

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: 2014–08–21 10:22:35

SpecLibDolphin2011 version 0.5–4

OrgMassSpecR version 0.4–4

png version 0.1–7

R version 3.1.0 (2014–04–10)

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

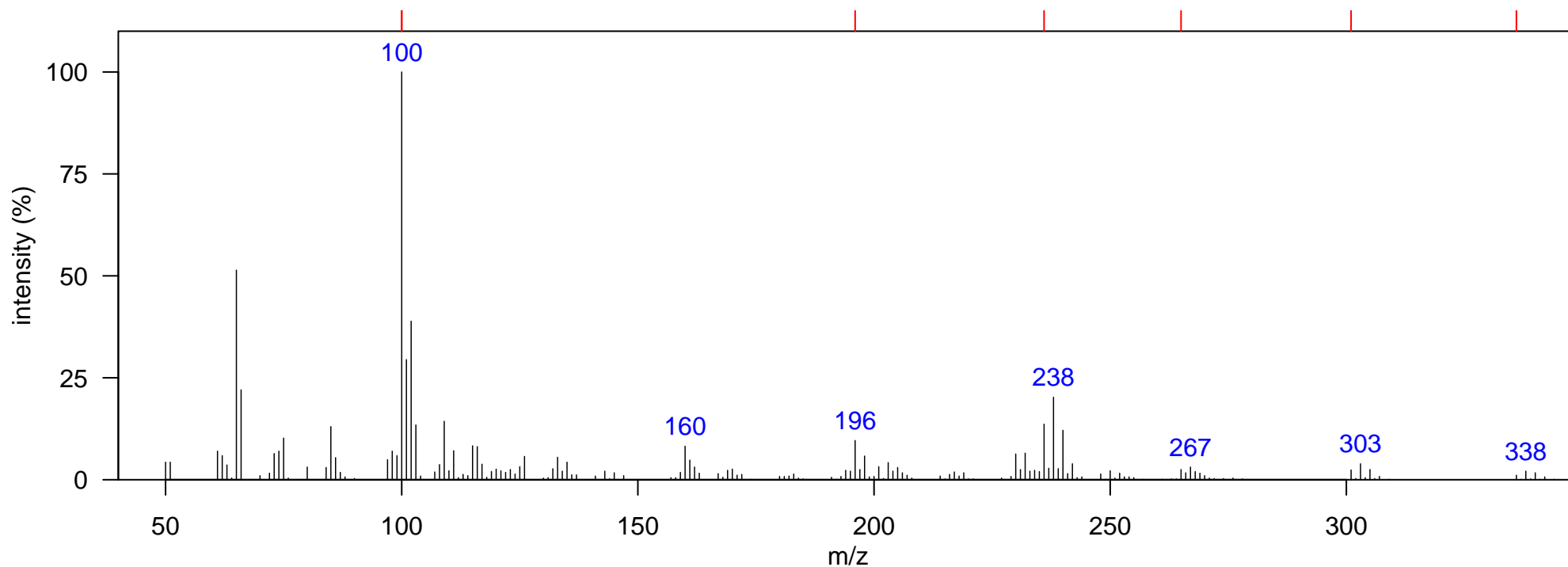
Comment:

Elemental Formula: C₁₀H₆Cl₆

Source: anthropogenic

Class: chlordane related

Identification: Manual



m/z	Identity
100	[C ₅ H ₅ Cl] ⁺
196	[M-4Cl] ⁺
236	[C ₅ HCl ₅] ⁺
265	[M-HCl ₂] ⁺
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

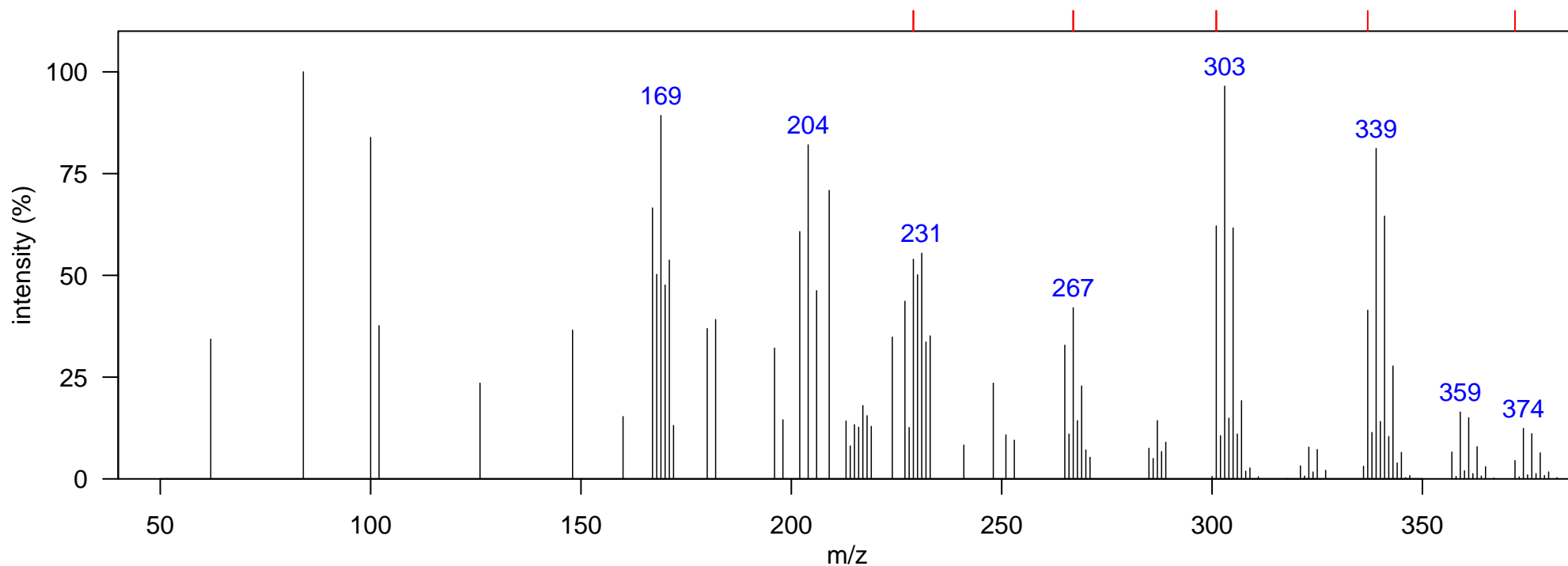
Comment:

Elemental Formula: C₁₀H₇Cl₇

Source: anthropogenic

Class: chlordane related

Identification: Manual



m/z	Identity
229	[M-H ₃ Cl ₄] ⁺
267	[M-H ₂ Cl ₃] ⁺
301	[M-HCl ₂] ⁺
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

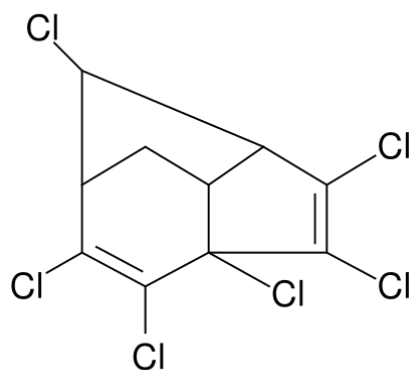
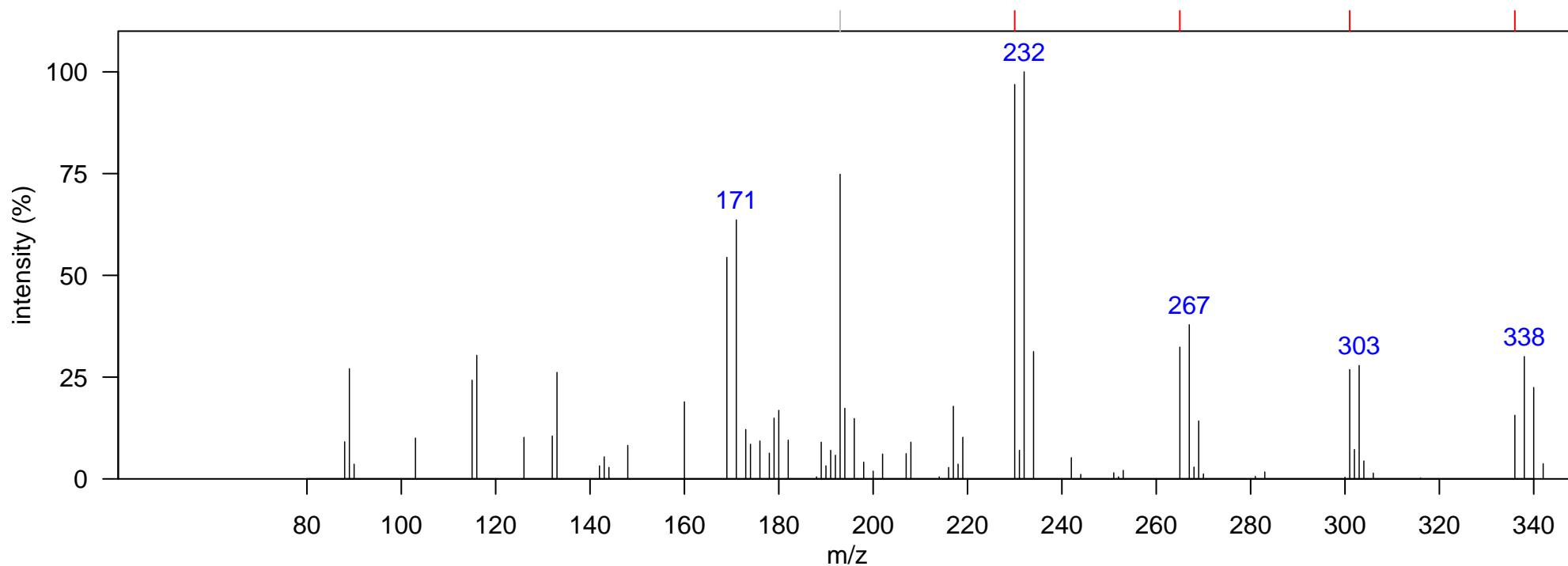
Comment:

Elemental Formula: C₁₀H₆Cl₆

Source: anthropogenic

Class: chlordane related

Identification: Reference Database MS



m/z	Identity
193	interference
230	[M-HCl ₃] ⁺
265	[M-HCl ₂] ⁺
301	[M-Cl] ⁺
336	M ⁺

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

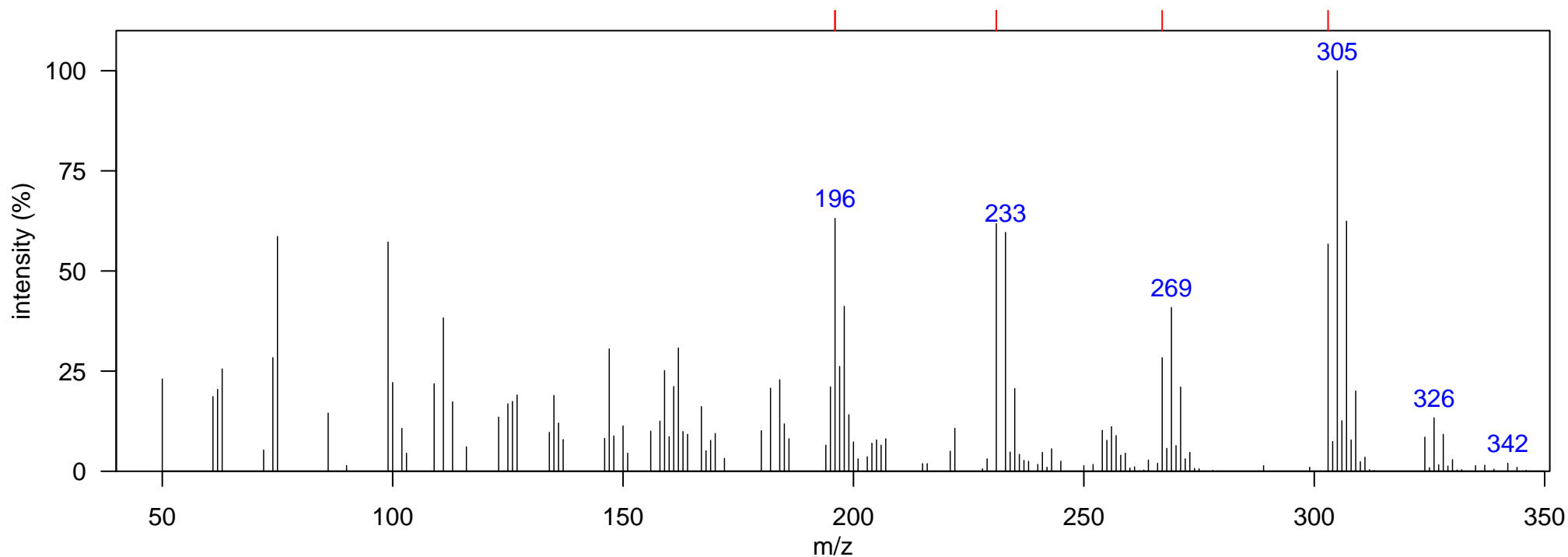
Comment: Suggested elemental formula is C₁₀H₈Cl₆.

Elemental Formula: C₁₀H₈Cl₆

Source: anthropogenic

Class: chlordane related

Identification: Manual



m/z	Identity
196	[Frag-H ₂ Cl ₃] ⁺
231	[Frag-H ₂ Cl ₂] ⁺
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

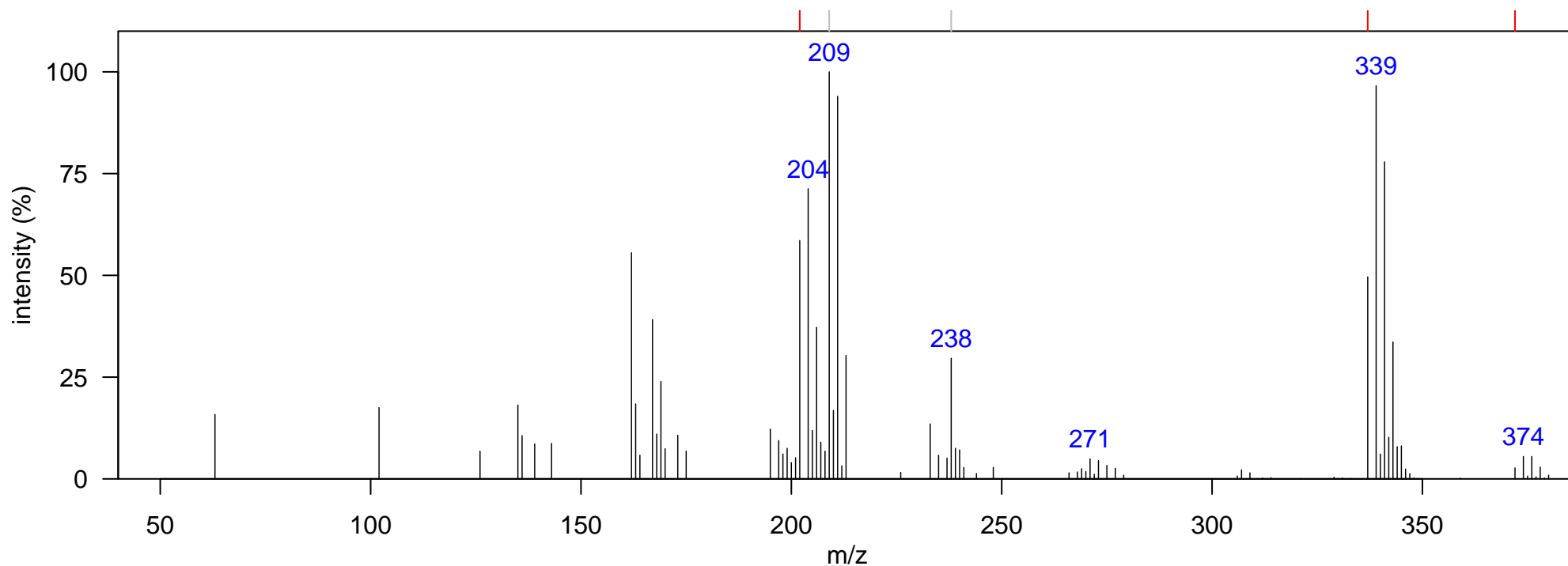
Comment:

Elemental Formula: C₁₀H₇Cl₇

Source: anthropogenic

Class: chlordane related

Identification: Manual – Congener Group



m/z	Identity
202	[C ₅ H ₂ Cl ₄] ⁺
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

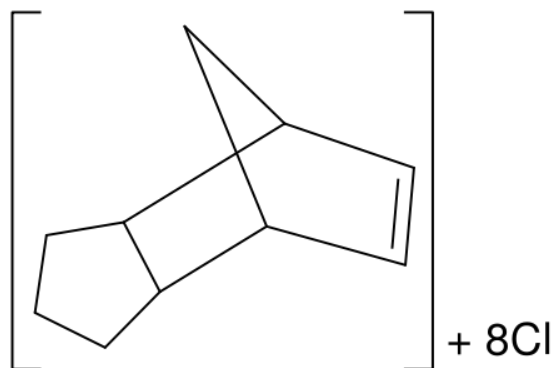
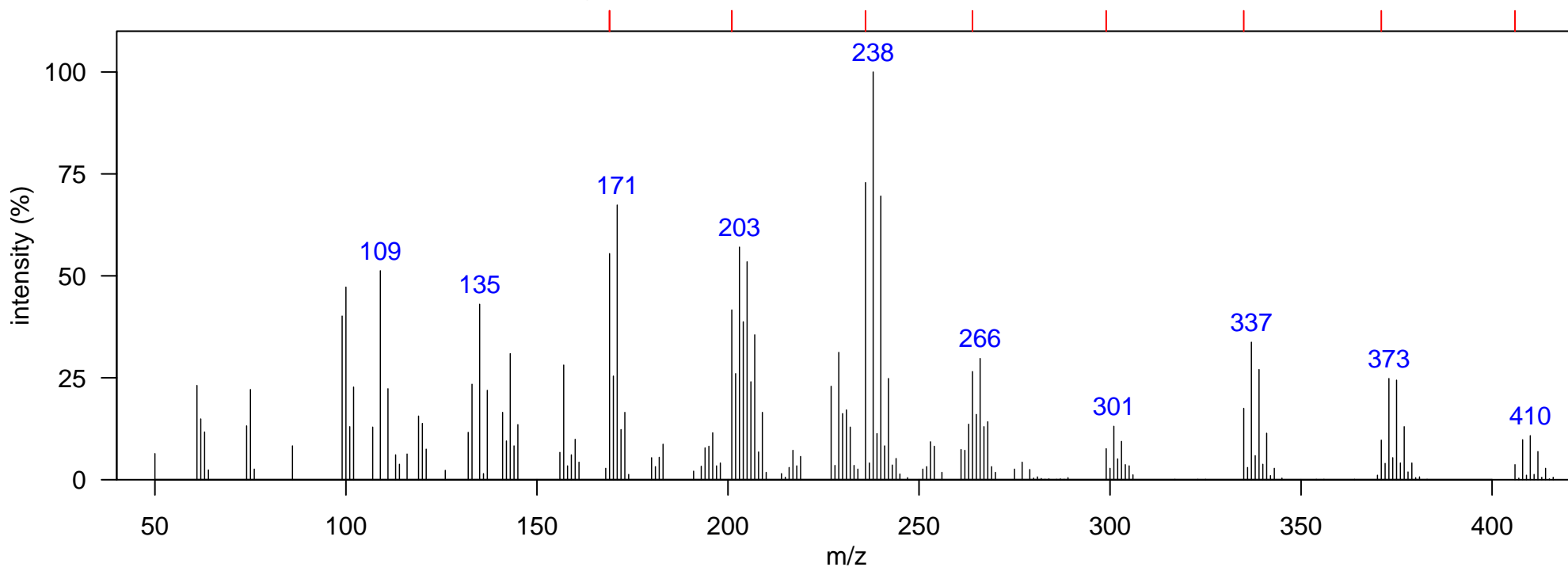
Comment: Similar to chlordane, but different fragment ion intensities,

Elemental Formula: C₁₀H₆Cl₈

Source: anthropogenic

Class: chlordane related

Identification: Manual – Congener Group



m/z	Identity
169	[C ₅ H ₄ Cl ₃] ⁺
201	[C ₅ HCl ₄] ⁺
236	[C ₅ HCl ₅] ⁺
264	[M-H ₂ Cl ₄] ⁺
299	[M-HCl ₃] ⁺
335	[M-HCl ₂] ⁺
371	[M-Cl] ⁺
406	[M] ⁺

Name: chlordanes related 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

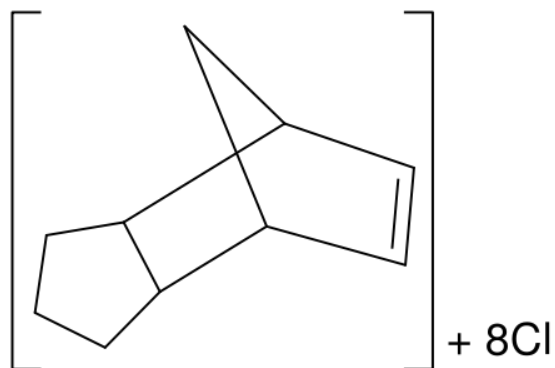
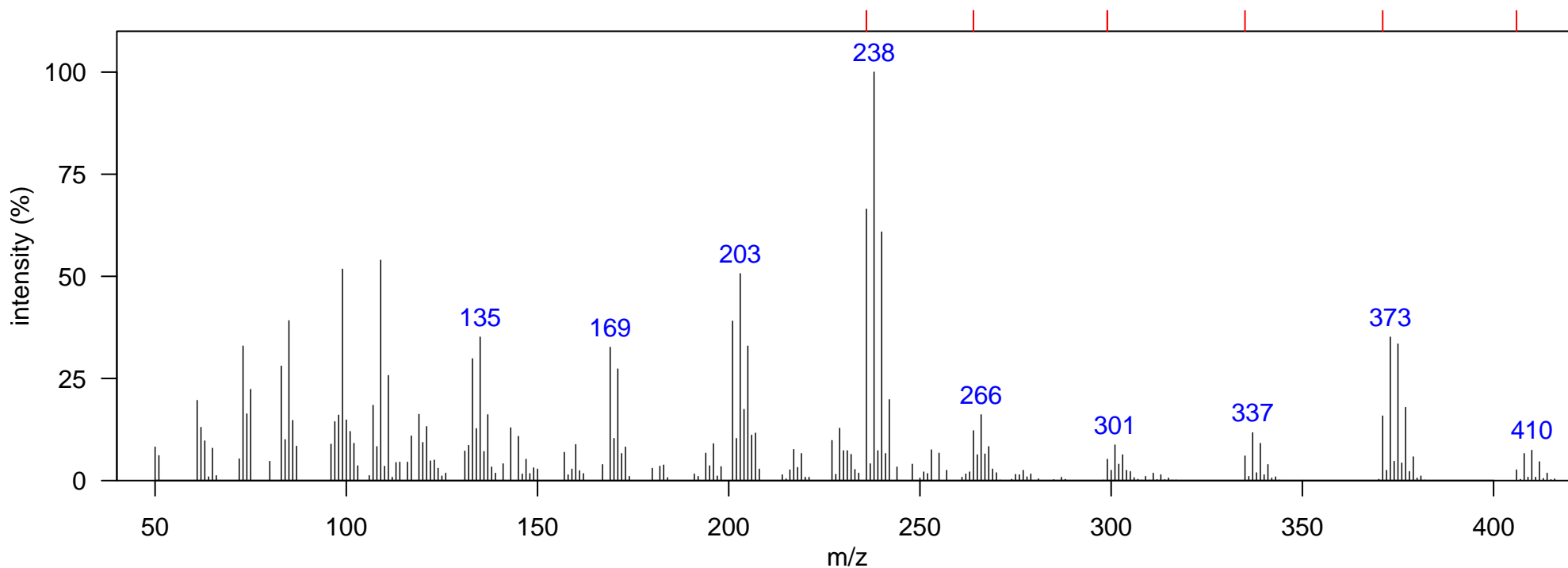
Comment: Similar to chlordanes, but ion cluster at m/z 272 is not present.

Elemental Formula: C₁₀H₆Cl₈

Source: anthropogenic

Class: chlordanes related

Identification: Manual – Congener Group



m/z	Identity
236	[C ₅ HCl ₅] ⁺
264	[M-H ₂ Cl ₃] ⁺
299	[M-H ₂ Cl ₃] ⁺
335	[M-HCl ₂] ⁺
371	[M-Cl] ⁺
406	M ⁺

Name: oxychlordanes

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

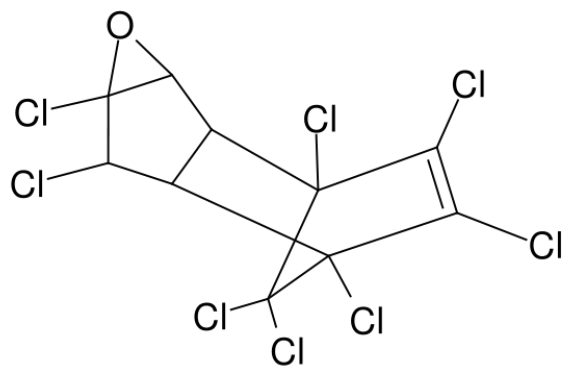
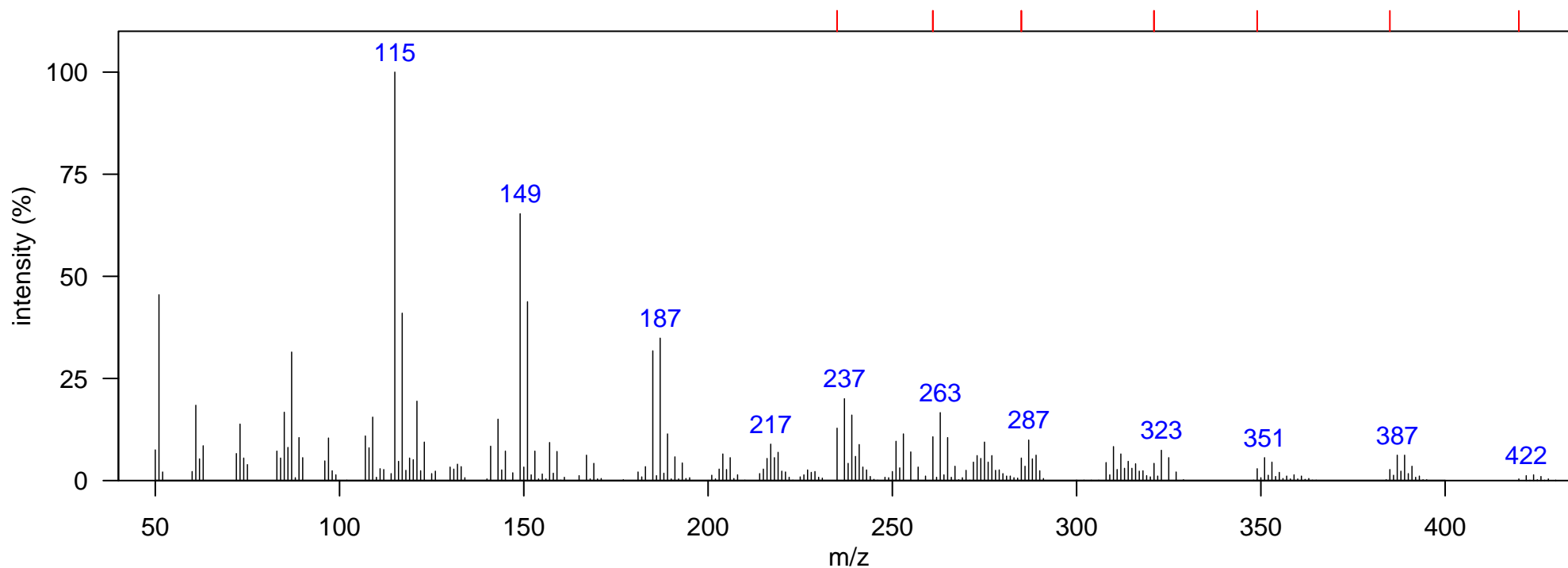
Comment:

Elemental Formula: C₁₀H₄Cl₈O

Source: anthropogenic

Class: chlordanes related

Identification: Reference Database MS



m/z	Identity
235	[C ₅ Cl ₅] ⁺
261	[C ₇ H ₂ Cl ₅] ⁺
285	[M-H ₂ Cl ₃ -CO] ⁺
321	[M-HCl ₂ -CO] ⁺
349	[M-HCl ₂] ⁺
385	[M-Cl] ⁺
420	[M] ⁺

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

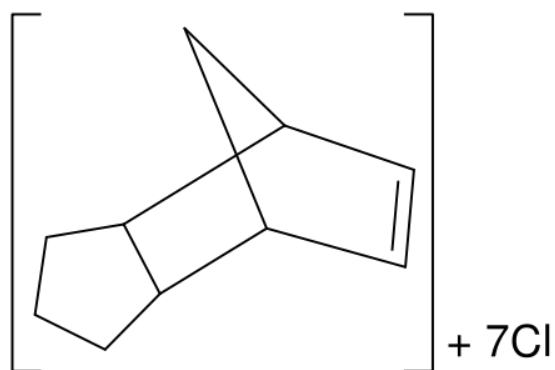
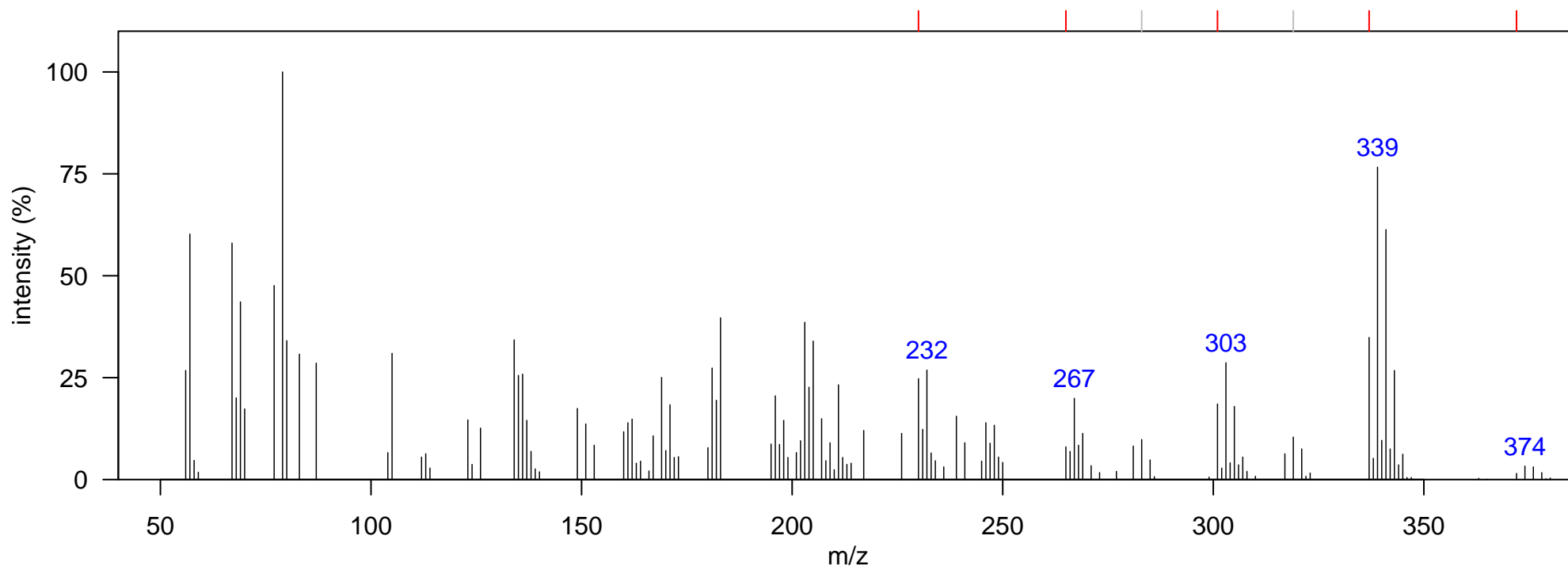
Comment: Similar to heptachlor, but ion cluster at m/z 272 is not present.

Elemental Formula: C₁₀H₇Cl₇

Source: anthropogenic

Class: chlordane related

Identification: Manual – Congener Group



m/z	Identity
230	[M-H ₂ Cl ₄] ⁺
265	[M-H ₂ Cl ₃] ⁺
283	interference
301	[M-HCl ₂] ⁺
319	interference
337	[M-Cl] ⁺
372	M ⁺

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

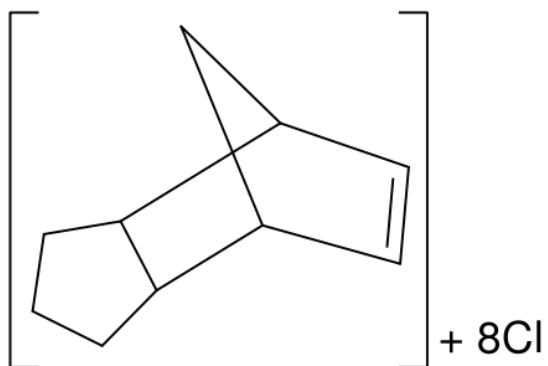
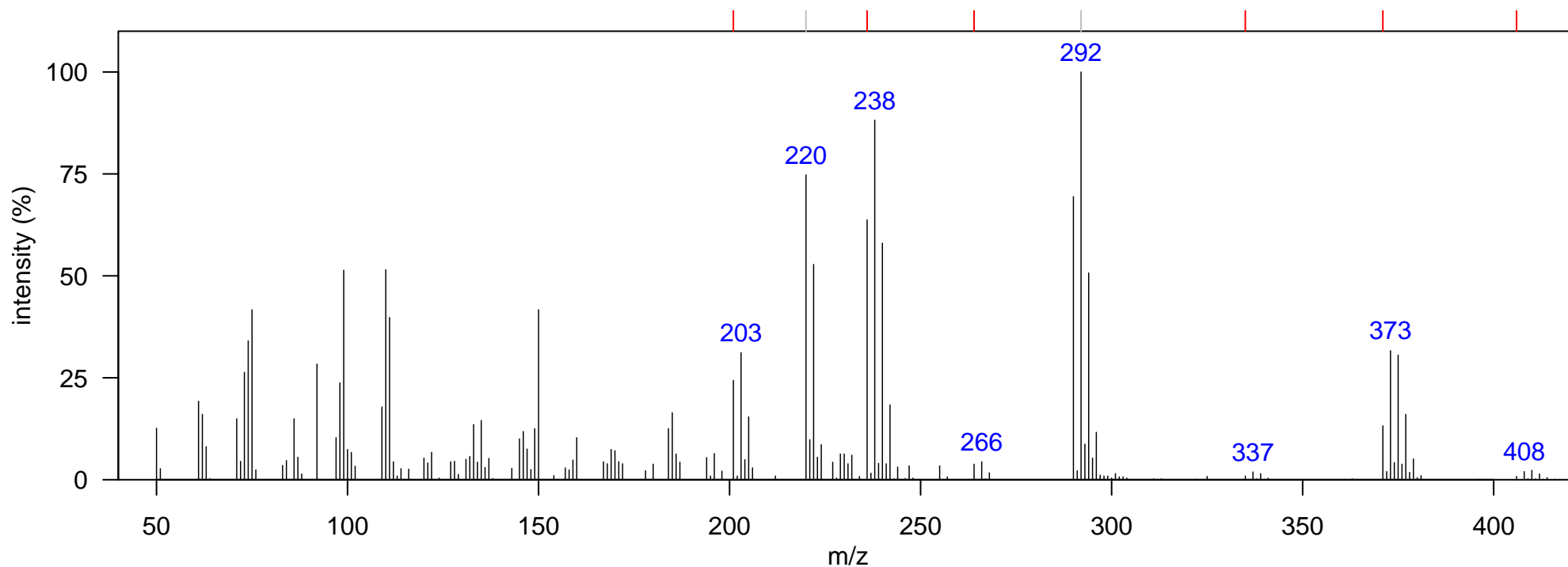
Comment: Similar to chlordane.

Elemental Formula: C₁₀H₆Cl₈

Source: anthropogenic

Class: chlordane related

Identification: Manual – Congener Group



m/z	Identity
201	[C ₅ HCl ₄] ⁺
220	PCB interference
236	[C ₅ HCl ₅] ⁺
264	[M-H ₂ Cl ₄] ⁺
292	PCB interference
335	[M-HCl ₂] ⁺
371	[M-Cl] ⁺
406	M ⁺

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

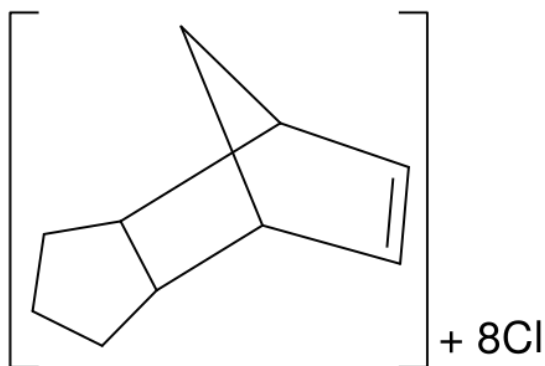
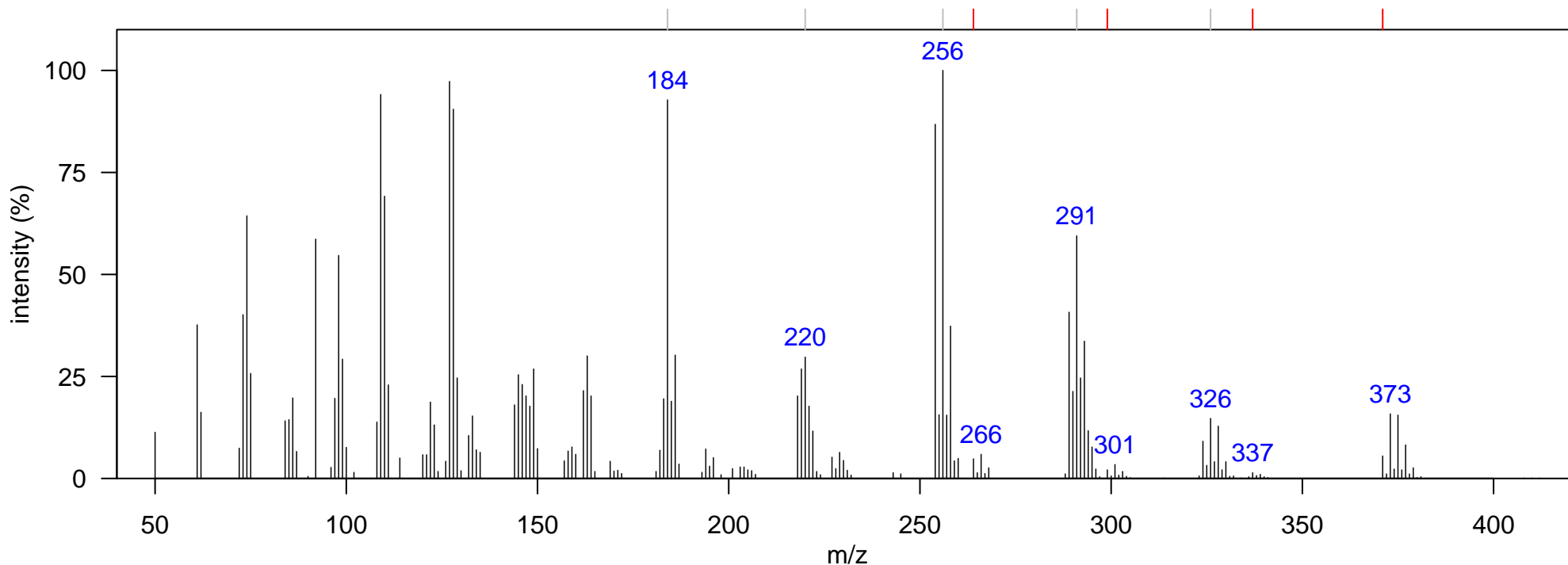
Comment: Ion cluster at m/z 373 related to chlordane. M+ not detected.

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-H ₂ Cl ₄] ⁺
291	PCB interference
299	[M-H ₂ Cl ₃] ⁺
326	PCB interference
337	[M-HCl ₂] ⁺ (not monoisotopic)
371	[M-Cl] ⁺

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

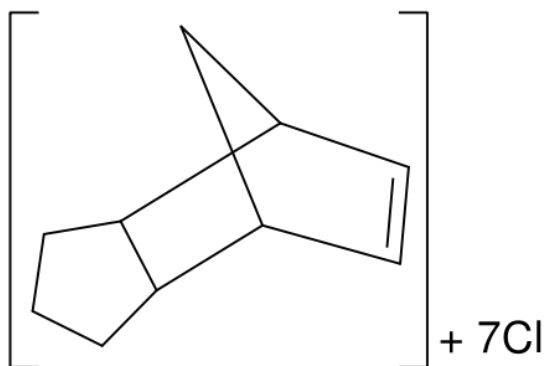
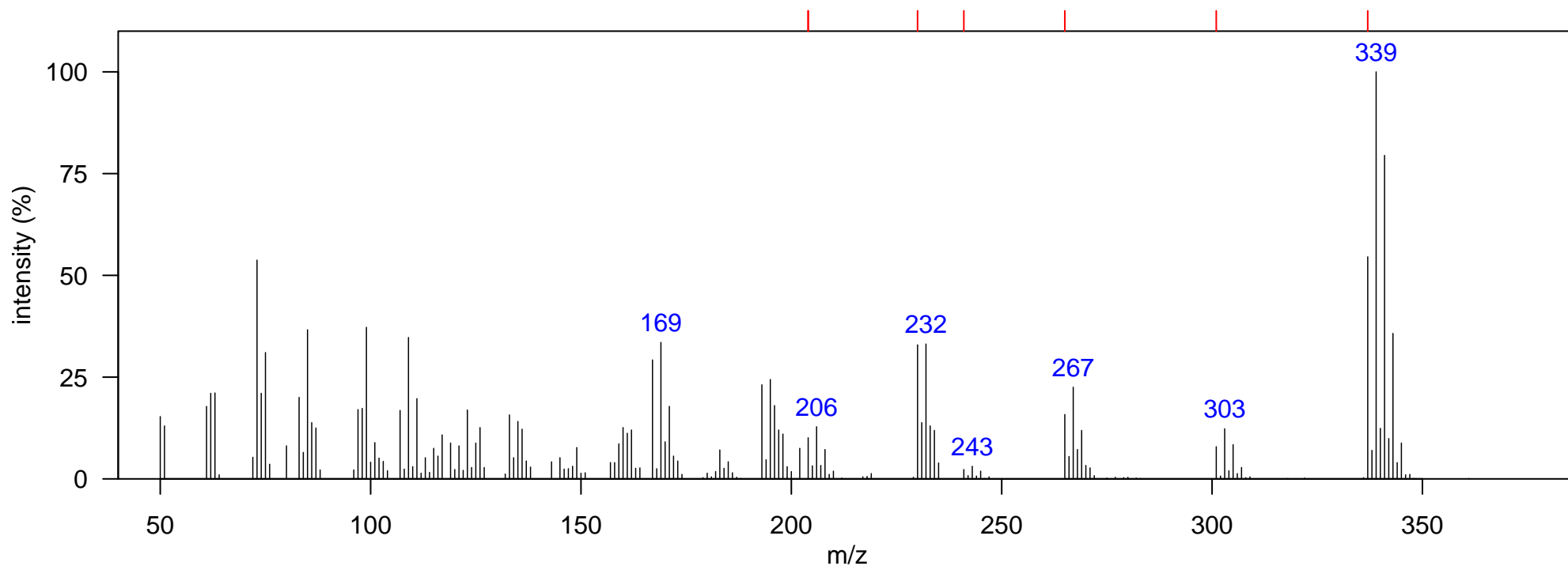
Comment: Ion cluster at m/z 339 suggests C₁₀H₆Cl₆. M⁺ not detected.

Elemental Formula: C₁₀H₇Cl₇

Source: anthropogenic

Class: chlordane related

Identification: Manual



m/z	Identity
204	[C ₅ H ₄ Cl ₄] ⁺
230	[M-H ₂ Cl ₄] ⁺
241	[C ₅ H ₆ Cl ₅] ⁺
265	[M-H ₂ Cl ₃] ⁺
301	[M-HCl ₂] ⁺
337	[M-Cl] ⁺

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

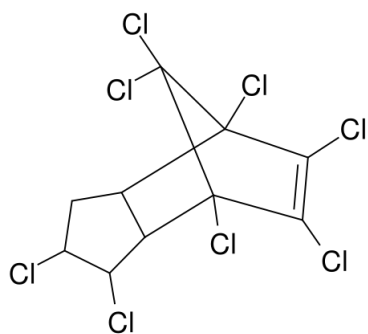
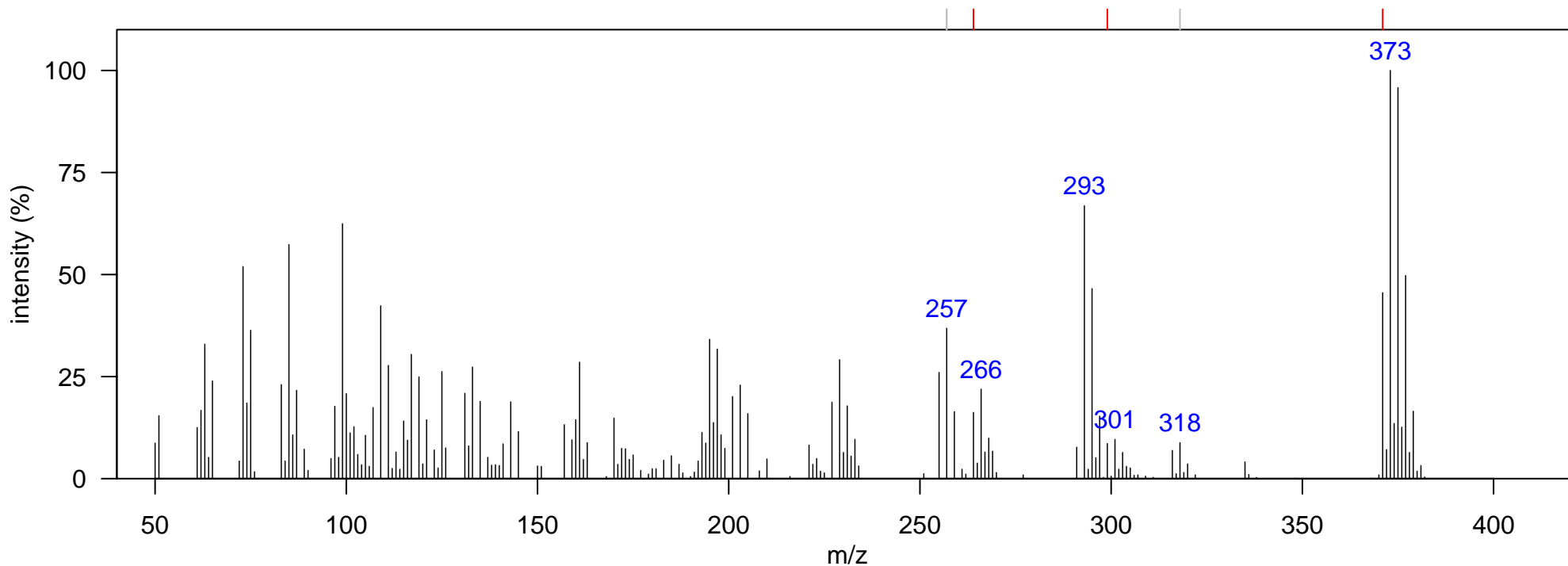
Comment: M+ not present in the "peak true" mass spectrum, but is present in the caliper mass spectrum.

Elemental Formula: C₁₀H₆Cl₈

Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT



(stereochemistry not shown)

m/z	Identity
257	interference
264	[M-H ₂ Cl ₄] ⁺
299	[M-H ₂ Cl ₃] ⁺
318	DDE interference
371	[M-Cl] ⁺

Name: alpha-chlordane

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

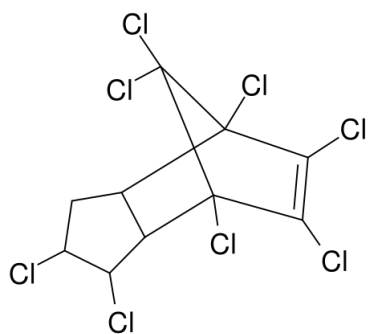
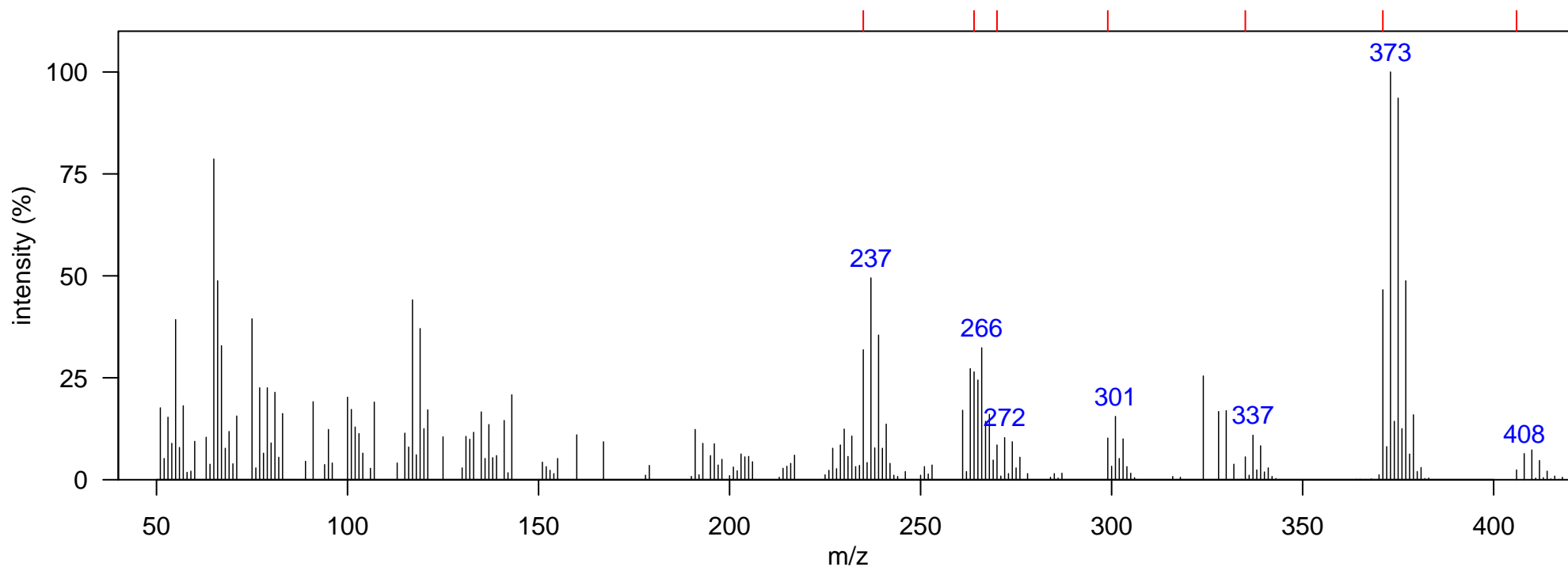
Comment:

Elemental Formula: C₁₀H₆Cl₈

Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT



(stereochemistry not shown)

m/z	Identity
235	[C ₅ Cl ₅] ⁺
264	[M-H ₂ Cl ₄] ⁺
270	[C ₅ Cl ₆] ⁺
299	[M-H ₂ Cl ₃] ⁺
335	[M-HCl ₂] ⁺
371	[M-Cl] ⁺
406	M ⁺

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

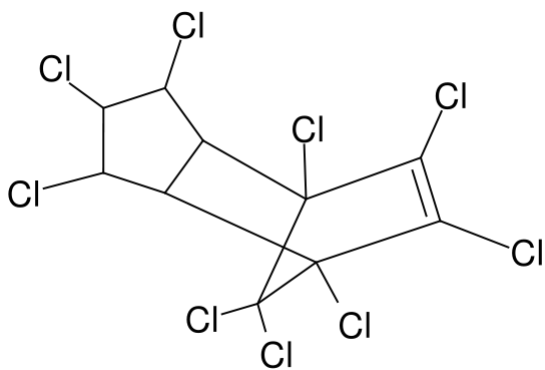
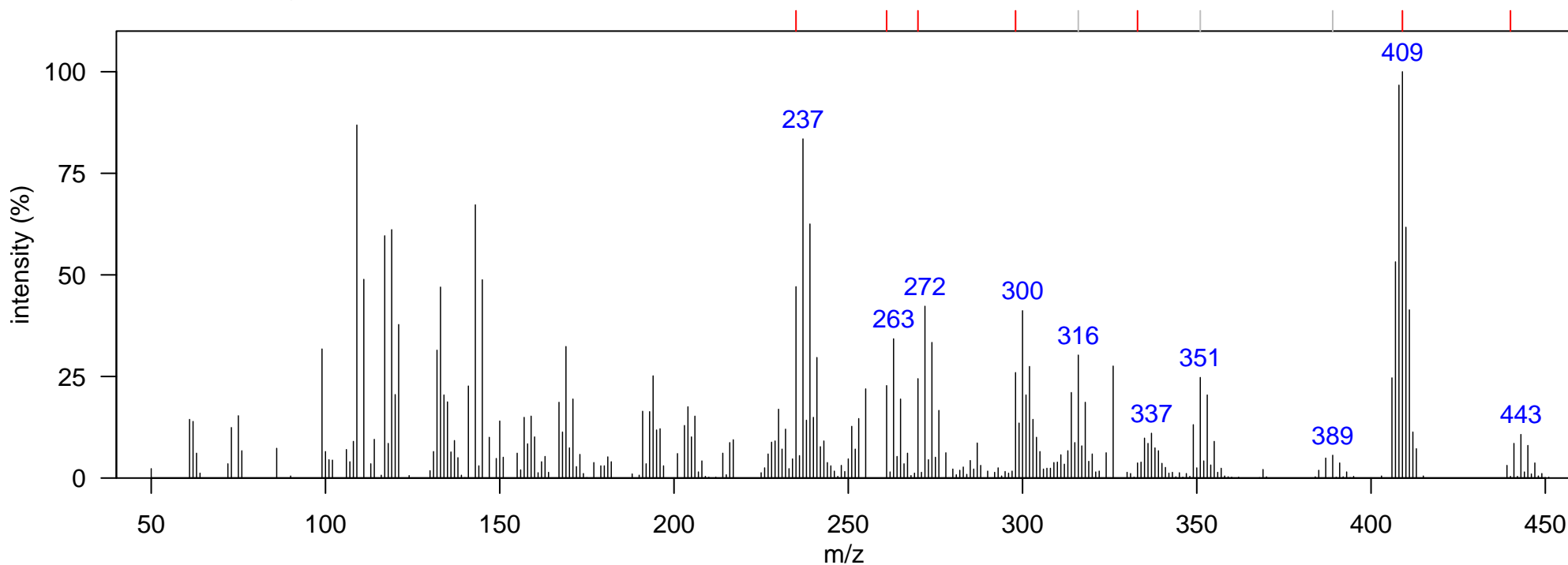
Comment: Chromatographic peak is saturated.

Elemental Formula: C₁₀H₅Cl₉

Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT



m/z	Identity
235	[C ₅ Cl ₅] ⁺
261	[M-H ₄ Cl ₅] ⁺
270	[C ₅ Cl ₆] ⁺
298	[M-H ₂ Cl ₄] ⁺
316	interference MBP(7Cl)
333	[M-H ₂ Cl ₃] ⁺
351	interference MBP(7Cl)
389	interference MBP(7Cl)
409	[M-Cl] ⁺ (not monoisotopic)
440	M ⁺

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

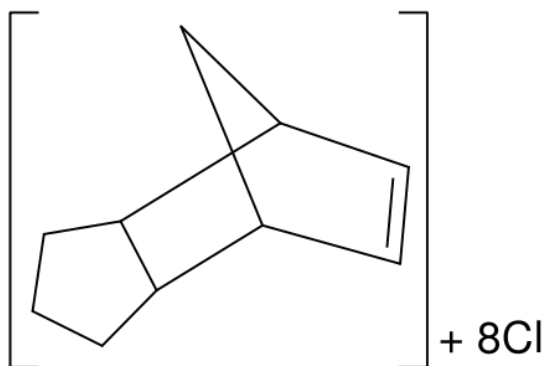
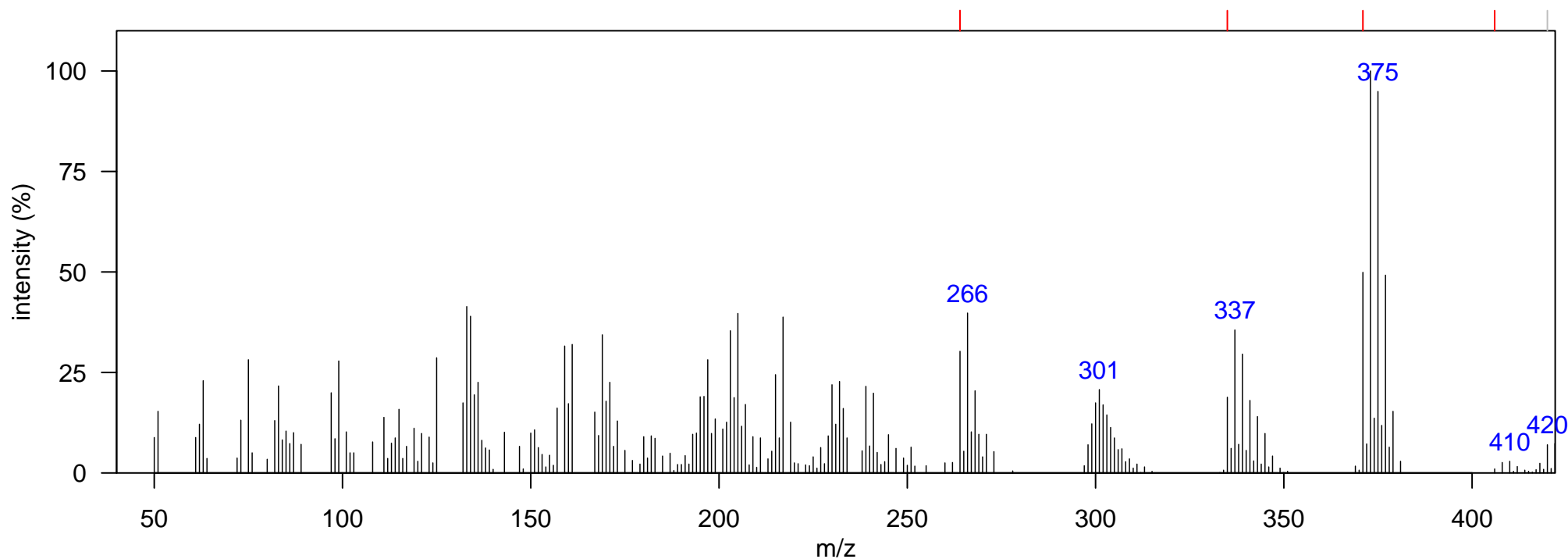
Comment: Chlordane isomer.

Elemental Formula: C₁₀H₆Cl₈

Source: anthropogenic

Class: chlordane related

Identification: Manual – Congener Group



m/z	Identity
264	[M-H ₂ Cl ₄] ⁺
335	[M-HCl ₂] ⁺
371	[M-Cl] ⁺
406	M ⁺
420	interference
452	interference

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

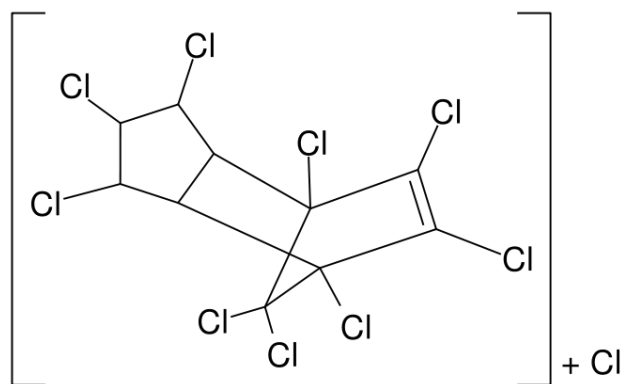
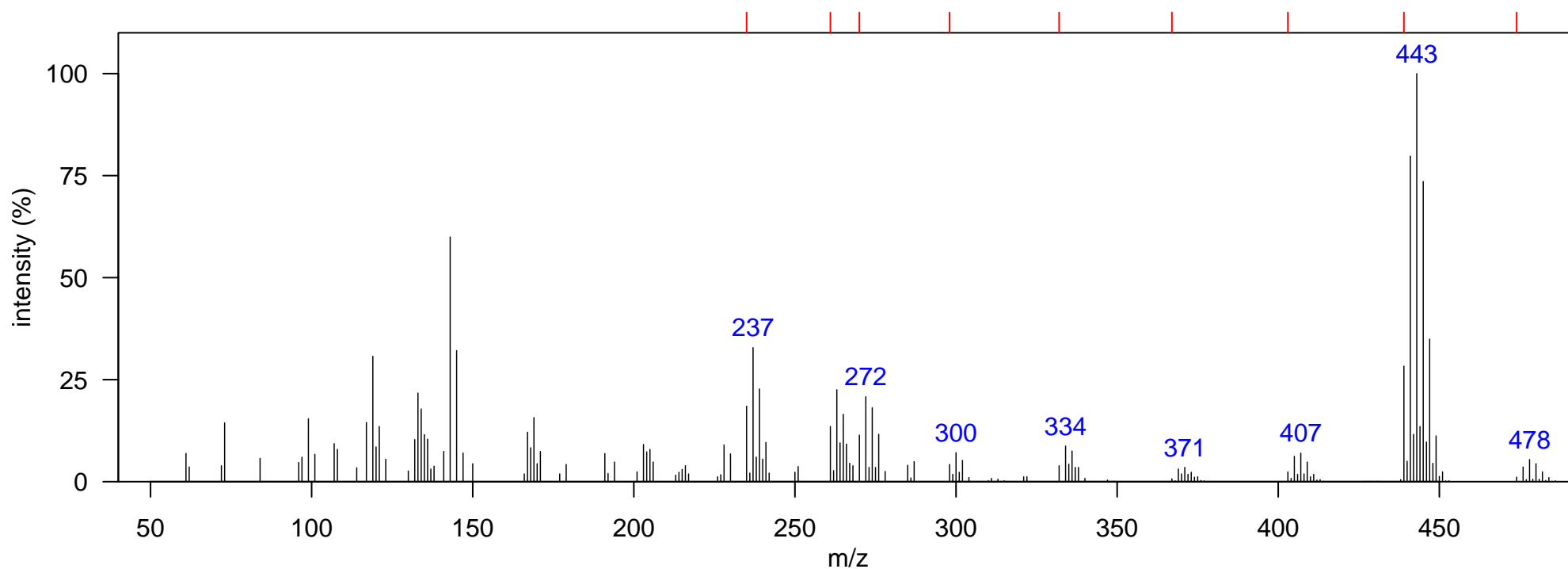
Comment:

Elemental Formula: C₁₀H₄Cl₁₀

Source: anthropogenic

Class: chlordane related

Identification: Manual – Congener Group



m/z	Identity
235	[C ₅ Cl ₅] ⁺
261	[C ₇ H ₂ Cl ₅] ⁺
270	[C ₅ Cl ₆] ⁺
298	[M-HCl ₅] ⁺
332	[M-H ₂ Cl ₄] ⁺
367	[M-H ₂ Cl ₃] ⁺
403	[M-HCl ₂] ⁺
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

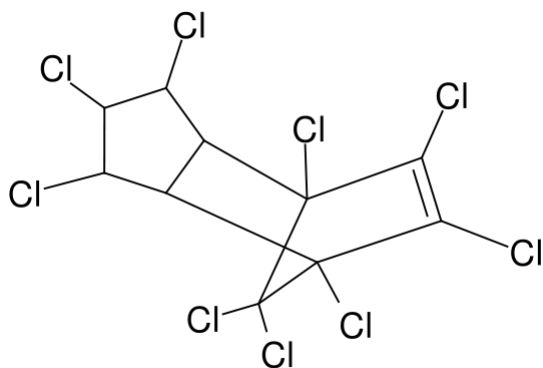
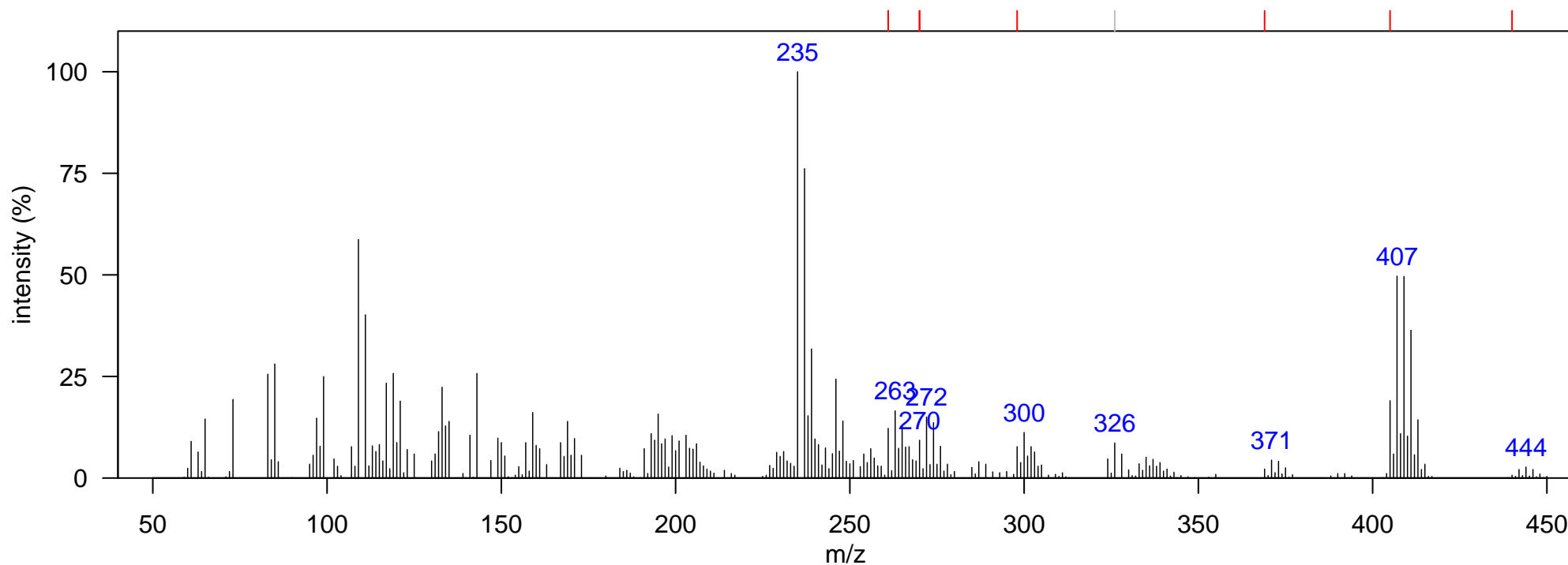
Comment:

Elemental Formula: C₁₀H₅Cl₉

Source: anthropogenic

Class: chlordane related

Identification: Authentic MS RT



m/z	Identity
261	[M-H ₄ Cl ₅] ⁺
270	[C ₅ Cl ₆] ⁺
298	[M-H ₂ Cl ₄] ⁺
326	PCB interference
369	[M-HCl ₂] ⁺
405	[M-Cl] ⁺
440	M ⁺

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

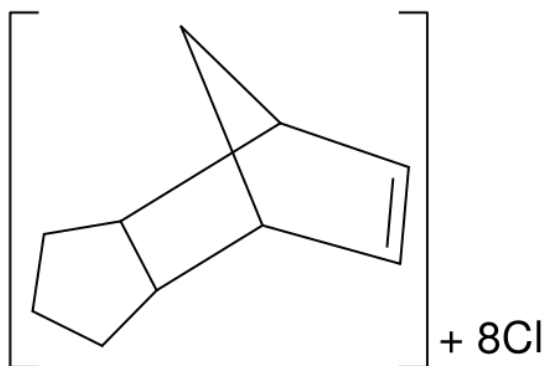
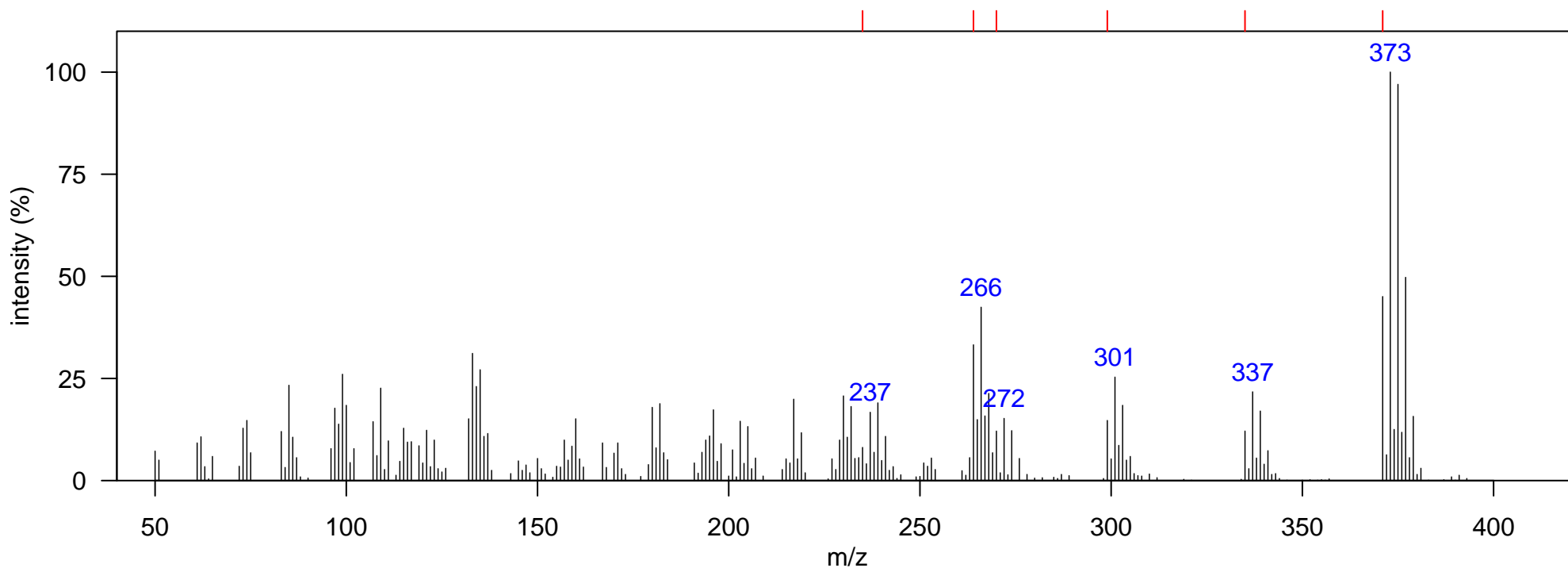
Comment: Chlordane isomer. M+ is not detected.

Elemental Formula: C₁₀H₆Cl₈

Source: anthropogenic

Class: chlordane related

Identification: Manual – Congener Group



m/z	Identity
235	[C ₅ Cl ₅] ⁺
264	[M-H ₂ Cl ₄] ⁺
270	[C ₅ Cl ₆] ⁺
299	[M-H ₂ Cl ₃] ⁺
335	[M-HCl ₂] ⁺
371	[M-Cl] ⁺

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

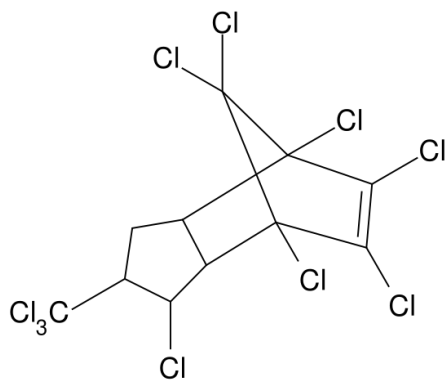
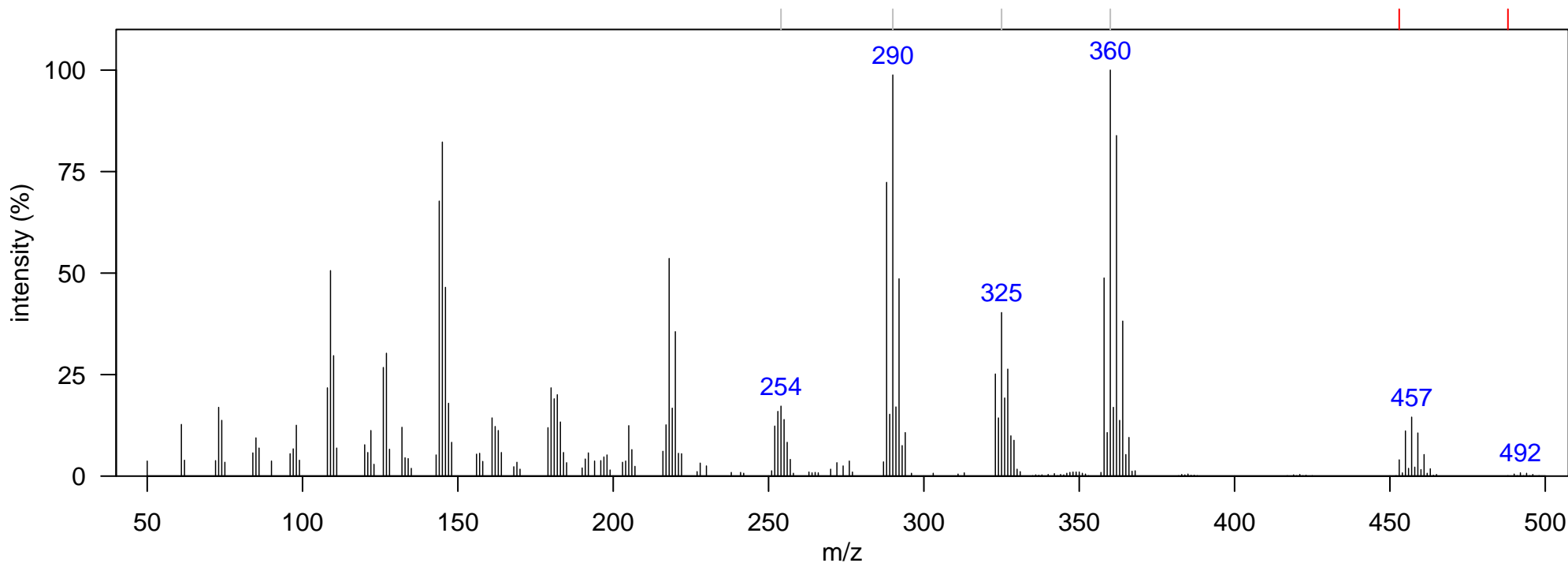
Comment: Ref: ES&T. 1991, 25, 245-254.

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 ⁺

Name: 2 co-eluting: 1-hydroxychlordeane (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

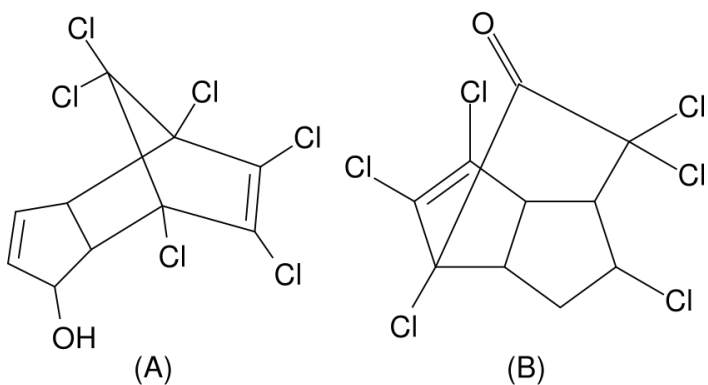
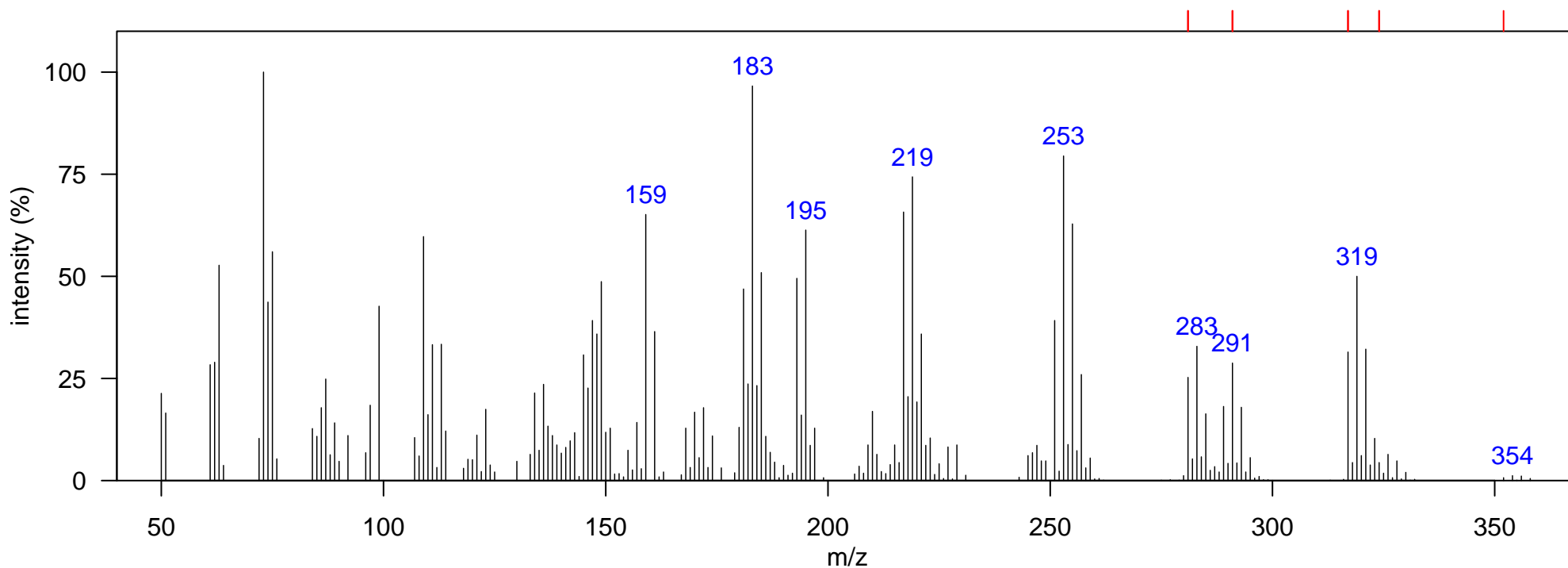
Comment: C₁₀H₆Cl₆O (A); C₁₀H₆Cl₆O (B)

Elemental Formula: NA

Source: anthropogenic

Class: heptachlor related

Identification: Reference Database MS



m/z	Identity
281	[M-HCl ₂] ⁺ (compound A)
291	[M-CO-Cl] ⁺ (compound B)
317	[M-Cl] ⁺ (compound A)
324	[M-CO] ⁺ (compound B)
352	M ⁺ (compound B)

Name: heptachlor

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

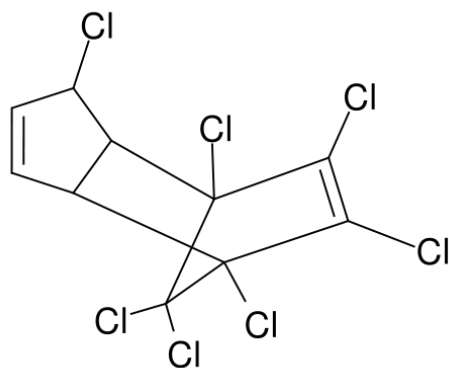
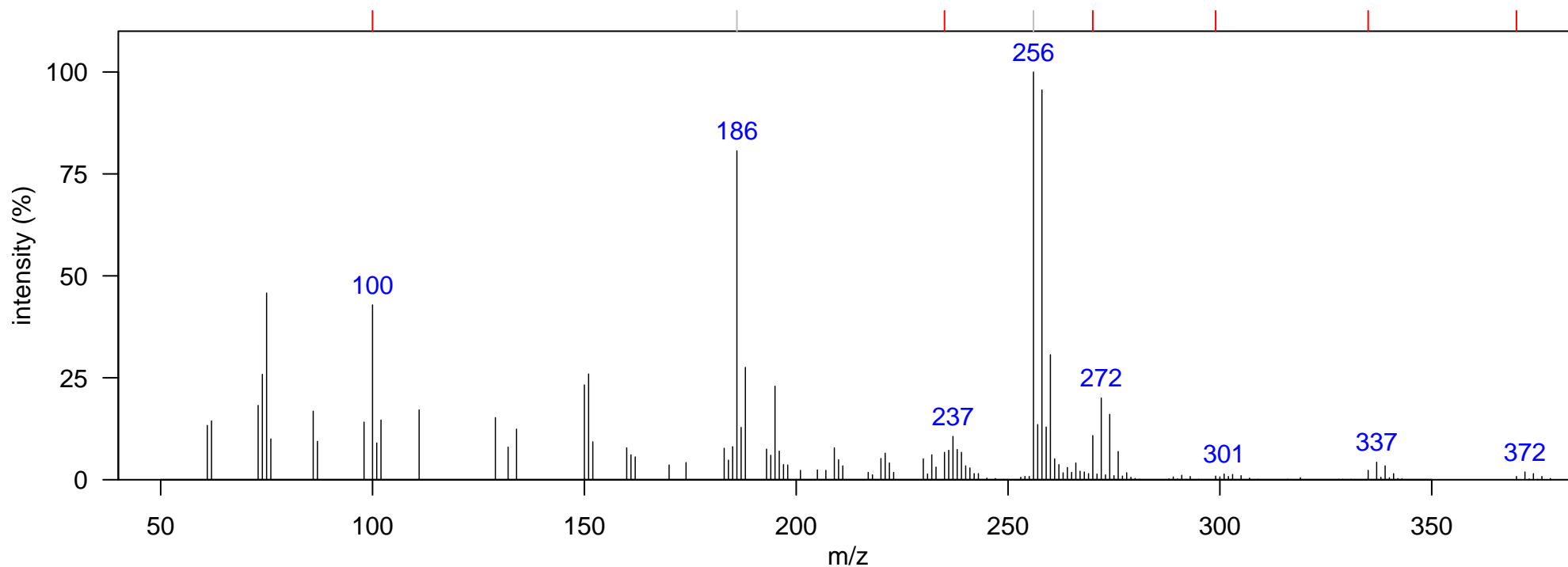
Comment: Low intensity, but visible in raw data. Interference from trichlorobiphenyl.

Elemental Formula: C₁₀H₅Cl₇

Source: anthropogenic

Class: heptachlor related

Identification: Authentic MS RT



m/z	Identity
100	[C ₅ H ₅ Cl] ⁺
186	interference PCB
235	[C ₅ Cl ₅] ⁺
256	interference PCB
270	[C ₅ Cl ₆] ⁺
299	[M-HCl ₂] ⁺
335	[M-Cl] ⁺
370	M ⁺

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

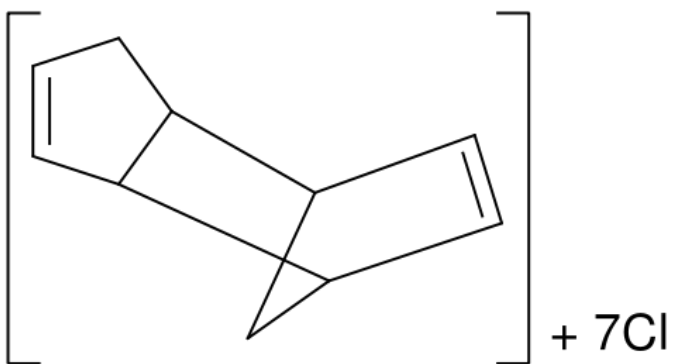
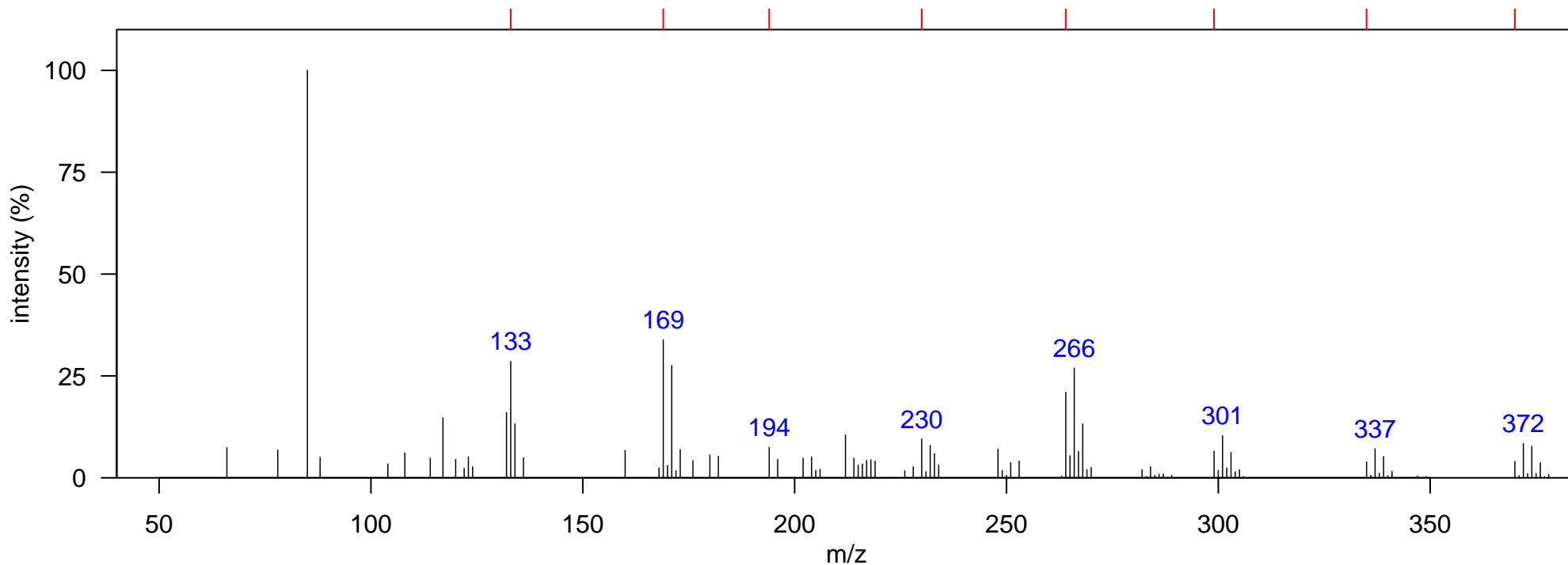
Comment: Similar to heptachlor, but ion cluster at m/z 272 is not present.

Elemental Formula: C₁₀H₅Cl₇

Source: anthropogenic

Class: heptachlor related

Identification: Manual – Congener Group



m/z	Identity
133	[M-HCl ₃] ²⁺
169	[C ₈ H ₃ Cl ₂] ⁺
194	[M-HCl ₅] ⁺
230	[M-4Cl] ⁺
264	[M-HCl ₃] ⁺
299	[M-HCl ₂] ⁺
335	[M-Cl] ⁺
370	[M] ⁺

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

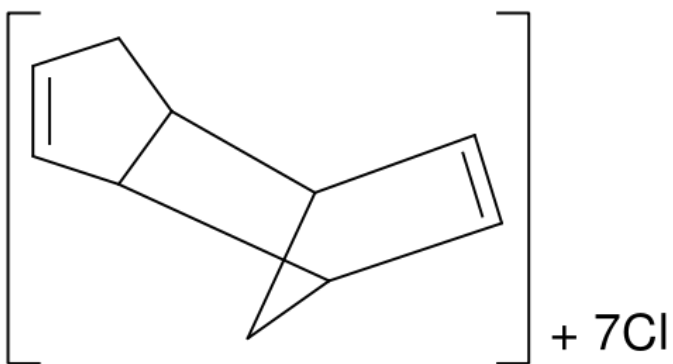
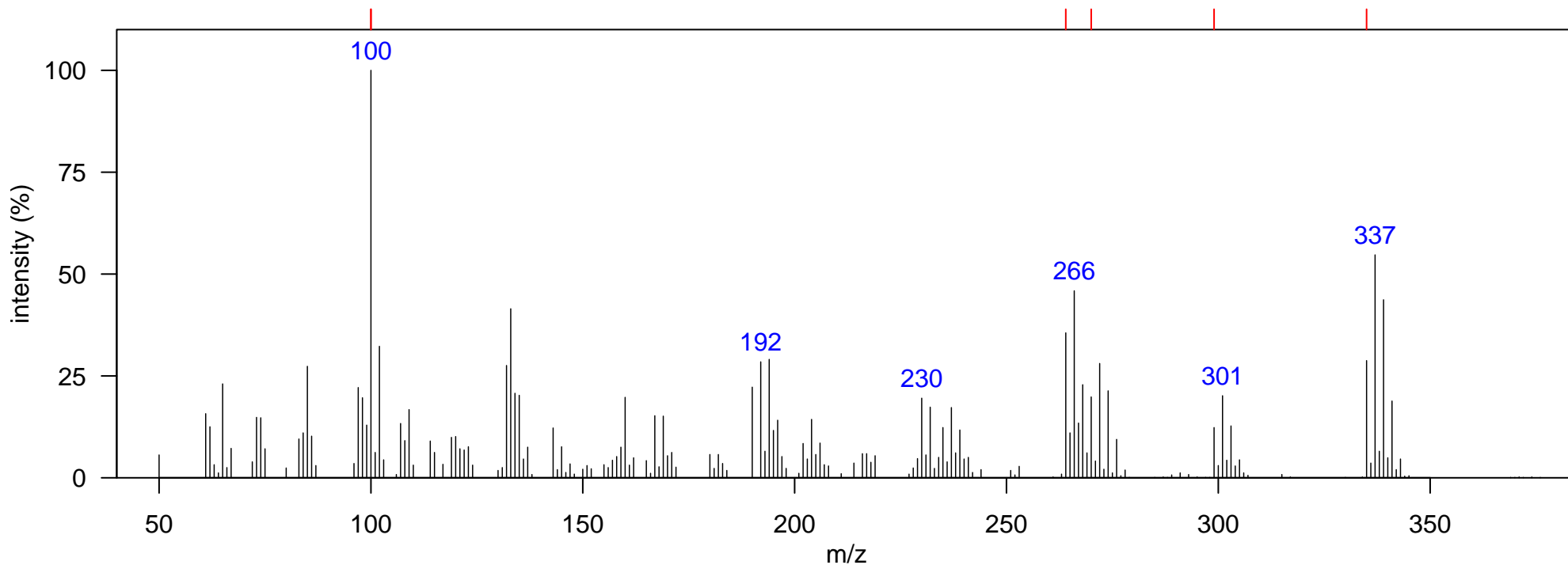
Comment:

Elemental Formula: C₁₀H₅Cl₇

Source: anthropogenic

Class: heptachlor related

Identification: Manual – Congener Group



m/z	Identity
100	[C ₅ H ₅ Cl] ⁺
264	[M-HCl ₃] ⁺
270	[C ₅ Cl ₆] ⁺
299	[M-HCl ₂] ⁺
335	[M-Cl] ⁺

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

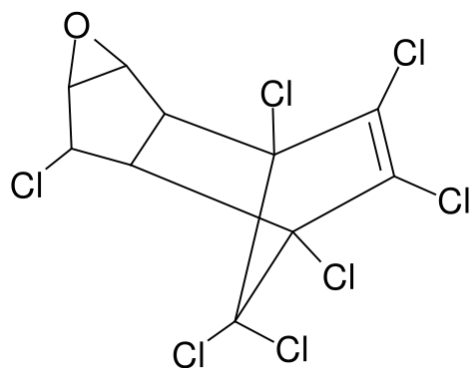
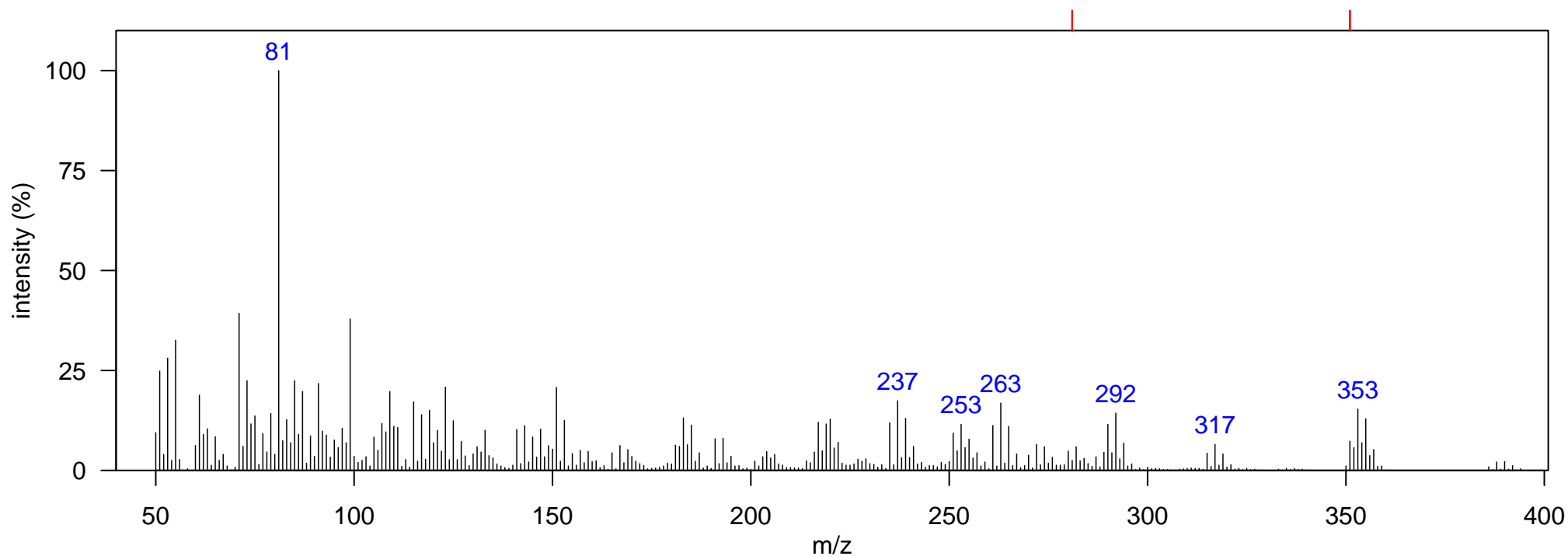
Comment:

Elemental Formula: C₁₀H₅Cl₇O

Source: anthropogenic

Class: heptachlor related

Identification: Authentic MS RT



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

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

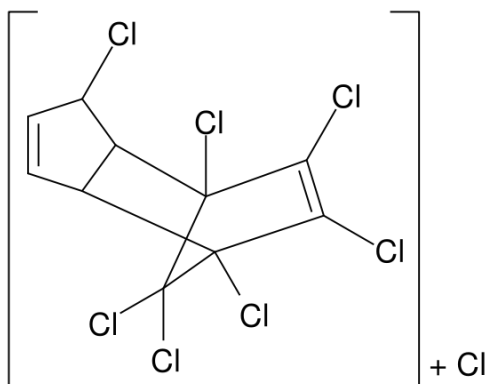
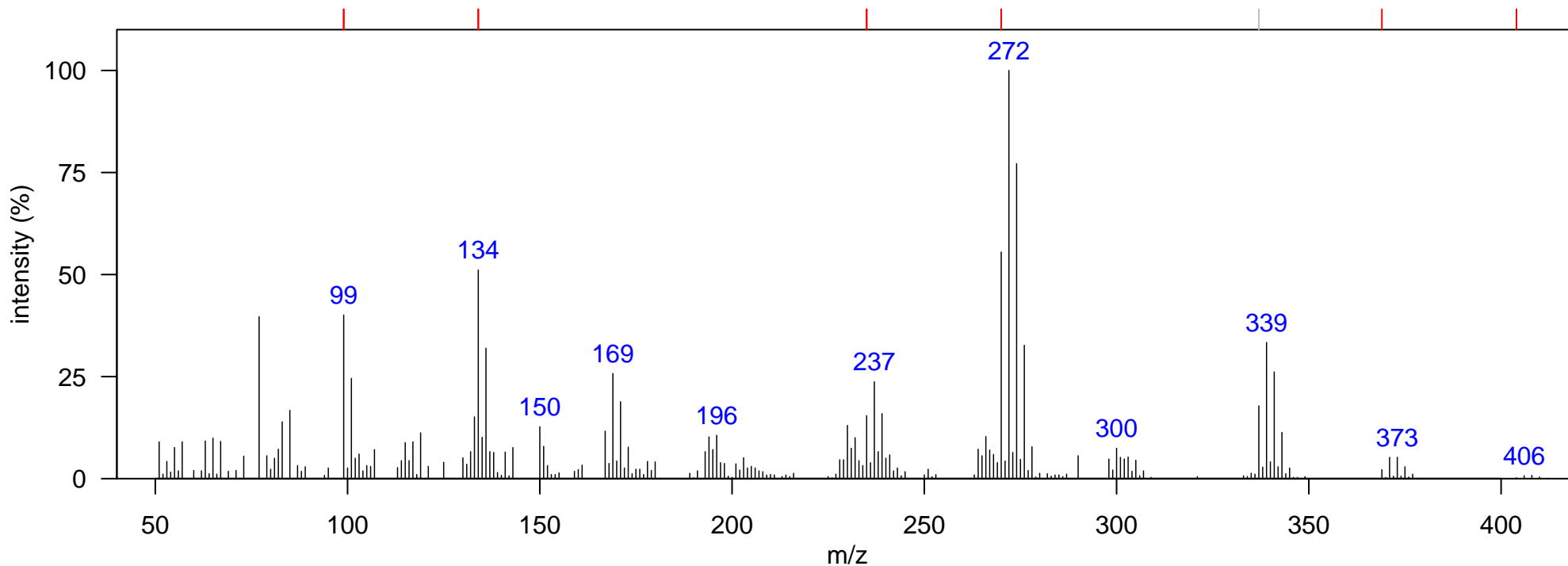
Comment:

Elemental Formula: C₁₀H₄Cl₈

Source: anthropogenic

Class: heptachlor related

Identification: Manual – Congener Group



m/z	Identity
99	[C ₅ H ₄ Cl] ⁺
134	[C ₅ H ₄ Cl ₂] ⁺
235	[C ₅ Cl ₅] ⁺
270	[C ₅ Cl ₆] ⁺
337	interference
369	[M-Cl] ⁺
404	M ⁺

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

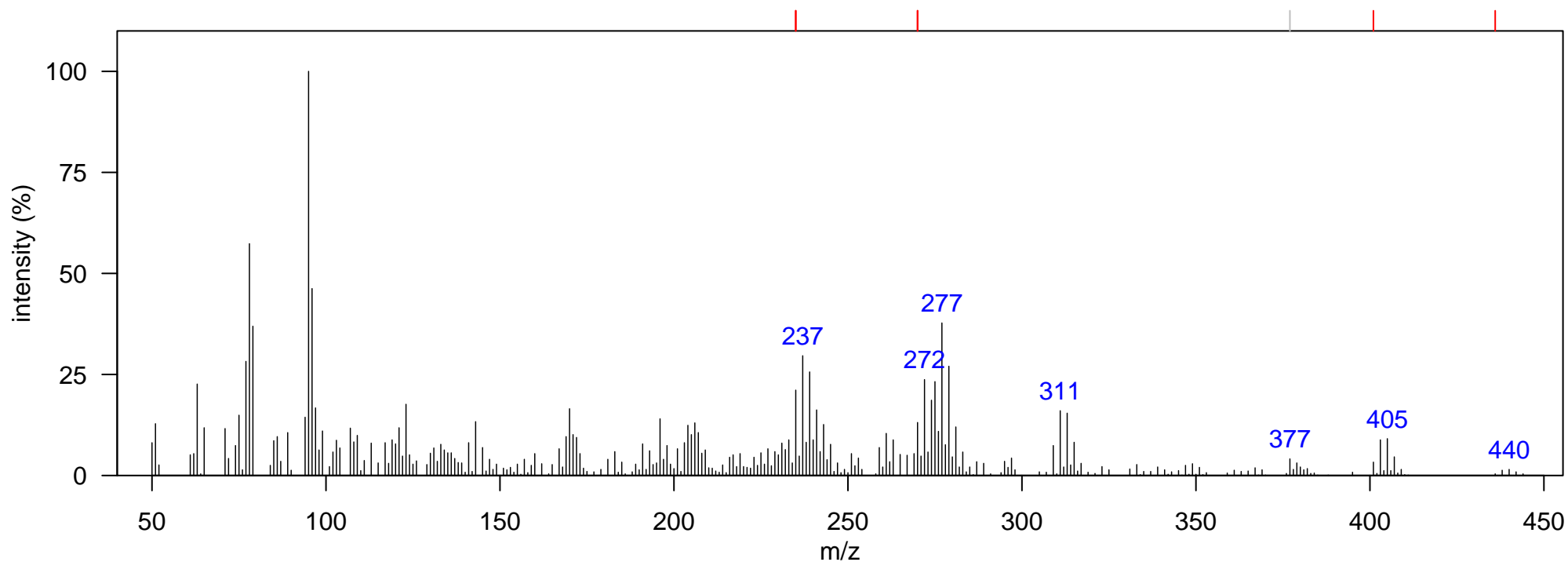
Comment: PM = Possible Molecular Ion

Elemental Formula: C₁₀H₃Cl₉

Source: anthropogenic

Class: heptachlor related

Identification: Manual – Congener Group



m/z	Identity
235	[C ₅ Cl ₅] ⁺
270	[C ₅ Cl ₆] ⁺
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

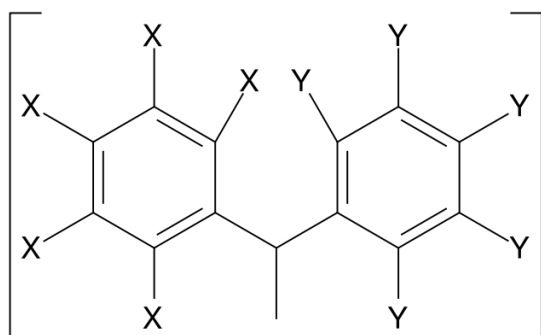
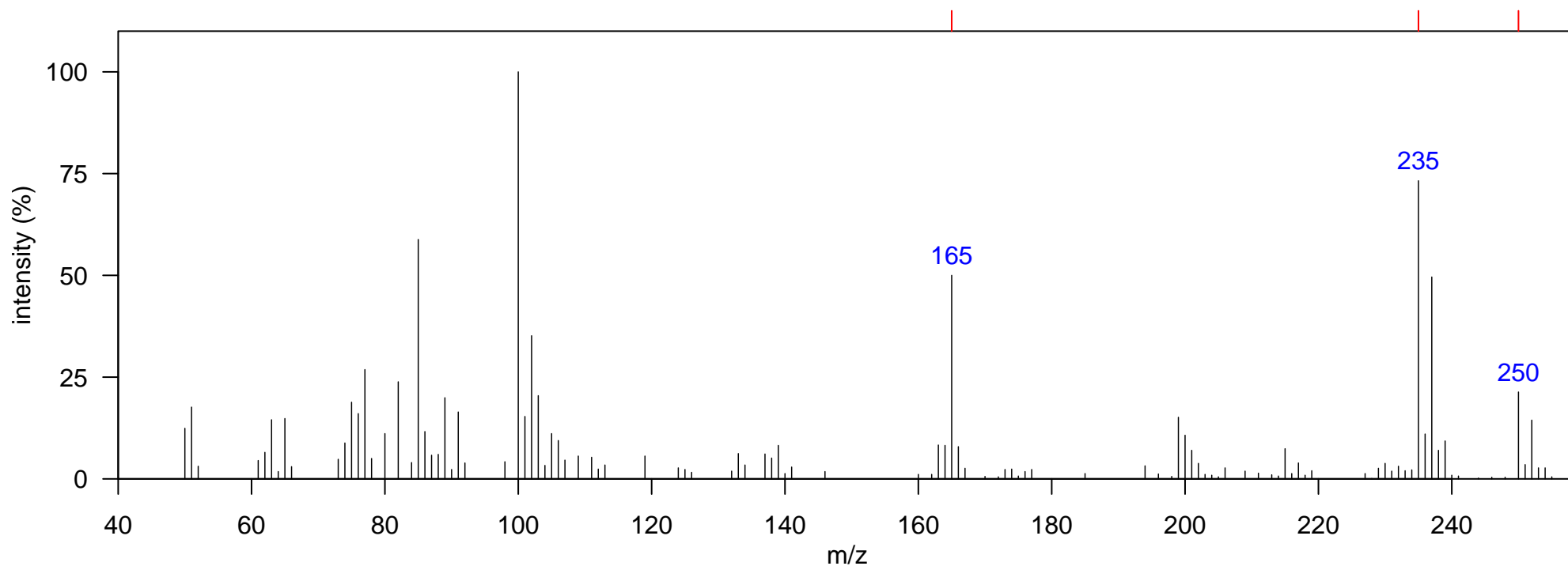
Comment:

Elemental Formula: C₁₄H₁₂Cl₂

Source: anthropogenic

Class: DDT related

Identification: Reference Database MS



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

m/z	Identity
165	[M-CH ₃ -2Cl] ⁺
235	[M-CH ₃] ⁺
250	M ⁺

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

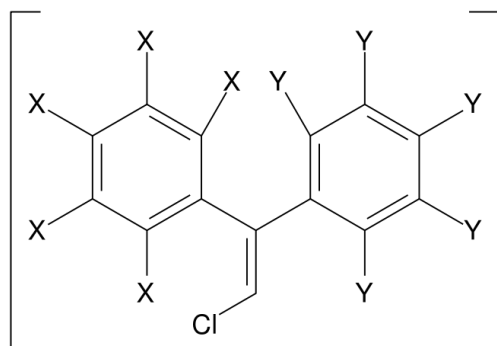
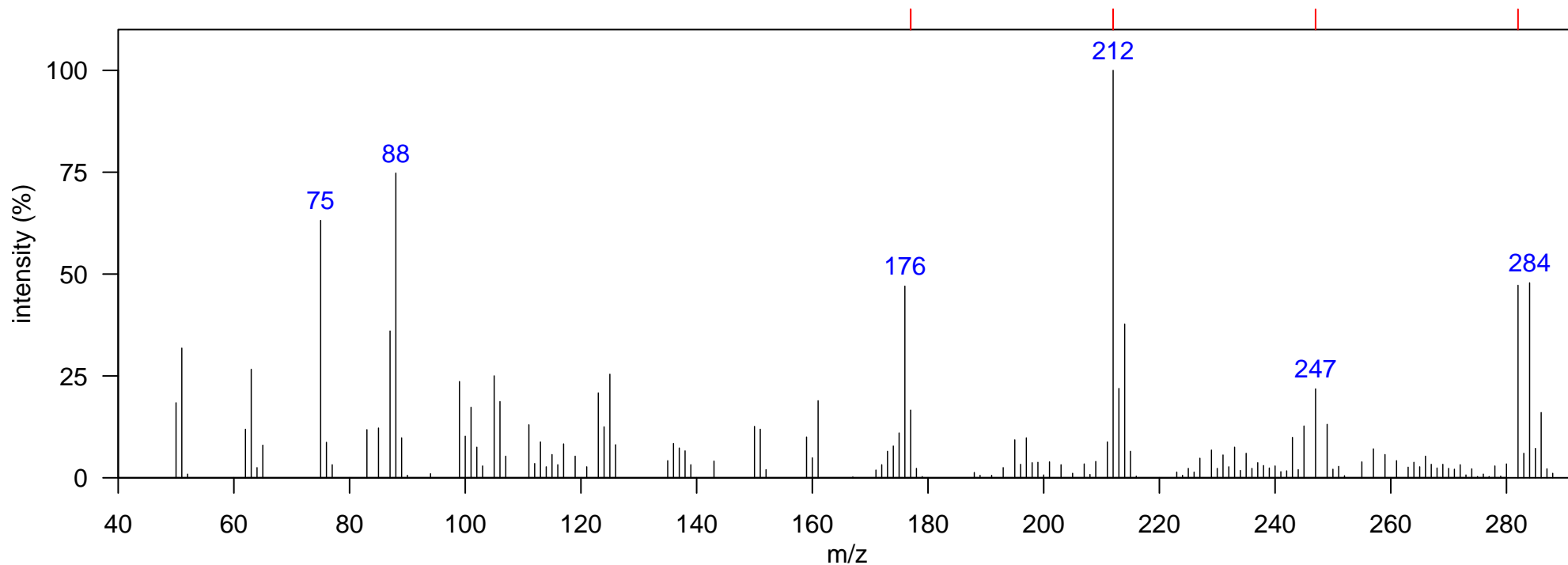
Comment:

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 ⁺

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

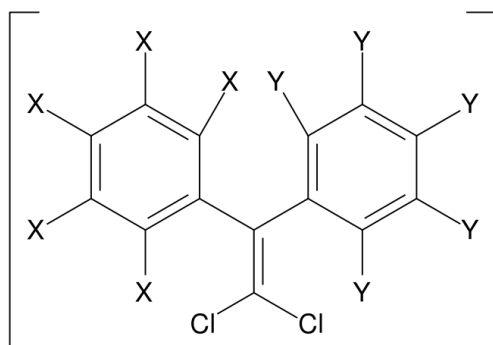
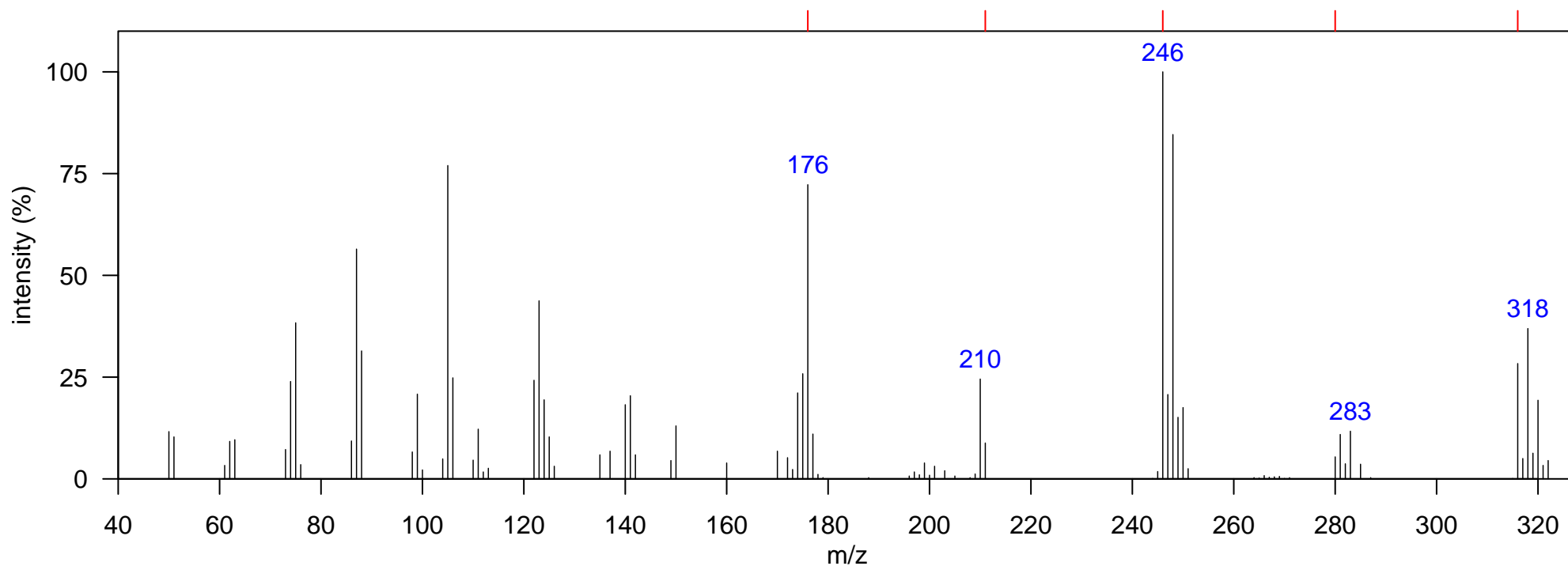
Comment:

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 ⁺

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

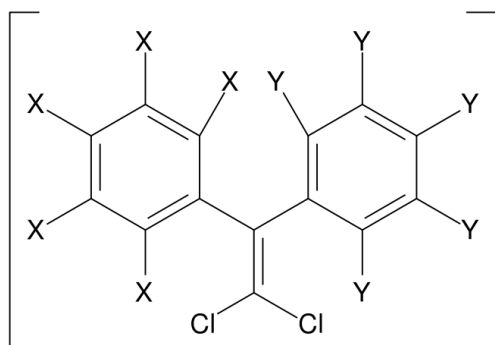
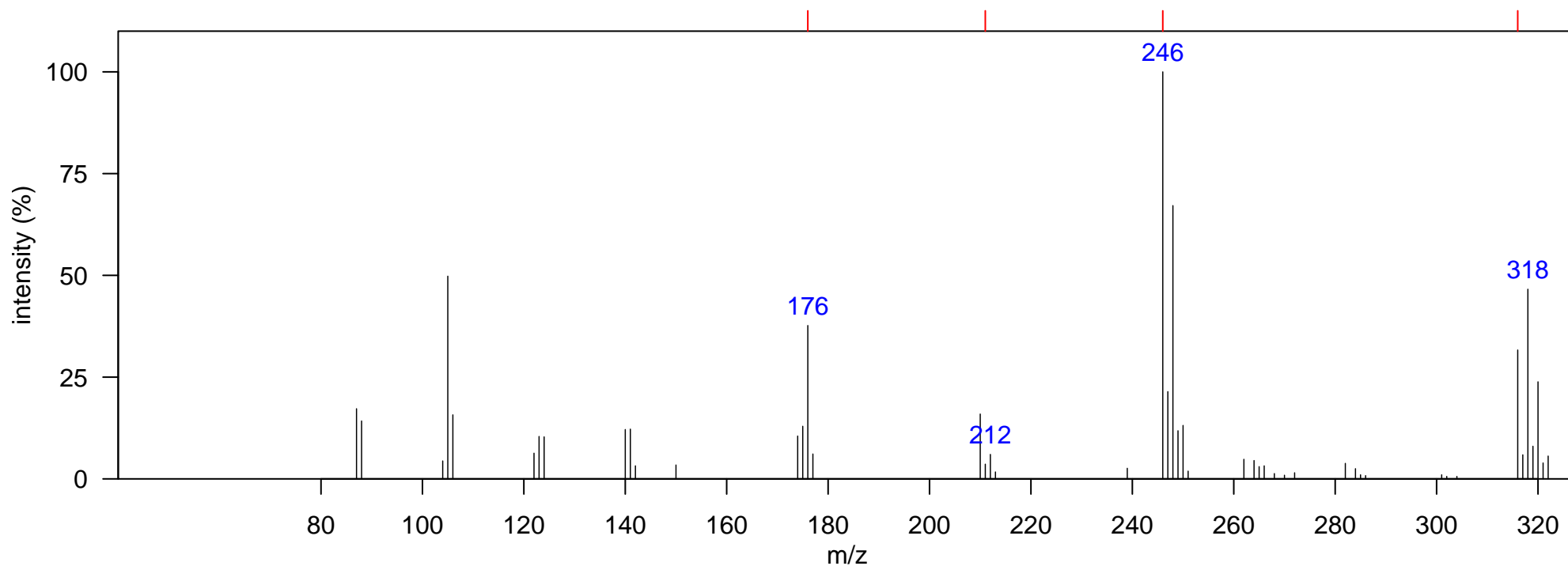
Comment:

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 ⁺

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

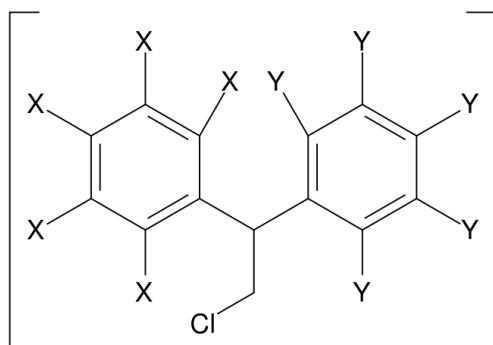
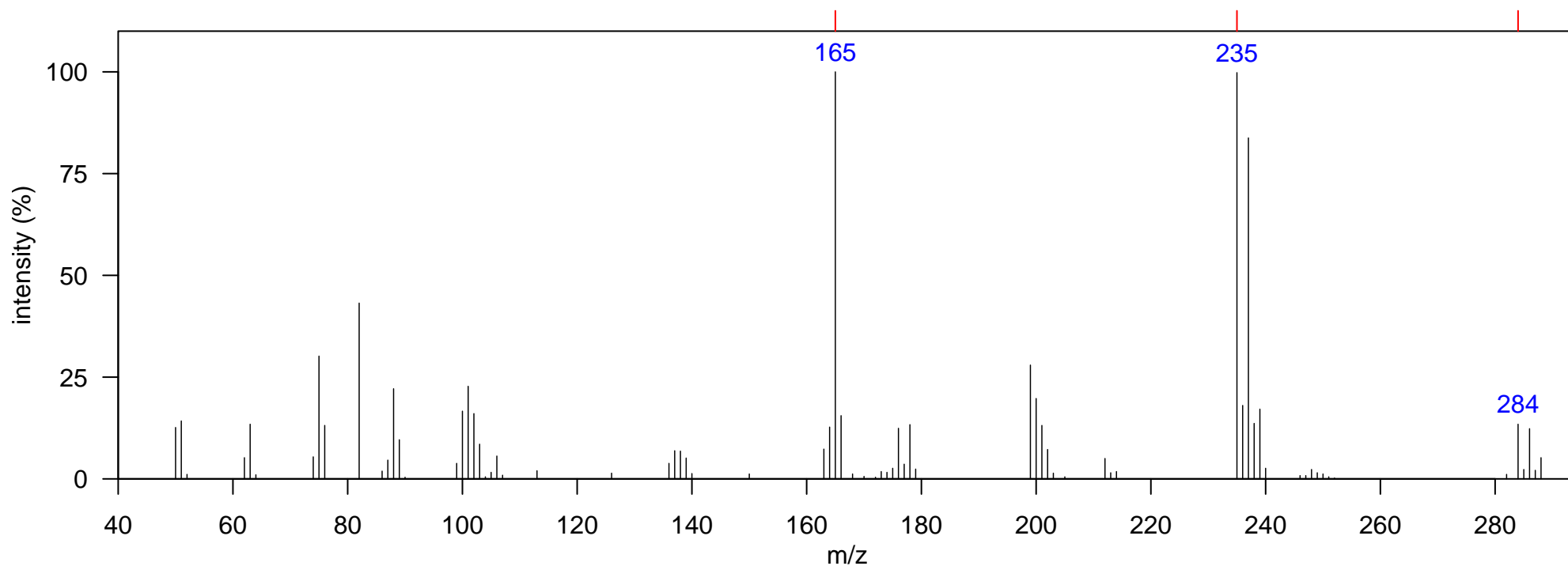
Comment:

Elemental Formula: C₁₄H₁₁Cl₃

Source: anthropogenic

Class: DDT related

Identification: Reference Database MS



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

m/z	Identity
165	[M-CH ₂ Cl-2Cl] ⁺
235	[M-CH ₂ Cl] ⁺
284	M ⁺

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

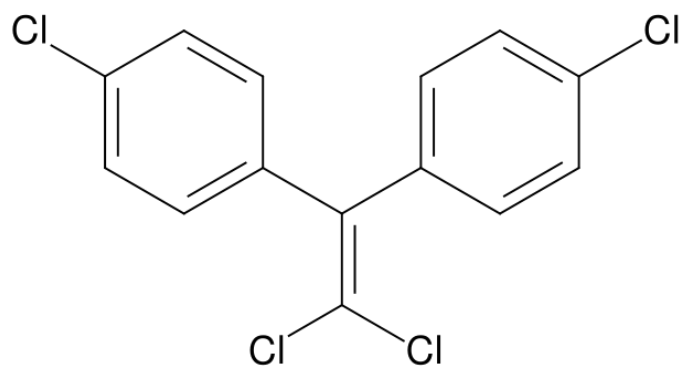
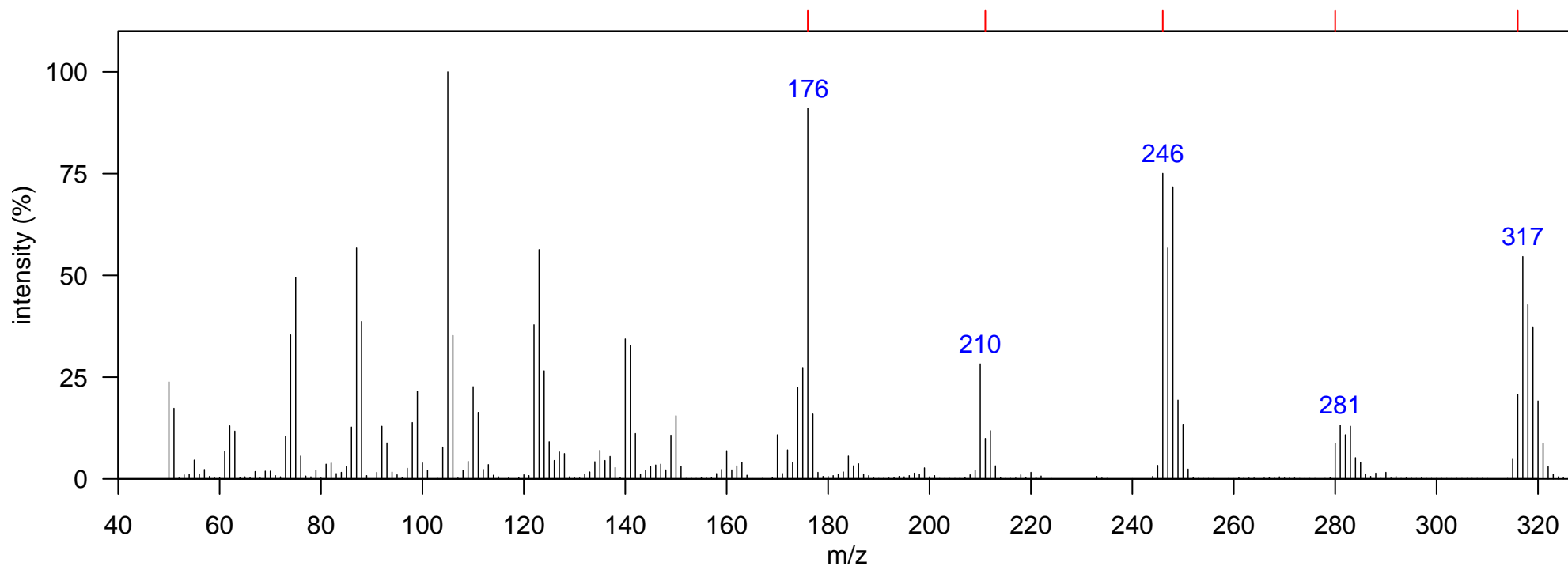
Comment:

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 ⁺

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

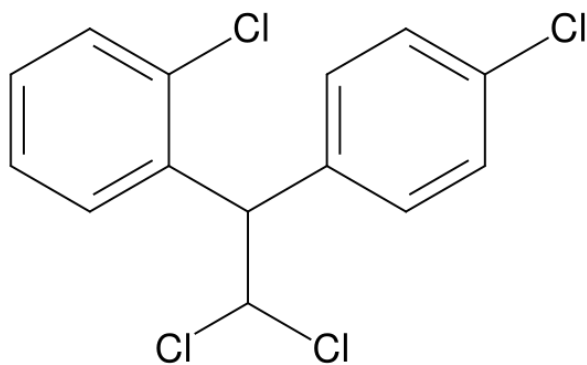
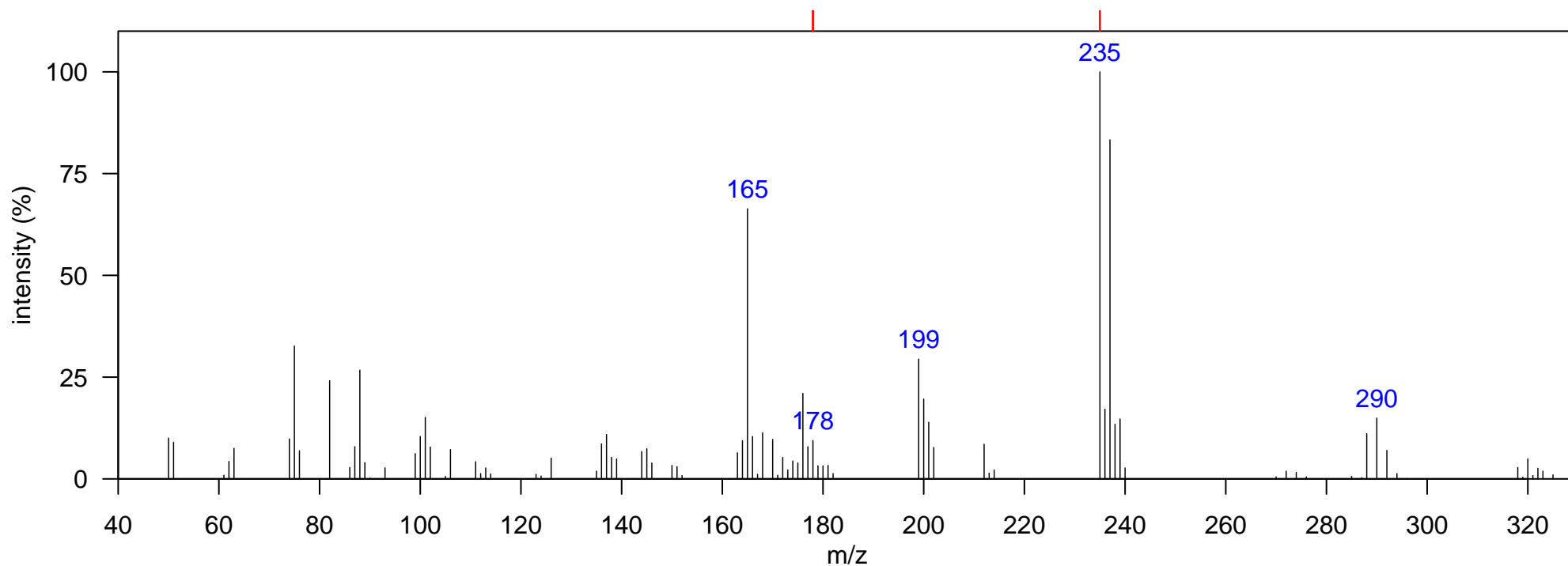
Comment:

Elemental Formula: C₁₄H₁₀Cl₄

Source: anthropogenic

Class: DDT related

Identification: Authentic MS RT



m/z	Identity
178	[M-4Cl] ⁺
235	[M-CHCl ₂] ⁺

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

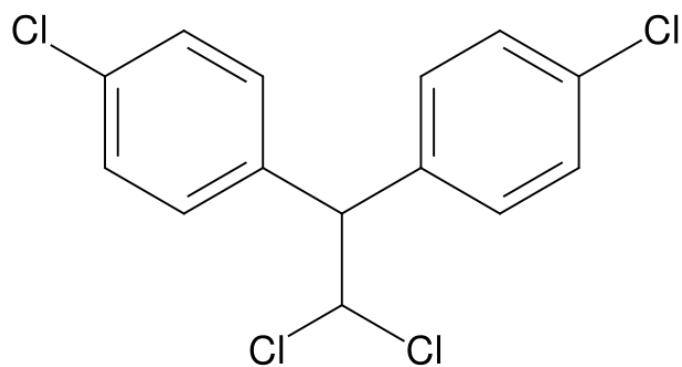
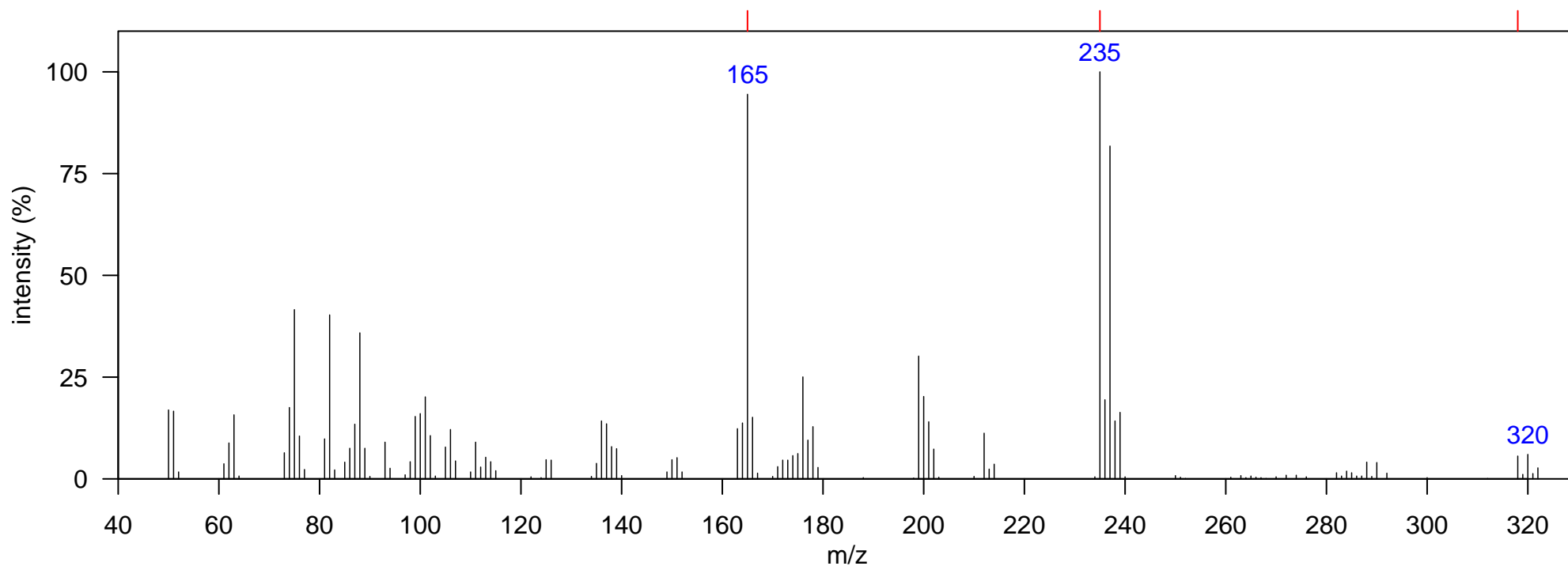
Comment:

Elemental Formula: C₁₄H₁₀Cl₄

Source: anthropogenic

Class: DDT related

Identification: Authentic MS RT



m/z	Identity
165	[M-CHCl ₂ -HCl] ⁺
235	[M-CHCl ₂] ⁺
318	M ⁺

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

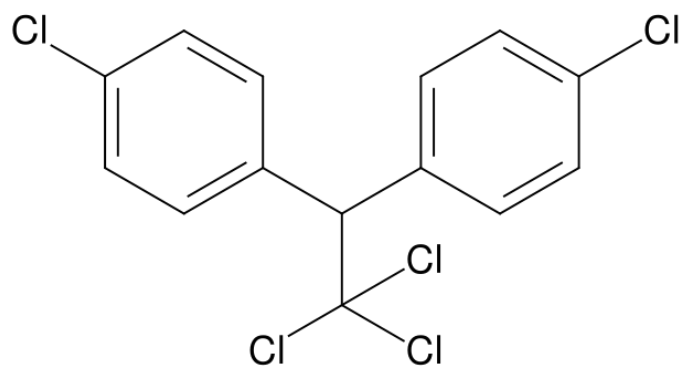
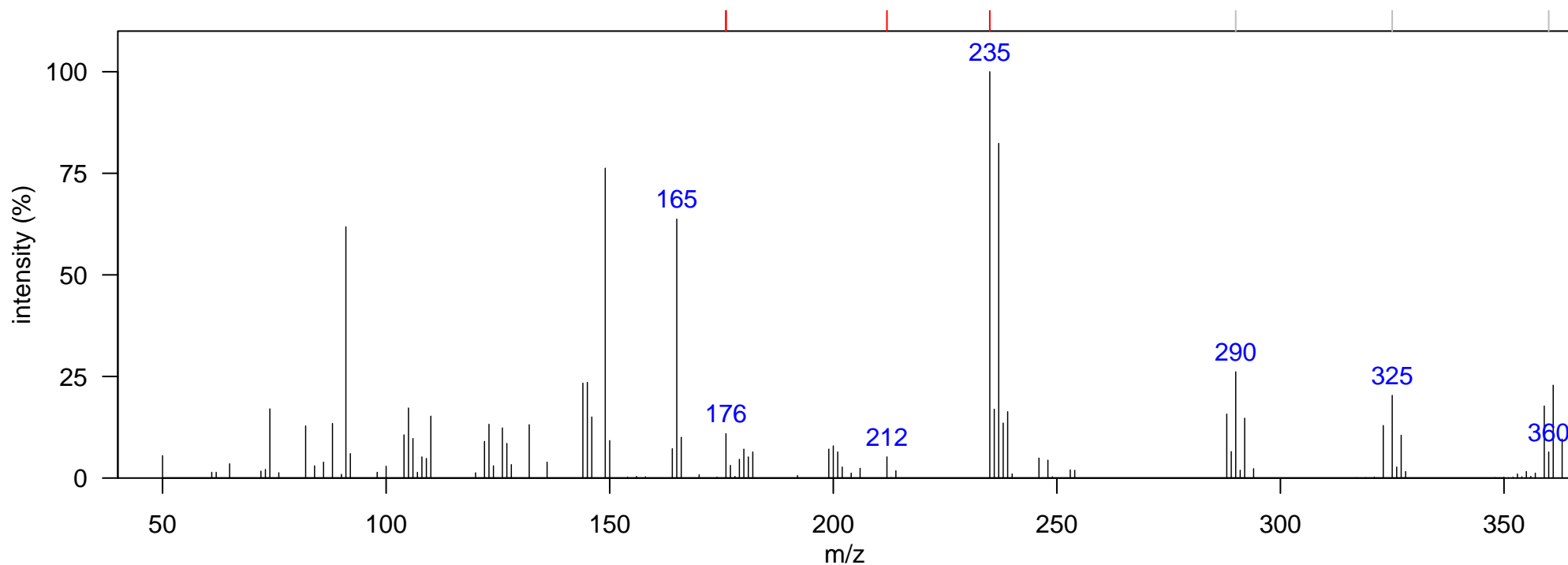
Comment:

Elemental Formula: C₁₄H₉Cl₅

Source: anthropogenic

Class: DDT related

Identification: Authentic MS RT



m/z	Identity
176	[M-HCl ₅] ⁺
212	[M-4Cl] ⁺
235	[M-CCl ₃] ⁺
290	interference PCB
325	interference PCB
360	interference PCB

Name: DDT related 1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

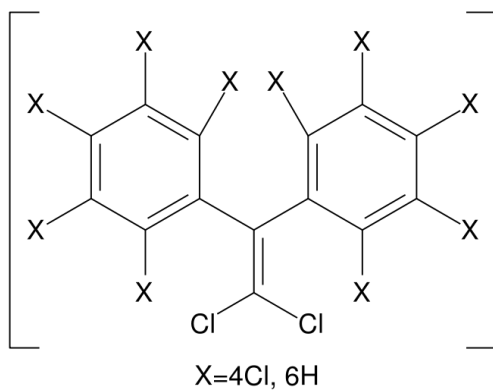
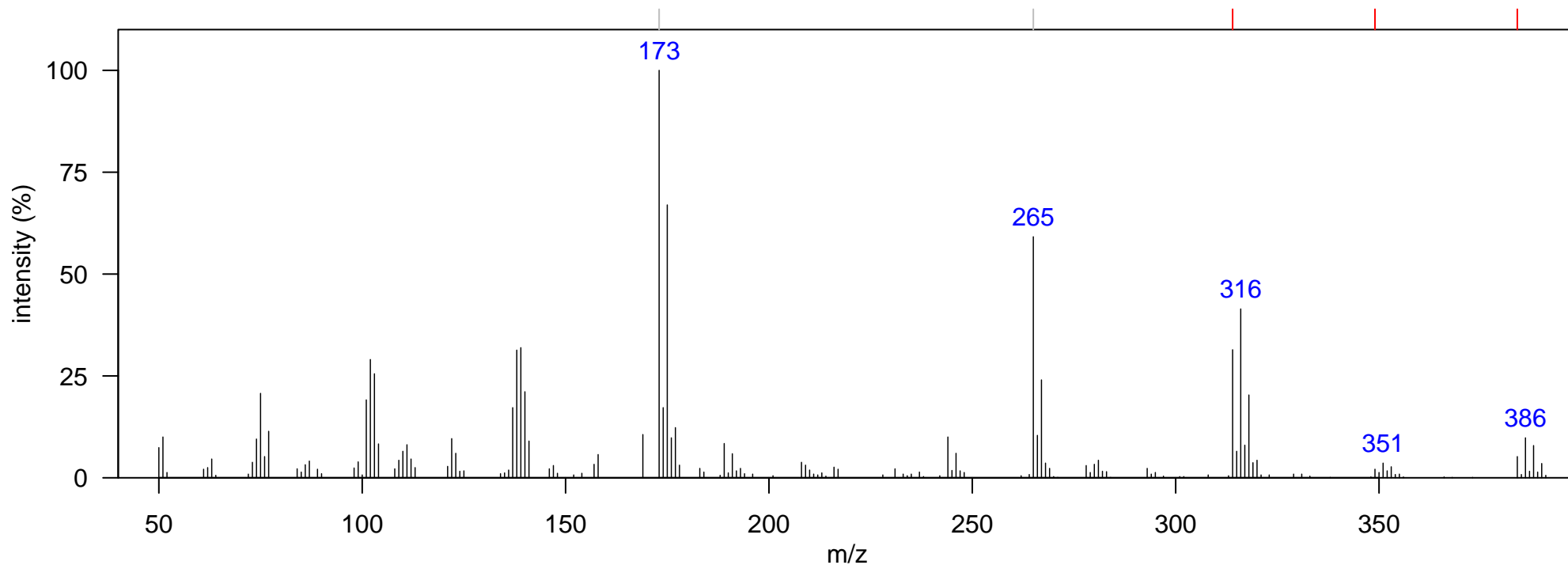
Comment: Suggested DDE backbone structure, but containing 6 chlorines.

Elemental Formula: C₁₄H₆Cl₆

Source: anthropogenic

Class: DDT related

Identification: Manual – Congener Group



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

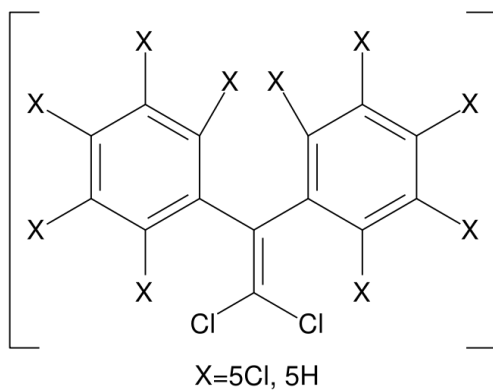
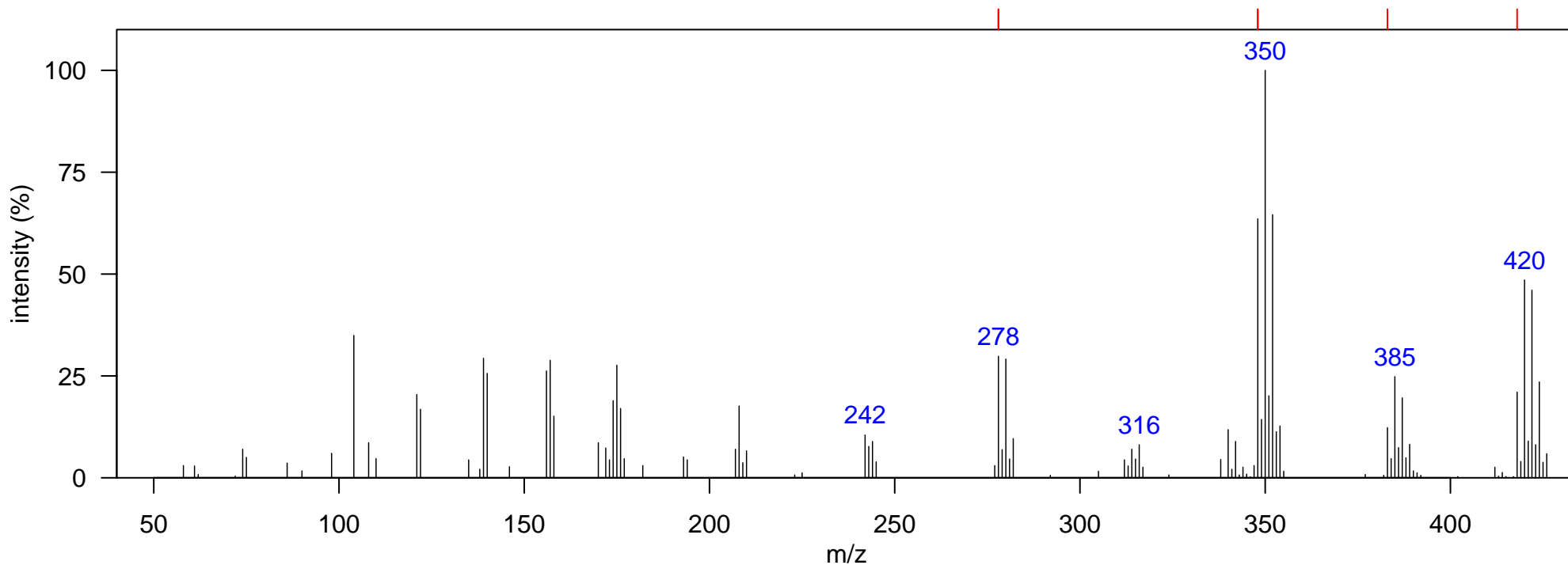
Comment: Suggested DDE backbone structure, but containing 7 chlorines.

Elemental Formula: C₁₄H₅Cl₇

Source: anthropogenic

Class: DDT related

Identification: Manual – Congener Group



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

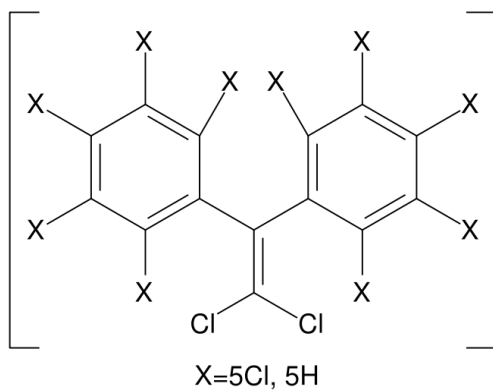
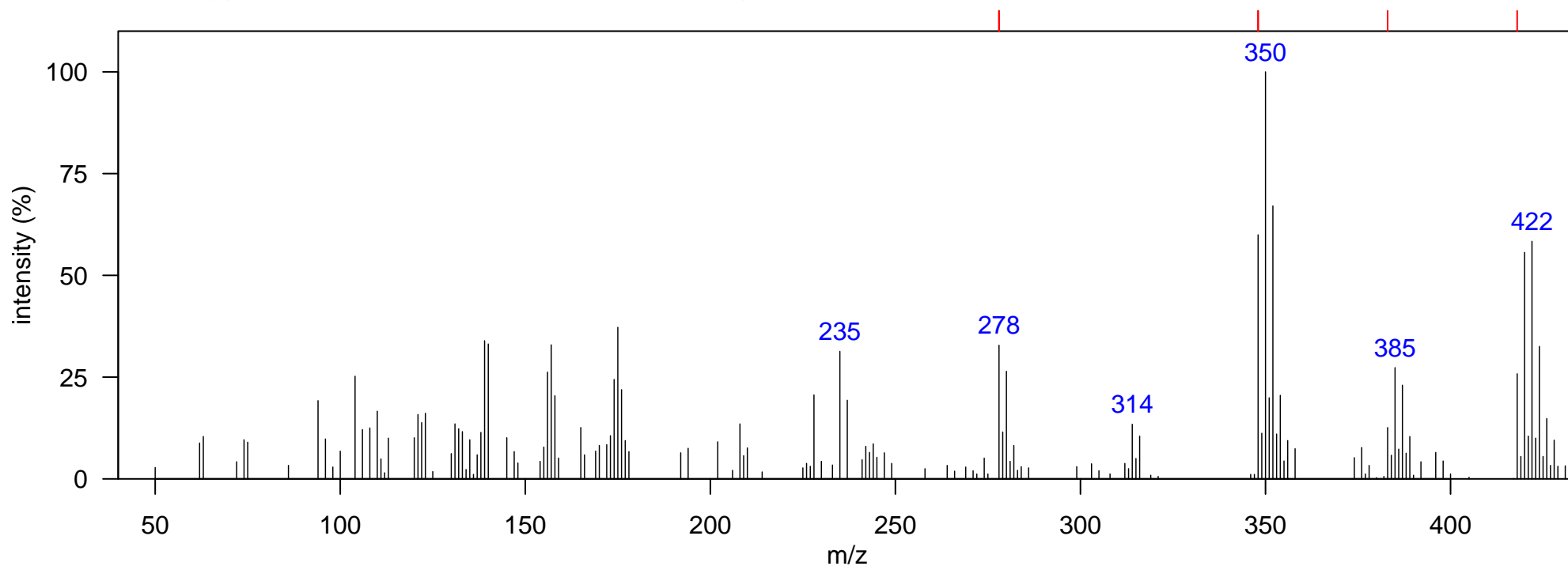
Comment: Suggested DDE backbone structure, but containing 7 chlorines.

Elemental Formula: C₁₄H₅Cl₇

Source: anthropogenic

Class: DDT related

Identification: Manual – Congener Group



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

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

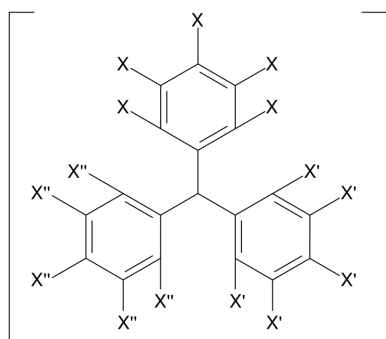
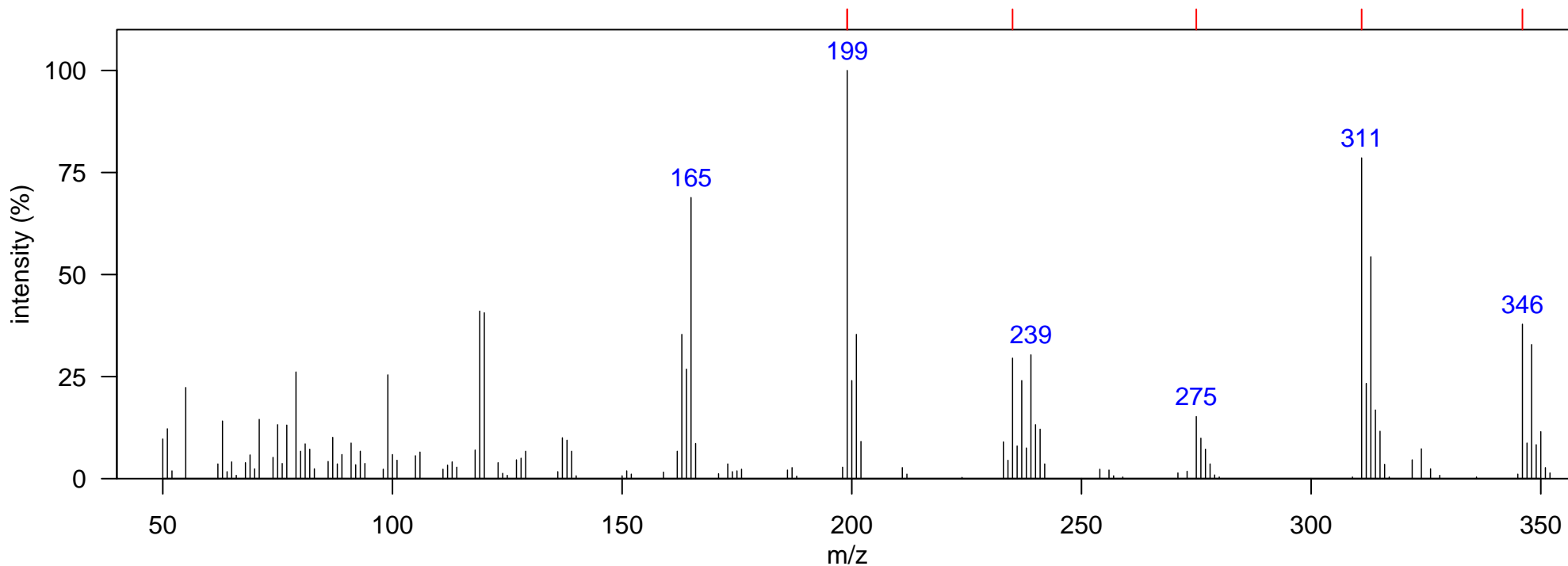
Comment: Ref: ES&T. 1995, 29, 2133-2139. At least one 2-chloro ring based on 235/239 ratio.

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-C ₆ H ₄ Cl-HCl] ⁺
235	[M-C ₆ H ₄ Cl] ⁺
275	[M-HCl ₂] ⁺
311	[M-Cl] ⁺
346	M ⁺

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

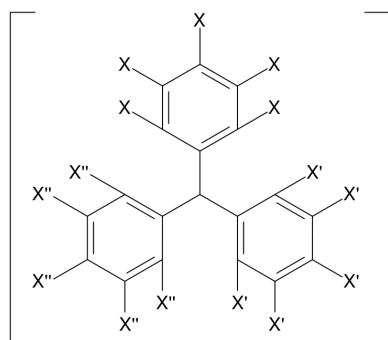
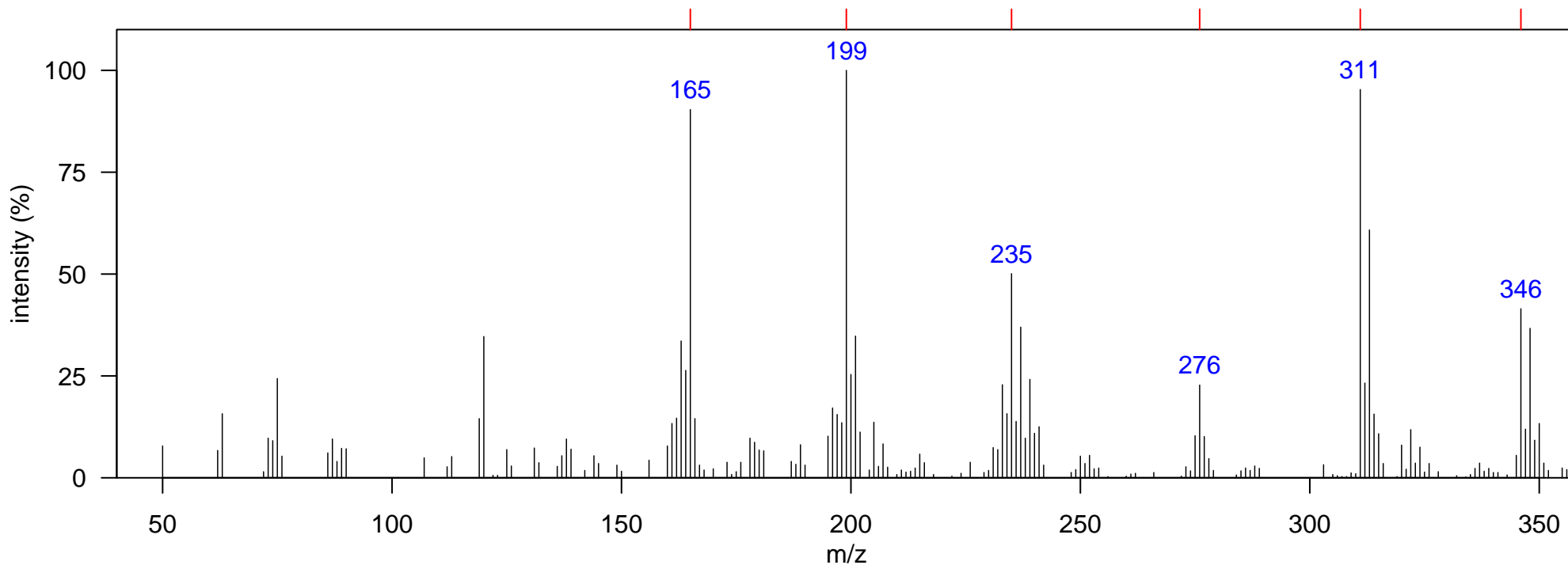
Comment: Ref: ES&T. 1995, 29, 2133-2139. Only 3/4-chloro ring based on 235/239 ratio.

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	[C ₁₃ H ₉] ⁺ = [M-3Cl-C ₆ H ₄] ⁺
199	[M-C ₆ H ₄ Cl-HCl] ⁺
235	[M-C ₆ H ₄ Cl] ⁺
276	[M-Cl ₂] ⁺
311	[M-Cl] ⁺
346	M ⁺

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

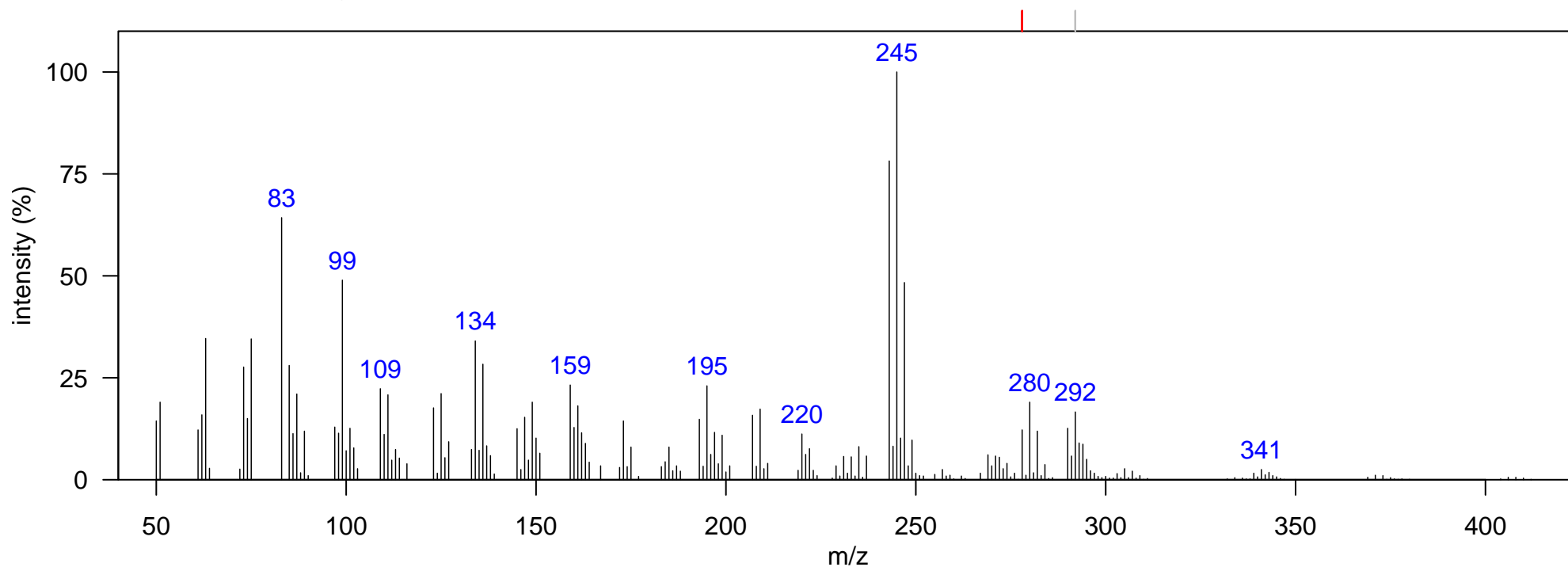
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: NA

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



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

Name: toxaphene 2

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

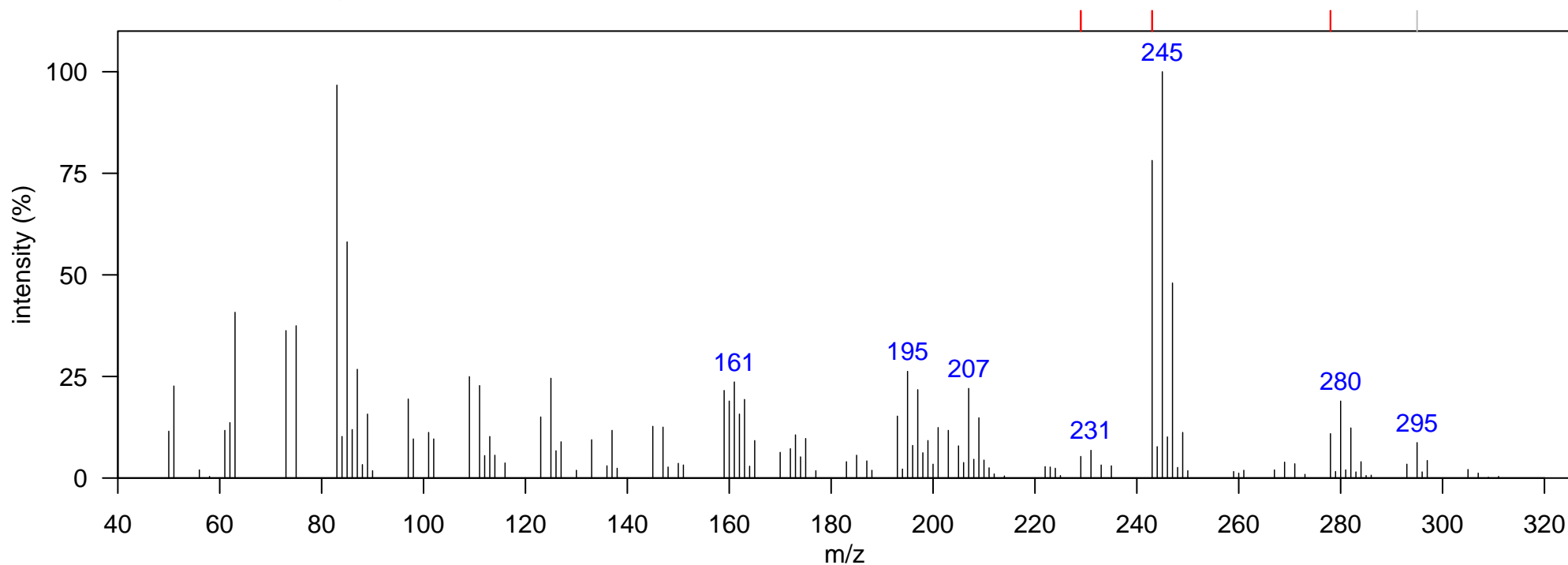
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₈H₇Cl₆

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
229	[PM-CH ₂ Cl] ⁺
243	[PM-Cl] ⁺
278	[PM] ⁺ contains 5Cl
295	interference
382	interference

Name: toxaphene 3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

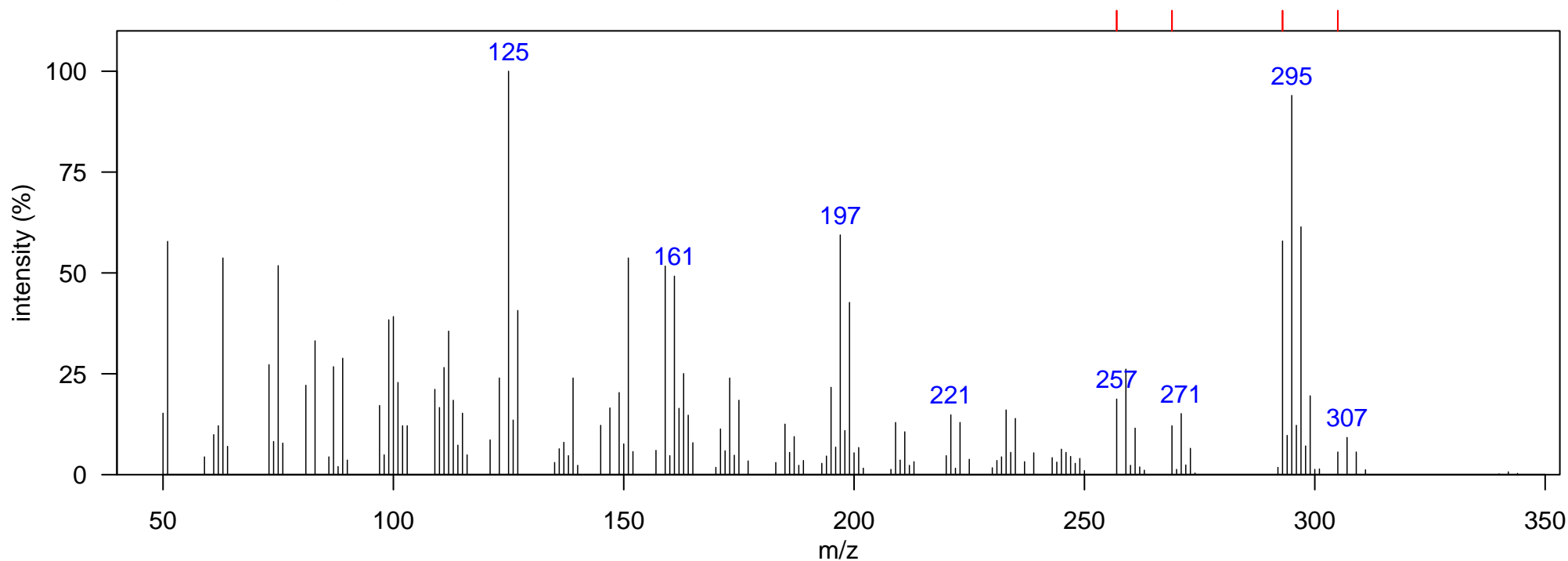
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₁₀H₁₀Cl₆

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
257	[Frag-HCl-CH ₂] ⁺
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

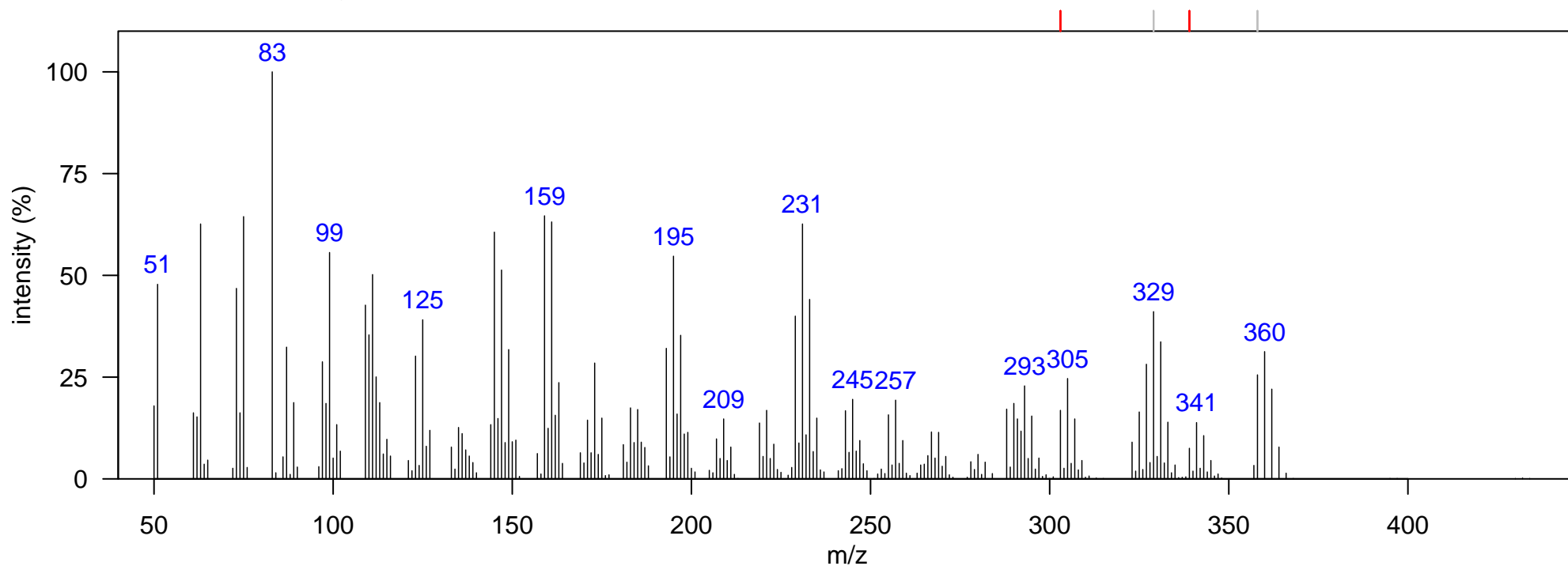
Comment: Toxaphene fragmentation pattern.

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

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

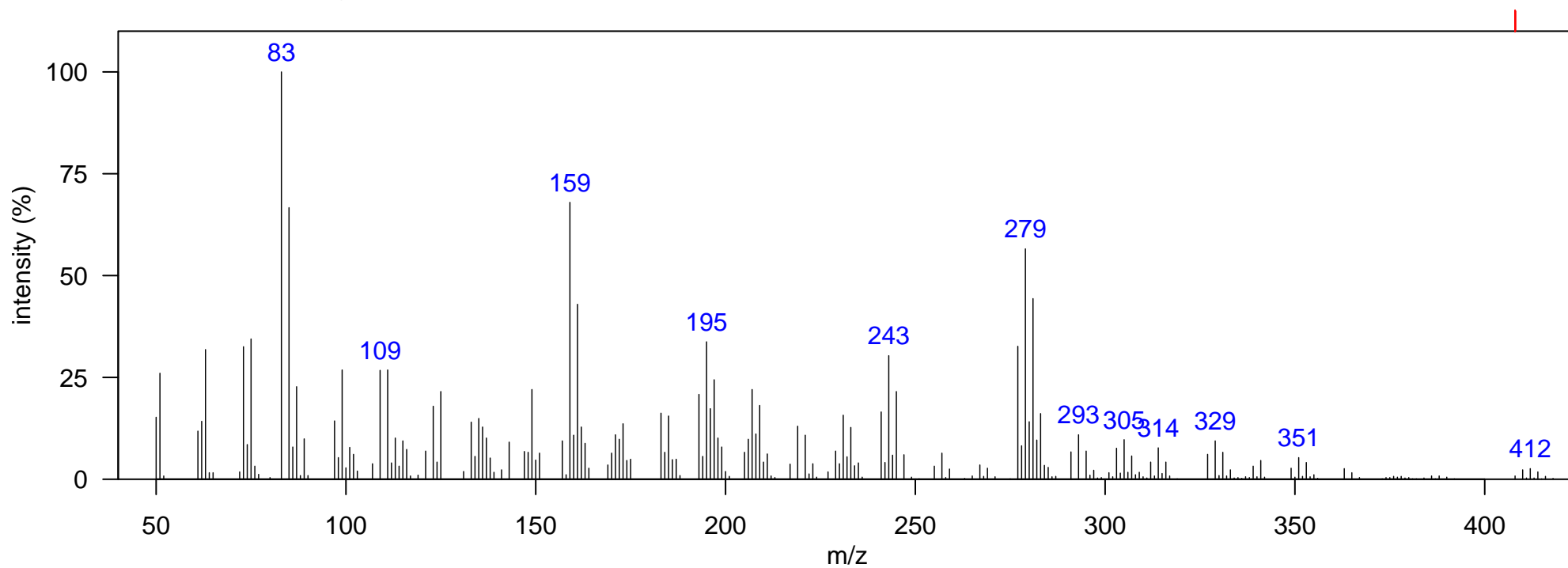
Comment: Toxaphene fragmentation pattern.

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

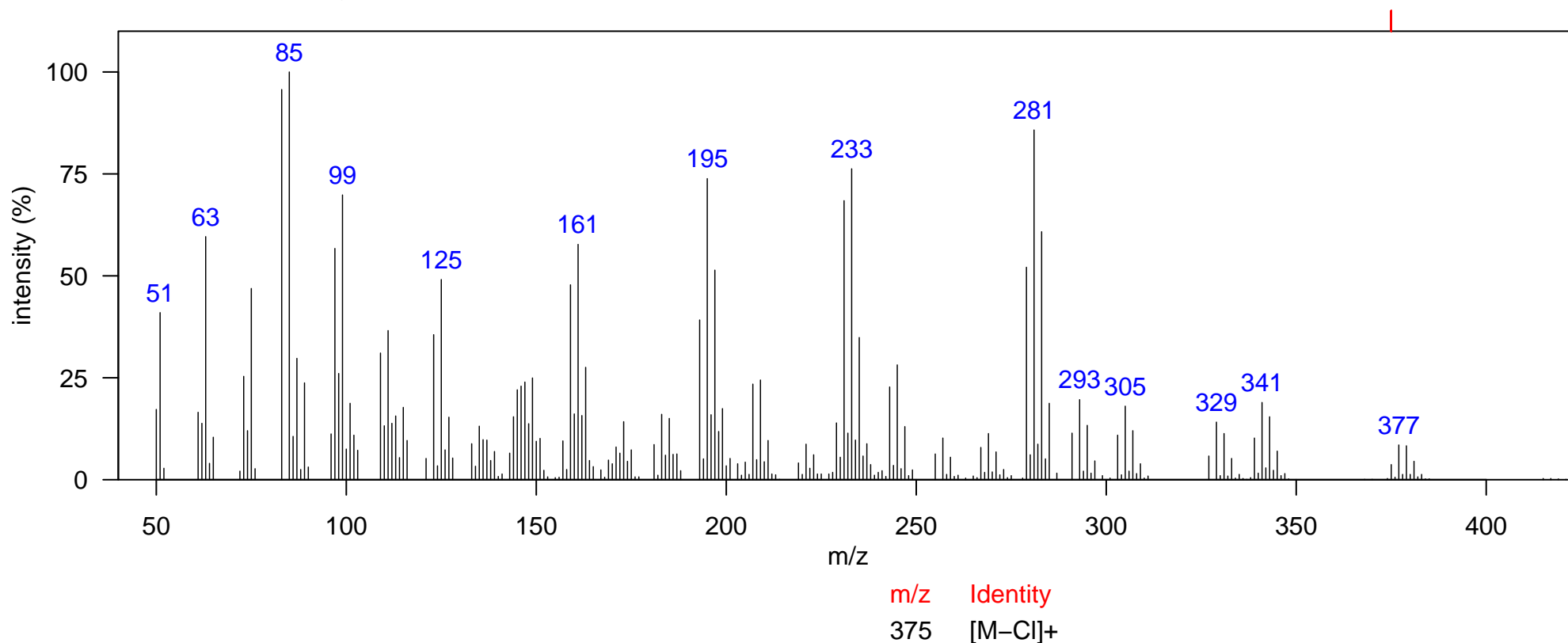
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₁₀H₈Cl₈

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



Name: toxaphene 7

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

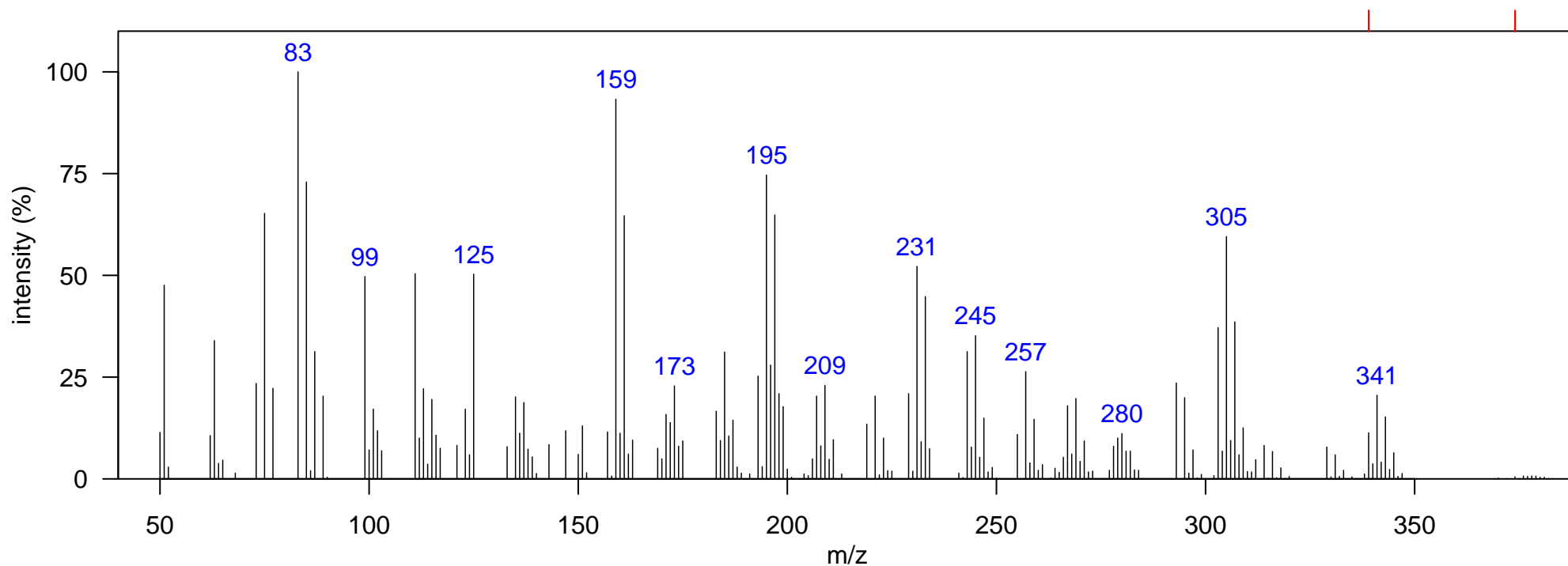
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₁₀H₉Cl₇

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



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

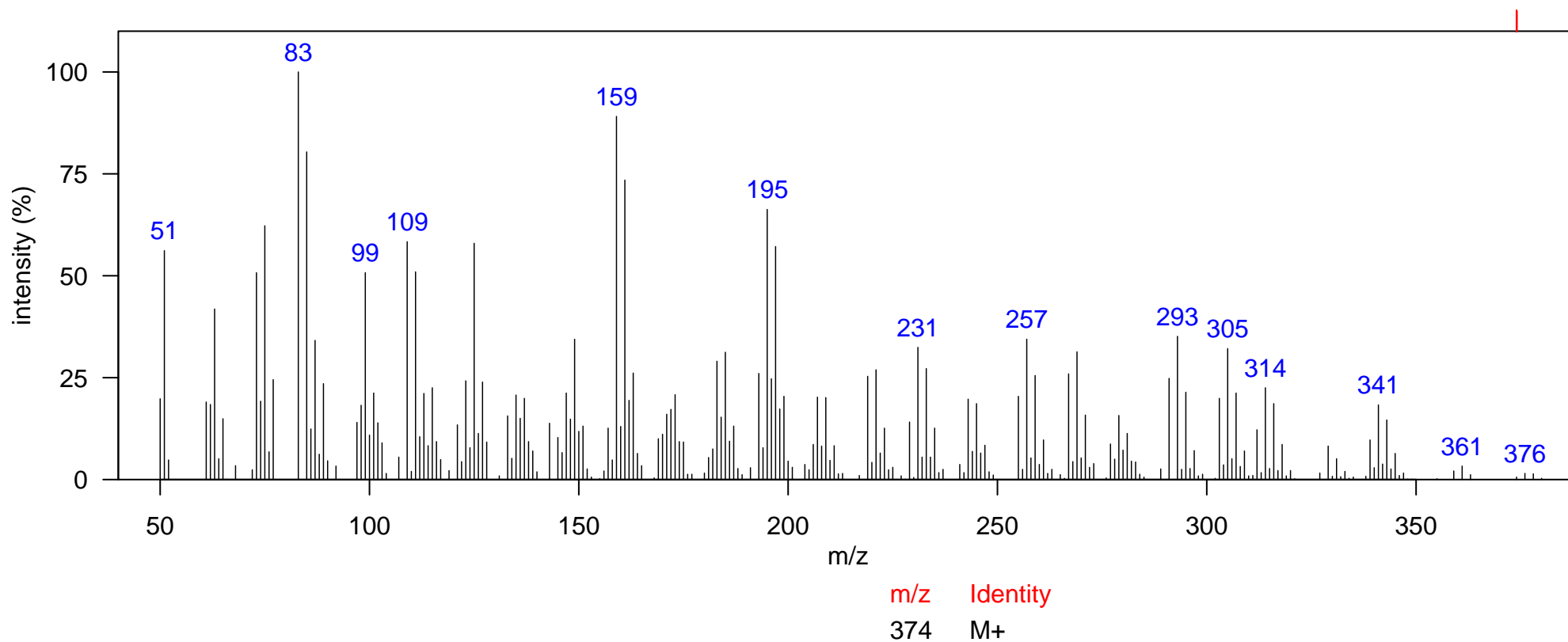
Comment: Toxaphene fragmentation pattern.

Elemental Formula: C₁₀H₉Cl₇

Source: anthropogenic

Class: toxaphene related

Identification: Manual



Name: toxaphene 9

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

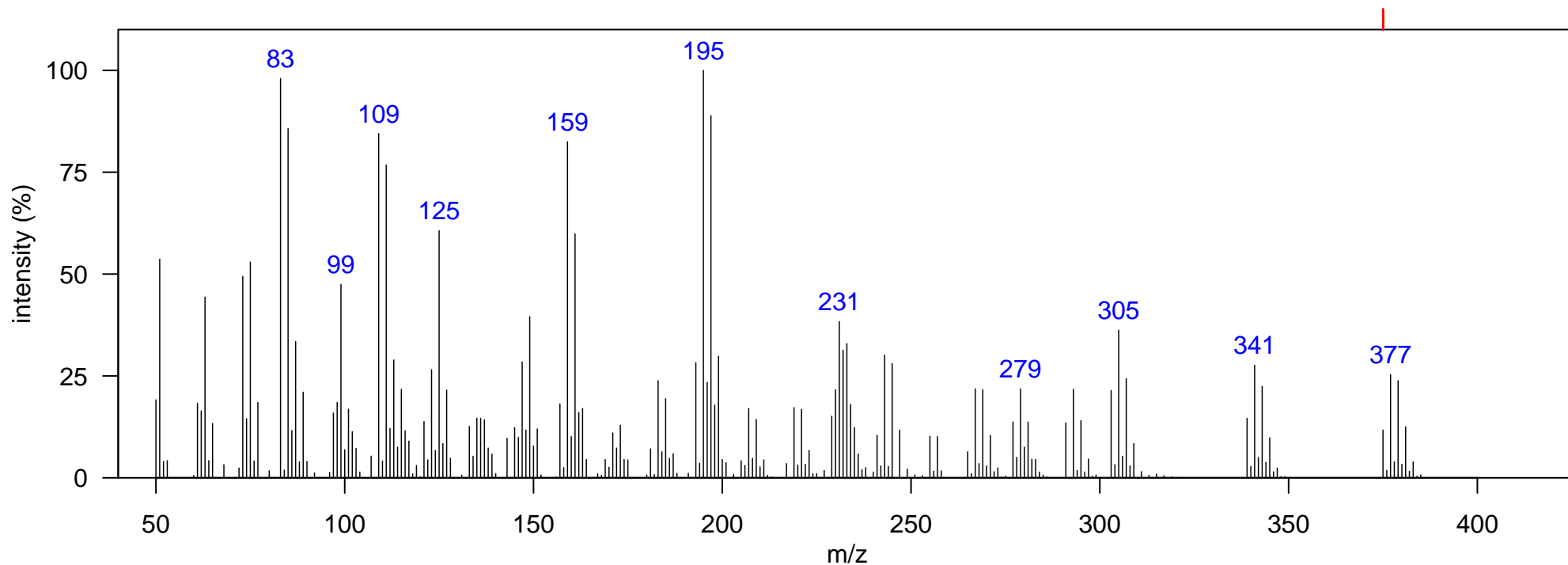
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₁₀H₁₀Cl₈

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
375	[M-Cl] ⁺

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

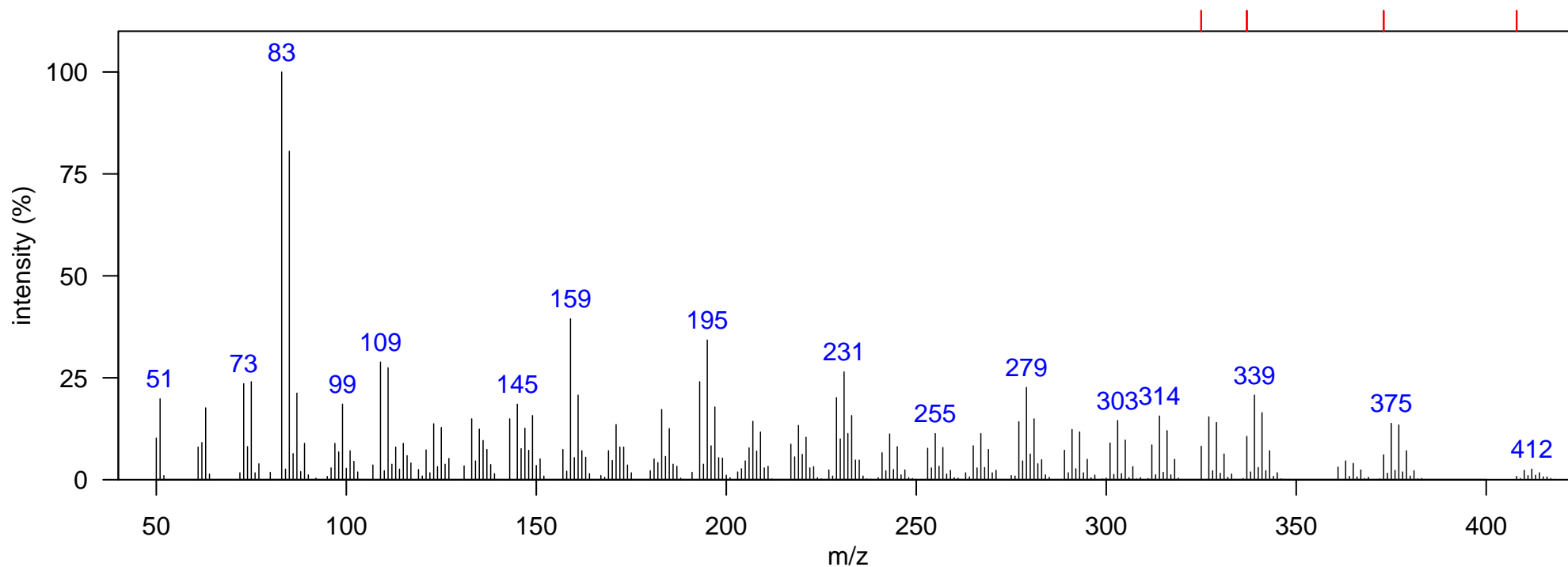
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₁₀H₈Cl₈

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
325	[M-CHCl ₂] ⁺
337	[M-2Cl] ⁺
373	[M-Cl] ⁺
408	M ⁺

Name: toxaphene 11

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

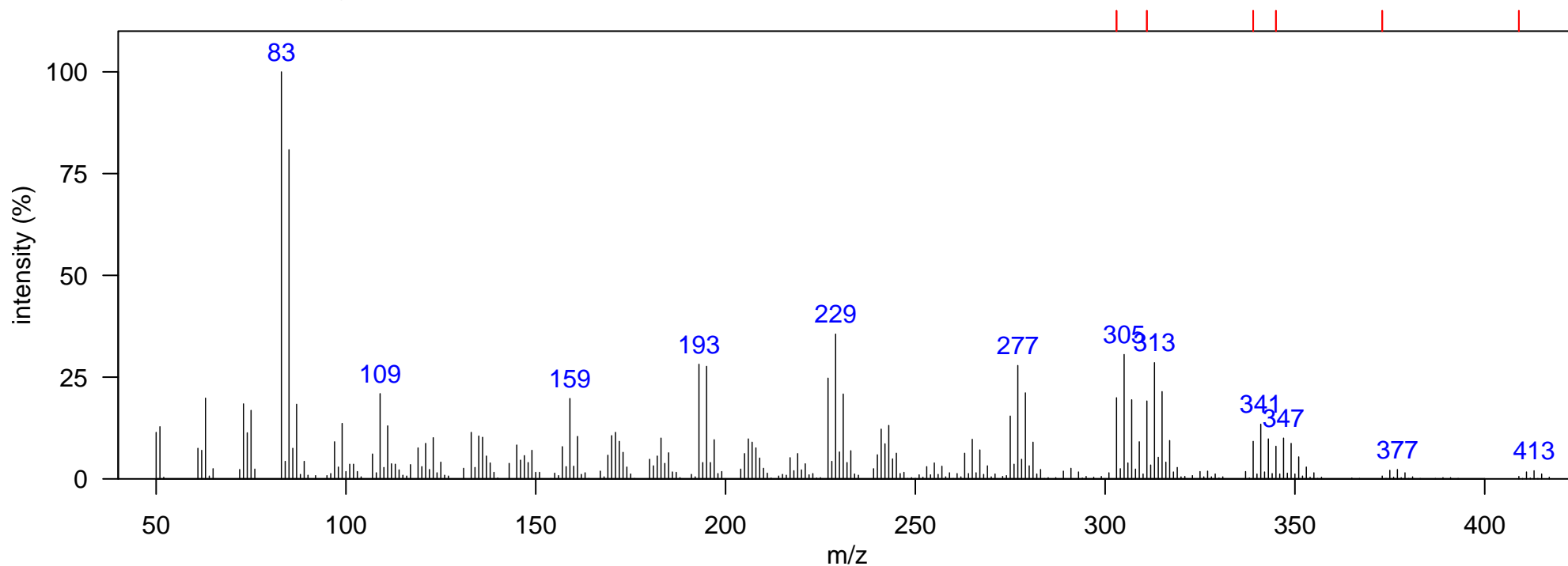
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₁₀H₈Cl₈

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



m/z	Identity
303	[M-HCl ₄] ⁺
311	[M-3Cl-C ₂ H ₄] ⁺
339	[M-3Cl] ⁺
345	[M-HCl ₂ -C ₂ H ₄] ⁺
373	[M-HCl ₂] ⁺
409	[M-Cl] ⁺

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

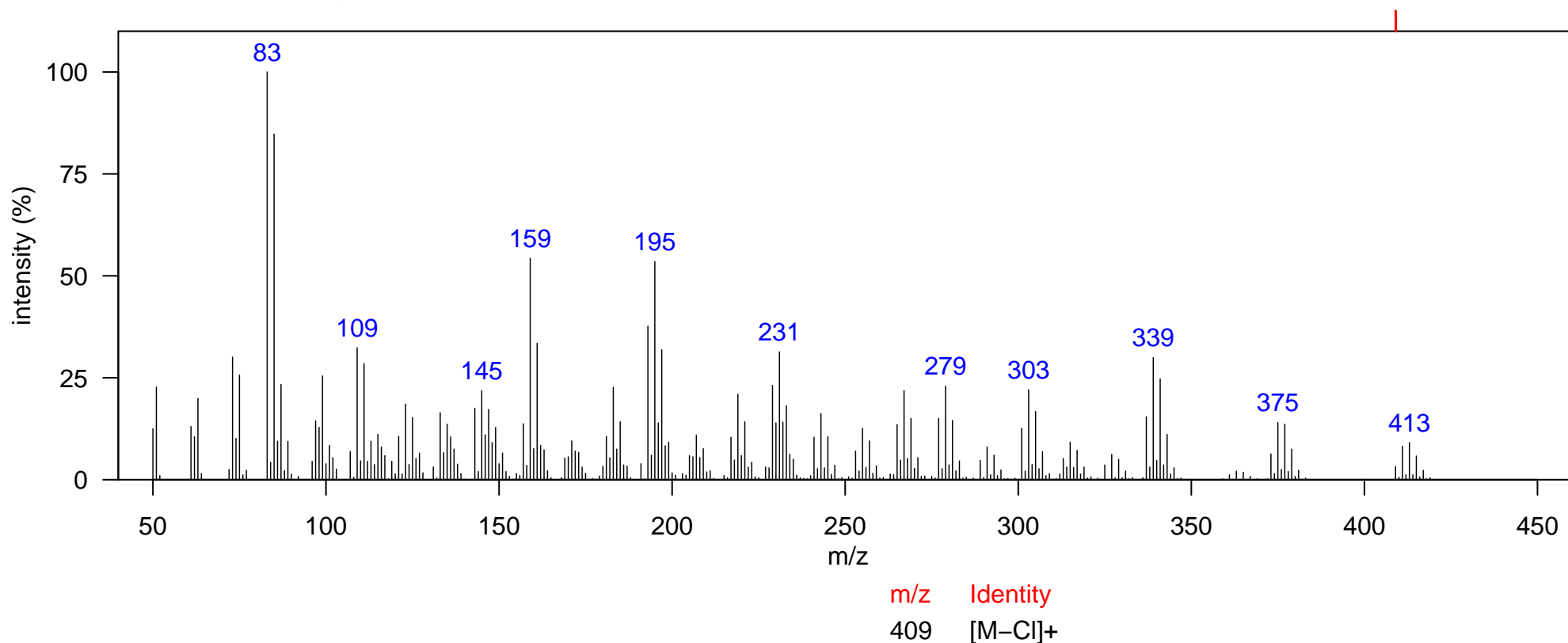
Comment: Toxaphene fragmentation pattern. Detected in toxaphene tech. mix.

Elemental Formula: C₁₀H₉Cl₉

Source: anthropogenic

Class: toxaphene related

Identification: Authentic MS RT



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

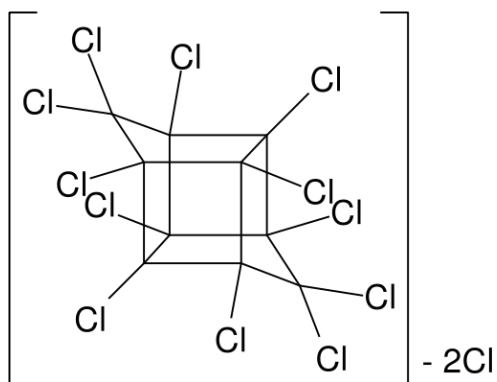
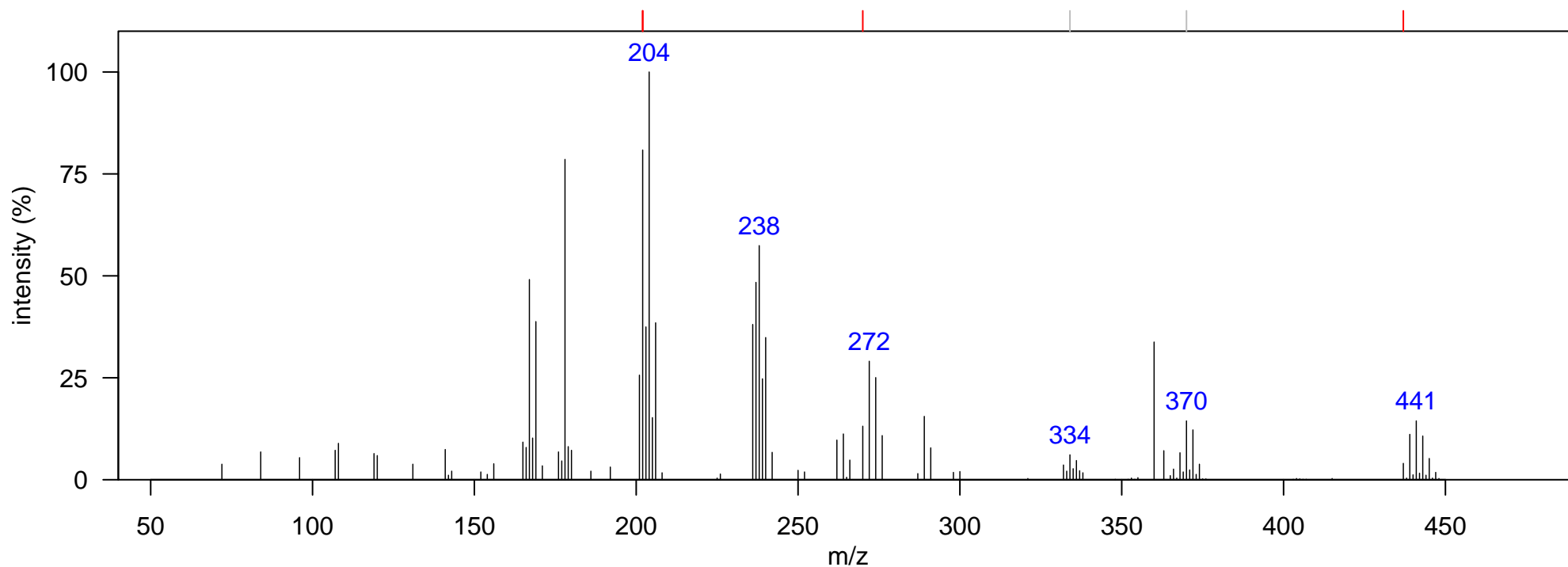
Comment:

Elemental Formula: C₁₀H₂Cl₁₀

Source: anthropogenic

Class: mirex

Identification: Manual – Congener Group



m/z	Identity
202	[C ₅ H ₂ Cl ₄] ⁺
270	[C ₅ Cl ₆] ⁺
334	interference
370	interference from MBP-Br ₄ Cl ₂
437	[M-Cl] ⁺

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

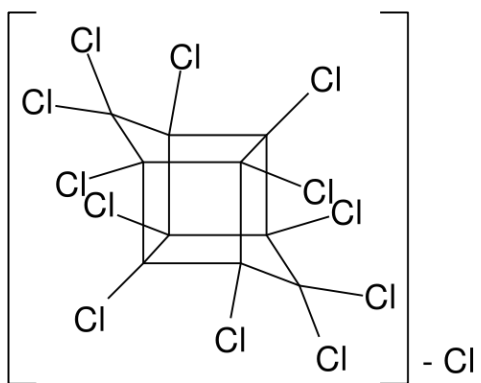
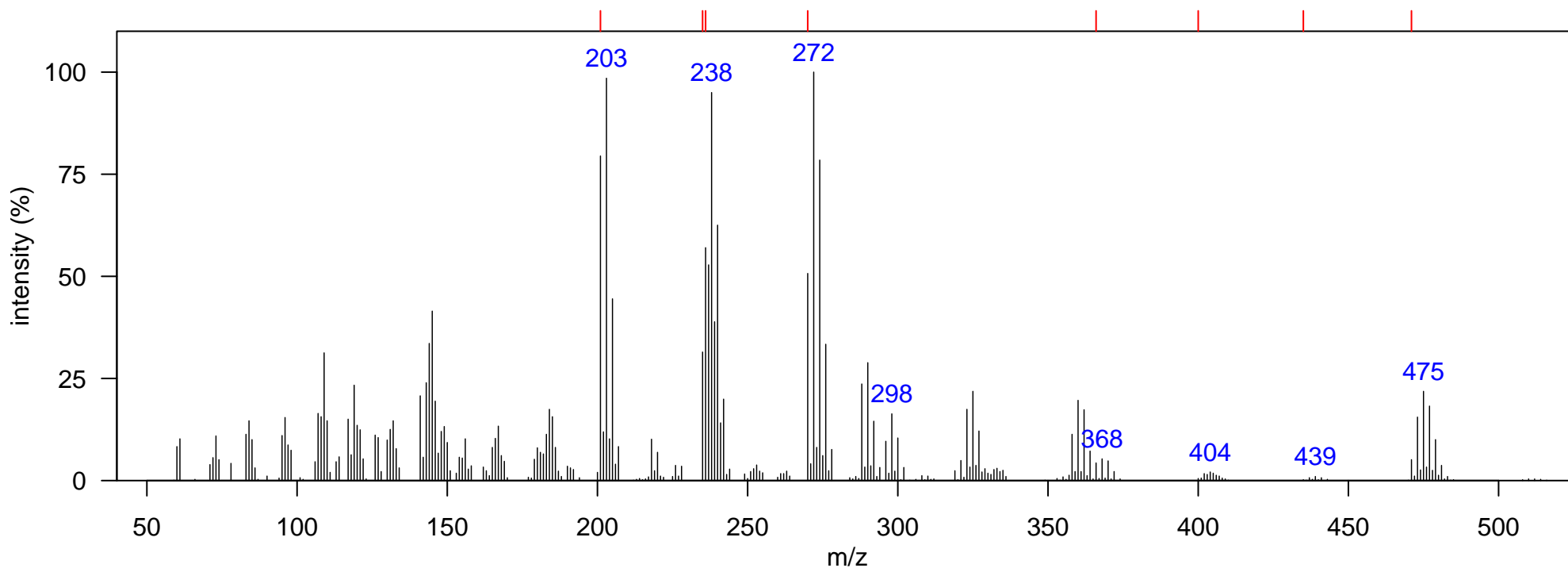
Comment:

Elemental Formula: C₁₀HCl₁₁

Source: anthropogenic

Class: mirex

Identification: Manual – Congener Group



m/z	Identity
201	[C ₅ HCl ₄] ⁺
235	[C ₅ Cl ₅] ⁺
236	[C ₅ HCl ₅] ⁺
270	[C ₅ Cl ₆] ⁺
366	[M-4Cl] ⁺
400	[M-HCl ₃] ⁺
435	[M-HCl ₂] ⁺
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

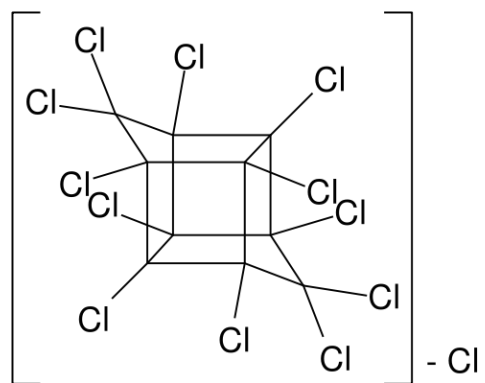
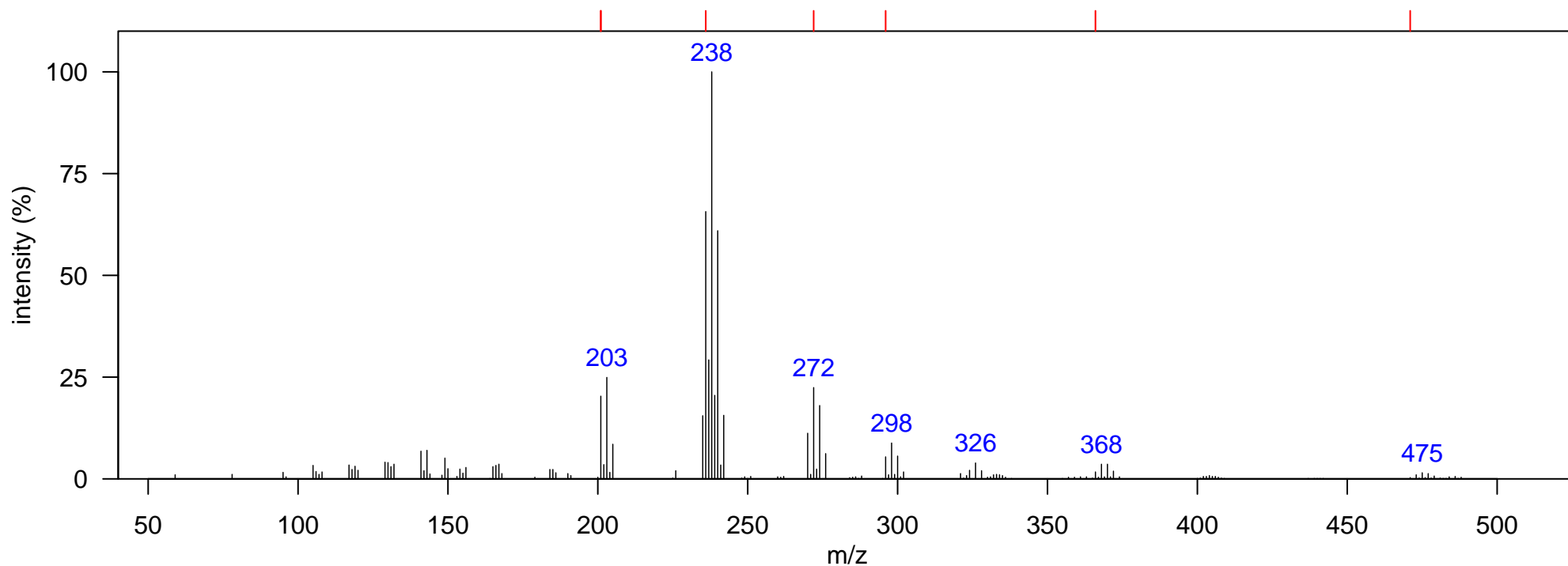
Comment:

Elemental Formula: C₁₀HCl₁₁

Source: anthropogenic

Class: mirex

Identification: Manual – Congener Group



m/z	Identity
201	[C ₅ HCl ₄] ⁺
236	[C ₅ HCl ₅] ⁺
272	[C ₅ Cl ₆] ⁺
296	[C ₁₀ HCl ₅] ⁺
366	[C ₁₀ HCl ₇] ⁺
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

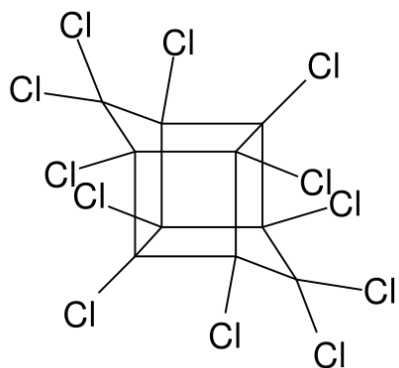
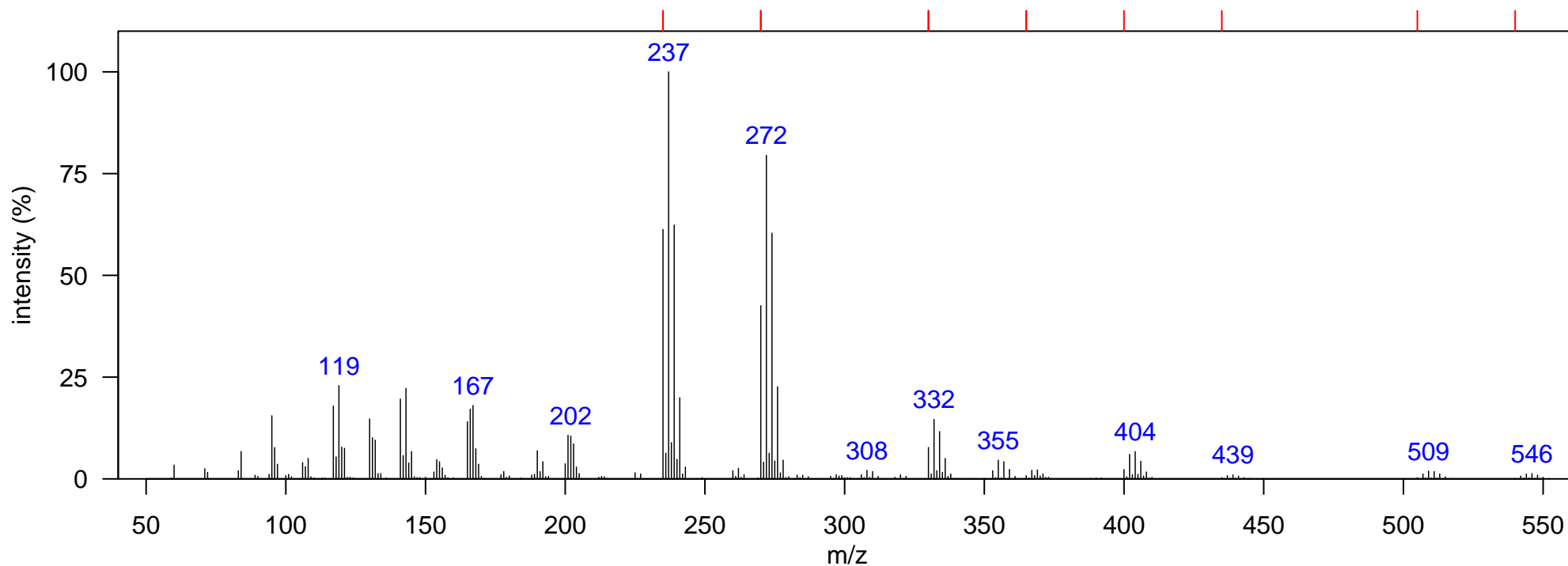
Comment:

Elemental Formula: C₁₀Cl₁₂

Source: anthropogenic

Class: mirex

Identification: Reference Database MS



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

Name: dieldrin

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

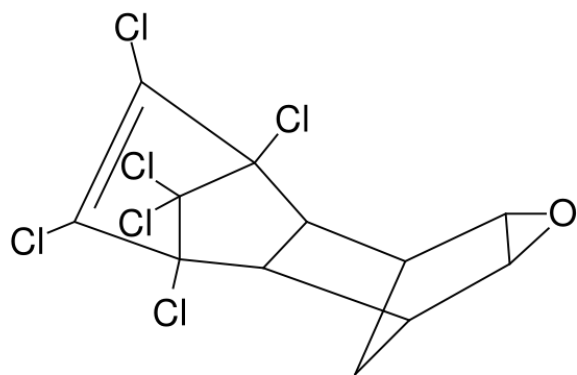
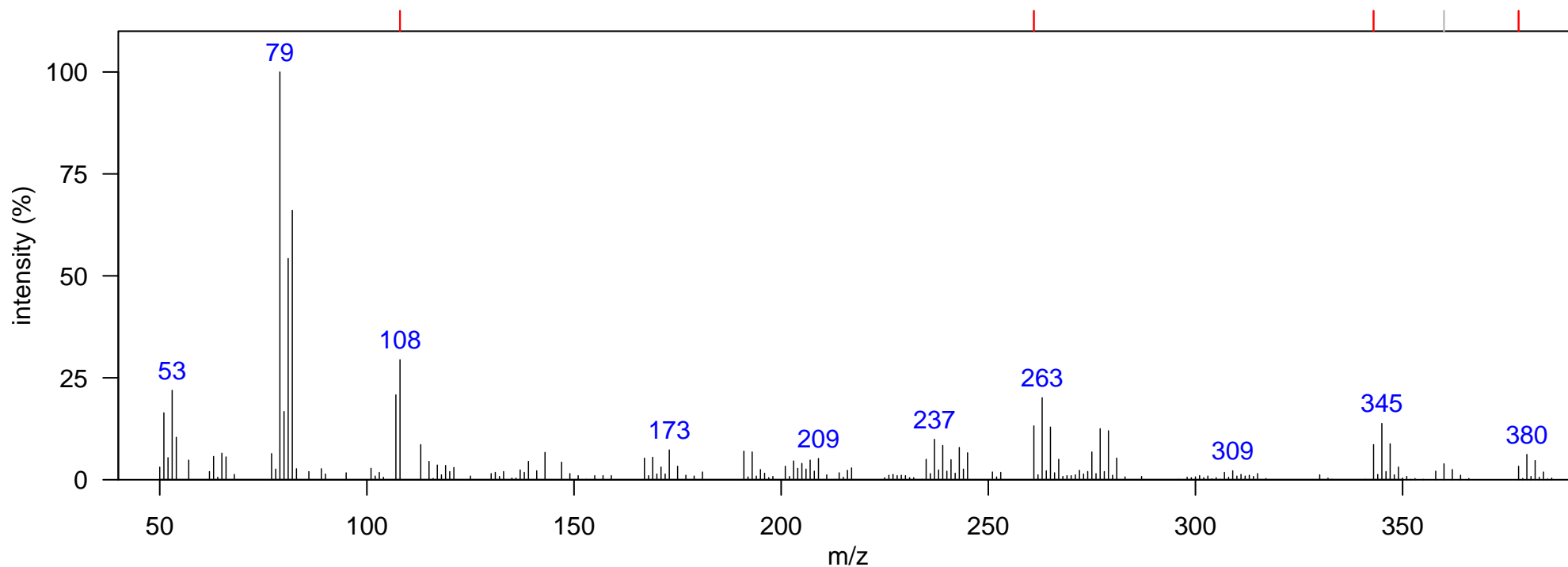
Comment:

Elemental Formula: C₁₂H₈Cl₆O

Source: anthropogenic

Class: pesticide

Identification: Authentic MS RT



m/z	Identity
108	[C ₇ H ₈ O] ⁺
261	[C ₇ H ₂ Cl ₅] ⁺
343	[M-Cl] ⁺
360	PCB interference
378	M ⁺

Name: pentachlorobenzene

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

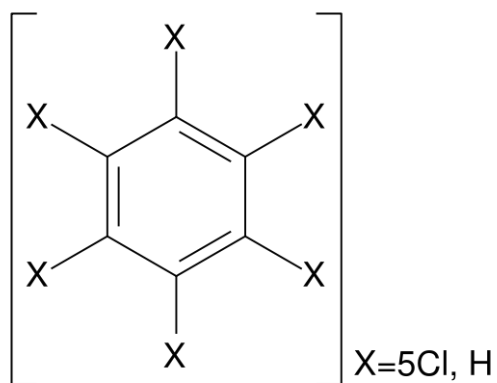
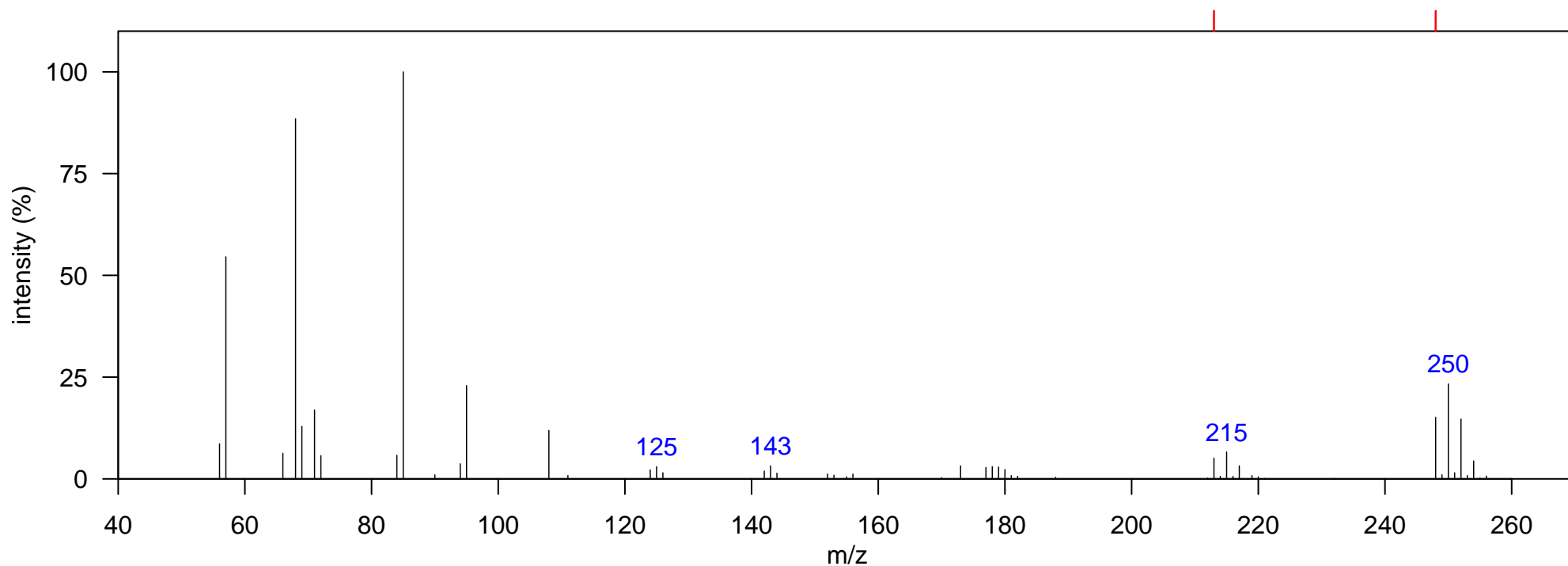
Comment:

Elemental Formula: C₆HCl₅

Source: anthropogenic

Class: pesticide

Identification: Manual – Congener Group



m/z	Identity
213	[M-Cl] ⁺
248	M ⁺

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

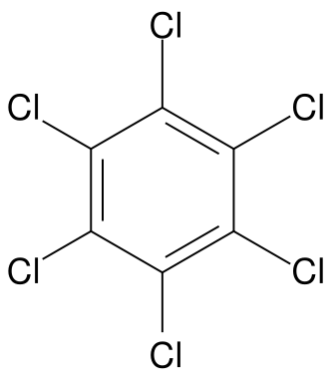
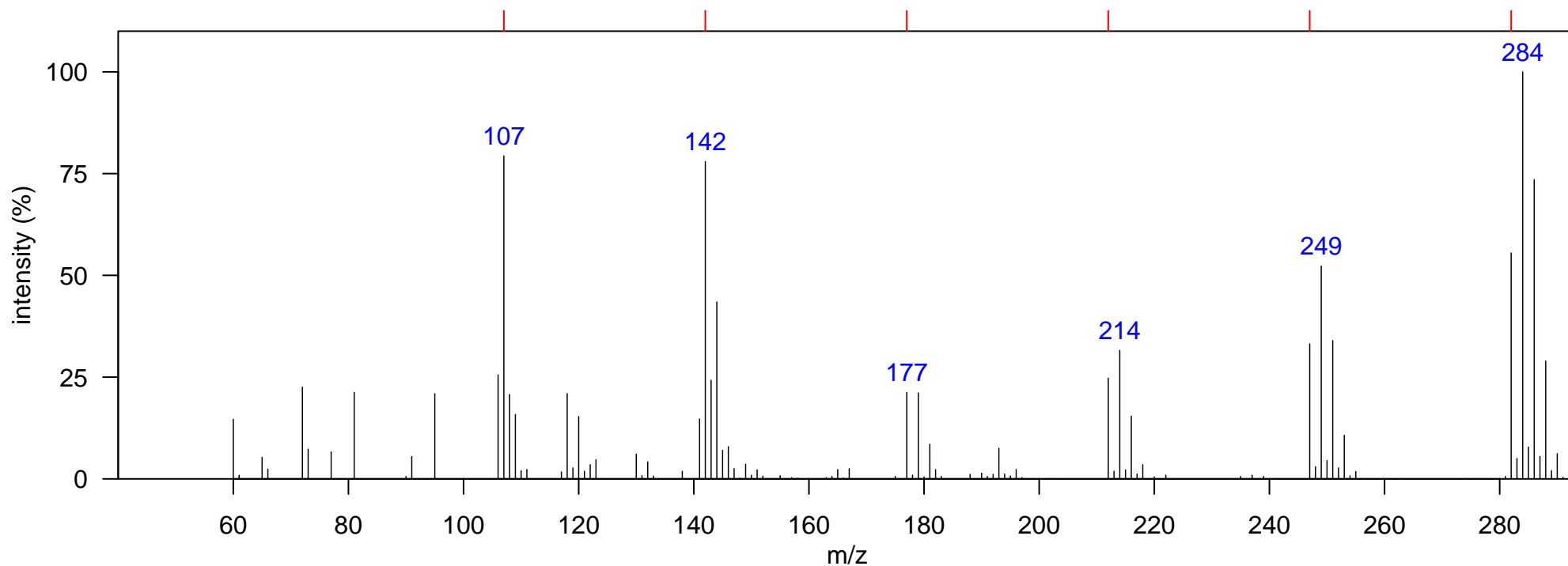
Comment:

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⁺

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

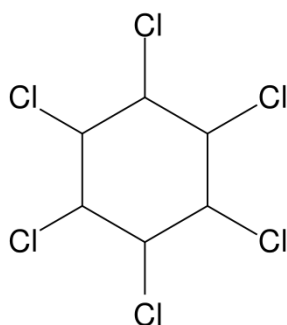
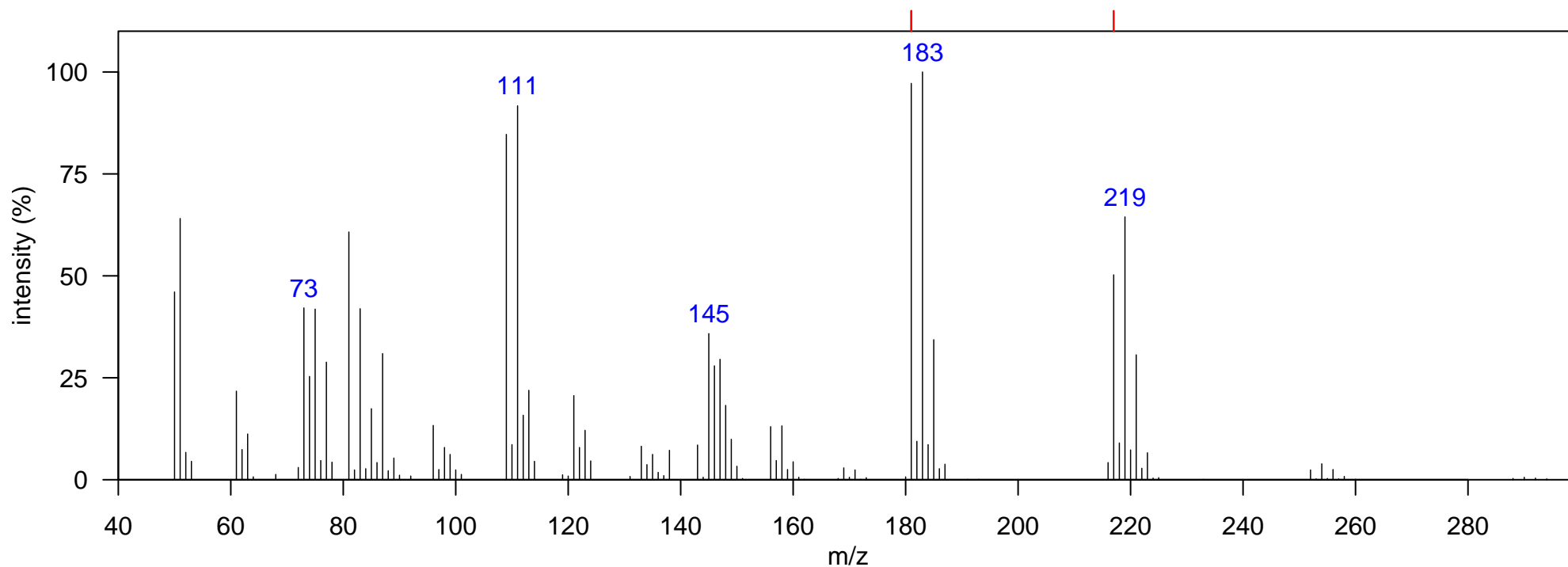
Comment:

Elemental Formula: C₆H₆Cl₆

Source: anthropogenic

Class: pesticide

Identification: Authentic MS RT



(stereochemistry not shown)

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

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

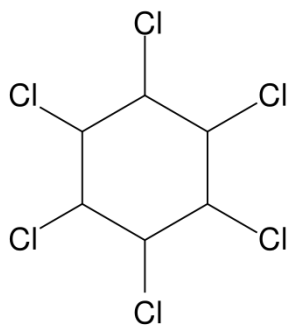
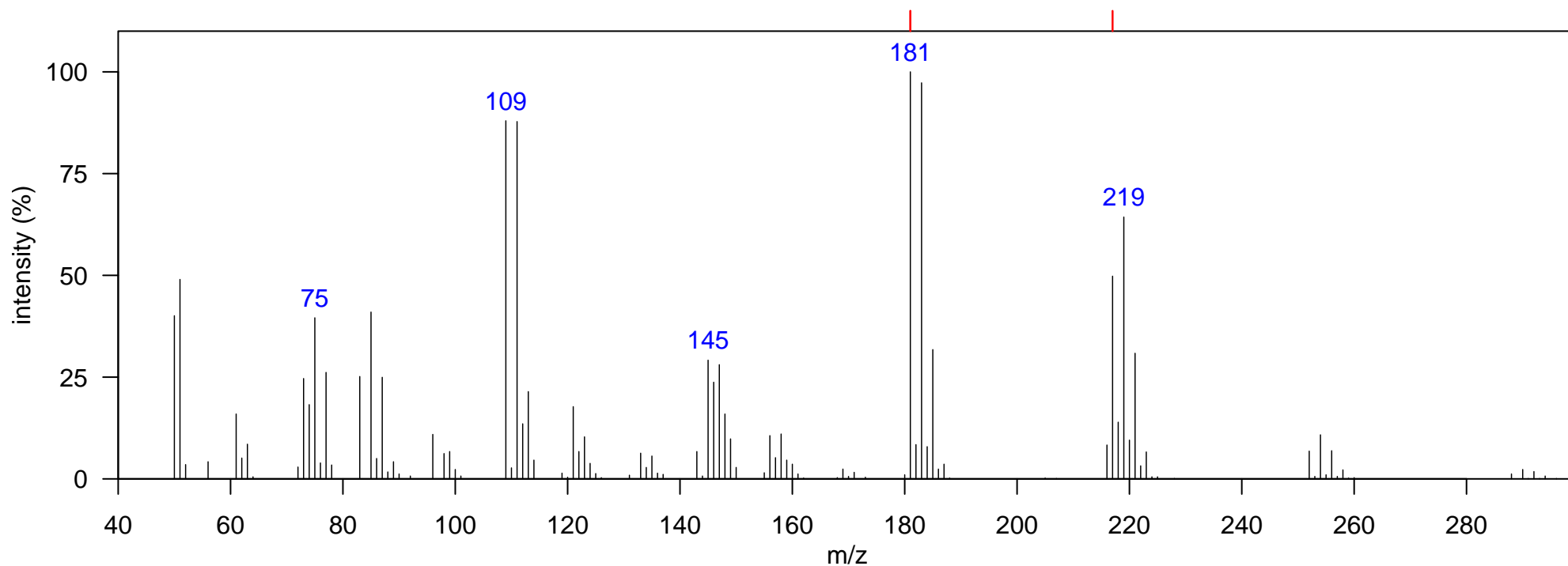
Comment:

Elemental Formula: C₆H₆Cl₆

Source: anthropogenic

Class: pesticide

Identification: Authentic MS RT



(stereochemistry not shown)

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

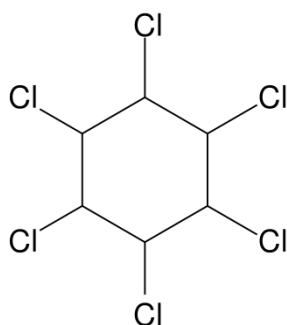
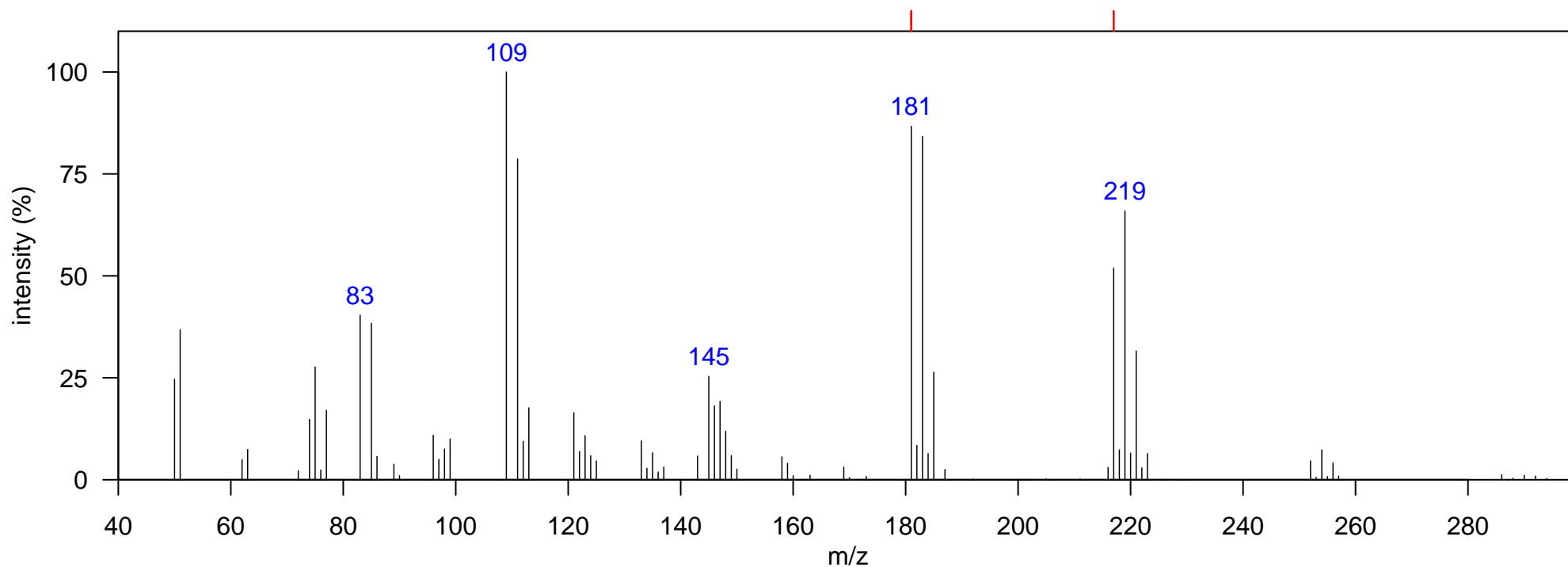
Comment:

Elemental Formula: C₆H₆Cl₆

Source: anthropogenic

Class: pesticide

Identification: Authentic MS



(stereochemistry not shown)

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

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

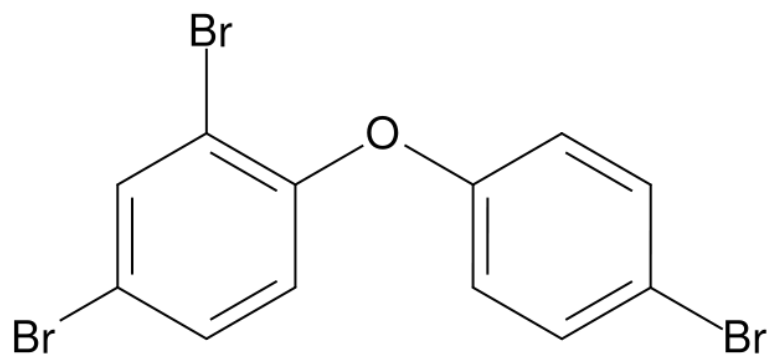
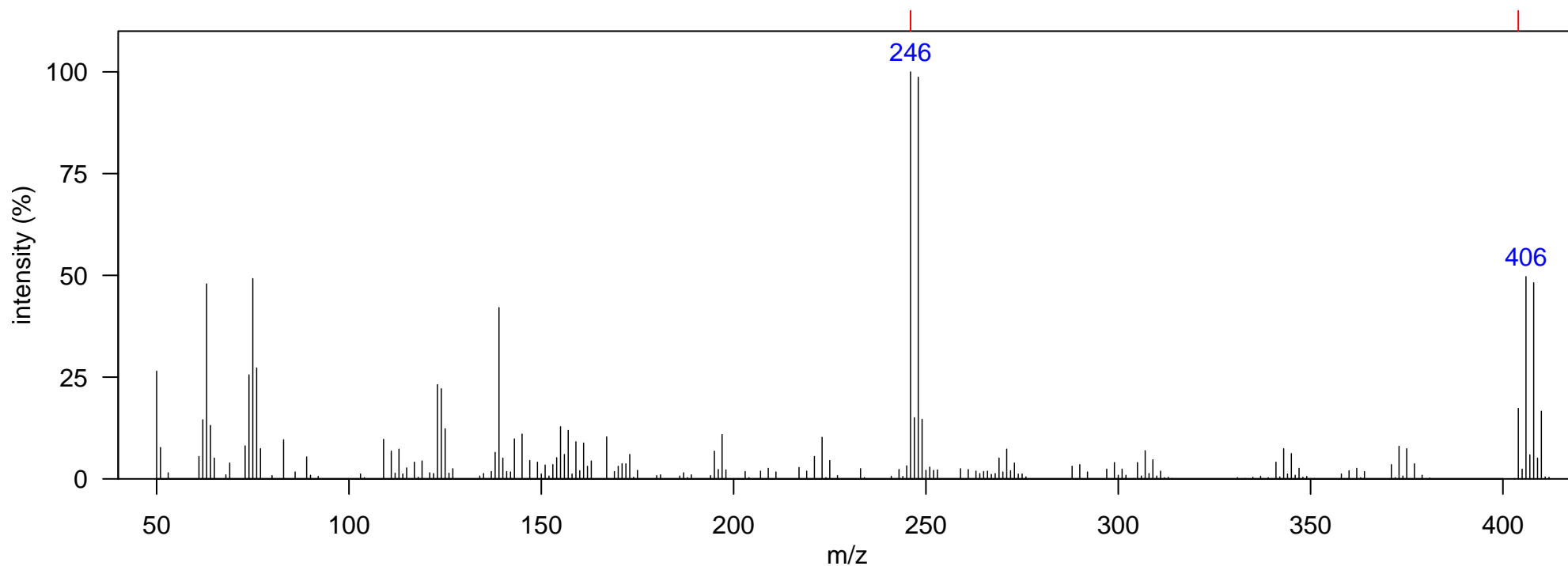
Comment:

Elemental Formula: C₁₂H₇Br₃O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT



m/z	Identity
246	[M-2Br] ⁺
404	M ⁺

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

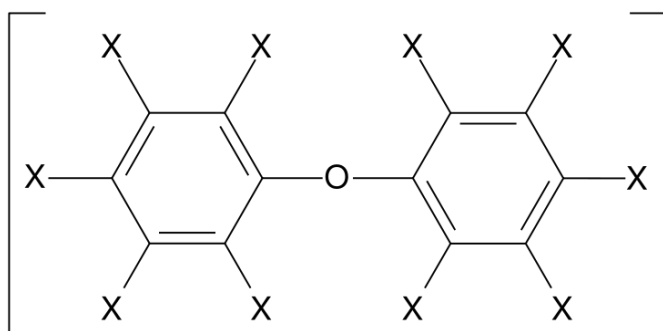
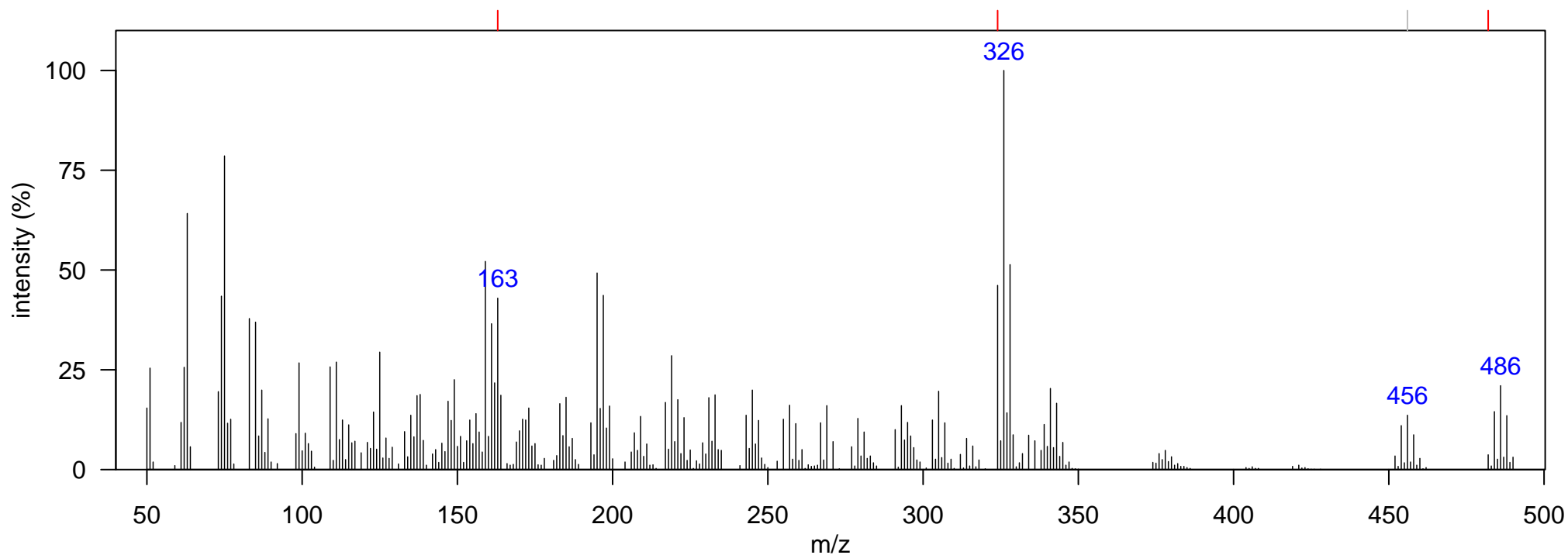
Comment:

Elemental Formula: C₁₂H₆Br₄O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS



X=4Br, 6H

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

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

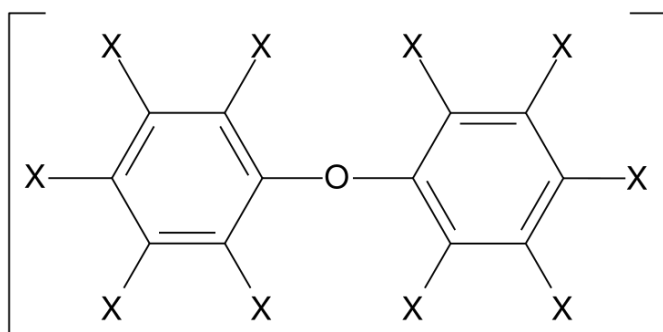
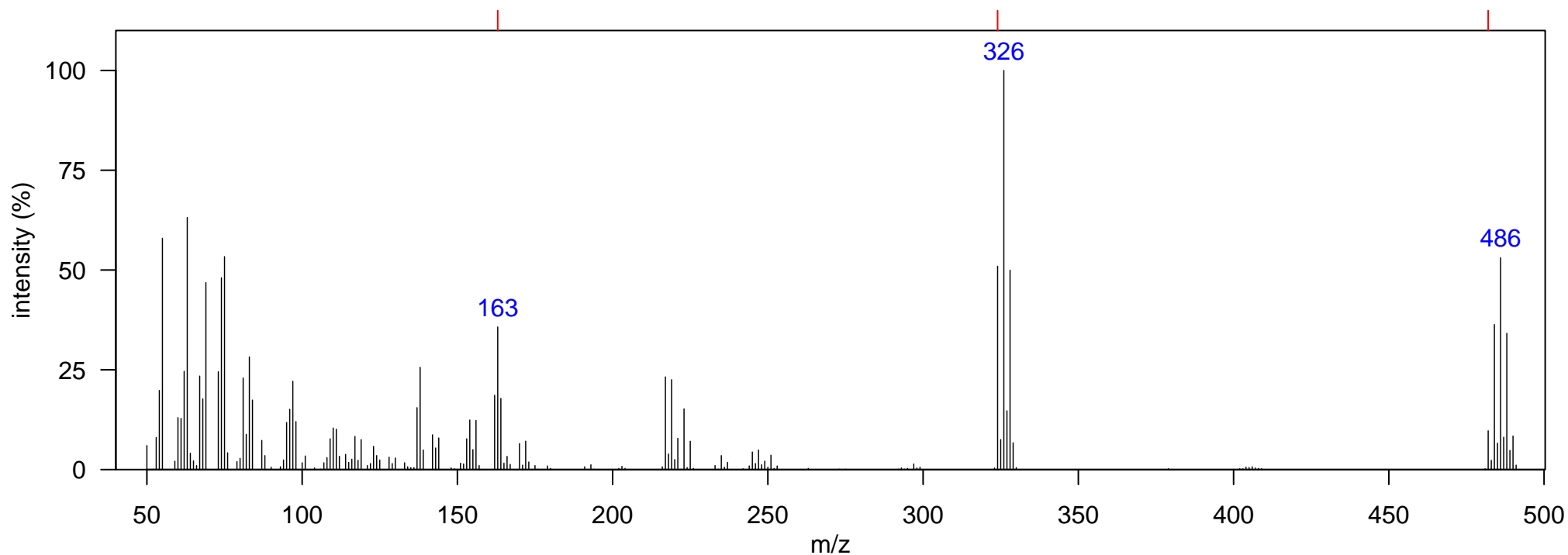
Comment:

Elemental Formula: C₁₂H₆Br₄O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS



X=4Br, 6H

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

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

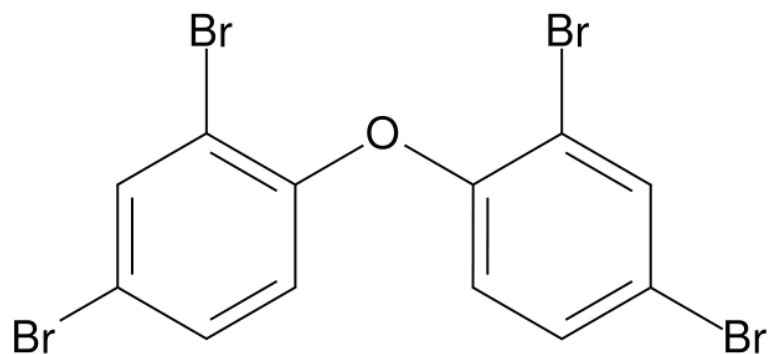
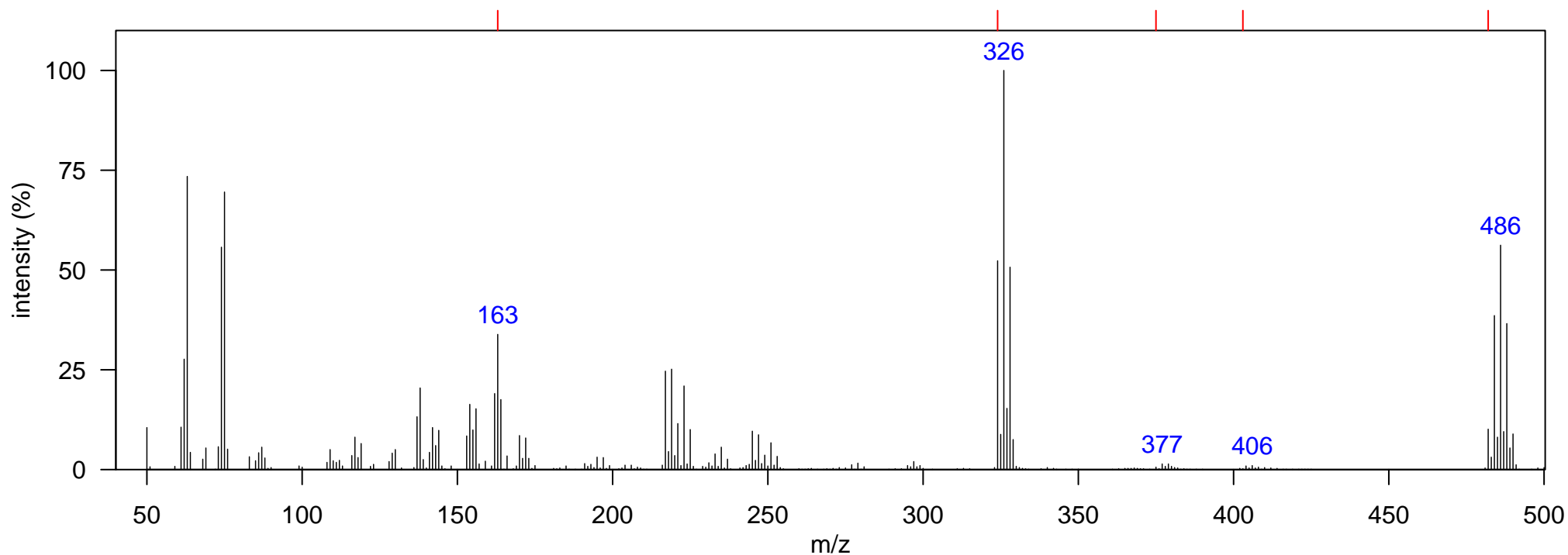
Comment:

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 ⁺

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

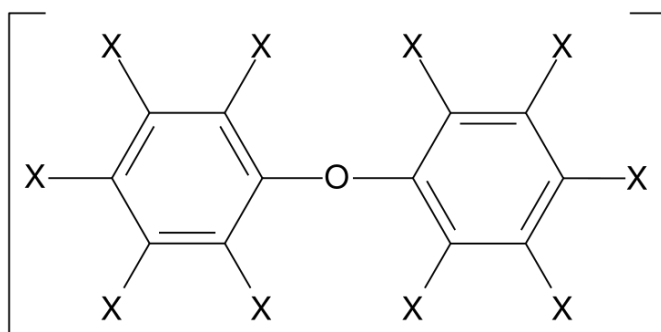
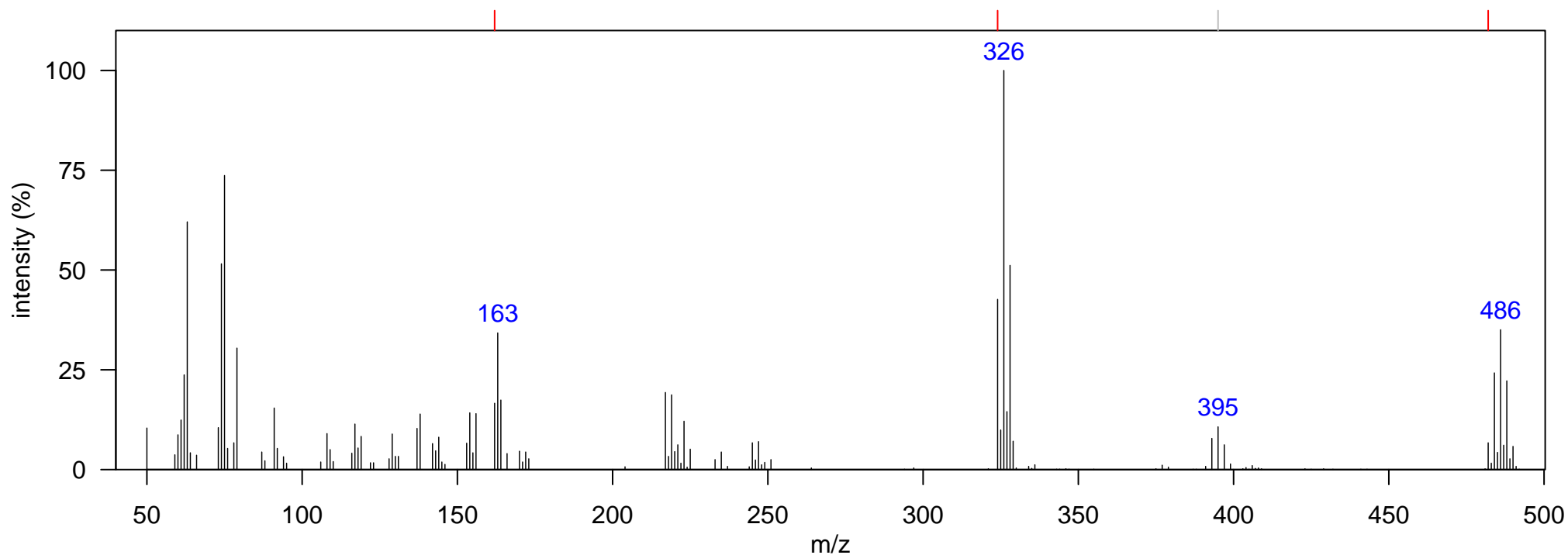
Comment:

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 ⁺

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

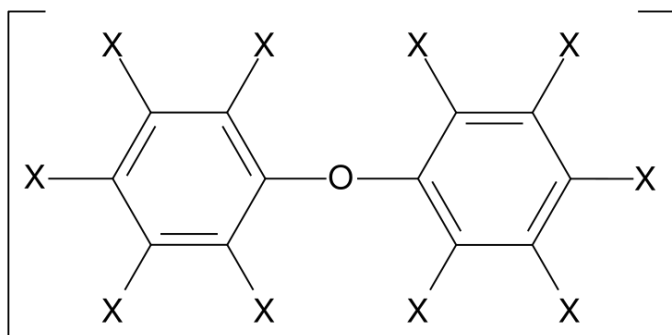
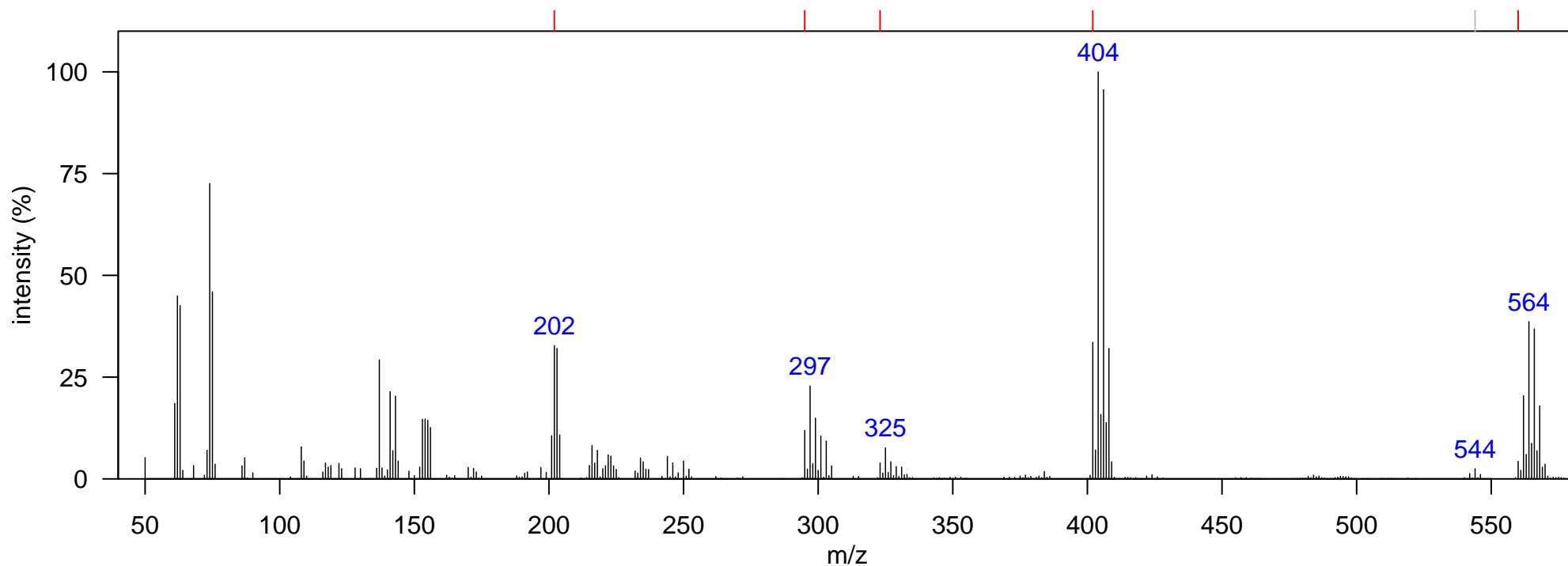
Comment:

Elemental Formula: C₁₂H₅Br₅O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS



X=5Br, 5H

m/z	Identity
202	[M-2Br] ²⁺
295	[M-3Br-CO] ⁺
323	[M-3Br] ⁺
402	[M-2Br] ⁺
544	DMBP Br ₄ Cl ₂ 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

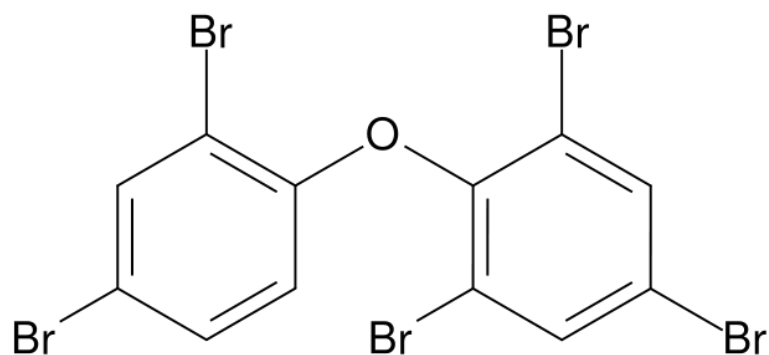
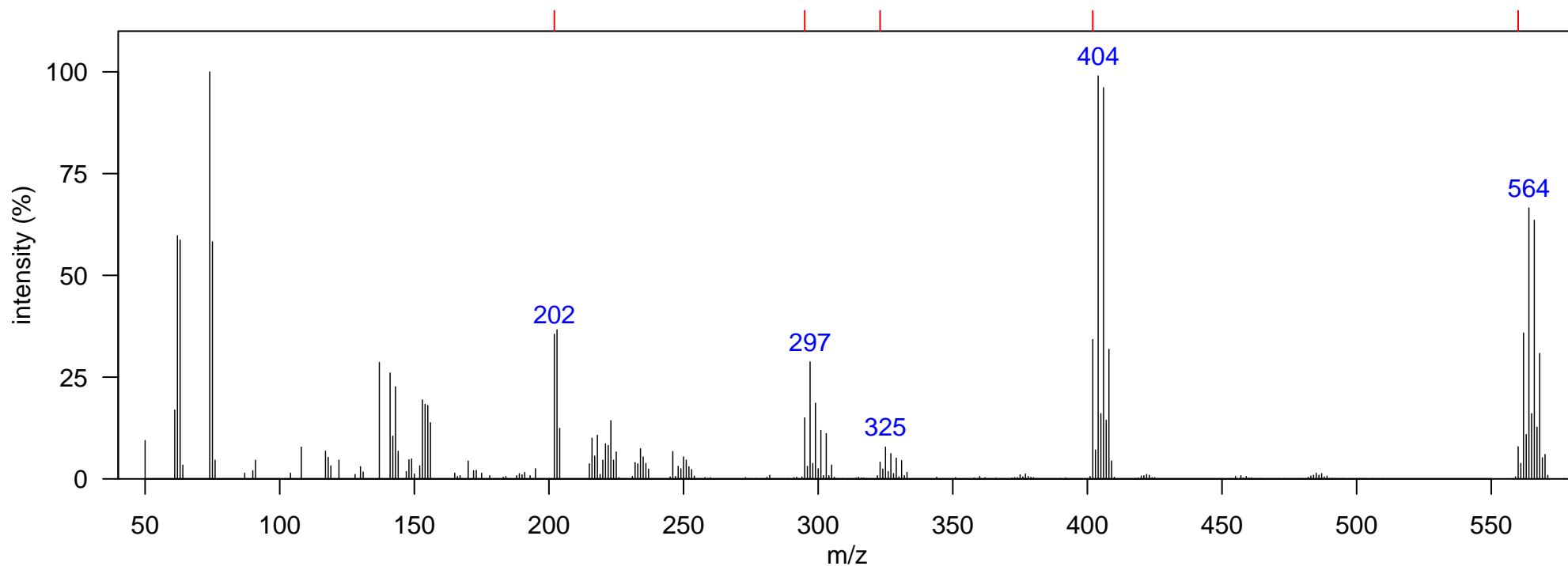
Comment:

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 ⁺

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

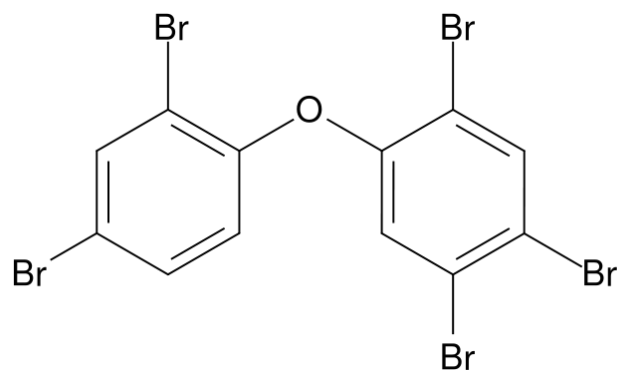
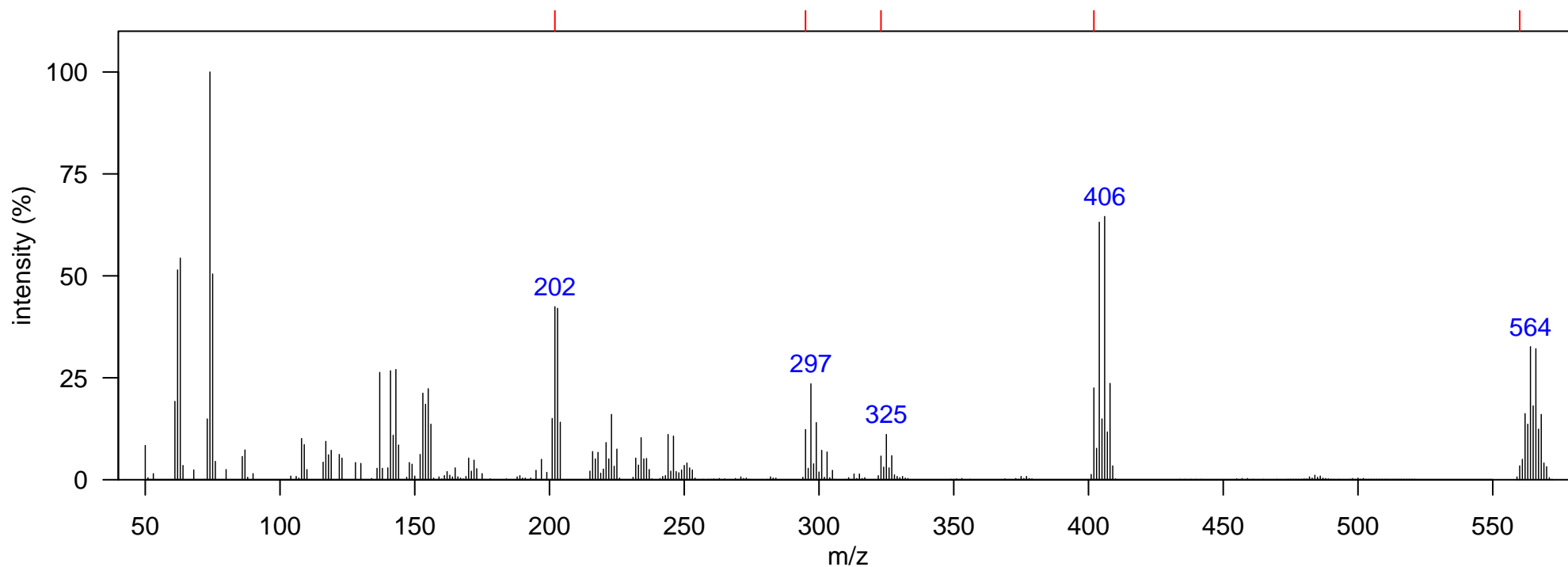
Comment:

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 ⁺

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

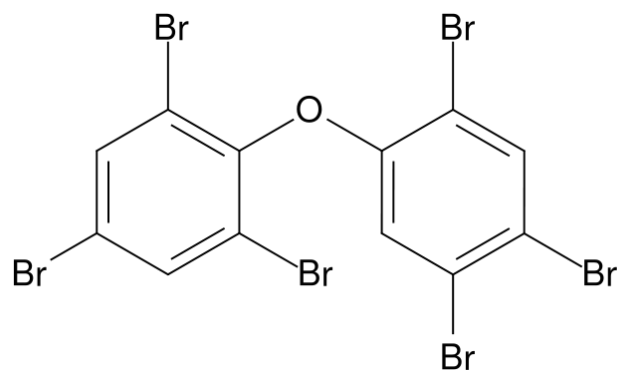
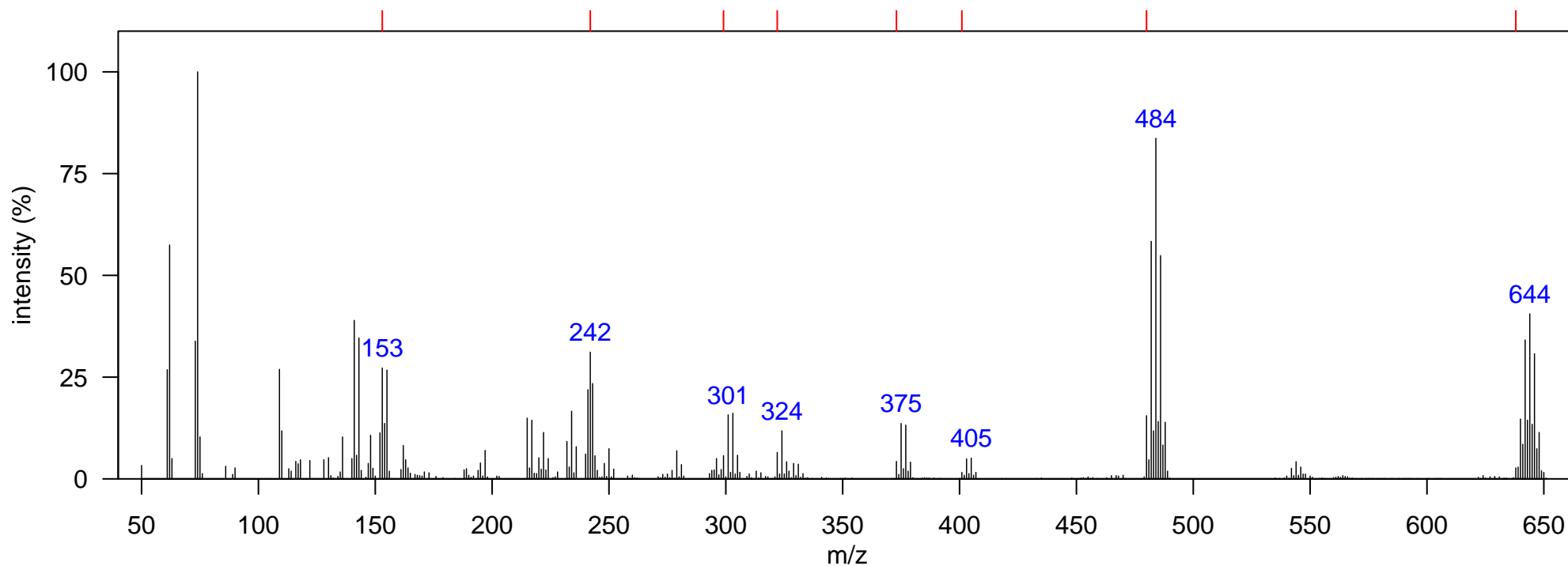
Comment:

Elemental Formula: C₁₂H₅Br₆O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT



m/z	Identity
153	[C ₆ H ₂ Br] ⁺
242	[M-2Br] ₂ ⁺
299	[M-CO-C ₆ H ₂ Br ₃] ⁺ = [C ₅ H ₂ Br ₃] ⁺
322	[M-4Br] ⁺
373	[M-3Br-CO] ⁺
401	[M-3Br] ⁺
480	[M-2Br] ⁺
638	M ⁺

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

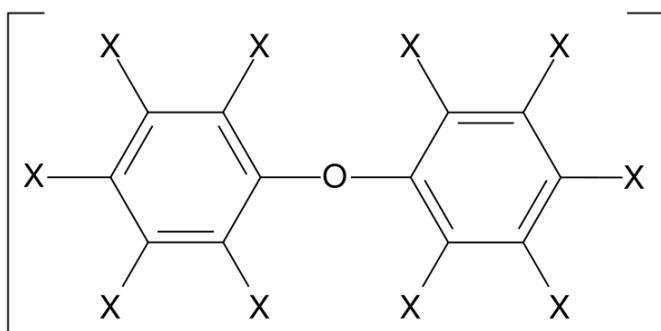
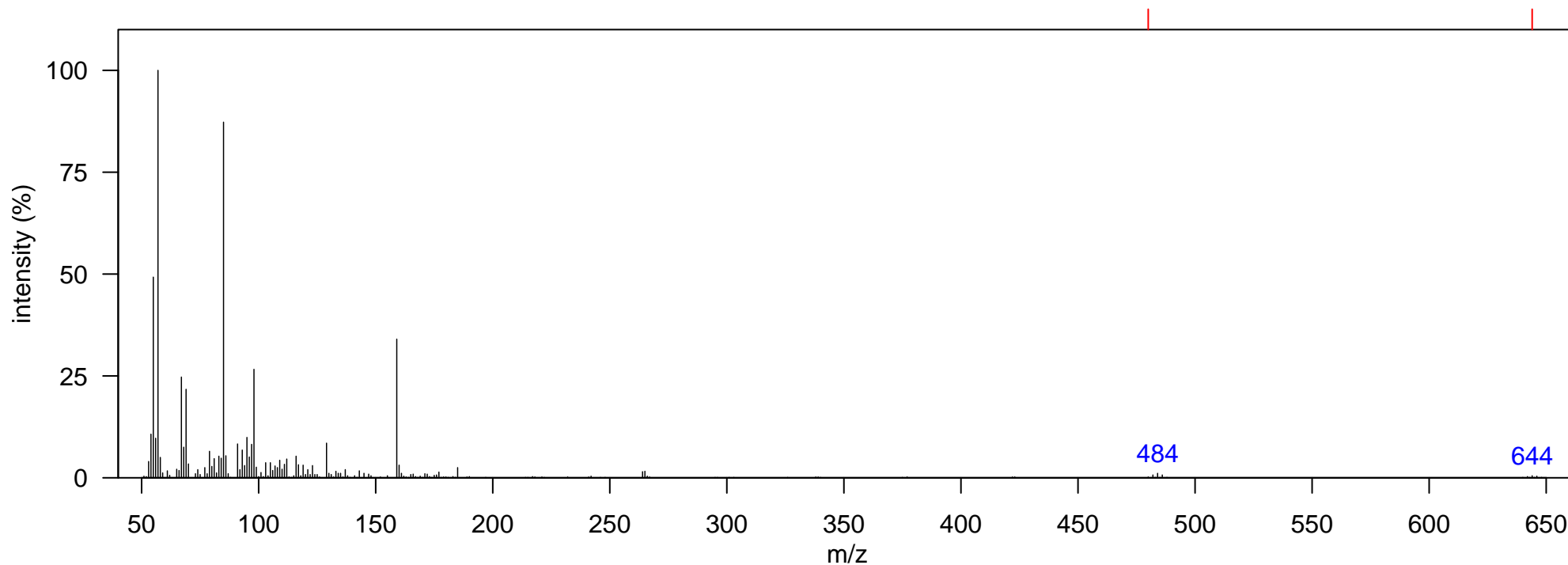
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₁₂H₄Br₆O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS



X=6Br, 4H

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

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

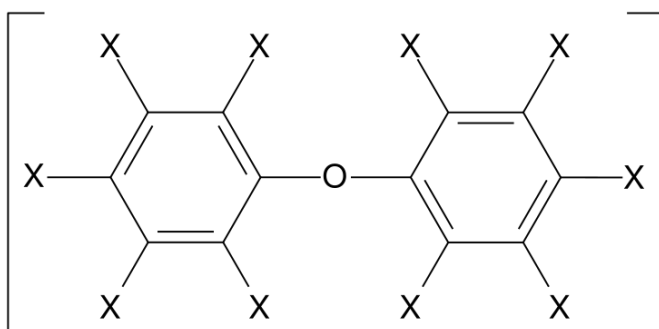
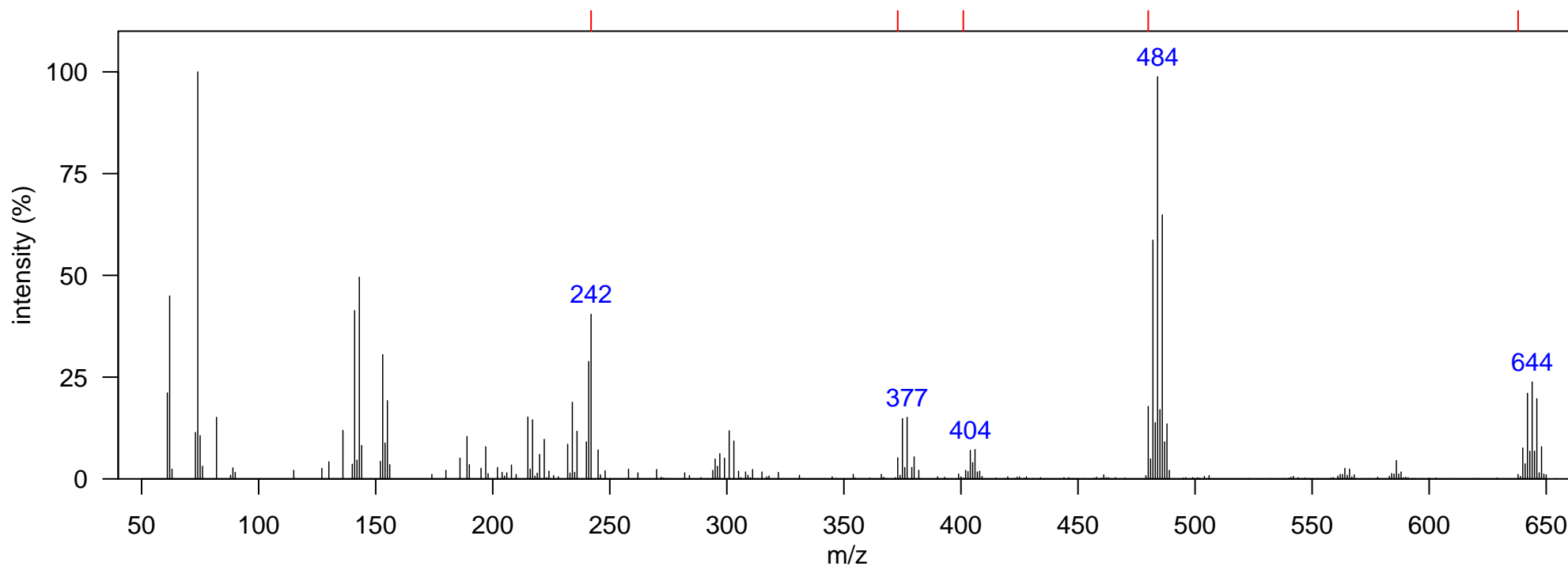
Comment:

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

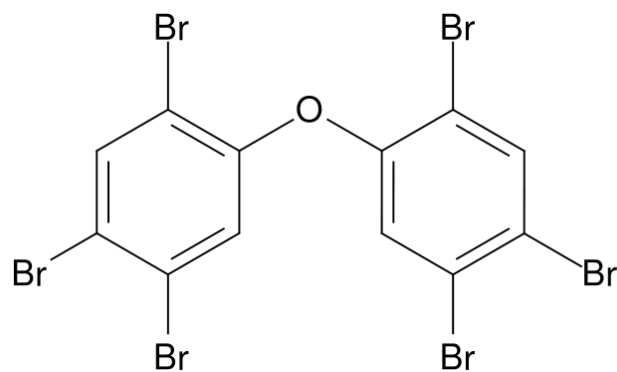
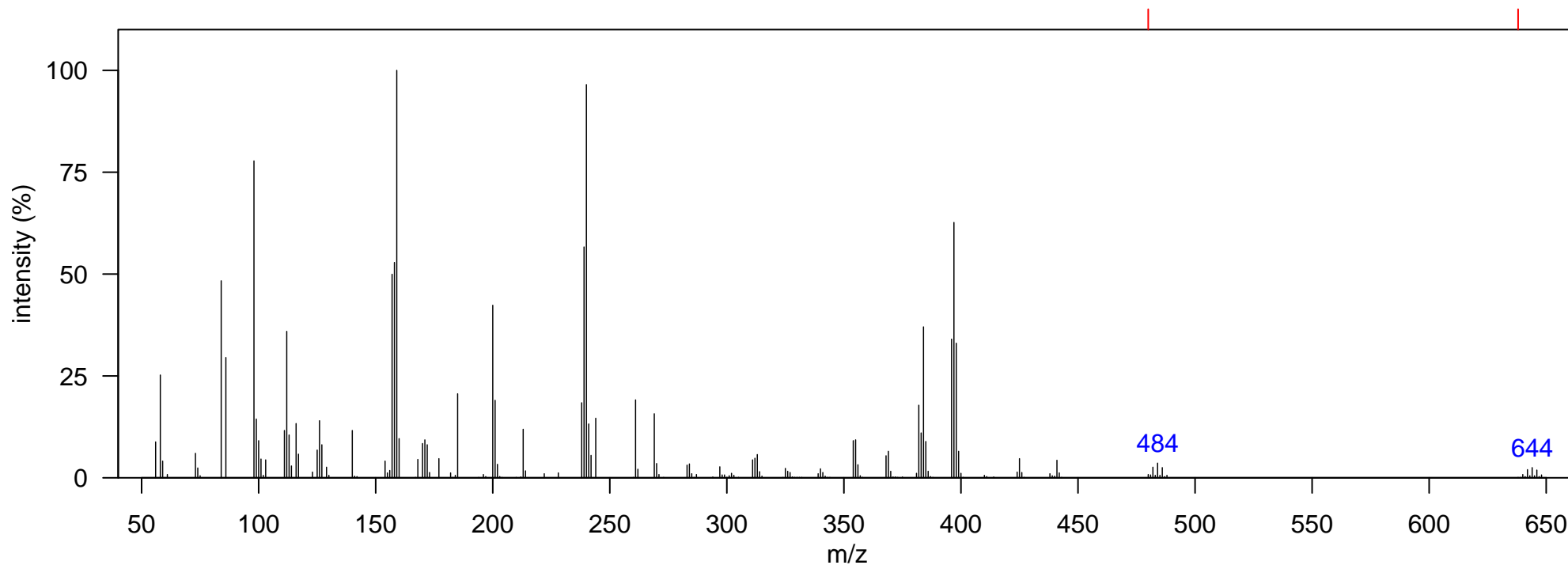
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₁₂H₄Br₆O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT



m/z	Identity
480	[M-2Br] ⁺
638	M ⁺

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

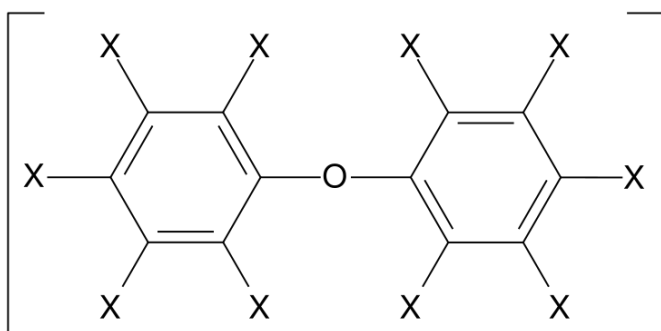
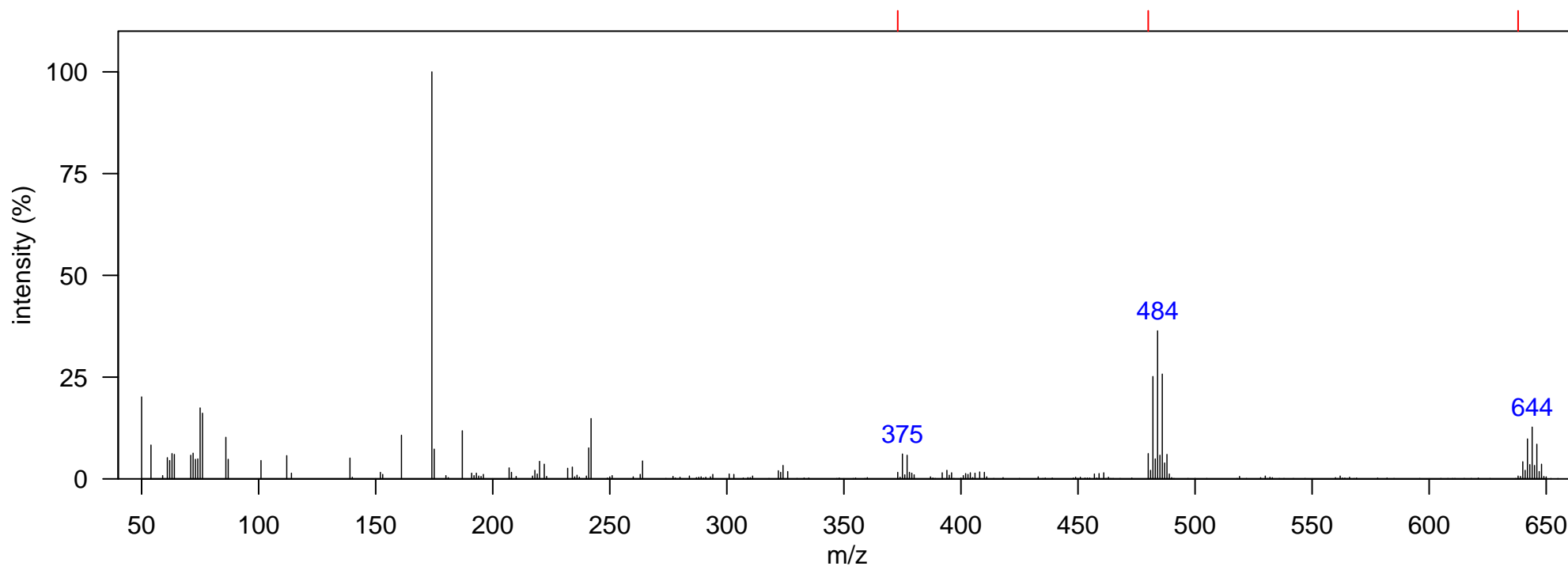
Comment:

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 ⁺

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

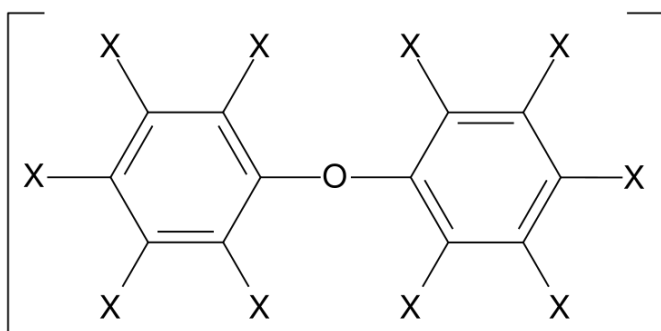
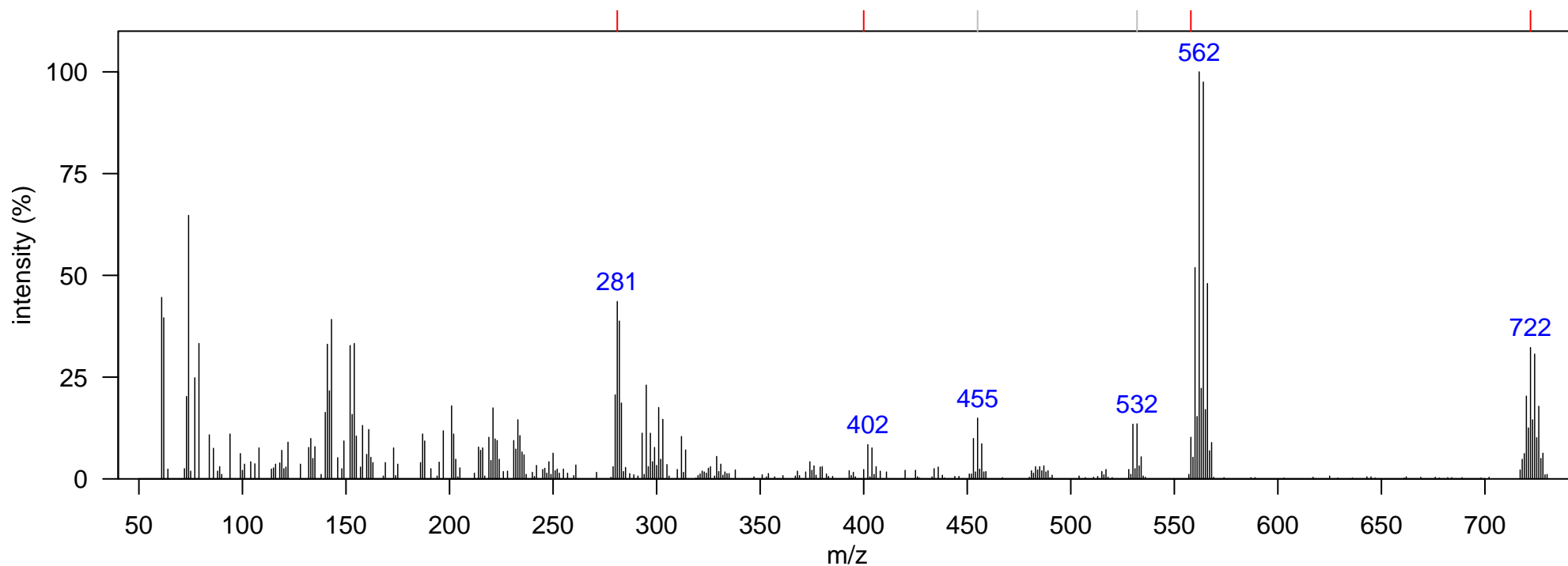
Comment:

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)

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

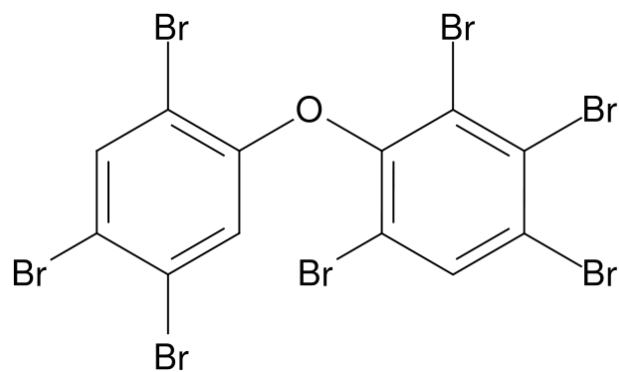
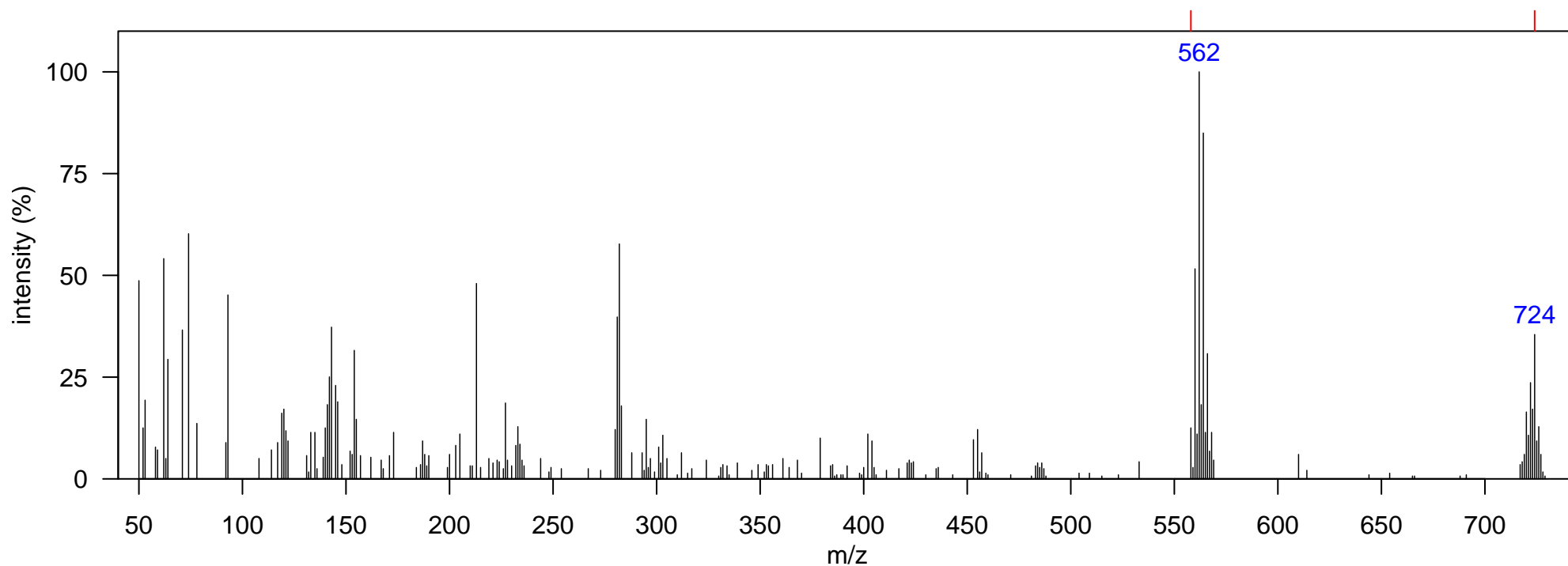
Comment:

Elemental Formula: C₁₂H₃Br₇O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS RT



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

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

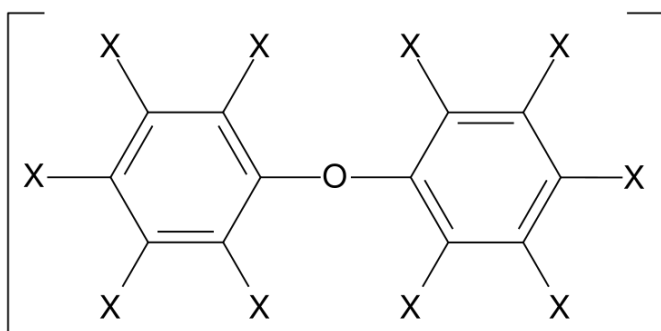
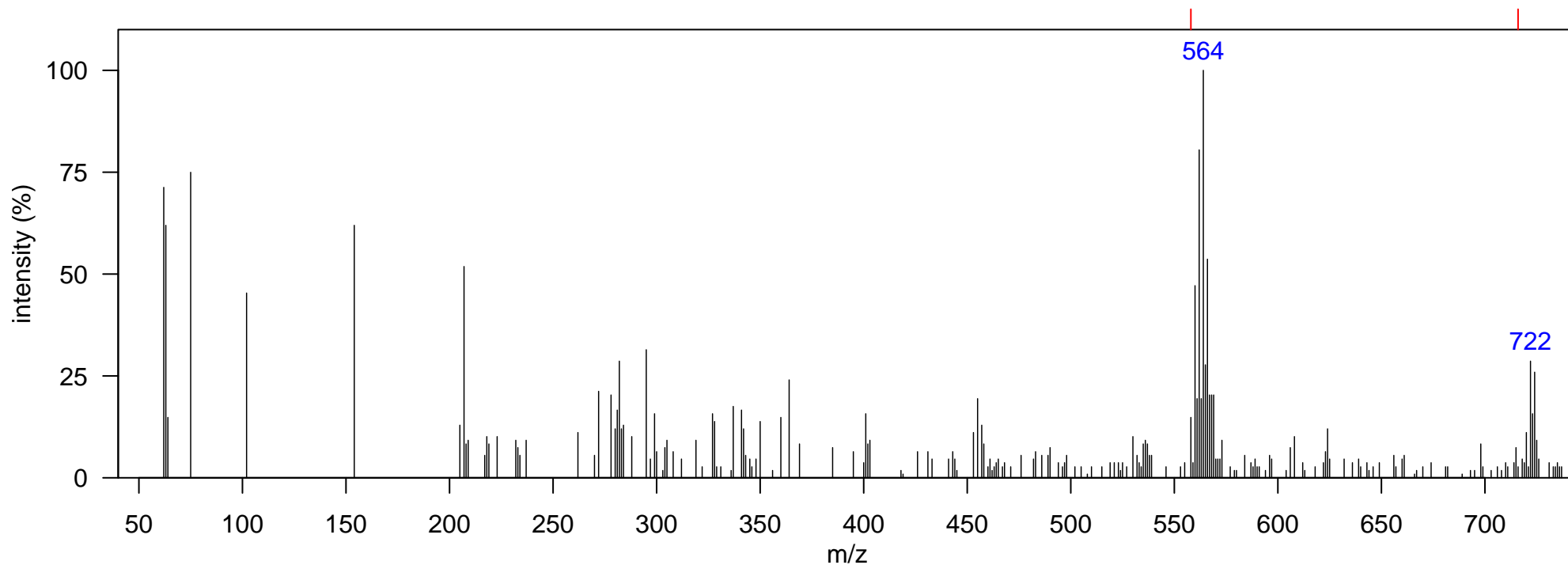
Comment:

Elemental Formula: C₁₂H₃Br₇O

Source: anthropogenic

Class: PBDE

Identification: Authentic MS



X=7Br, 3H

m/z	Identity
558	[M-2Br] ⁺
716	M ⁺

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

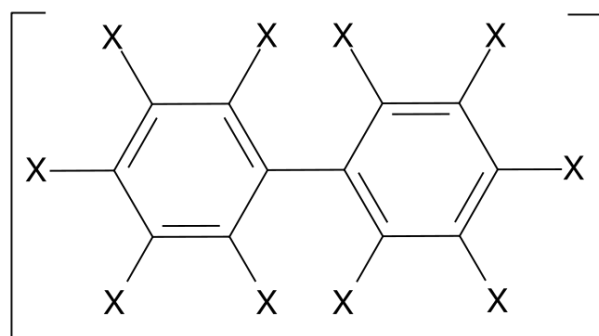
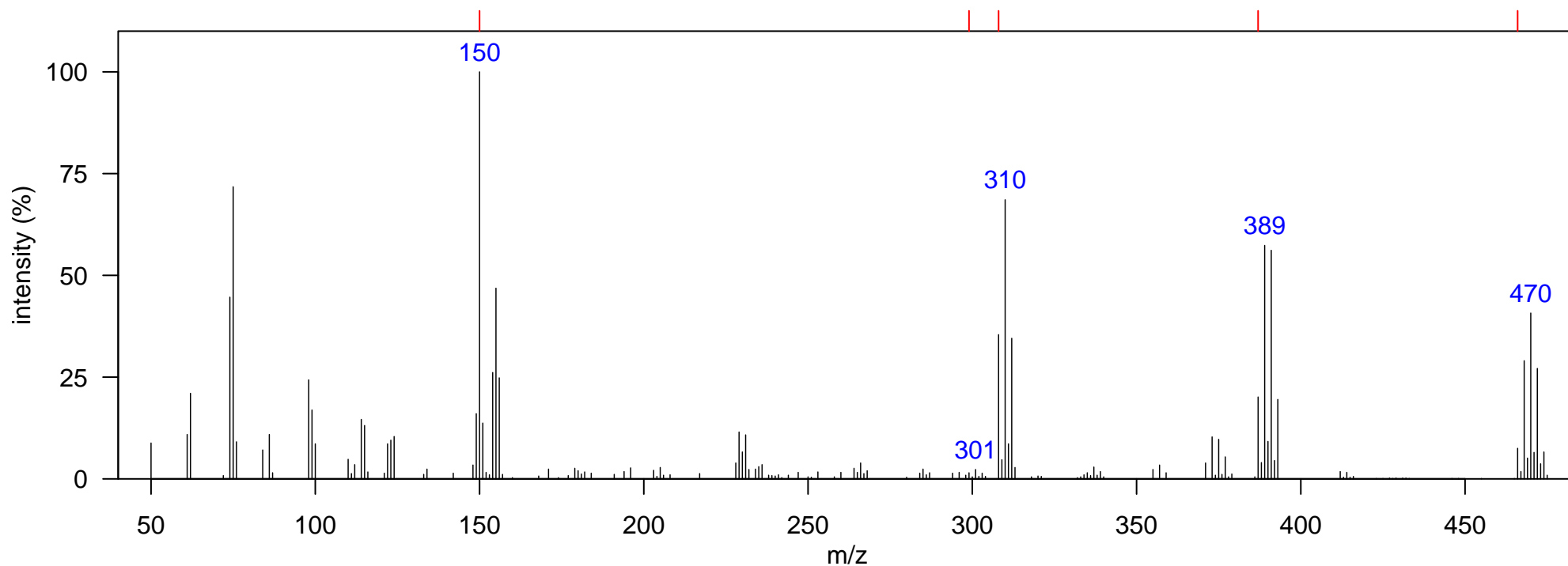
Comment:

Elemental Formula: C₁₂H₆Br₄

Source: anthropogenic

Class: PBB

Identification: Manual – Congener Group



X = 4Br, 6H

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

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

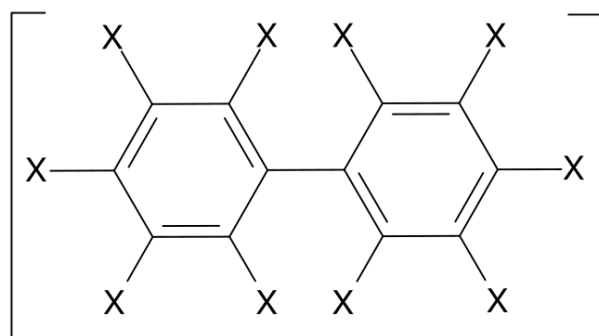
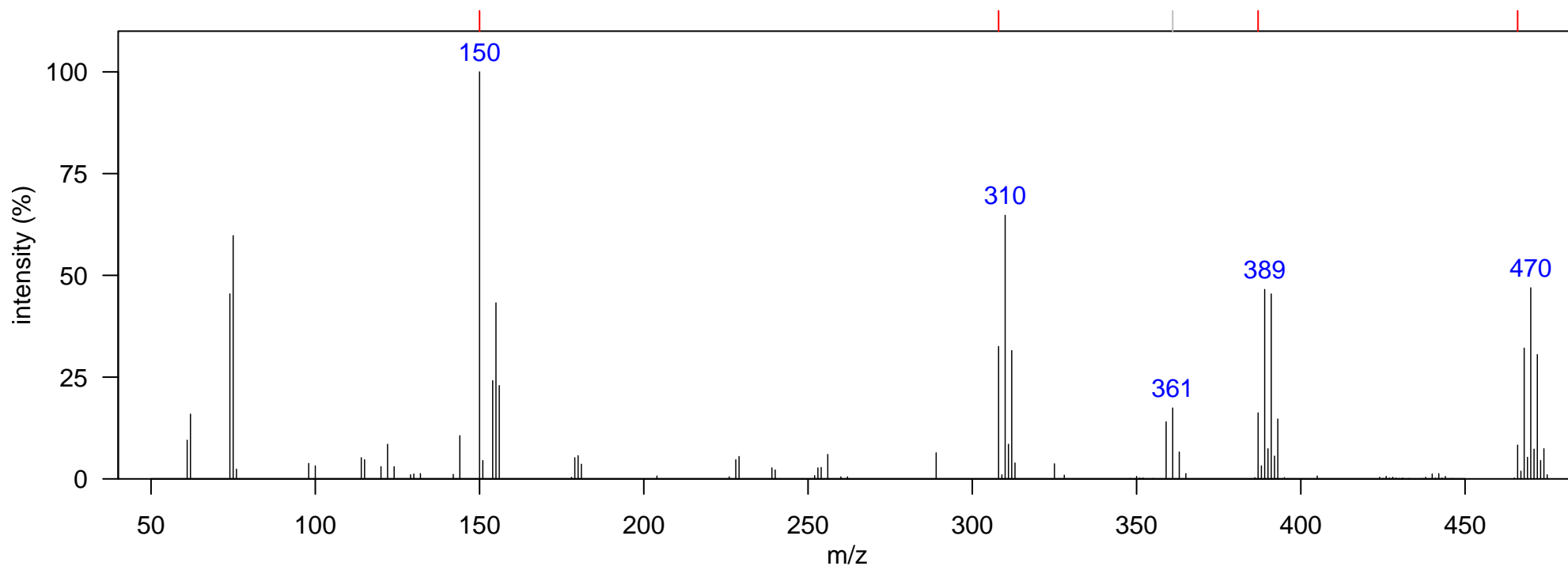
Comment:

Elemental Formula: C₁₂H₆Br₄

Source: anthropogenic

Class: PBB

Identification: Manual – Congener Group



X = 4Br, 6H

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

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

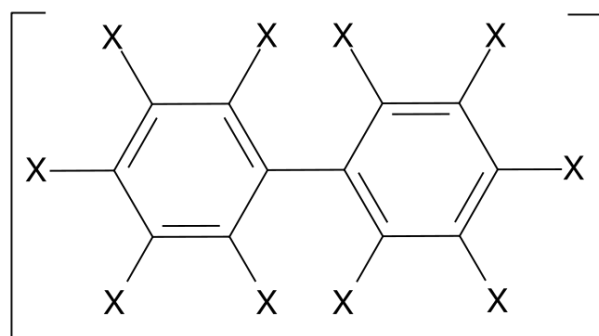
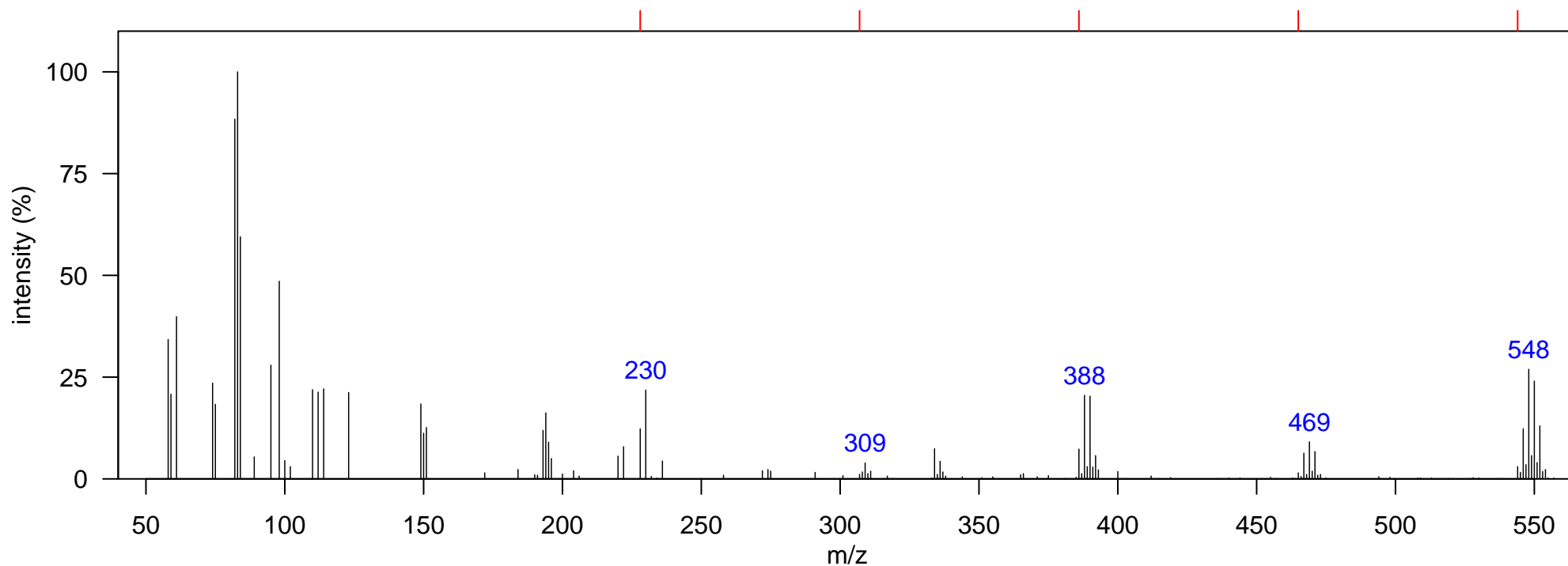
Comment:

Elemental Formula: C₁₂H₅Br₅

Source: anthropogenic

Class: PBB

Identification: Manual – Congener Group



X = 5Br, 5H

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

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

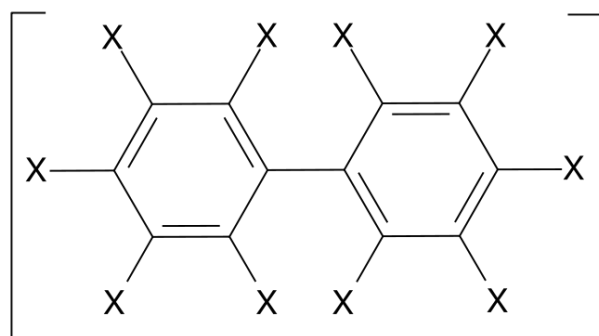
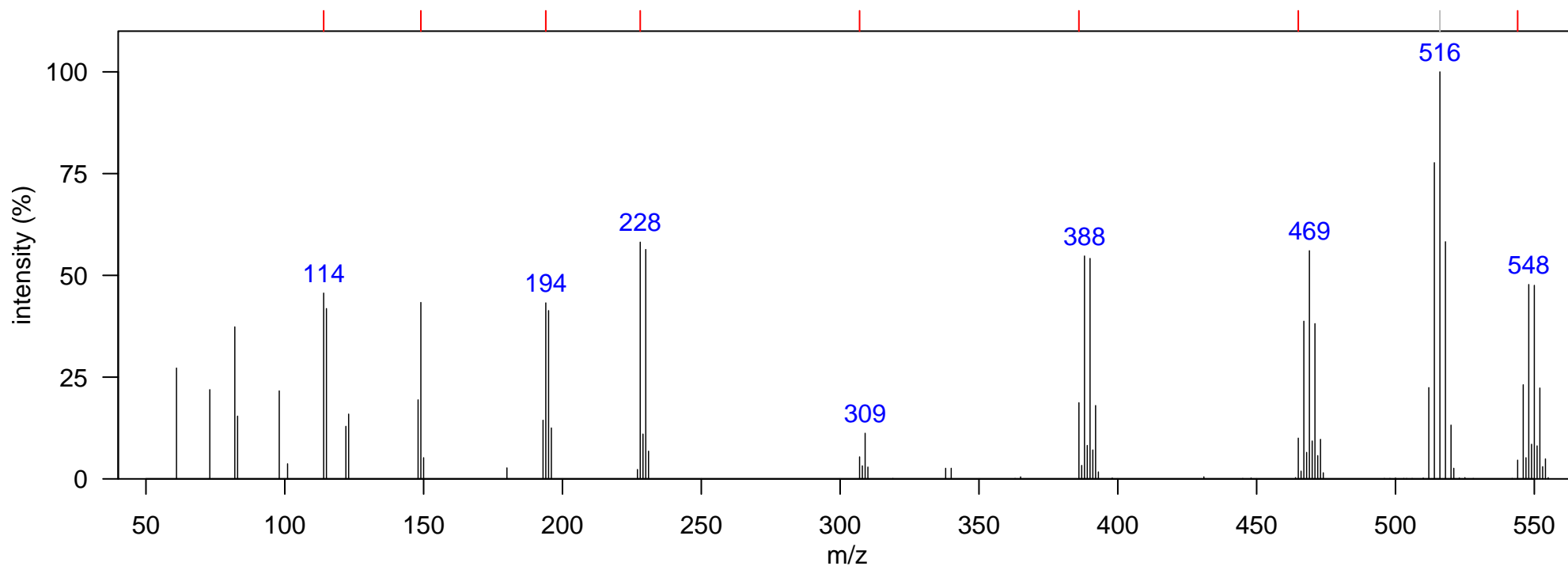
Comment:

Elemental Formula: C₁₂H₅Br₅

Source: anthropogenic

Class: PBB

Identification: Manual – Congener Group



X = 5Br, 5H

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 ⁺

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

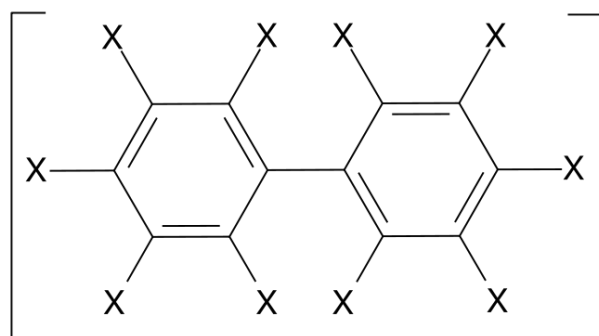
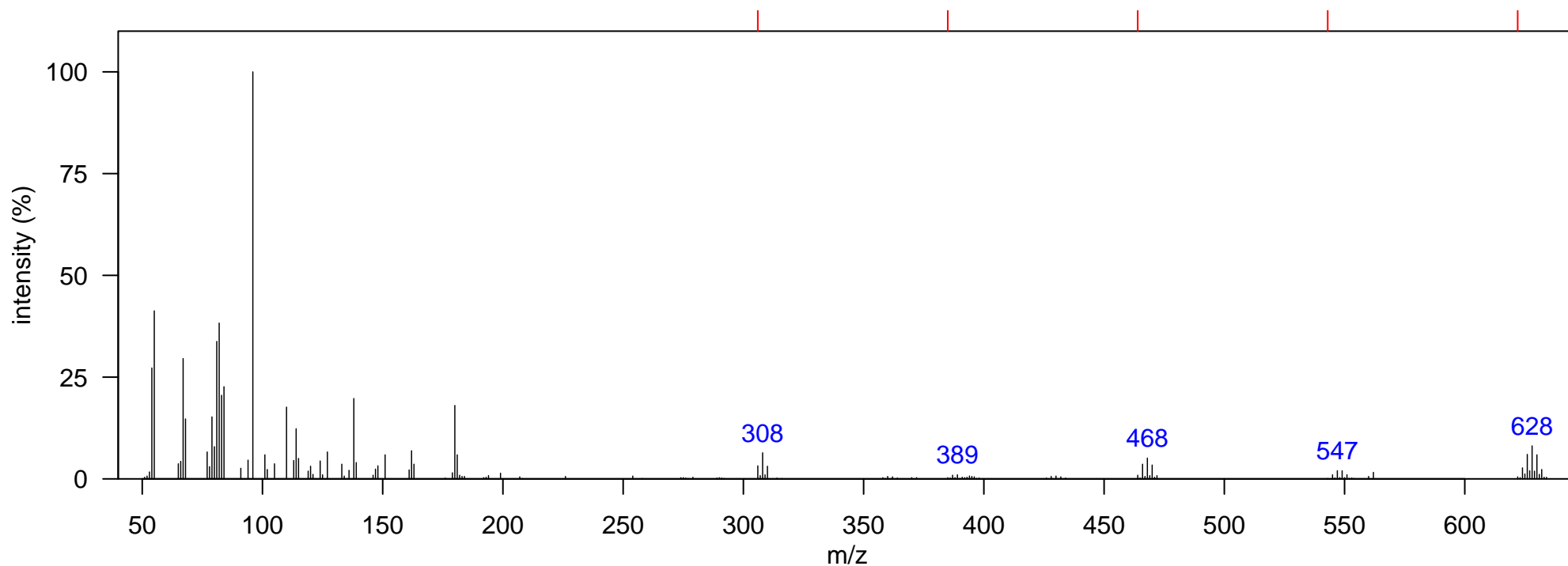
Comment:

Elemental Formula: C₁₂H₄Br₆

Source: anthropogenic

Class: PBB

Identification: Authentic MS



X = 6Br, 4H

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

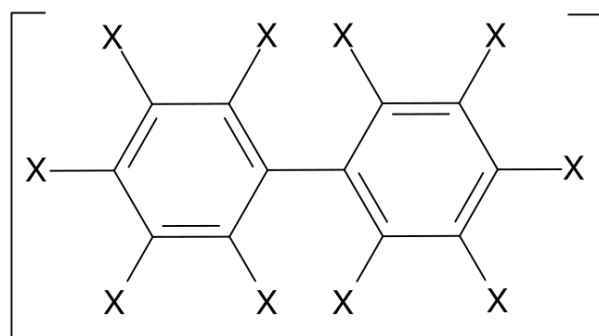
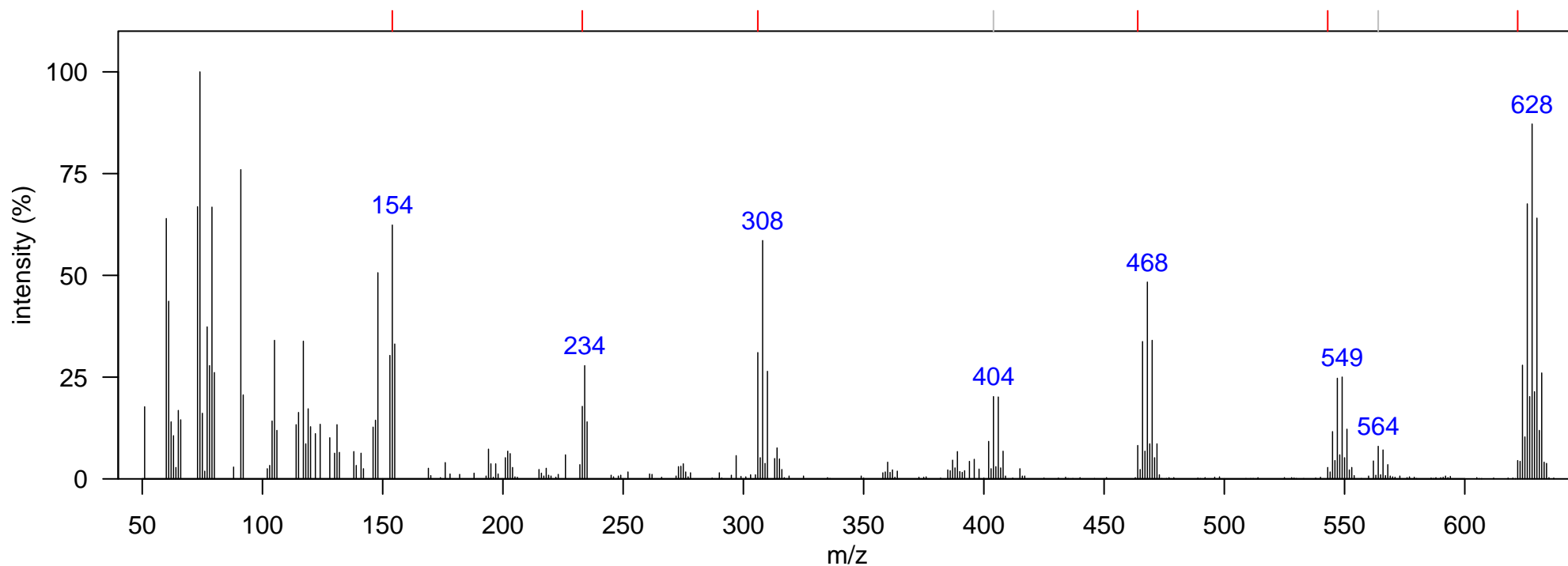
Comment:

Elemental Formula: C₁₂H₄Br₆

Source: anthropogenic

Class: PBB

Identification: Authentic MS



X = 6Br, 4H

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 ⁺

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

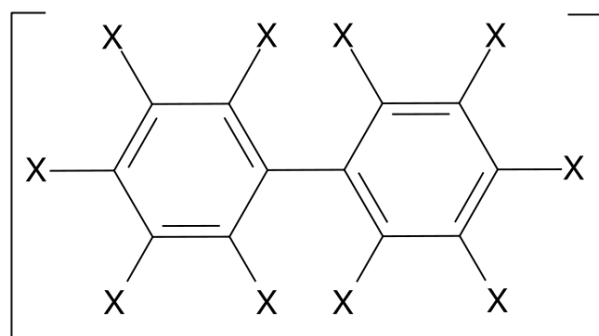
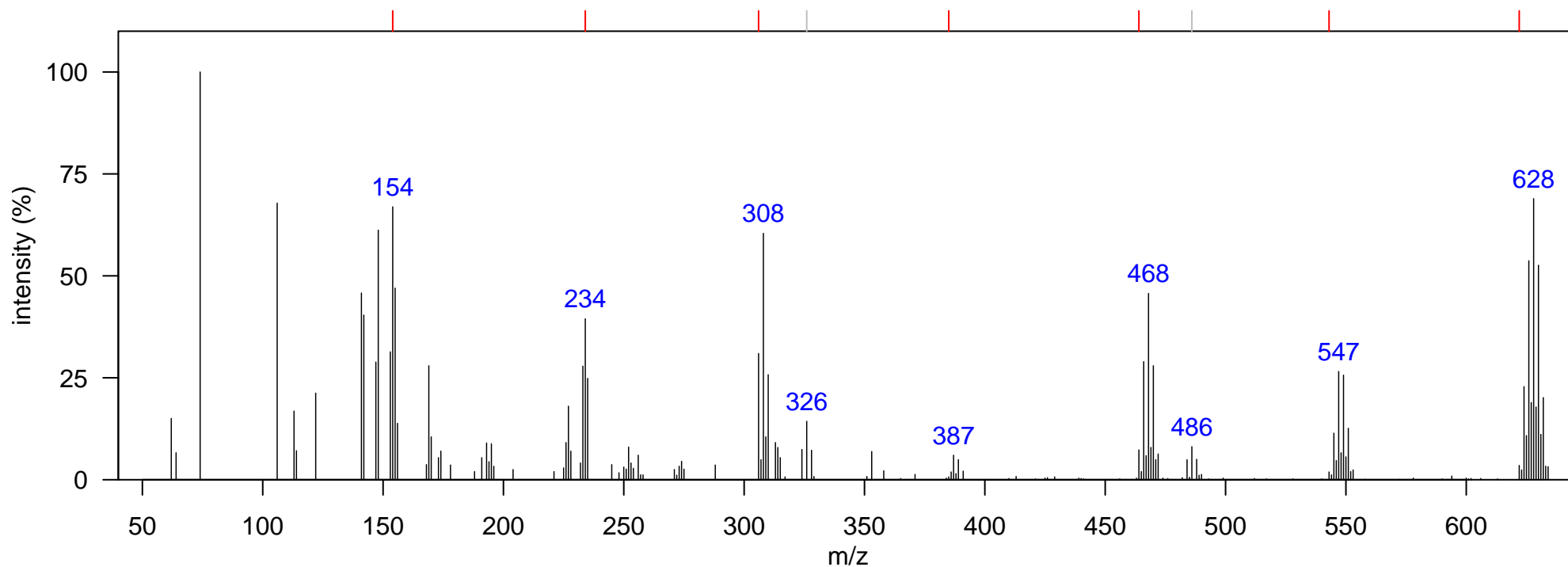
Comment:

Elemental Formula: C₁₂H₄Br₆

Source: anthropogenic

Class: PBB

Identification: Authentic MS



X = 6Br, 4H

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 ⁺

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

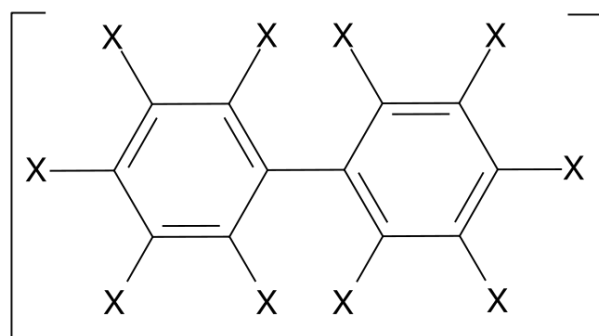
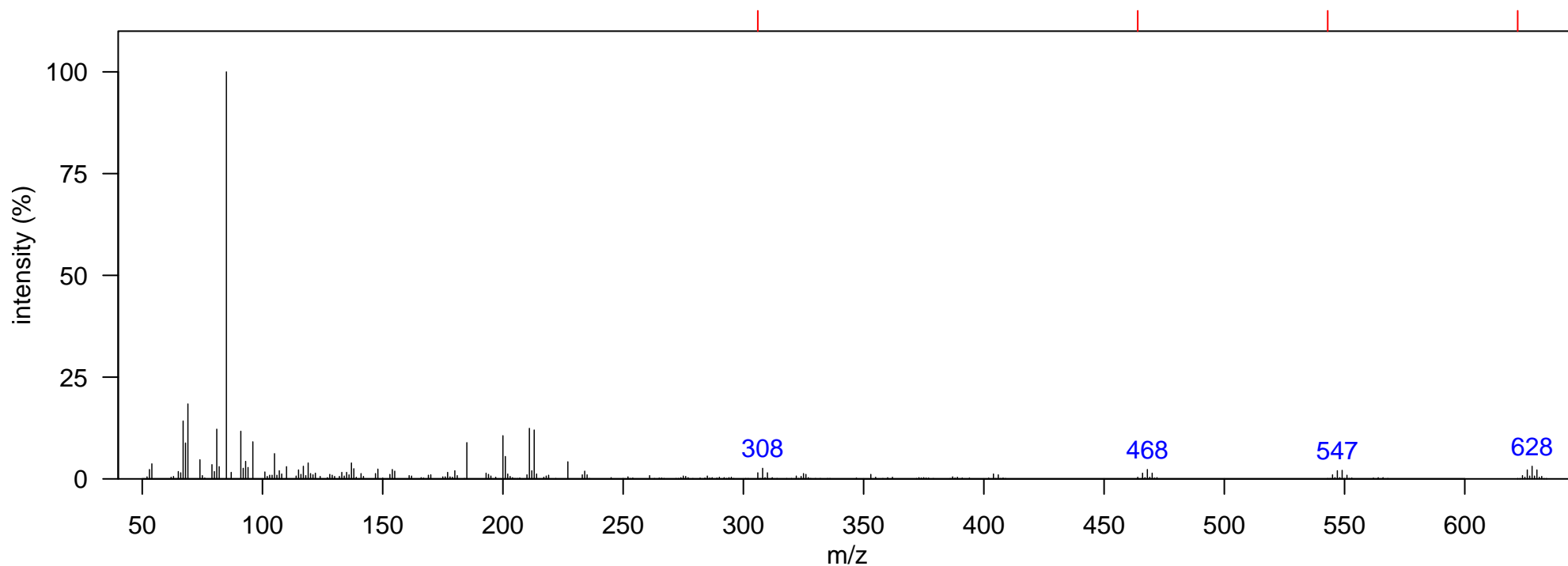
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₁₂H₄Br₆

Source: anthropogenic

Class: PBB

Identification: Authentic MS



X = 6Br, 4H

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

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

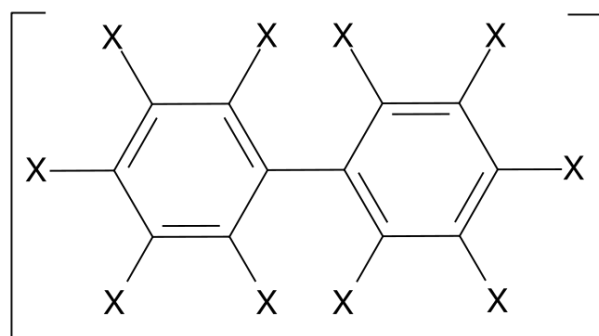
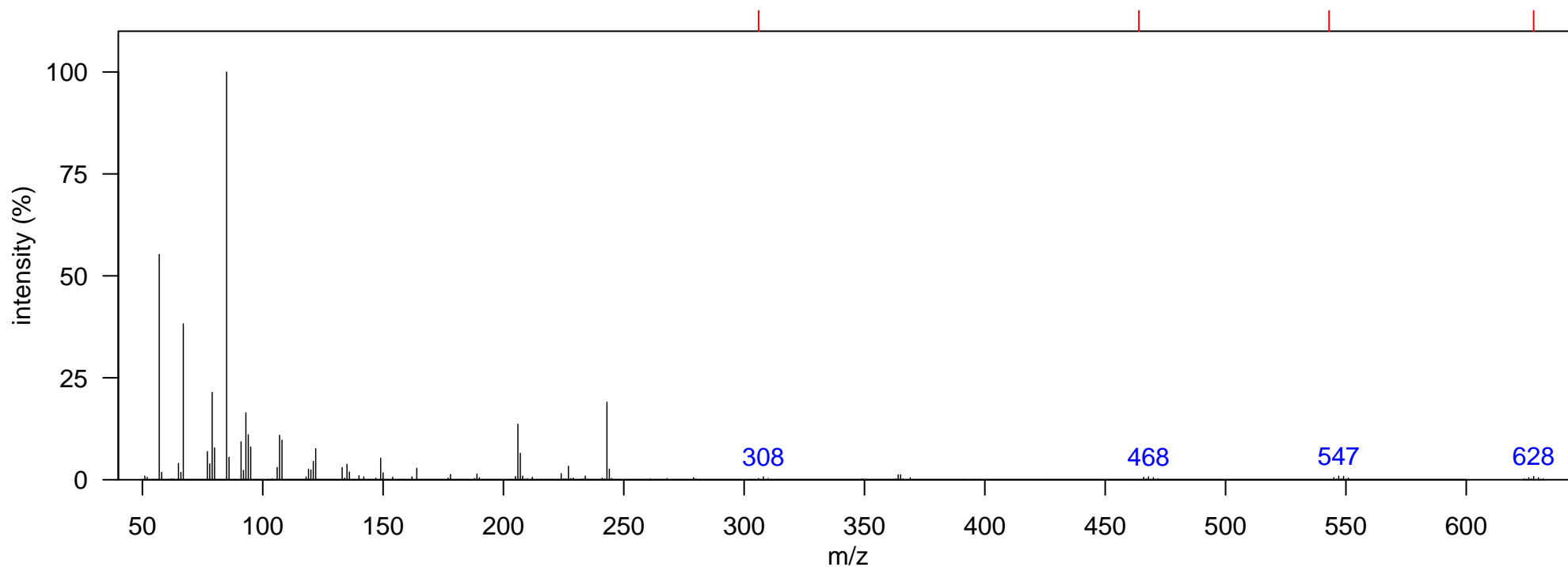
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₁₂H₄Br₆

Source: anthropogenic

Class: PBB

Identification: Authentic MS



X = 6Br, 4H

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

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

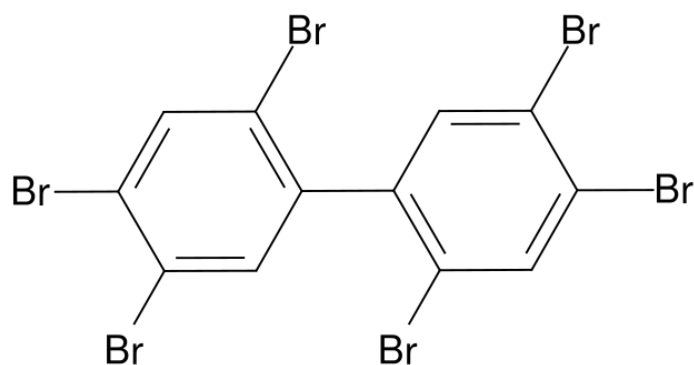
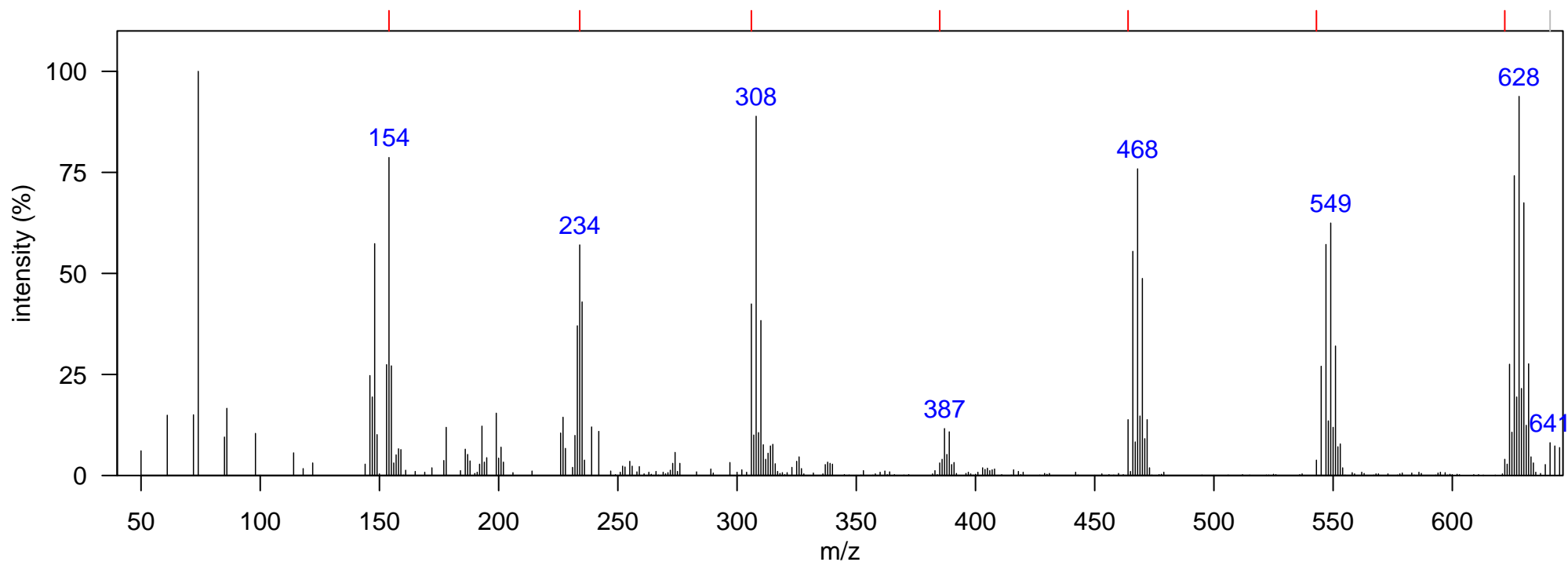
Comment:

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

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

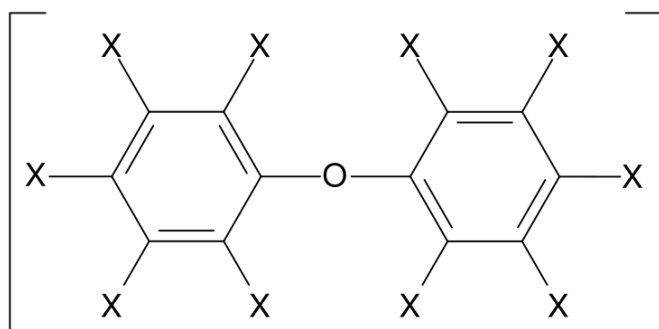
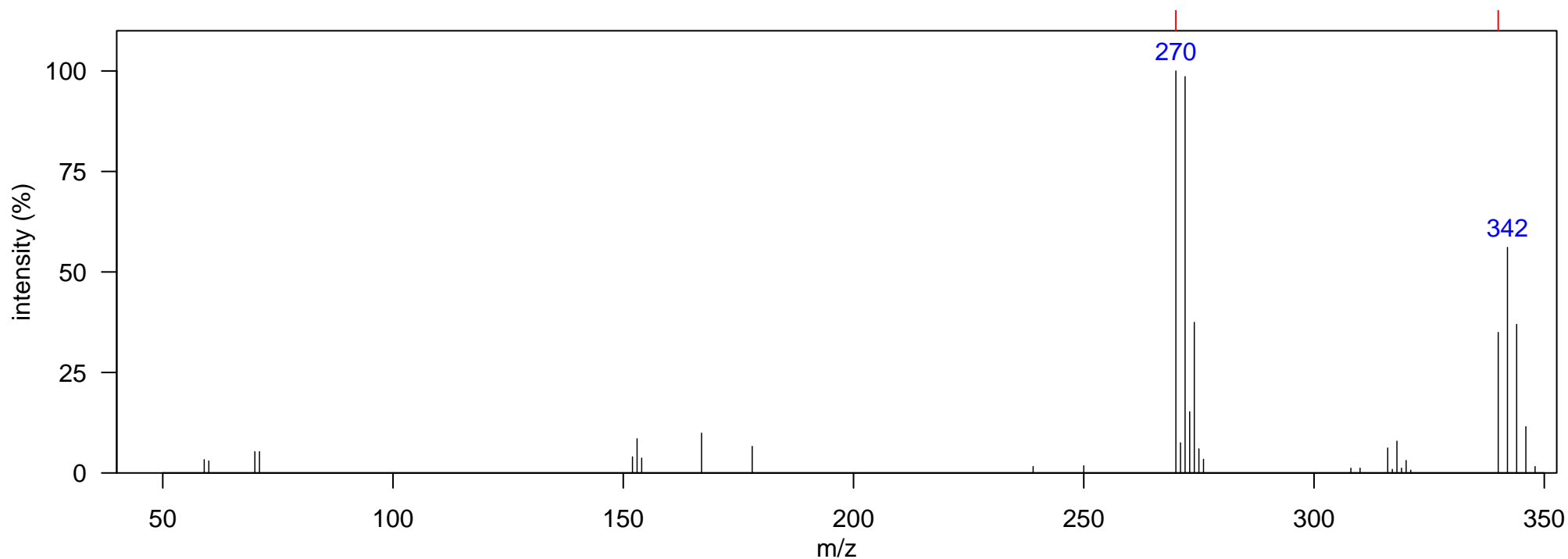
Comment:

Elemental Formula: C₁₂H₅Cl₅O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=5Cl, 5H

m/z	Identity
270	[M-2Cl] ⁺
340	M ⁺

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

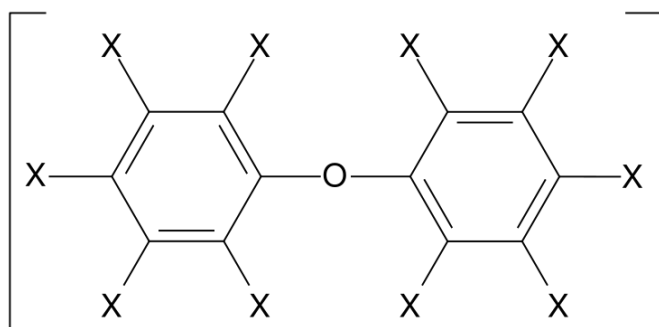
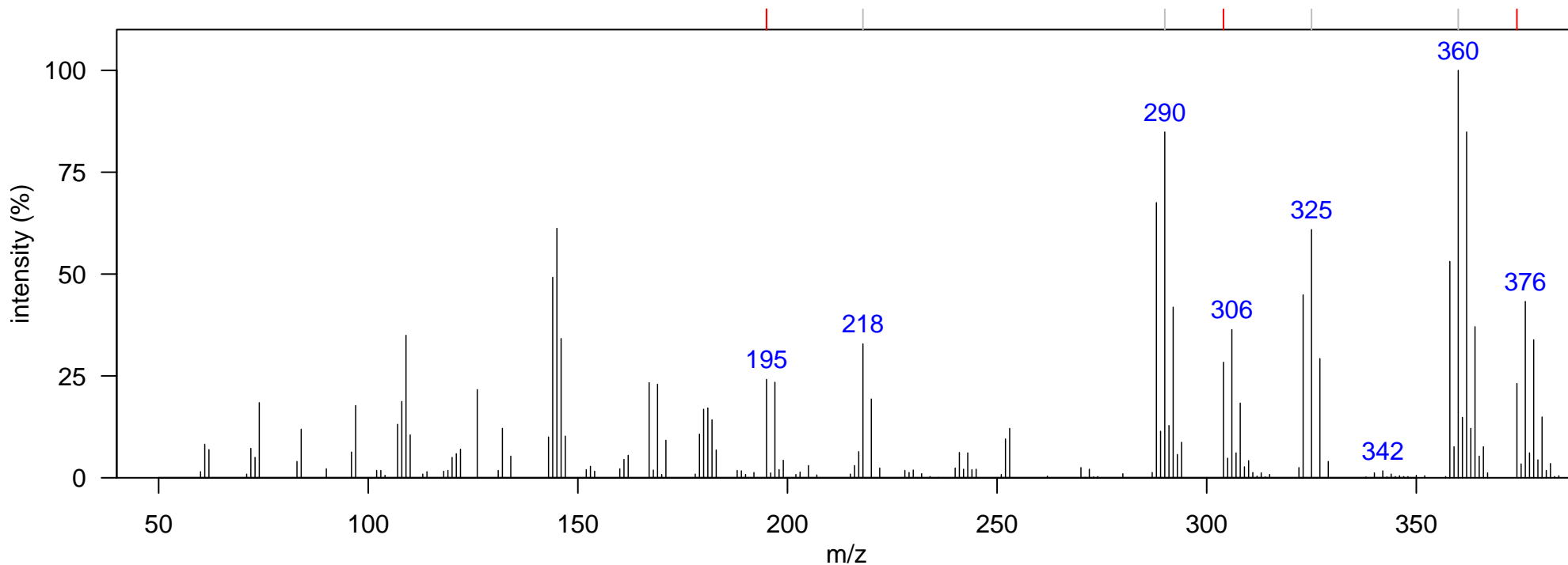
Comment:

Elemental Formula: C₁₂H₄Cl₆O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=6Cl, 4H

m/z	Identity
195	[C ₅ H ₂ OC ₃] ⁺
218	interference PCB
290	PCB interference
304	[M-2Cl] ⁺
325	PCB interference
360	PCB interference
374	M ⁺

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

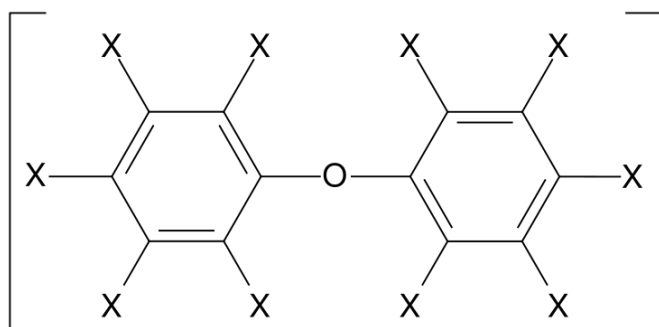
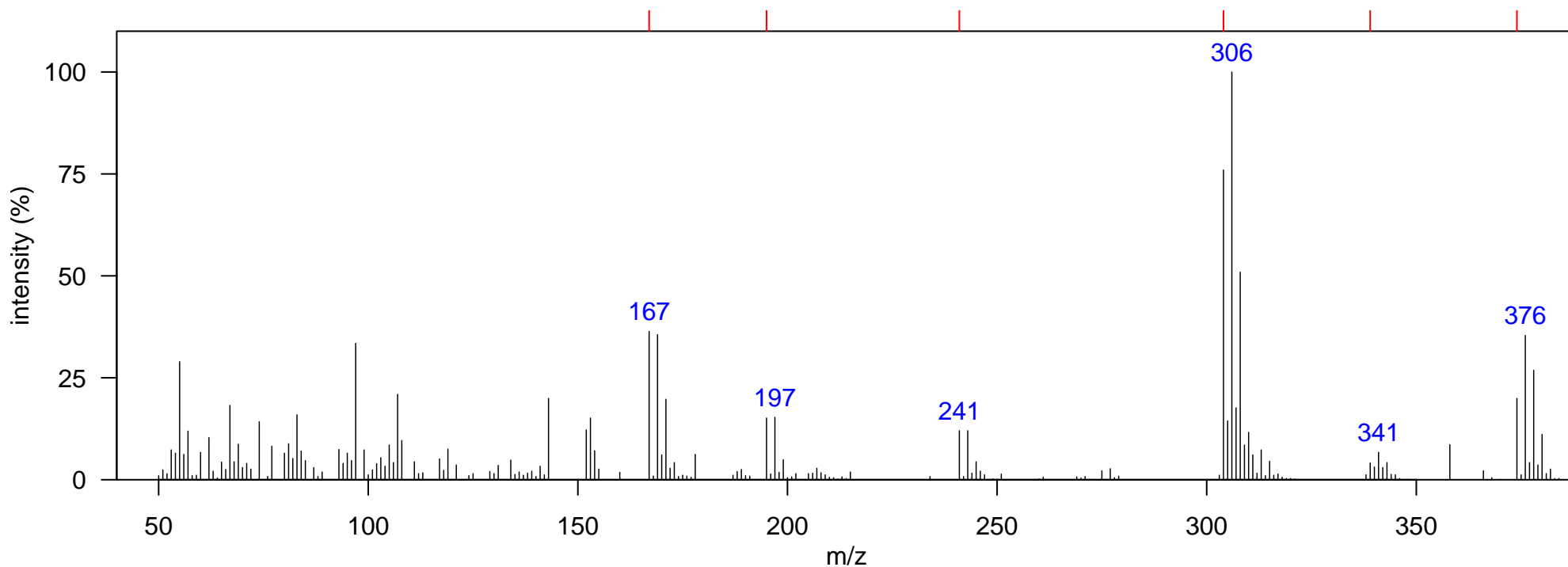
Comment:

Elemental Formula: C₁₂H₄Cl₆O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=6Cl, 4H

m/z	Identity
167	[C ₅ H ₂ Cl ₃] ⁺
195	[C ₆ H ₂ OC ₃] ⁺
241	[M-3Cl-CO] ⁺
304	[M-2Cl] ⁺
339	[M-Cl] ⁺
374	M ⁺

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

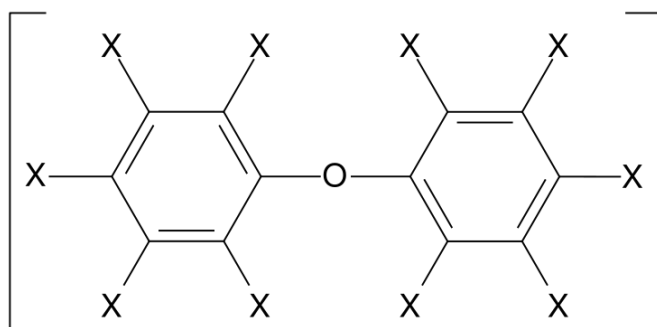
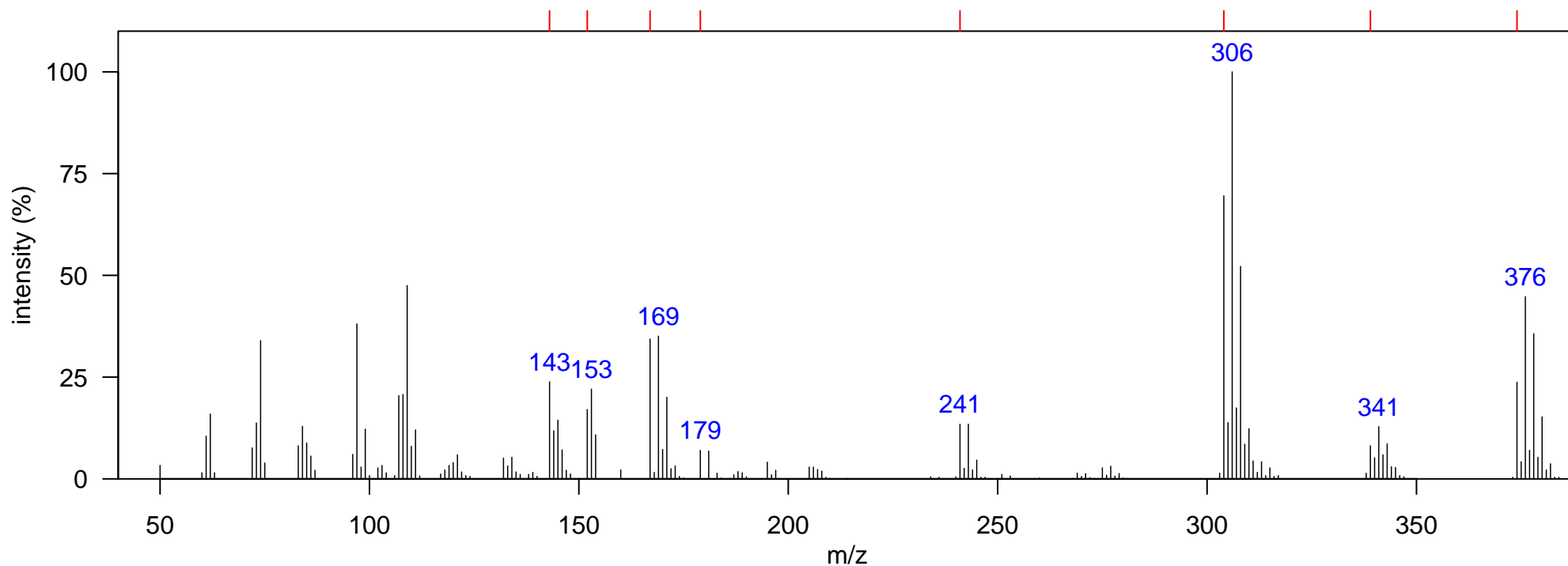
Comment:

Elemental Formula: C₁₂H₄Cl₆O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=6Cl, 4H

m/z	Identity
143	[C ₆ Cl ₂ H] ⁺
152	[M-2Cl] ₂ ⁺
167	[C ₅ Cl ₃ H ₂] ⁺
179	[C ₆ Cl ₃ H ₂] ⁺
241	[M-3Cl-CO] ⁺
304	[M-2Cl] ⁺
339	[M-Cl] ⁺
374	M ⁺

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

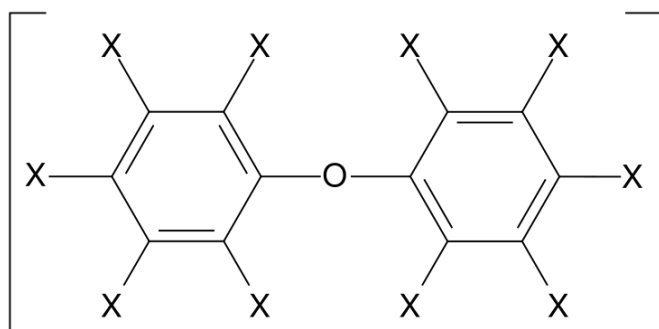
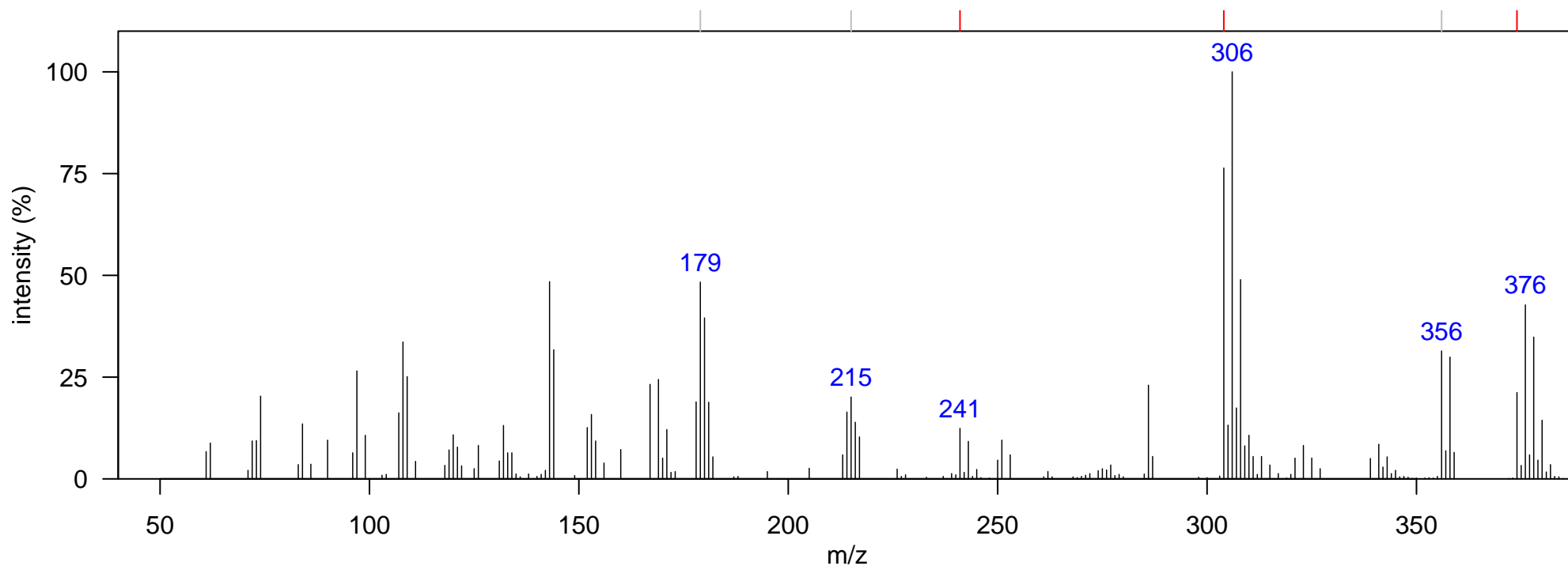
Comment:

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

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

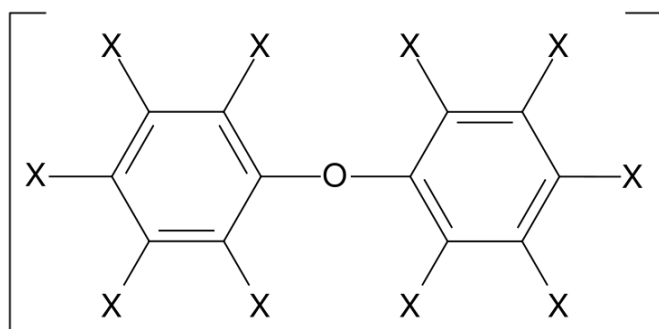
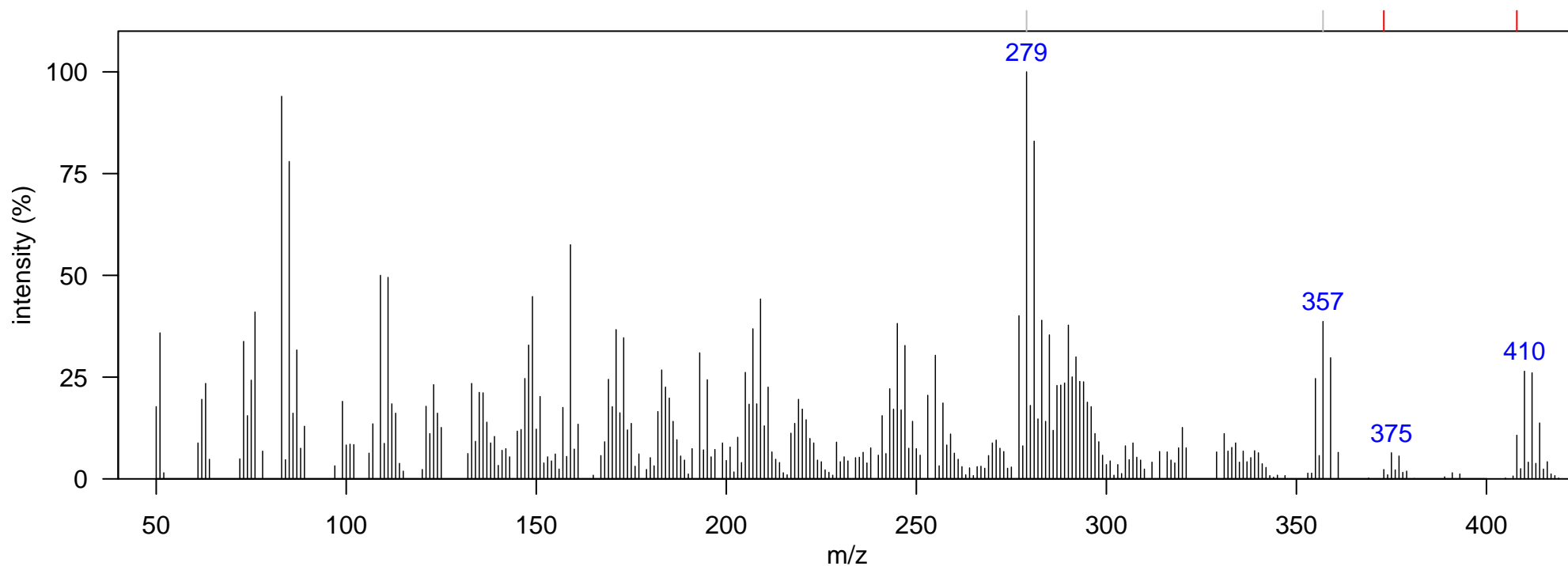
Comment: Likely PCDE, but low intensity.

Elemental Formula: C₁₂H₃Cl₇O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=7Cl, 3H

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

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

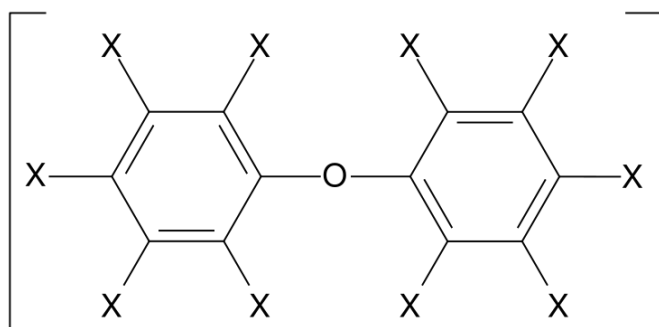
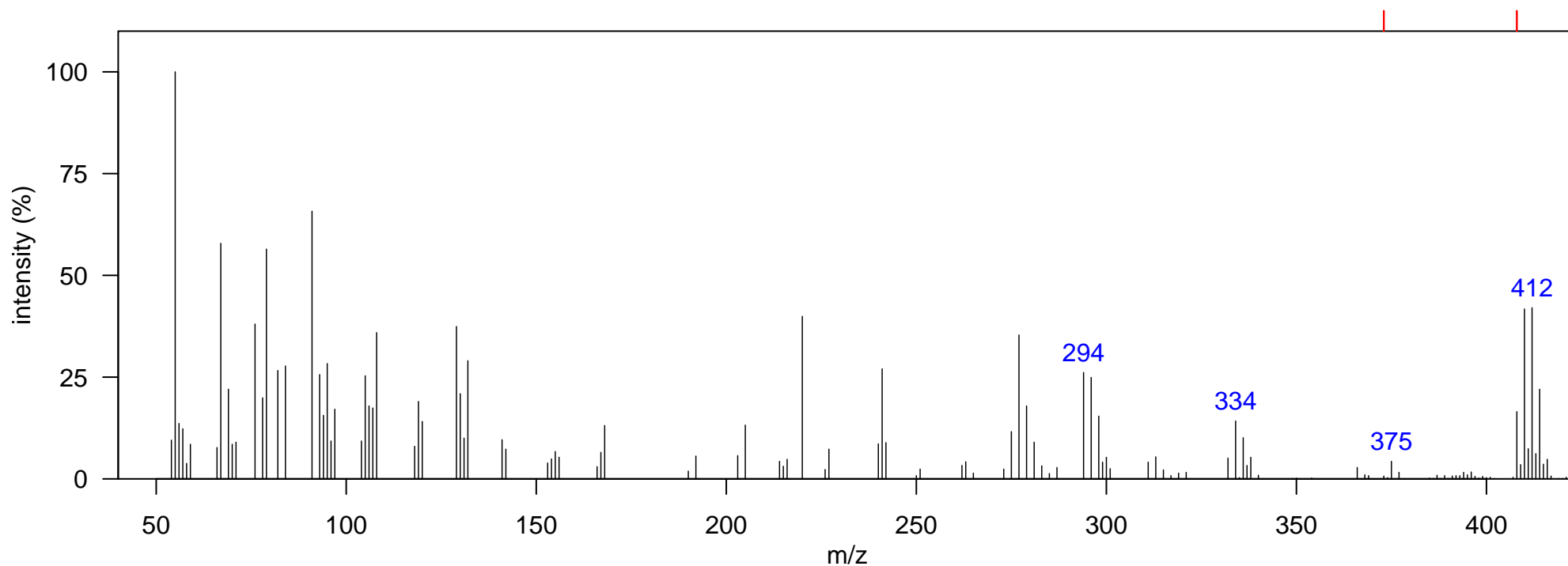
Comment: Likely PCDE, but low intensity.

Elemental Formula: C₁₂H₃Cl₇O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=7Cl, 3H

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

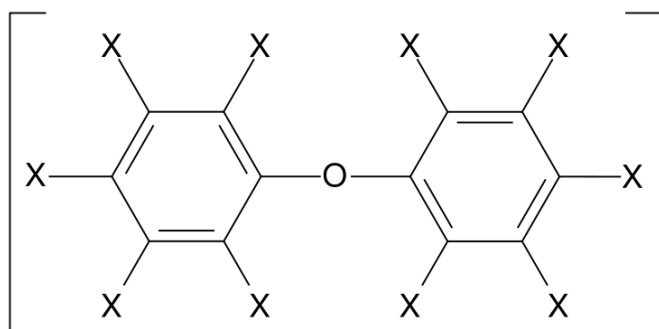
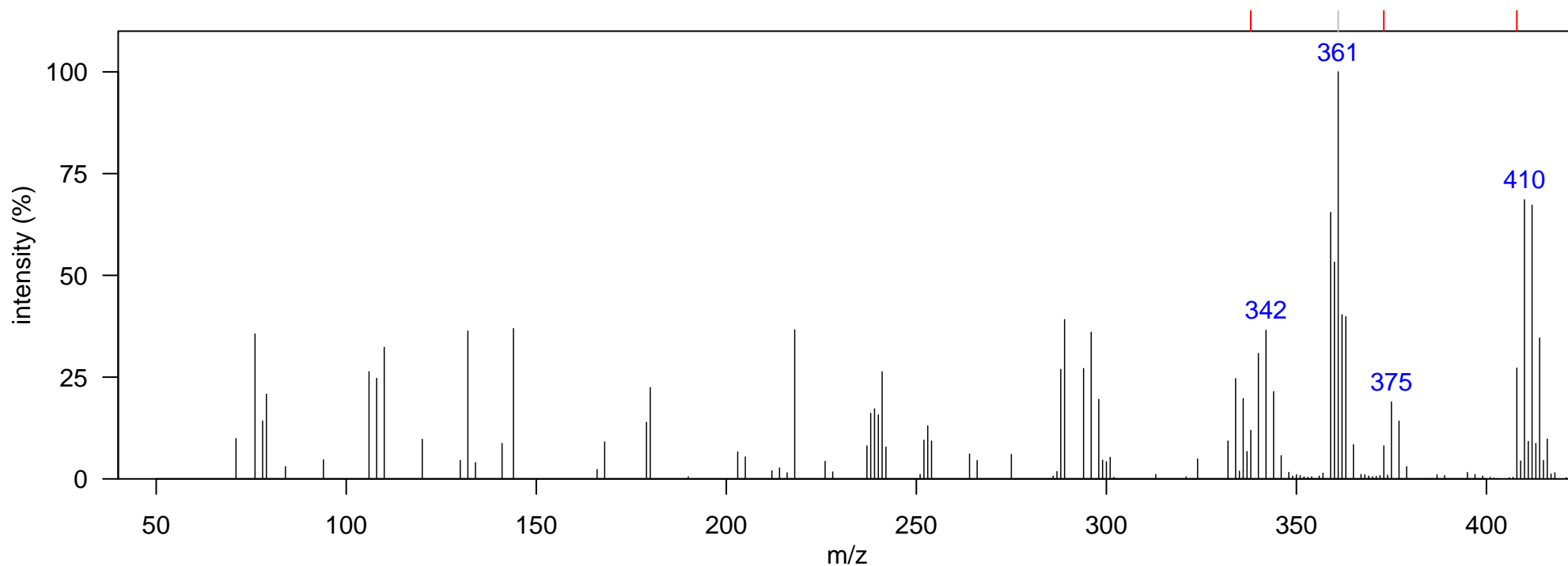
Comment: Likely PCDE, but low intensity.

Elemental Formula: C₁₂H₃Cl₇O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=7Cl, 3H

m/z	Identity
338	[M-Cl ₂] ⁺
361	interference
373	[M-Cl] ⁺
408	M ⁺

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

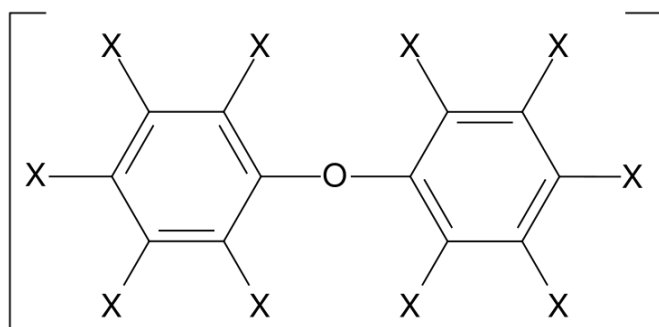
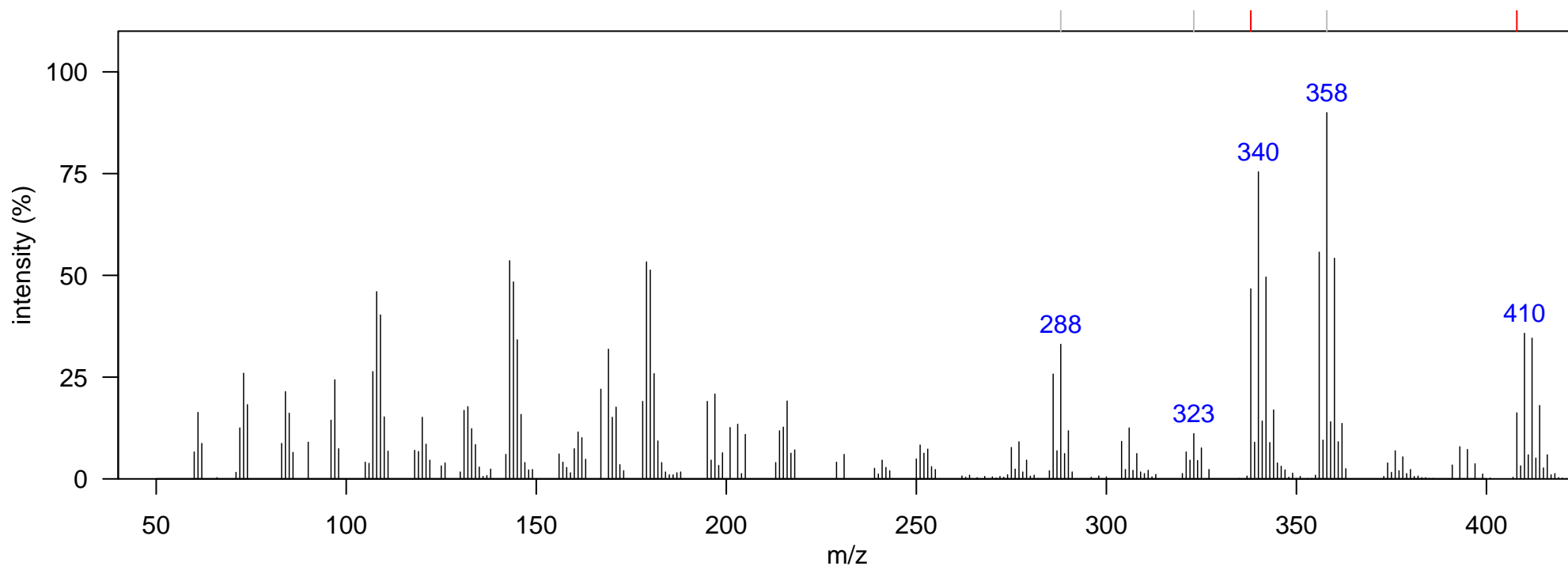
Comment:

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

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

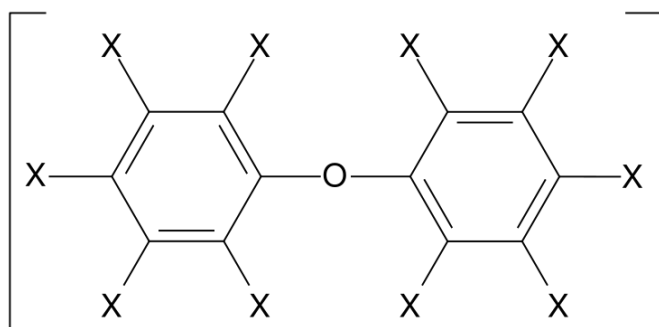
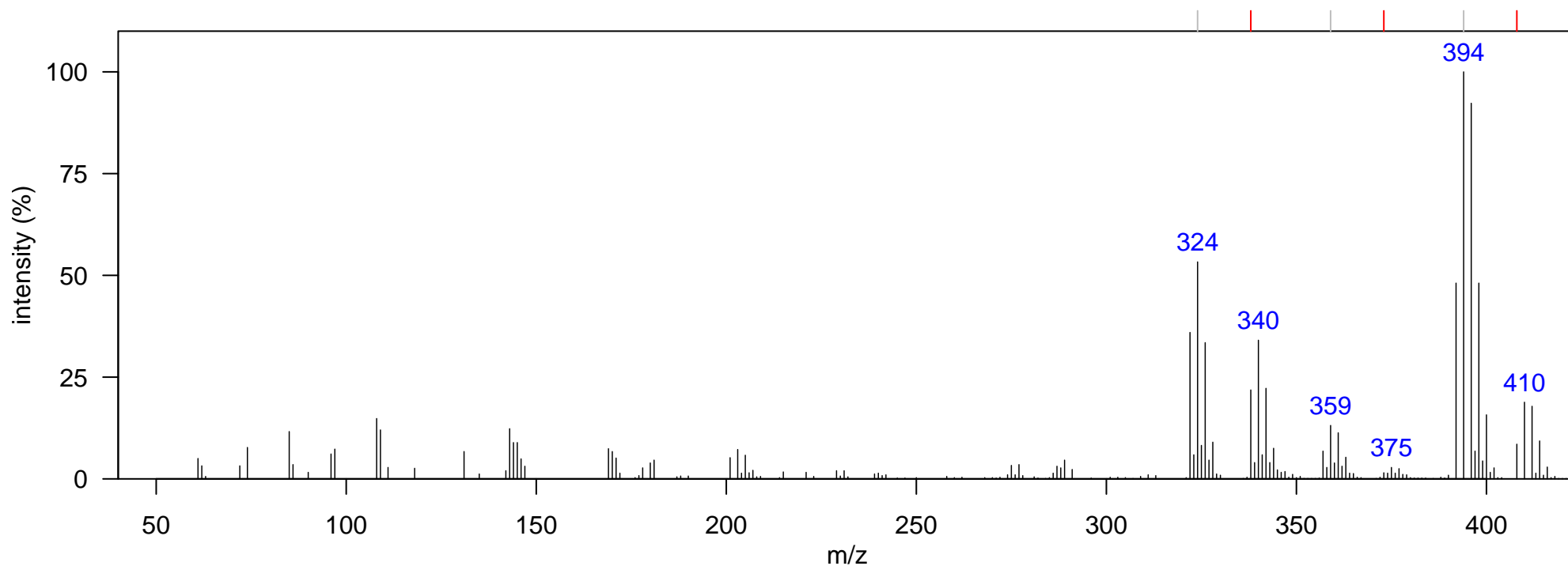
Comment:

Elemental Formula: C₁₂H₃Cl₇O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=7Cl, 3H

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

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

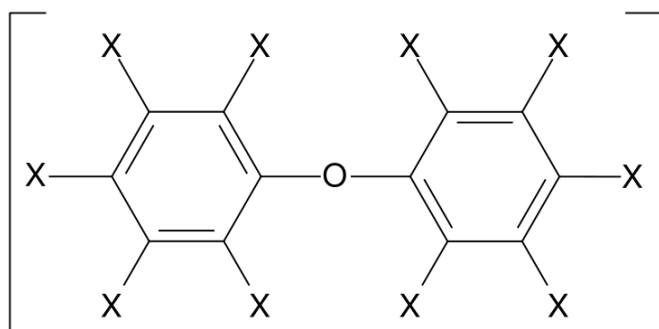
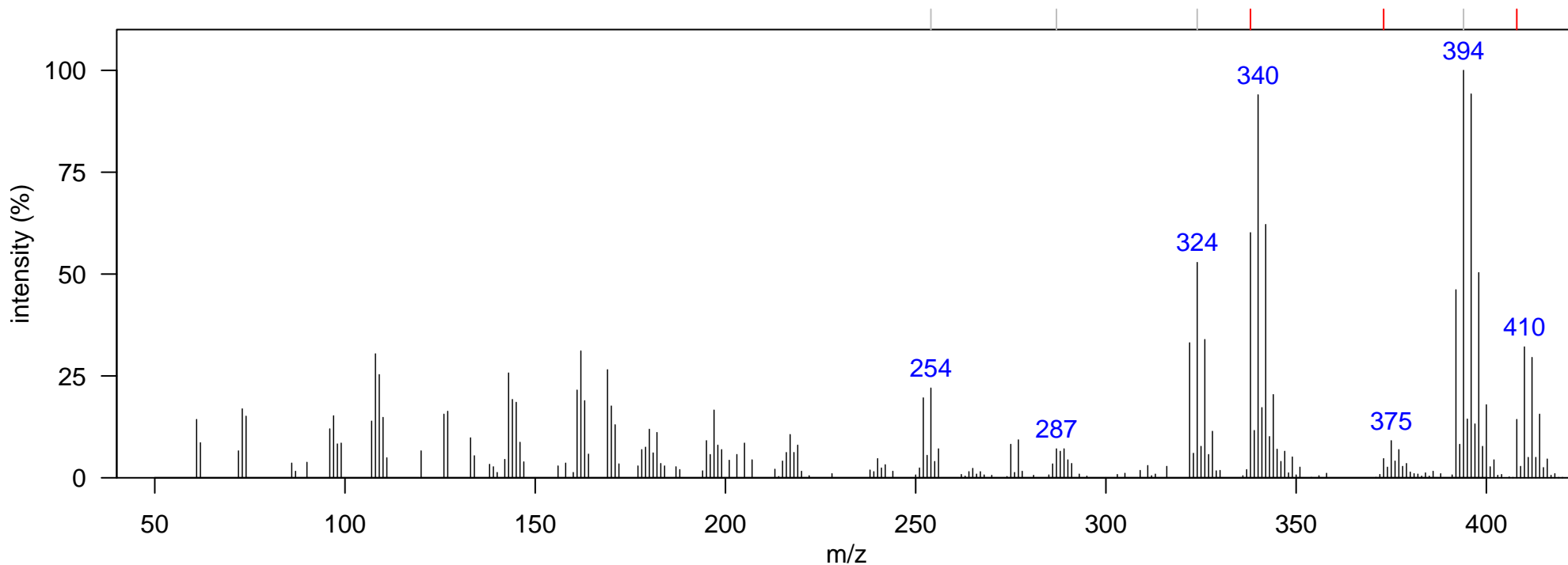
Comment:

Elemental Formula: C₁₂H₃Cl₇O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=7Cl, 3H

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

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

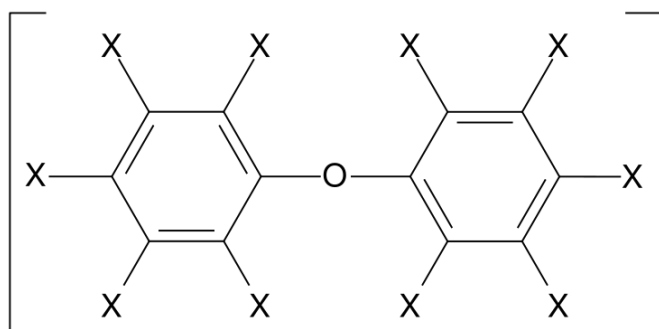
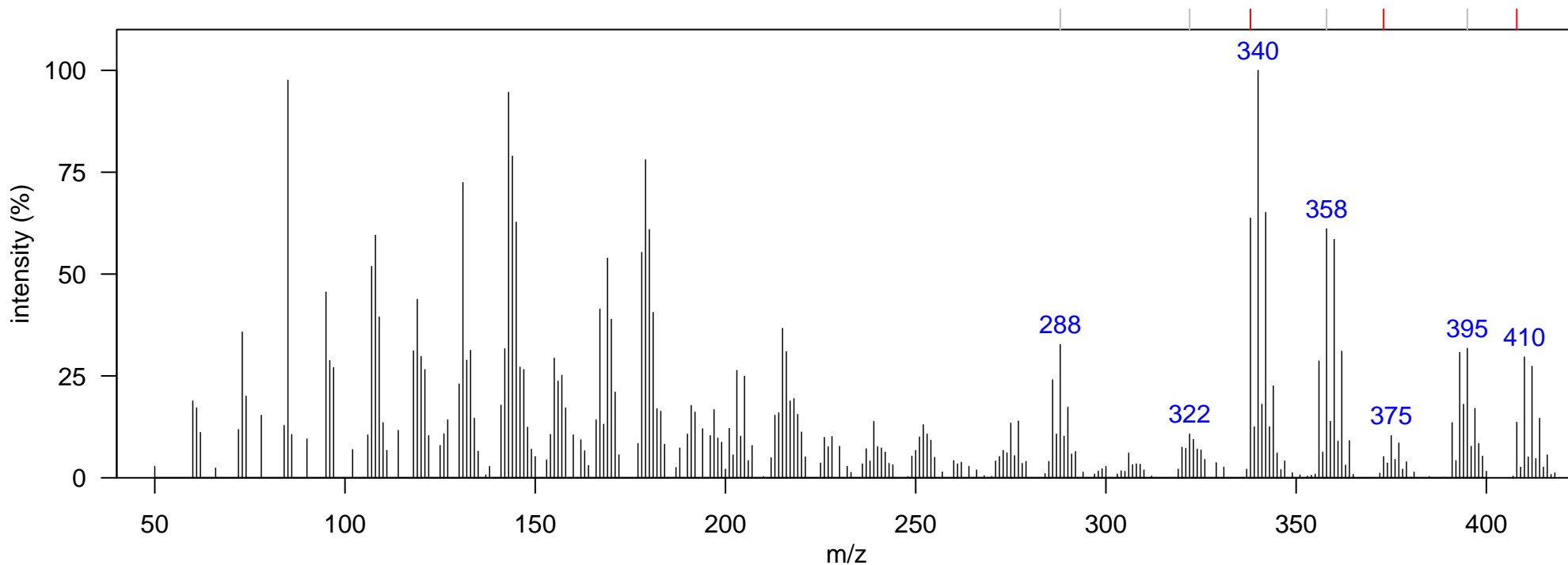
Comment:

Elemental Formula: C₁₂H₃Cl₇O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=7Cl, 3H

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

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

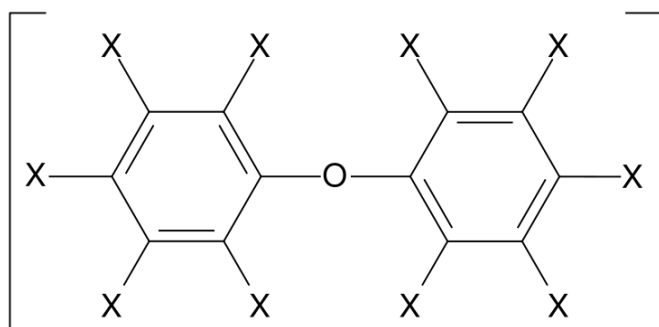
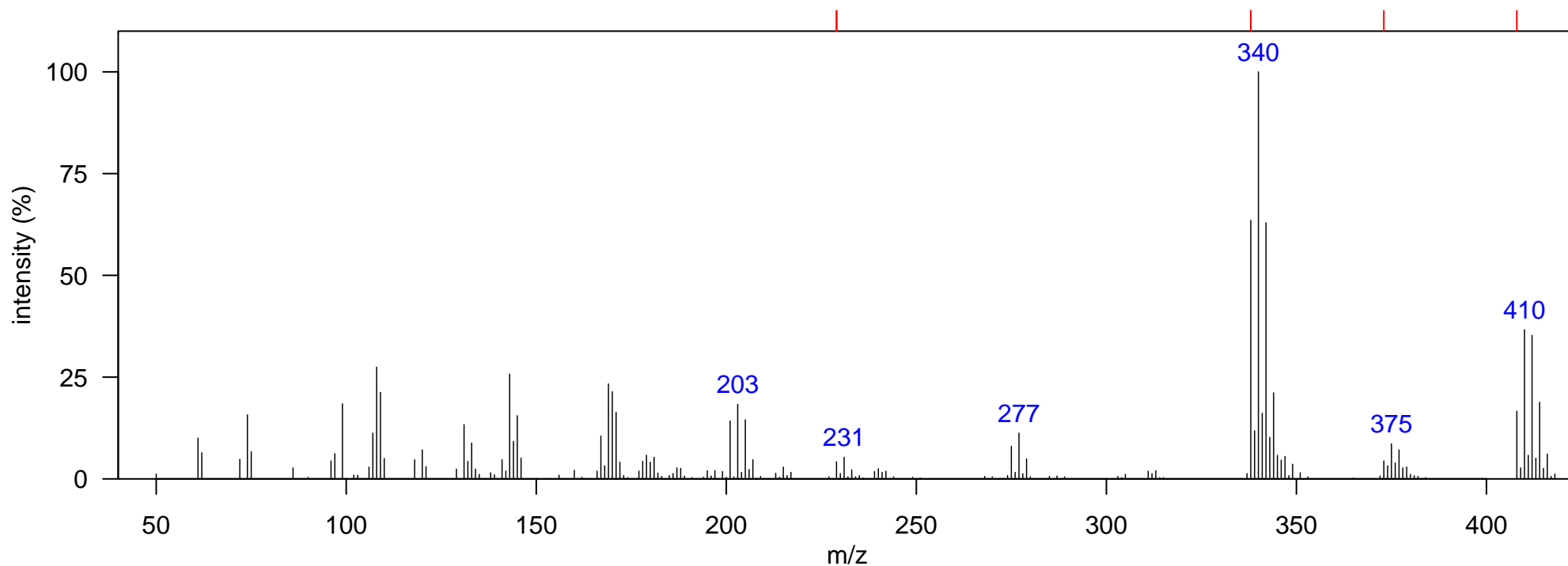
Comment:

Elemental Formula: C₁₂H₃Cl₇O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=7Cl, 3H

m/z	Identity
229	[M-3Cl-C ₆ H ₂] ⁺
338	[M-2Cl] ⁺
373	[M-Cl] ⁺
408	M ⁺

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

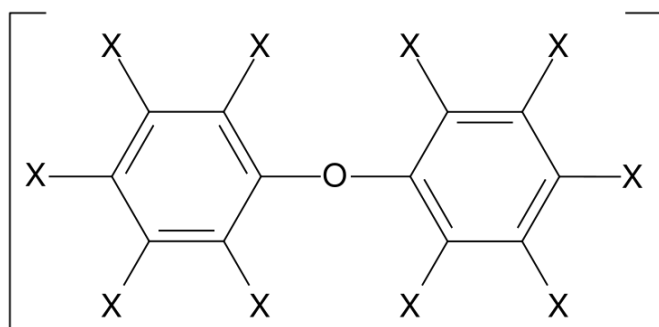
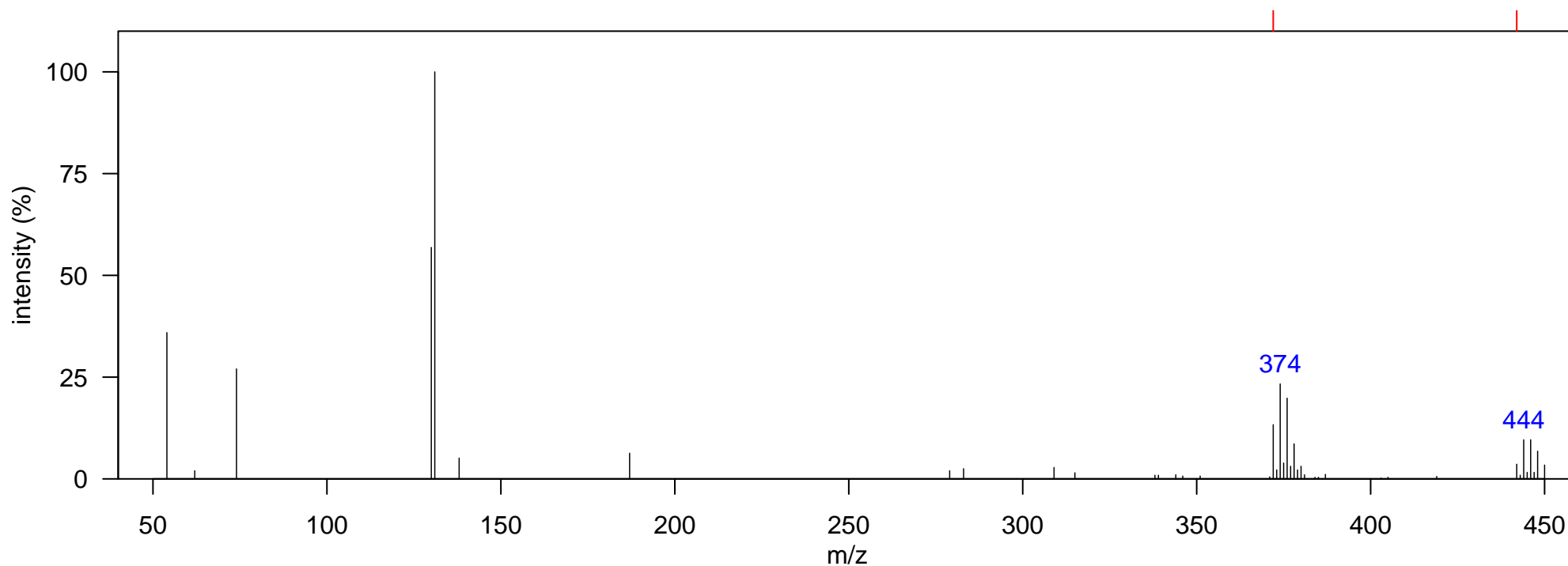
Comment:

Elemental Formula: C₁₂H₂Cl₈O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=8Cl, 2H

m/z	Identity
372	[M-2Cl] ⁺
442	M ⁺

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

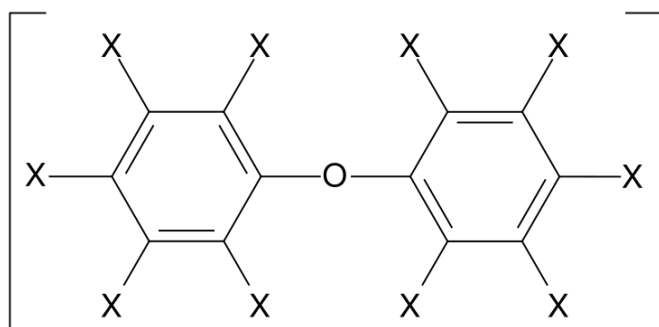
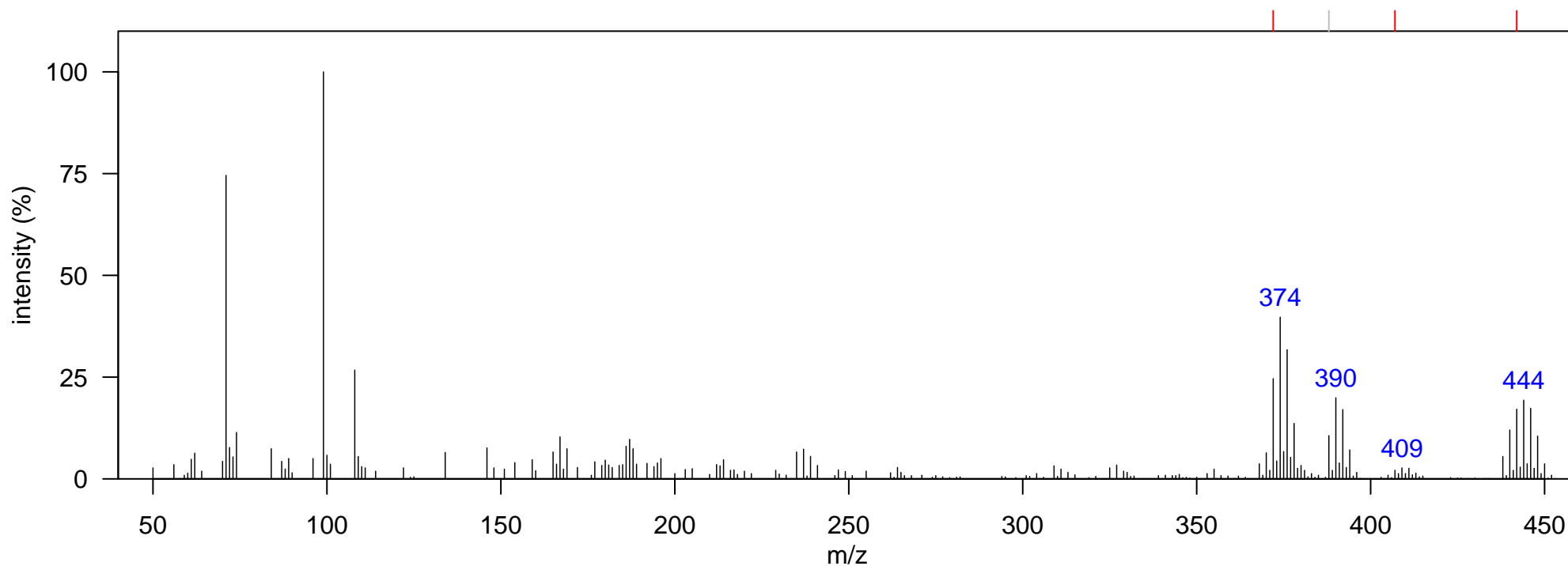
Comment:

Elemental Formula: C₁₂H₂Cl₈O

Source: anthropogenic

Class: PCDE

Identification: Manual – Congener Group



X=8Cl, 2H

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

Name: trichlorostyrene (PCS)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

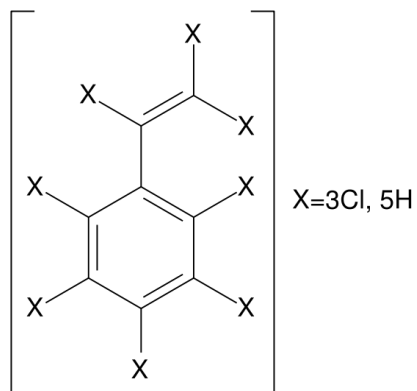
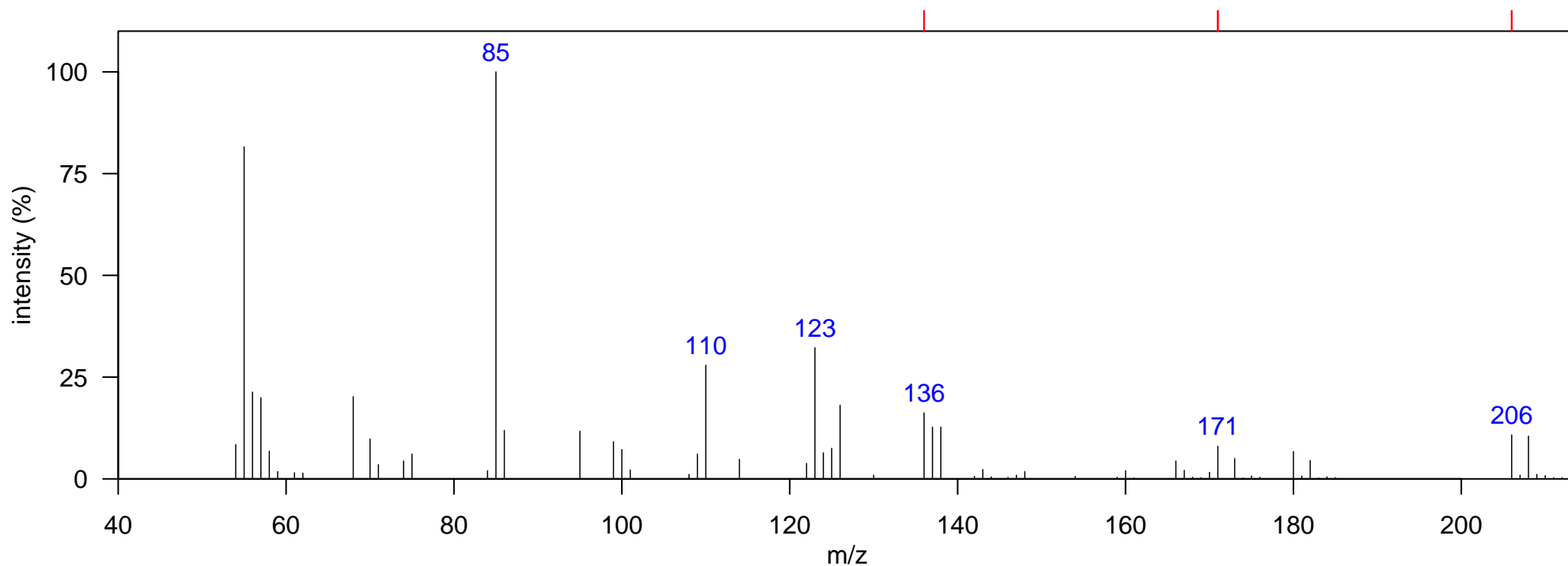
Comment:

Elemental Formula: C₈H₅Cl₃

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual – Congener Group



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

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

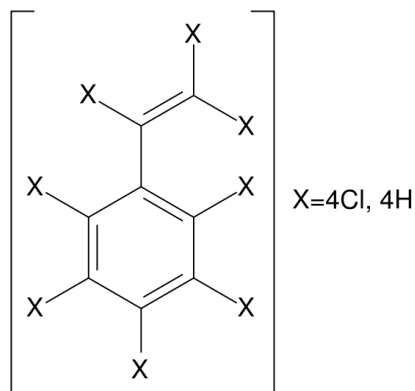
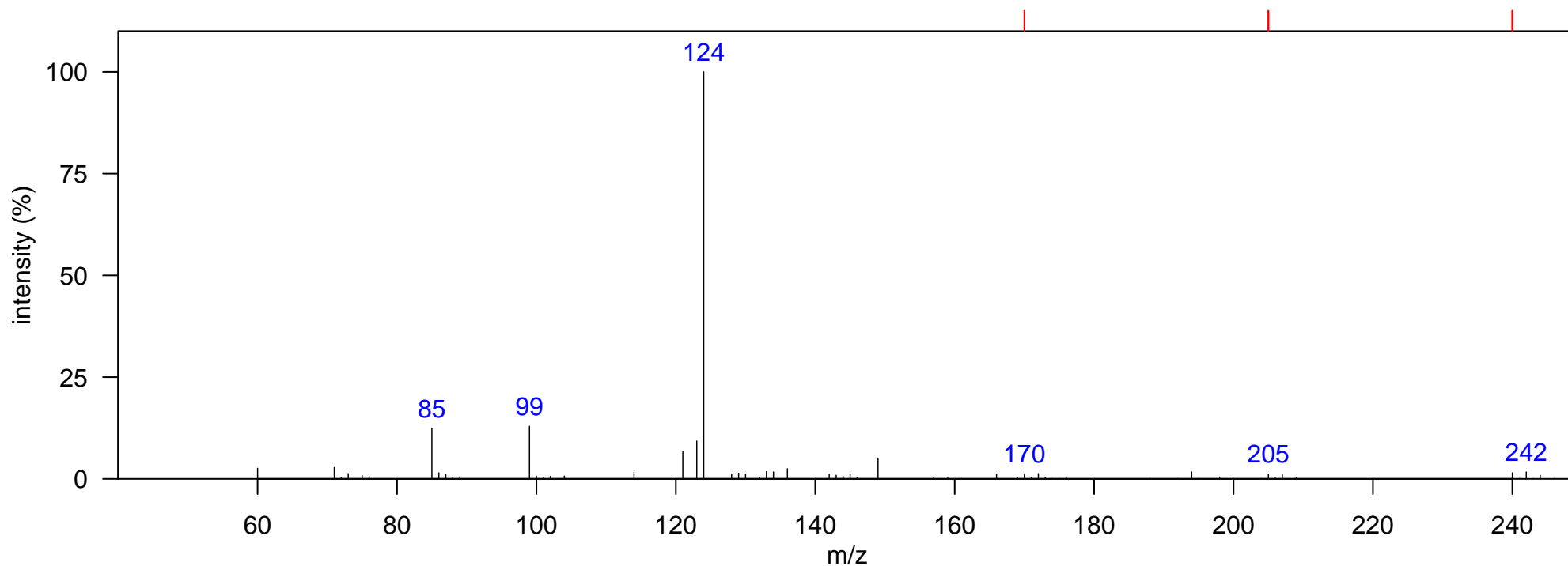
Comment:

Elemental Formula: C₈H₄Cl₄

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual – Congener Group



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

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

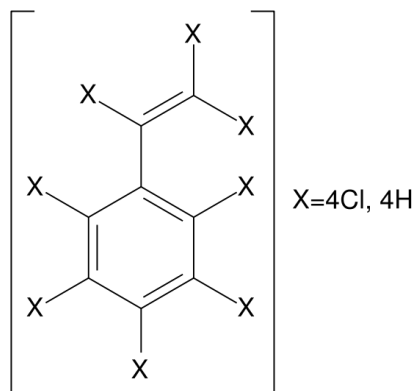
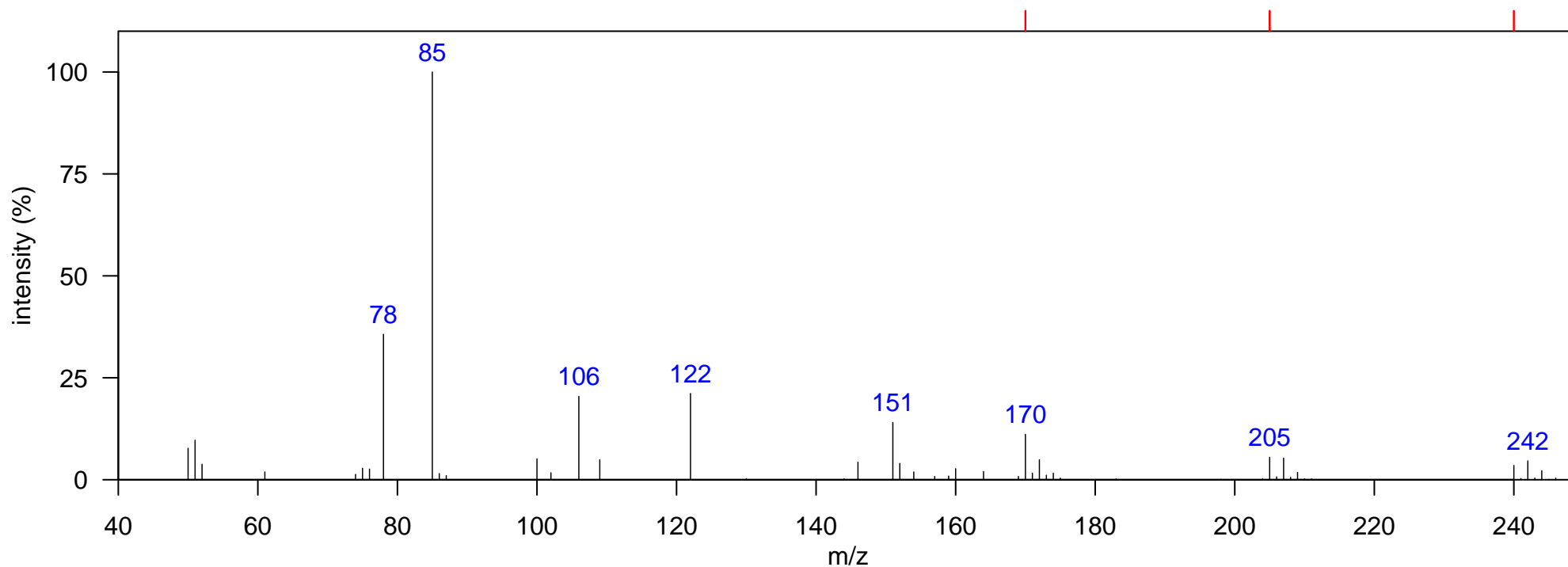
Comment:

Elemental Formula: C₈H₄Cl₄

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual – Congener Group



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

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

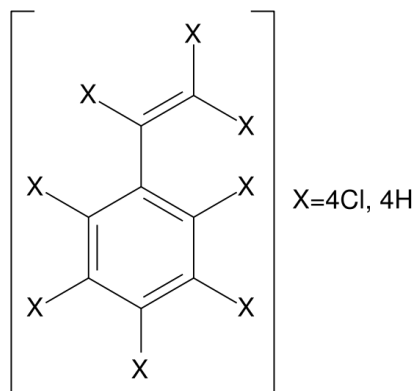
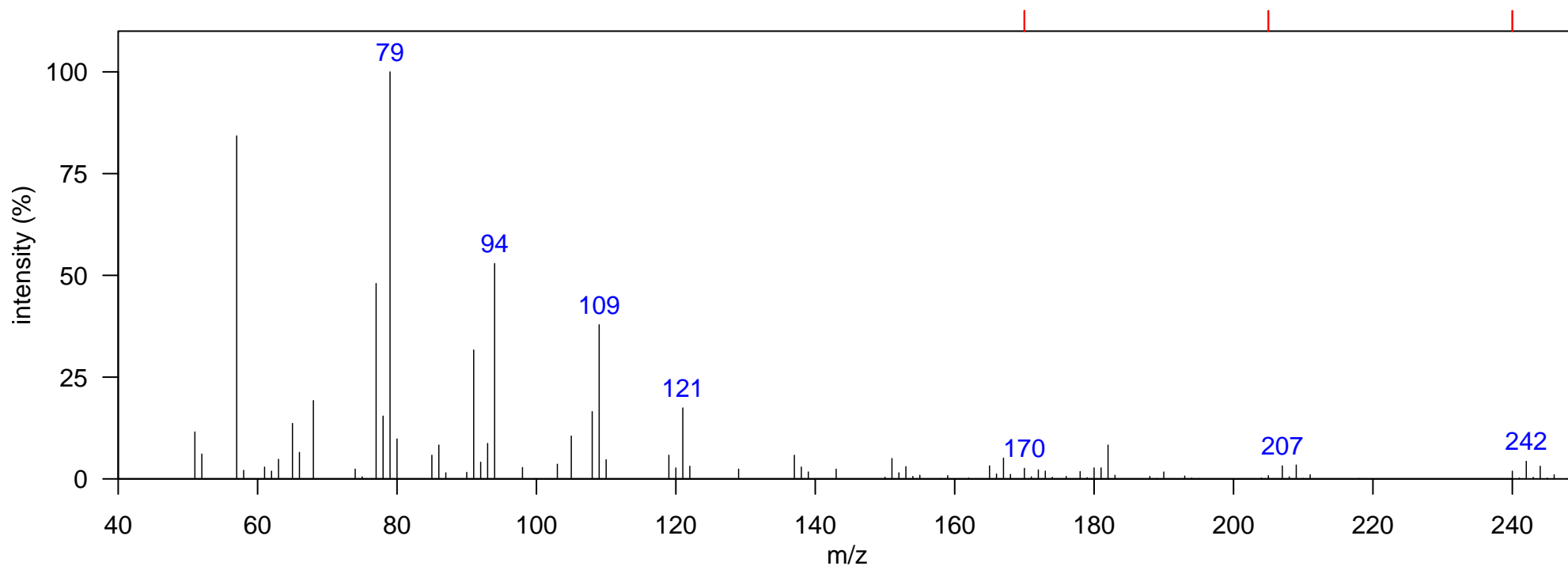
Comment:

Elemental Formula: C₈H₄Cl₄

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual – Congener Group



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

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

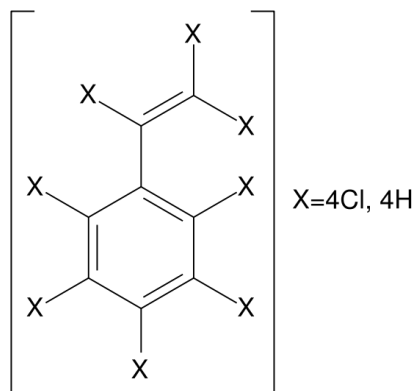
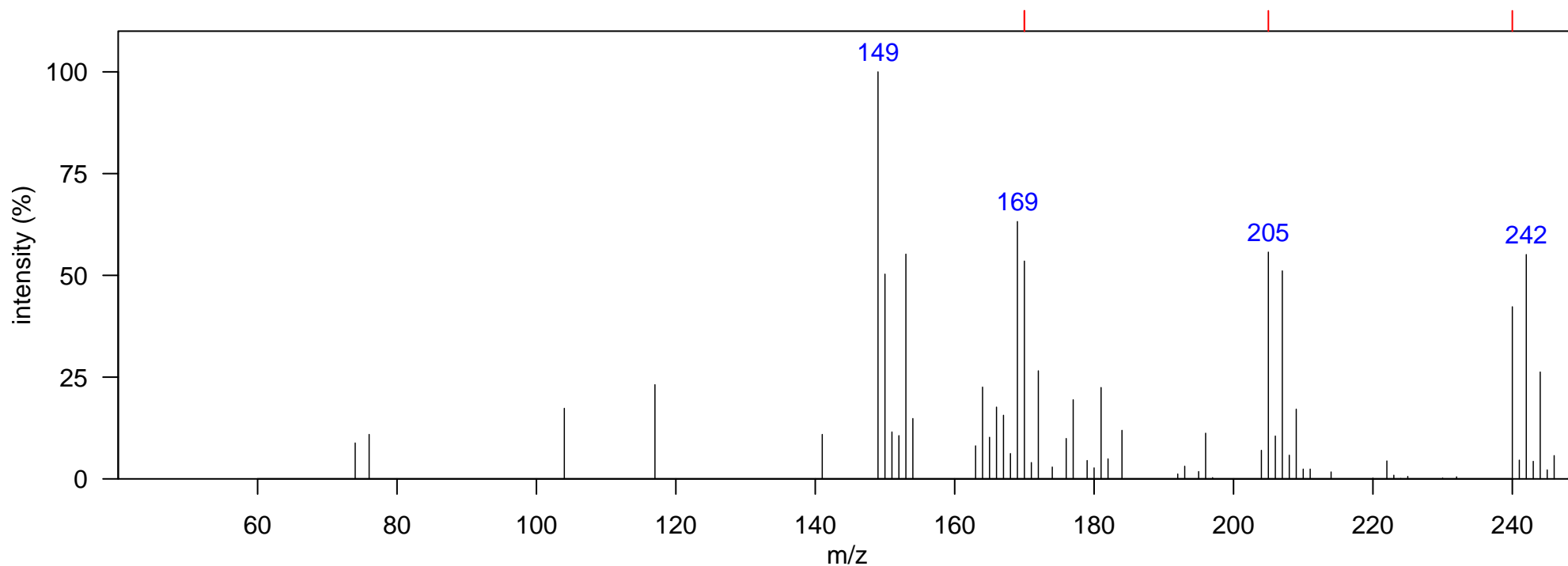
Comment:

Elemental Formula: C₈H₄Cl₄

Source: anthropogenic

Class: chlorinated styrene

Identification: Manual – Congener Group



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

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

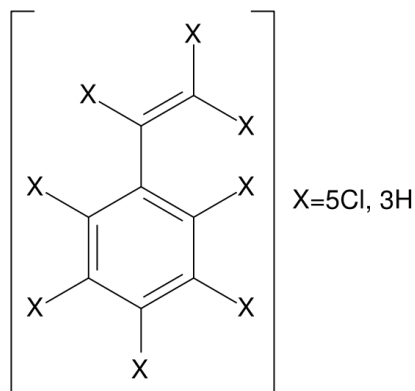
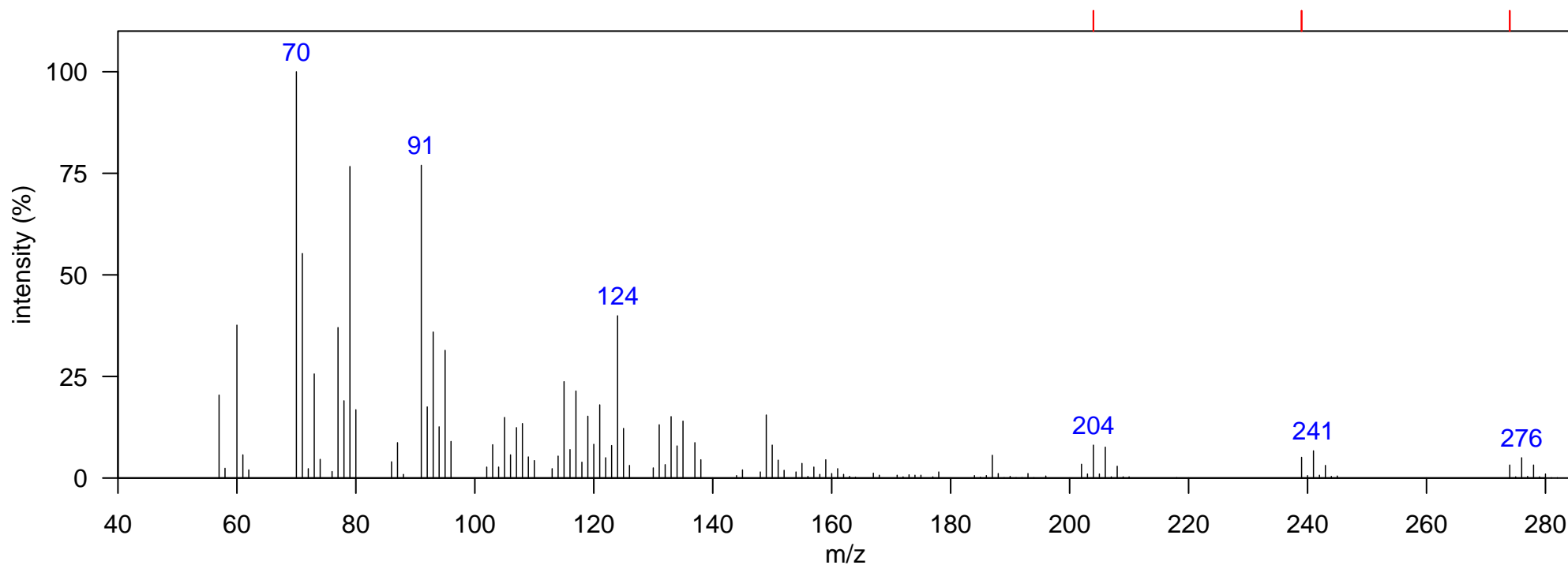
Comment:

Elemental Formula: C₈H₃Cl₅

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



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

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

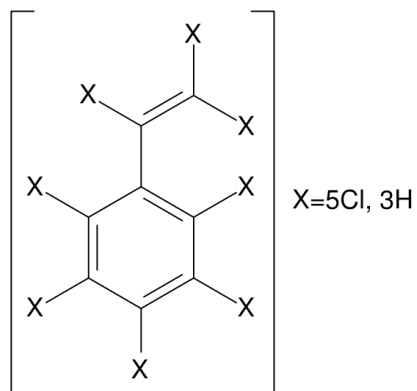
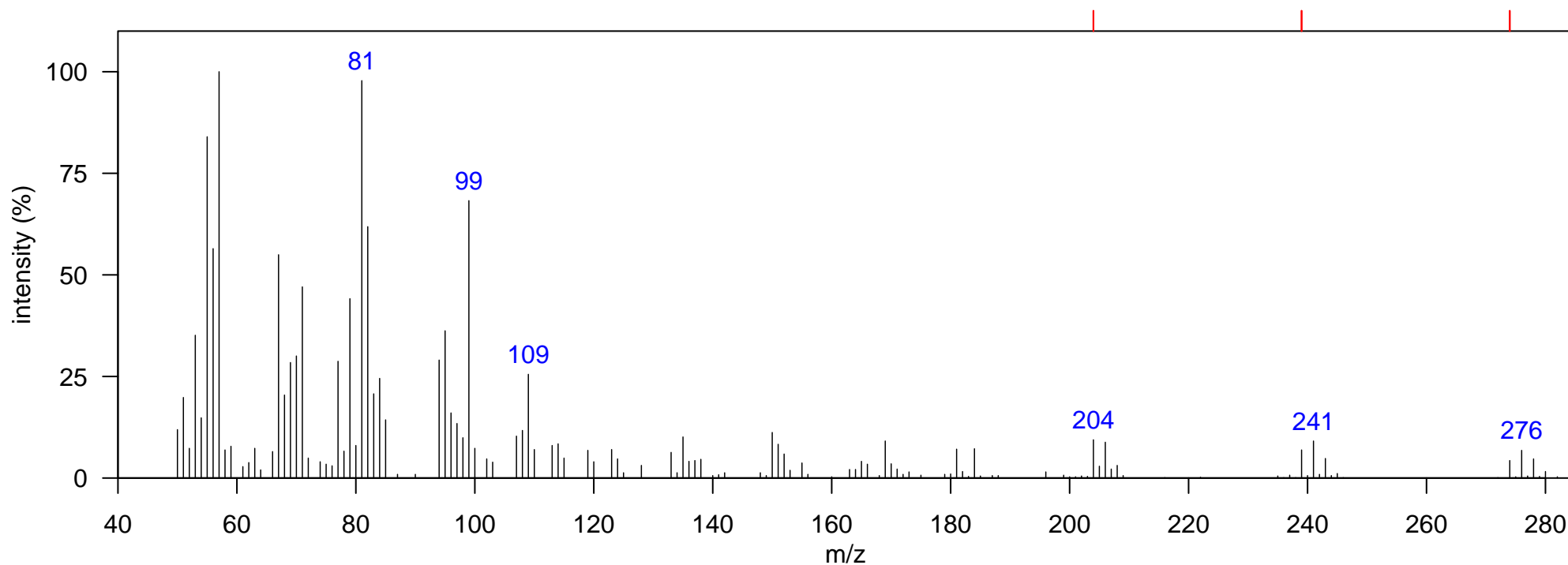
Comment:

Elemental Formula: C₈H₃Cl₅

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



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

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

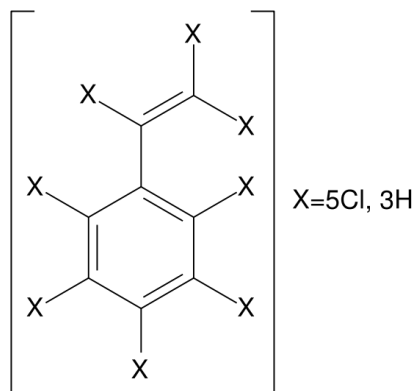
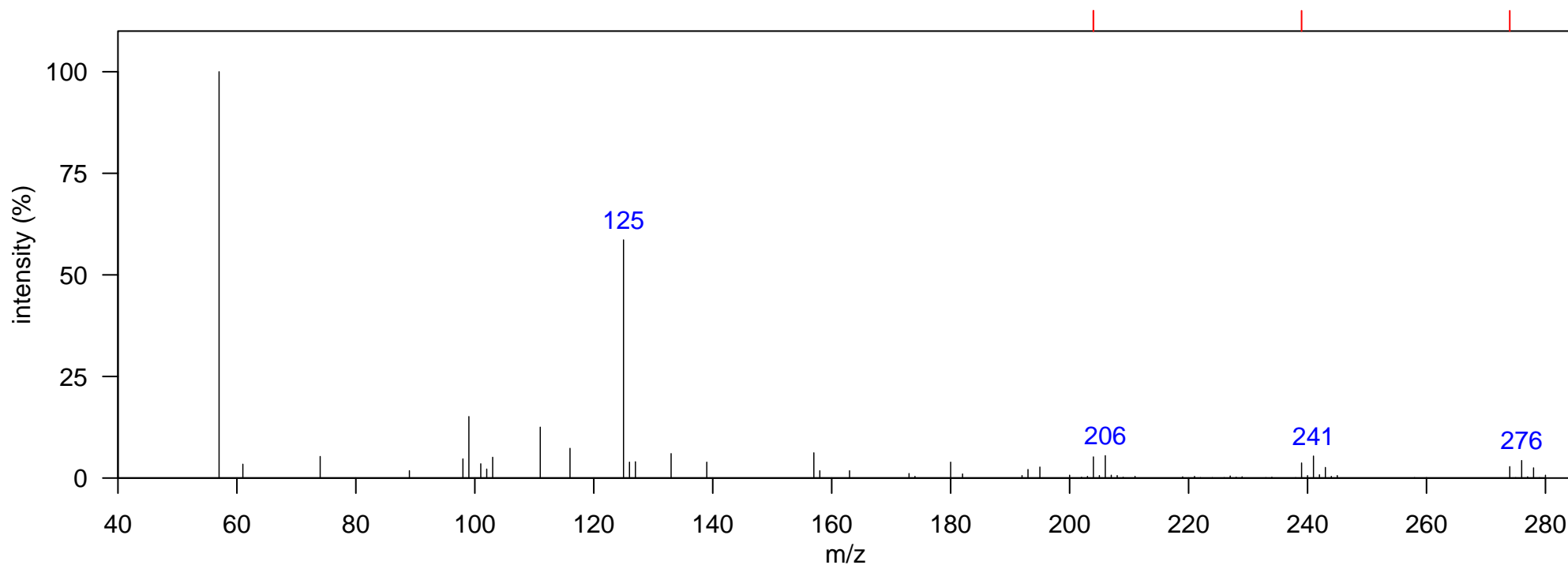
Comment:

Elemental Formula: C₈H₃Cl₅

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



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

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

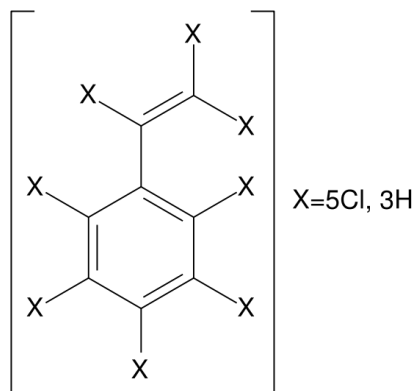
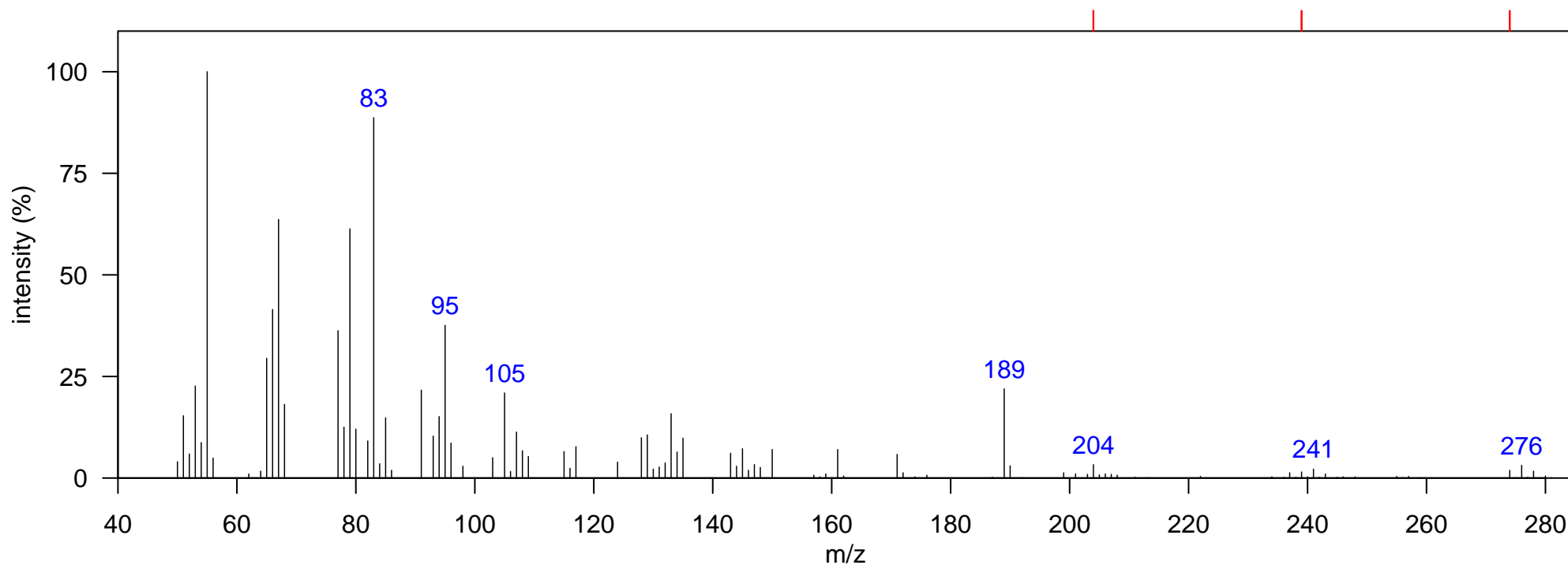
Comment:

Elemental Formula: C₈H₃Cl₅

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



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

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

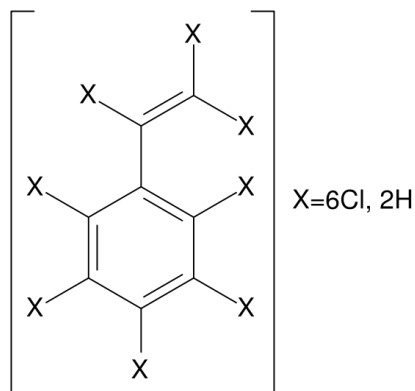
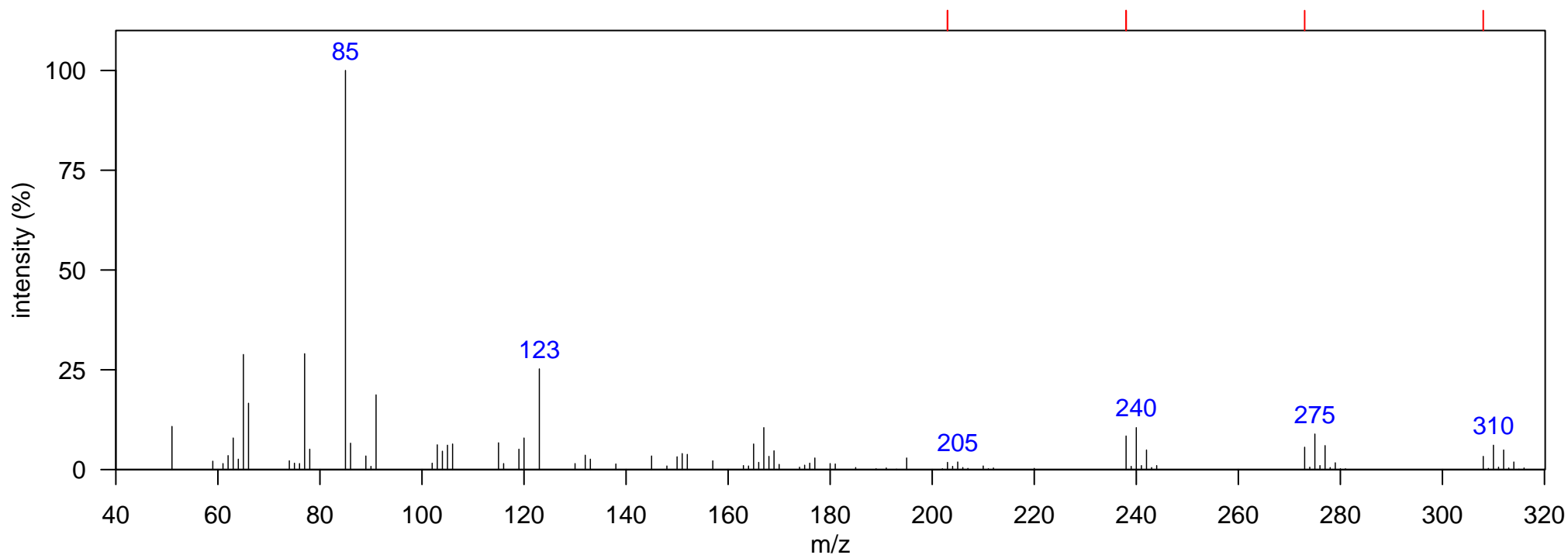
Comment:

Elemental Formula: C₈H₂Cl₆

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



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

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

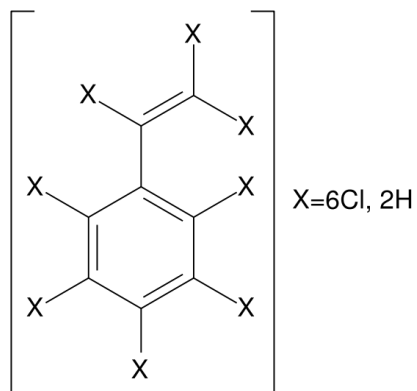
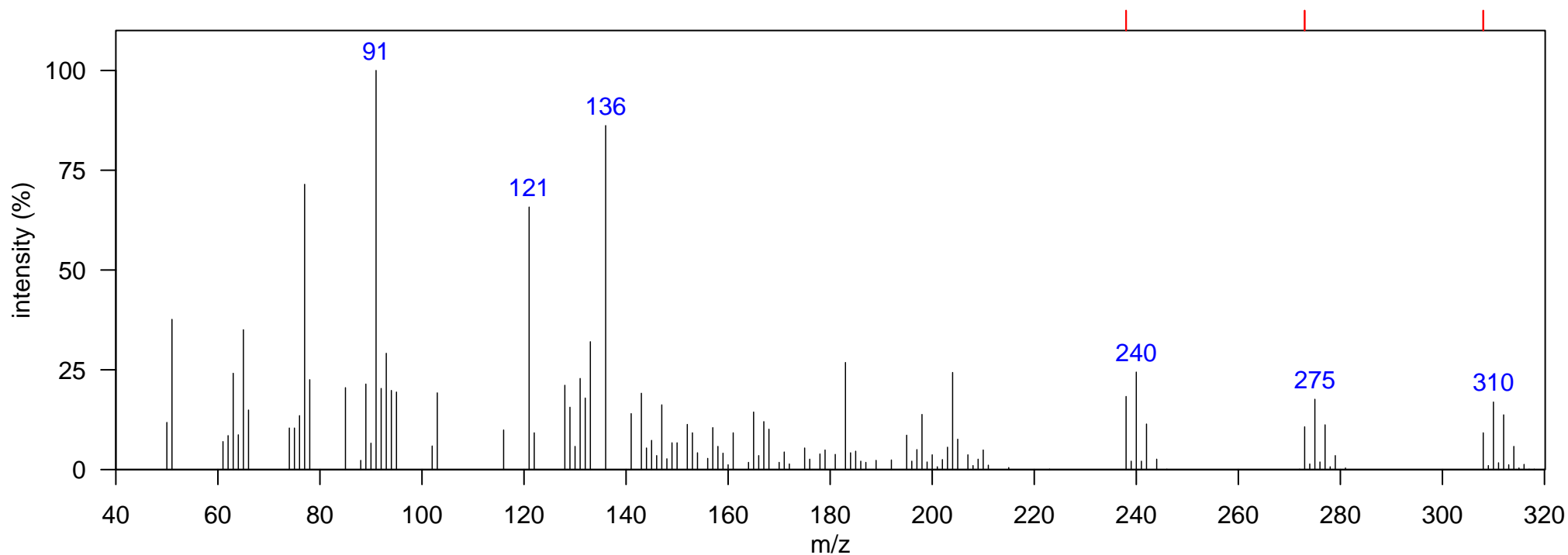
Comment:

Elemental Formula: C₈H₂Cl₆

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



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

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

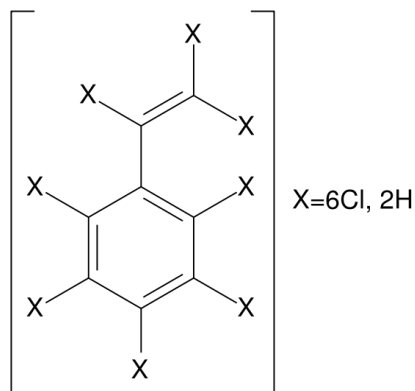
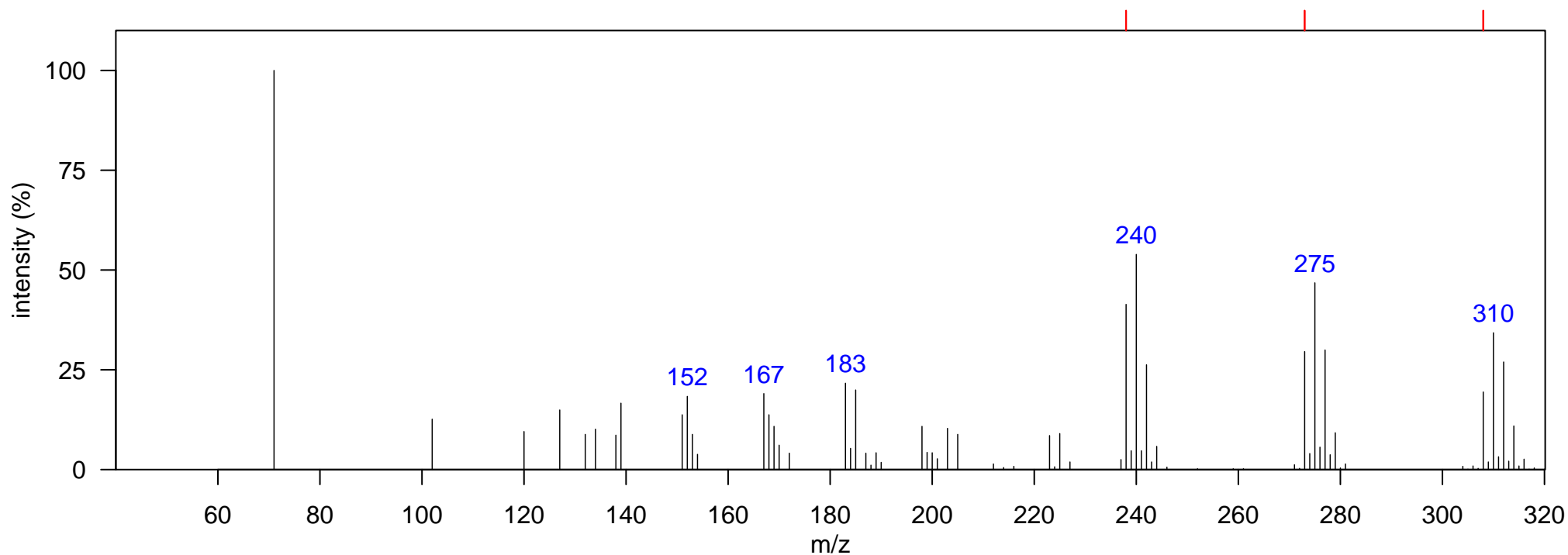
Comment:

Elemental Formula: C₈H₂Cl₆

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



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

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

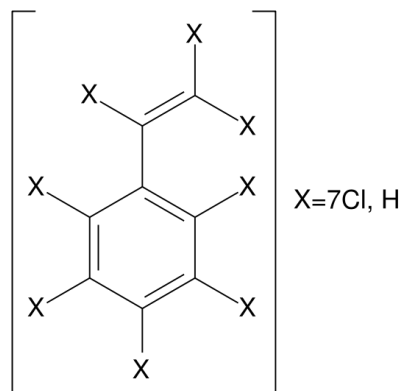
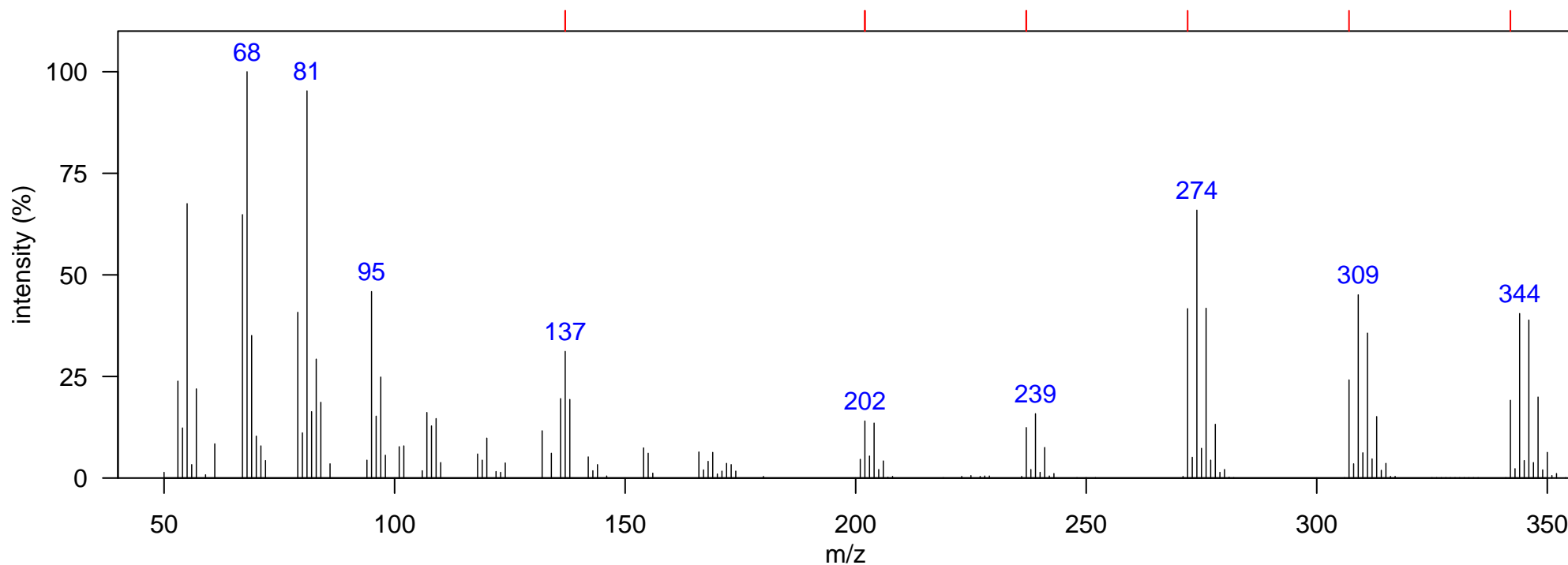
Comment:

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 ⁺

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

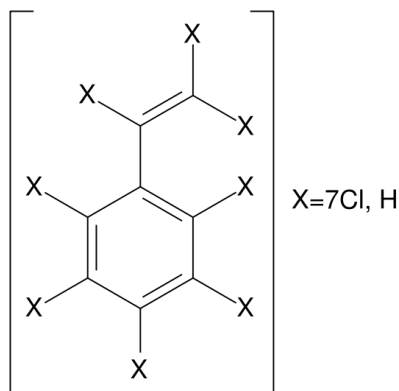
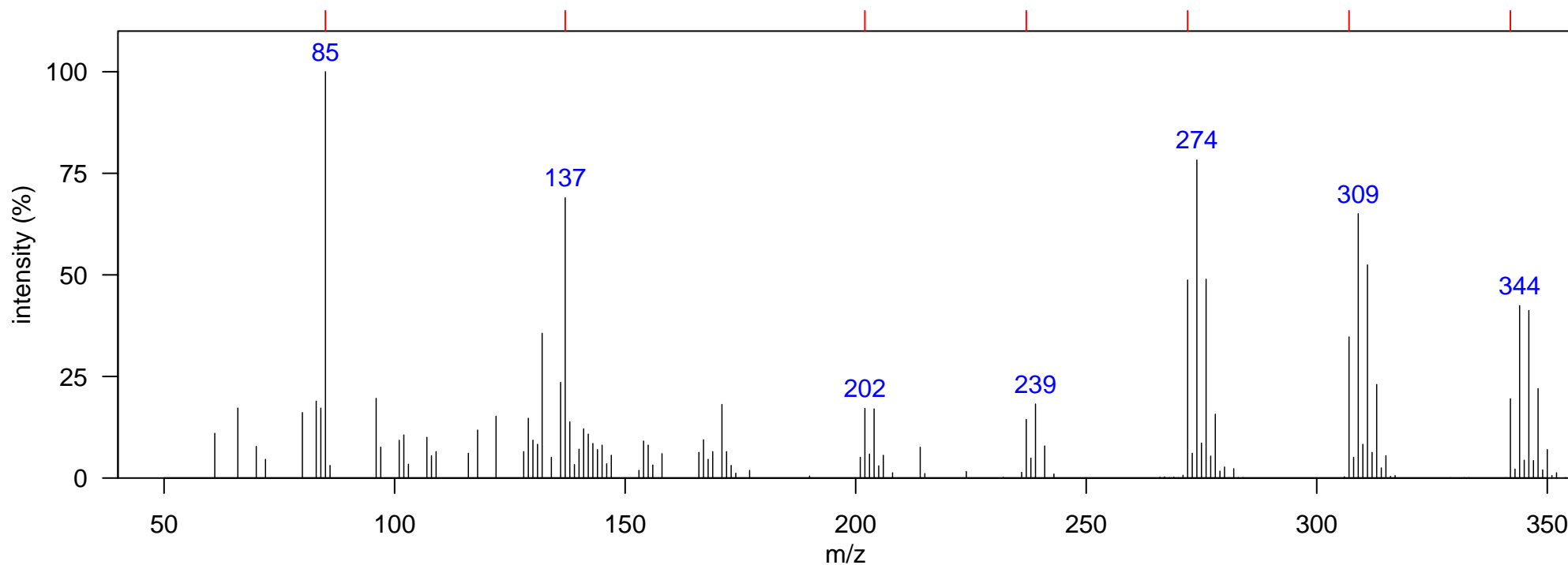
Comment:

Elemental Formula: C₈HCl₇

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



m/z	Identity
85	[C ₇ H] ⁺
137	[M-2Cl] ₂ ⁺
202	[M-4Cl] ⁺
237	[M-3Cl] ⁺
272	[M-2Cl] ⁺
307	[M-Cl] ⁺
342	M ⁺

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

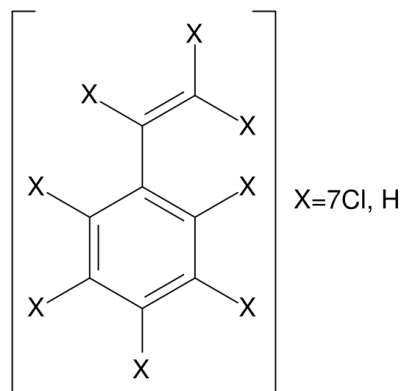
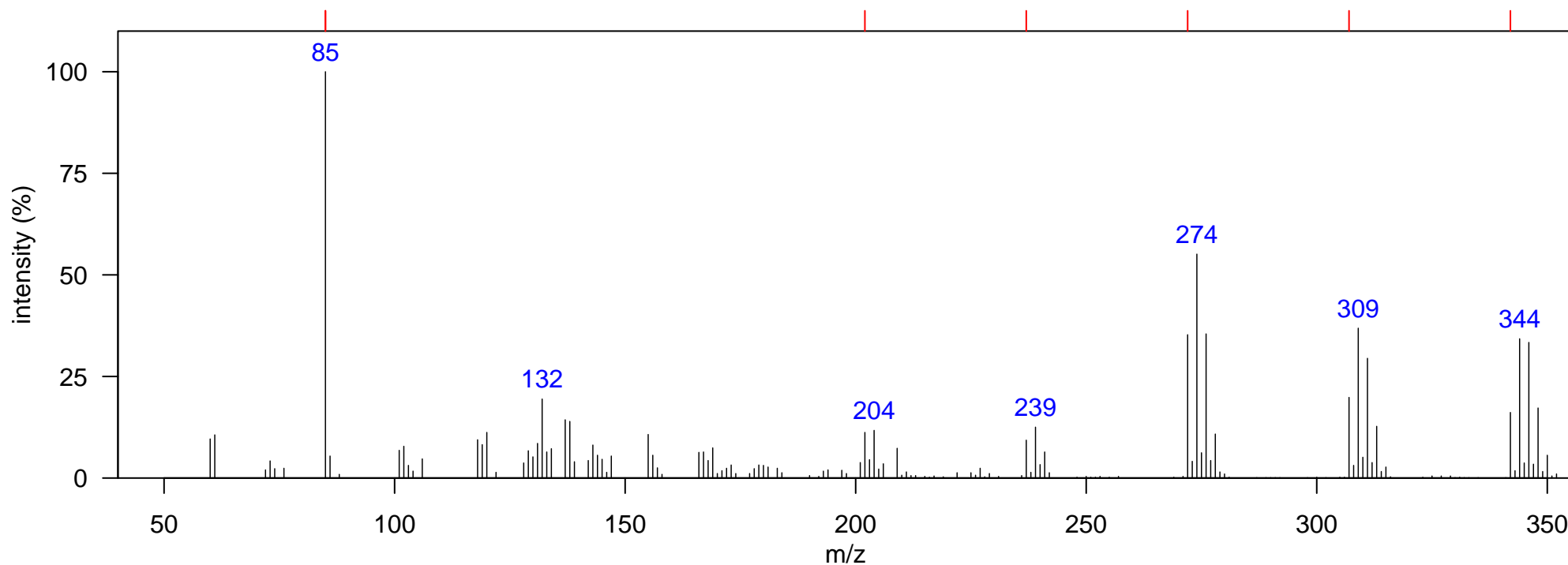
Comment:

Elemental Formula: C₈HCl₇

Source: anthropogenic

Class: chlorinated styrene

Identification: Literature MS



m/z	Identity
85	[C ₇ H] ⁺
202	[M-4Cl] ⁺
237	[M-3Cl] ⁺
272	[M-2Cl] ⁺
307	[M-Cl] ⁺
342	M ⁺

Name: octachlorostyrene (PCS)

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

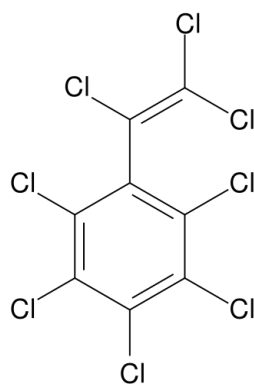
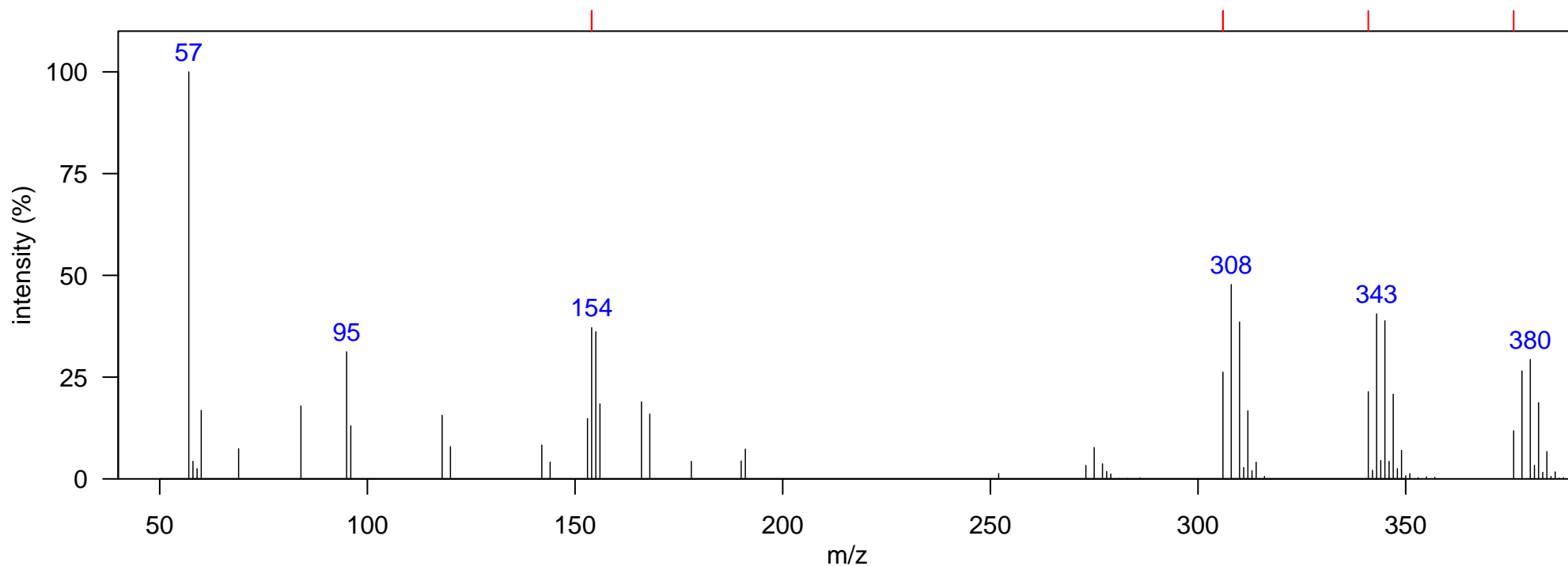
Comment:

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 ⁺

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

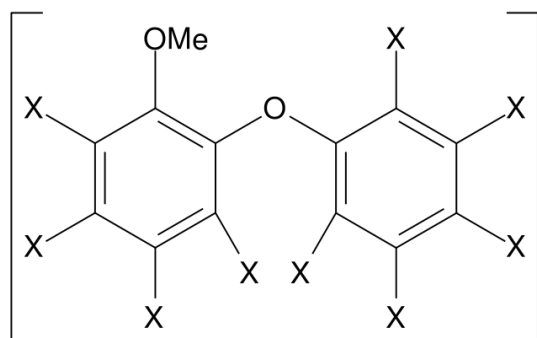
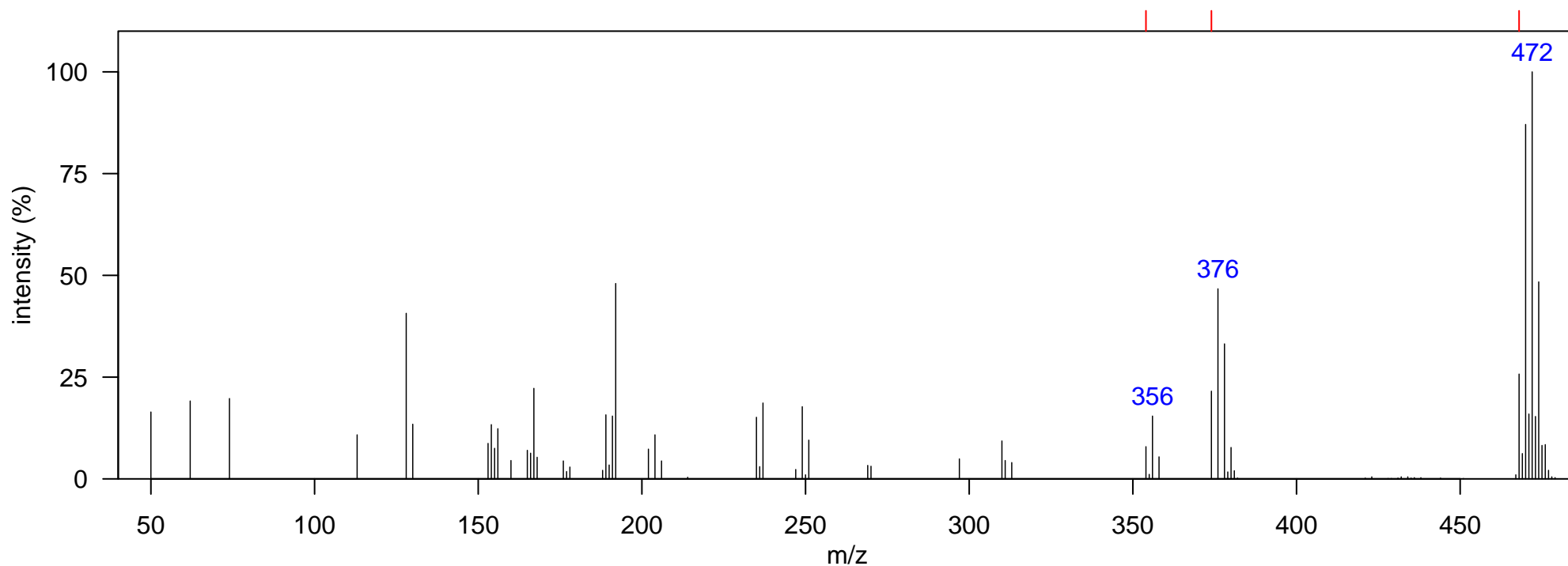
Comment:

Elemental Formula: C₁₃H₈Br₃ClO₂

Source: natural

Class: MeO–B/CDE

Identification: Manual – Congener Group



X=3Br, Cl, 5H

m/z	Identity
354	[M–Br–Cl] ⁺
374	[M–Br–CH ₃] ⁺
468	M ⁺

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

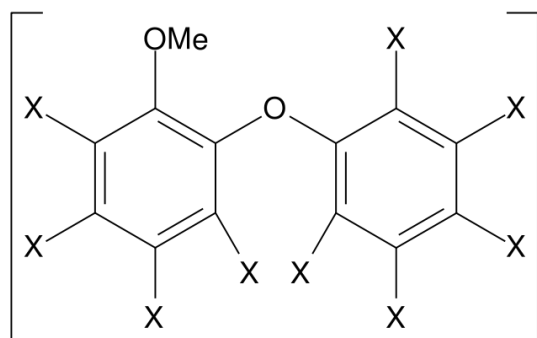
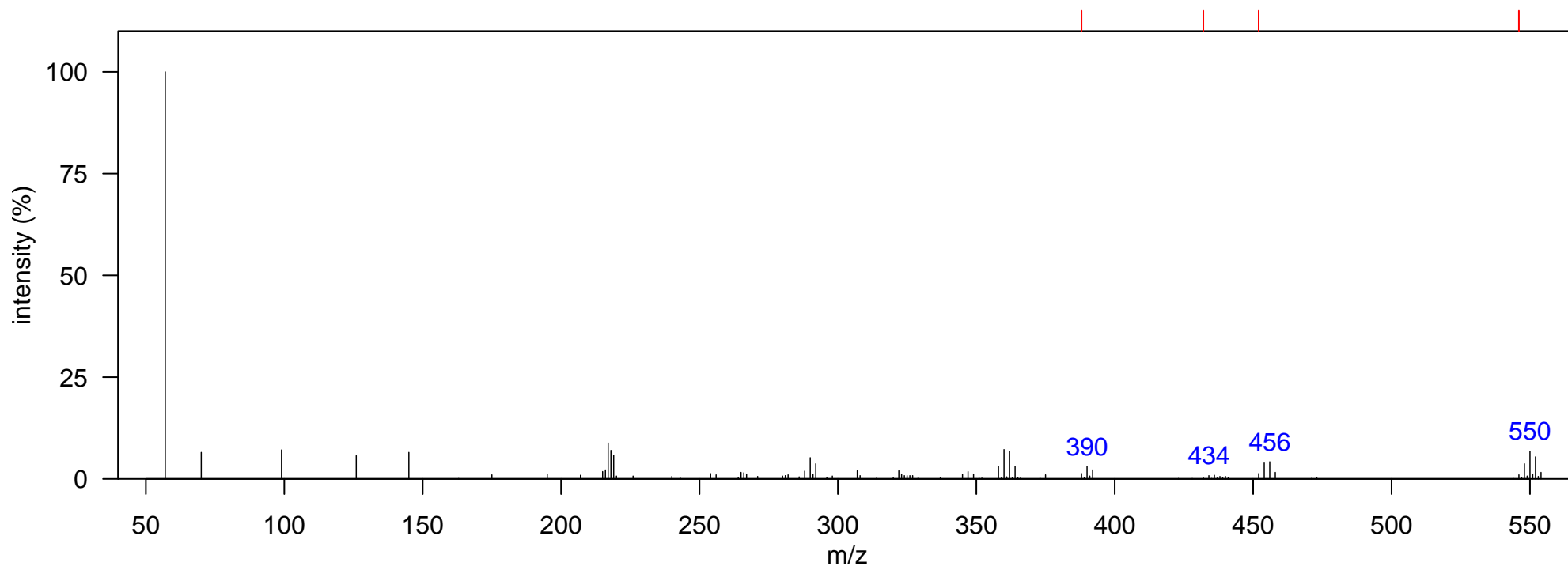
Comment: Ref: J.Mass.Spectrum, 2006, 41, 790–801.

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–CH ₃] ⁺
546	M ⁺

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

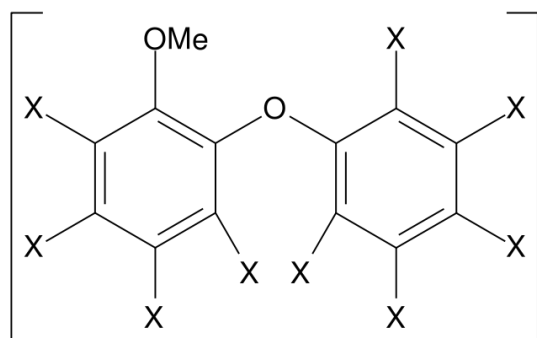
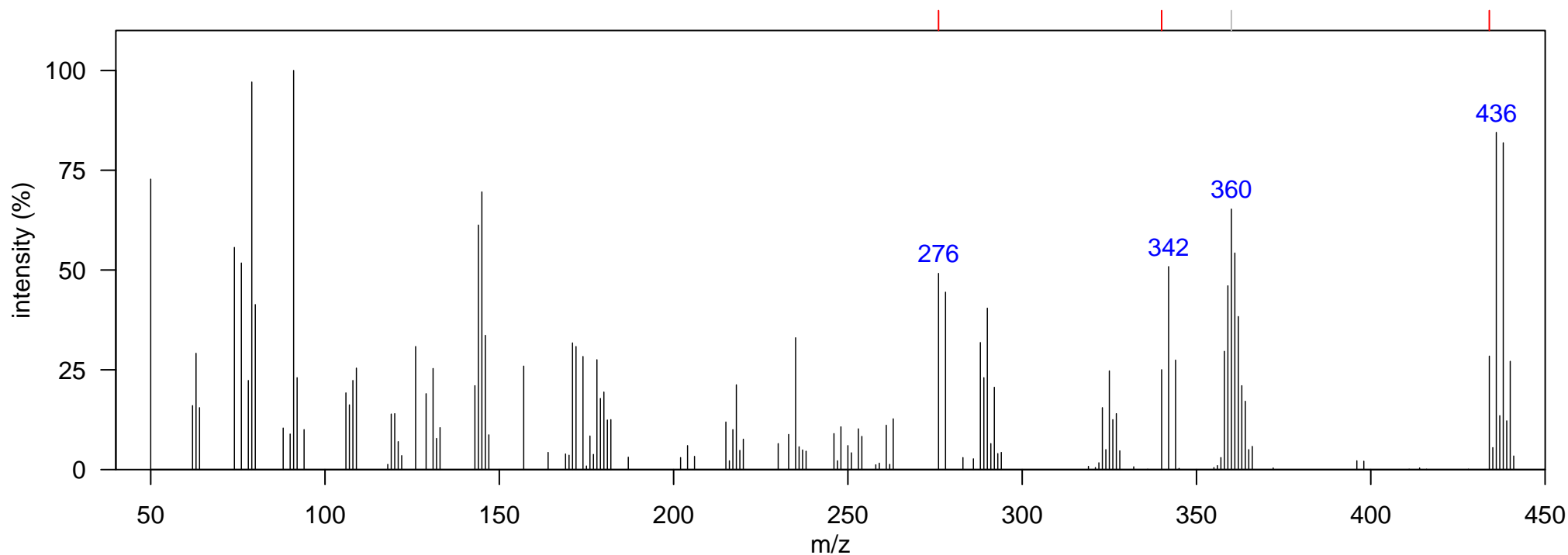
Comment:

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-CH ₃] ⁺
360	interference
434	M ⁺

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

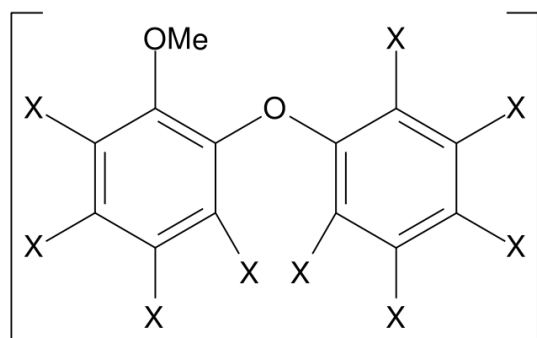
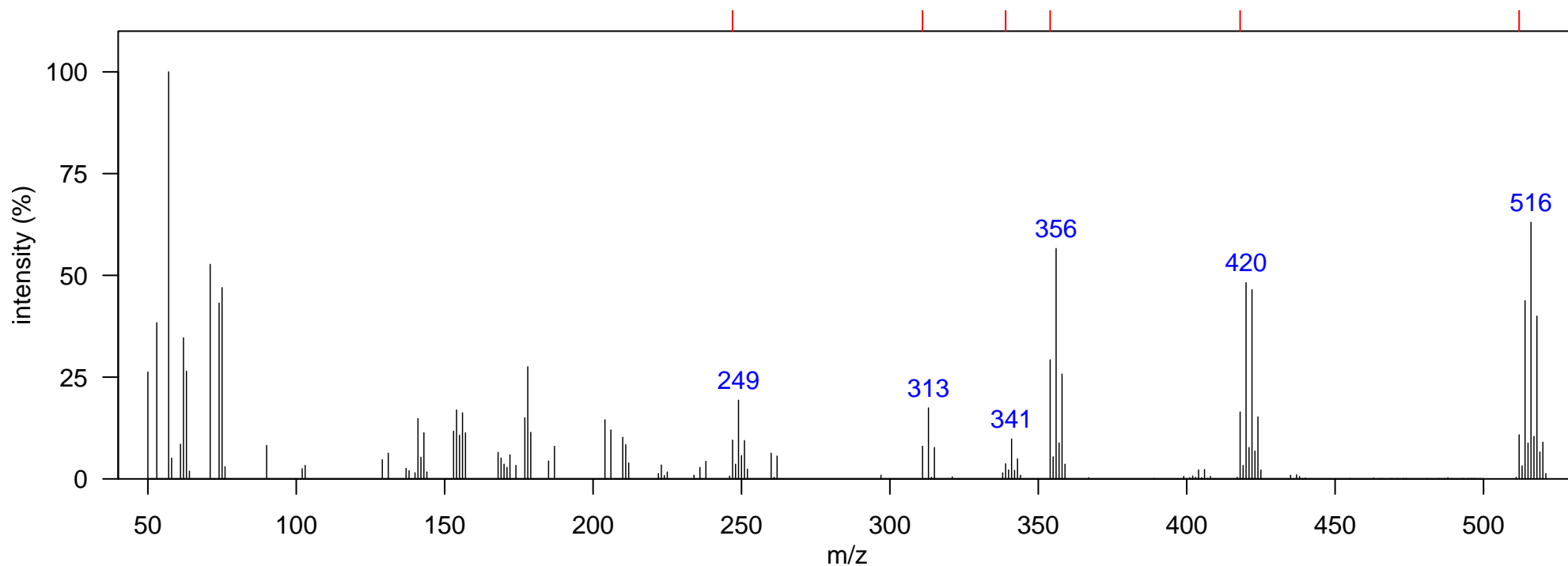
Comment:

Elemental Formula: C₁₃H₈Br₄O₂

Source: natural

Class: MeO-B/CDE

Identification: Manual – Congener Group



X=4Br, 5H

m/z	Identity
247	[C ₆ Br ₂ HO] ⁺
311	[M-2Br-CH ₃ -CO] ⁺
339	[M-2Br-CH ₃] ⁺
354	[M-2Br] ⁺
418	[M-Br-CH ₃] ⁺
512	M ⁺

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

Elemental Formula: C₁₃H₈Br₄O₂

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: natural

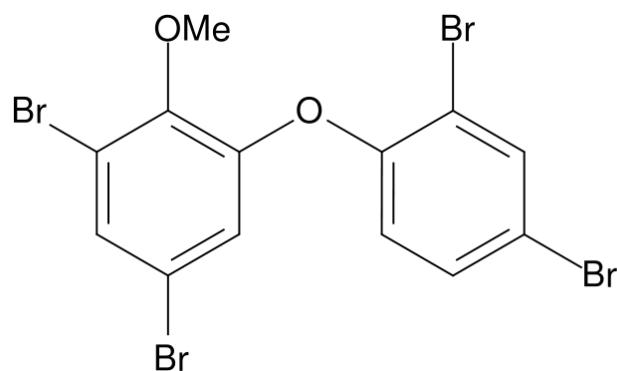
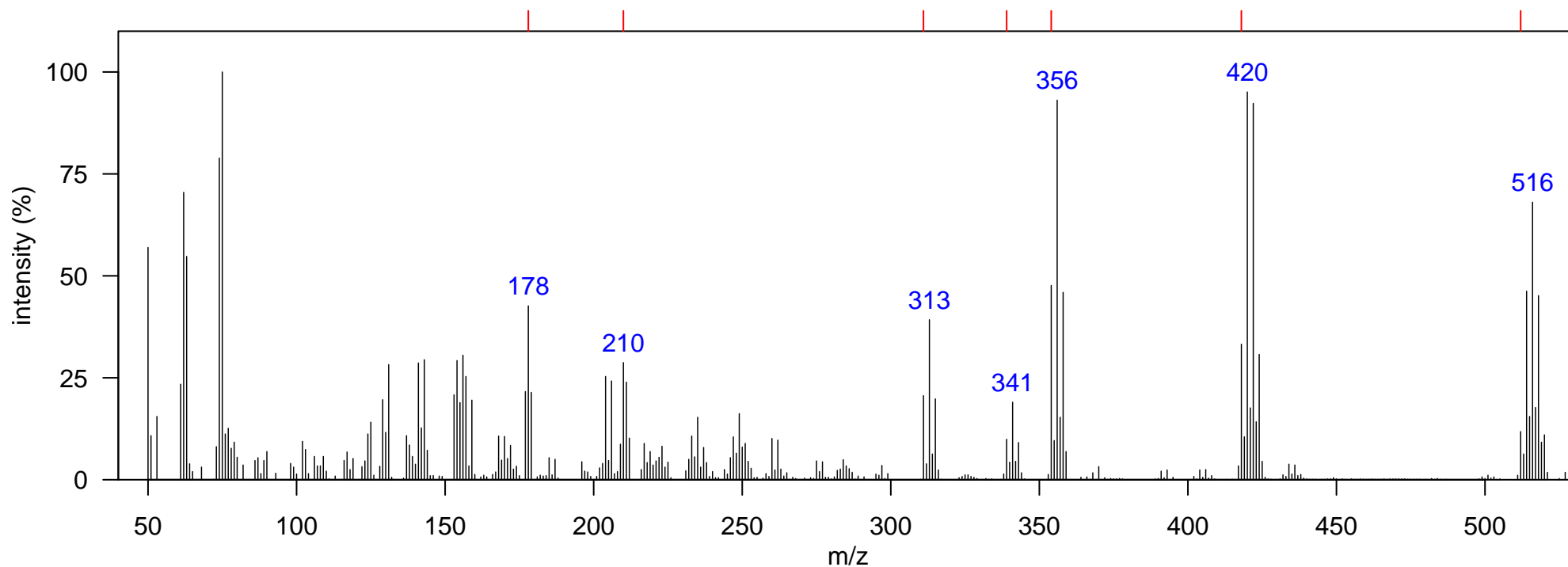
Instrument: GCxGC-TOF, electron impact

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-CH ₃] ²⁺
311	[M-2Br-CH ₃ -CO] ⁺
339	[M-2Br-CH ₃] ⁺
354	[M-2Br] ⁺
418	[M-CH ₃ Br] ⁺
512	M ⁺

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

Elemental Formula: C₁₃H₈Br₄O₂

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Source: natural

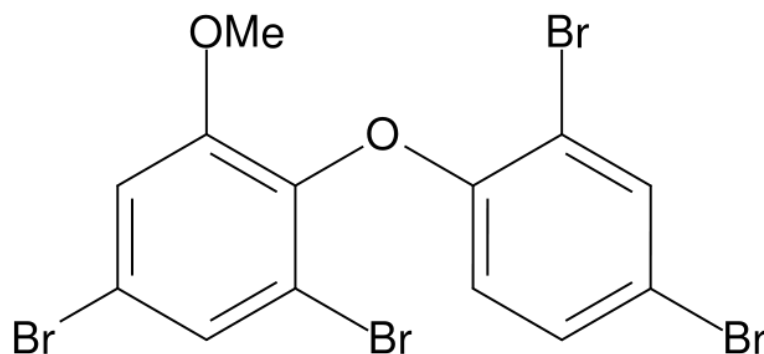
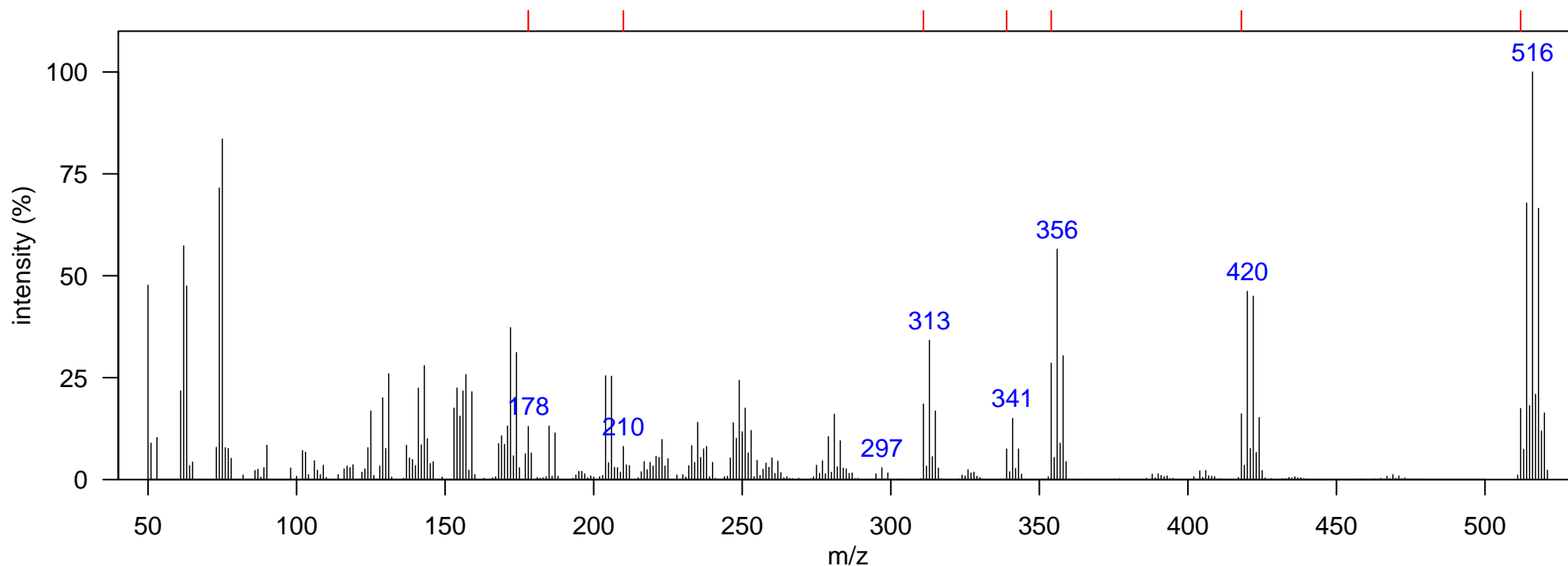
Instrument: GCxGC-TOF, electron impact

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-CH ₃] ₂ ⁺
311	[M-2Br-CH ₃ -CO] ⁺
339	[M-2Br-CH ₃] ⁺
354	[M-2Br] ⁺
418	[M-Br-CH ₃] ⁺
512	M ⁺

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

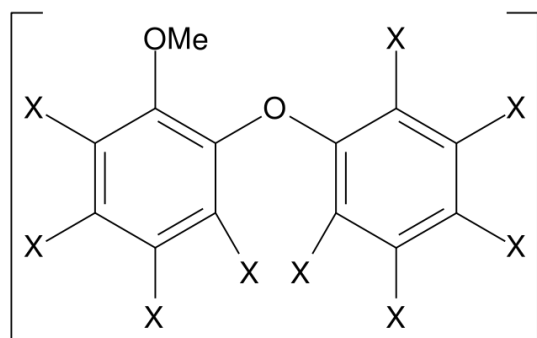
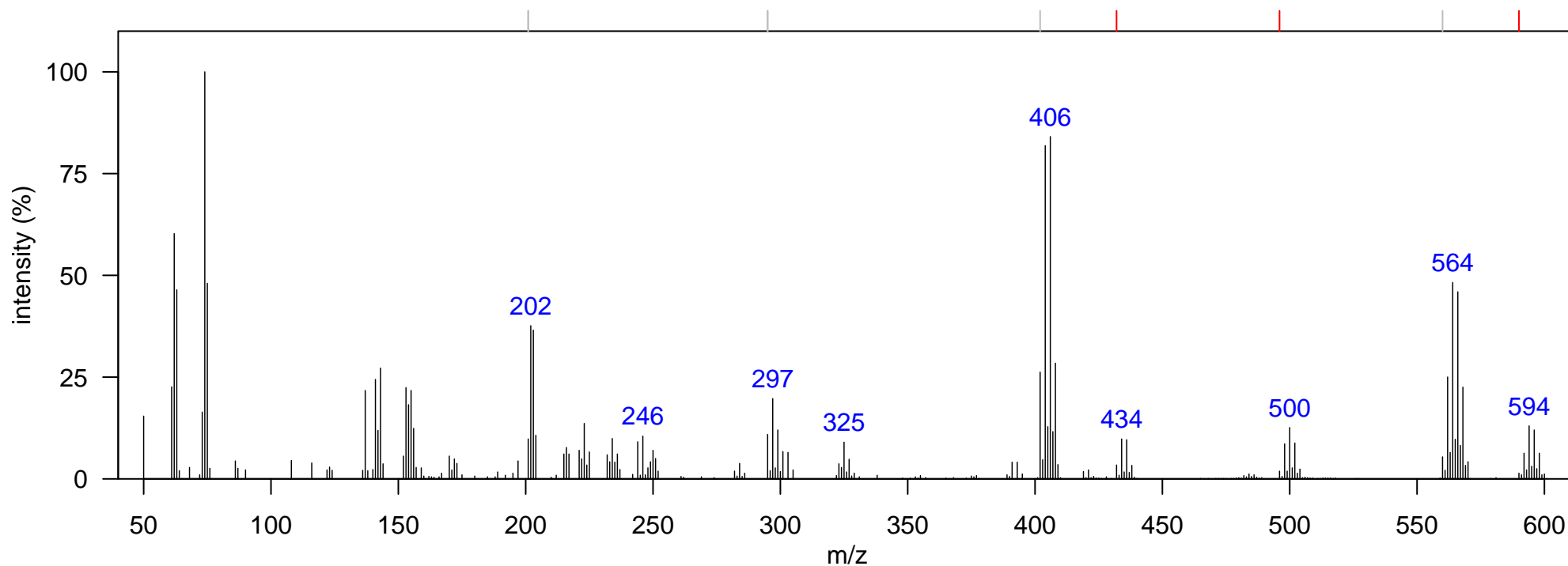
Comment:

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-CH ₃] ⁺
560	interference BDE-99
590	M ⁺

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

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

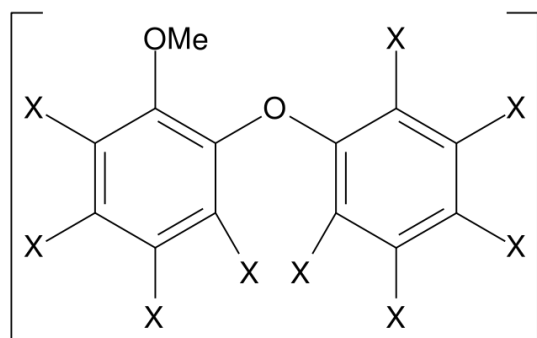
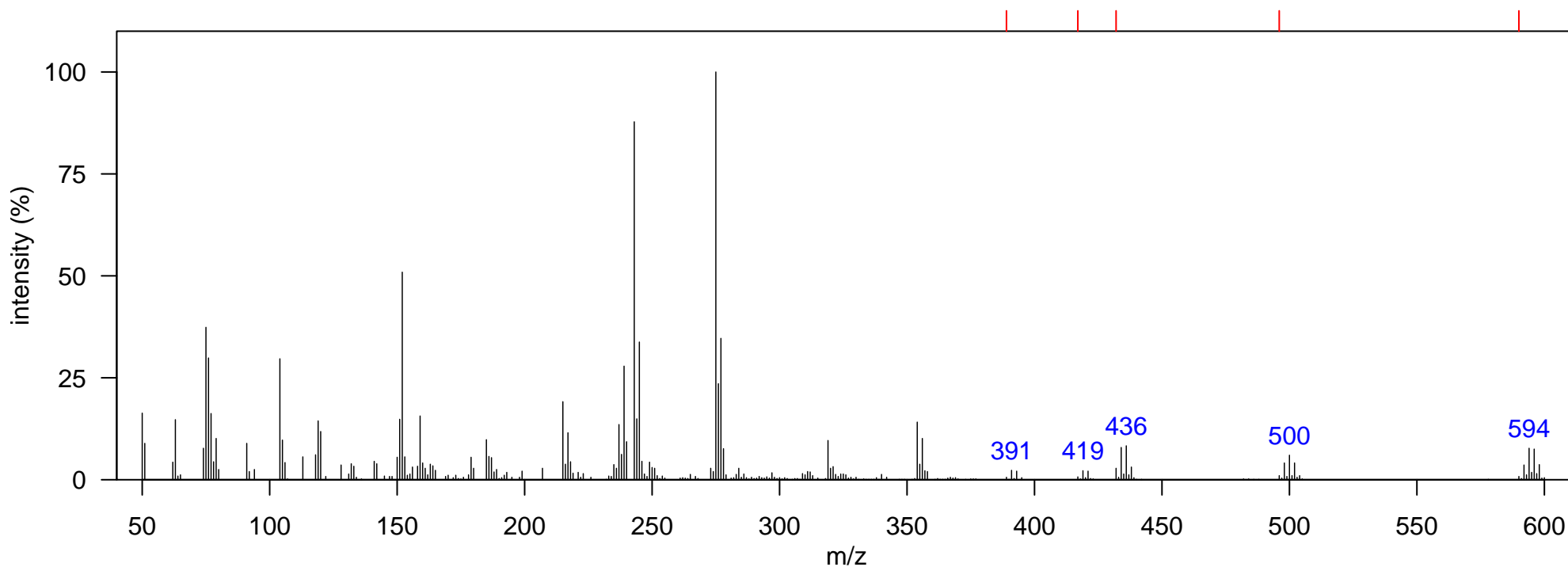
Comment:

Elemental Formula: C₁₃H₇Br₅O₂

Source: natural

Class: MeO-B/CDE

Identification: Manual – Congener Group



X=5Br, 4H

m/z	Identity
389	[M-2Br-CH ₃ -CO] ⁺
417	[M-2Br-CH ₃] ⁺
432	[M-2Br] ⁺
496	[M-Br-CH ₃] ⁺
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

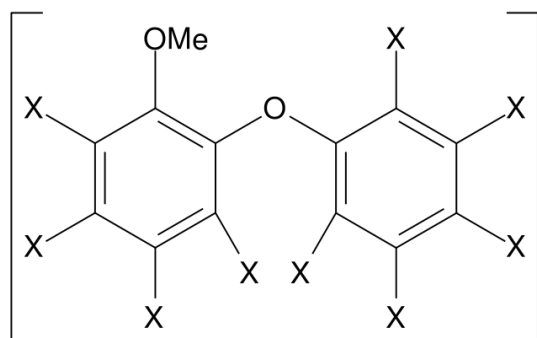
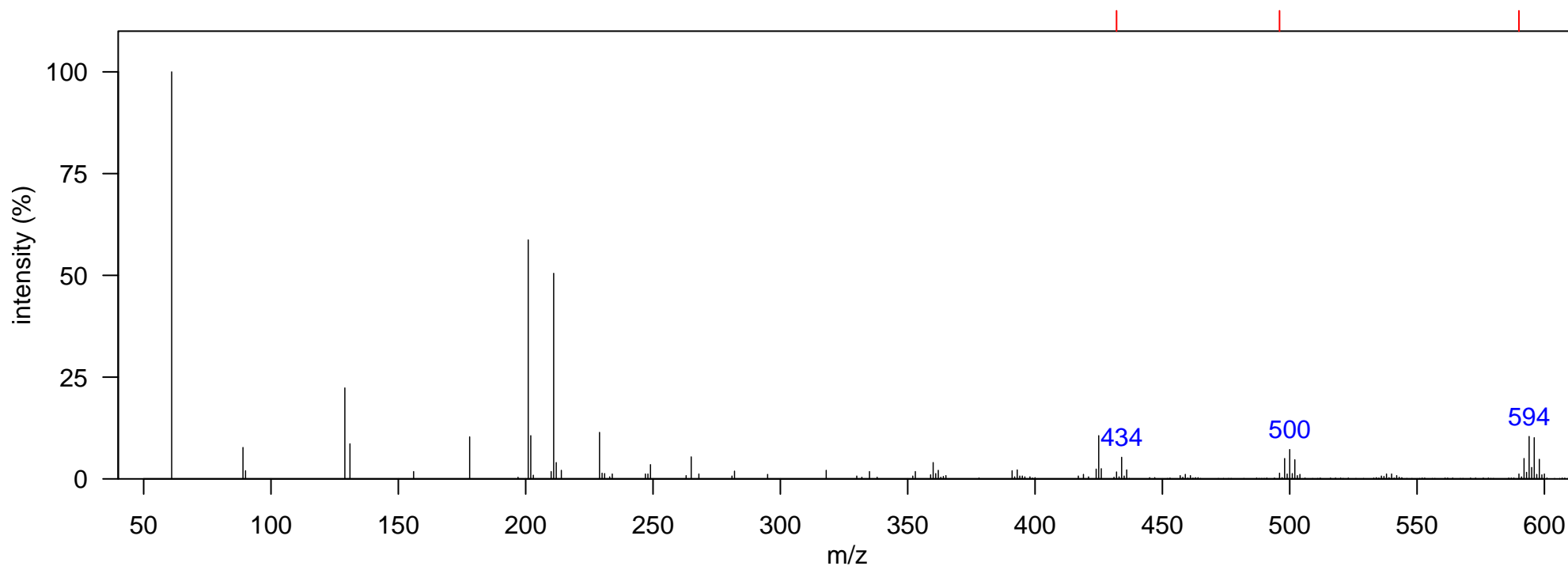
Comment:

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-CH ₃] ⁺
590	M ⁺

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

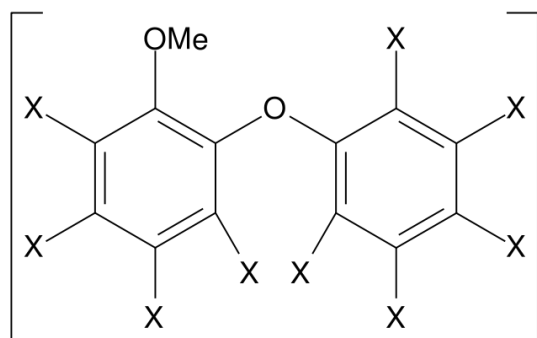
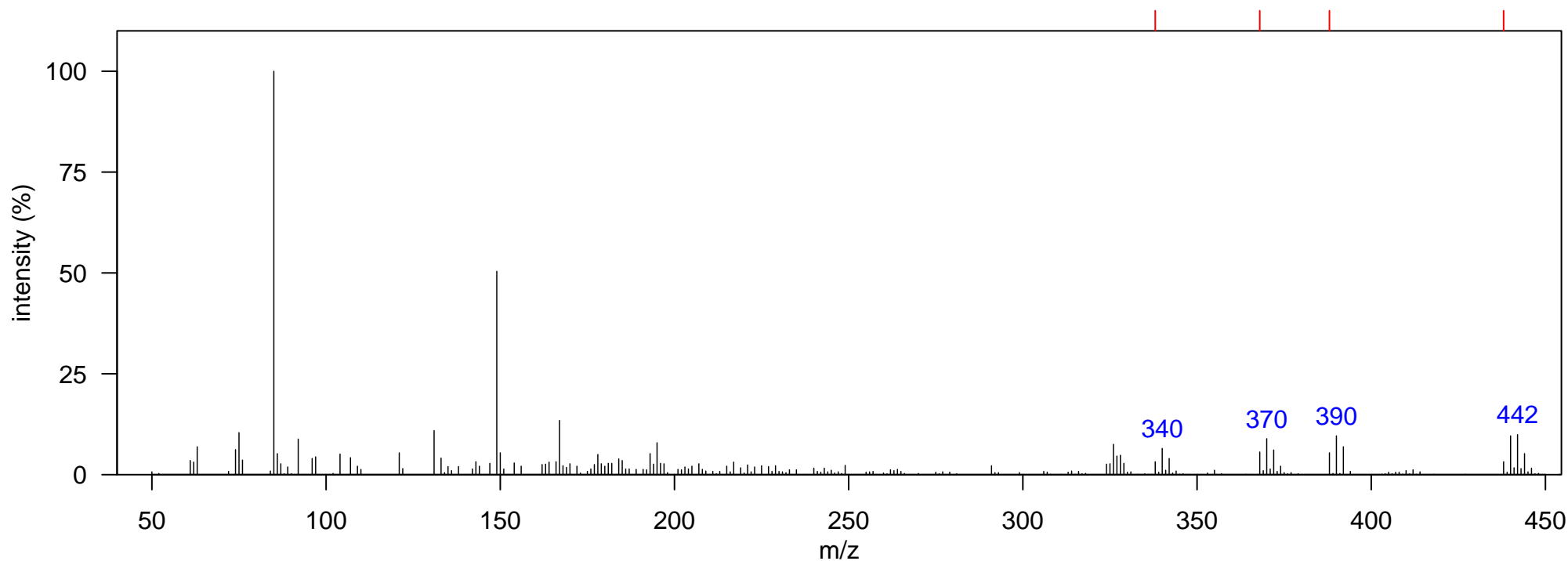
Comment:

Elemental Formula: C₁₃H₅Cl₇O₂

Source: anthropogenic

Class: MeO-CDE

Identification: Manual – Congener Group



X=7Cl, 2H

m/z	Identity
338	[M-2Cl-OCH ₂] ⁺
368	[M-2Cl] ⁺
388	[M-Cl-CH ₃] ⁺
438	M ⁺
486	BDE interference

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

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

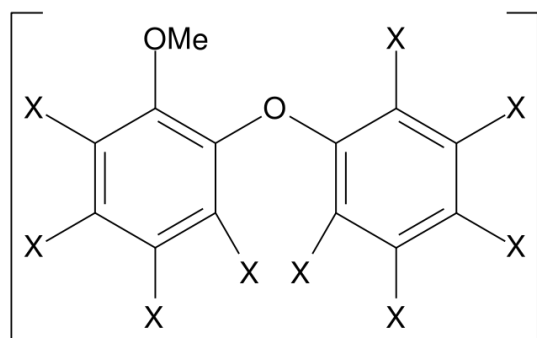
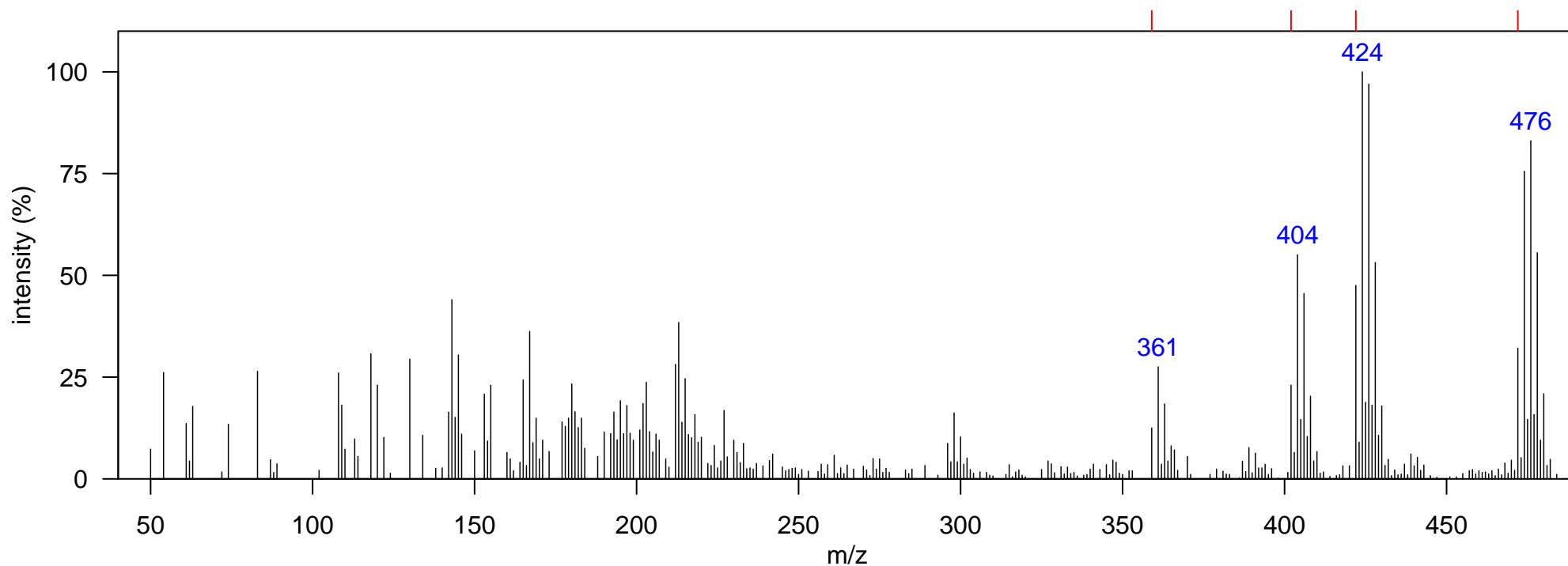
Comment:

Elemental Formula: C₁₃H₄Cl₈O₂

Source: anthropogenic

Class: MeO-CDE

Identification: Manual – Congener Group



X=8Cl, H

m/z	Identity
359	[M-2Cl-CH ₃ -CO] ⁺
402	[M-2Cl] ⁺
422	[M-Cl-CH ₃] ⁺
472	M ⁺
501	interference
536	interference
568	interference

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

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

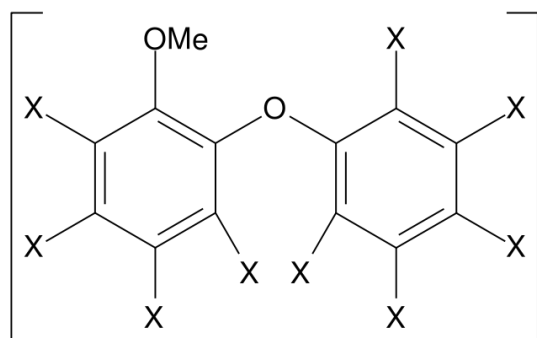
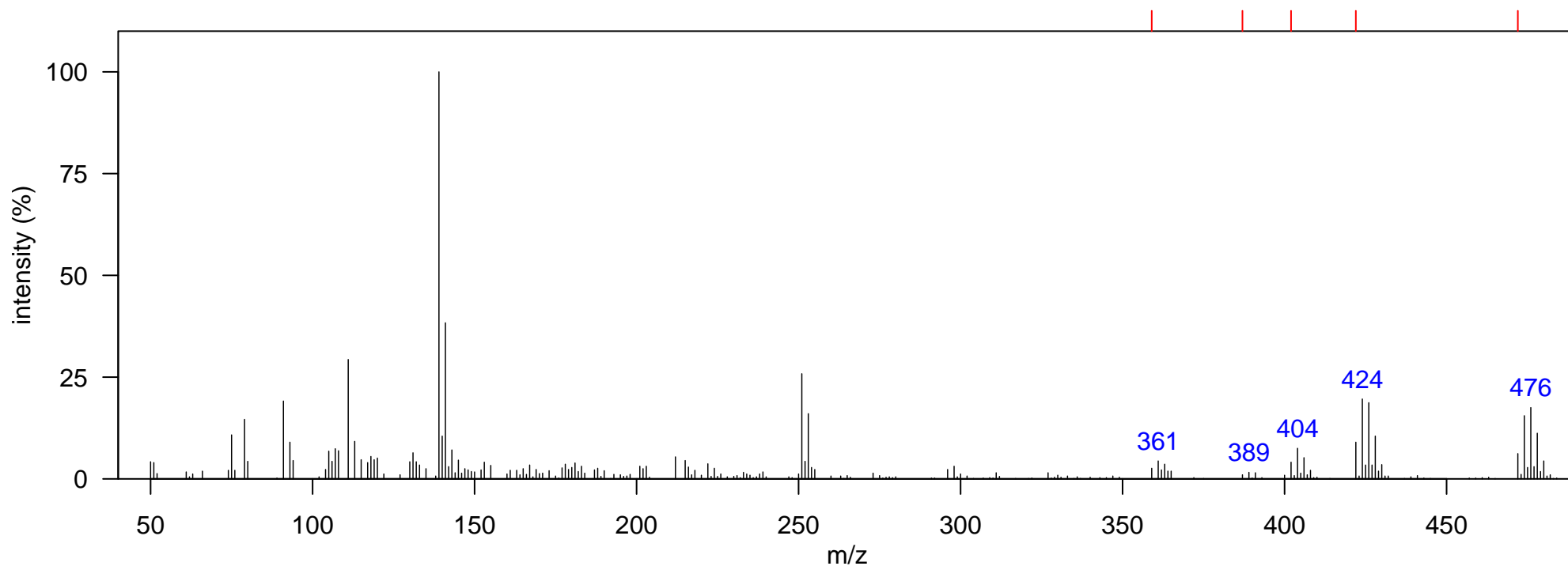
Comment:

Elemental Formula: C₁₃H₄Cl₈O₂

Source: anthropogenic

Class: MeO-CDE

Identification: Manual – Congener Group



X=8Cl, H

m/z	Identity
359	[M-2Cl-CH ₃ -CO] ⁺
387	[M-2Cl-CH ₃] ⁺
402	[M-2Cl] ⁺
422	[M-Cl-CH ₃] ⁺
472	M ⁺

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

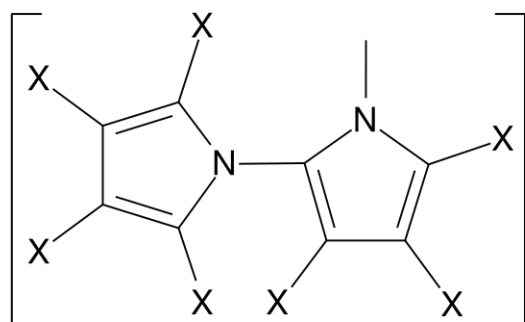
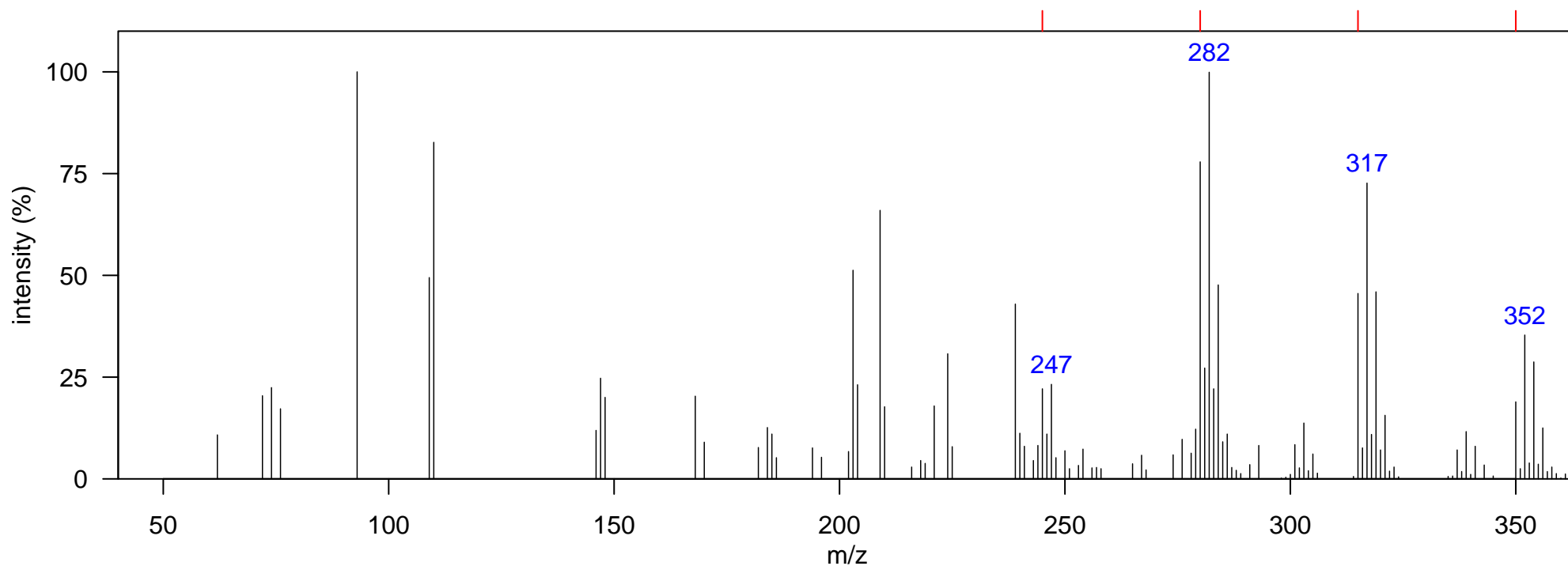
Comment: Ref: Chemosphere, 2008, 70, 1721-1729.

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 ⁺

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

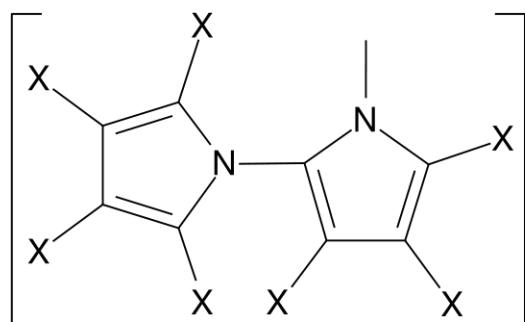
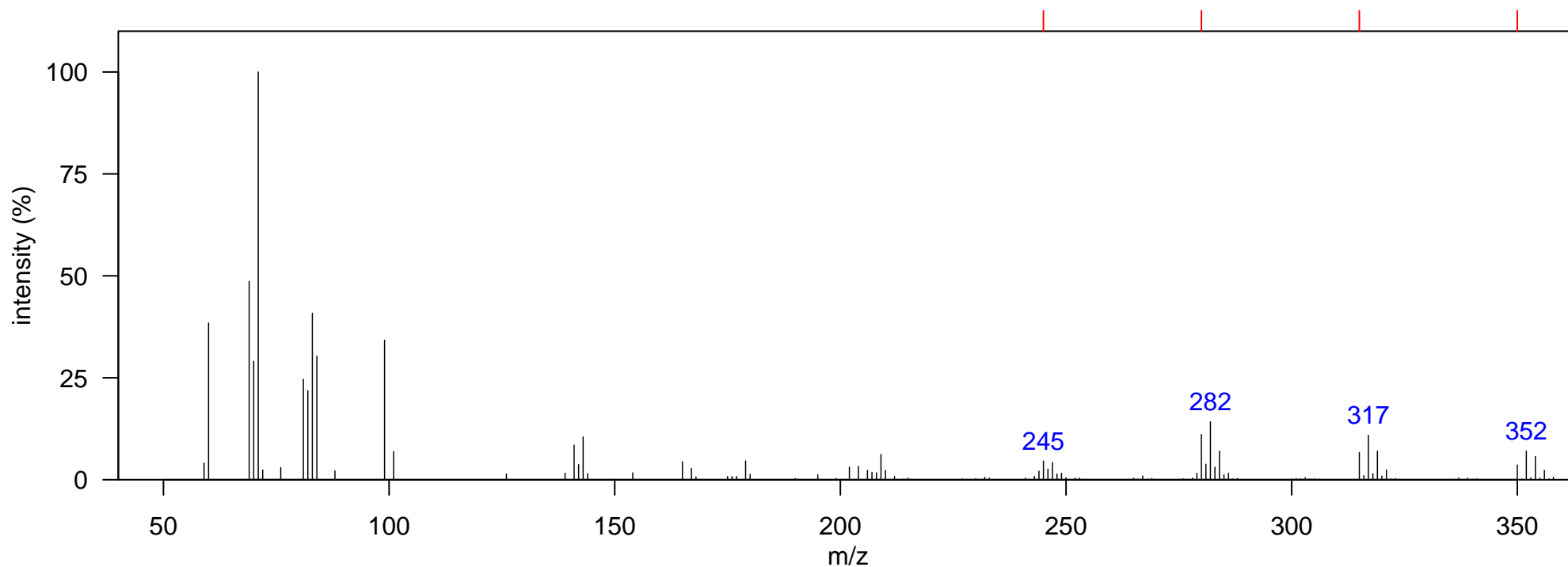
Comment: Ref: Chemosphere, 2008, 70, 1721-1729.

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 ⁺

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

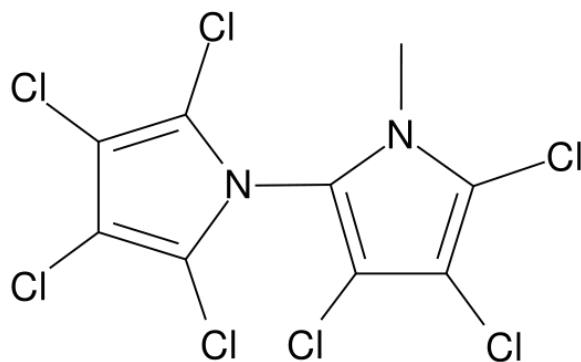
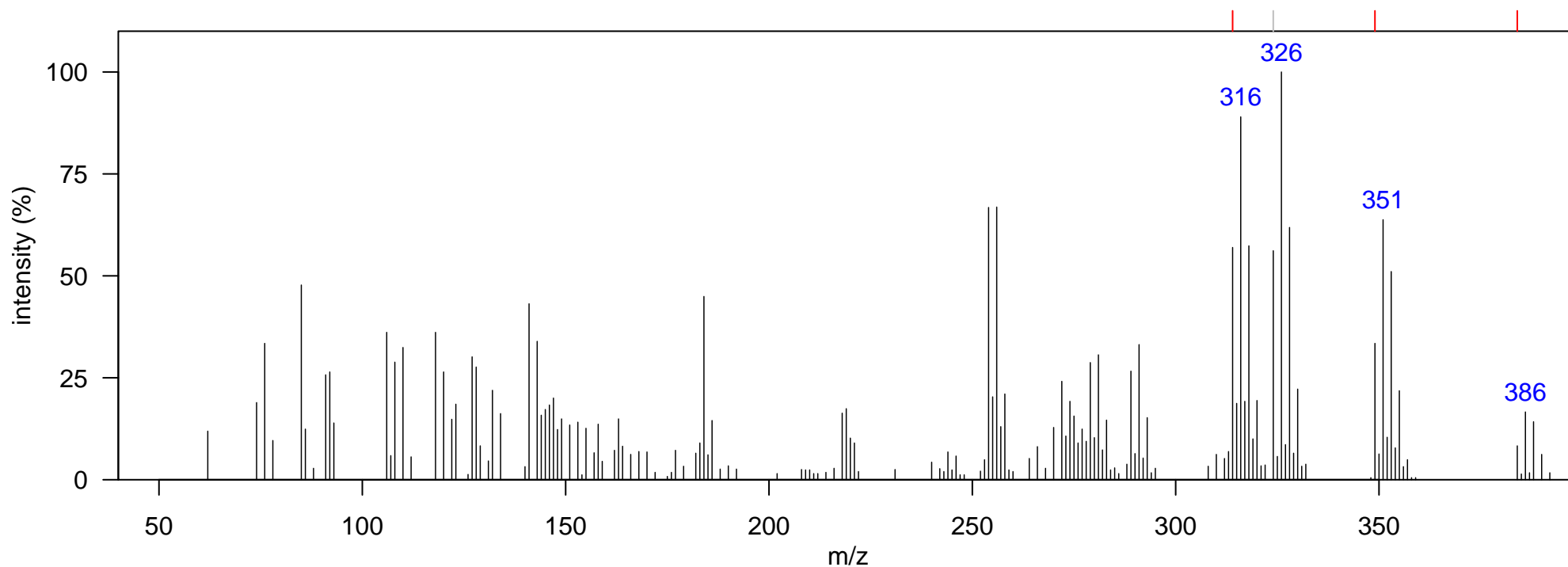
Comment: Also referred to as Q1.

Elemental Formula: C₉H₃Cl₇N₂

Source: natural

Class: MBP

Identification: Authentic MS RT



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

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

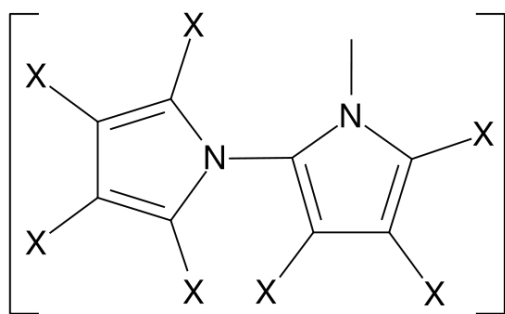
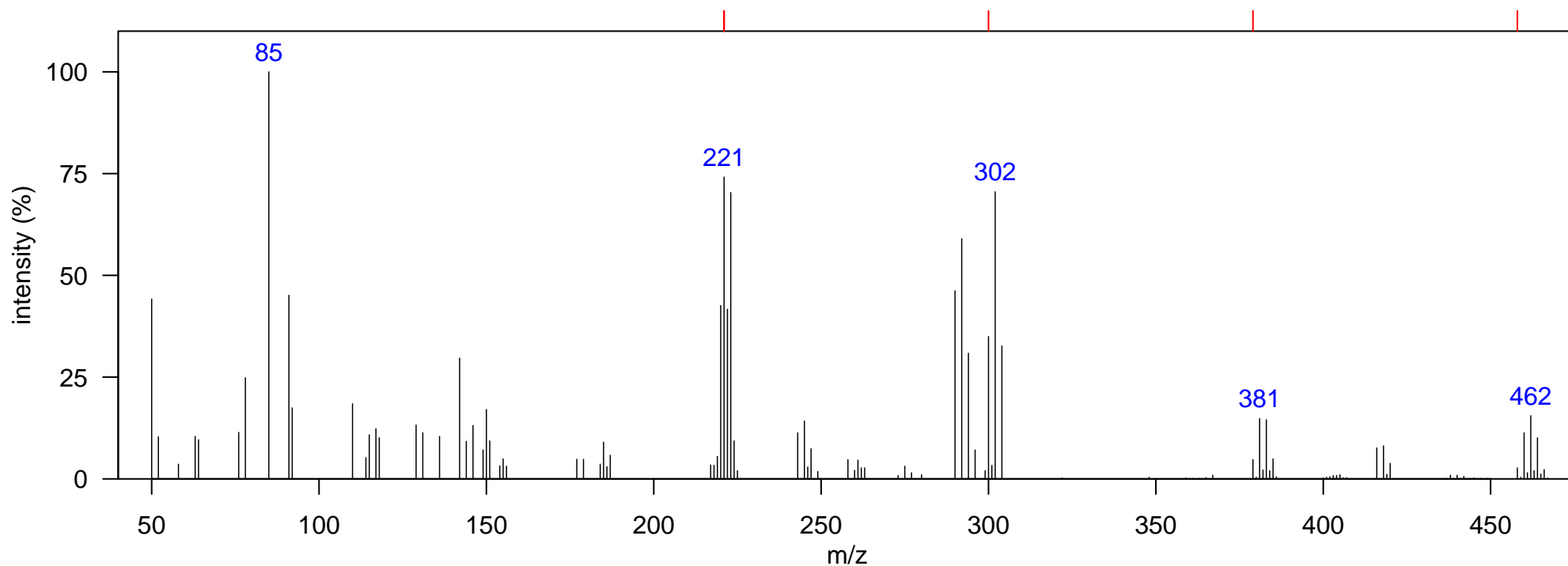
Comment:

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 ⁺

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

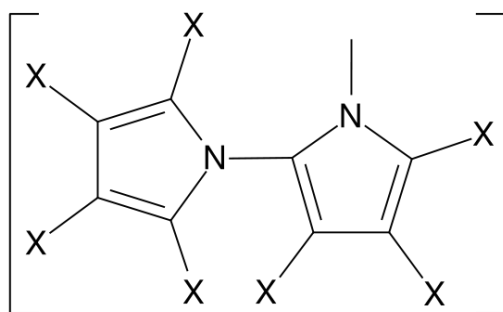
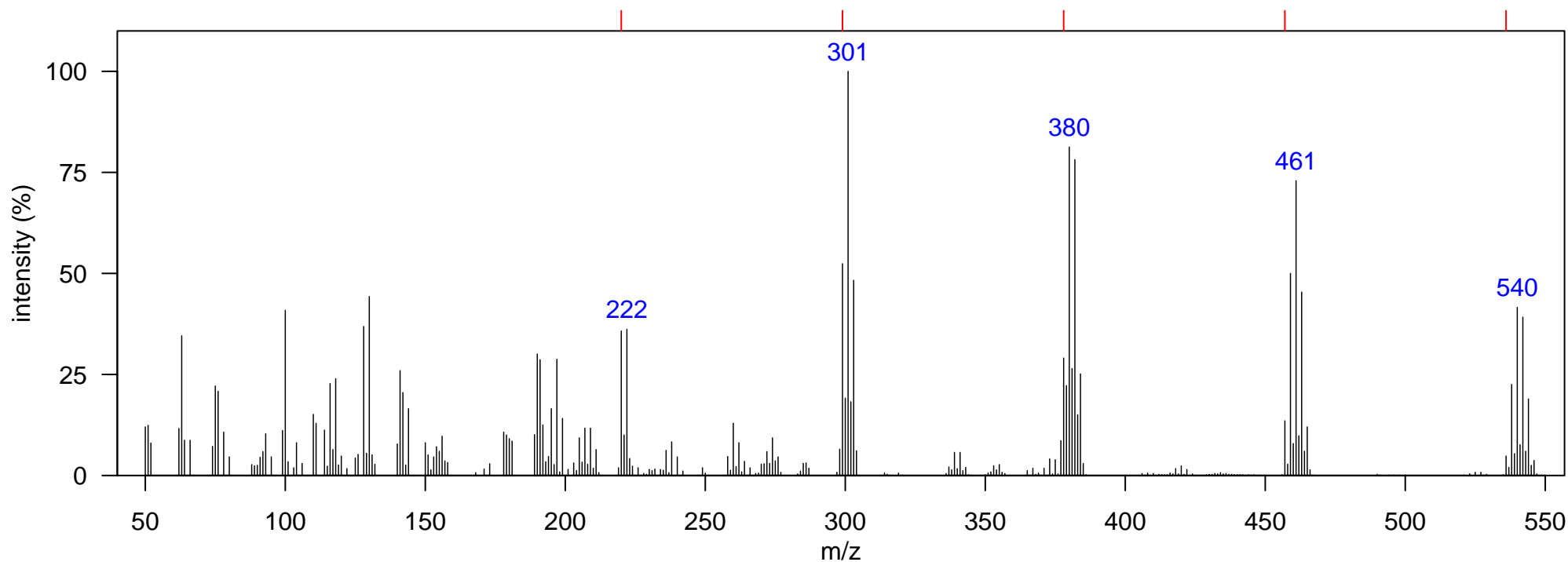
Comment:

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 ⁺

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

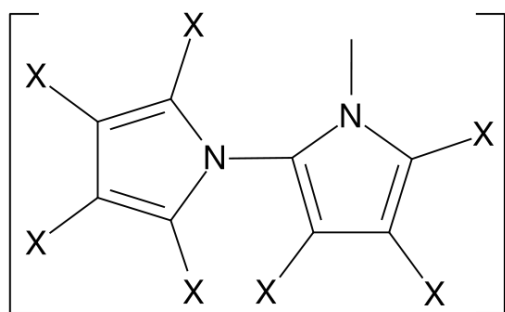
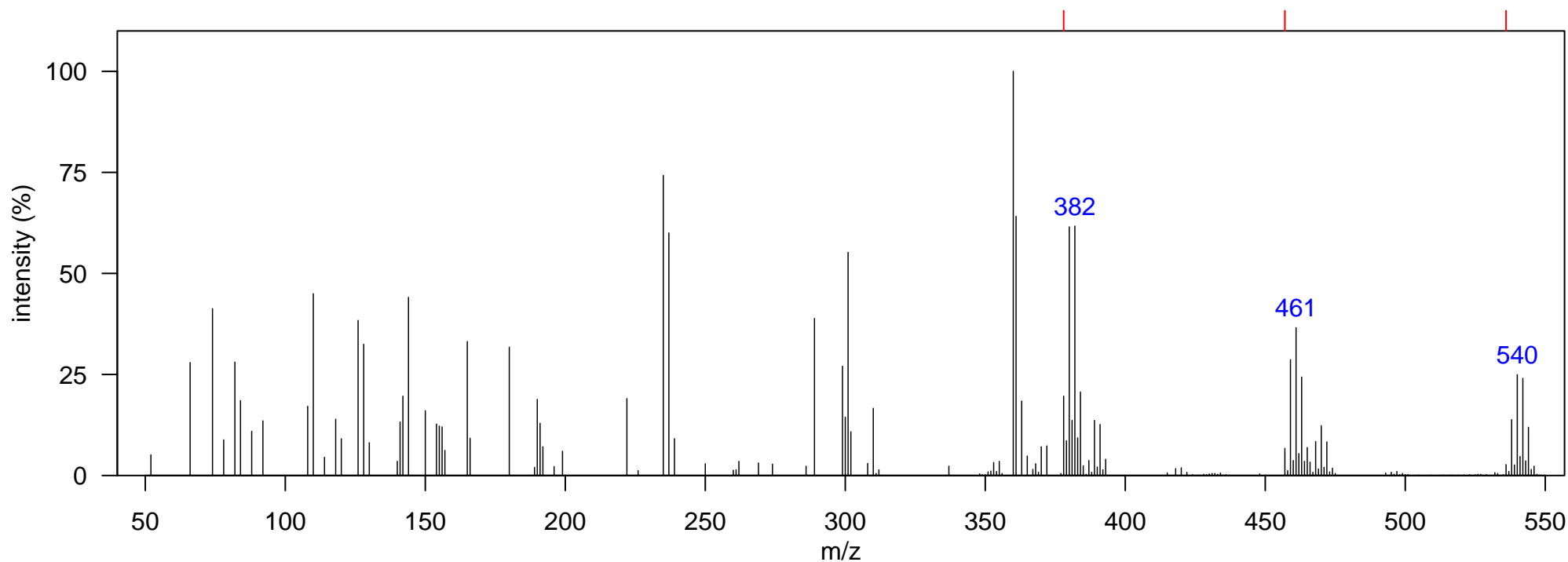
Comment:

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 ⁺

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

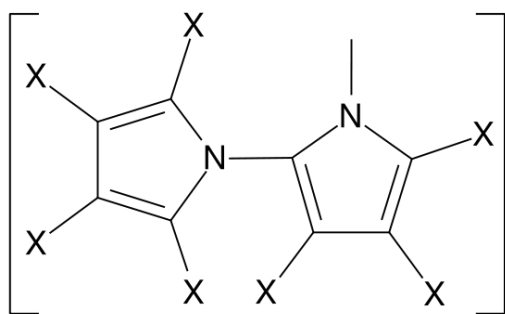
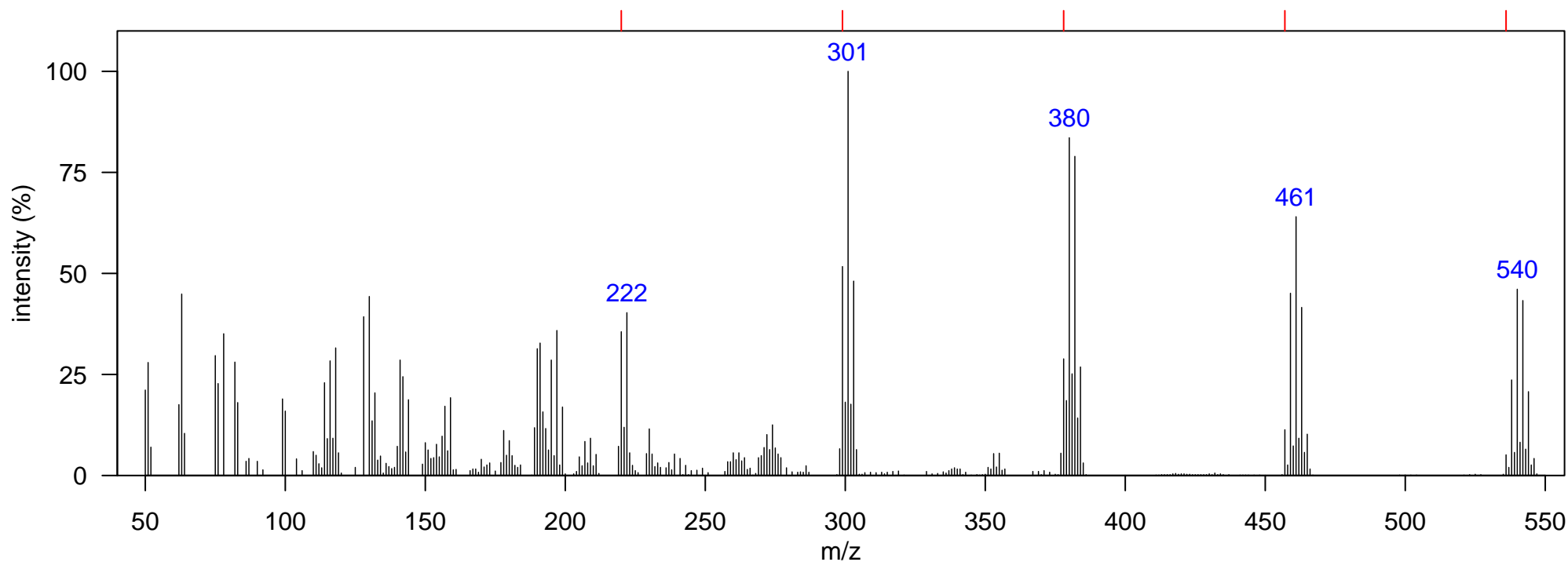
Comment:

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 ⁺

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

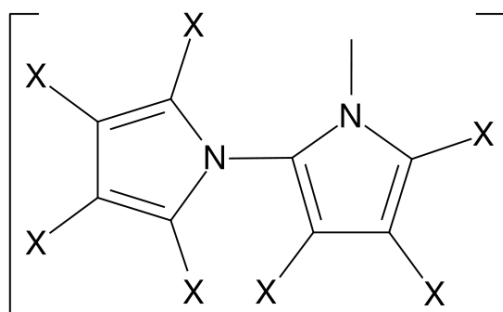
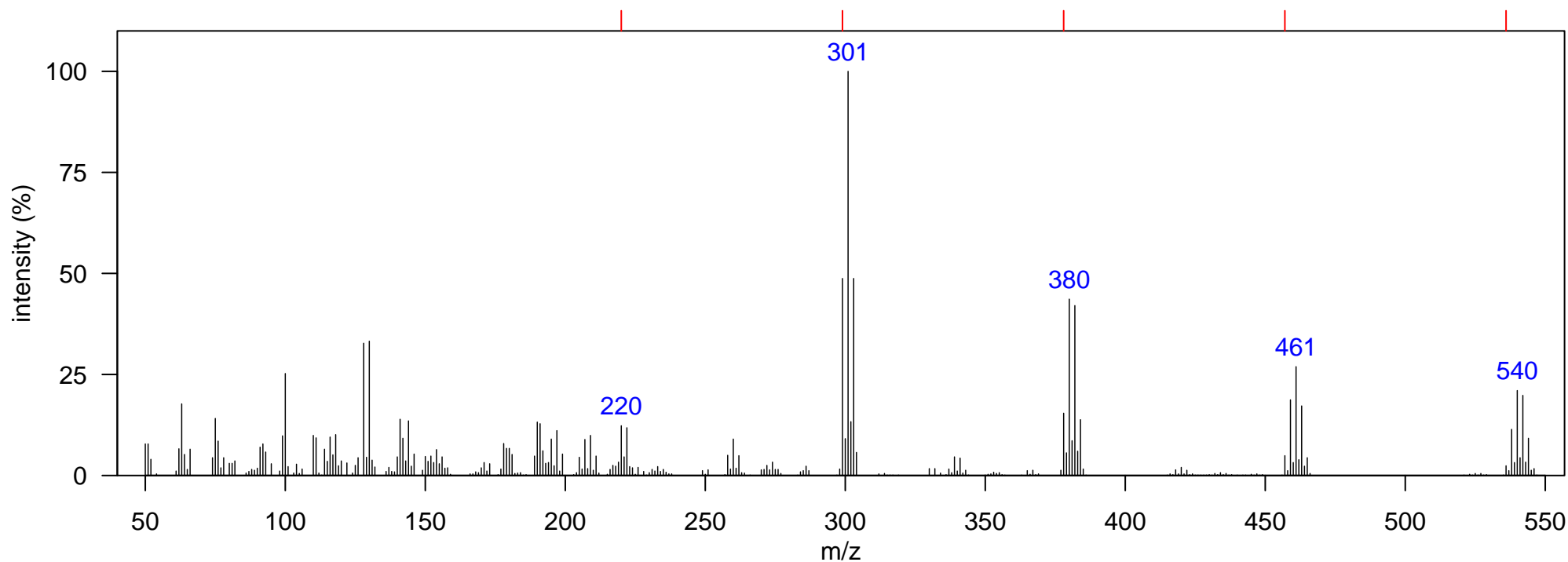
Comment:

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 ⁺

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

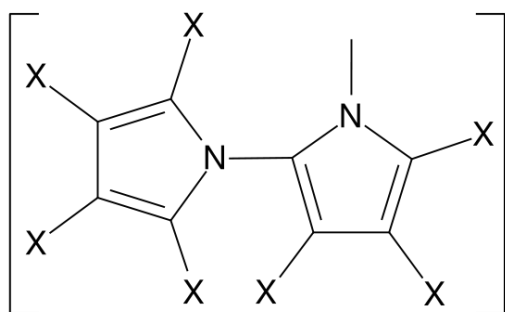
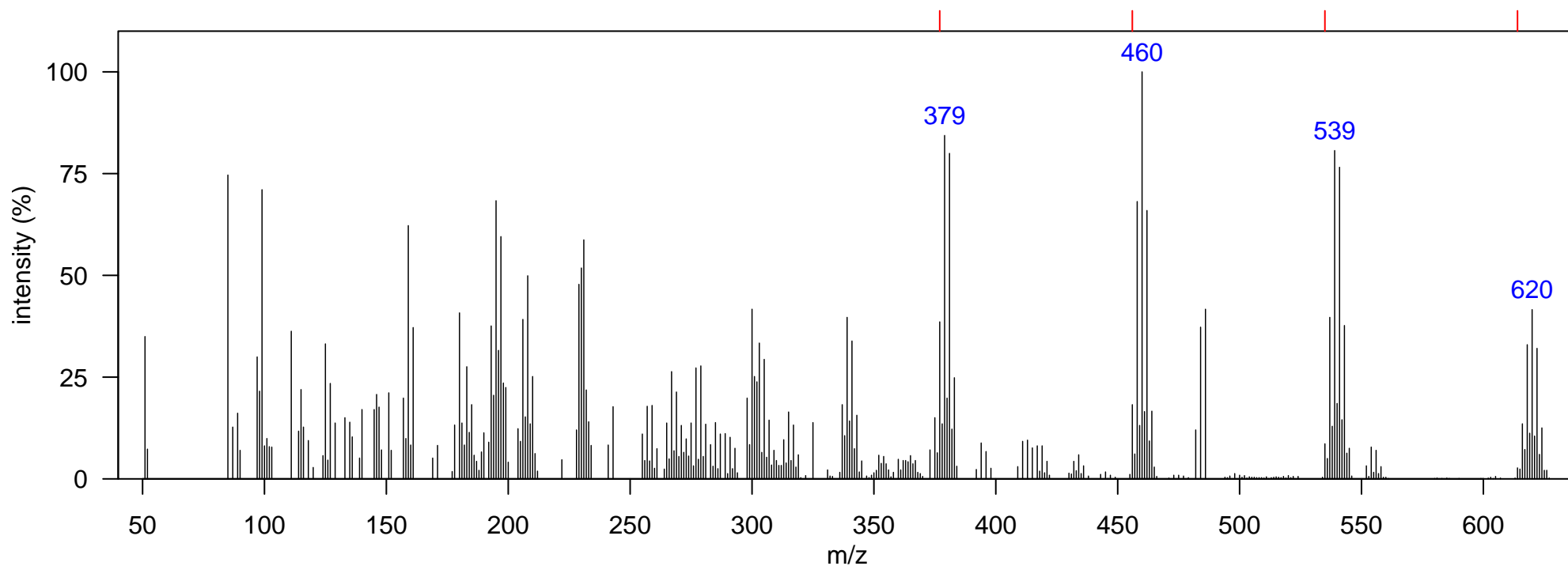
Comment:

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 ⁺

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

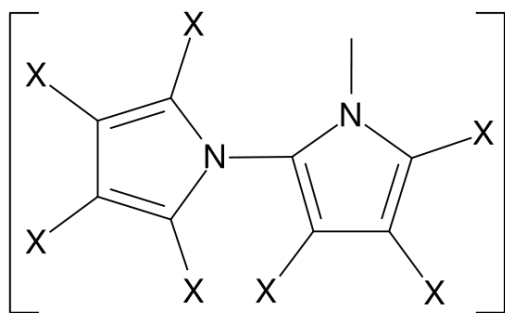
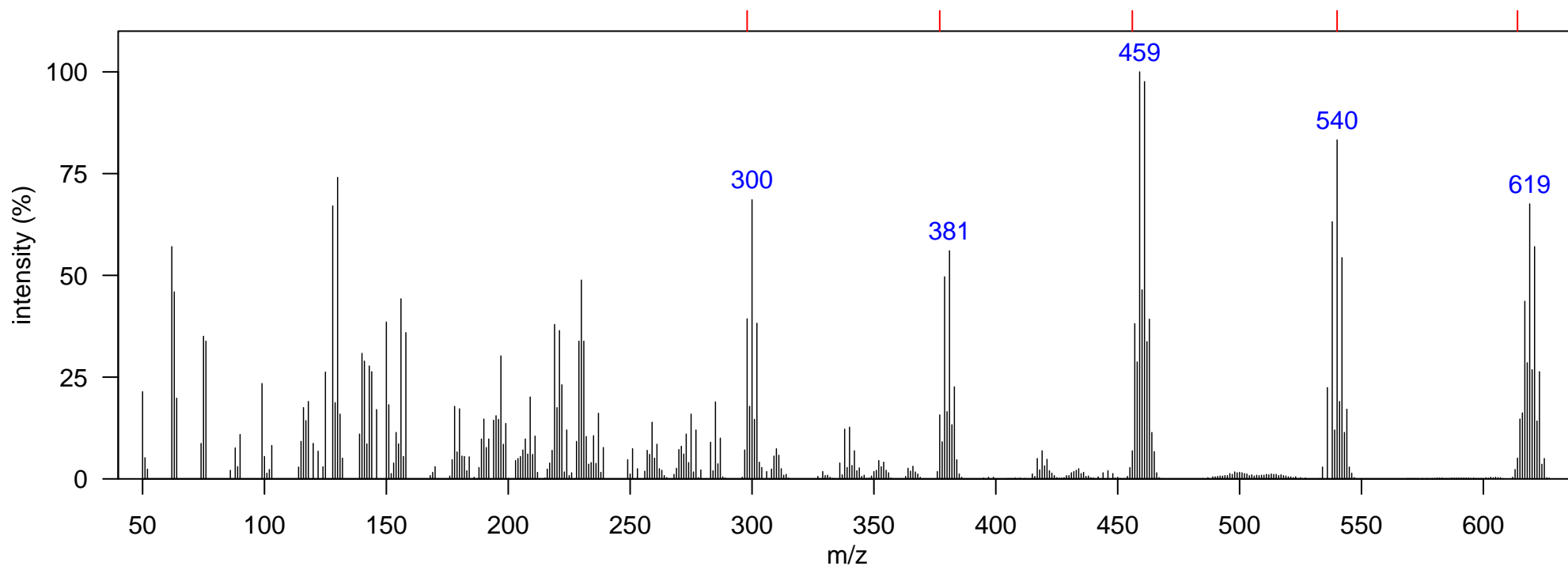
Comment:

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 ⁺

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

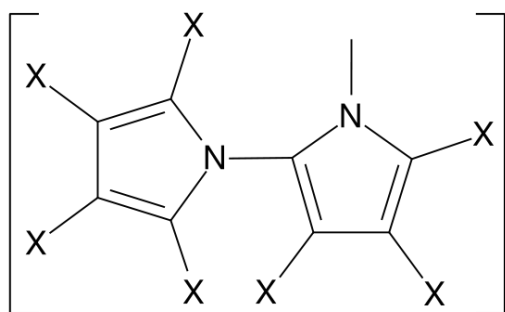
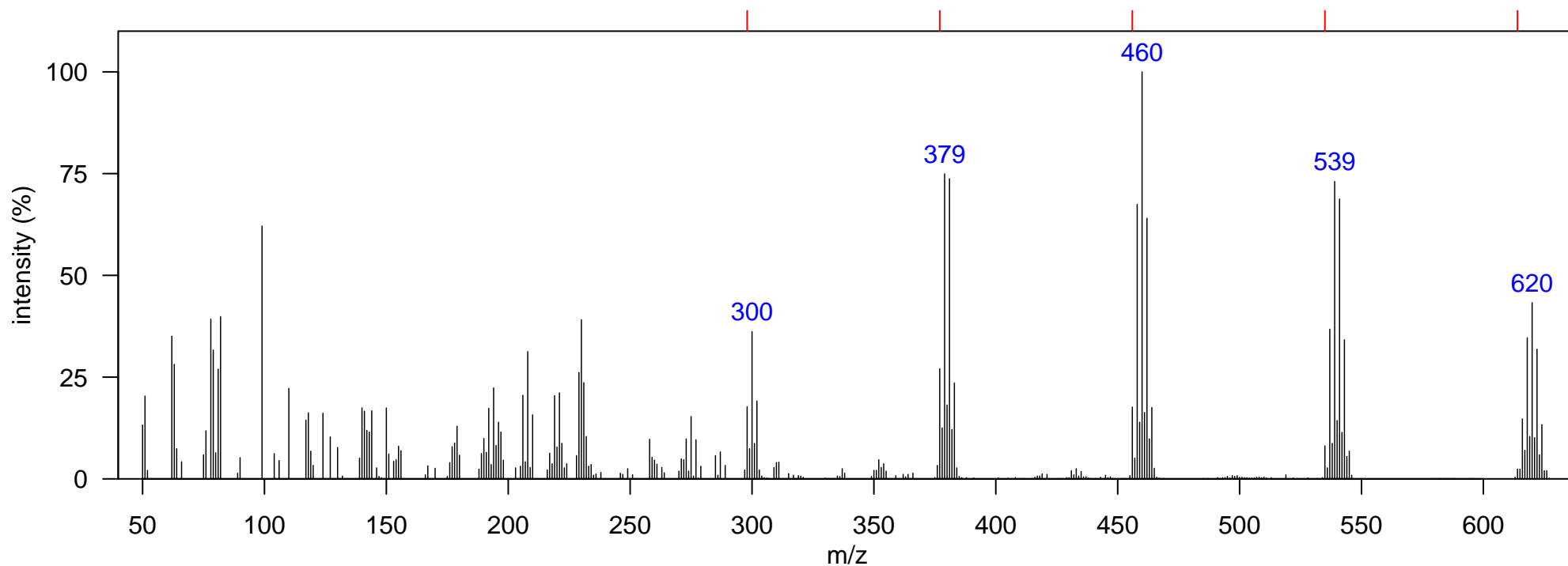
Comment:

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 ⁺

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

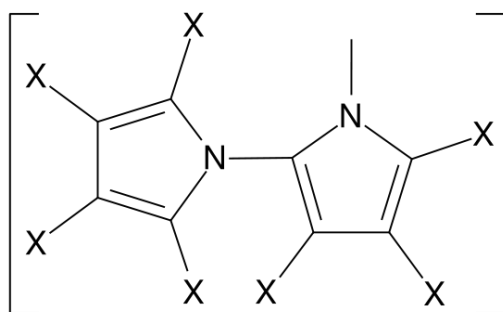
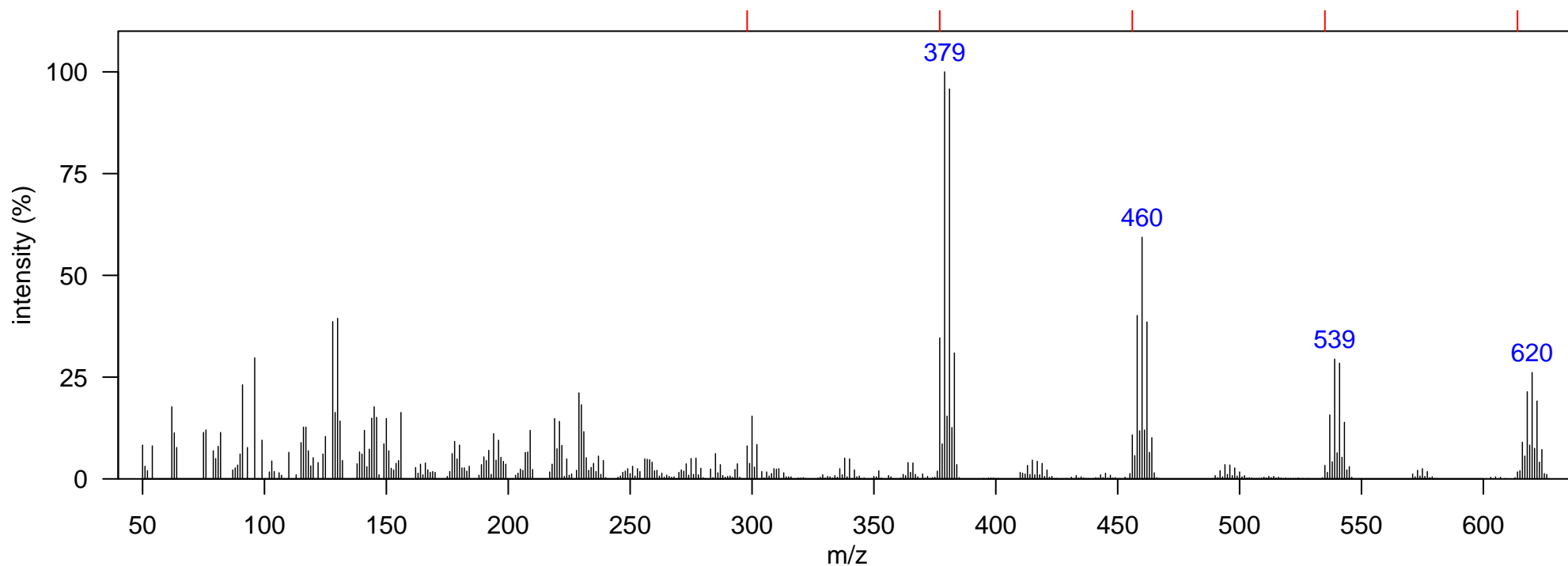
Comment:

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 ⁺

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

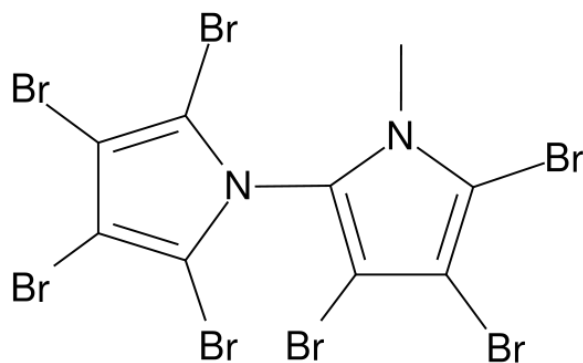
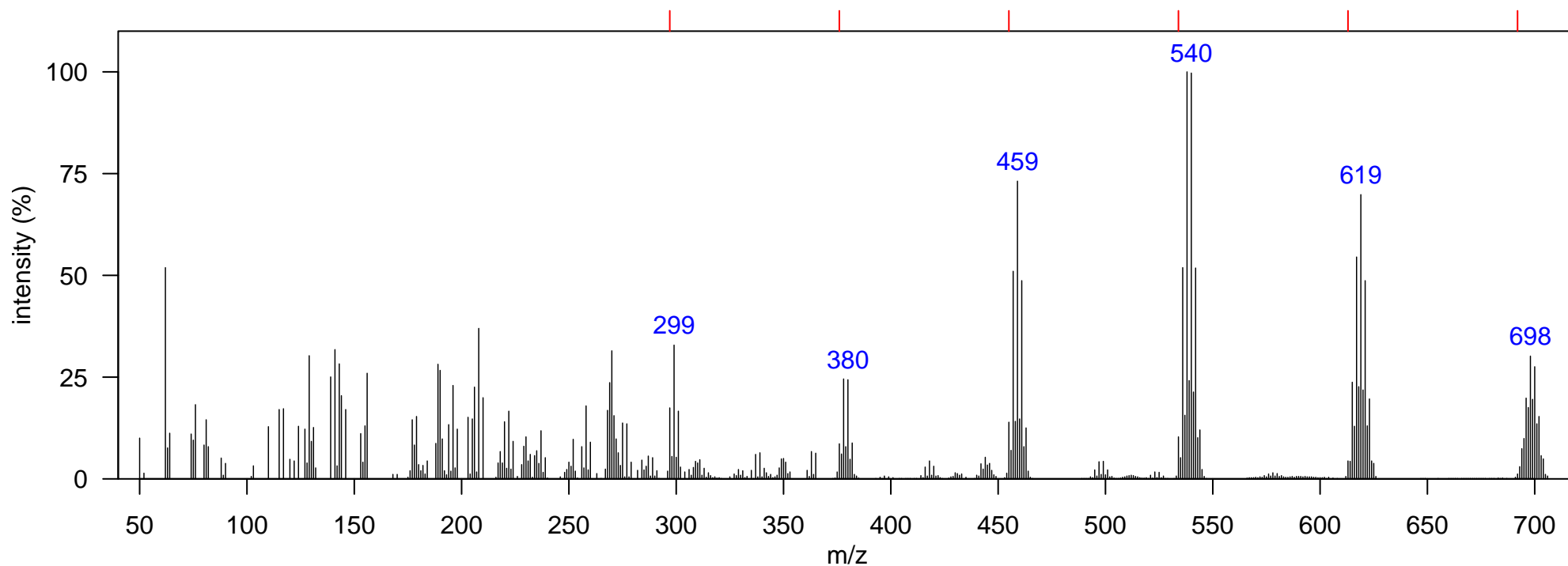
Comment:

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 ⁺

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

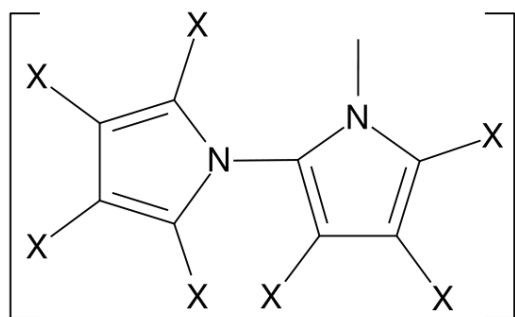
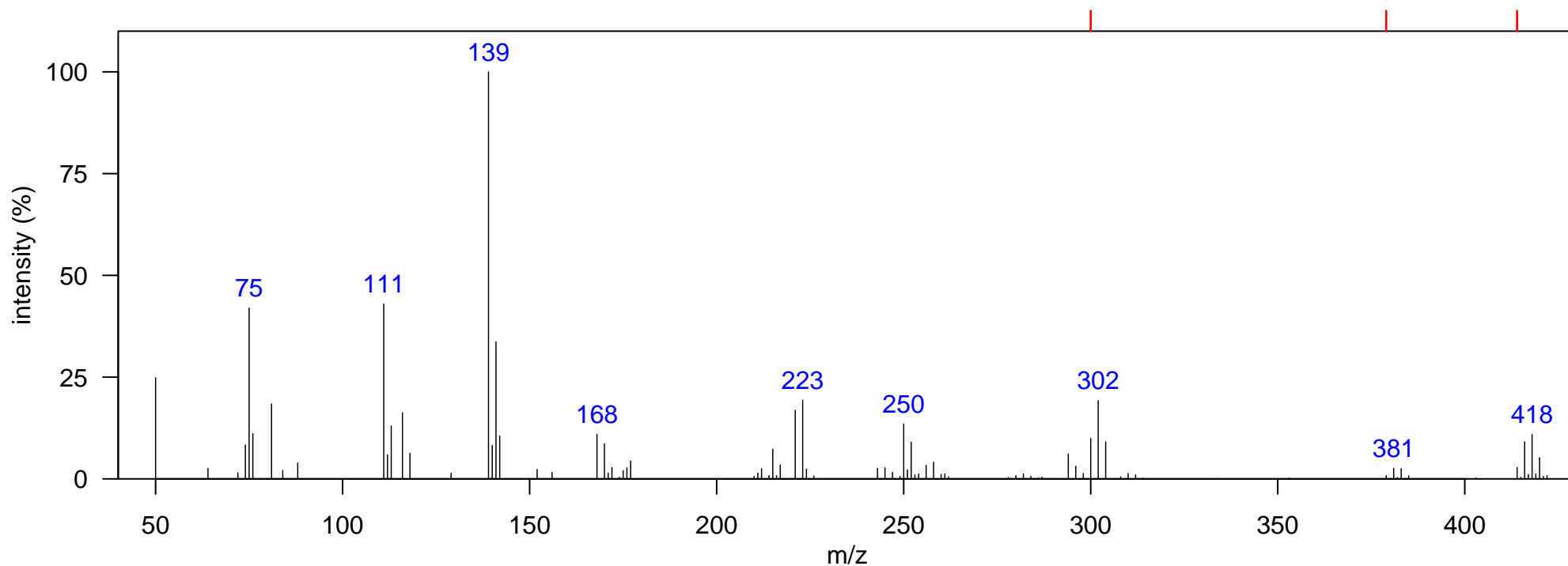
Comment:

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 ⁺

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

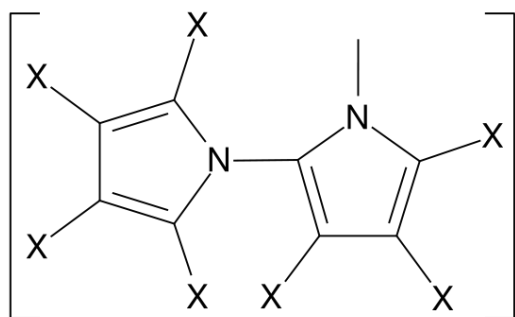
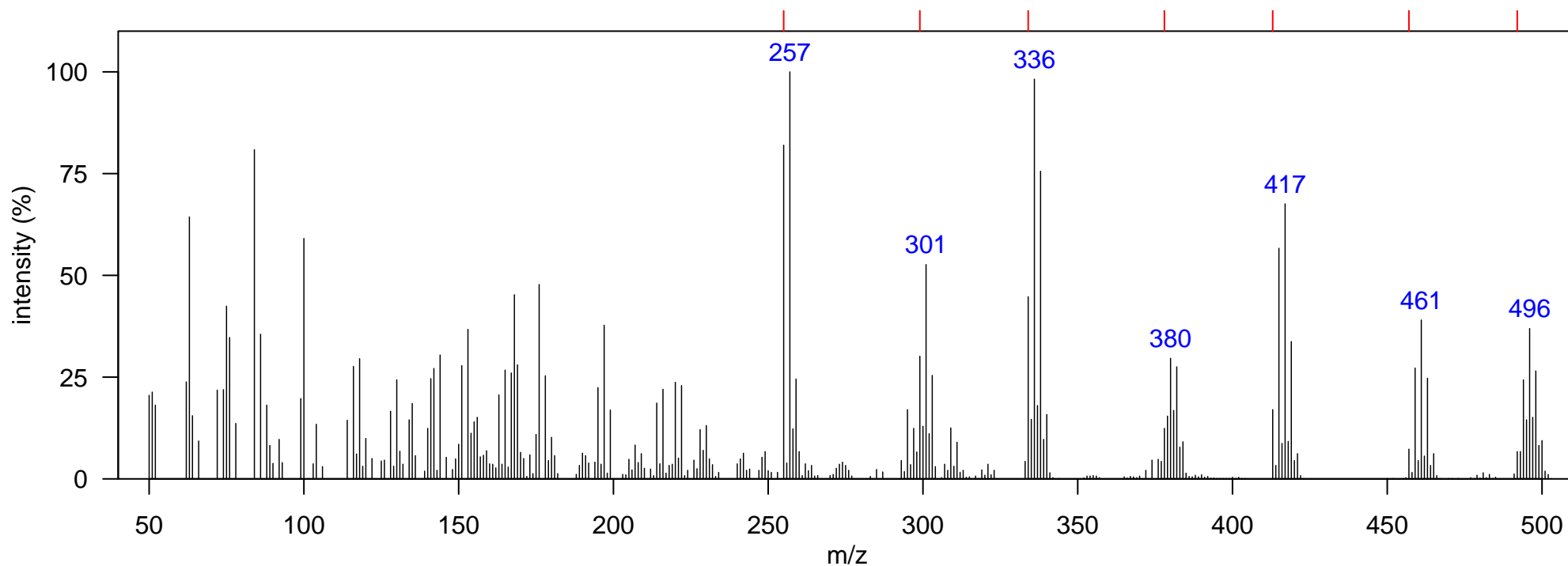
Comment:

Elemental Formula: C₉H₅Br₄ClN₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, Cl, 2H

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

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

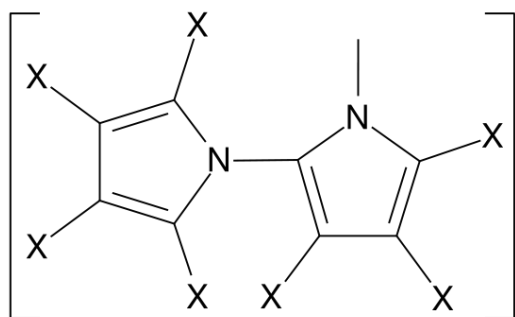
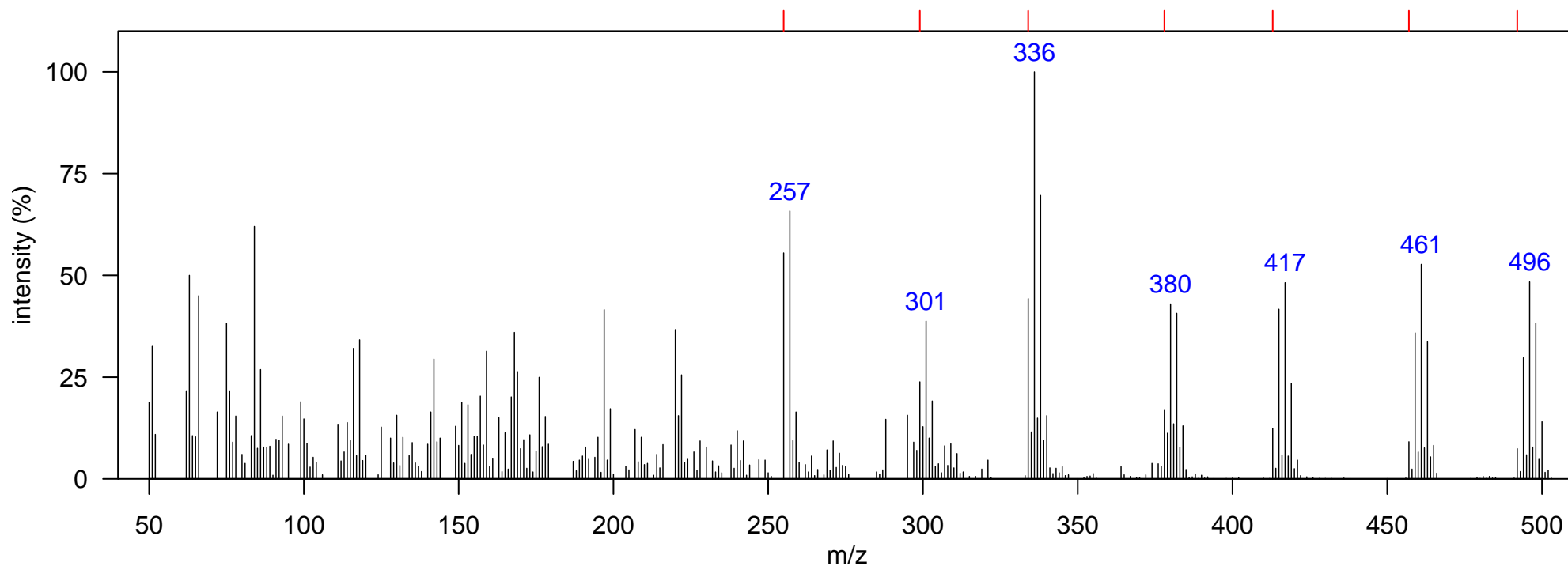
Comment:

Elemental Formula: C₉H₅Br₄ClN₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, Cl, 2H

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

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

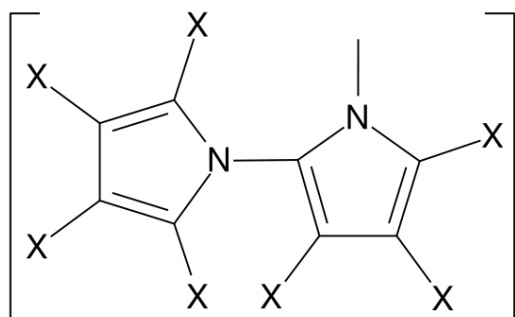
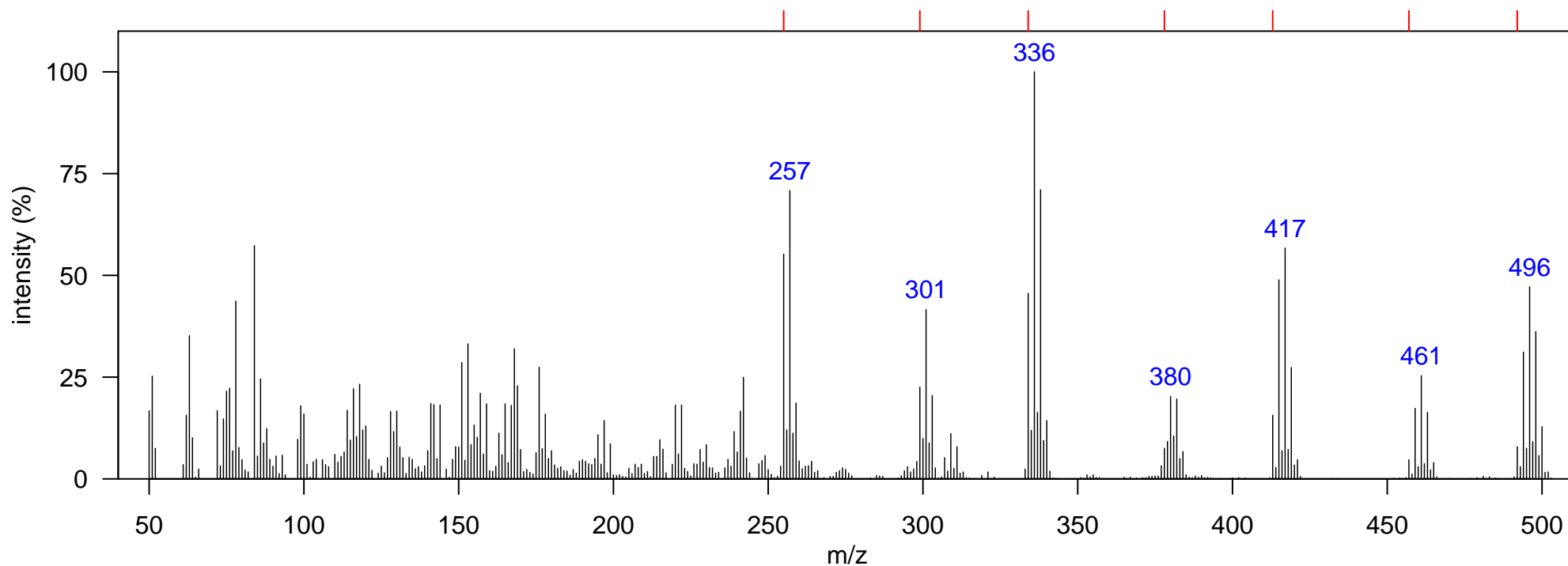
Comment:

Elemental Formula: C₉H₅Br₄ClN₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, Cl, 2H

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

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

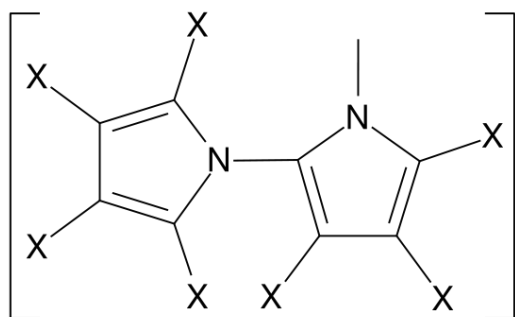
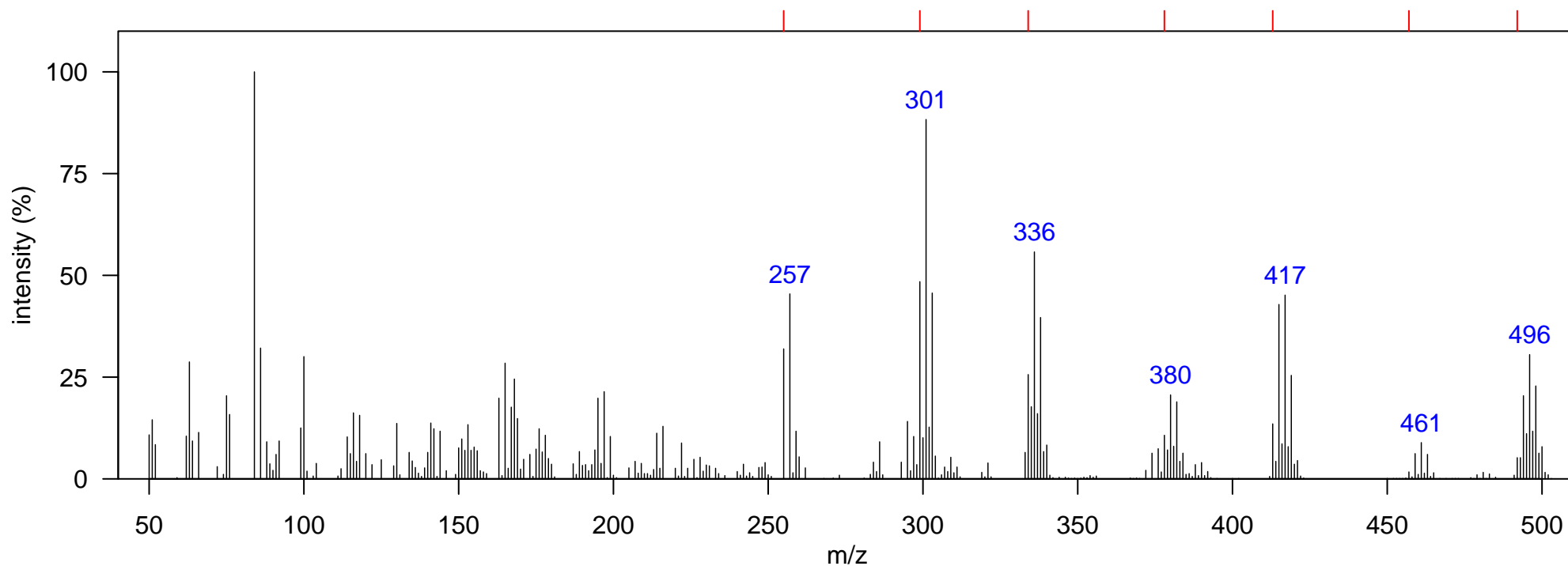
Comment:

Elemental Formula: C₉H₅Br₄ClN₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, Cl, 2H

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

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

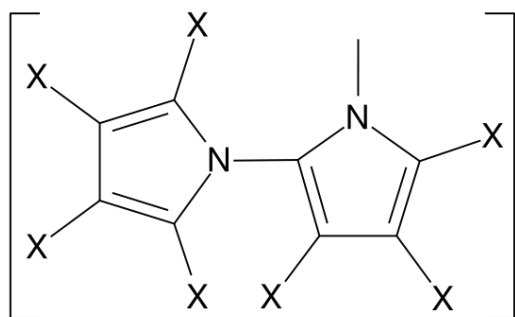
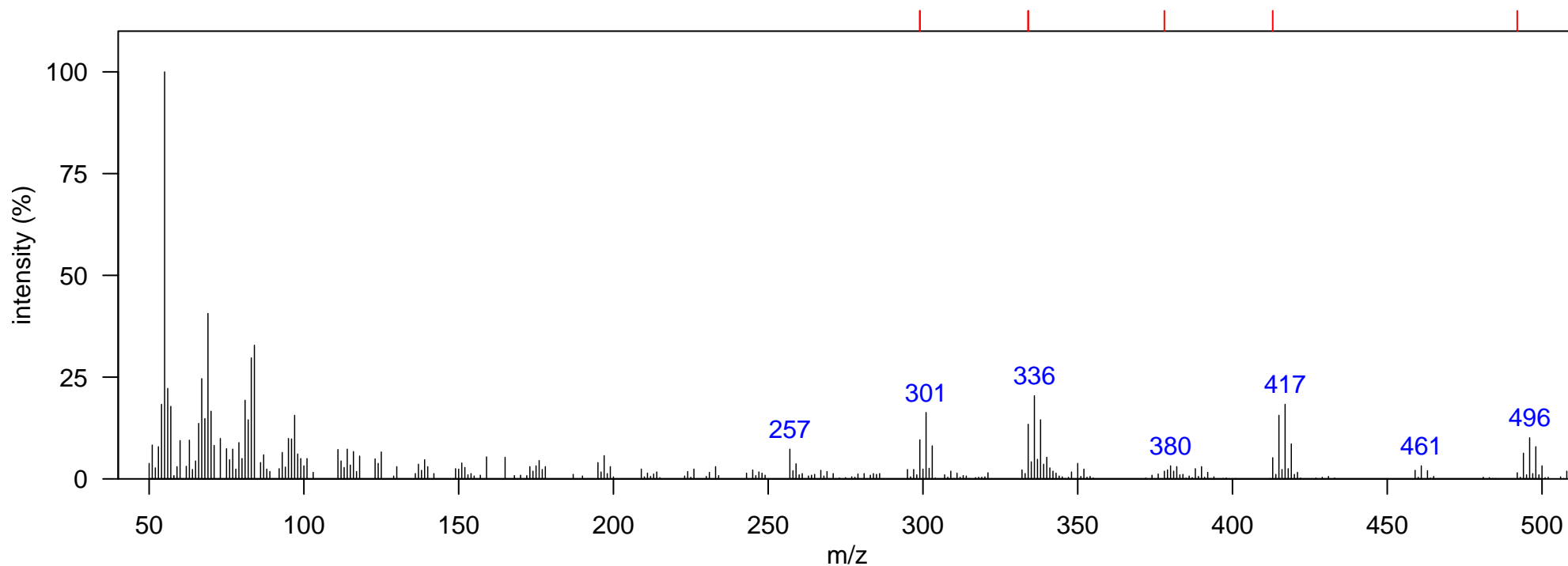
Comment:

Elemental Formula: C₉H₅Br₄ClN₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, Cl, 2H

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

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

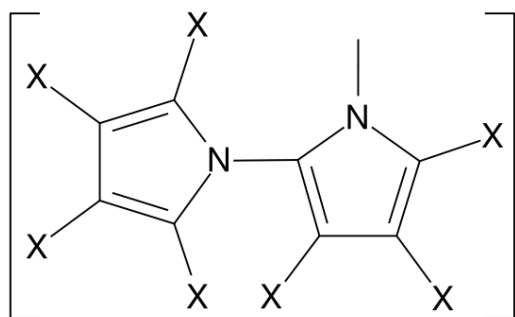
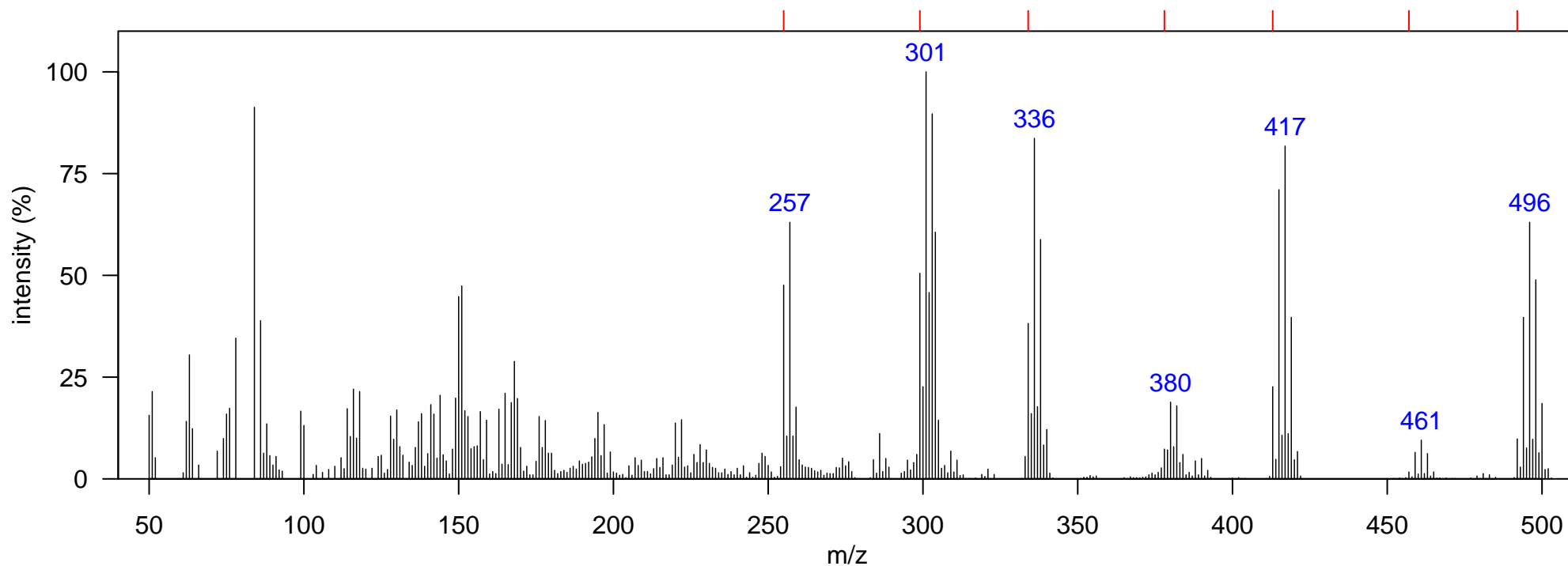
Comment:

Elemental Formula: C₉H₅Br₄ClN₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, Cl, 2H

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

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

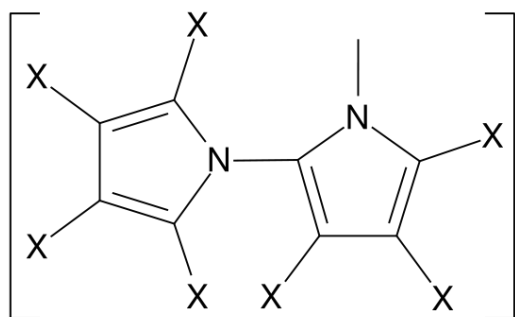
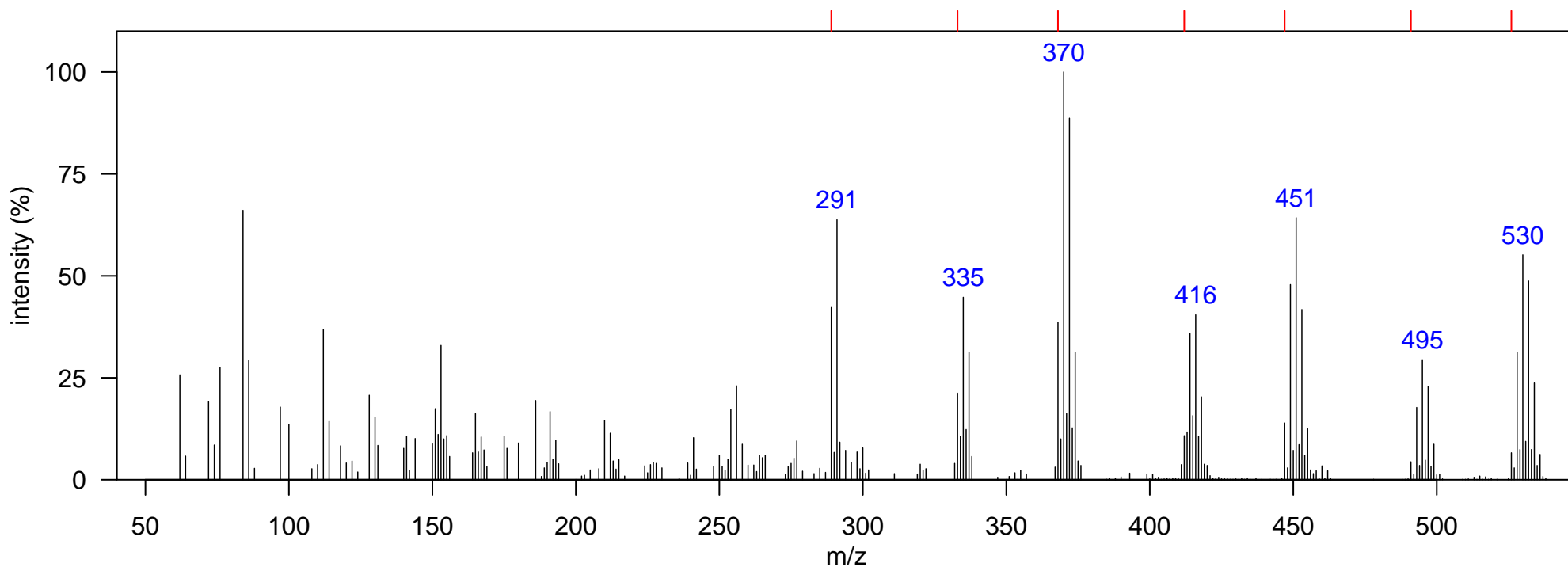
Comment:

Elemental Formula: C₉H₆Br₄Cl₂N₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, 2Cl, H

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

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

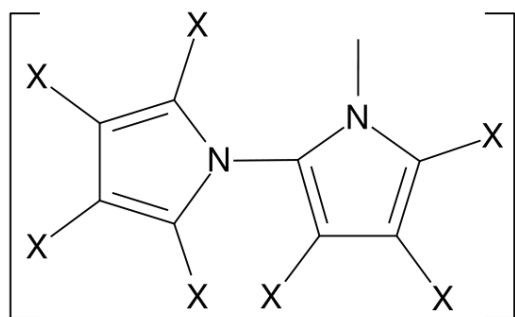
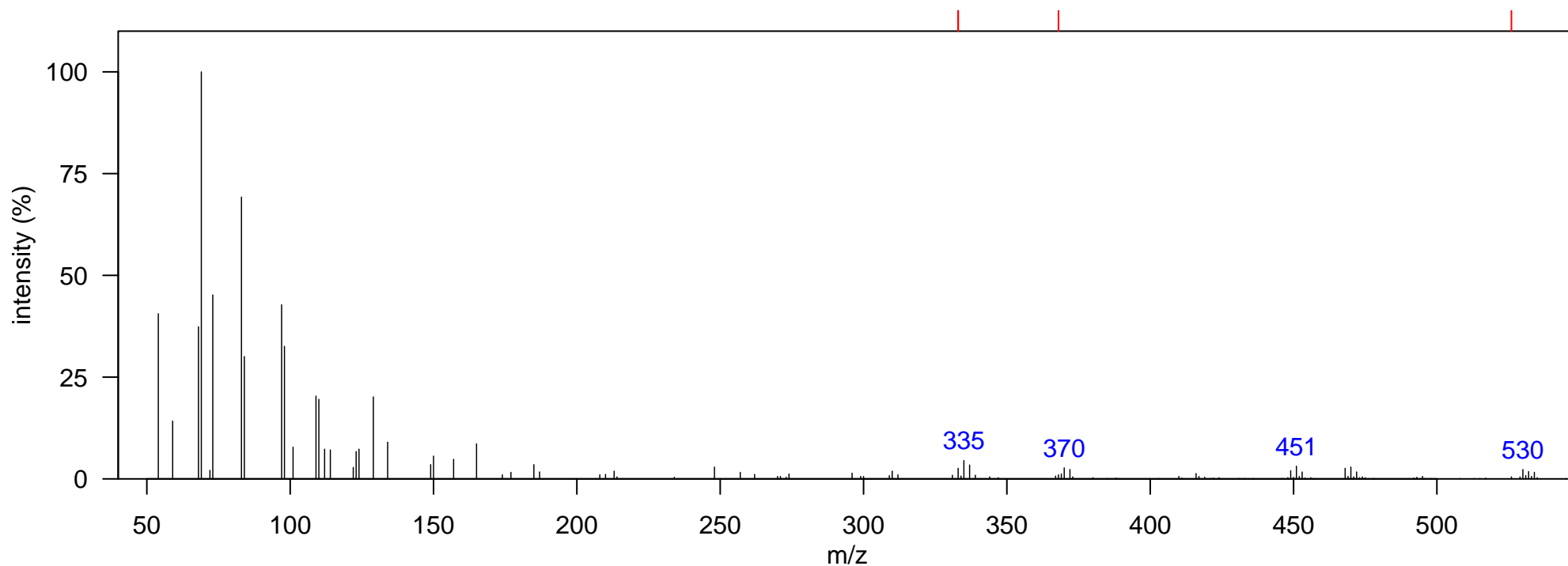
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₉H₆Br₄Cl₂N₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=4Br, 2Cl, H

m/z	Identity
333	[M-Br ₂ Cl] ⁺
368	[M-2Br] ⁺
526	M ⁺

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

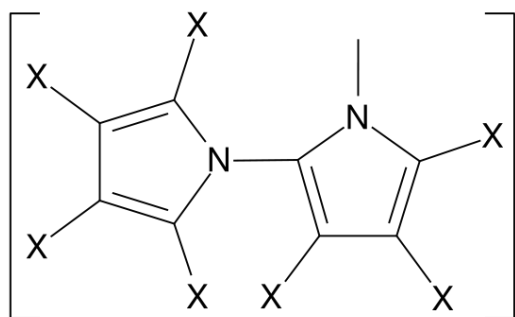
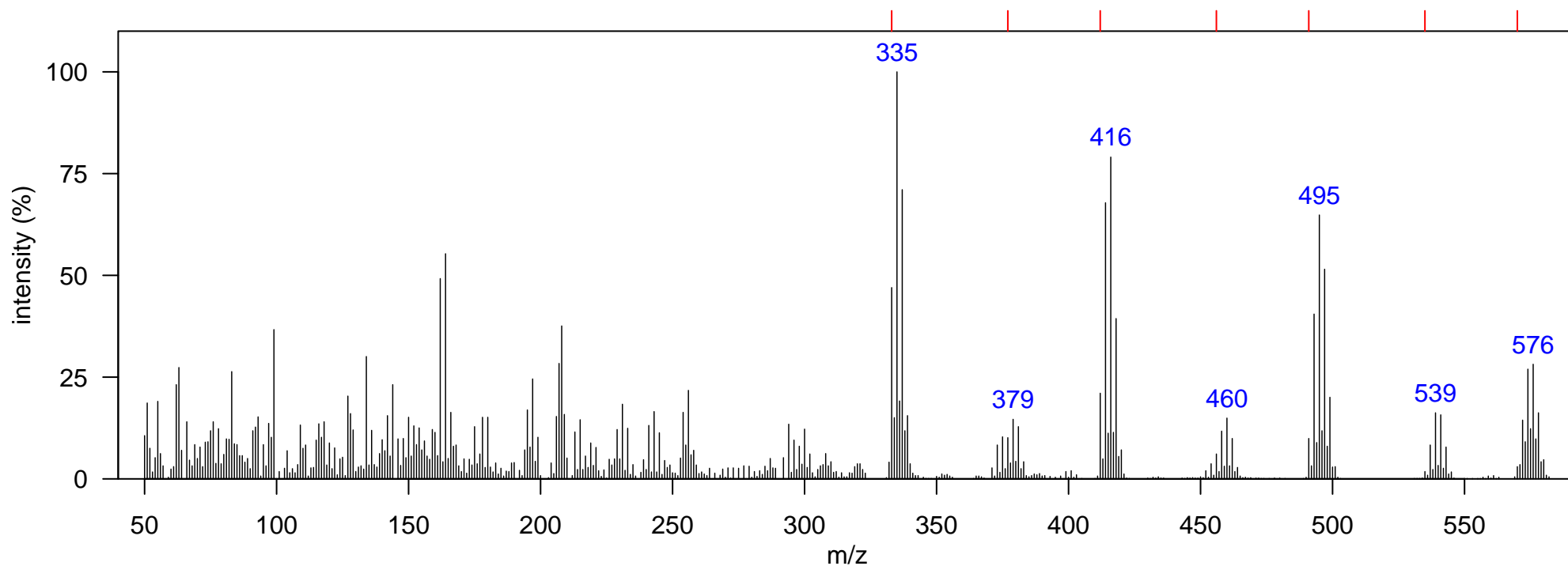
Comment:

Elemental Formula: C₉H₄Br₅ClN₂

Source: natural

Class: MBP

Identification: Authentic MS RT



X=5Br, Cl, H

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

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

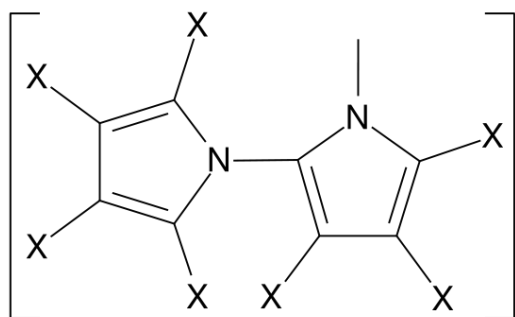
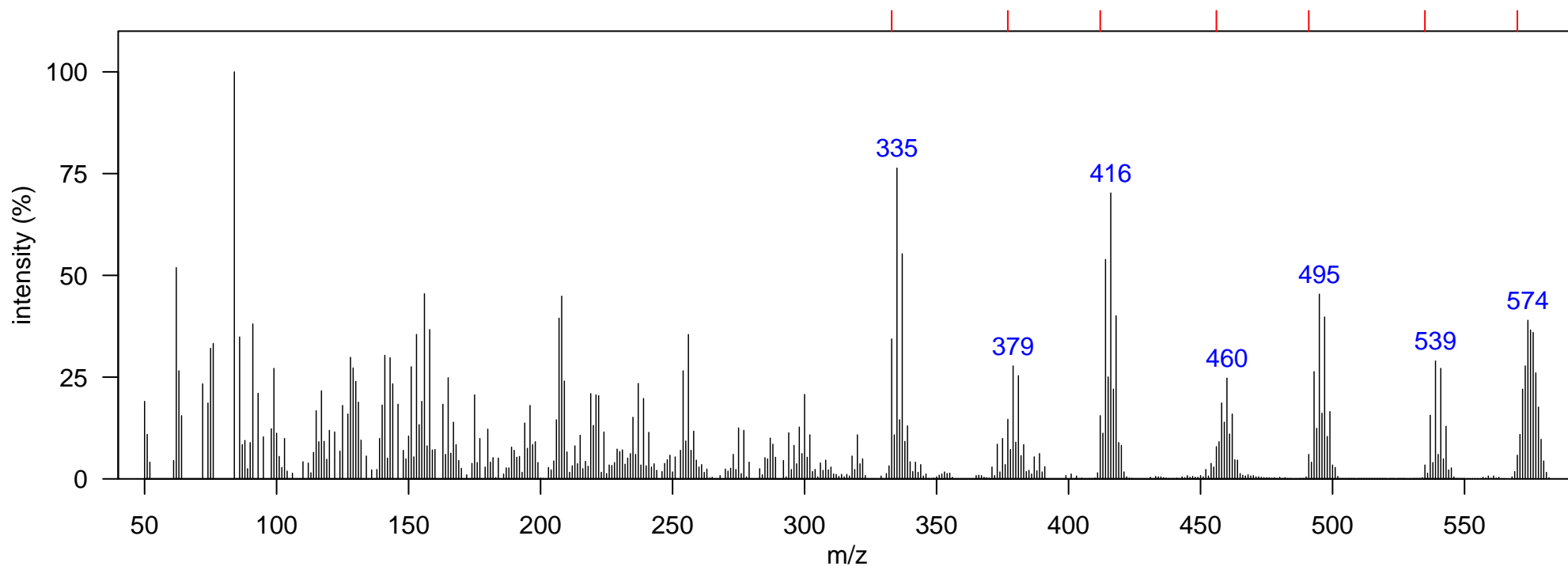
Comment:

Elemental Formula: C₉H₄Br₅ClN₂

Source: natural

Class: MBP

Identification: Authentic MS



X=5Br, Cl, H

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

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

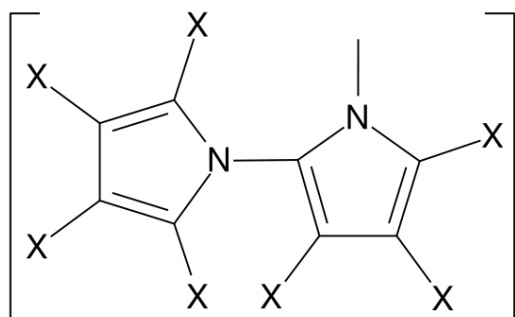
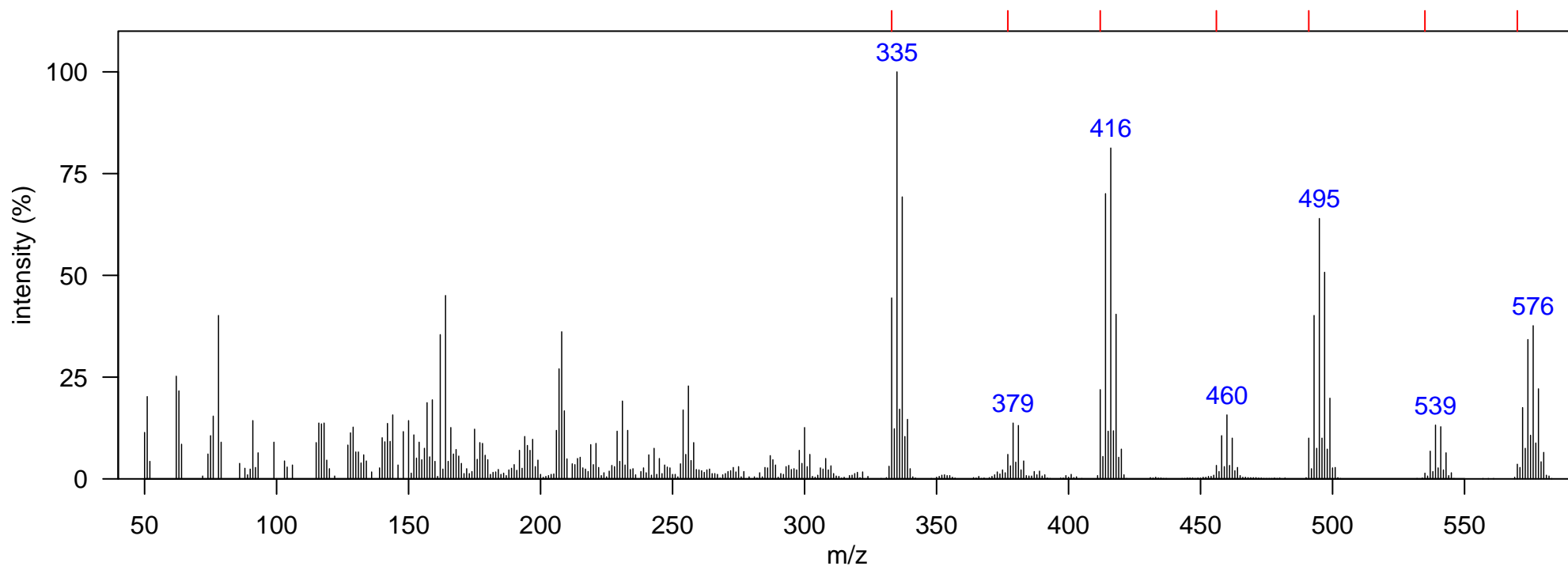
Comment:

Elemental Formula: C₉H₄Br₅ClN₂

Source: natural

Class: MBP

Identification: Authentic MS RT



X=5Br, Cl, H

m/z	Identity
333	[M-3Br] ⁺
377	[M-Br ₂ Cl] ⁺
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

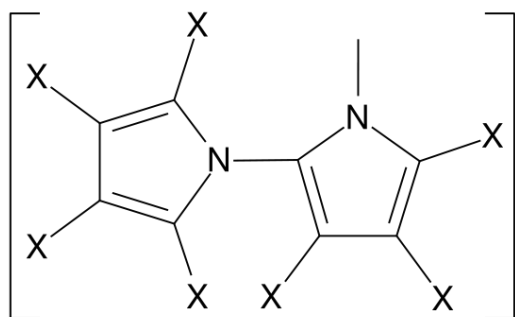
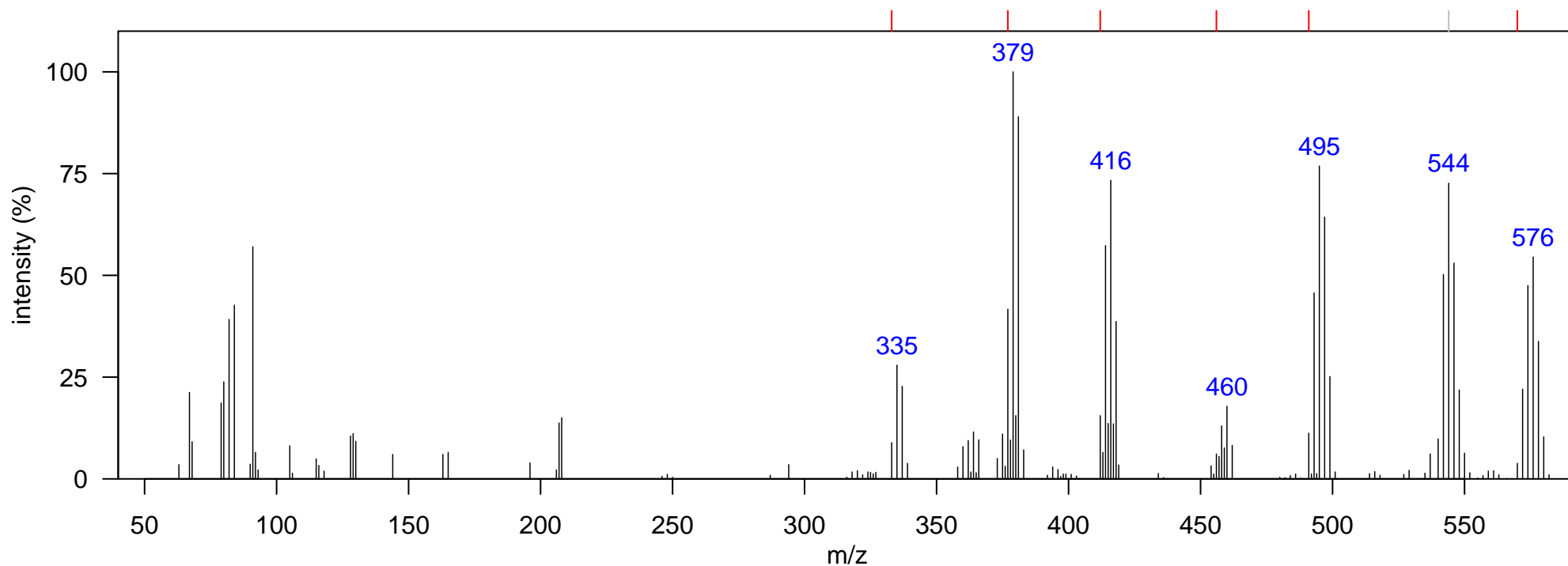
Comment:

Elemental Formula: C₉H₄Br₅ClN₂

Source: natural

Class: MBP

Identification: Authentic MS



X=5Br, Cl, H

m/z	Identity
333	[M-3Br] ⁺
377	[M-Br ₂ Cl] ⁺
412	[M-2Br] ⁺
456	[M-BrCl] ⁺
491	[M-Br] ⁺
544	interference DMBPBr ₄ Cl ₂
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

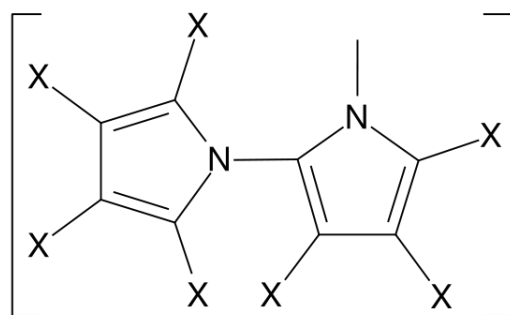
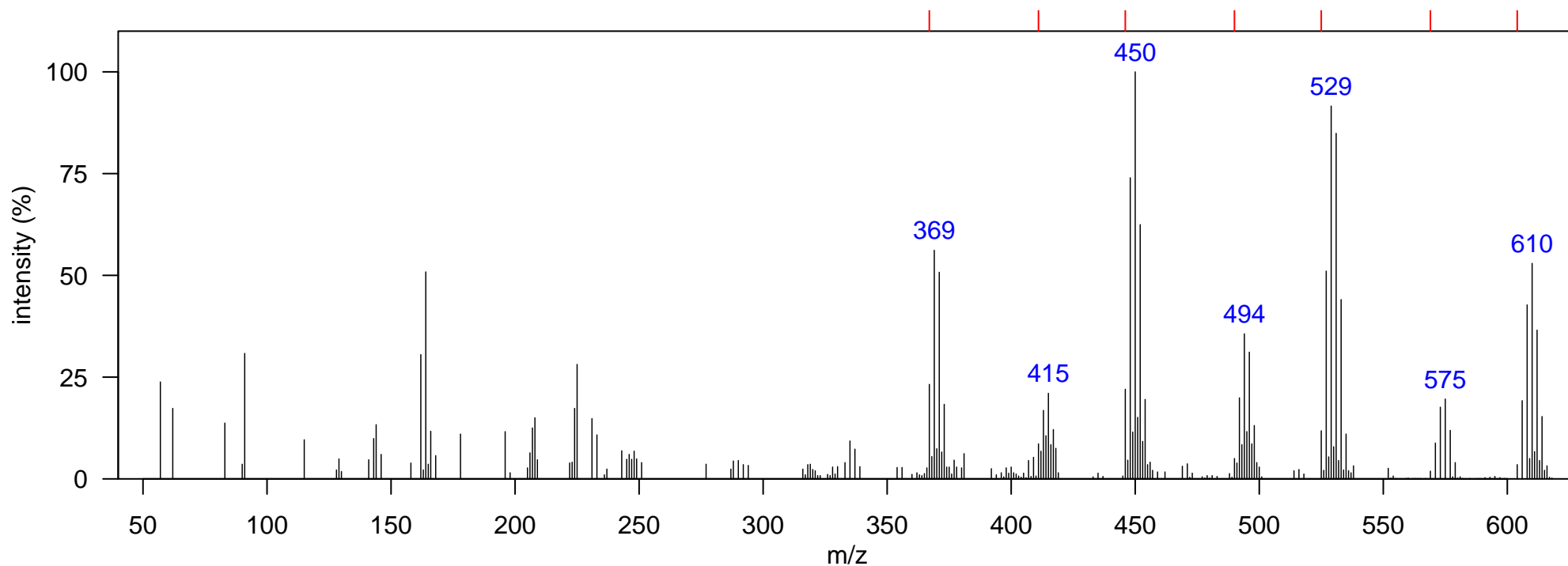
Comment:

Elemental Formula: C₉H₃Br₅Cl₂N₂

Source: natural

Class: MBP

Identification: Manual – Congener Group



X=5Br, 2Cl

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

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

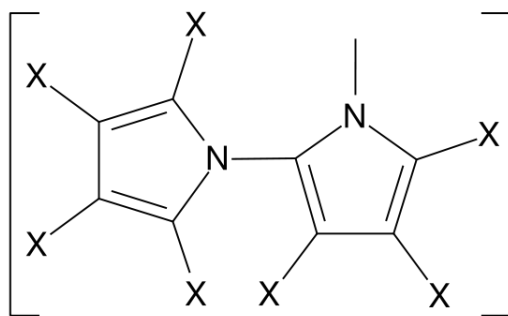
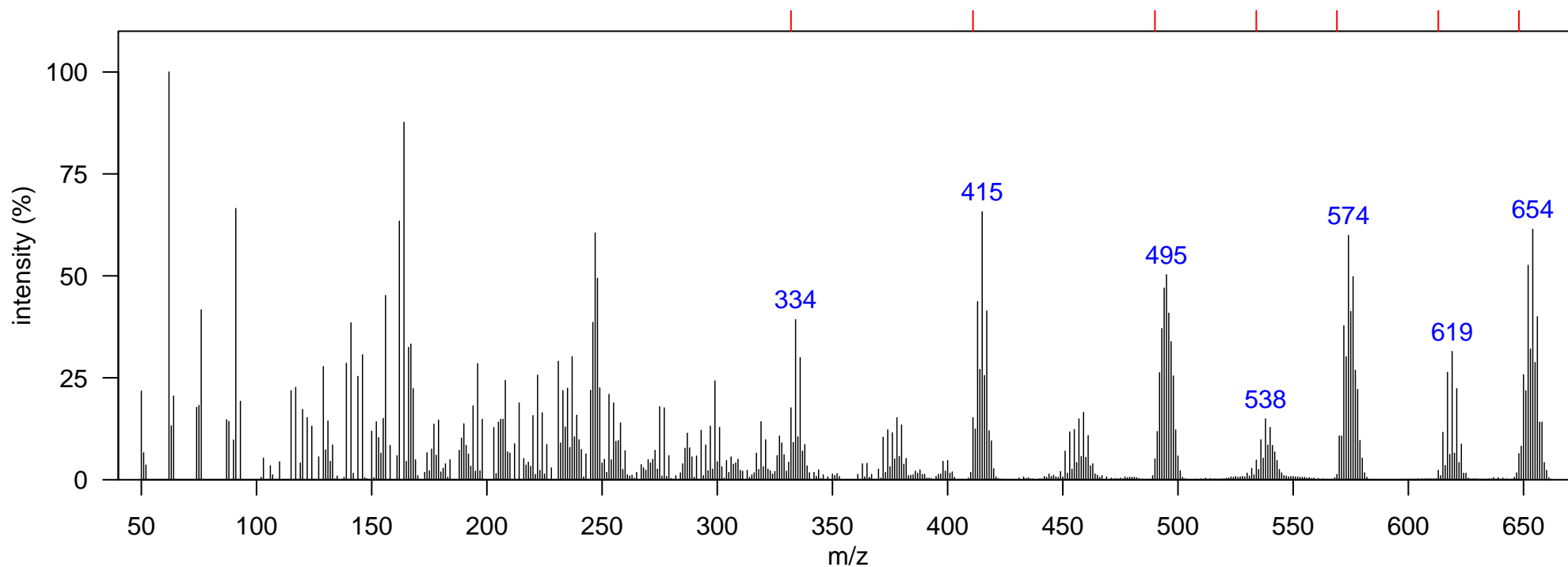
Comment:

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 ⁺

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

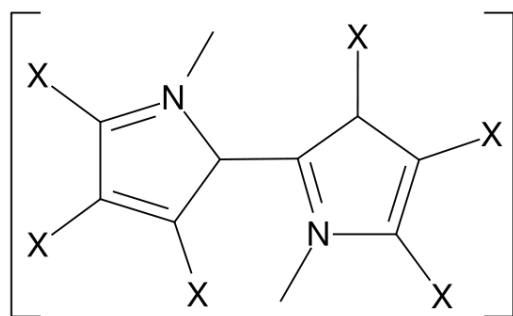
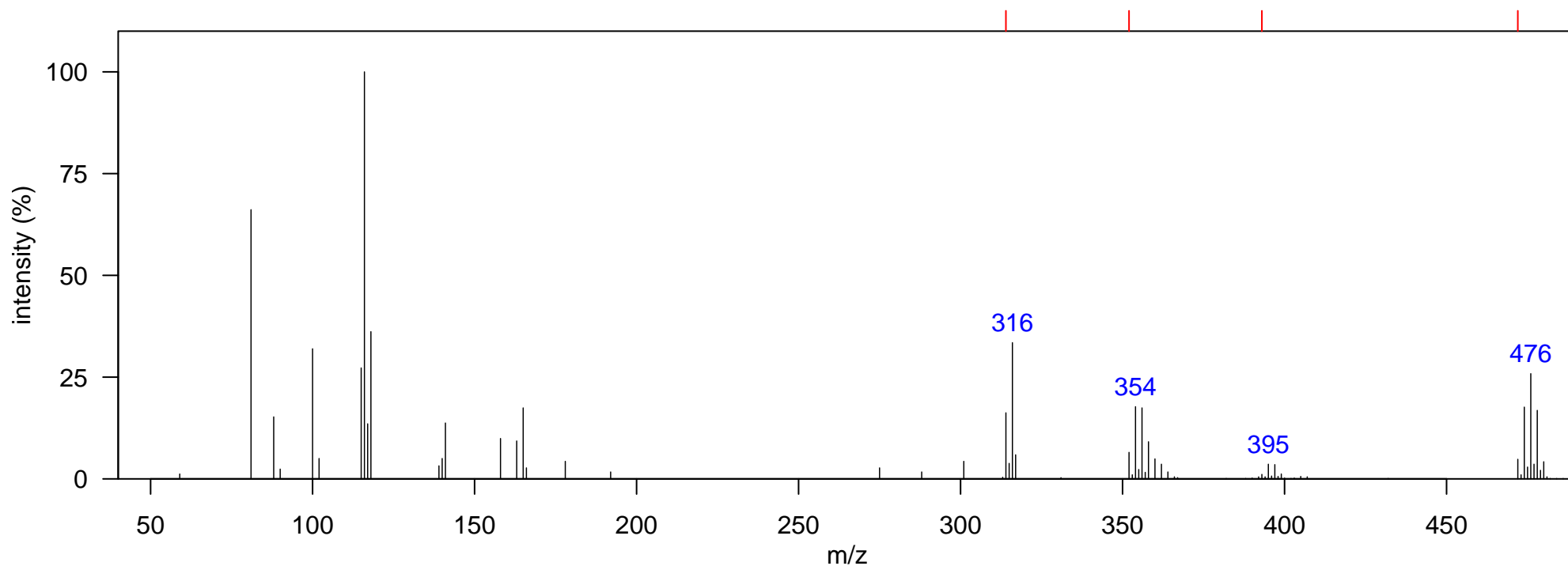
Comment:

Elemental Formula: C₁₀H₈Br₄N₂

Source: natural

Class: DMBP

Identification: Manual – Congener Group



X=4Br, 2H

m/z	Identity
314	[M-2Br] ⁺
352	[M-BrCNCH ₃] ⁺
393	[M-Br] ⁺
472	M ⁺

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

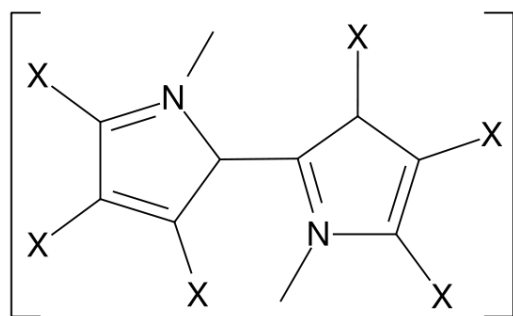
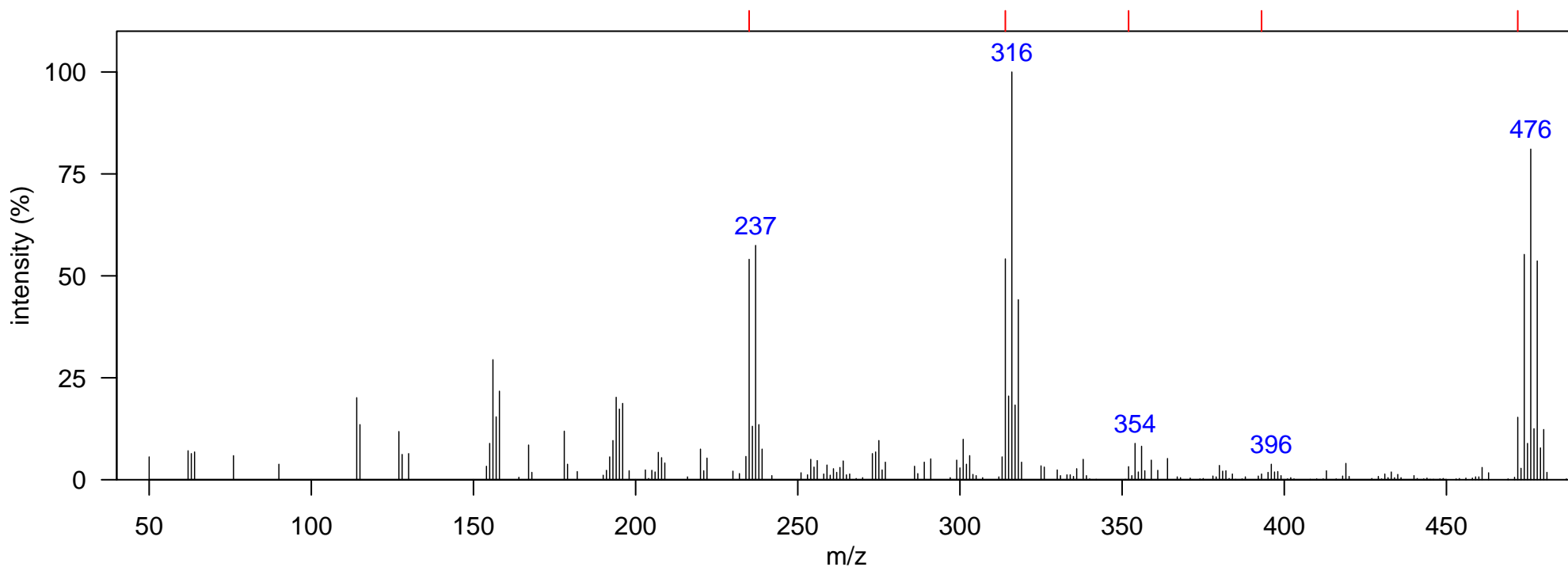
Comment:

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-BrCNCH ₃] ⁺
393	[M-Br] ⁺
472	M ⁺
498	interference

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

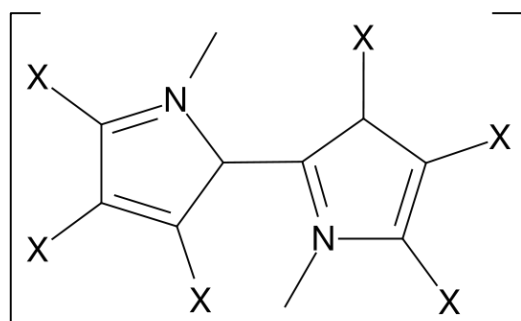
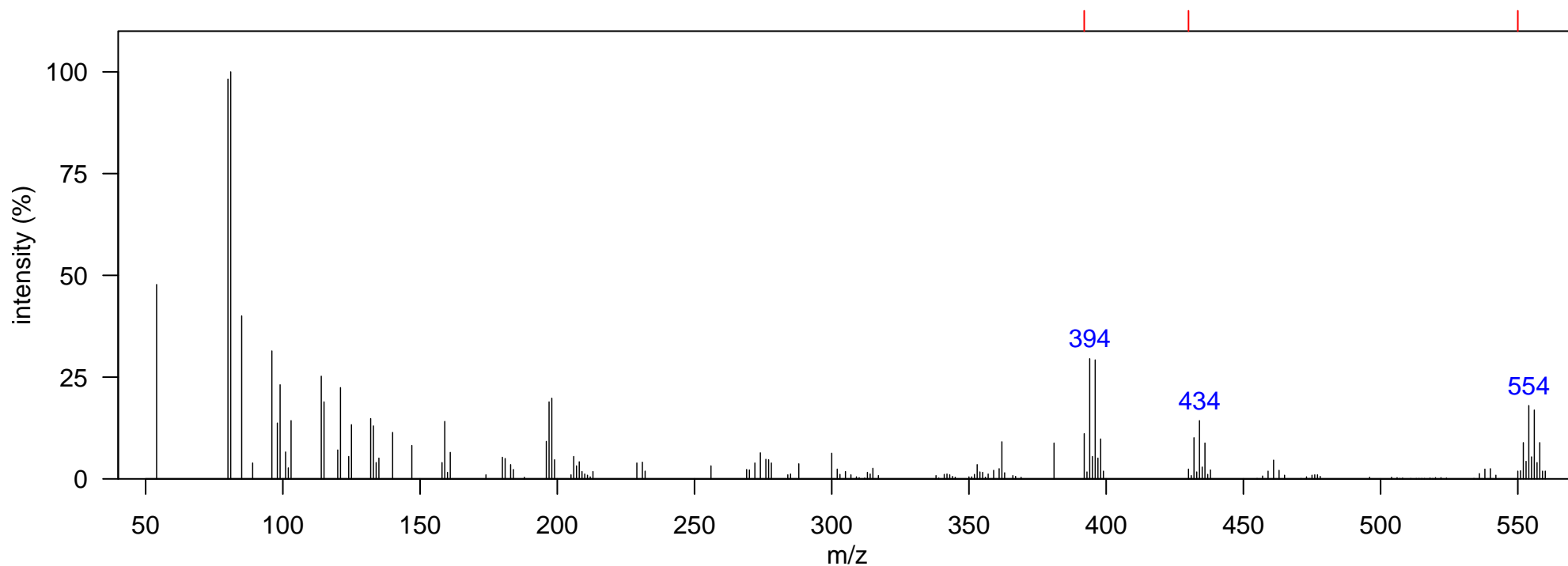
Comment:

Elemental Formula: C₁₀H₇Br₅N₂

Source: natural

Class: DMBP

Identification: Manual – Congener Group



X=5Br, H

m/z	Identity
392	[M-2Br] ⁺
430	[M-BrCNCH ₃] ⁺
550	M ⁺

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

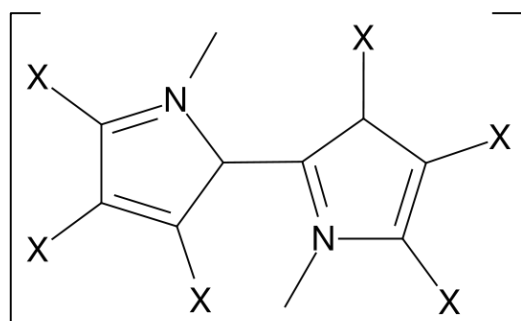
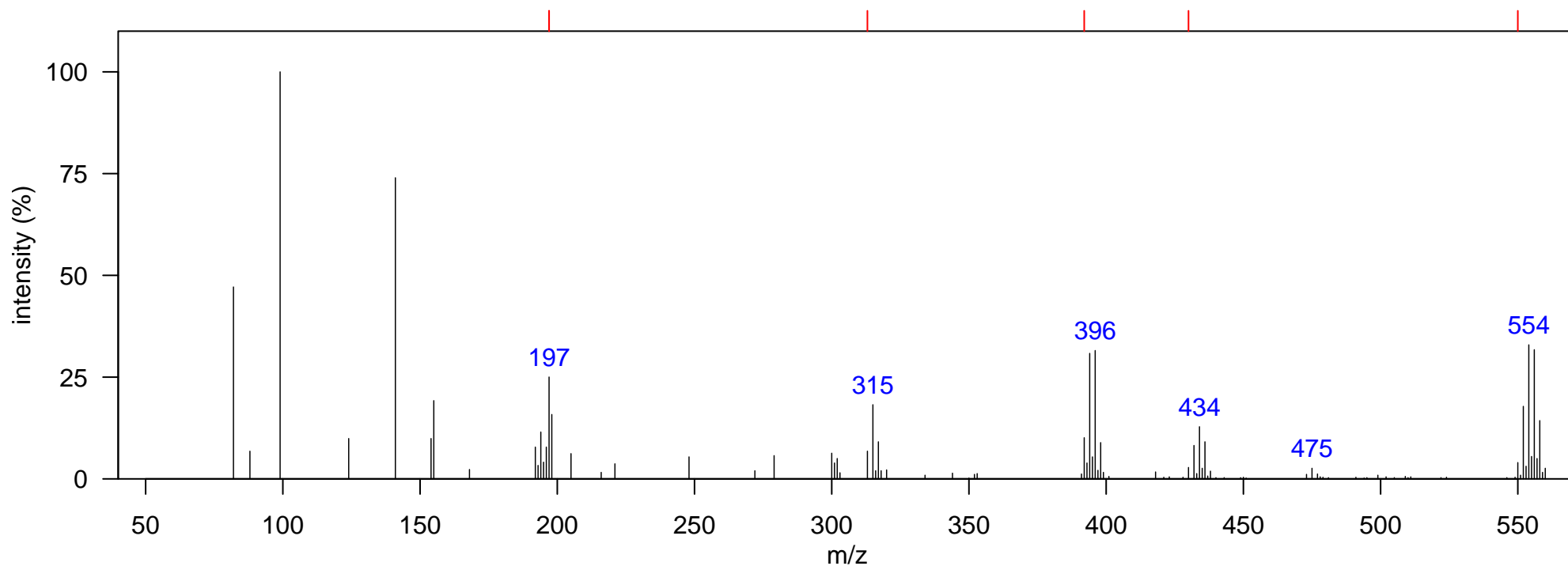
Comment:

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-BrCNCH ₃] ⁺
550	M ⁺

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

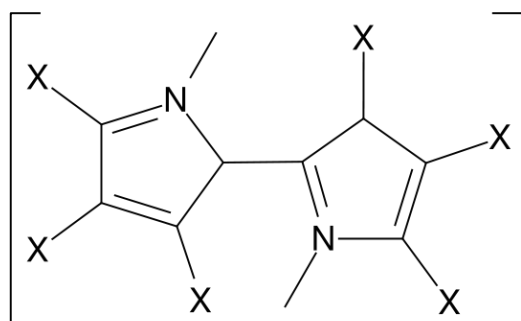
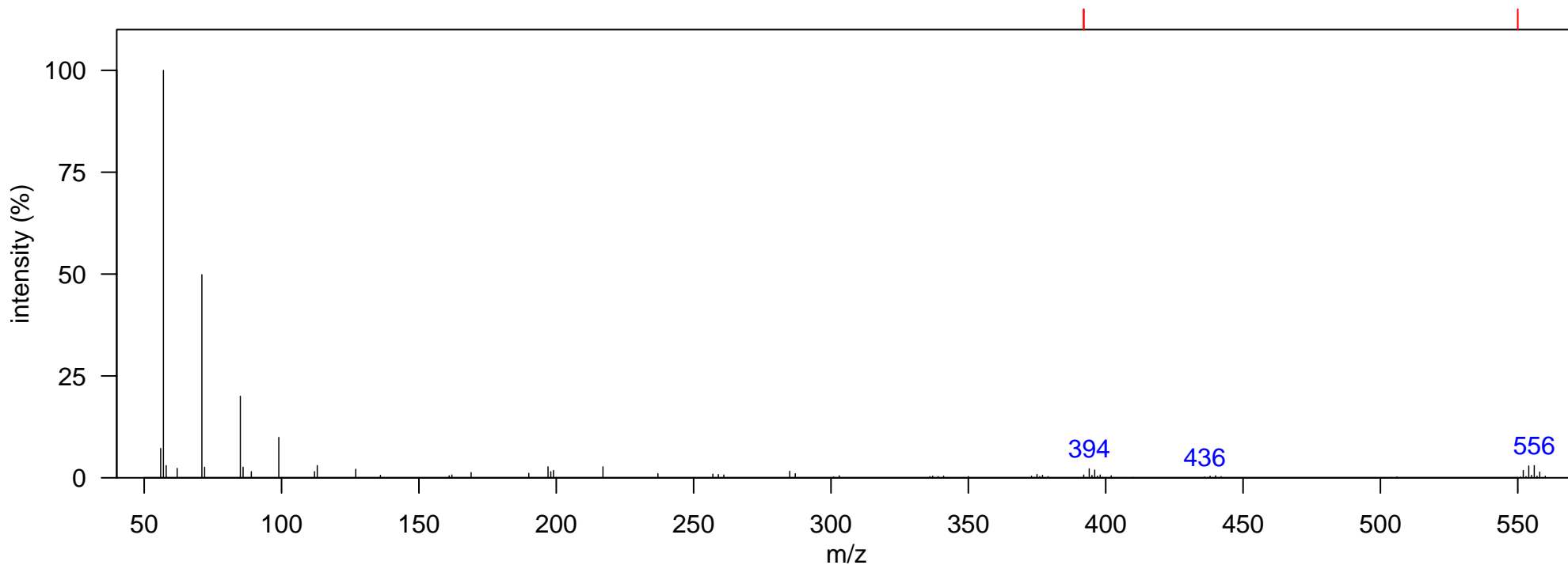
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₁₀H₇Br₅N₂

Source: natural

Class: DMBP

Identification: Manual – Congener Group



X=5Br, H

m/z	Identity
392	[M-2Br] ⁺
550	M ⁺

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

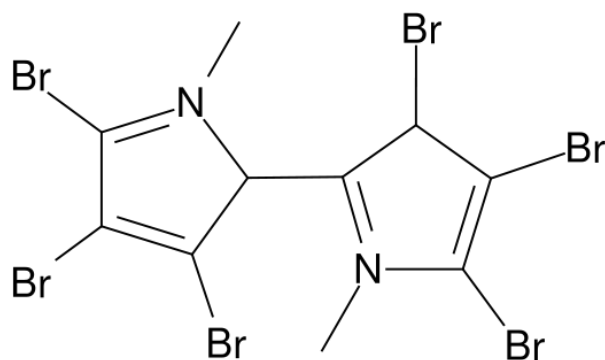
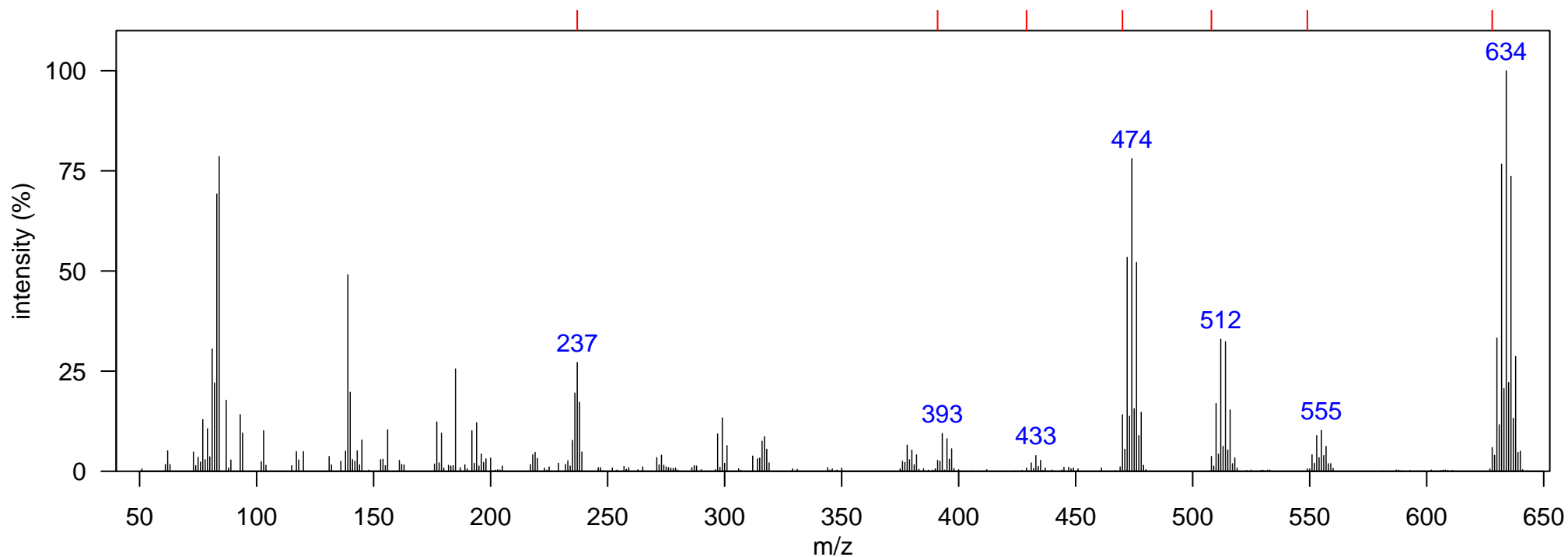
Comment:

Elemental Formula: C₁₀H₆Br₆N₂

Source: natural

Class: DMBP

Identification: Authentic MS RT



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

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

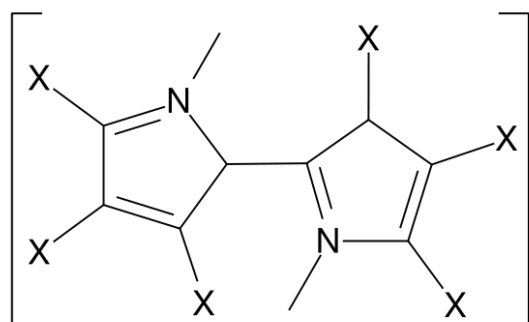
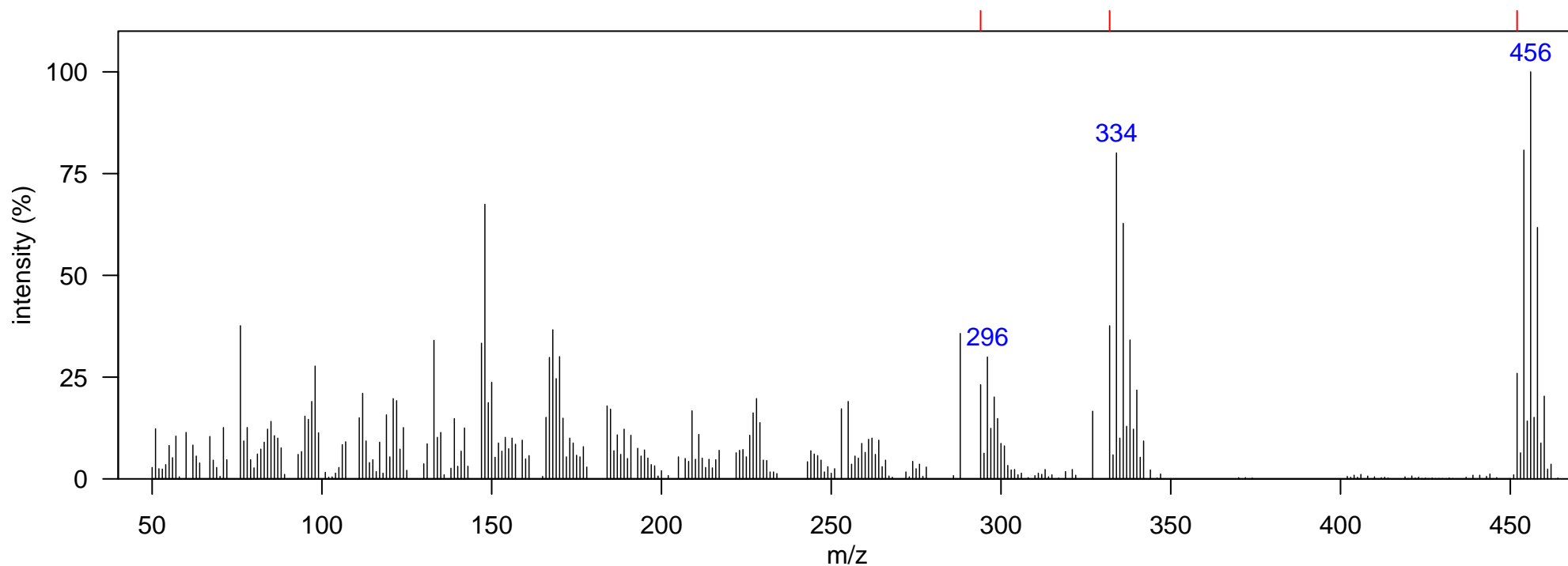
Comment:

Elemental Formula: C₁₀H₆Br₂Cl₄N₂

Source: natural

Class: DMBP

Identification: Manual – Congener Group



X=2Br, 4Cl

m/z	Identity
294	[M-2Br] ⁺
332	[M-BrCNCH ₃]
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

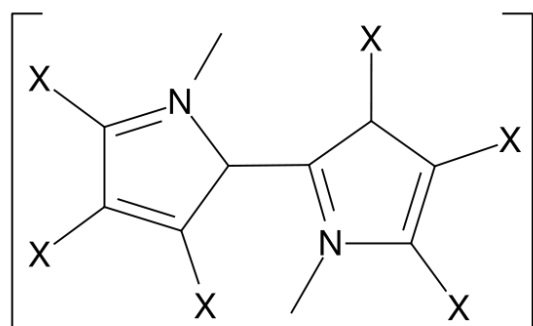
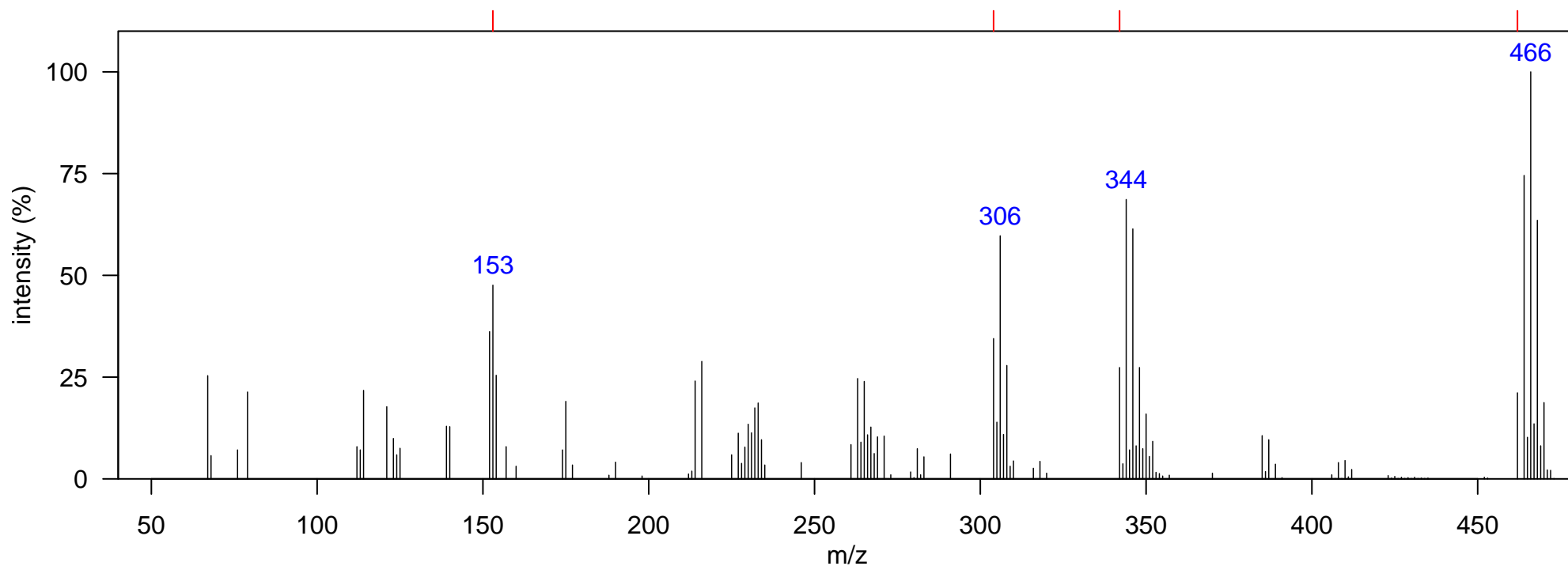
Comment:

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-BrCNCH ₃] ⁺
462	M ⁺

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

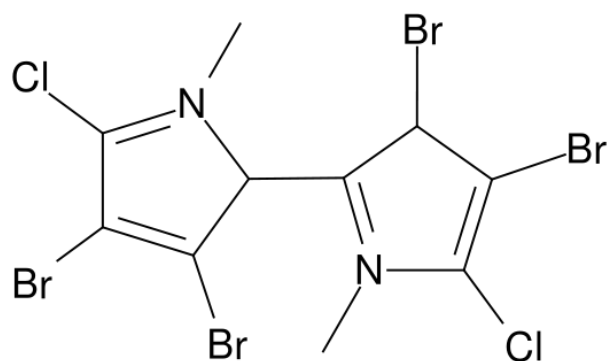
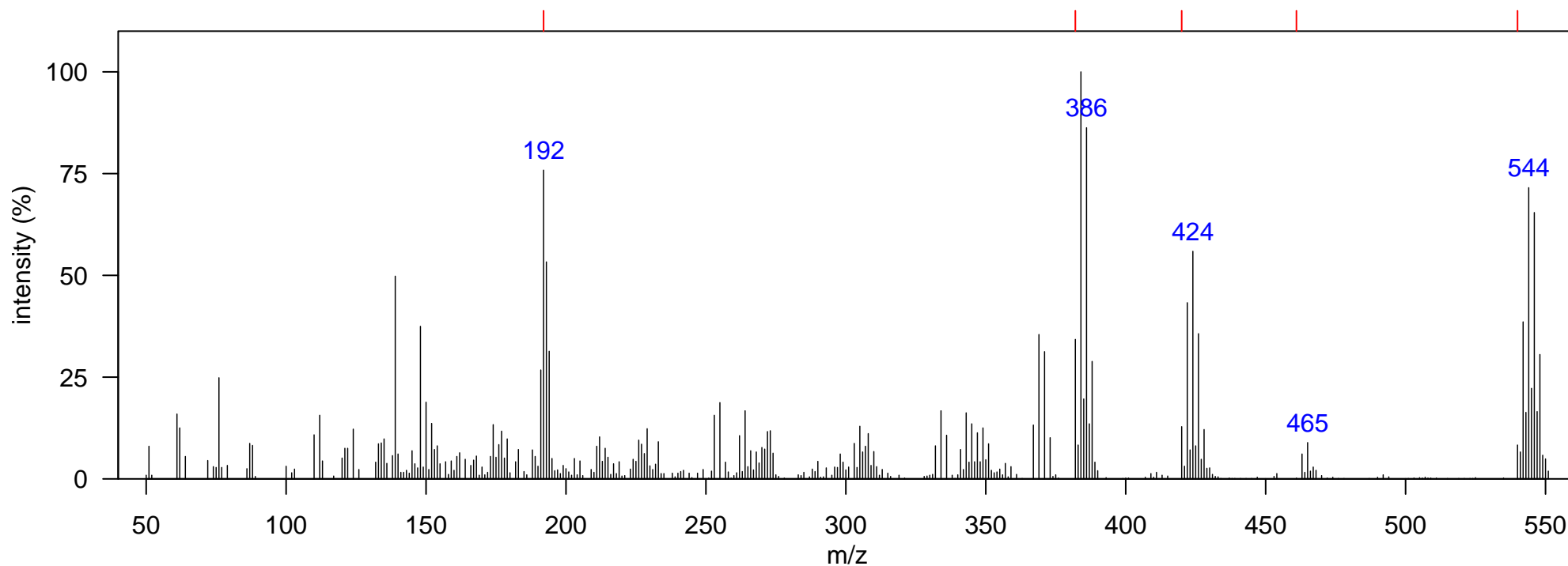
Comment:

Elemental Formula: C₁₀H₆Br₄Cl₂N₂

Source: natural

Class: DMBP

Identification: Authentic MS RT



m/z	Identity
192	[M-2Br] ²⁺
382	[M-2Br] ⁺
420	[M-BrCNCH ₃] ⁺
461	[M-Br] ⁺
540	M ⁺

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

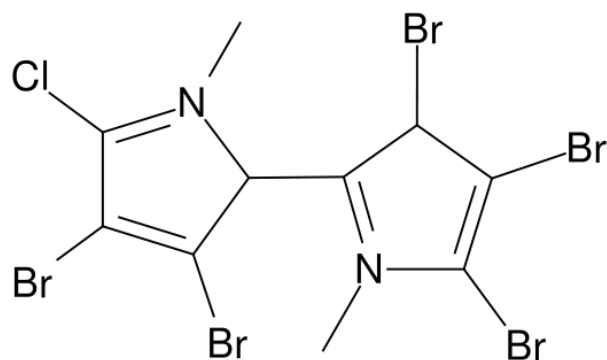
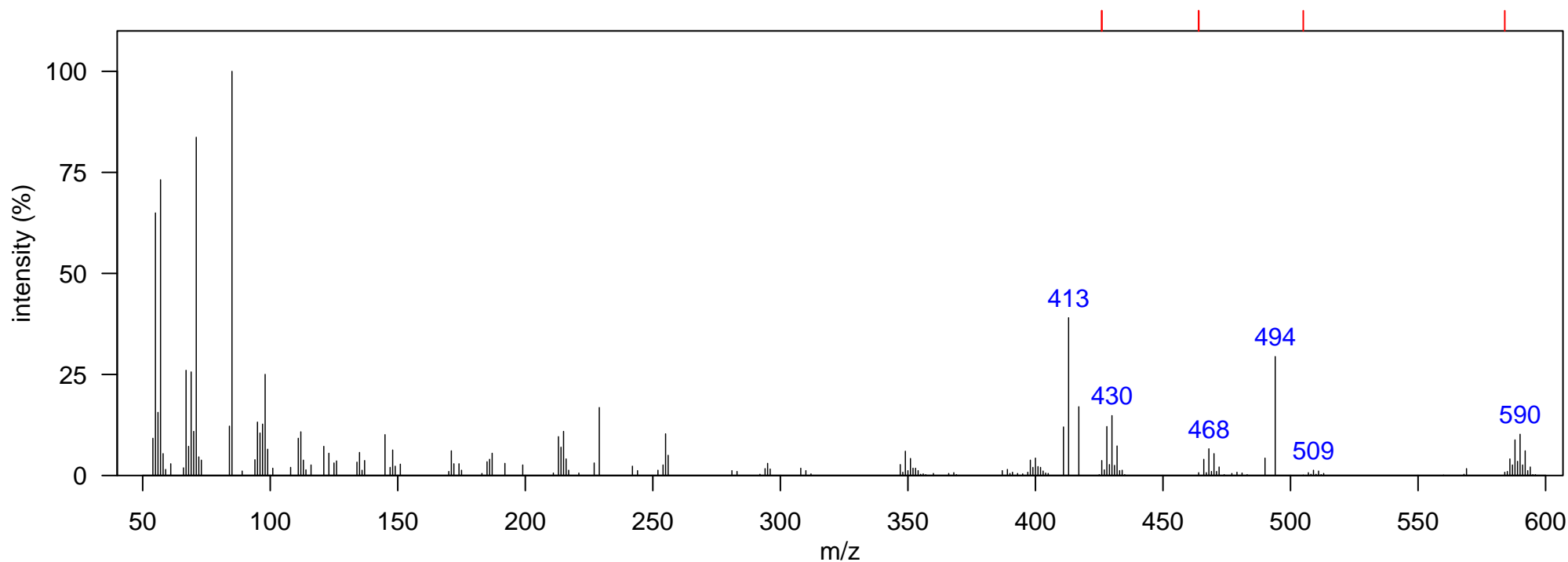
Comment:

Elemental Formula: C₁₀H₆Br₅ClN₂

Source: natural

Class: DMBP

Identification: Authentic MS RT



m/z	Identity
426	[M-2Br] ⁺
464	[M-BrCNCH ₃] ⁺
505	[M-Br] ⁺
584	M ⁺

Name: tribromophenol

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

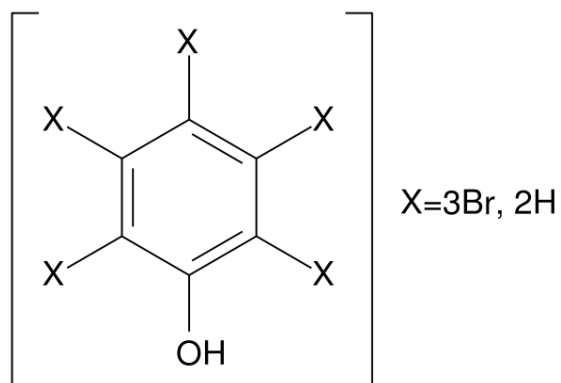
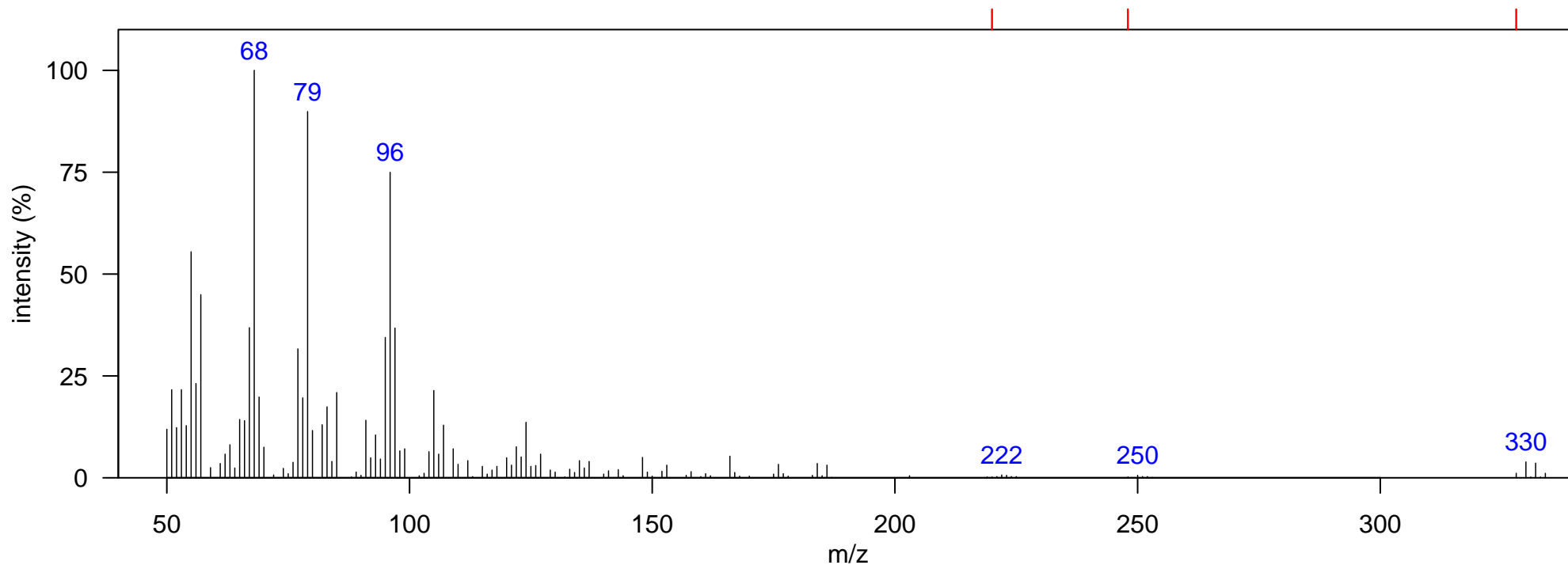
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₆H₃Br₃O

Source: natural/anthropogenic

Class: bromophenol

Identification: Reference Database MS



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

Name: tribromoanisoole: 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

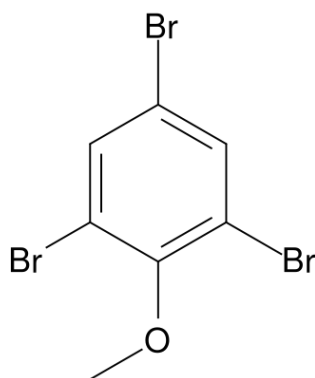
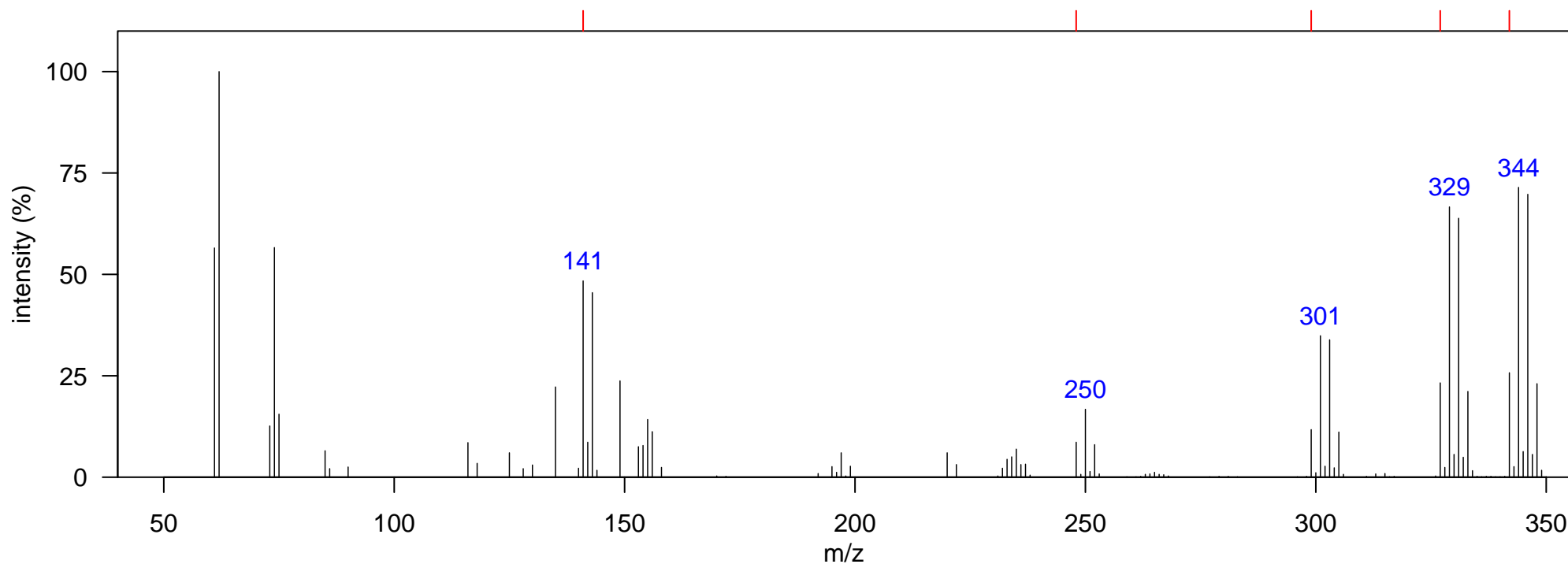
Comment:

Elemental Formula: C₇H₅Br₃O

Source: natural

Class: brominated anisole

Identification: Authentic MS RT



m/z	Identity
141	[C ₅ H ₂ Br] ⁺
248	[M-Br-CH ₃] ⁺
299	[M-CH ₃ -CO] ⁺
327	[M-CH ₃] ⁺
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

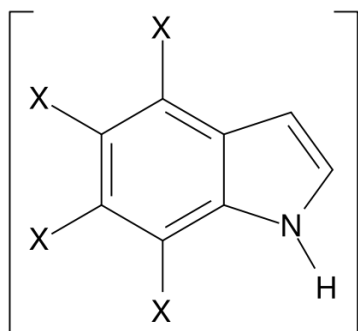
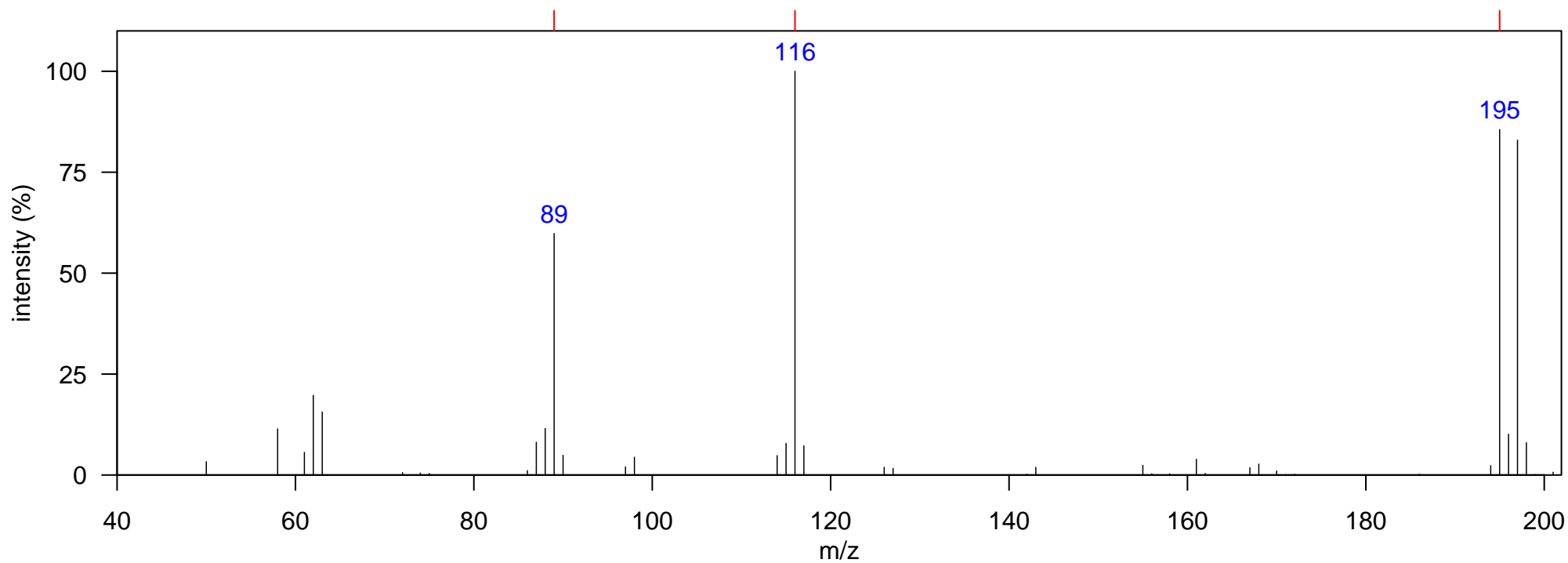
Comment:

Elemental Formula: C₈H₆BrN

Source: natural

Class: brominated indole

Identification: Authentic MS



X=Br, 3H

m/z	Identity
89	[M-Br-CN ⁺ H]
116	[M-Br] ⁺
195	M ⁺

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

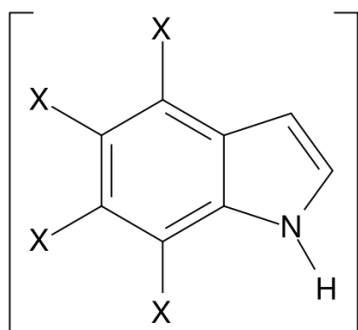
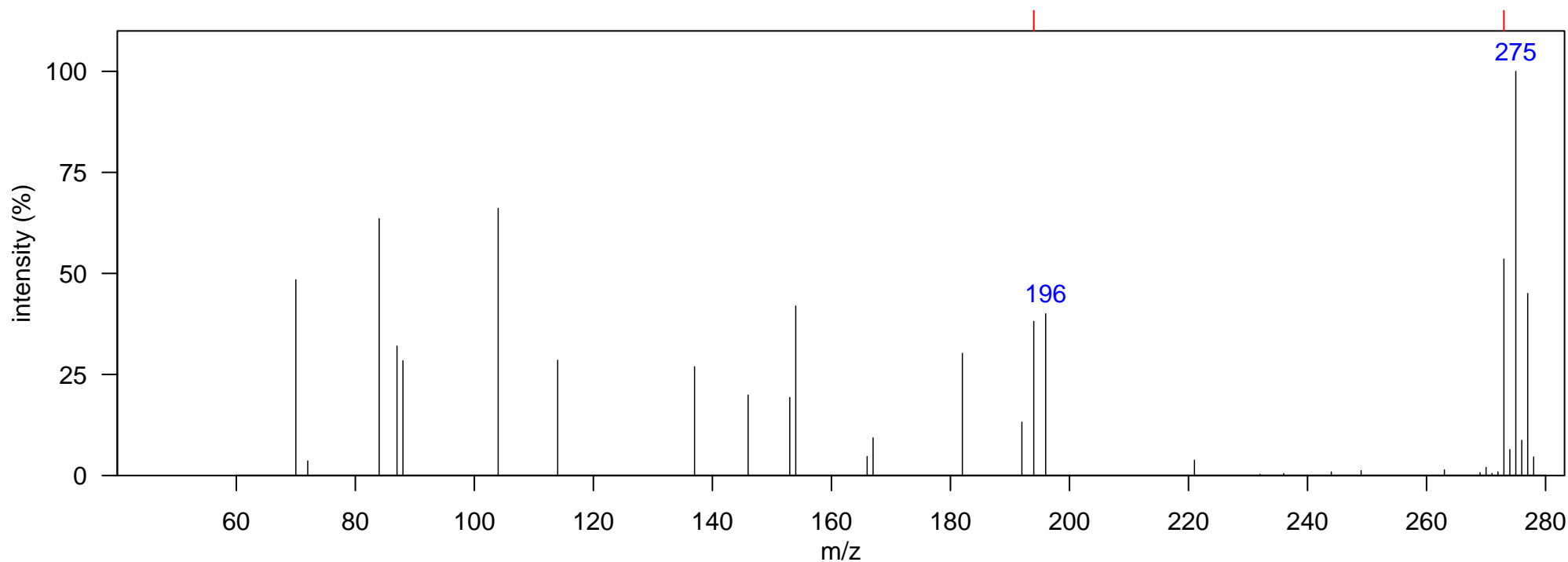
Comment:

Elemental Formula: C₈H₅Br₂N

Source: natural

Class: brominated indole

Identification: Authentic MS



X=2Br, 2H

m/z	Identity
194	[M-Br] ⁺
273	M ⁺

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

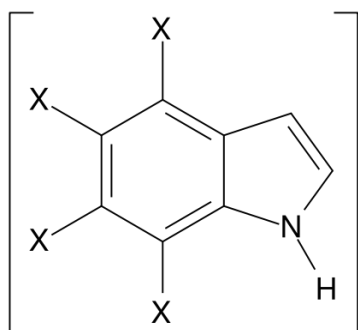
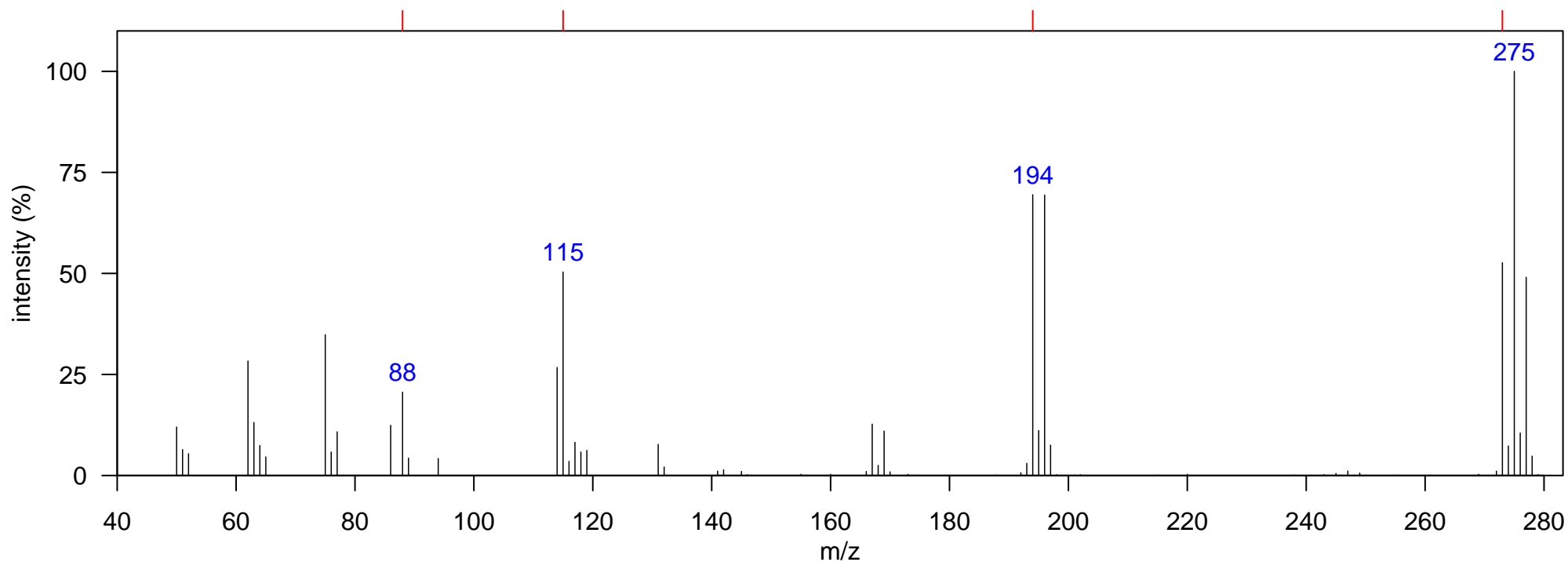
Comment:

Elemental Formula: C₈H₅Br₂N

Source: natural

Class: brominated indole

Identification: Authentic MS



X=2Br, 2H

m/z	Identity
88	[M-2Br-CN _H] ⁺
115	[M-2Br] ⁺
194	[M-Br] ⁺
273	M ⁺

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

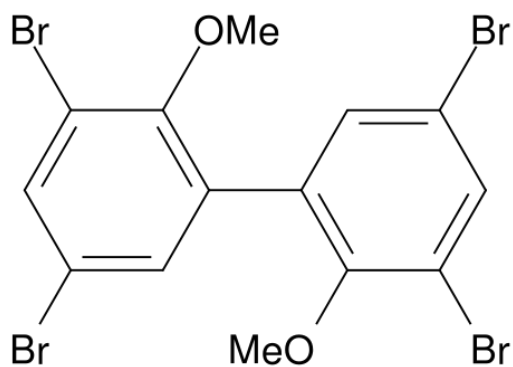
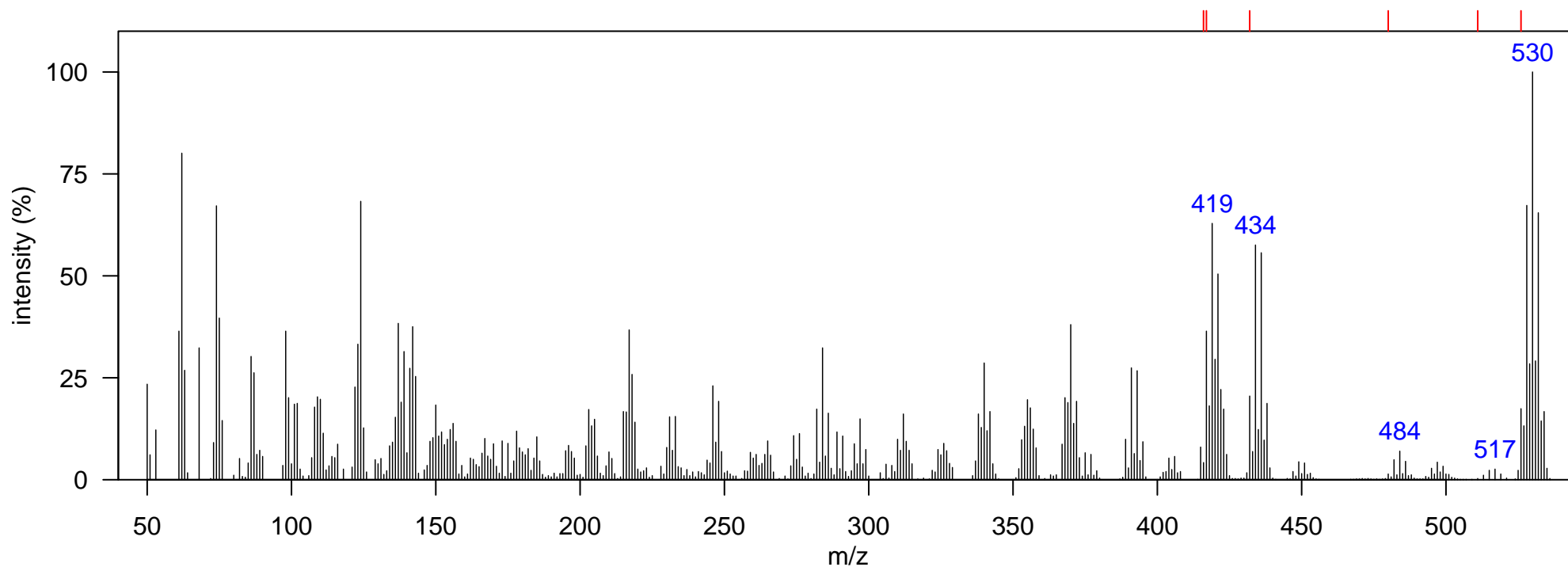
Comment:

Elemental Formula: C₁₄H₁₀Br₄O₂

Source: natural

Class: 2MeO–BB

Identification: Authentic MS RT



m/z	Identity
416	[M–CH ₃ –Br–O] ⁺
417	[M–CH ₃ –CH ₃ –Br] ⁺
432	[M–CH ₃ –Br] ⁺
480	[M–CH ₃ –CH ₃ –O] ⁺
511	[M–CH ₃] ⁺
526	M ⁺

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

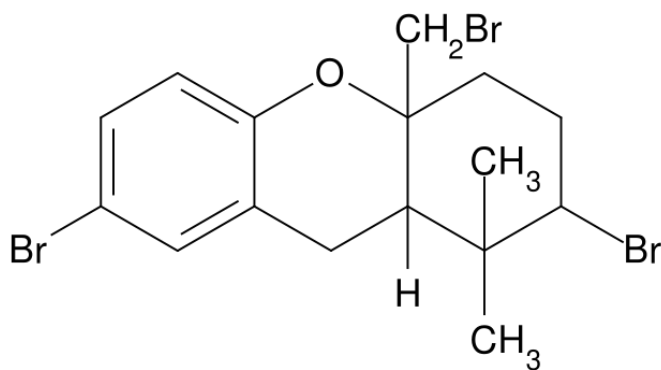
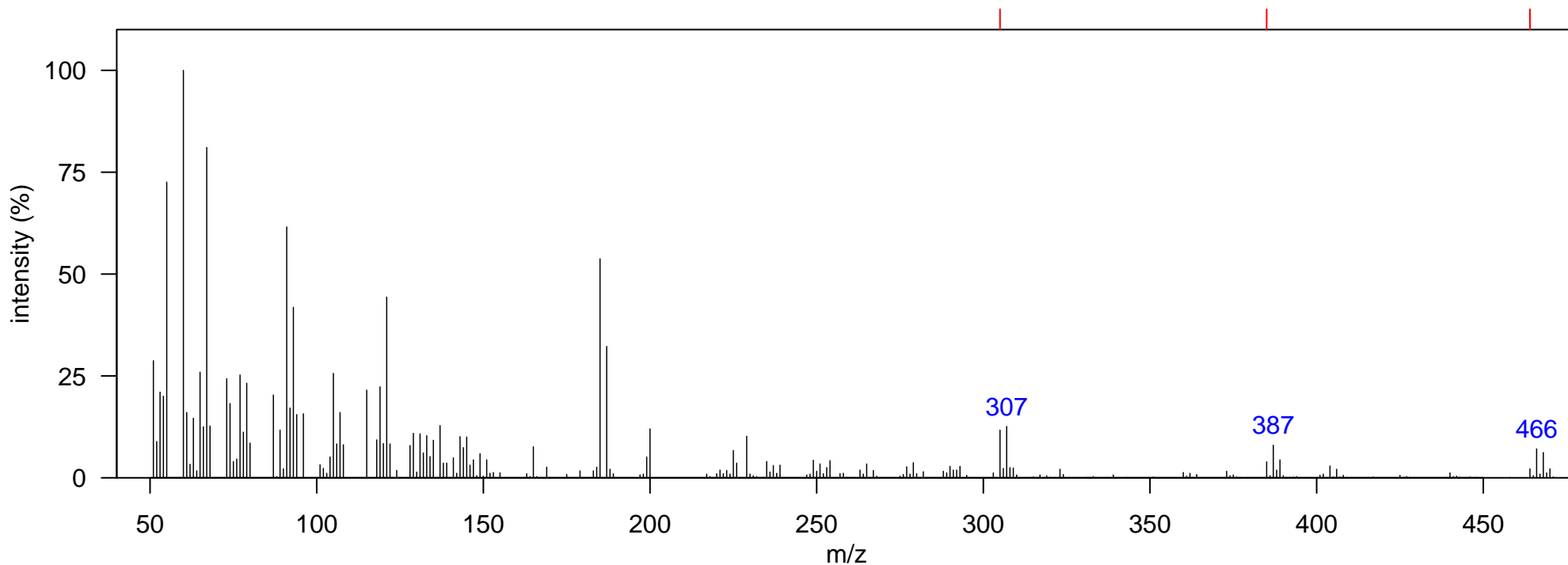
Comment: Low intensity, but visible in raw data.

Elemental Formula: C₁₆H₁₆Br₃O

Source: natural

Class: PBHD

Identification: Authentic MS RT



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

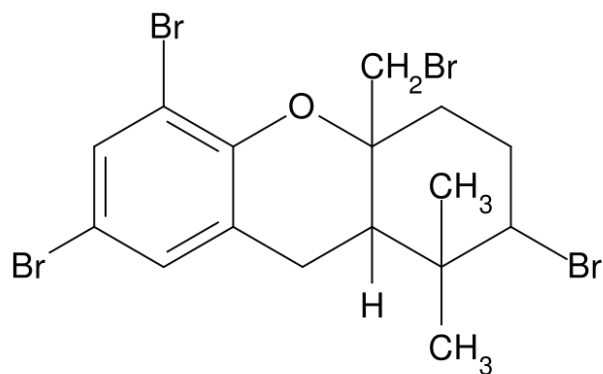
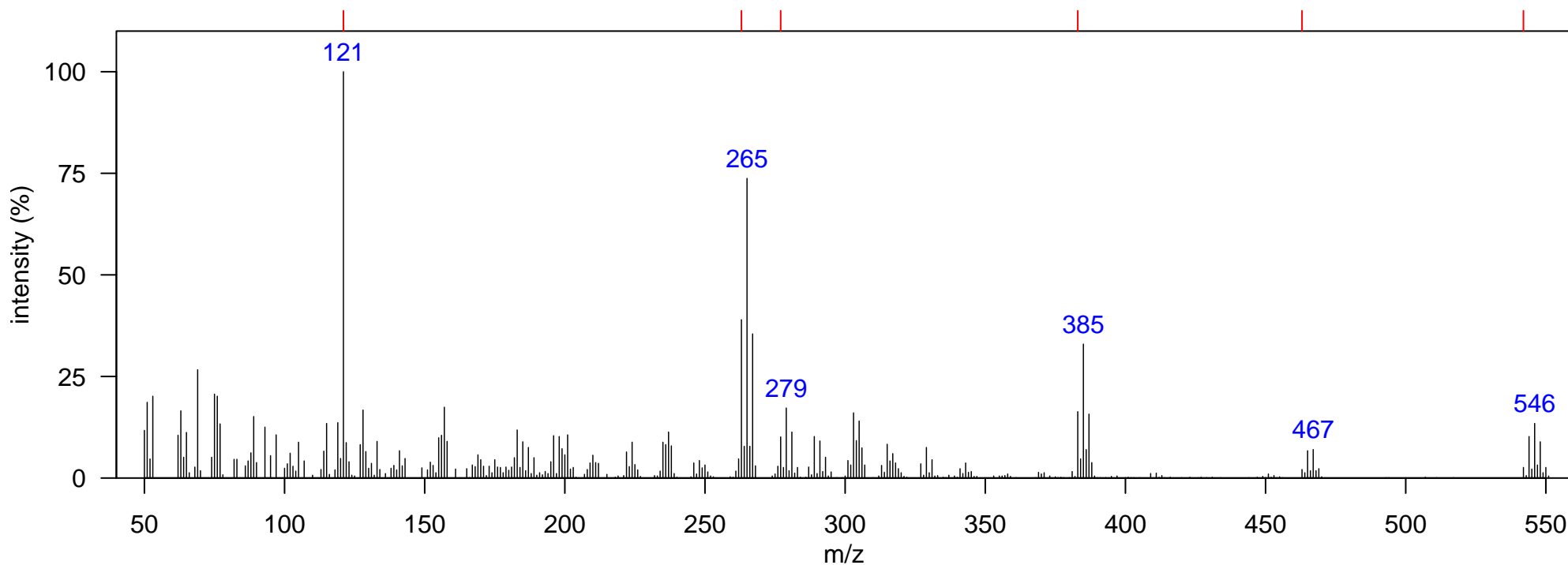
Comment:

Elemental Formula: C₁₆H₁₅Br₄O

Source: natural

Class: PBHD

Identification: Authentic MS RT



m/z	Identity
121	[C ₉ H ₁₃] ⁺
263	[C ₇ H ₅ OBr ₂] ⁺
277	[C ₉ H ₁₁ Br ₂] ⁺
383	[M-HBr ₂] ⁺
463	[M-Br] ⁺
542	M ⁺

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

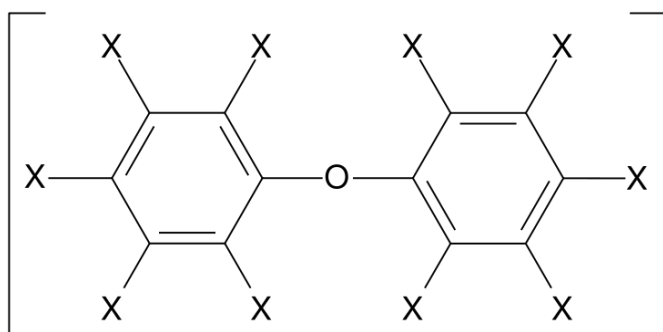
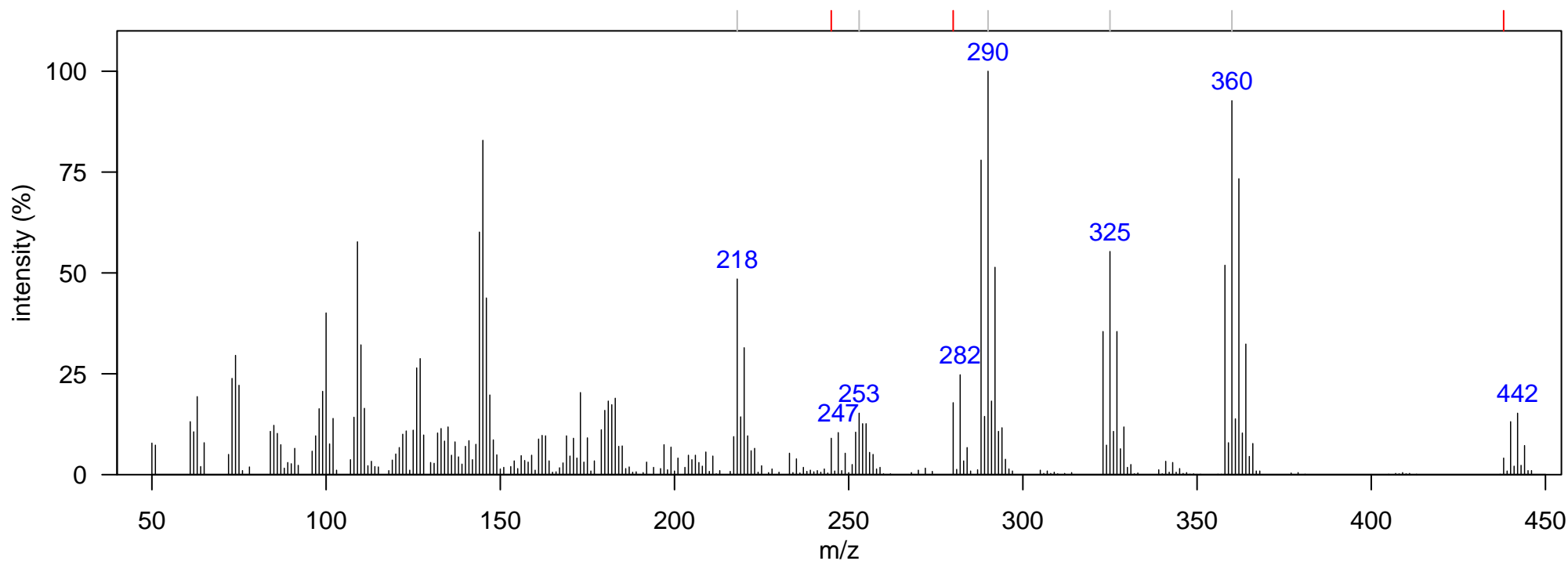
Comment:

Elemental Formula: C₁₂H₆Br₃ClO

Source: unknown

Class: B/CDE

Identification: Manual – Congener Group



X=3Br, Cl, 6H

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 ⁺

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

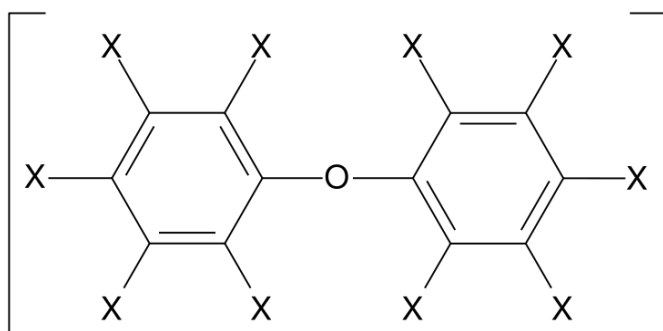
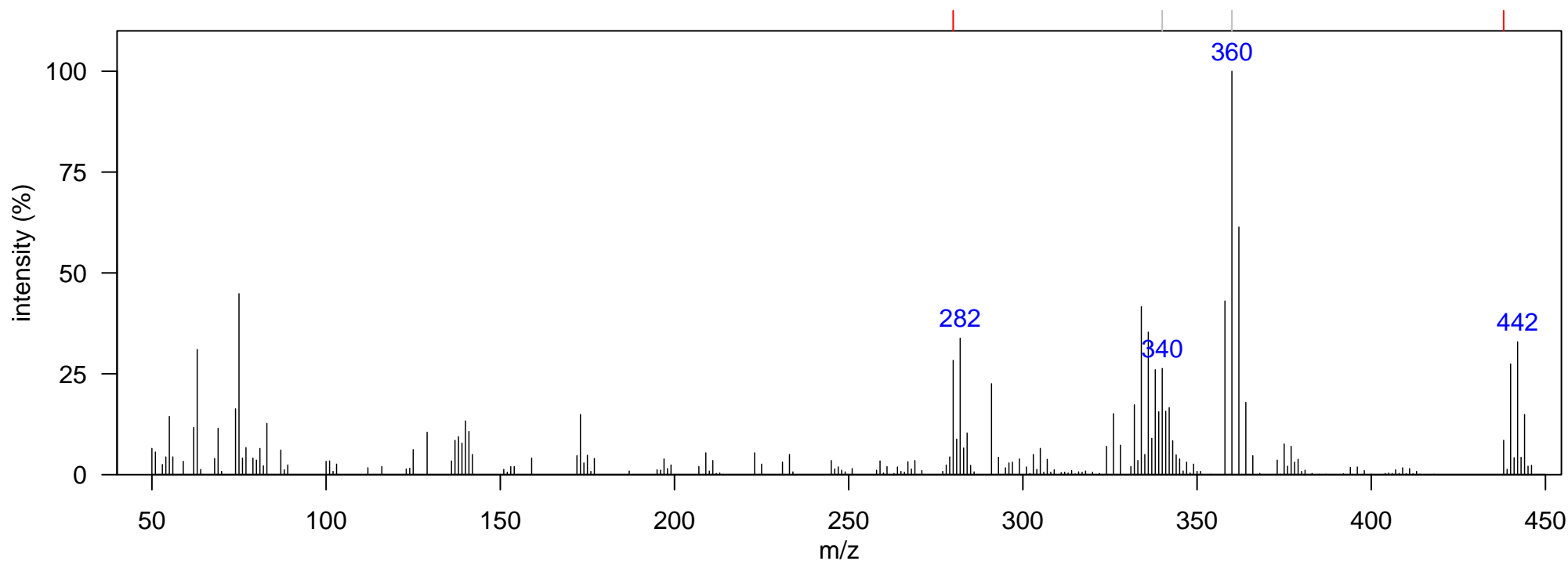
Comment:

Elemental Formula: C₁₂H₆Br₃ClO

Source: unknown

Class: B/CDE

Identification: Manual – Congener Group



X=3Br, Cl, 6H

m/z	Identity
280	[M-2Br] ⁺
340	interference MeO-BB Br ₃ Cl
360	PCB interference
438	M ⁺

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

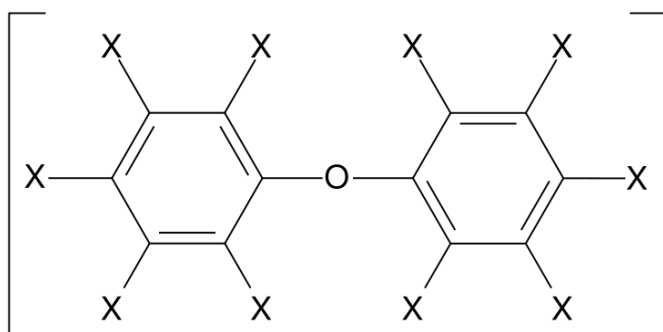
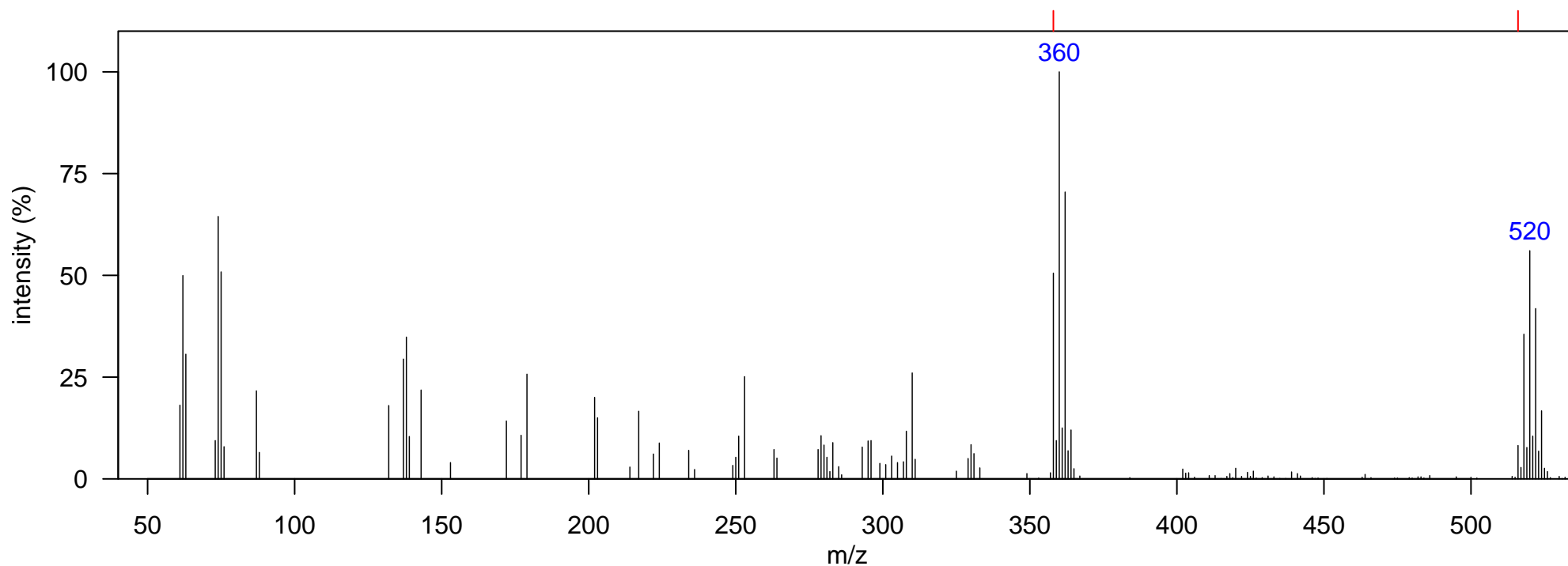
Comment:

Elemental Formula: C₁₂H₅Br₄ClO

Source: unknown

Class: B/CDE

Identification: Manual – Congener Group



X=4Br, Cl, 5H

m/z	Identity
358	[M-2Br] ⁺
516	M ⁺

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

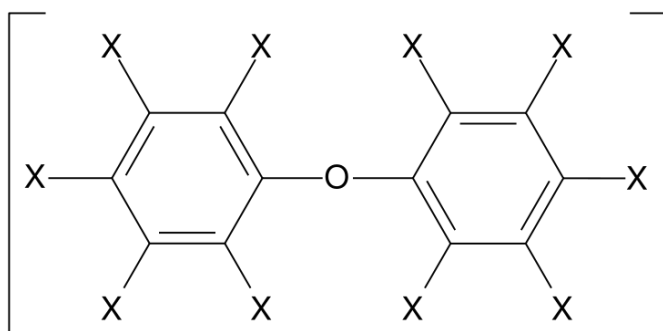
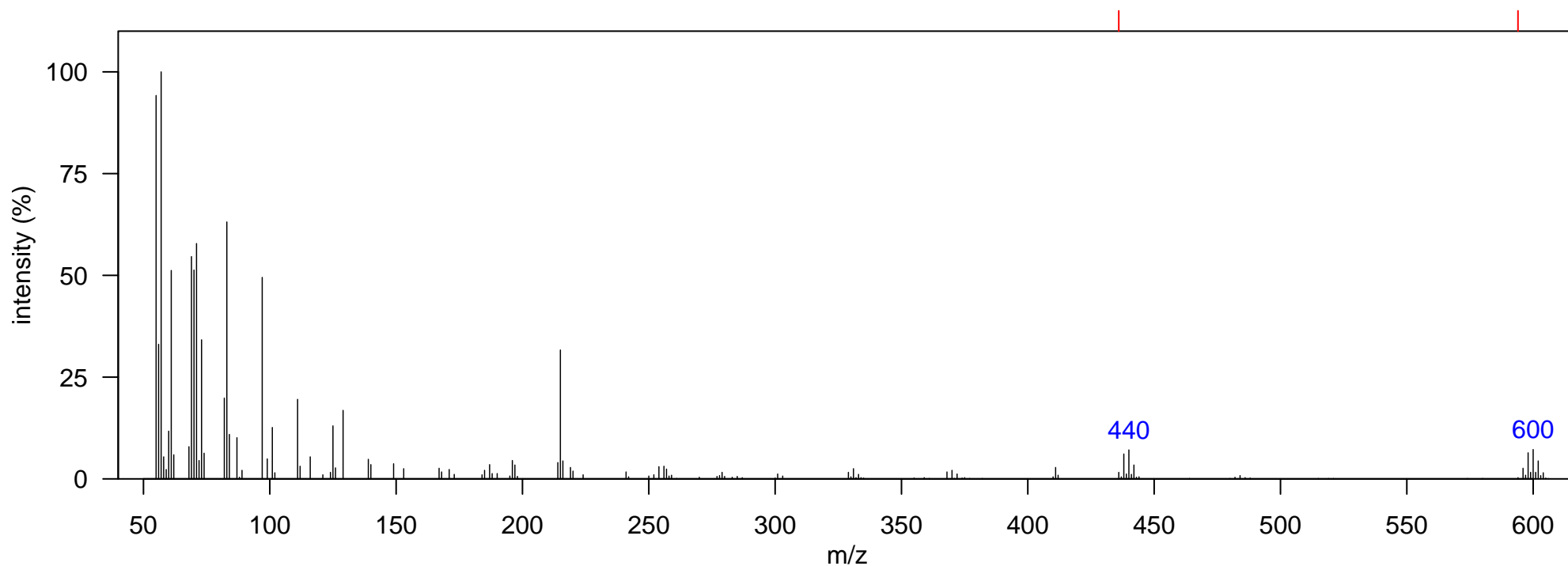
Comment:

Elemental Formula: C₁₂H₄Br₅ClO

Source: unknown

Class: B/CDE

Identification: Manual – Congener Group



X=5Br, Cl, 4H

m/z	Identity
436	[M-2Br] ⁺
594	M ⁺

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

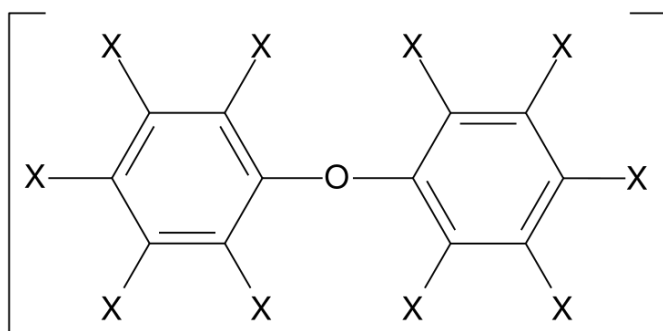
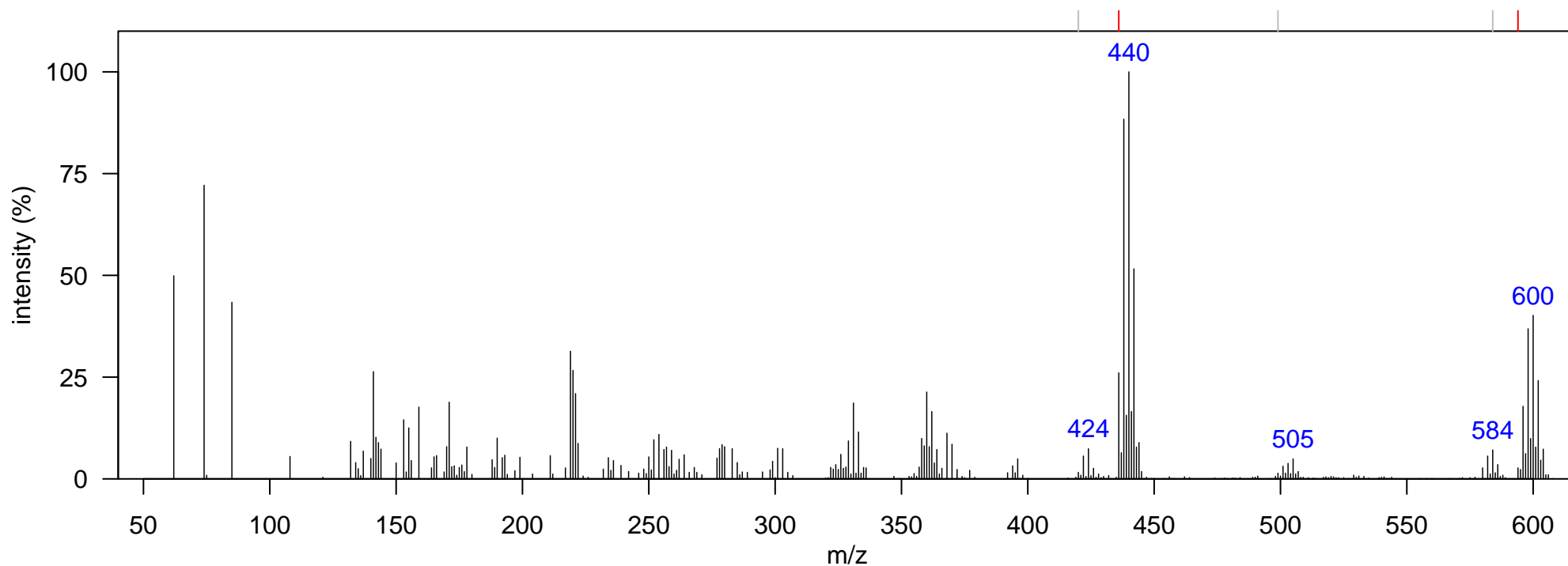
Comment:

Elemental Formula: C₁₂H₄Br₅ClO

Source: unknown

Class: B/CDE

Identification: Manual – Congener Group



X=5Br, Cl, 4H

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

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

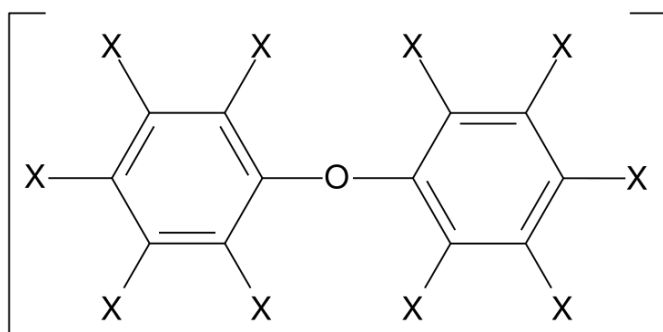
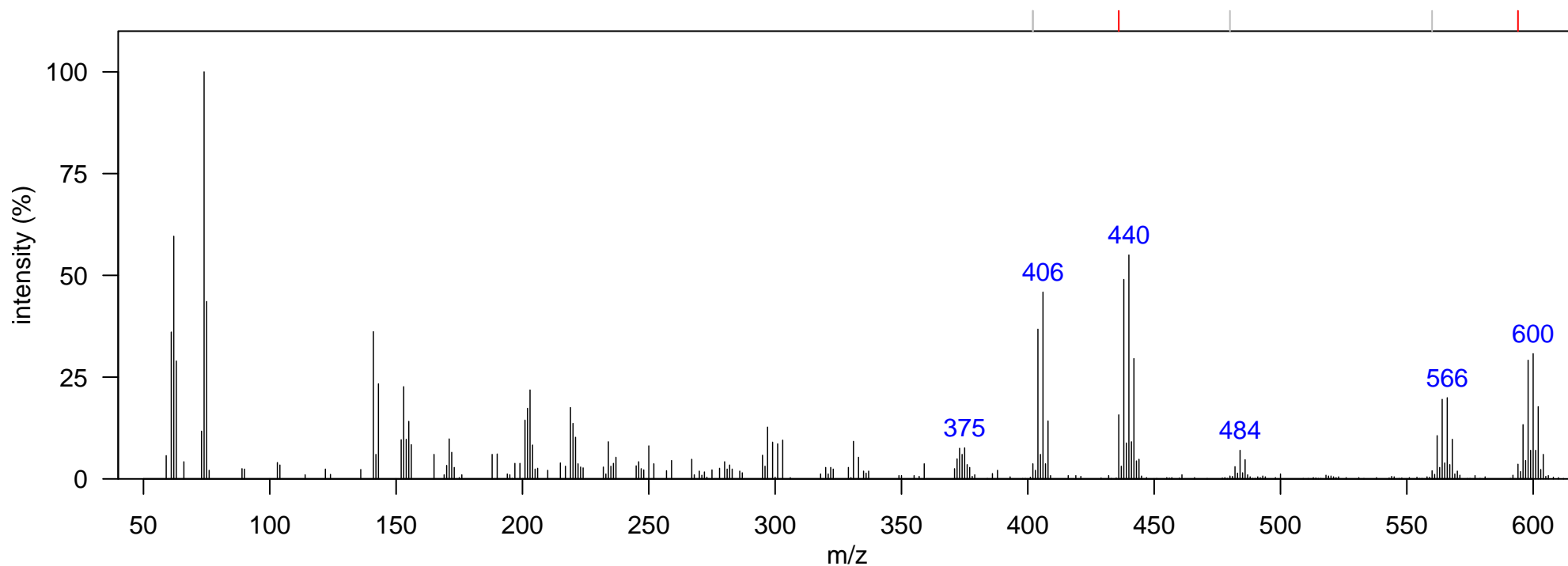
Comment: Co-elution with PBDE (5Br) isomer.

Elemental Formula: C₁₂H₄Br₅ClO

Source: unknown

Class: B/CDE

Identification: Manual – Congener Group



X=5Br, Cl, 4H

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

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

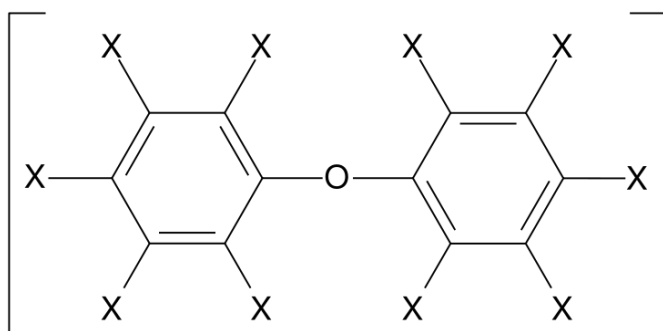
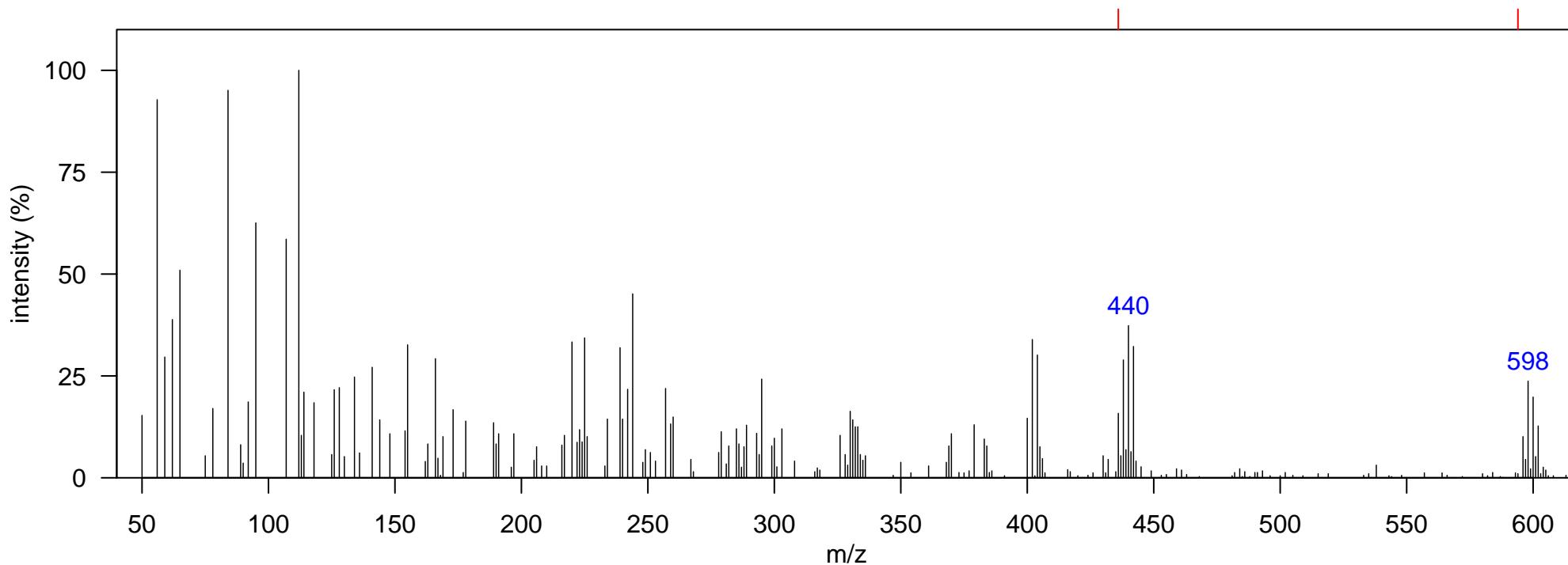
Comment:

Elemental Formula: C₁₂H₄Br₅ClO

Source: unknown

Class: B/CDE

Identification: Manual – Congener Group



X=5Br, Cl, 4H

m/z	Identity
436	[M-2Br] ⁺
594	M ⁺

Name: pentachloroethylbenzene

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

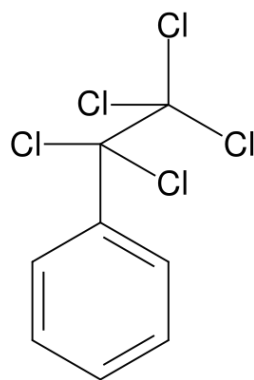
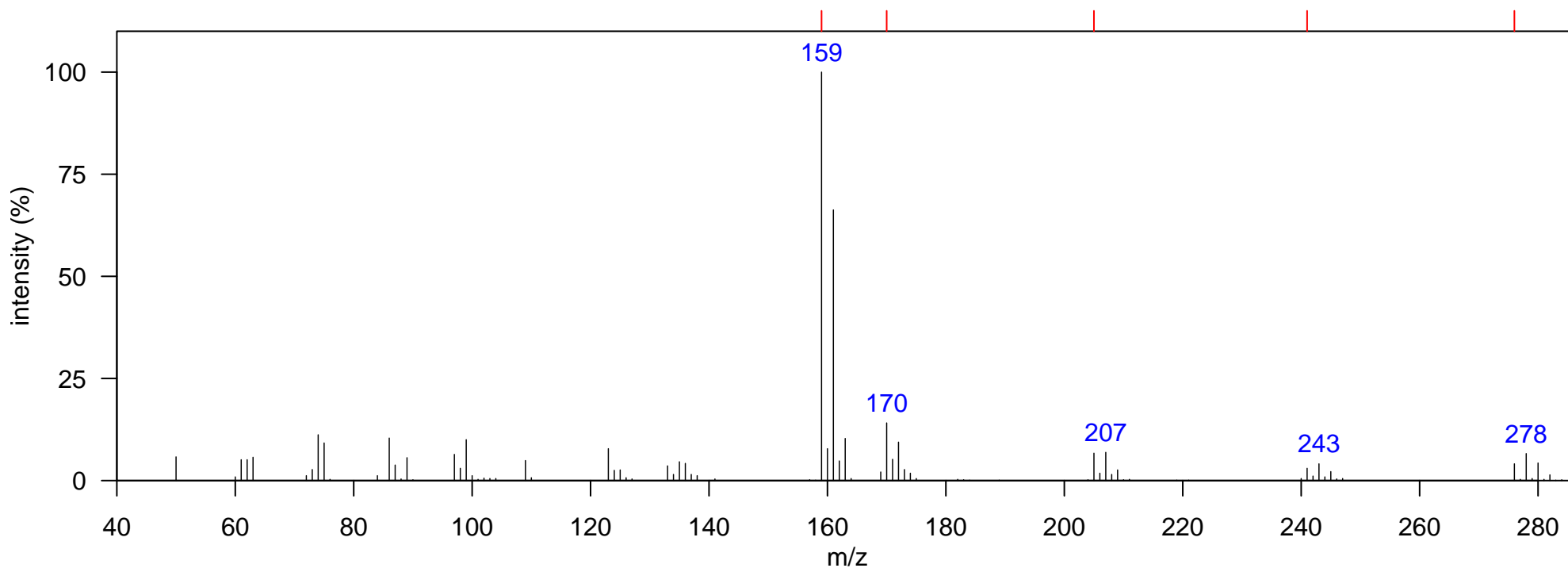
Comment:

Elemental Formula: C₈H₅Cl₅

Source: unknown

Class: ethylbenzene

Identification: Reference Database MS



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

Name: hexachloroethylbenzene

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

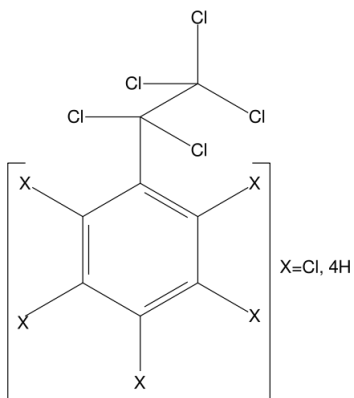
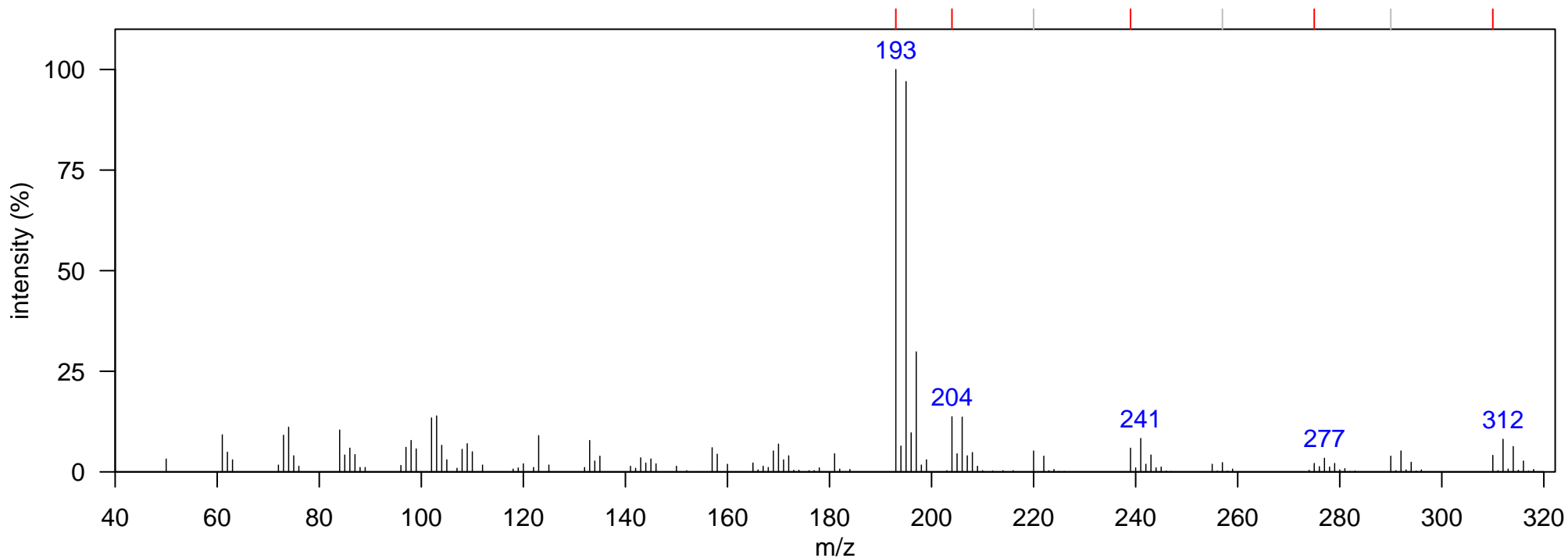
Comment:

Elemental Formula: C₈H₄Cl₆

Source: unknown

Class: ethylbenzene

Identification: Manual – Congener Group



m/z	Identity
193	[M-CCl ₃] ⁺
204	[M-HCl ₃] ⁺
220	PCB interference
239	[M-HCl ₂] ⁺
257	PCB interference
275	[M-Cl] ⁺
290	PCB interference
310	M ⁺

Name: tetraphenyltin

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

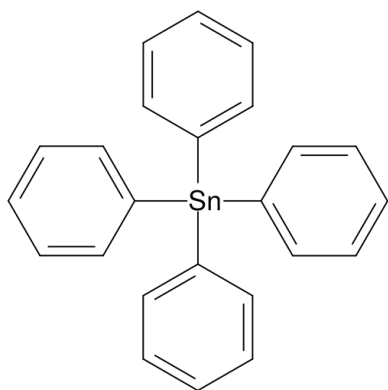
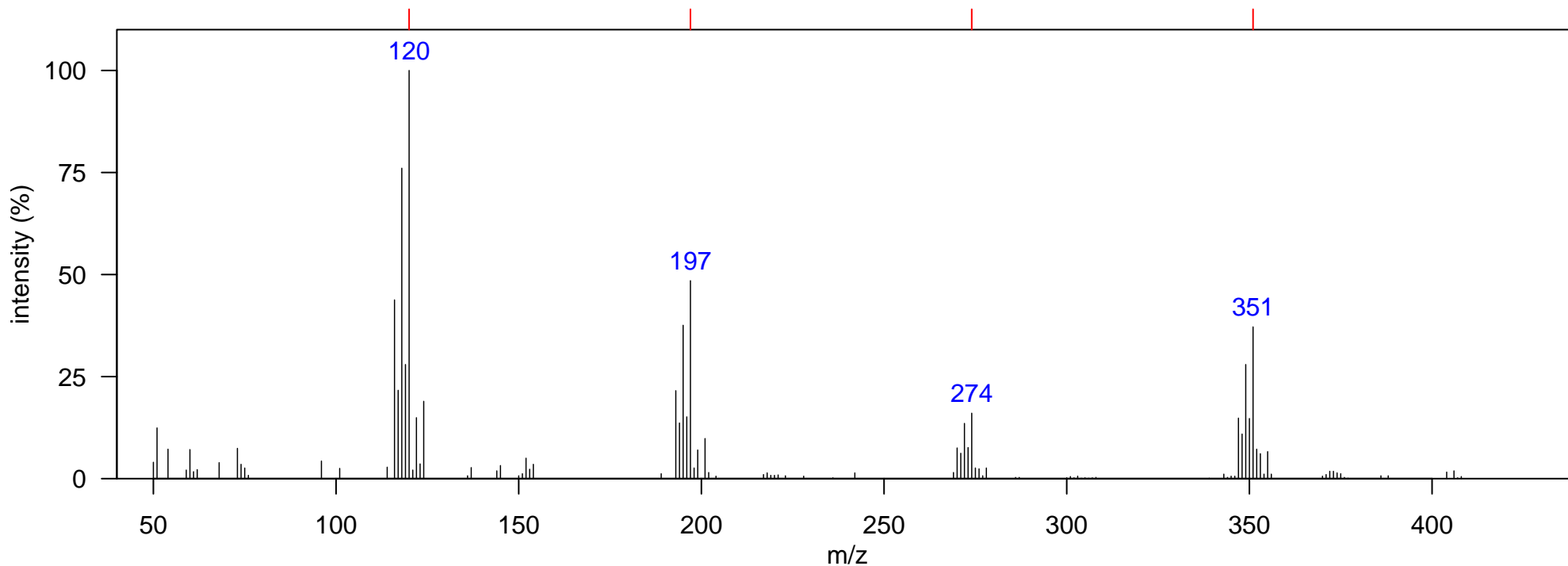
Comment:

Elemental Formula: C₂₄H₂₀Sn

Source: anthropogenic

Class: organotin

Identification: Reference Database MS



m/z	Identity
120	Sn ⁺
197	[M-3(C ₆ H ₅)] ⁺
274	[M-2(C ₆ H ₅)] ⁺
351	[M-C ₆ H ₅] ⁺

Name: unknown 1-1

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

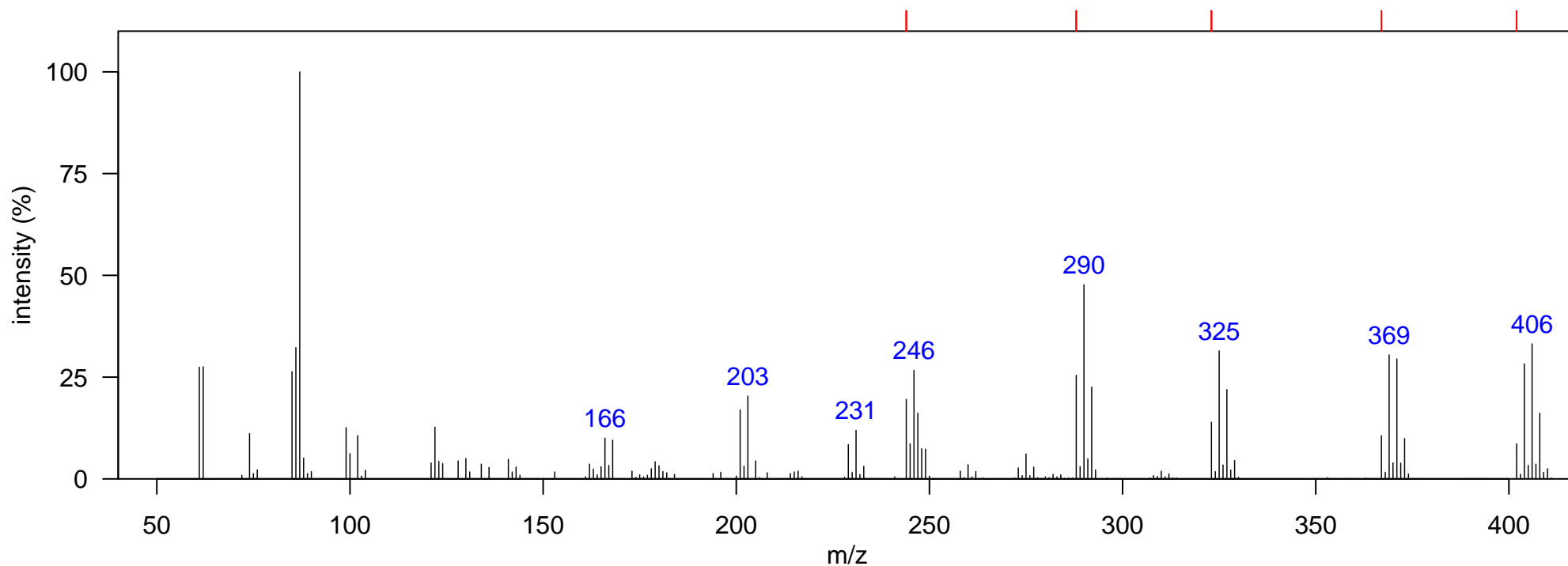
Comment: Ref: ES&T, 2009, 43, 3240-3247. Unknowns 1-(1-4) seem to share the same backbone.

Elemental Formula: C₉H₆OBr₃Cl

Source: unknown

Class: unknown

Identification: Literature MS



m/z	Identity
244	[M-Br ₂] ⁺
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

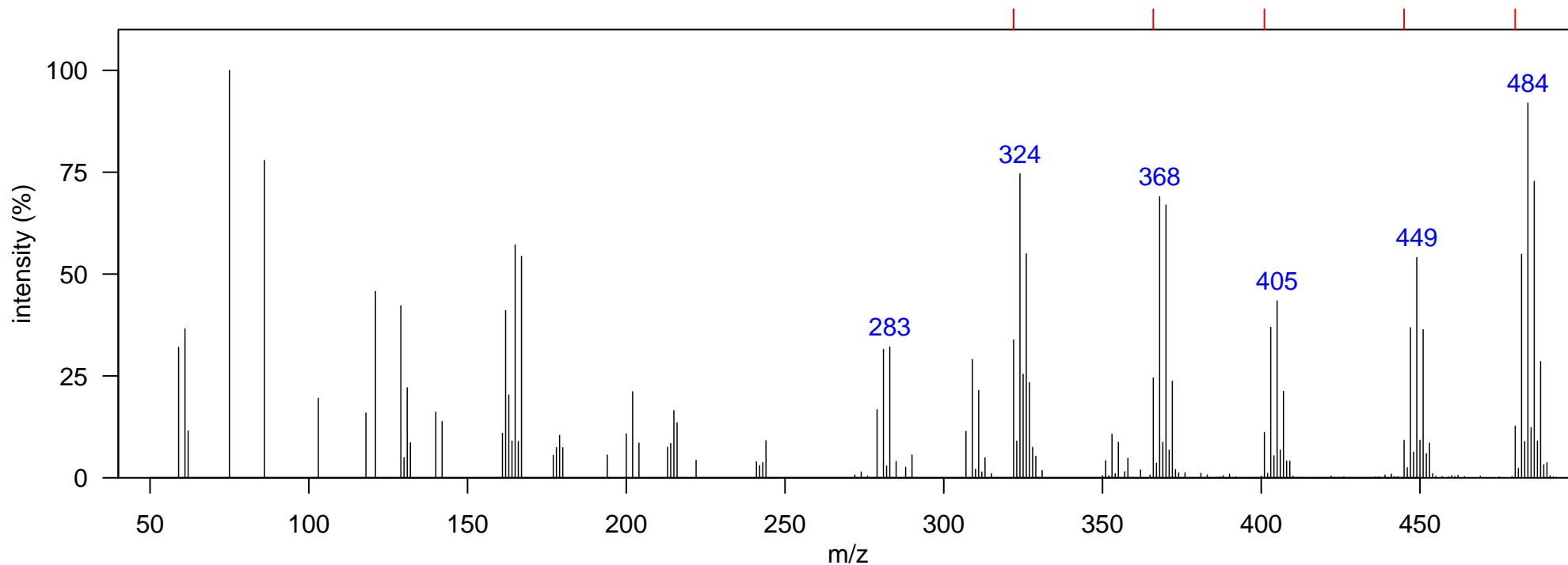
Comment: Ref: ES&T, 2009, 43, 3240–3247. Unknowns 1–(1–4) seem to share the same backbone.

Elemental Formula: C₉H₆OBr₄Cl

Source: unknown

Class: unknown

Identification: Literature MS



m/z	Identity
322	[M–Br ₂] ⁺
366	[M–BrCl] ⁺
401	[M–Br] ⁺
445	[M–Cl] ⁺
480	M ⁺

Name: unknown 1–3

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC–TOF, electron impact

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

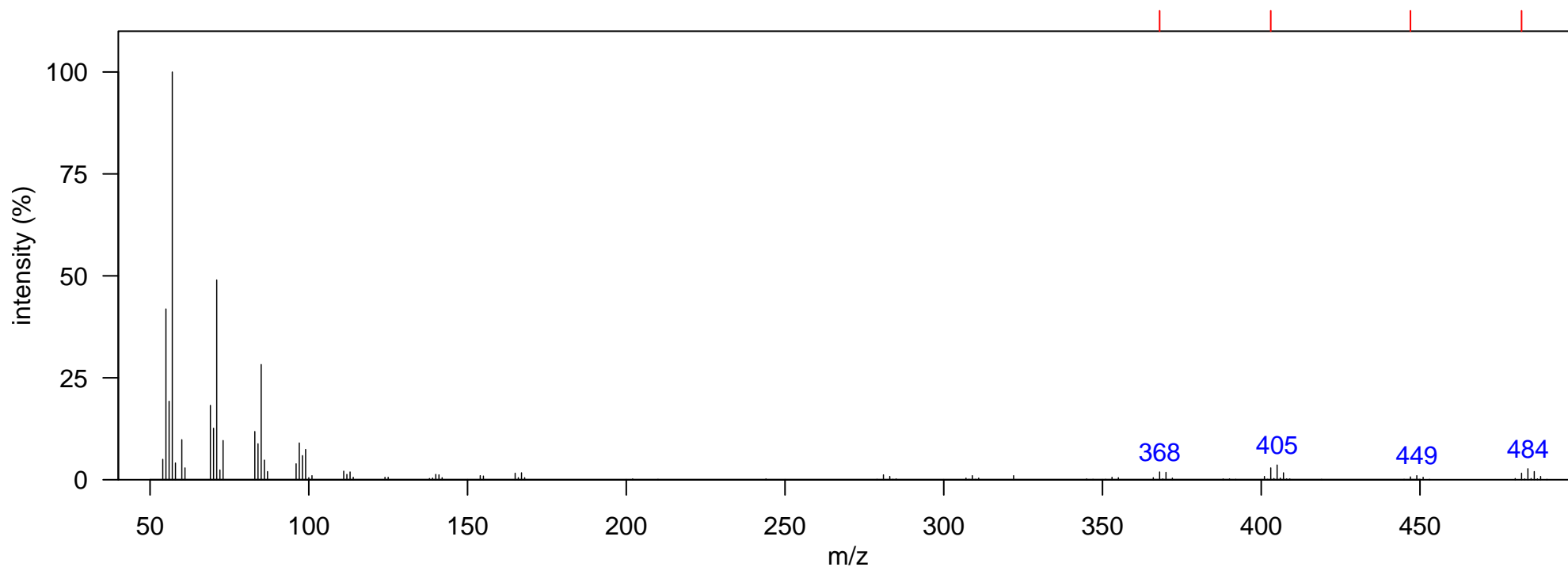
Comment: Ref: ES&T, 2009, 43, 3240–3247. Unknowns 1–(1–4) seem to share the same backbone.

Elemental Formula: C₉H₆OBr₄Cl

Source: unknown

Class: unknown

Identification: Literature MS



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

Name: unknown 1–4

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC–TOF, electron impact

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

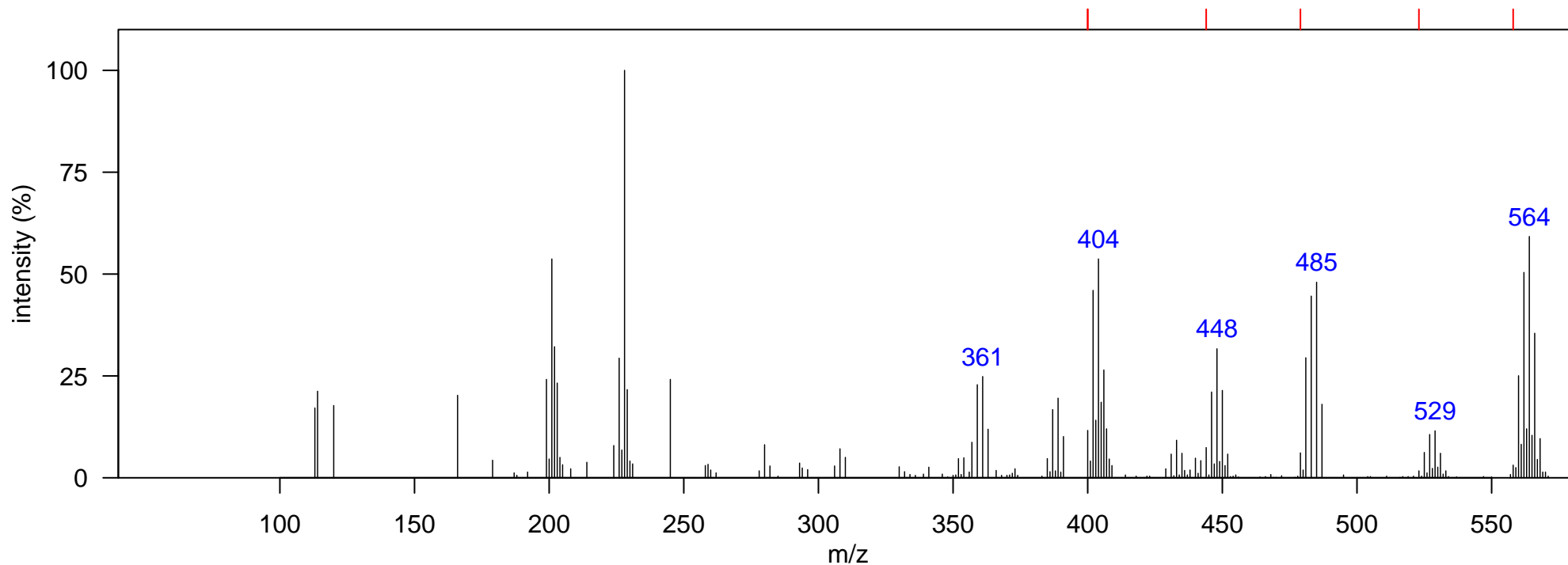
Comment: Ref: ES&T, 2009, 43, 3240–3247. Unknowns 1–(1–4) seem to share the same backbone.

Elemental Formula: C₉H₆OBr₅Cl

Source: unknown

Class: unknown

Identification: Literature MS



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

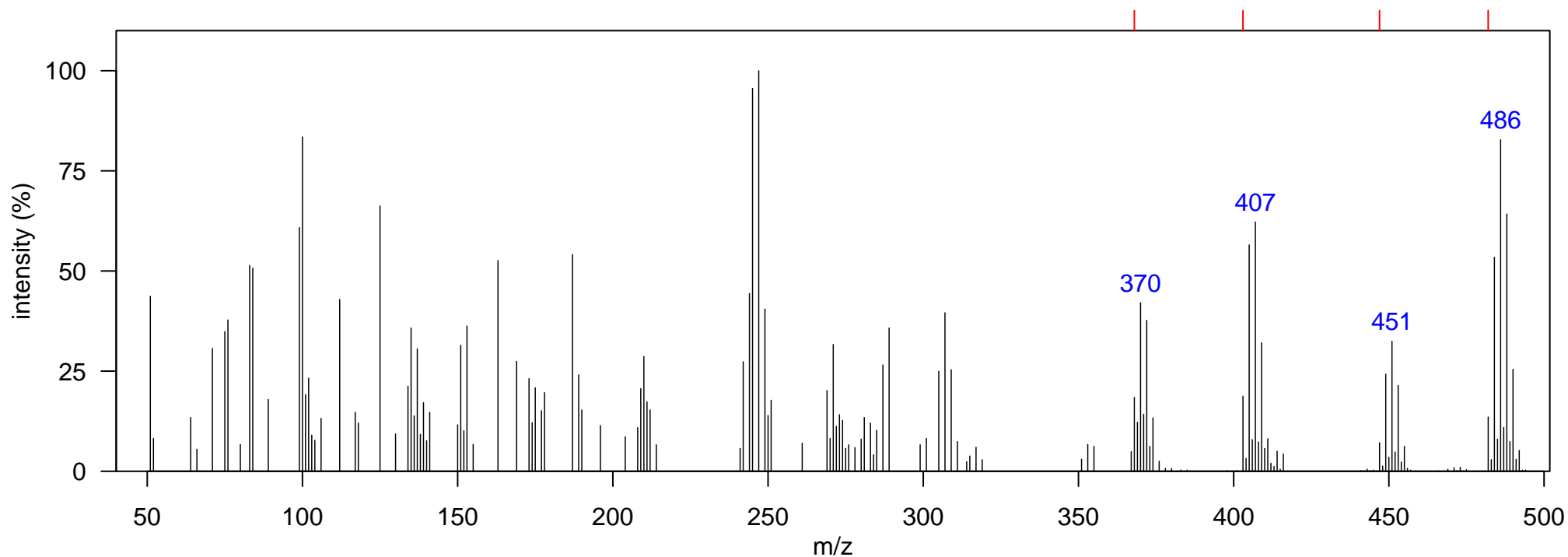
Comment: Related to unknown 1 family of compounds.

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

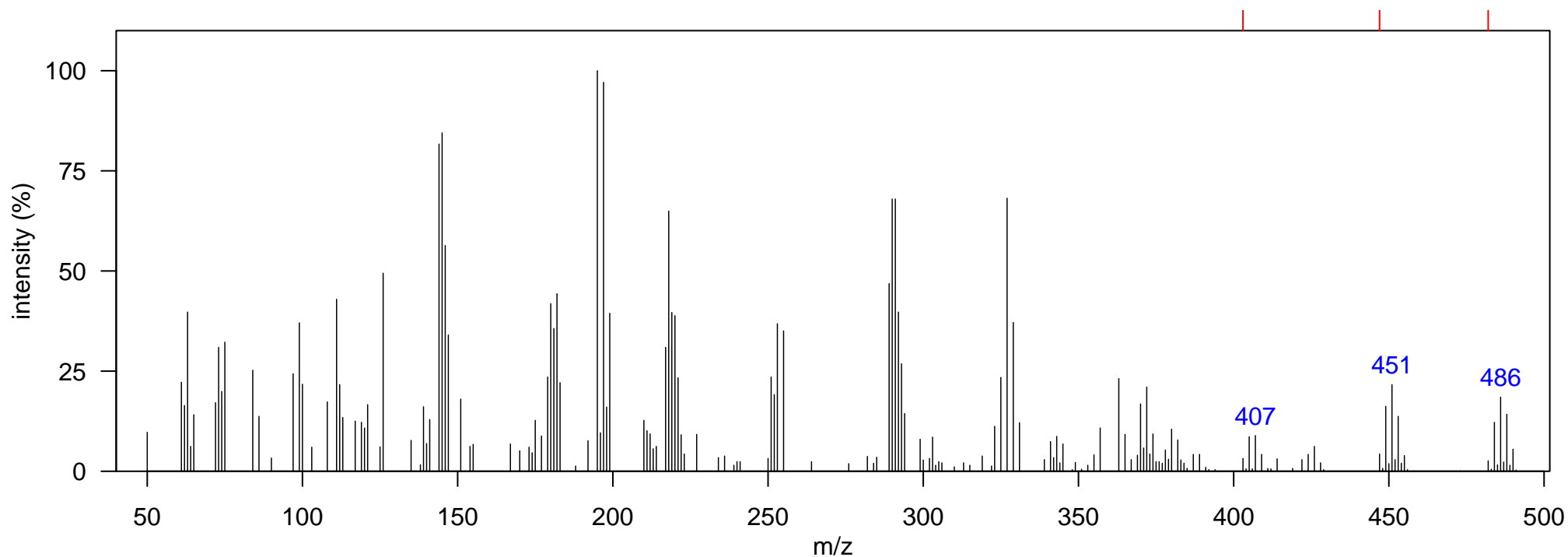
Comment: Related to unknown 1 family of compounds.

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

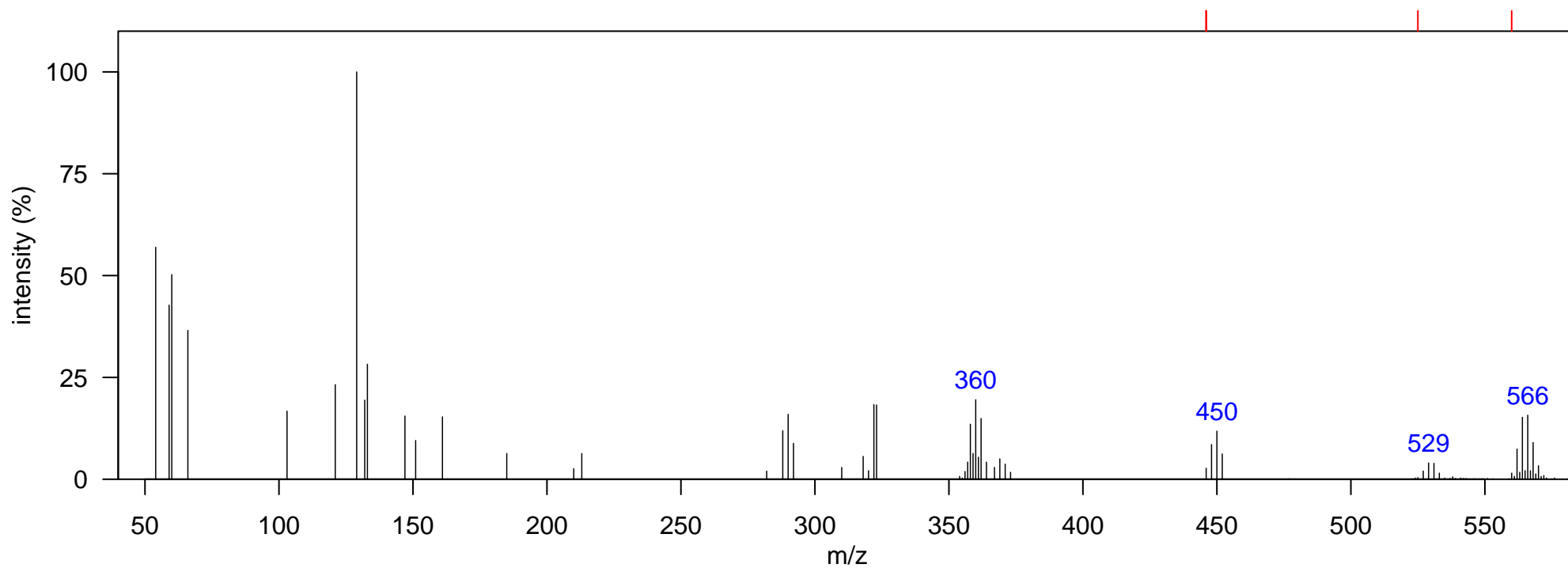
Comment: Related to unknown 1 family of compounds.

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

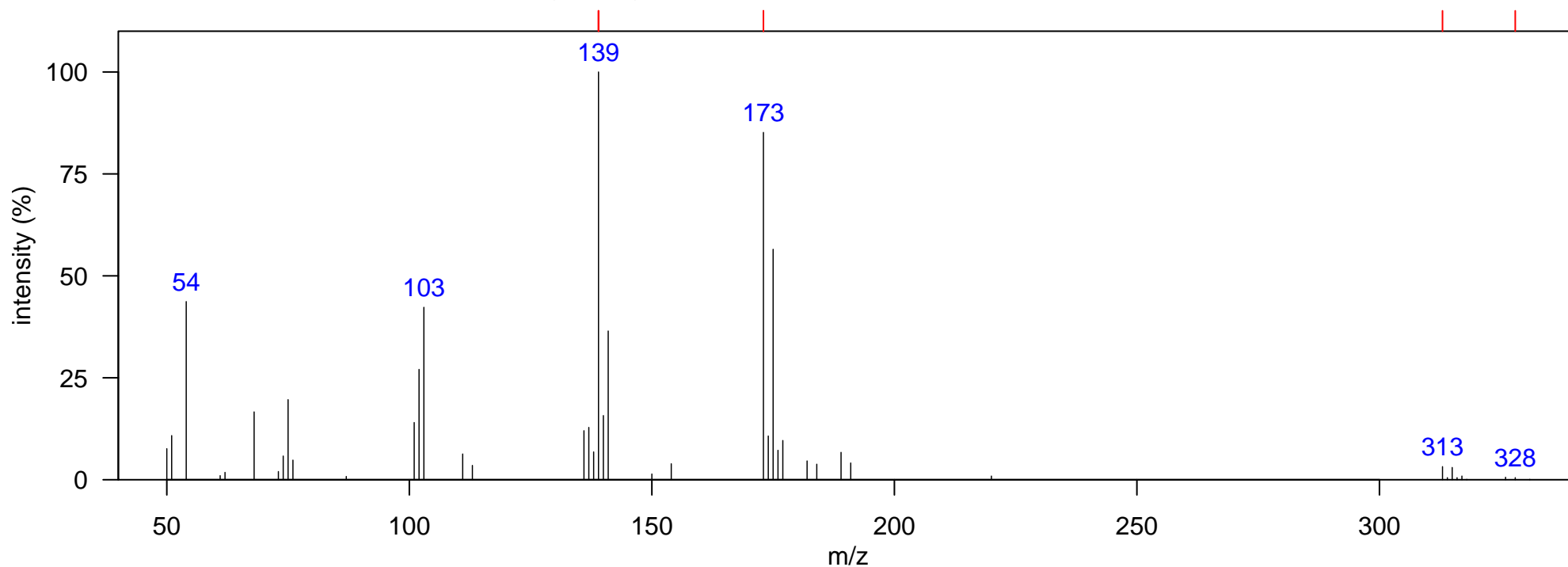
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion. Unknowns 3-(1-3) are related.

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

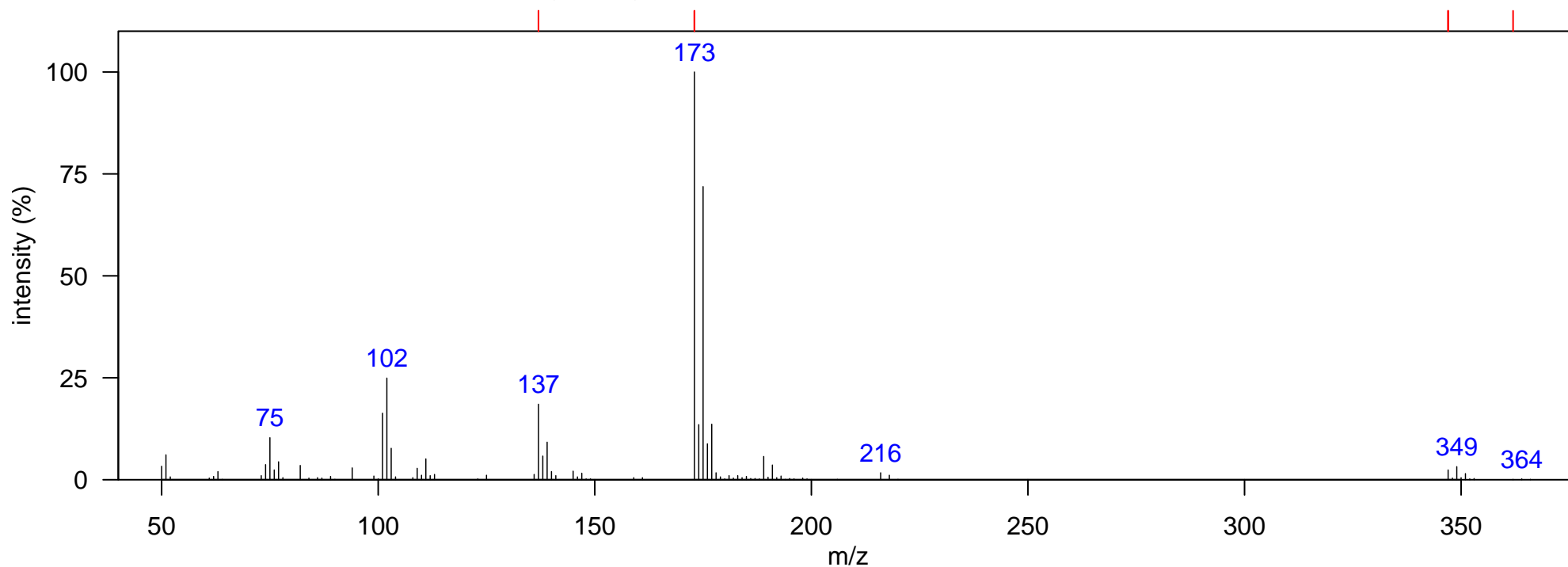
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion. Unknowns 3-(1-3) are related.

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

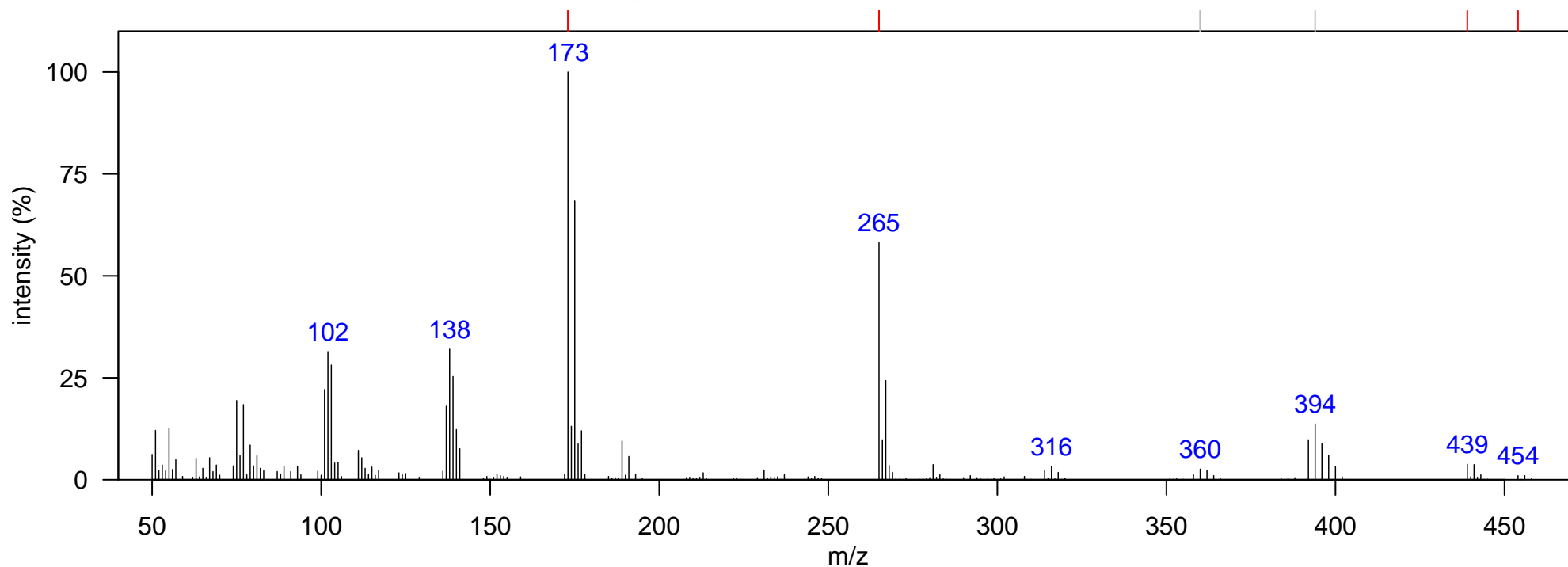
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion. Unknowns 3-(1-3) are related.

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

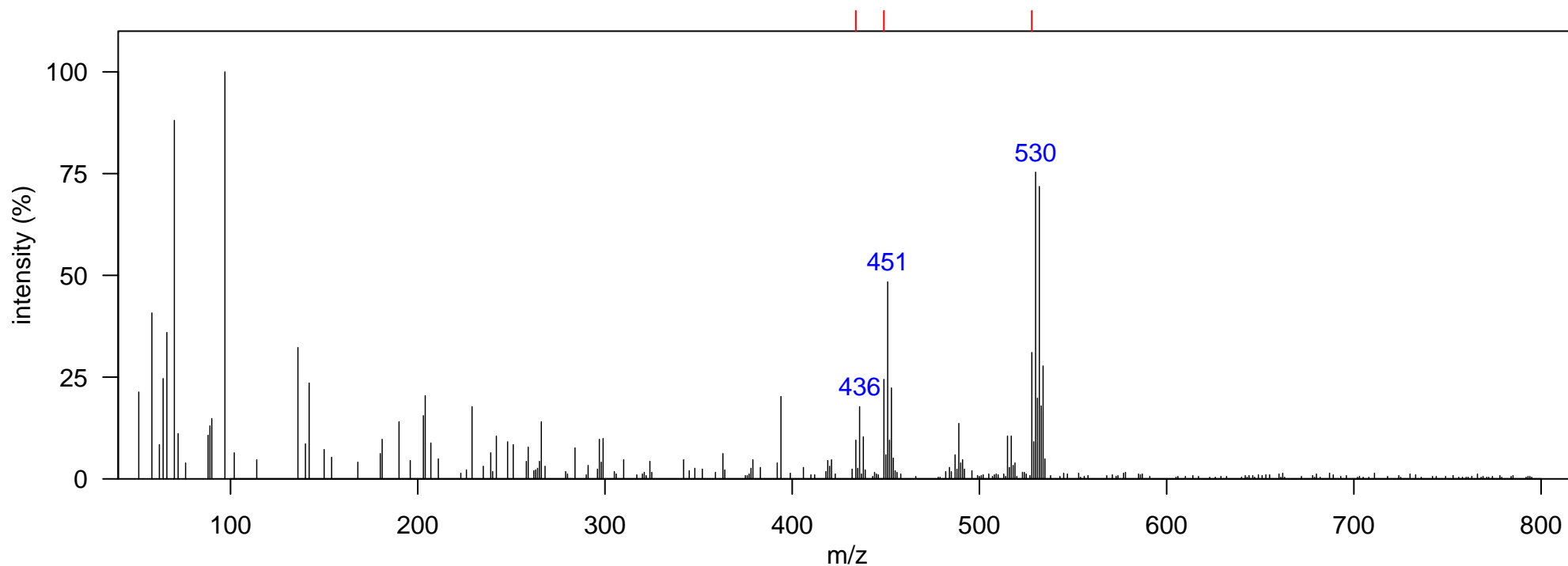
Comment: PM = Possible Molecular Ion. Unknowns 4-(1-4) seem to share the same backbone.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
434	[PM-Br-15] ⁺ = [PM-Br-CH ₃] ⁺
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

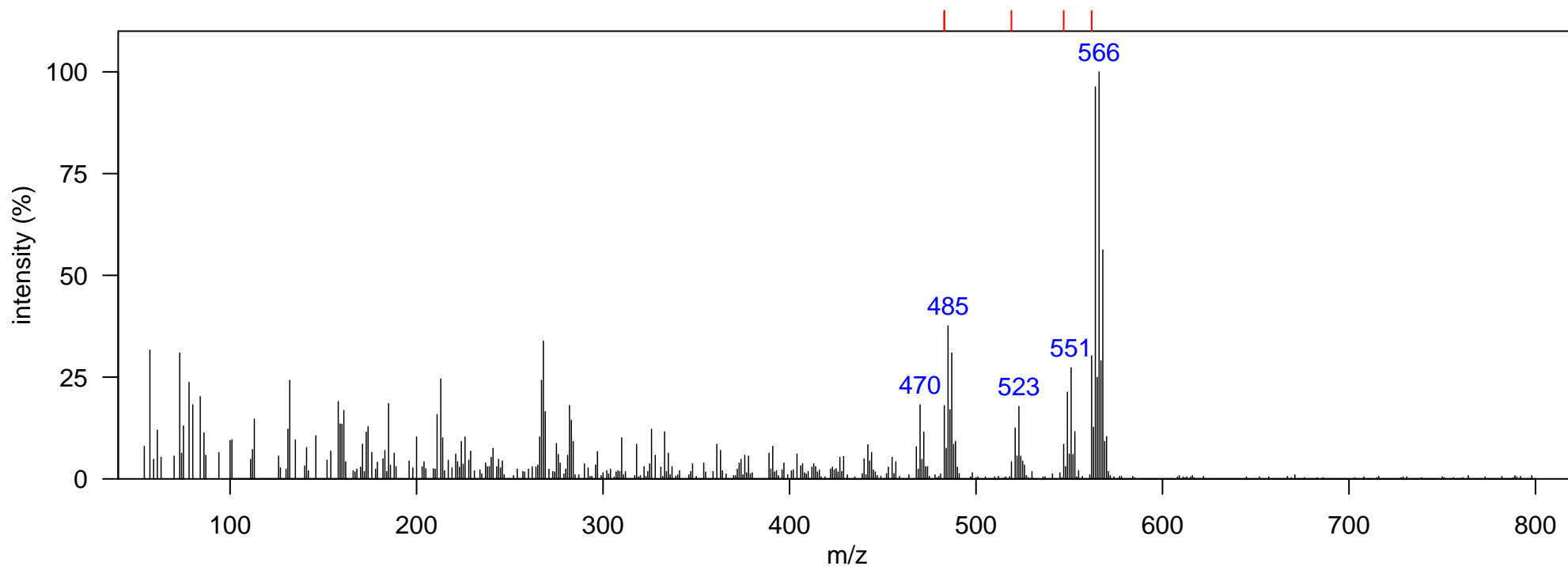
Comment: PM = Possible Molecular Ion. Unknowns 4-(1-4) seem to share the same backbone.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
483	[PM-Br] ⁺
519	[PM-43] ⁺ = [PM-C ₃ H ₇] ⁺
547	[PM-15] ⁺ = [PM-CH ₃] ⁺
562	[PM] ⁺ contains Br ₃ Cl

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

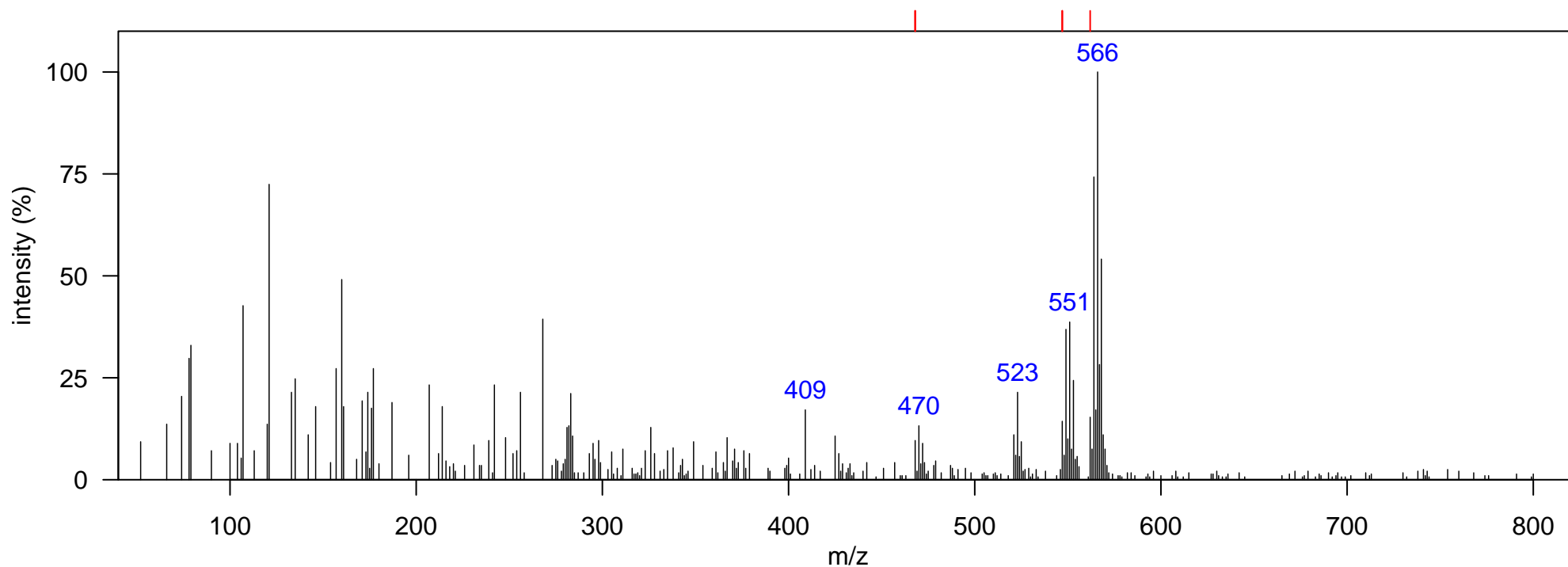
Comment: PM = Possible Molecular Ion. Unknowns 4-(1-4) seem to share the same backbone.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
468	[PM-Br-15] ⁺ = [PM-Br-CH ₃] ⁺
547	[PM-15] ⁺ = [PM-CH ₃] ⁺
562	[PM] ⁺ contains Br ₃ Cl

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

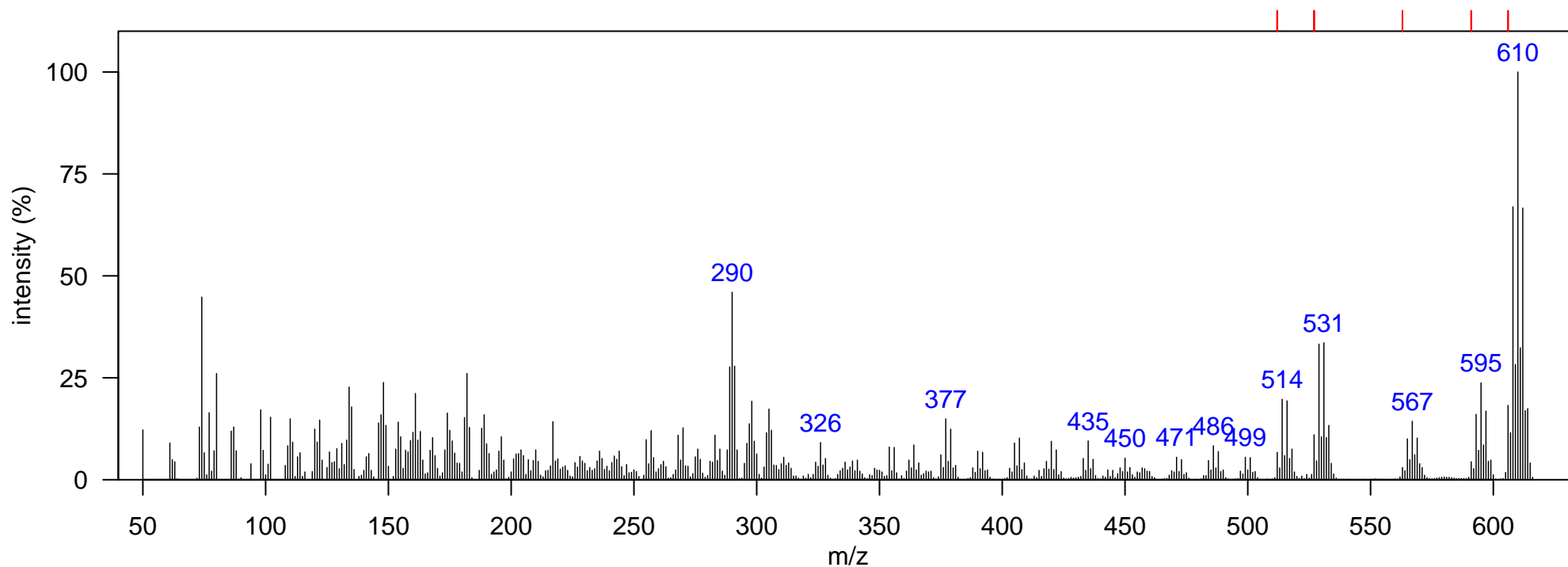
Comment: PM = Possible Molecular Ion. Unknowns 4-(1-4) seem to share the same backbone.

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

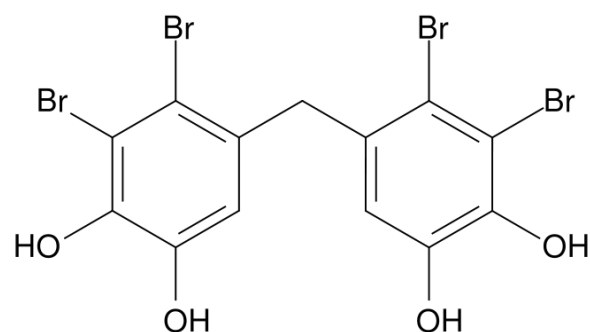
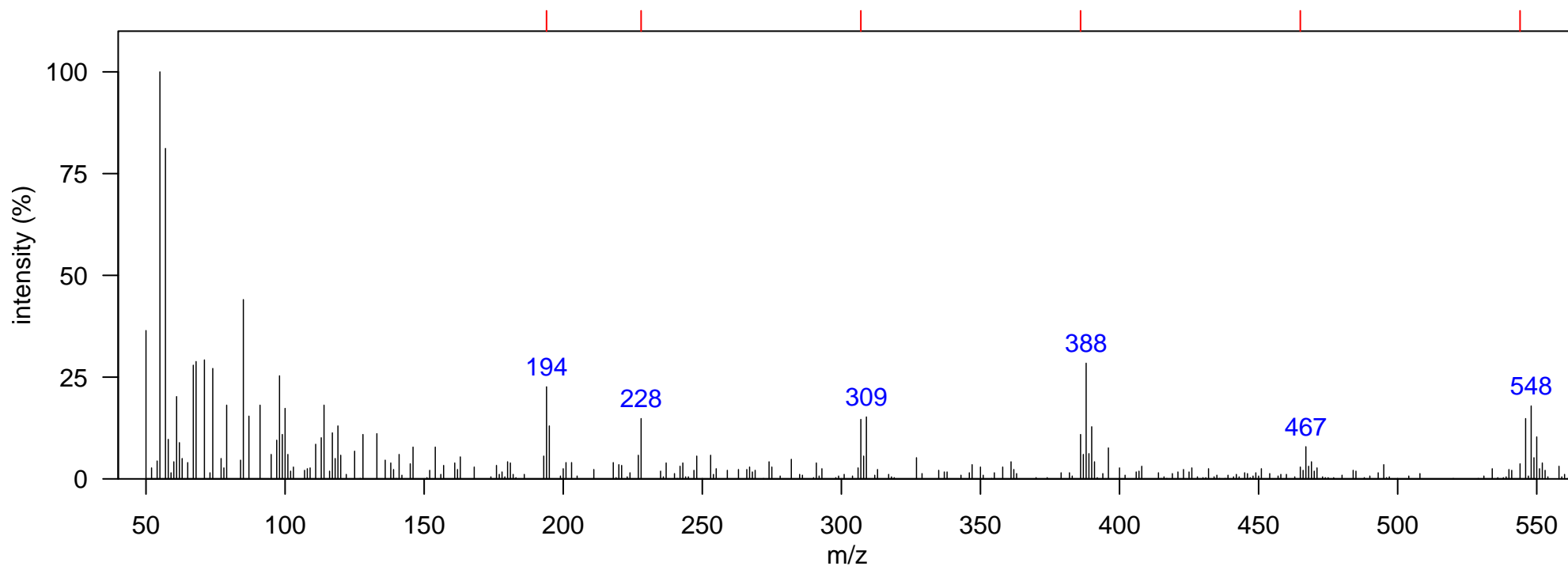
Comment: Ref: ES&T, 2009, 43, 3240-3247. Possible structure shown.

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 ⁺

Name: unknown 6

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

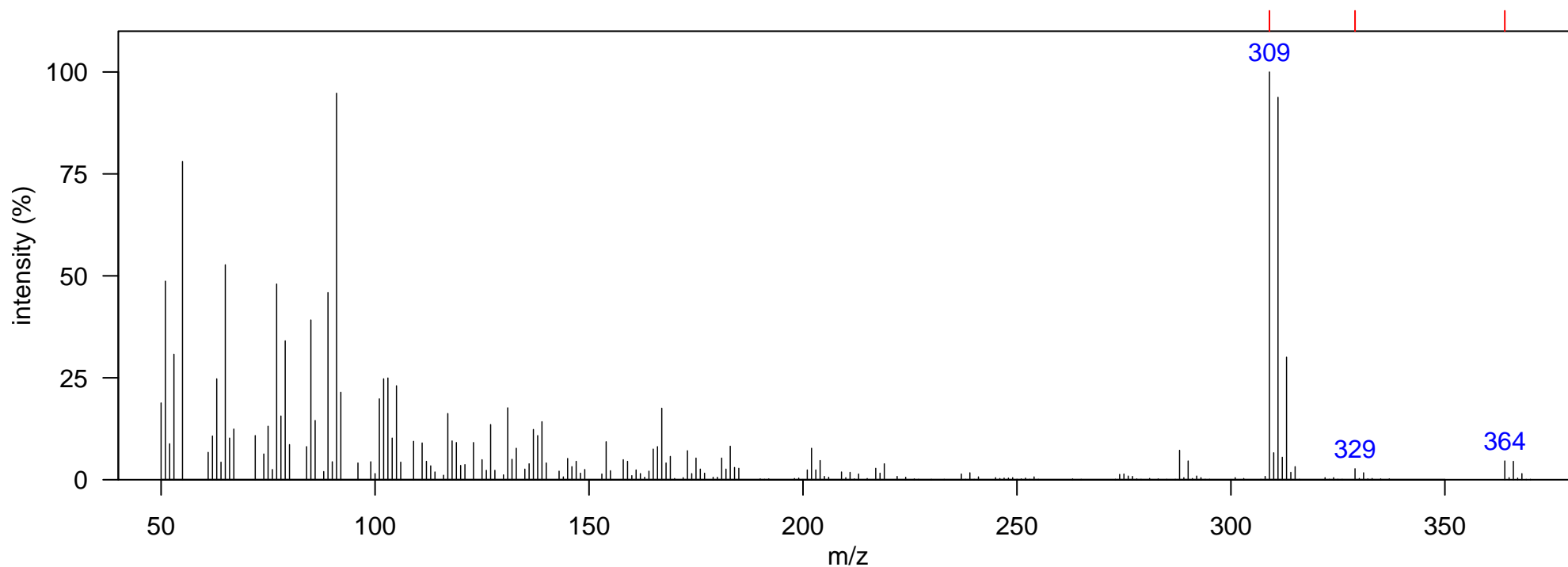
Comment: PM = Possible Molecular Ion

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

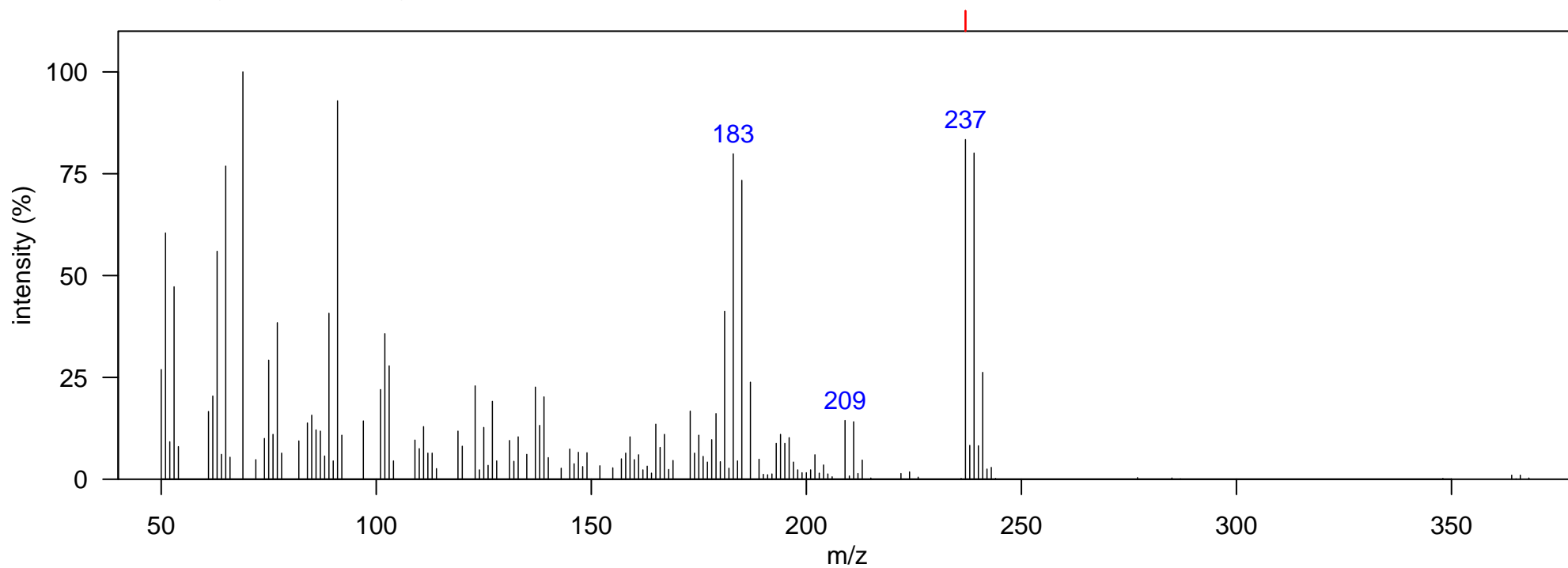
Comment: Frag = Possible Fragment Ion

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

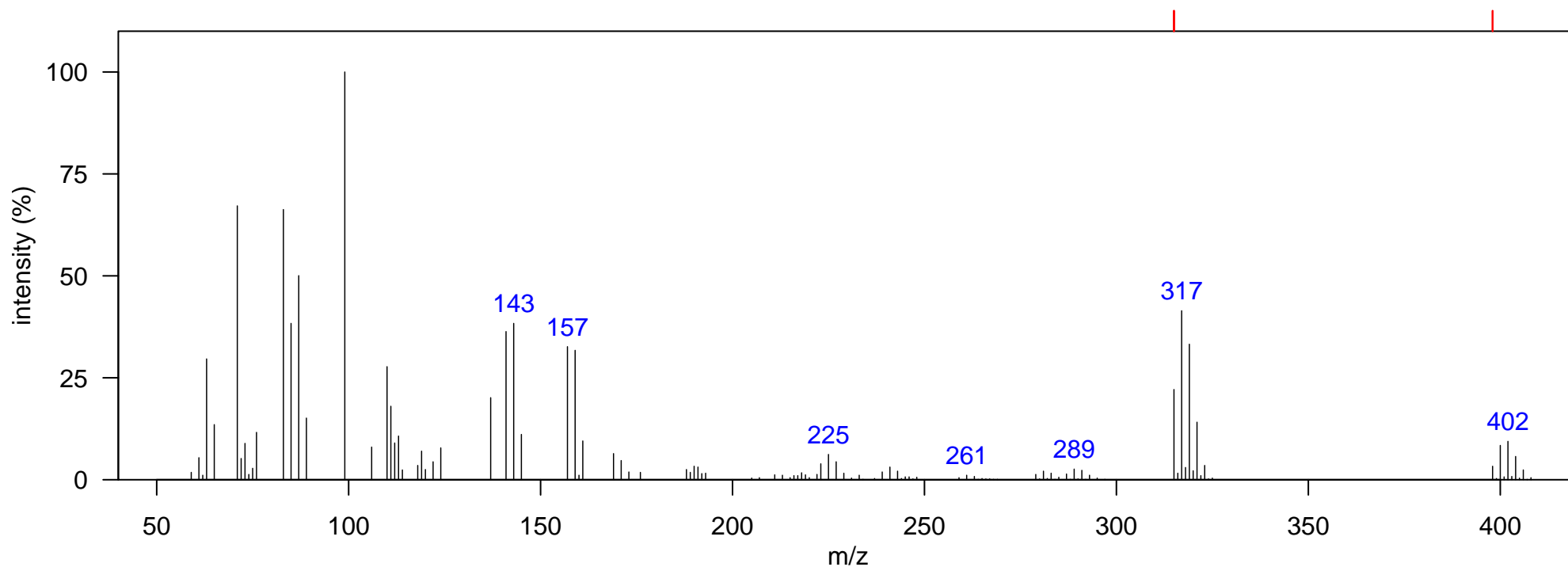
Comment: PM = Possible Molecular Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
315	[PM-CHCl ₂] ⁺
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

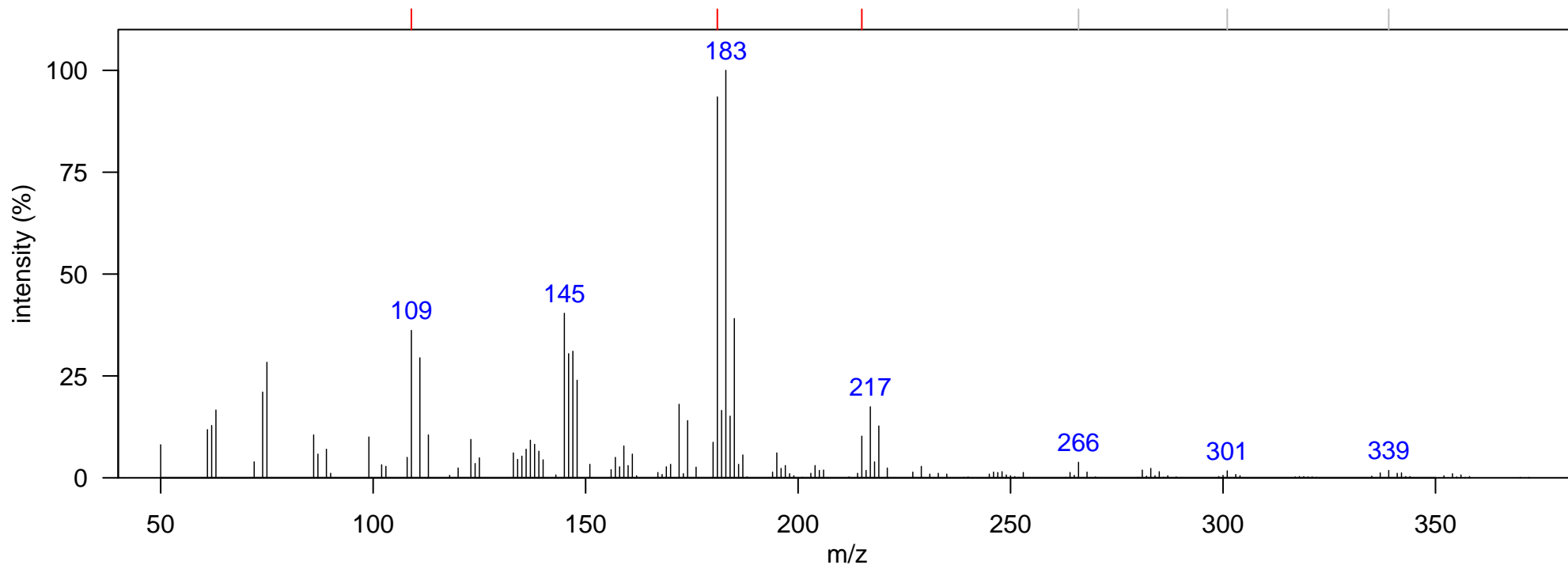
Comment: Frag1 and Frag2 = fragments

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

Name: unknown 10

Sample: Delphinus delphis blubber, Atlantic Ocean, 2006

Instrument: GCxGC-TOF, electron impact

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

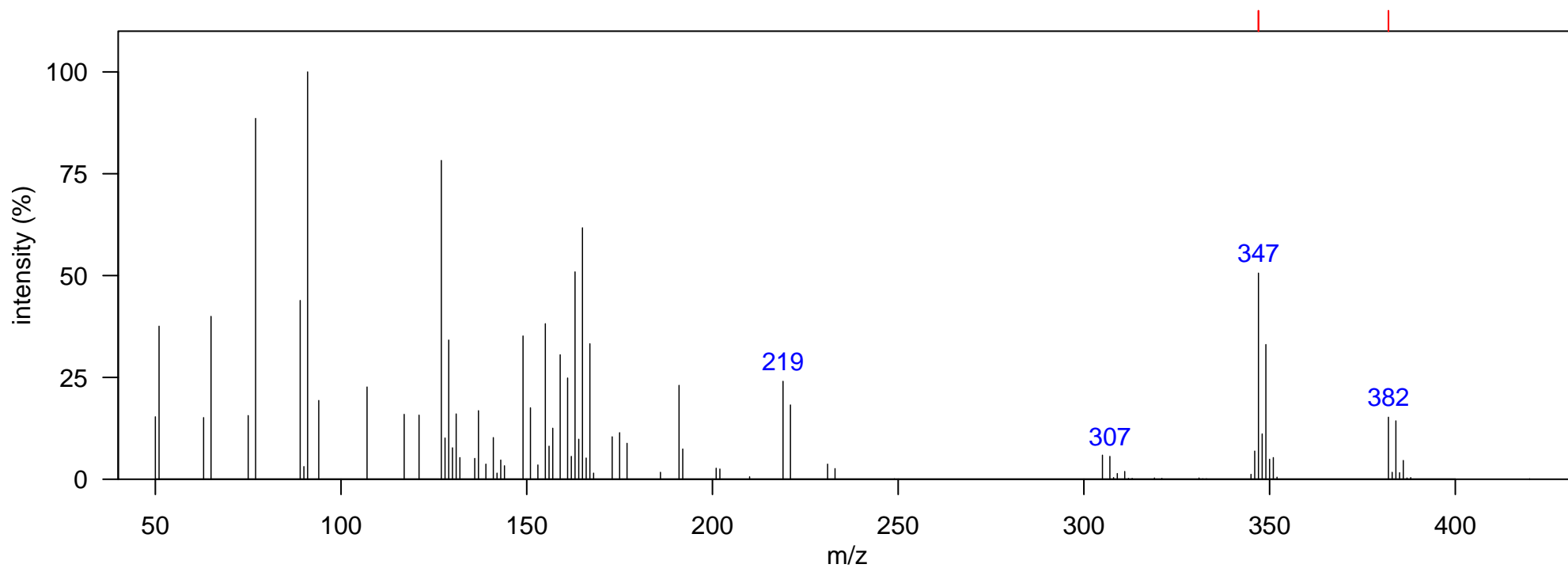
Comment: PM = Possible Molecular Ion

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

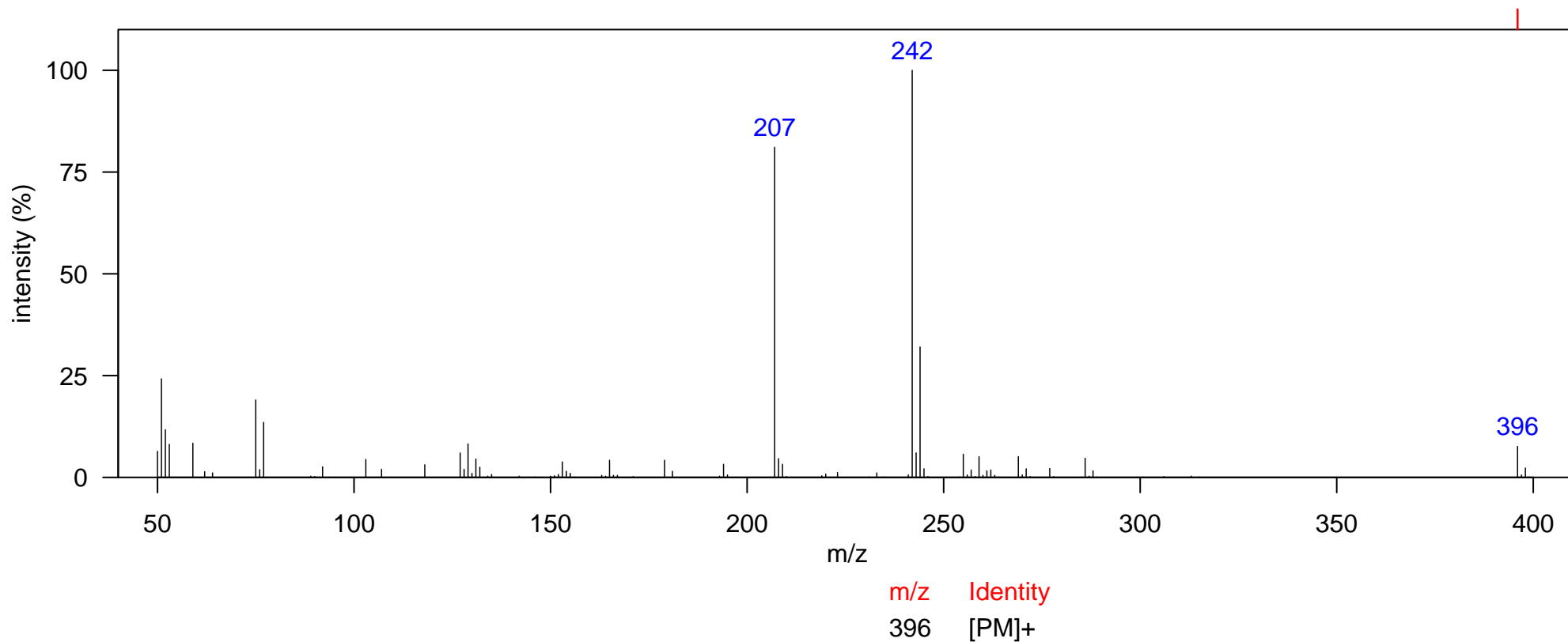
Comment: PM = Possible Molecular Ion. Contains chlorine.

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



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

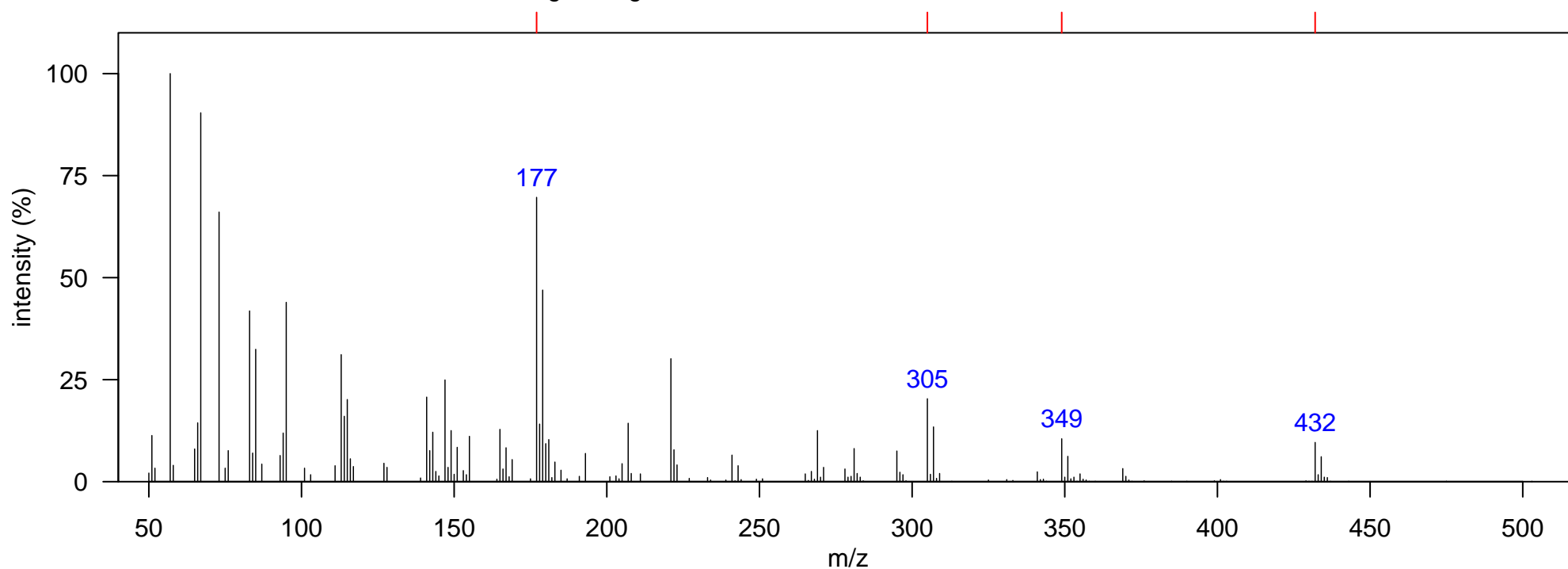
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion

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

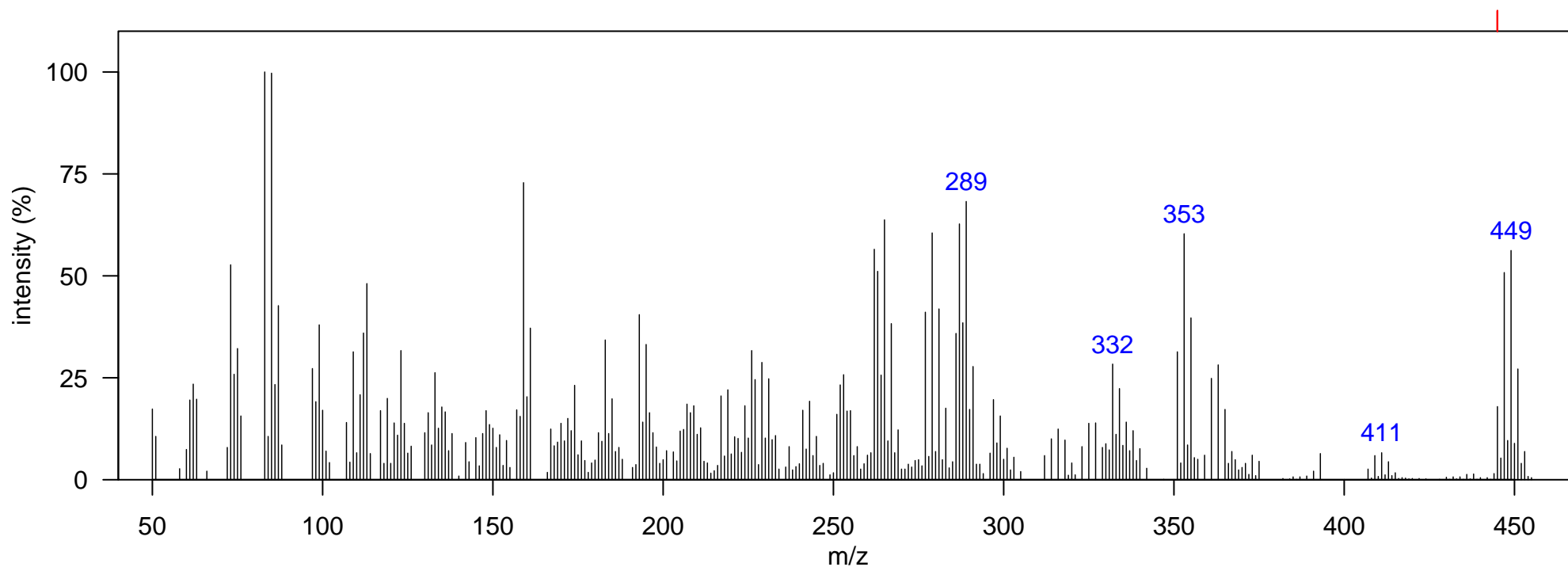
Comment: PM = Possible Molecular Ion

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

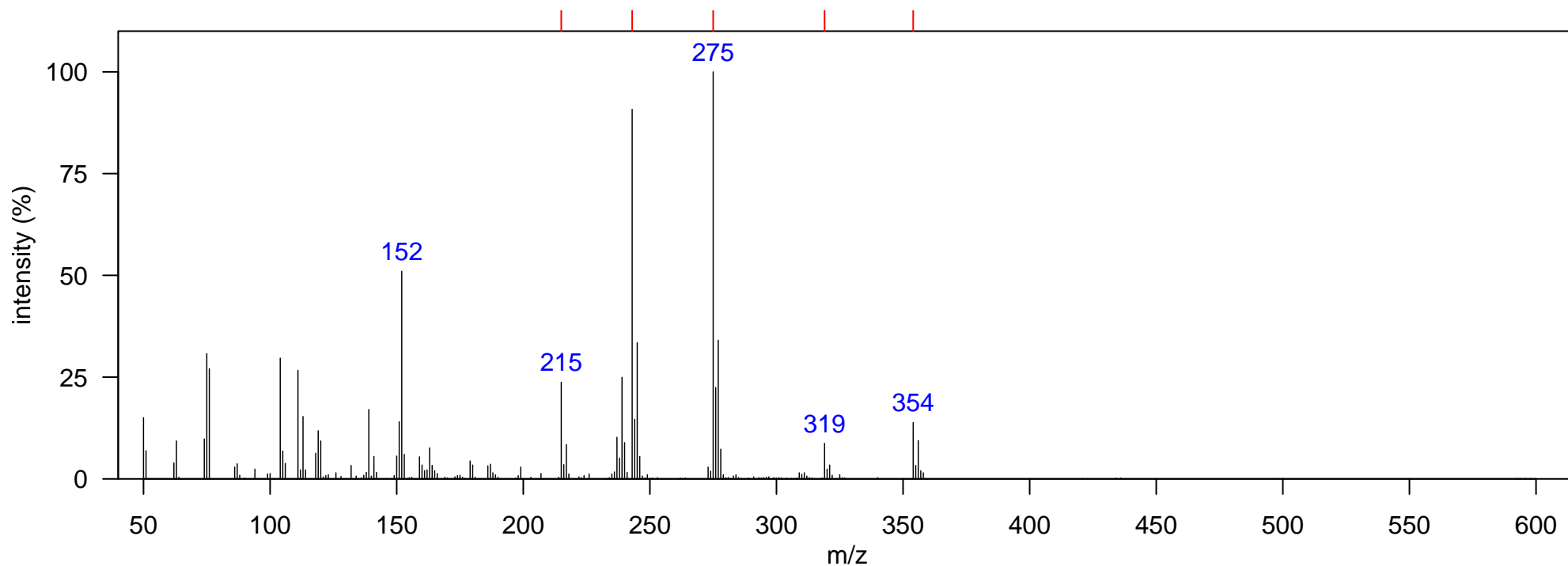
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion

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

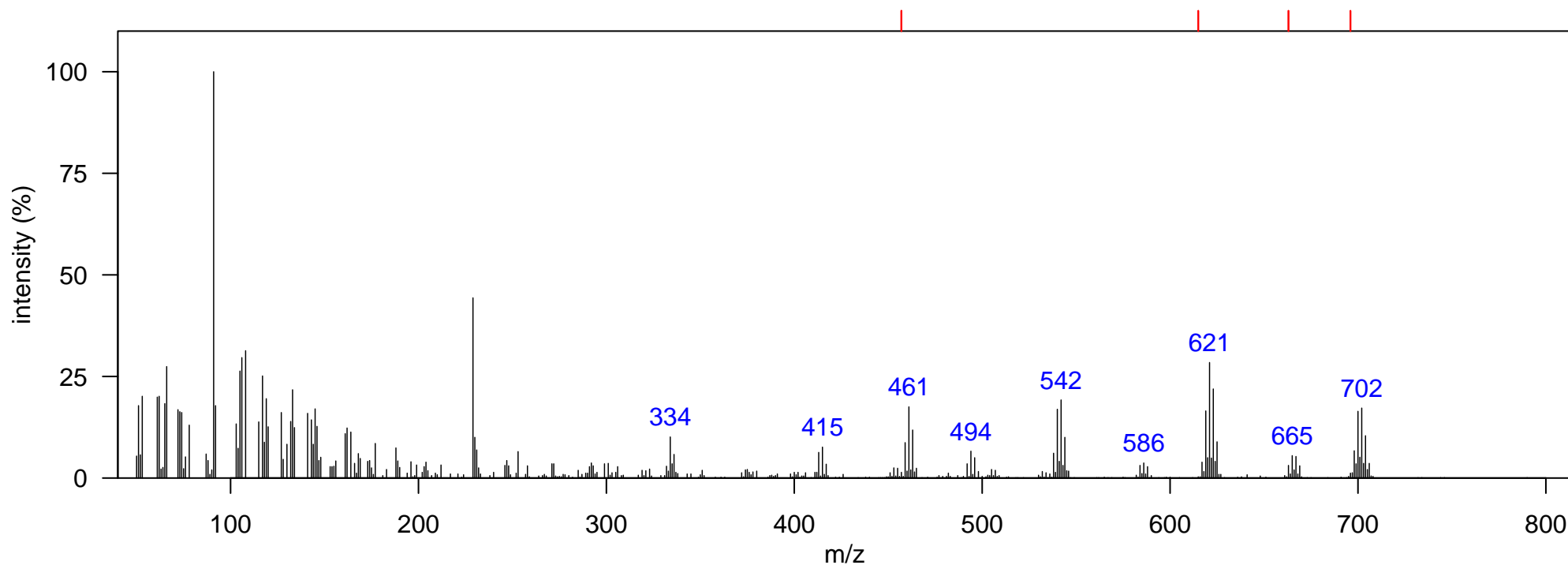
Comment: PM = Possible Molecular Ion. Contains Br7Cl.

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

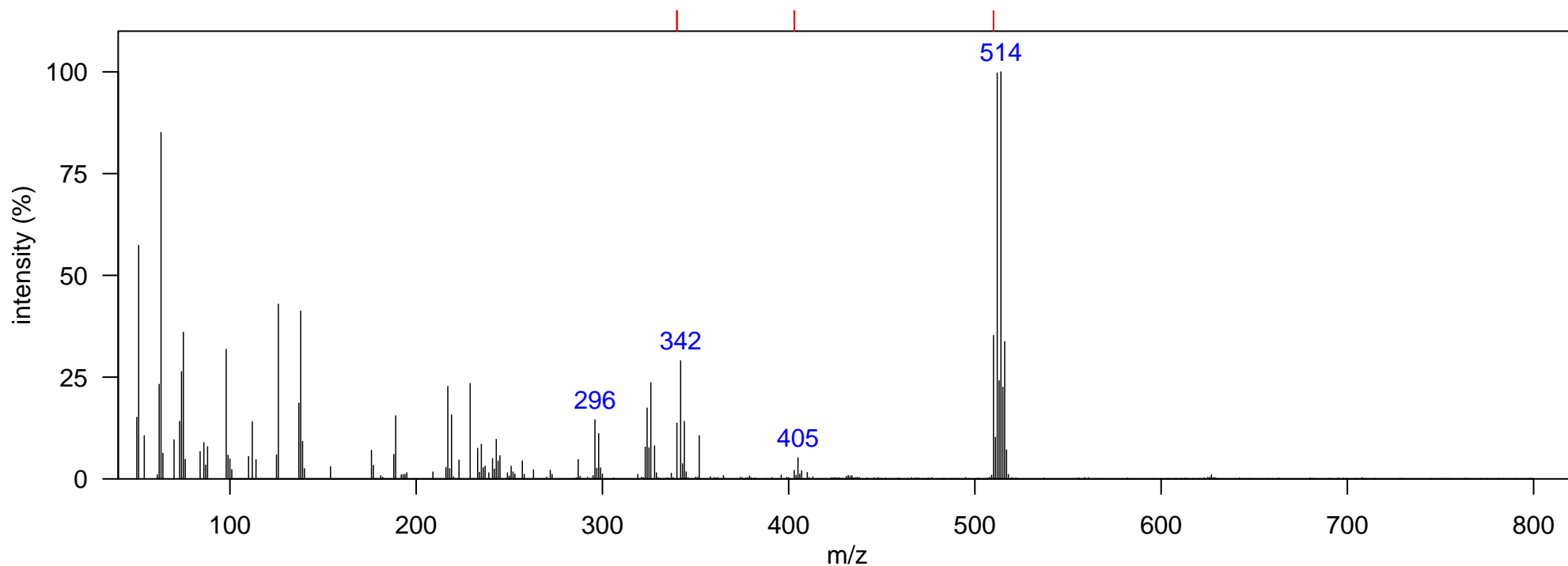
Comment: PM = Possible Molecular Ion, Frag = Fragment Ion

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

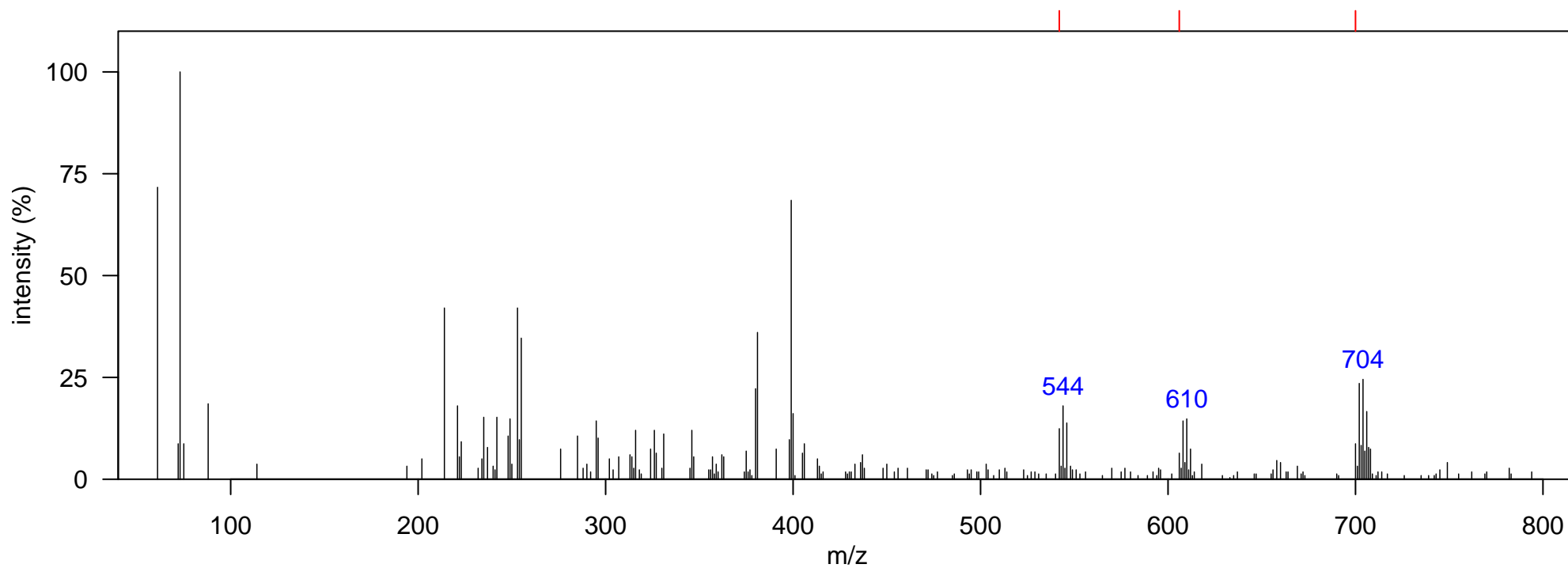
Comment: PM = Possible Molecular Ion

Elemental Formula: NA

Source: unknown

Class: unknown

Identification: Unknown



m/z	Identity
542	[PM-2Br] ⁺
606	[PM-Br-15] ⁺ = [PM-Br-CH ₃] ⁺
700	[PM] ⁺