

San Diego Bay Black Skimmer Eggs

Identifying Bioaccumulative Halogenated Organic Compounds Using a Nontargeted Analytical Approach:
Seabirds as Sentinels.

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Web Reference: <http://OrgMassSpec.github.io>

Prepared: 2015-03-02 18:21:15
SpecLibBlackSkimmerEgg2014 version 0.1-2
OrgMassSpecR version 0.4-4
png version 0.1-7
R version 3.1.0 (2014-04-10)

Name: Heptachloro-1'-methyl-1,2'-bipyrrole

Class: MBP

Matrix: SD Bay Black Skimmer Egg

In Samples: All

Group: Not Typically Monitored

Comment: Also referred to as Q1.

Instrument: GCxGC-TOF, EI, 70 eV

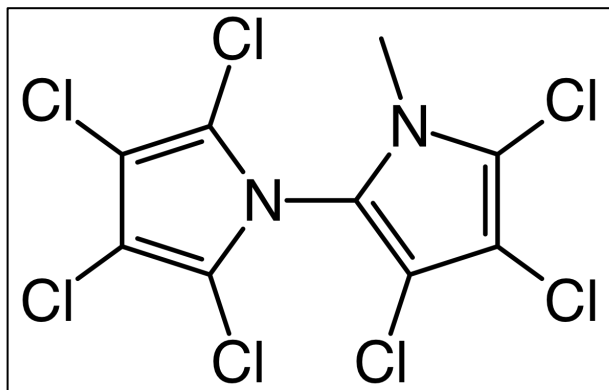
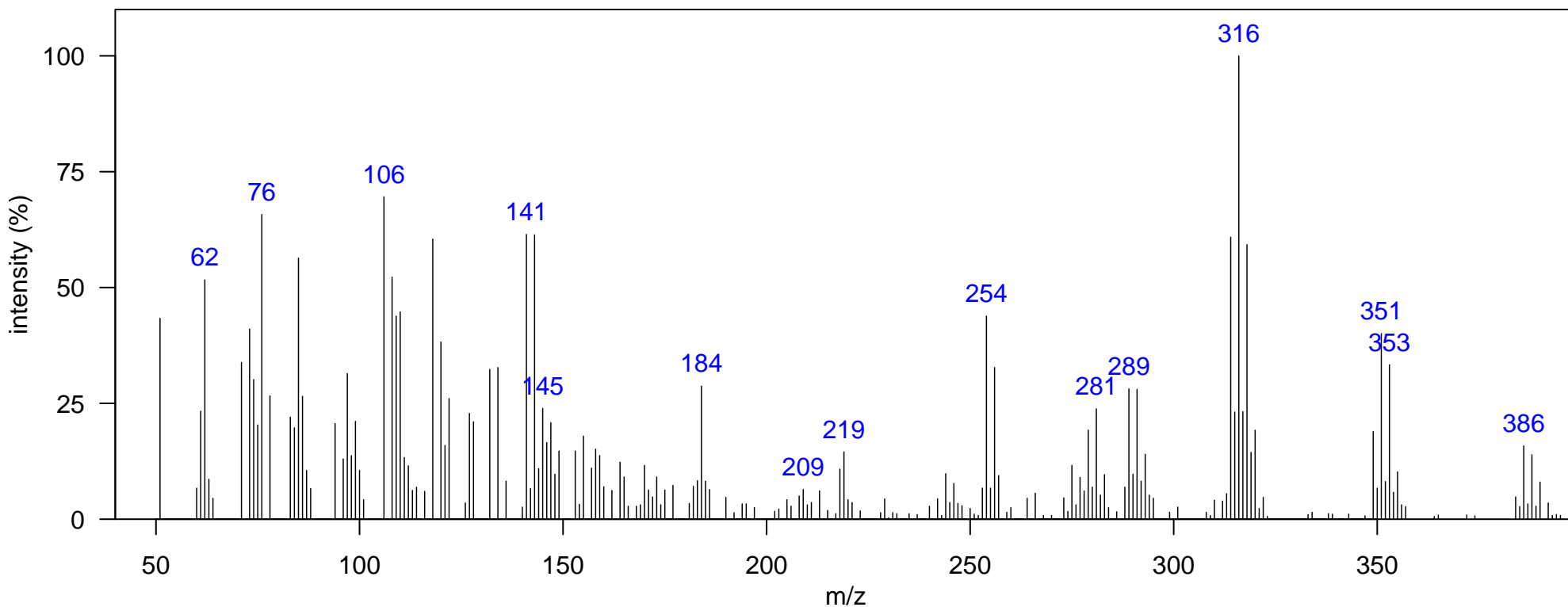
1D RT, 2D RT (s): 1988.71, 1.561

Quantitative Ion m/z: 316

Elemental Formula: C₉H₃Cl₇N₂

Source: Natural

Identification: Authentic MS RT



m/z [Fragment]
314 [M-Cl ₂] ⁺
349 [M-Cl] ⁺
384 M ⁺

Name: DDT-related 1

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₇H₅ClO

In Samples: A, B, C

1D RT, 2D RT (s): 830.868, 1.32

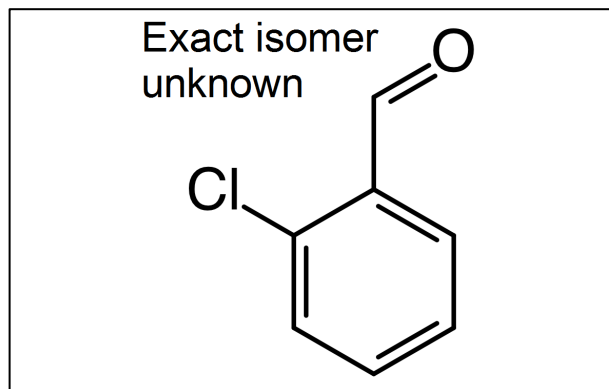
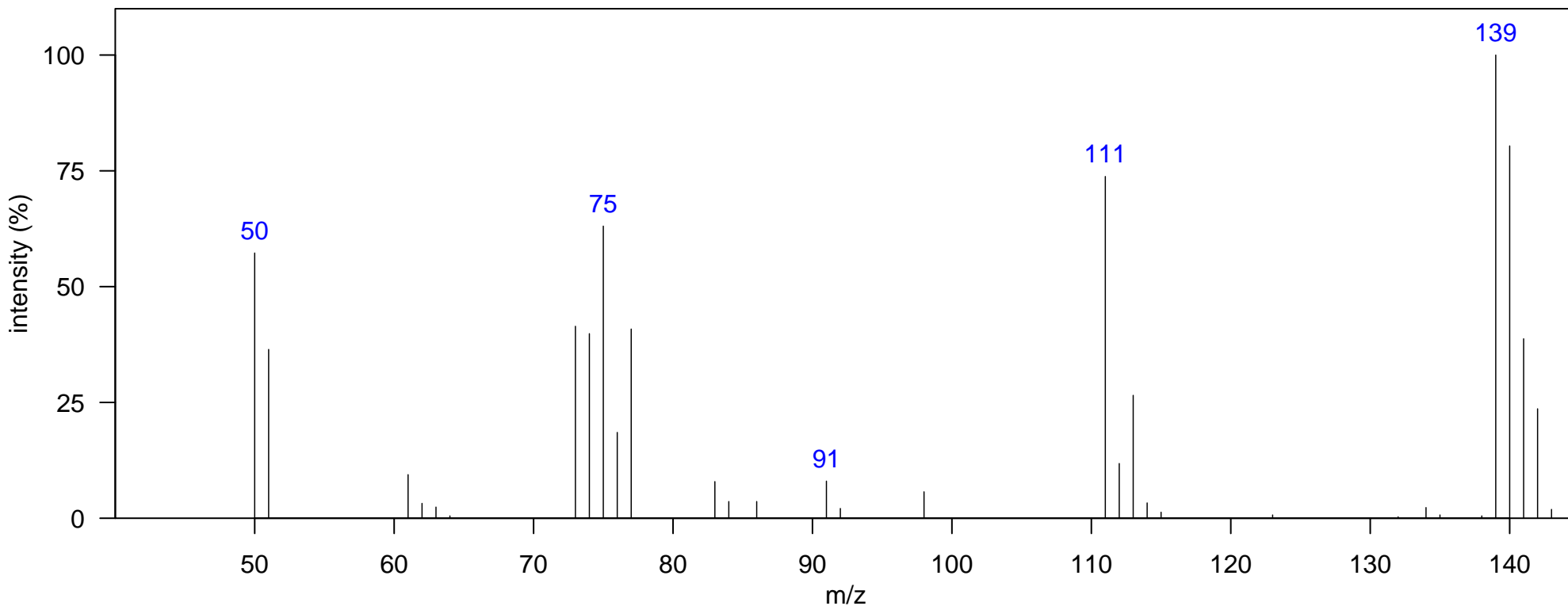
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 139

Identification: Authentic MS RT

Comment: NIST I.D. is 2-Chlorobenzaldehyde. Detected in DDT tech. mix.



m/z [Fragment]
76 [M-CHClO] ⁺
112 [M-CO] ⁺
140 M ⁺

Name: DDT-related 2

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₉H₄ClO

In Samples: A, B

1D RT, 2D RT (s): 1114.21, 1.327

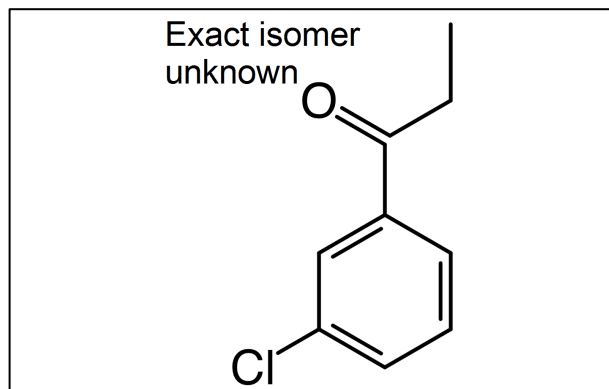
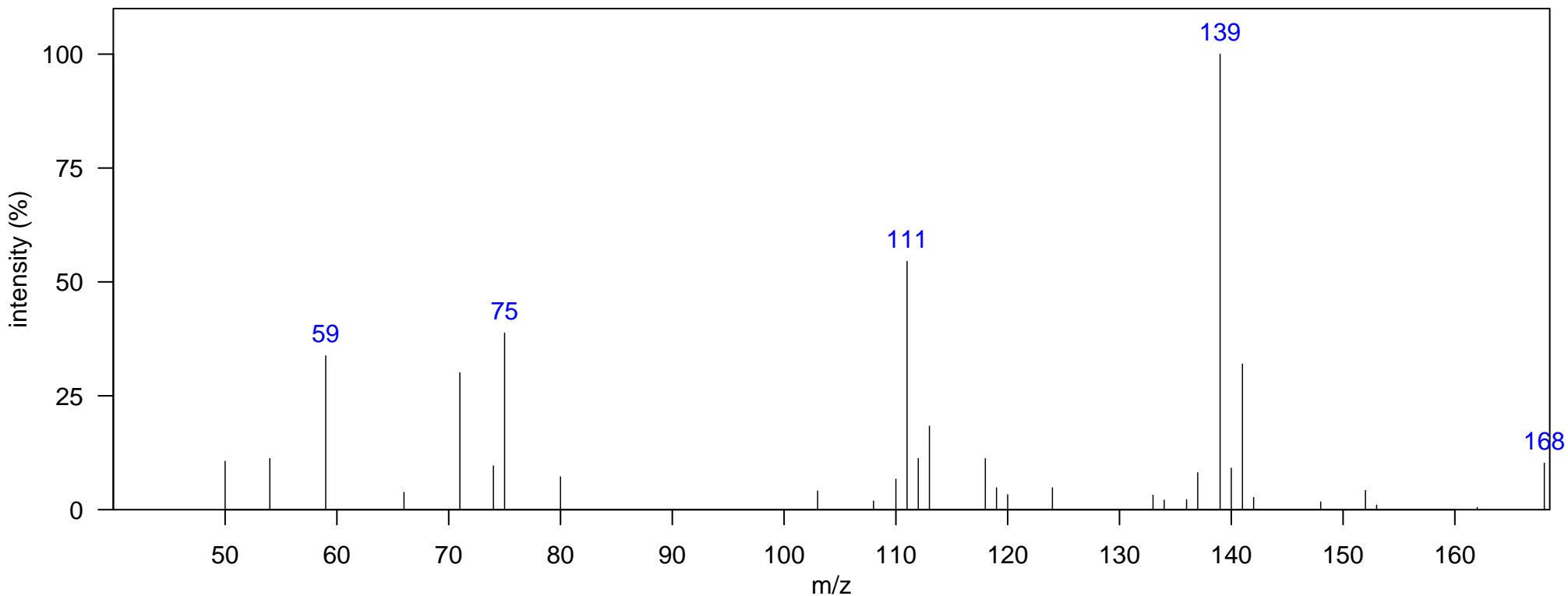
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 139

Identification: Reference Database MS

Comment: NIST I.D. is m-Chloropropiophenone.



m/z [Fragment]
112 [M-C ₃ H ₄ O] ⁺
140 [M-C ₂ H ₄] ⁺
168 M ⁺

Name: 1,1-Bis(p-chlorophenyl)-ethane (DDeT)

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₁₄H₁₂Cl₂

In Samples: A, B

1D RT, 2D RT (s): 1778.83, 1.485

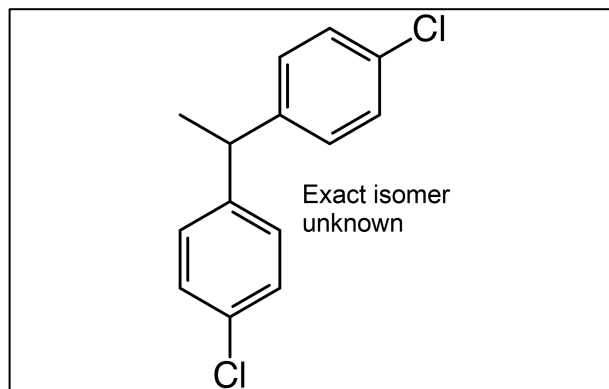
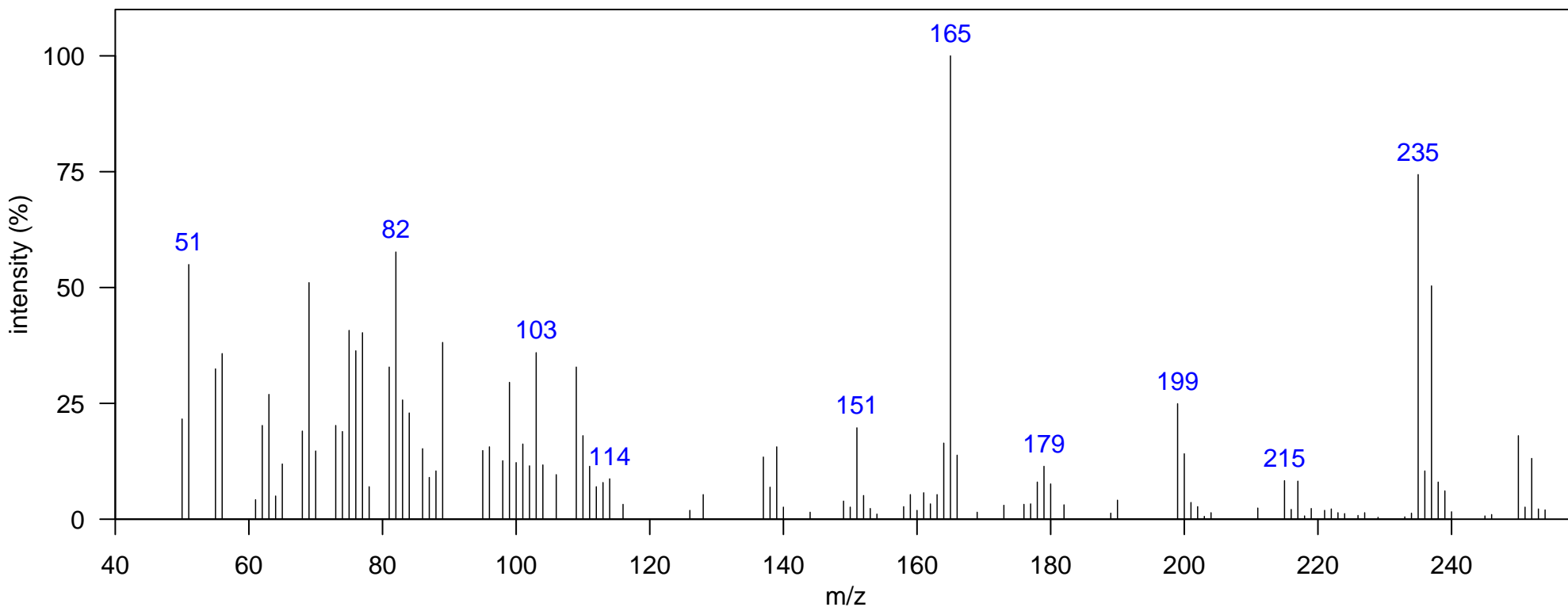
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 235

Identification: Reference Database MS

Comment: NIST I.D. is 1,1-Bis(p-chlorophenyl)ethane.



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

Name: Chlordane Related 1

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₁₀H₆Cl₈

In Samples: All

1D RT, 2D RT (s): 1950.23, 1.498

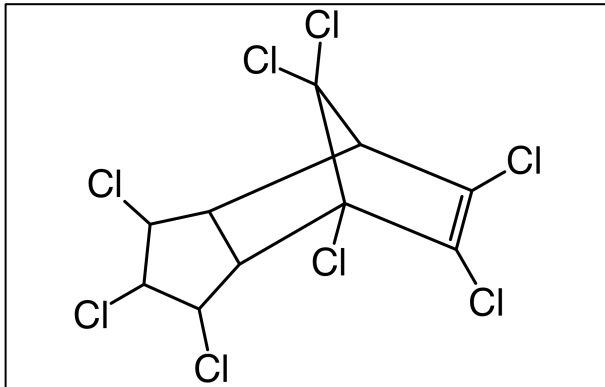
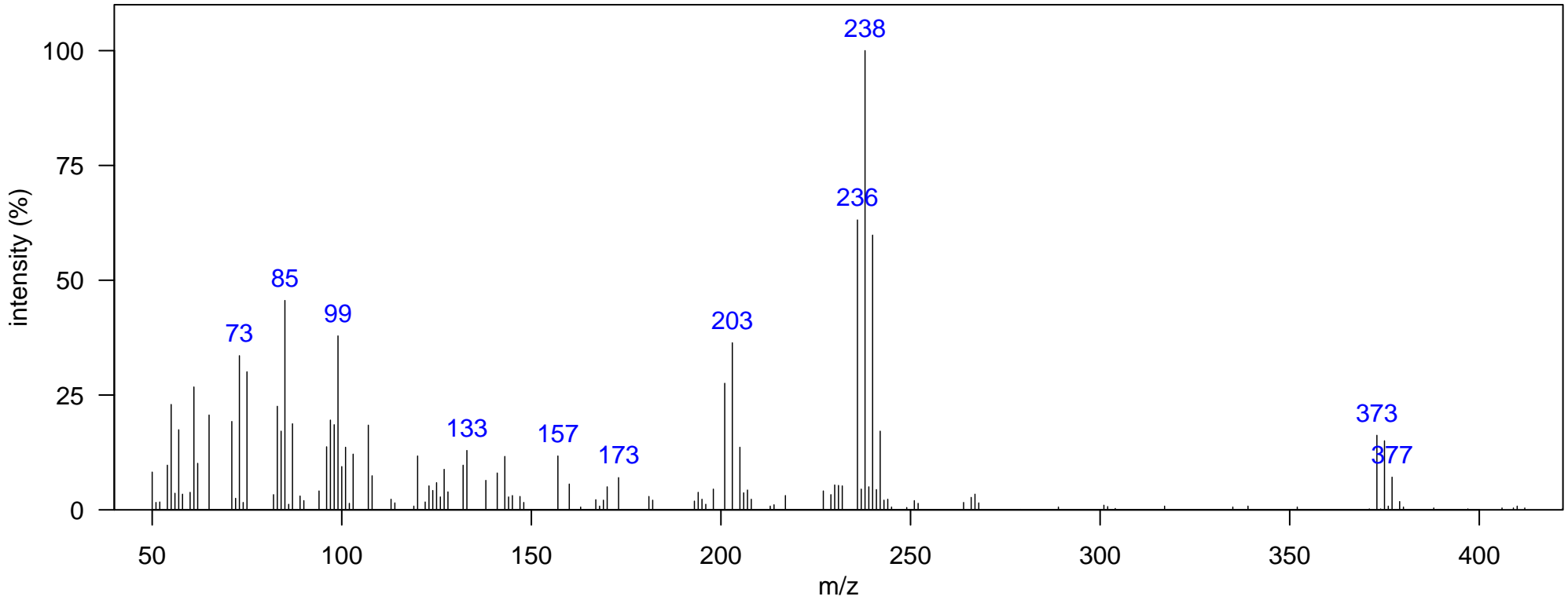
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 238

Identification: Literature MS

Comment: M⁺ is not detected. Tentatively identified as U82 (Environ. Sci. Technol., 1999, 33, 1353-1358).



m/z [Fragment]
236 [C ₅ HCl ₅] ⁺
371 [M-Cl] ⁺
406 M ⁺

Name: Chlordane Related 2

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₁₀H₇Cl₇

In Samples: All

1D RT, 2D RT (s): 1957.22, 1.67

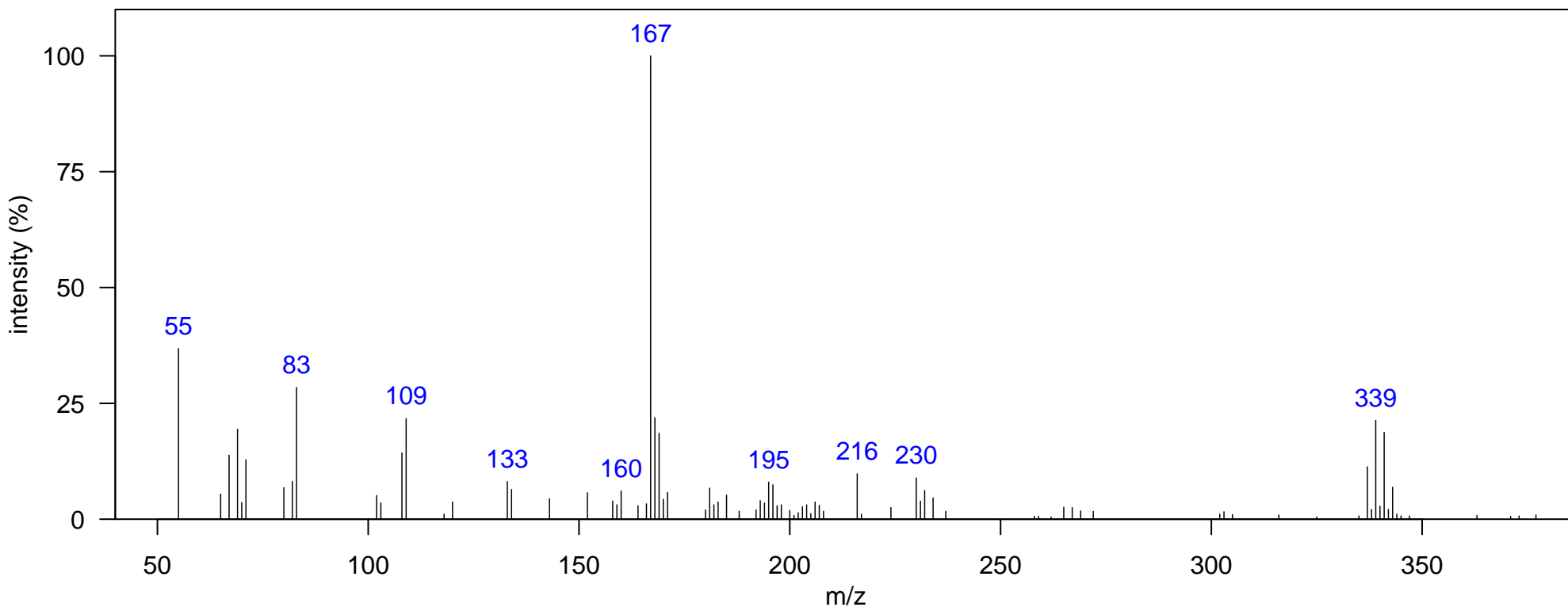
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 339

Identification: Manual Congener Group

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



m/z [Fragment]
337 [M-Cl] ⁺
372 M ⁺

Name: DDT-related 3

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₁₄H₁₂Cl₃

In Samples: A, B, C

1D RT, 2D RT (s): 1999.2, 1.663

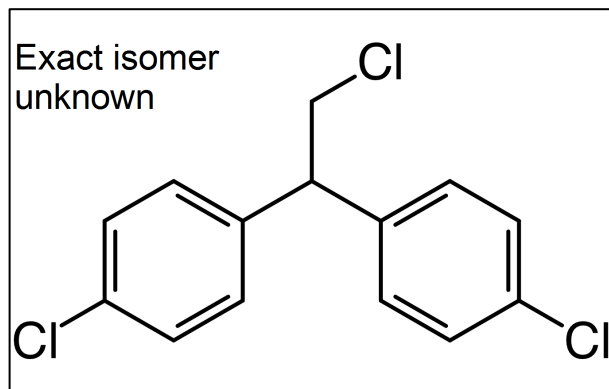
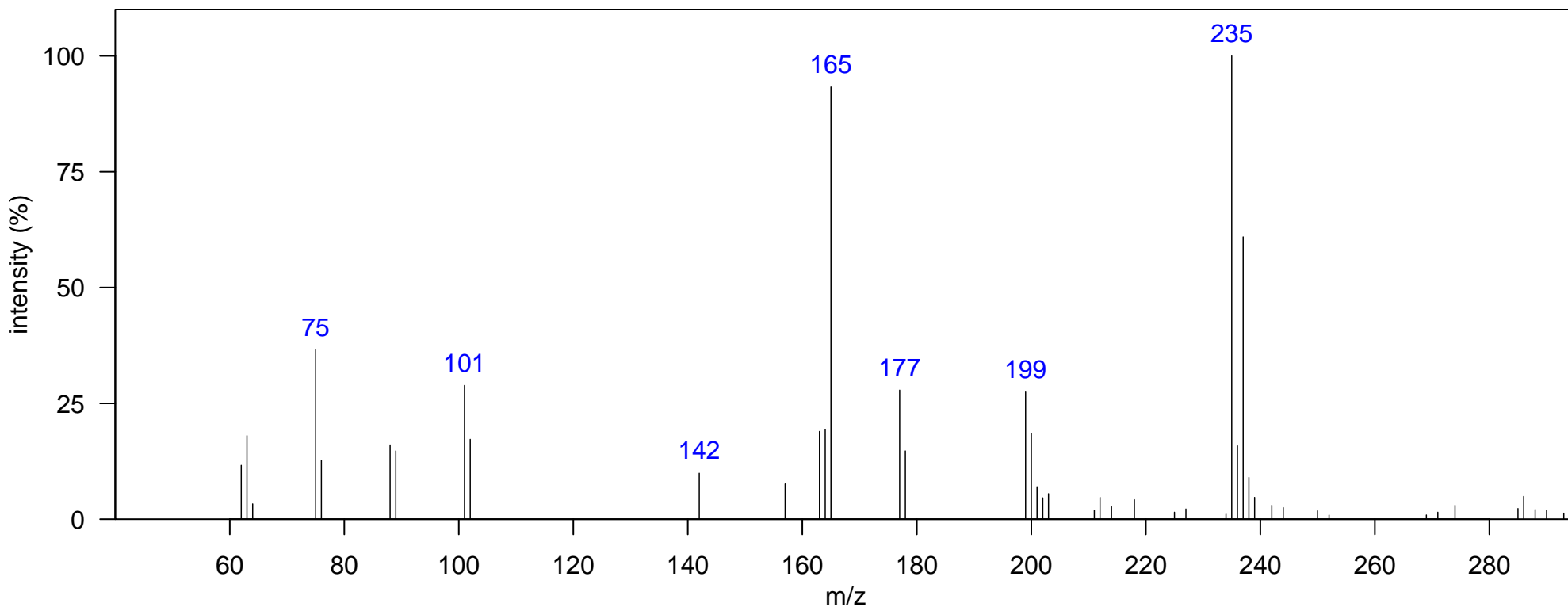
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 235

Identification: Reference Database MS

Comment: NIST I.D. is 1-Chloro-2,2-Bis(p-chlorophenyl)ethane.



m/z [Fragment]
166 [M-CH ₂ Cl ₃] ⁺
201 [M-CH ₂ Cl ₂] ⁺
236 [M-CH ₂ Cl] ⁺
285 M ⁺

Name: DDT-related 4

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

In Samples: All

Group: Not Typically Monitored

Comment: DDE Isomer.

Instrument: GCxGC-TOF, EI, 70 eV

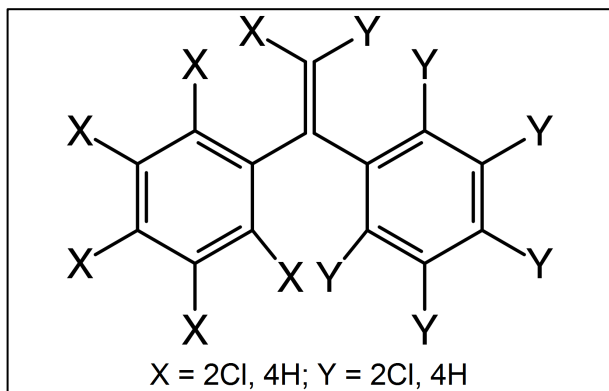
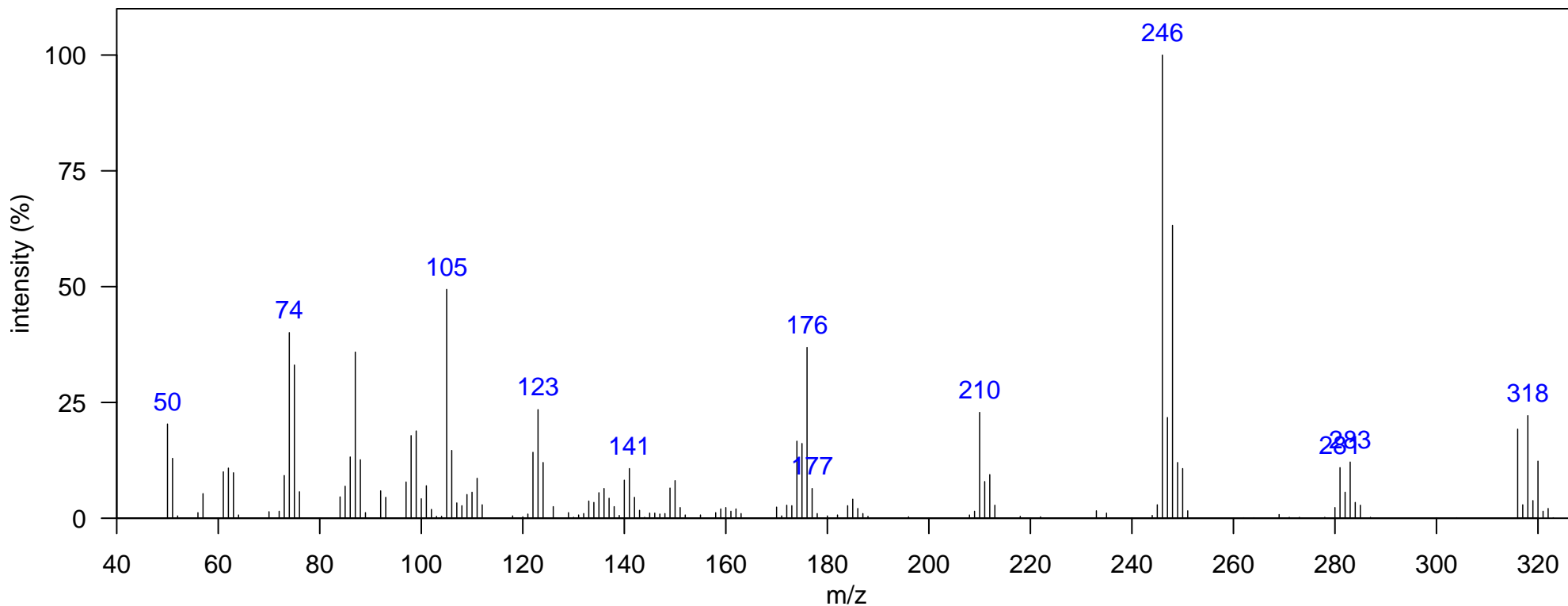
1D RT, 2D RT (s): 2051.67, 1.597

Quantitative Ion m/z: 318

Elemental Formula: C₁₄H₈Cl₄

Source: Anthropogenic

Identification: Authentic MS



m/z [Fragment]
176 [M-C ₁₄] ⁺
211 [M-C ₁₃] ⁺
246 [M-C ₁₂] ⁺
280 [M-Cl] ⁺
316 M ⁺

Name: Tris(4-chlorophenyl)methane (TCPM)

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₁₉H₁₃Cl₃

In Samples: All

1D RT, 2D RT (s): 2397.97, 1.855

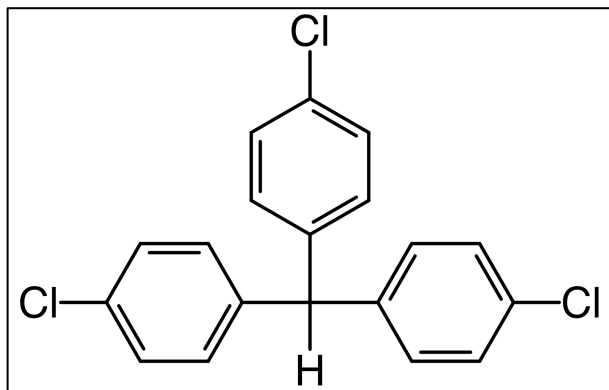
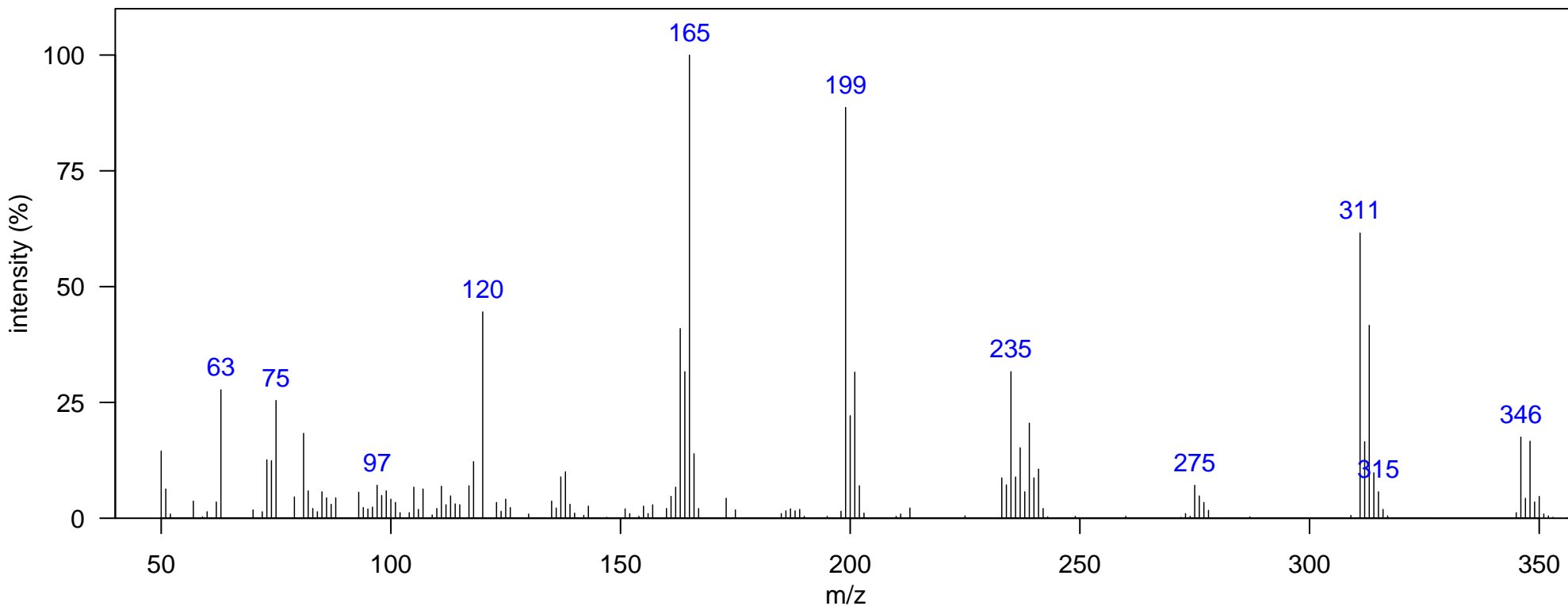
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 311

Identification: Authentic MS RT

Comment:



m/z [Fragment]
275 [M-HCl ₂] ⁺
311 [M-Cl] ⁺
346 M ⁺

Name: Tris(4-chlorophenyl)methanol (TCPMOH)

Class: OC pesticide

Matrix: SD Bay Black Skimmer Egg

In Samples: All

Group: Not Typically Monitored

Comment: M+ is not detected.

Instrument: GCxGC-TOF, EI, 70 eV

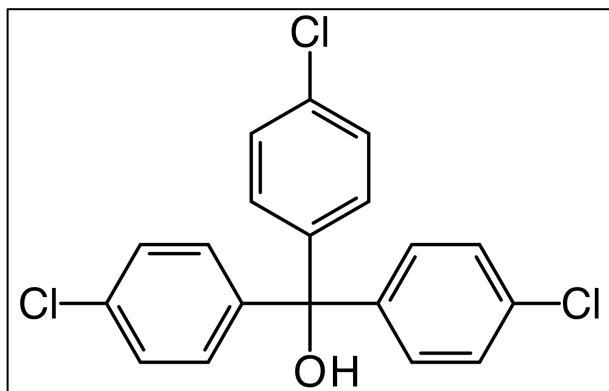
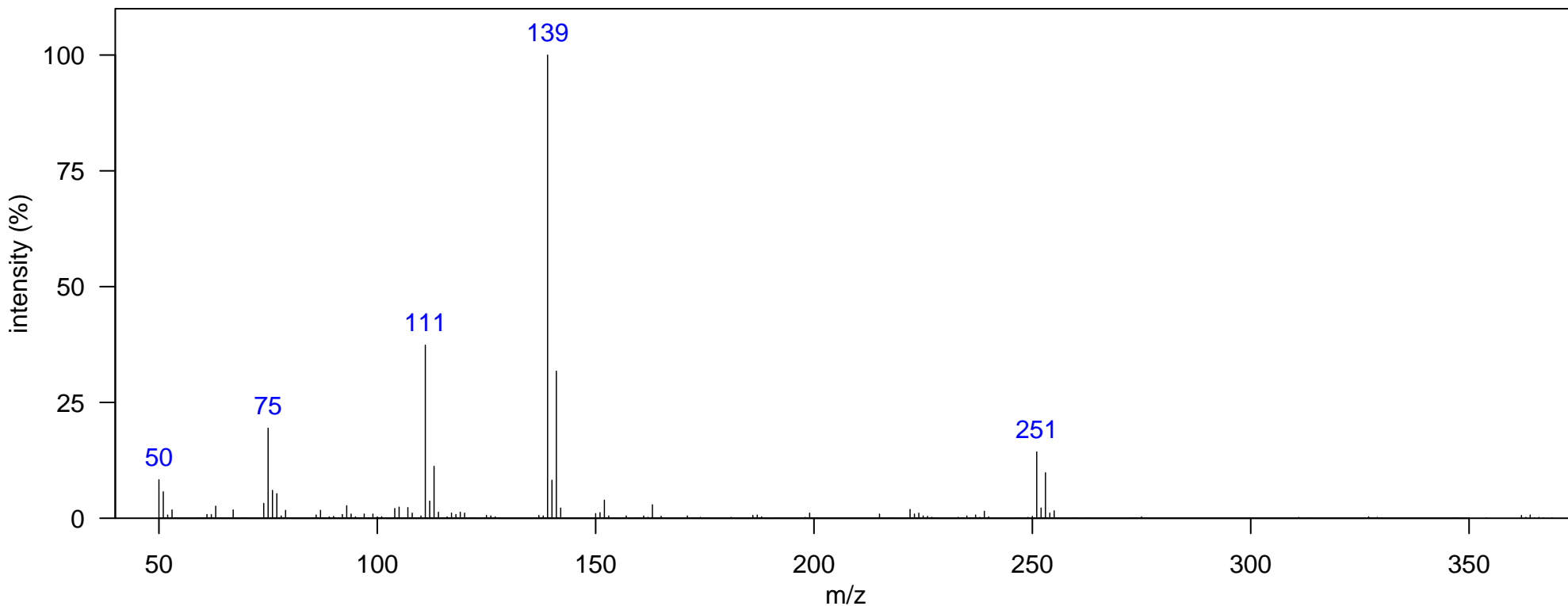
1D RT, 2D RT (s): 2499.41, 2.125

Quantitative Ion m/z: 139

Elemental Formula: C₁₉H₁₃Cl₃O

Source: Anthropogenic

Identification: Authentic MS RT



m/z [Fragment]
251 [M-C ₂ HCl ₂ O] ⁺
311 [M-HClO] ⁺
362 M ⁺

Name: Methylmercuric iodide

Class: Other

Matrix: SD Bay Black Skimmer Egg

In Samples: A, B, C

Group: Not Typically Monitored

Comment: NIST I.D. is Methylmercuric iodide. Formula is CH₃HgI.

Instrument: GCxGC-TOF, EI, 70 eV

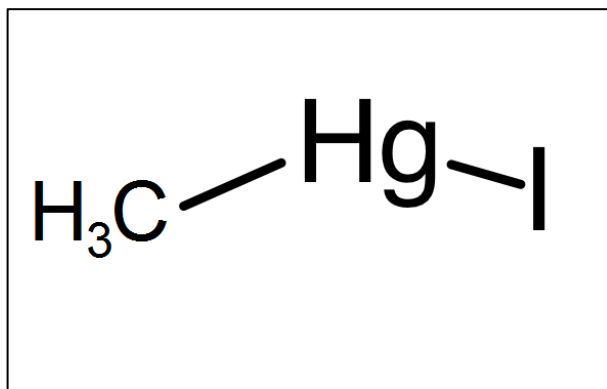
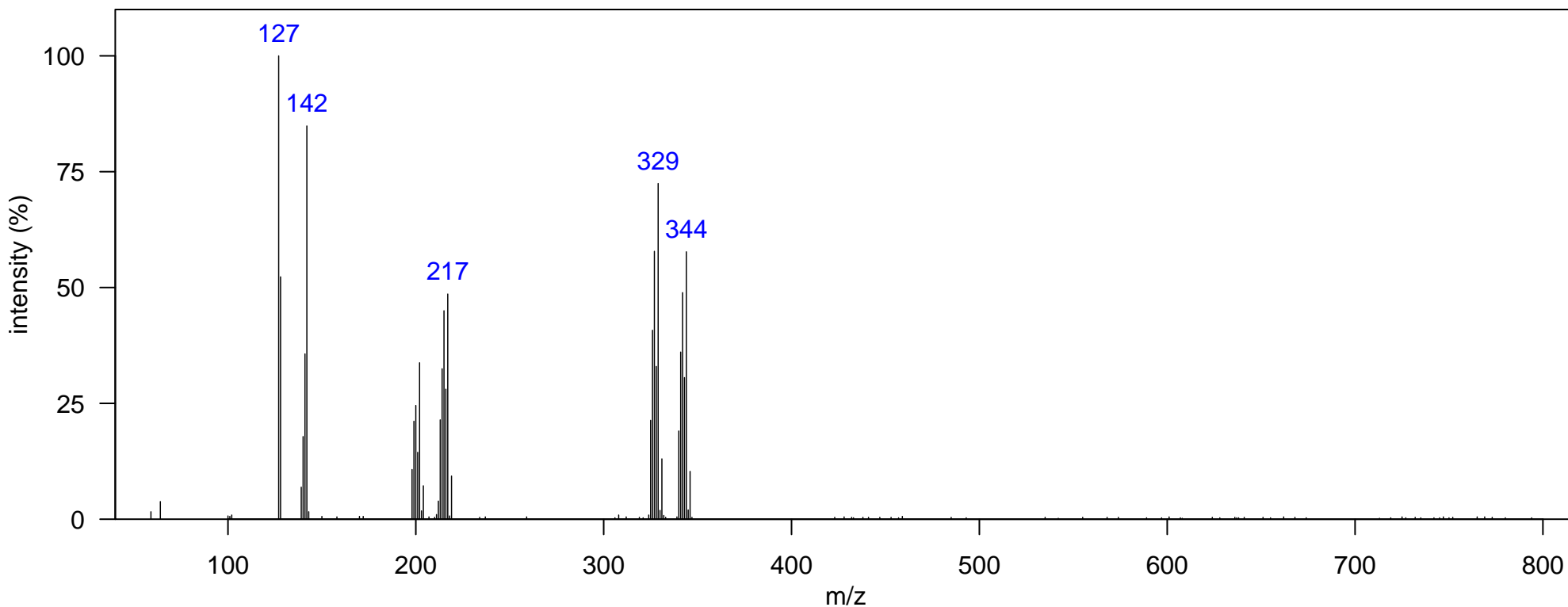
1D RT, 2D RT (s): 753.912, 1.551

Quantitative Ion m/z: 329

Elemental Formula:

Source: Unknown

Identification: Authentic MS RT



m/z [Fragment]
325 [M-CH ₃] ⁺
340 M ⁺

Name: 2-Bromo-1,3-diphenyl-1,3-propanedione

Class: Other

Matrix: SD Bay Black Skimmer Egg

In Samples: All

Group: Not Typically Monitored

Comment: M+ is not detected.

Instrument: GCxGC-TOF, EI, 70 eV

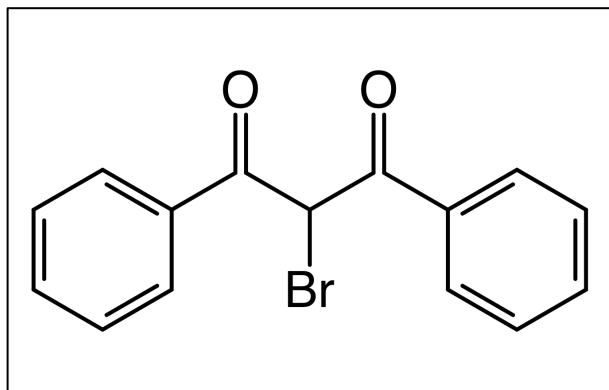
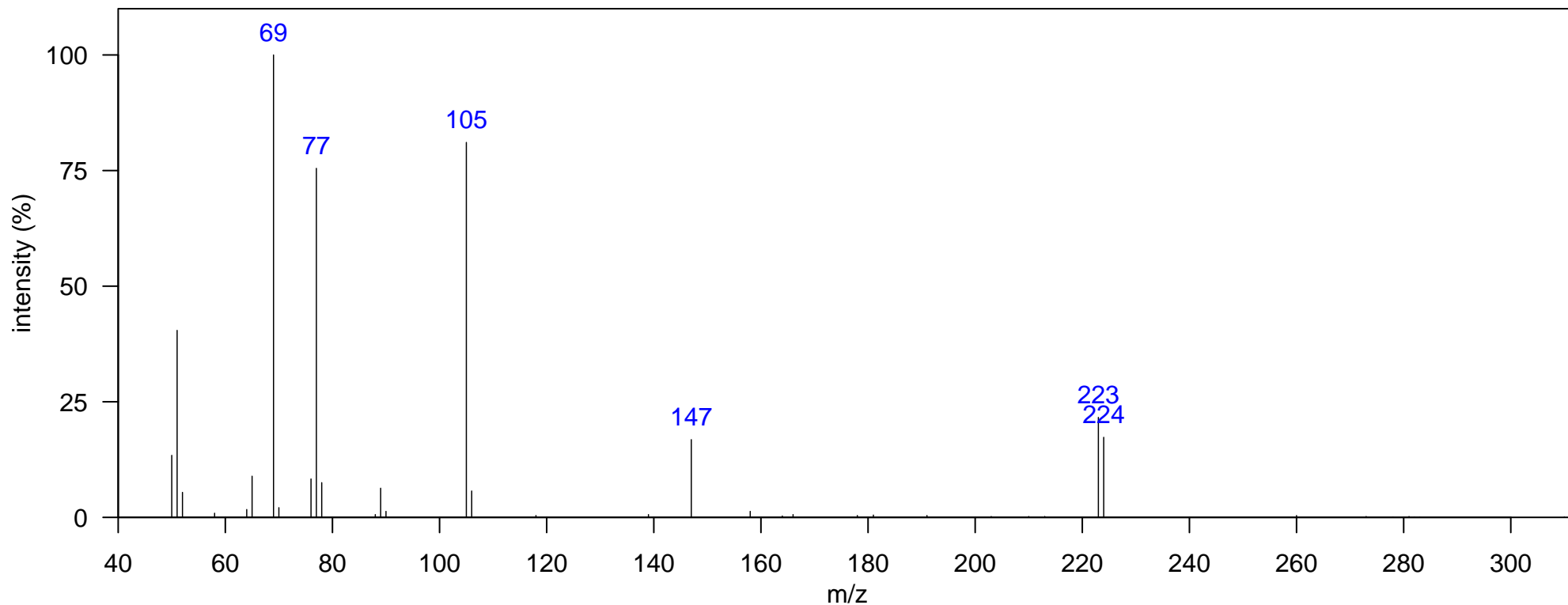
1D RT, 2D RT (s): 1932.74, 1.67

Quantitative Ion m/z: 223

Elemental Formula: C₁₅H₁₁BrO₂

Source: Unknown

Identification: Authentic MS RT



m/z [Fragment]
223 [M-Br] ⁺
302 M ⁺

Name: p,p'-Dichlorodiphenyl sulfone

Class: Other

Matrix: SD Bay Black Skimmer Egg

In Samples: A, C, D

Group: Not Typically Monitored

Comment:

Instrument: GCxGC-TOF, EI, 70 eV

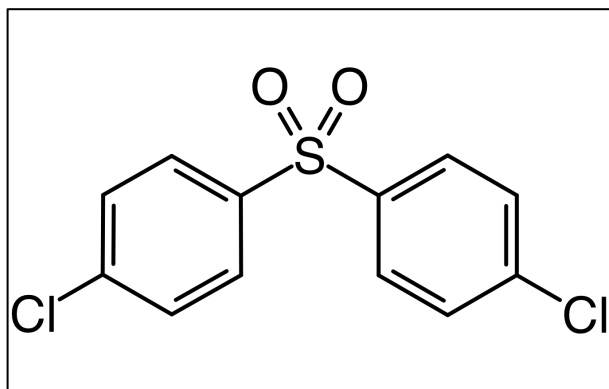
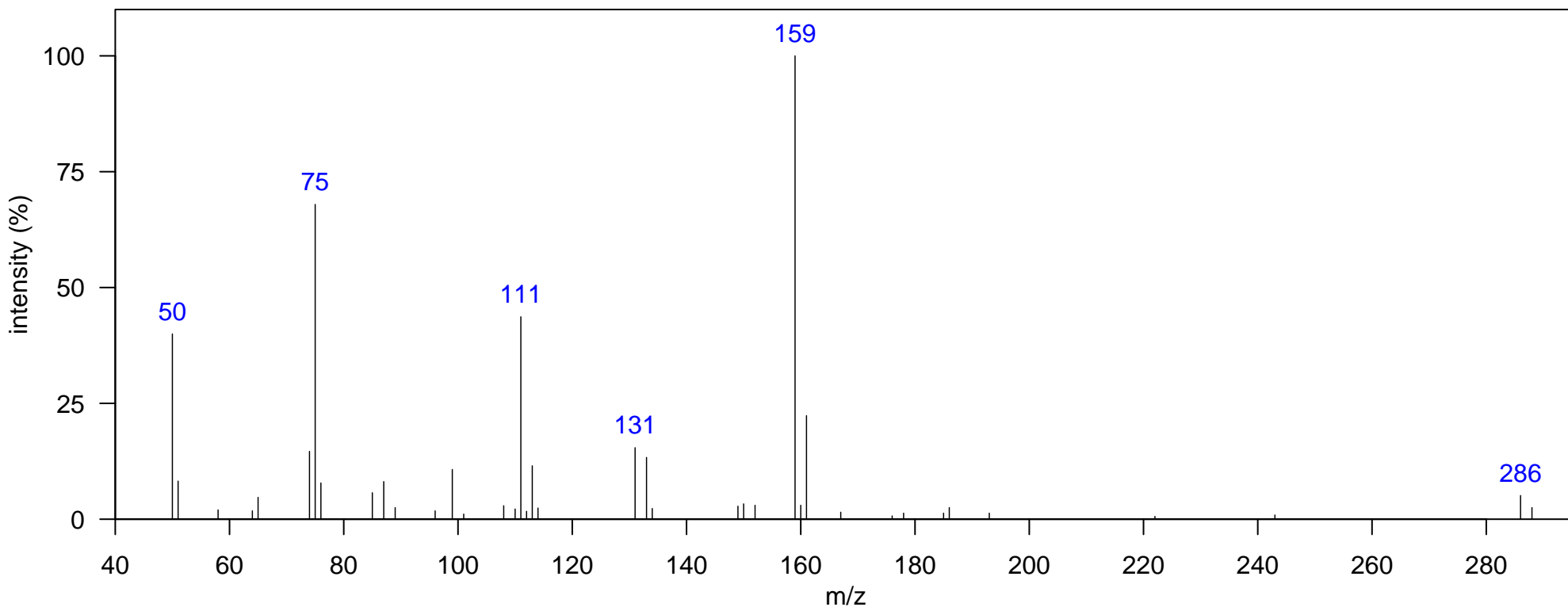
1D RT, 2D RT (s): 2072.66, 1.855

Quantitative Ion m/z: 159

Elemental Formula: C₁₂H₈Cl₂O₂S

Source: Unknown

Identification: Authentic MS RT



m/z [Fragment]
159 [M-C ₆ H ₄ ClSO] ⁺
286 M ⁺

Name: Parachlorophenol

Class: Phenol A

Matrix: SD Bay Black Skimmer Egg

In Samples: A, B, C

Group: Not Typically Monitored

Comment: NIST I.D. is Parachlorophenol.

Instrument: GCxGC-TOF, EI, 70 eV

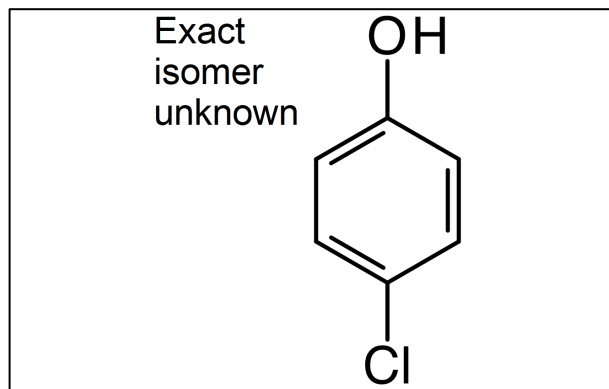
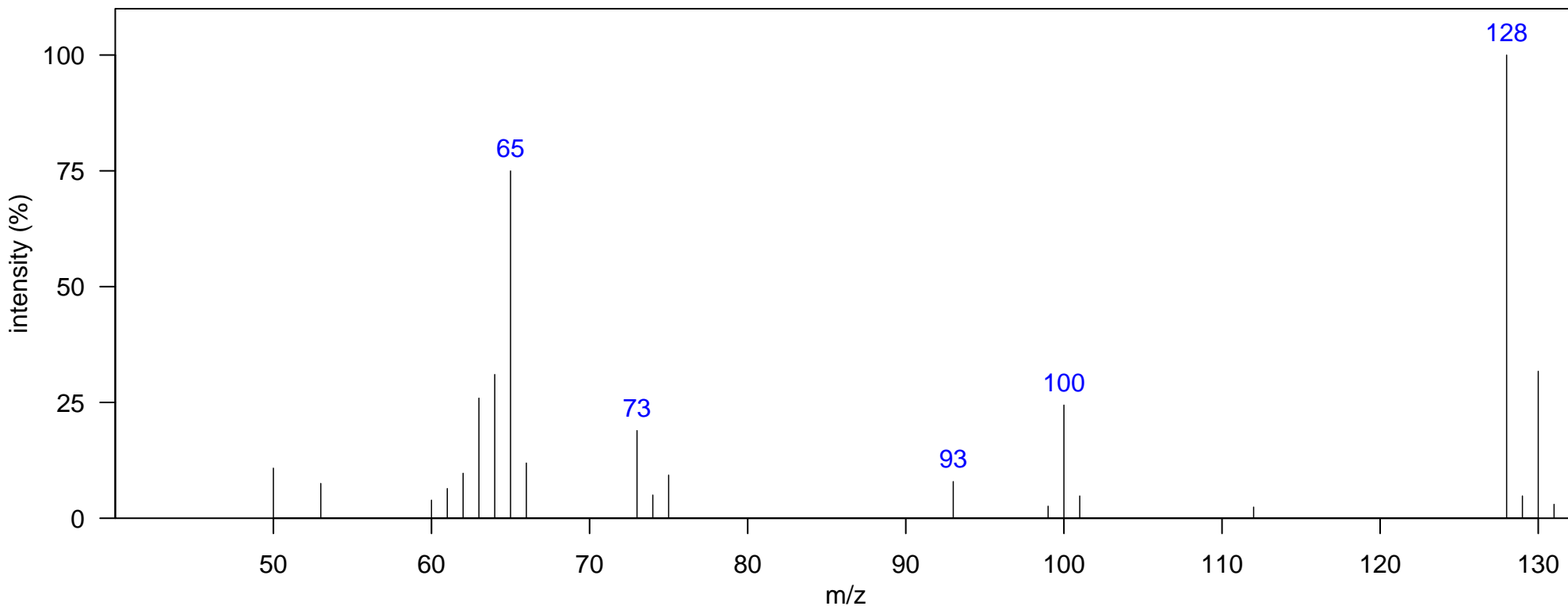
1D RT, 2D RT (s): 939.306, 1.307

Quantitative Ion m/z: 128

Elemental Formula: C₆H₅ClO

Source: Anthropogenic

Identification: Reference Database MS



m/z [Fragment]
128 M+

Name: 4-Bromophenol

Class: Phenol N

Matrix: SD Bay Black Skimmer Egg

In Samples: All

Group: Not Typically Monitored

Comment:

Instrument: GCxGC-TOF, EI, 70 eV

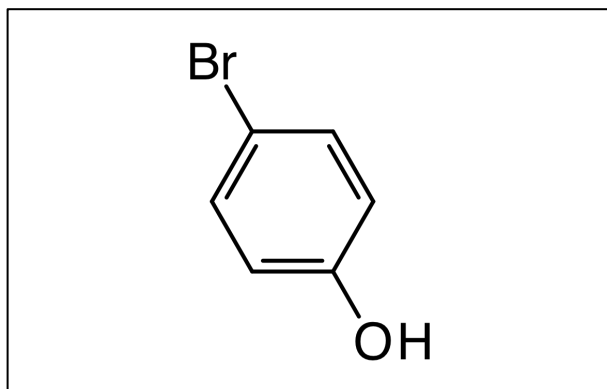
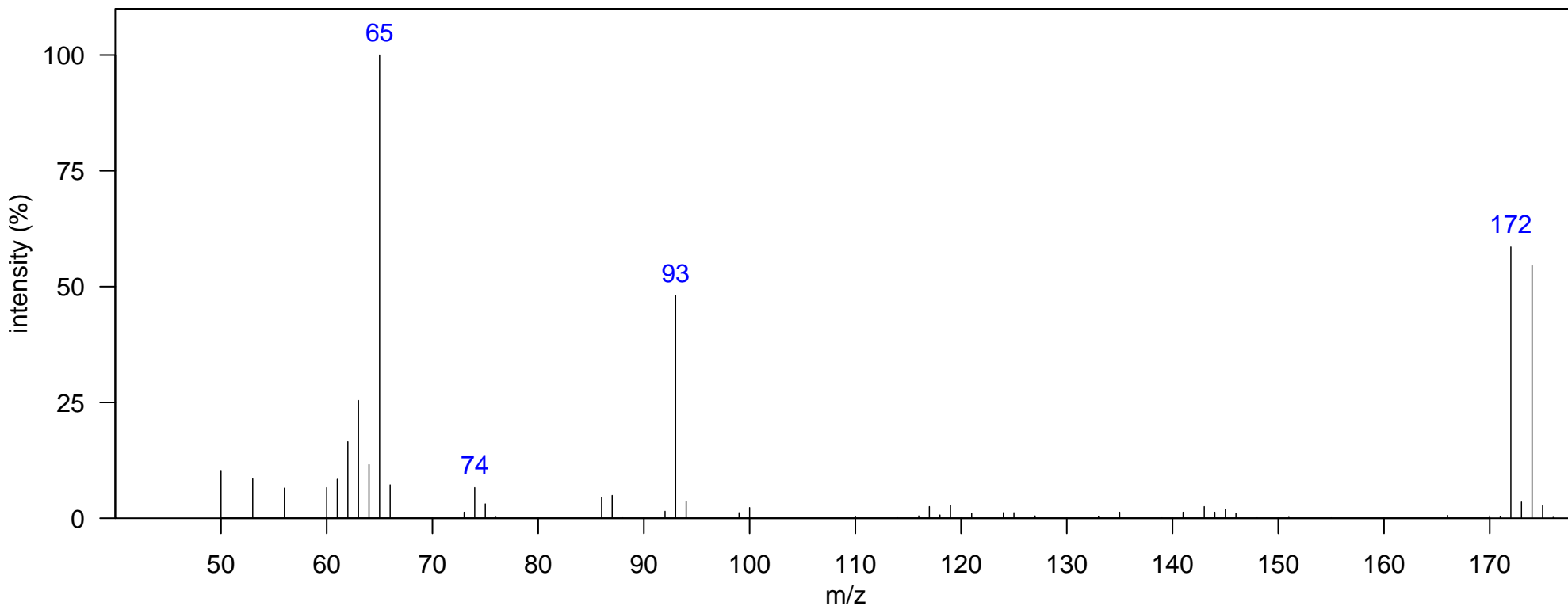
1D RT, 2D RT (s): 1065.23, 1.386

Quantitative Ion m/z: 172

Elemental Formula: C₆H₅BrO

Source: Natural

Identification: Authentic MS RT



m/z [Fragment]
93 [M-Br] ⁺
172 M ⁺

Name: 4-Chlorocatechol

Class: Phenol A

Matrix: SD Bay Black Skimmer Egg

In Samples: A, B, C

Group: Not Typically Monitored

Comment:

Instrument: GCxGC-TOF, EI, 70 eV

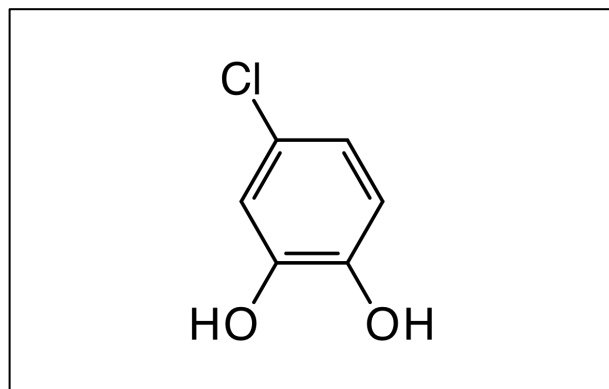
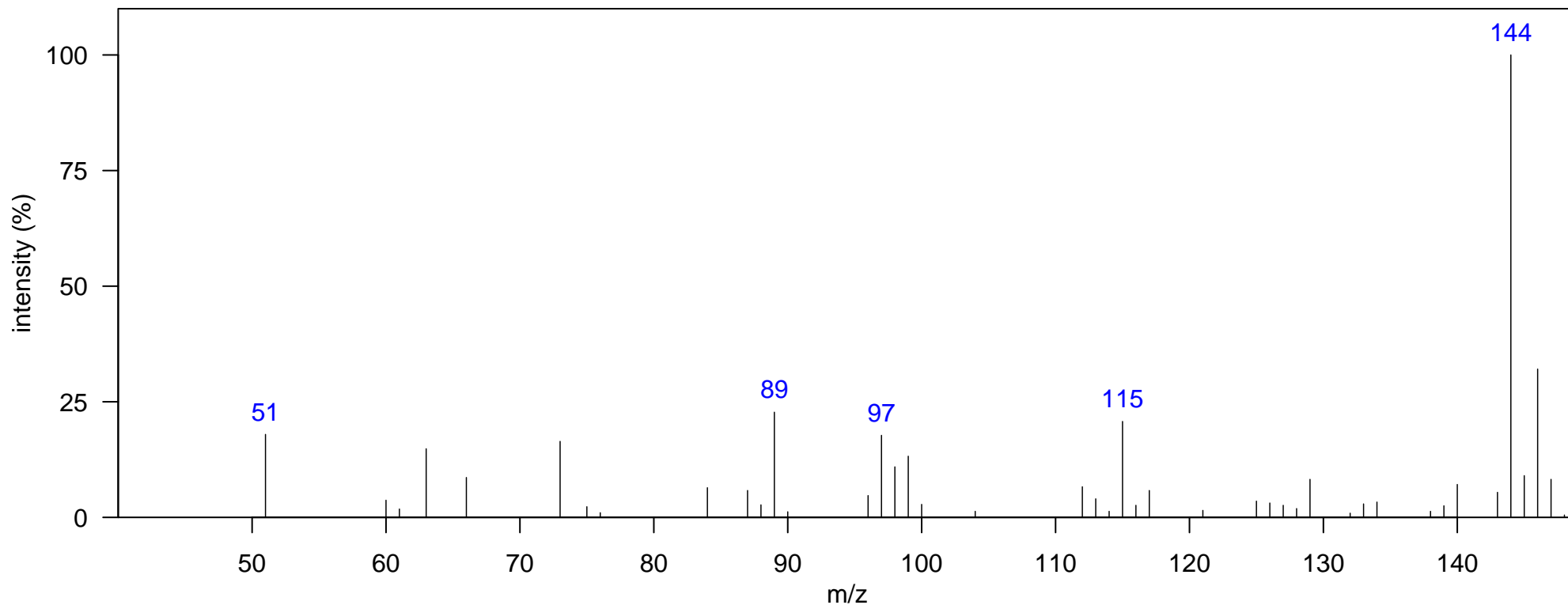
1D RT, 2D RT (s): 1233.14, 1.287

Quantitative Ion m/z: 144

Elemental Formula: C₆H₅ClO₂

Source: Anthropogenic

Identification: Authentic MS RT



m/z [Fragment]
144 M+

Name: 4-Chlorocatechol isomer

Class: Phenol A

Matrix: SD Bay Black Skimmer Egg

In Samples: A, B, C

Group: Not Typically Monitored

Comment:

Instrument: GCxGC-TOF, EI, 70 eV

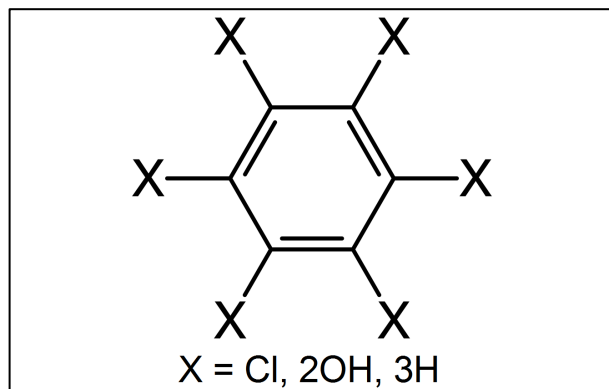
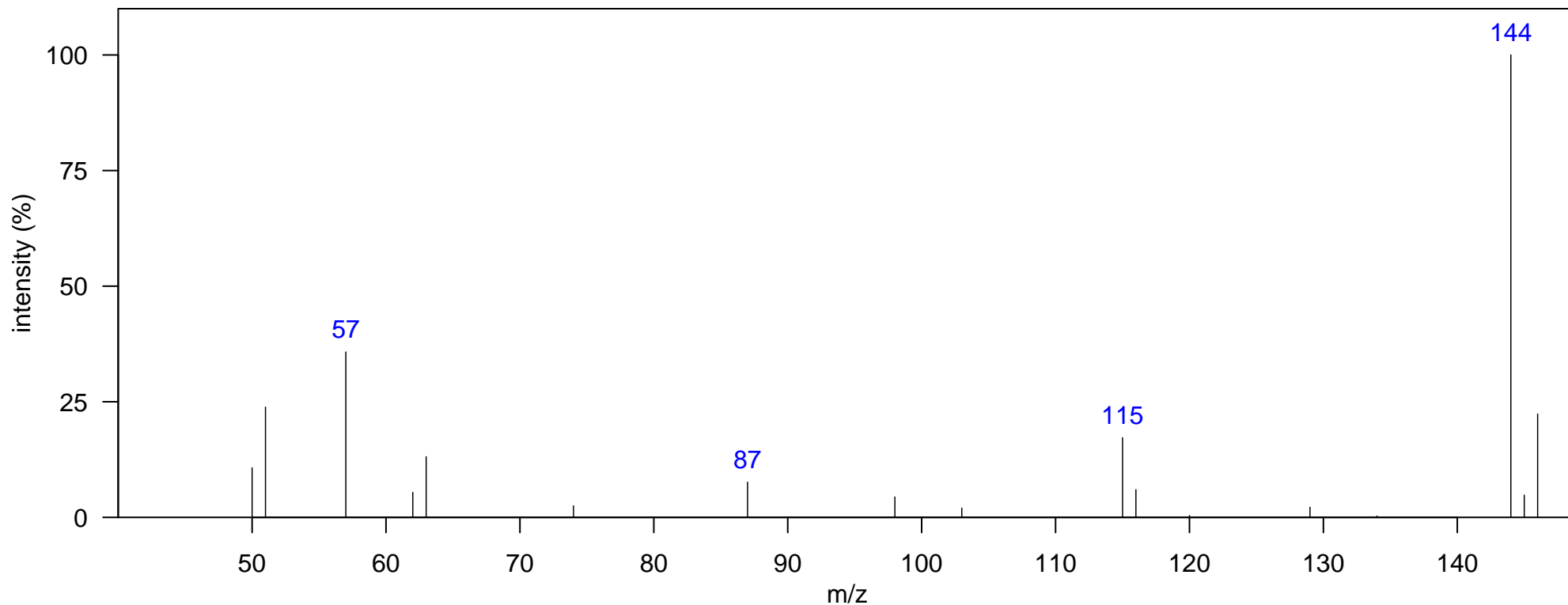
1D RT, 2D RT (s): 1355.57, 1.28

Quantitative Ion m/z: 144

Elemental Formula: C₆H₅ClO₂

Source: Anthropogenic

Identification: Authentic MS



m/z [Fragment]
144 M+

Name: 2,4,6-Tribromoanisole

Class: Phenol M

Matrix: SD Bay Black Skimmer Egg

In Samples: A, C

Group: Not Typically Monitored

Comment:

Instrument: GCxGC-TOF, EI, 70 eV

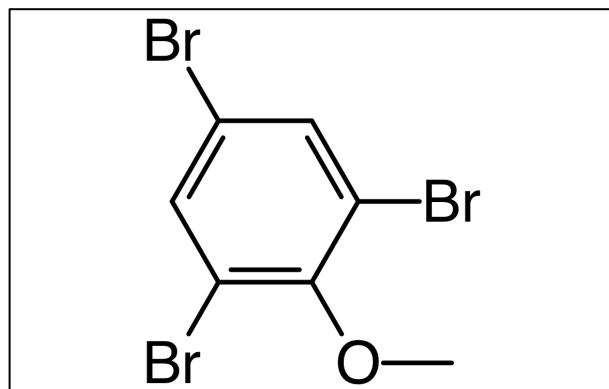
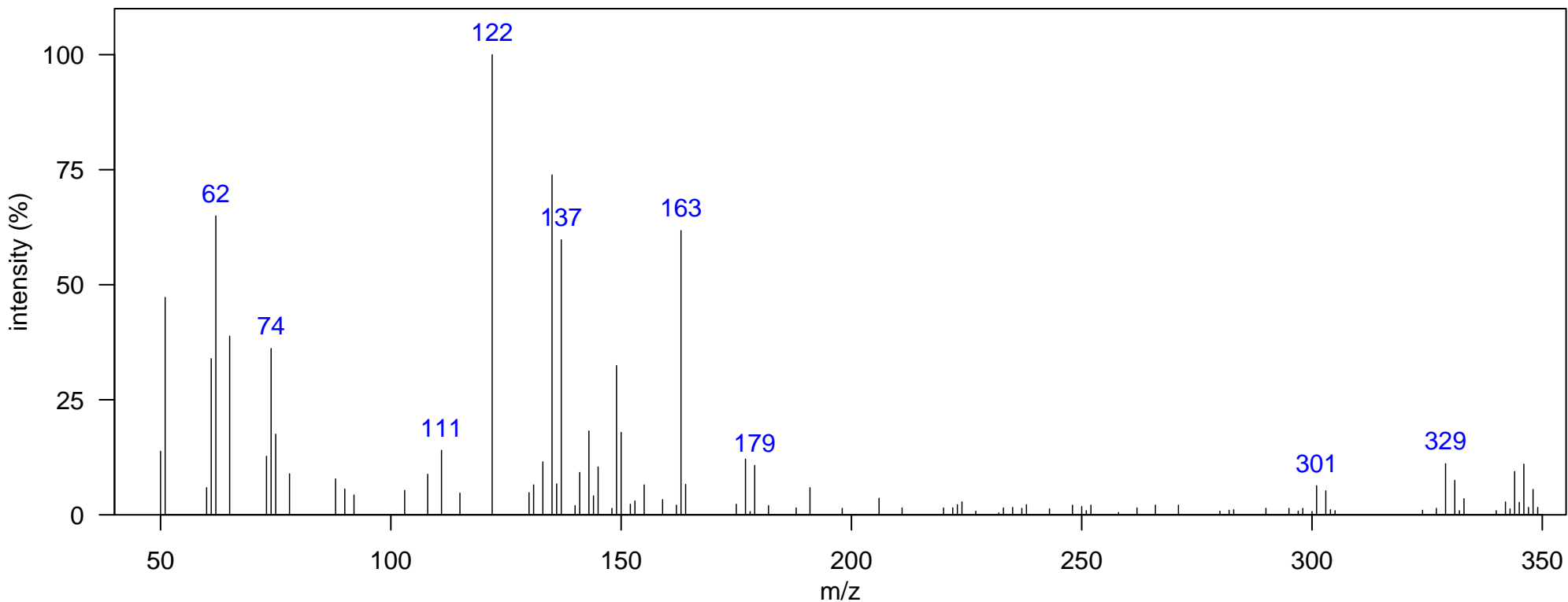
1D RT, 2D RT (s): 1478, 1.465

Quantitative Ion m/z: 331

Elemental Formula: C₇H₅Br₃O

Source: Mixed

Identification: Authentic MS RT



m/z [Fragment]
299 [M-C ₂ H ₃ O] ⁺
327 [M-CH ₃] ⁺
342 M ⁺

Name: p-Chloroanisole

Class: Phenol A

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₇H₇ClO

In Samples: A, C, D

1D RT, 2D RT (s): 1596.93, 1.082

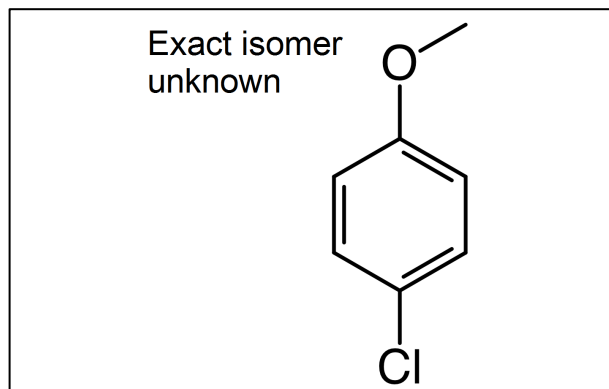
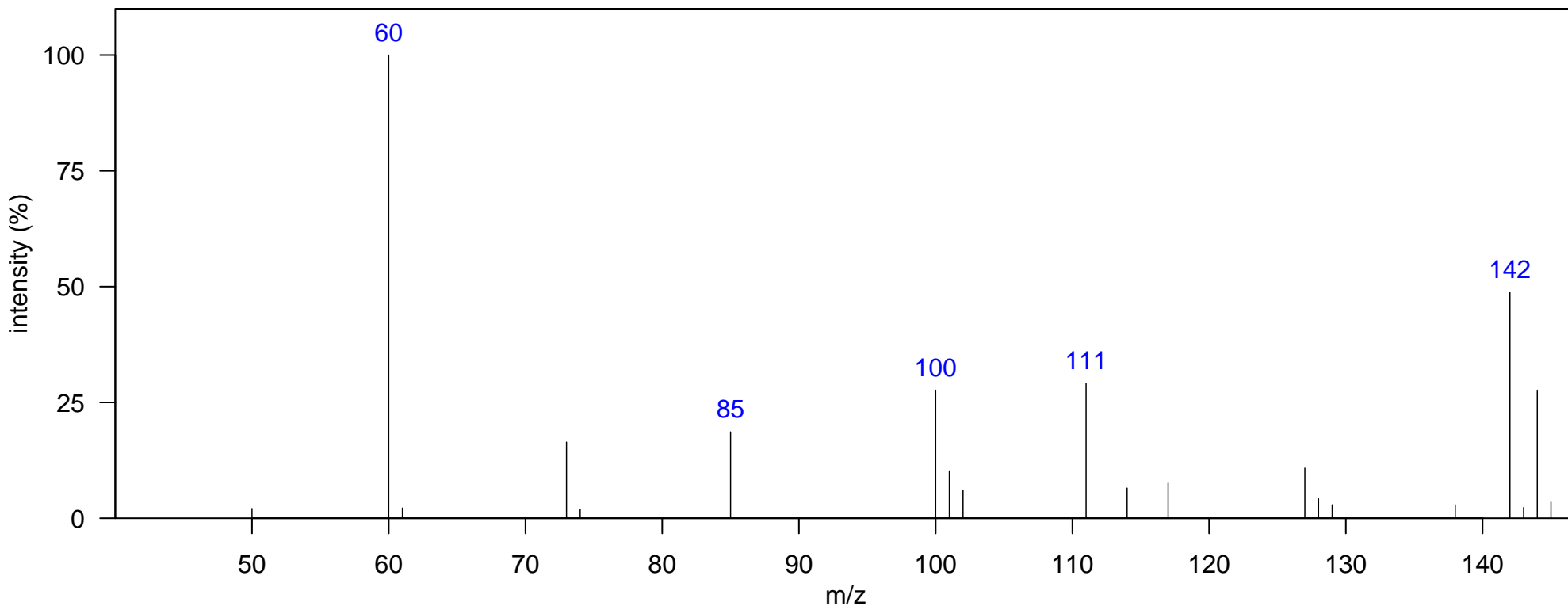
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 142

Identification: Reference Database MS

Comment: NIST I.D. is 1-Chloro-4-methoxybenzene.



m/z [Fragment]
142 M+

Name: Triclosan

Class: Phenol A

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₁₂H₇Cl₃O₂

In Samples: All

1D RT, 2D RT (s): 1960.72, 1.61

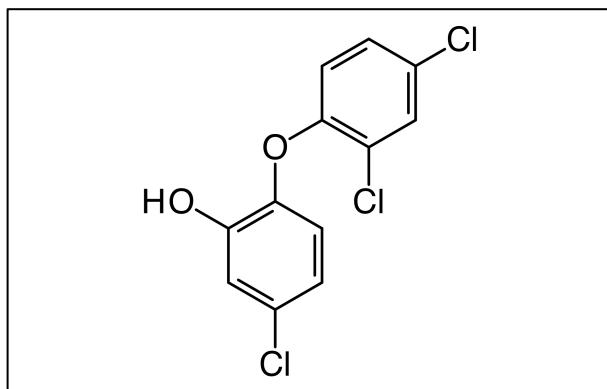
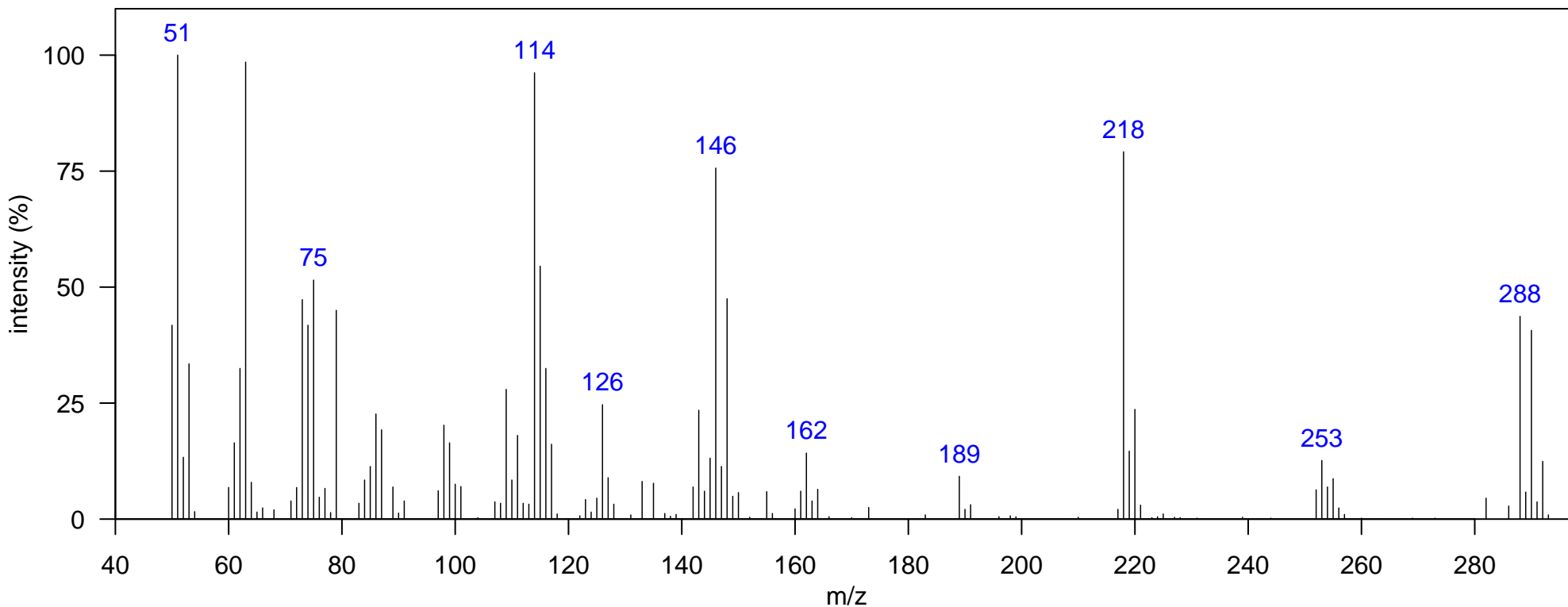
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 288

Identification: Authentic MS RT

Comment:



m/z [Fragment]
218 [M-Cl ₂] ⁺
253 [M-Cl] ⁺
288 M ⁺

Name: Permethrin 1

Class: Pyrethroid

Matrix: SD Bay Black Skimmer Egg

In Samples: A, D

Group: Not Typically Monitored

Comment: M+ is not detected.

Instrument: GCxGC-TOF, EI, 70 eV

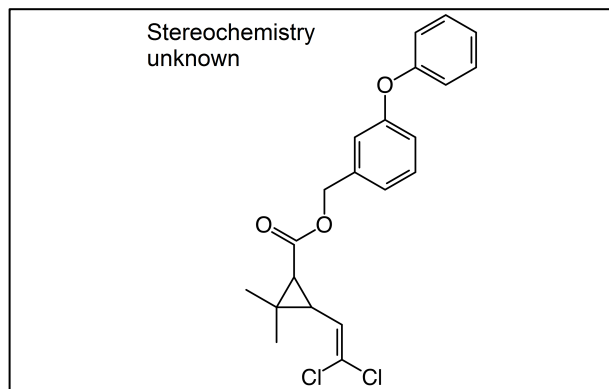
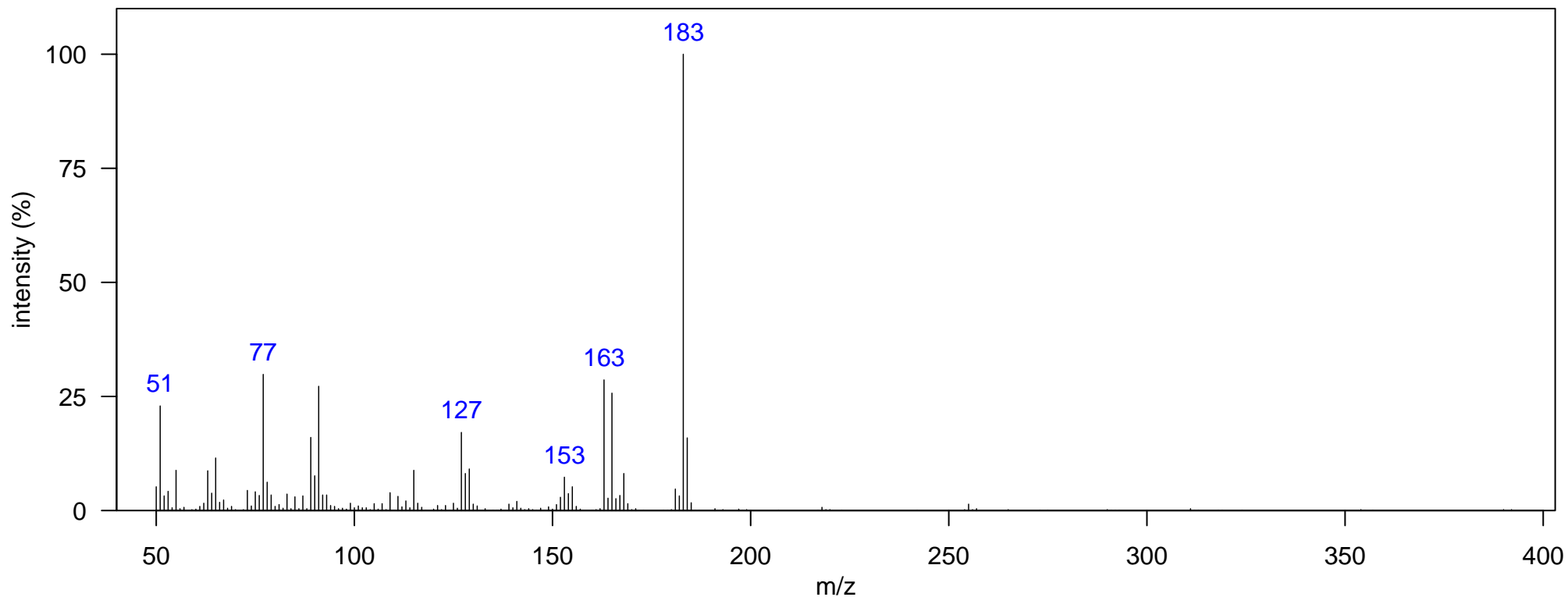
1D RT, 2D RT (s): 2408.47, 1.855

Quantitative Ion m/z: 183

Elemental Formula: C₂₁H₂₀Cl₂O₃

Source: Anthropogenic

Identification: Authentic MS RT



m/z [Fragment]
390 M+

Name: Permethrin 2

Class: Pyrethroid

Matrix: SD Bay Black Skimmer Egg

In Samples: A, D

Group: Not Typically Monitored

Comment: M+ is not detected.

Instrument: GCxGC-TOF, EI, 70 eV

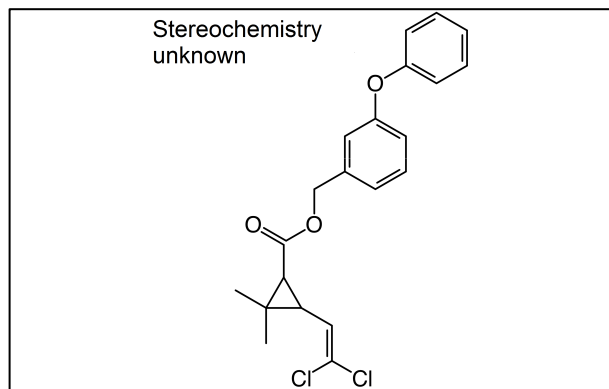
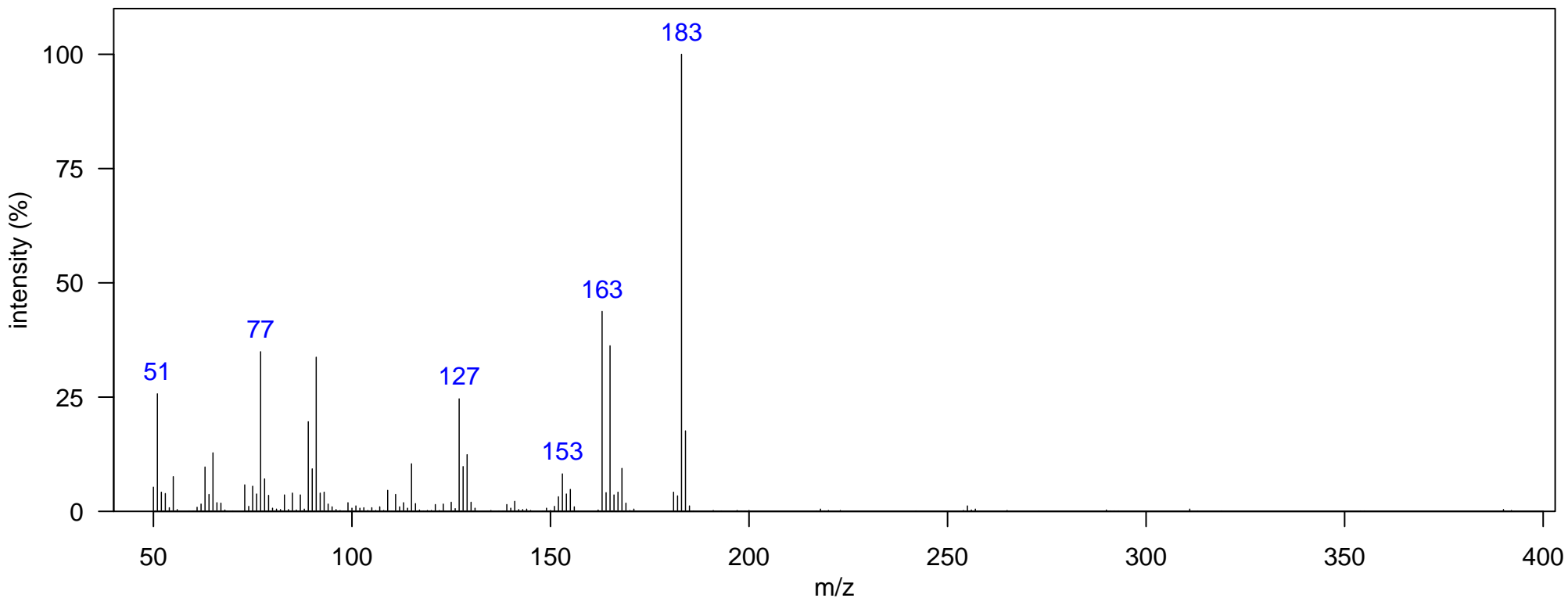
1D RT, 2D RT (s): 2418.96, 1.868

Quantitative Ion m/z: 183

Elemental Formula: C₂₁H₂₀Cl₂O₃

Source: Anthropogenic

Identification: Authentic MS RT



m/z [Fragment]
390 M+

Name: Cypermethrin

Class: Pyrethroid

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula: C₂₂H₁₉Cl₂NO₃

In Samples: A

1D RT, 2D RT (s): 2499.41, 1.987

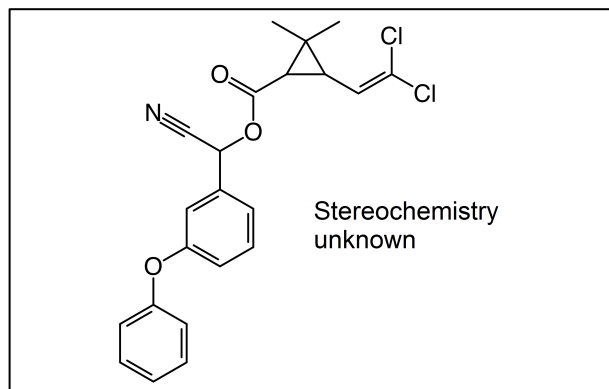
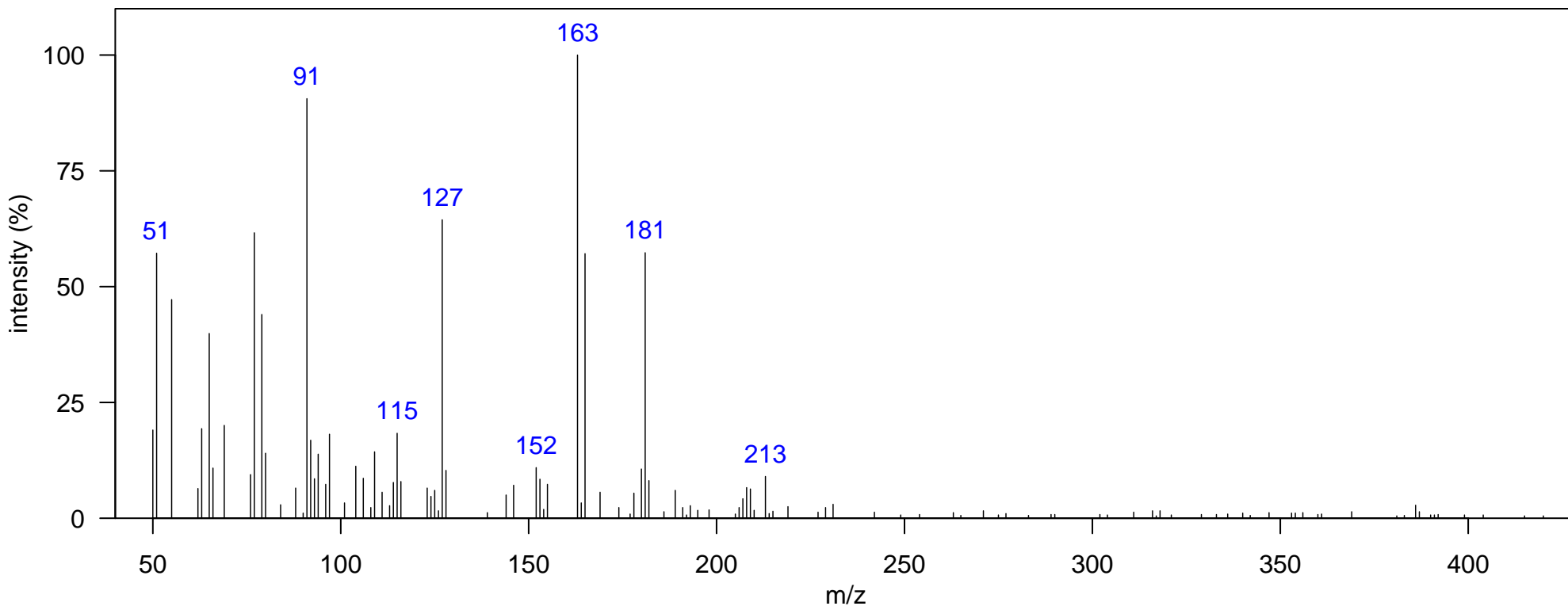
Source: Anthropogenic

Group: Not Typically Monitored

Quantitative Ion m/z: 181

Identification: Reference Database MS

Comment: NIST I.D. is Cypermethrin. M+ is not detected.



m/z [Fragment]
415 M+

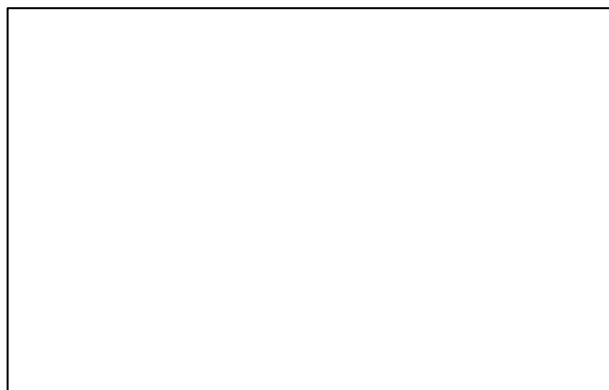
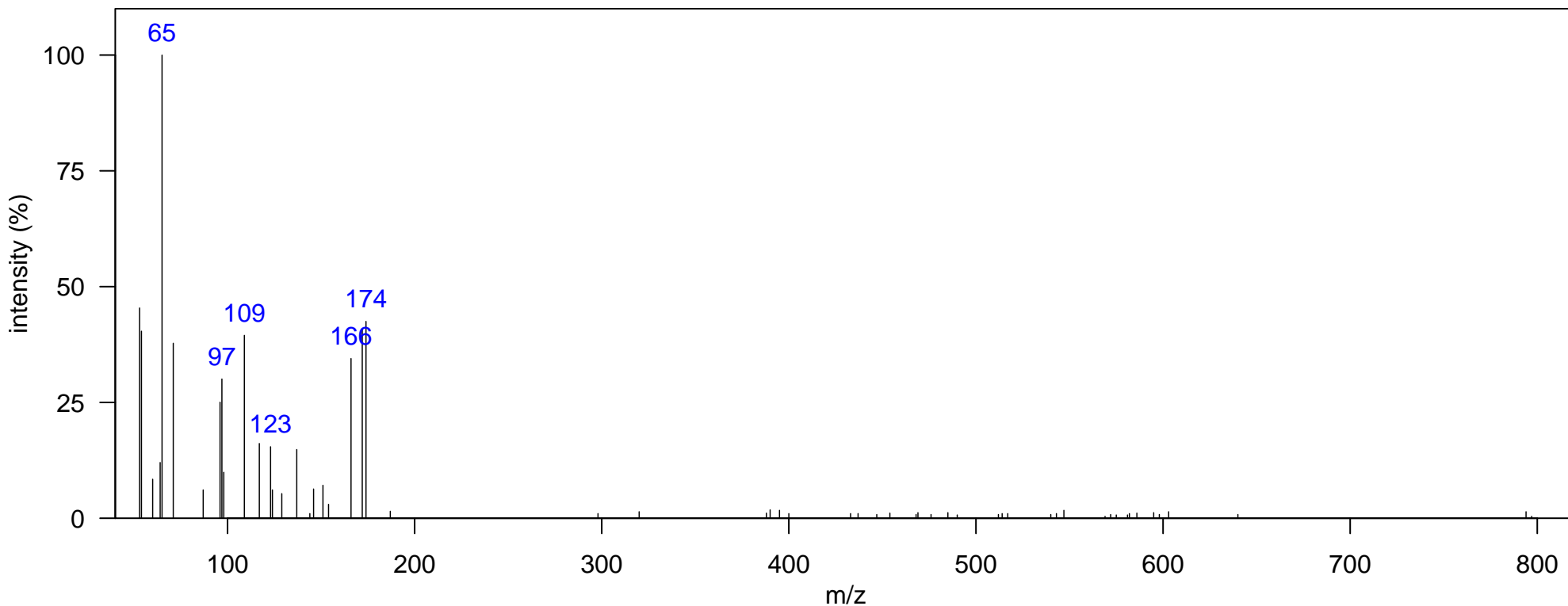
Name: Unknown 1

Class: Unknown

Matrix: SD Bay Black Skimmer Egg
In Samples: All
Group: Not Typically Monitored
Comment:

Instrument: GCxGC-TOF, EI, 70 eV
1D RT, 2D RT (s): 1089.72, 1.339
Quantitative Ion m/z: 172

Elemental Formula:
Source: Unknown
Identification: Unknown



m/z [Fragment]

Name: Unknown 2A

Class: Unknown

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula:

In Samples: All

1D RT, 2D RT (s): 1645.9, 1.445

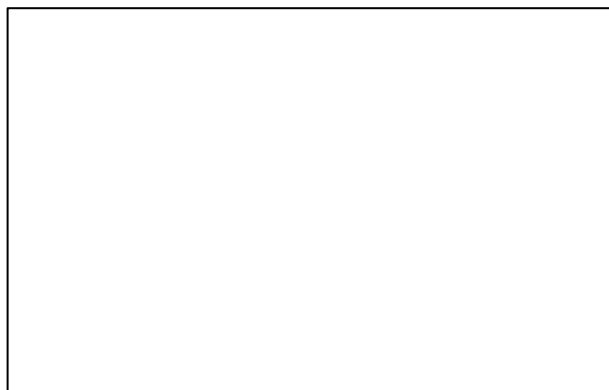
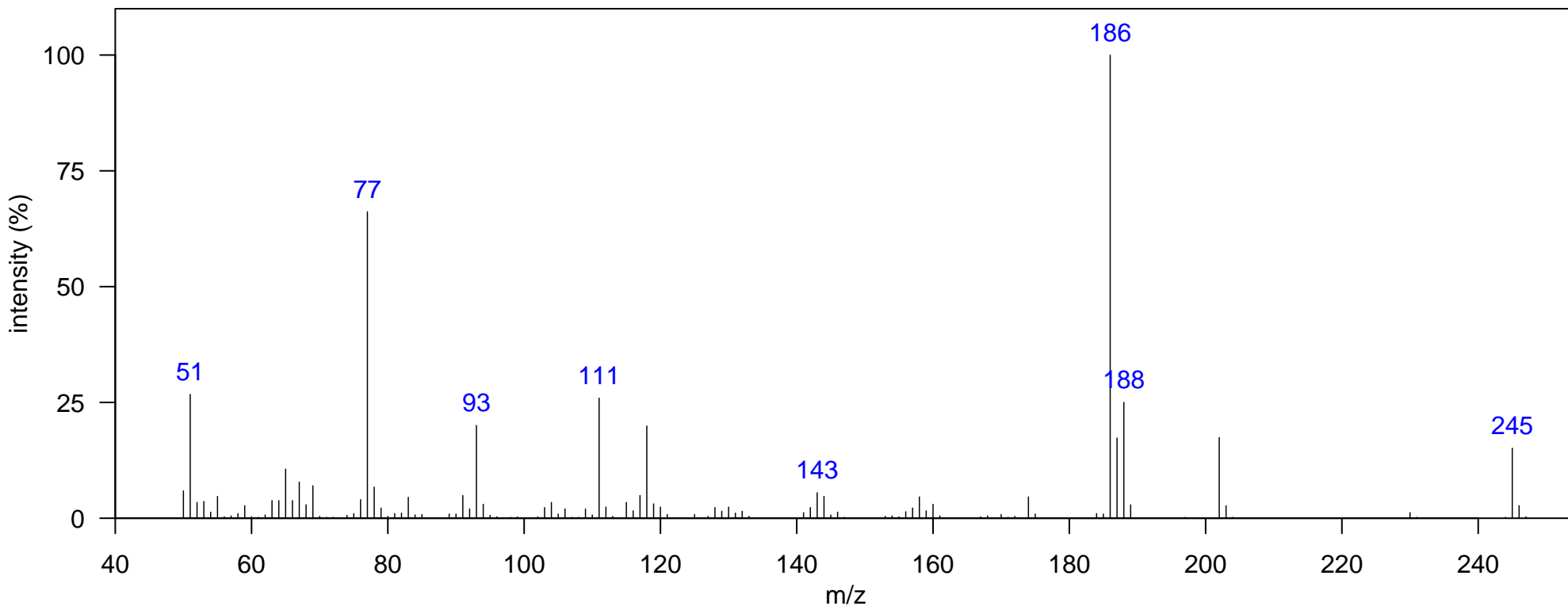
Source: Unknown

Group: Not Typically Monitored

Quantitative Ion m/z: 186

Identification: Unknown

Comment:



m/z [Fragment]

Name: Unknown 2B

Class: Unknown

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula:

In Samples: All

1D RT, 2D RT (s): 1736.85, 1.432

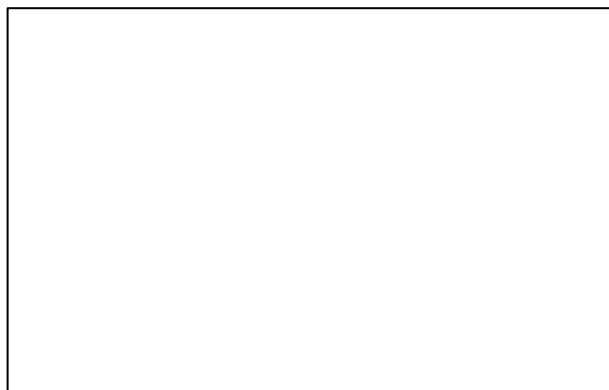
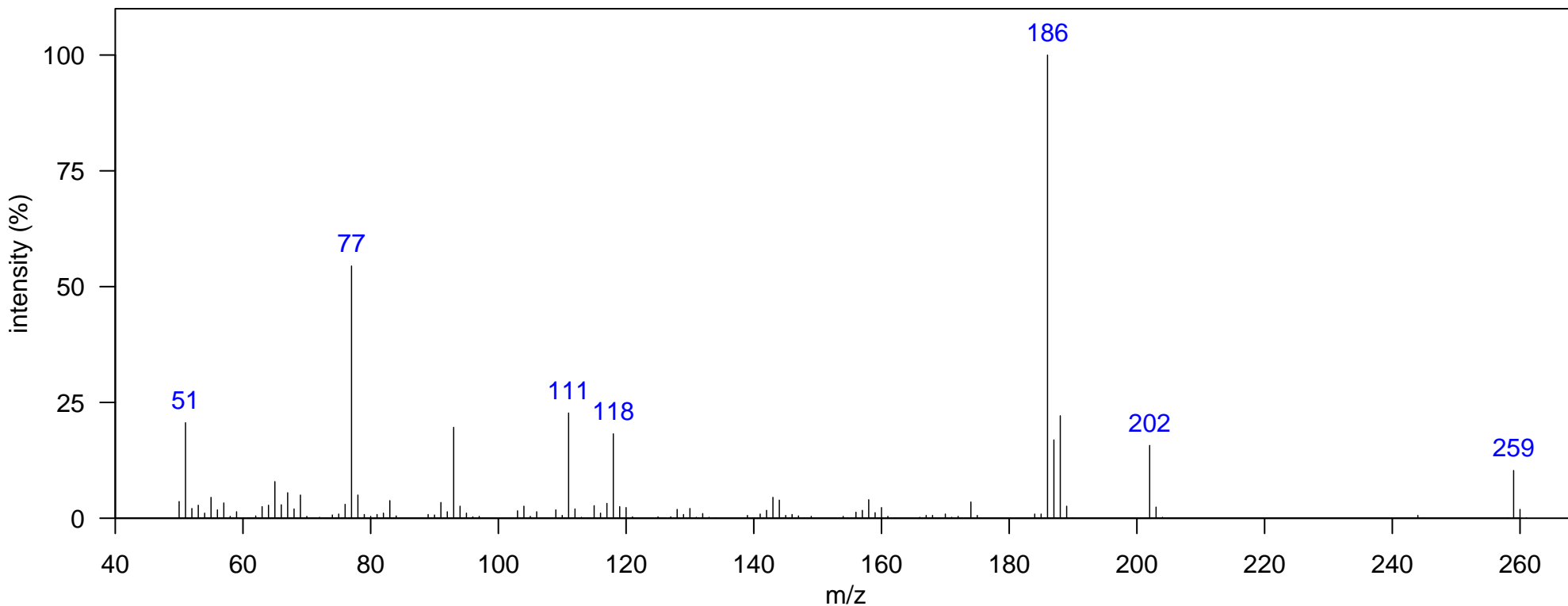
Source: Unknown

Group: Not Typically Monitored

Quantitative Ion m/z: 186

Identification: Unknown

Comment:



m/z [Fragment]

Name: Unknown 3

Class: Unknown

Matrix: SD Bay Black Skimmer Egg

Instrument: GCxGC-TOF, EI, 70 eV

Elemental Formula:

In Samples: All

1D RT, 2D RT (s): 2167.1, 1.656

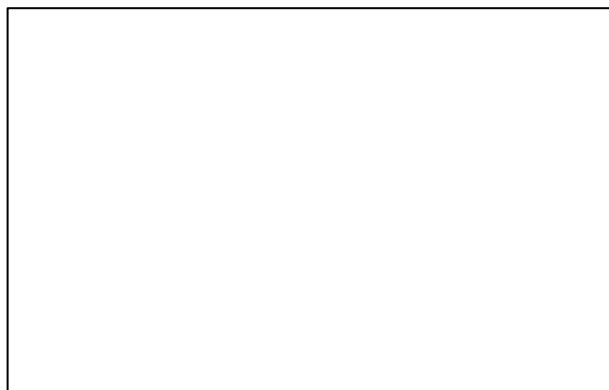
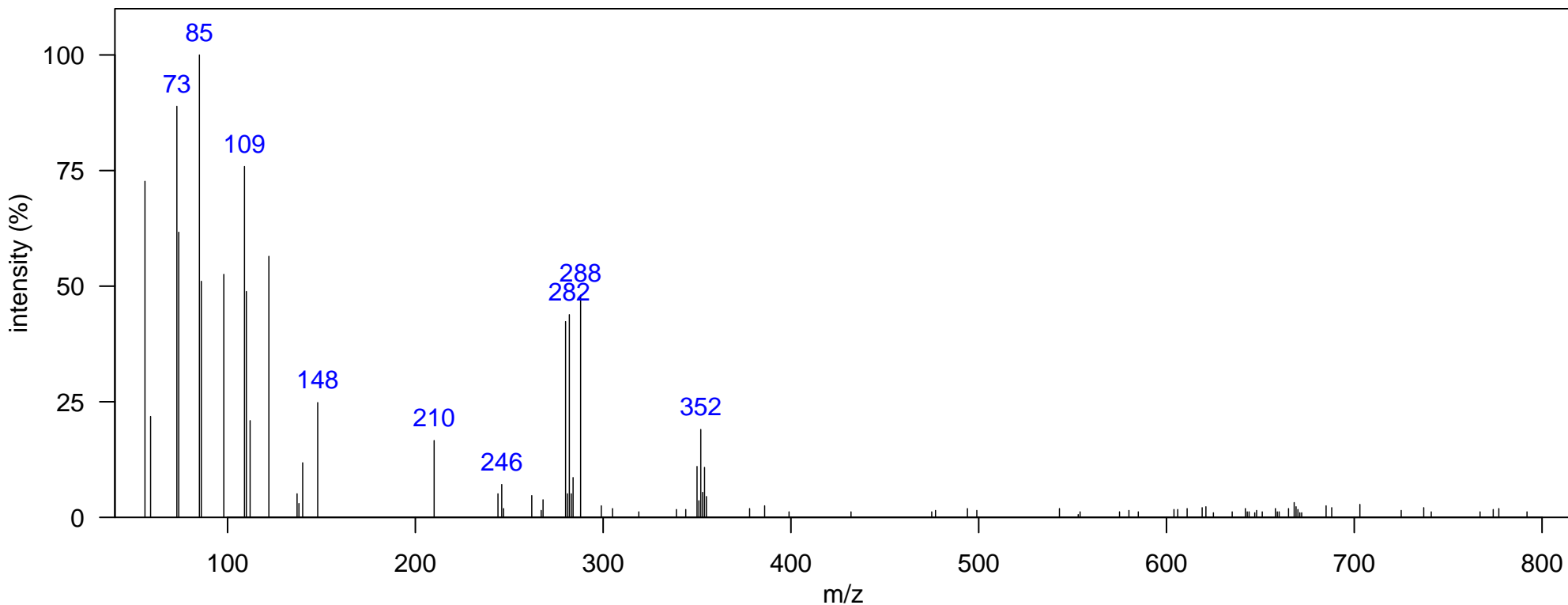
Source: Unknown

Group: Not Typically Monitored

Quantitative Ion m/z: 282

Identification: Unknown

Comment:



m/z [Fragment]
