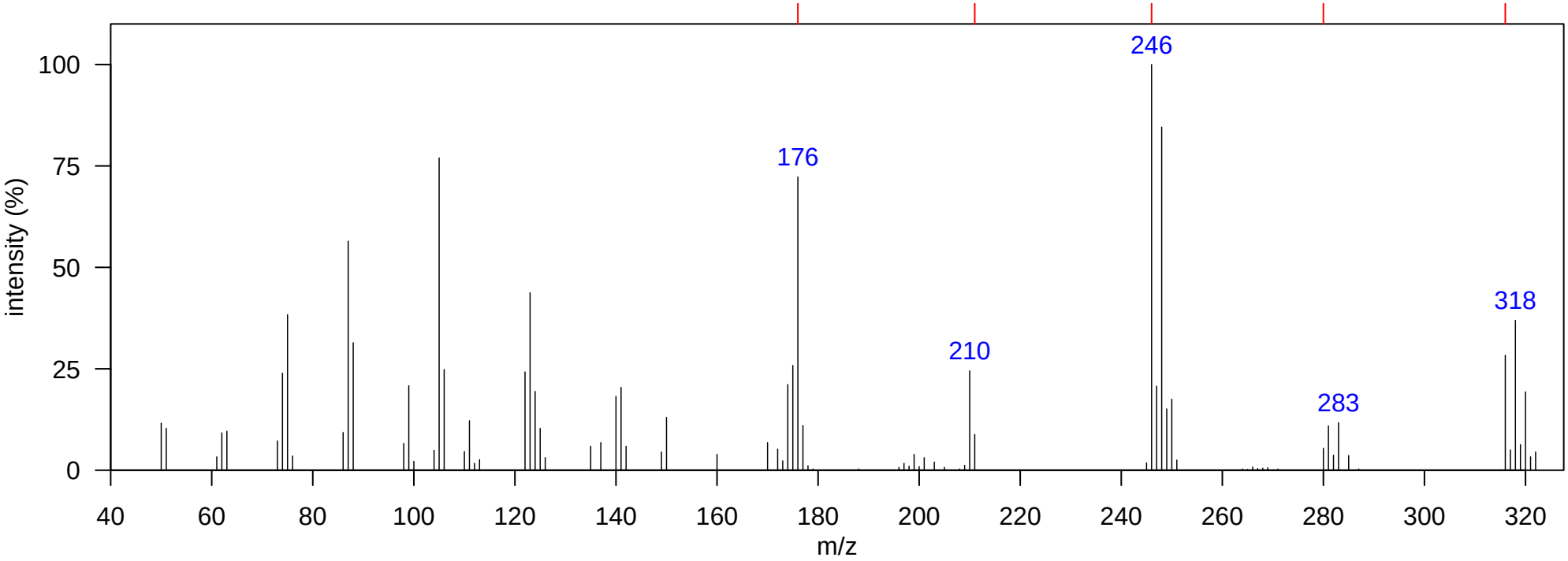
Comment:

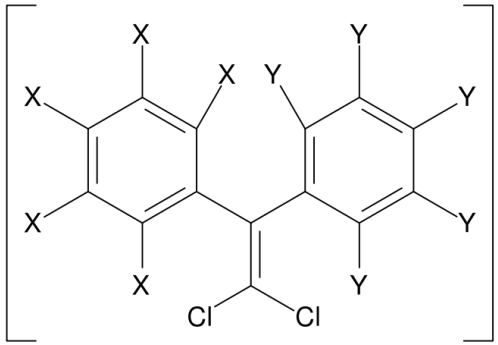
Elemental Formula: C14H8Cl4

Source: anthropogenic

Class: DDT related

Identification: Authentic MS





X=Cl, 4H; Y=Cl, 4H

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

Filename: DDE_isomer_1

Name: dichlorodiphenyldichloroethylene (DDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1486.5, RT (s) (2D): 1.242

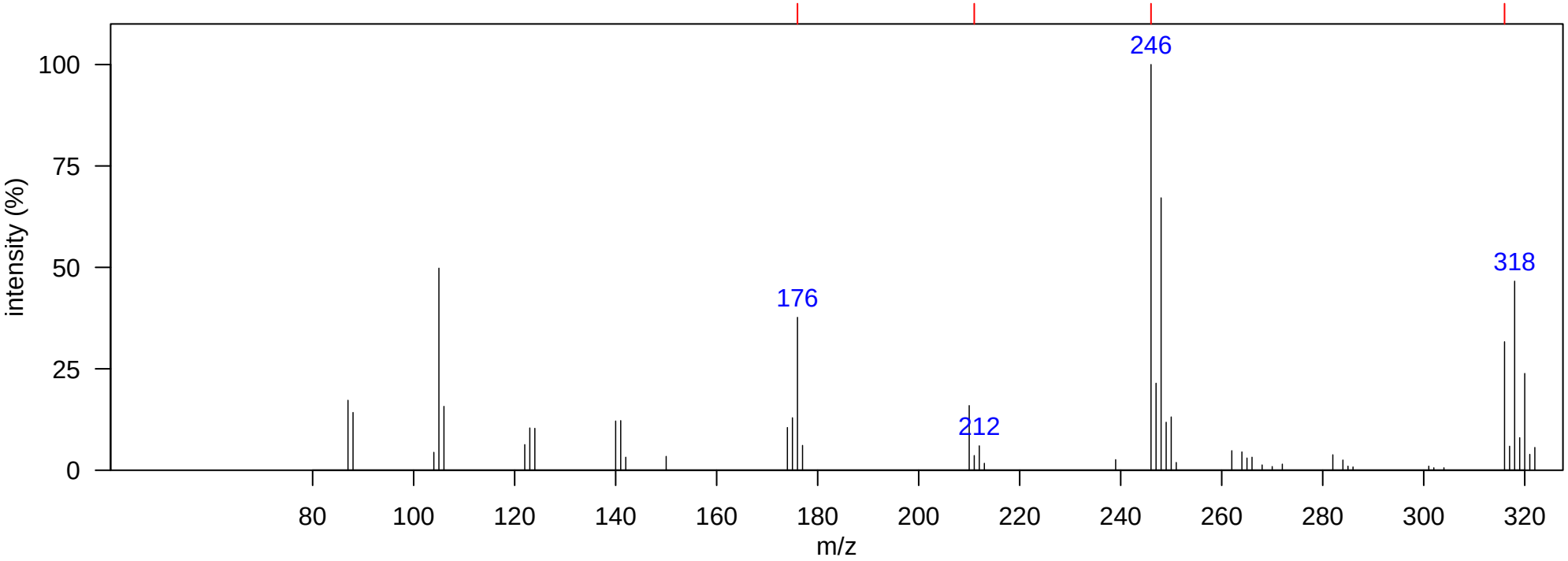
Comment:

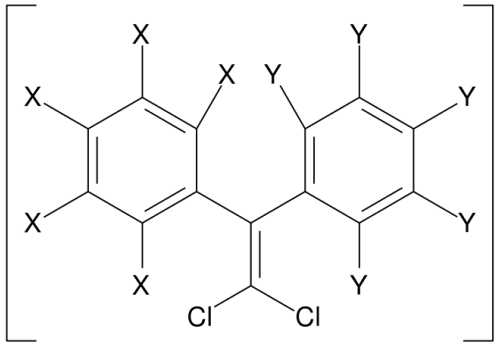
Elemental Formula: C14H8Cl4

Source: anthropogenic

Class: DDT related

Identification: Authentic MS





X=Cl, 4H; Y=Cl, 4H

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

Filename: DDE_isomer_2

Name: 1−chloro−2,2−bis(p−chlorophenyl)ethane (DDM)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1490, RT (s) (2D): 1.58

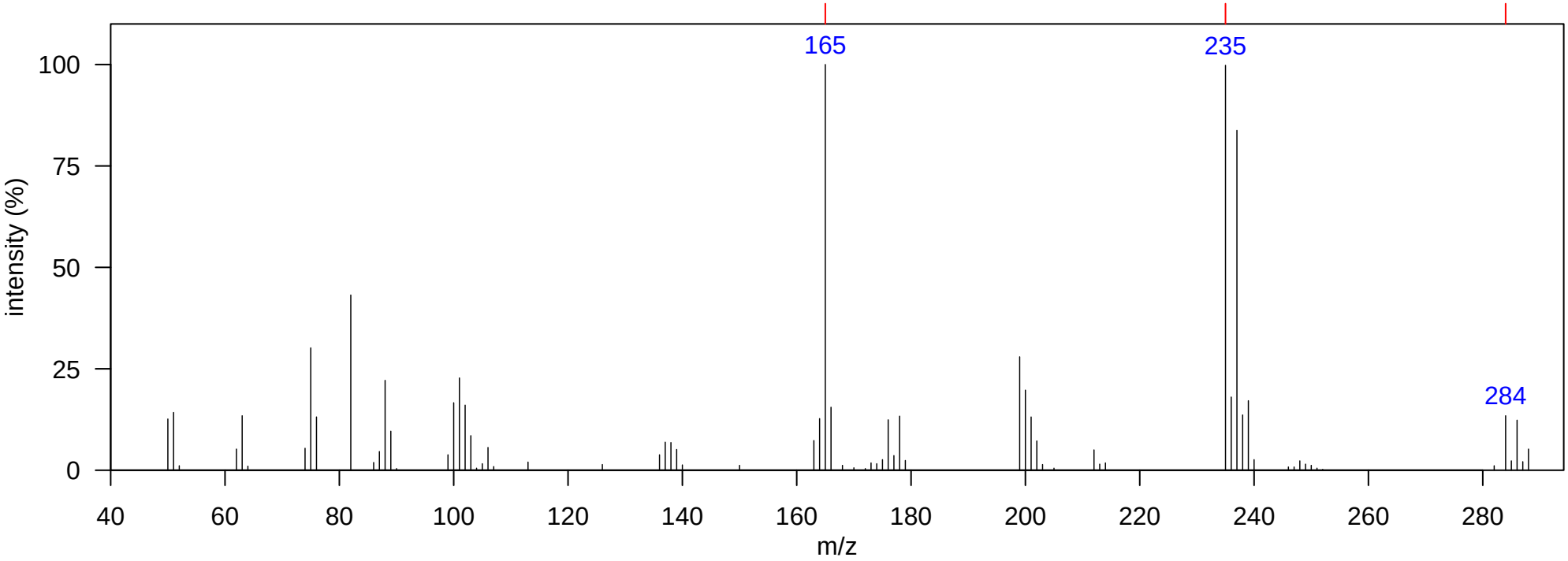
Comment:

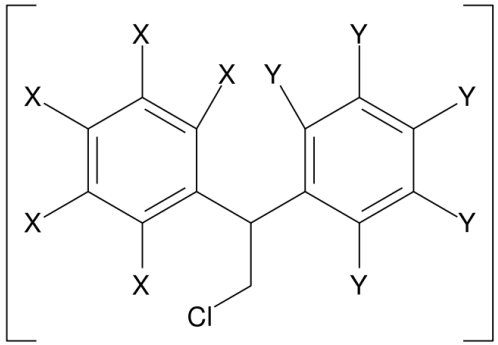
Elemental Formula: C14H11Cl3

Source: anthropogenic

Class: DDT related

Identification: Reference Database MS





X=Cl, 4H; Y=Cl, 4H

m/z	Identity
165	[M−CH2Cl−2Cl]+
235	[M−CH2Cl]+
284	M+

Filename: DDM

Name: p,p'−dichlorodiphenyldichloroethylene (p,p'−DDE)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1514.5, RT (s) (2D): 1.077

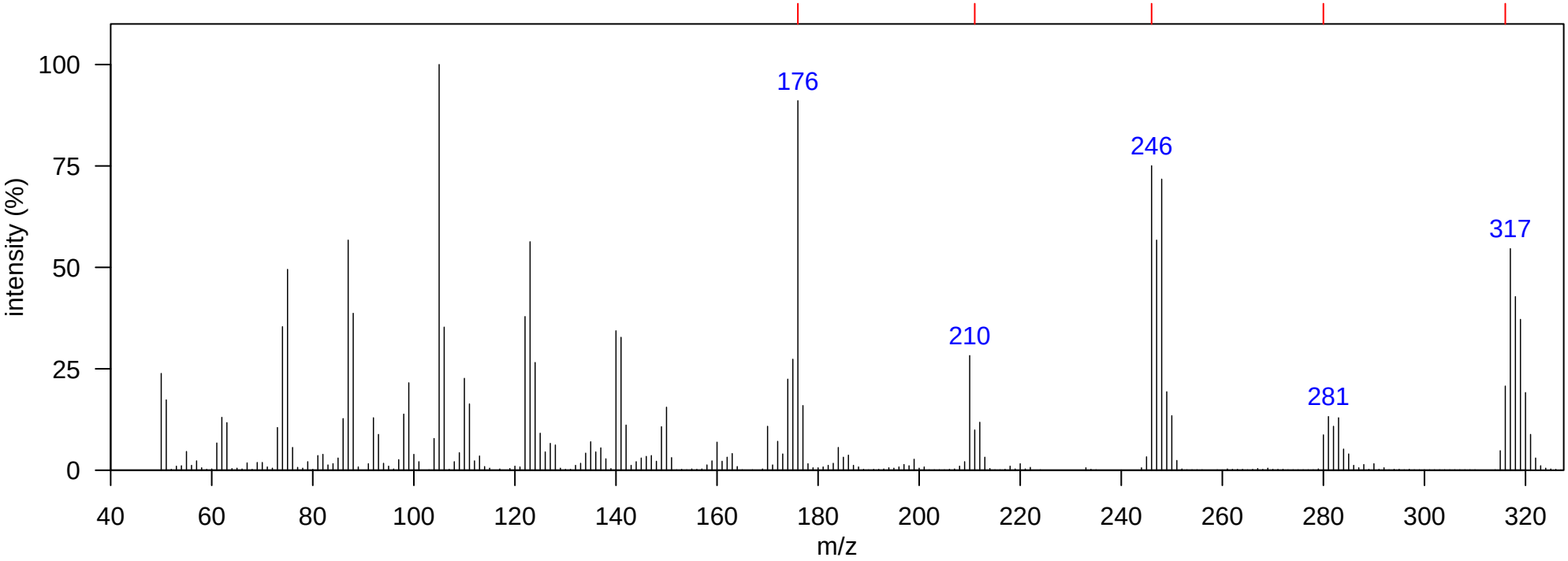
Comment:

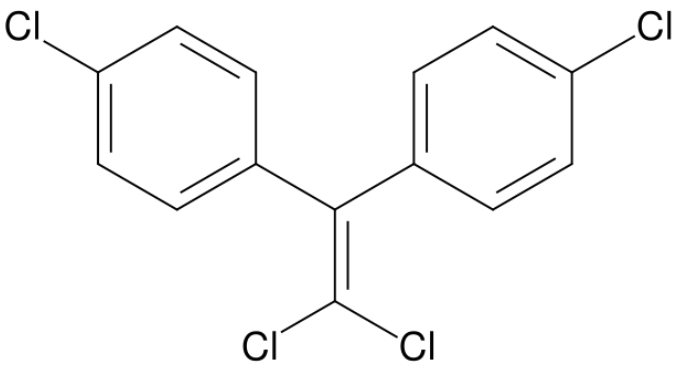
Elemental Formula: C14H8Cl4

Source: anthropogenic

Class: DDT related

Identification: Authentic MS RT





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

Filename: ppDDE

Name: o,p'−dichlorodiphenyldichloroethane (o,p'−DDD)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1514.5, RT (s) (2D): 1.616

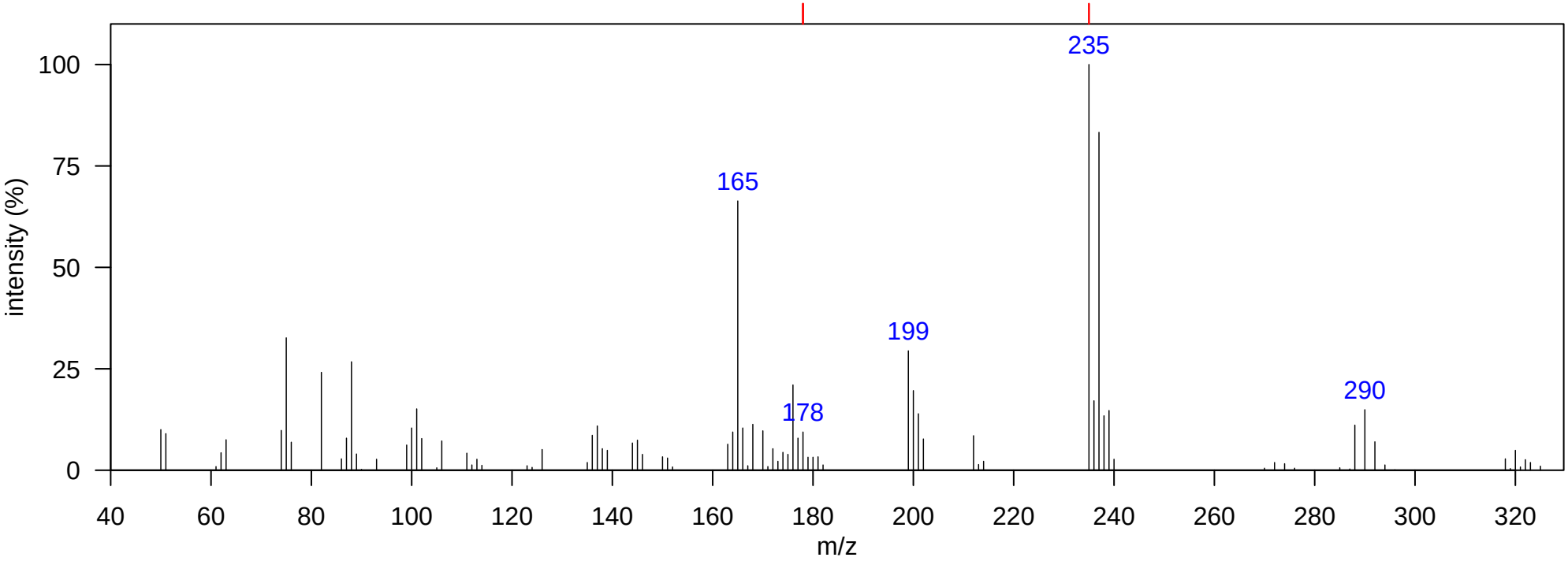
Comment:

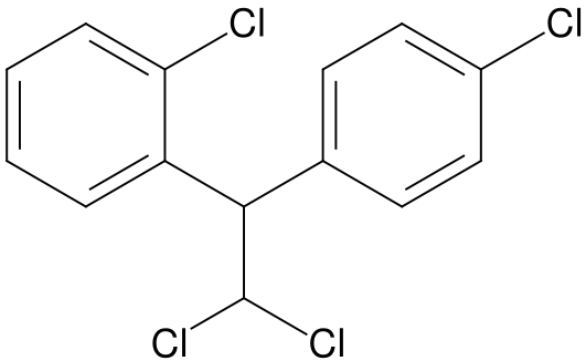
Elemental Formula: C14H10Cl4

Source: anthropogenic

Class: DDT related

Identification: Authentic MS RT





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

Filename: opDDD

Name: p,p'−DDD

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1553, RT (s) (2D): 1.715

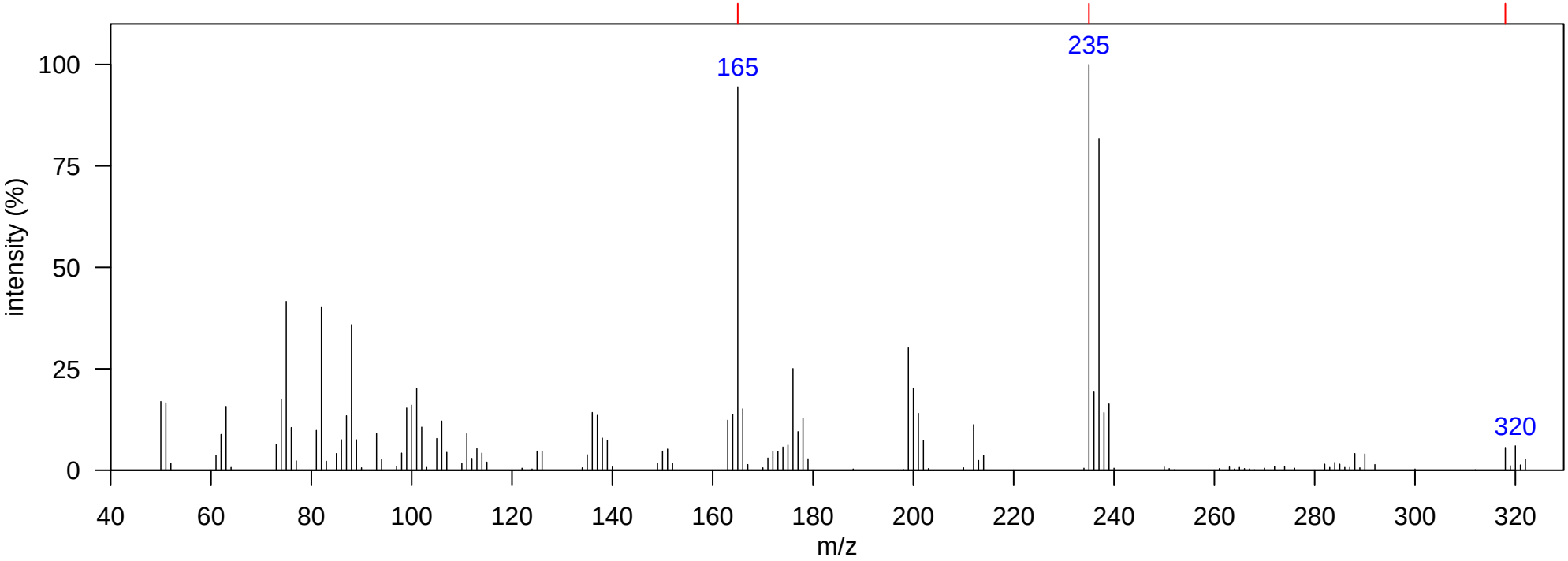
Comment:

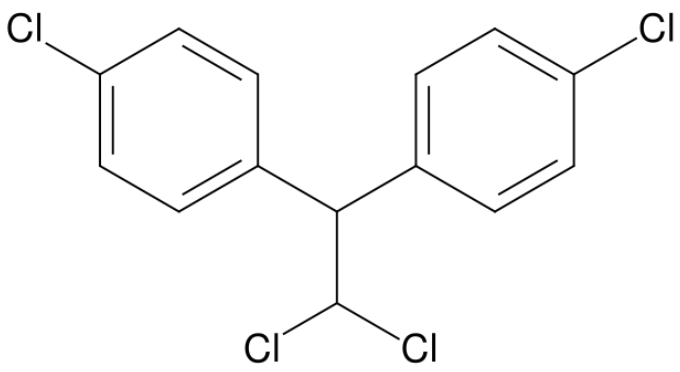
Elemental Formula: C14H10Cl4

Source: anthropogenic

Class: DDT related

Identification: Authentic MS RT





m/z	Identity
165	[M−CHCl2−HCl2]+
235	[M−CHCl2]+
318	M+

Filename: ppDDD

Name: p,p'−DDT

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1591.5, RT (s) (2D): 1.792

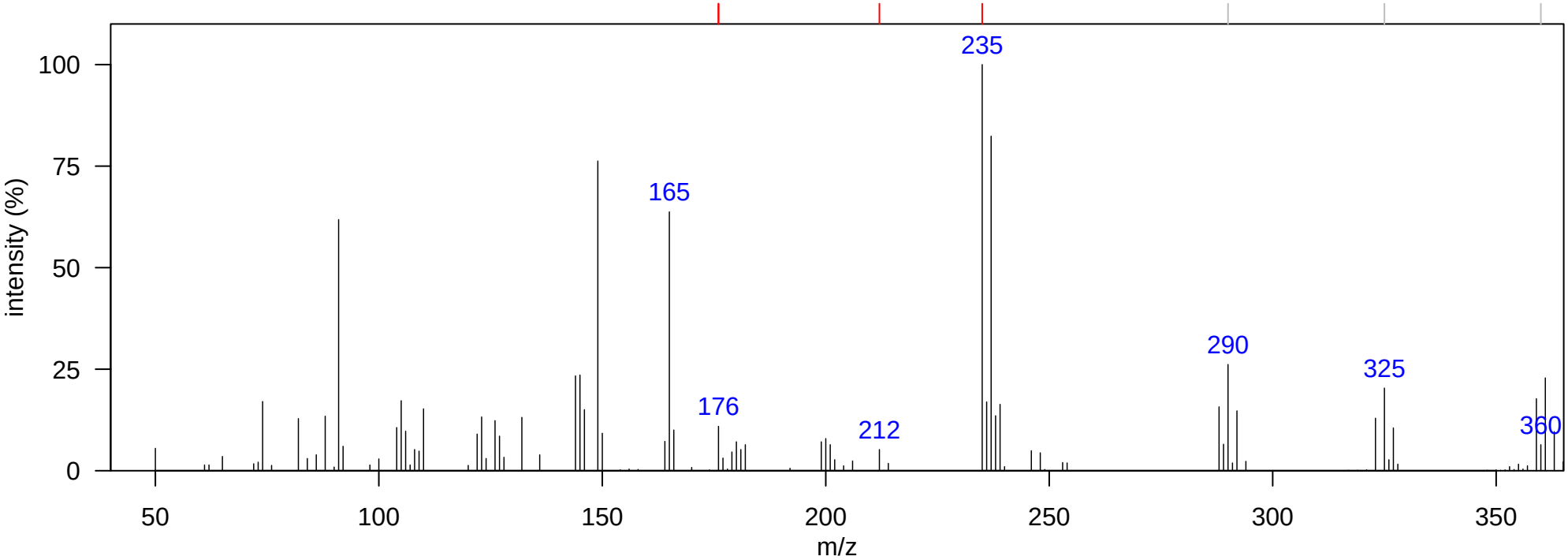
Comment:

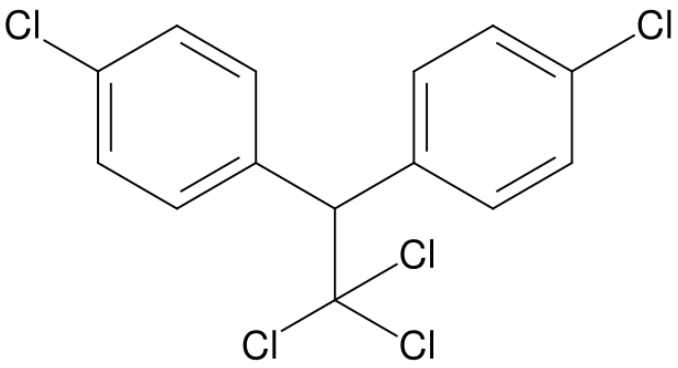
Elemental Formula: C14H9Cl5

Source: anthropogenic

Class: DDT related

Identification: Authentic MS RT





m/z	Identity
176	[M−HCl5]+
212	[M−4Cl]+
235	[M−CCl3]+
290	interference PCB
325	interference PCB
360	interference PCB

Filename: ppDDT

Name: DDT related 1

Elemental Formula: C14H6Cl6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: anthropogenic

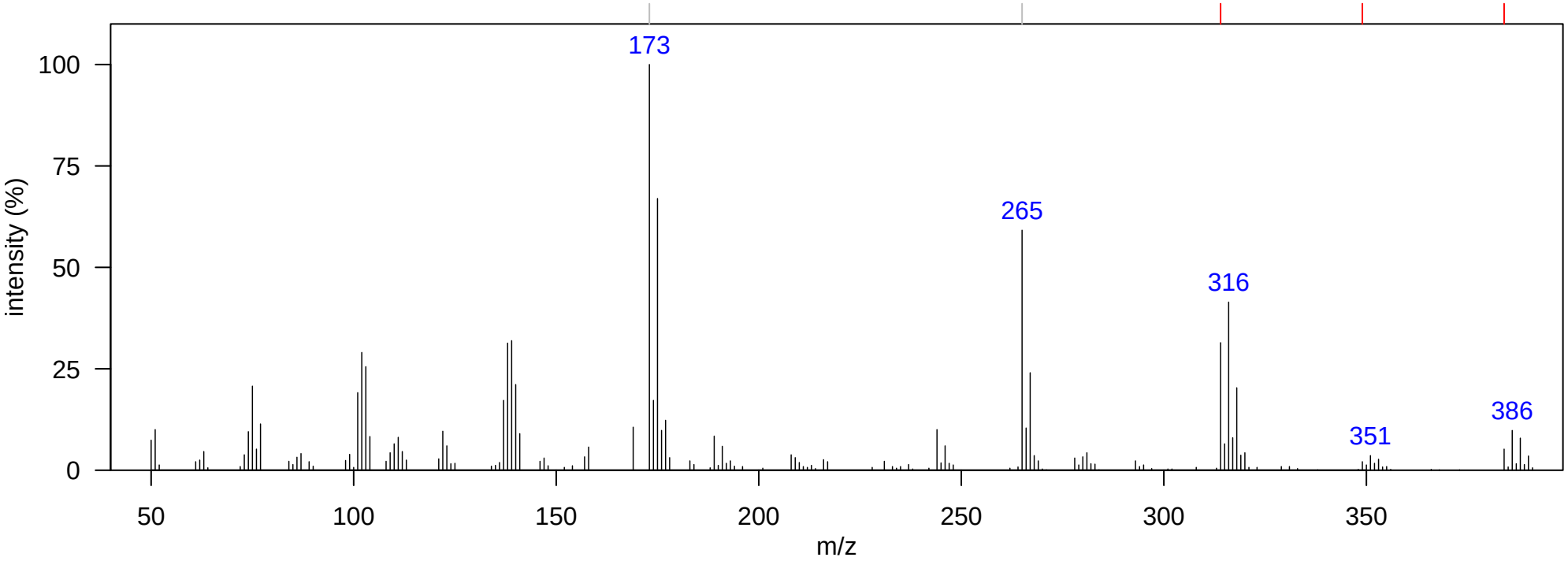
Instrument: GCxGC−TOF, electron impact

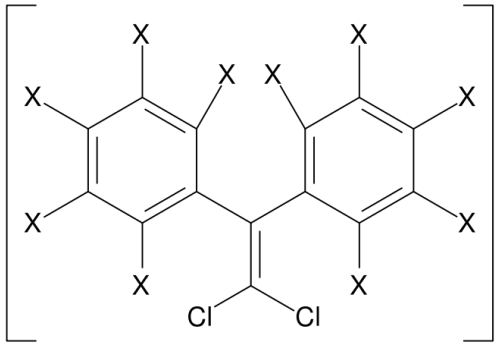
Class: DDT related

RT (s) (1D): 1619.5, RT (s) (2D): 1.254

Identification: Manual − Congener Group

Comment: Suggested DDE backbone structure, but containing 6 chlorines.





X=4Cl, 6H

m/z	Identity
173	interference unknown12
265	interference unknown12
314	[M−2Cl]+
349	[M−Cl]+
384	M+

Name: DDT related 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1686, RT (s) (2D): 1.537

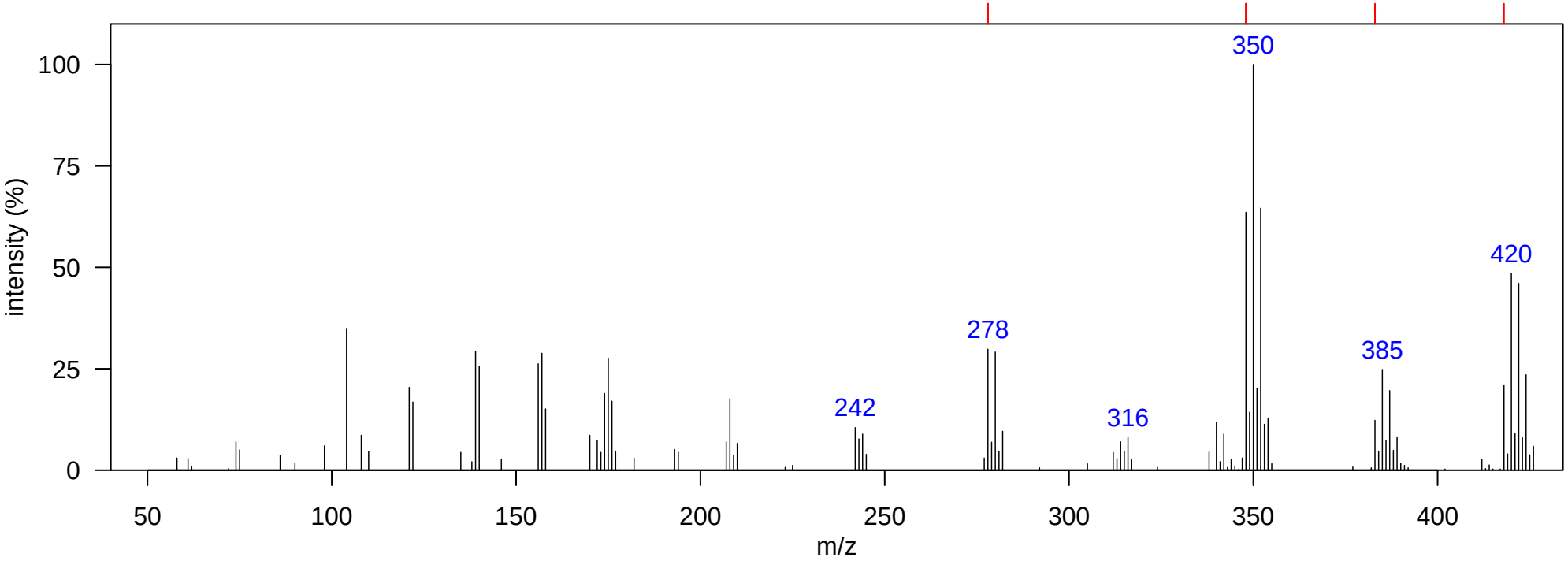
Comment: Suggested DDE backbone structure, but containing 7 chlorines.

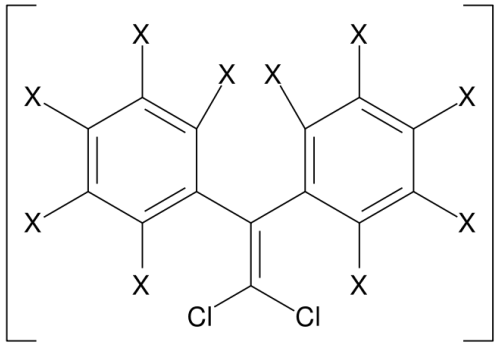
Elemental Formula: C14H5Cl7

Source: anthropogenic

Class: DDT related

Identification: Manual − Congener Group





X=5Cl, 5H

m/z	Identity
278	[M−4Cl]+
348	[M−2Cl]+
383	[M−Cl]+
418	M+

Name: DDT related 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1693, RT (s) (2D): 1.609

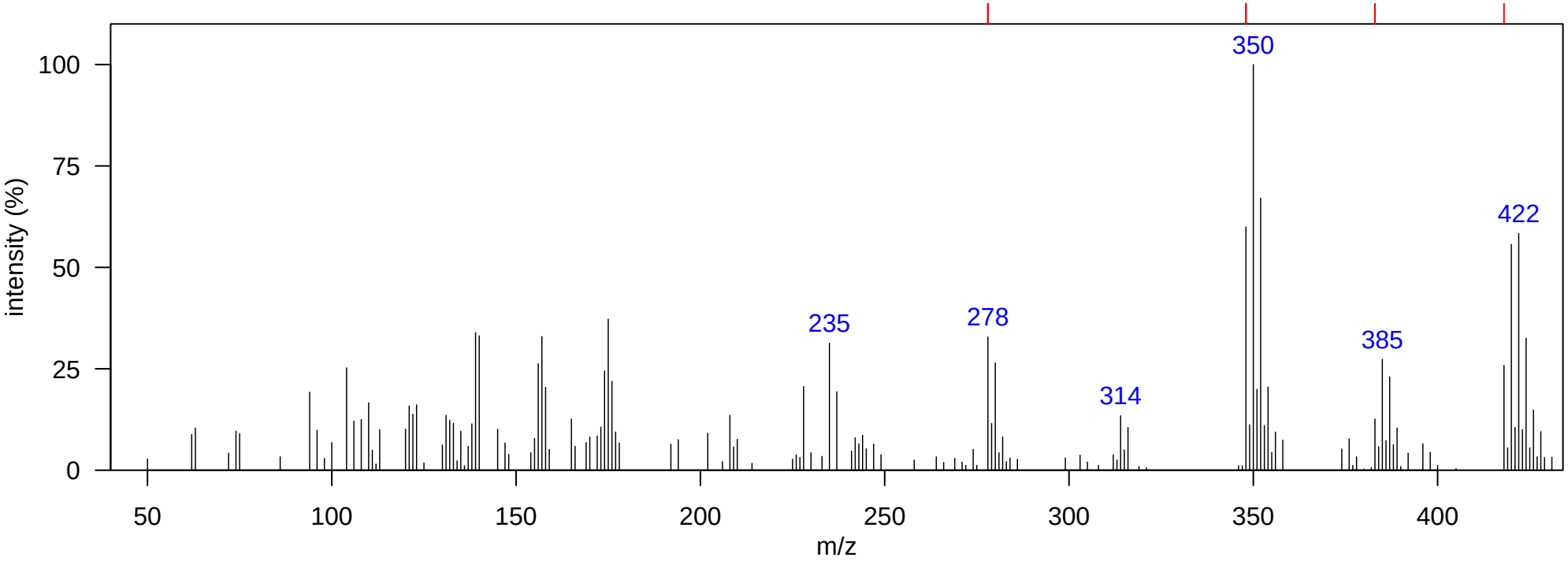
Comment: Suggested DDE backbone structure, but containing 7 chlorines.

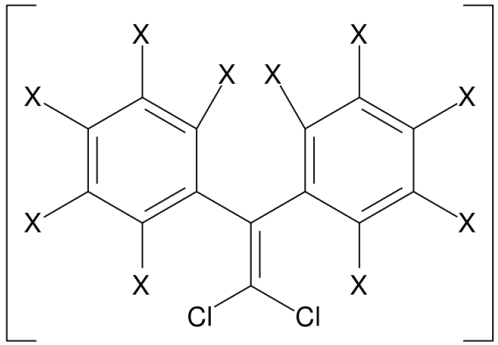
Elemental Formula: C14H5Cl7

Source: anthropogenic

Class: DDT related

Identification: Manual − Congener Group





X=5Cl, 5H

m/z	Identity
278	[M−4Cl]+
348	[M−2Cl]+
383	[M−Cl]+
418	M+

Filename: DDT_related_3

Name: tris(chlorophenyl)methane (TCPM) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1700, RT (s) (2D): 1.917

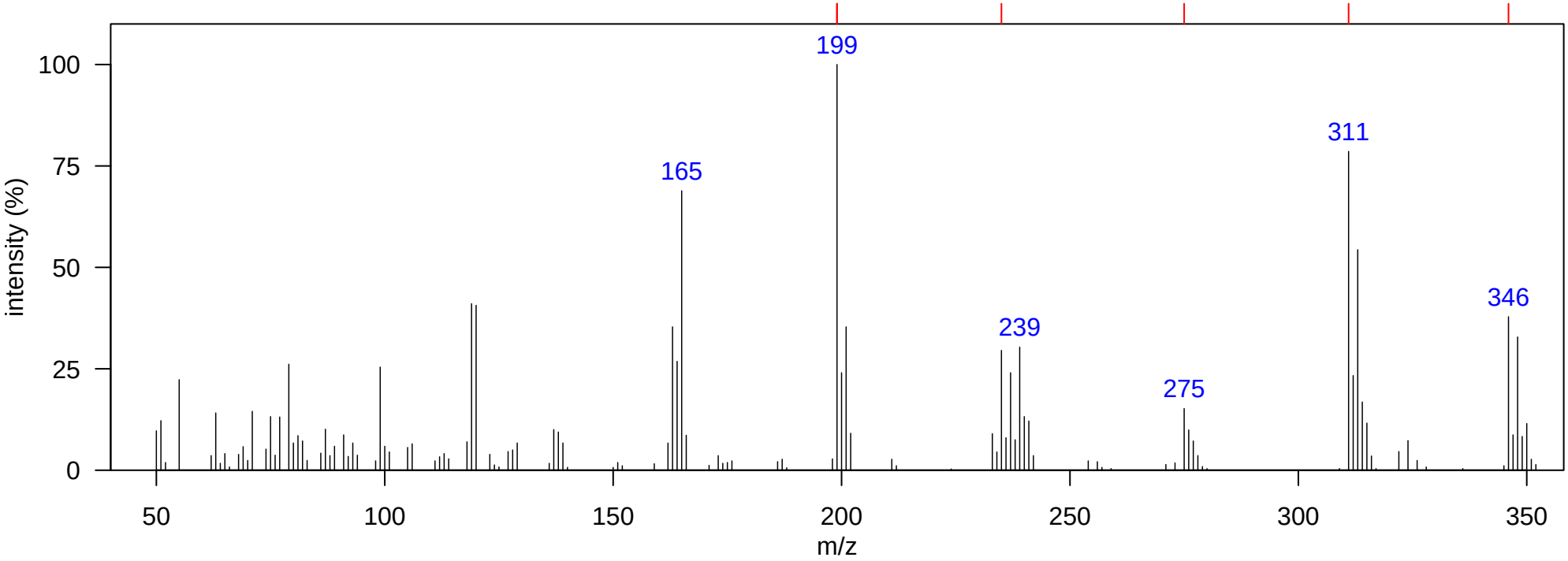
Comment: Ref: ES&T. 1995, 29, 2133−2139. At least one 2−chloro ring based on 235/239 ratio.

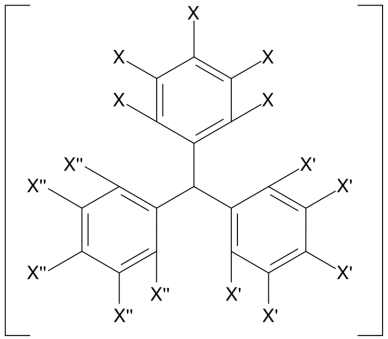
Elemental Formula: C19H13Cl3

Source: anthropogenic

Class: DDT related

Identification: Literature MS





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]+
275	[M−HCl2]+
311	[M−Cl]+
346	M+

Filename: TCPM_isomer_1

Name: tris(chlorophenyl)methane (TCPM) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1738.5, RT (s) (2D): 1.96

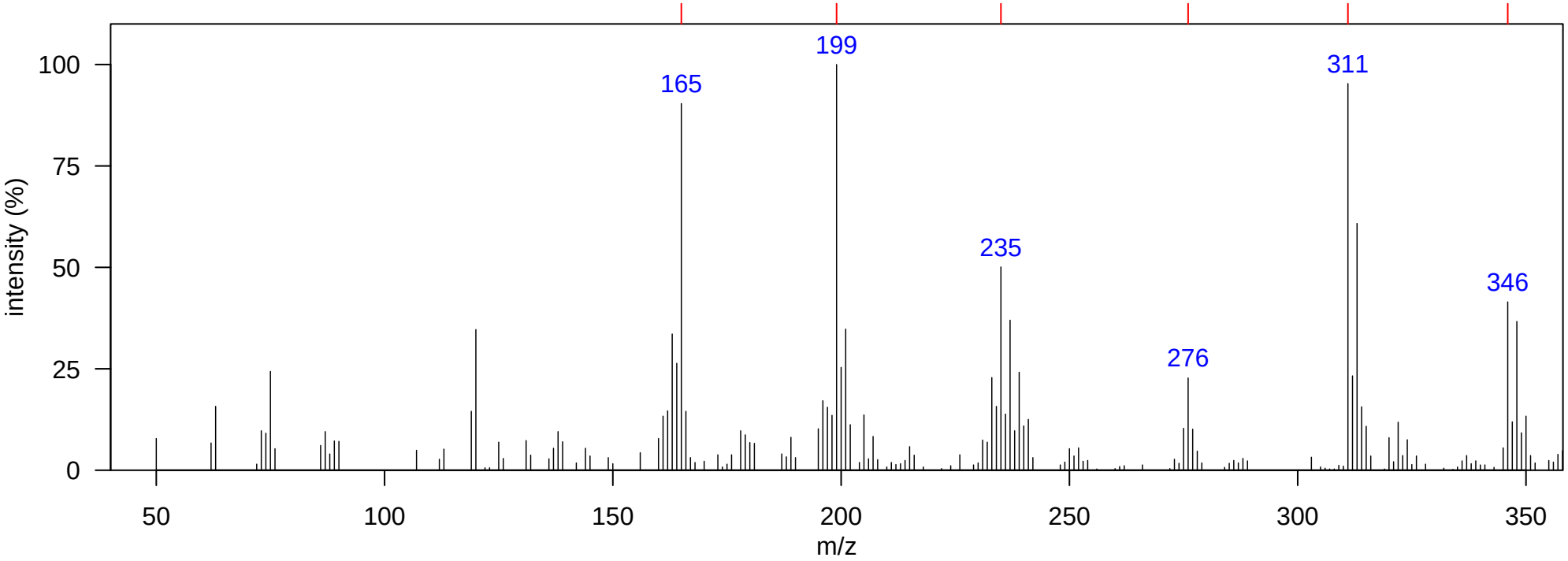
Comment: Ref: ES&T. 1995, 29, 2133−2139. Only 3/4−chloro ring based on 235/239 ratio.

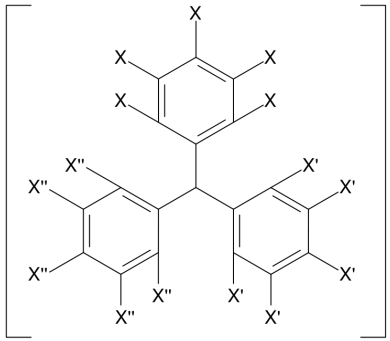
Elemental Formula: C19H13Cl3

Source: anthropogenic

Class: DDT related

Identification: Literature MS





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

No ortho-Cl present.

m/z	Identity
165	[C13H9]+ = [M−3Cl−C6H4]+
199	[M−C6H4Cl−HCl]+
235	[M−C6H4Cl]+
276	[M−Cl2]+
311	[M−Cl]+
346	M+

Filename: TCPM_isomer_2

Name: toxaphene 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1402.5, RT (s) (2D): 0.91

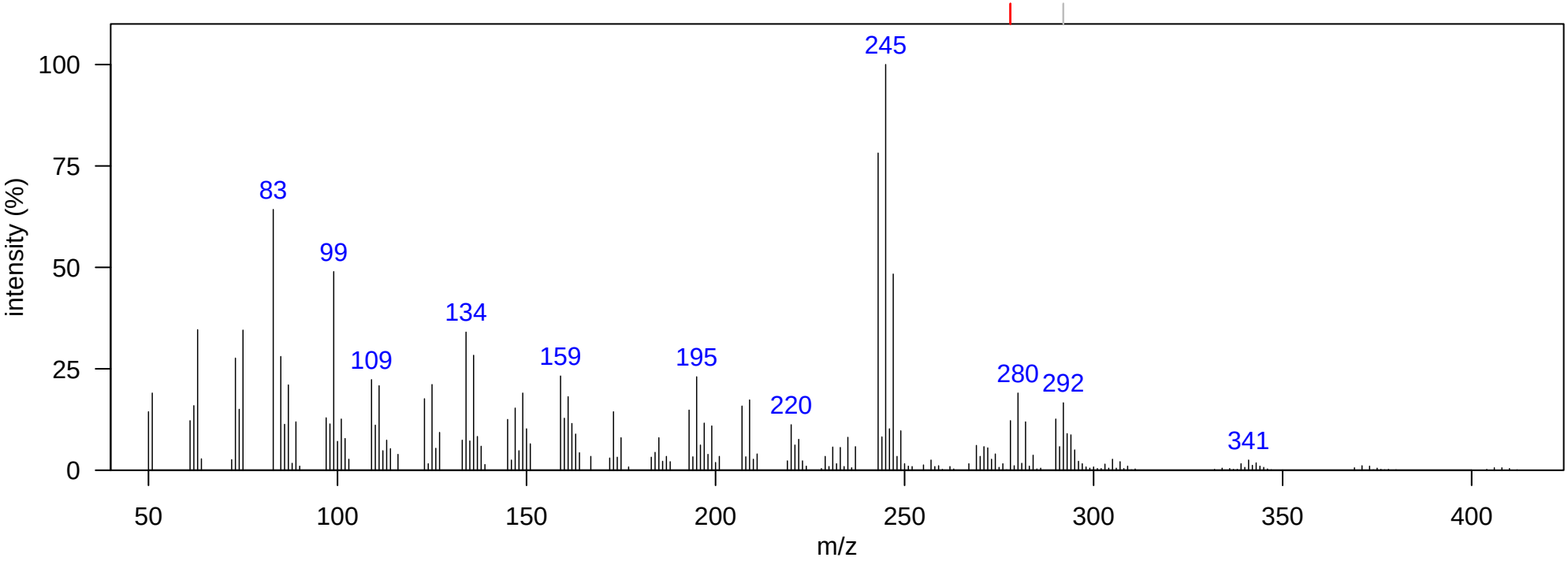
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: NA

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
278	[PM]+
292	interference from PCB

Filename: toxaphene_1

Name: toxaphene 2

Elemental Formula: C8H7Cl6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: anthropogenic

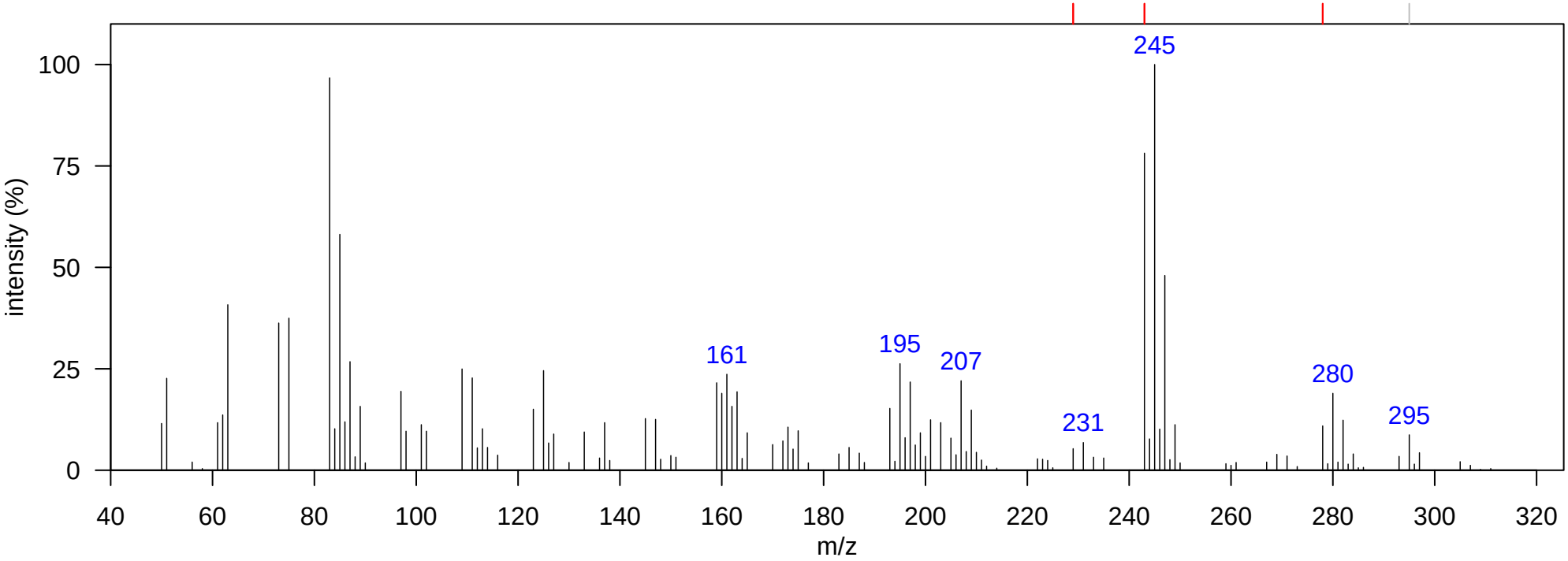
Instrument: GCxGC−TOF, electron impact

Class: toxaphene related

RT (s) (1D): 1416.5, RT (s) (2D): 0.999

Identification: Authentic MS RT

Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.



m/z	Identity
229	[PM−CH2Cl]+
243	[PM−Cl]+
278	[PM]+ contains 5Cl
295	interference
382	interference

Filename: toxaphene_2

Name: toxaphene 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1420, RT (s) (2D): 1.002

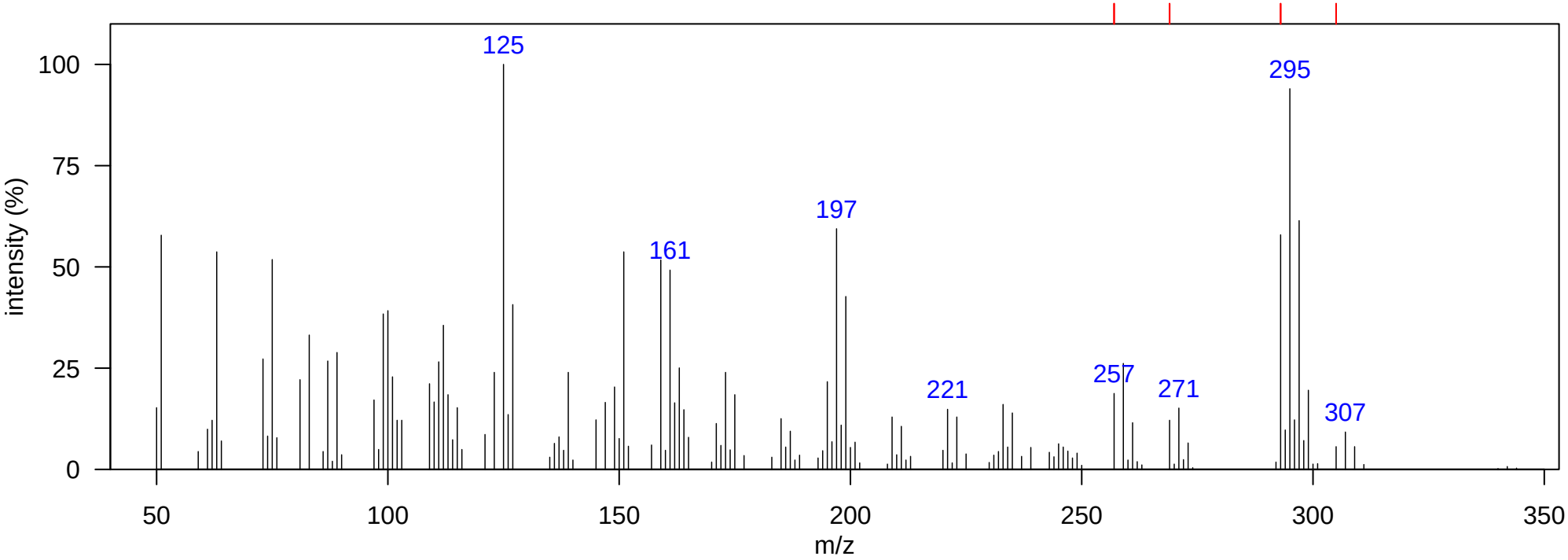
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C10H10Cl6

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
257	[Frag−HCl−CH2]+
269	[Frag−HCl]+
293	[Frag−12]+
305	[Frag]+

Name: toxaphene 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1525, RT (s) (2D): 1.238

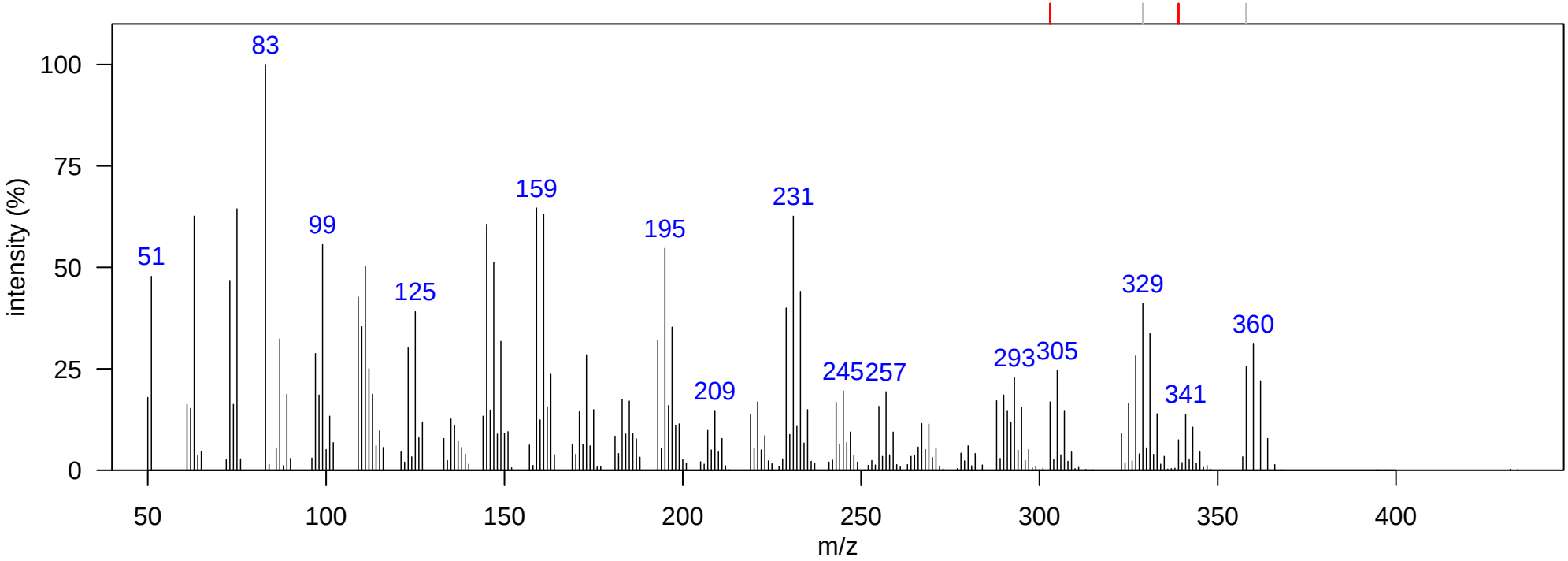
Comment: Toxaphene fragmentation pattern.

Elemental Formula: NA

Source: anthropogenic

Class: toxaphene related

Identification: Manual



m/z	Identity
303	[F−HCl]+
329	interference from PCB
339	[F]+
358	interference from PCB

Filename: toxaphene_4

Name: toxaphene 5

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1528.5, RT (s) (2D): 1.515

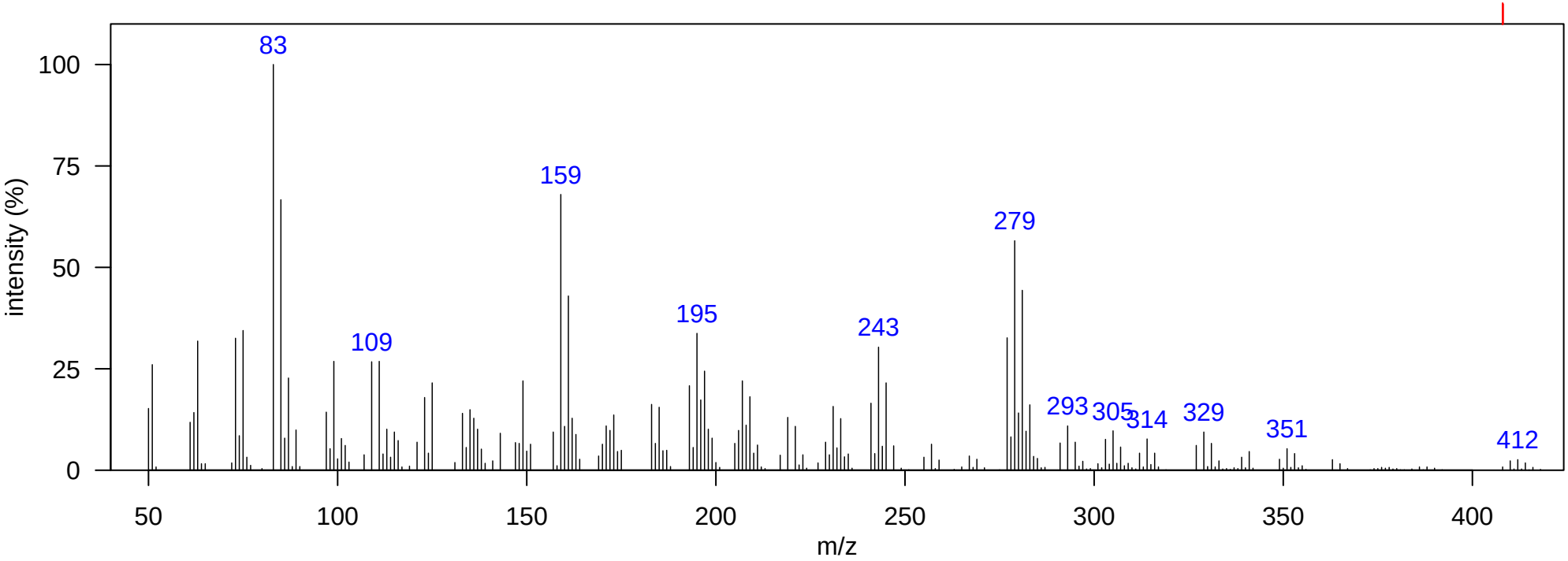
Comment: Toxaphene fragmentation pattern.

Elemental Formula: C10H8Cl8

Source: anthropogenic

Class: toxaphene related

Identification: Manual



m/z	Identity
408	M+

Name: toxaphene 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1577.5, RT (s) (2D): 1.913

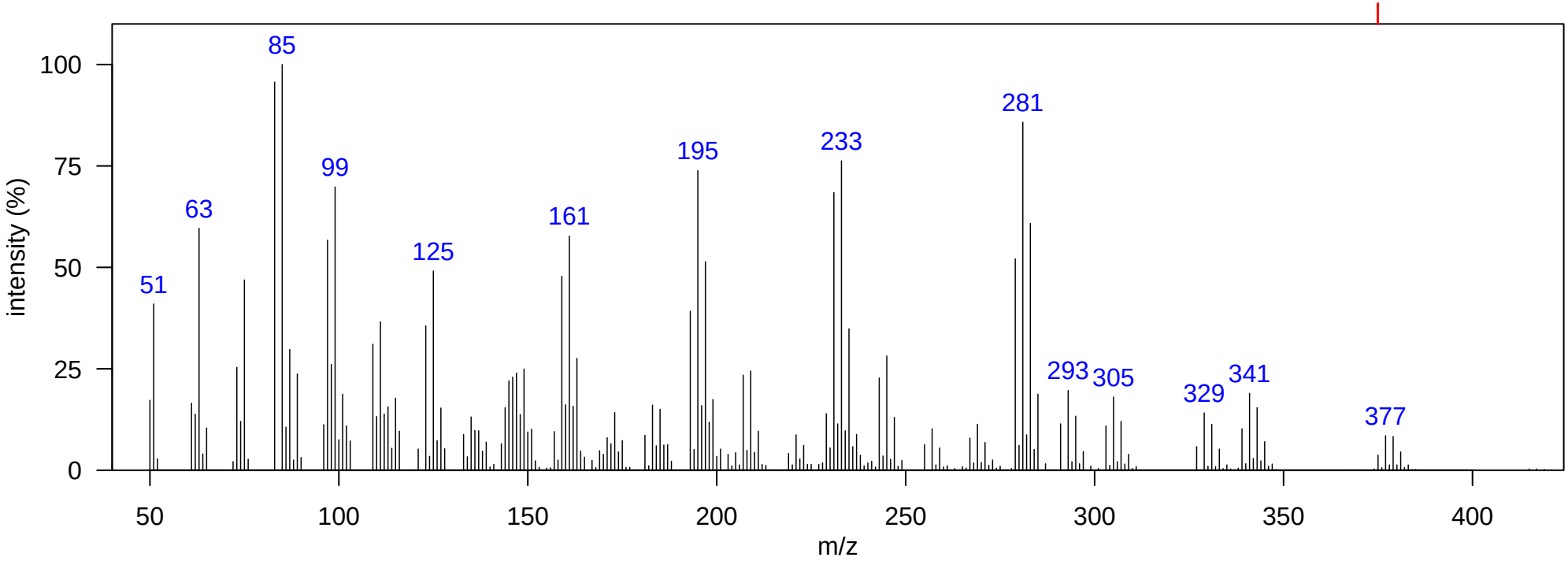
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C10H8Cl8

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
375	[M−Cl]+

Name: toxaphene 7

Elemental Formula: C10H9Cl7

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: anthropogenic

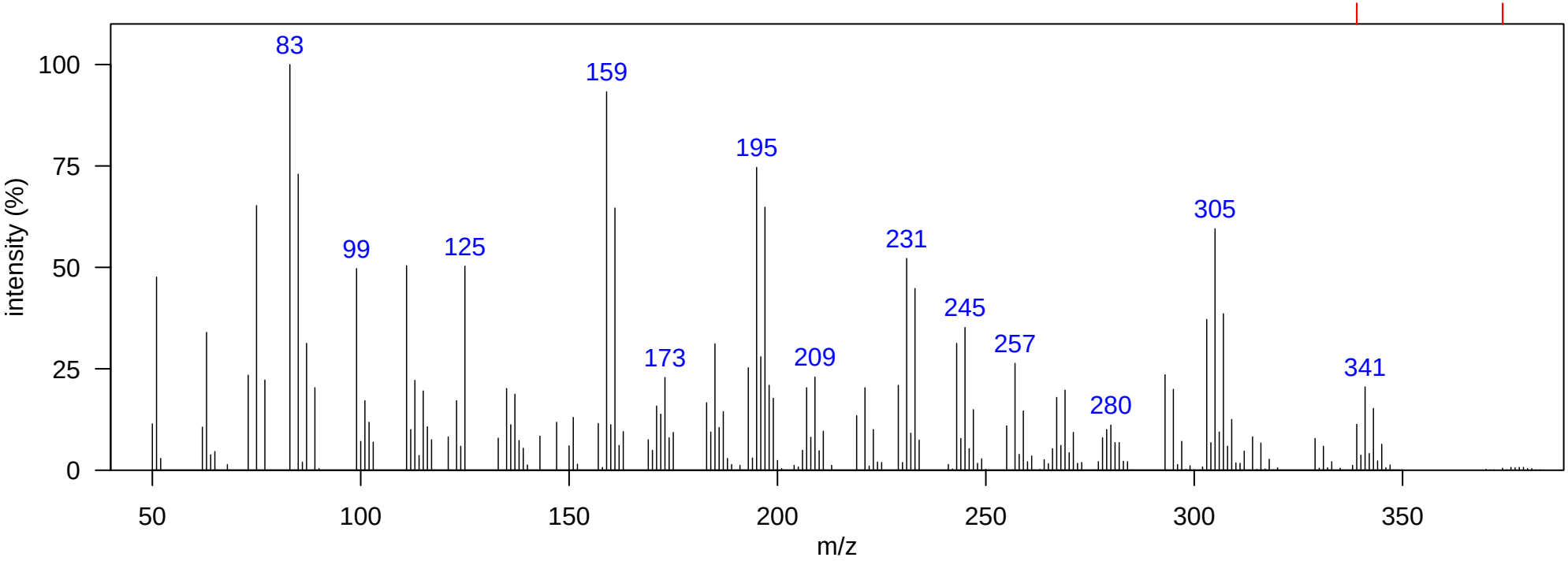
Instrument: GCxGC−TOF, electron impact

Class: toxaphene related

RT (s) (1D): 1591.5, RT (s) (2D): 1.948

Identification: Authentic MS RT

Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.



m/z	Identity
339	[M−Cl]+
374	M+

Name: toxaphene 8

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1598.5, RT (s) (2D): 2.083

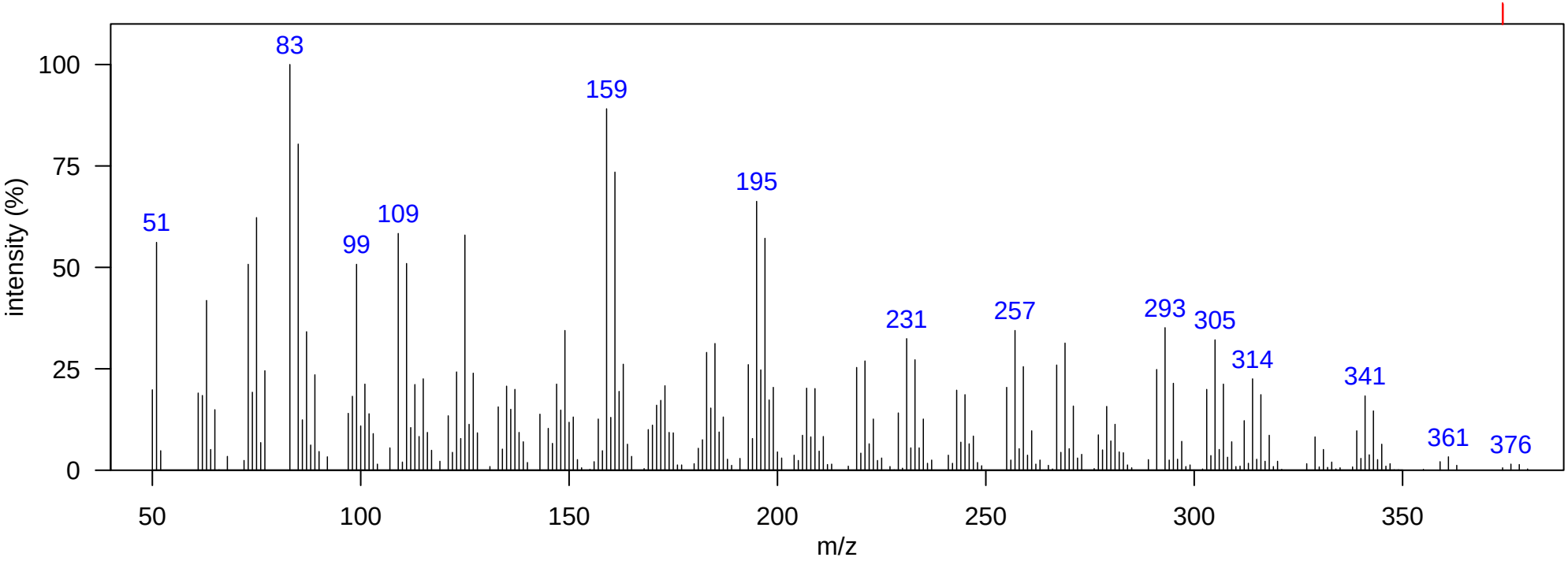
Comment: Toxaphene fragmentation pattern.

Elemental Formula: C10H9Cl7

Source: anthropogenic

Class: toxaphene related

Identification: Manual



m/z	Identity
374	M+

Name: toxaphene 9

Elemental Formula: C10H10Cl8

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: anthropogenic

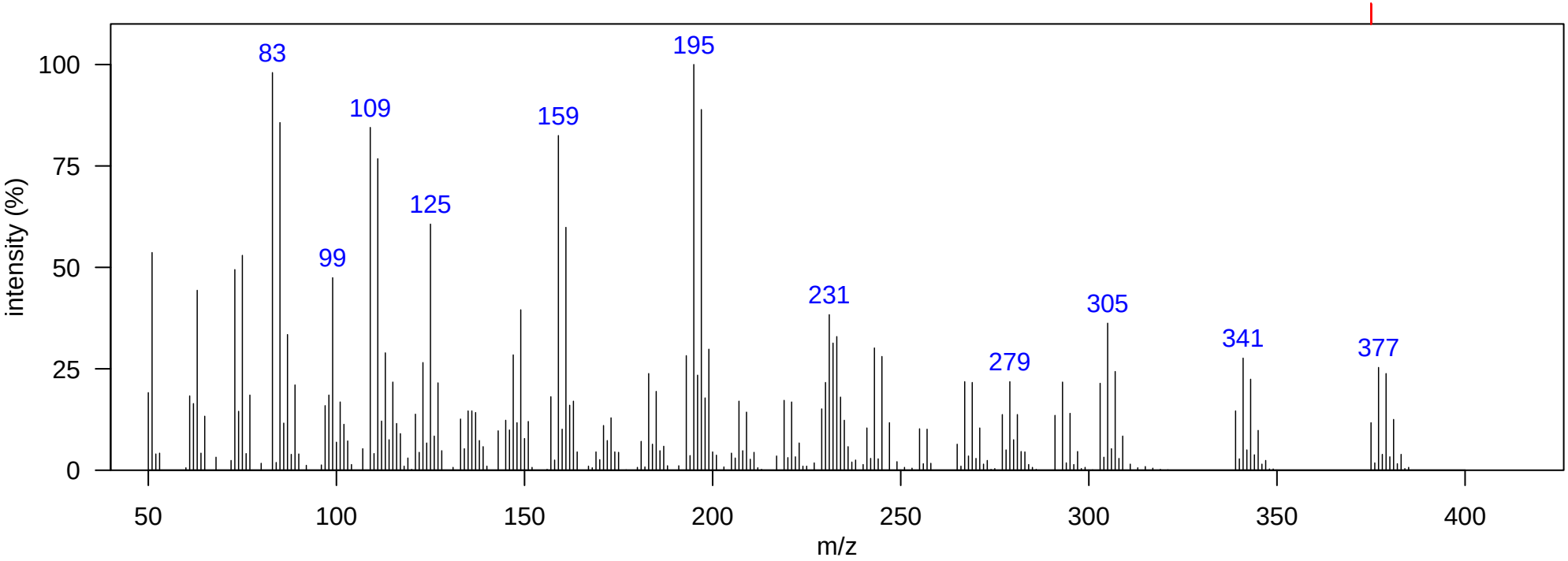
Instrument: GCxGC−TOF, electron impact

Class: toxaphene related

RT (s) (1D): 1602, RT (s) (2D): 2.085

Identification: Authentic MS RT

Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.



m/z	Identity
375	[M−Cl]+

Filename: toxaphene_9

Name: toxaphene 10

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1619.5, RT (s) (2D): 1.777

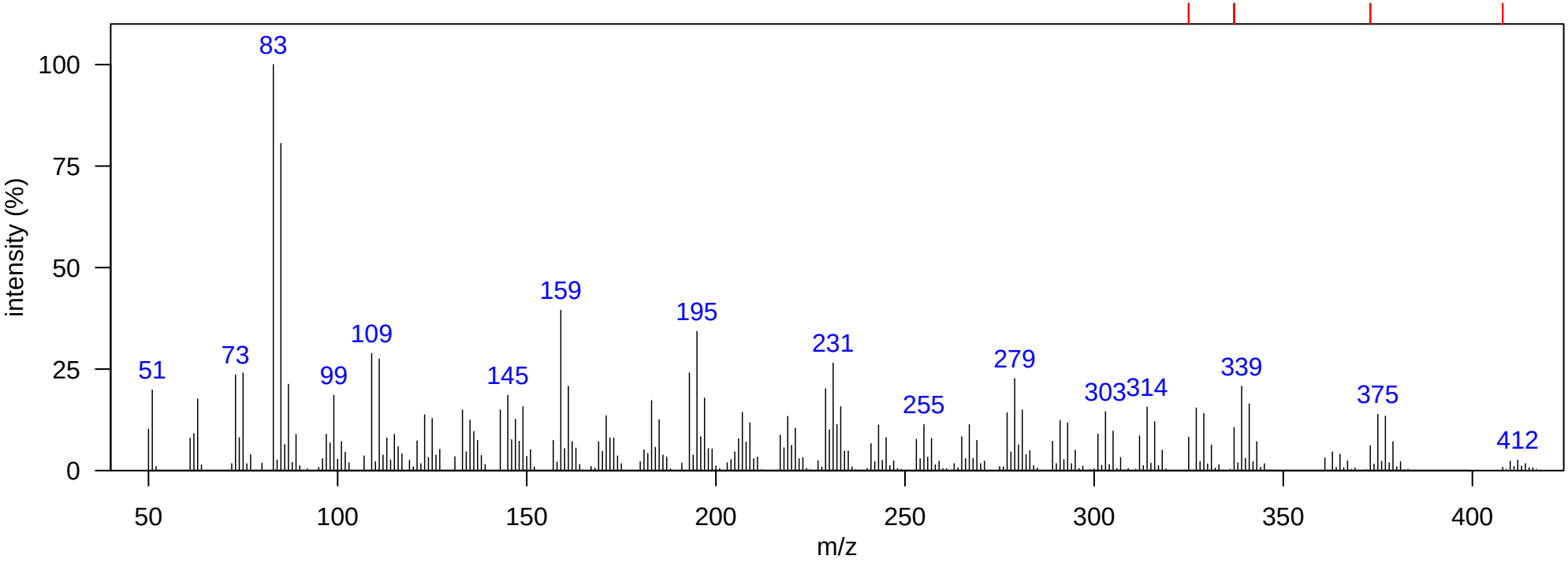
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C10H8Cl8

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
325	[M−CHCl2]+
337	[M−2Cl]+
373	[M−Cl]+
408	M+

Name: toxaphene 11

Elemental Formula: C10H8Cl8

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: anthropogenic

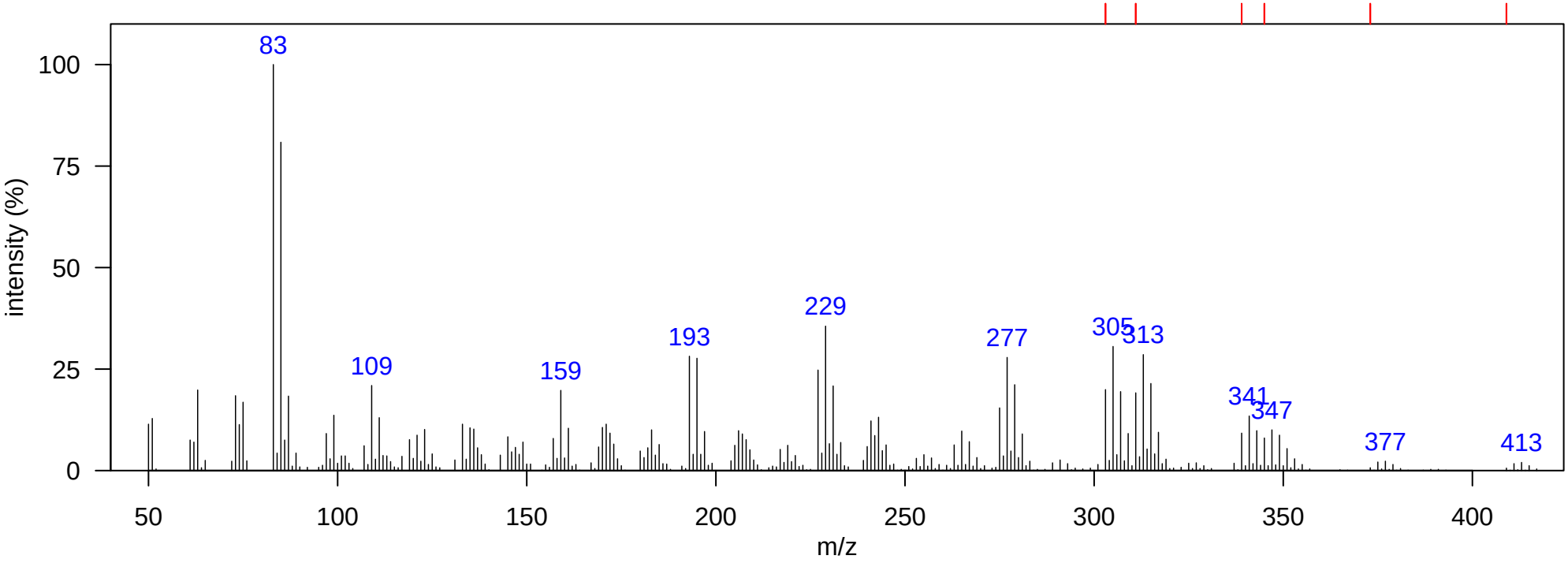
Instrument: GCxGC−TOF, electron impact

Class: toxaphene related

RT (s) (1D): 1651, RT (s) (2D): 2.059

Identification: Authentic MS RT

Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.



m/z	Identity
303	[M−HCl4]+
311	[M−3Cl−C2H4]+
339	[M−3Cl]+
345	[M−HCl2−C2H4]+
373	[M−HCl2]+
409	[M−Cl]+

Filename: toxaphene_11

Name: toxaphene 12

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1682.5, RT (s) (2D): 2.543

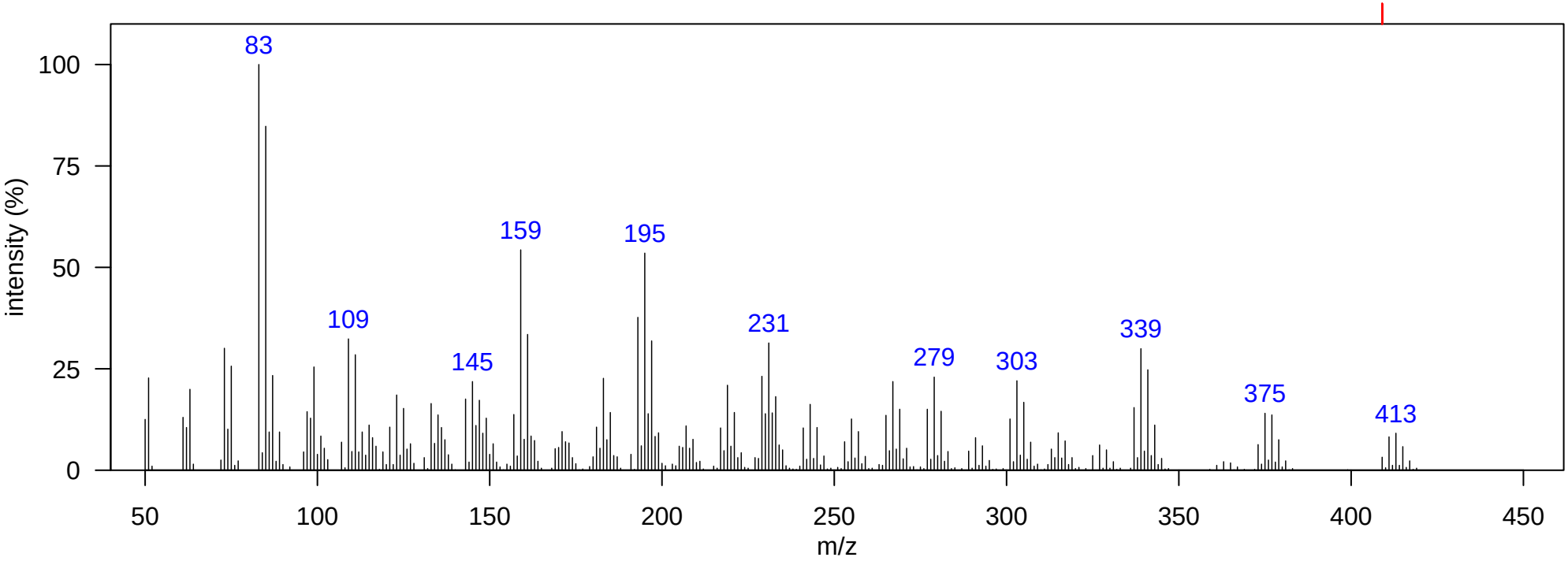
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C10H9Cl9

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
409	[M−Cl]+

Name: mirex−2Cl

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1591.5, RT (s) (2D): 2.13

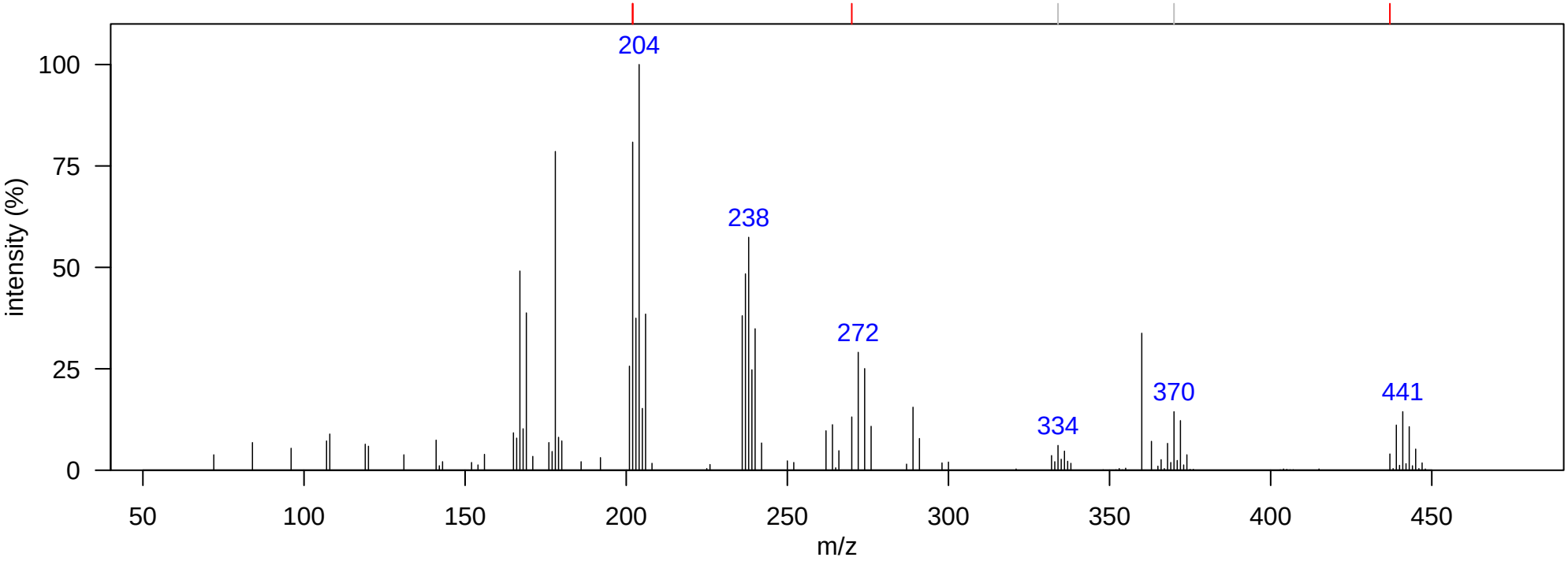
Comment:

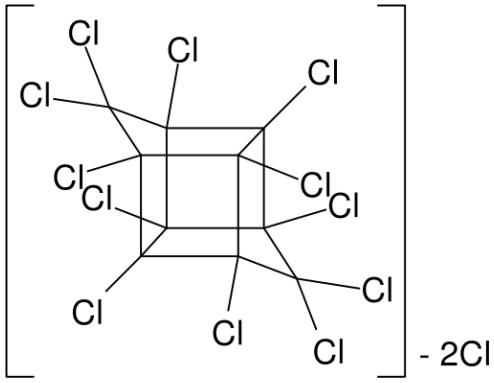
Elemental Formula: C10H2Cl10

Source: anthropogenic

Class: mirex

Identification: Manual − Congener Group





m/z	Identity
202	[C5H2Cl4]+
270	[C5Cl6]+
334	interference
370	interference from MBP−Br4Cl2
437	[M−Cl]+

Filename: mirex2Cl

Name: mirex−Cl isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1626.5, RT (s) (2D): 1.985

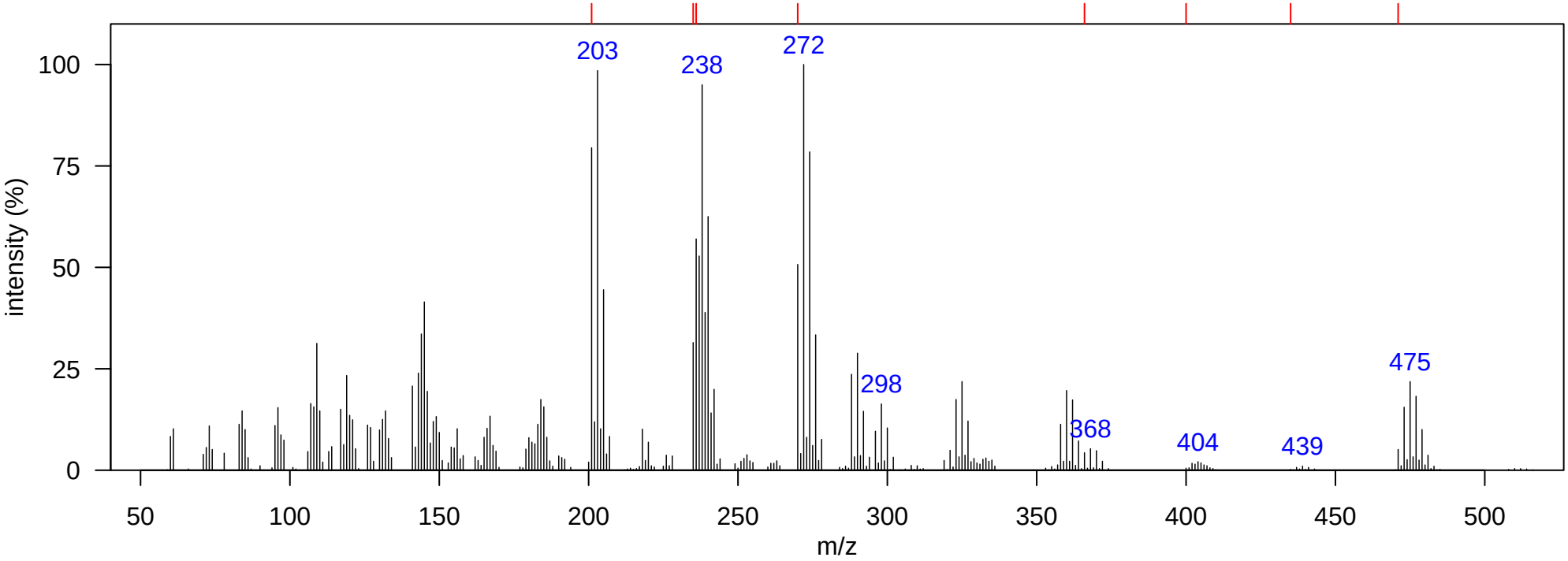
Comment:

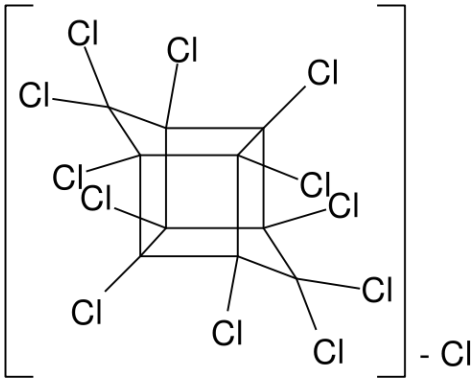
Elemental Formula: C10HCl11

Source: anthropogenic

Class: mirex

Identification: Manual − Congener Group





m/z	Identity
201	[C5HCl4]+
235	[C5Cl5]+
236	[C5HCl5]+
270	[C5Cl6]+
366	[M−4Cl]+
400	[M−HCl3]+
435	[M−HCl2]+
471	[M−Cl]+

Name: mirex−Cl isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1651, RT (s) (2D): 2.148

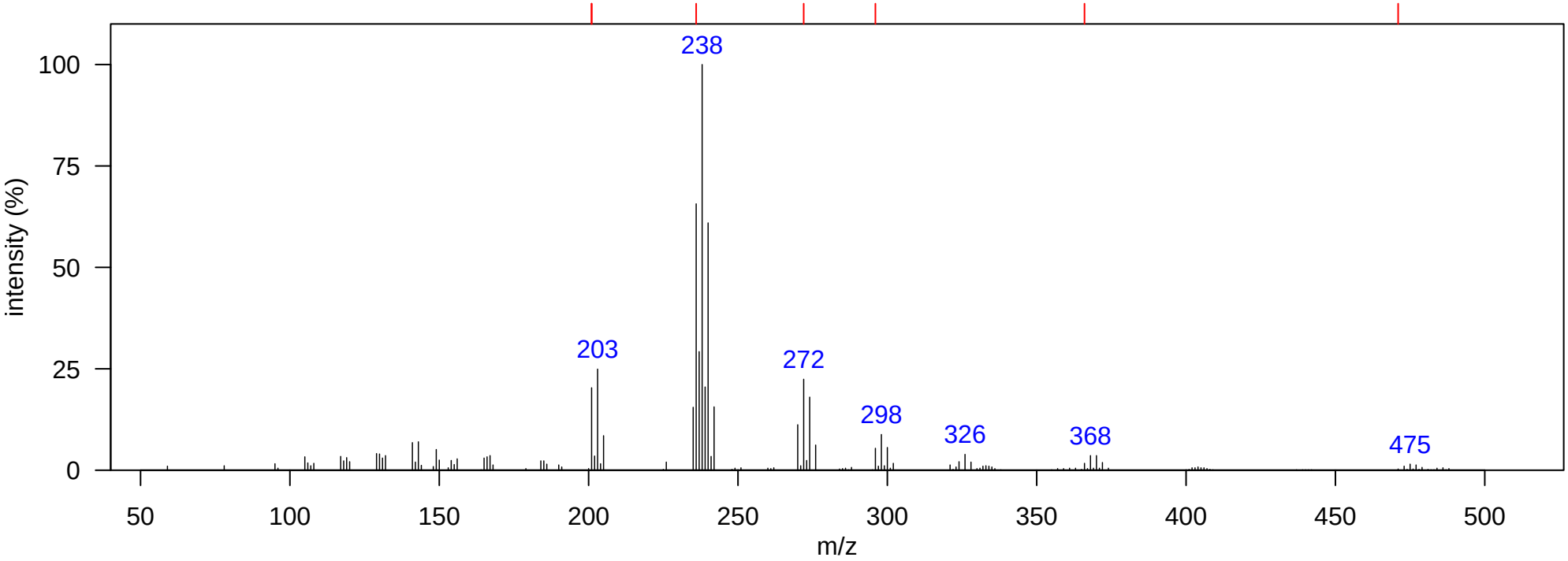
Comment:

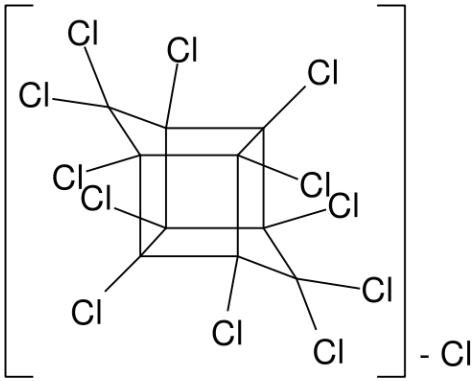
Elemental Formula: C10HCl11

Source: anthropogenic

Class: mirex

Identification: Manual − Congener Group





m/z	Identity
201	[C5HCl4]+
236	[C5HCl5]+
272	[C5Cl6]+
296	[C10HC5]+
366	[C10HCl7]+
471	[M−Cl]+

Name: mirex

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1700, RT (s) (2D): 2.312

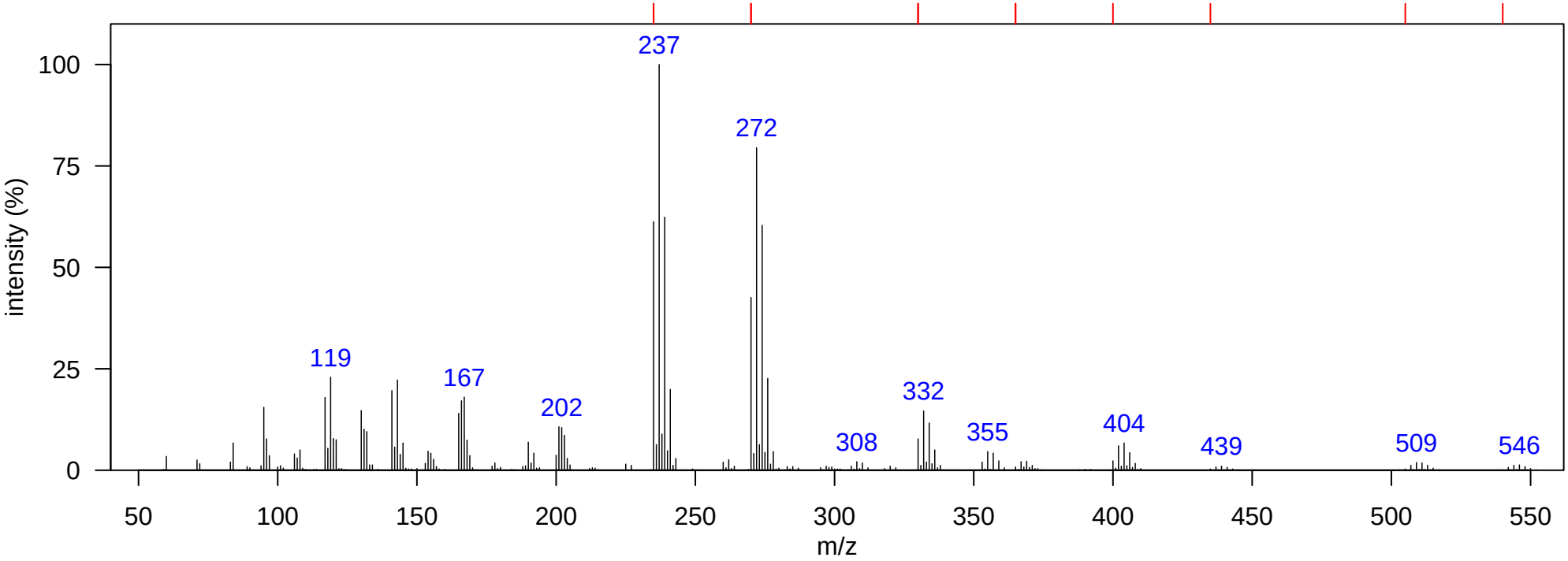
Comment:

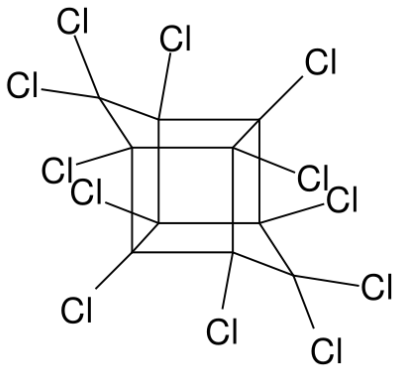
Elemental Formula: C10Cl12

Source: anthropogenic

Class: mirex

Identification: Reference Database MS





m/z	Identity
235	[C5Cl5]+
270	[C5Cl6]+
330	[M−6Cl]+
365	[M−5Cl]+
400	[M−4Cl]+
435	[M−3Cl]+
505	[M−Cl]+
540	M+

Filename: mirex

Name: dieldrin

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1507.5, RT (s) (2D): 1.749

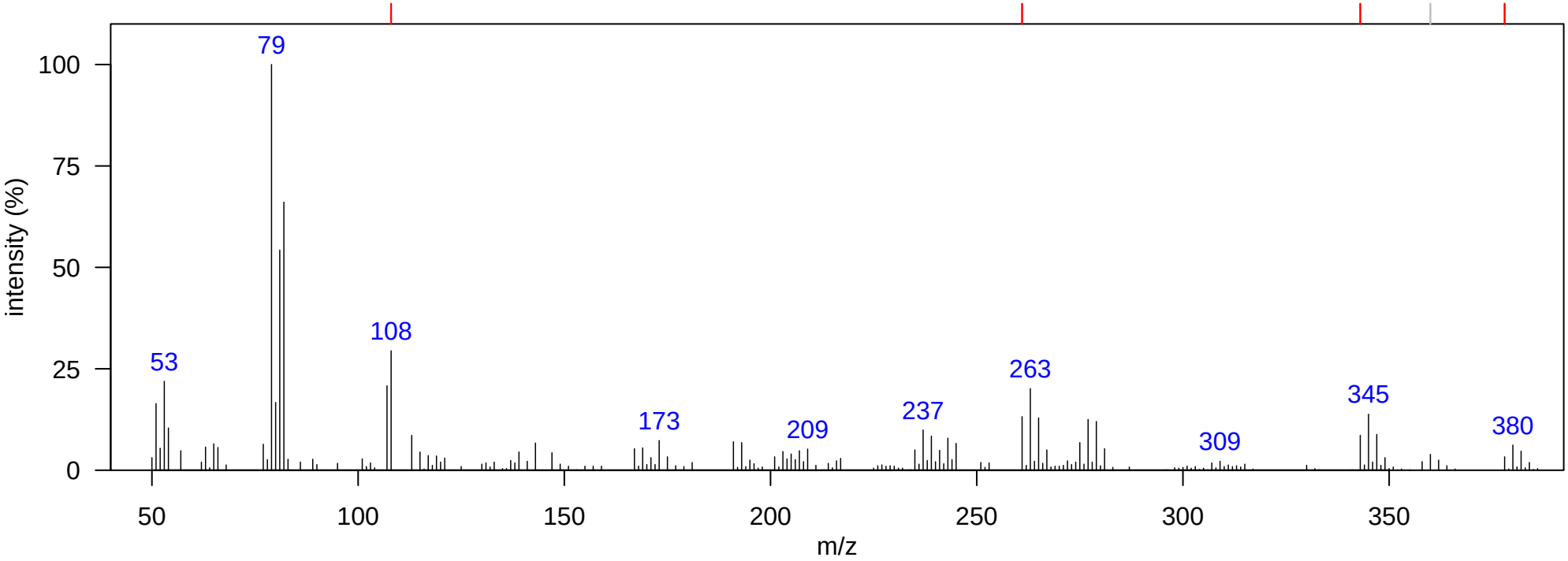
Comment:

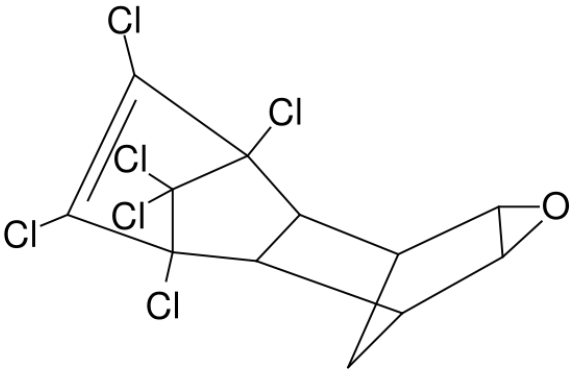
Elemental Formula: C12H8Cl6O

Source: anthropogenic

Class: pesticide

Identification: Authentic MS RT





m/z	Identity
108	[C7H8O]+
261	[C7H2Cl5]+
343	[M−Cl]+
360	PCB interference
378	M+

Filename: dieldrin

Name: pentachlorobenzene

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1077, RT (s) (2D): 2.581

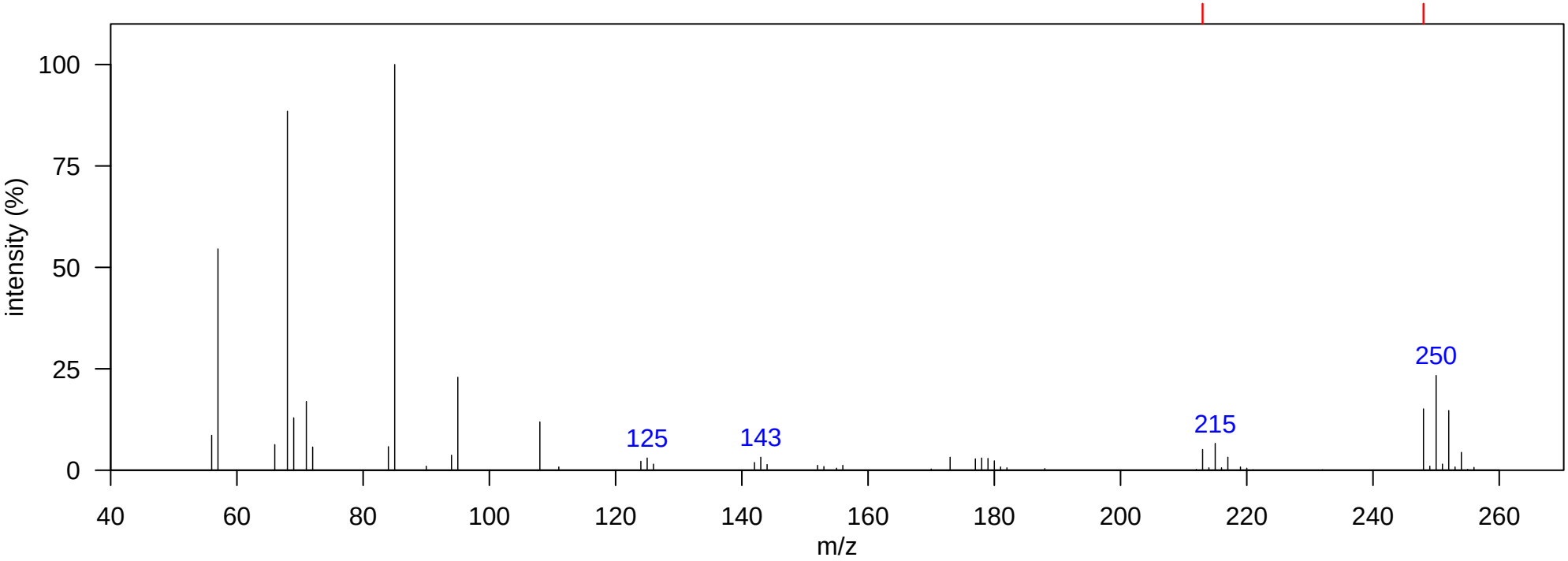
Comment:

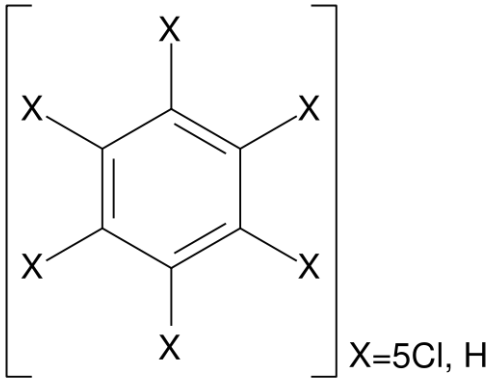
Elemental Formula: C6CHCl5

Source: anthropogenic

Class: pesticide

Identification: Manual − Congener Group





m/z	Identity
213	[M−Cl]+
248	M+

Filename: pentachlorobenzene

Name: hexachlorobenzene (HCB)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1213.5, RT (s) (2D): 1.031

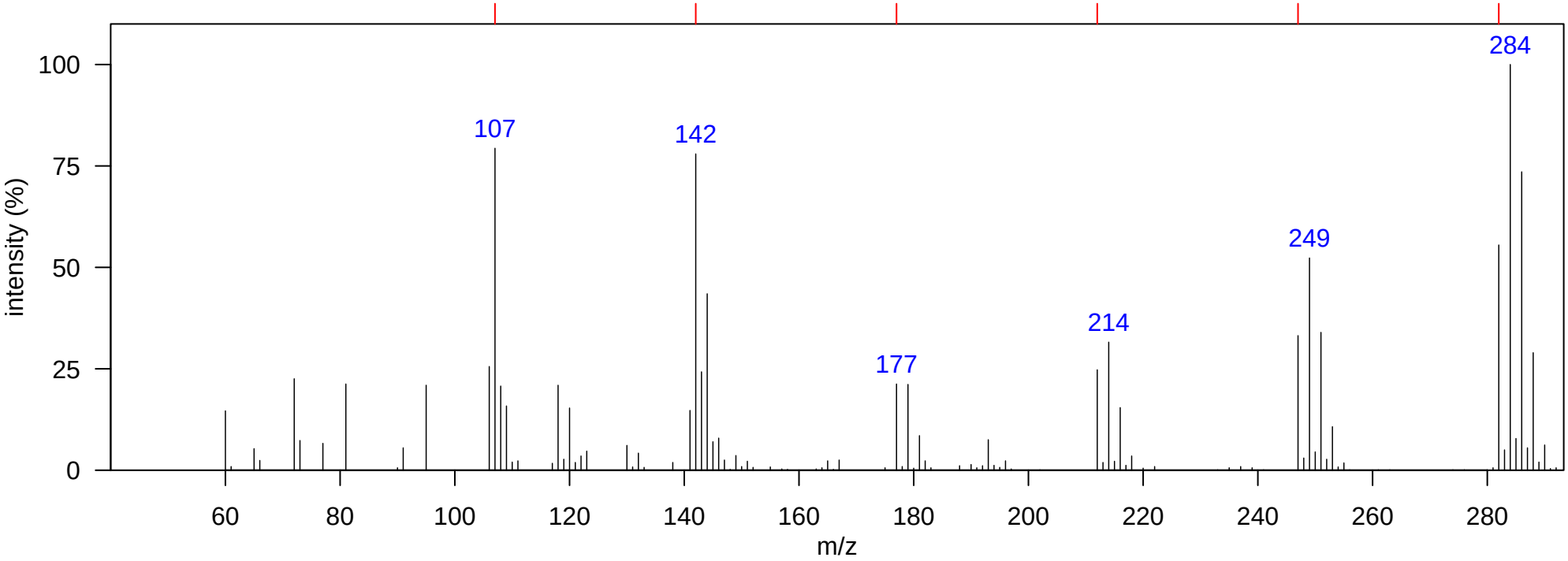
Comment:

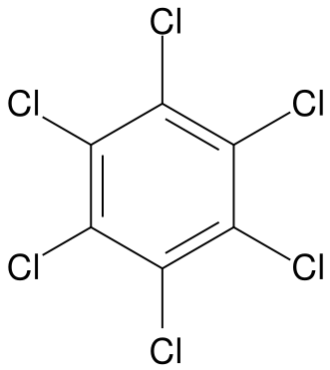
Elemental Formula: C6Cl6

Source: anthropogenic

Class: pesticide

Identification: Authentic MS RT





m/z	Identity
107	[M−5Cl]+
142	[M−4Cl]+
177	[M−3Cl]+
212	[M−2Cl]+
247	[M−Cl]+
282	M+

Filename: hexachlorobenzene

Name: hexachlorocyclohexane (HCH) isomer 1, alpha−HCH

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1210, RT (s) (2D): 1.377

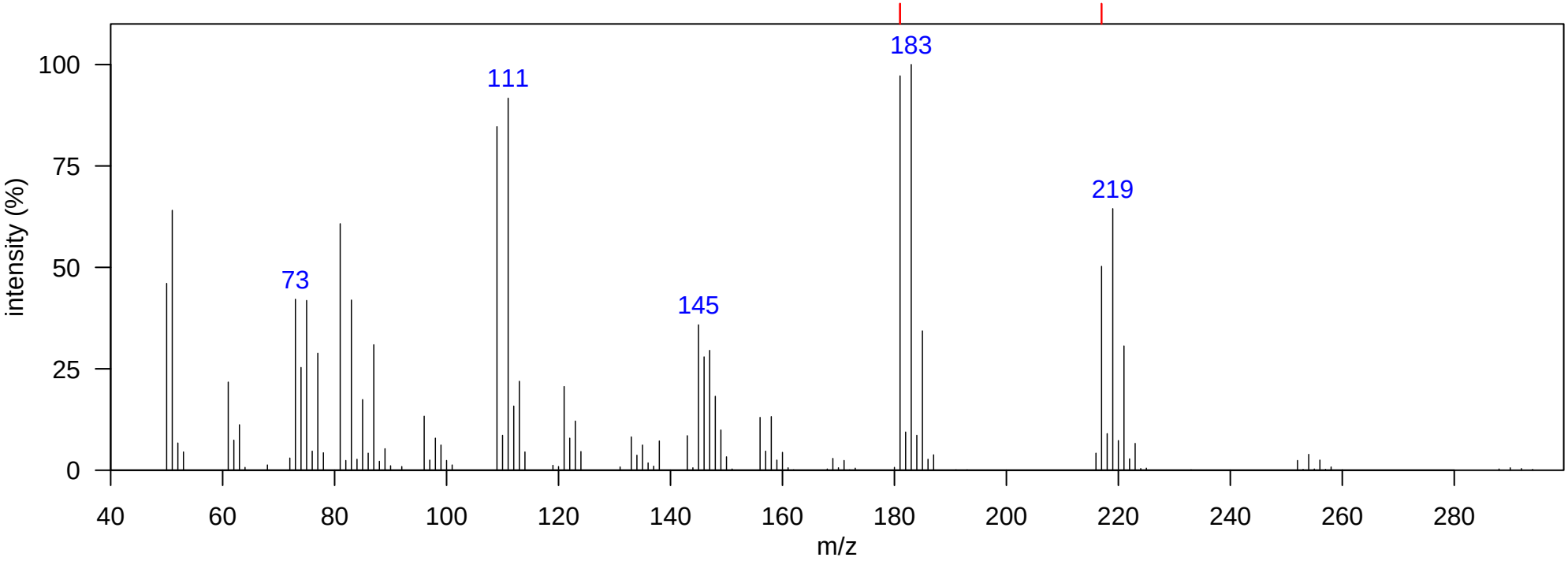
Comment:

Elemental Formula: C6H6Cl6

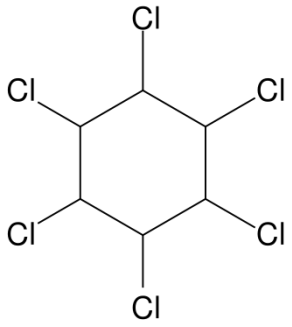
Source: anthropogenic

Class: pesticide

Identification: Authentic MS RT



m/z	Identity
181	[M−H2Cl3]+
217	[M−HCl2]+



(stereochemistry not shown)

Filename: HCH_isomer_1

Name: hexachlorocyclohexane (HCH) isomer 2, gamma−HCH

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1255.5, RT (s) (2D): 1.5656

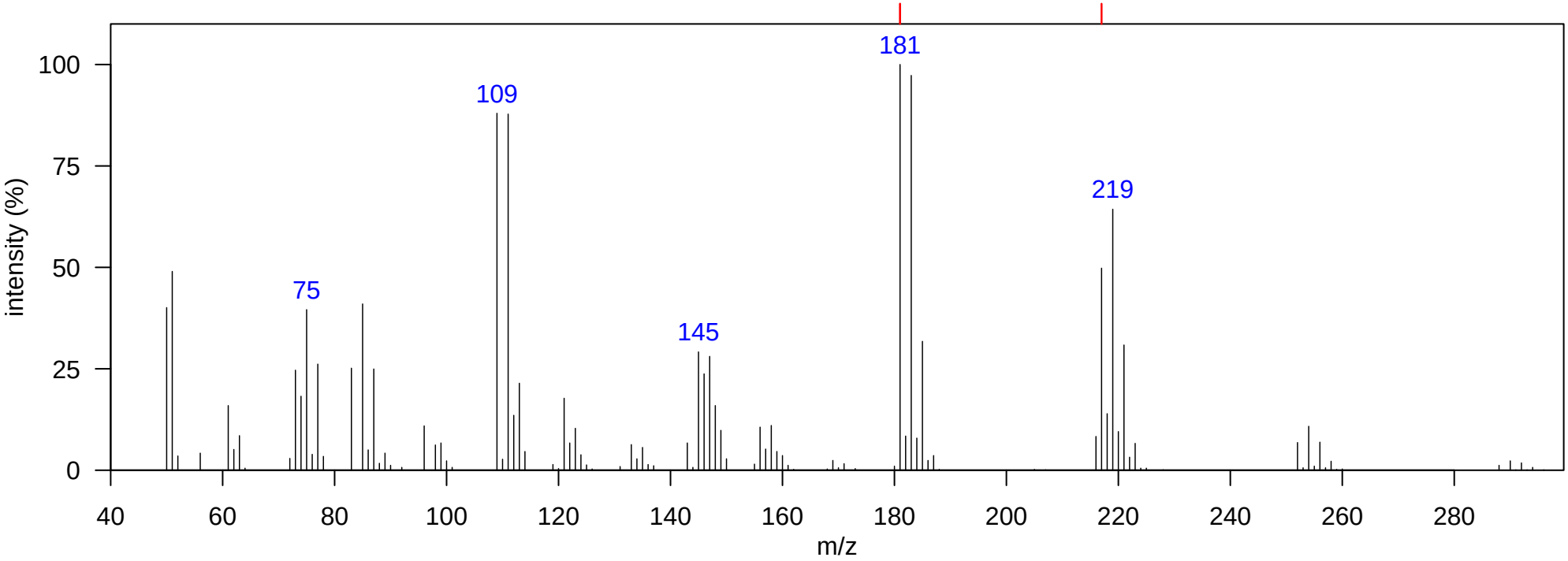
Comment:

Elemental Formula: C6H6Cl6

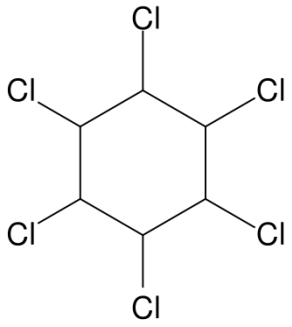
Source: anthropogenic

Class: pesticide

Identification: Authentic MS RT



m/z	Identity
181	[M−H2Cl3]+
217	[M−HCl2]+



(stereochemistry not shown)

Filename: HCH_isomer_2

Name: hexachlorocyclohexane (HCH) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1266, RT (s) (2D): 1.803

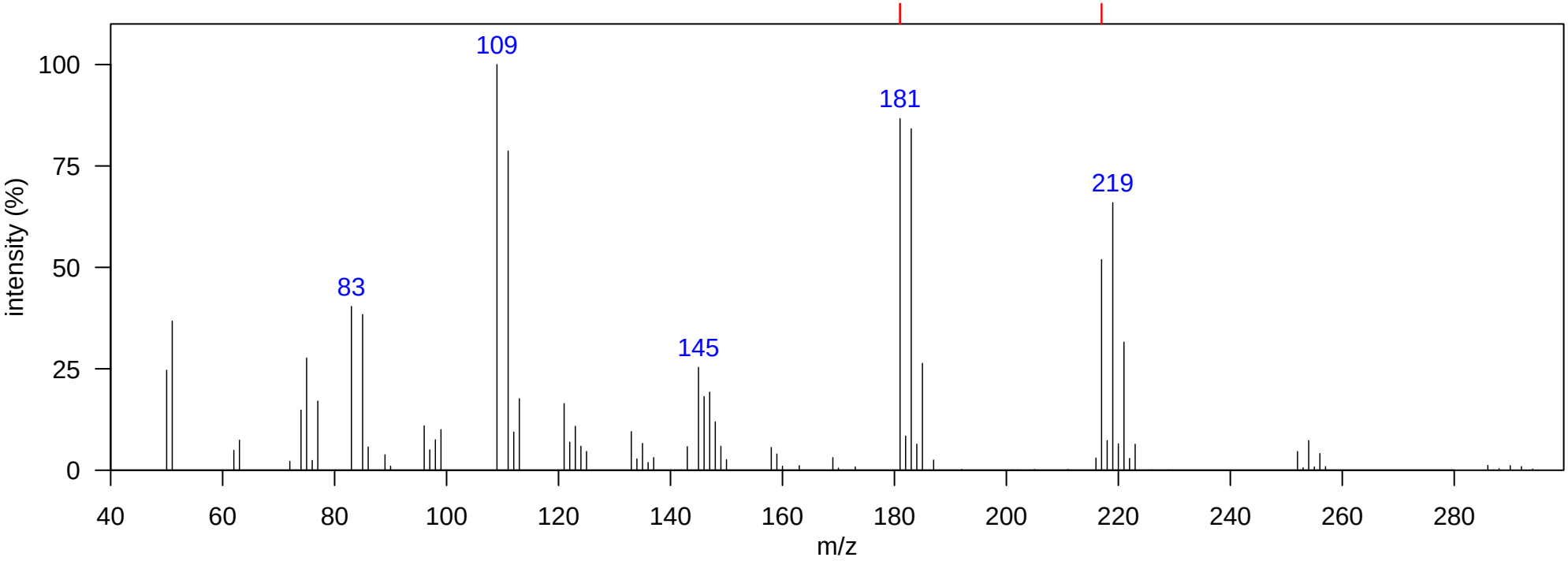
Comment:

Elemental Formula: C6H6Cl6

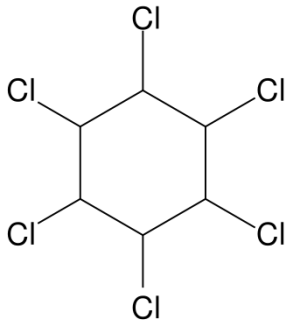
Source: anthropogenic

Class: pesticide

Identification: Authentic MS



m/z	Identity
181	[M−H2Cl3]+
217	[M−HCl2]+



(stereochemistry not shown)

Filename: HCH_isomer_3

Name: polybrominated diphenyl ether 3Br (PBDE), BDE−28

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1546, RT (s) (2D): 2.027

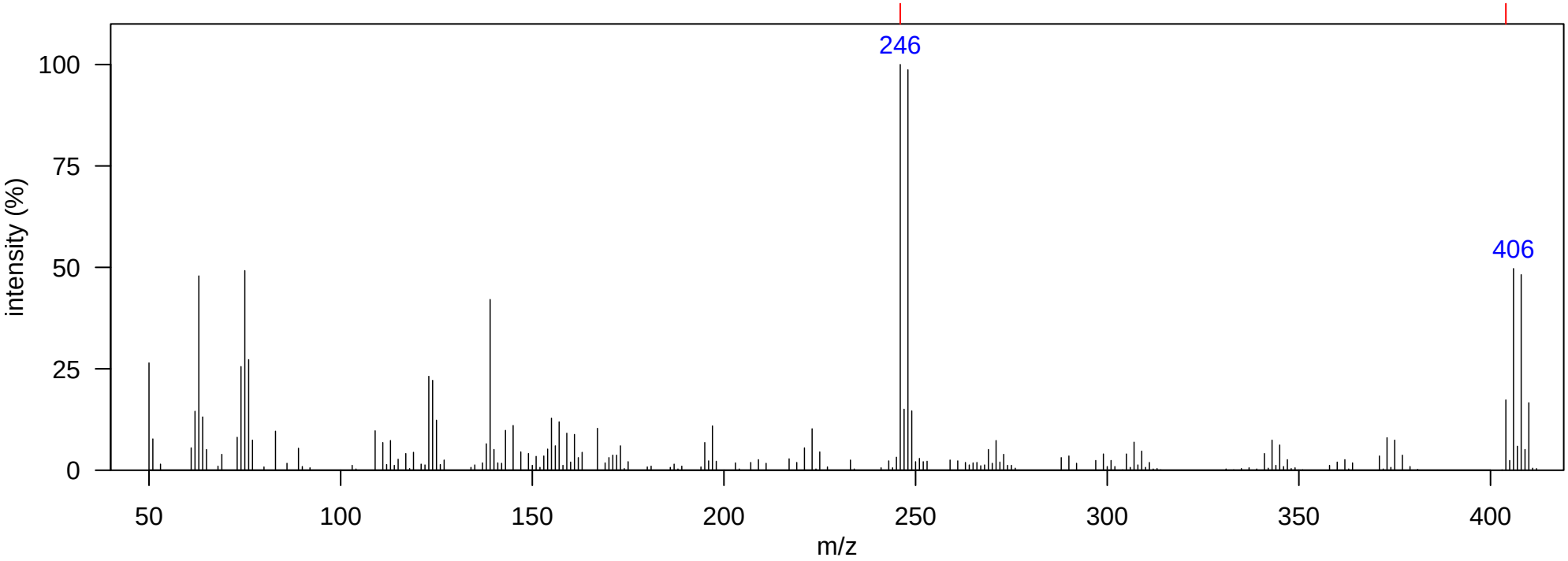
Comment:

Elemental Formula: C12H7Br3O

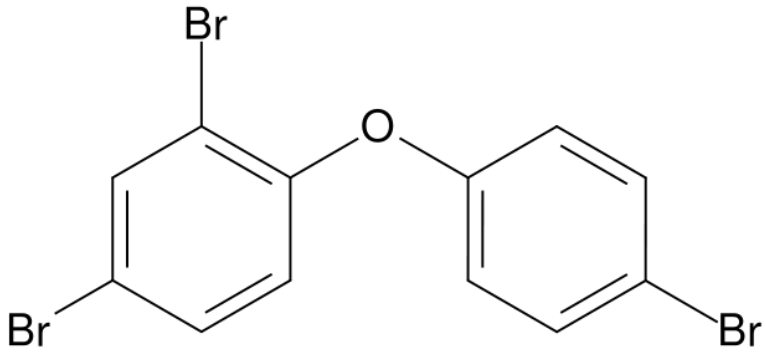
Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT



m/z	Identity
246	[M−2Br]+
404	M+



Filename: 3Br_PBDE

Name: polybrominated diphenyl ether 4Br (PBDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1633.5, RT (s) (2D): 2.199

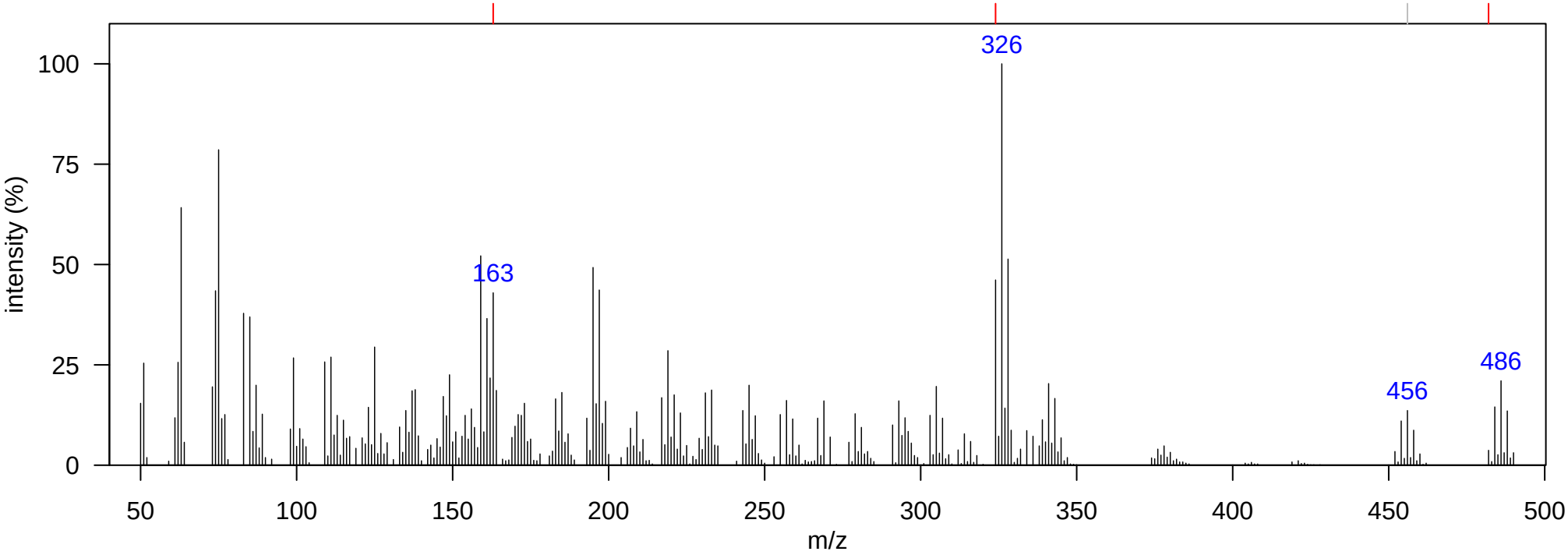
Comment:

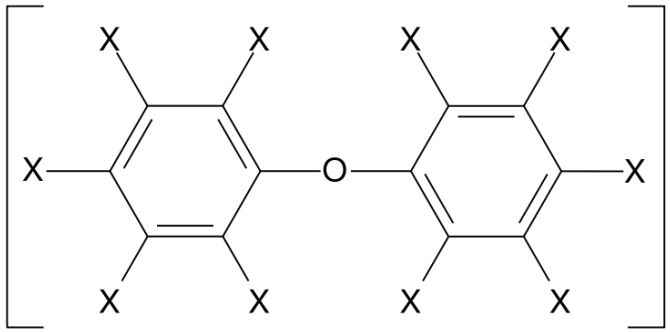
Elemental Formula: C12H6Br4O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





m/z	Identity
163	[M−2Br]2+
324	[M−2Br]+
456	interference
482	M+

Filename: 4Br_PBDE_isomer_1

Name: polybrominated diphenyl ether 4Br (PBDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1644, RT (s) (2D): 2.738

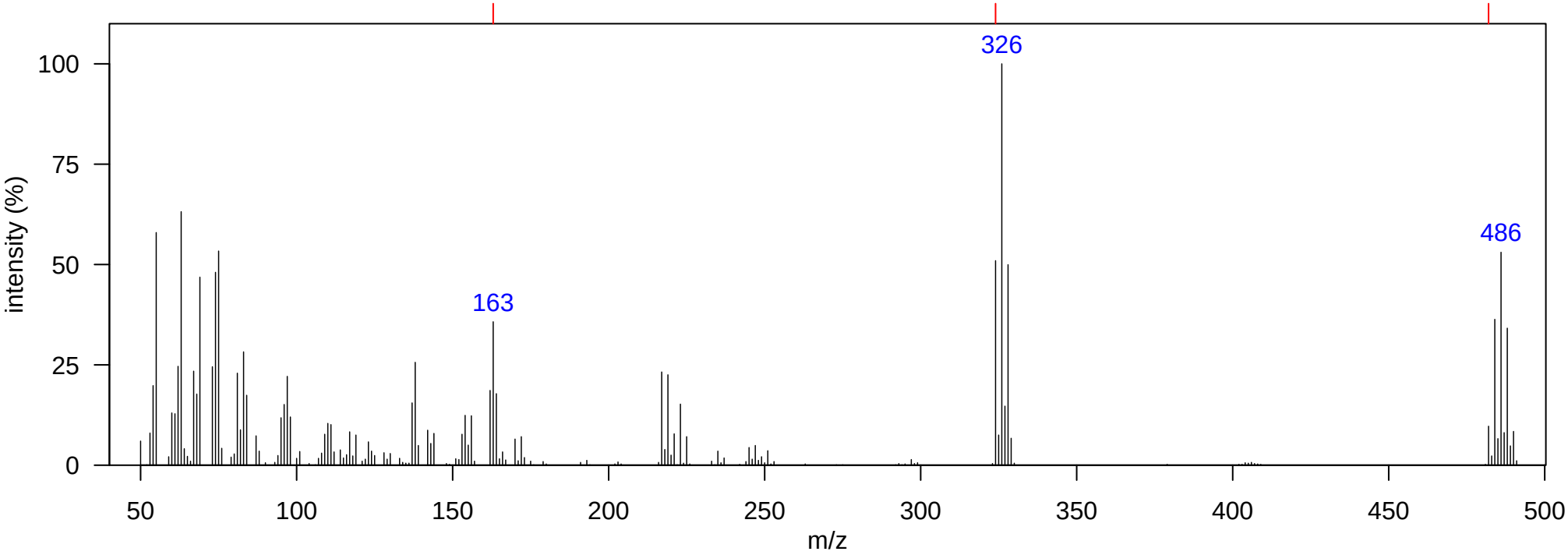
Comment:

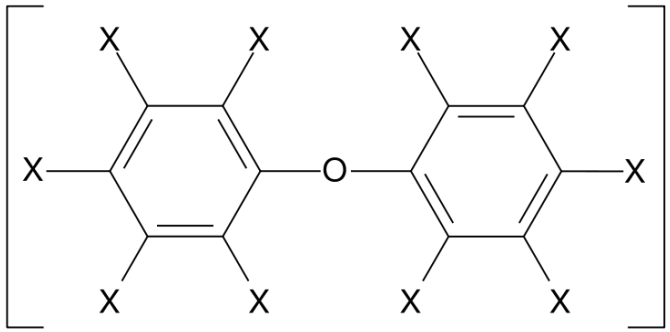
Elemental Formula: C12H6Br4O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





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

Filename: 4Br_PBDE_isomer_2

Name: polybrominated diphenyl ether 4Br (PBDE) isomer 3, BDE−47

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1672, RT (s) (2D): 2.647

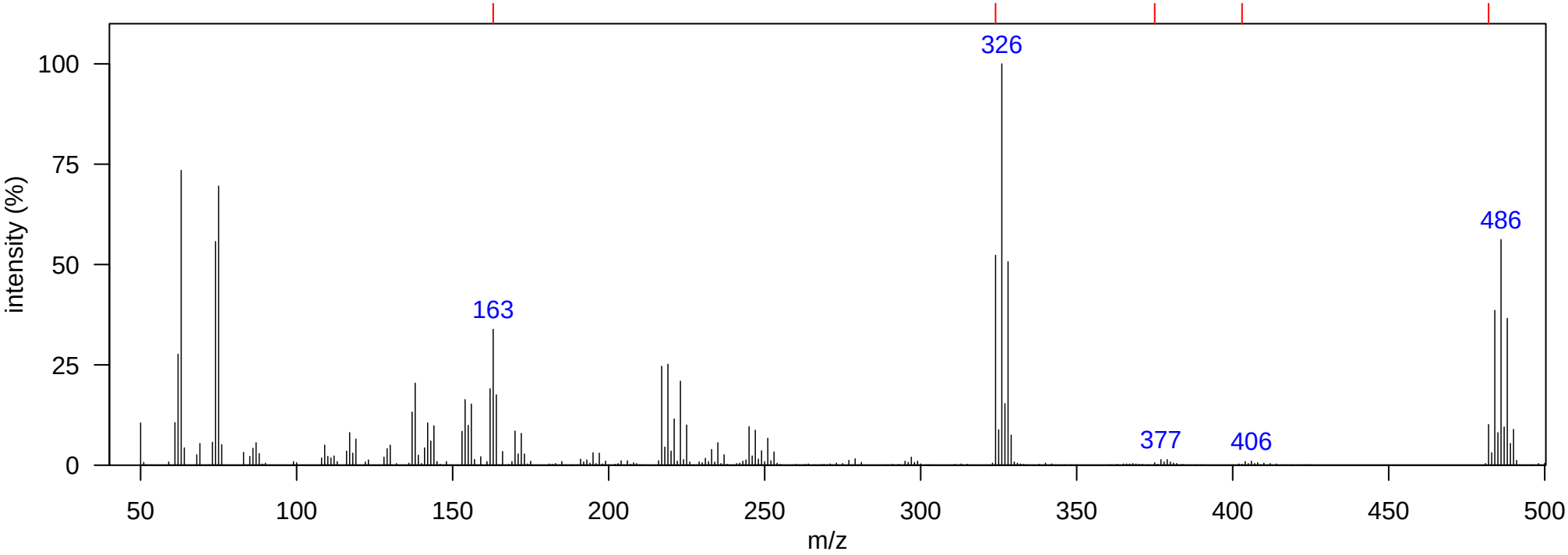
Comment:

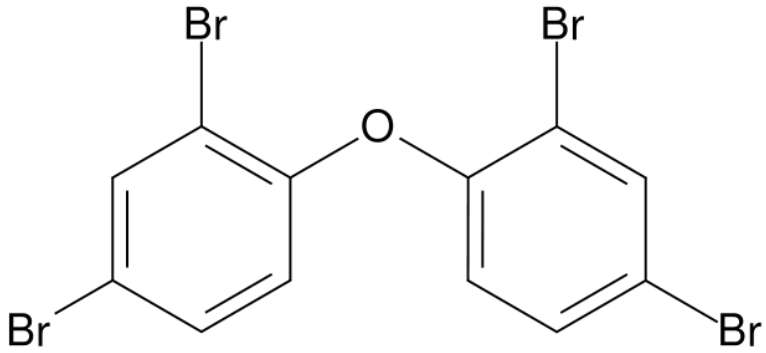
Elemental Formula: C12H6Br4O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT





m/z	Identity
163	[M−2Br]2+
324	[M−2Br]+
375	[M−Br−CO]+
403	[M−Br]+
482	M+

Filename: 4Br_PBDE_isomer_3

Name: polybrominated diphenyl ether 4Br (PBDE) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1693, RT (s) (2D): 2.55

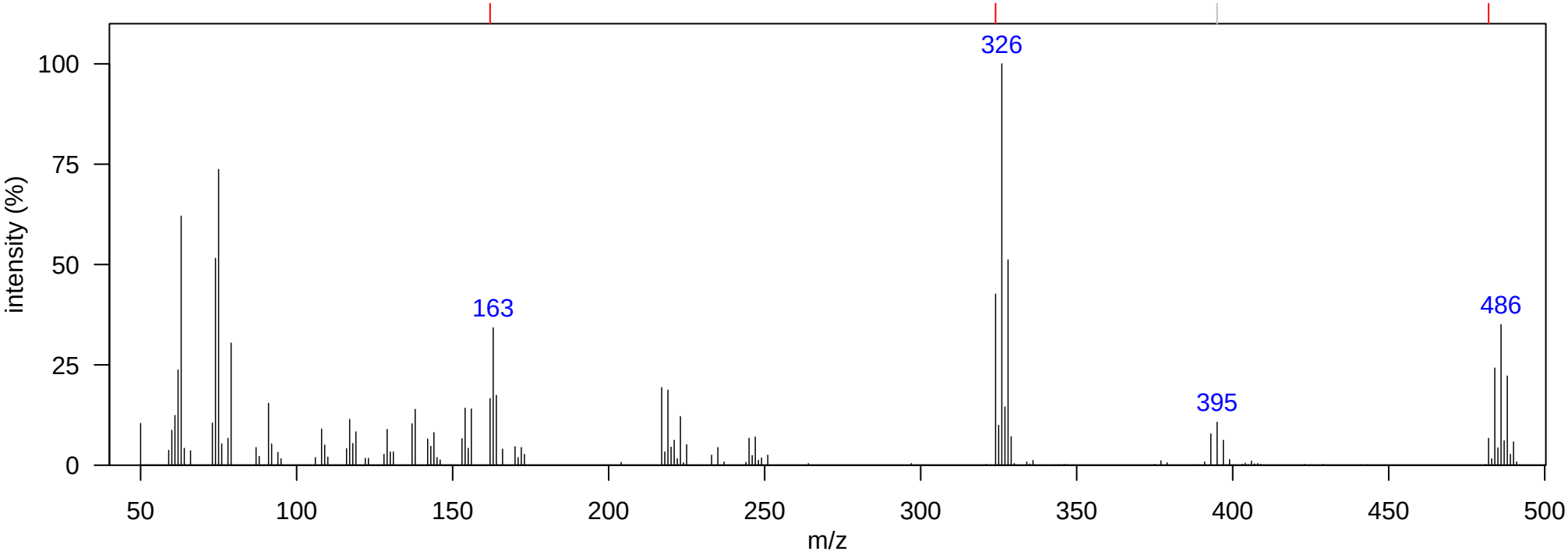
Comment:

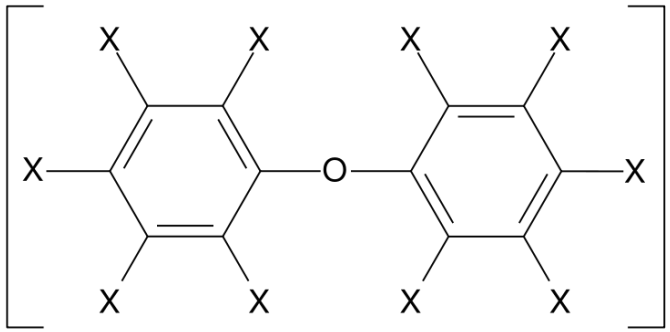
Elemental Formula: C12H6Br4O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





X=4Br, 6H

m/z	Identity
162	[M−2Br]2+
324	[M−2Br]+
395	PCB interference
482	M+

Filename: 4Br_PBDE_isomer_4

Name: polybrominated diphenyl ether 5Br (PBDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1728, RT (s) (2D): 2.802

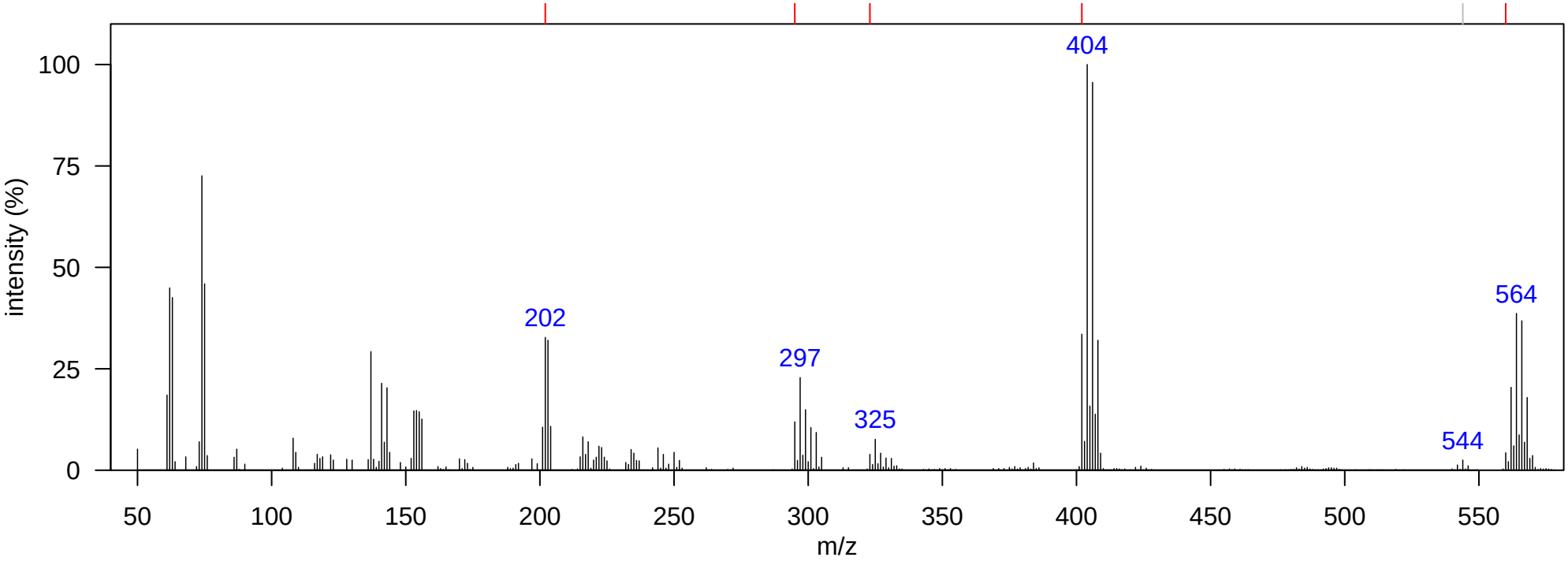
Comment:

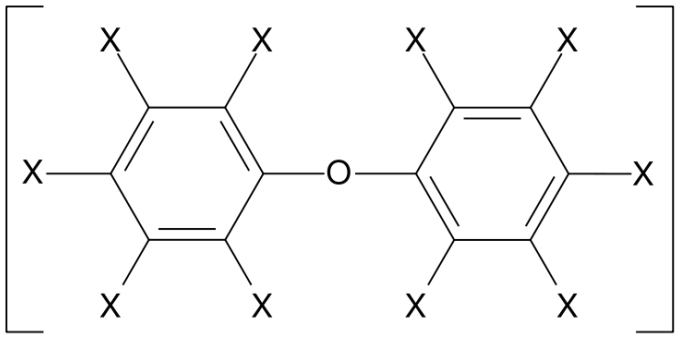
Elemental Formula: C12H5Br5O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





m/z	Identity
202	[M−2Br]2+
295	[M−3Br−CO]+
323	[M−3Br]+
402	[M−2Br]+
544	DMBP Br4Cl2 interference
560	M+

Name: polybrominated diphenyl ether 5Br (PBDE) isomer 2, BDE−100

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1763, RT (s) (2D): 2.936

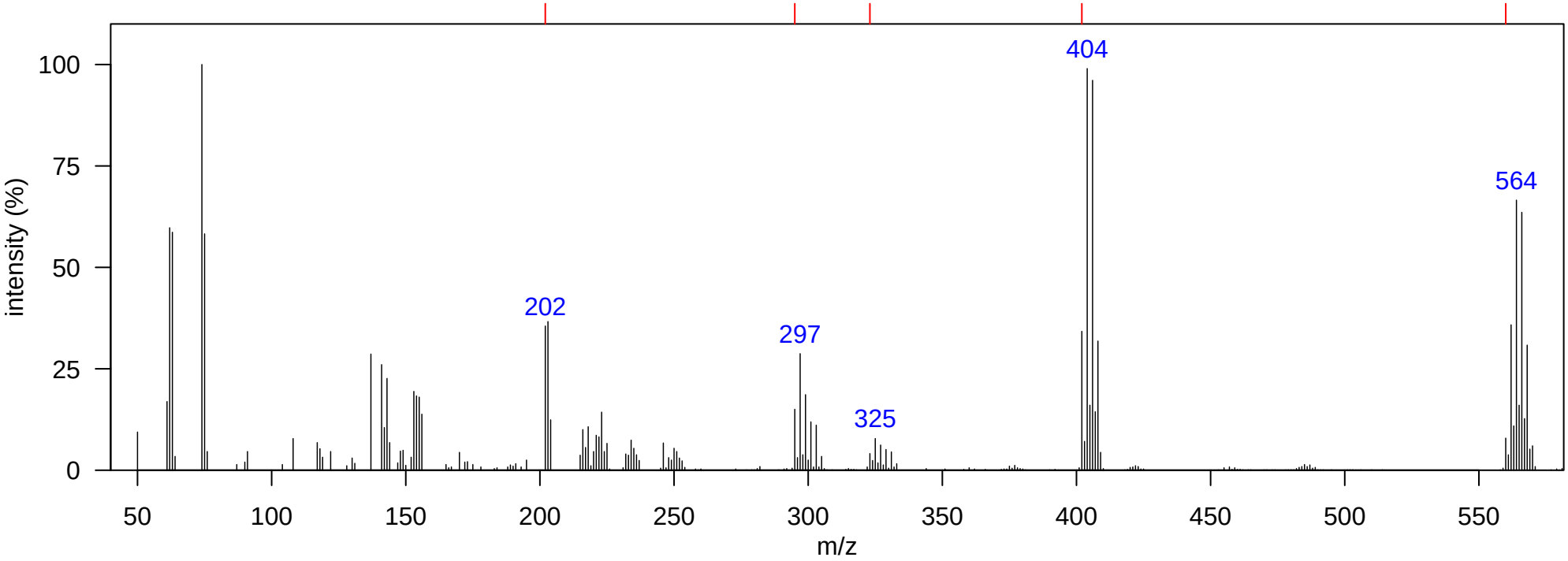
Comment:

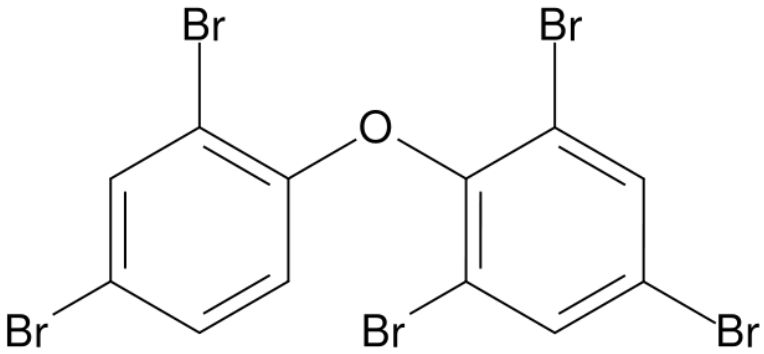
Elemental Formula: C12H5Br5O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT





m/z	Identity
202	[M−2Br]2+
295	[M−3Br−CO]+
323	[M−3Br]+
402	[M−2Br]+
560	M+

Filename: 5Br_PBDE_isomer_2

Name: polybrominated diphenyl ether 5Br (PBDE) isomer 3, BDE−99

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1791, RT (s) (2D): 2.957

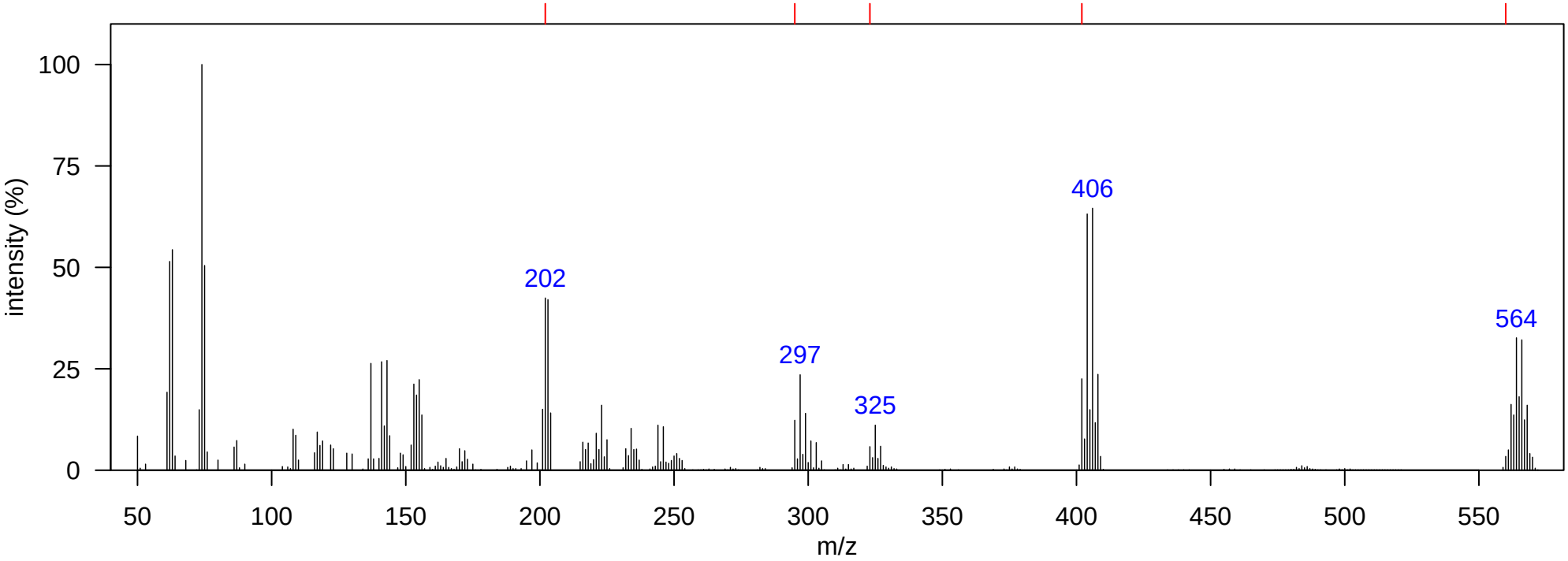
Comment:

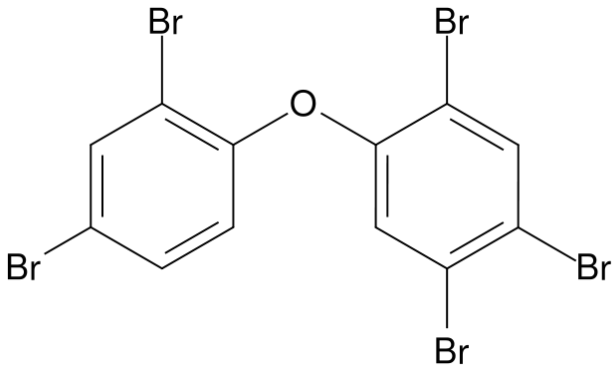
Elemental Formula: C12H5Br5O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT





m/z	Identity
202	[M−2Br]2+
295	[M−3Br−CO]+
323	[M−3Br]+
402	[M−2Br]+
560	M+

Filename: 5Br_PBDE_isomer_3

Name: polybrominated diphenyl ether 6Br (PBDE) isomer 1, BDE−154

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1864.5, RT (s) (2D): 3.37

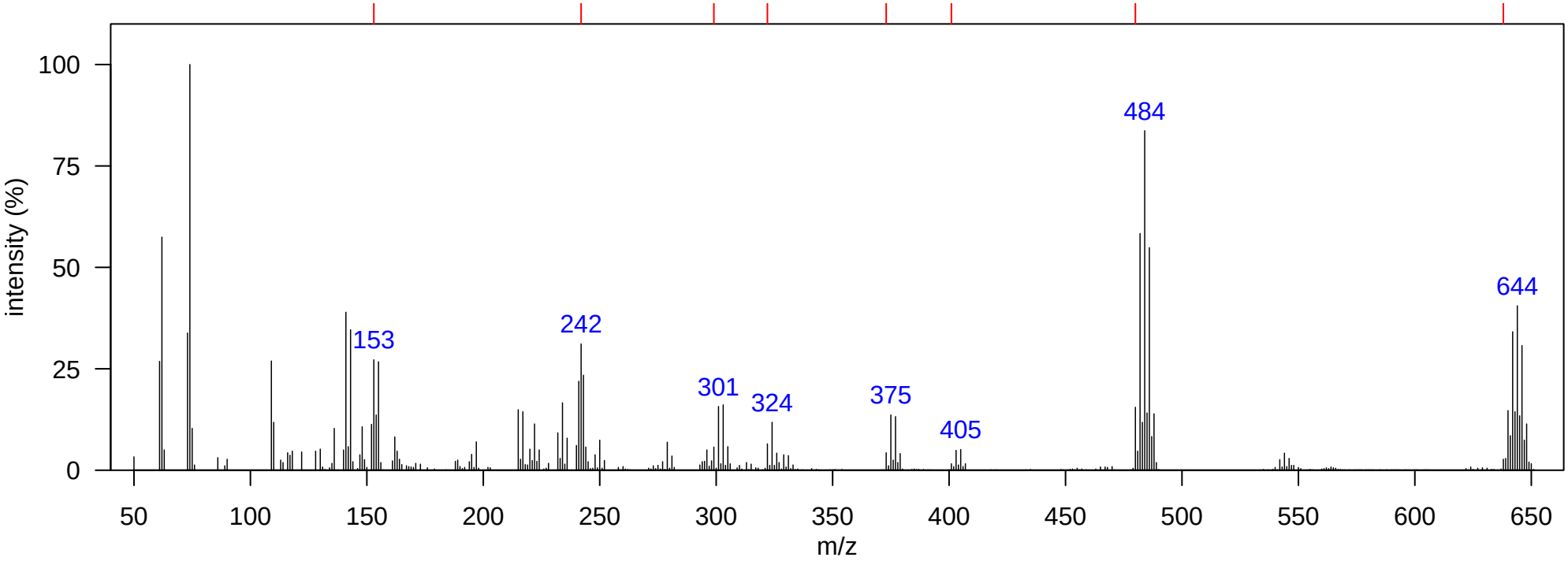
Comment:

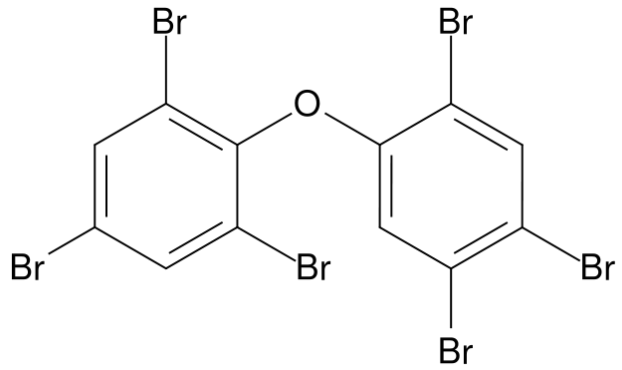
Elemental Formula: C12H5Br6O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT





m/z	Identity
153	[C6H2Br]+
242	[M−2Br]2+
299	[M−CO−C6H2Br3]+ = [C5H2Br3]+
322	[M−4Br]+
373	[M−3Br−CO]+
401	[M−3Br]+
480	[M−2Br]+
638	M+

Filename: 6Br_PBDE_isomer_1

Name: polybrominated diphenyl ether 6Br (PBDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1871.5, RT (s) (2D): 0.311

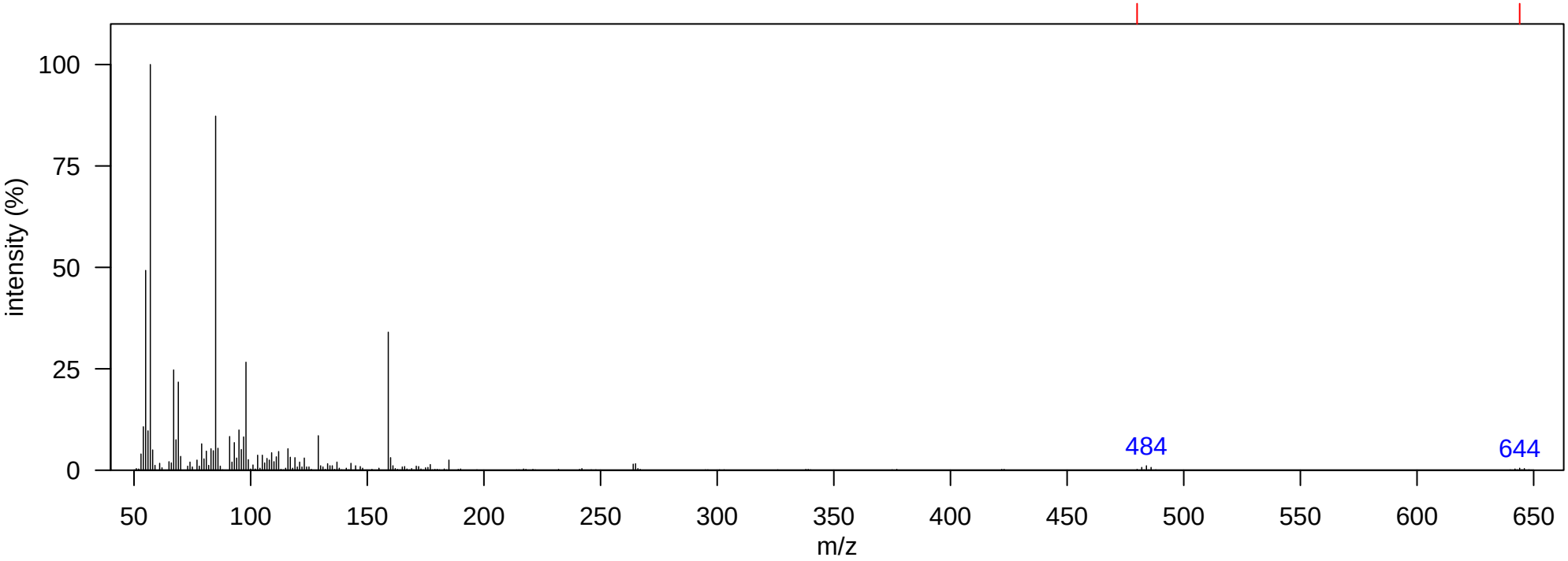
Comment: Low intensity, but visible in raw data.

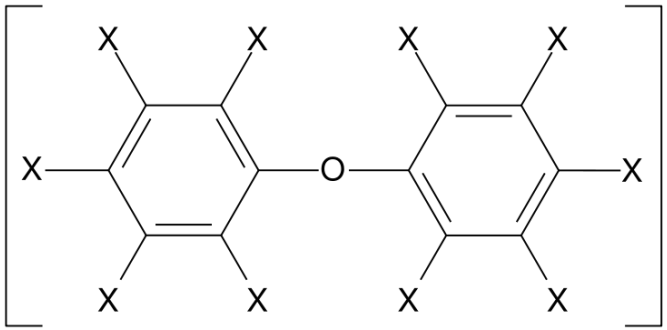
Elemental Formula: C12H4Br6O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





X=6Br, 4H

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

Filename: 6Br_PBDE_isomer_2

Name: polybrominated diphenyl ether 6Br (PBDE) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1885.5, RT (s) (2D): 1.029

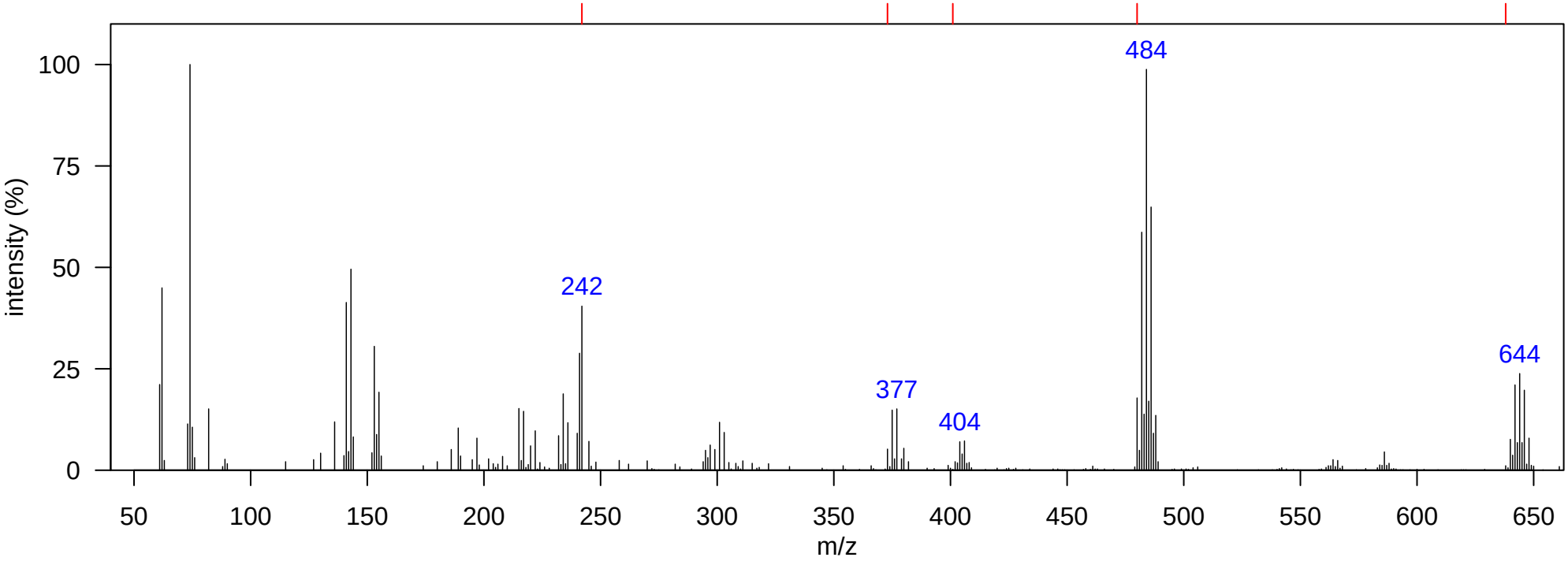
Comment:

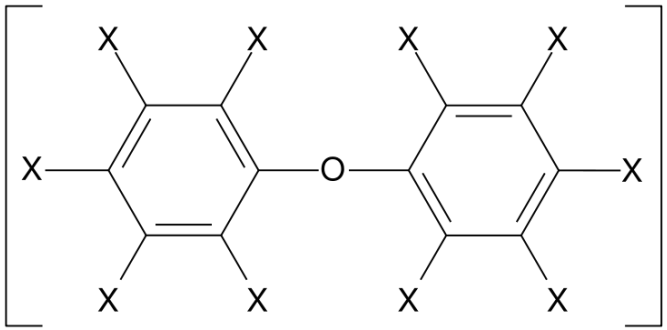
Elemental Formula: C12H4Br6O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





X=6Br, 4H

m/z	Identity
242	[M−2Br]2+
373	[M−3Br−CO]+
401	[M−3Br]+
480	[M−2Br]+
638	M+
665	interference

Name: polybrominated diphenyl ether 6Br (PBDE) isomer 4, BDE−153

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1906.5, RT (s) (2D): 0.166

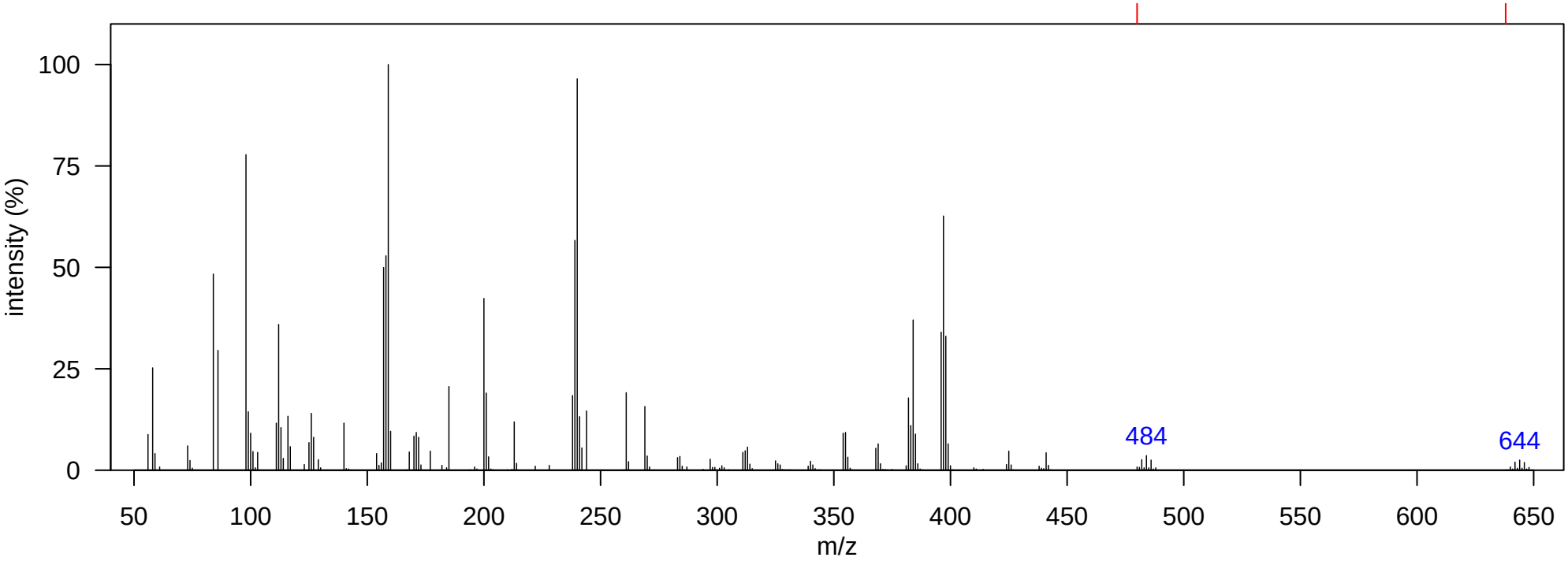
Comment: Low intensity, but visible in raw data.

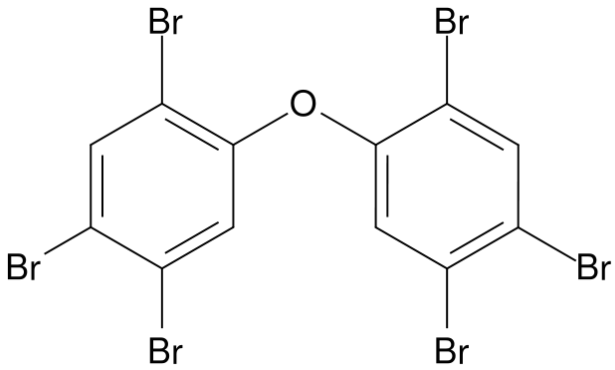
Elemental Formula: C12H4Br6O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT





m/z	Identity
480	[M−2Br]+
638	M+

Filename: 6Br_PBDE_isomer_4

Name: polybrominated diphenyl ether 6Br (PBDE) isomer 5

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1966, RT (s) (2D): 2.934

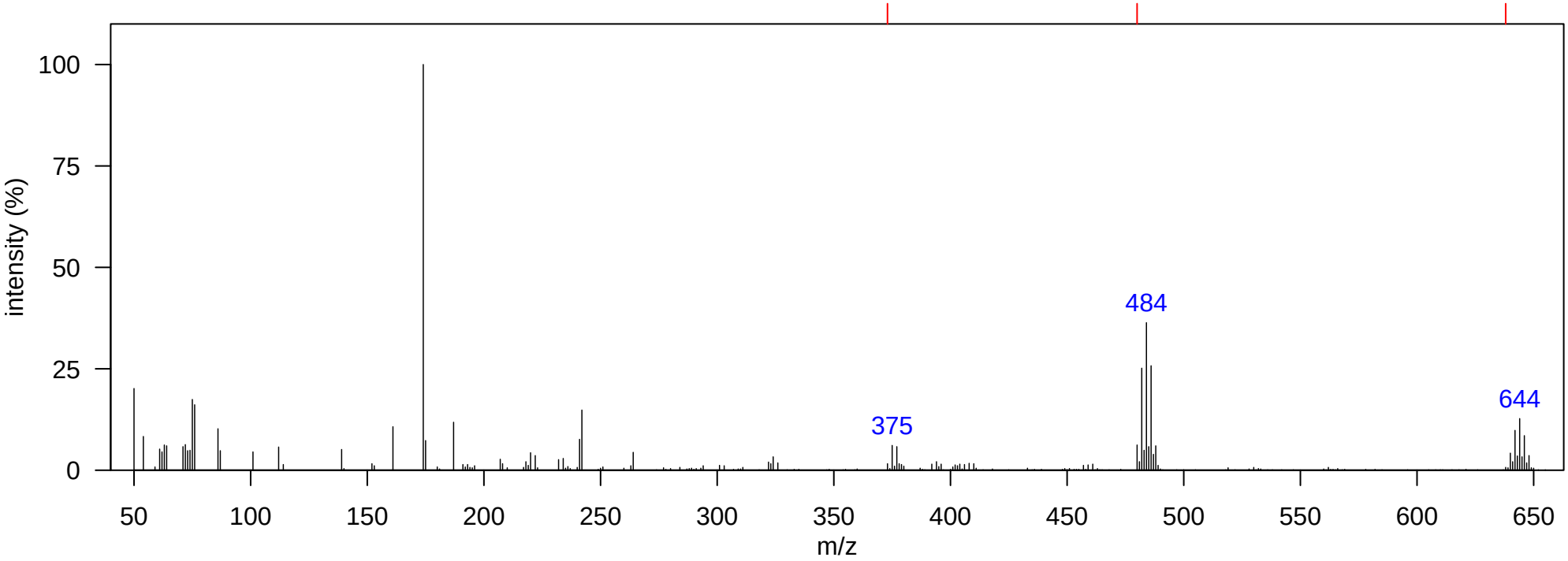
Comment:

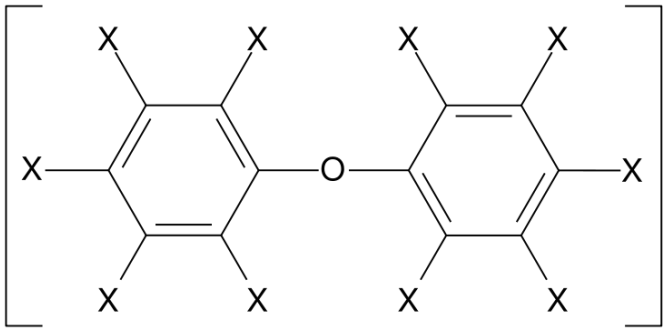
Elemental Formula: C12H4Br6O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





X=6Br, 4H

m/z	Identity
373	[M−3Br−CO]+
480	[M−2Br]+
638	M+

Filename: 6Br_PBDE_isomer_5

Name: polybrominated diphenyl ether 7Br (PBDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1994, RT (s) (2D): 0.22

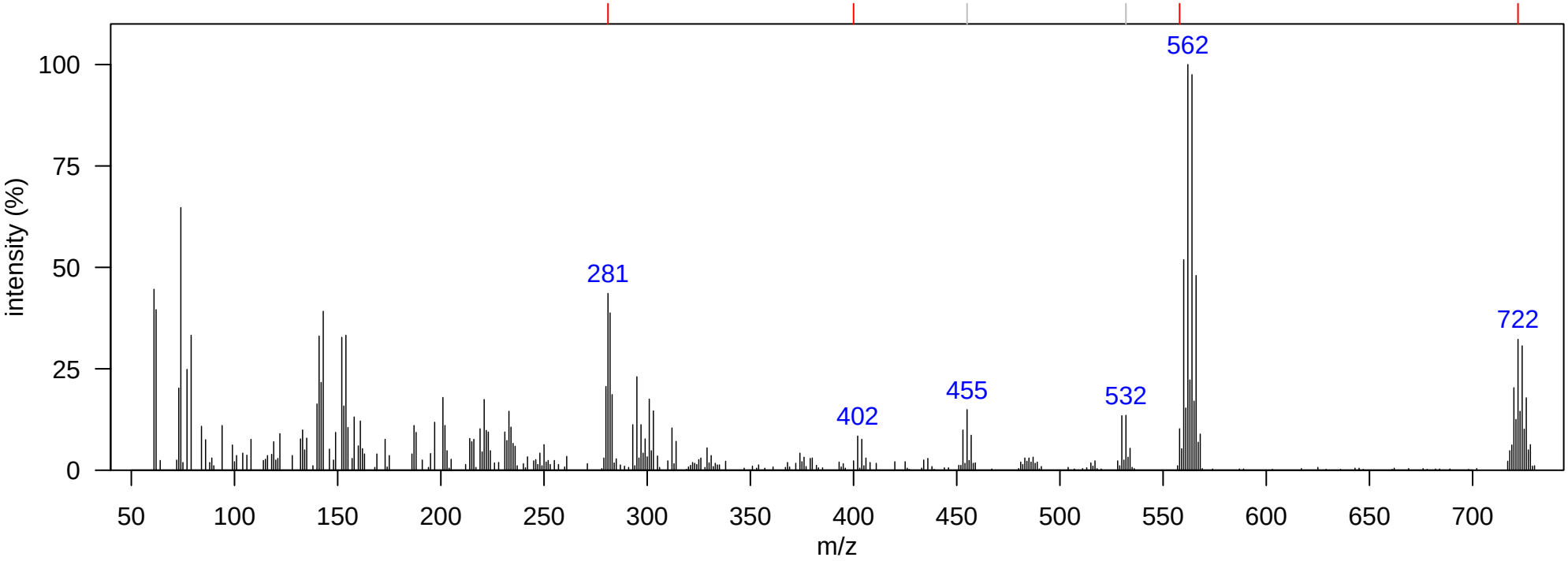
Comment:

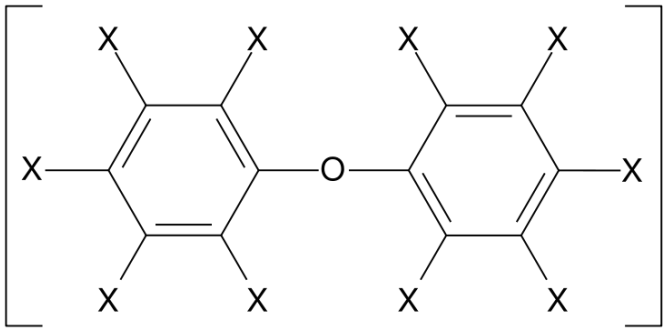
Elemental Formula: C12H3Br7O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





X=7Br, 3H

m/z	Identity
281	[M−2Br]2+
400	[M−4Br]+
455	interference
532	interference
558	[M−2Br]+
722	M+ (not monoisotopic)

Filename: 7Br_PBDE_isomer_1

Name: polybrominated diphenyl ether 7Br (PBDE) isomer 2, BDE−183

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 2018.5, RT (s) (2D): 0.717

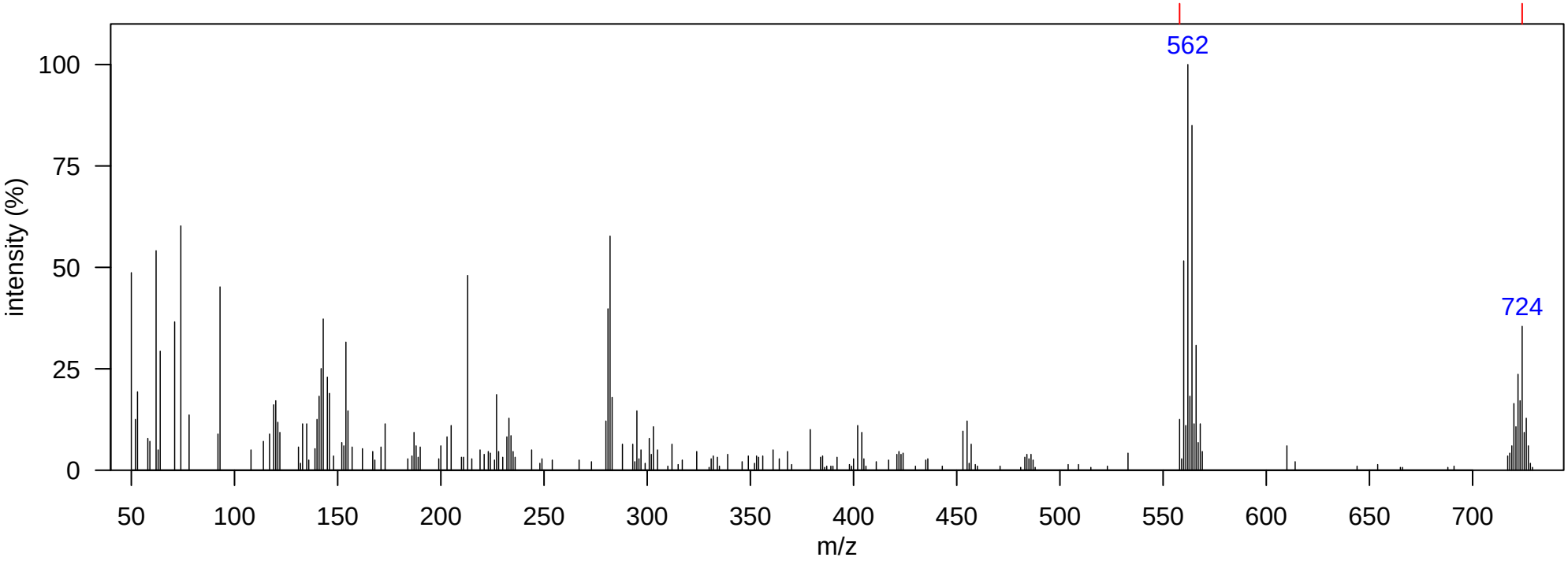
Comment:

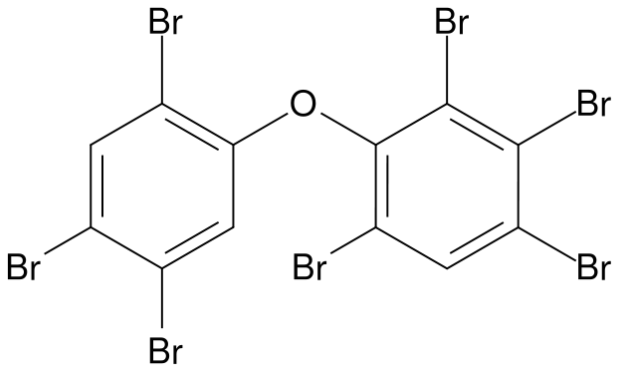
Elemental Formula: C12H3Br7O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT





m/z	Identity
558	[M−2Br]+
724	M+ (not monoisotopic)

Filename: 7Br_PBDE_isomer_2

Name: polybrominated diphenyl ether 7Br (PBDE) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 2018.5, RT (s) (2D): 1.889

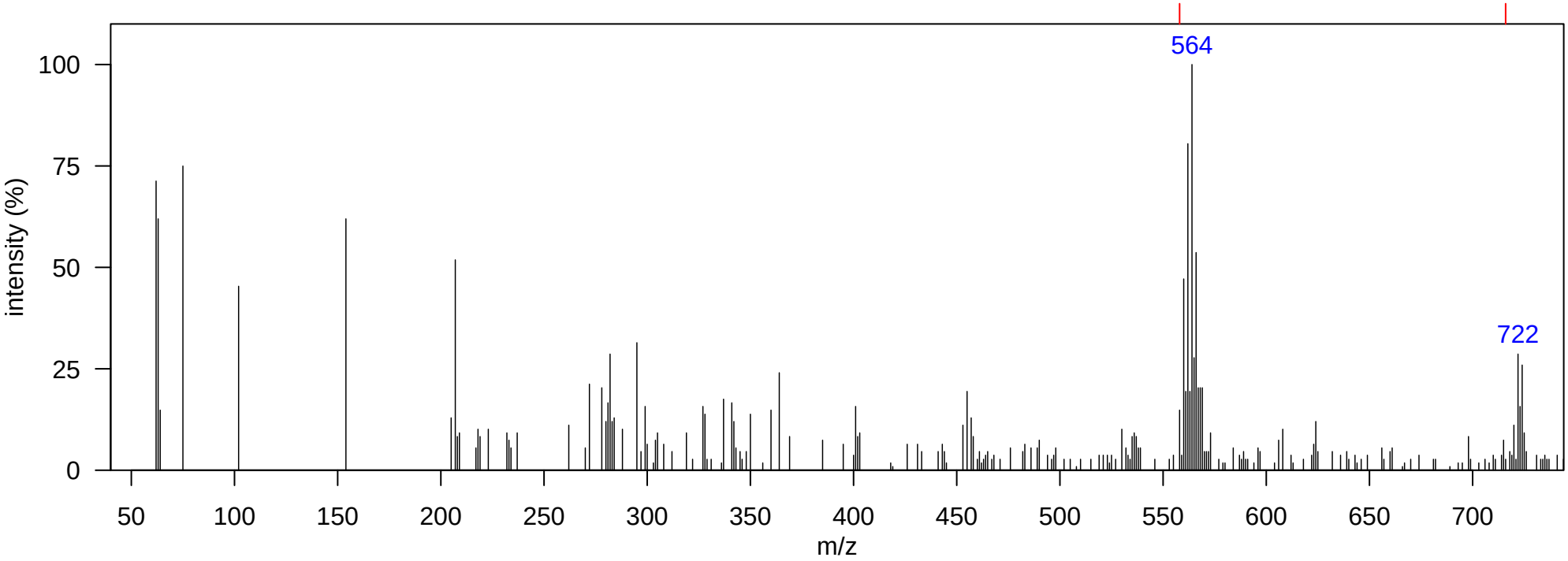
Comment:

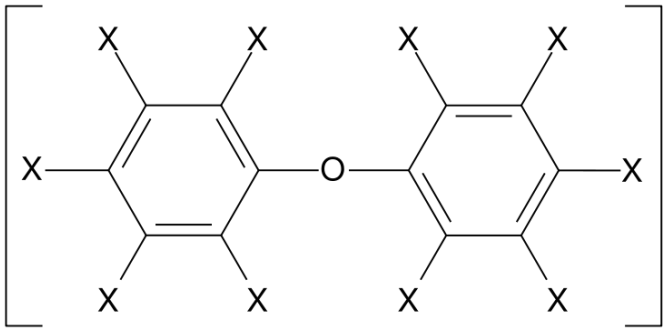
Elemental Formula: C12H3Br7O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS





m/z	Identity
558	[M−2Br]+
716	M+

Filename: 7Br_PBDE_isomer_3

Name: polybrominated biphenyl 4Br (PBB) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1581, RT (s) (2D): 2.151

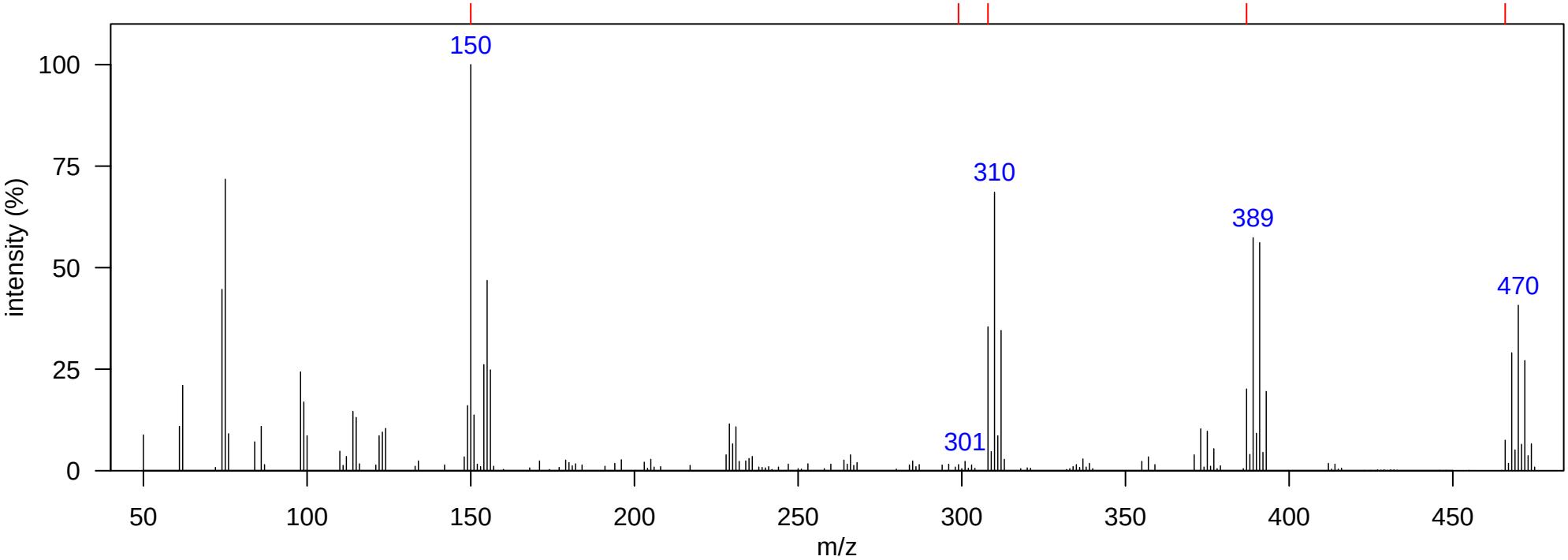
Comment:

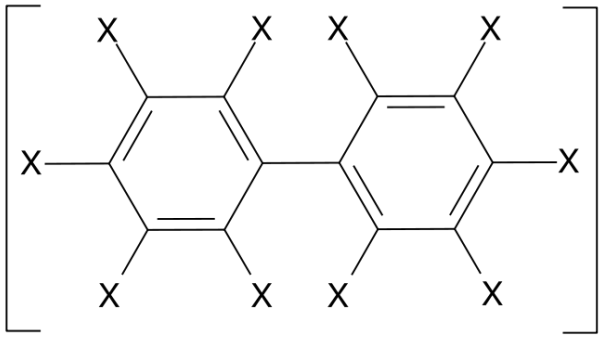
Elemental Formula: C12H6Br4

Source: anthropogenic

Class: PBB

Identification: Manual − Congener Group





m/z	Identity
150	[M−4Br]+
299	[M−3Br]+
308	[M−2Br]+
387	[M−Br]+
466	M+

Filename: 4Br_PBB_isomer_1

Name: polybrominated biphenyl 4Br (PBB) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1598.5, RT (s) (2D): 2.357

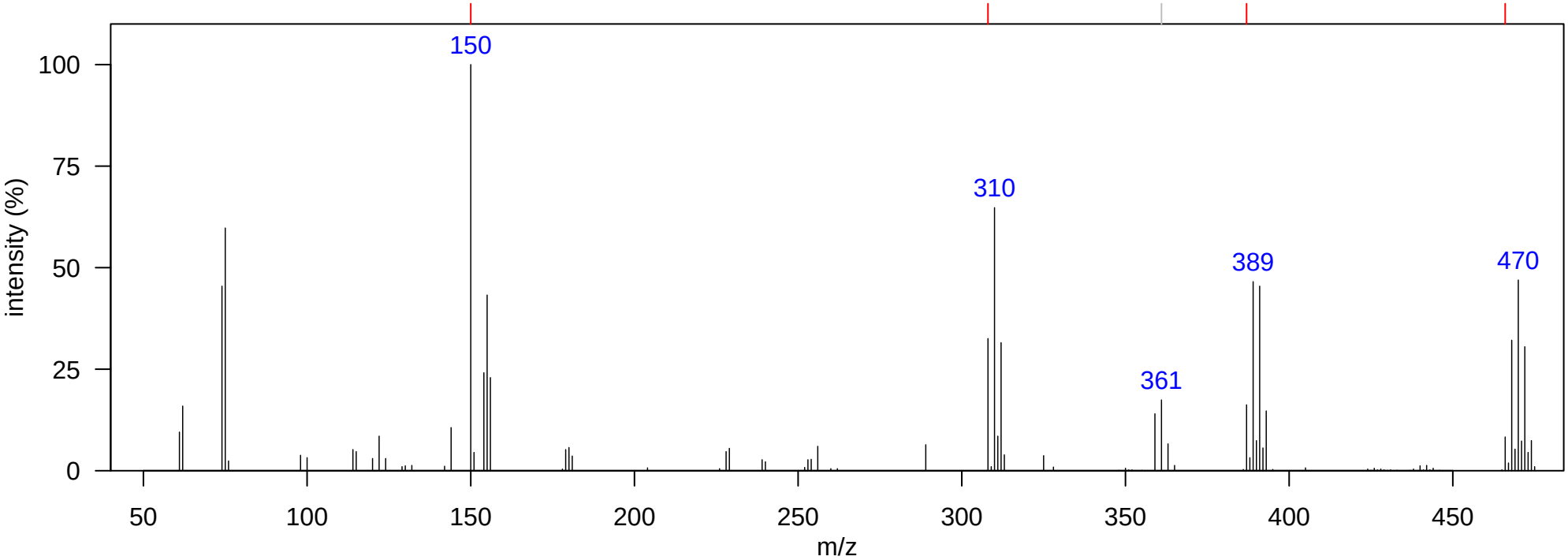
Comment:

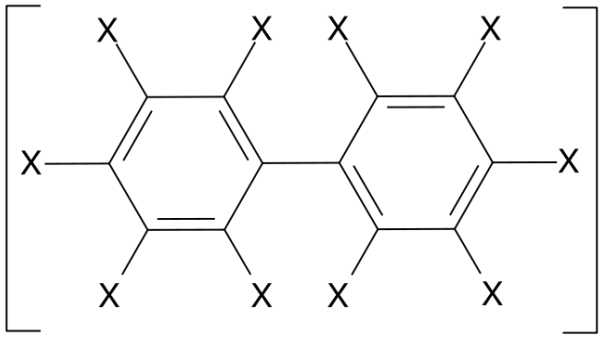
Elemental Formula: C12H6Br4

Source: anthropogenic

Class: PBB

Identification: Manual − Congener Group





m/z	Identity
150	[M−4Br]+
308	[M−2Br]+
361	PCB interference
387	[M−Br]+
466	M+

Filename: 4Br_PBB_isomer_2

Name: polybrominated biphenyl 5Br (PBB) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1644, RT (s) (2D): 2.92

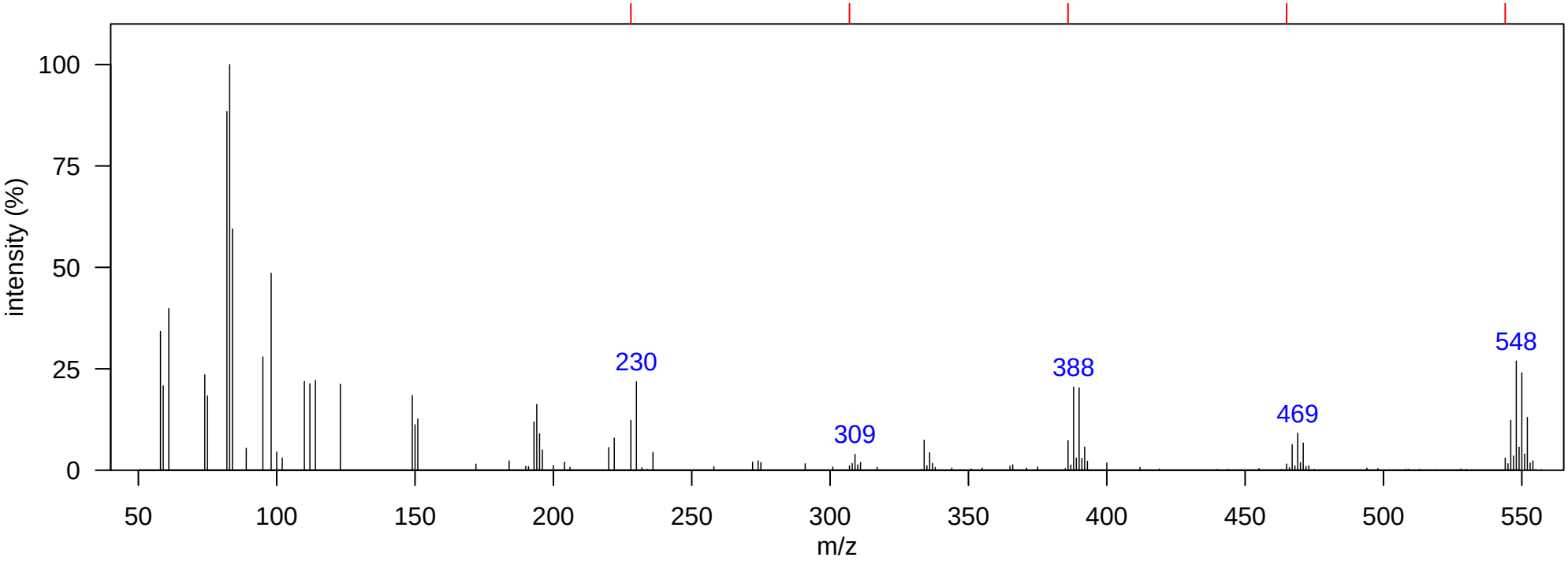
Comment:

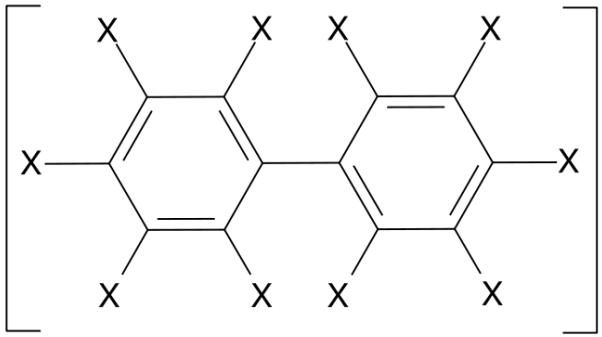
Elemental Formula: C12H5Br5

Source: anthropogenic

Class: PBB

Identification: Manual − Congener Group





m/z	Identity
228	[M−4Br]+
307	[M−3Br]+
386	[M−2Br]+
465	[M−Br]+
544	M+

Filename: 5Br_PBB_isomer_1

Name: polybrominated biphenyl 5Br (PBB) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1735, RT (s) (2D): 2.921

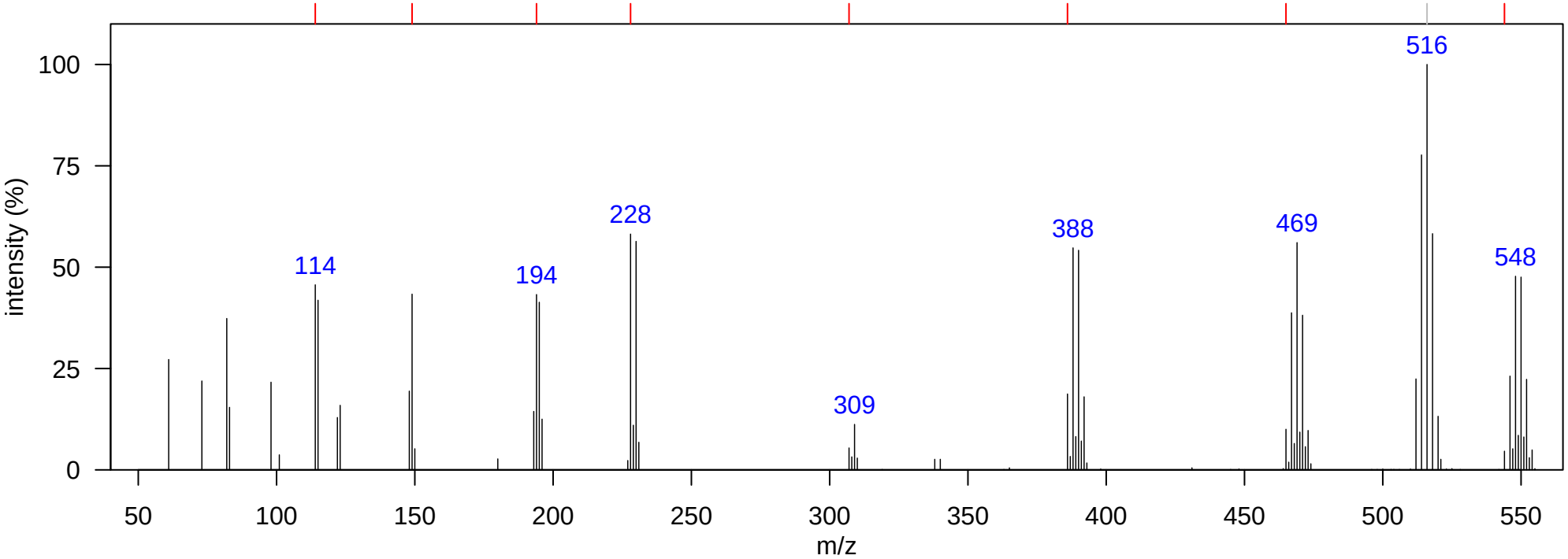
Comment:

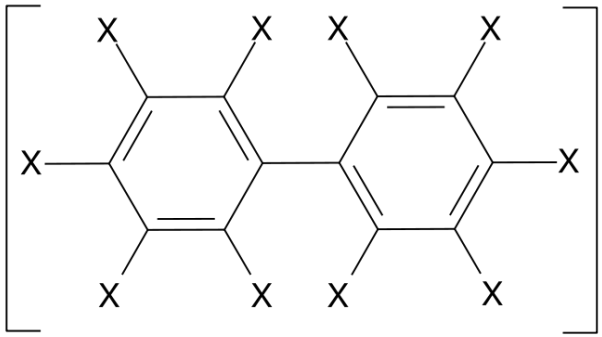
Elemental Formula: C12H5Br5

Source: anthropogenic

Class: PBB

Identification: Manual − Congener Group





m/z	Identity
114	[M−4Br]2+
149	[M−5Br]+
194	[M−2Br]2+
228	[M−4Br]+
307	[M−3Br]+
386	[M−2Br]+
465	[M−Br]+
516	MeO−BDE (4Br) interference
544	M+

Filename: 5Br_PBB_isomer_2

Name: polybrominated biphenyl 6Br (PBB) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1759.5, RT (s) (2D): 3.149

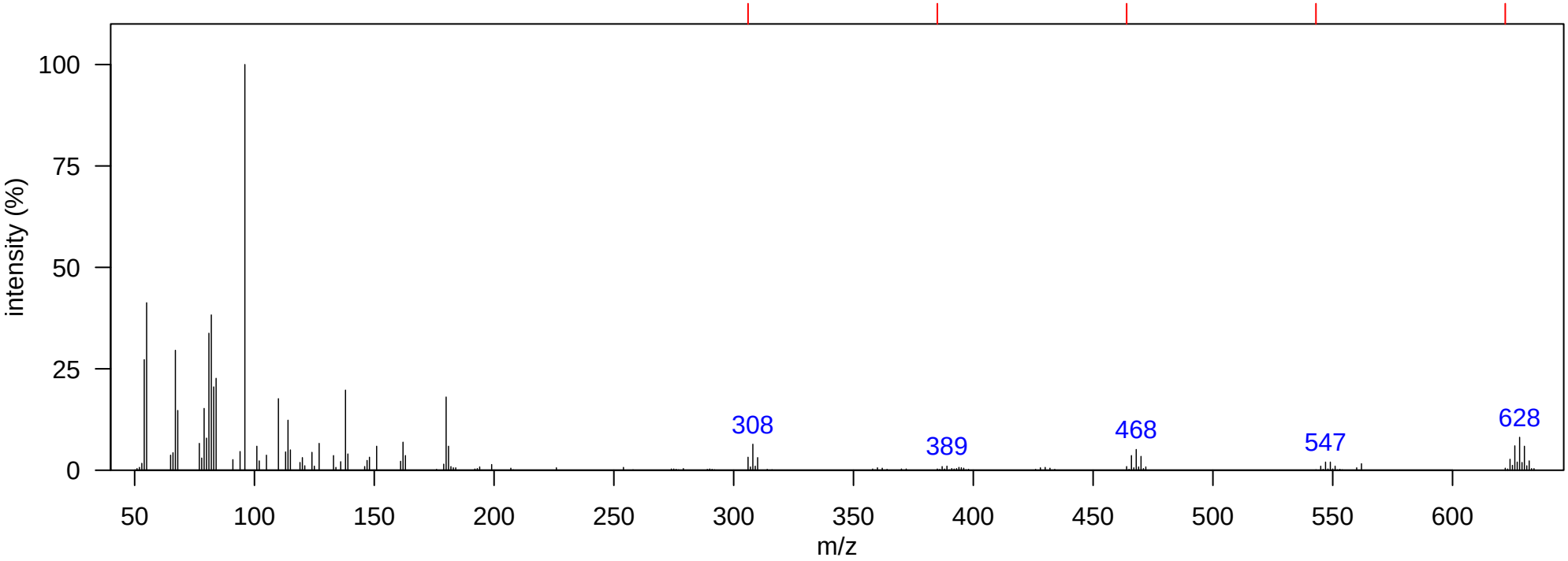
Comment:

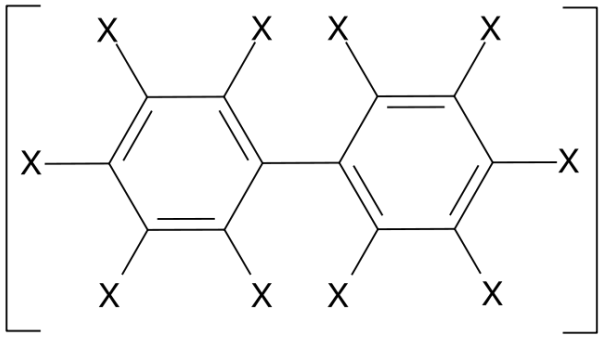
Elemental Formula: C12H4Br6

Source: anthropogenic

Class: PBB

Identification: Authentic MS





m/z	Identity
306	[M−4Br]+
385	[M−3Br]+
464	[M−2Br]+
543	[M−Br]+
622	M+

Name: polybrominated biphenyl 6Br (PBB) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1780.5, RT (s) (2D): 0.168

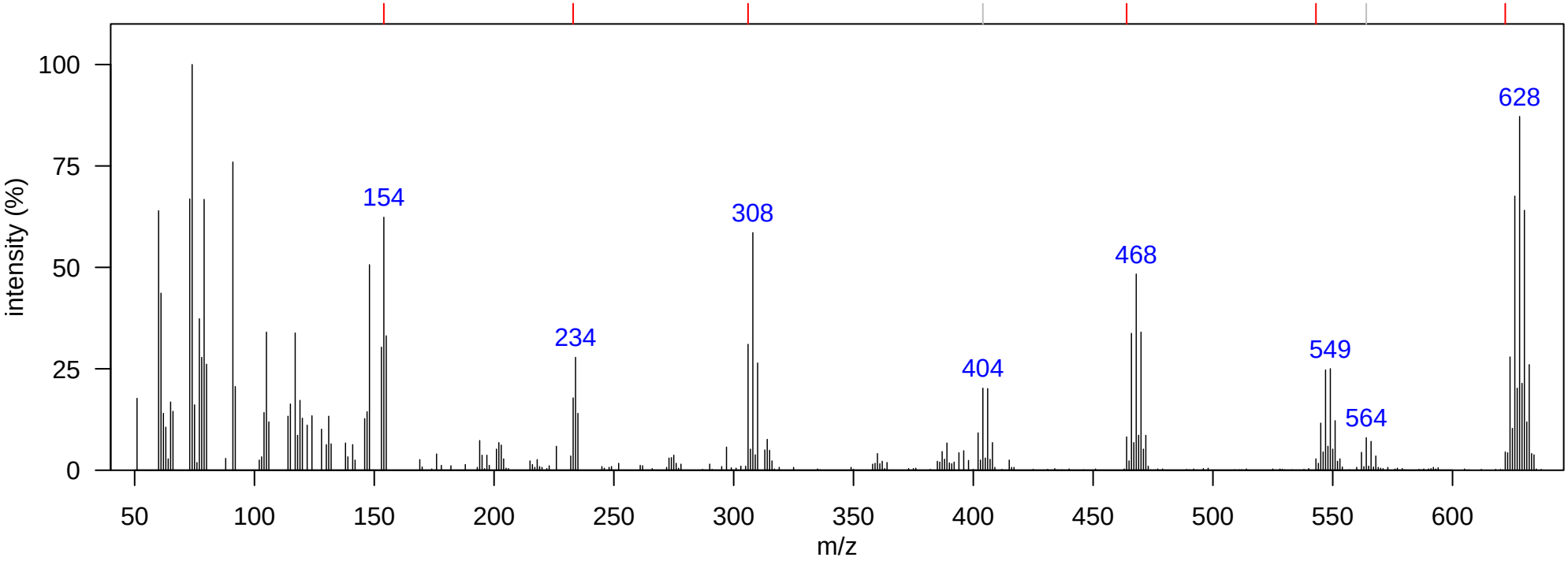
Comment:

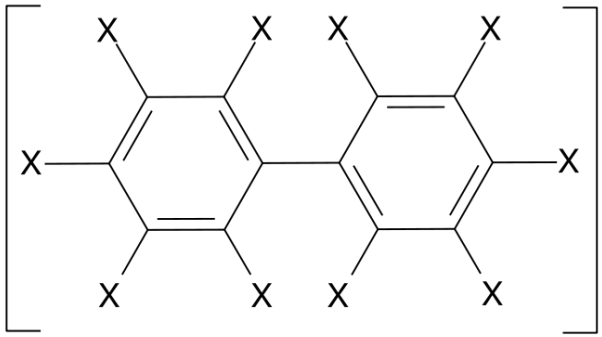
Elemental Formula: C12H4Br6

Source: anthropogenic

Class: PBB

Identification: Authentic MS





m/z	Identity
154	[M−4Br]2+
233	[M−2Br]2+
306	[M−4Br]+
404	PBDE interference
464	[M−2Br]+
543	[M−Br]+
564	PBDE interference
622	M+

Filename: 6Br_PBB_isomer_2

Name: polybrominated biphenyl 6Br (PBB) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1798, RT (s) (2D): 0.682

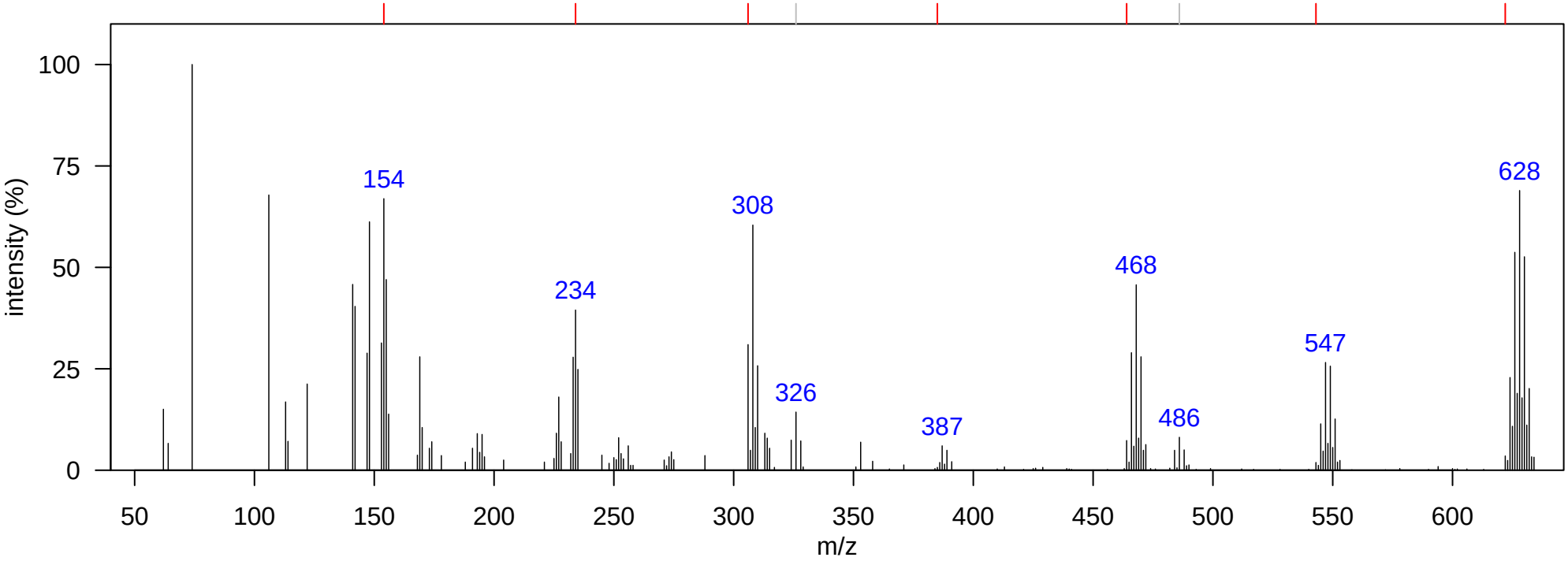
Comment:

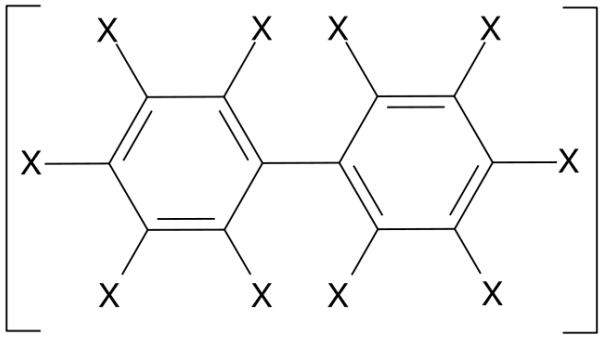
Elemental Formula: C12H4Br6

Source: anthropogenic

Class: PBB

Identification: Authentic MS





m/z	Identity
154	[M−4Br]2+
234	[M−2Br]2+
306	[M−4Br]+
326	PBDE interference
385	[M−3Br]+
464	[M−2Br]+
486	PBDE interference
543	[M−Br]+
622	M+

Filename: 6Br_PBB_isomer_3

Name: polybrominated biphenyl 6Br (PBB) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1808.5, RT (s) (2D): 3.188

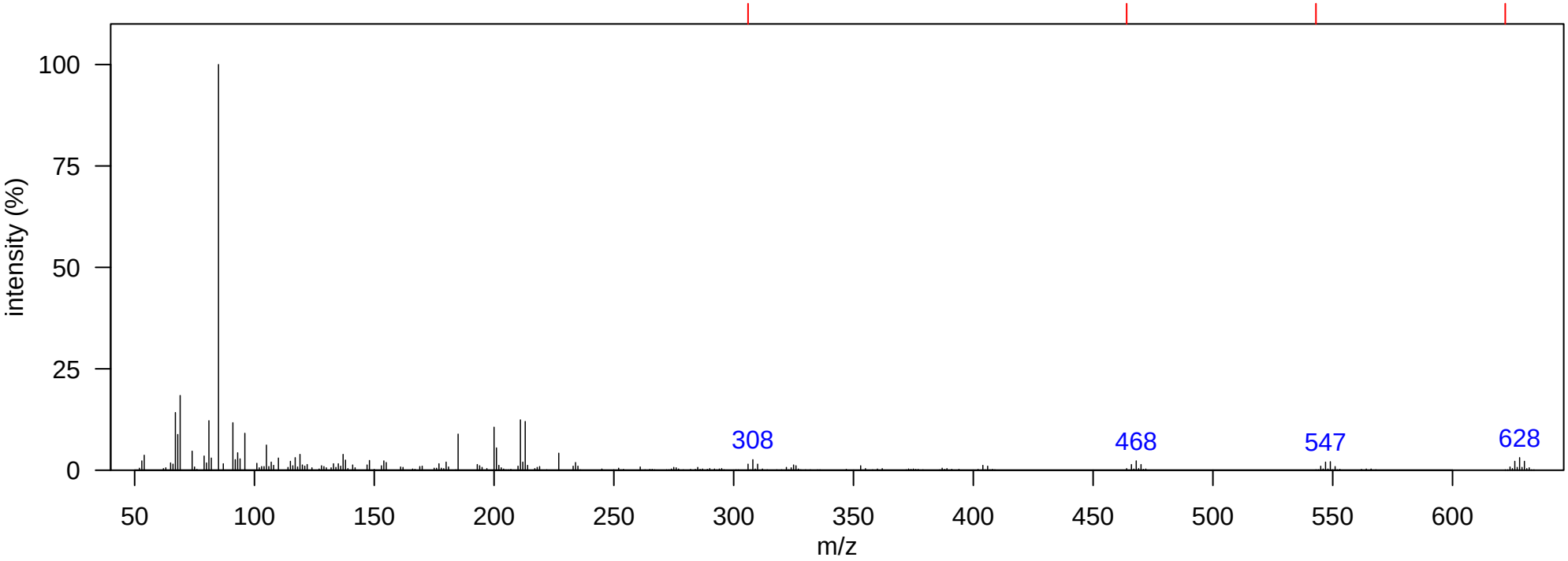
Comment: Low intensity, but visible in raw data.

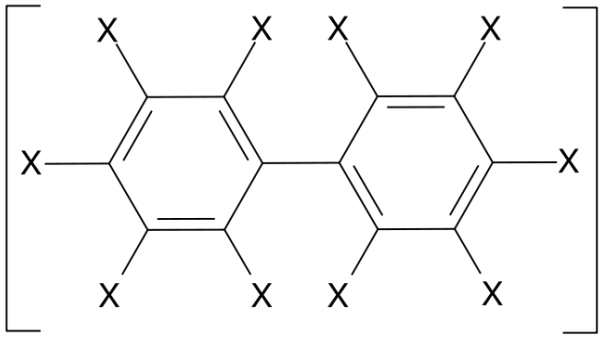
Elemental Formula: C12H4Br6

Source: anthropogenic

Class: PBB

Identification: Authentic MS





m/z	Identity
306	[M−4Br]+
464	[M−2Br]+
543	[M−Br]+
622	M+

Filename: 6Br_PBB_isomer_4

Name: polybrominated biphenyl 6Br (PBB) isomer 5

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1836.5, RT (s) (2D): 0.135

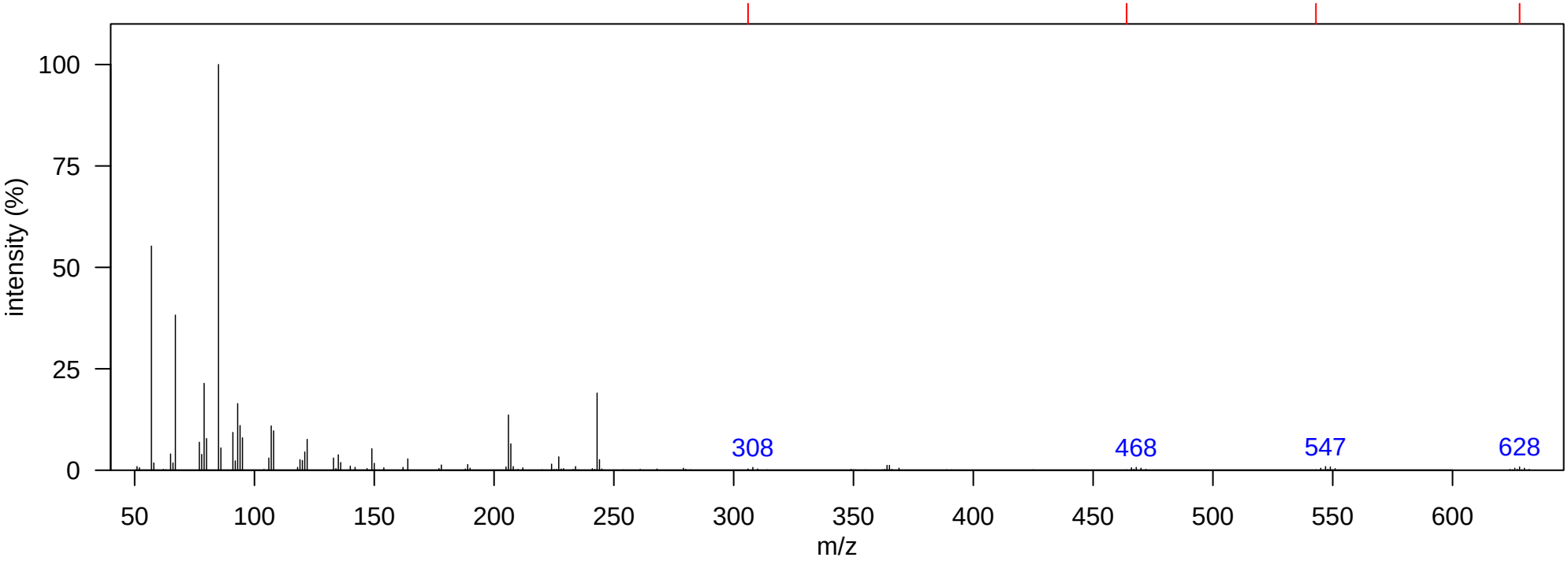
Comment: Low intensity, but visible in raw data.

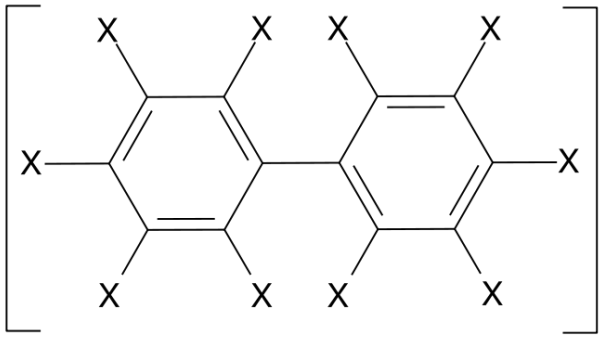
Elemental Formula: C12H4Br6

Source: anthropogenic

Class: PBB

Identification: Authentic MS





m/z	Identity
306	[M−4Br]+
464	[M−2Br]+
543	[M−Br]+
628	M+ (not monoisotopic)

Filename: 6Br_PBB_isomer_5

Name: polybrominated biphenyl 6Br (BB−153) isomer 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1868, RT (s) (2D): 3.312

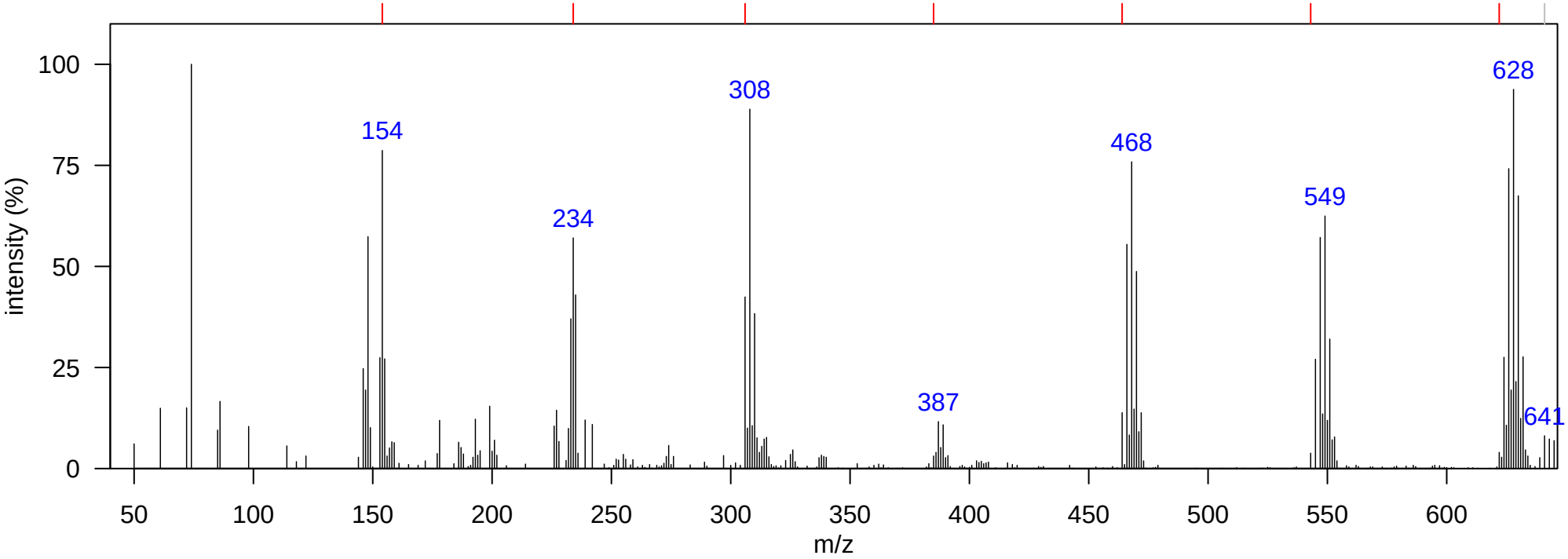
Comment:

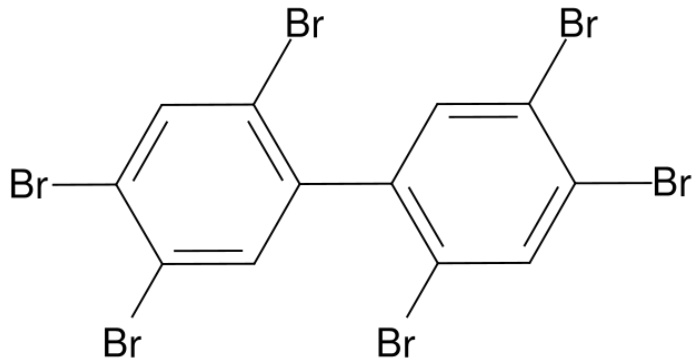
Elemental Formula: C12H4Br6

Source: anthropogenic

Class: PBB

Identification: Authentic MS RT





m/z	Identity
154	[M−4Br]2+
234	[M−2Br]2+
306	[M−4Br]+
385	[M−3Br]+
464	[M−2Br]+
543	[M−Br]+
622	M+
641	PBDE interference

Filename: 6Br_PBB_isomer_6

Name: polychlorinated diphenyl ether 5Cl (PCDE)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1535.5, RT (s) (2D): 1.247

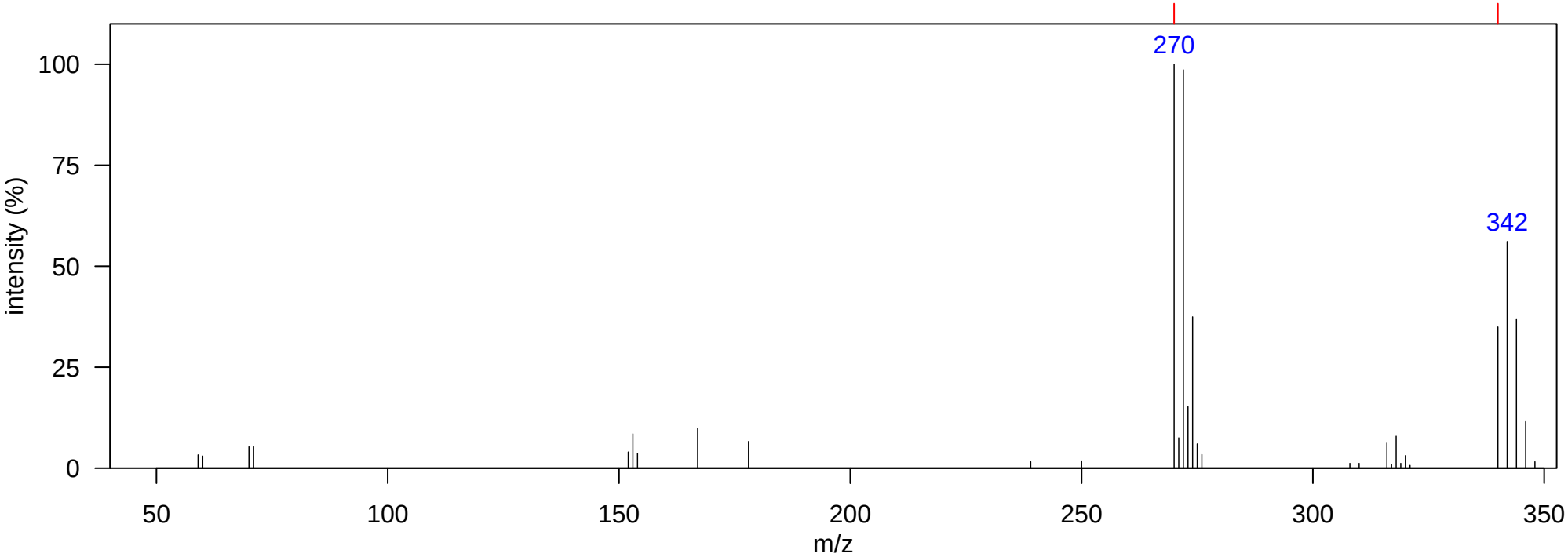
Comment:

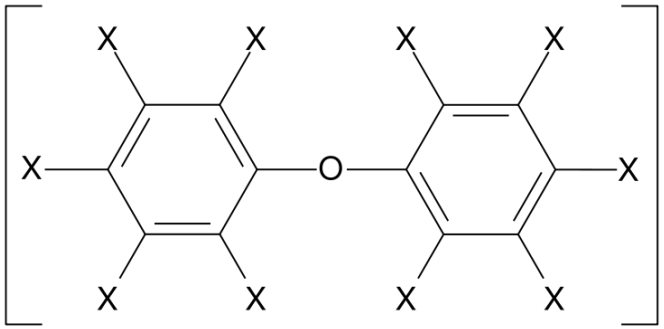
Elemental Formula: C12H5Cl5O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
270	[M−2Cl]+
340	M+

Filename: 5Cl_PCDE

Name: polychlorinated diphenyl ether 6Cl (PCDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1549.5, RT (s) (2D): 1.339

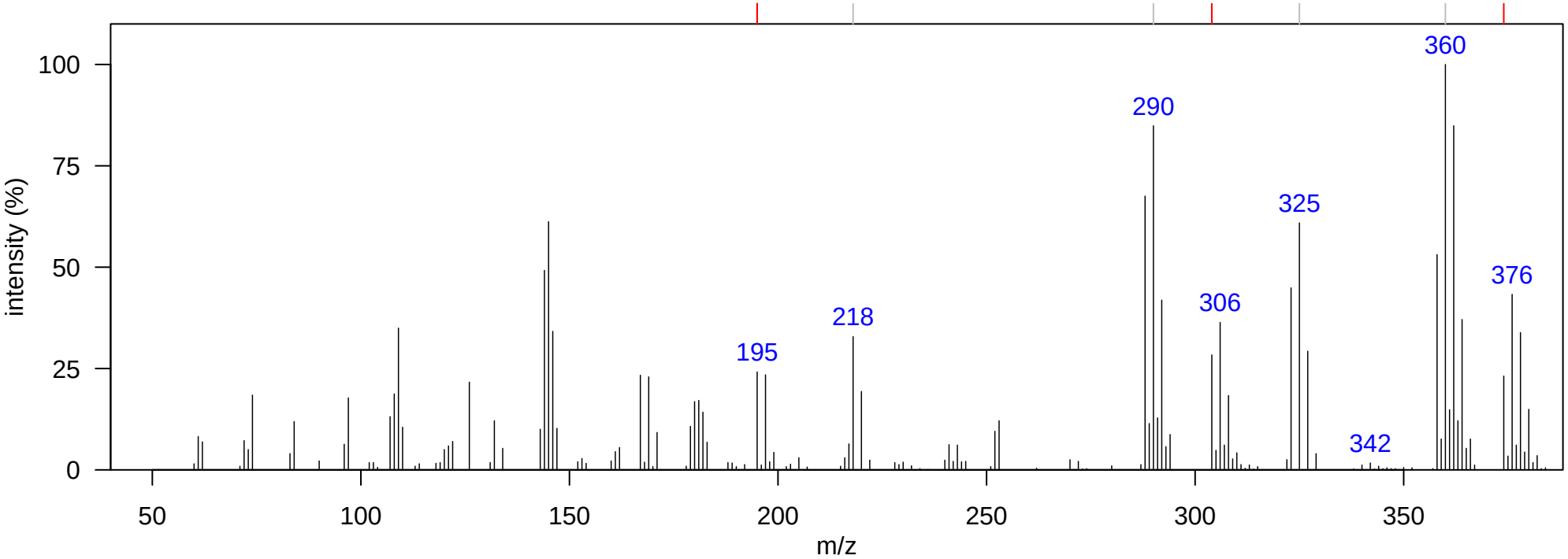
Comment:

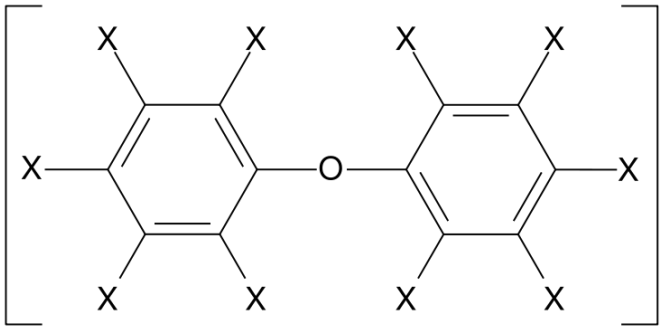
Elemental Formula: C12H4Cl6O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
195	[C5H2OCl3]+
218	interference PCB
290	PCB interference
304	[M−2Cl]+
325	PCB interference
360	PCB interference
374	M+

Filename: 6Cl_PCDE_isomer_1

Name: polychlorinated diphenyl ether 6Cl (PCDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1570.5, RT (s) (2D): 1.254

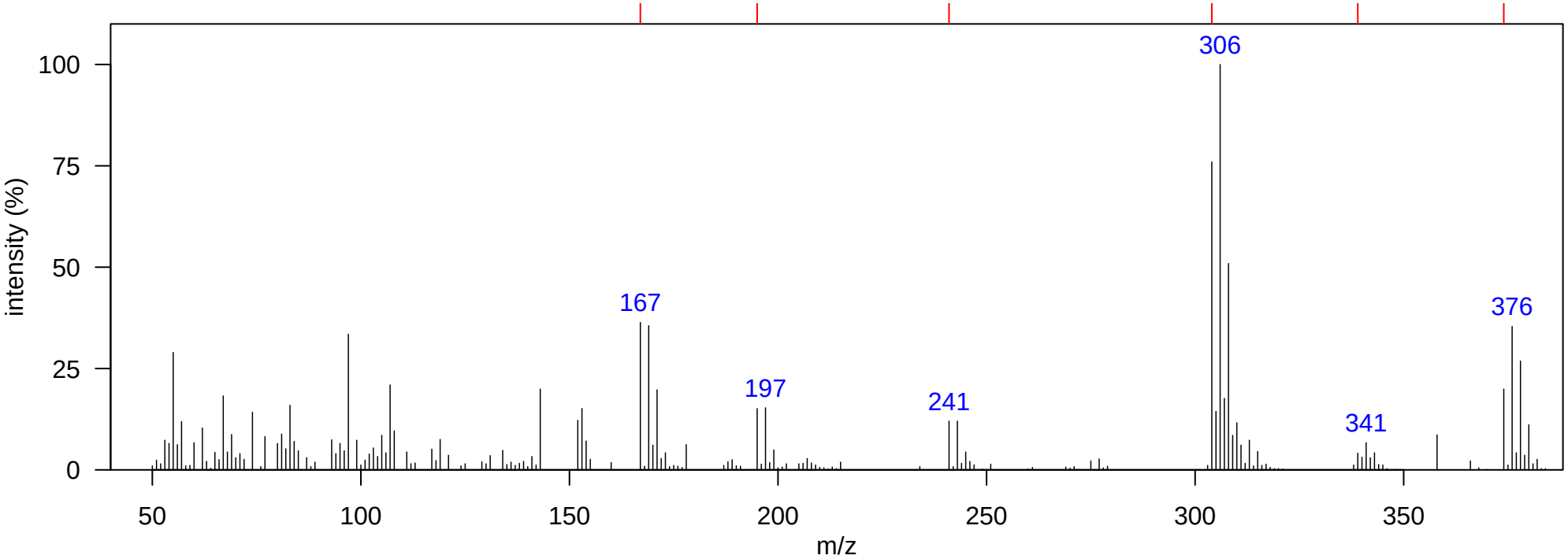
Comment:

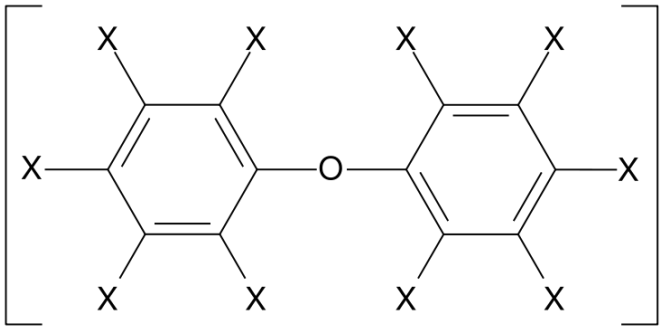
Elemental Formula: C12H4Cl6O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





X=6Cl, 4H

m/z	Identity
167	[C5H2Cl3]+
195	[C6H2OCl3]+
241	[M−3Cl−CO]+
304	[M−2Cl]+
339	[M−Cl]+
374	M+

Filename: 6Cl_PCDE_isomer_2

Name: polychlorinated diphenyl ether 6Cl (PCDE) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1605.5, RT (s) (2D): 1.21

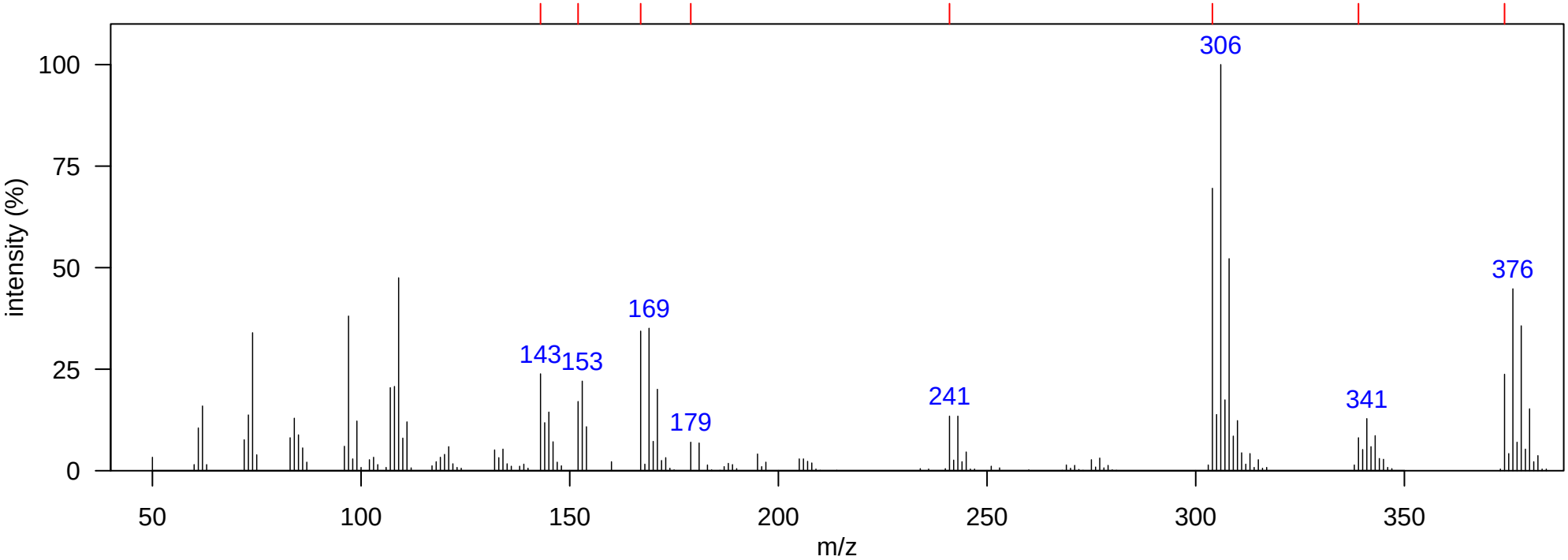
Comment:

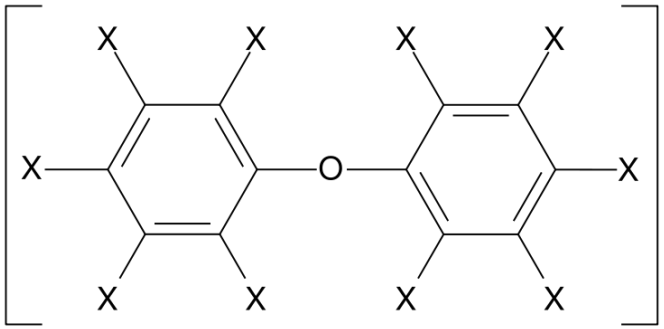
Elemental Formula: C12H4Cl6O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





X=6Cl, 4H

m/z	Identity
143	[C6Cl2H]+
152	[M−2Cl]2+
167	[C5Cl3H2]+
179	[C6Cl3H2]+
241	[M−3Cl−CO]+
304	[M−2Cl]+
339	[M−Cl]+
374	M+

Filename: 6Cl_PCDE_isomer_3

Name: polychlorinated diphenyl ether 6Cl (PCDE) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1644, RT (s) (2D): 1.67

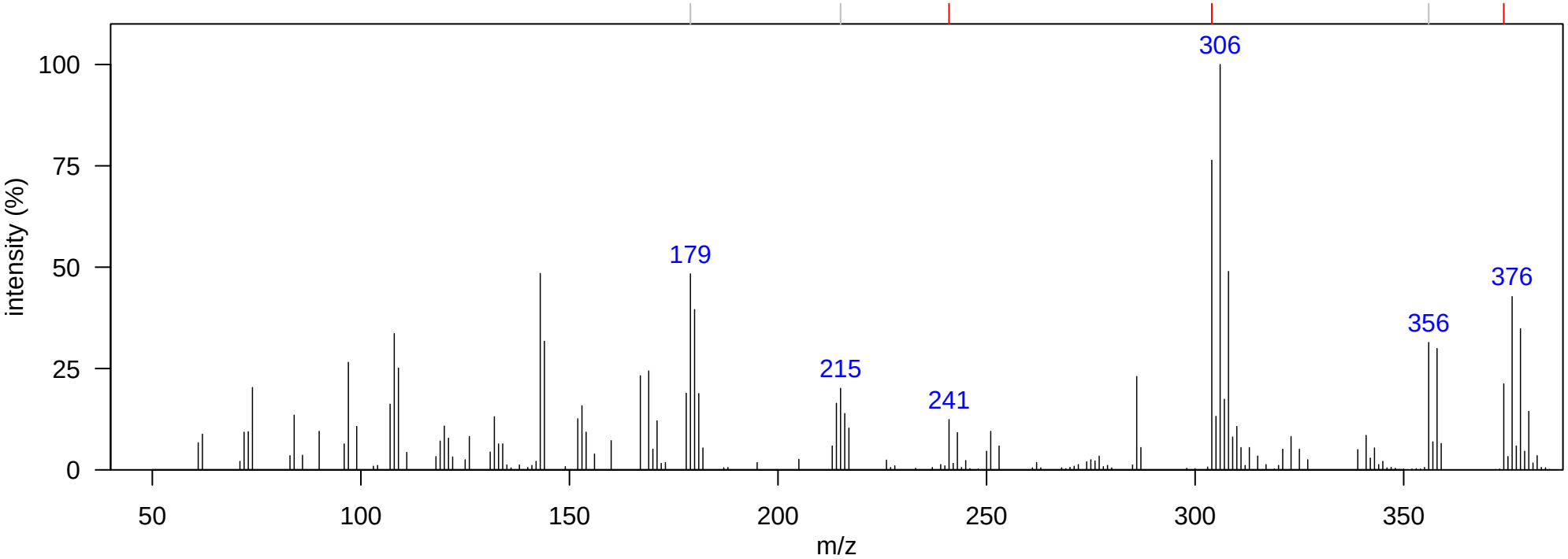
Comment:

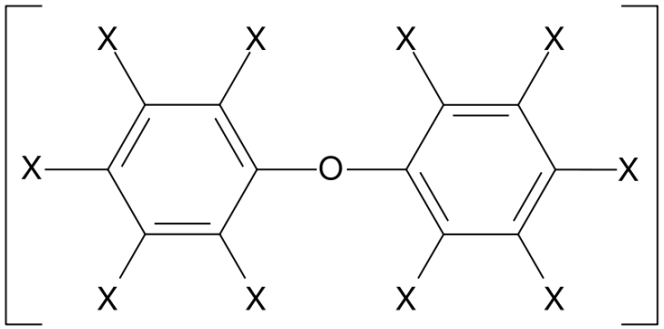
Elemental Formula: C12H4Cl6O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





X=6Cl, 4H

m/z	Identity
179	PCB interference
215	PCB interference
241	[M−3Cl−CO]+
304	[M−2Cl]+
356	PCB interference
374	M+
430	PCB interference

Filename: 6Cl_PCDE_isomer_4

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1588, RT (s) (2D): 1.86

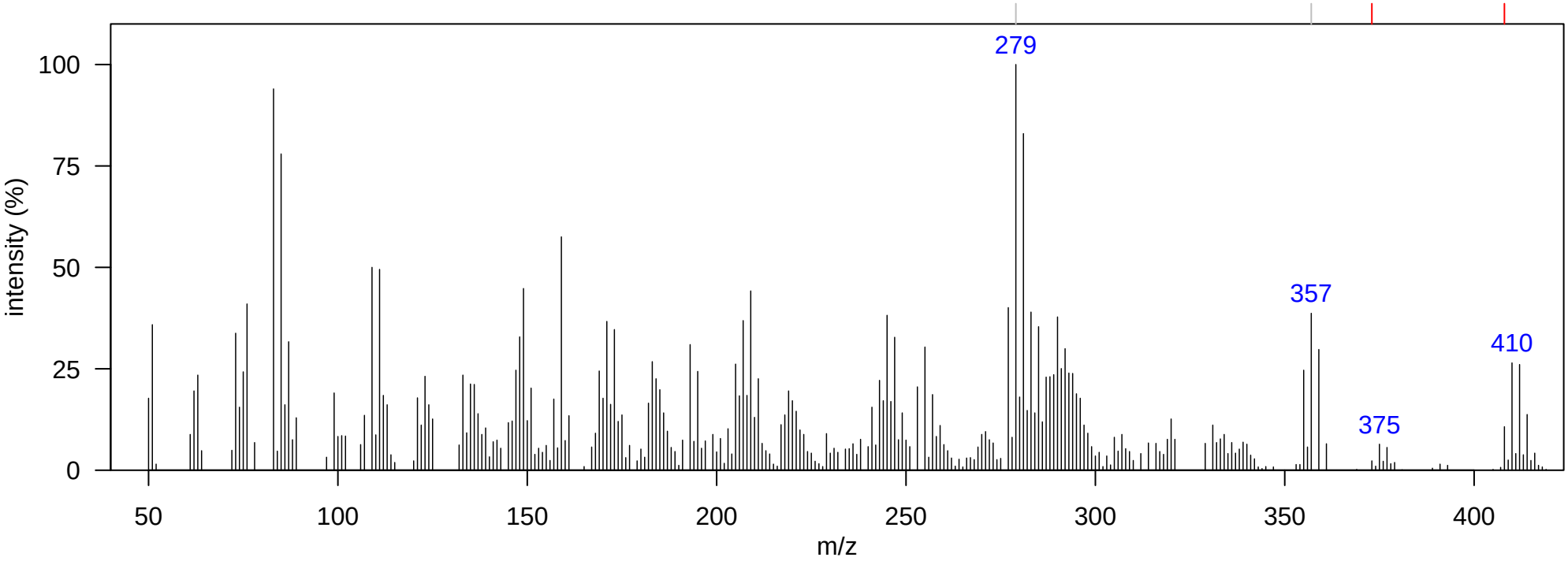
Comment: Likely PCDE, but low intensity.

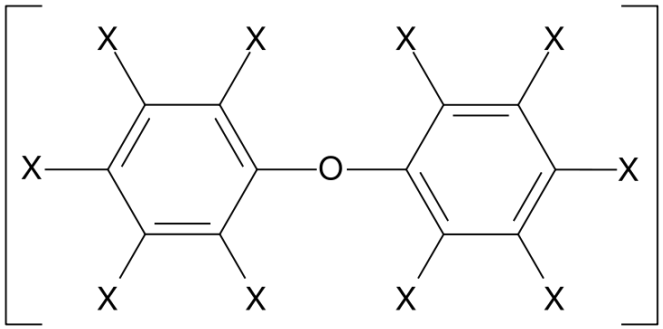
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
279	interference
357	interference
373	[M−Cl]+
408	M+

Filename: 7Cl_PCDE_isomer_1

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1595, RT (s) (2D): 2.019

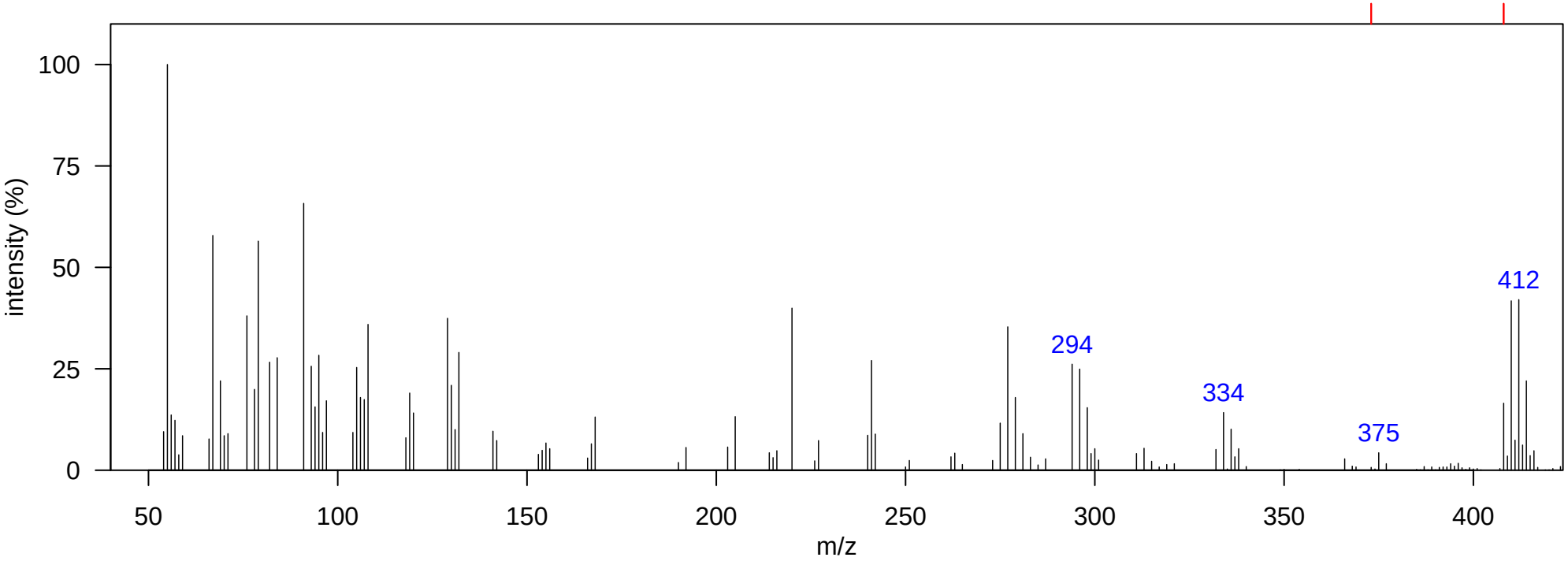
Comment: Likely PCDE, but low intensity.

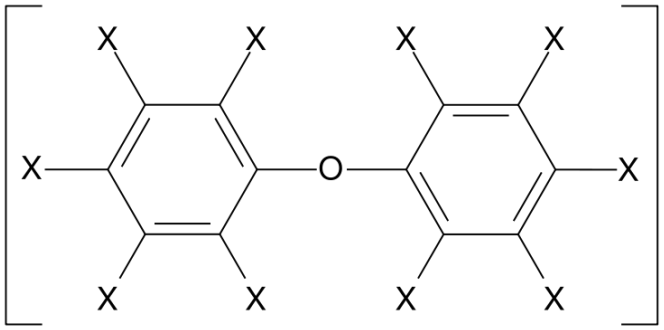
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
373	[M−Cl]+
408	M+

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1598.5, RT (s) (2D): 1.888

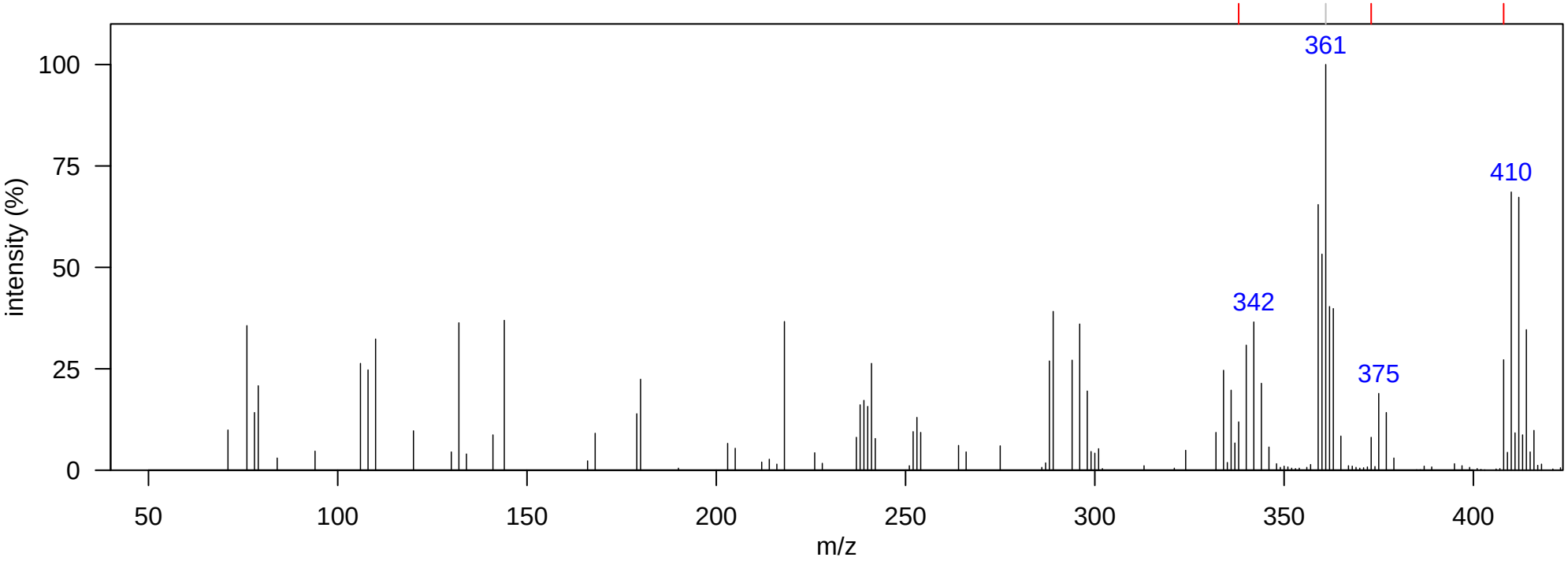
Comment: Likely PCDE, but low intensity.

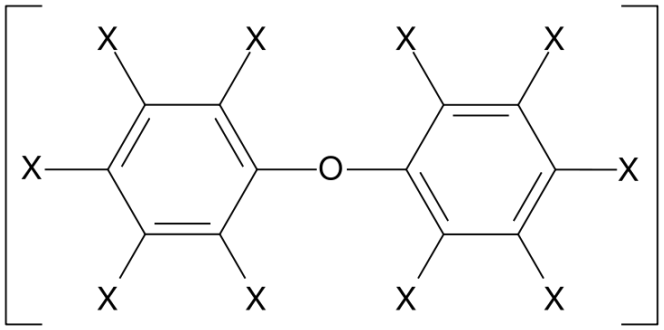
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
338	[M−Cl2]+
361	interference
373	[M−Cl]+
408	M+

Filename: 7Cl_PCDE_isomer_3

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1647.5, RT (s) (2D): 1.54

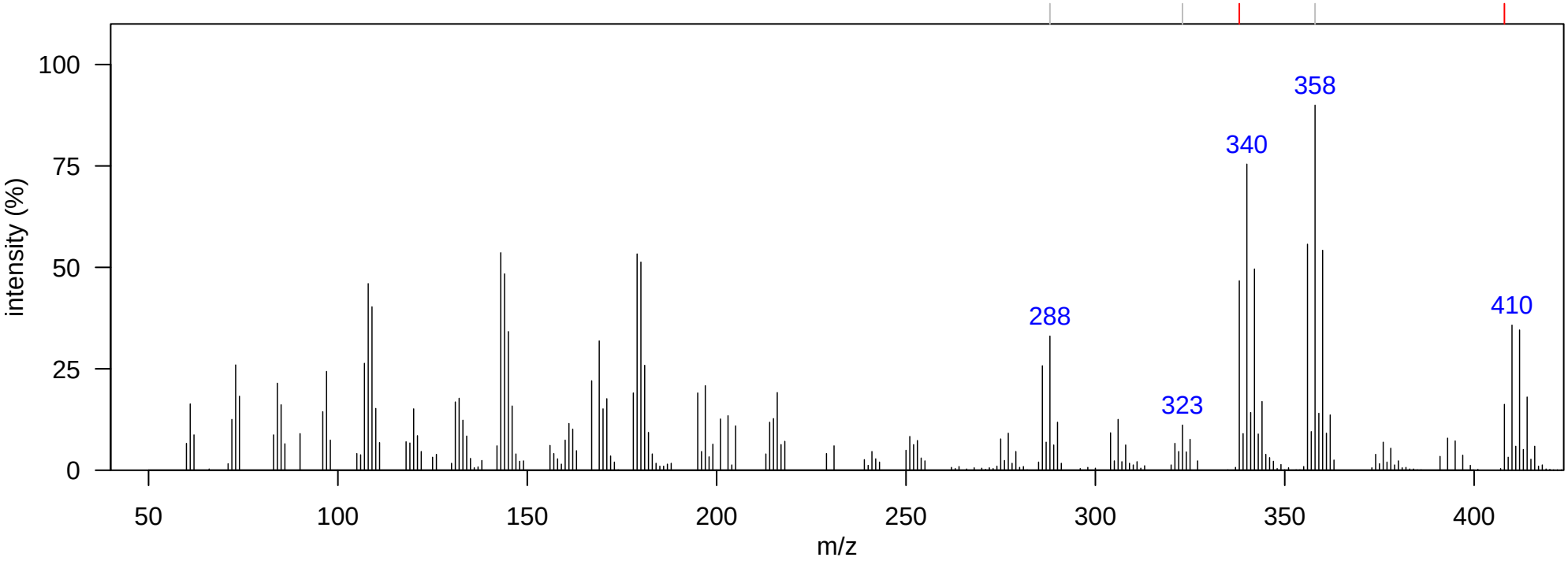
Comment:

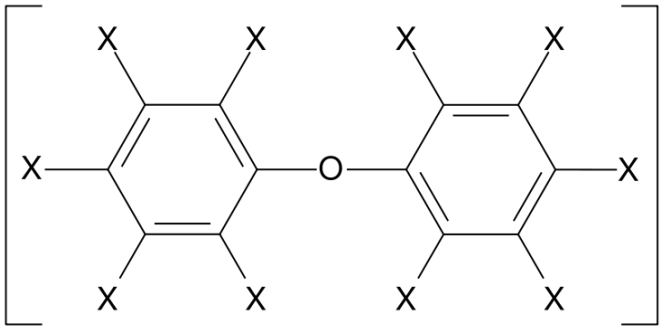
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





X=7Cl, 3H

m/z	Identity
288	PCB interference
323	PCB interference
338	[M−2Cl]+
358	PCB interference
408	M+
430	PCB interference

Filename: 7Cl_PCDE_isomer_4

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 5

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1668.5, RT (s) (2D): 1.372

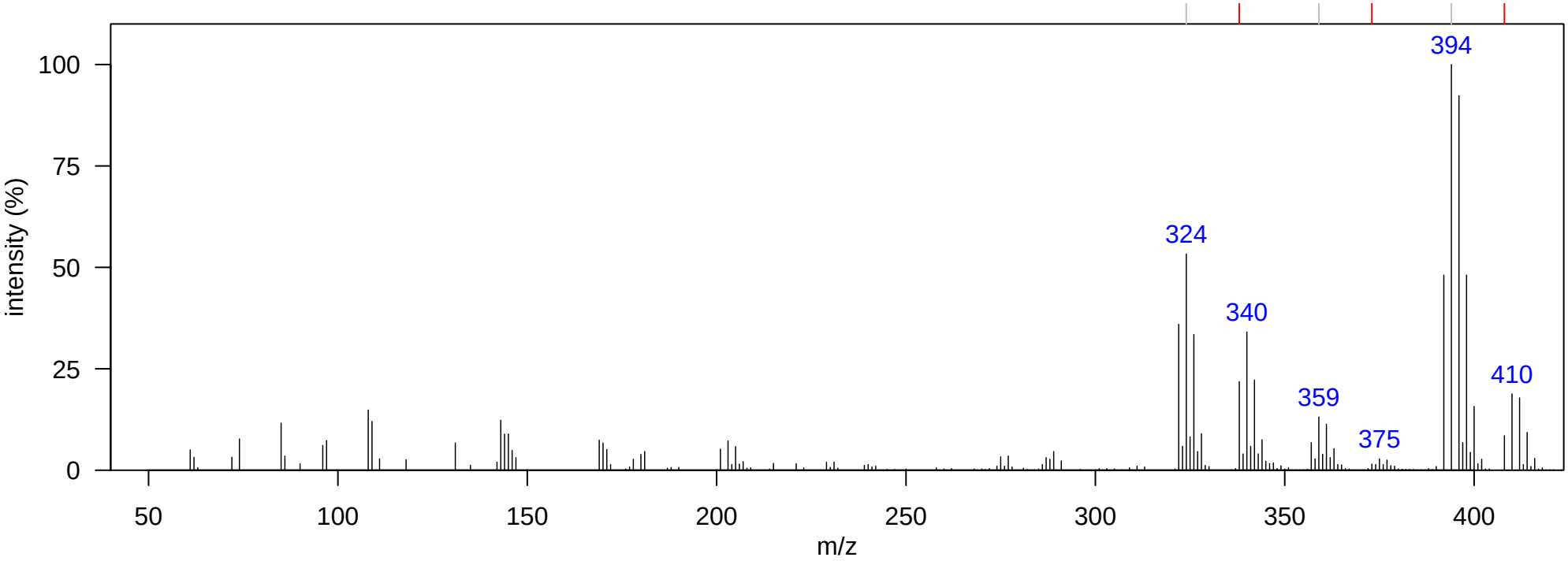
Comment:

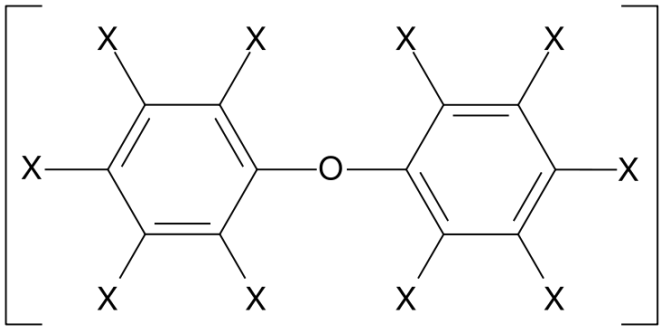
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
324	PCB interference
338	[M−2Cl]+
359	PCB interference
373	[M−Cl]+
394	PCB interference
408	M+

Filename: 7Cl_PCDE_isomer_5

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1672, RT (s) (2D): 1.521

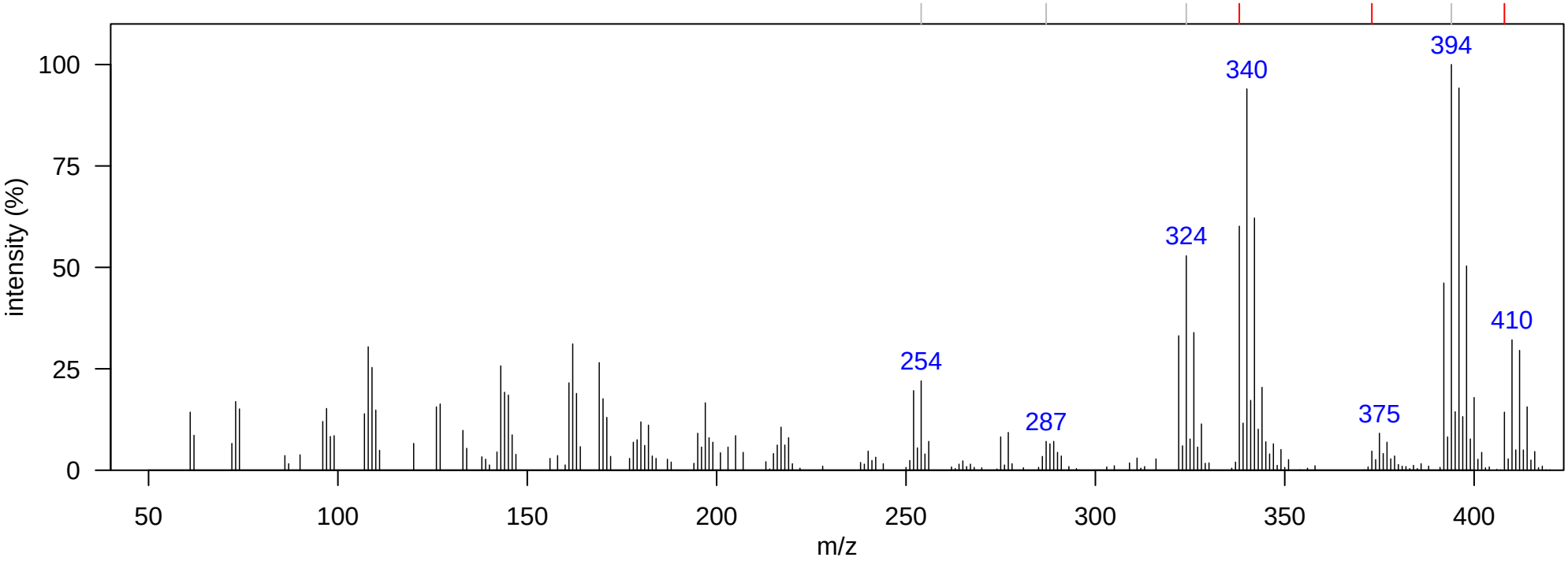
Comment:

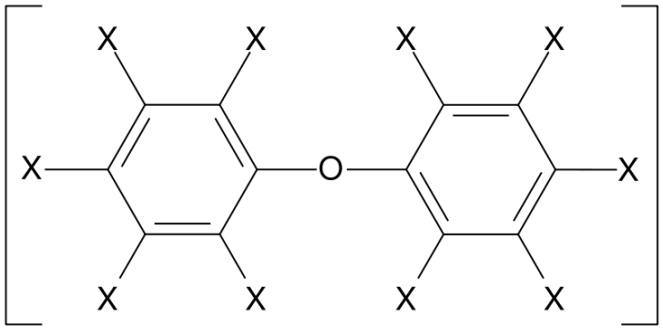
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
254	PCB interference
287	PCB interference
324	PCB interference
338	[M−2Cl]+
373	[M−Cl]+
394	PCB interference
408	M+

Filename: 7Cl_PCDE_isomer_6

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 7

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1703.5, RT (s) (2D): 1.449

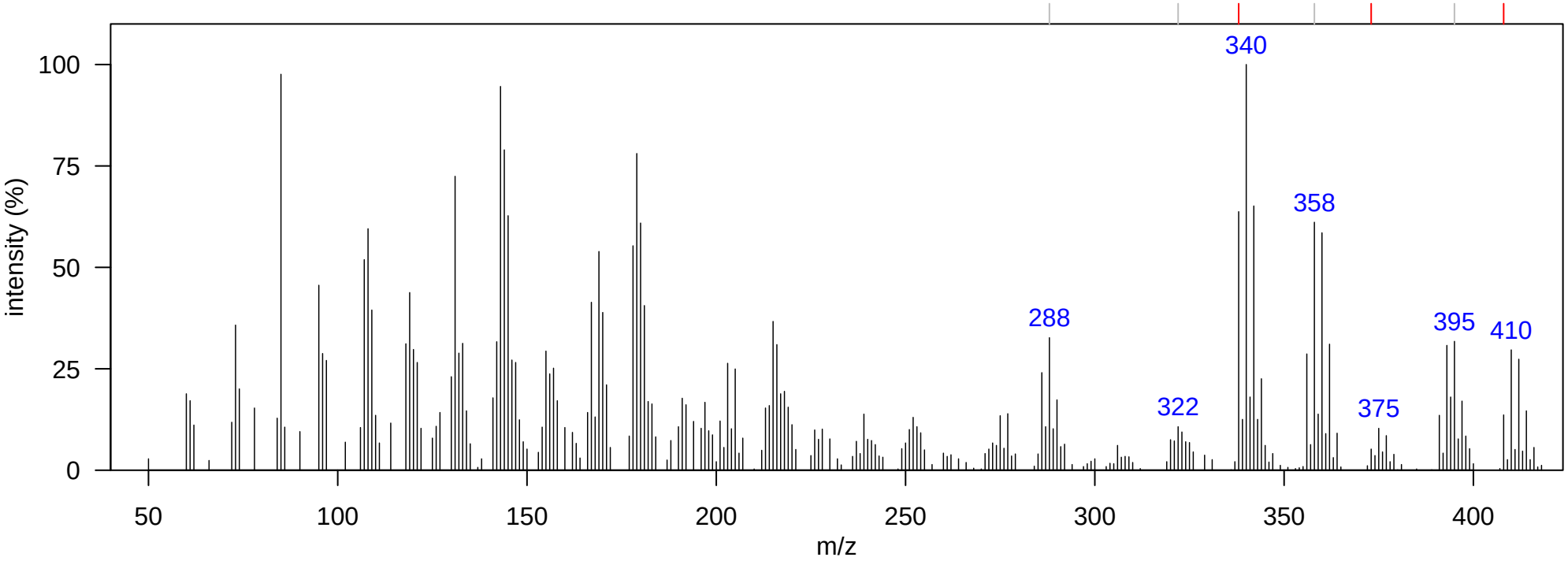
Comment:

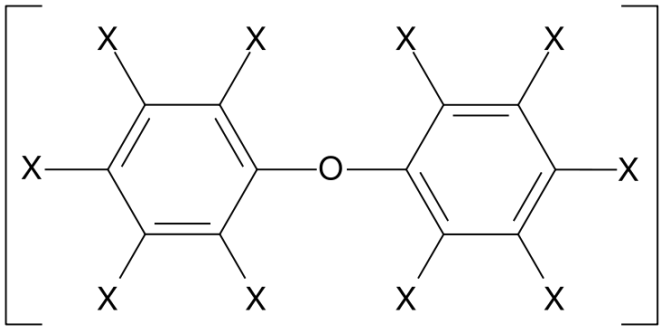
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
288	PCB interference
322	PCB interference
338	[M−2Cl]+
358	PCB interference
373	[M−Cl]+
395	PCB interference
408	M+
431	PCB interference

Filename: 7Cl_PCDE_isomer_7

Name: polychlorinated diphenyl ether 7Cl (PCDE) isomer 8

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1717.5, RT (s) (2D): 1.991

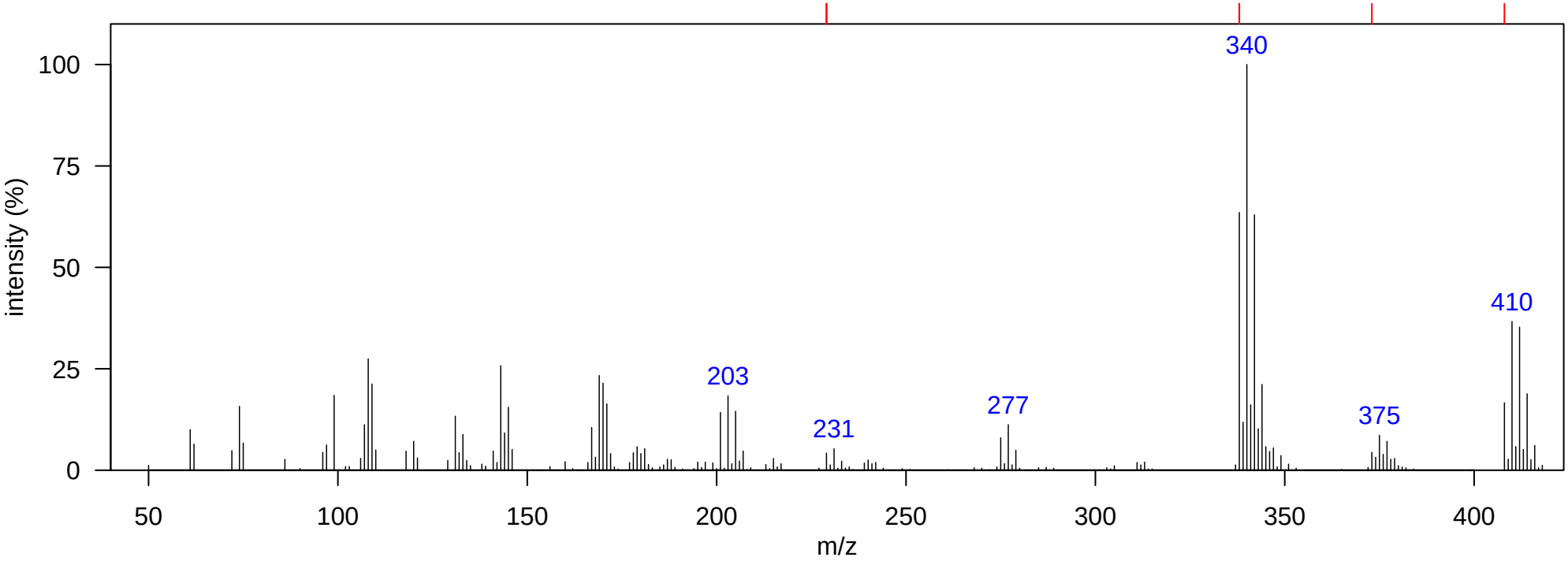
Comment:

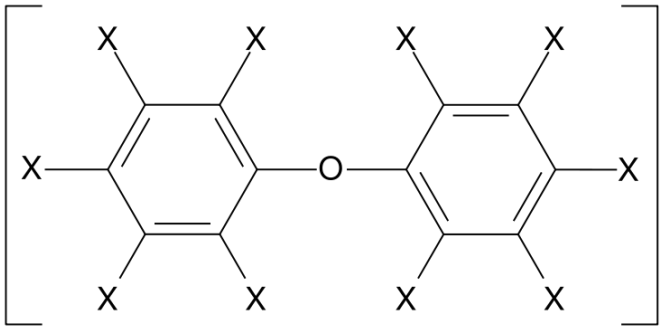
Elemental Formula: C12H3Cl7O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
229	[M−3Cl−C6H2]+
338	[M−2Cl]+
373	[M−Cl]+
408	M+

Filename: 7Cl_PCDE_isomer_8

Name: polychlorinated diphenyl ether 8Cl (PCDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1731.5, RT (s) (2D): 1.848

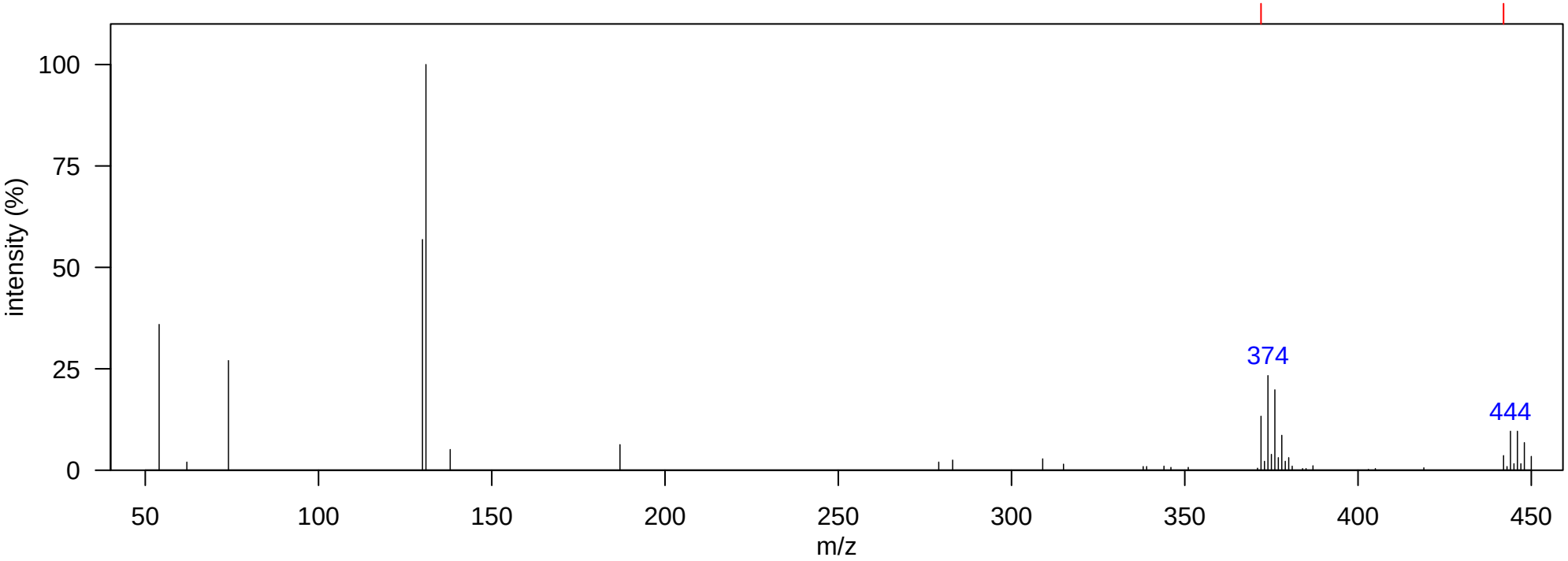
Comment:

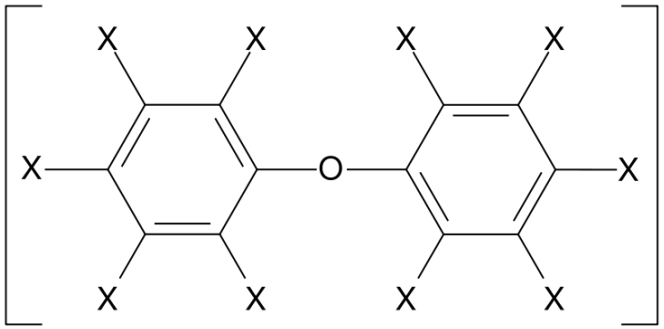
Elemental Formula: C12H2Cl8O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
372	[M−2Cl]+
442	M+

Filename: 8Cl_PCDE_isomer_1

Name: polychlorinated diphenyl ether 8Cl (PCDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1749, RT (s) (2D): 1.658

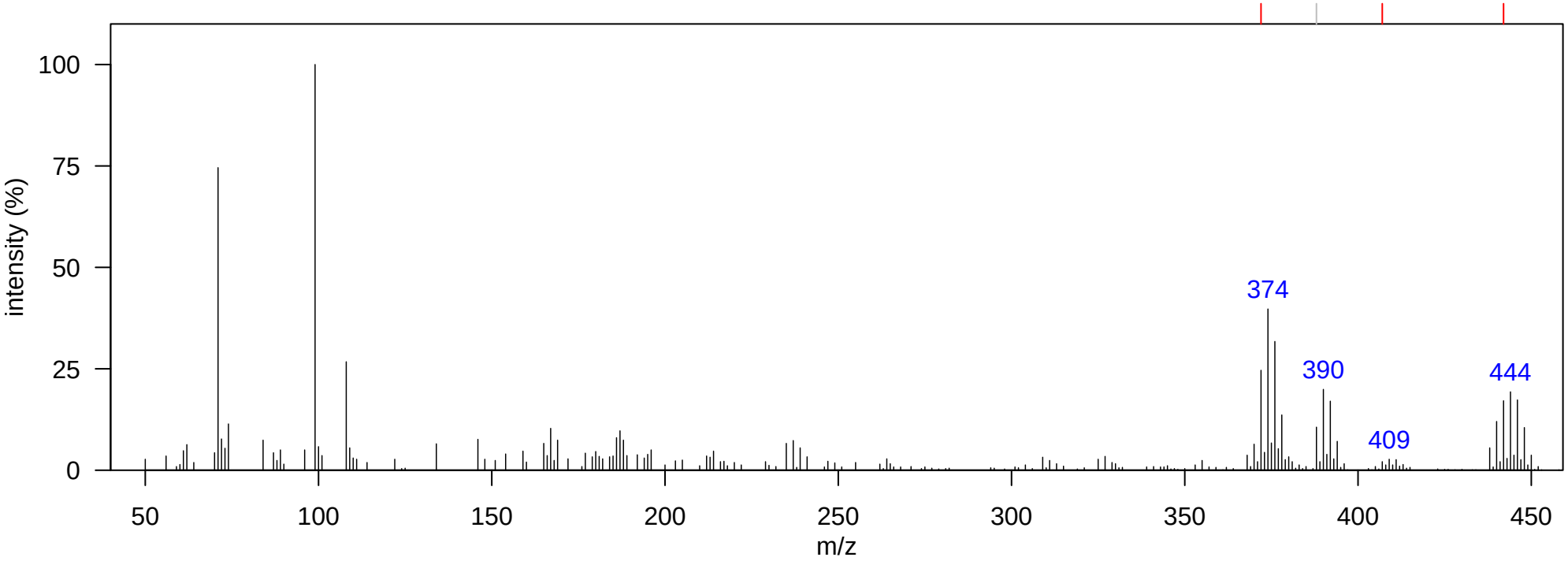
Comment:

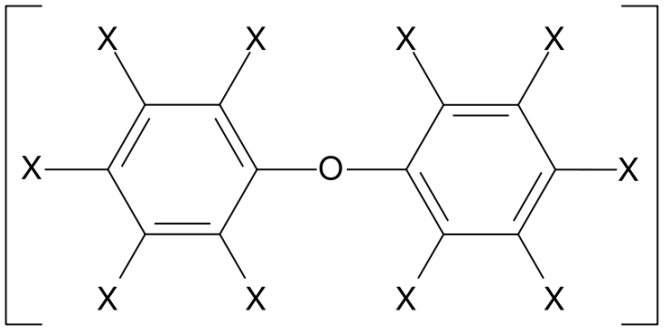
Elemental Formula: C12H2Cl8O

Source: anthropogenic

Class: PCDE

Identification: Manual − Congener Group





m/z	Identity
372	[M−2Cl]+
388	PCB interference
407	[M−Cl]+
442	M+

Filename: 8Cl_PCDE_isomer_2

Name: trichlorostyrene (PCS)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1014, RT (s) (2D): 0.594

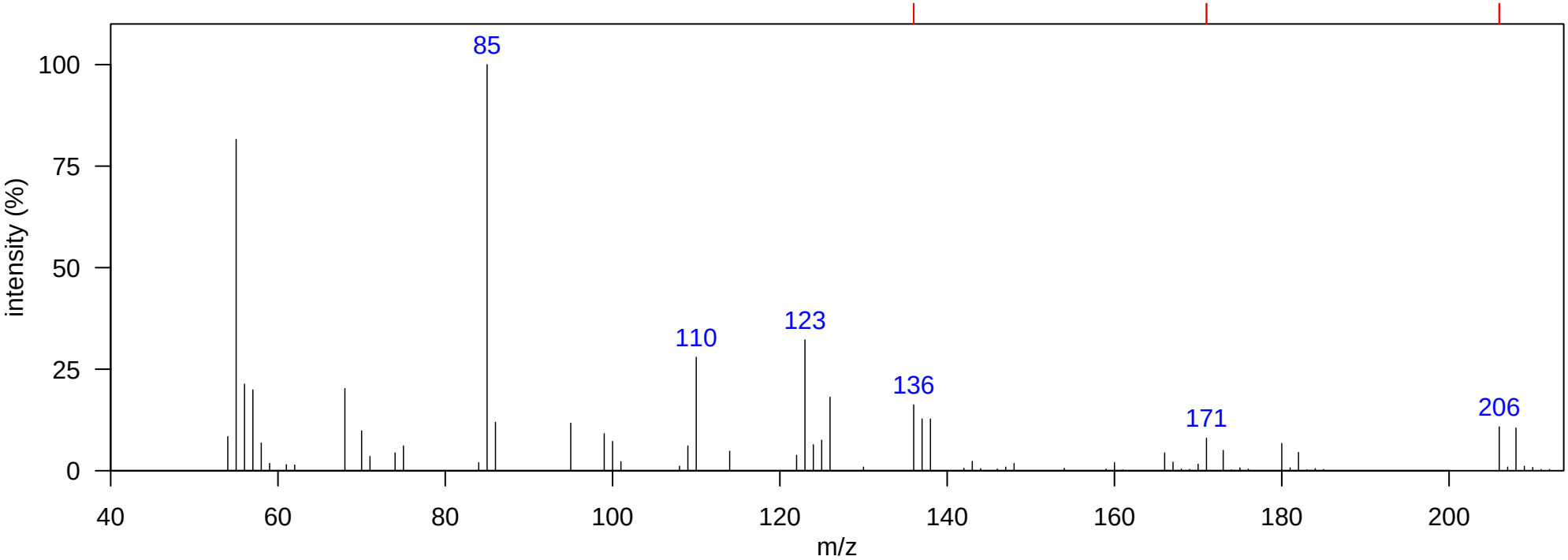
Comment:

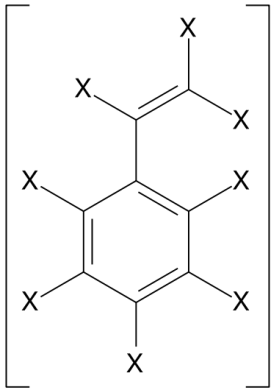
Elemental Formula: C8H5Cl3

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual − Congener Group





X=3Cl, 5H

m/z	Identity
136	[M−2Cl]+
171	[M−Cl]+
206	M+

Filename: 3Cl_PCS

Name: tetrachlorostyrene (PCS) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1087.5, RT (s) (2D): 0.523

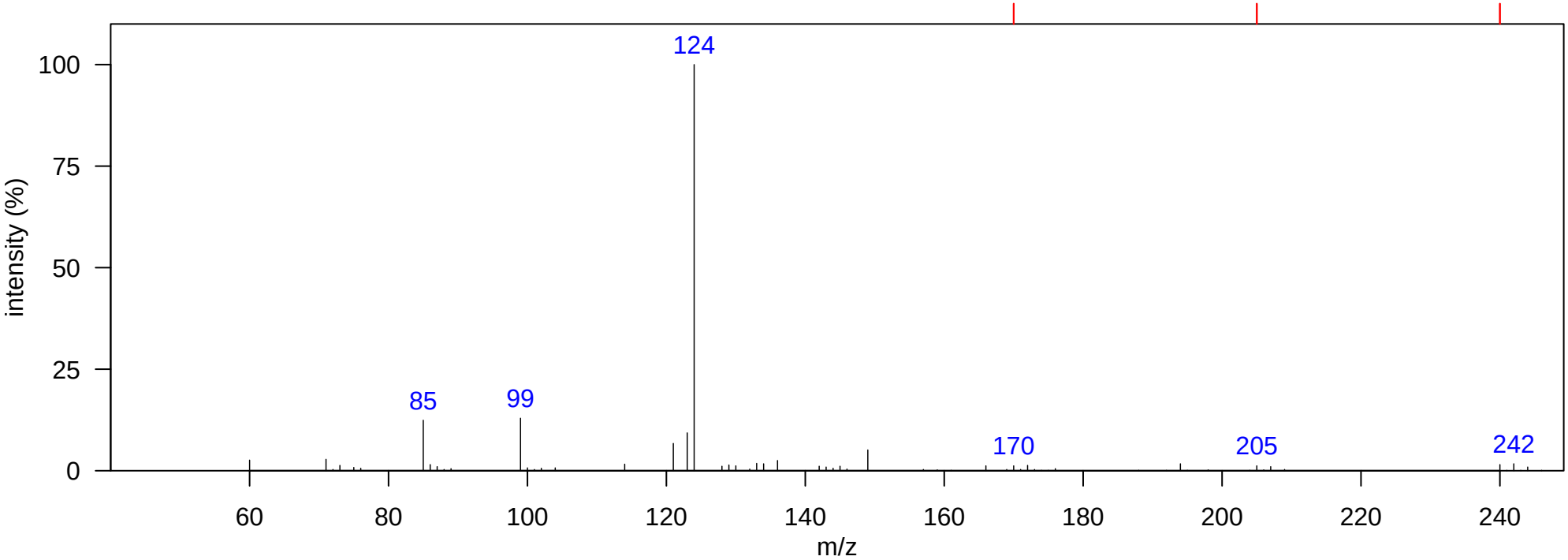
Comment:

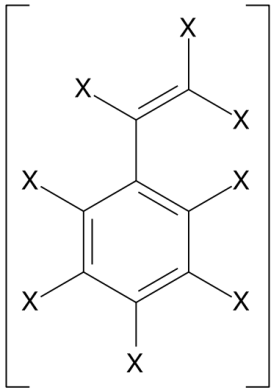
Elemental Formula: C8H4Cl4

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual − Congener Group





X=4Cl, 4H

m/z	Identity
170	[M−2Cl]+
205	[M−Cl]+
240	M+

Filename: 4Cl_PCS_isomer_1

Name: tetrachlorostyrene (PCS) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1105, RT (s) (2D): 0.642

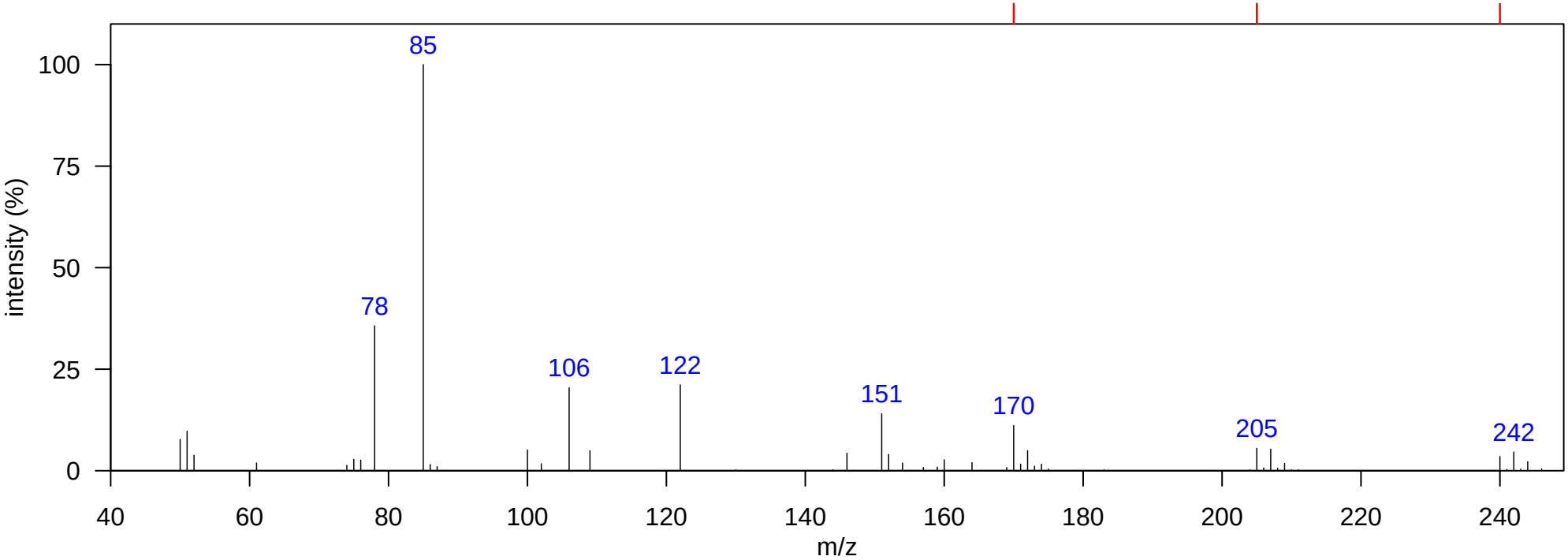
Comment:

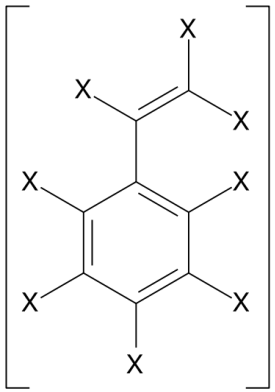
Elemental Formula: C8H4Cl4

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual − Congener Group





X=4Cl, 4H

m/z	Identity
170	[M−2Cl]+
205	[M−Cl]+
240	M+

Filename: 4Cl_PCS_isomer_2

Name: tetrachlorostyrene (PCS) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1150.5, RT (s) (2D): 0.722

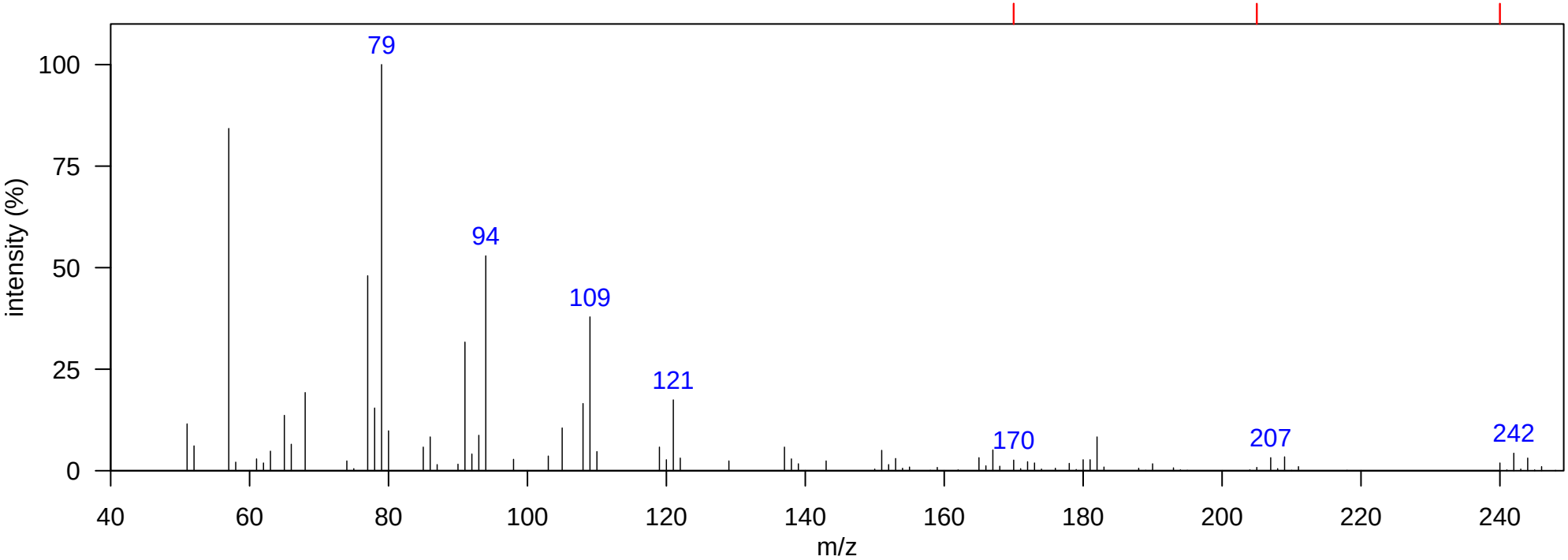
Comment:

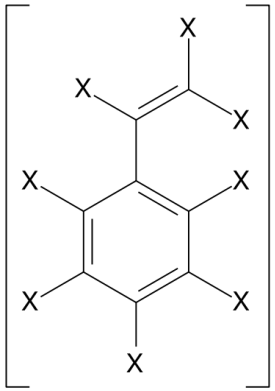
Elemental Formula: C8H4Cl4

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual − Congener Group





X=4Cl, 4H

m/z	Identity
170	[M−2Cl]+
205	[M−Cl]+
240	M+

Filename: 4Cl_PCS_isomer_3

Name: tetrachlorostyrene (PCS) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1157.5, RT (s) (2D): 0.669

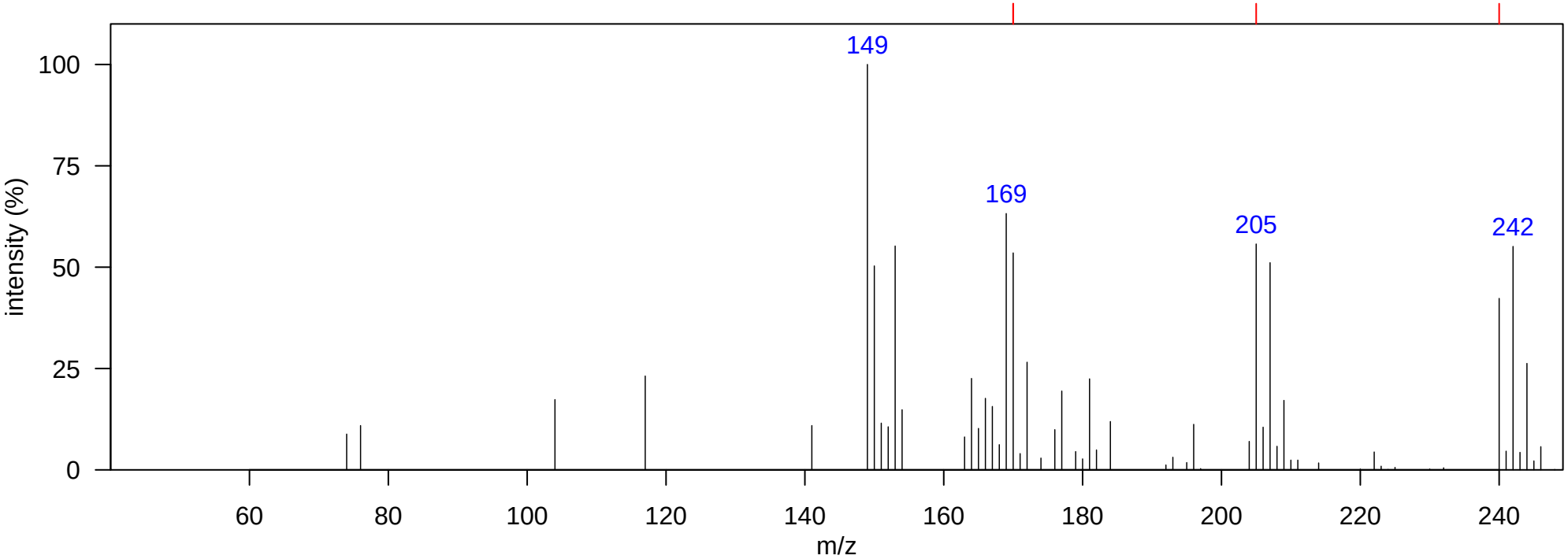
Comment:

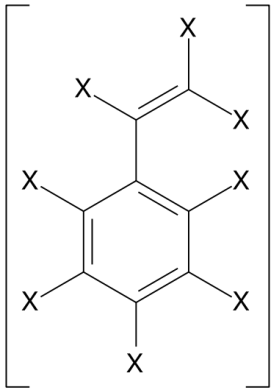
Elemental Formula: C8H4Cl4

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual − Congener Group





X=4Cl, 4H

m/z	Identity
170	[M−2Cl]+
205	[M−Cl]+
240	M+

Filename: 4Cl_PCS_isomer_4

Name: pentachlorostyrene (PCS) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1129.5, RT (s) (2D): 0.617

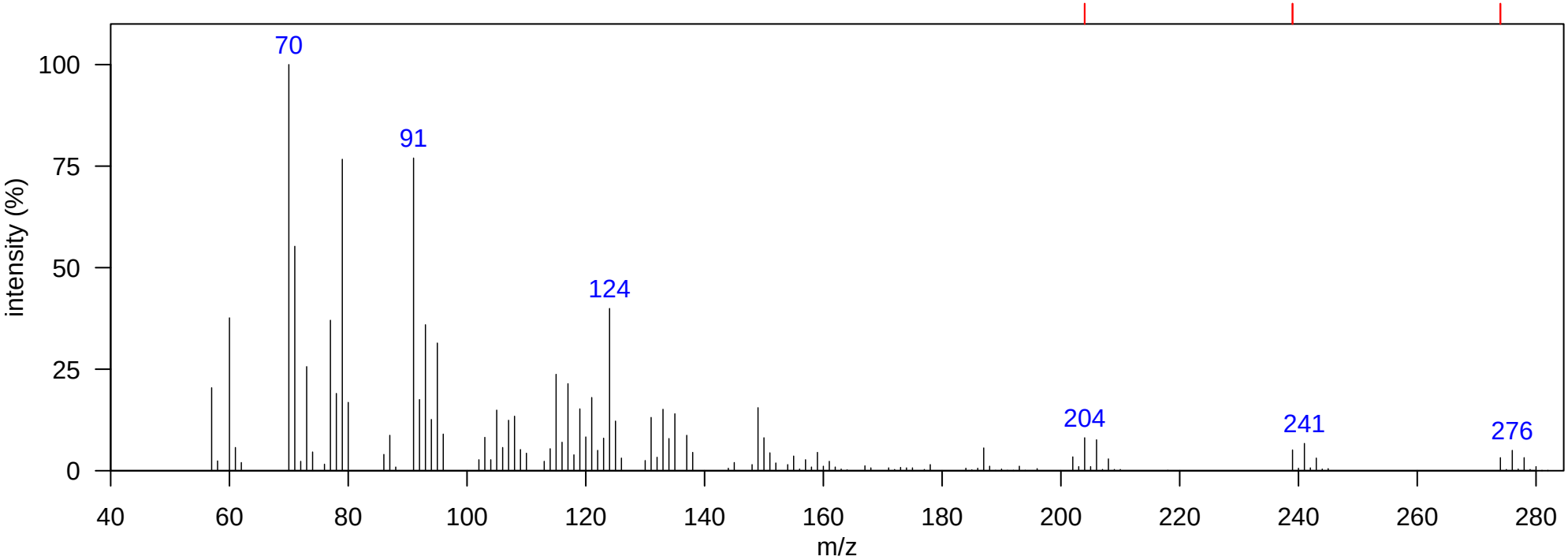
Comment:

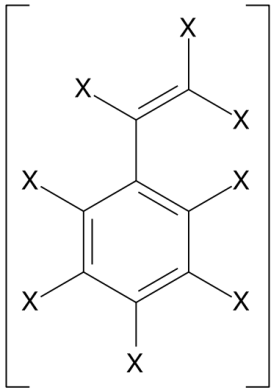
Elemental Formula: C8H3Cl5

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





m/z	Identity
204	[M−2Cl]+
239	[M−Cl]+
274	M+

Filename: 5Cl_PCS_isomer_1

Name: pentachlorostyrene (PCS) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1161, RT (s) (2D): 0.551

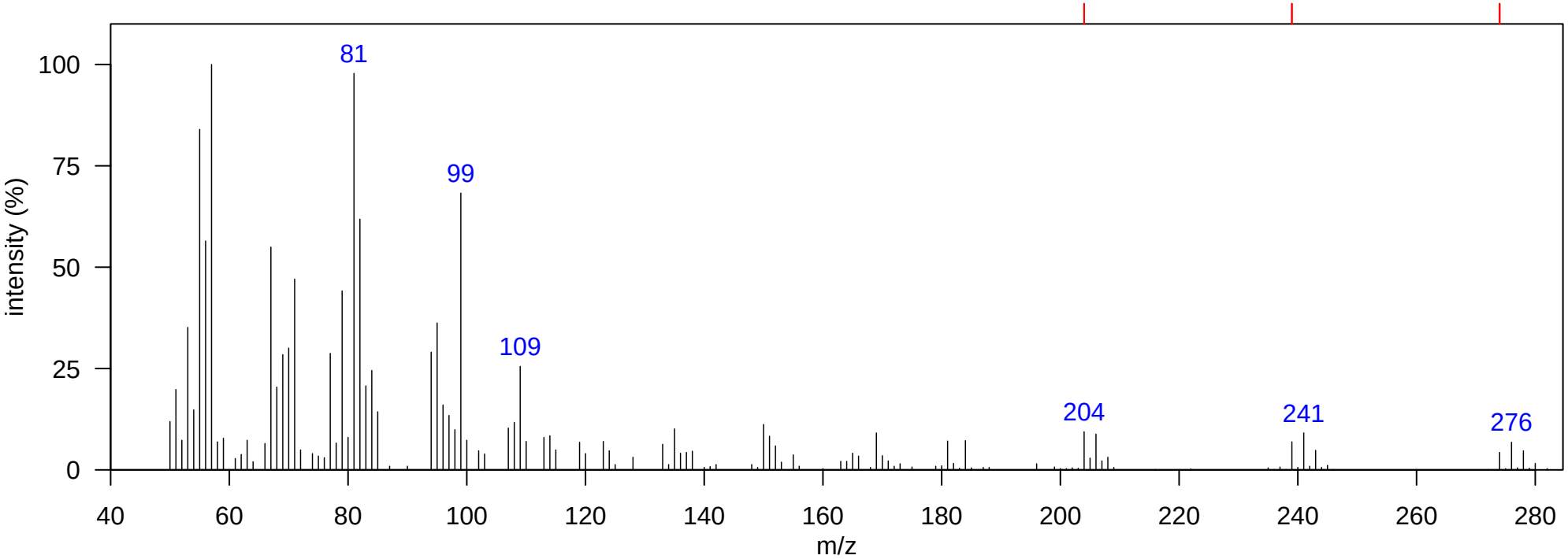
Comment:

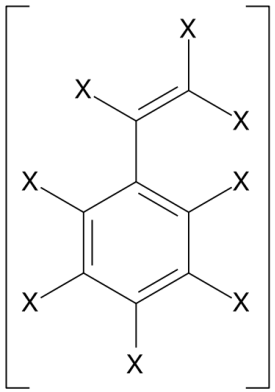
Elemental Formula: C8H3Cl5

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





X=5Cl, 3H

m/z	Identity
204	[M−2Cl]+
239	[M−Cl]+
274	M+

Filename: 5Cl_PCS_isomer_2

Name: pentachlorostyrene (PCS) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1213.5, RT (s) (2D): 0.807

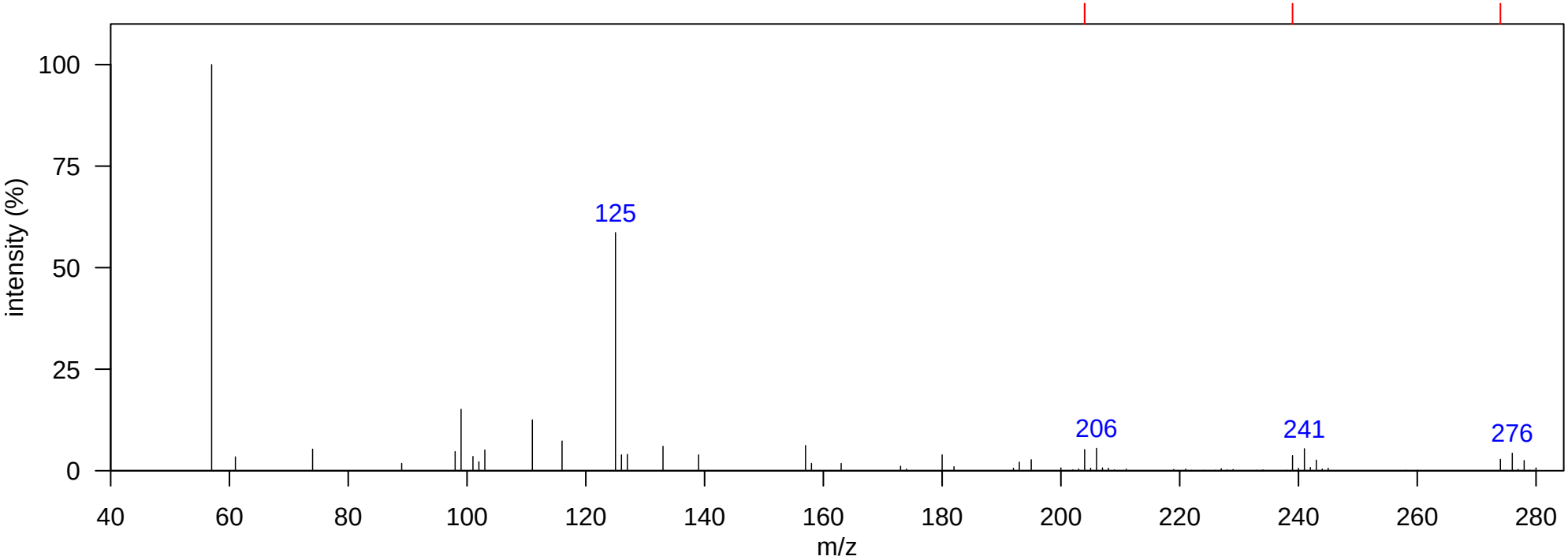
Comment:

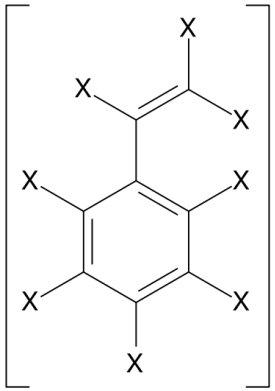
Elemental Formula: C8H3Cl5

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





X=5Cl, 3H

m/z	Identity
204	[M−2Cl]+
239	[M−Cl]+
274	M+

Filename: 5Cl_PCS_isomer_3

Name: pentachlorostyrene (PCS) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1234.5, RT (s) (2D): 0.878

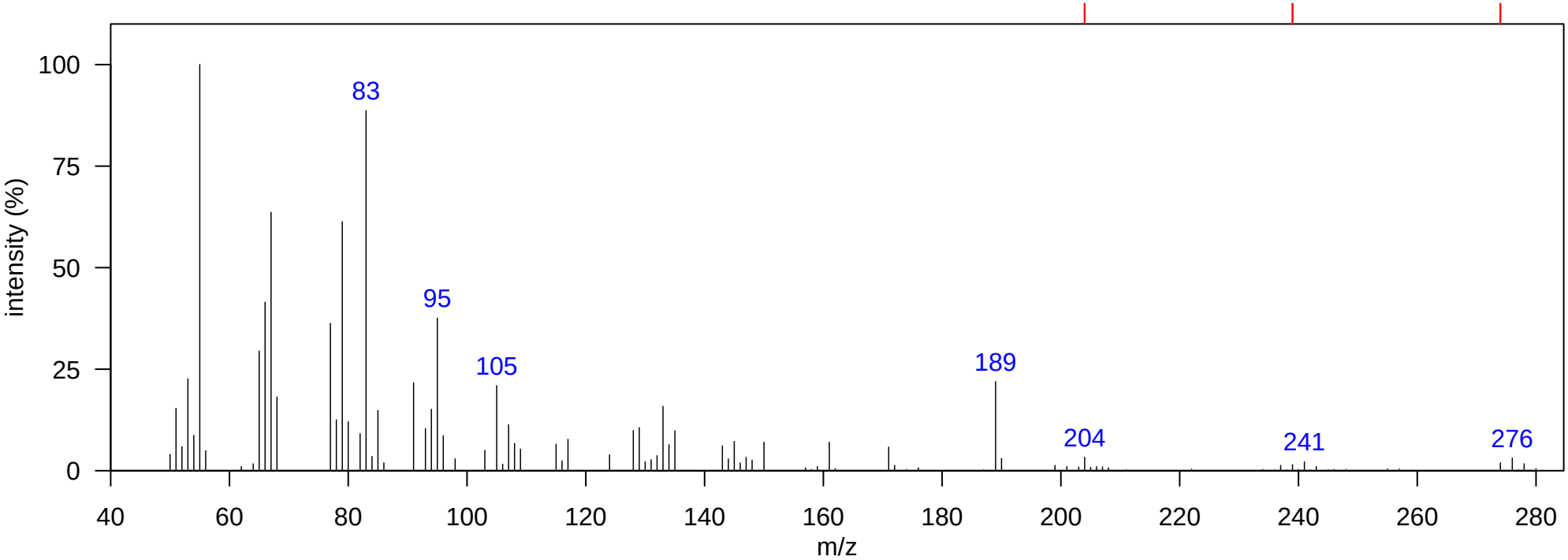
Comment:

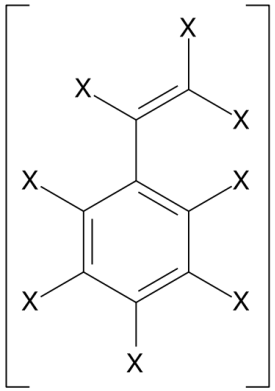
Elemental Formula: C8H3Cl5

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





m/z	Identity
204	[M−2Cl]+
239	[M−Cl]+
274	M+

Filename: 5Cl_PCS_isomer_4

Name: hexachlorostyrene (PCS) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1189, RT (s) (2D): 0.572

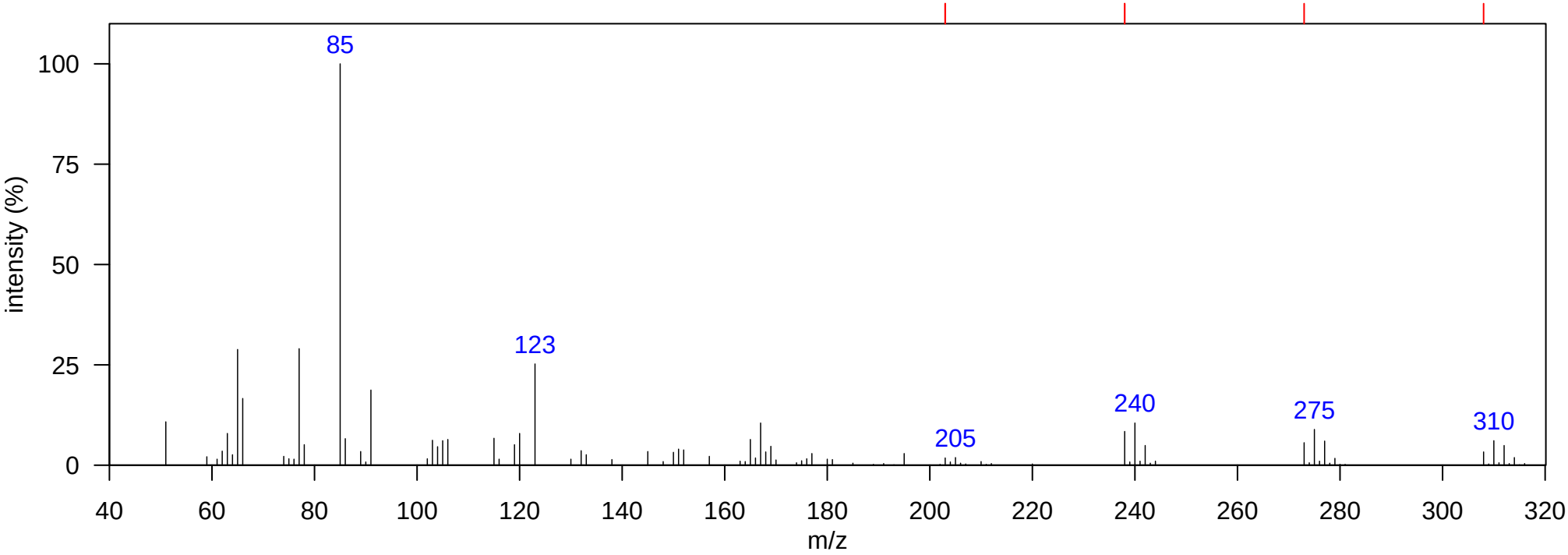
Comment:

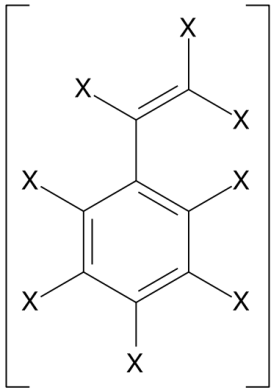
Elemental Formula: C8H2Cl6

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





X=6Cl, 2H

m/z	Identity
203	[M−3Cl]+
238	[M−2Cl]+
273	[M−Cl]+
308	M+

Filename: 6Cl_PCS_isomer_1

Name: hexachlorostyrene (PCS) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1231, RT (s) (2D): 0.605

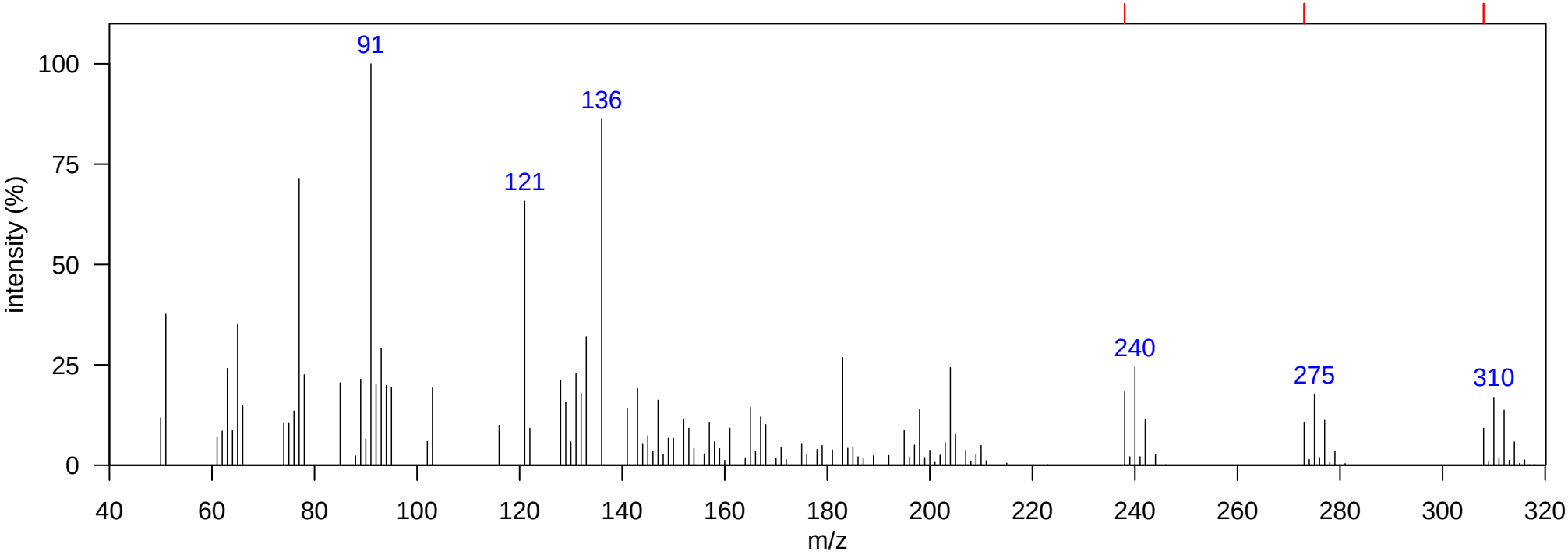
Comment:

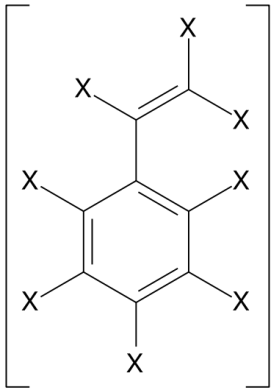
Elemental Formula: C8H2Cl6

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





X=6Cl, 2H

m/z	Identity
238	[M−2Cl]+
273	[M−Cl]+
308	M+

Filename: 6Cl_PCS_isomer_2

Name: hexachlorostyrene (PCS) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1266, RT (s) (2D): 0.925

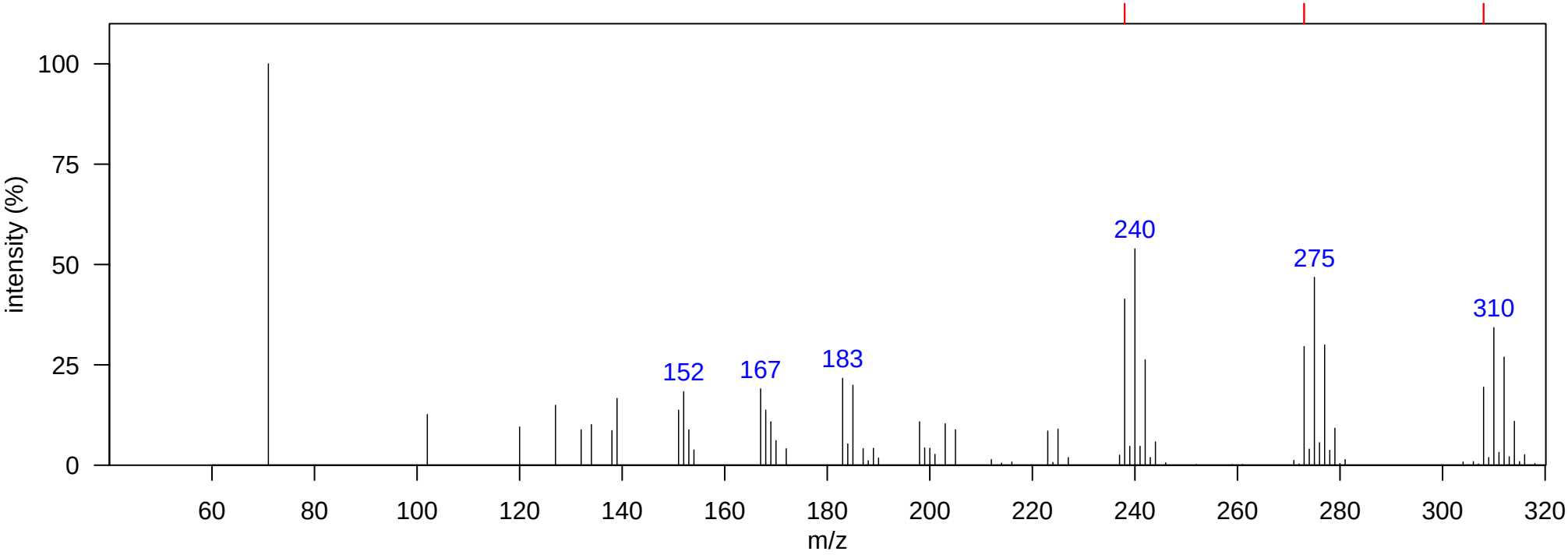
Comment:

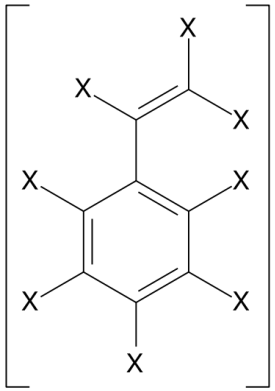
Elemental Formula: C8H2Cl6

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





X=6Cl, 2H

m/z	Identity
238	[M−2Cl]+
273	[M−Cl]+
308	M+

Filename: 6Cl_PCS_isomer_3

Name: heptachlorostyrene (PCS) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1304.5, RT (s) (2D): 0.783

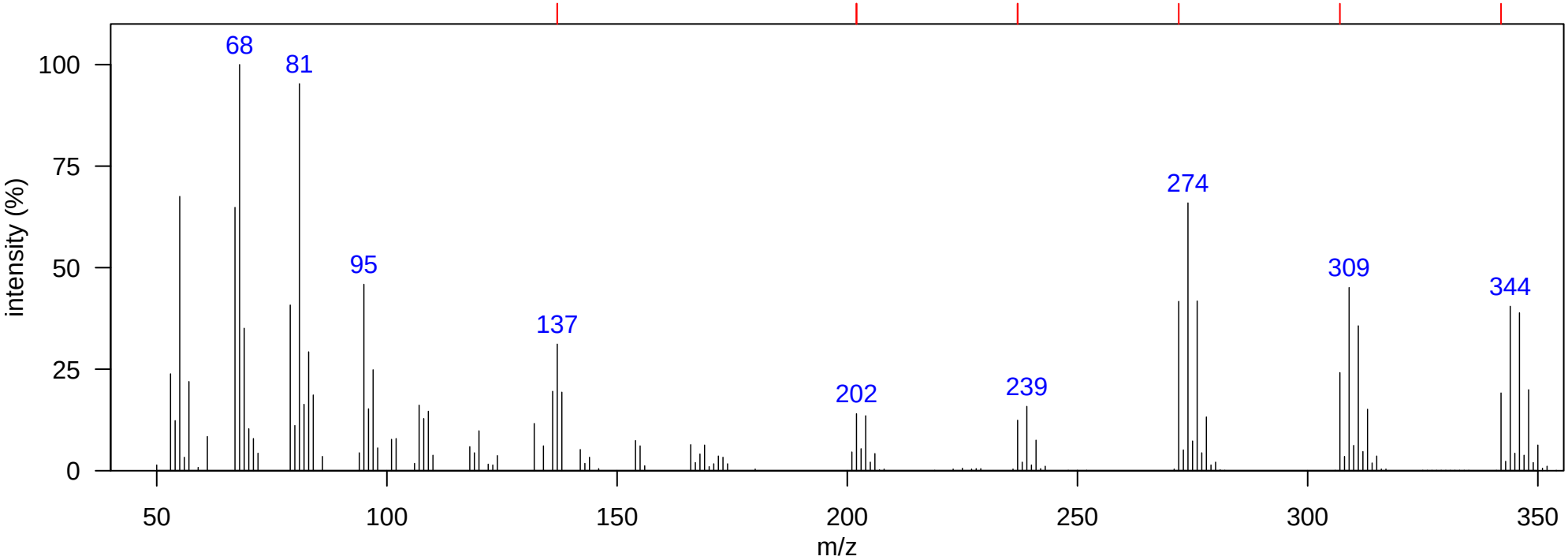
Comment:

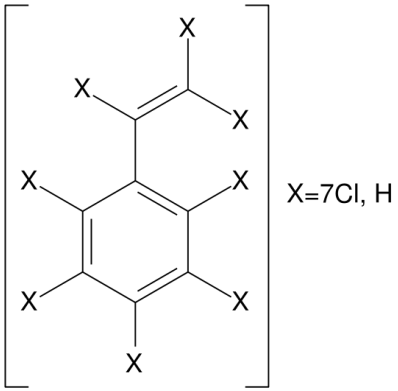
Elemental Formula: C8HCl7

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





m/z	Identity
137	[M−2Cl]2+
202	[M−4Cl]+
237	[M−3Cl]+
272	[M−2Cl]+
307	[M−Cl]+
342	M+

Filename: 7Cl_PCS_isomer_1

Name: heptachlorostyrene (PCS) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1311.5, RT (s) (2D): 0.79

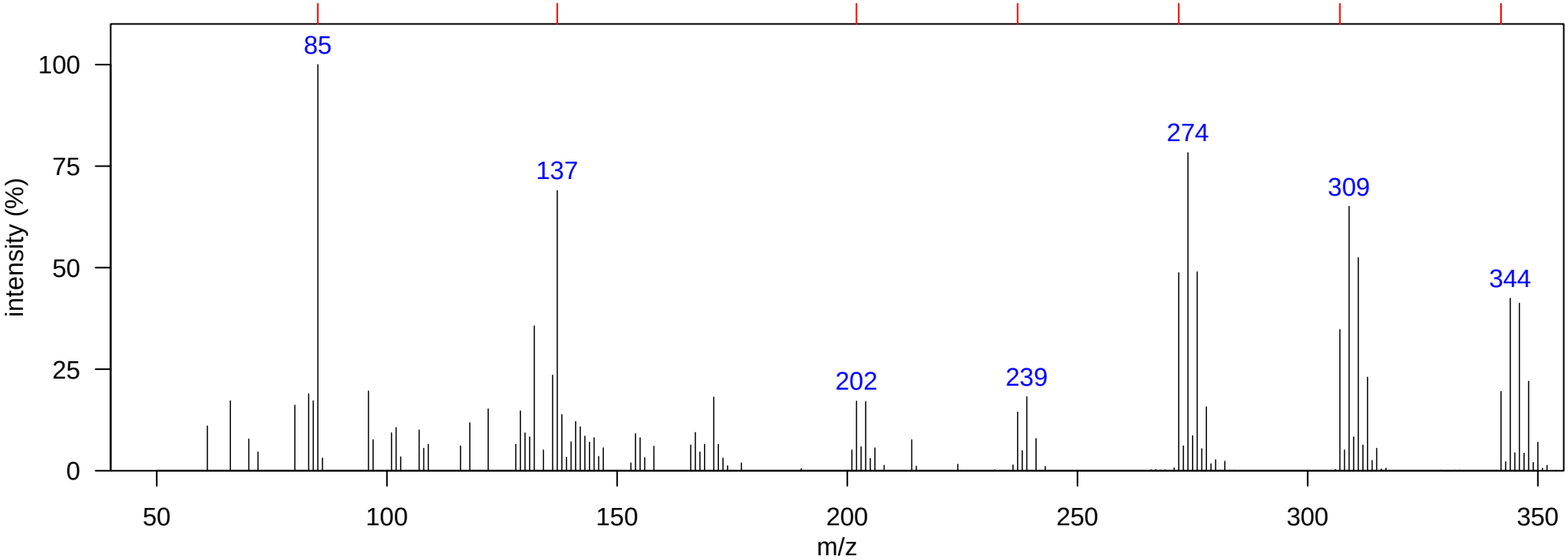
Comment:

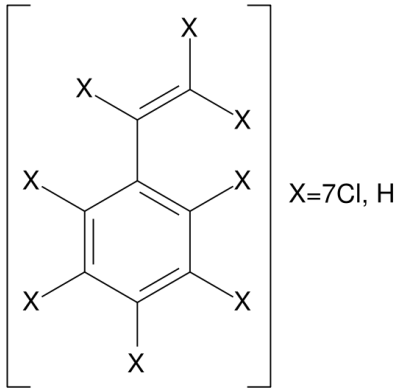
Elemental Formula: C8HCl7

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





m/z	Identity
85	[C7H]+
137	[M−2Cl]2+
202	[M−4Cl]+
237	[M−3Cl]+
272	[M−2Cl]+
307	[M−Cl]+
342	M+

Filename: 7Cl_PCS_isomer_2

Name: heptachlorostyrene (PCS) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1346.5, RT (s) (2D): 0.83

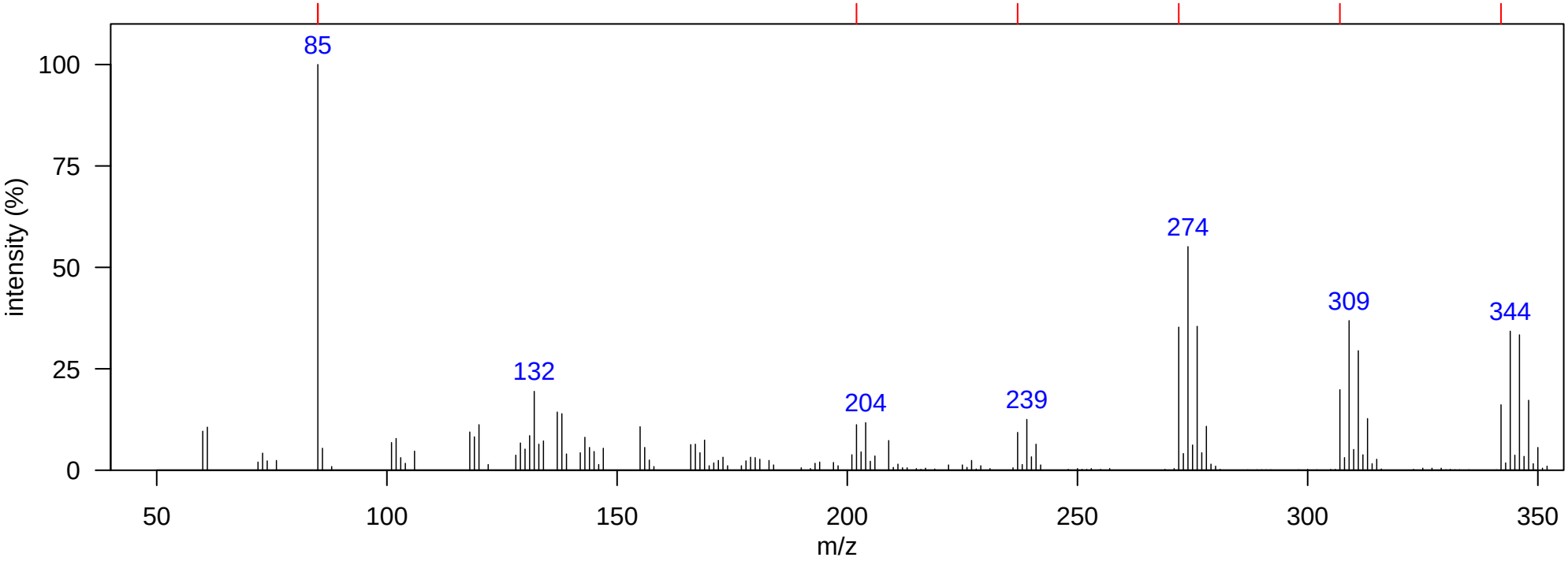
Comment:

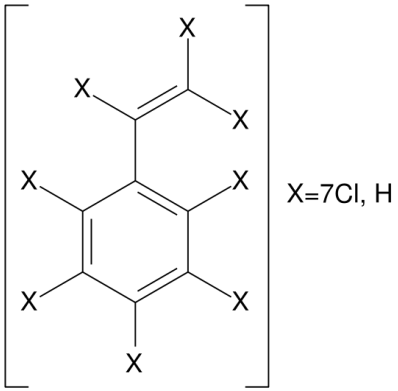
Elemental Formula: C8HCl7

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS





m/z	Identity
85	[C7H]+
202	[M−4Cl]+
237	[M−3Cl]+
272	[M−2Cl]+
307	[M−Cl]+
342	M+

Filename: 7Cl_PCS_isomer_3

Name: octachlorostyrene (PCS)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1420, RT (s) (2D): 0.92

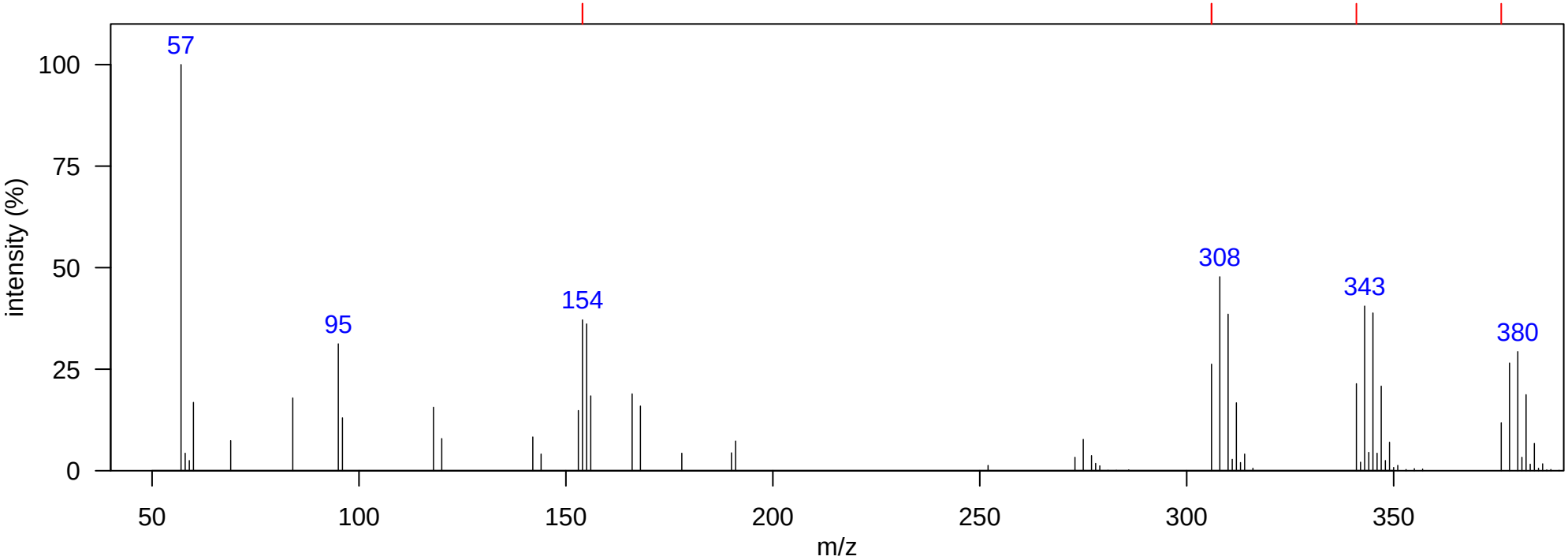
Comment:

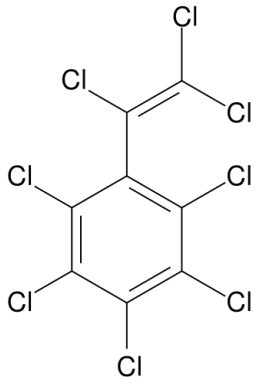
Elemental Formula: C8Cl8

Source: anthropogenic

Class: chlorinated styrene

Identification: Authentic MS RT





m/z	Identity
154	[M−2Cl]2+
306	[M−2Cl]+
341	[M−Cl]+
376	M+

Filename: 8Cl_PCS

Name: methoxy diphenyl ether Br3Cl (MeO−B/CDE)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1689.5, RT (s) (2D): 2.445

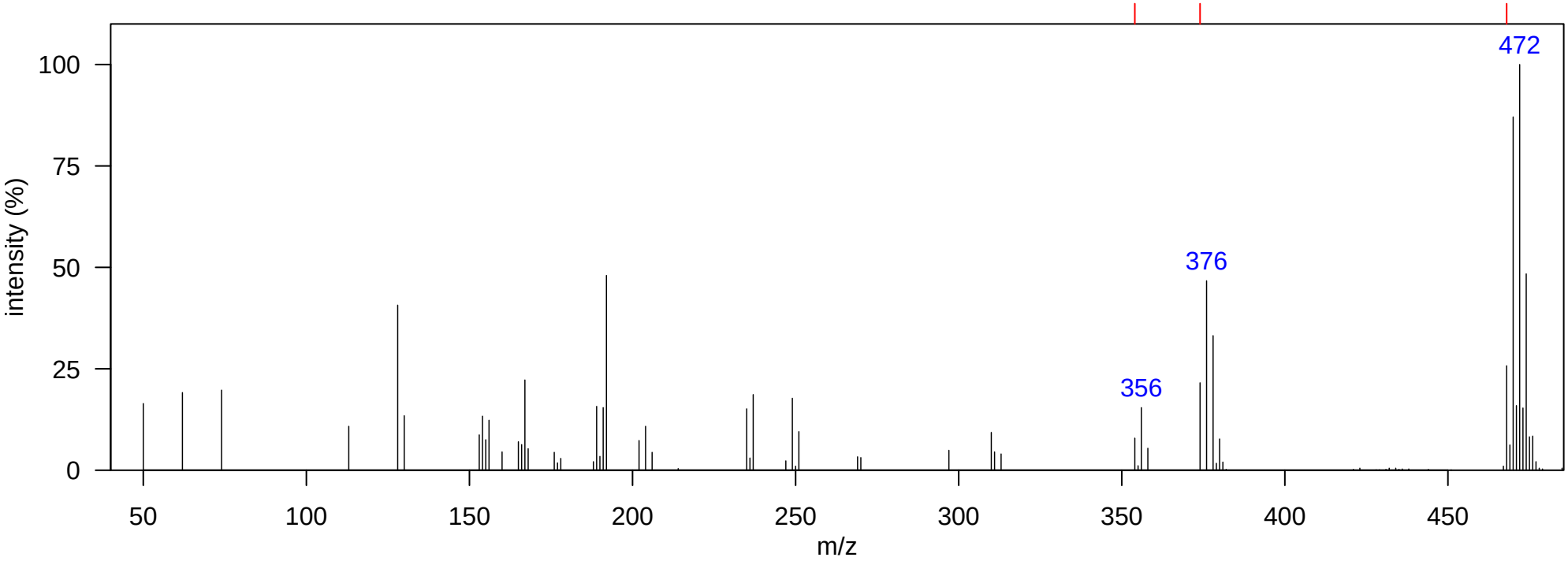
Comment:

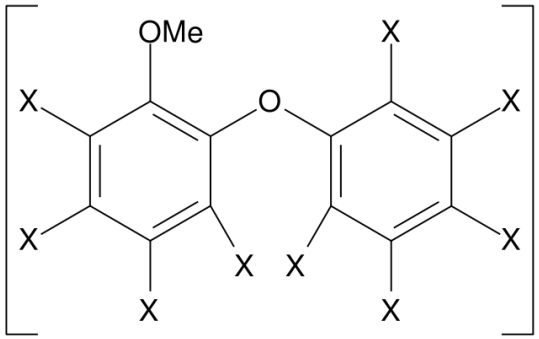
Elemental Formula: C13H8Br3ClO2

Source: natural

Class: MeO−B/CDE

Identification: Manual − Congener Group





m/z	Identity
354	[M−Br−Cl]+
374	[M−Br−CH3]+
468	M+

Filename: methoxy_DE_Br3Cl

Name: methoxy diphenyl ether Br4Cl (MeO−B/CDE)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1787.5, RT (s) (2D): 2.723

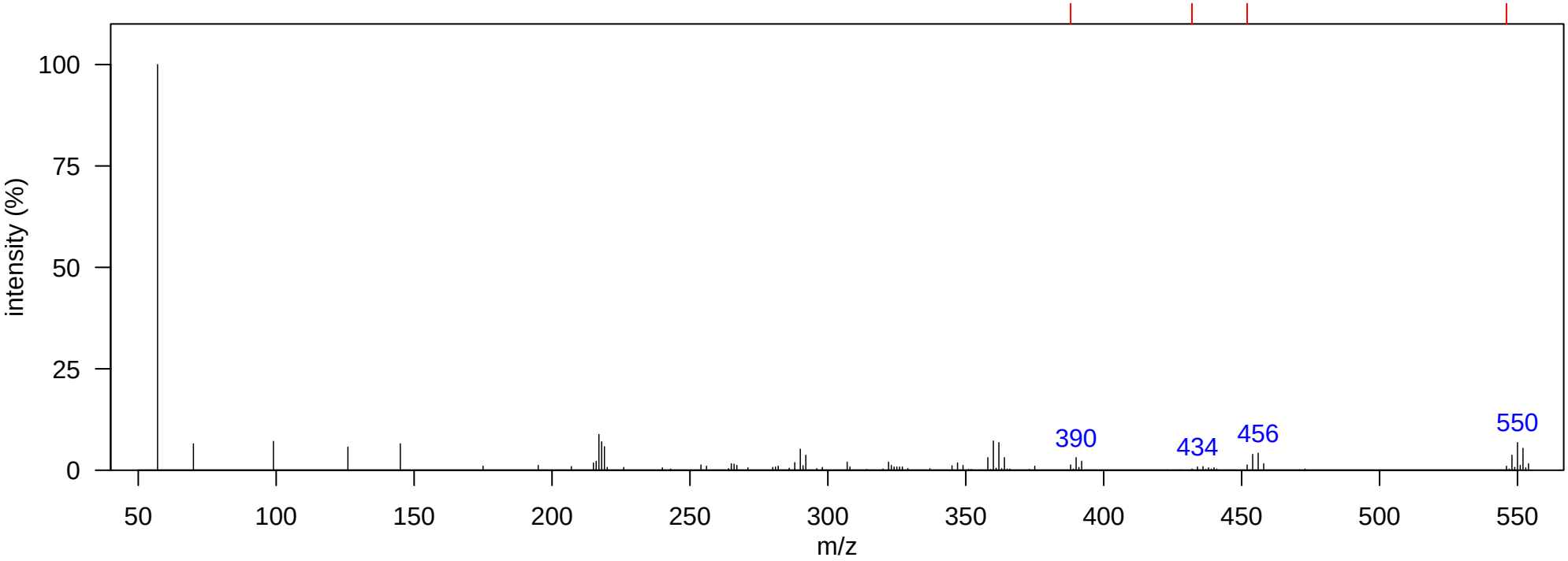
Comment: Ref: J.Mass.Spectrum, 2006, 41, 790−801.

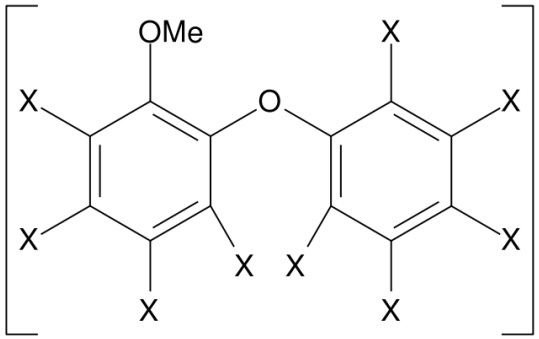
Elemental Formula: C13H7Br4ClO2

Source: natural

Class: MeO−B/CDE

Identification: Literature MS





X=4Br, Cl, 4H

m/z	Identity
388	[M−2Br]+
432	[M−Br−Cl]+
452	[M−Br−CH3]+
546	M+

Filename: methoxy_DE_Br4Cl

Name: methoxy brominated diphenyl ether 3Br (MeO−BDE)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1598.5, RT (s) (2D): 2.519

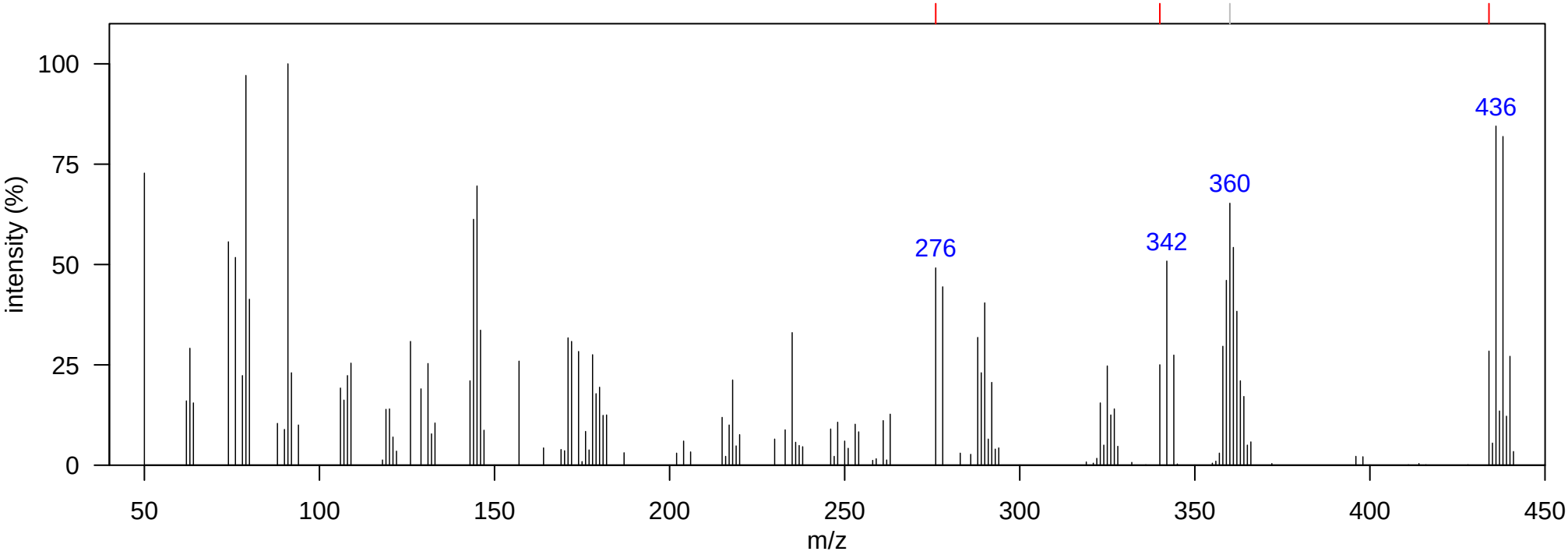
Comment:

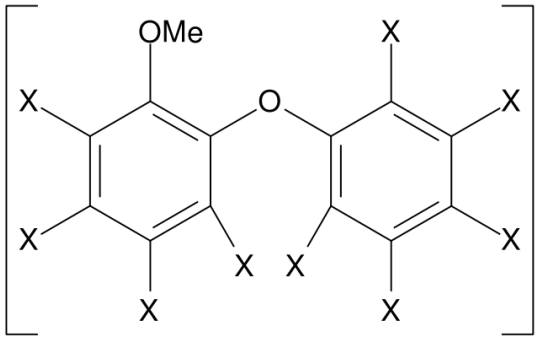
Elemental Formula: C13H9Br3O2

Source: natural

Class: MeO−B/CDE

Identification: Manual − Congener Group





X=3Br, 6H

m/z	Identity
276	[M−2Br]+
340	[M−Br−CH3]+
360	interference
434	M+

Filename: 3Br_MeOBDE

Name: methoxy brominated diphenyl ether 4Br (MeO−BDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1700, RT (s) (2D): 2.583

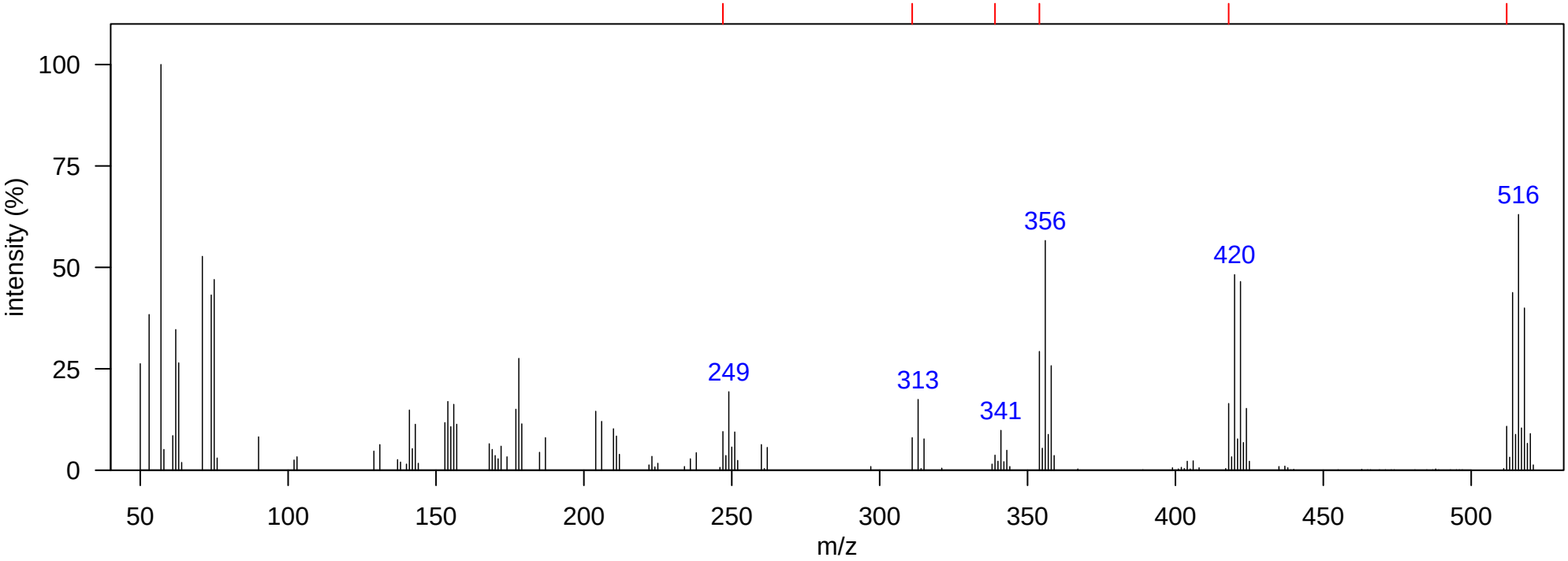
Comment:

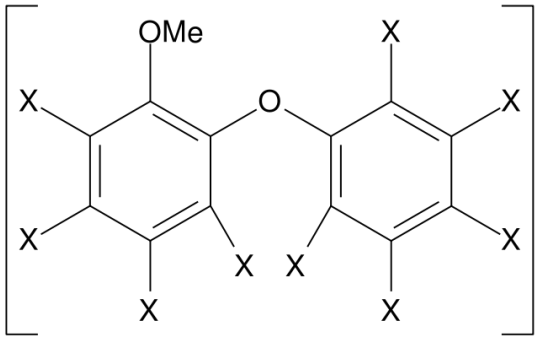
Elemental Formula: C13H8Br4O2

Source: natural

Class: MeO−B/CDE

Identification: Manual − Congener Group





X=4Br, 5H

m/z	Identity
247	[C6Br2HO]+
311	[M−2Br−CH3−CO]+
339	[M−2Br−CH3]+
354	[M−2Br]+
418	[M−Br−CH3]+
512	M+

Filename: 4Br_MeOBDE_isomer_1

Name: methoxy brominated diphenyl ether 4Br (2'−MeO−BDE68) isomer 2

Elemental Formula: C13H8Br4O2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: natural

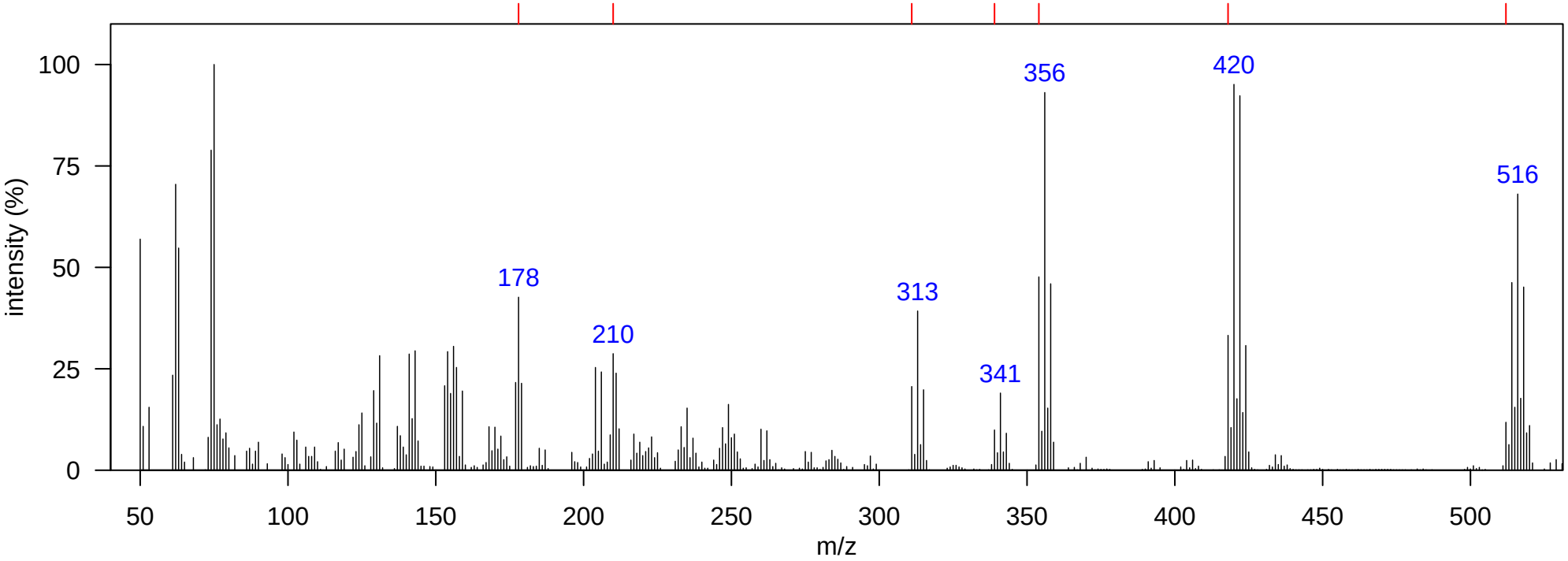
Instrument: GCxGC−TOF, electron impact

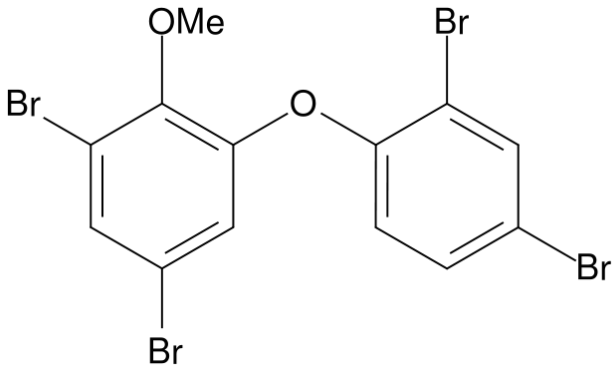
Class: MeO−B/CDE

RT (s) (1D): 1717.5, RT (s) (2D): 2.356

Identification: Authentic MS RT

Comment:





m/z	Identity
178	[M−2Br]2+
210	[M−Br−CH3]2+
311	[M−2Br−CH3−CO]+
339	[M−2Br−CH3]+
354	[M−2Br]+
418	[M−CH3Br]+
512	M+

Filename: 4Br_MeOBDE68_isomer_2

Name: methoxy brominated diphenyl ether 4Br (6'−MeO−BDE47) isomer 3

Elemental Formula: C13H8Br4O2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: natural

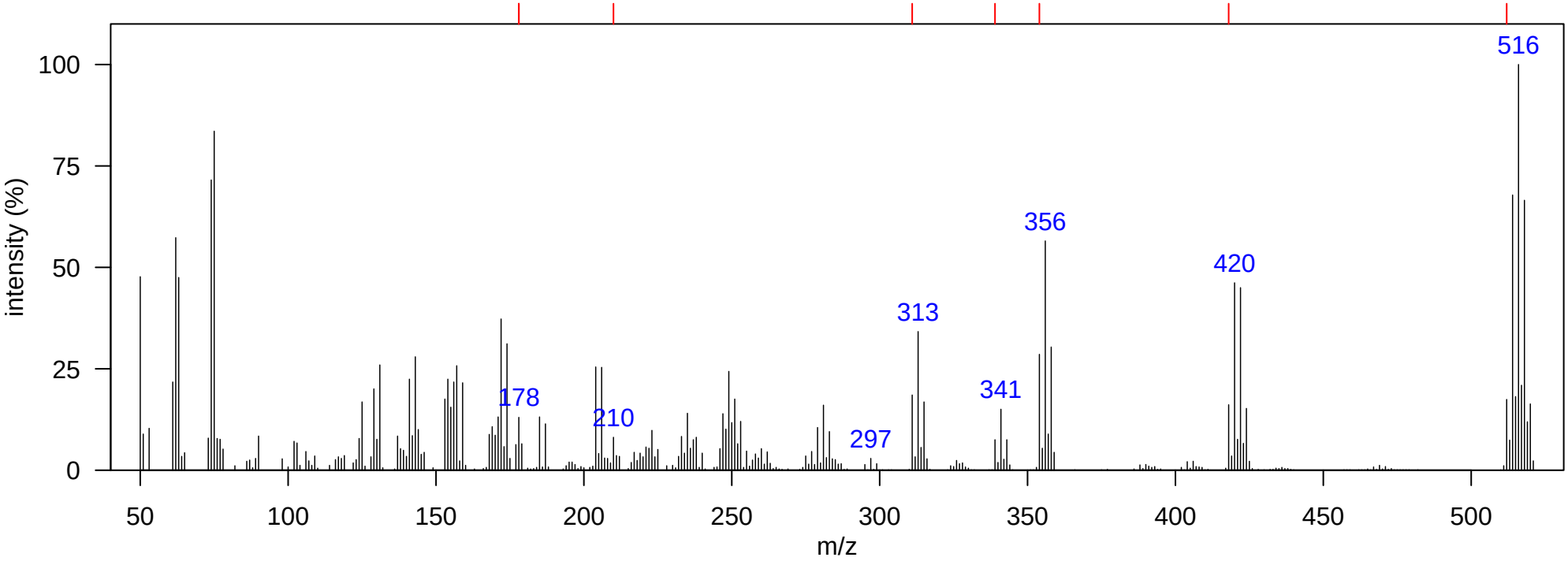
Instrument: GCxGC−TOF, electron impact

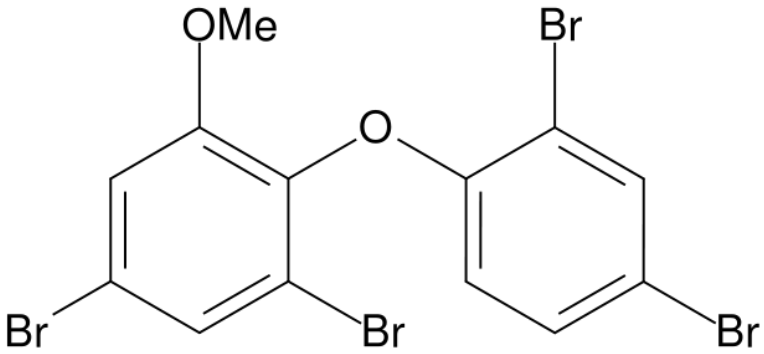
Class: MeO−B/CDE

RT (s) (1D): 1735, RT (s) (2D): 2.813

Identification: Authentic MS RT

Comment:





m/z	Identity
178	[M−2Br]2+
210	[M−Br−CH3]2+
311	[M−2Br−CH3−CO]+
339	[M−2Br−CH3]+
354	[M−2Br]+
418	[M−Br−CH3]+
512	M+

Filename: 4Br_MeOBDE47_isomer_3

Name: methoxy brominated diphenyl ether 5Br (MeO−BDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1798, RT (s) (2D): 2.824

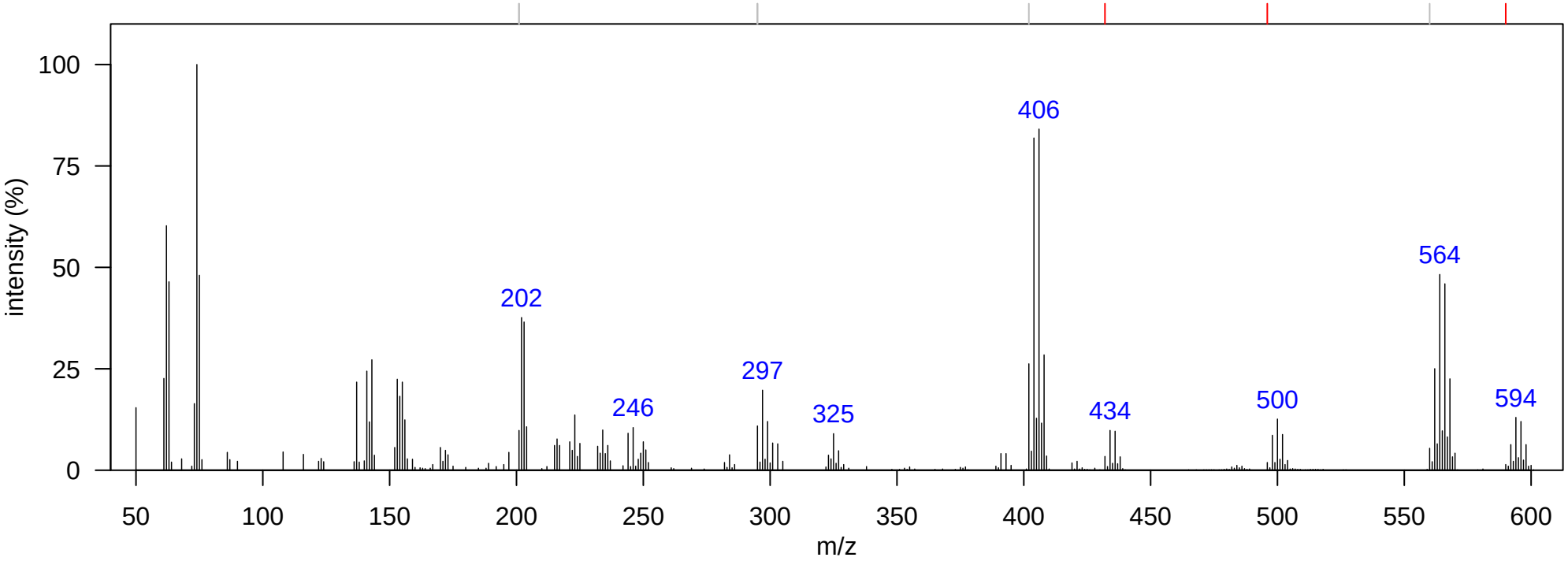
Comment:

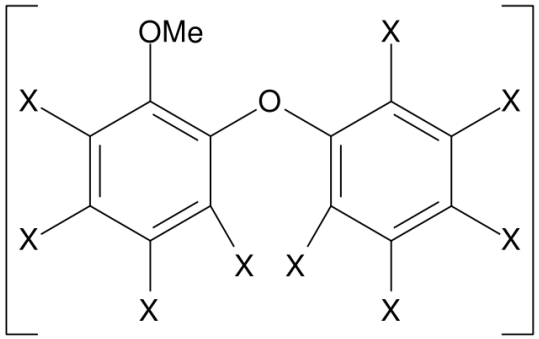
Elemental Formula: C13H7Br5O2

Source: natural

Class: MeO−B/CDE

Identification: Manual − Congener Group





X=5Br, 4H

m/z	Identity
201	interference BDE−99
295	interference BDE−99
402	interference BDE−99
432	[M−2Br]+
496	[M−Br−CH3]+
560	interference BDE−99
590	M+

Filename: 5Br_MeOBDE_isomer_1

Name: methoxy brominated diphenyl ether 5Br (MeO−BDE) isomer 2

Elemental Formula: C13H7Br5O2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: natural

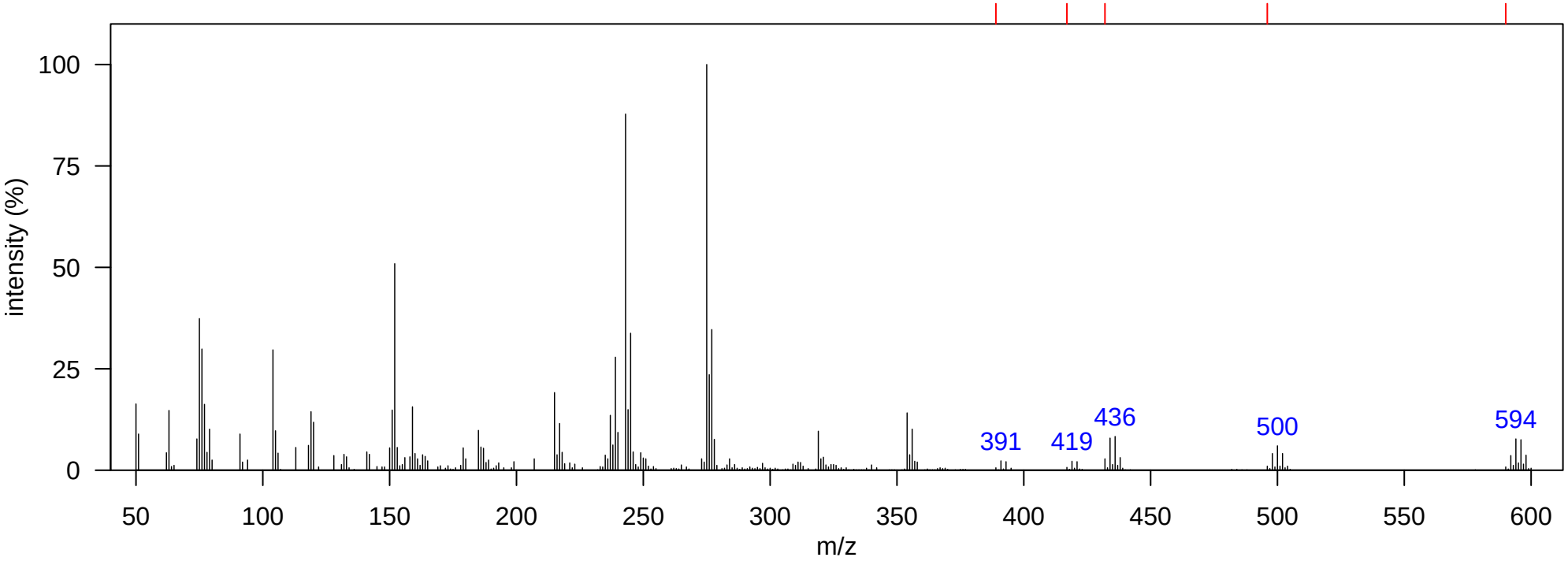
Instrument: GCxGC−TOF, electron impact

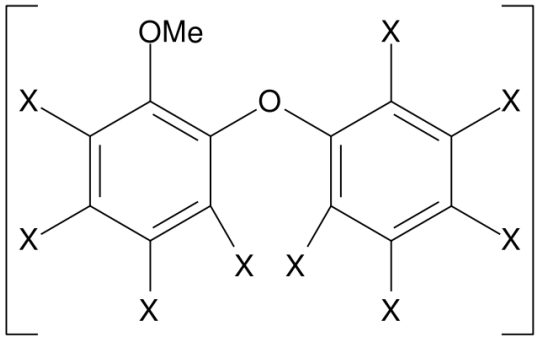
Class: MeO−B/CDE

RT (s) (1D): 1836.5, RT (s) (2D): 2.991

Identification: Manual − Congener Group

Comment:





X=5Br, 4H

m/z	Identity
389	[M−2Br−CH3−CO]+
417	[M−2Br−CH3]+
432	[M−2Br]+
496	[M−Br−CH3]+
590	M+

Name: methoxy brominated diphenyl ether 5Br (MeO−BDE) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1840, RT (s) (2D): 3.115

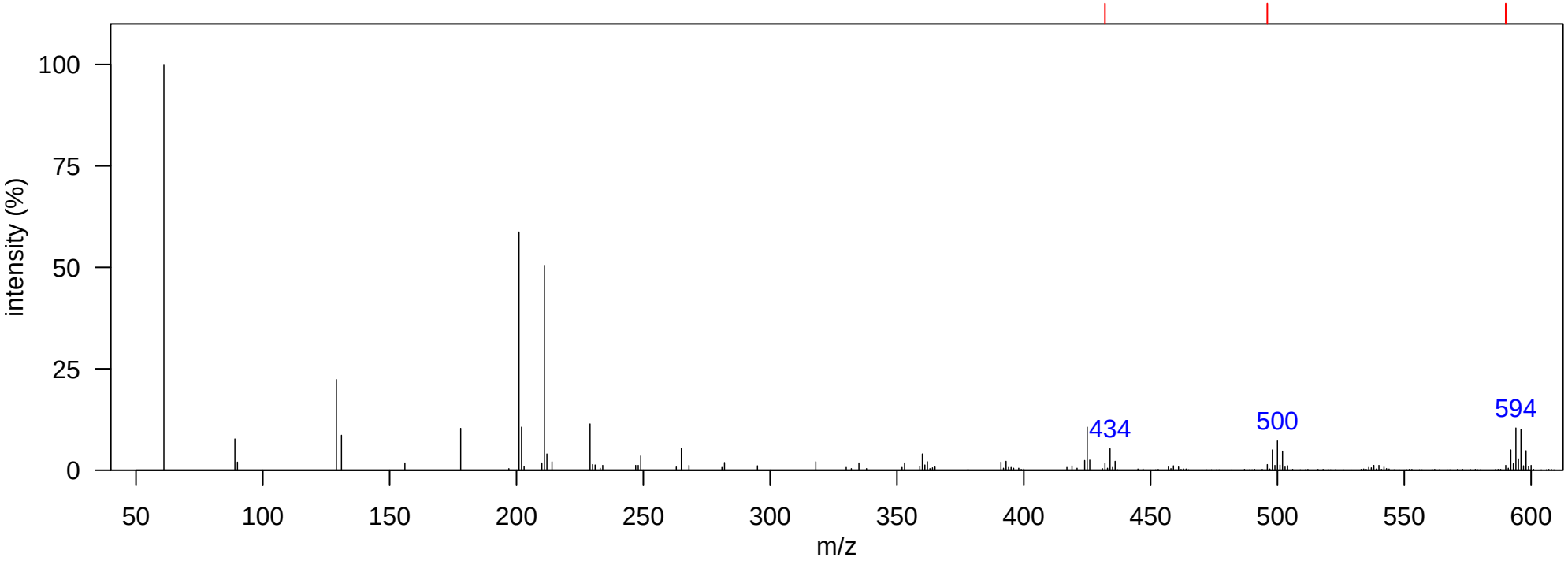
Comment:

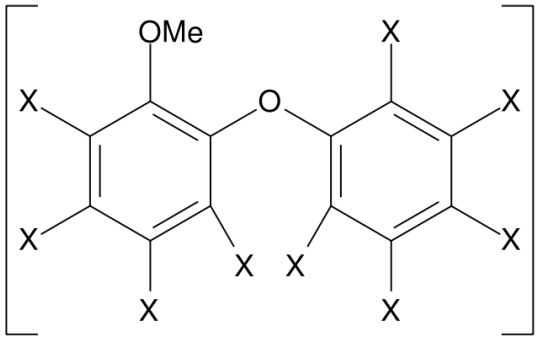
Elemental Formula: C13H7Br5O2

Source: natural

Class: MeO−B/CDE

Identification: Manual − Congener Group





X=5Br, 4H

m/z	Identity
432	[M−2Br]+
496	[M−Br−CH3]+
590	M+

Filename: 5Br_MeOBDE_isomer_3

Name: methoxy chlorinated diphenyl ether 7Cl (MeO−CDE)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1714, RT (s) (2D): 1.788

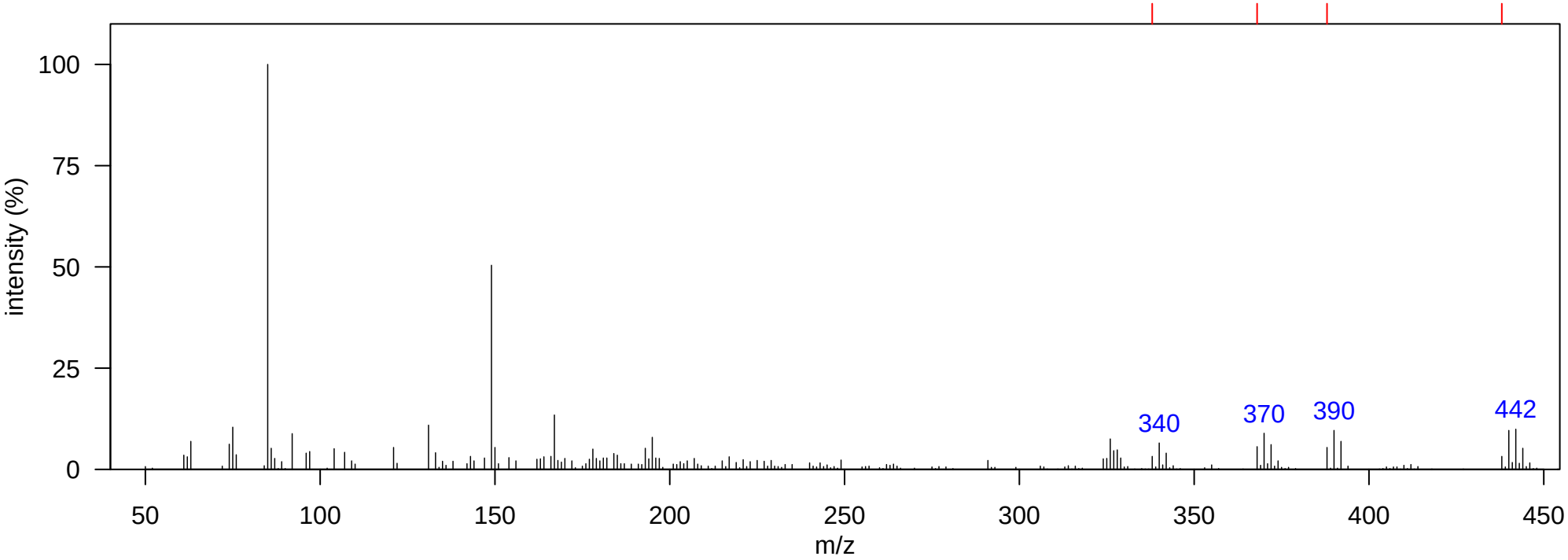
Comment:

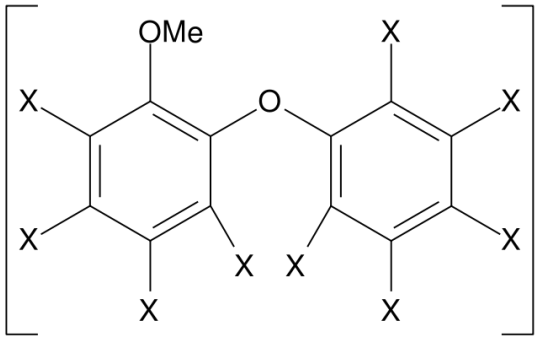
Elemental Formula: C13H5Cl7O2

Source: anthropogenic

Class: MeO−CDE

Identification: Manual − Congener Group





m/z	Identity
338	[M−2Cl−OCH2]+
368	[M−2Cl]+
388	[M−Cl−CH3]+
438	M+
486	BDE interference

Filename: 7Cl_MeOCDE

Name: methoxy chlorinated diphenyl ether 8Cl (MeO−CDE) isomer 1

Elemental Formula: C13H4Cl8O2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: anthropogenic

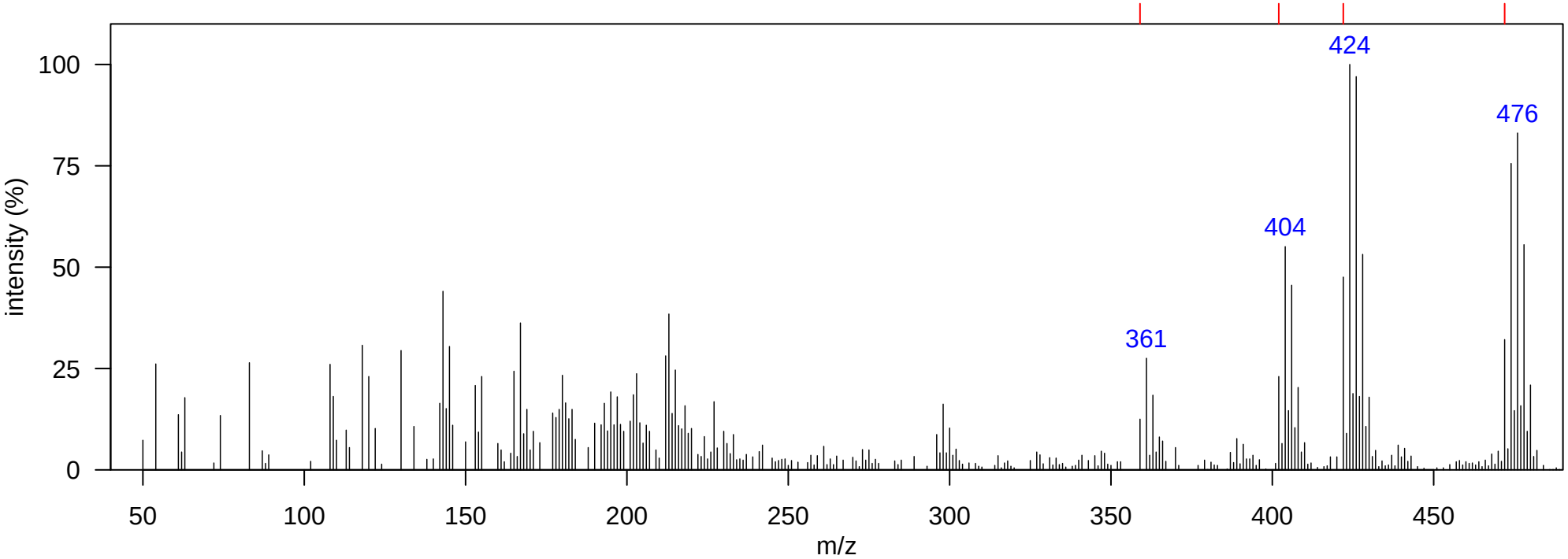
Instrument: GCxGC−TOF, electron impact

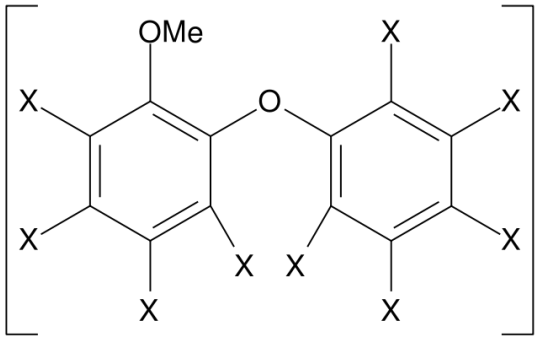
Class: MeO−CDE

RT (s) (1D): 1805, RT (s) (2D): 2.103

Identification: Manual − Congener Group

Comment:





m/z	Identity
359	[M−2Cl−CH3−CO]+
402	[M−2Cl]+
422	[M−Cl−CH3]+
472	M+
501	interference
536	interference
568	interference

Filename: 8Cl_MeOCDE_isomer_1

Name: methoxy chlorinated diphenyl ether 8Cl (MeO−CDE) isomer 2

Elemental Formula: C13H4Cl8O2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: anthropogenic

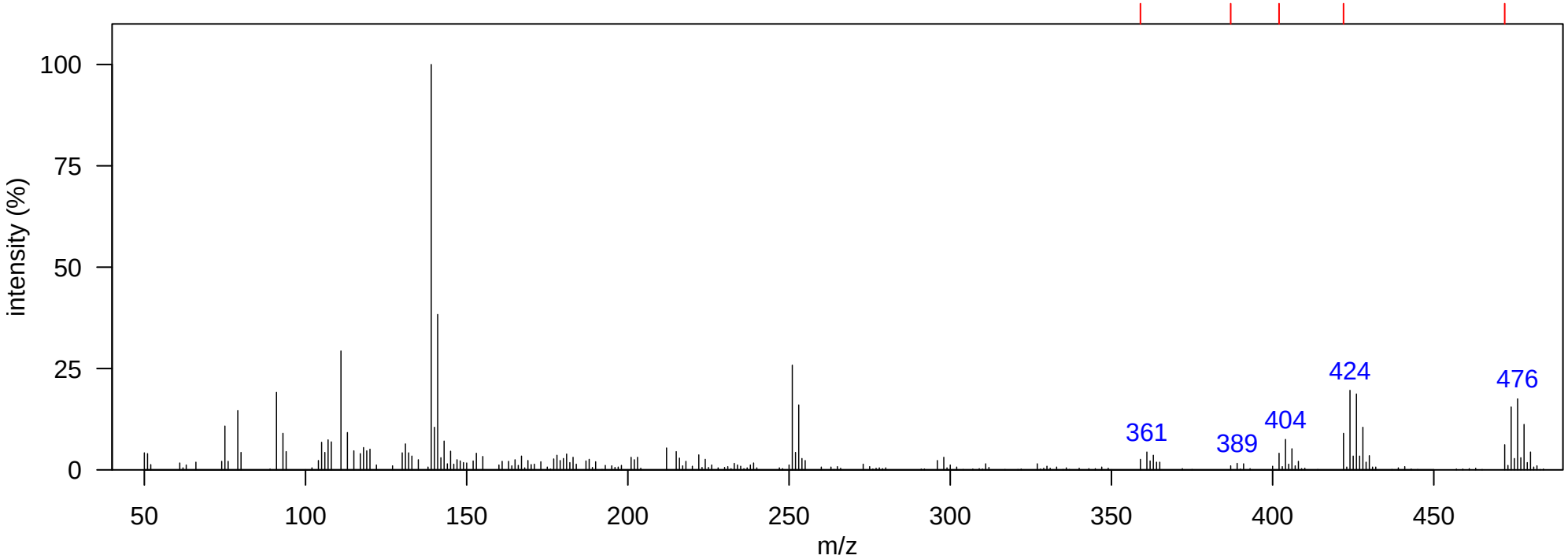
Instrument: GCxGC−TOF, electron impact

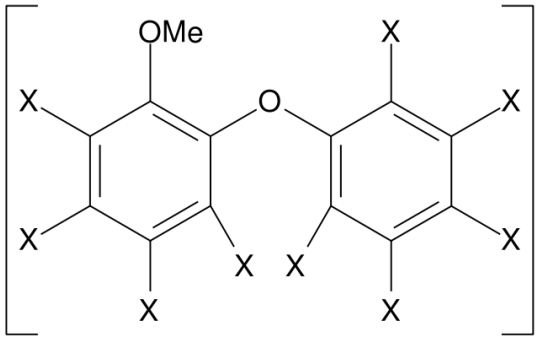
Class: MeO−CDE

RT (s) (1D): 1815.5, RT (s) (2D): 2.197

Identification: Manual − Congener Group

Comment:





m/z	Identity
359	[M−2Cl−CH3−CO]+
387	[M−2Cl−CH3]+
402	[M−2Cl]+
422	[M−Cl−CH3]+
472	M+

Filename: 8Cl_MeOCDE_isomer_2

Name: methyl bipyrrole 6Cl (MBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1367.5, RT (s) (2D): 0.861

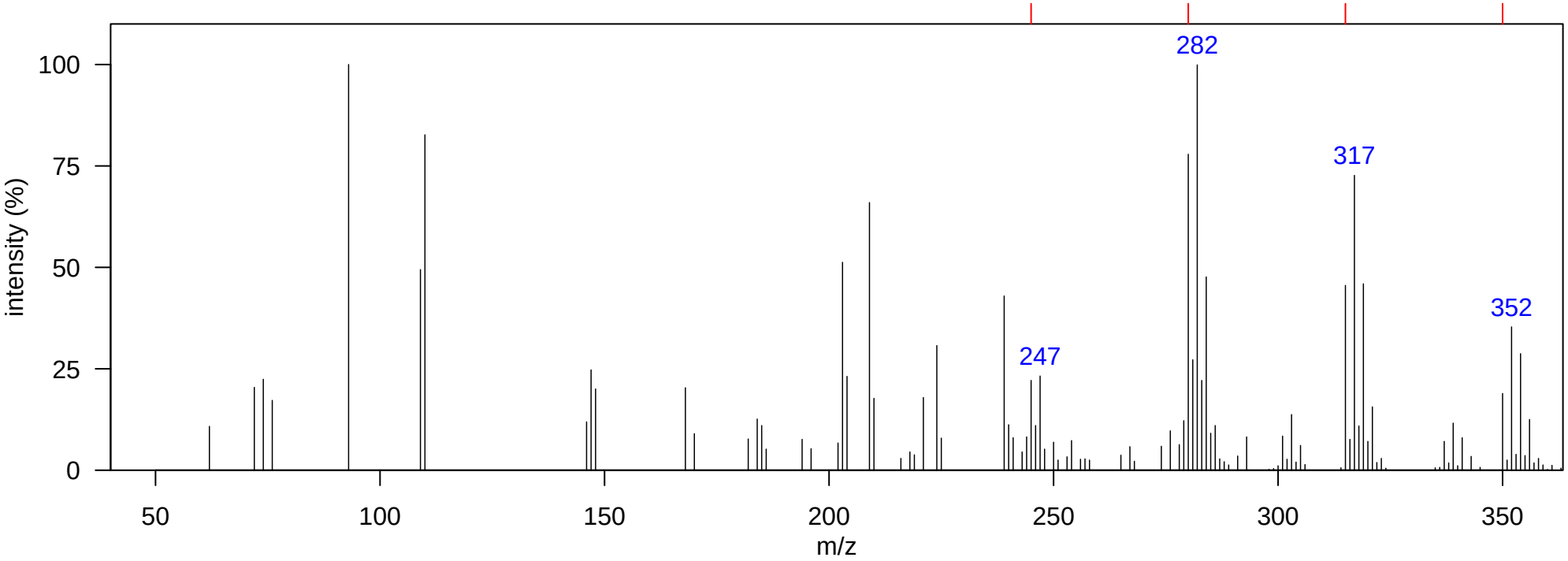
Comment: Ref: Chemosphere, 2008, 70, 1721−1729.

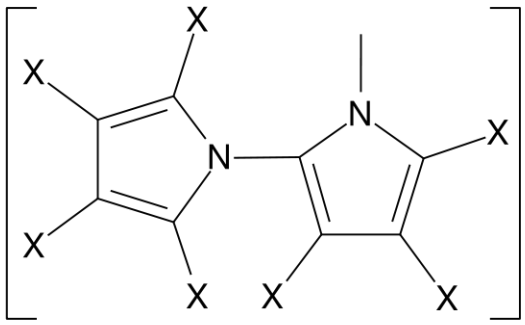
Elemental Formula: C9H4Cl6N2

Source: natural

Class: MBP

Identification: Literature MS





X=6Cl, H

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

Filename: 6Cl_MBP_isomer_1

Name: methyl bipyrrole 6Cl (MBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1381.5, RT (s) (2D): 0.969

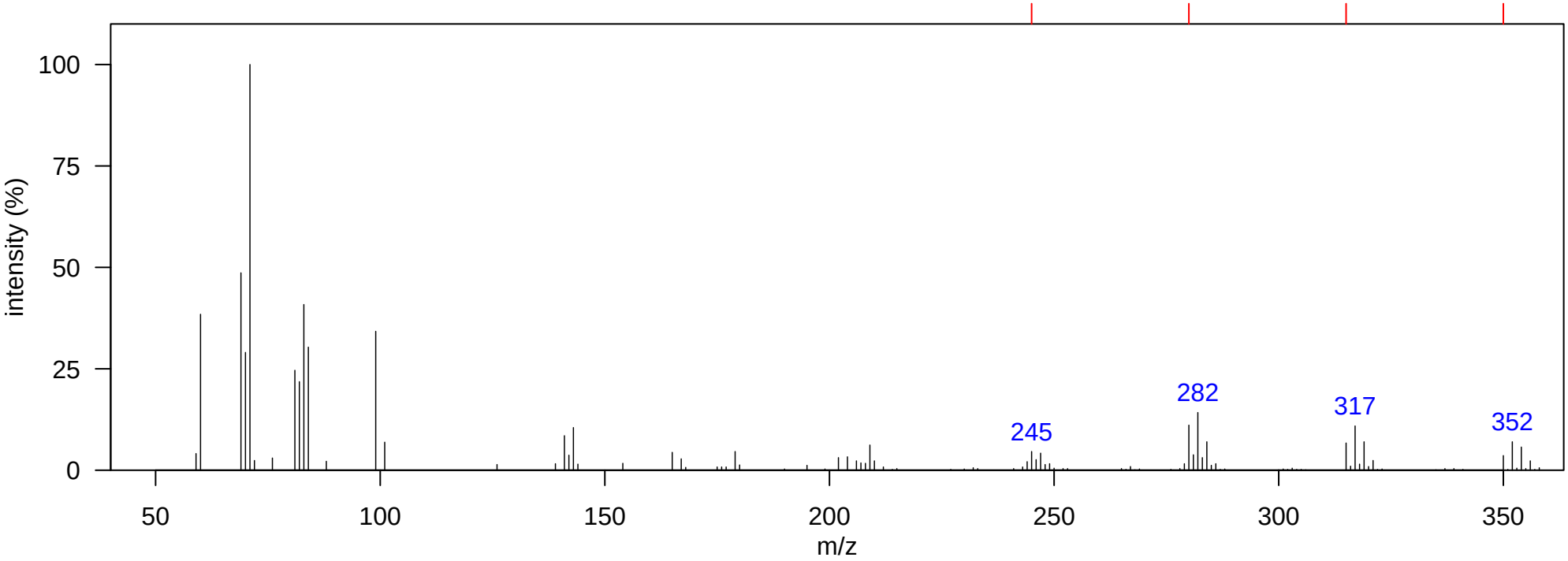
Comment: Ref: Chemosphere, 2008, 70, 1721−1729.

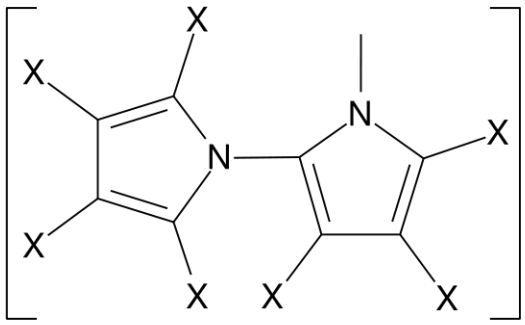
Elemental Formula: C9H4Cl6N2

Source: natural

Class: MBP

Identification: Literature MS





X=6Cl, H

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

Filename: 6Cl_MBP_isomer_2

Name: methyl bipyrrole 7Cl (MBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1472.5, RT (s) (2D): 1.138

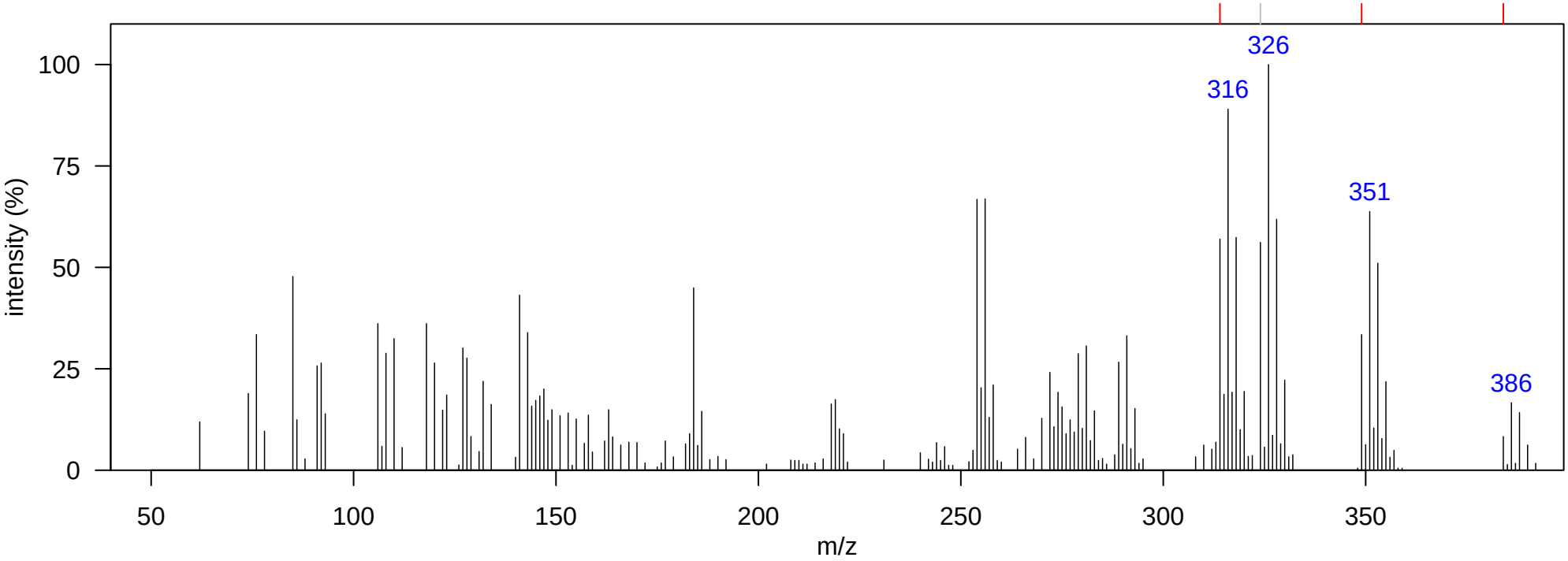
Comment: Also referred to as Q1.

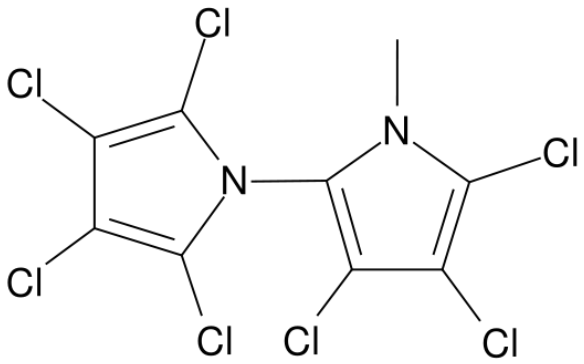
Elemental Formula: C9H3Cl7N2

Source: natural

Class: MBP

Identification: Authentic MS RT





m/z	Identity
314	[M−2Cl]+
324	interference
349	[M−Cl]+
384	M+

Filename: 7Cl_MBP

Name: methyl bipyrrole 4Br (MBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1455, RT (s) (2D): 1.729

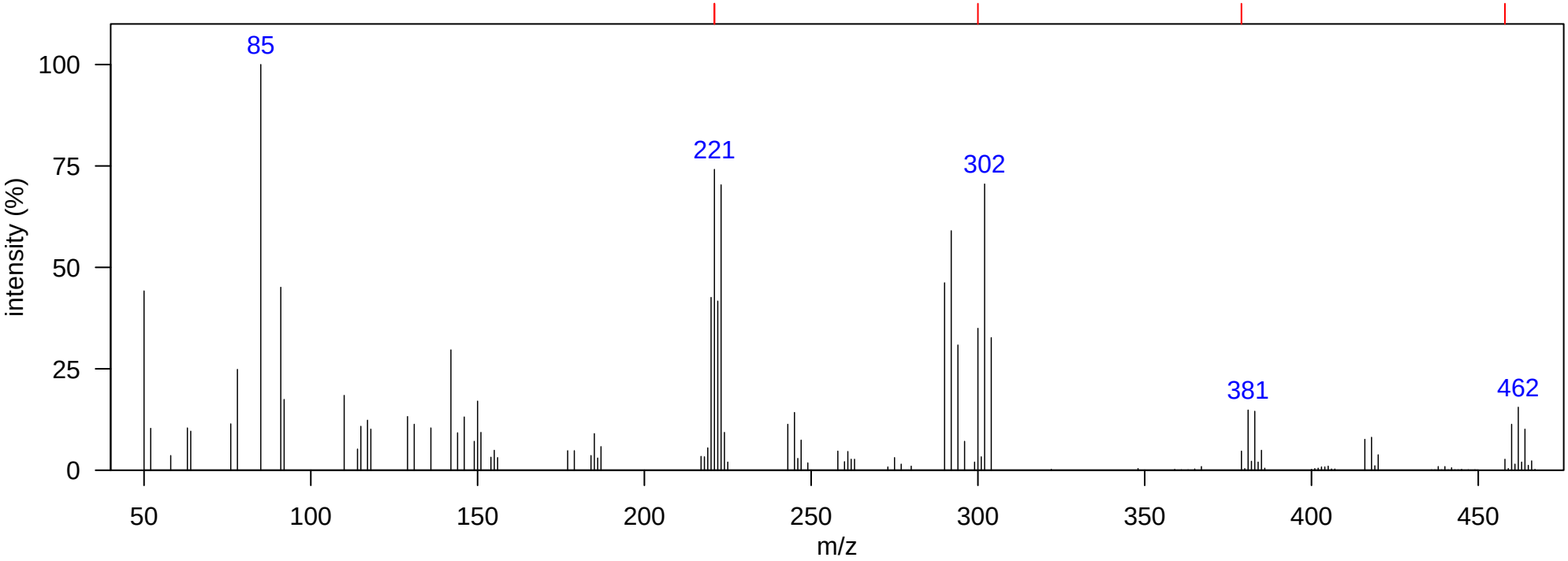
Comment:

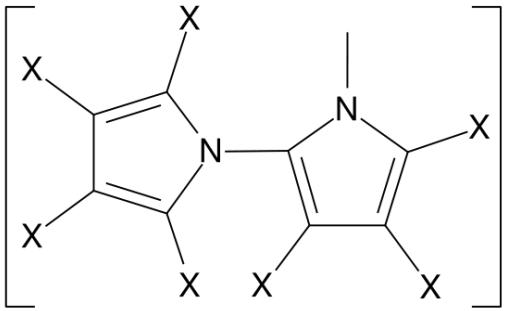
Elemental Formula: C9H6Br4N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, 3H

m/z	Identity
221	[M−3Br]+
300	[M−2Br]+
379	[M−Br]+
458	M+

Filename: 4Br_MBP

Name: methyl bipyrrole 5Br (MBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1535.5, RT (s) (2D): 2.037

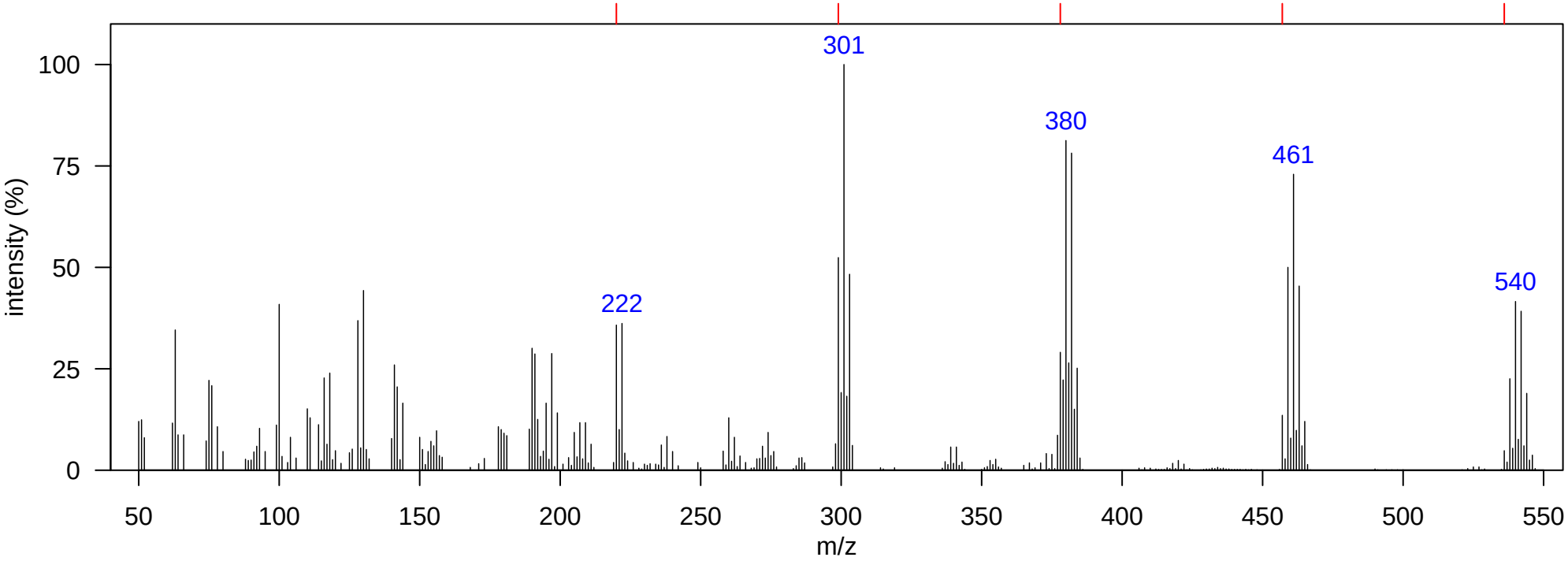
Comment:

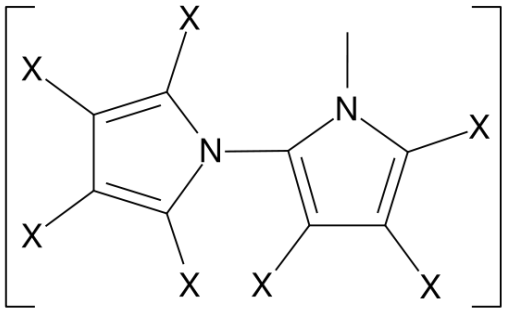
Elemental Formula: C9H5Br5N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=5Br, 2H

m/z	Identity
220	[M−4Br]+
299	[M−3Br]+
378	[M−2Br]+
457	[M−Br]+
536	M+

Filename: 5Br_MBP_isomer_1

Name: methyl bipyrrole 5Br (MBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1591.5, RT (s) (2D): 2.26

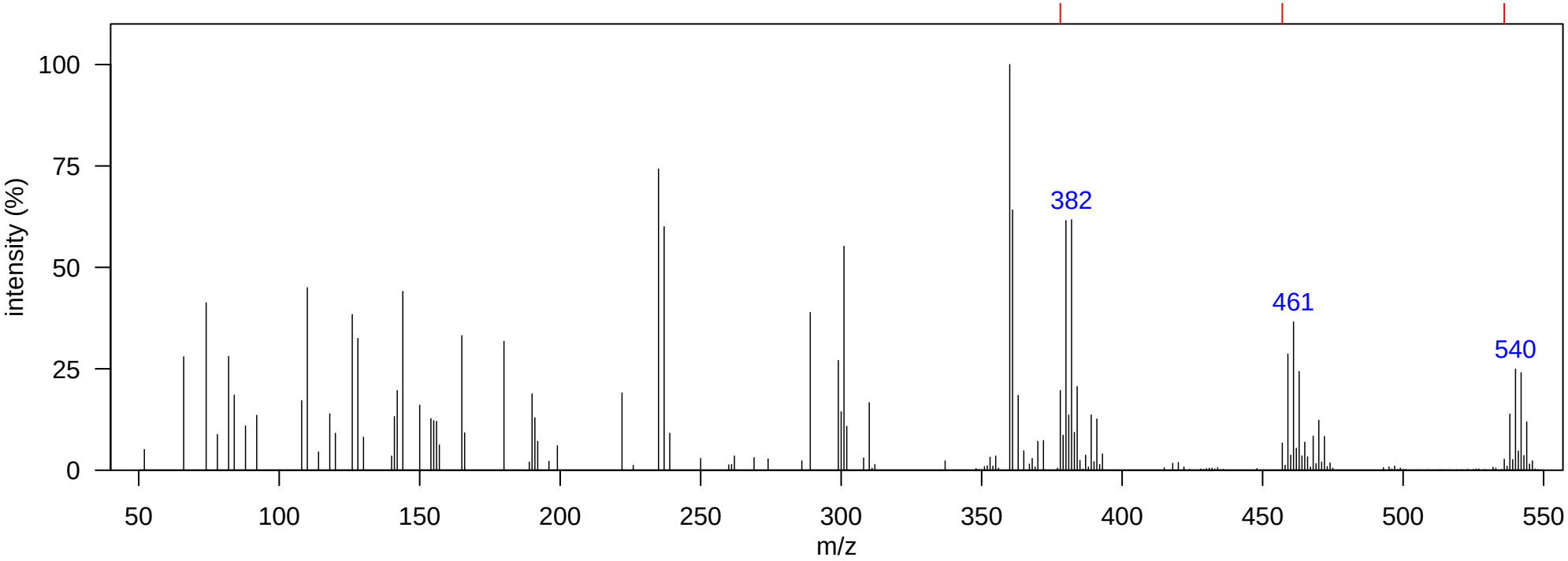
Comment:

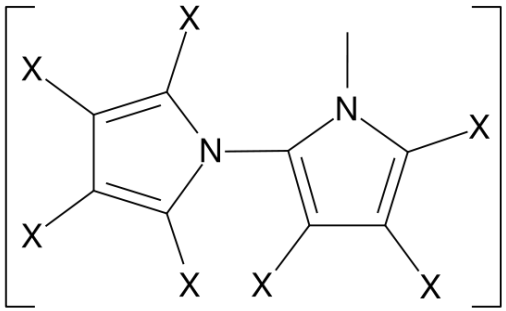
Elemental Formula: C9H5Br5N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=5Br, 2H

m/z	Identity
378	[M−2Br]+
457	[M−Br]+
536	M+

Filename: 5Br_MBP_isomer_2

Name: methyl bipyrrole 5Br (MBP) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1595, RT (s) (2D): 2.802

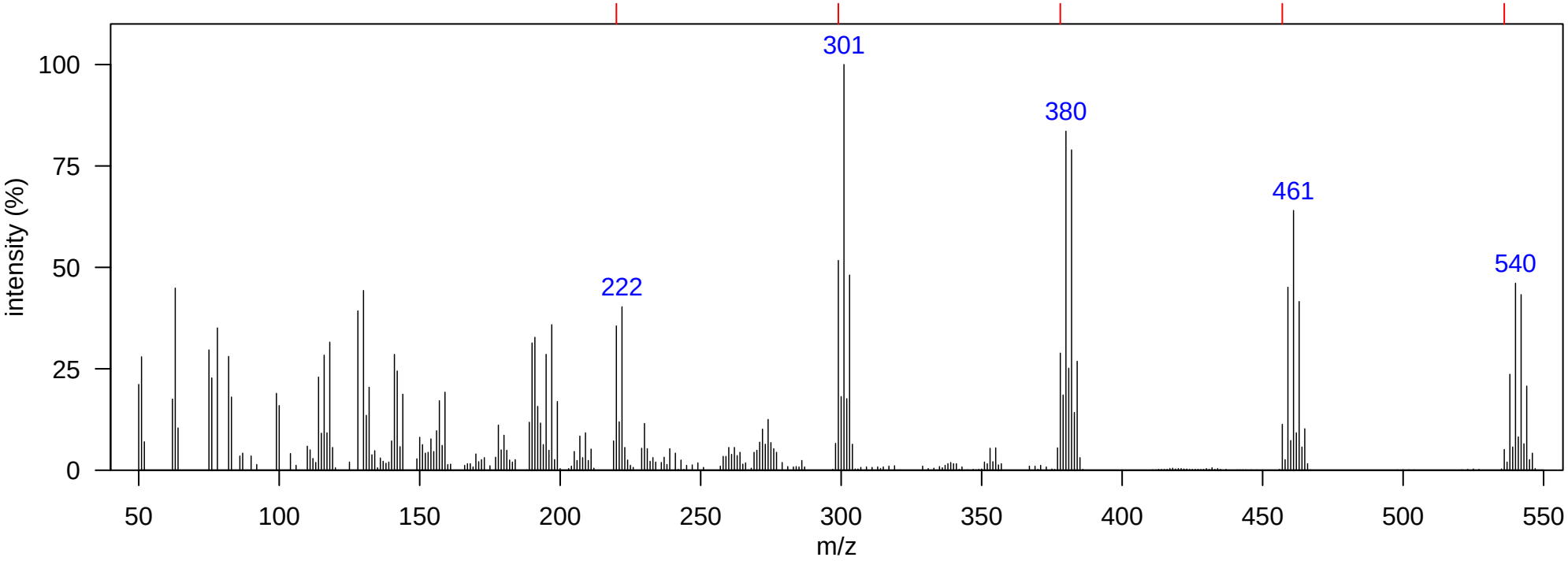
Comment:

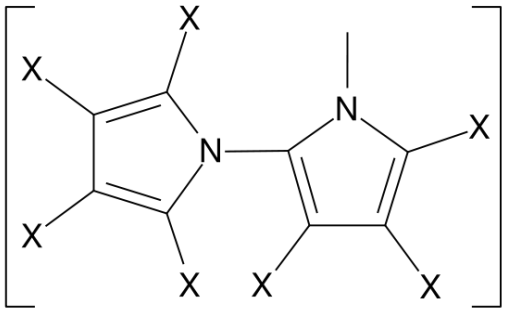
Elemental Formula: C9H5Br5N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=5Br, 2H

m/z	Identity
220	[M−4Br]+
299	[M−3Br]+
378	[M−2Br]+
457	[M−Br]+
536	M+

Filename: 5Br_MBP_isomer_3

Name: methyl bipyrrole 5Br (MBP) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1616, RT (s) (2D): 2.413

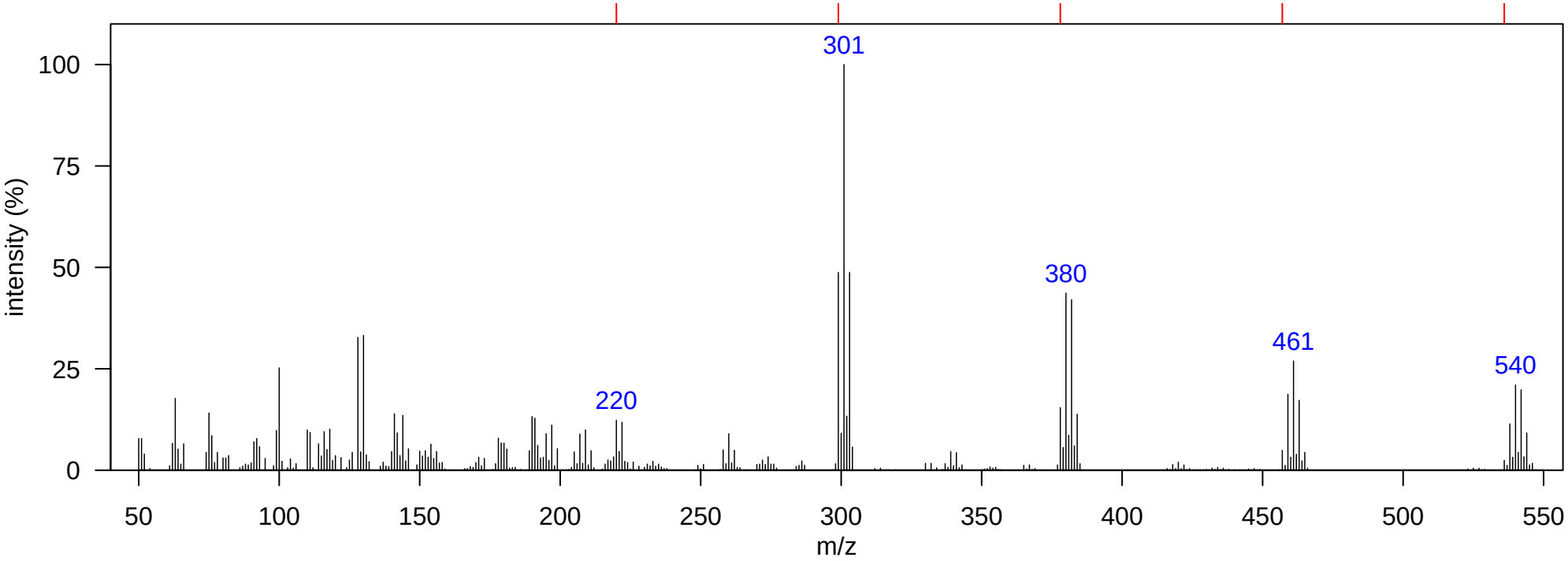
Comment:

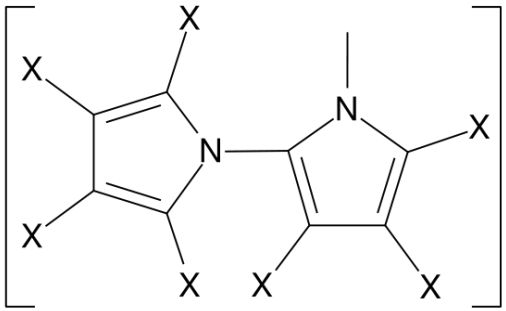
Elemental Formula: C9H5Br5N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=5Br, 2H

m/z	Identity
220	[M−4Br]+
299	[M−3Br]+
378	[M−2Br]+
457	[M−Br]+
536	M+

Filename: 5Br_MBP_isomer_4

Name: methyl bipyrrole 6Br (MBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1675.5, RT (s) (2D): 2.756

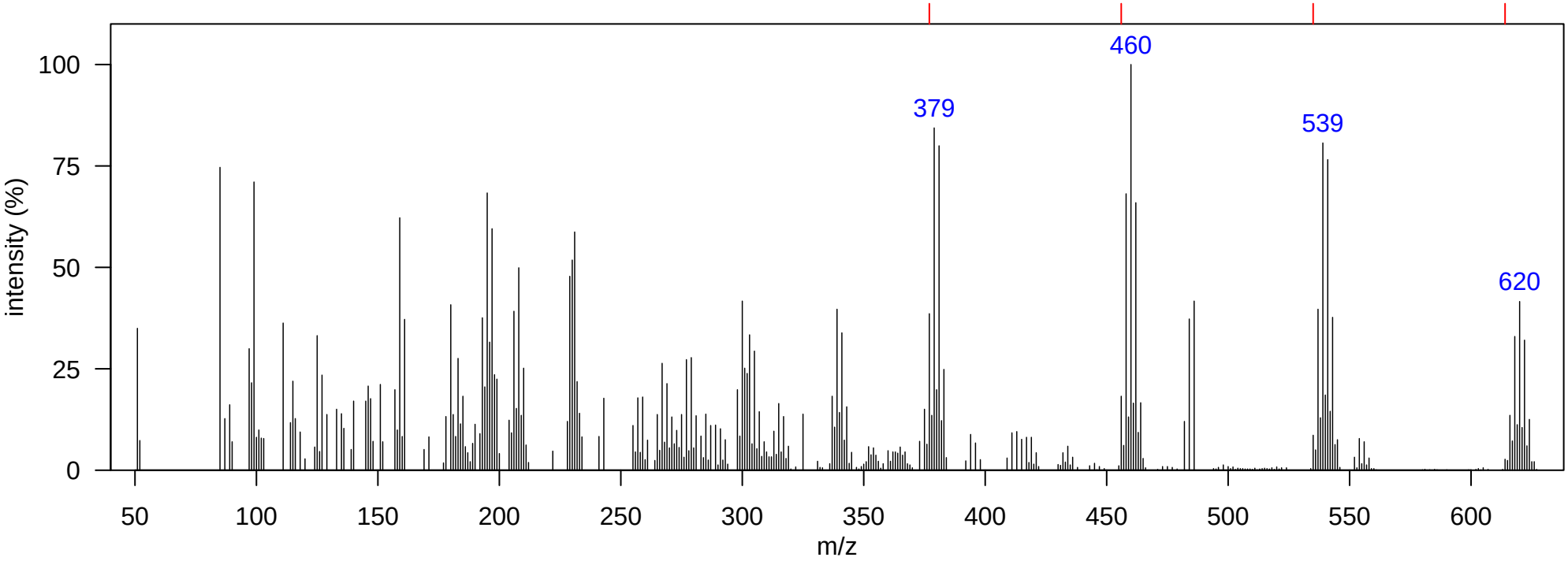
Comment:

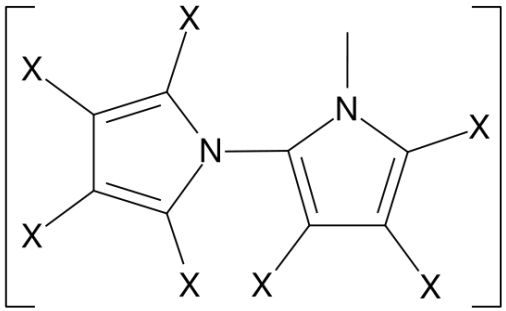
Elemental Formula: C9H4Br6N2

Source: natural

Class: MBP

Identification: Authentic MS RT





X=6Br, H

m/z	Identity
377	[M−3Br]+
456	[M−2Br]+
535	[M−Br]+
614	M+

Filename: 6Br_MBP_isomer_1

Name: methyl bipyrrole 6Br (MBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1682.5, RT (s) (2D): 2.881

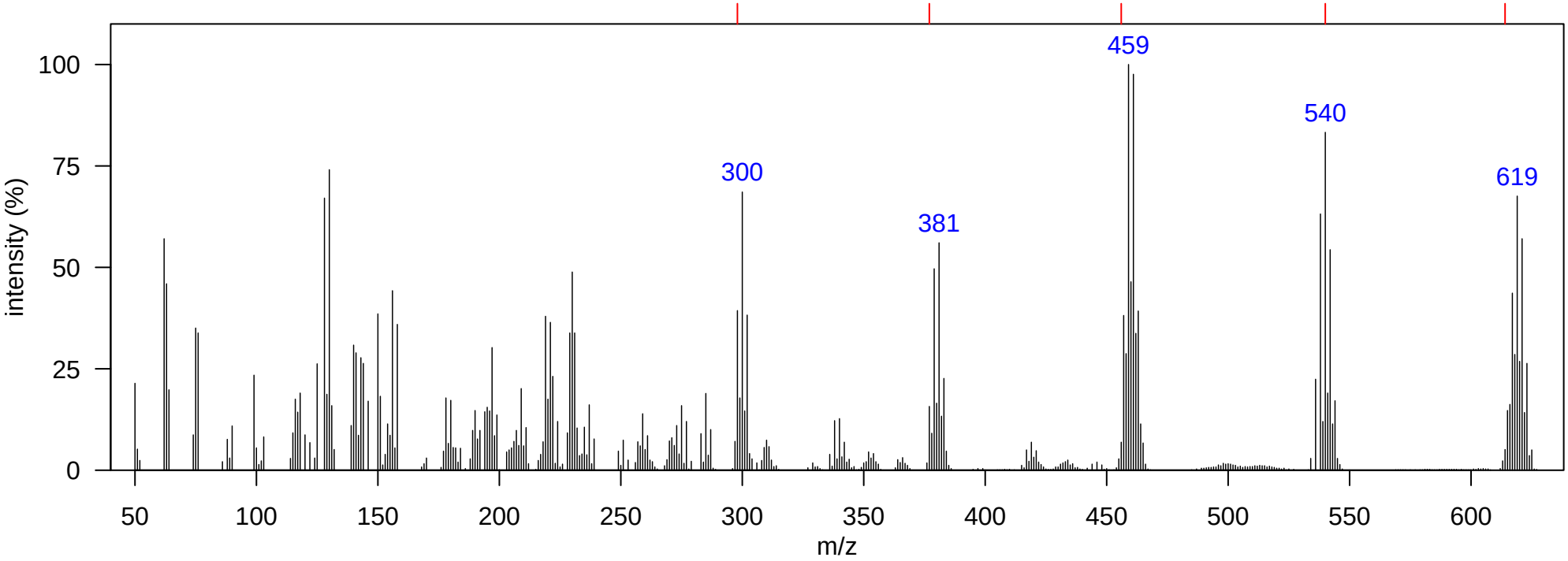
Comment:

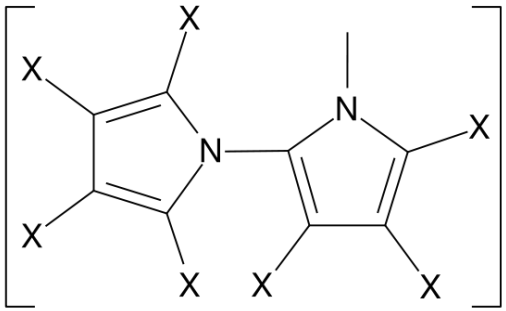
Elemental Formula: C9H4Br6N2

Source: natural

Class: MBP

Identification: Authentic MS





X=6Br, H

m/z	Identity
298	[M−4Br]+
377	[M−3Br]+
456	[M−2Br]+
540	[M−Br]+ (not monoisotopic)
614	M+

Filename: 6Br_MBP_isomer_2

Name: methyl bipyrrole 6Br (MBP) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1735, RT (s) (2D): 0.138

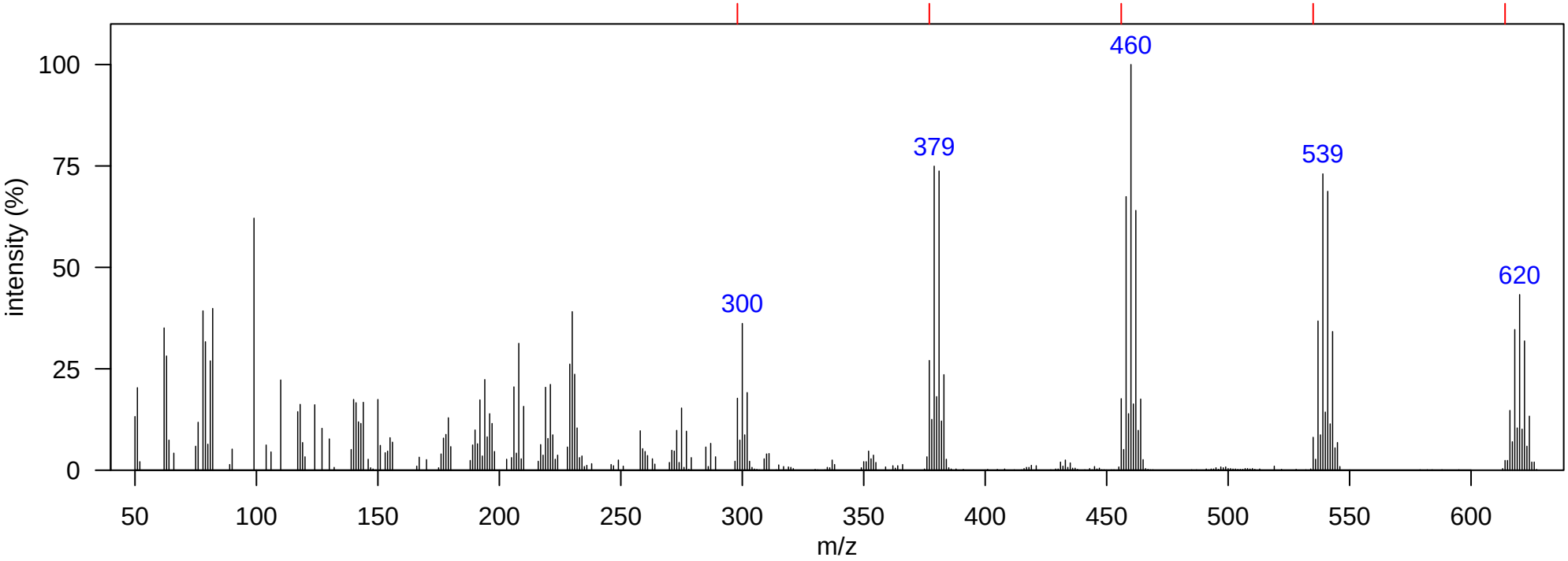
Comment:

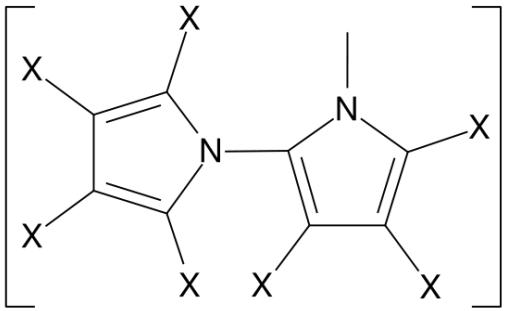
Elemental Formula: C9H4Br6N2

Source: natural

Class: MBP

Identification: Authentic MS





X=6Br, H

m/z	Identity
298	[M−4Br]+
377	[M−3Br]+
456	[M−2Br]+
535	[M−Br]+
614	M+

Filename: 6Br_MBP_isomer_3

Name: methyl bipyrrole 6Br (MBP) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1763, RT (s) (2D): 3.437

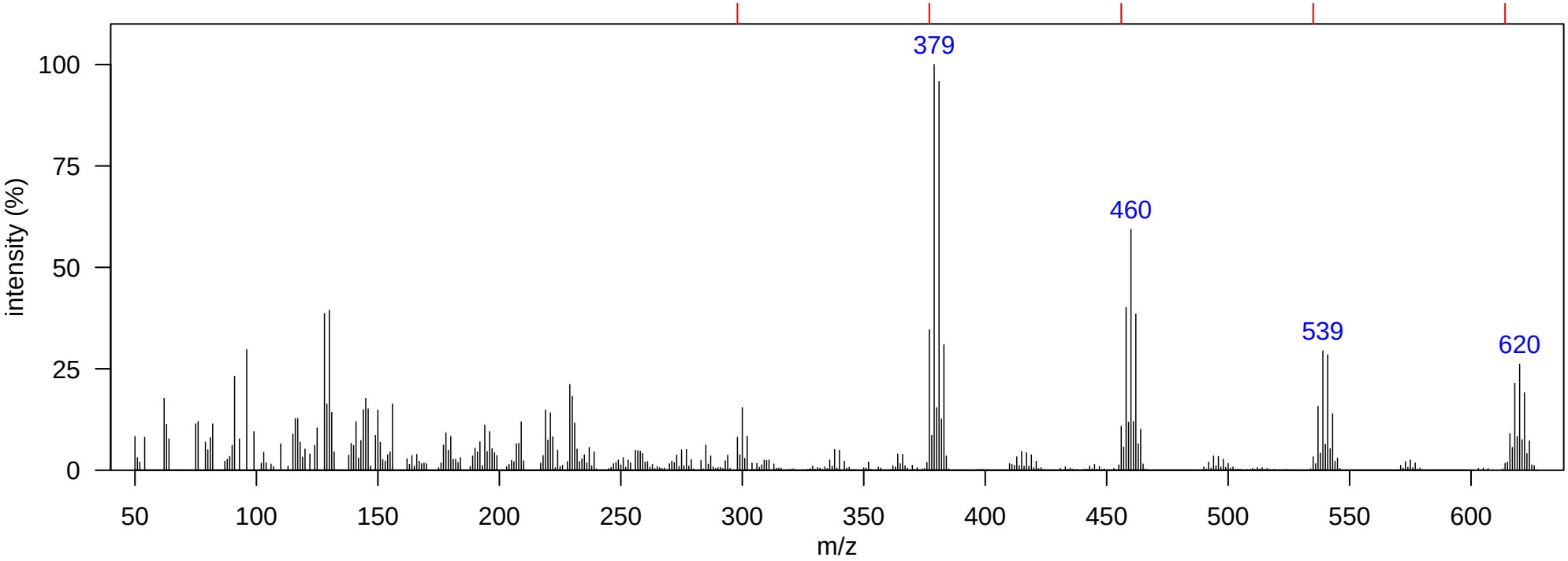
Comment:

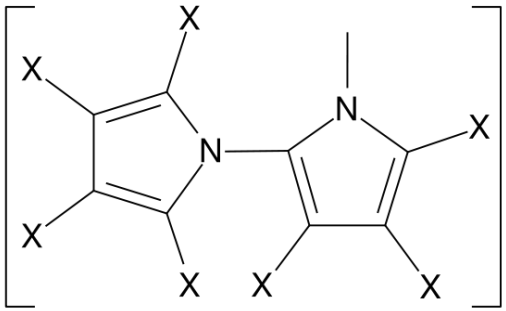
Elemental Formula: C9H4Br6N2

Source: natural

Class: MBP

Identification: Authentic MS





X=6Br, H

m/z	Identity
298	[M−4Br]+
377	[M−3Br]+
456	[M−2Br]+
535	[M−Br]+
614	M+

Filename: 6Br_MBP_isomer_4

Name: methyl bipyrrole 7Br (MBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1815.5, RT (s) (2D): 0.322

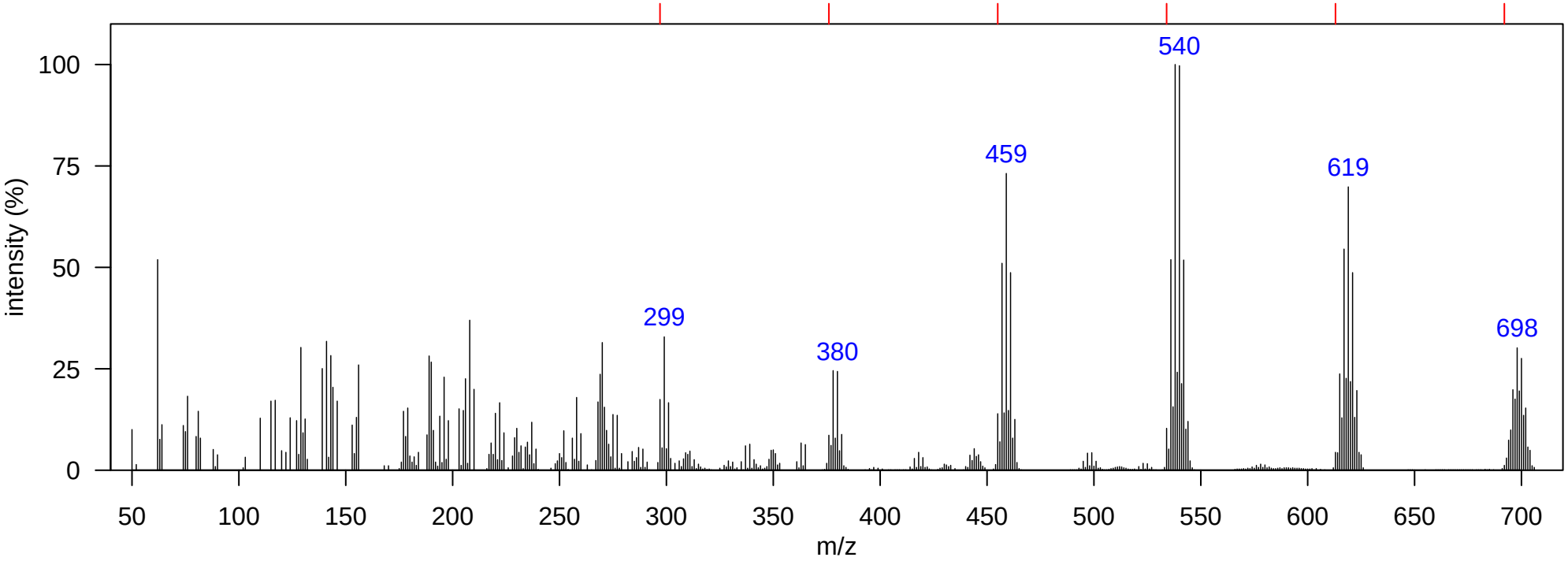
Comment:

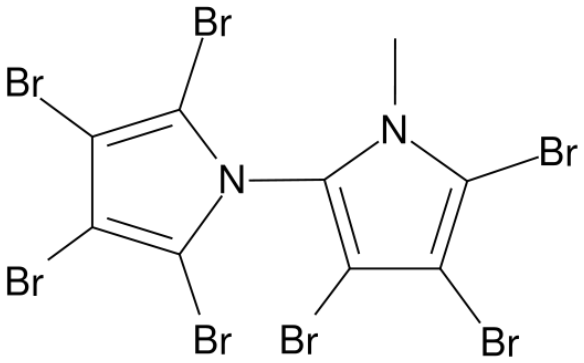
Elemental Formula: C9H3Br7N2

Source: natural

Class: MBP

Identification: Authentic MS RT





m/z	Identity
297	[M−5Br]+
376	[M−4Br]+
455	[M−3Br]+
534	[M−2Br]+
613	[M−Br]+
692	M+

Filename: 7Br_MBP

Name: methyl bipyrrole Br3Cl (MBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1406, RT (s) (2D): 1.481

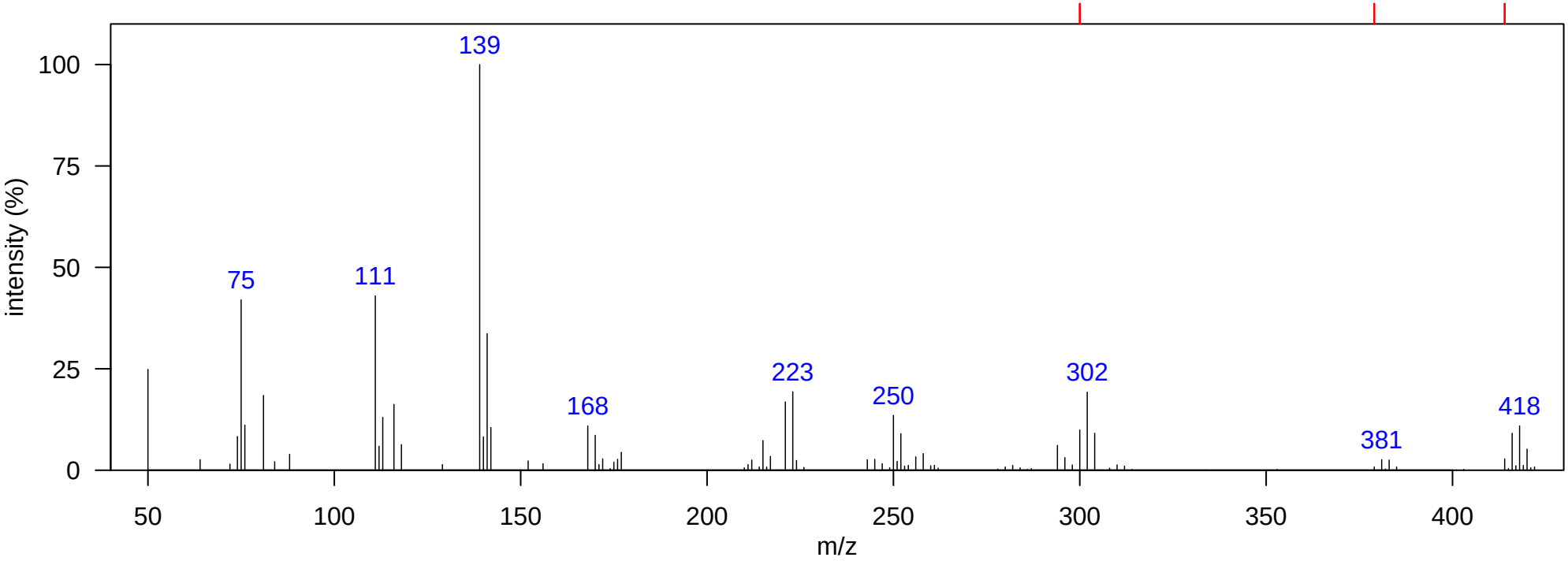
Comment:

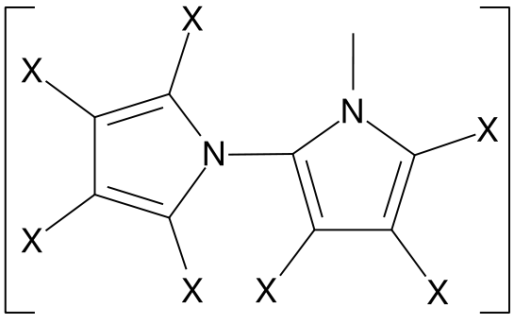
Elemental Formula: C9H6Br3ClN2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=3Br, Cl, 3H

m/z	Identity
300	[M−BrCl]+
379	[M−Cl]+
414	M+

Filename: Br3Cl_MBP

Name: methyl bipyrrole Br4Cl (MBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1483, RT (s) (2D): 1.802

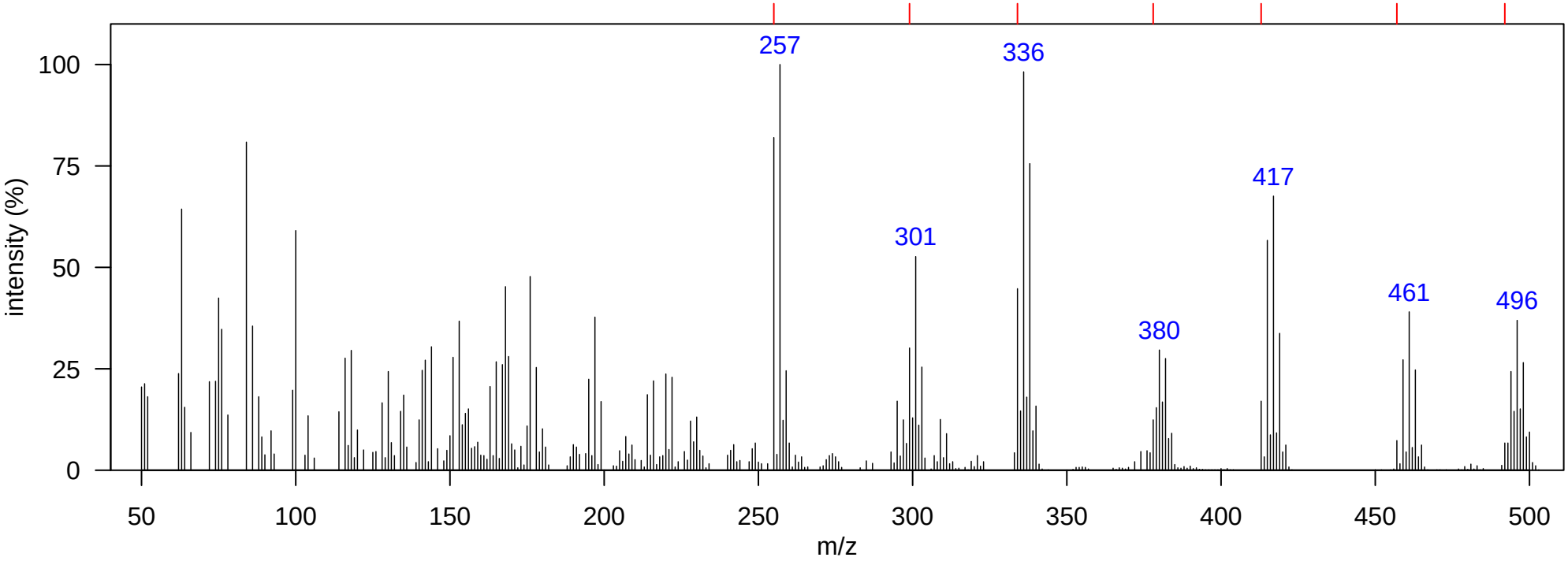
Comment:

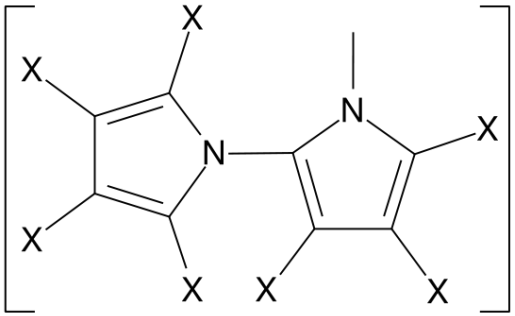
Elemental Formula: C9H5Br4ClN2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, Cl, 2H

m/z	Identity
255	[M−3Br]+
299	[M−Br2Cl]+
334	[M−2Br]+
378	[M−BrCl]+
413	[M−Br]+
457	[M−Cl]+
492	M+

Filename: Br4Cl_MBP_isomer_1

Name: methyl bipyrrole Br4Cl (MBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1542.5, RT (s) (2D): 1.921

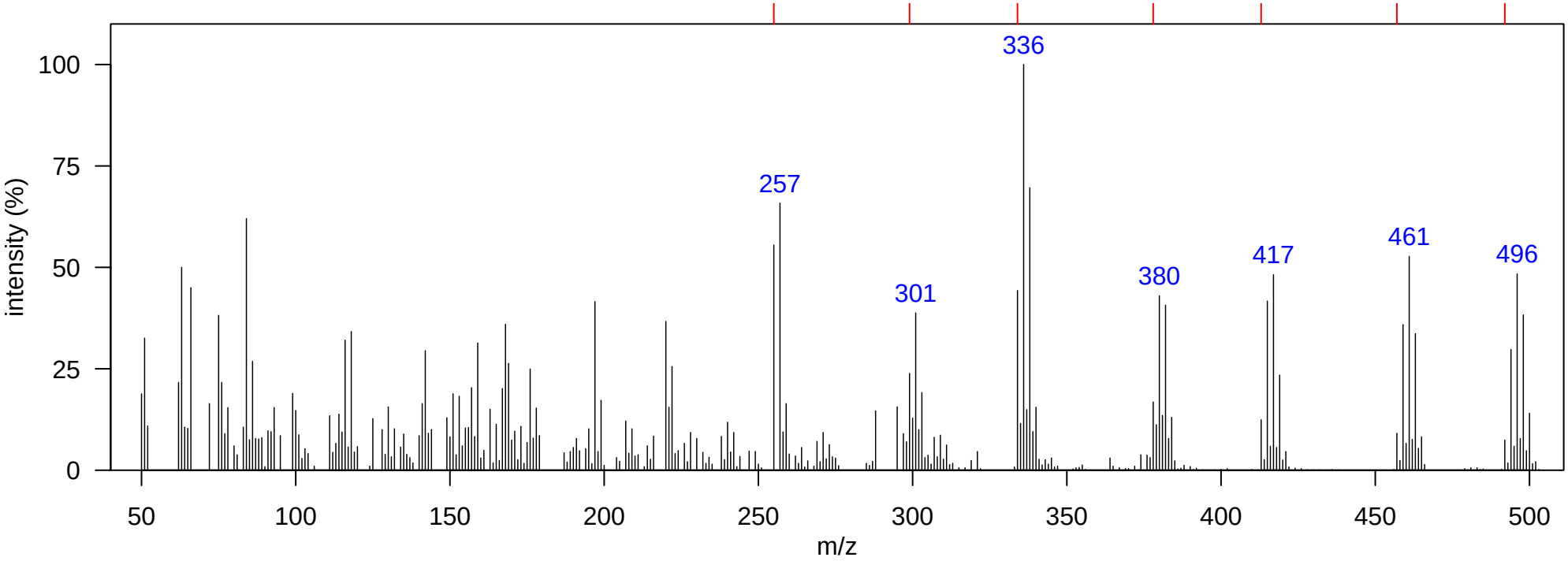
Comment:

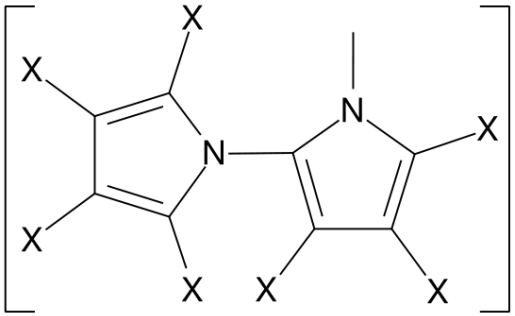
Elemental Formula: C9H5Br4ClN2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, Cl, 2H

m/z	Identity
255	[M−3Br]+
299	[M−Br2Cl]+
334	[M−2Br]+
378	[M−BrCl]+
413	[M−Br]+
457	[M−Cl]+
492	M+

Filename: Br4Cl_MBP_isomer_2

Name: methyl bipyrrole Br4Cl (MBP) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1546, RT (s) (2D): 2.491

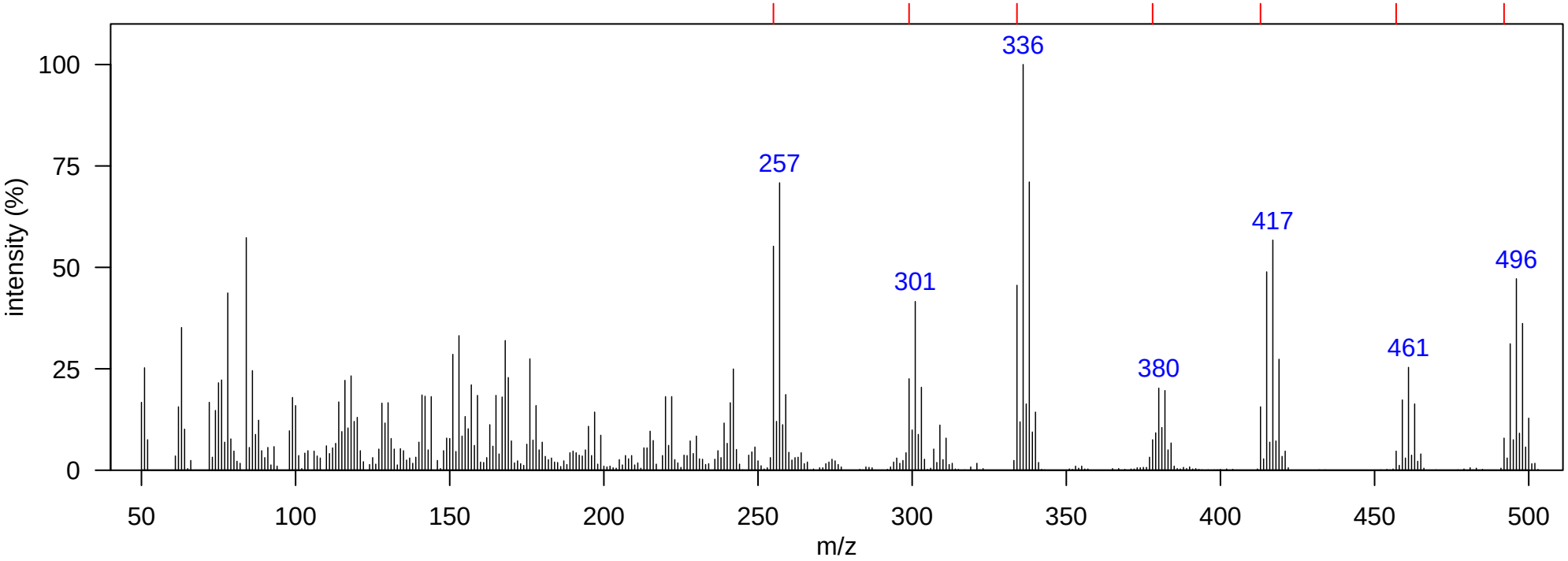
Comment:

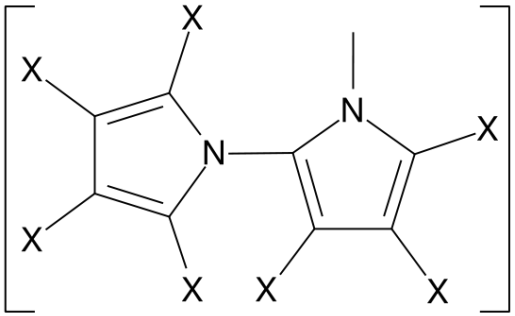
Elemental Formula: C9H5Br4ClN2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, Cl, 2H

m/z	Identity
255	[M−3Br]+
299	[M−Br2Cl]+
334	[M−2Br]+
378	[M−BrCl]+
413	[M−Br]+
457	[M−Cl]+
492	M+

Filename: Br4Cl_MBP_isomer_3

Name: methyl bipyrrole Br4Cl (MBP) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1570.5, RT (s) (2D): 2.083

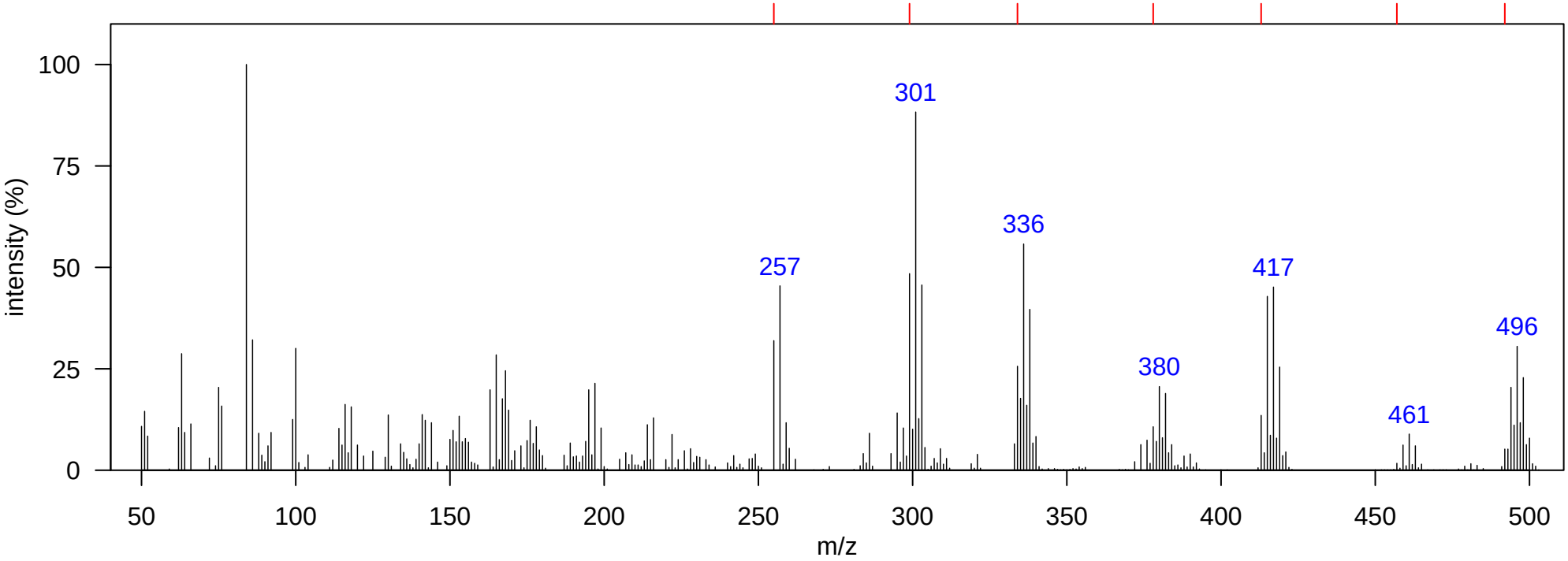
Comment:

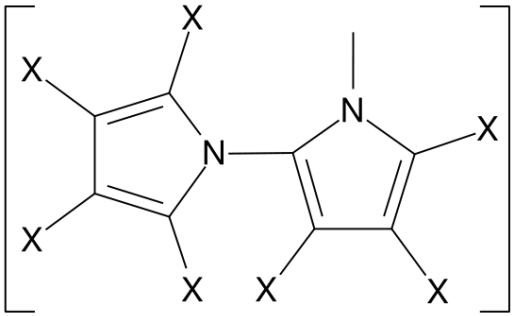
Elemental Formula: C9H5Br4ClN2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, Cl, 2H

m/z	Identity
255	[M−3Br]+
299	[M−Br2Cl]+
334	[M−2Br]+
378	[M−BrCl]+
413	[M−Br]+
457	[M−Cl]+
492	M+

Filename: Br4Cl_MBP_isomer_4

Name: methyl bipyrrole Br4Cl (MBP) isomer 5

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1623, RT (s) (2D): 2.358

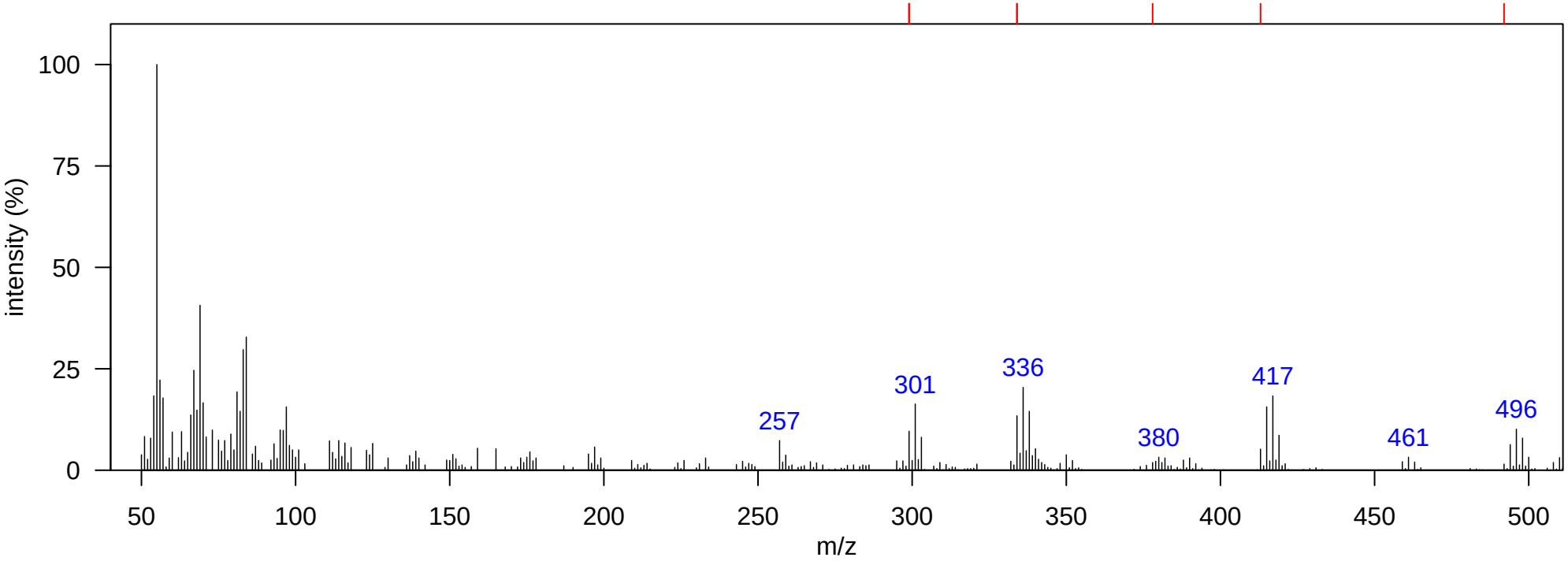
Comment:

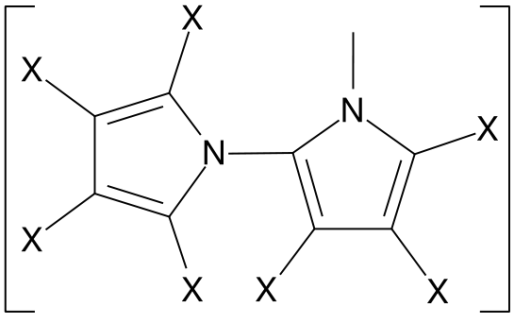
Elemental Formula: C9H5Br4ClN2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, Cl, 2H

m/z	Identity
299	[M−Br2Cl]+
334	[M−2Br]+
378	[M−BrCl]+
413	[M−Br]+
492	M+

Filename: Br4Cl_MBP_isomer_5

Name: methyl bipyrrole Br4Cl (MBP) isomer 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1630, RT (s) (2D): 2.912

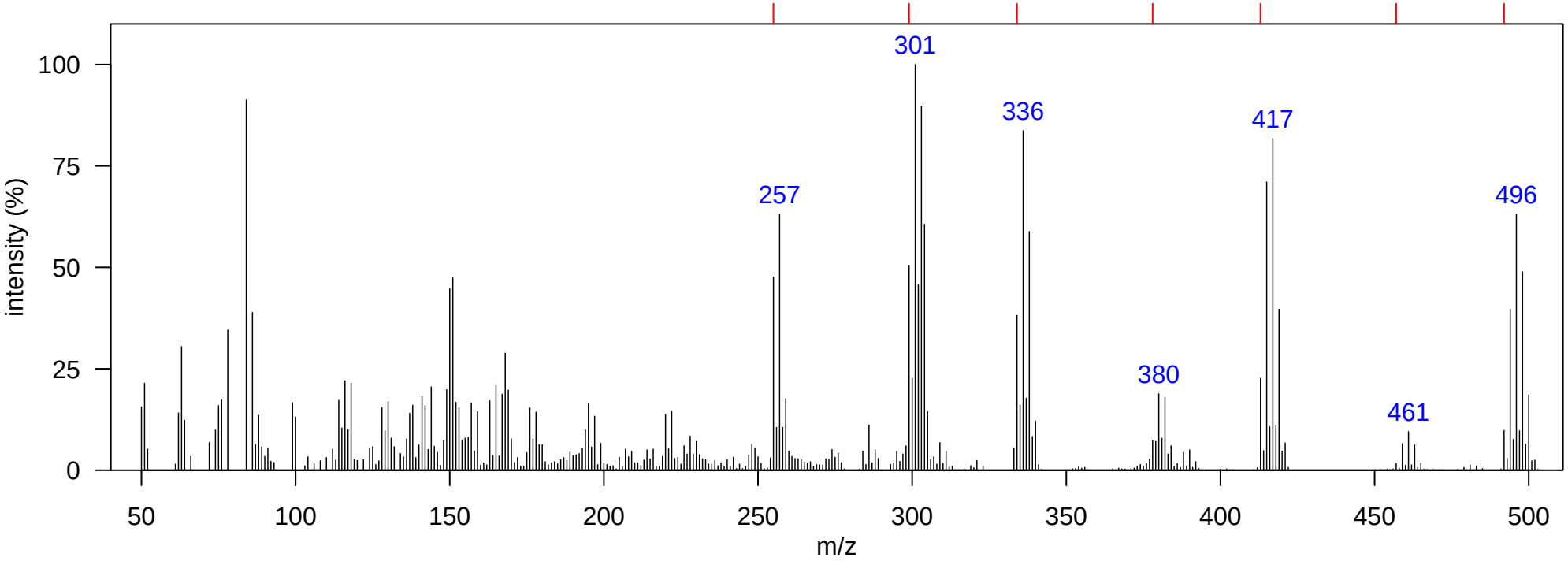
Comment:

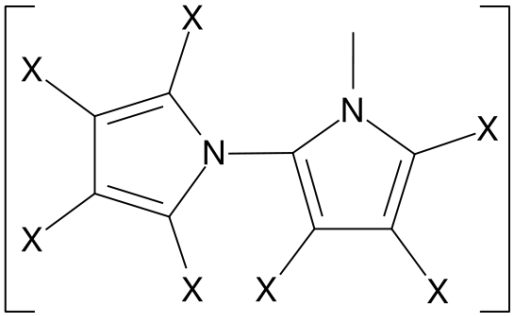
Elemental Formula: C9H5Br4ClN2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, Cl, 2H

m/z	Identity
255	[M−3Br]+
299	[M−Br2Cl]+
334	[M−2Br]+
378	[M−BrCl]+
413	[M−Br]+
457	[M−Cl]+
492	M+

Filename: Br4Cl_MBP_isomer_6

Name: methyl bipyrrole Br4Cl2 (MBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1584.5, RT (s) (2D): 2.128

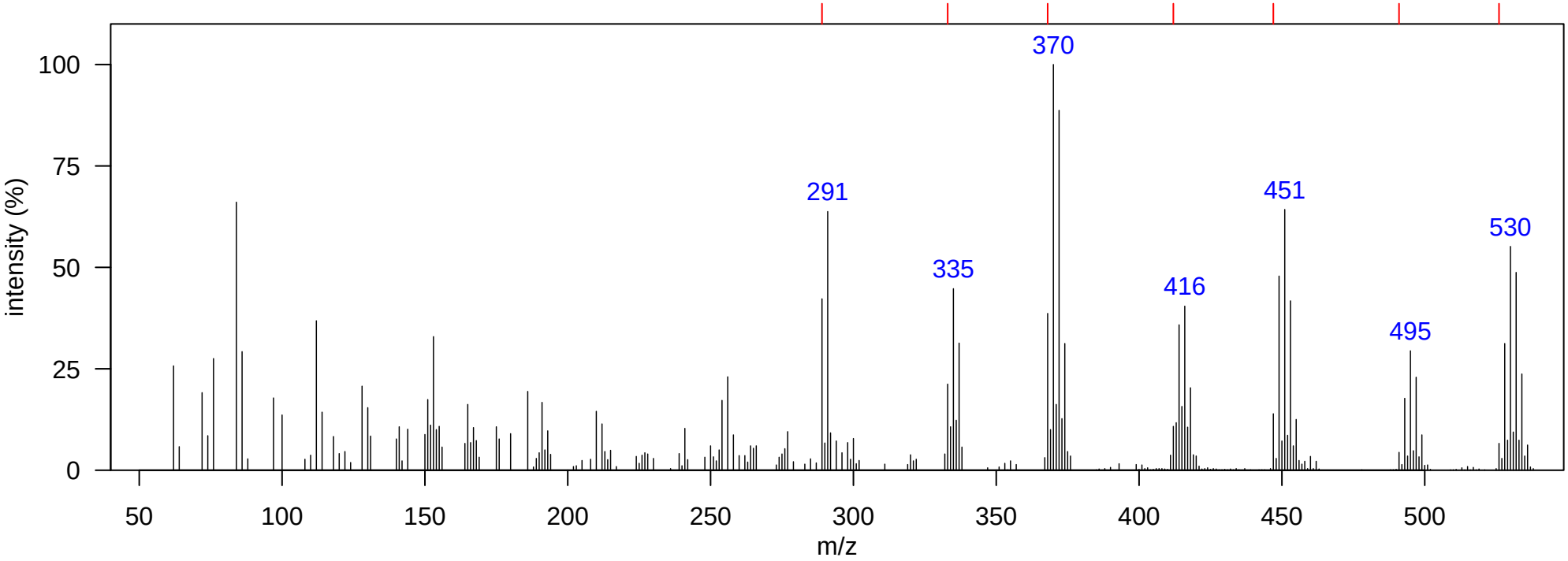
Comment:

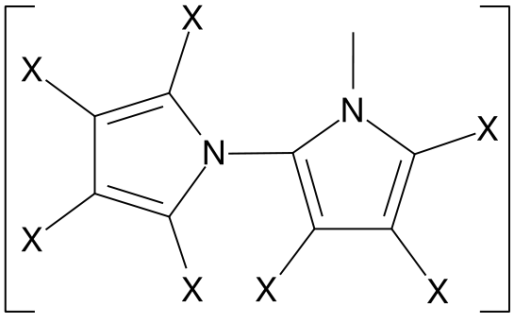
Elemental Formula: C9H6Br4Cl2N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, 2Cl, H

m/z	Identity
289	[M−3Br]+
333	[M−Br2Cl]+
368	[M−2Br]+
412	[M−BrCl]+
447	[M−Br]+
491	[M−Cl]+
526	M+

Filename: Br4Cl2_MBP_isomer_1

Name: methyl bipyrrole Br4Cl2 (MBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1665, RT (s) (2D): 2.671

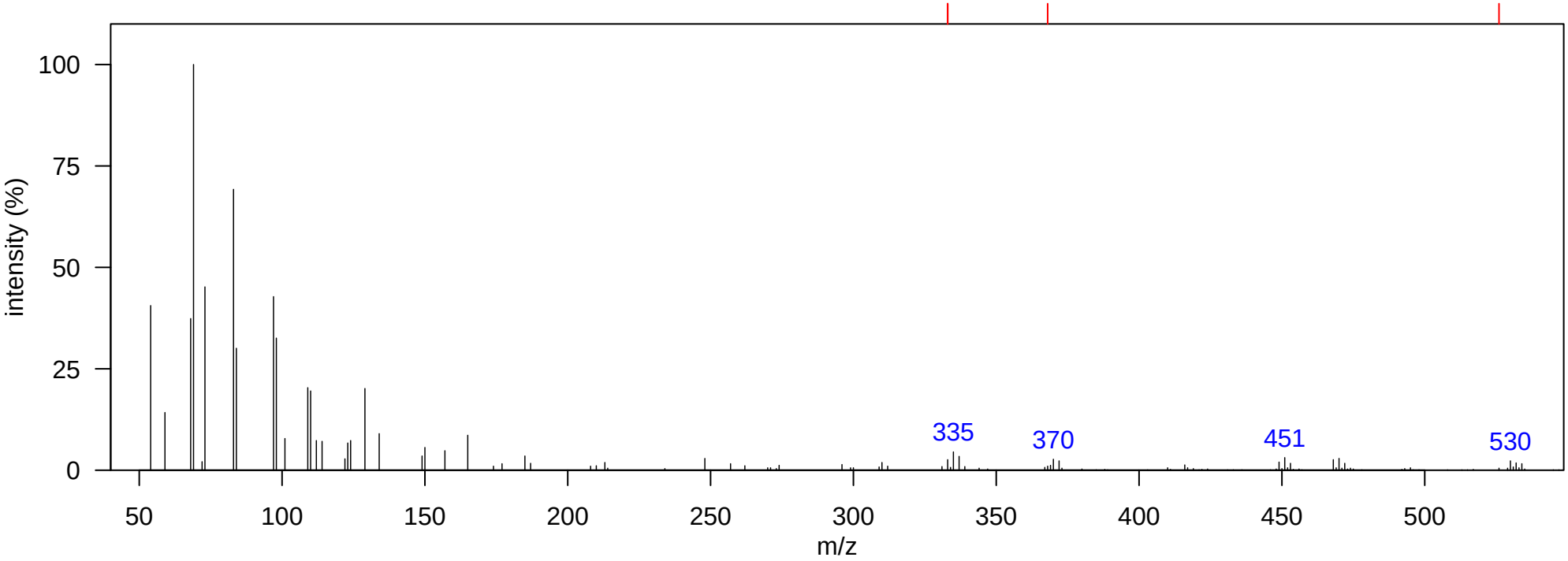
Comment: Low intensity, but visible in raw data.

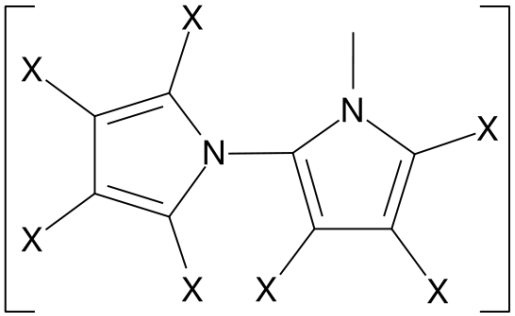
Elemental Formula: C9H6Br4Cl2N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=4Br, 2Cl, H

m/z	Identity
333	[M−Br2Cl]+
368	[M−2Br]+
526	M+

Filename: Br4Cl2_MBP_isomer_2

Name: methyl bipyrrole Br5Cl (MBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1630, RT (s) (2D): 2.34

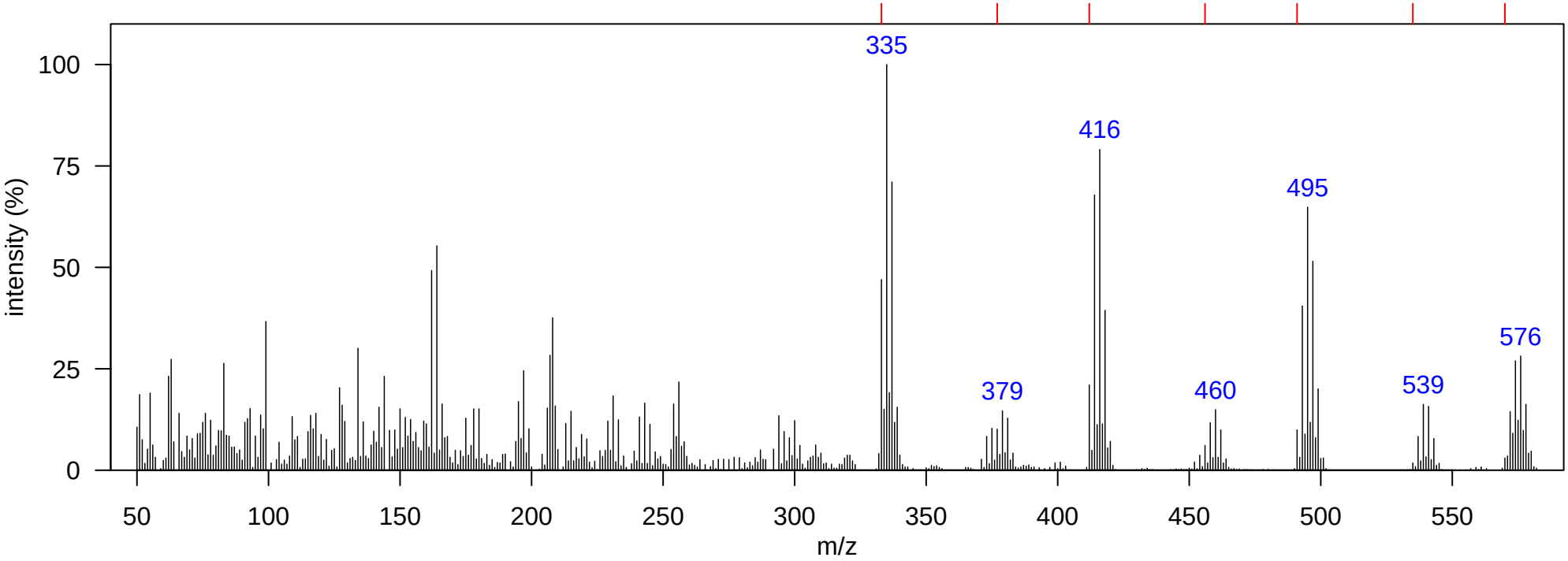
Comment:

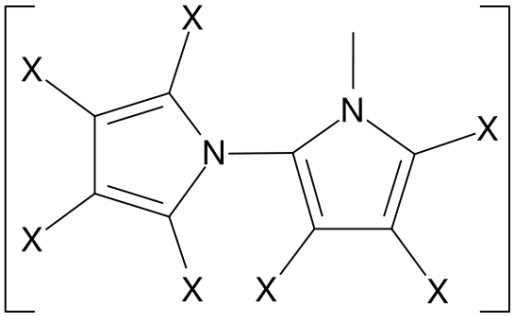
Elemental Formula: C9H4Br5ClN2

Source: natural

Class: MBP

Identification: Authentic MS RT





X=5Br, Cl, H

m/z	Identity
333	[M−3Br]+
377	[M−Br2Cl]+
412	[M−2Br]+
456	[M−BrCl]+
491	[M−Br]+
535	[M−Cl]+
570	M+

Filename: Br5Cl_MBP_isomer_1

Name: methyl bipyrrole Br5Cl (MBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1640.5, RT (s) (2D): 2.462

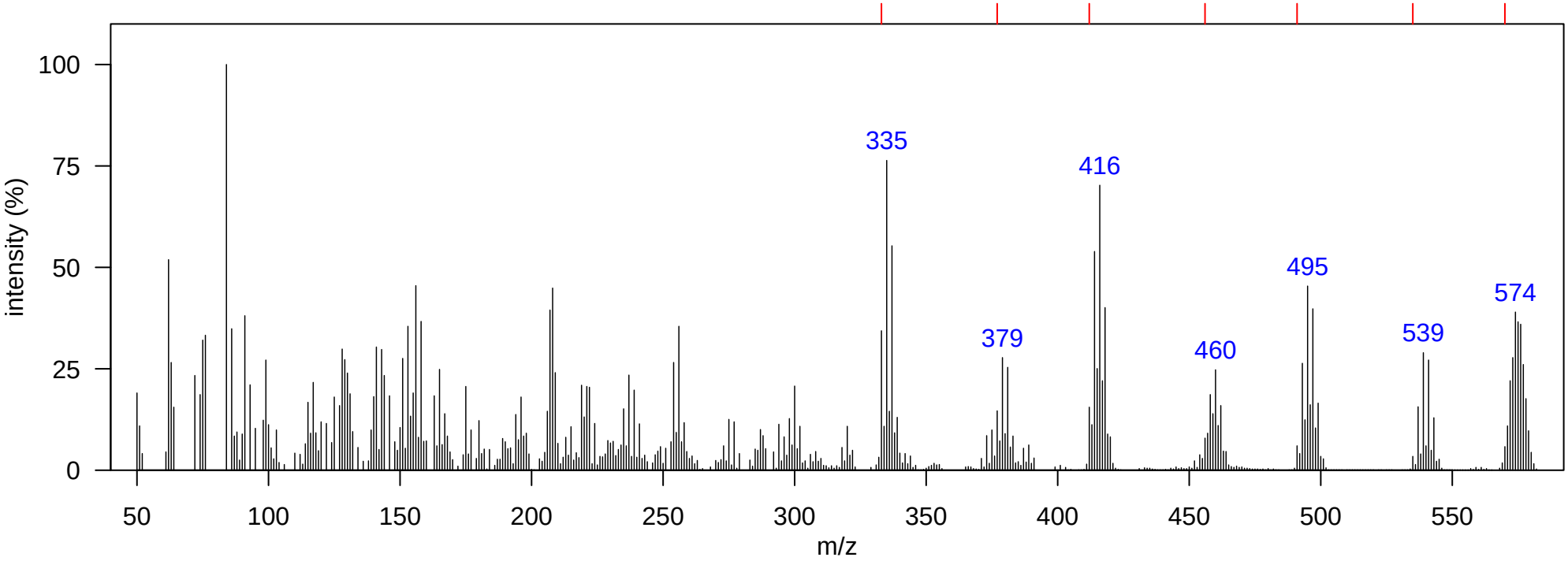
Comment:

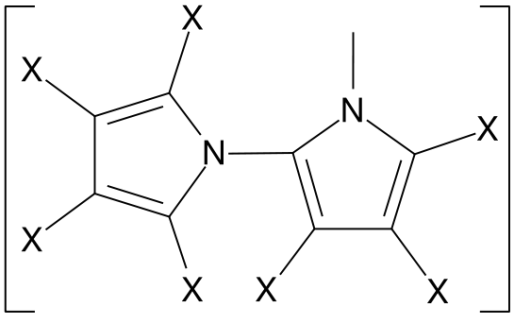
Elemental Formula: C9H4Br5ClN2

Source: natural

Class: MBP

Identification: Authentic MS





X=5Br, Cl, H

m/z	Identity
333	[M−3Br]+
377	[M−Br2Cl]+
412	[M−2Br]+
456	[M−BrCl]+
491	[M−Br]+
535	[M−Cl]+
570	M+

Filename: Br5Cl_MBP_isomer_2

Name: methyl bipyrrole Br5Cl (MBP) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1686, RT (s) (2D): 3.216

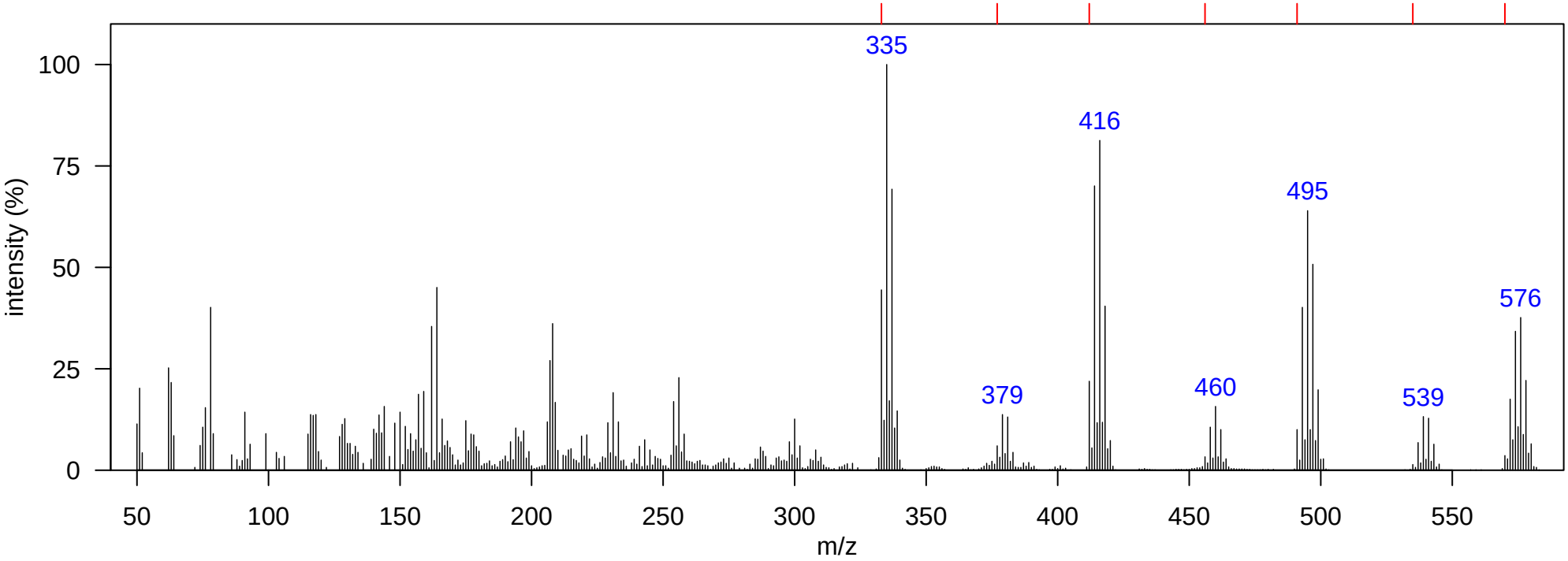
Comment:

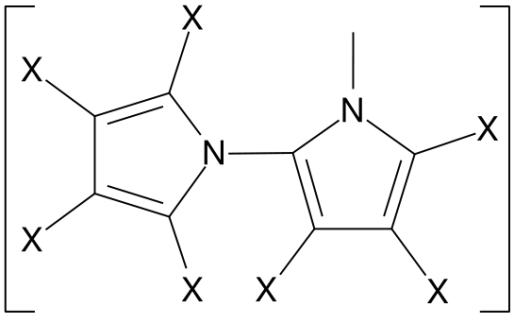
Elemental Formula: C9H4Br5ClN2

Source: natural

Class: MBP

Identification: Authentic MS RT





X=5Br, Cl, H

m/z	Identity
333	[M−3Br]+
377	[M−Br2Cl]+
412	[M−2Br]+
456	[M−BrCl]+
491	[M−Br]+
535	[M−Cl]+
570	M+

Name: methyl bipyrrole Br5Cl (MBP) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1721, RT (s) (2D): 3.08

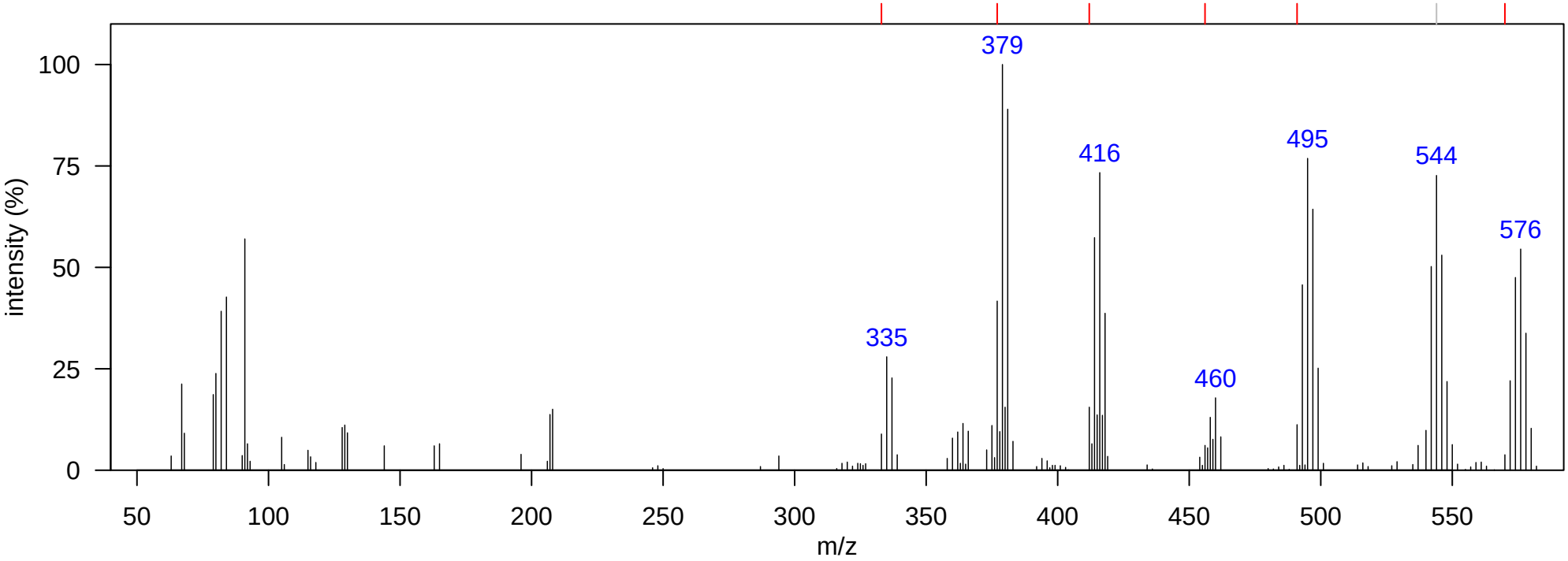
Comment:

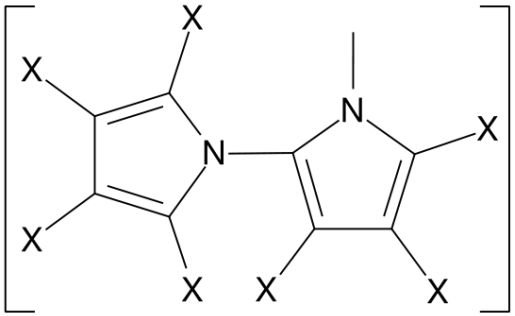
Elemental Formula: C9H4Br5ClN2

Source: natural

Class: MBP

Identification: Authentic MS





X=5Br, Cl, H

m/z	Identity
333	[M−3Br]+
377	[M−Br2Cl]+
412	[M−2Br]+
456	[M−BrCl]+
491	[M−Br]+
544	interference DMBPBr4Cl2
570	M+

Name: methyl bipyrrole Br5Cl2 (MBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1721, RT (s) (2D): 2.788

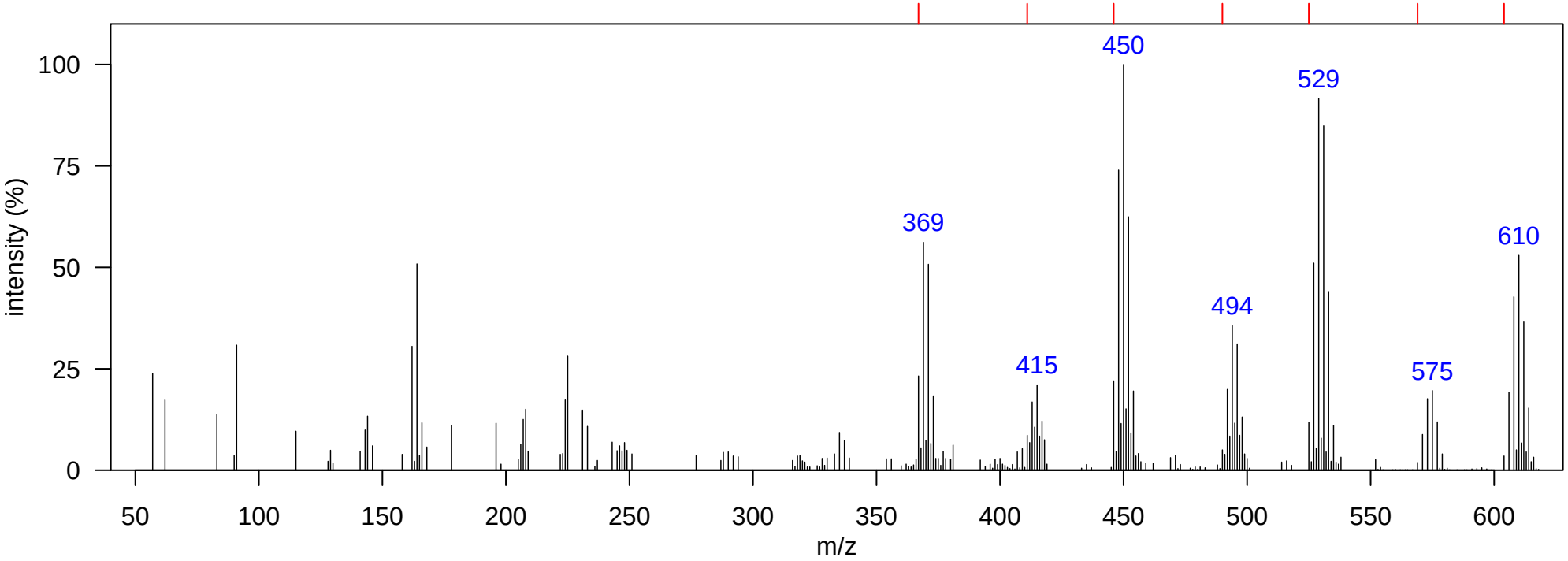
Comment:

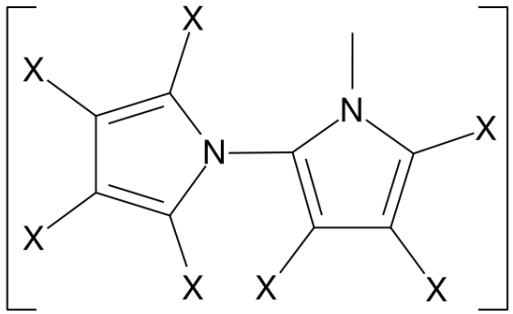
Elemental Formula: C9H3Br5Cl2N2

Source: natural

Class: MBP

Identification: Manual − Congener Group





X=5Br, 2Cl

m/z	Identity
367	[M−3Br]+
411	[M−Br2Cl]+
446	[M−2Br]+
490	[M−BrCl]+
525	[M−Br]+
569	[M−Cl]+
604	M+

Filename: Br5Cl2_MBP

Name: methyl bipyrrole Br6Cl (MBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1773.5, RT (s) (2D): 3.238

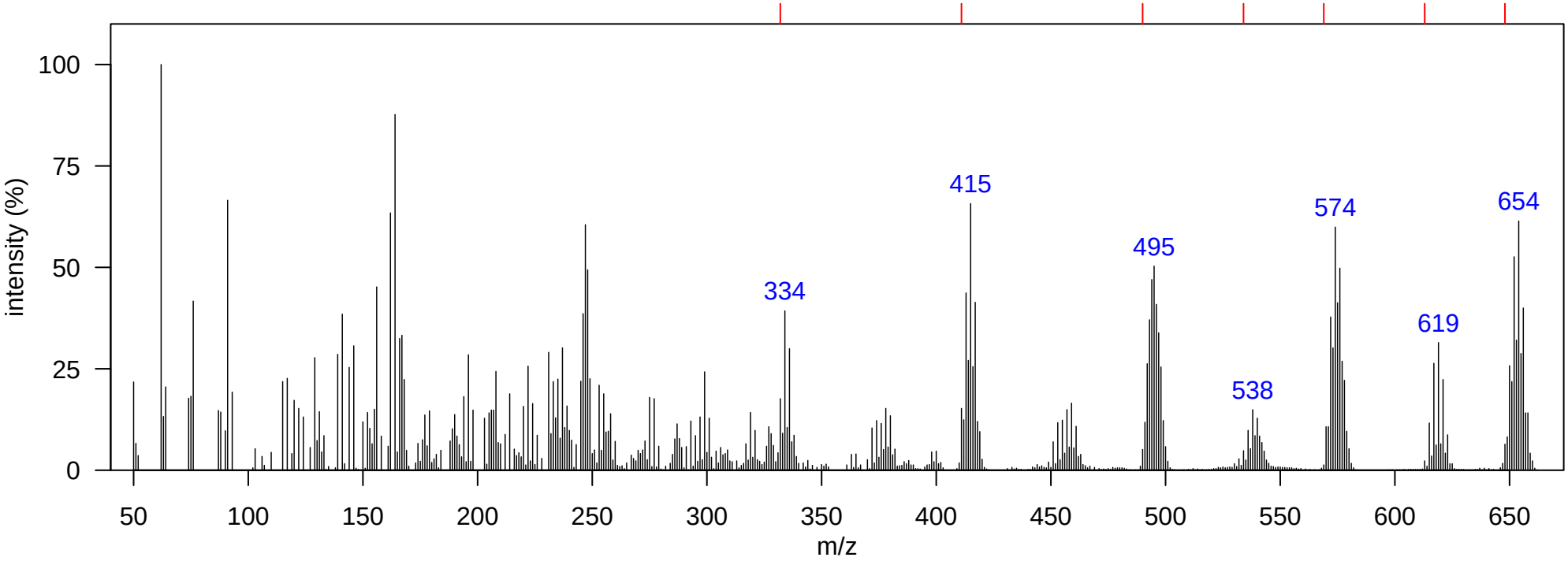
Comment:

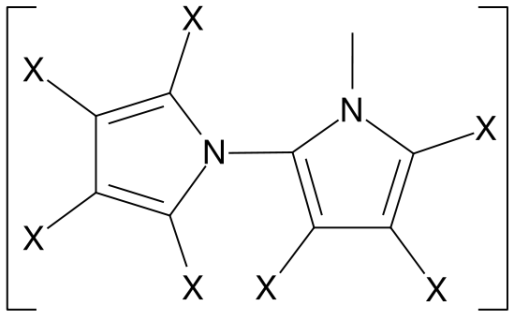
Elemental Formula: C9H3Br6ClN2

Source: natural

Class: MBP

Identification: Authentic MS RT





X=6Br, Cl

m/z	Identity
332	[M−4Br]+
411	[M−3Br]+
490	[M−2Br]+
534	[M−BrCl]+
569	[M−Br]+
613	[M−Cl]+
648	M+

Filename: Br6Cl_MBP

Name: dimethyl bipyrrole 4Br (DMBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1514.5, RT (s) (2D): 1.885

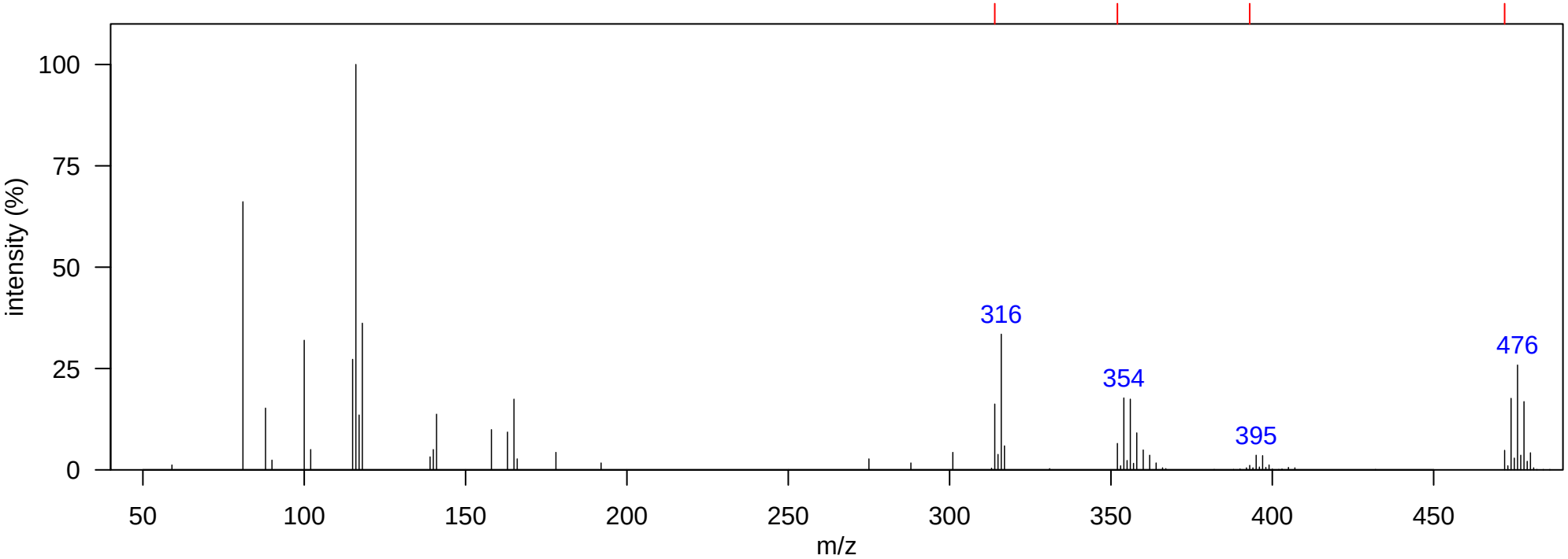
Comment:

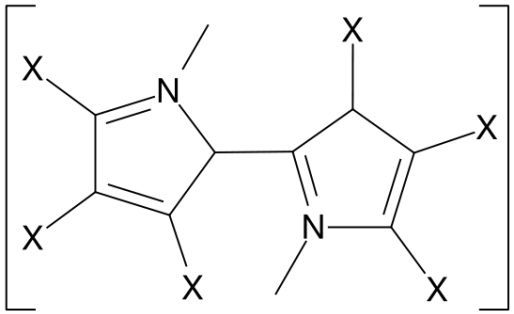
Elemental Formula: C10H8Br4N2

Source: natural

Class: DMBP

Identification: Manual − Congener Group





X=4Br, 2H

m/z	Identity
314	[M−2Br]+
352	[M−BrCNCH3]+
393	[M−Br]+
472	M+

Filename: 4Br_DMBP_isomer_1

Name: dimethyl bipyrrole 4Br (DMBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1626.5, RT (s) (2D): 3.491

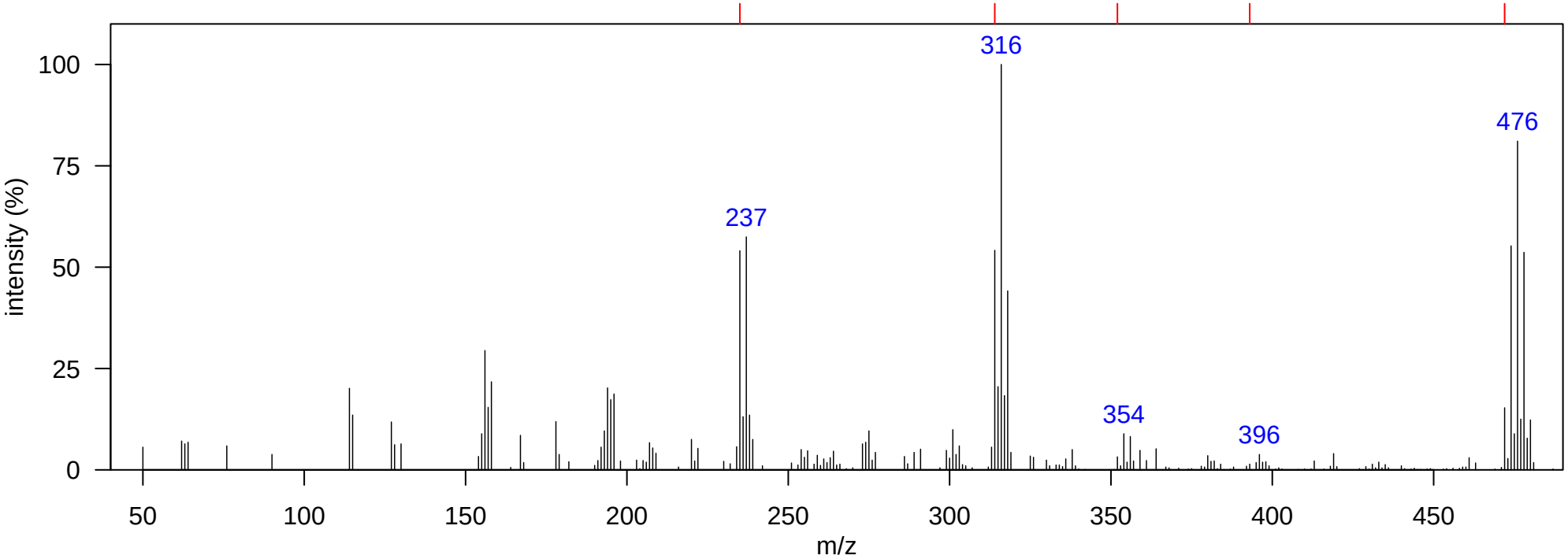
Comment:

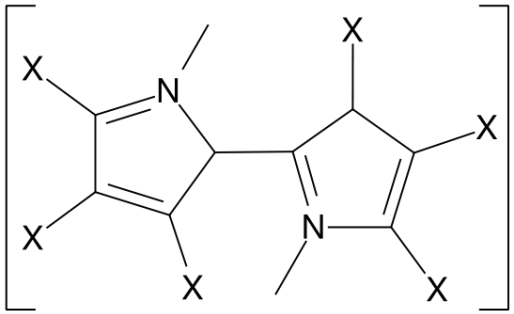
Elemental Formula: C10H8Br4N2

Source: natural

Class: DMBP

Identification: Manual − Congener Group





X=4Br, 2H

m/z	Identity
235	[M−3Br]+
314	[M−2Br]+
352	[M−BrCNCH3]+
393	[M−Br]+
472	M+
498	interference

Filename: 4Br_DMBP_isomer_2

Name: dimethyl bipyrrole 5Br (DMBP) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1672, RT (s) (2D): 2.831

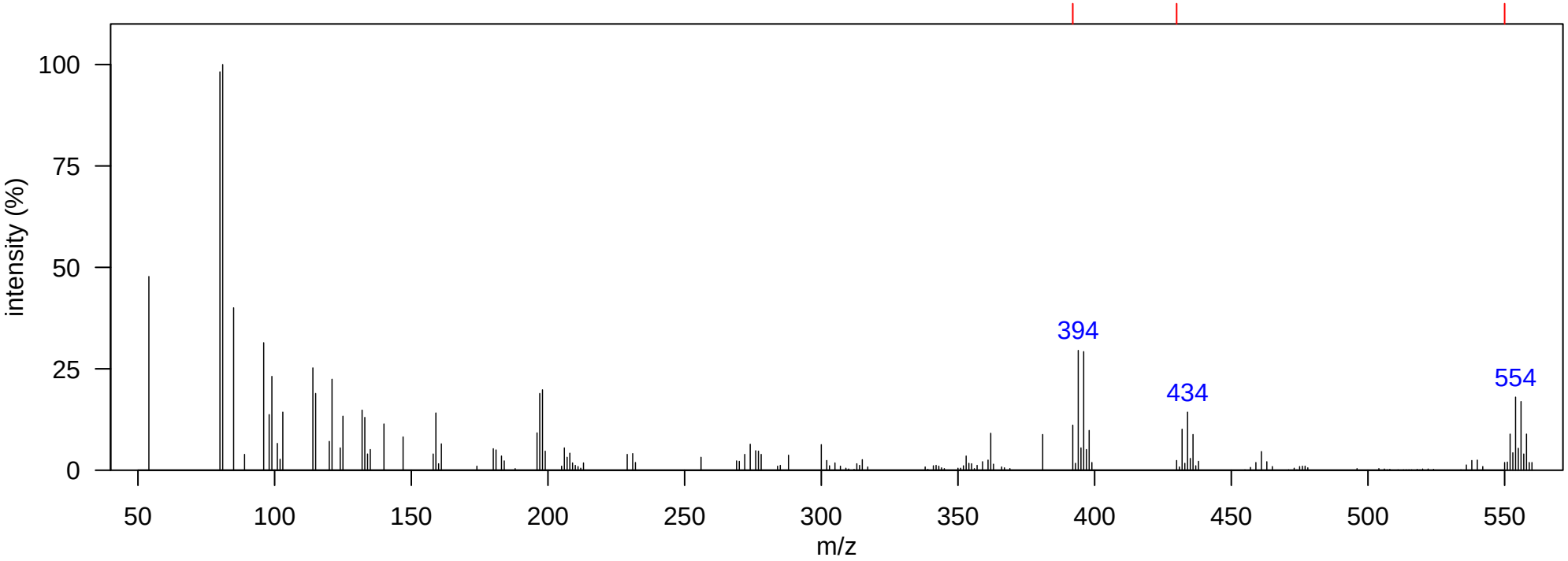
Comment:

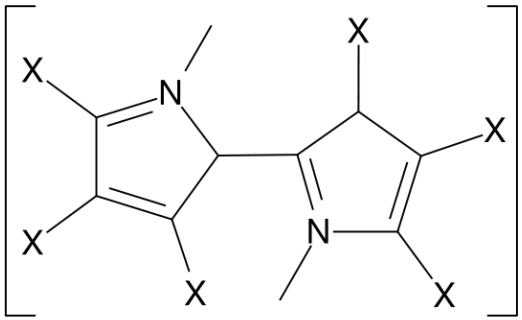
Elemental Formula: C10H7Br5N2

Source: natural

Class: DMBP

Identification: Manual − Congener Group





X=5Br, H

m/z	Identity
392	[M−2Br]+
430	[M−BrCNCH3]+
550	M+

Filename: 5Br_DMBP_isomer_1

Name: dimethyl bipyrrole 5Br (DMBP) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1731.5, RT (s) (2D): 0.123

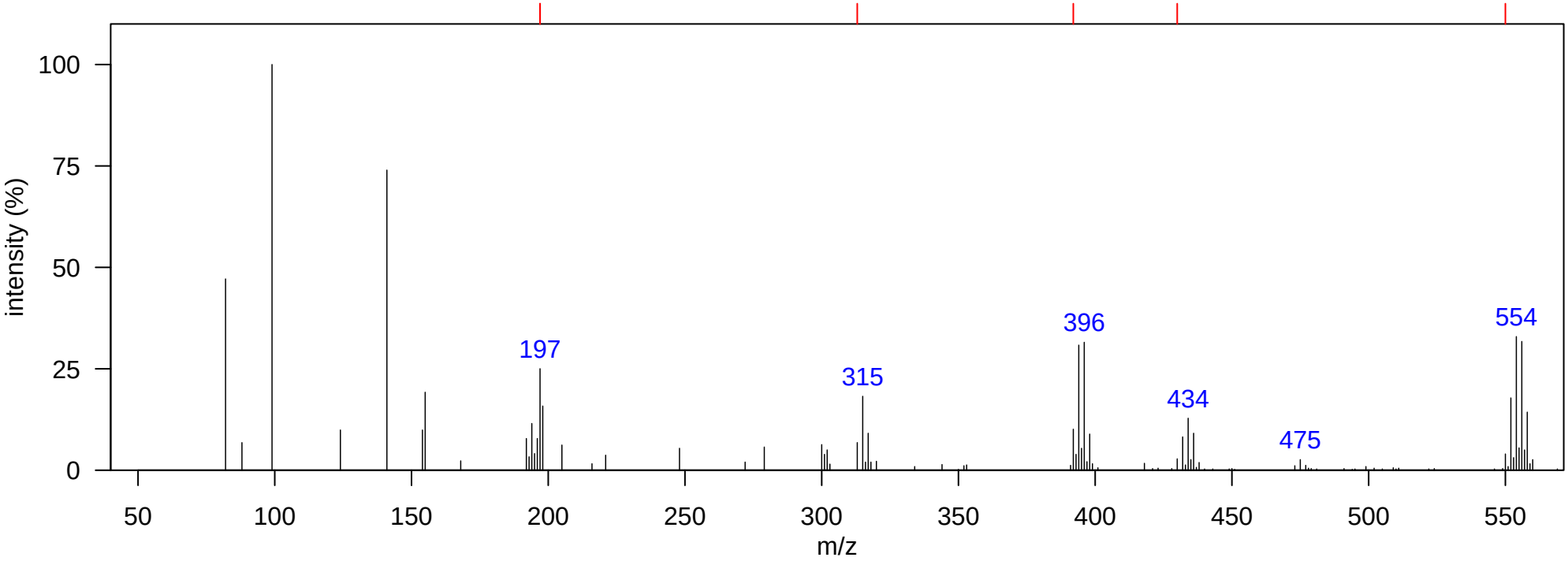
Comment:

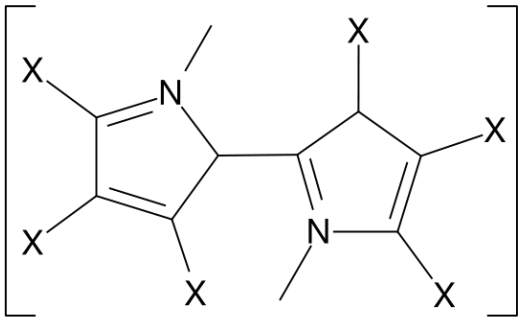
Elemental Formula: C10H7Br5N2

Source: natural

Class: DMBP

Identification: Manual − Congener Group





X=5Br, H

m/z	Identity
197	[M−2Br]2+
313	[M−3Br]+
392	[M−2Br]+
430	[M−BrCNCH3]+
550	M+

Filename: 5Br_DMBP_isomer_2

Name: dimethyl bipyrrole 5Br (DMBP) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1752.5, RT (s) (2D): 2.665

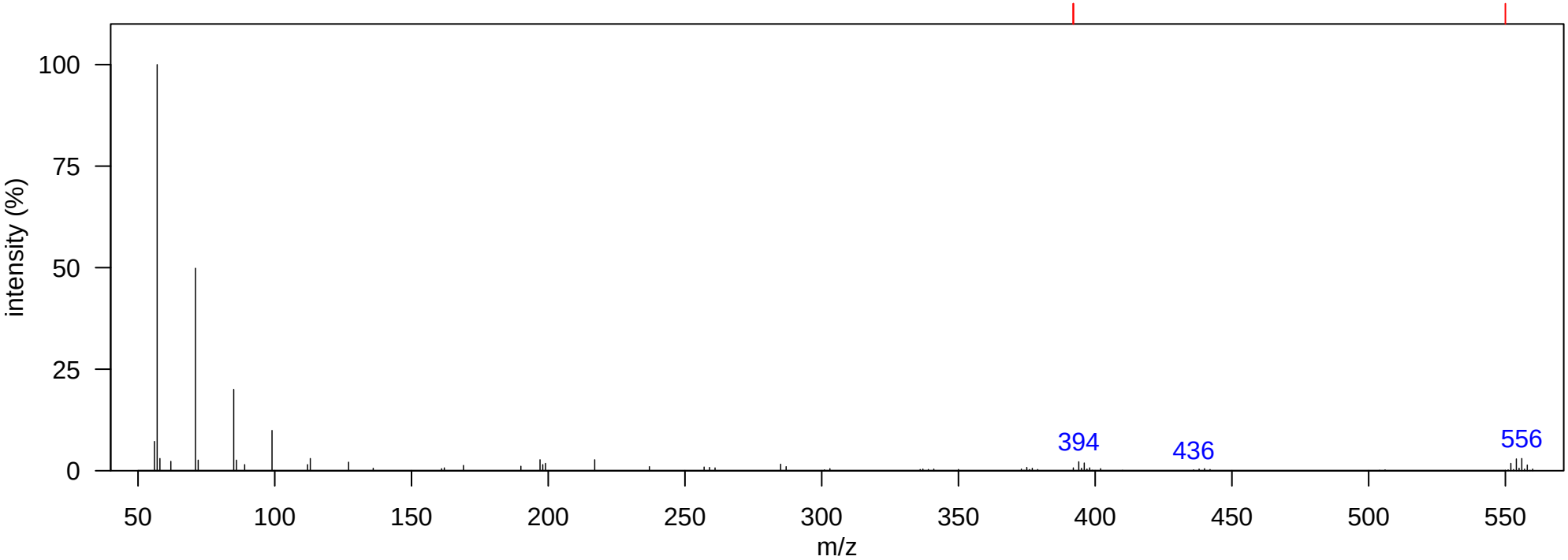
Comment: Low intensity, but visible in raw data.

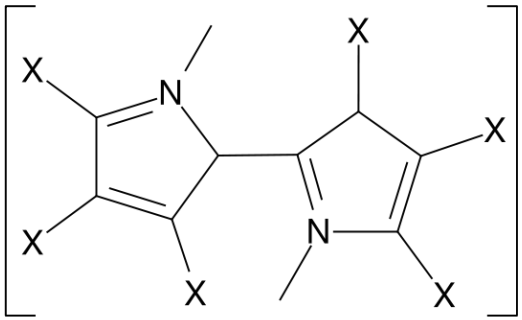
Elemental Formula: C10H7Br5N2

Source: natural

Class: DMBP

Identification: Manual − Congener Group





X=5Br, H

m/z	Identity
392	[M−2Br]+
550	M+

Filename: 5Br_DMBP_isomer_3

Name: dimethyl bipyrrole 6Br (DMBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1822.5, RT (s) (2D): 0.451

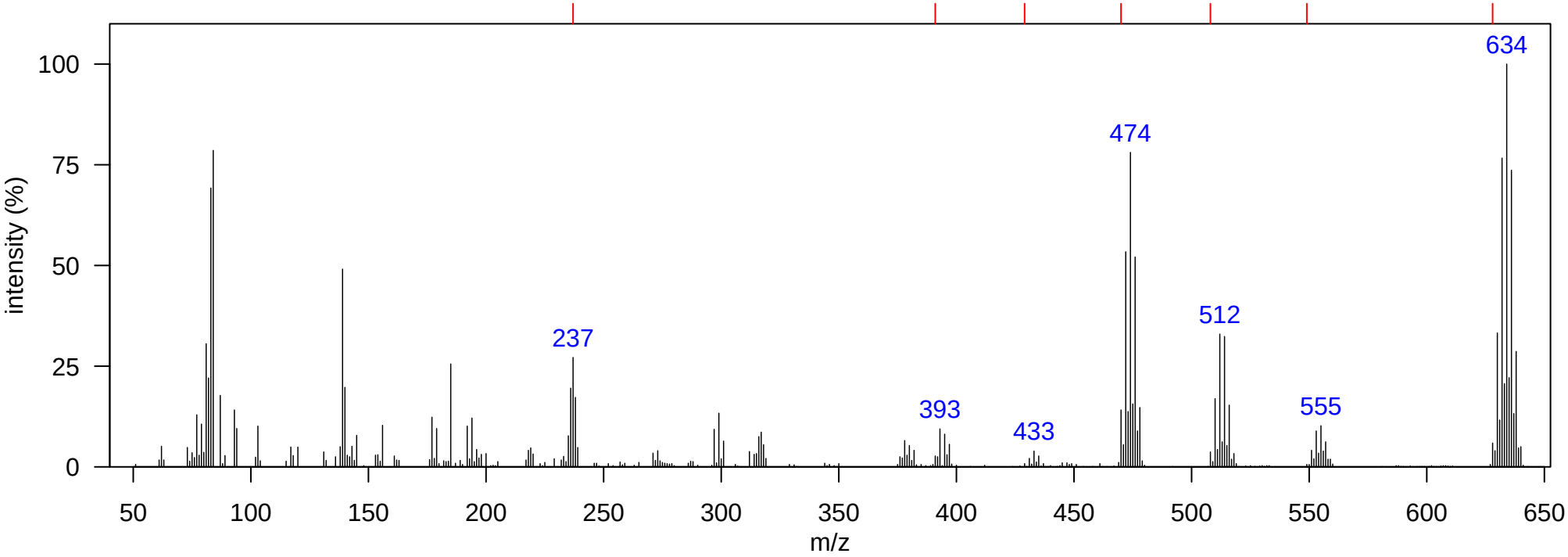
Comment:

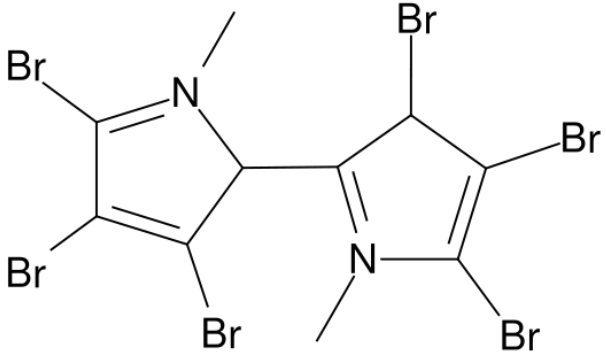
Elemental Formula: C10H6Br6N2

Source: natural

Class: DMBP

Identification: Authentic MS RT





m/z	Identity
237	[M−2Br]2+
391	[M−3Br]+
429	[M−BrCNCH3−Br]+
470	[M−2Br]+
508	[M−BrCNCH3]+
549	[M−Br]+
628	M+

Filename: 6Br_DMBP

Name: dimethyl bipyrrole Br2Cl4 (DMBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1623, RT (s) (2D): 2.19

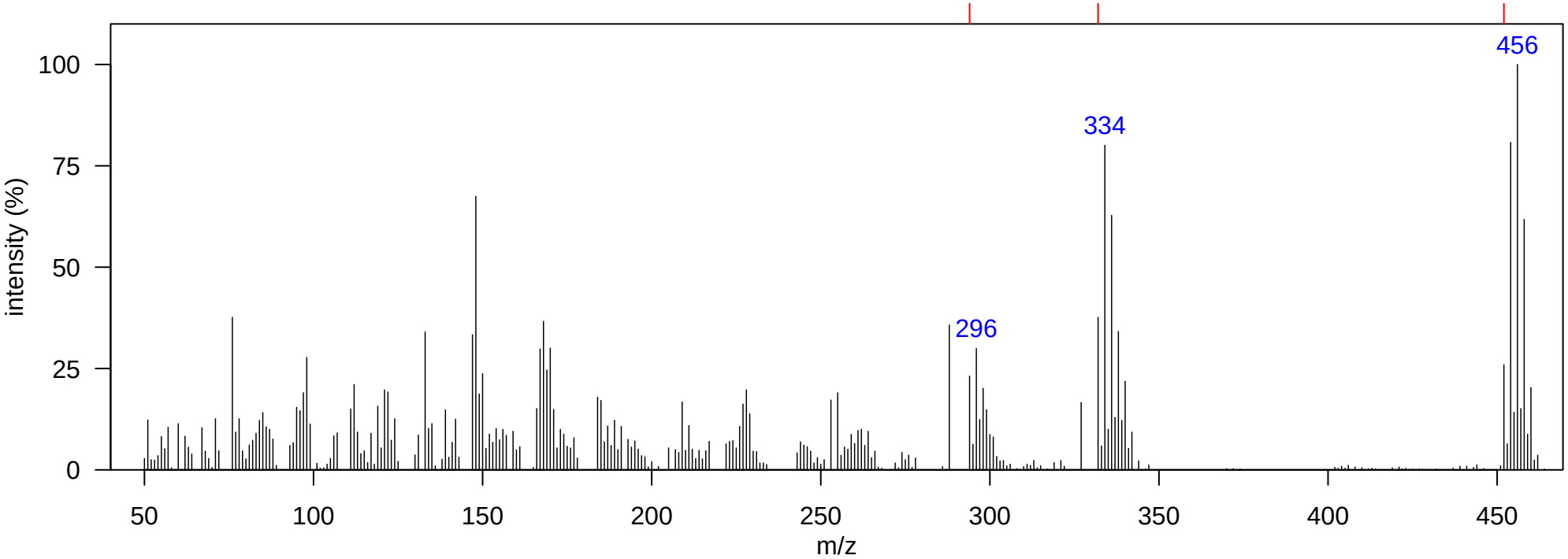
Comment:

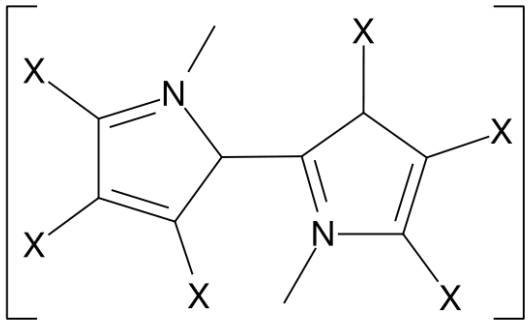
Elemental Formula: C10H6Br2Cl4N2

Source: natural

Class: DMBP

Identification: Manual − Congener Group





X=2Br, 4Cl

m/z	Identity
294	[M−2Br]+
332	[M−BrCNCH3]
452	M+

Name: dimethyl bipyrrole Br3Cl2 (DMBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1570.5, RT (s) (2D): 1.986

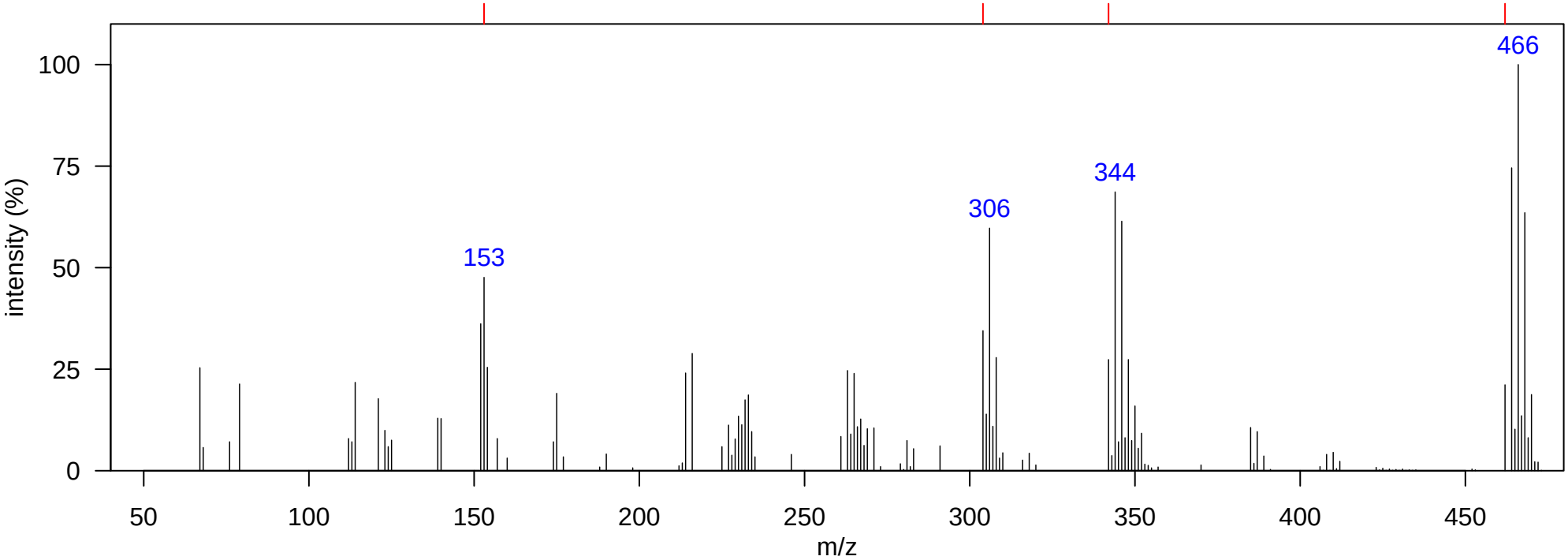
Comment:

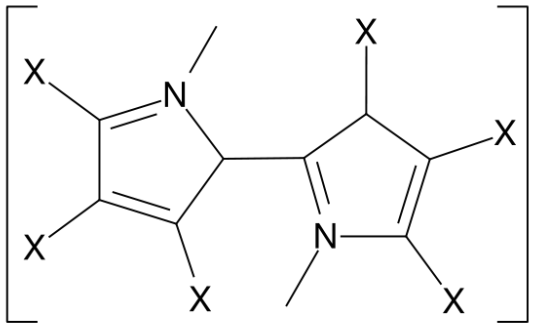
Elemental Formula: C10H7Br3Cl2N2

Source: natural

Class: DMBP

Identification: Manual − Congener Group





X=3Br, 2Cl, H

m/z	Identity
153	[M−2Br]2+
304	[M−2Br]+
342	[M−BrCNCH3]+
462	M+

Filename: Br3Cl2_DMBP

Name: dimethyl bipyrrole Br4Cl2 (DMBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1721, RT (s) (2D): 2.944

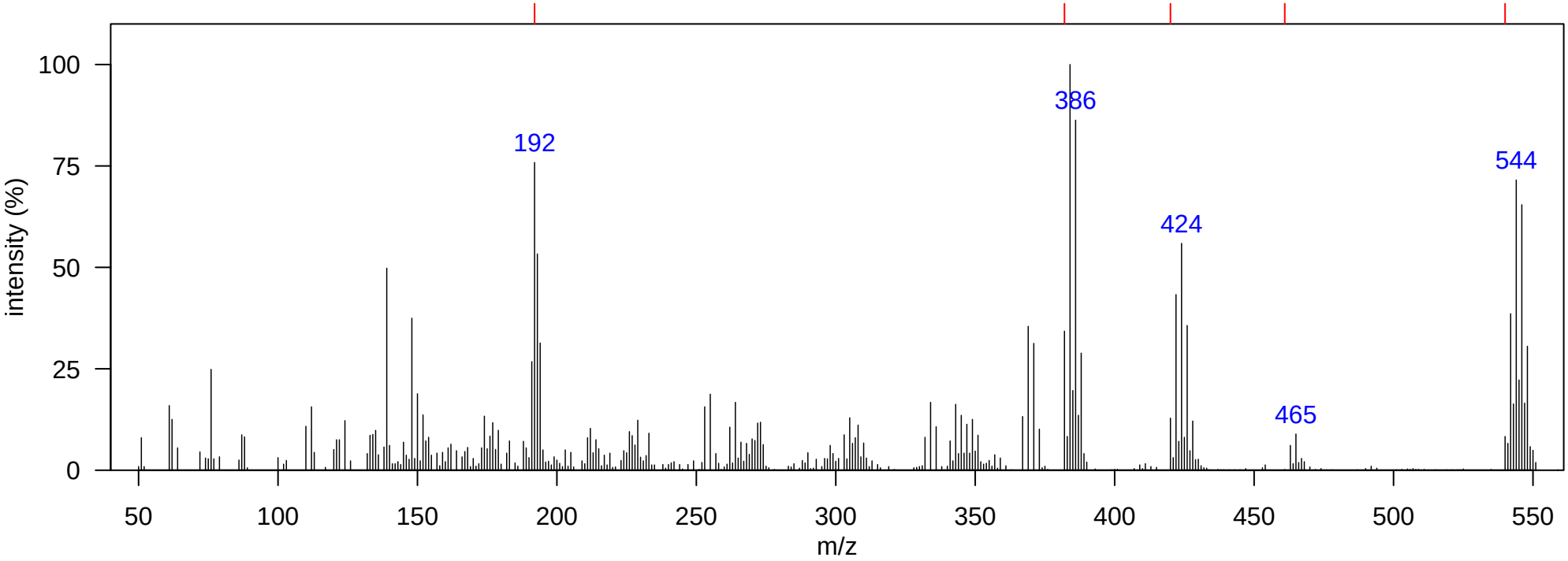
Comment:

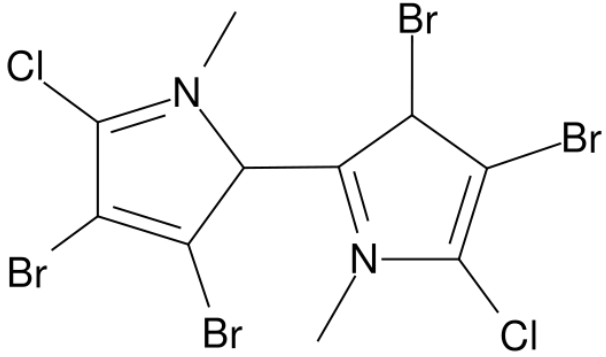
Elemental Formula: C10H6Br4Cl2N2

Source: natural

Class: DMBP

Identification: Authentic MS RT





m/z	Identity
192	[M−2Br]2+
382	[M−2Br]+
420	[M−BrCNCH3]+
461	[M−Br]+
540	M+

Filename: Br4Cl2_DMBP

Name: dimethyl bipyrrole Br5Cl (DMBP)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1773.5, RT (s) (2D): 0.058

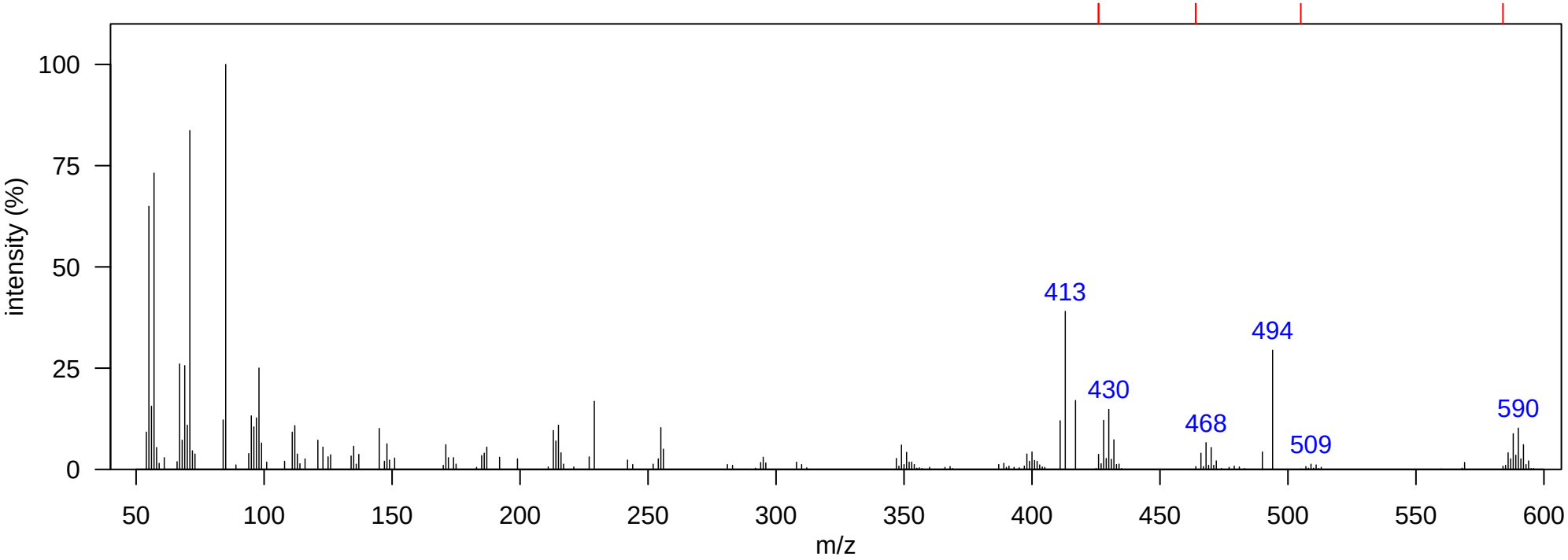
Comment:

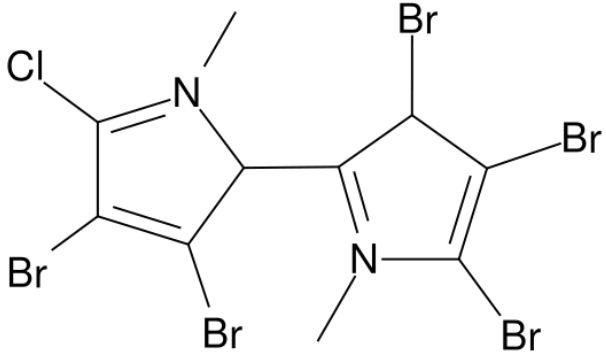
Elemental Formula: C10H6Br5ClN2

Source: natural

Class: DMBP

Identification: Authentic MS RT





m/z	Identity
426	[M−2Br]+
464	[M−BrCNCH3]+
505	[M−Br]+
584	M+

Filename: Br5Cl_DMBP

Name: tribromophenol

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1171.5, RT (s) (2D): 1.59

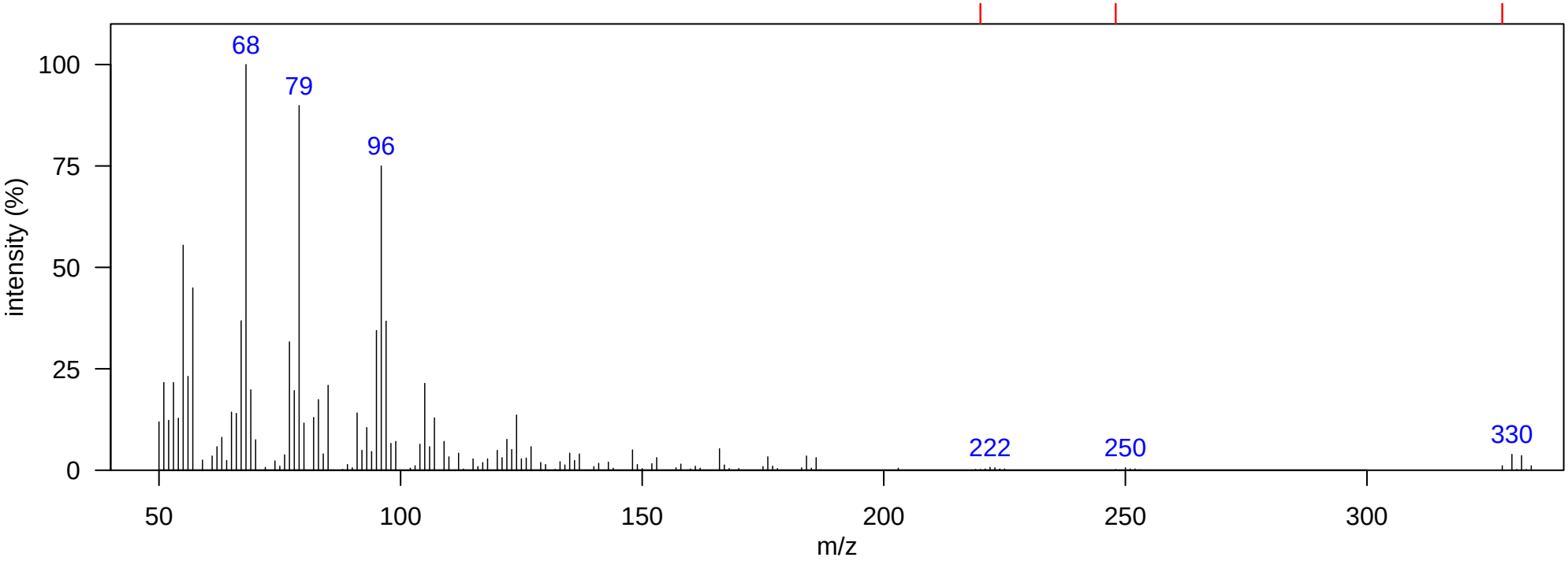
Comment: Low intensity, but visible in raw data.

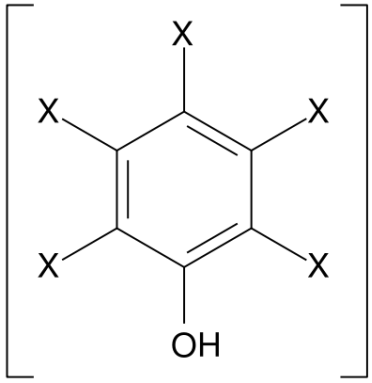
Elemental Formula: C6H3Br3O

Source: natural/anthropogenic

Class: bromophenol

Identification: Reference Database MS





X=3Br, 2H

m/z	Identity
220	[M−H−Br−CO]+
248	[M−HBr]+
328	M+

Filename: tribromophenol

Name: tribromoanisole: Benzene, 1,3,5−tribromo−2−methoxy−

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1154, RT (s) (2D): 1.161

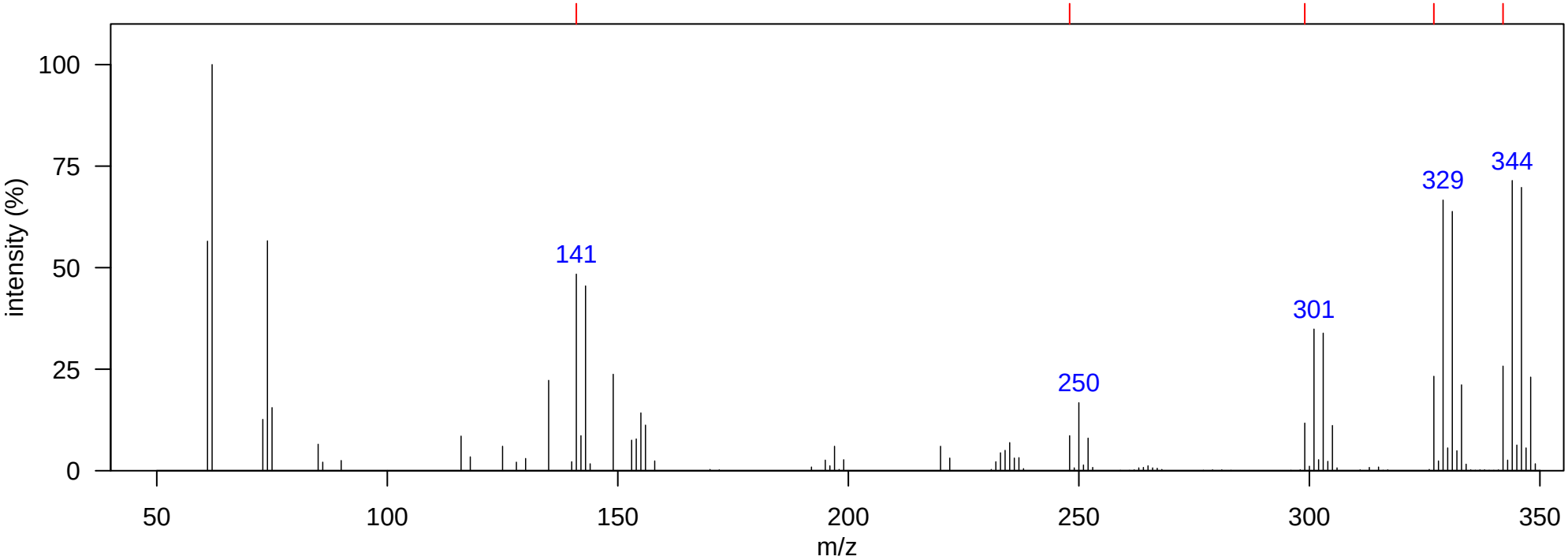
Comment:

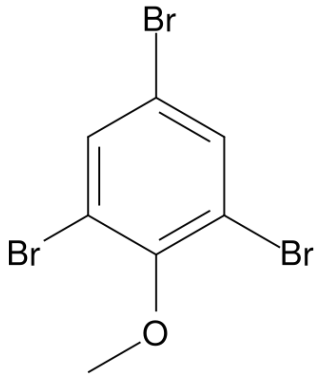
Elemental Formula: C7H5Br3O

Source: natural

Class: brominated anisole

Identification: Authentic MS RT





m/z	Identity
141	[C5H2Br]+
248	[M−Br−CH3]+
299	[M−CH3−CO]+
327	[M−CH3]+
342	M+

Name: bromoindole

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1175, RT (s) (2D): 2.139

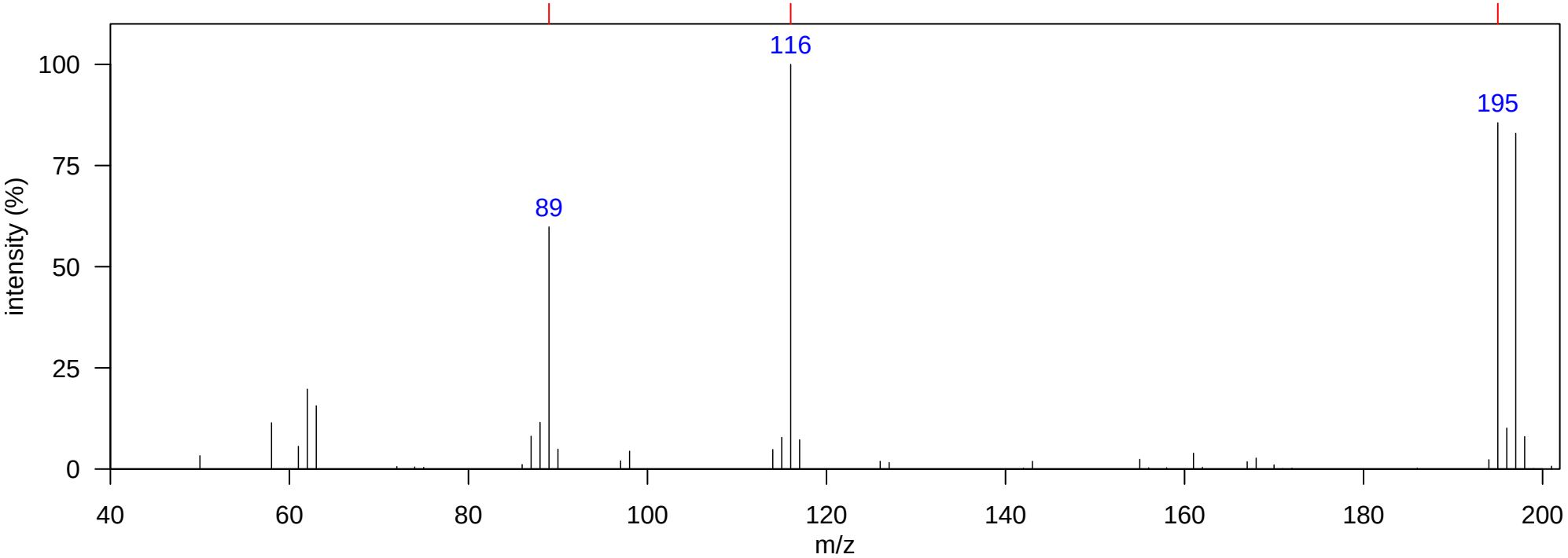
Comment:

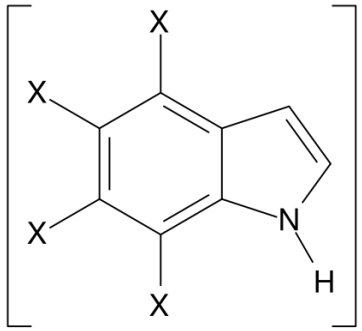
Elemental Formula: C8H6BrN

Source: natural

Class: brominated indole

Identification: Authentic MS





X=Br, 3H

m/z	Identity
89	[M−Br−CNH]+
116	[M−Br]+
195	M+

Filename: bromoindole

Name: dibromoindole isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1325.5, RT (s) (2D): 1.88

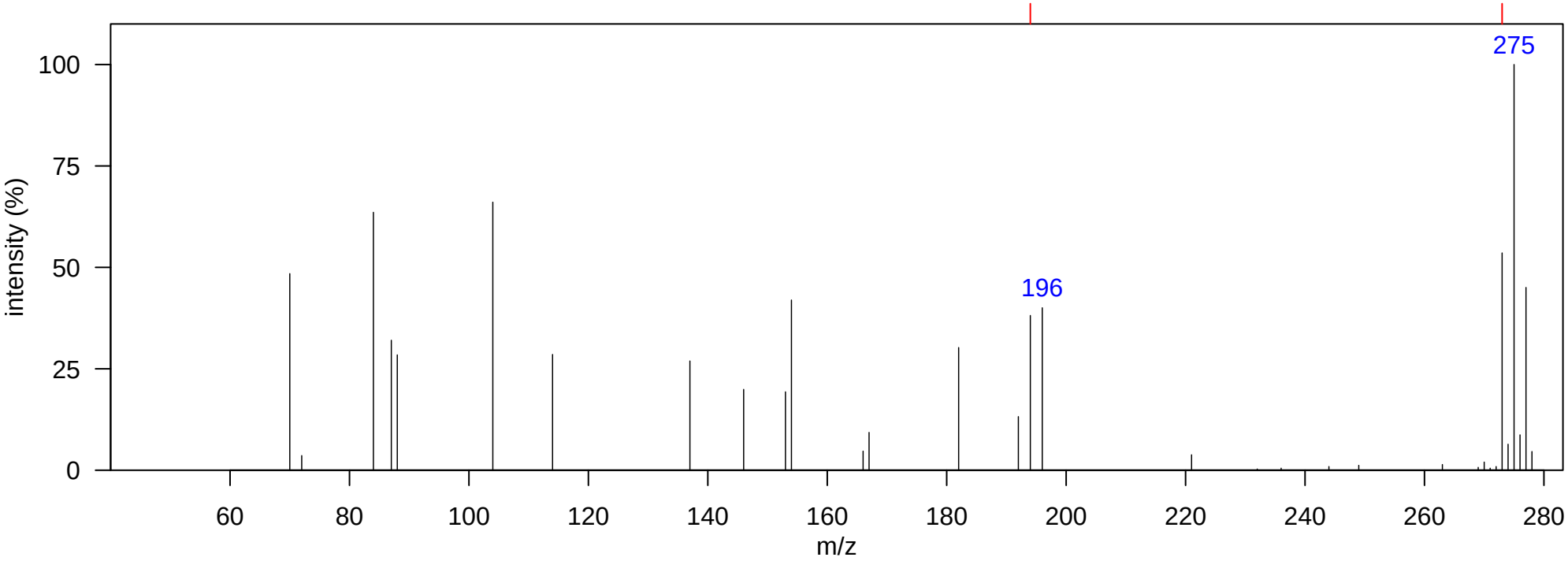
Comment:

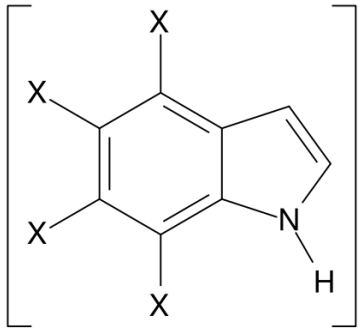
Elemental Formula: C8H5Br2N

Source: natural

Class: brominated indole

Identification: Authentic MS





X=2Br, 2H

m/z	Identity
194	[M−Br]+
273	M+

Filename: dibromoindole_isomer_1

Name: dibromoindole isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1406, RT (s) (2D): 2.674

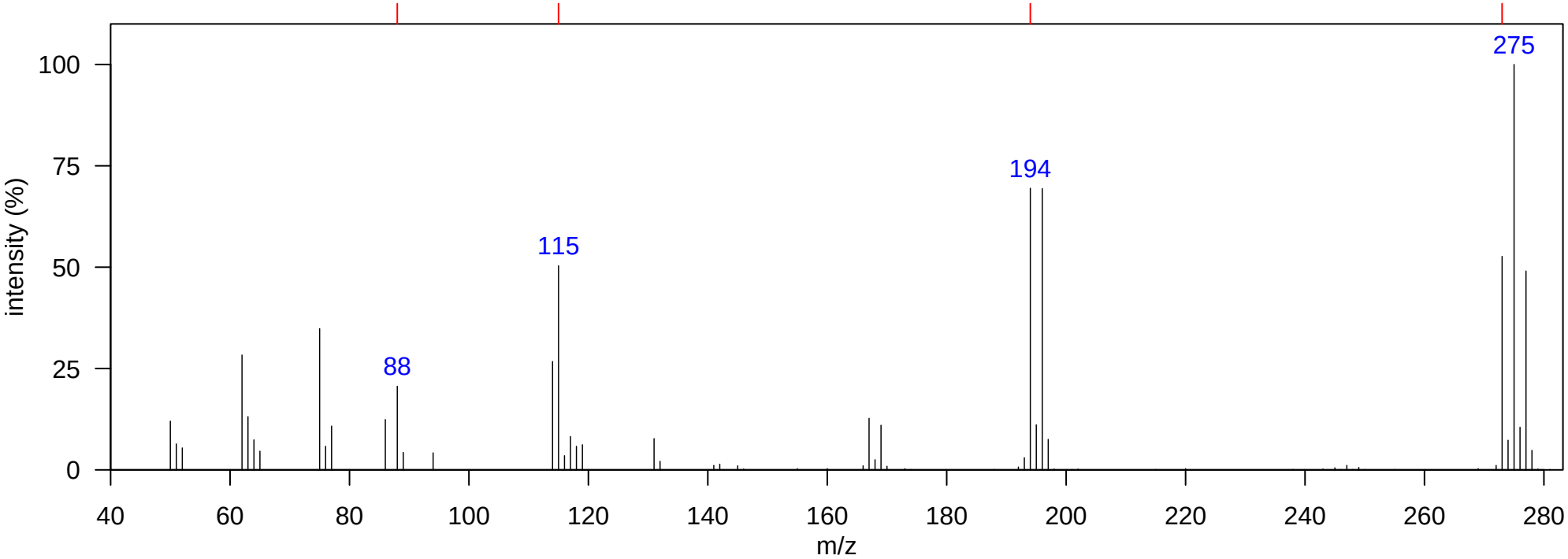
Comment:

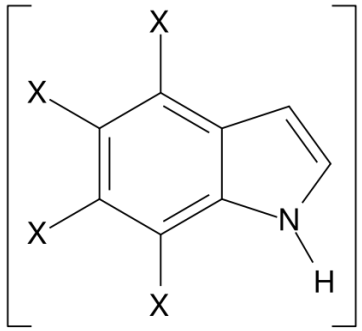
Elemental Formula: C8H5Br2N

Source: natural

Class: brominated indole

Identification: Authentic MS





X=2Br, 2H

m/z	Identity
88	[M−2Br−CNH]+
115	[M−2Br]+
194	[M−Br]+
273	M+

Filename: dibromoindole_isomer_2

Name: dimethoxy brominated biphenyl 4Br (2MeO−BB−80)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1721, RT (s) (2D): 2.209

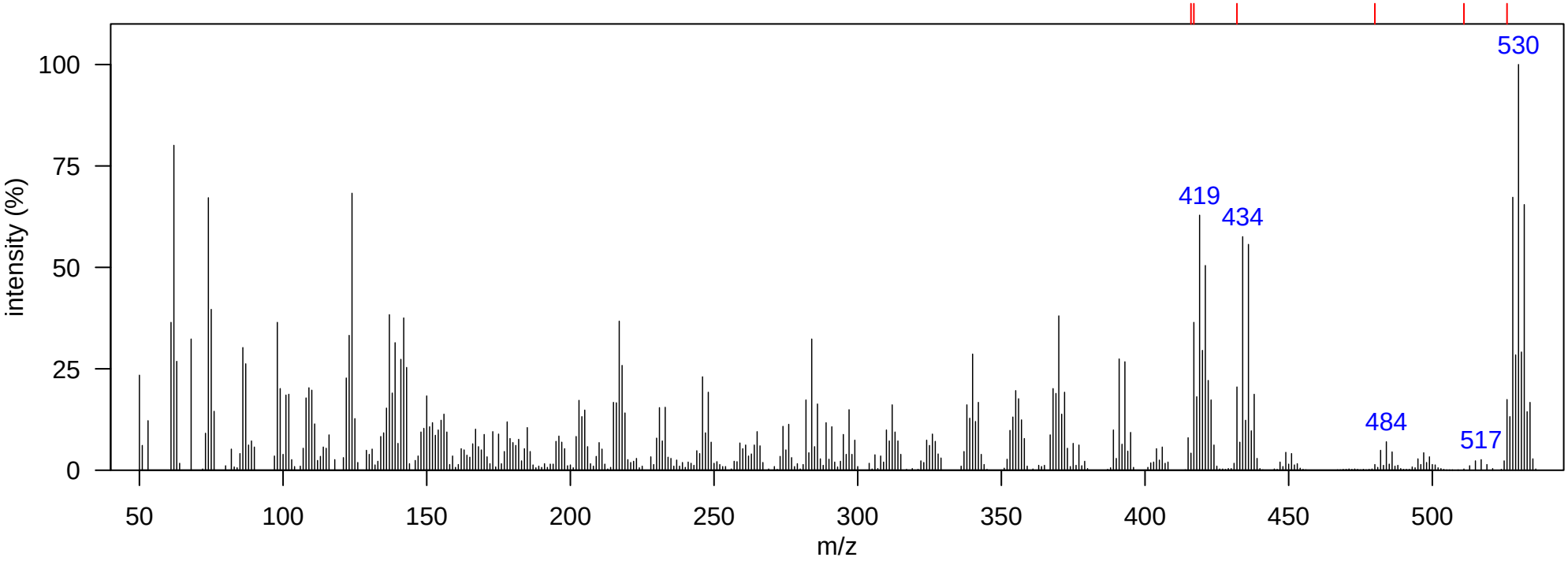
Comment:

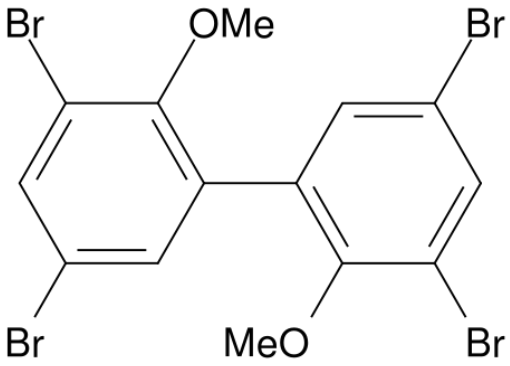
Elemental Formula: C14H10Br4O2

Source: natural

Class: 2MeO−BB

Identification: Authentic MS RT





m/z	Identity
416	[M−CH3−Br−O]+
417	[M−CH3−CH3−Br]+
432	[M−CH3−Br]+
480	[M−CH3−CH3−O]+
511	[M−CH3]+
526	M+

Filename: 4Br_2MeOBB80

Name: polybrominated hexahydroxanthene 3Br (PBHD)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1819, RT (s) (2D): 3.242

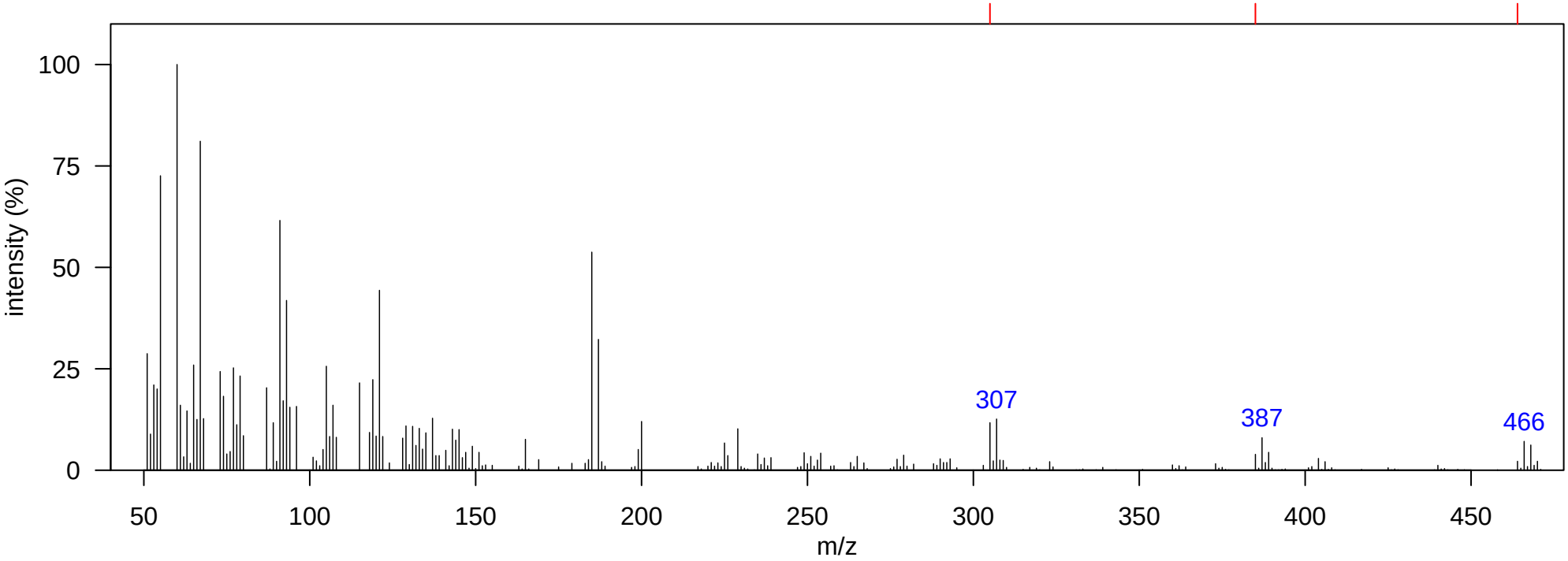
Comment: Low intensity, but visible in raw data.

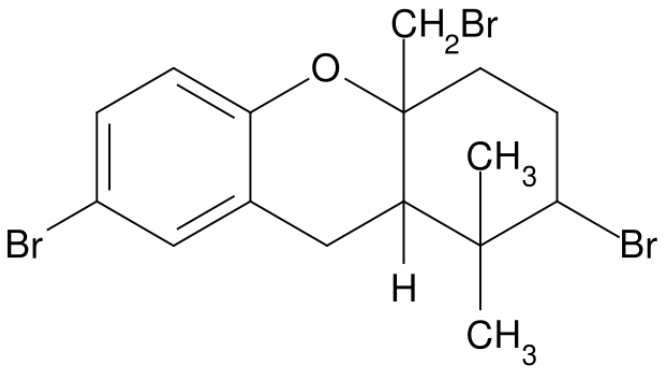
Elemental Formula: C16H16Br3O

Source: natural

Class: PBHD

Identification: Authentic MS RT





m/z	Identity
305	[M−HBr2]+
385	[M−Br]+
464	M+

Filename: 3Br_PBHD

Name: polybrominated hexahydroxanthene 4Br (PBHD)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1955.5, RT (s) (2D): 5.659

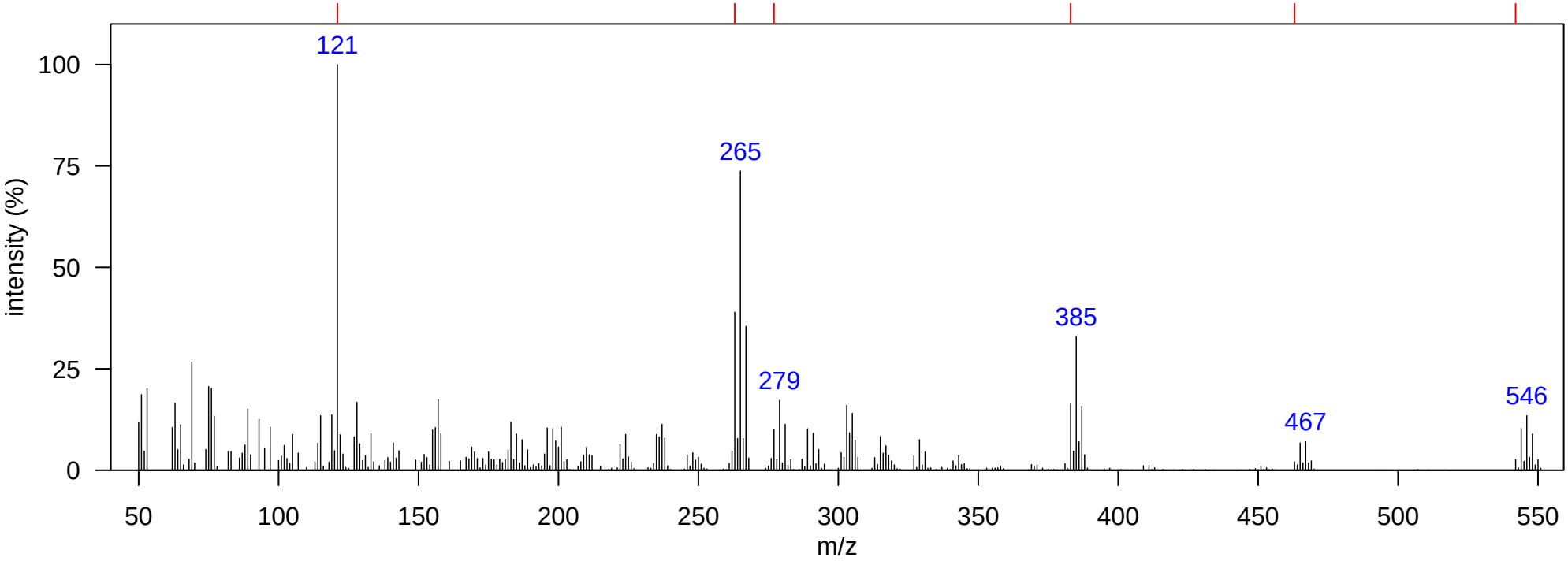
Comment:

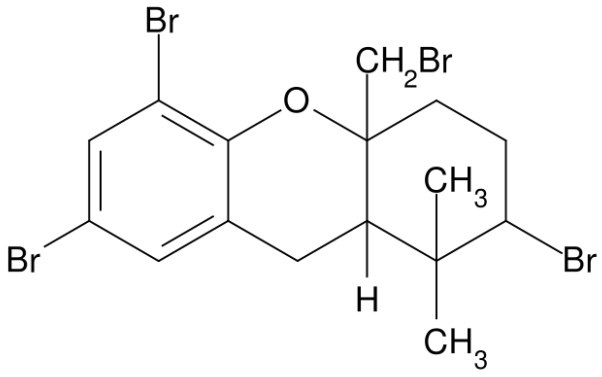
Elemental Formula: C16H15Br4O

Source: natural

Class: PBHD

Identification: Authentic MS RT





m/z	Identity
121	[C9H13]+
263	[C7H5OBr2]+
277	[C9H11Br2]+
383	[M−HBr2]+
463	[M−Br]+
542	M+

Filename: 4Br_PBHD

Name: diphenyl ether Br3Cl (B/CDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1623, RT (s) (2D): 2.088

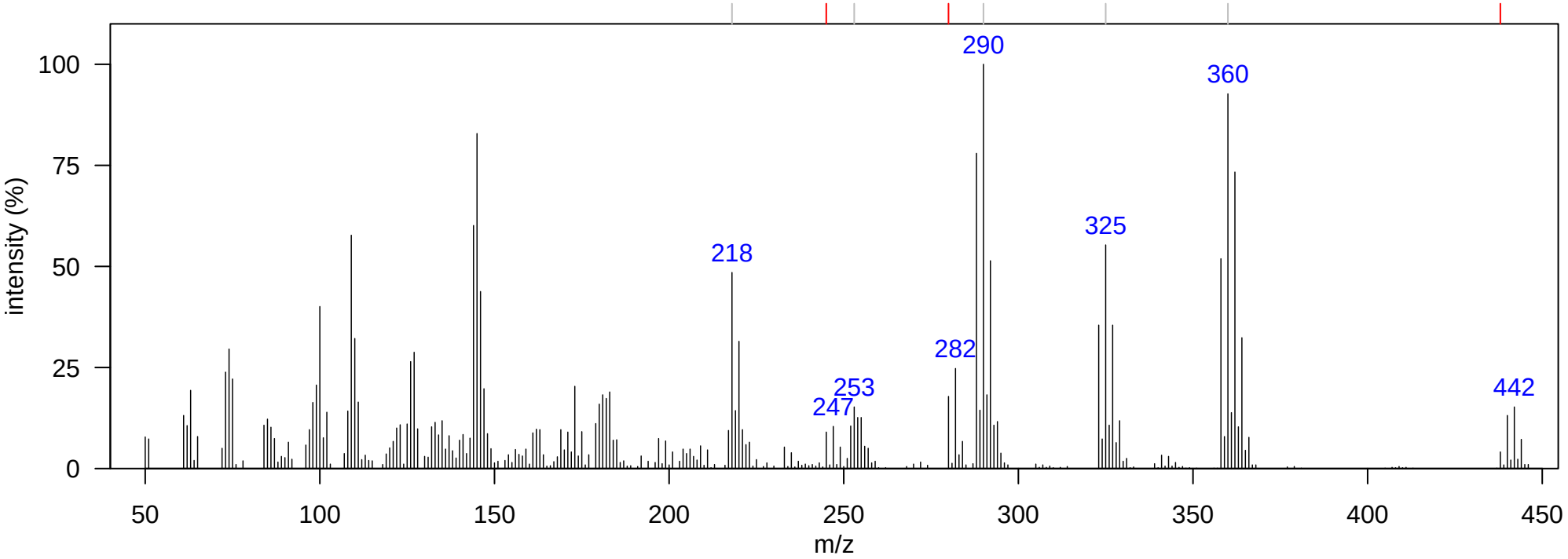
Comment:

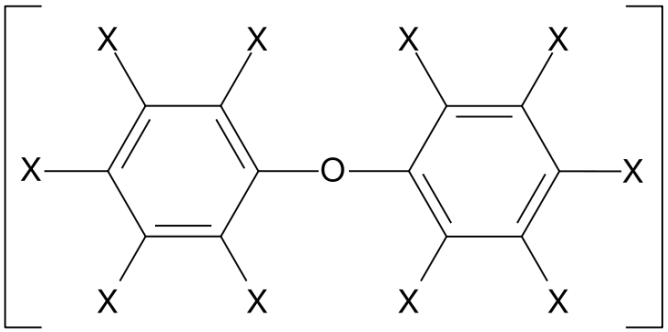
Elemental Formula: C12H6Br3ClO

Source: unknown

Class: B/CDE

Identification: Manual − Congener Group





m/z	Identity
218	PCB interference
245	[M−2Br−Cl]+
253	PCB interference
280	[M−2Br]+
290	PCB interference
325	PCB interference
360	PCB interference
438	M+

Filename: Br3Cl_BCDE_isomer_1

Name: diphenyl ether Br3Cl (B/CDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1623, RT (s) (2D): 2.217

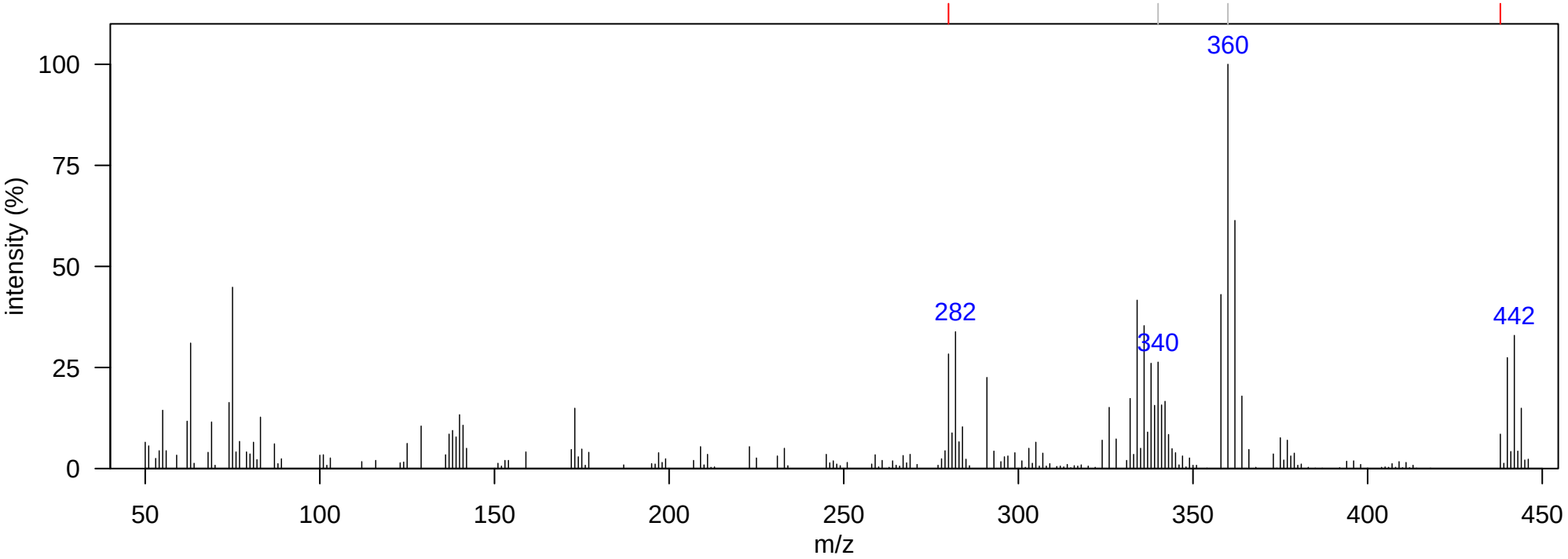
Comment:

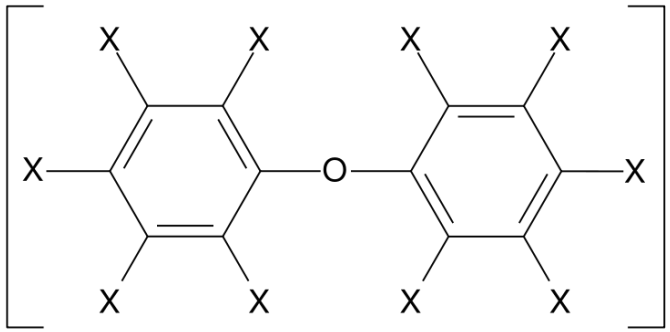
Elemental Formula: C12H6Br3ClO

Source: unknown

Class: B/CDE

Identification: Manual − Congener Group





m/z	Identity
280	[M−2Br]+
340	interference MeO−BB Br3Cl
360	PCB interference
438	M+

Filename: Br3Cl_BCDE_isomer_2

Name: diphenyl ether Br4Cl (B/CDE)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1707, RT (s) (2D): 2.547

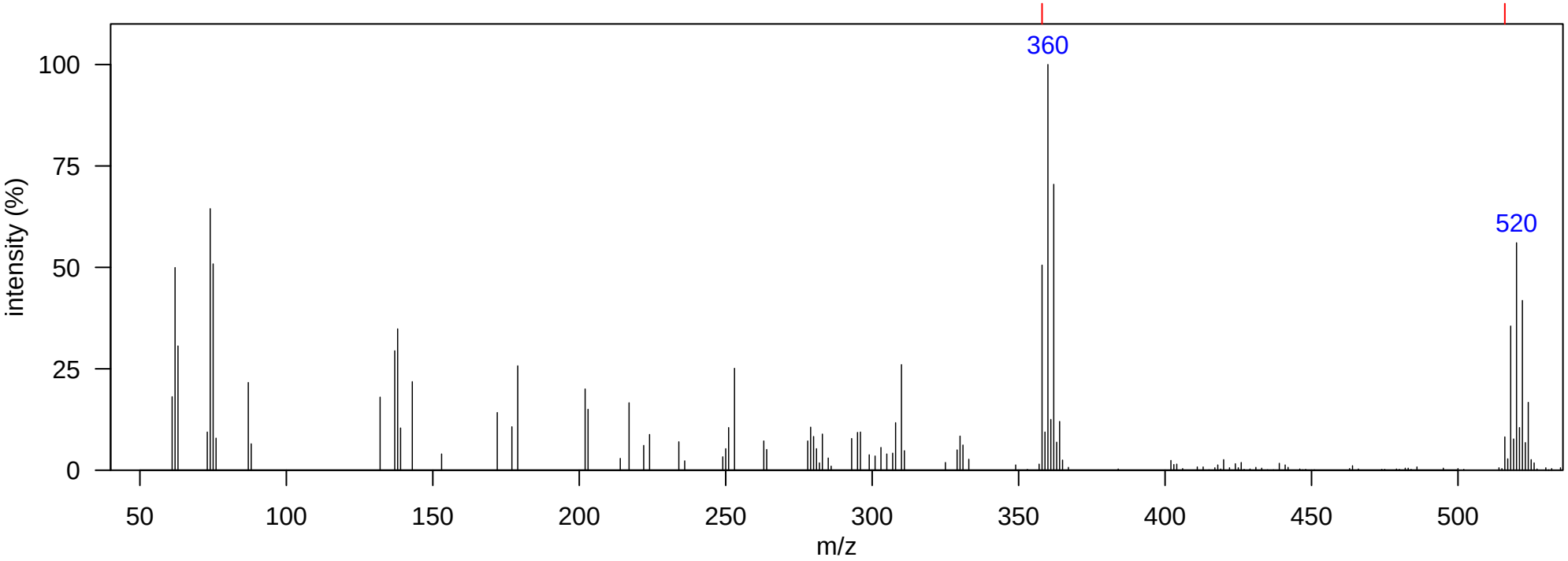
Comment:

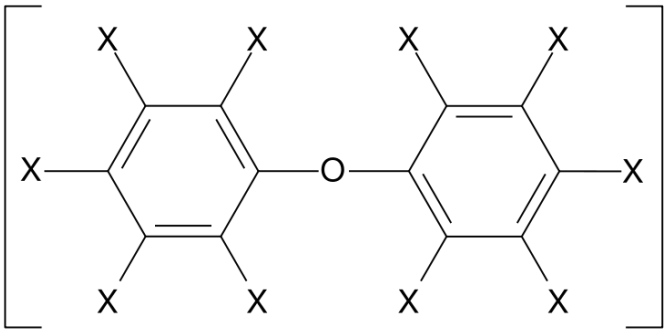
Elemental Formula: C12H5Br4ClO

Source: unknown

Class: B/CDE

Identification: Manual − Congener Group





X=4Br, Cl, 5H

m/z	Identity
358	[M−2Br]+
516	M+

Filename: Br4Cl_BCDE

Name: diphenyl ether Br5Cl (B/CDE) isomer 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1798, RT (s) (2D): 3.069

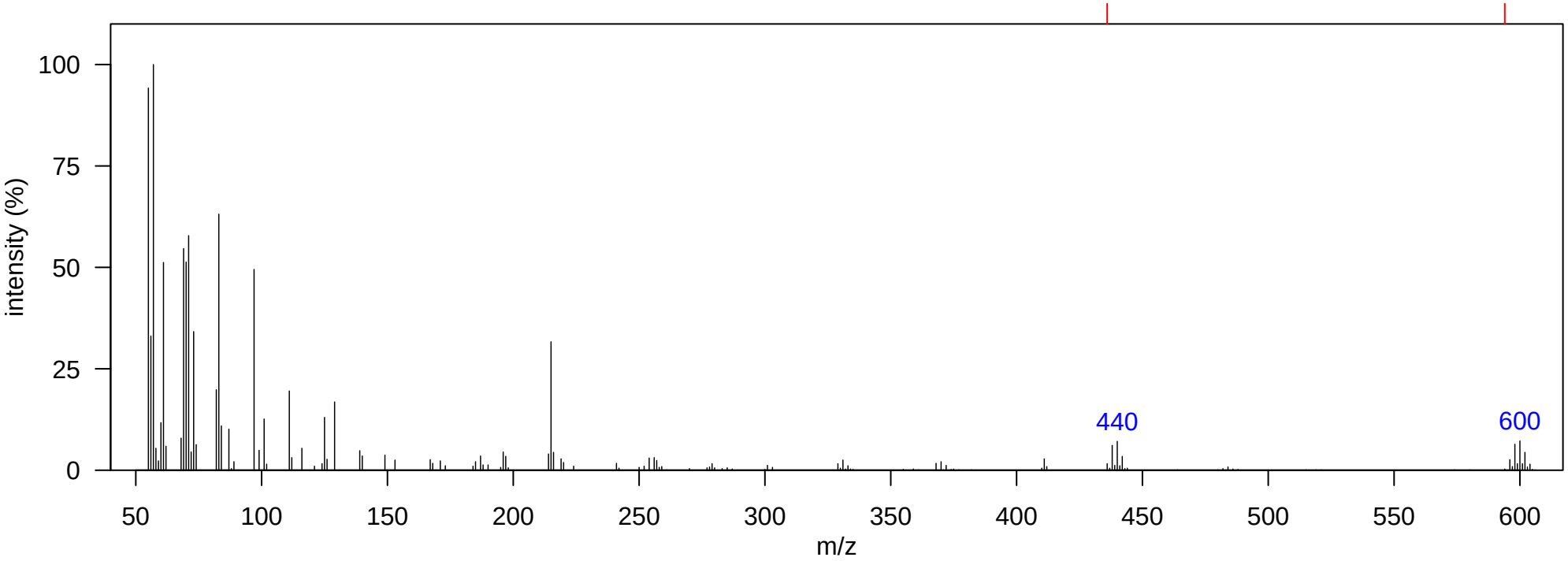
Comment:

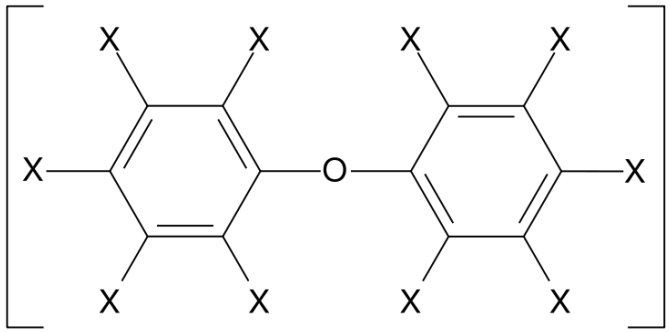
Elemental Formula: C12H4Br5ClO

Source: unknown

Class: B/CDE

Identification: Manual − Congener Group





m/z	Identity
436	[M−2Br]+
594	M+

Filename: Br5Cl_BCDE_isomer_1

Name: diphenyl ether Br5Cl (B/CDE) isomer 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1808.5, RT (s) (2D): 2.947

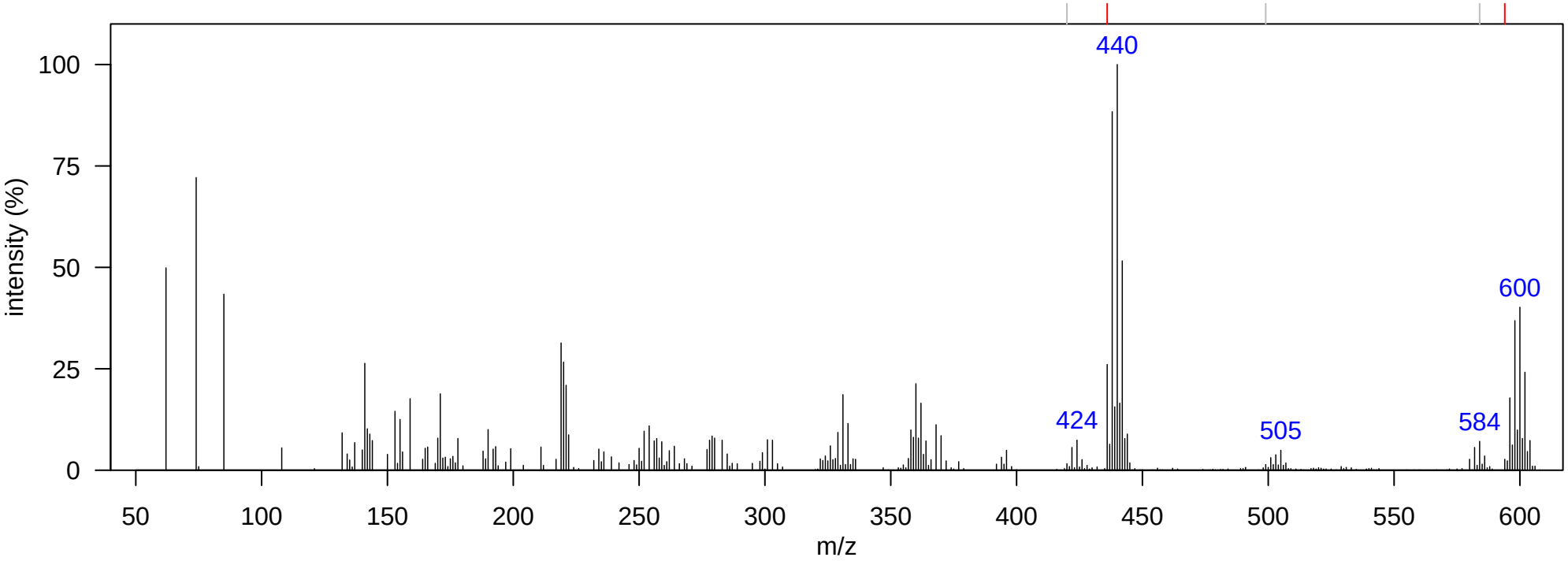
Comment:

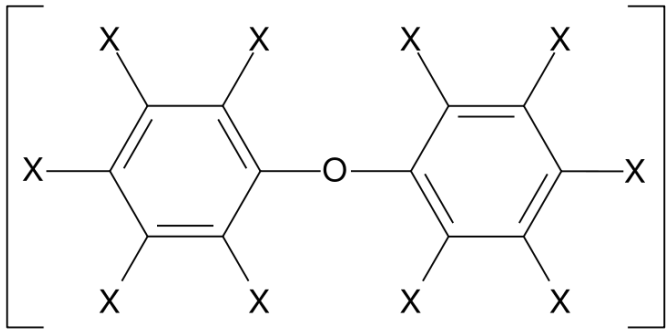
Elemental Formula: C12H4Br5ClO

Source: unknown

Class: B/CDE

Identification: Manual − Congener Group





m/z	Identity
420	likely interference
436	[M−2Br]+
499	likely interference
584	likely interference
594	M+

Filename: Br5Cl_BCDE_isomer_2

Name: diphenyl ether Br5Cl (B/CDE) isomer 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1815.5, RT (s) (2D): 3.042

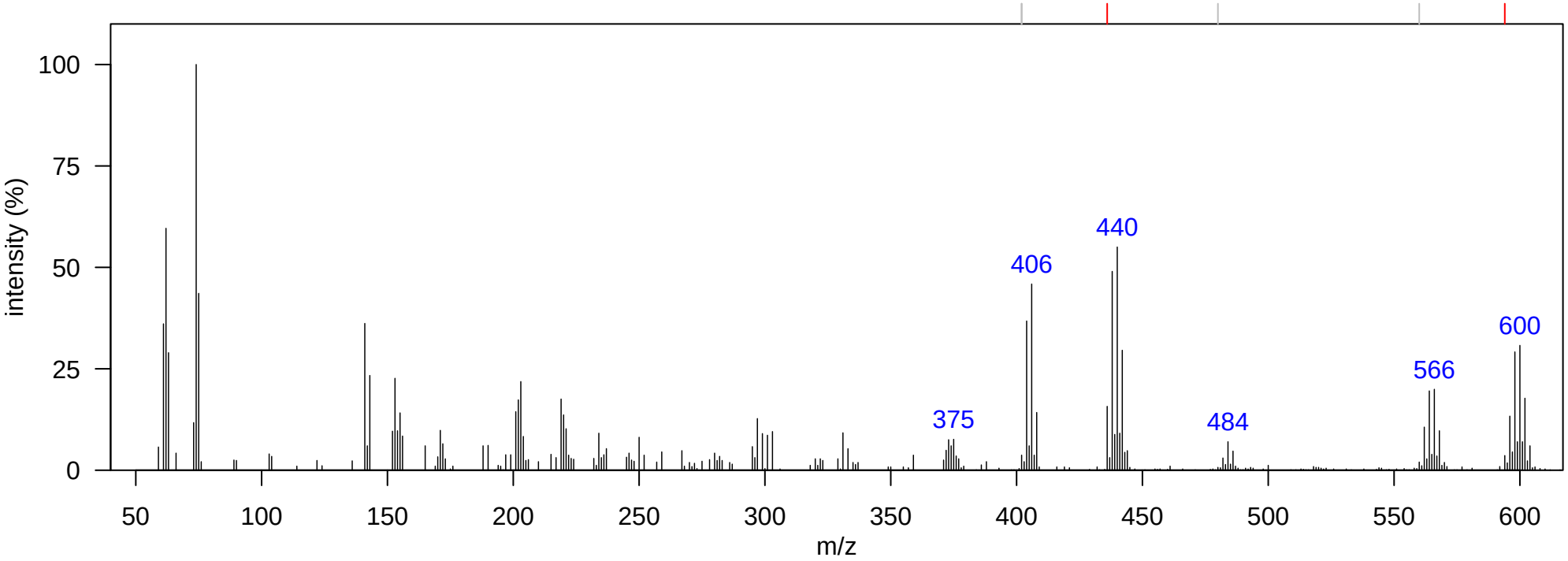
Comment: Co−elution with PBDE (5Br) isomer.

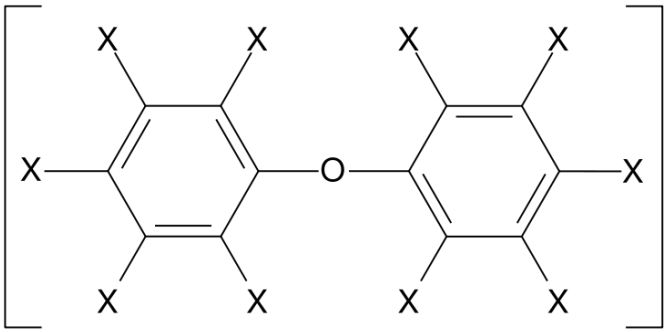
Elemental Formula: C12H4Br5ClO

Source: unknown

Class: B/CDE

Identification: Manual − Congener Group





m/z	Identity
402	interference PBDE(5Br)
436	[M−2Br]+
480	interference PBDE(5Br)
560	interference PBDE(5Br)
594	M+

Filename: Br5Cl_BCDE_isomer_3

Name: diphenyl ether Br5Cl (B/CDE) isomer 4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1857.5, RT (s) (2D): 2.914

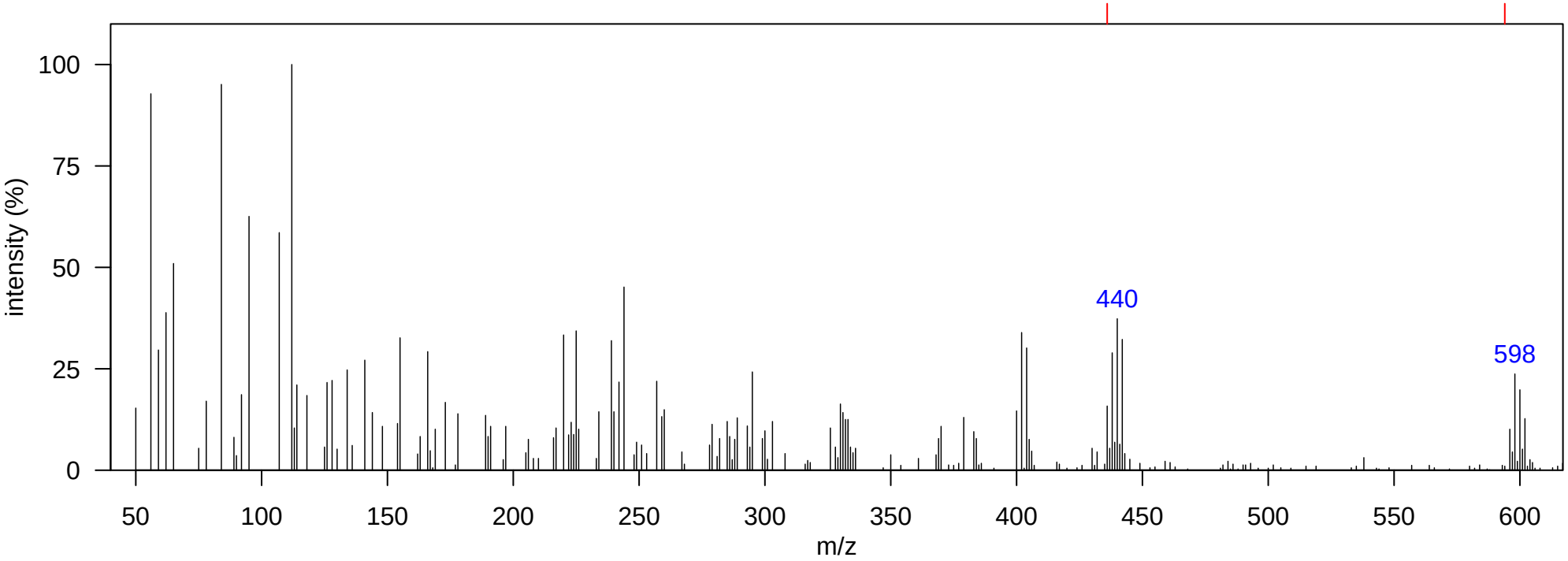
Comment:

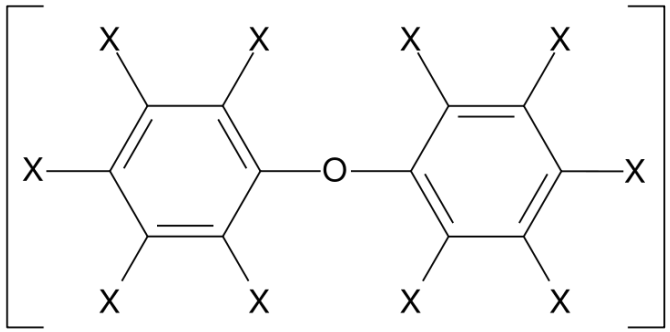
Elemental Formula: C12H4Br5ClO

Source: unknown

Class: B/CDE

Identification: Manual − Congener Group





m/z	Identity
436	[M−2Br]+
594	M+

Filename: Br5Cl_BCDE_isomer_4

Name: pentachloroethylbenzene

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1178.5, RT (s) (2D): 0.779

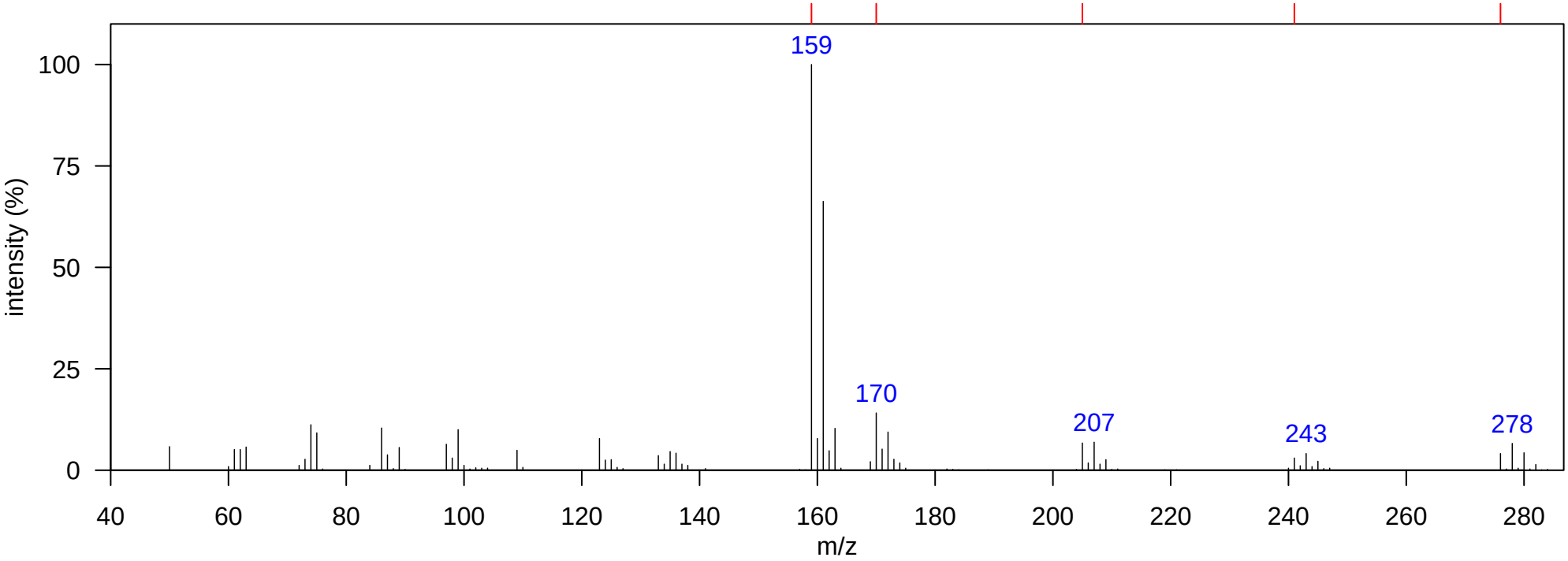
Comment:

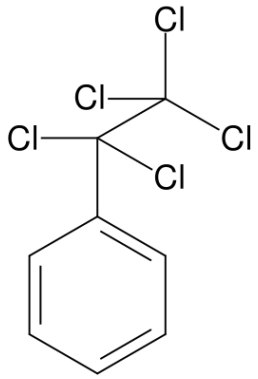
Elemental Formula: C8H5Cl5

Source: unknown

Class: ethylbenzene

Identification: Reference Database MS





m/z	Identity
159	[M−CCl3]+
170	[M−3Cl]+
205	[M−2Cl]+
241	[M−Cl]+
276	M+

Filename: pentachloroethylbenzene

Name: hexachloroethylbenzene

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1318.5, RT (s) (2D): 1.252

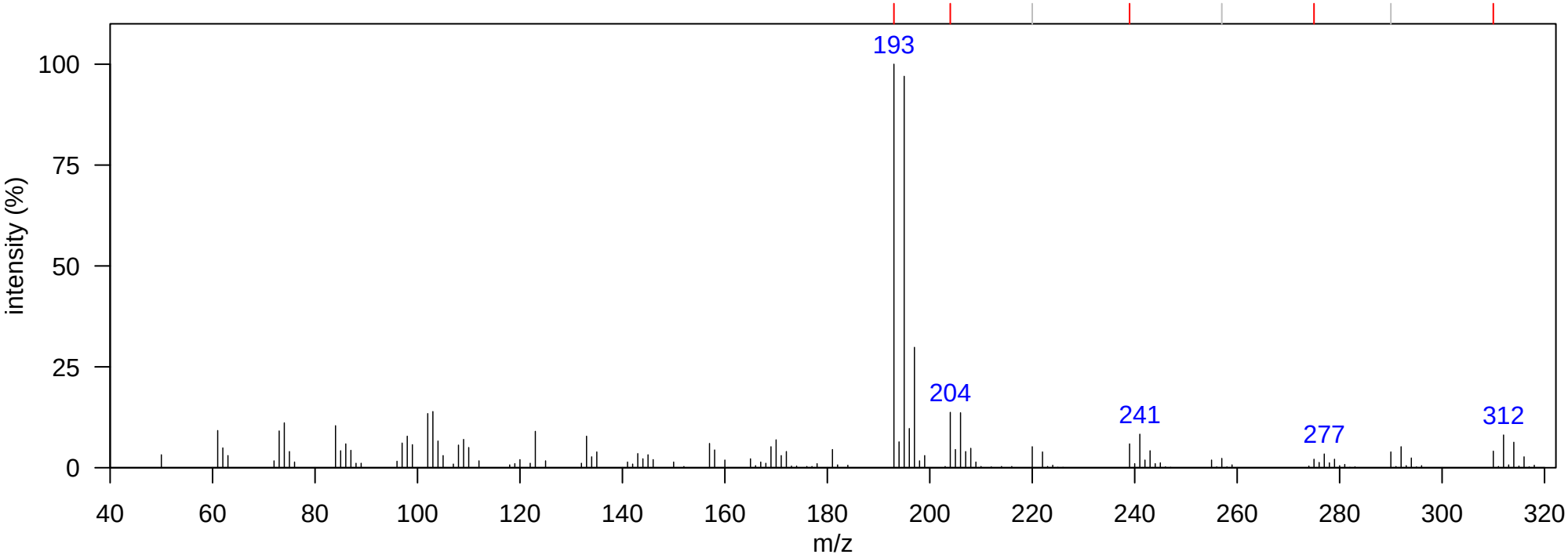
Comment:

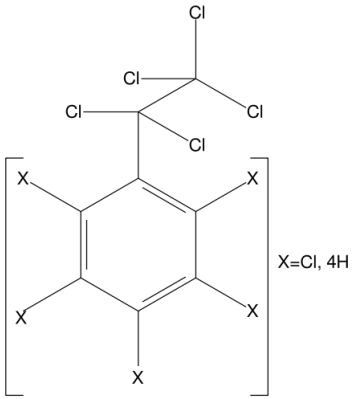
Elemental Formula: C8H4Cl6

Source: unknown

Class: ethylbenzene

Identification: Manual − Congener Group





m/z	Identity
193	[M−CCl3]+
204	[M−HCl3]+
220	PCB interference
239	[M−HCl2]+
257	PCB interference
275	[M−Cl]+
290	PCB interference
310	M+

Filename: hexachloro_ethylbenzene

Name: tetraphenyltin

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1777, RT (s) (2D): 2.614

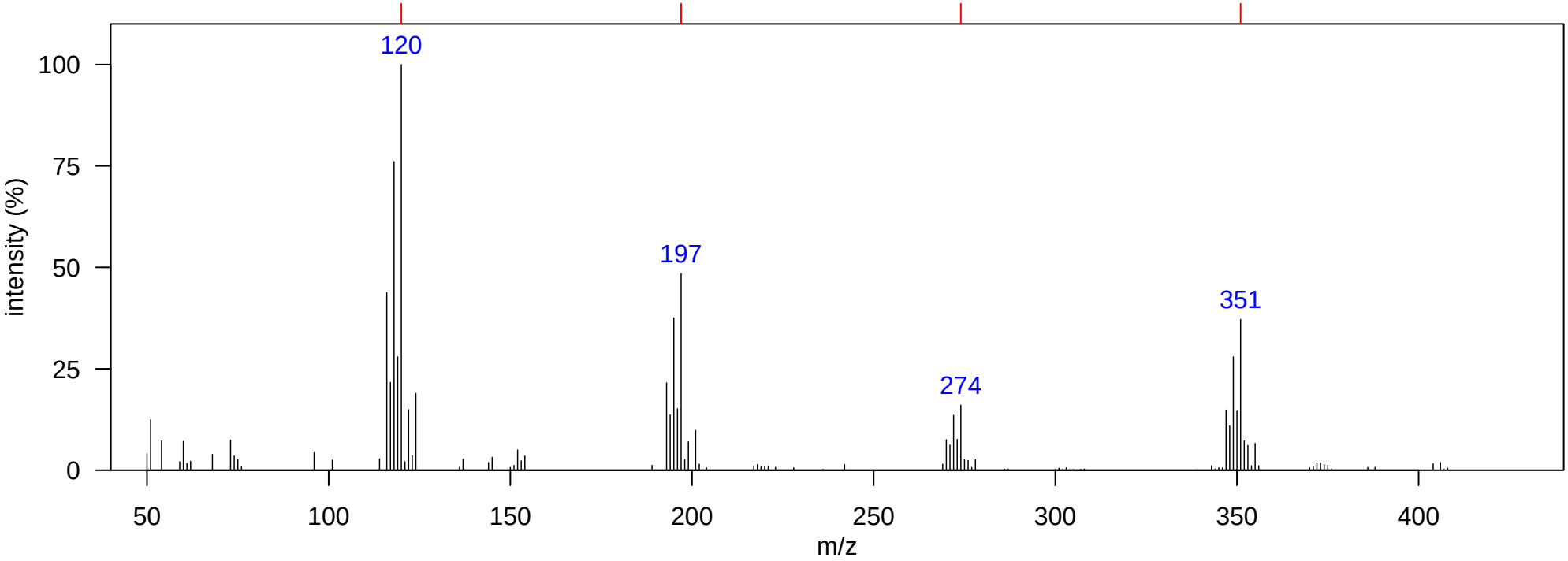
Comment:

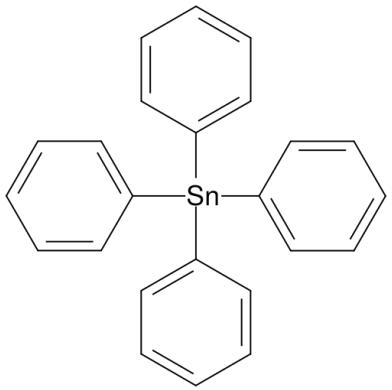
Elemental Formula: C24H20Sn

Source: anthropogenic

Class: organotin

Identification: Reference Database MS





m/z	Identity
120	Sn+
197	[M−3(C6H5)]+
274	[M−2(C6H5)]+
351	[M−C6H5]+

Name: unknown 1−1

Elemental Formula: C9H6OBr3Cl

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: unknown

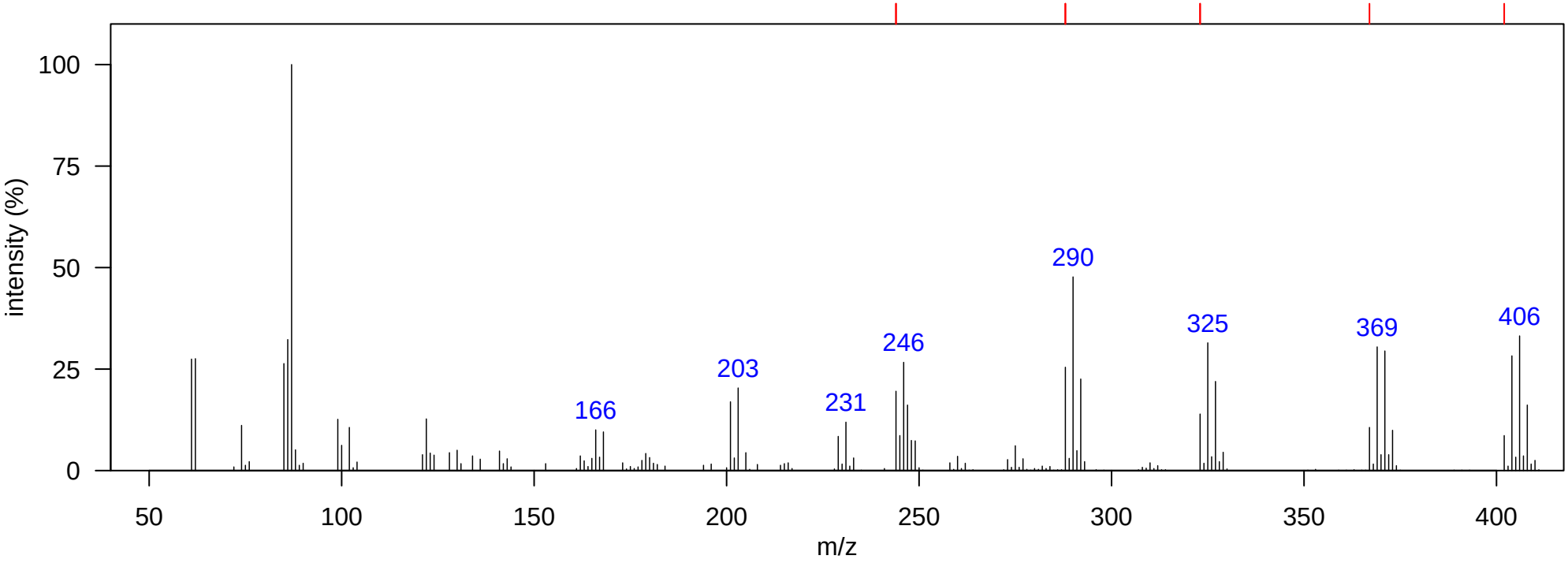
Instrument: GCxGC−TOF, electron impact

Class: unknown

RT (s) (1D): 1392, RT (s) (2D): 1.85

Identification: Literature MS

Comment: Ref: ES&T, 2009, 43, 3240−3247. Unknowns 1−(1−4) seem to share the same backbone.



m/z	Identity
244	[M−Br2]+
288	[M−BrCl]+
323	[M−Br]+
367	[M−Cl]+
402	M+

Name: unknown 1−2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1514.5, RT (s) (2D): 2.189

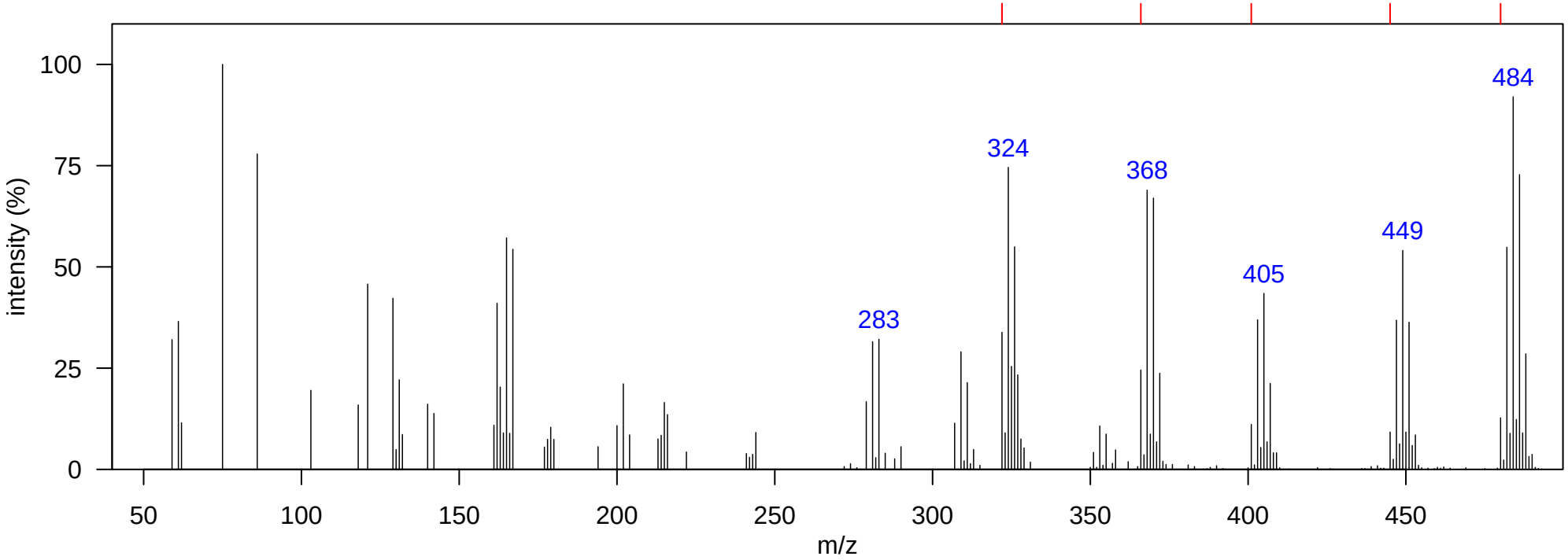
Elemental Formula: C9H6OBr4Cl

Source: unknown

Class: unknown

Identification: Literature MS

Comment: Ref: ES&T, 2009, 43, 3240−3247. Unknowns 1−(1−4) seem to share the same backbone.



m/z	Identity
322	[M−Br2]+
366	[M−BrCl]+
401	[M−Br]+
445	[M−Cl]+
480	M+

Name: unknown 1−3

Elemental Formula: C9H6OBr4Cl

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: unknown

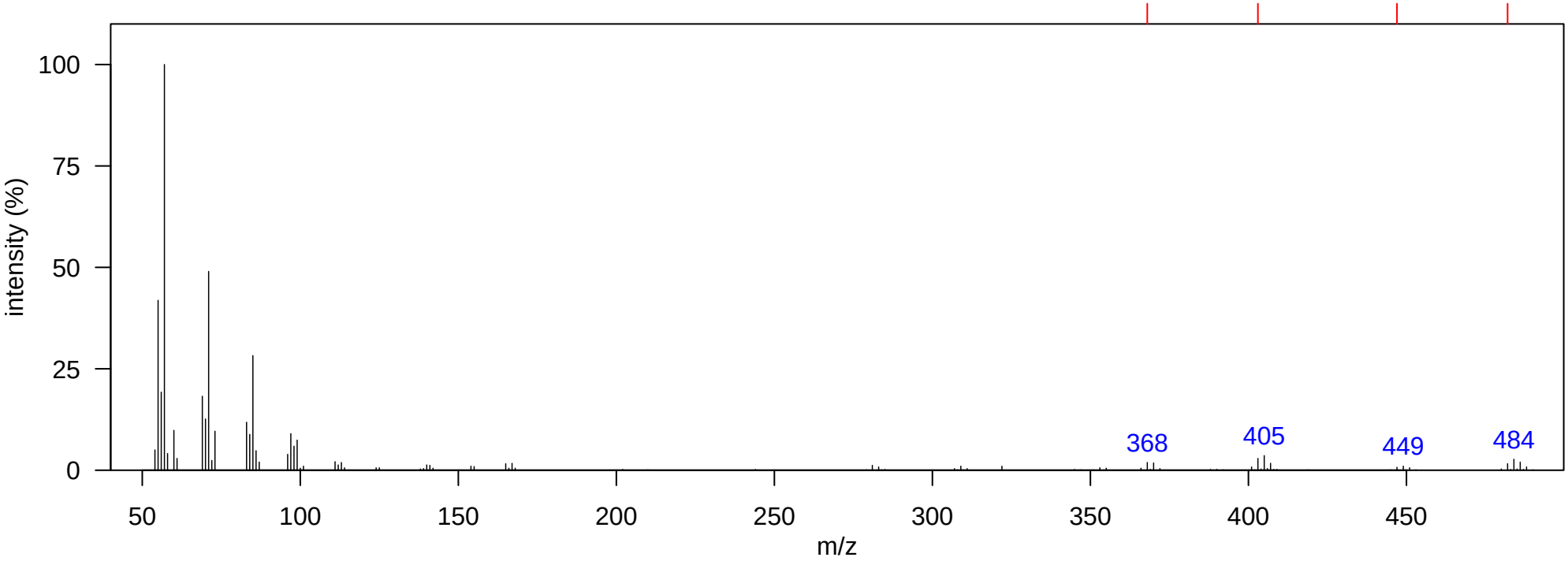
Instrument: GCxGC−TOF, electron impact

Class: unknown

RT (s) (1D): 1567, RT (s) (2D): 2.553

Identification: Literature MS

Comment: Ref: ES&T, 2009, 43, 3240−3247. Unknowns 1−(1−4) seem to share the same backbone.



m/z	Identity
368	[M−BrCl]+
403	[M−Br]+
447	[M−Cl]+
482	M+

Name: unknown 1−4

Elemental Formula: C9H6OBr5Cl

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: unknown

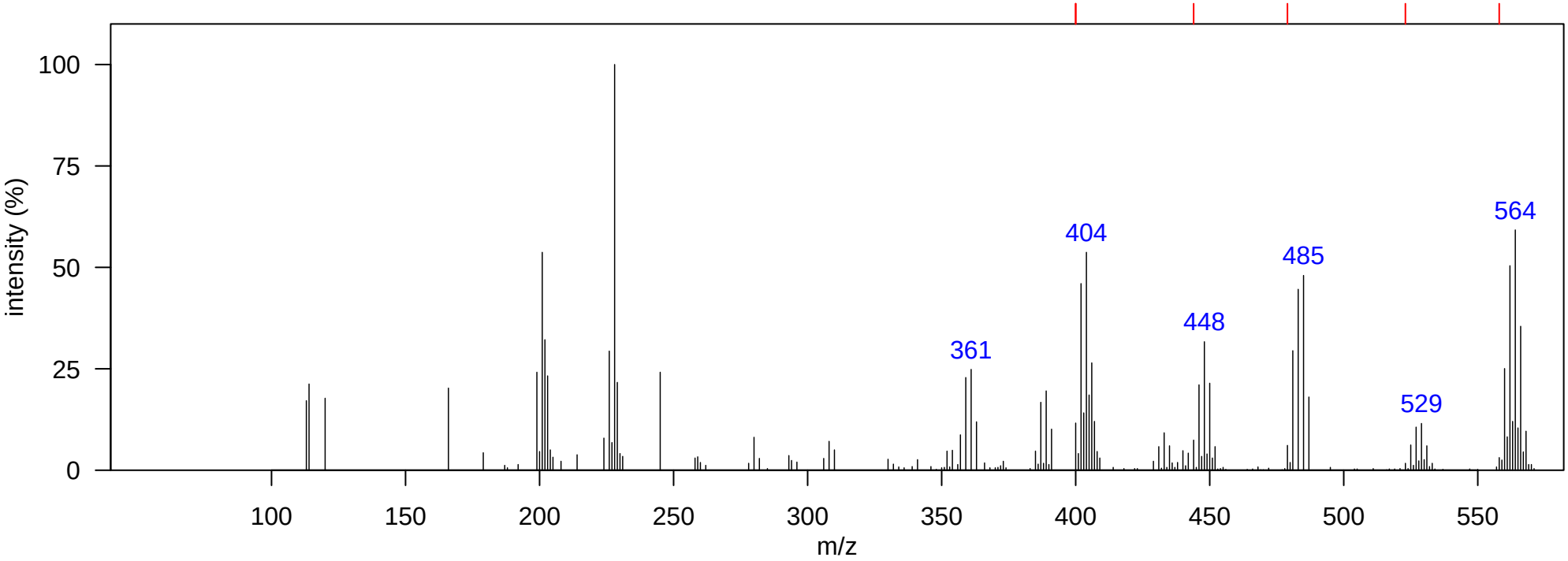
Instrument: GCxGC−TOF, electron impact

Class: unknown

RT (s) (1D): 1668.5, RT (s) (2D): 3.128

Identification: Literature MS

Comment: Ref: ES&T, 2009, 43, 3240−3247. Unknowns 1−(1−4) seem to share the same backbone.



m/z	Identity
400	[M−2Br]+
444	[M−BrCl]+
479	[M−Br]+
523	[M−Cl]+
558	M+

Name: unknown 2−1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1539, RT (s) (2D): 1.697

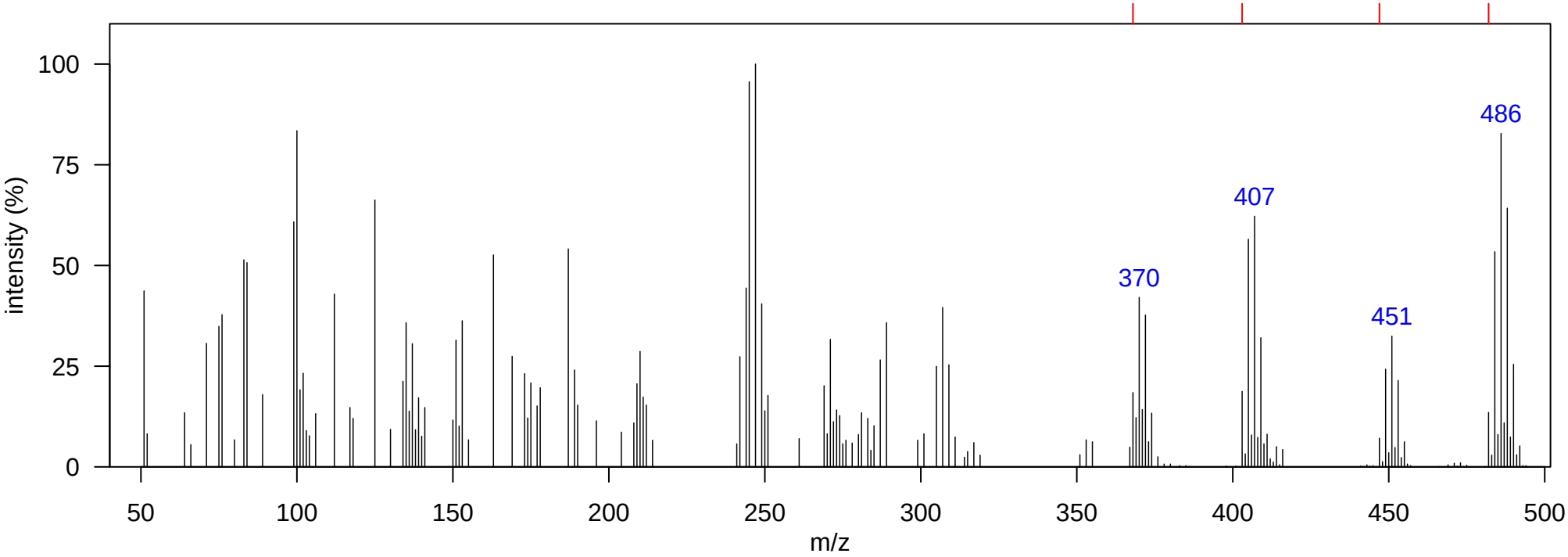
Comment: Related to unknown 1 family of compounds.

Elemental Formula: C9H8OBr4Cl

Source: unknown

Class: unknown

Identification: Manual



m/z	Identity
368	[M−BrCl]+
403	[M−Br]+
447	[M−Cl]+
482	M+

Name: unknown 2−2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1539, RT (s) (2D): 1.828

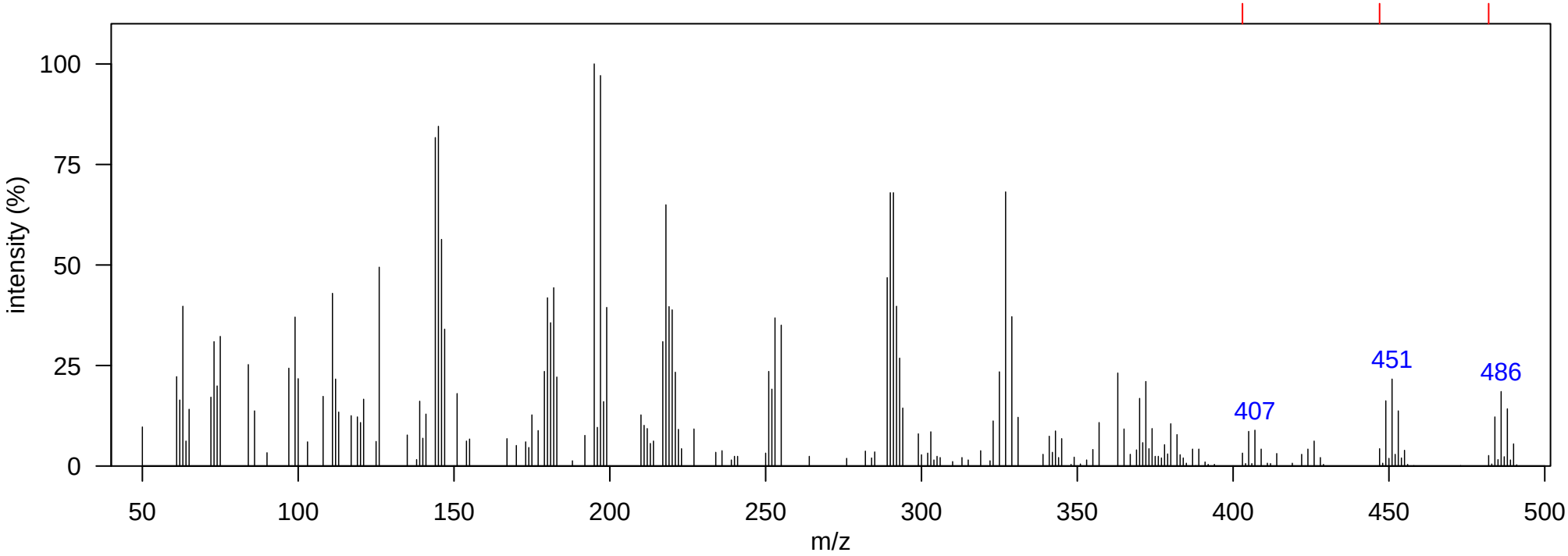
Comment: Related to unknown 1 family of compounds.

Elemental Formula: C9H8OBr4Cl

Source: unknown

Class: unknown

Identification: Manual



m/z	Identity
403	[M−Br]+
447	[PM−Cl]+
482	[PM]+

Name: unknown 2−3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1672, RT (s) (2D): 2.387

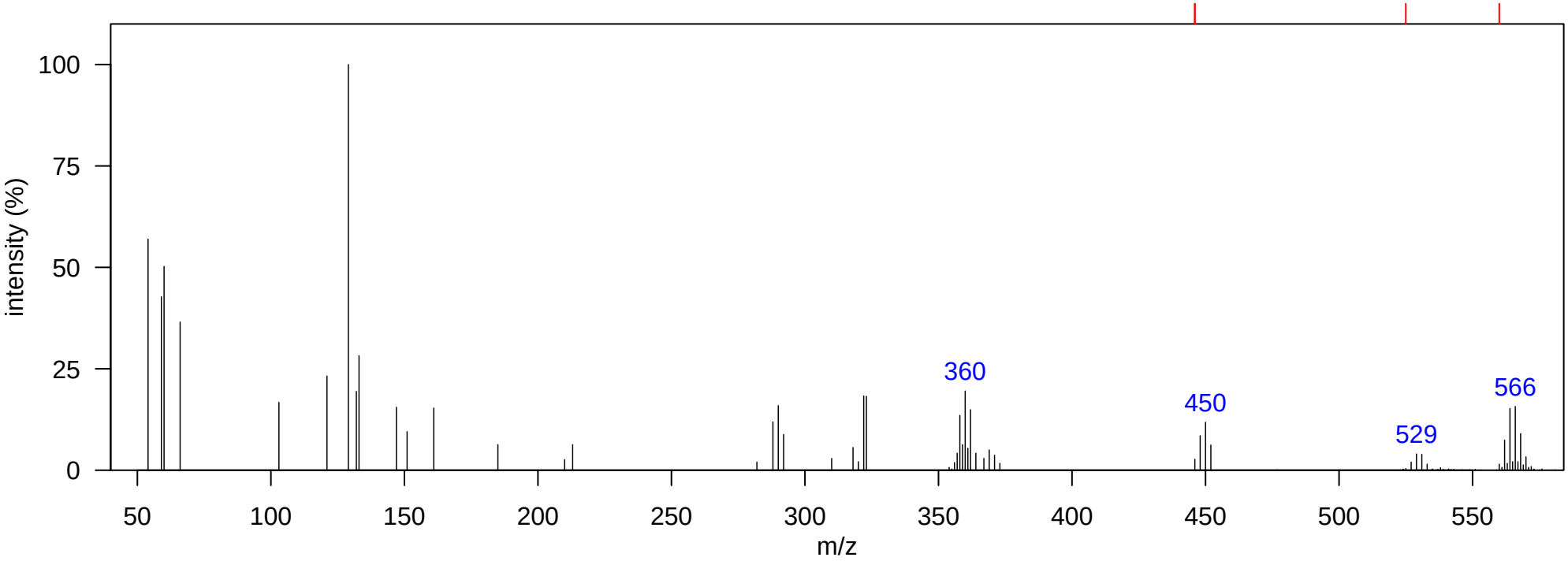
Comment: Related to unknown 1 family of compounds.

Elemental Formula: C9H8OBr5Cl

Source: unknown

Class: unknown

Identification: Manual



m/z	Identity
446	[M−BrCl]+
525	[M−Cl]+
560	M+

Name: unknown 3−1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1458.5, RT (s) (2D): 0.703

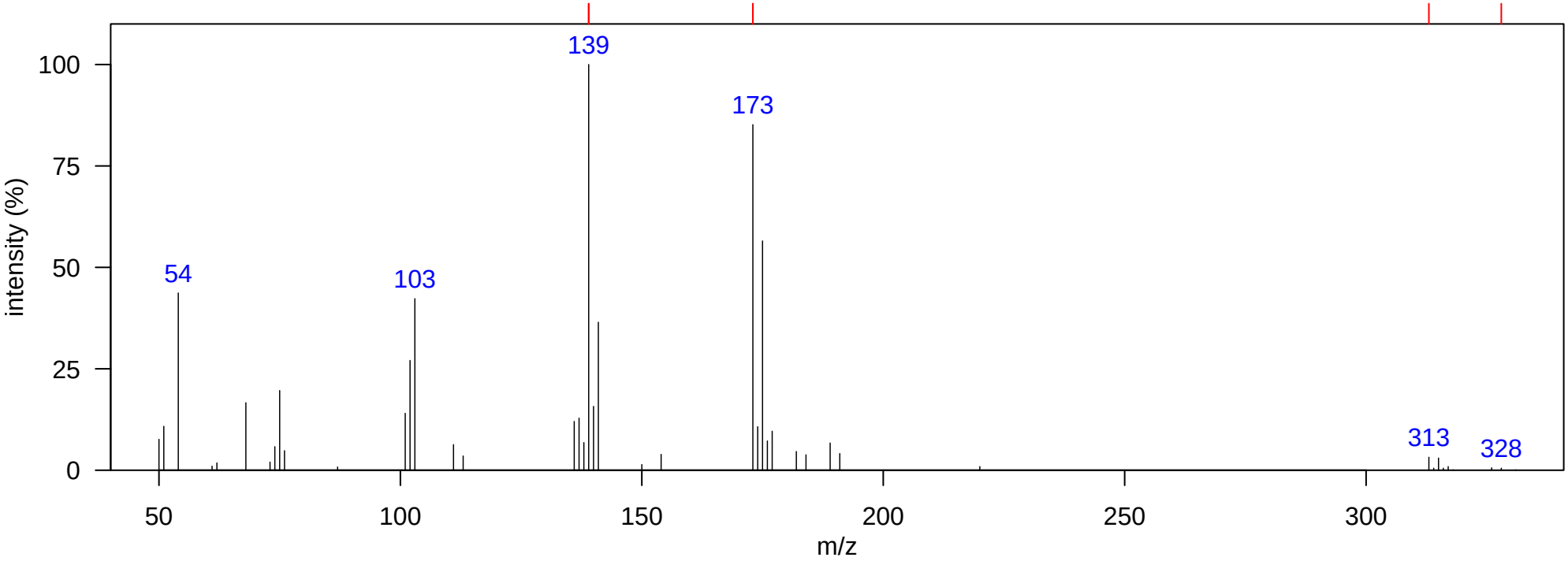
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion. Unknowns 3−(1−3) are related.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
139	[Frag2]+ contains 1Cl
173	[Frag]+ contains 2Cl
313	[PM−15]+ contains 3Cl
328	[PM]+

Name: unknown 3−2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1518, RT (s) (2D): 0.693

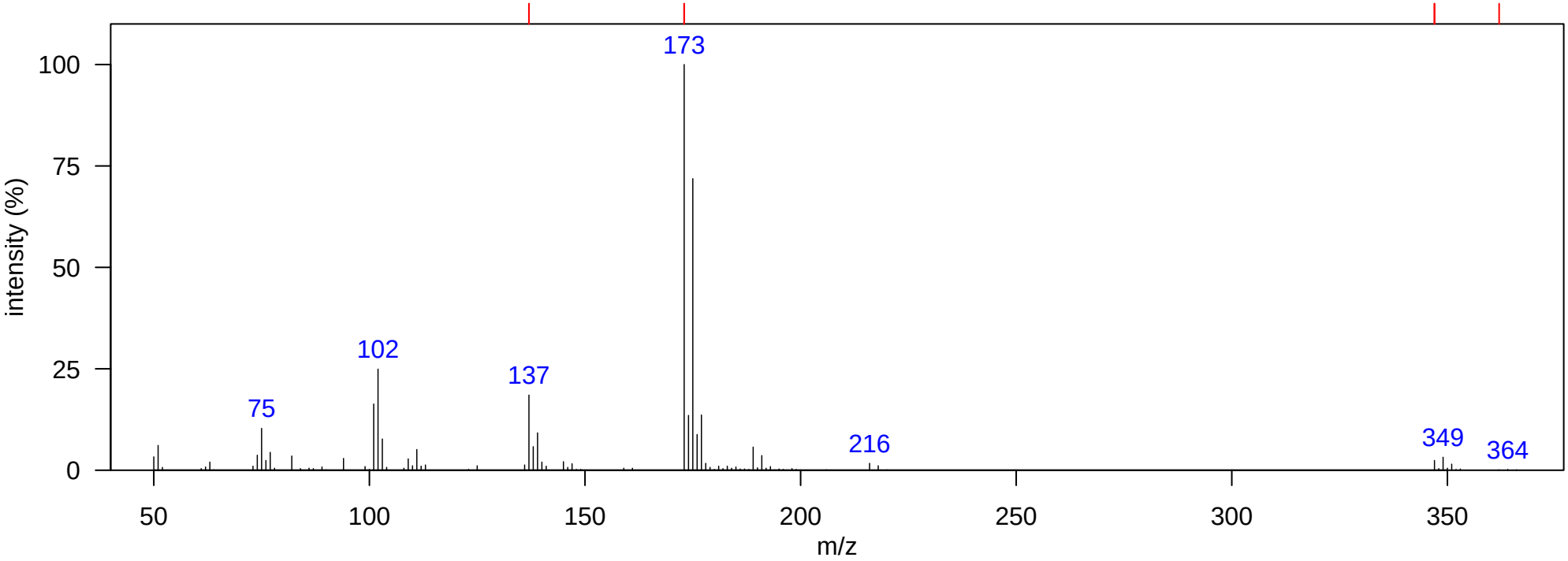
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion. Unknowns 3−(1−3) are related.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
137	[Frag−HCl]+
173	[Frag]+ contains 2Cl
347	[PM−15]+ contains 4Cl
362	[PM]+

Name: unknown 3−3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1616, RT (s) (2D): 1.281

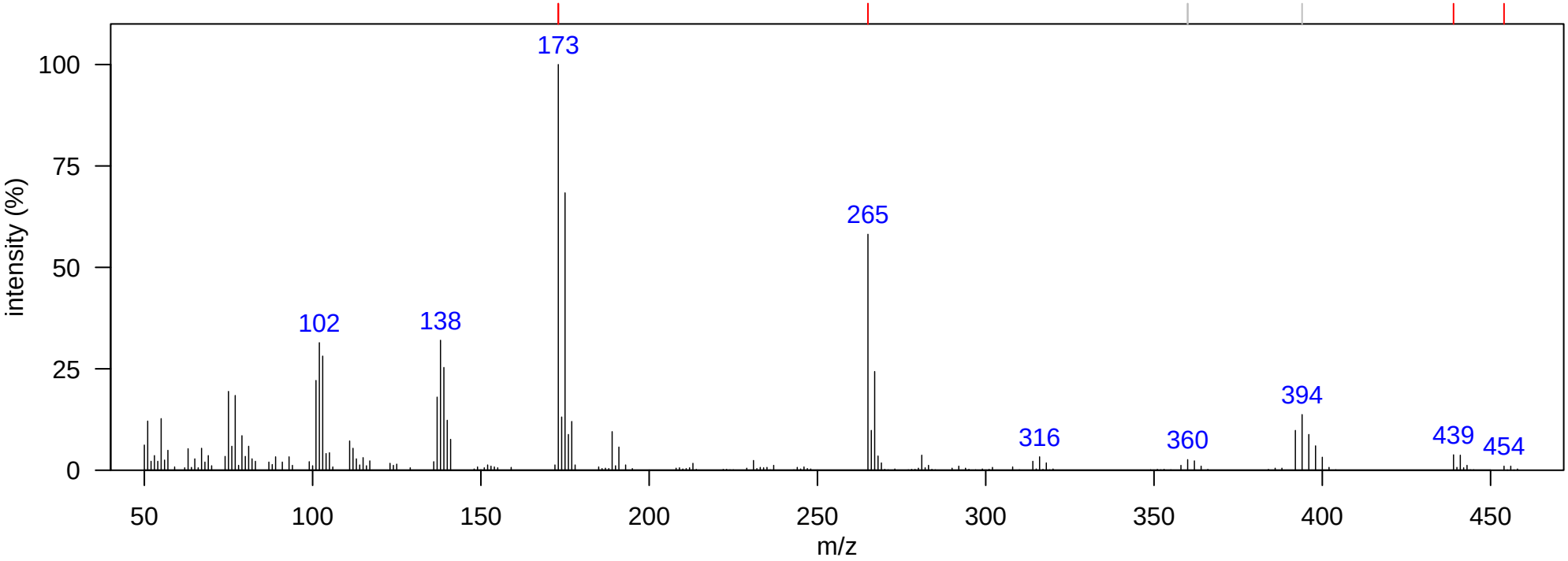
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion. Unknowns 3−(1−3) are related.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
173	[Frag]+ contains 2Cl
265	[Frag]+ contains Cl
360	interference
394	interference
439	[PM−15]+ contains 3Cl
454	[PM]+

Name: unknown 4−1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1931, RT (s) (2D): 2.882

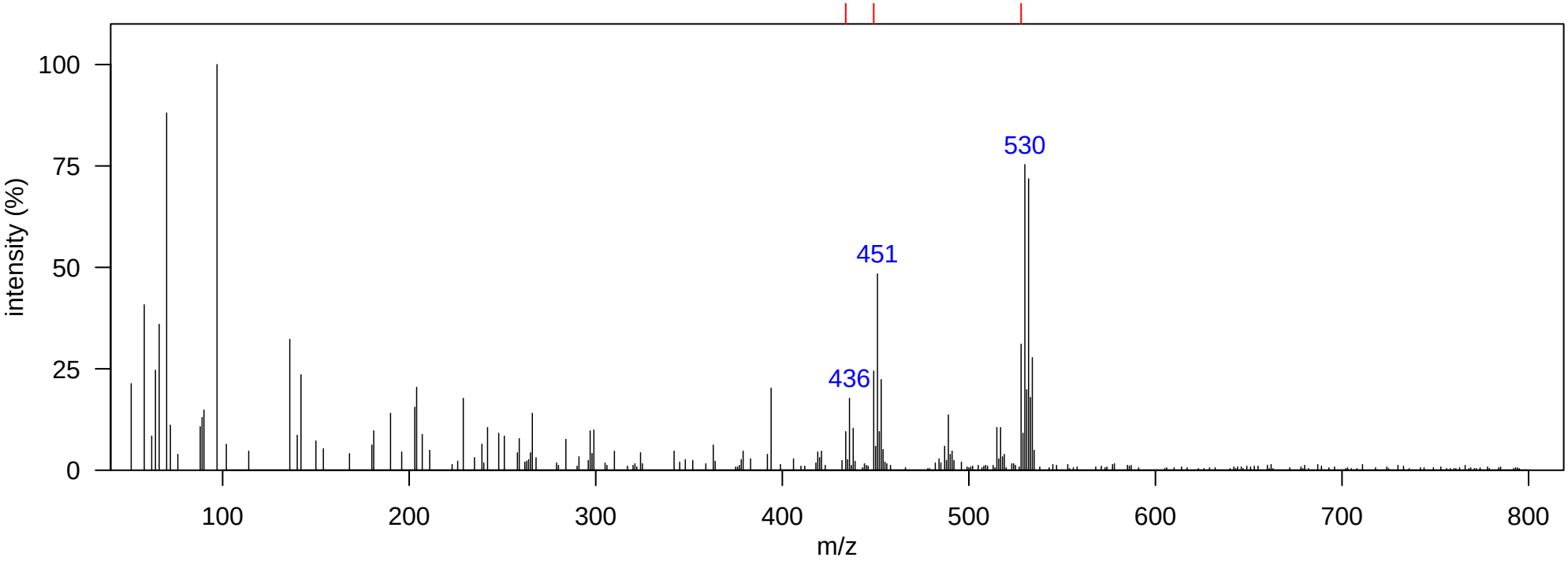
Comment: PM = Possible Molecular Ion. Unknowns 4−(1−4) seem to share the same backbone.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
434	[PM−Br−15]+ = [PM−Br−CH3]+
449	[PM−Br]+
528	[PM]+ contains 3Br

Name: unknown 4−2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1959, RT (s) (2D): 3.321

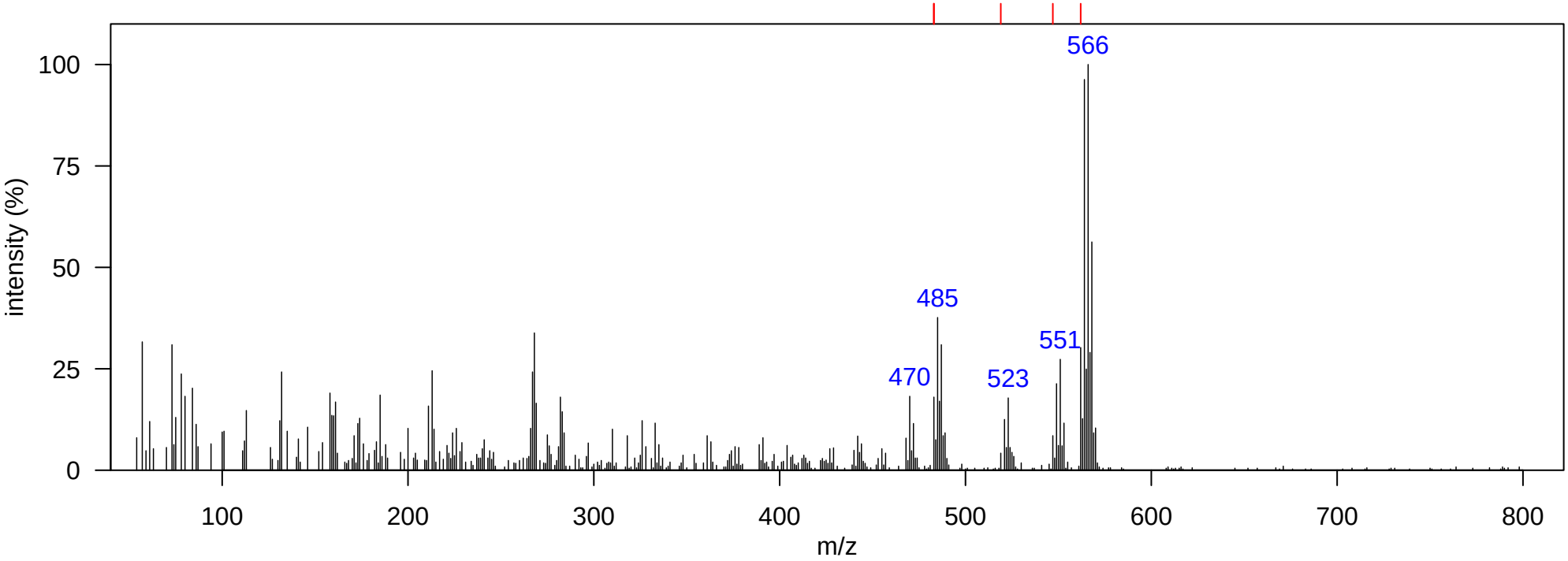
Comment: PM = Possible Molecular Ion. Unknowns 4−(1−4) seem to share the same backbone.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
483	[PM−Br]+
519	[PM−43]+ = [PM−C3H7]+
547	[PM−15]+ = [PM−CH3]+
562	[PM]+ contains Br3Cl

Name: unknown 4−3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1976.5, RT (s) (2D): 0.431

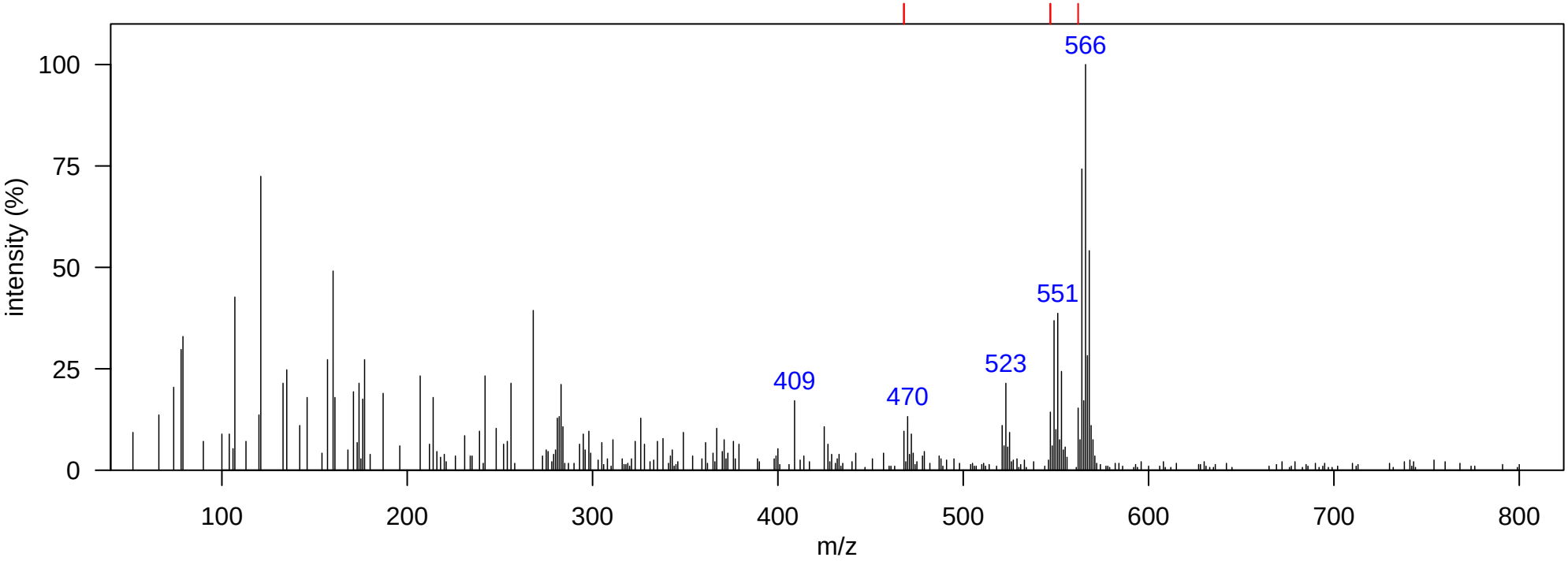
Comment: PM = Possible Molecular Ion. Unknowns 4−(1−4) seem to share the same backbone.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
468	[PM−Br−15]+ = [PM−Br−CH3]+
547	[PM−15]+ = [PM−CH3]+
562	[PM]+ contains Br3Cl

Name: unknown 4−4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 2018.5, RT (s) (2D): 2.764

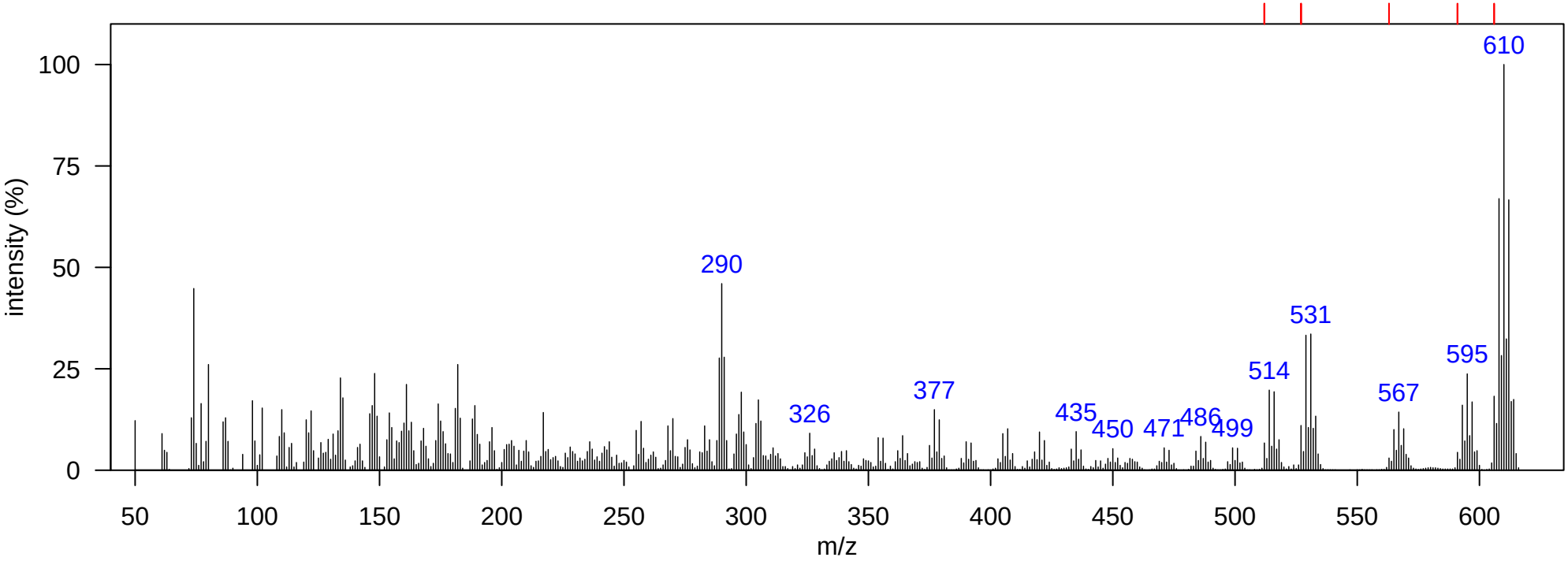
Comment: PM = Possible Molecular Ion. Unknowns 4−(1−4) seem to share the same backbone.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
512	[PM−Br−CH3]+
527	[PM−Br]+
563	[PM−C3H7]+
591	[PM−CH3]+
606	[PM]+ contains 4Br.

Name: unknown 5

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 2099, RT (s) (2D): 0.159

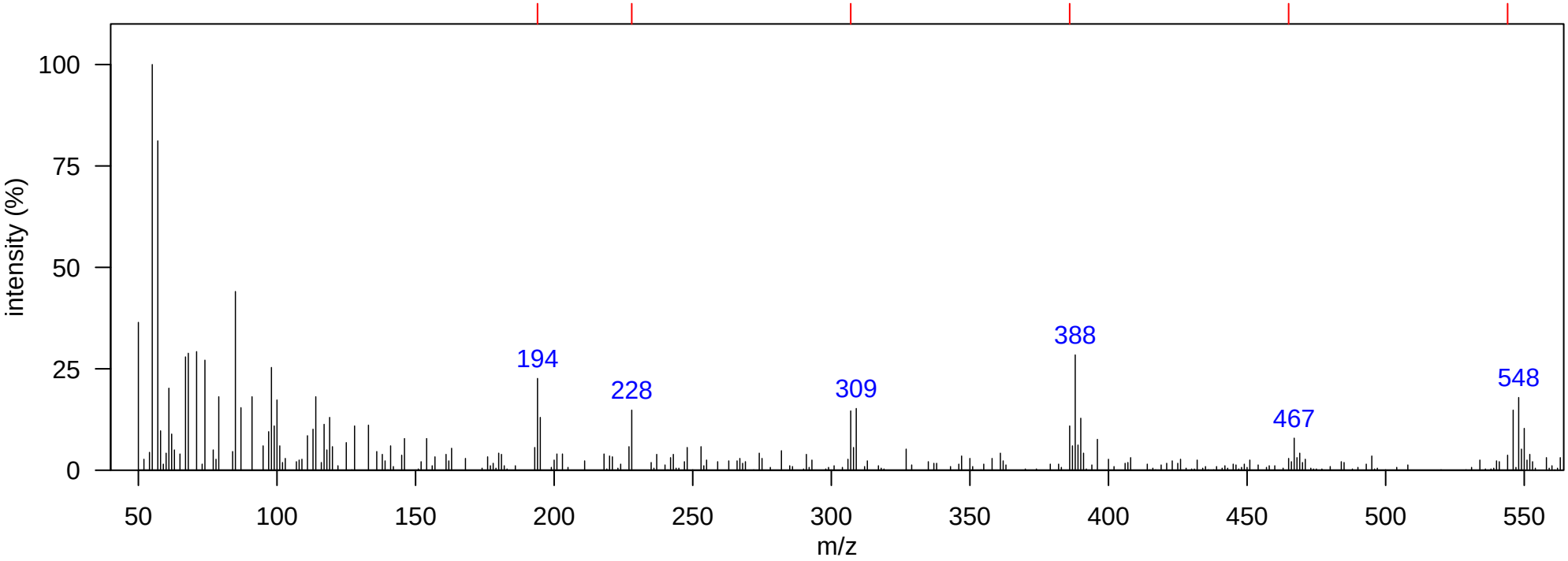
Comment: Ref: ES&T, 2009, 43, 3240−3247. Possible structure shown.

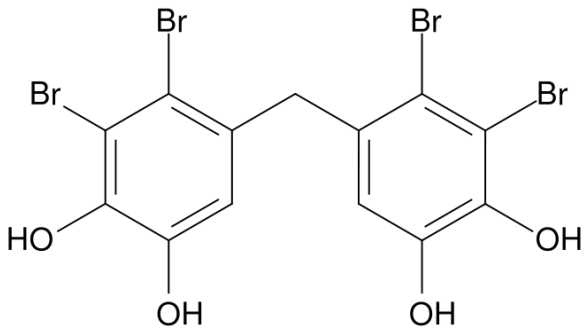
Elemental Formula: C13H8Br4O4

Source: natural

Class: unknown

Identification: Literature MS





possible structure

m/z	Identity
194	[M−2Br]2+
228	[M−4Br]+
307	[M−3Br]+
386	[M−2Br]+
465	[M−Br]+
544	M+

Filename: unknown_5

Name: unknown 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1273, RT (s) (2D): 1.248

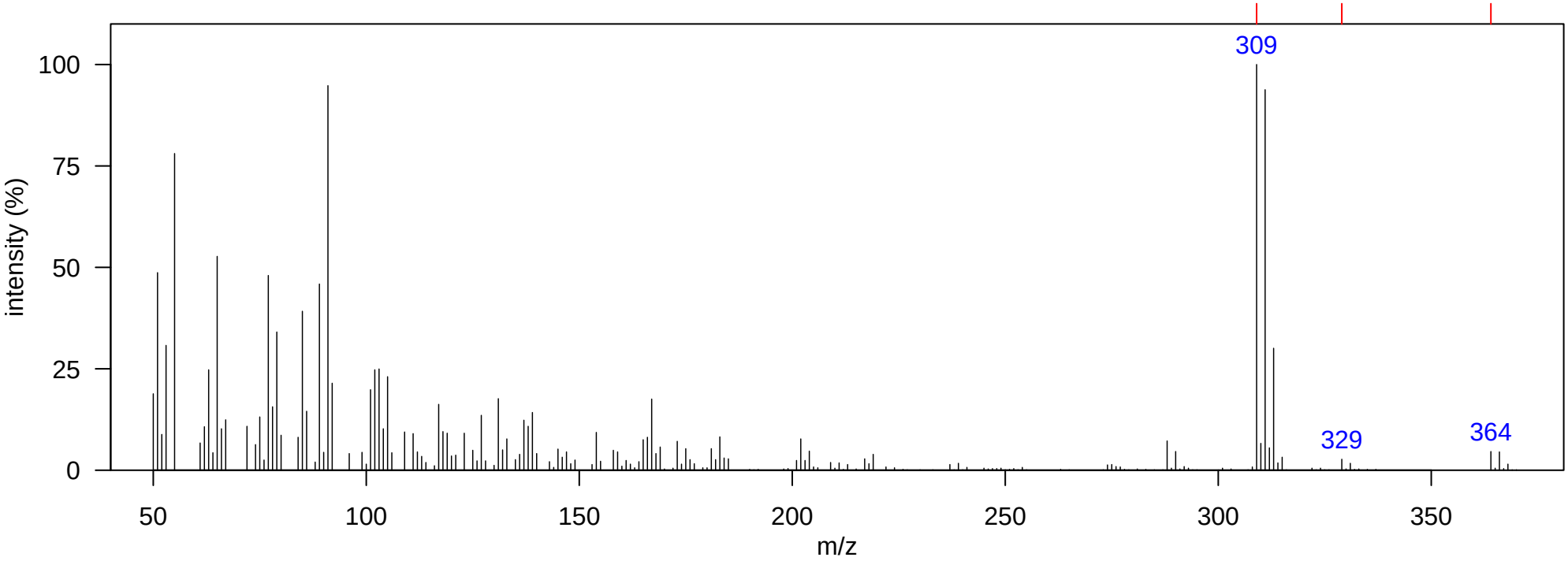
Comment: PM = Possible Molecular Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
309	[PM−55]+ (contains 3Cl)
329	[PM−Cl]+ (contains 2Cl)
364	PM+ (contains 3Cl)

Name: unknown 7

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1290.5, RT (s) (2D): 1.181

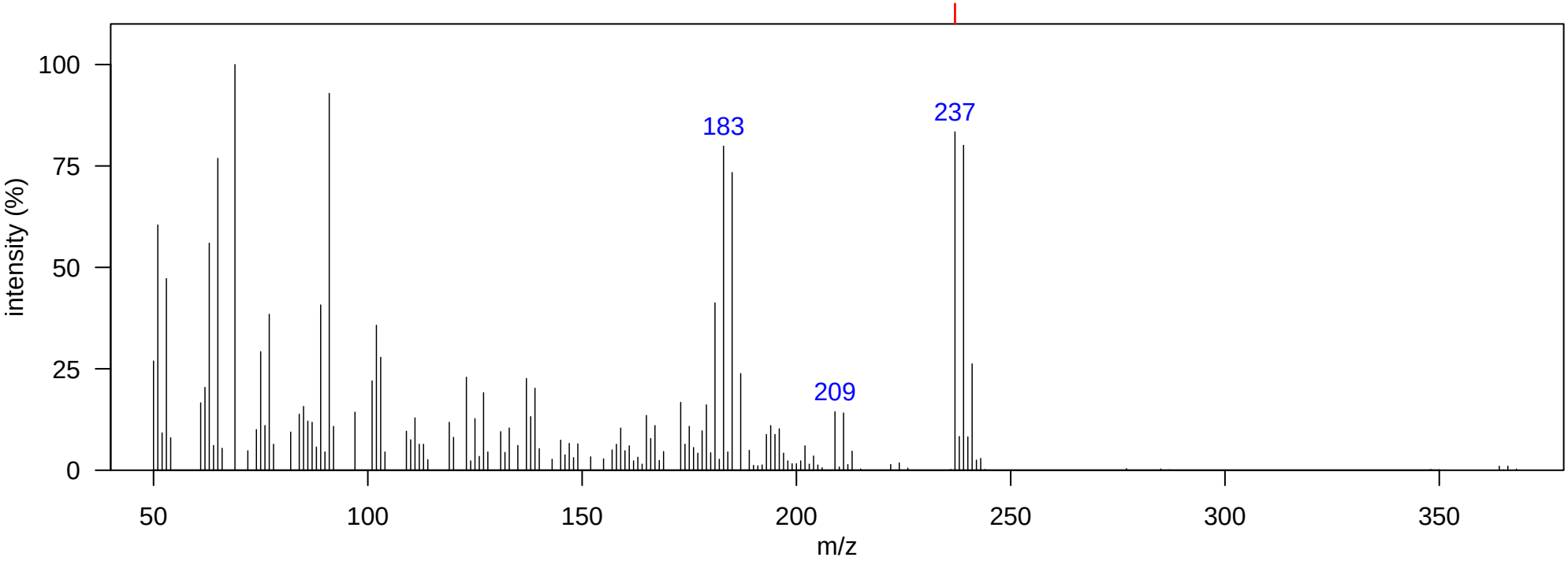
Comment: Frag = Possible Fragment Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
237	[Frag]+ containing 3Cl

Name: unknown 8

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1339.5, RT (s) (2D): 0.781

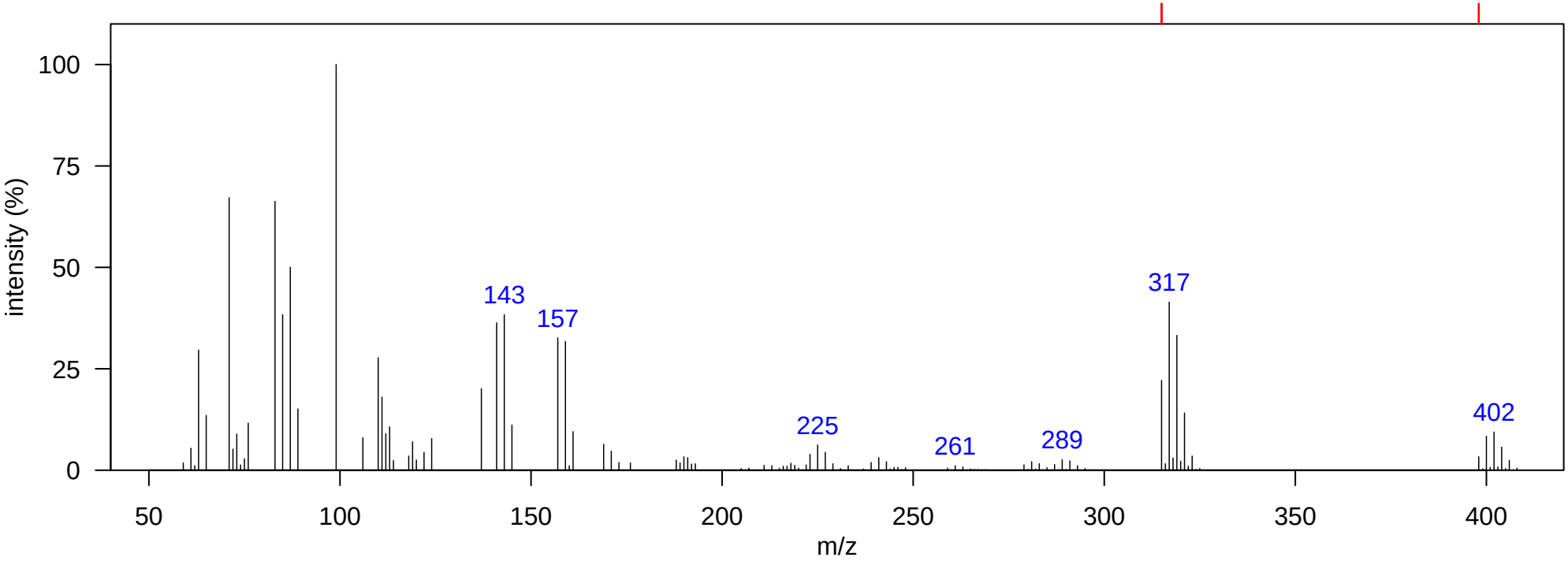
Comment: PM = Possible Molecular Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
315	[PM−CHCl2]+
398	[PM]+ containing 8Cl

Name: unknown 9

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1378, RT (s) (2D): 1.407

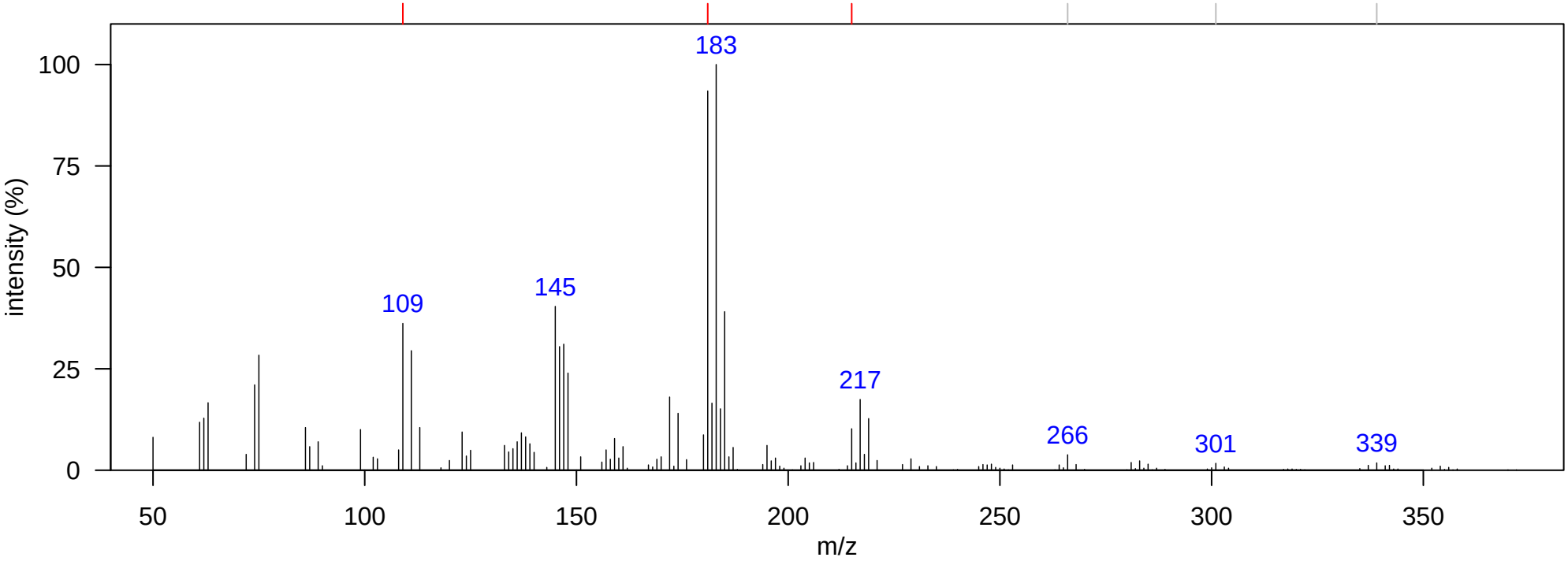
Comment: Frag1 and Frag2 = fragments

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
109	[Frag2 − H2Cl2]+ contains 2Cl
181	[Frag2]+ contains 4Cl
215	[Frag1] contains 5Cl
266	interference
301	interference
339	interference

Filename: unknown_9

Name: unknown 10

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1385, RT (s) (2D): 1.426

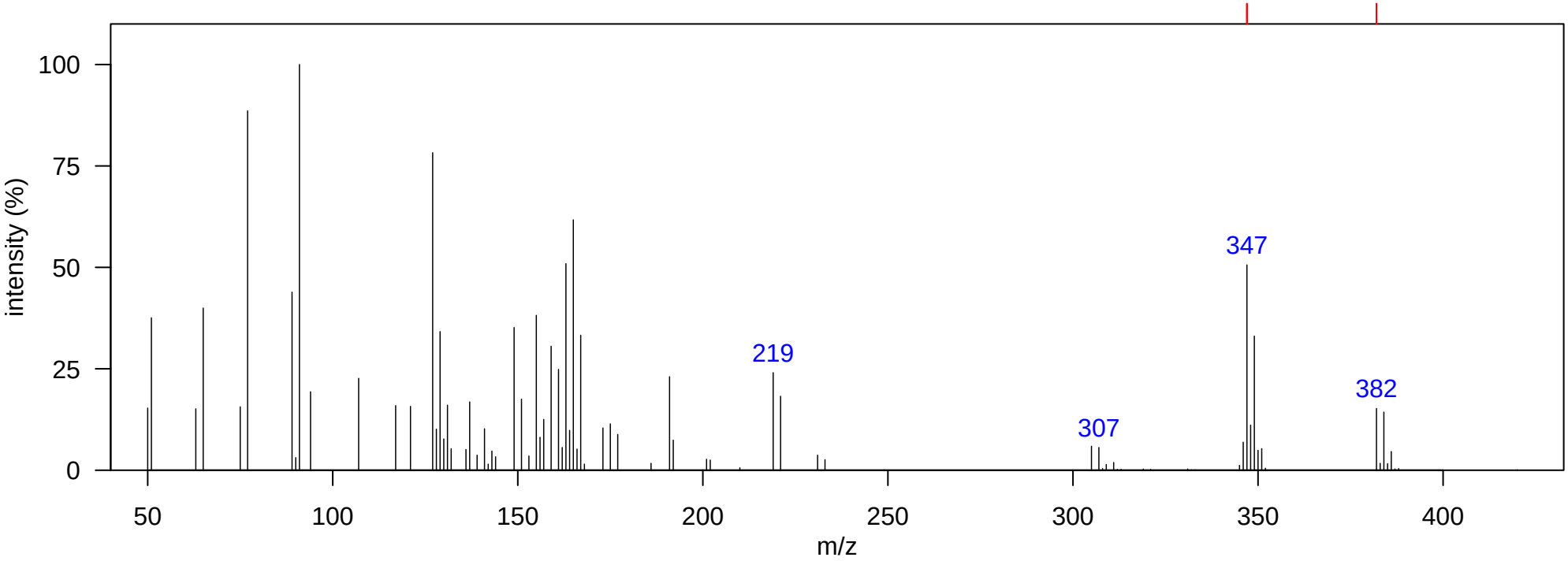
Comment: PM = Possible Molecular Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
347	[PM−Cl]+
382	[PM]+ contains 3Cl

Name: unknown 11

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1395.5, RT (s) (2D): 2.19

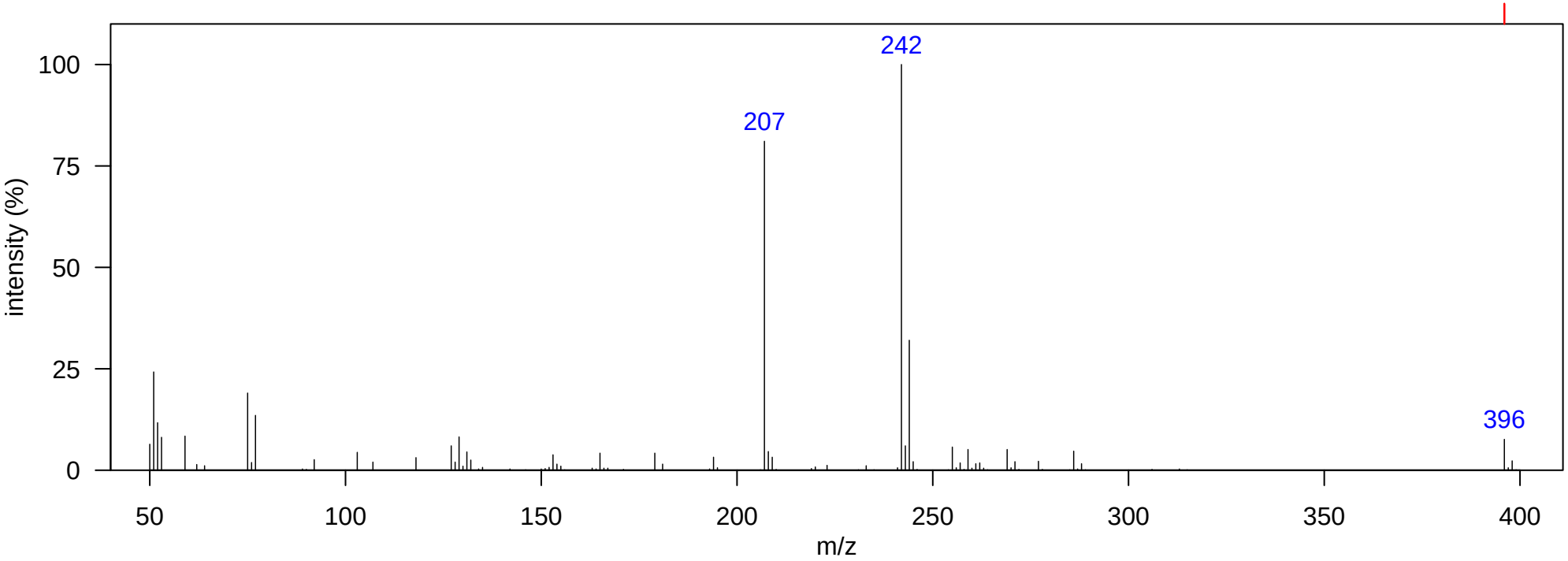
Comment: PM = Possible Molecular Ion. Contains chlorine.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
396	[PM]+

Name: unknown 12

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1479.5, RT (s) (2D): 1.923

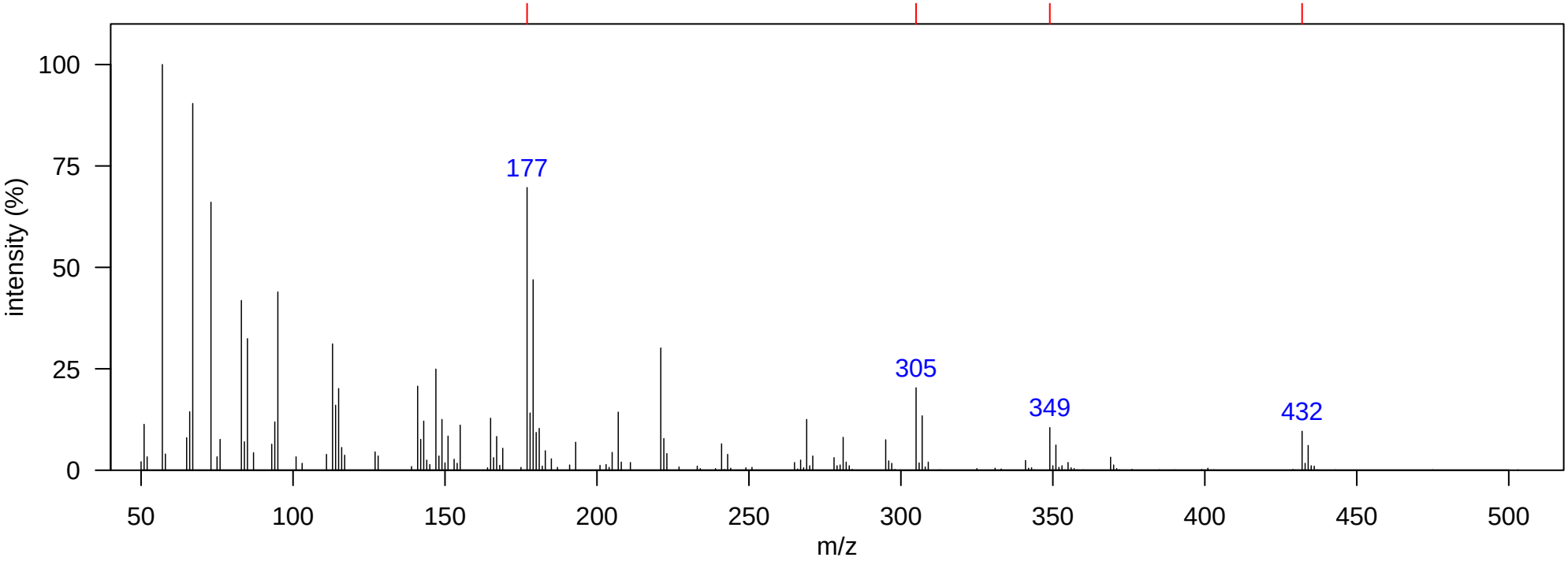
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
177	[Frag]+ contains 2Cl
305	[Frag]+ contains 2Cl
349	[Frag]+ contains 2Cl
432	[PM]+ contains 2Cl

Name: unknown 13

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1612.5, RT (s) (2D): 1.831

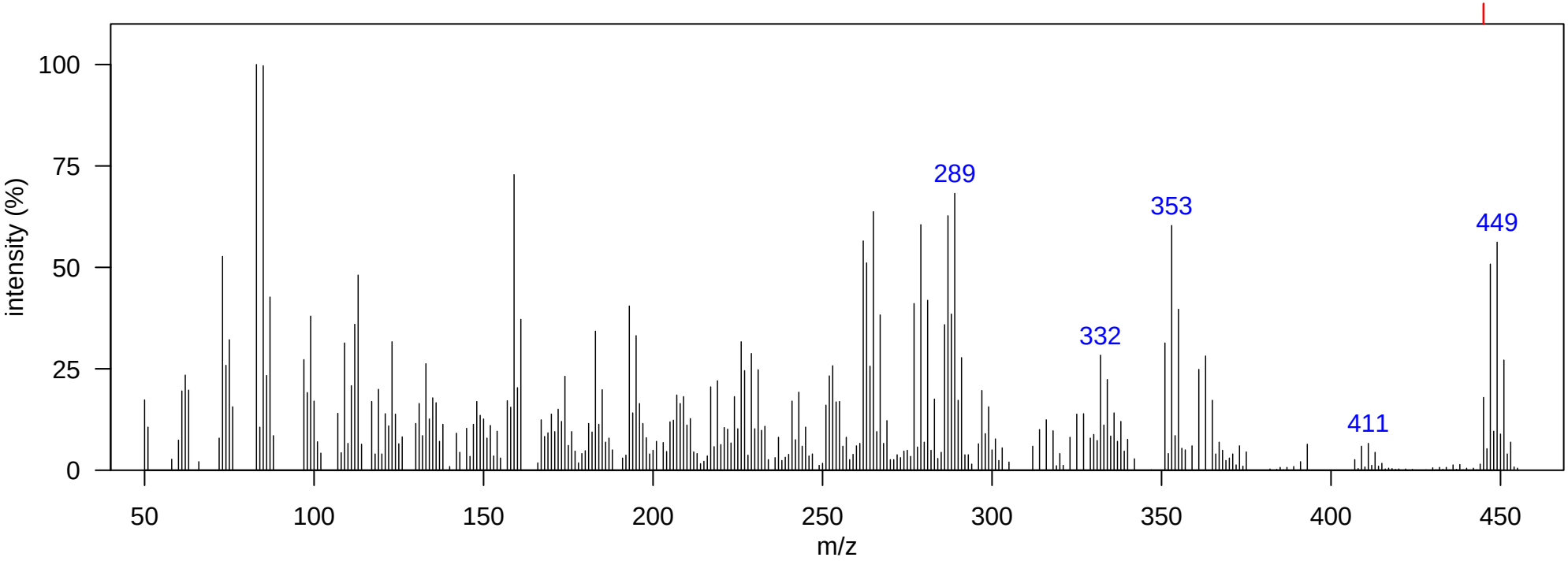
Comment: PM = Possible Molecular Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
445	[PM]+ contains 8Cl

Name: unknown 14

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1840, RT (s) (2D): 2.918

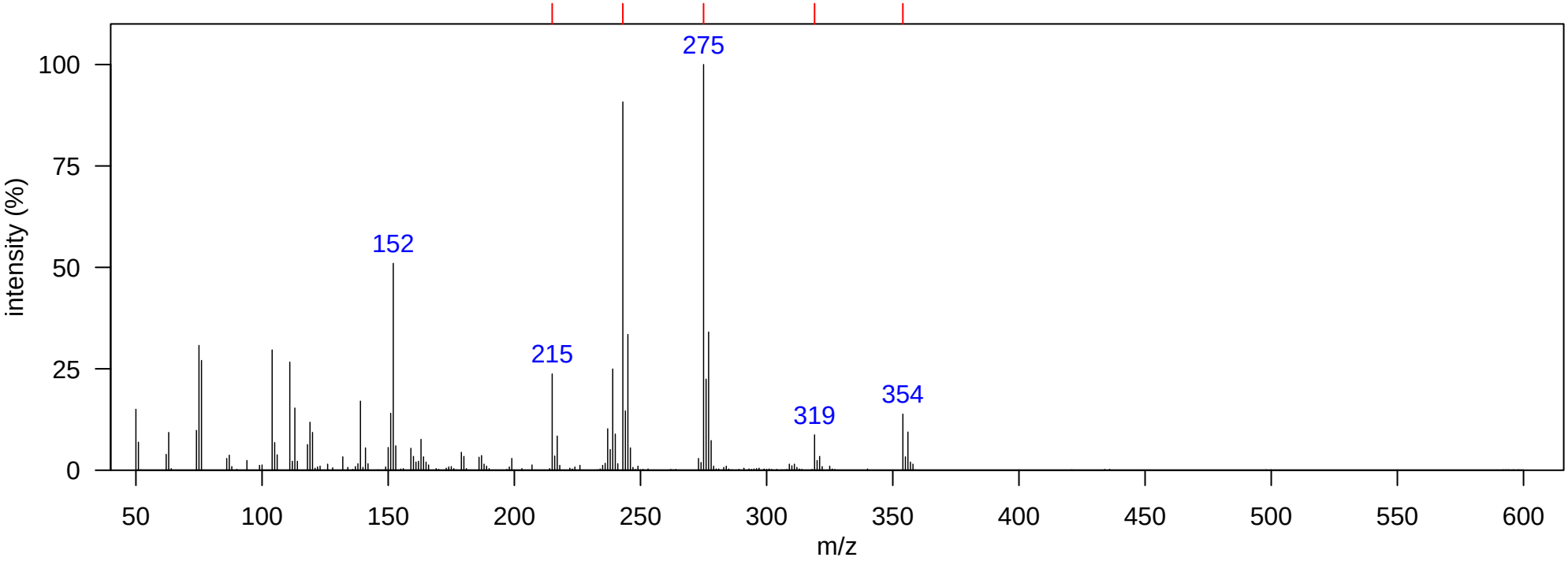
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
215	[Frag2 − 28]+ contains Cl
243	[Frag2]+ contains Cl
275	[Frag1]+ contains Cl
319	[PM−Cl]+
354	[PM]+ contains 2Cl

Name: unknown 15

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1847, RT (s) (2D): 0.401

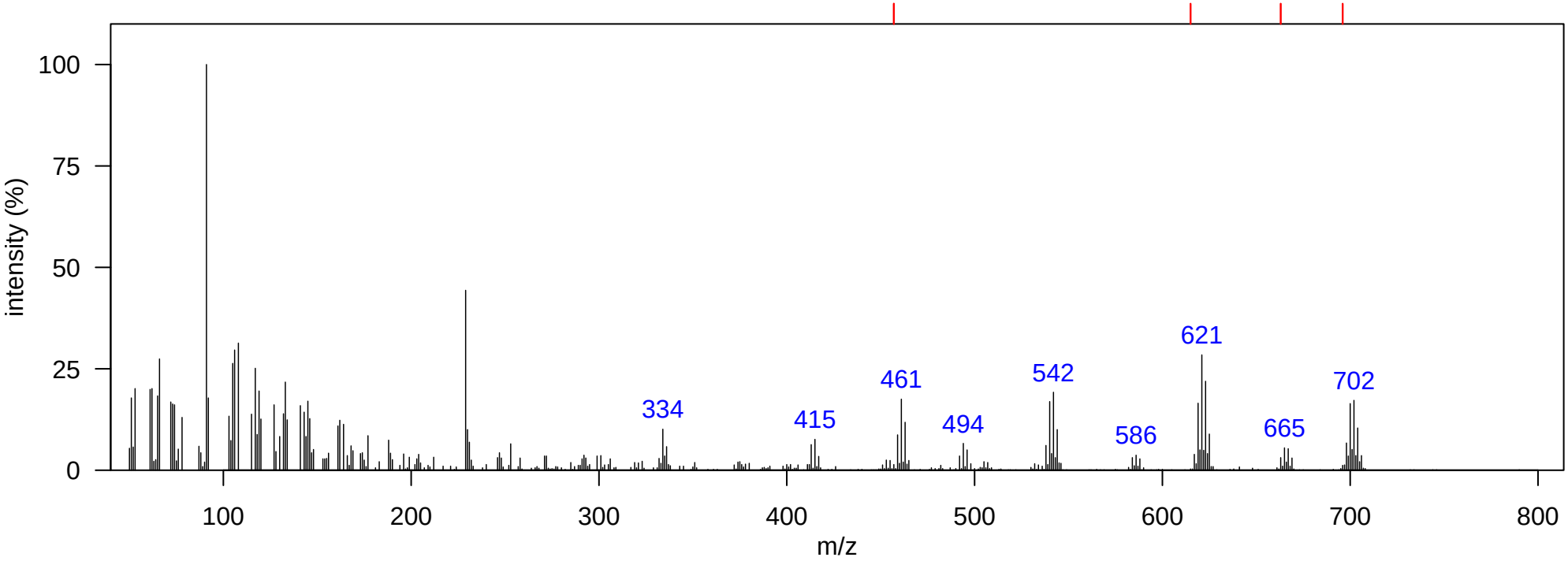
Comment: PM = Possible Molecular Ion. Contains Br7Cl.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
457	[PM−H2Br3]+
615	[PM−H2Br]+
663	[PM−Cl]+
696	[PM]+ contains Br7Cl

Name: unknown 16

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1948.5, RT (s) (2D): 5.491

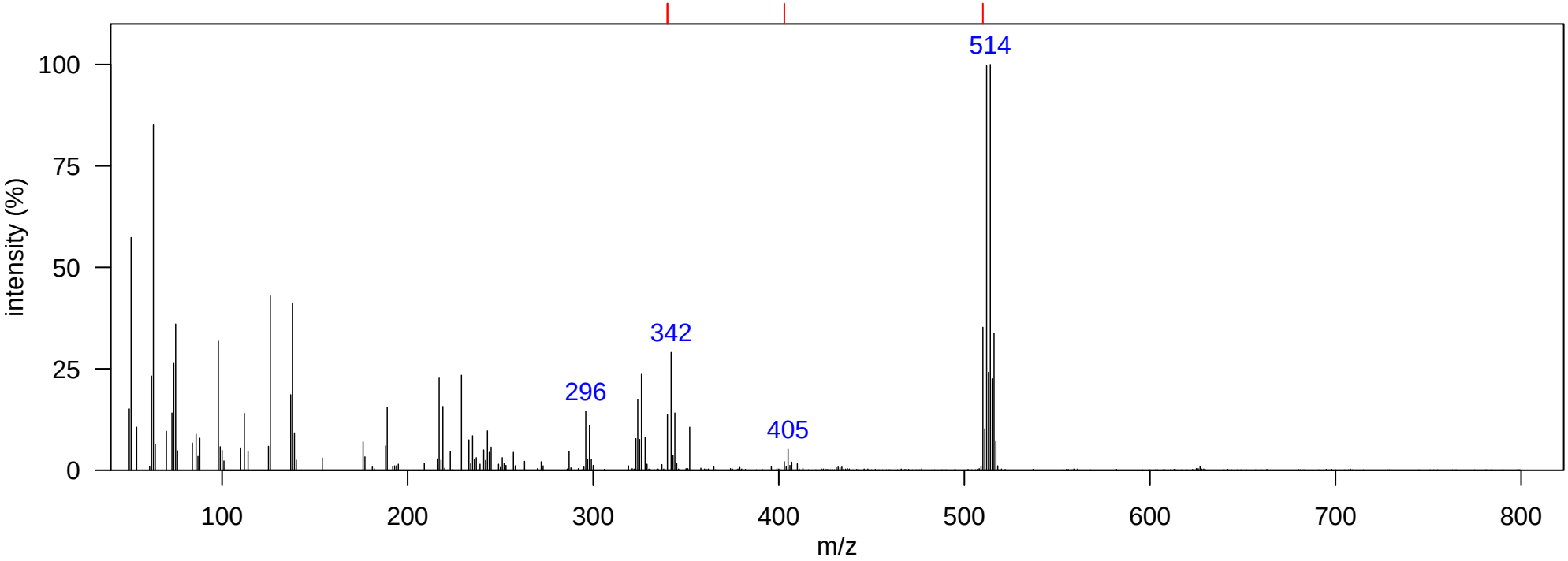
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
340	[Frag]+ contains 2Br
403	[PM−Br−28]+
510	[PM]+ contains 3Br

Name: unknown 17

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC−TOF, electron impact

RT (s) (1D): 1980, RT (s) (2D): 3.118

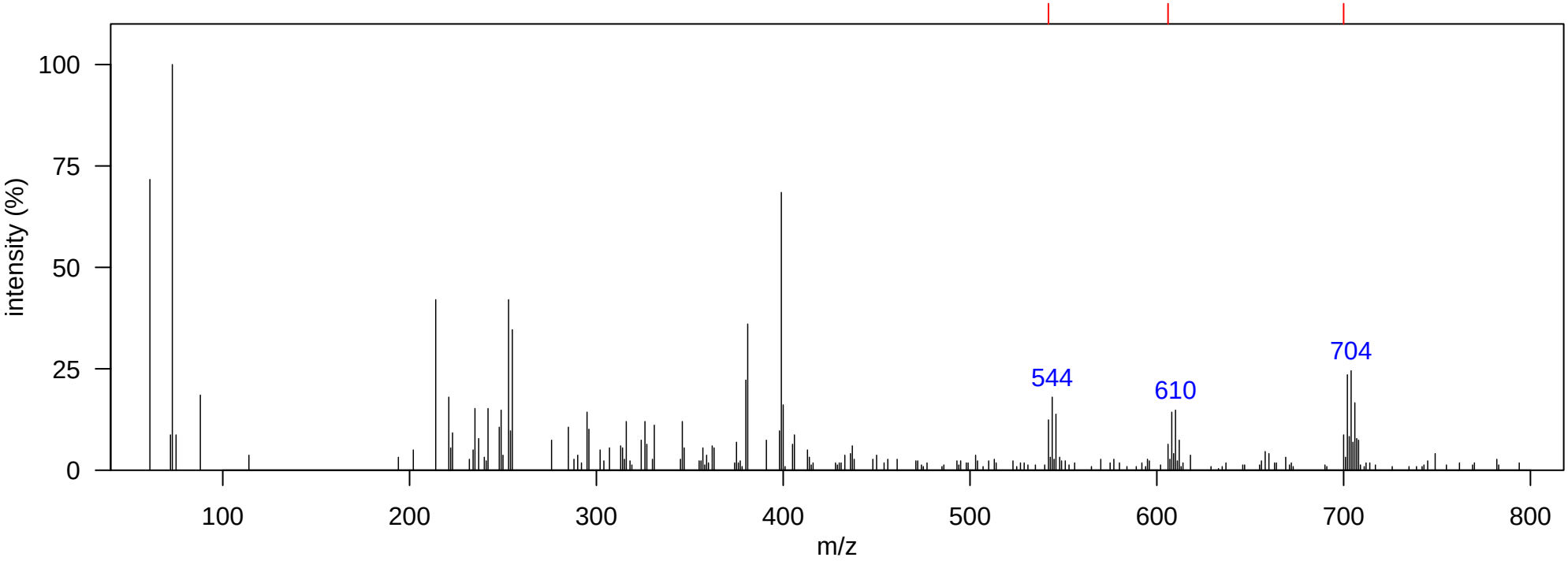
Comment: PM = Possible Molecular Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
542	[PM−2Br]+
606	[PM−Br−15]+ = [PM−Br−CH3]+
700	[PM]+