

## **SUPPORTING INFORMATION PART B**

### **Newly Identified DDT-Related Compounds Accumulating in Southern California**

#### **Bottlenose Dolphins**

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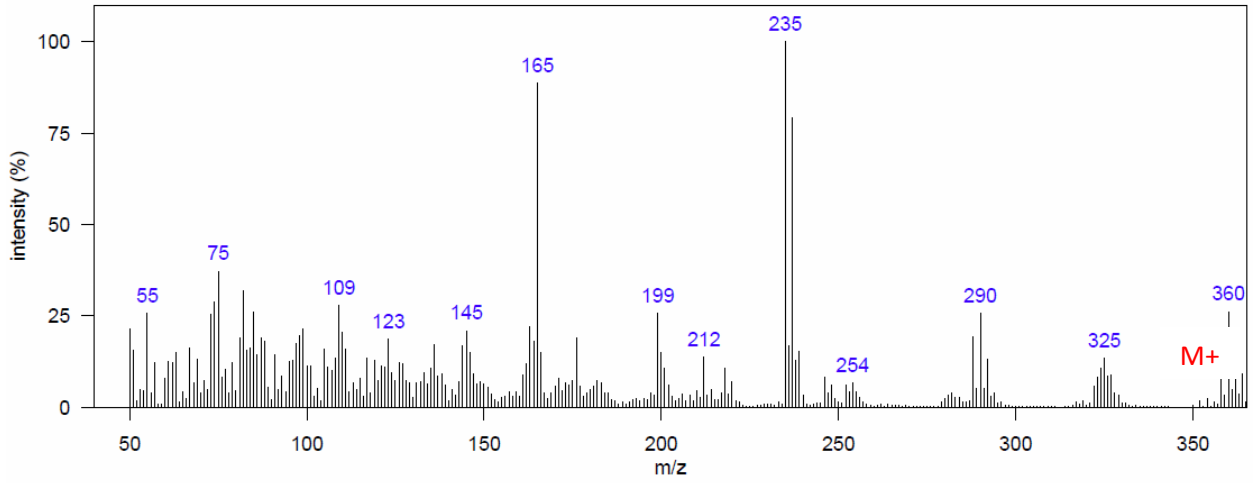
<sup>#</sup>Marine Mammal & Turtle Division, Southwest Fisheries Science Center, National Marine Fisheries Service, National Oceanic and Atmospheric Administration, 8901 La Jolla Shores Dr., La Jolla, CA, 92037, USA

#### **Supporting Information Summary**

Supporting Information Part B includes information associated with identification of the 45 DDT related compounds (mass spectra, interpretation of mass spectral fragmentation patterns, chromatographic retention times, and corresponding standards' mass spectra).

## p,p'-DDT

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: [M-CCl<sub>5</sub>]<sup>+</sup>

m/z 199: [M-CCl<sub>4</sub>]<sup>+</sup>

m/z 235: [M-CCl<sub>3</sub>]<sup>+</sup>

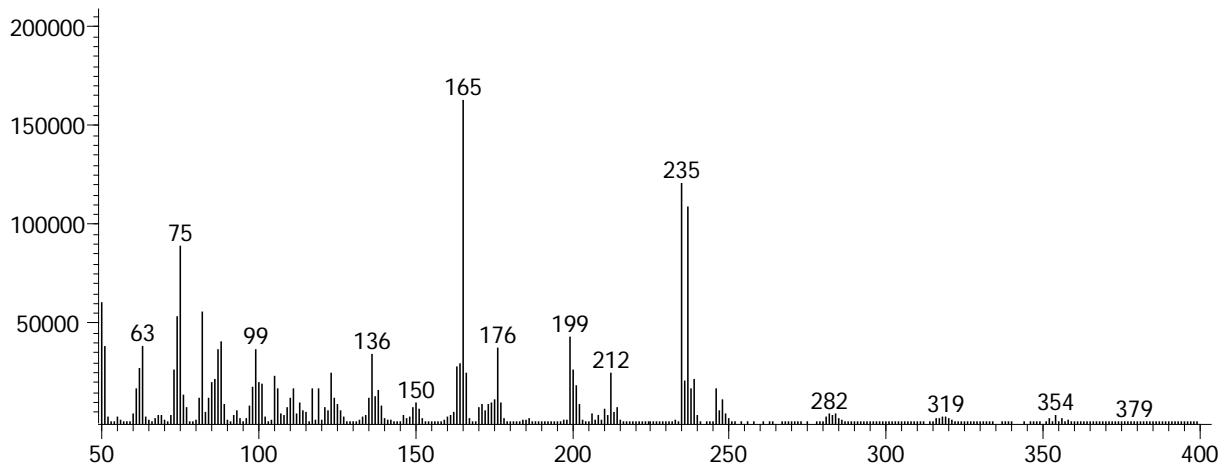
m/z 254, m/z 290, m/z 325, m/z 360: PCB interference

m/z 352: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1453.51 1.366

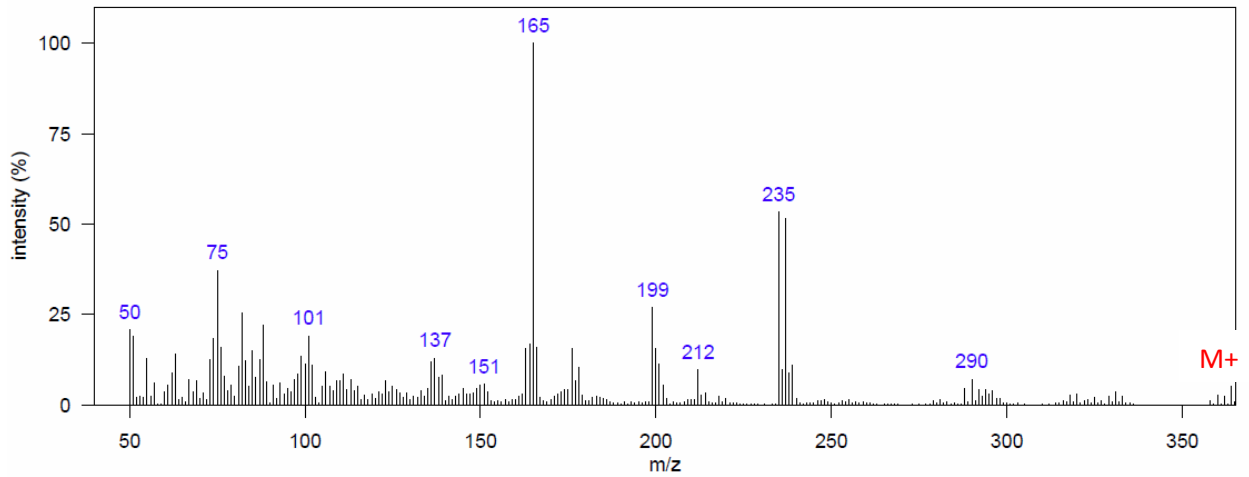
3. Identification: [1] Authentic MS/RT

### 4. Mass spectrum of p,p'-DDT standard



## ***o,p'*-DDT D1**

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: [M-CCl<sub>5</sub>]<sup>+</sup>

m/z 199: [M-CCl<sub>4</sub>]<sup>+</sup>

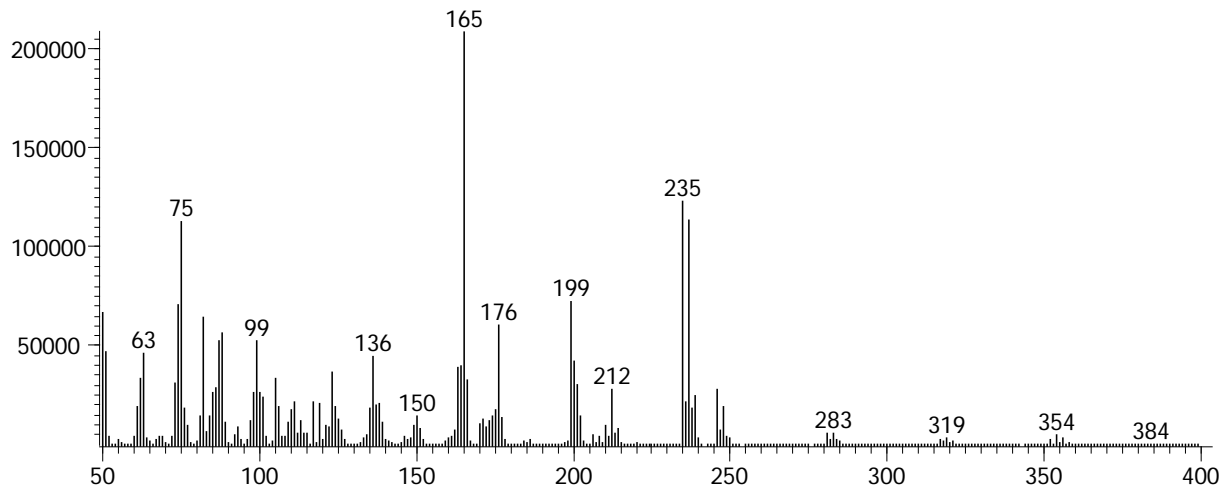
m/z 235: [M-CCl<sub>3</sub>]<sup>+</sup>

m/z 352: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1415.03 1.373

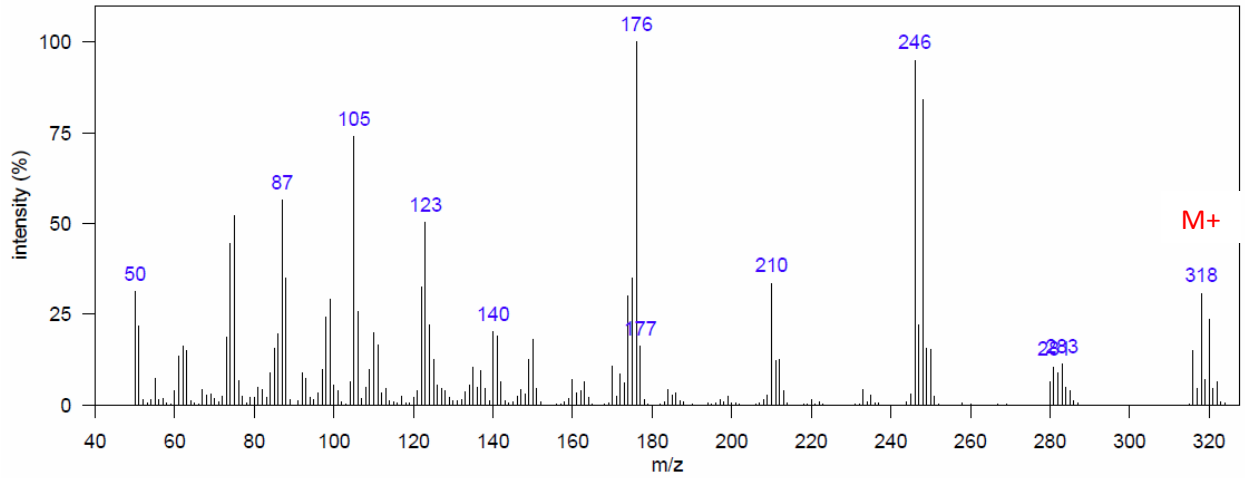
3. Identification: [1] Authentic MS/RT

4. Mass spectrum of *o,p'*-DDT standard



## p,p'-DDE

### 1. Mass Spectrum from SoCal dolphin blubber D4:



m/z 176: [M-Cl<sub>4</sub>]<sup>+</sup>

m/z 176: [M-Cl<sub>3</sub>]<sup>+</sup>

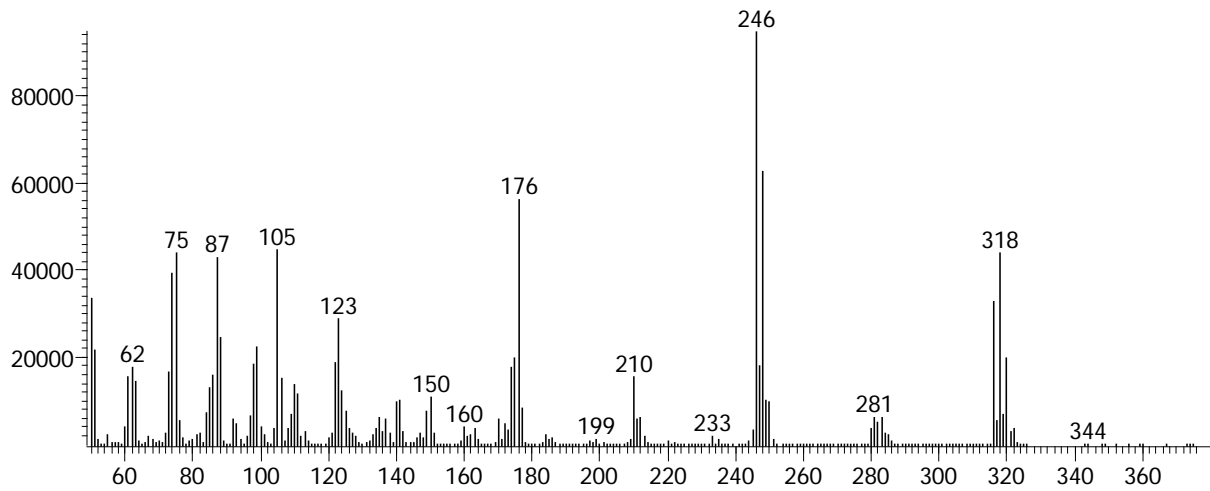
m/z 246: [M-Cl<sub>2</sub>]<sup>+</sup>

m/z 316: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1373.06 1.643

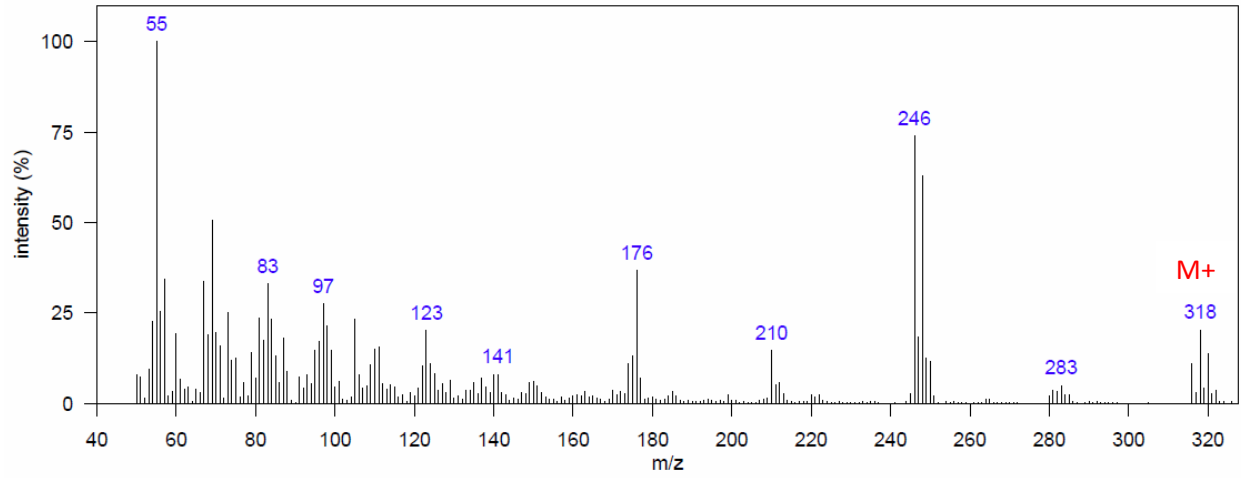
3. Identification: [1] Authentic MS/RT

4. Mass spectrum of p,p'-DDE standard



## **o,p'-DDE**

### 1. Mass Spectrum from SoCal dolphin blubber D1:

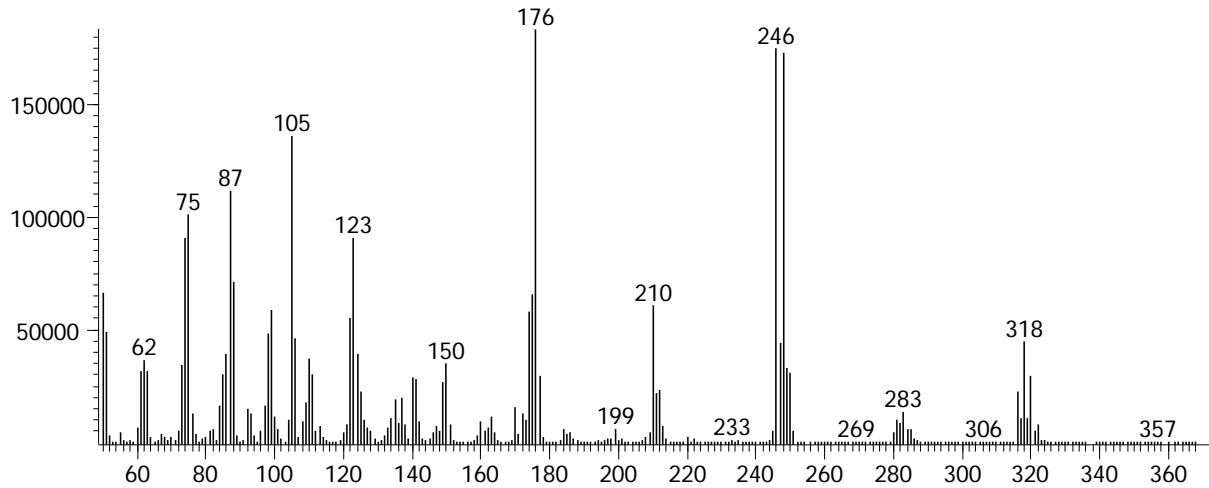


m/z 176: [M-Cl<sub>4</sub>]<sup>+</sup>  
m/z 176: [M-Cl<sub>3</sub>]<sup>+</sup>  
m/z 246: [M-Cl<sub>2</sub>]<sup>+</sup>  
m/z 316: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1331.08 1.373

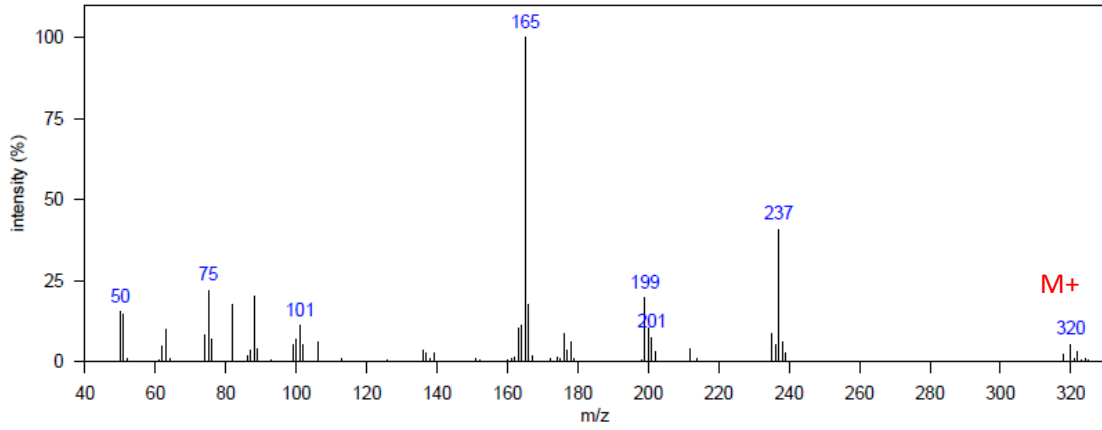
3. Identification: [1] Authentic MS/RT

4. Mass spectrum of o,p'-DDE standard



## p,p'-DDD

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: [M-CHCl<sub>4</sub>]<sup>+</sup>

m/z 199: [M-CHCl<sub>3</sub>]<sup>+</sup>

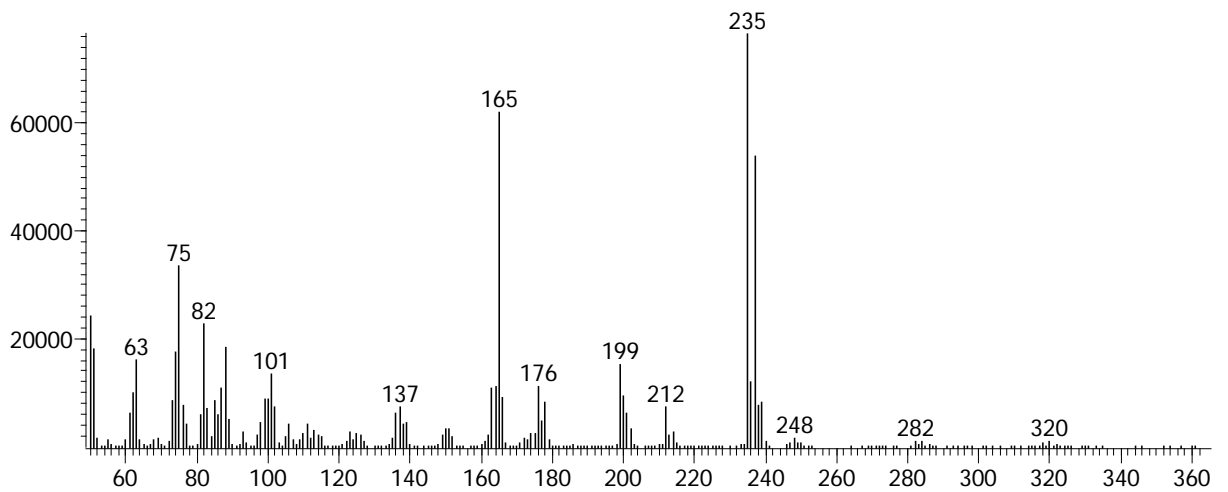
m/z 235: [M-CHCl<sub>2</sub>]<sup>+</sup>

m/z 318: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1411.54, 1.379

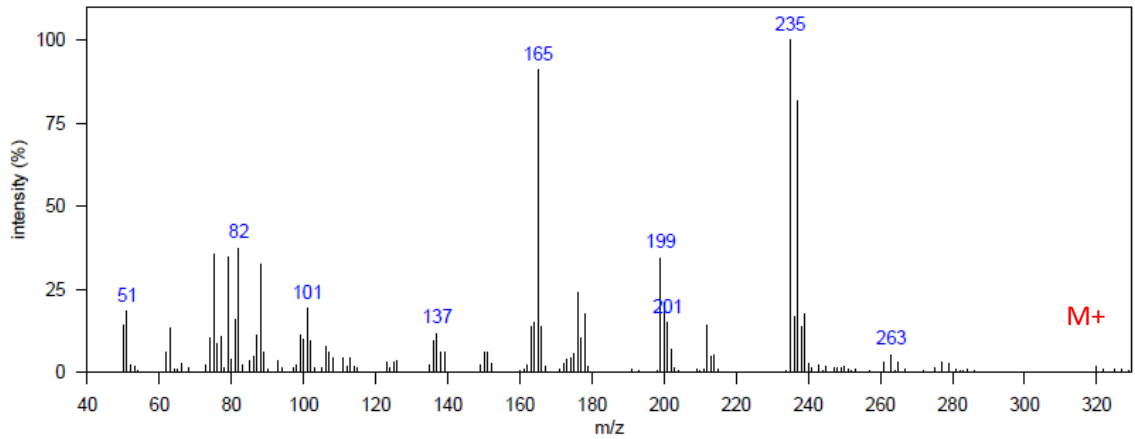
3. Identification: [1] Authentic MS/RT

4. Mass spectrum of p,p'-DDD standard



## **o,p'-DDD**

### 1. Mass Spectrum from SoCal dolphin blubber D6:



m/z 165: [M-CHCl<sub>4</sub>]<sup>+</sup>

m/z 199: [M-CHCl<sub>3</sub>]<sup>+</sup>

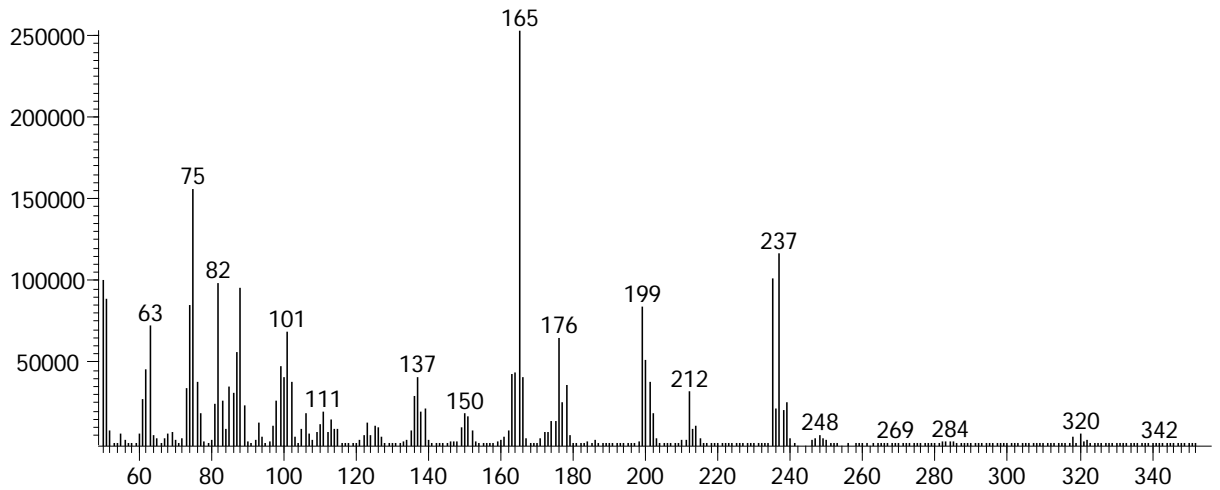
m/z 235: [M-CHCl<sub>2</sub>]<sup>+</sup>

m/z 318: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1376.56, 1.346

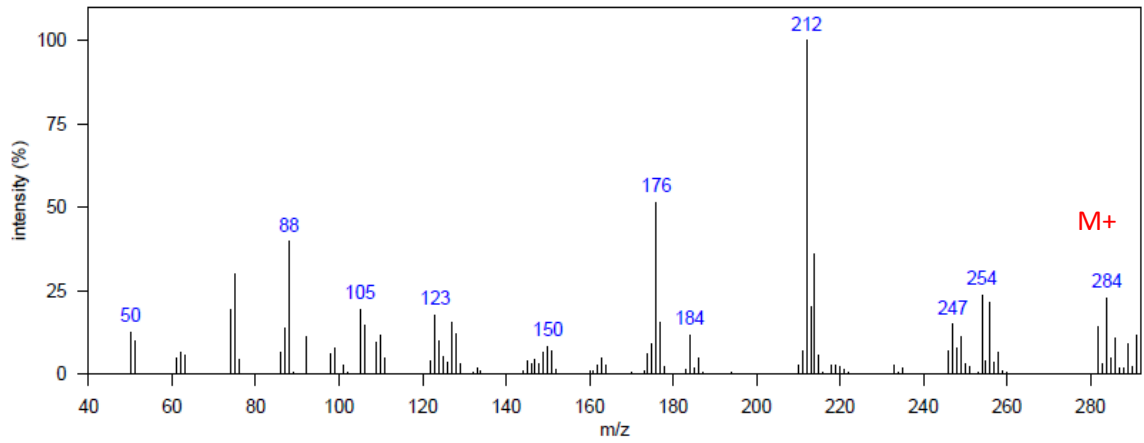
### 3. Identification: Authentic MS/RT

### 4. Mass spectrum of o,p'-DDD standard



## p,p'-DDMU

### 1. Mass Spectrum from SoCal dolphin blubber D5:



m/z 176: [M-HCl<sub>3</sub>]<sup>+</sup>

m/z 212: [M-Cl<sub>2</sub>]<sup>+</sup>

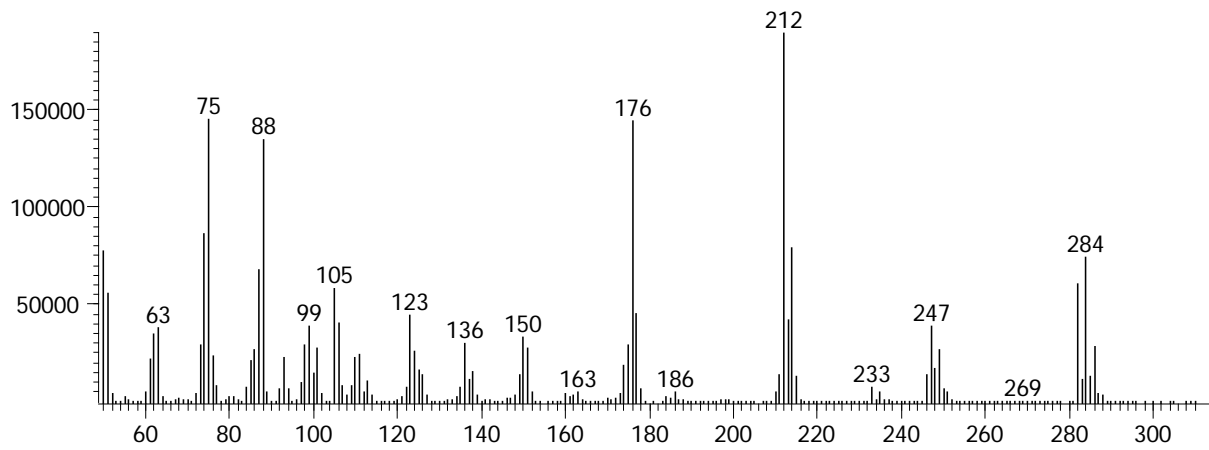
m/z 247: [M-Cl]<sup>+</sup>

m/z 282: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1331.08, 1.32

### 3. Identification: Authentic MS/RT

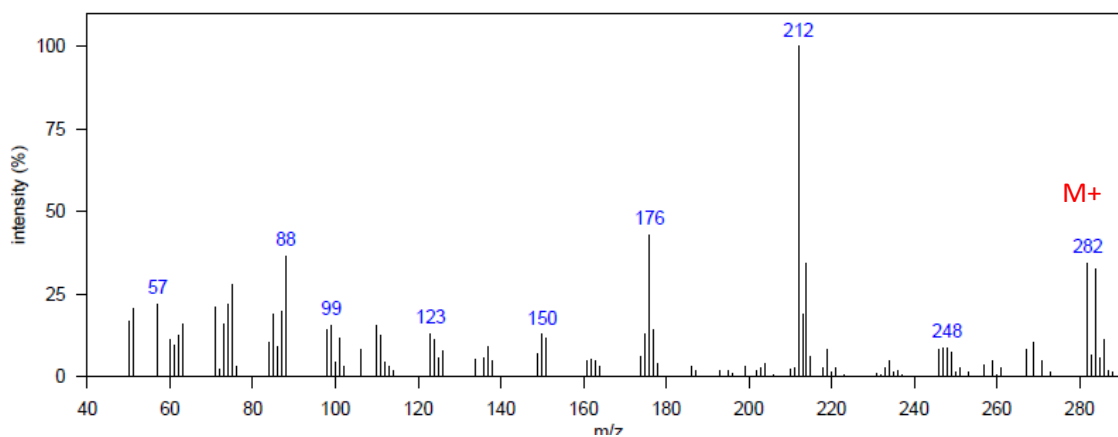
### 4. Mass spectrum of p,p'-DDMU standard





## DDMU 1

### 1. Mass Spectrum from SoCal dolphin blubber D4:



m/z 176: [M-HCl<sub>3</sub>]<sup>+</sup>

m/z 212: [M-Cl<sub>2</sub>]<sup>+</sup>

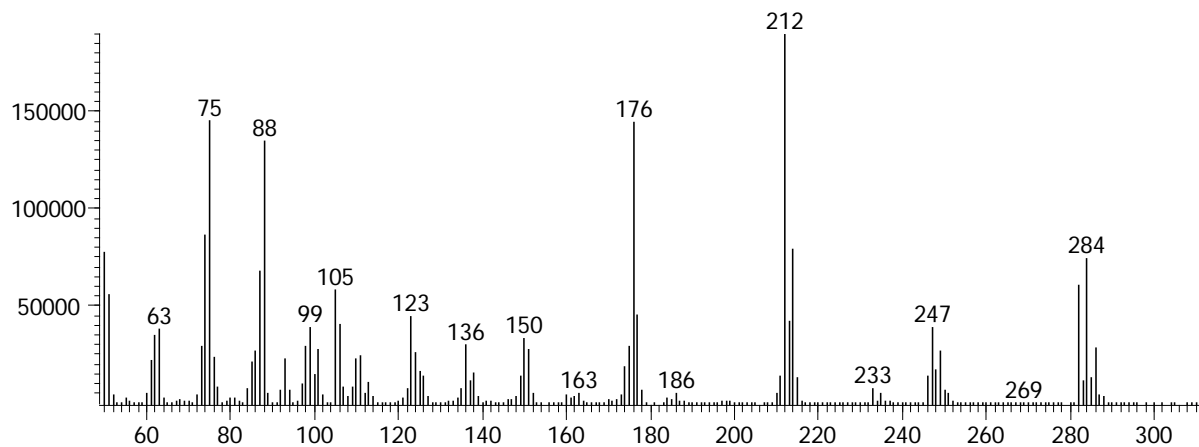
m/z 247: [M-Cl]<sup>+</sup>

m/z 282: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1254.13, 1.254

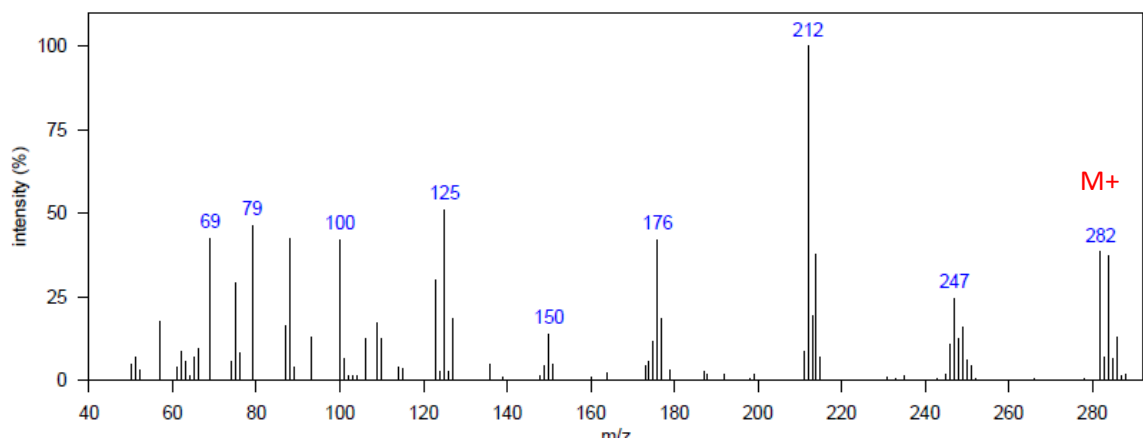
### 3. Identification: [2] Authentic MS (Isomer)

### 4. Mass spectrum of p,p'-DDMU standard



## DDMU 2

### 1. Mass Spectrum from SoCal dolphin blubber D5:



m/z 176: [M-HCl<sub>3</sub>]<sup>+</sup>

m/z 212: [M-Cl<sub>2</sub>]<sup>+</sup>

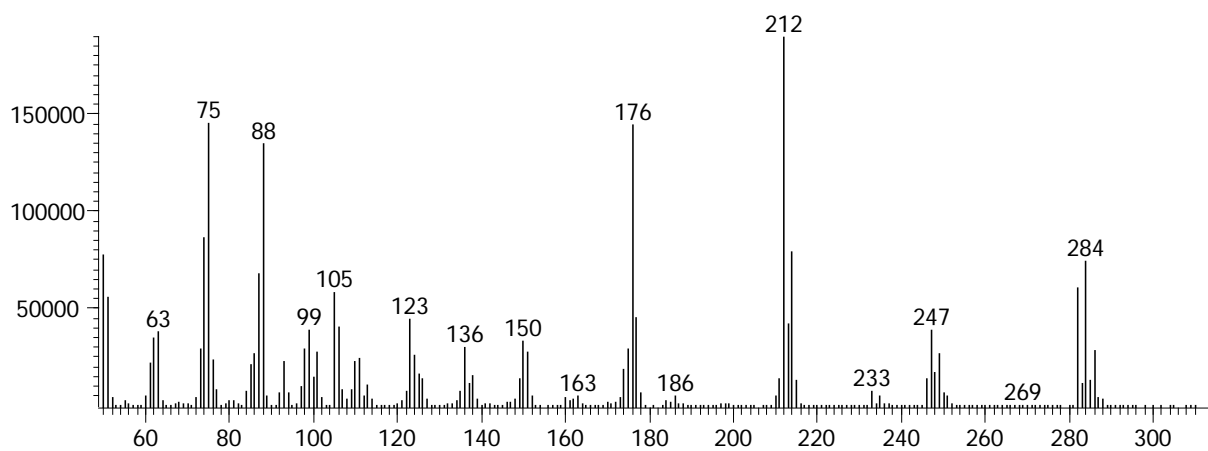
m/z 247: [M-Cl]<sup>+</sup>

m/z 282: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1296.1, 1.274

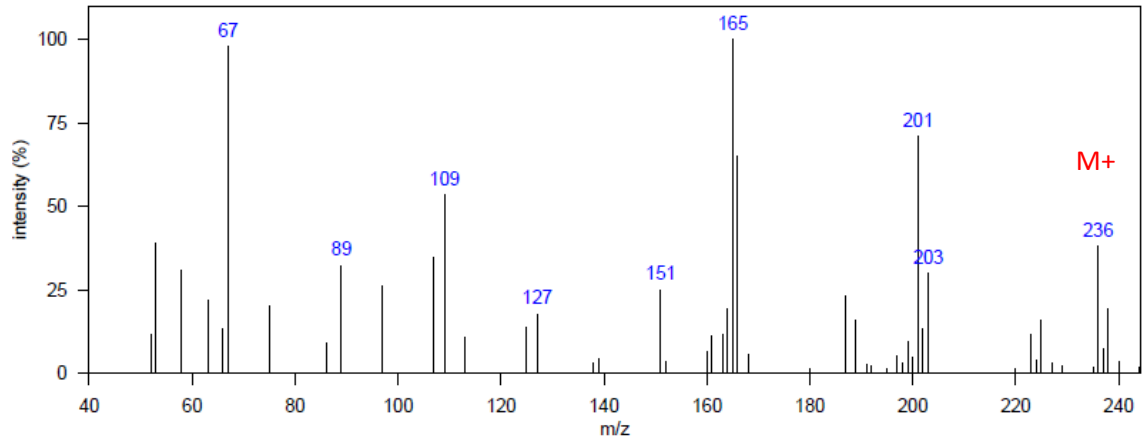
3. Identification: [2] Authentic MS (Isomer)

4. Mass spectrum of p,p'-DDMU standard



## p,p'-DDM

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: [M-HCl<sub>2</sub>]<sup>+</sup>

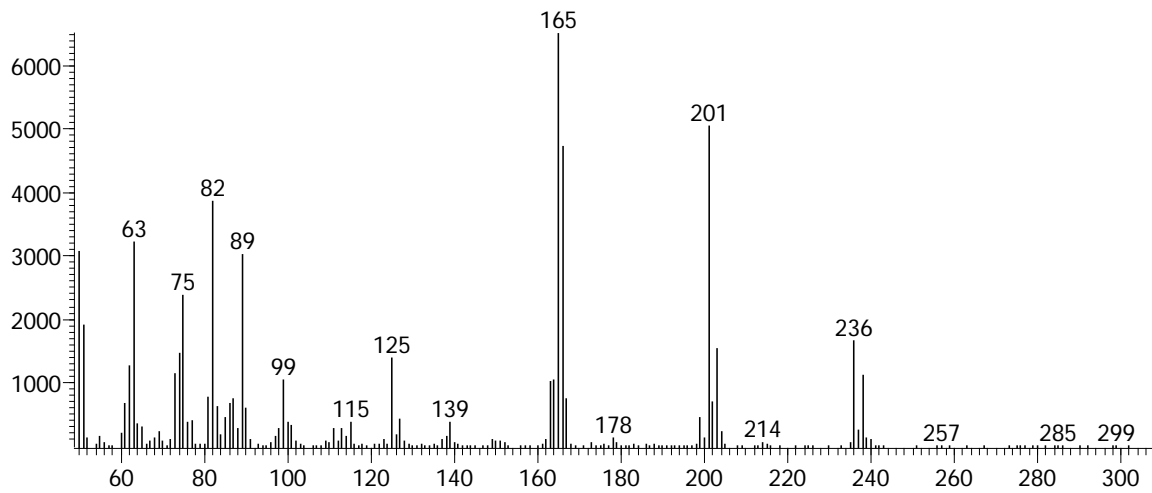
m/z 201: [M-Cl]<sup>+</sup>

m/z 236: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1187.66, 1.228

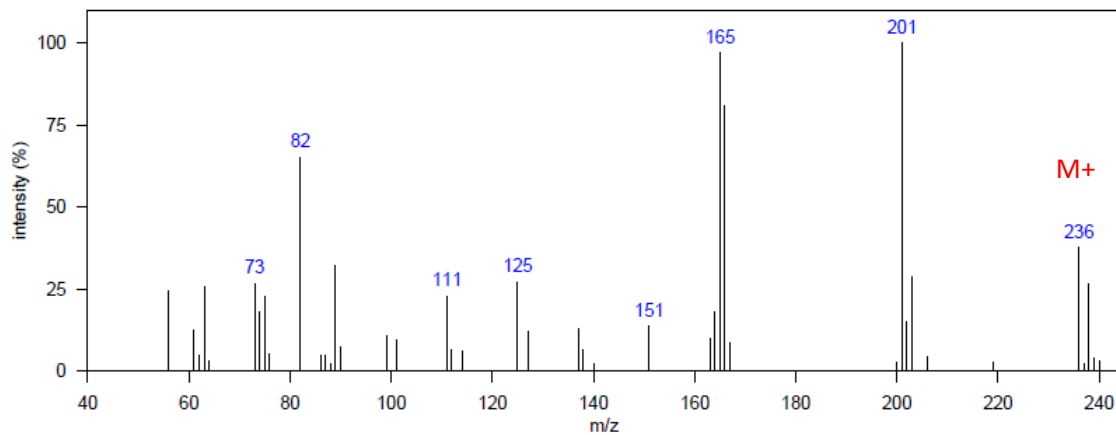
### 3. Identification: [1] Authentic MS/RT

### 4. Mass spectrum of p,p'-DDM standard



## DDM 1

### 1. Mass Spectrum from SoCal dolphin blubber D4:



m/z 165: [M-HCl<sub>2</sub>]<sup>+</sup>

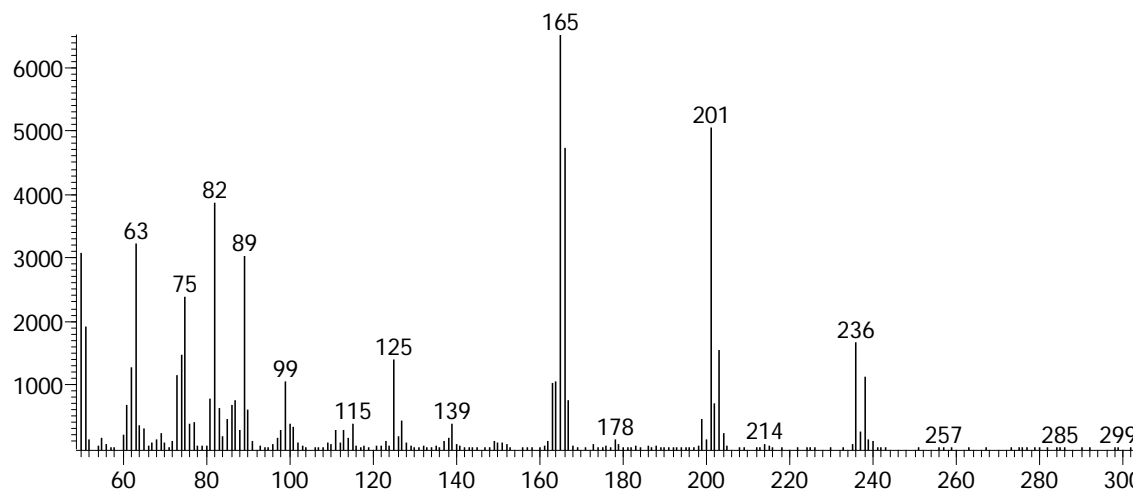
m/z 201: [M-Cl]<sup>+</sup>

m/z 236: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1166.68, 1.228

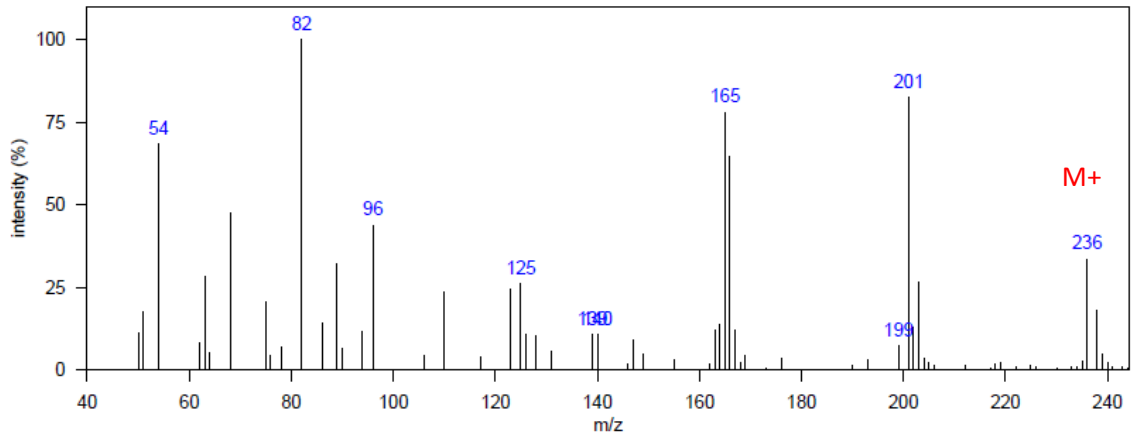
### 3. Identification: [2] Authentic MS (isomer)

### 4. Mass spectrum of p,p'-DDM standard



## DDM 2

### 1. Mass Spectrum from SoCal dolphin blubber D7:



m/z 165: [M-HCl<sub>2</sub>]<sup>+</sup>

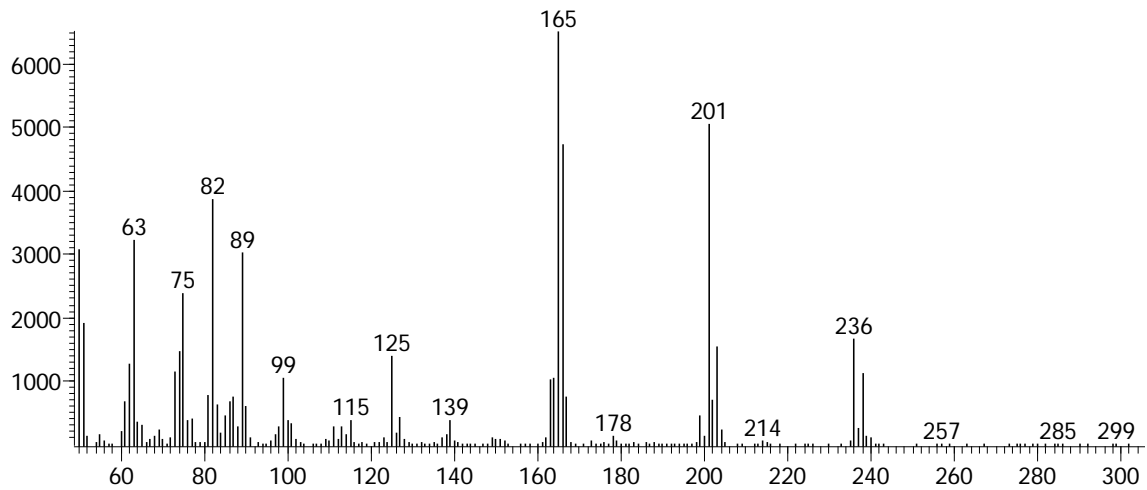
m/z 201: [M-Cl]<sup>+</sup>

m/z 236: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1411.54, 0.944

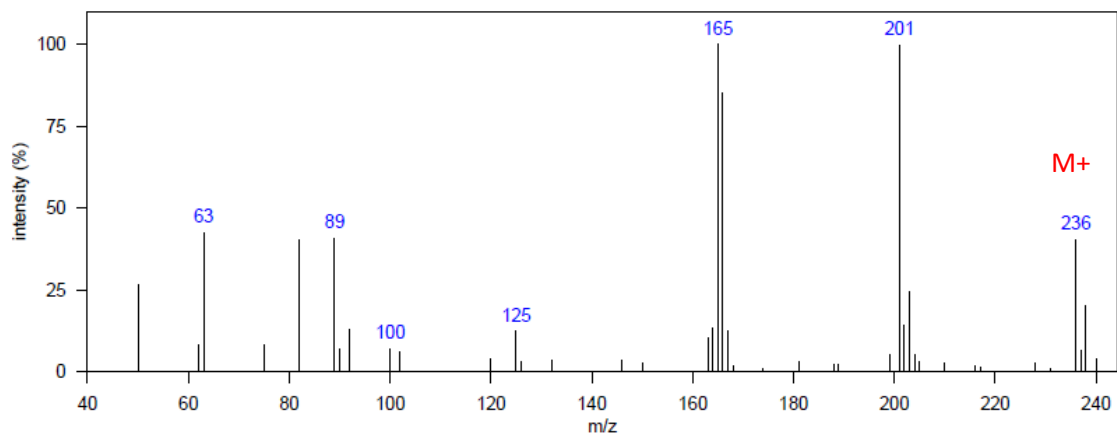
### 3. Identification: [2] Authentic MS (isomer)

### 4. Mass spectrum of p,p'-DDM standard



### DDM 3

#### 1. Mass Spectrum from SoCal dolphin blubber D8:



m/z 165: [M-HCl<sub>2</sub>]<sup>+</sup>

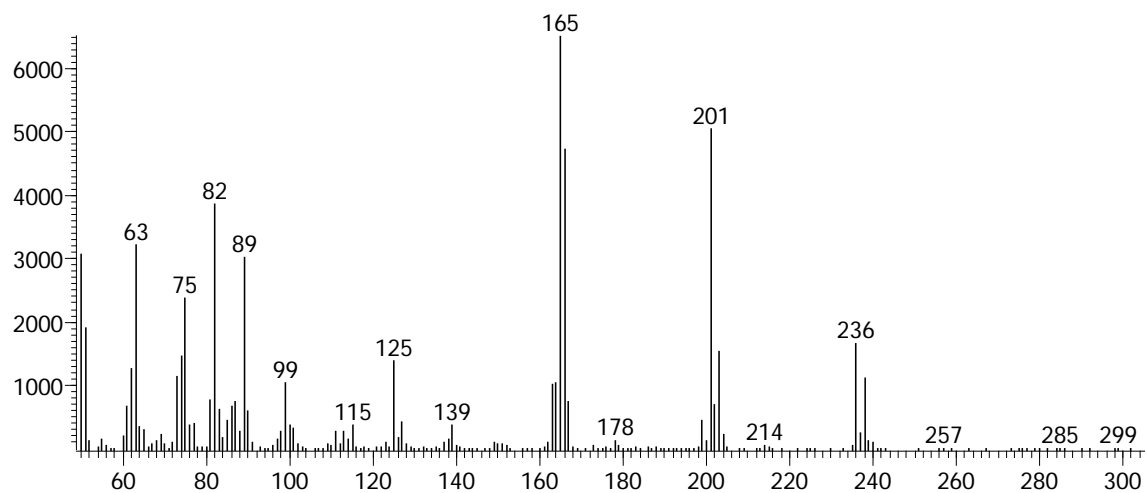
m/z 201: [M-Cl]<sup>+</sup>

m/z 236: M<sup>+</sup>

#### 2. 1D RT, 2D RT (s): 1450.01, 0.917

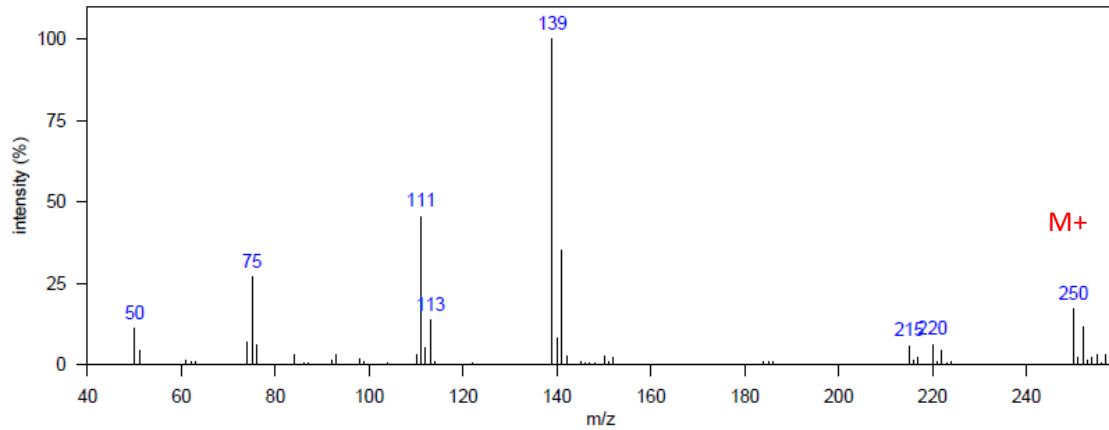
#### 3. Identification: [2] Authentic MS (isomer)

#### 4. Mass spectrum of p,p'-DDM standard



## p,p'-DBP

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 111: [M-C<sub>6</sub>H<sub>4</sub>Cl-CO]+

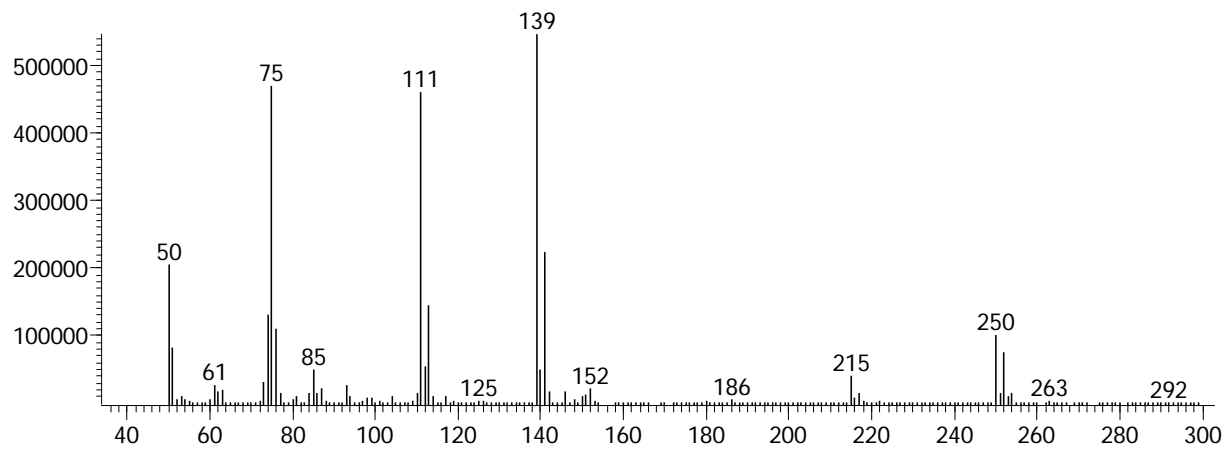
m/z 139: [M-Cl<sub>6</sub>HCl]+

m/z 250: M+

### 2. 1D RT, 2D RT (s): 1268.12, 1.287

### 3. Identification: [1] Authentic MS/RT

### 4. Mass spectrum of p,p'-DBP standard

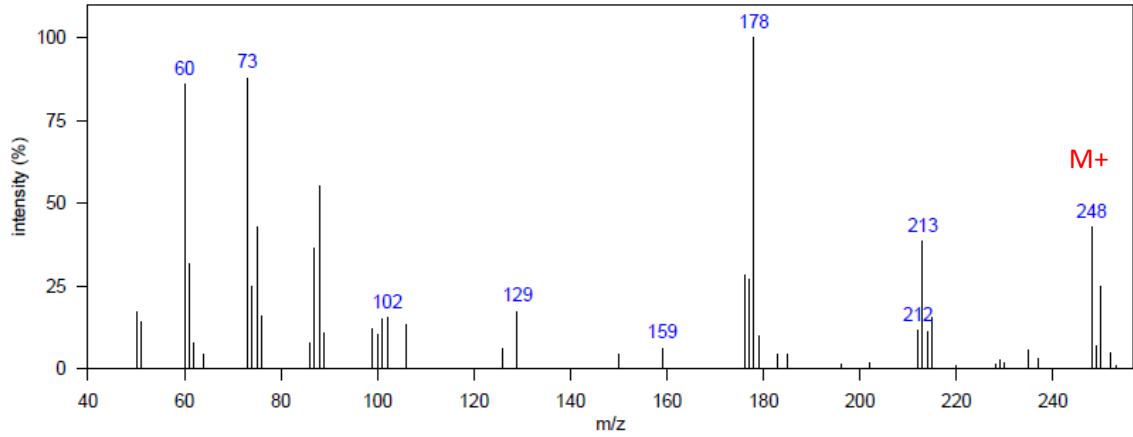






## p,p'-DDNU

### 1. Mass Spectrum from SoCal dolphin blubber D3:



m/z 178: [M-Cl<sub>2</sub>]<sup>+</sup>

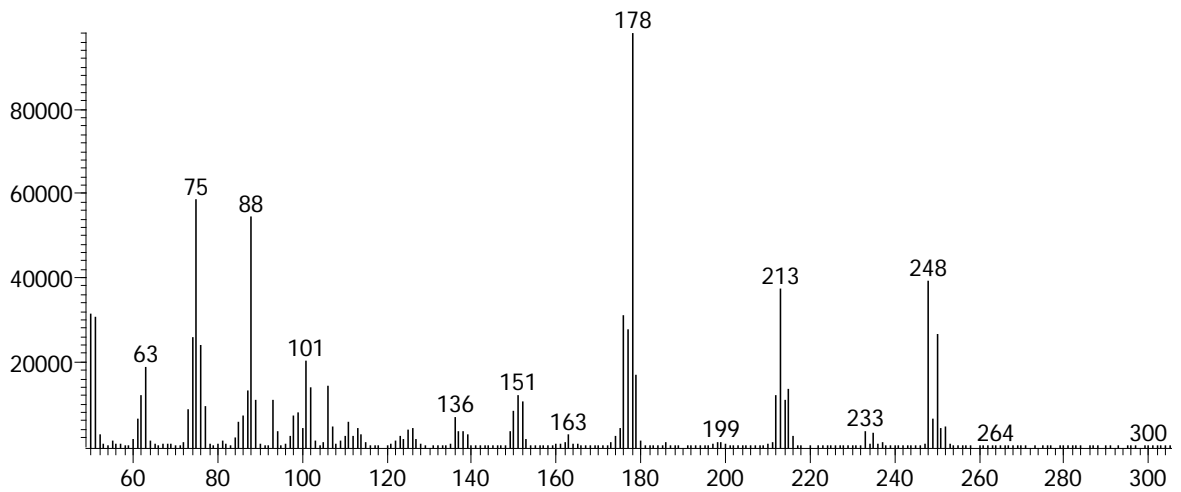
m/z 213: [M-Cl]<sup>+</sup>

m/z 248: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1222.64, 1.181

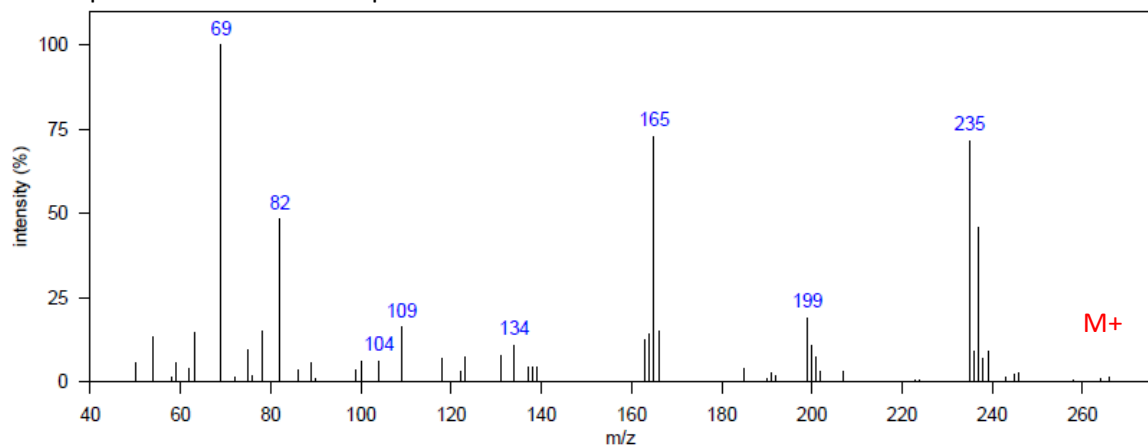
### 3. Identification: [1] Authentic MS/RT

### 4. Mass spectrum of p,p'-DDNU standard



## DDOH 1

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: [M-CH<sub>2</sub>OH-Cl<sub>2</sub>]<sup>+</sup>

m/z 199: [M-CH<sub>2</sub>OH-HCl]<sup>+</sup>

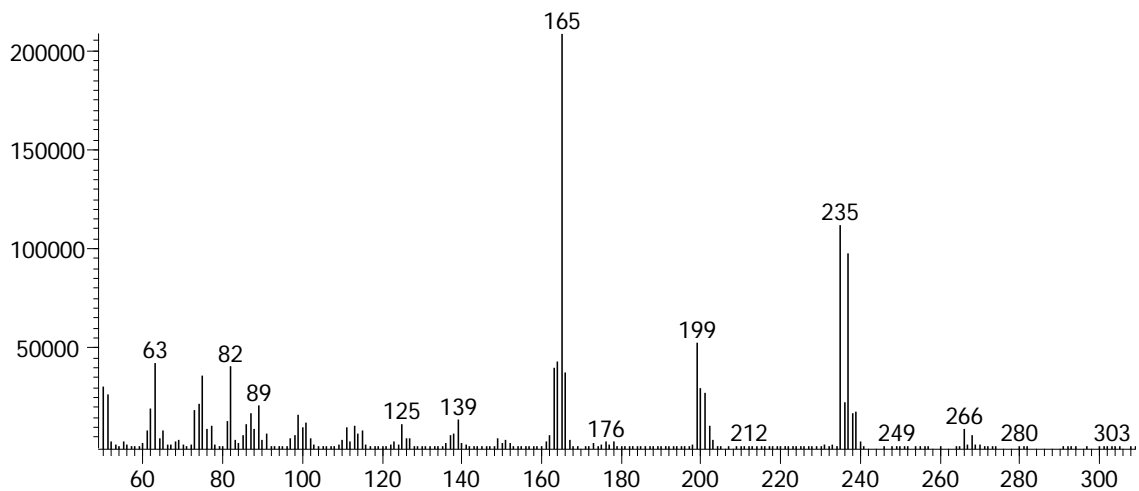
m/z 235: [M-CH<sub>2</sub>OH]<sup>+</sup>

m/z 266: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1464.01, 1.082

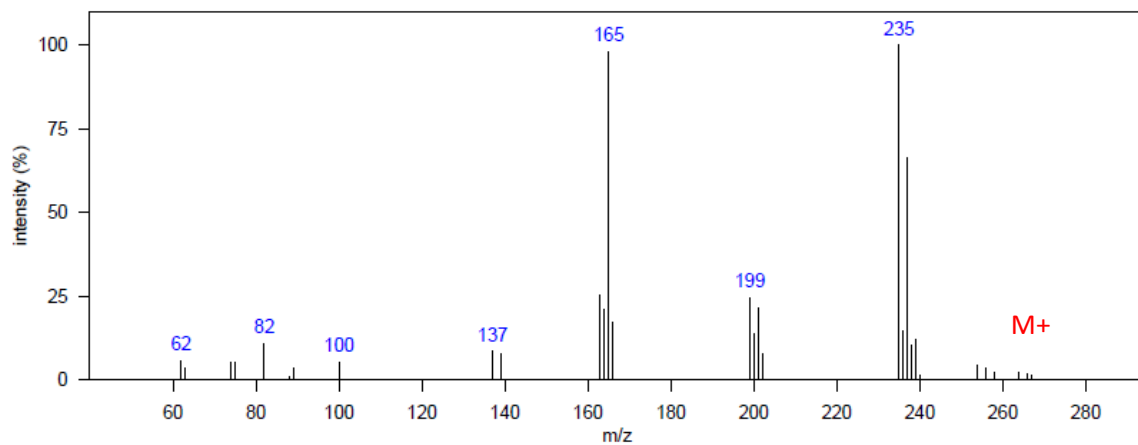
### 3. Identification: [2] Authentic MS (isomer)

### 4. Mass spectrum of p,p'-DDOH standard (IDRT and 2DRT: 1373.06, 1.188)



## DDOH 2

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: [M-CH<sub>2</sub>OH-Cl<sub>2</sub>]<sup>+</sup>

m/z 199: [M-CH<sub>2</sub>OH-HCl]<sup>+</sup>

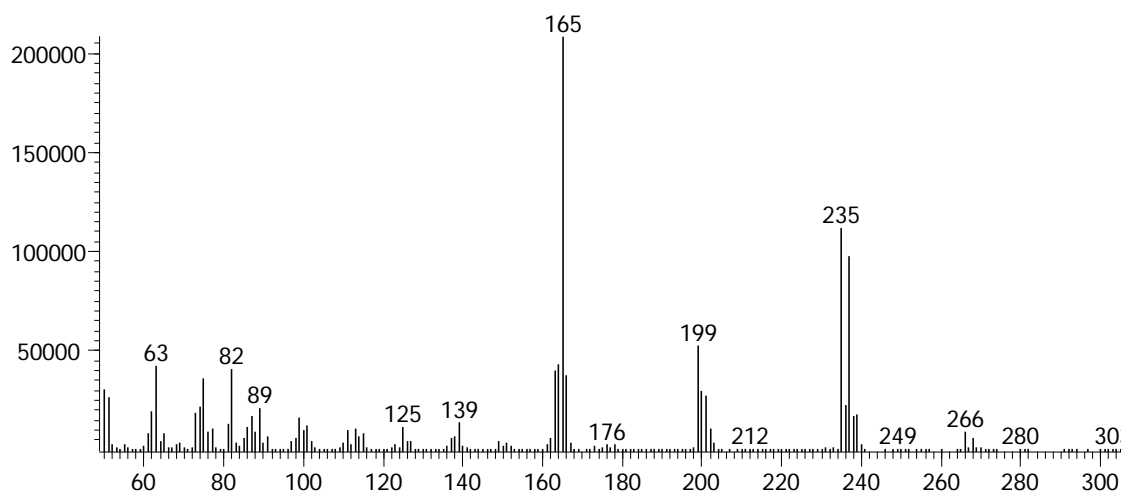
m/z 235: [M-CH<sub>2</sub>OH]<sup>+</sup>

m/z 266: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1317.09, 1.346

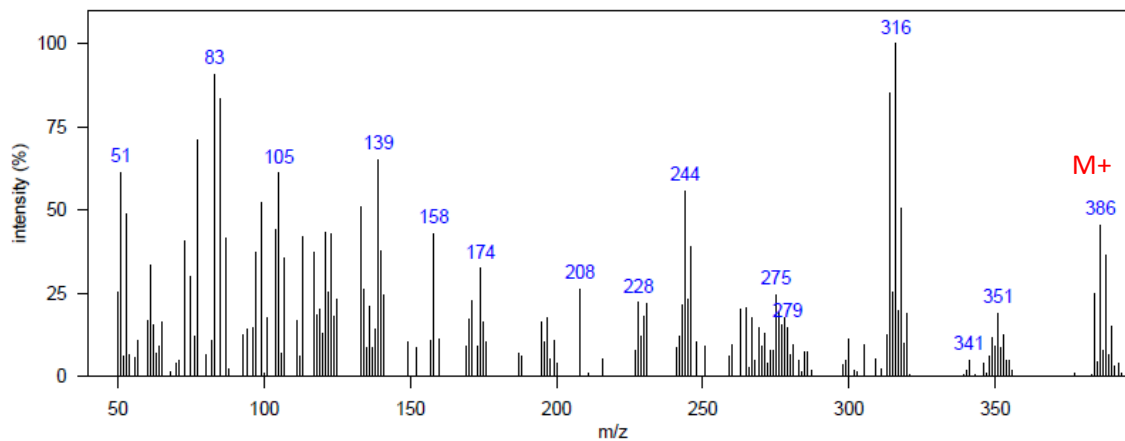
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of p,p'-DDOH standard (IDRT and 2DRT: 1373.06, 1.188)



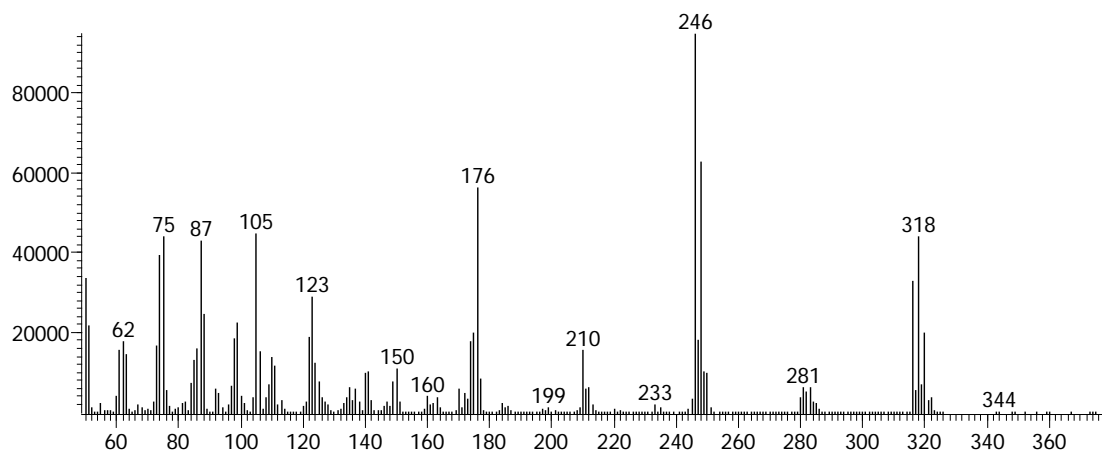
## DDE 6CI 1

### 1. Mass Spectrum from SoCal dolphin blubber D4:

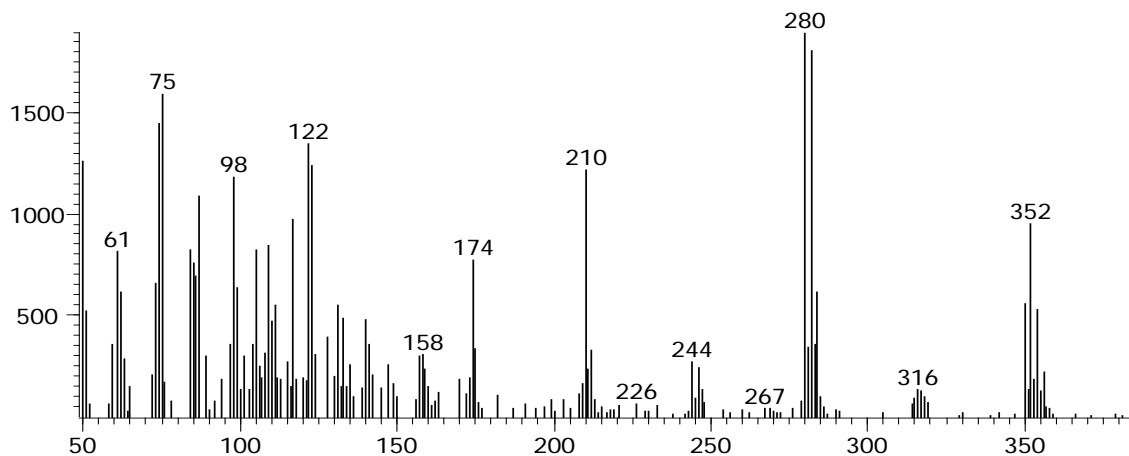


m/z 314: [M-Cl<sub>2</sub>]<sup>+</sup>, m/z 349: [M-Cl]<sup>+</sup>, m/z 384: M<sup>+</sup>

- 1D RT, 2D RT (s): 1484.99, 1.406
- Identification: [4] Congener MS
- Mass spectrum of p,p'-DDE standard

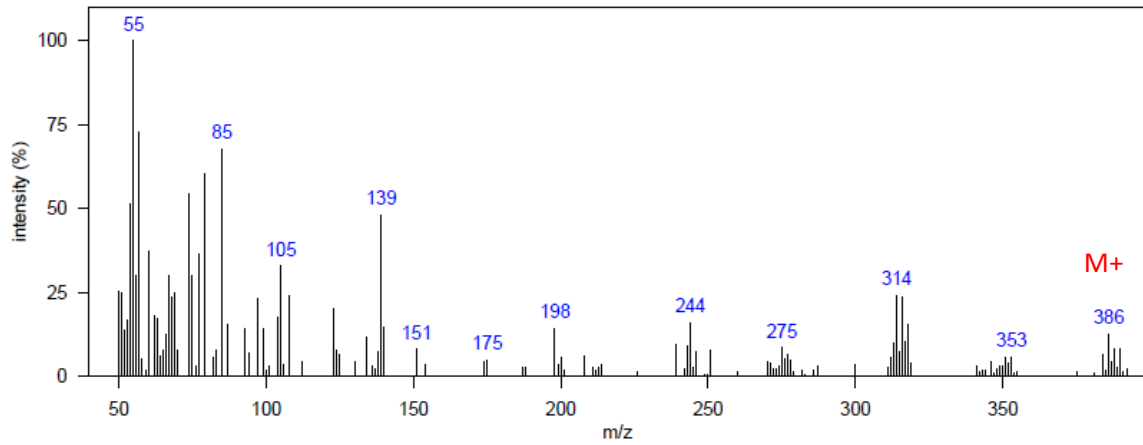


Pentachloro diphenylethene (DDE 5CI) found in p,p'-DDE std



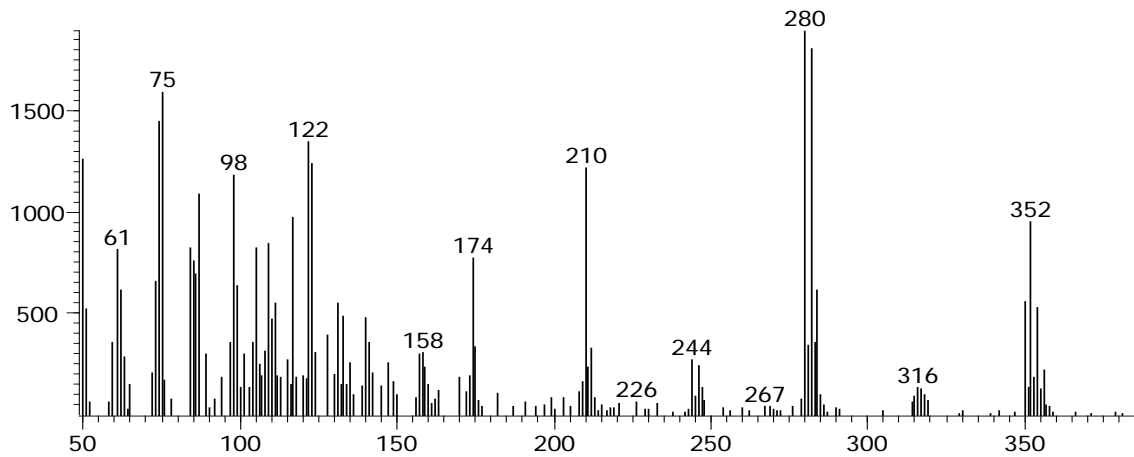
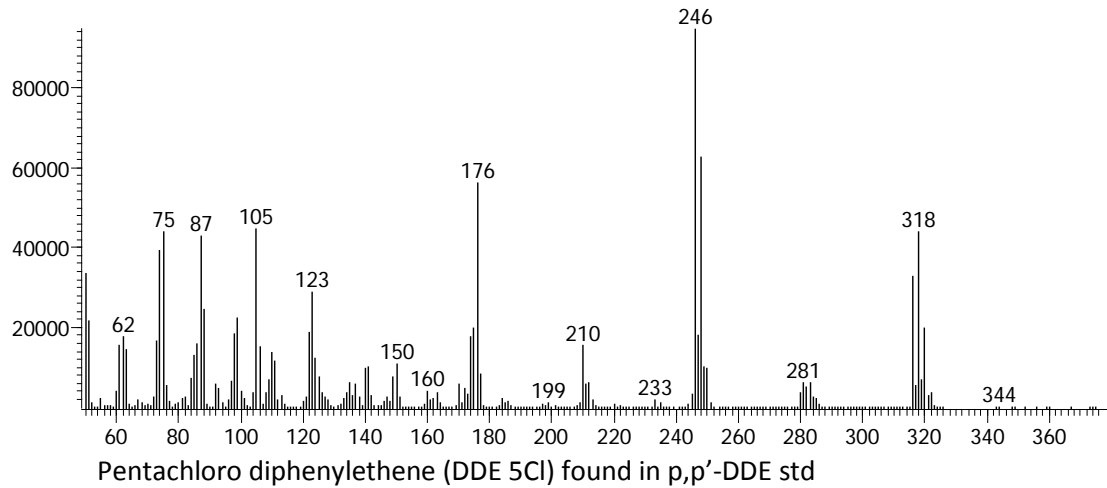
## DDE 6CI 2

### 1. Mass Spectrum from SoCal dolphin blubber D5:



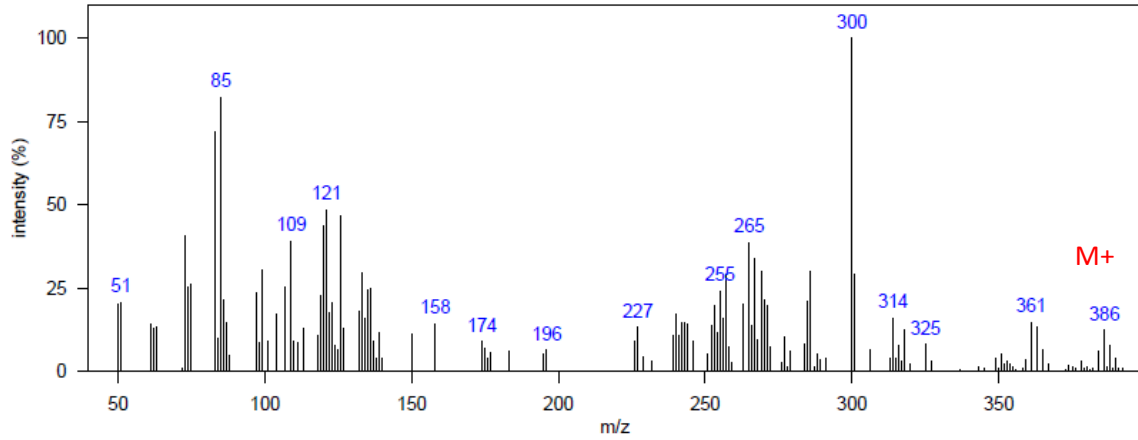
m/z 314: [M-Cl<sub>2</sub>]<sup>+</sup>      m/z 349: [M-Cl]<sup>+</sup>      m/z 384: M<sup>+</sup>

- 1D RT, 2D RT (s): 1488.49, 1.399
- Identification: [4] Congener MS
- Mass spectrum of p,p'-DDE standard



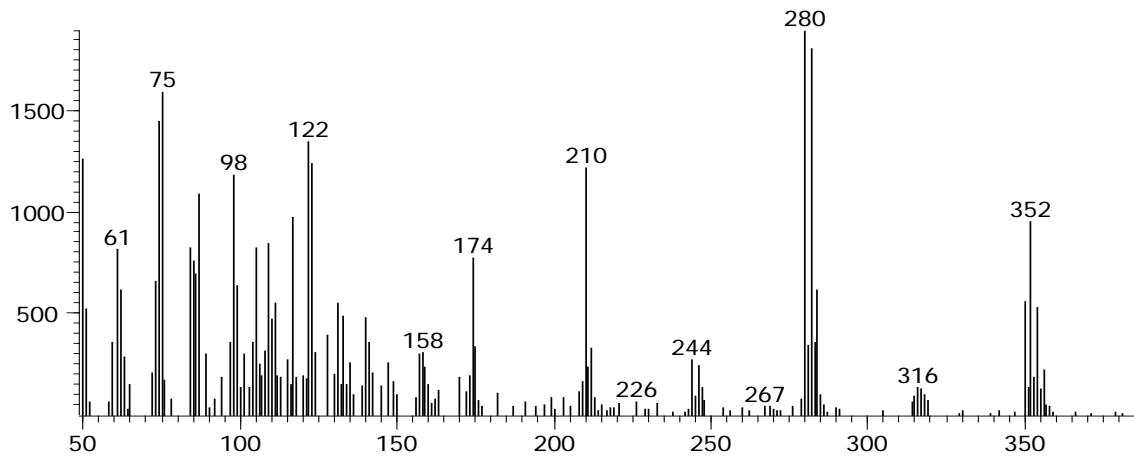
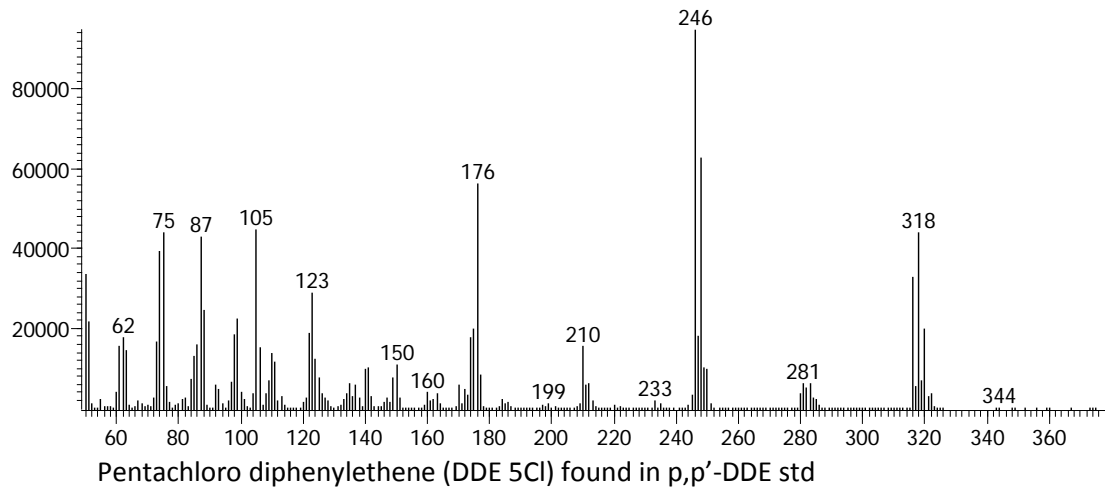
### DDE 6Cl 3

#### 1. Mass Spectrum from SoCal dolphin blubber D7:



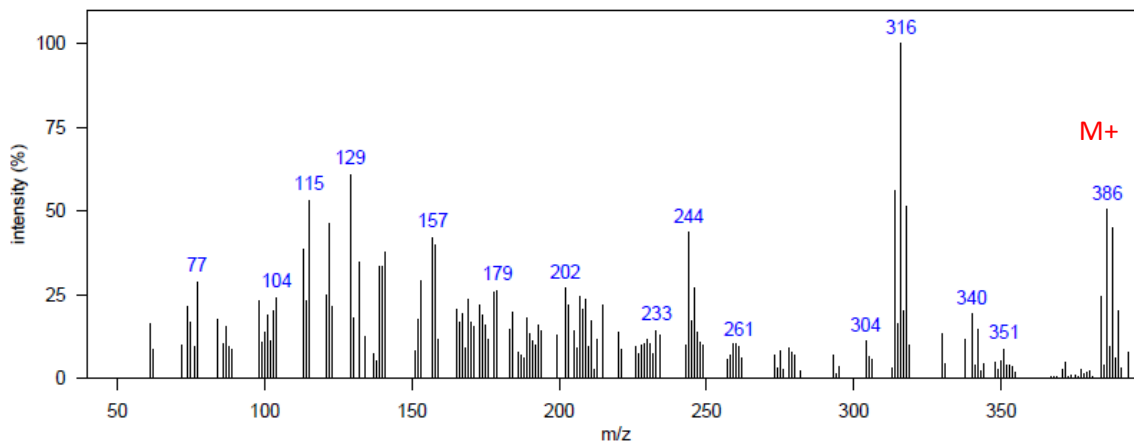
m/z 314: [M-Cl]<sup>+</sup>    m/z 349: [M-Cl]<sup>+</sup>    m/z 384: M<sup>+</sup>

- 1D RT, 2D RT (s): 1481.5, 1.399
- Identification: [4] Congener MS
- Mass spectrum of p,p'-DDE standard



## DDE 6Cl 4

### 1. Mass Spectrum from SoCal dolphin blubber D1:

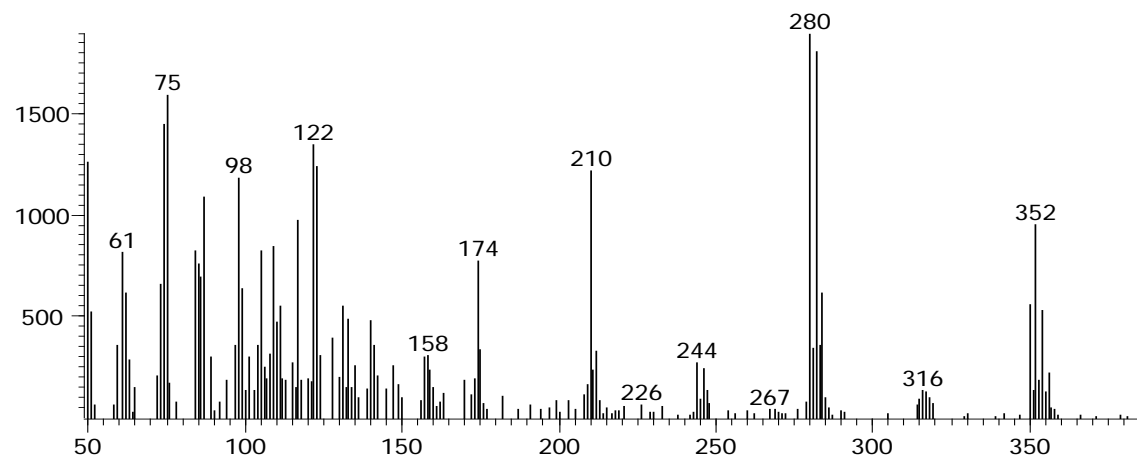
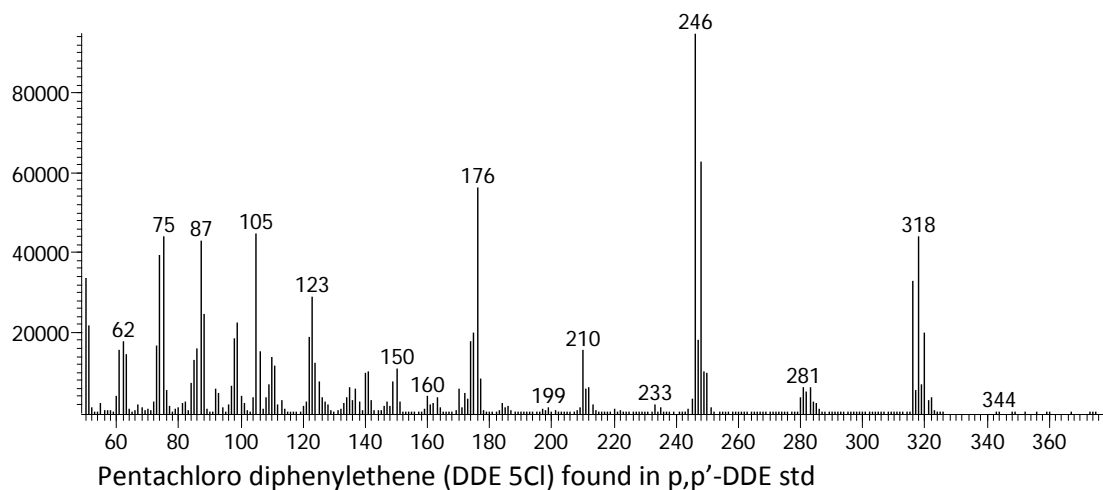


m/z 314: [M-Cl<sub>2</sub>]<sup>+</sup>    m/z 349: [M-Cl]<sup>+</sup>    m/z 384: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1523.47, 1.393

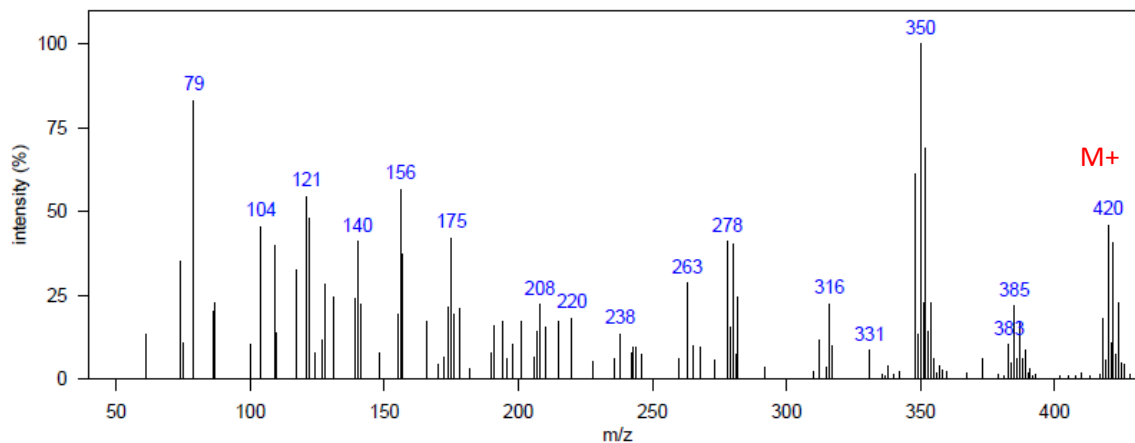
3. Identification: [4] Congener MS

4. Mass spectrum of p,p'-DDE standard



## DDE 7CI 1

### 1. Mass Spectrum from SoCal dolphin blubber D2:

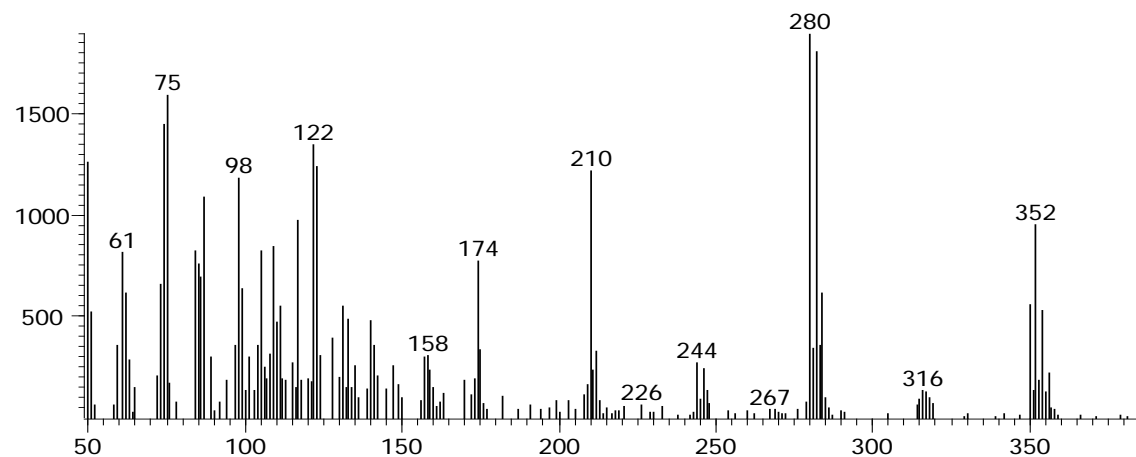
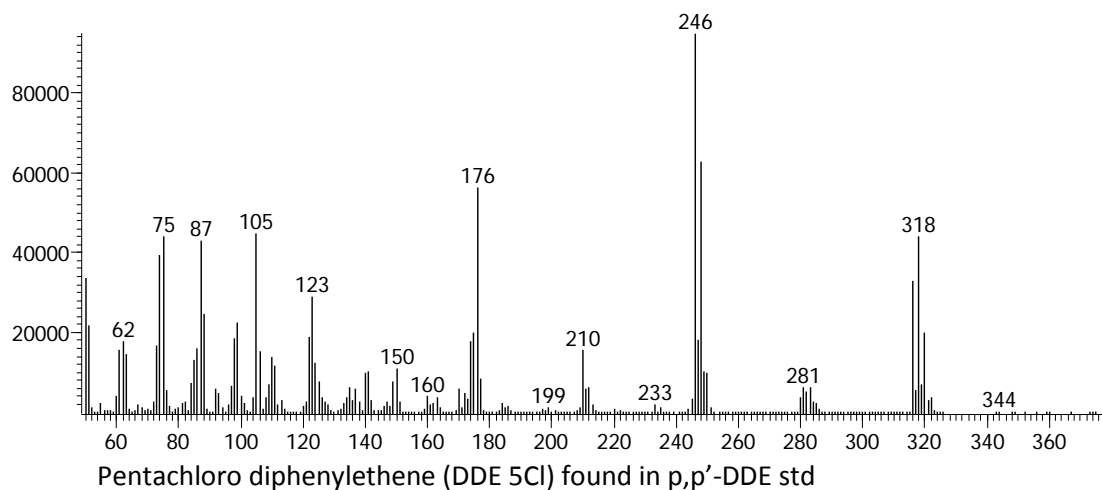


m/z 278: [M-Cl<sub>4</sub>]<sup>+</sup> m/z 348: [M-Cl<sub>2</sub>]<sup>+</sup> m/z 383: [M-Cl]<sup>+</sup> m/z 418: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1551.46, 1.485

3. Identification: [4] Congener MS

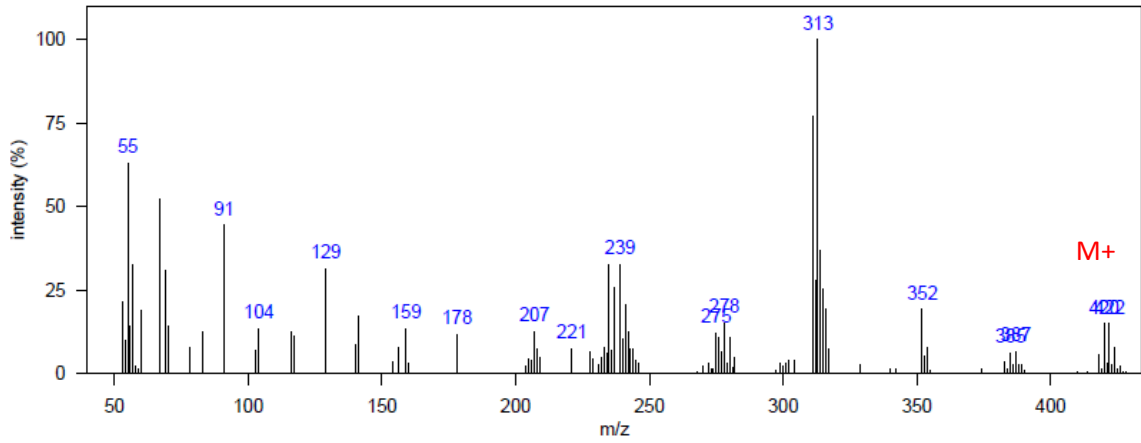
4. Mass spectrum of p,p'-DDE standard





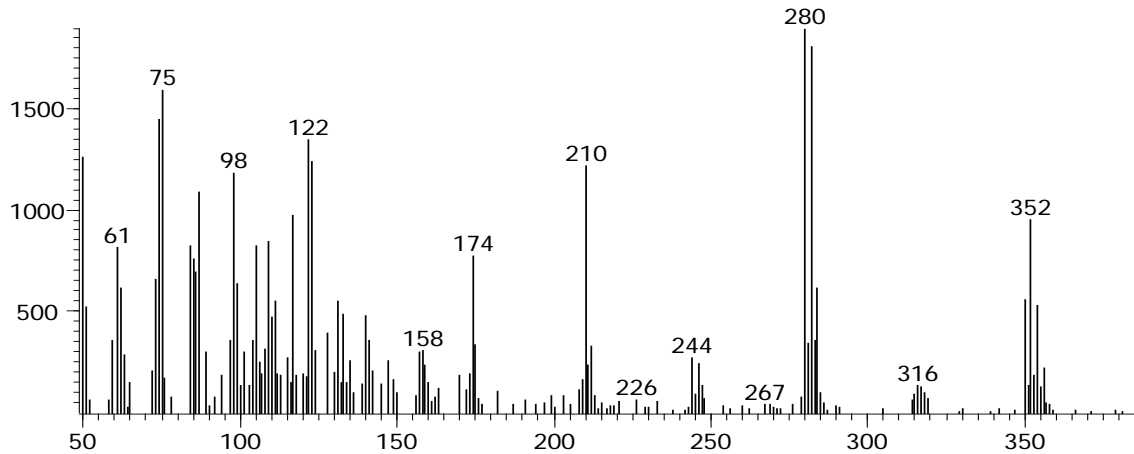
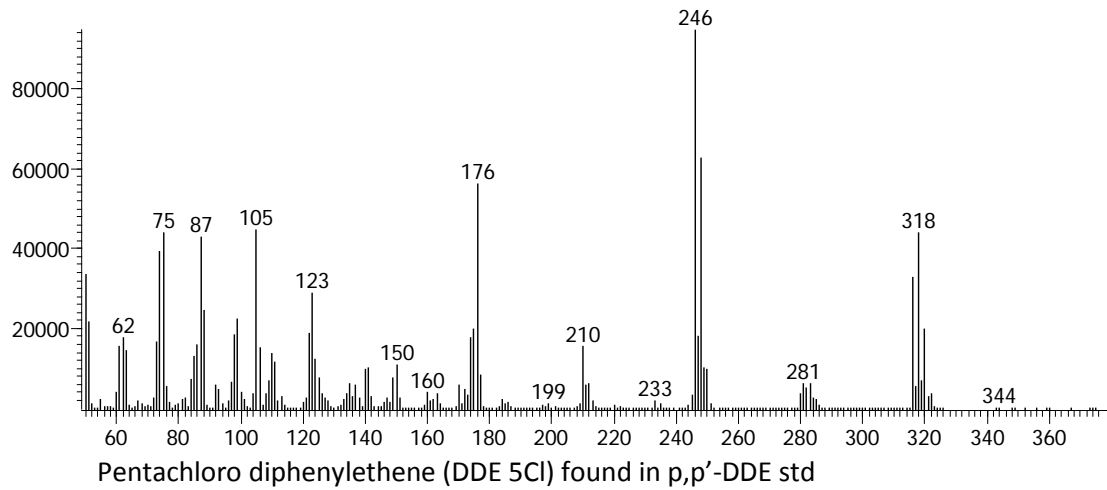
## DDE 7Cl 2

### 1. Mass Spectrum from SoCal dolphin blubber D1:



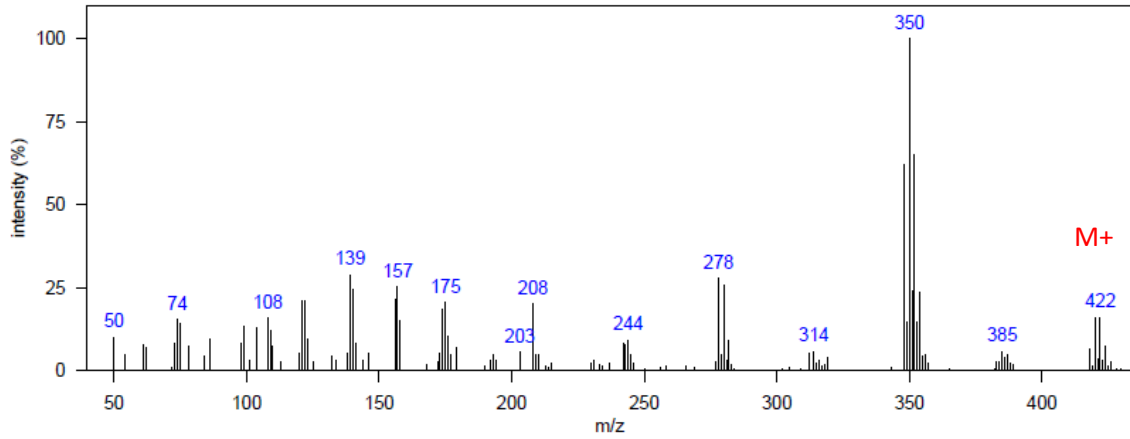
m/z 278: [M-Cl<sub>4</sub>]<sup>+</sup> m/z 348: [M-Cl<sub>2</sub>]<sup>+</sup> m/z 383: [M-Cl]<sup>+</sup> m/z 418: M<sup>+</sup>

- 1D RT, 2D RT (s): 1558.45, 1.525
- Identification: [4] Congener MS
- Mass spectrum of p,p'-DDE standard



### DDE 7Cl 3

#### 1. Mass Spectrum from SoCal dolphin blubber D1:

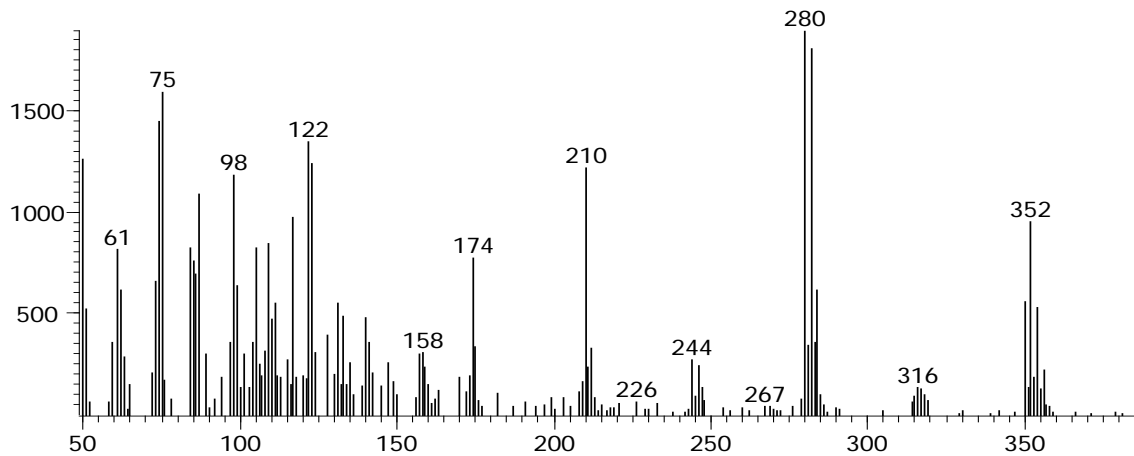
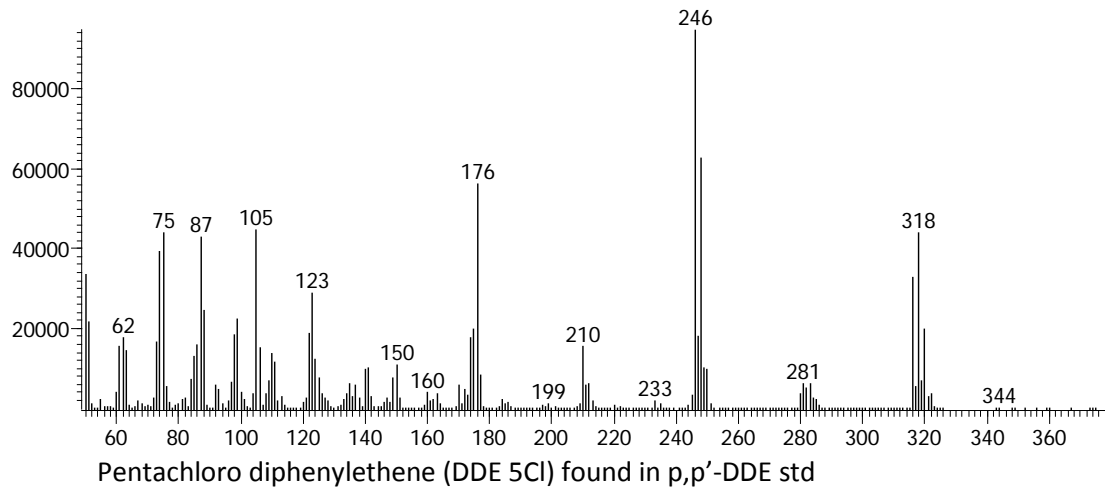


m/z 278: [M-Cl<sub>4</sub>]<sup>+</sup> m/z 348: [M-Cl<sub>2</sub>]<sup>+</sup> m/z 383: [M-Cl]<sup>+</sup> m/z 418: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1582.94, 1.571

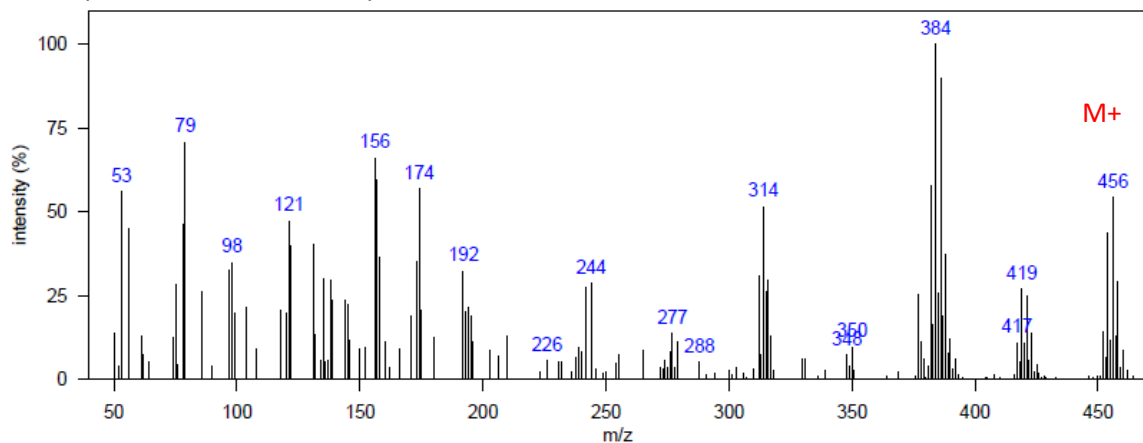
3. Identification: [4] Congener MS

4. Mass spectrum of p,p'-DDE standard



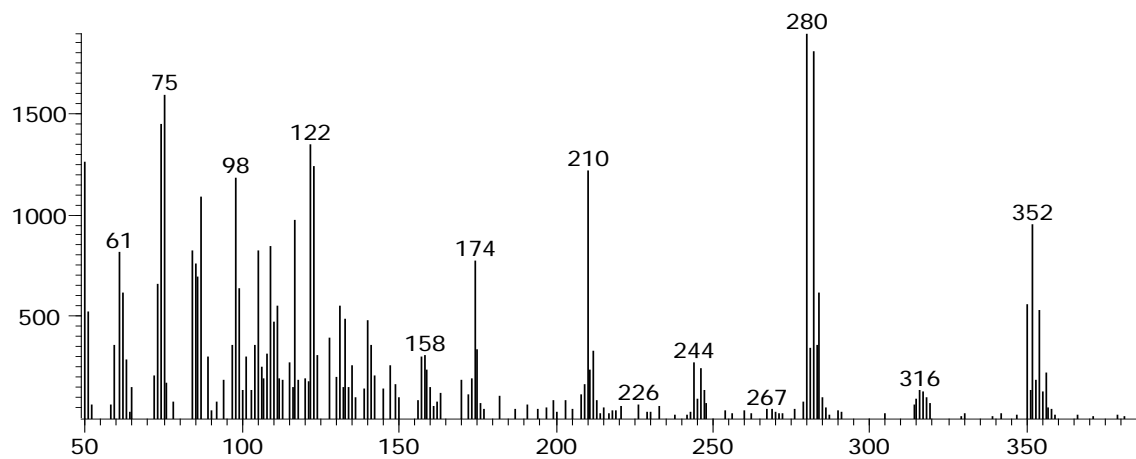
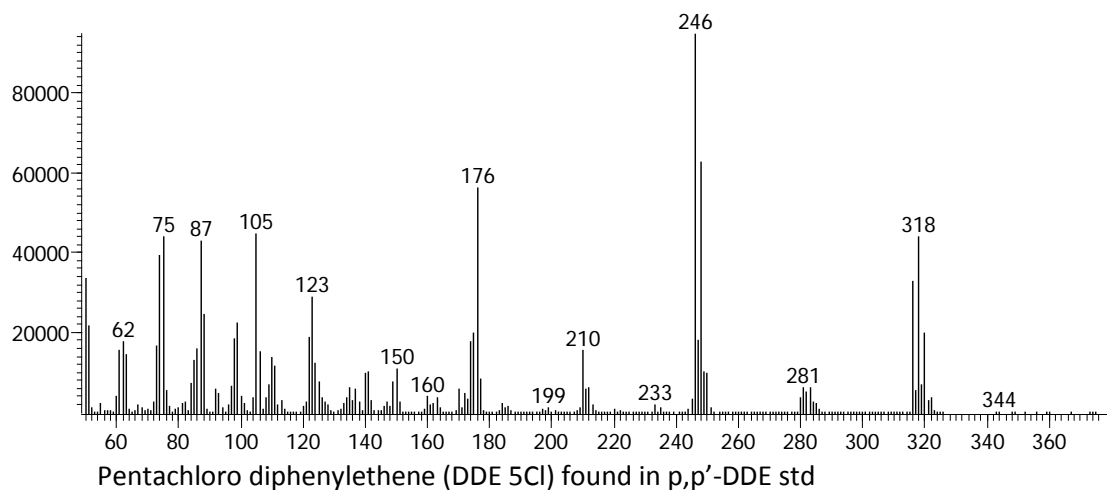
## DDE 8CI

### 1. Mass Spectrum from SoCal dolphin blubber D1:



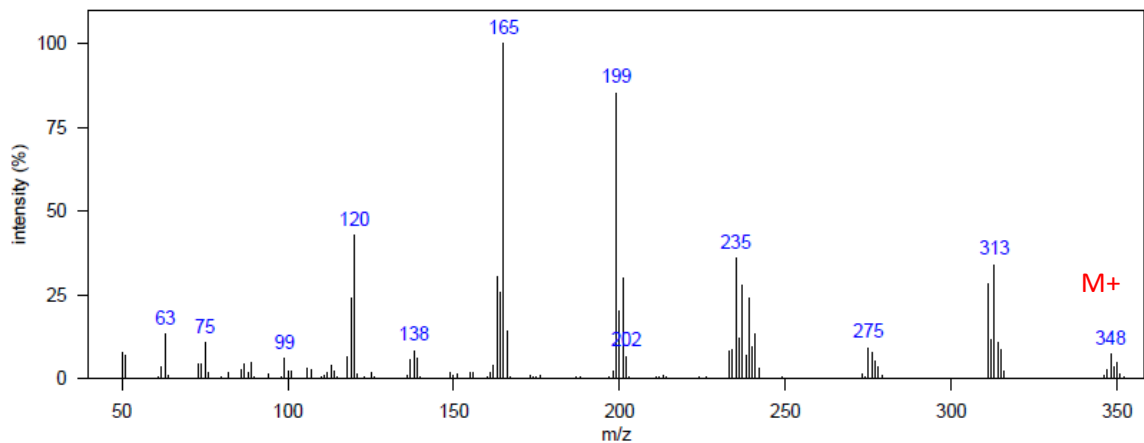
m/z 312: [M-Cl<sub>4</sub>]<sup>+</sup>    m/z 382: [M-Cl<sub>2</sub>]<sup>+</sup>    m/z 417: [M-Cl]<sup>+</sup>    m/z 452: M<sup>+</sup>

- 1D RT, 2D RT (s): 1659.89, 1.861
- Identification: [4] Congener MS
- Mass spectrum of p,p'-DDE standard



## 4,4',4''-TCPM

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>ClH<sub>8</sub><sup>+</sup>

m/z 235: C<sub>13</sub>Cl<sub>2</sub>H<sub>10</sub><sup>+</sup> or [M-C<sub>6</sub>ClH<sub>4</sub>]<sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

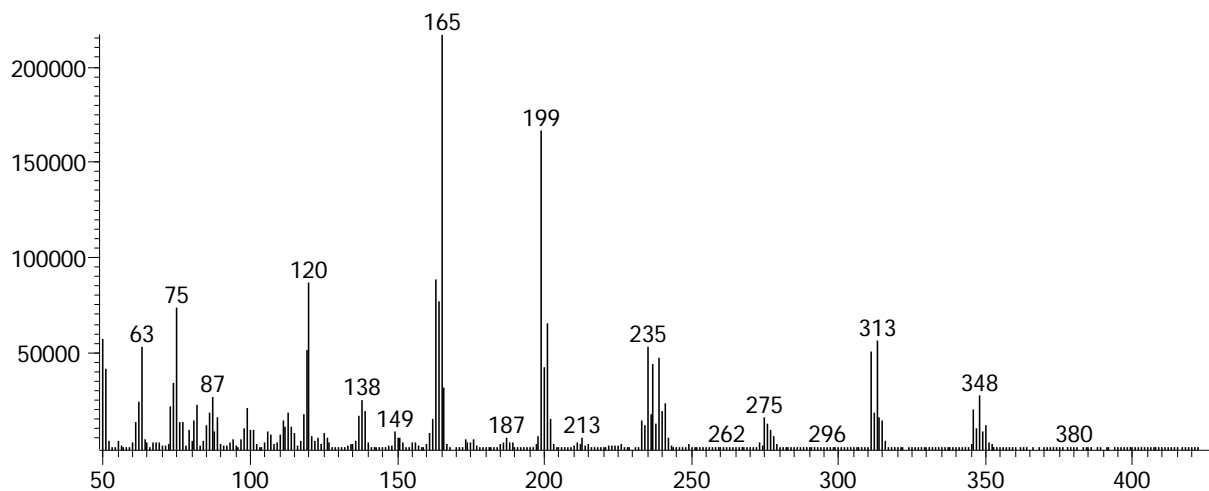
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1596.93, 1.723

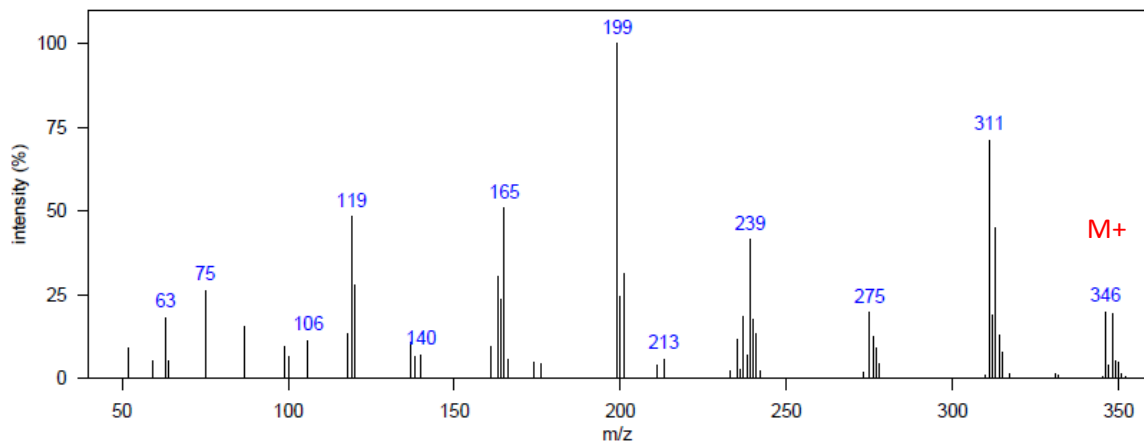
3. Identification: [1] Authentic MS/RT

4. Mass spectrum of 4,4',4''-TCPM standard



## TCPM 1

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>ClH<sub>8</sub><sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

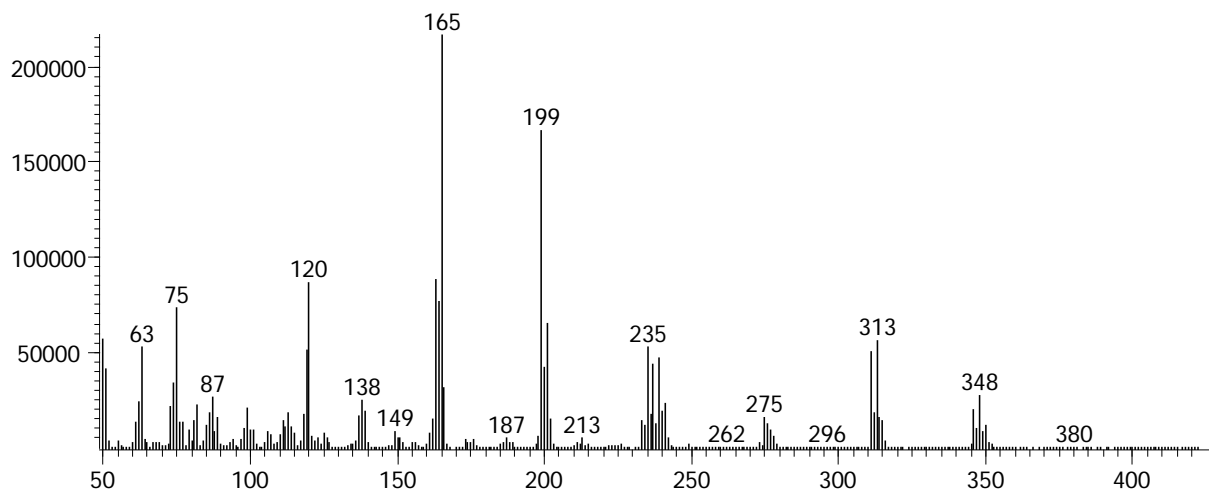
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1484.99, 1.531

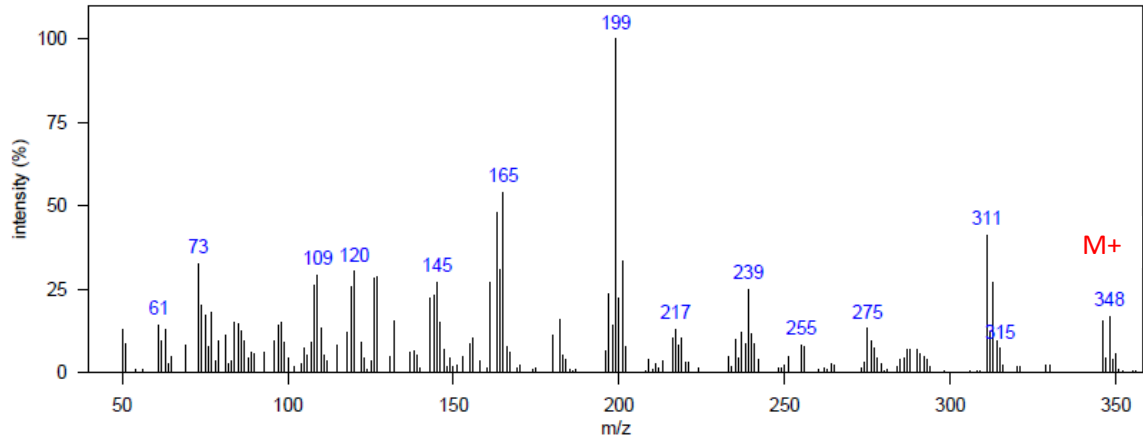
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPM standard



## TCPM 2

### 1. Mass Spectrum from SoCal dolphin blubber D4:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>ClH<sub>8</sub><sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

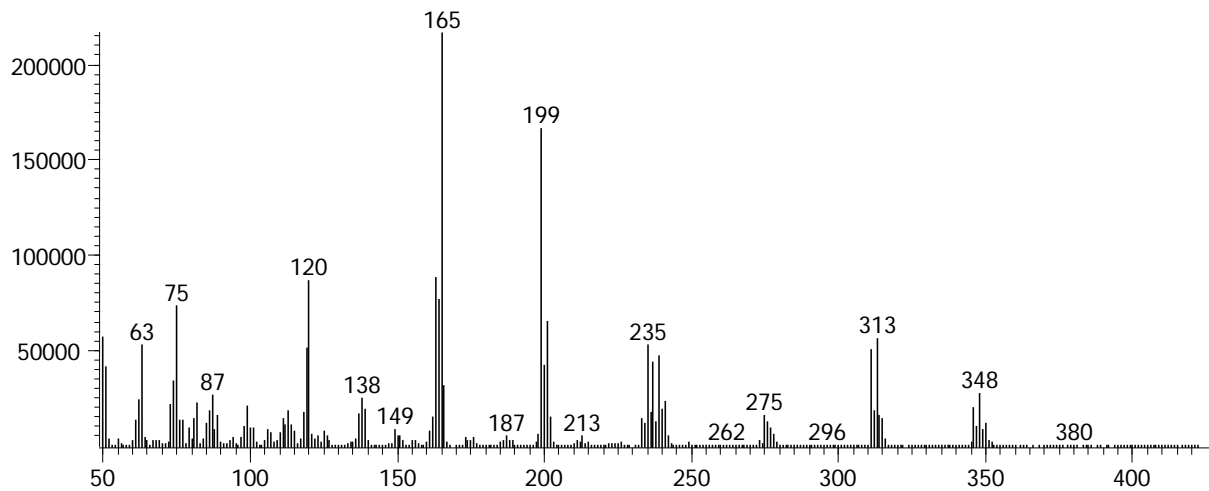
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1502.48, 1.498

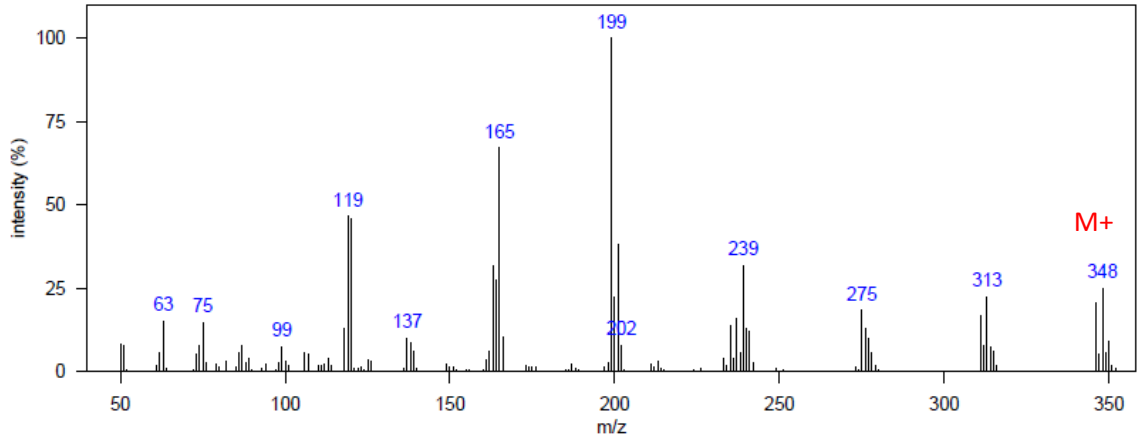
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPM standard



### TCPM 3

1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>ClH<sub>8</sub><sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

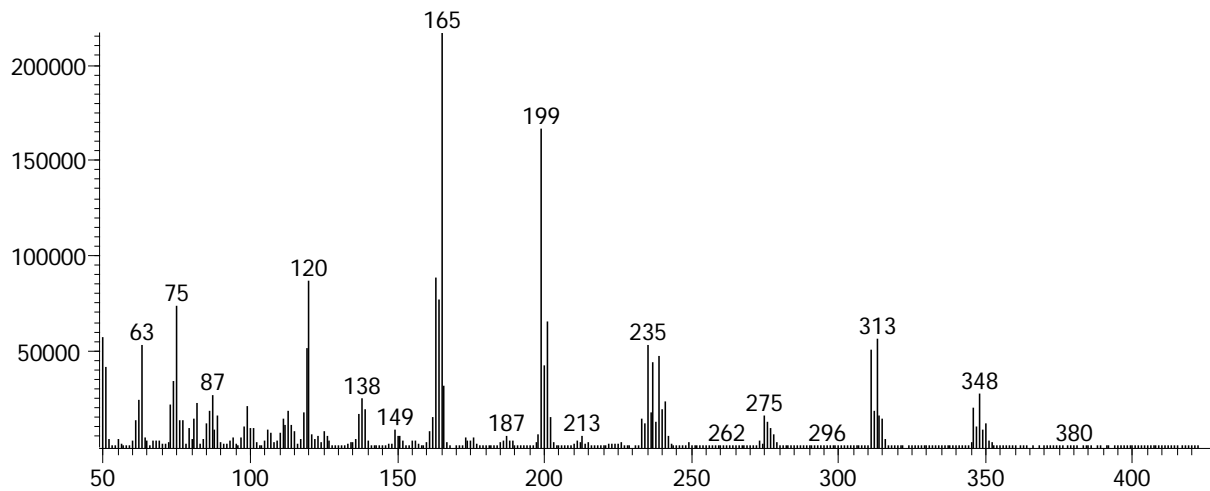
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1519.97, 1.538

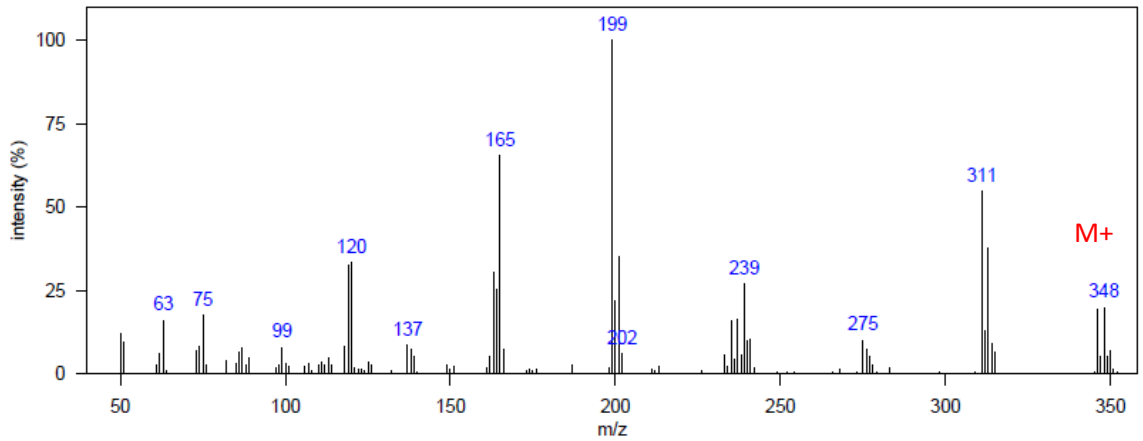
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPM standard



## TCPM 4

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>H<sub>8</sub><sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

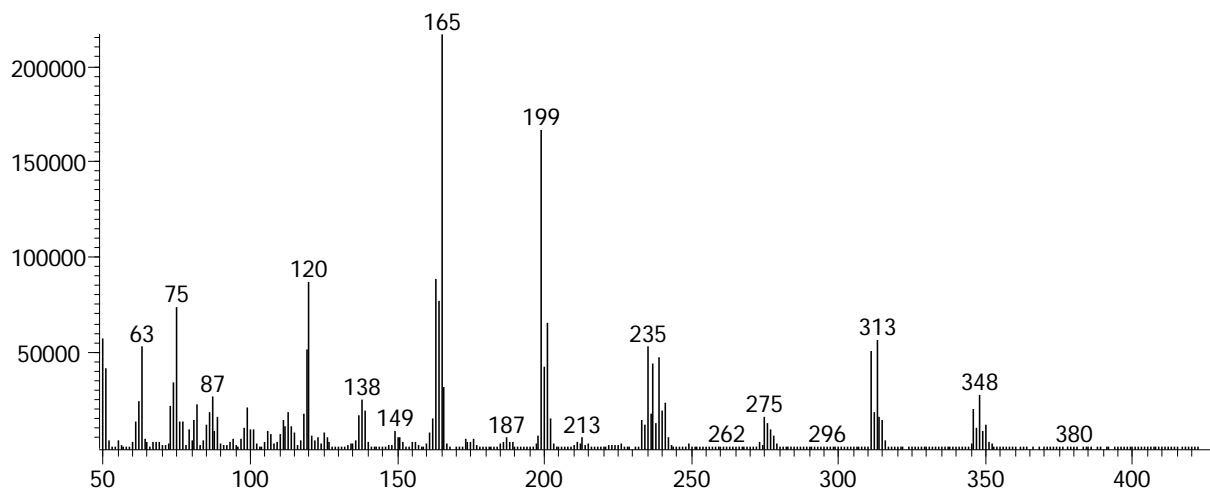
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1540.96, 1.544

3. Identification: [2] Authentic MS (isomer)

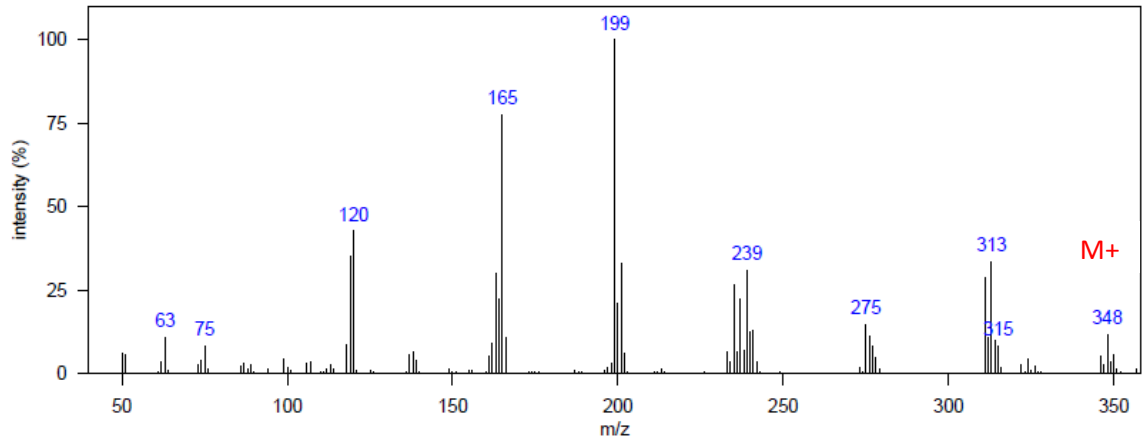
4. Mass spectrum of 4,4',4''-TCPM standard





## TCPM 5

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>ClH<sub>8</sub><sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

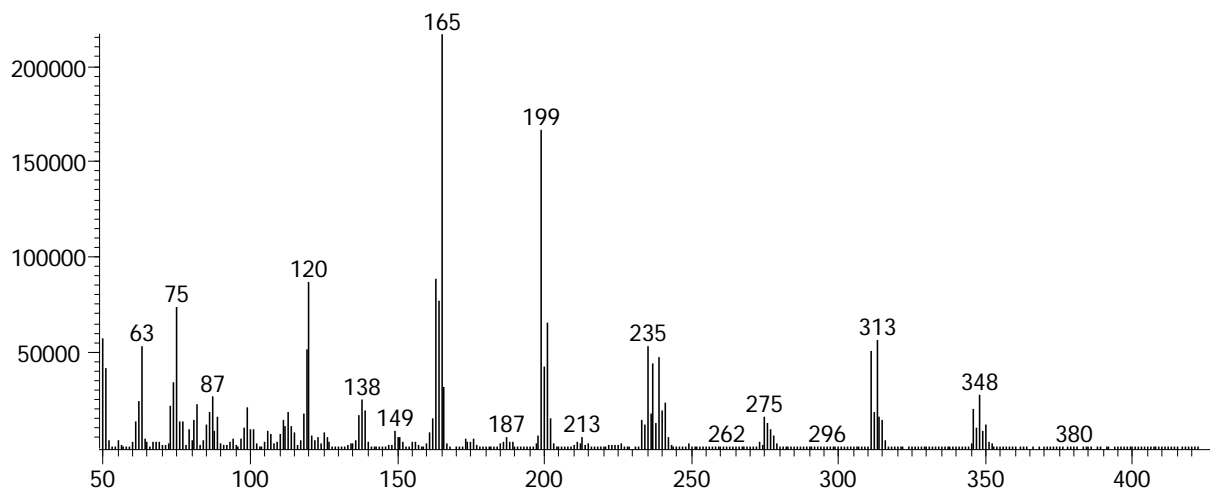
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1558.45, 1.61

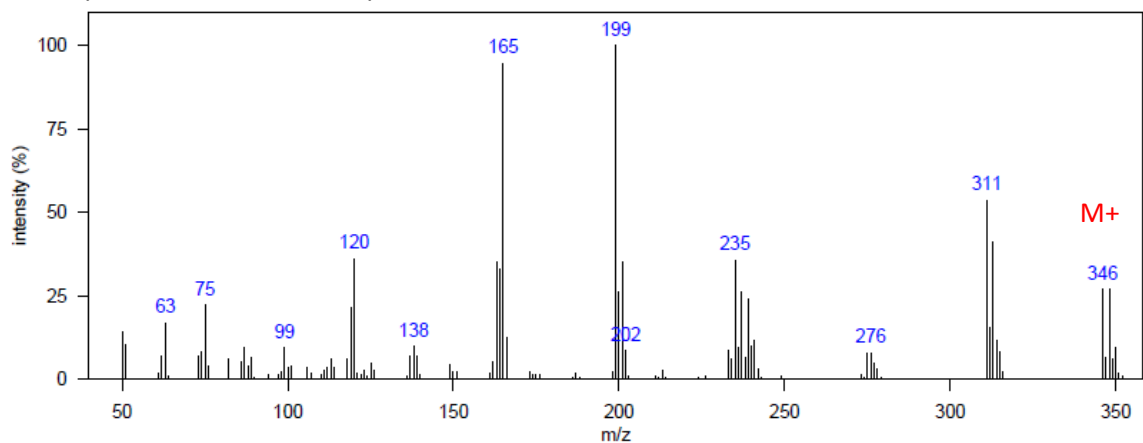
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPM standard



## TCPM 6

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>ClH<sub>8</sub><sup>+</sup>

m/z 235: C<sub>13</sub>Cl<sub>2</sub>H<sub>10</sub><sup>+</sup> or [M-C<sub>6</sub>ClH<sub>4</sub>]<sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

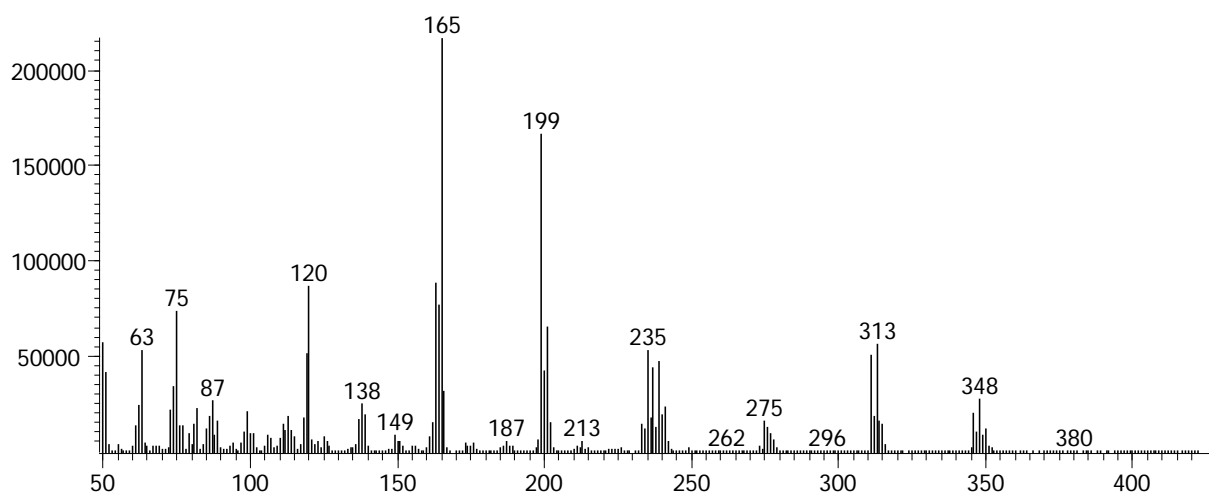
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1579.44, 1.65

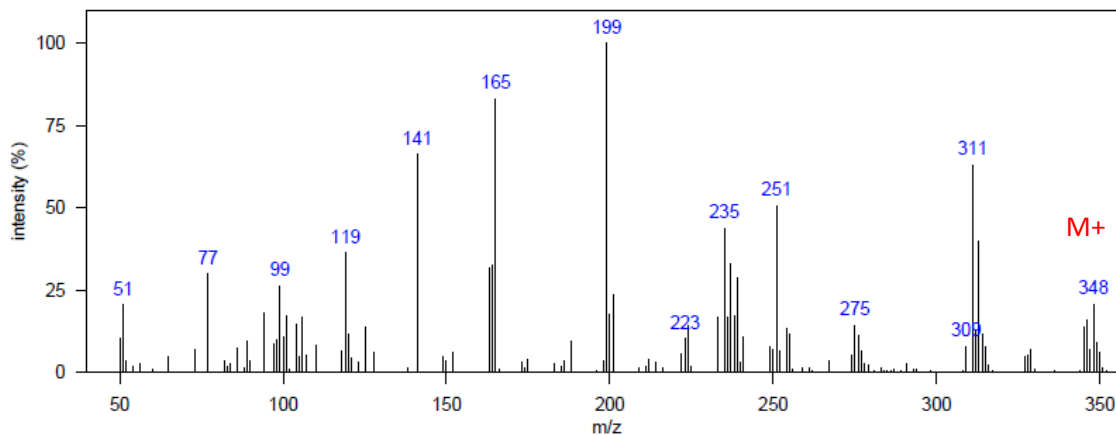
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPM standard



## TCPM 7

### 1. Mass Spectrum from SoCal dolphin blubber D8:



m/z 165: C<sub>13</sub>H<sub>9</sub><sup>+</sup>

m/z 199: C<sub>13</sub>ClH<sub>8</sub><sup>+</sup>

m/z 235: C<sub>13</sub>Cl<sub>2</sub>H<sub>10</sub><sup>+</sup> or [M-C<sub>6</sub>ClH<sub>4</sub>]<sup>+</sup>

m/z 239: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 275: [M-HCl<sub>2</sub>]<sup>+</sup>

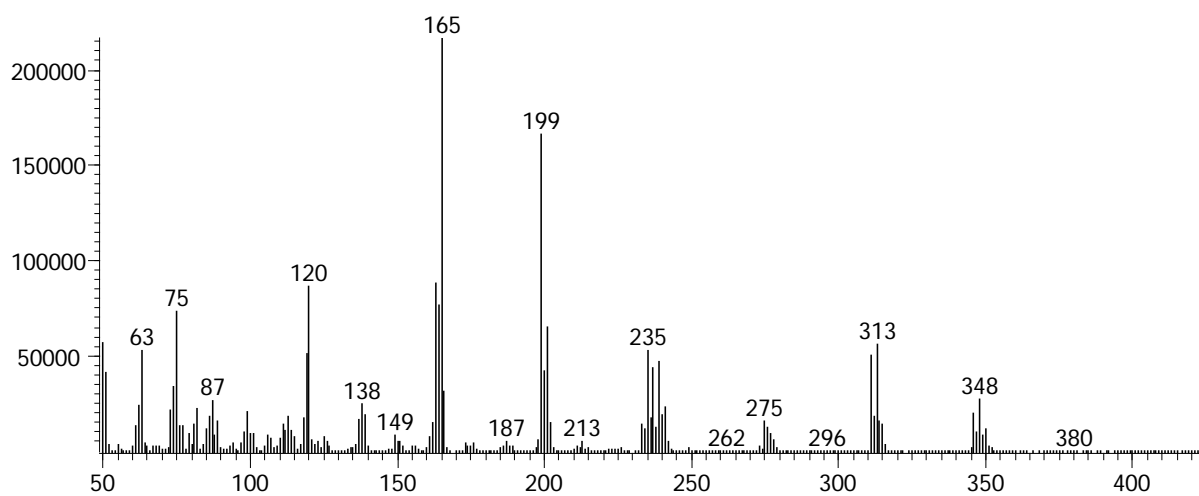
m/z 311: [M-Cl]<sup>+</sup>

m/z 346: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1673.89, 2.112

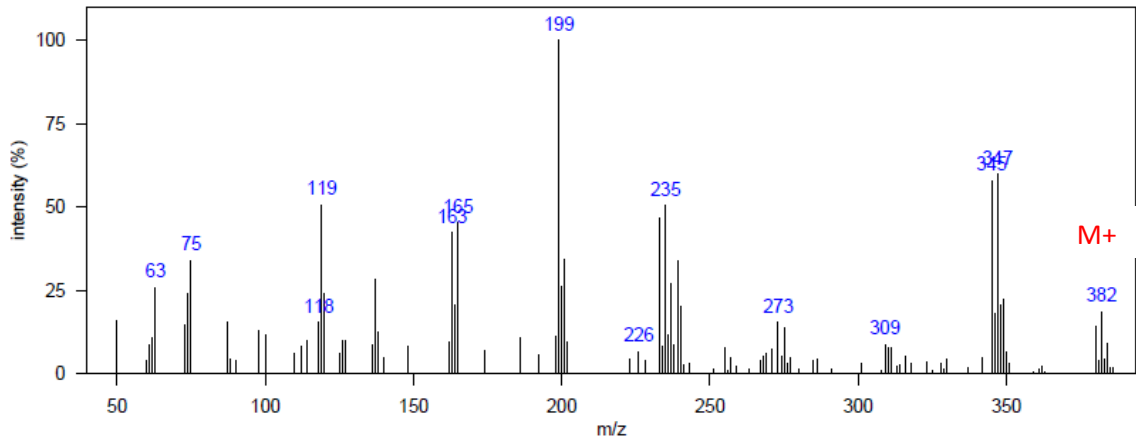
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPM standard



## TCPM 4Cl 1

### 1. Mass Spectrum from SoCal dolphin blubber D1:



m/z 199: C<sub>13</sub>H<sub>8</sub><sup>+</sup>

m/z 273: [M-H<sub>2</sub>Cl<sub>3</sub>]<sup>+</sup>

m/z 309: [M-HCl<sub>2</sub>]<sup>+</sup>

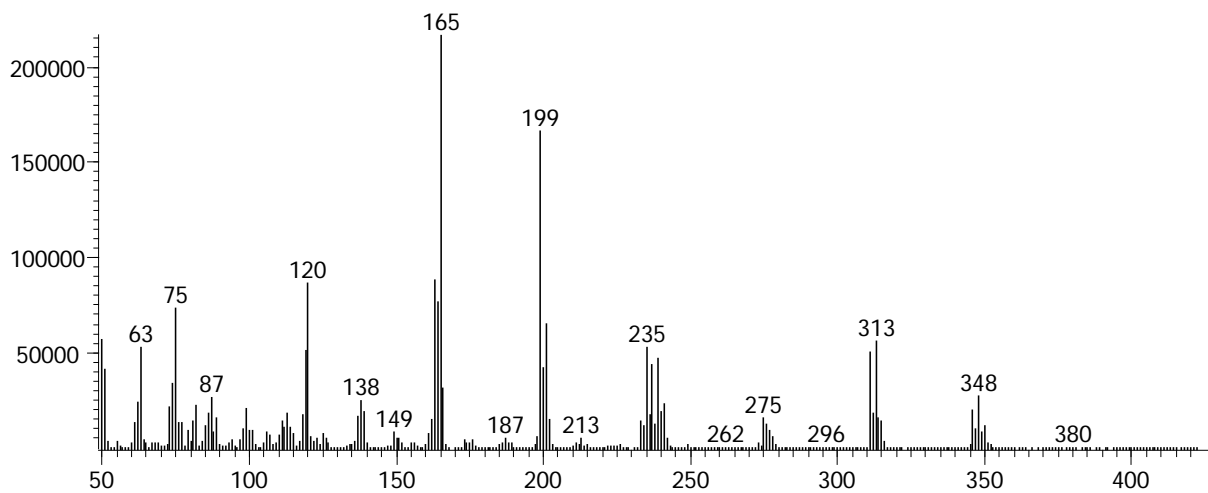
m/z 345: [M-Cl]<sup>+</sup>

m/z 380: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1624.91, 1.789

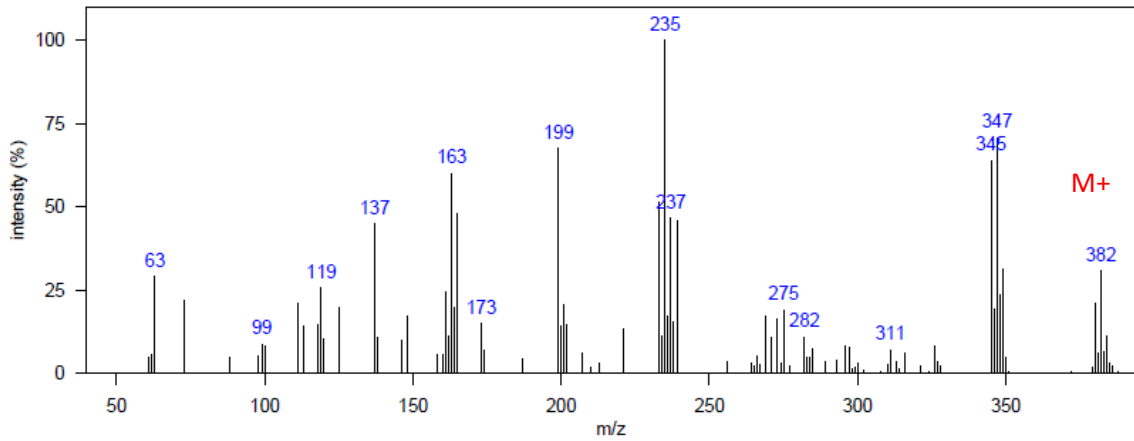
### 3. Identification: [4] Congener MS

### 4. Mass spectrum of 4,4',4''-TCPM standard



## TCPM 4Cl 2

### 1. Mass Spectrum from SoCal dolphin blubber D4:



m/z 199: C<sub>13</sub>H<sub>8</sub><sup>+</sup>

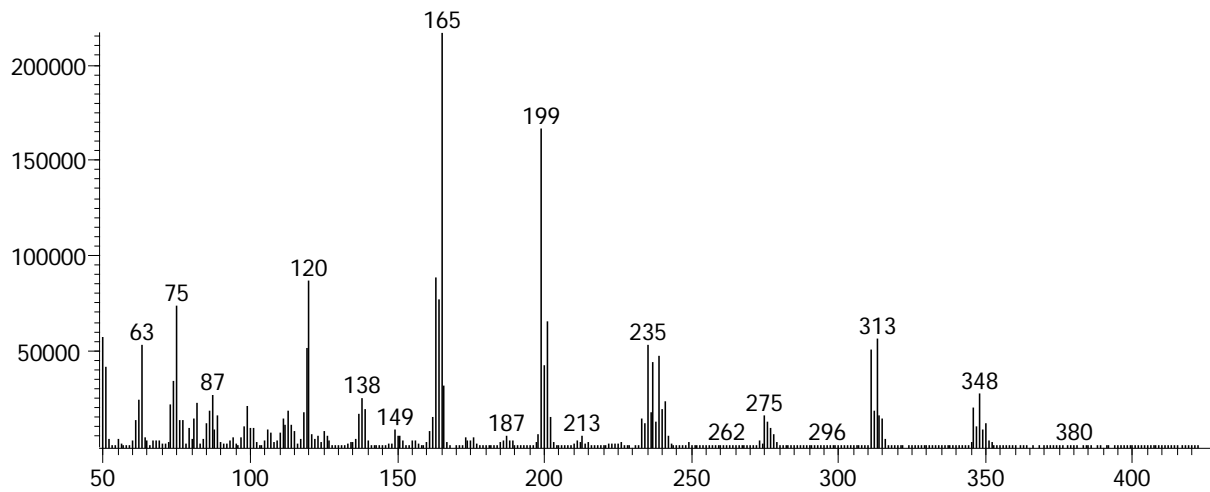
m/z 345: [M-Cl]<sup>+</sup>

m/z 380: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1652.9, 1.987

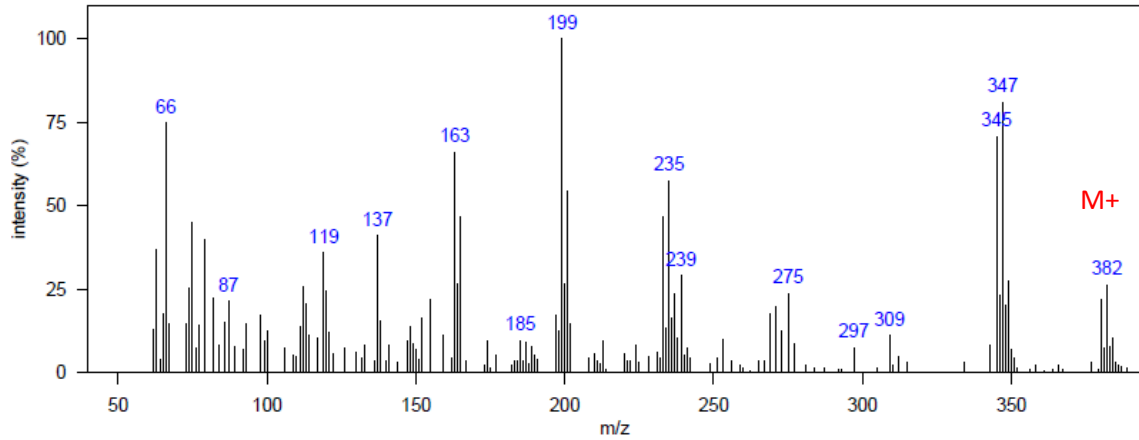
### 3. Identification: [4] Congener MS

### 4. Mass spectrum of 4,4',4''-TCPM standard



### TCPM 4CI 3

#### 1. Mass Spectrum from SoCal dolphin blubber D1:



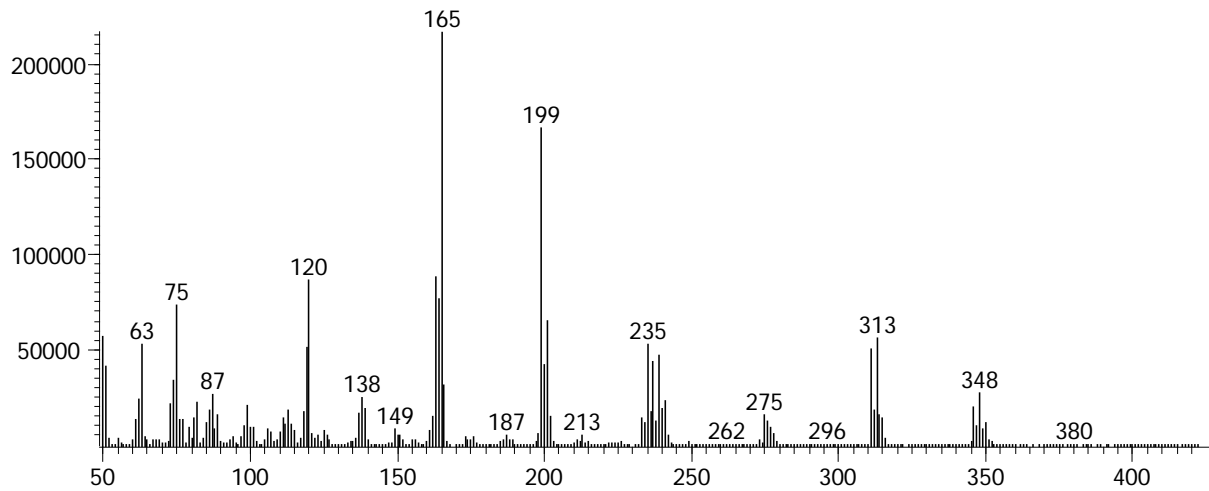
m/z 345: [M-Cl]+

m/z 380: M+

#### 2. 1D RT, 2D RT (s): 1705.37, 1.954

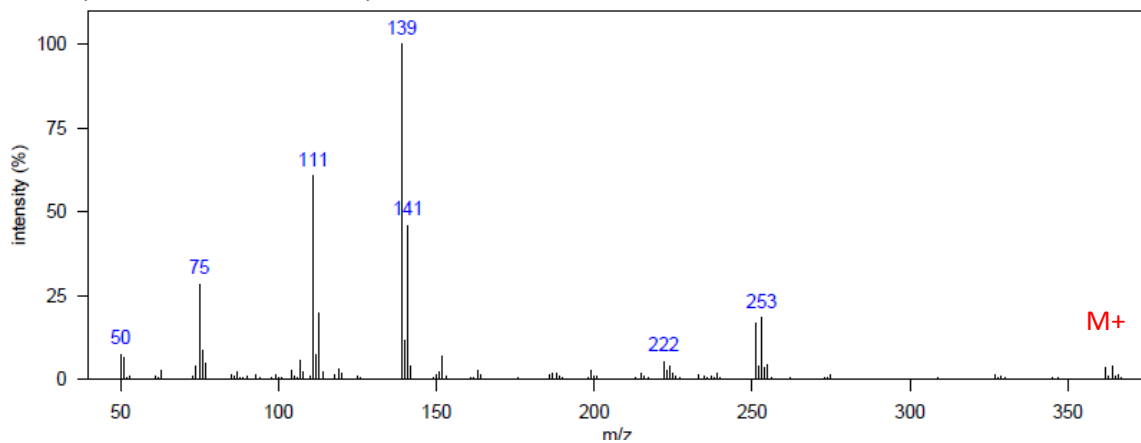
#### 3. Identification: [4] Congener MS

#### 4. Mass spectrum of 4,4',4''-TCPM standard



## 4,4',4''-TCPMOH

### 1. Mass Spectrum from SoCal dolphin blubber D4:



m/z 111: [M-C6H4Cl-C6H4Cl-COH]<sup>+</sup> or C6ClH4<sup>+</sup>

m/z 139: [M-C6H4Cl-C6H4Cl-H]<sup>+</sup> or C7ClOH4<sup>+</sup>

m/z 222: [M-C6H4Cl-COH]<sup>+</sup>

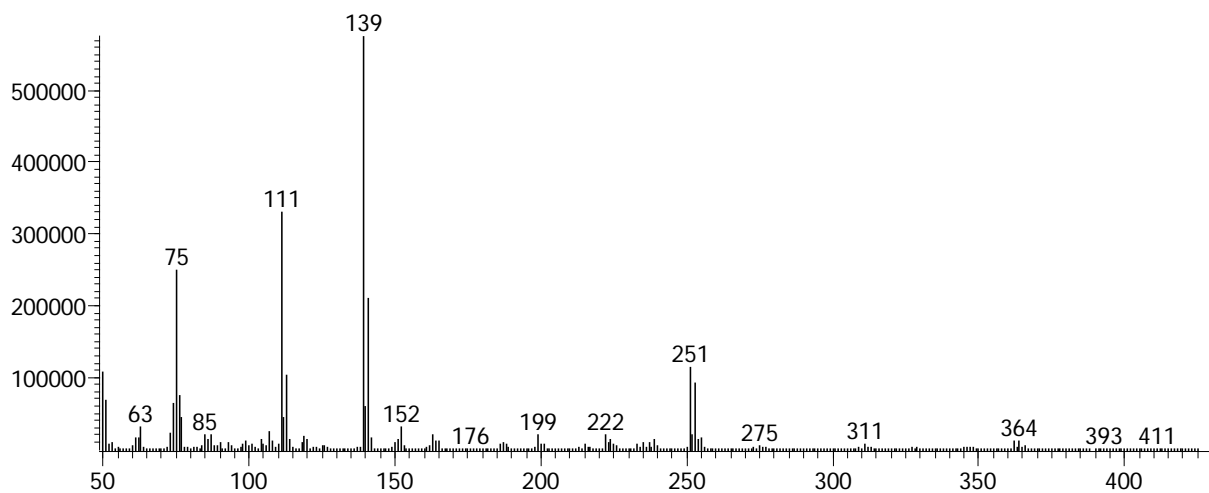
m/z 251: [M-C6H4Cl]<sup>+</sup>

m/z 362: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1677.38, 2.119

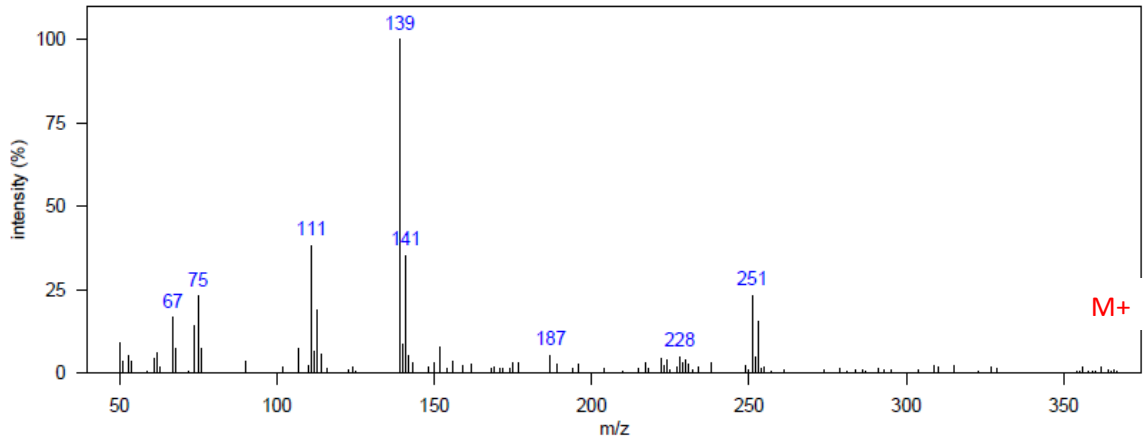
### 3. Identification: [1] Authentic MS/RT

### 4. Mass spectrum of 4,4',4''-TCPMOH standard



## TCPMOH 1

### 1. Mass Spectrum from SoCal dolphin blubber D5:



m/z 111: [M-C6H4Cl-C6H4Cl-COH]<sup>+</sup> or C6ClH4<sup>+</sup>

m/z 139: [M-C6H4Cl-C6H4Cl-H]<sup>+</sup> or C7ClOH4<sup>+</sup>

m/z 222: [M-C6H4Cl-COH]<sup>+</sup>

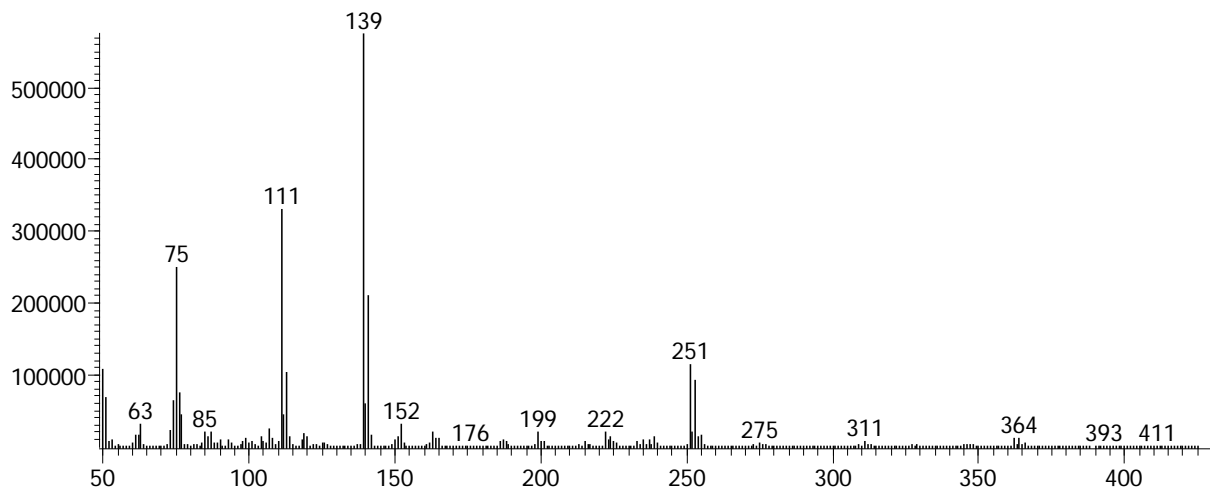
m/z 251: [M-C6H4Cl]<sup>+</sup>

m/z 362: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1603.93, 1.894

### 3. Identification: [2] Authentic MS (isomer)

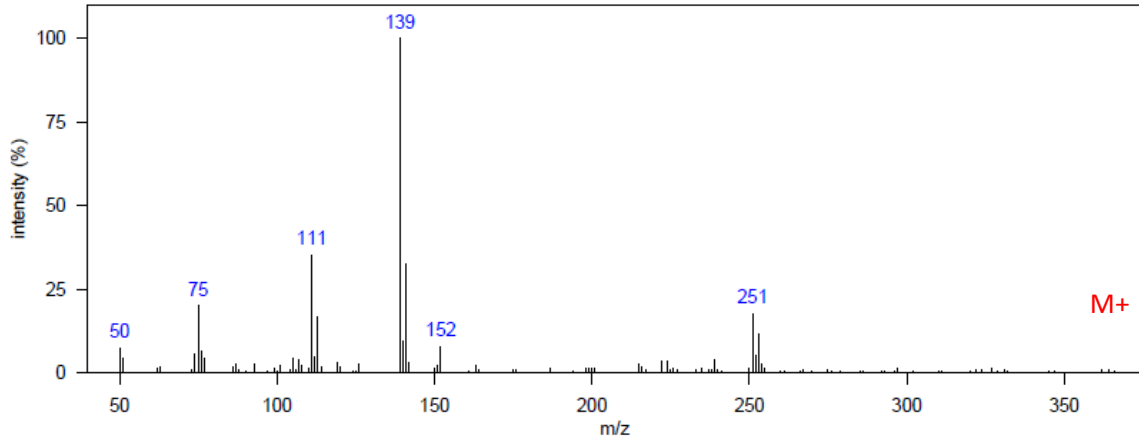
### 4. Mass spectrum of 4,4',4''-TCPMOH standard





## TCPMOH 2

### 1. Mass Spectrum from SoCal dolphin blubber D7:

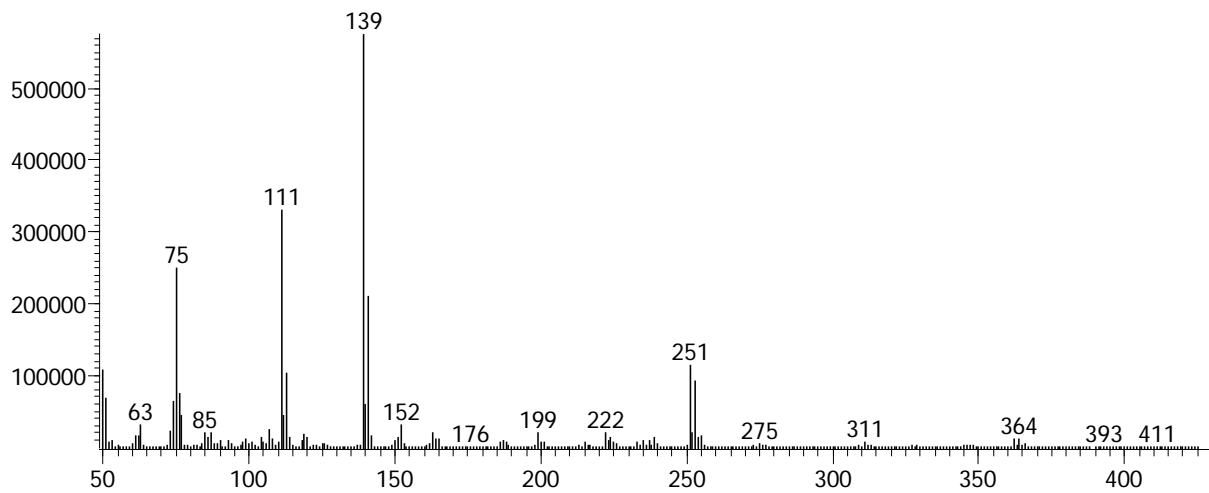


m/z 111: [M-C6H4Cl-C6H4Cl-COH]<sup>+</sup> or C6ClH4<sup>+</sup>  
m/z 139: [M-C6H4Cl-C6H4Cl-H]<sup>+</sup> or C7ClOH4<sup>+</sup>  
m/z 222: [M-C6H4Cl-COH]<sup>+</sup>  
m/z 251: [M-C6H4Cl]<sup>+</sup>  
m/z 362: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1621.42, 1.927

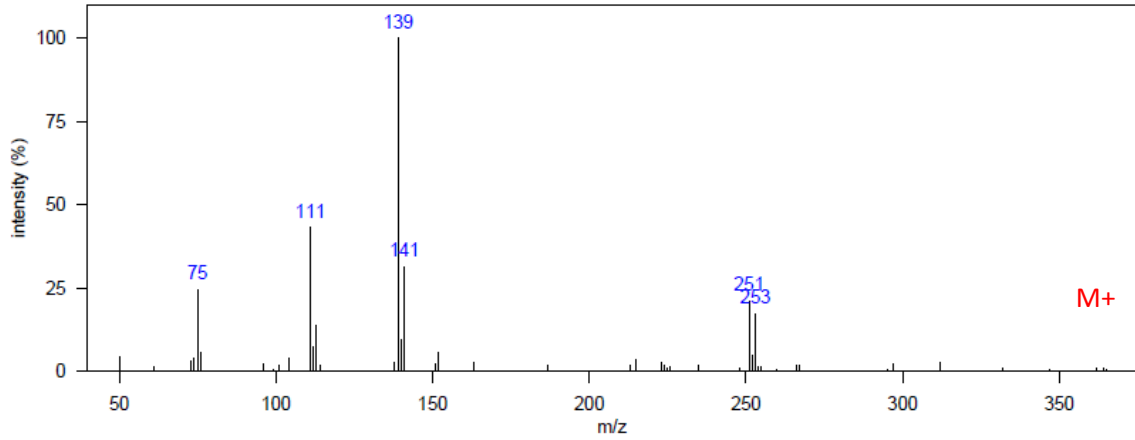
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPMOH standard



### TCPMOH 3

1. Mass Spectrum from SoCal dolphin blubber D7:

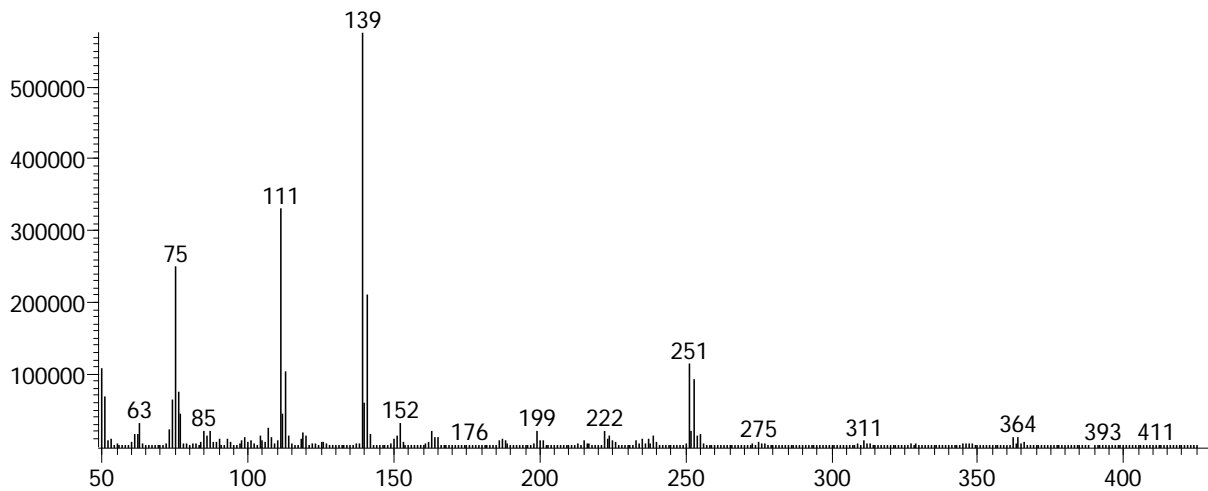


m/z 111: [M-C6H4Cl-C6H4Cl-COH]<sup>+</sup> or C6ClH4<sup>+</sup>  
m/z 139: [M-C6H4Cl-C6H4Cl-H]<sup>+</sup> or C7ClOH4<sup>+</sup>  
m/z 222: [M-C6H4Cl-COH]<sup>+</sup>  
m/z 251: [M-C6H4Cl]<sup>+</sup>  
m/z 362: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1652.9, 2.039

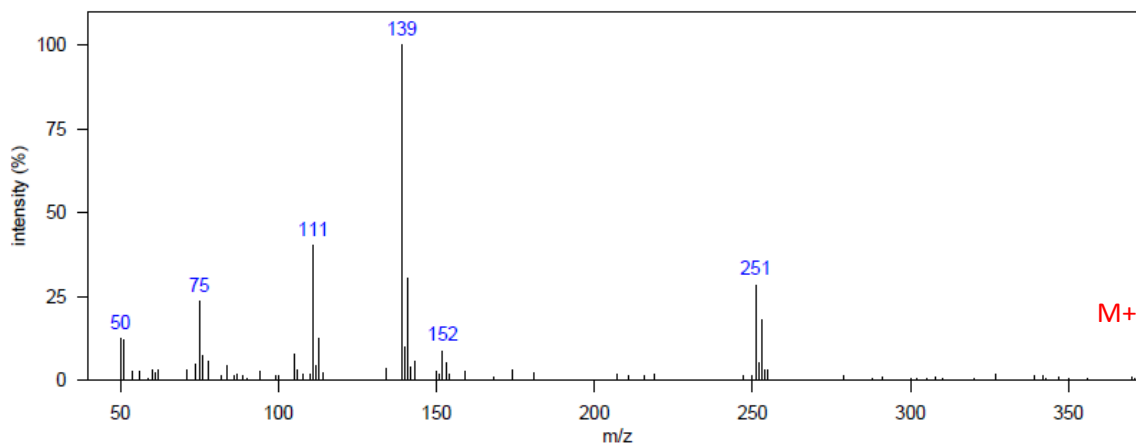
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPMOH standard



## TCPMOH 4

### 1. Mass Spectrum from SoCal dolphin blubber D4:



m/z 111: [M-C6H4Cl-C6H4Cl-COH]<sup>+</sup> or C6ClH4<sup>+</sup>

m/z 139: [M-C6H4Cl-C6H4Cl-H]<sup>+</sup> or C7ClOH4<sup>+</sup>

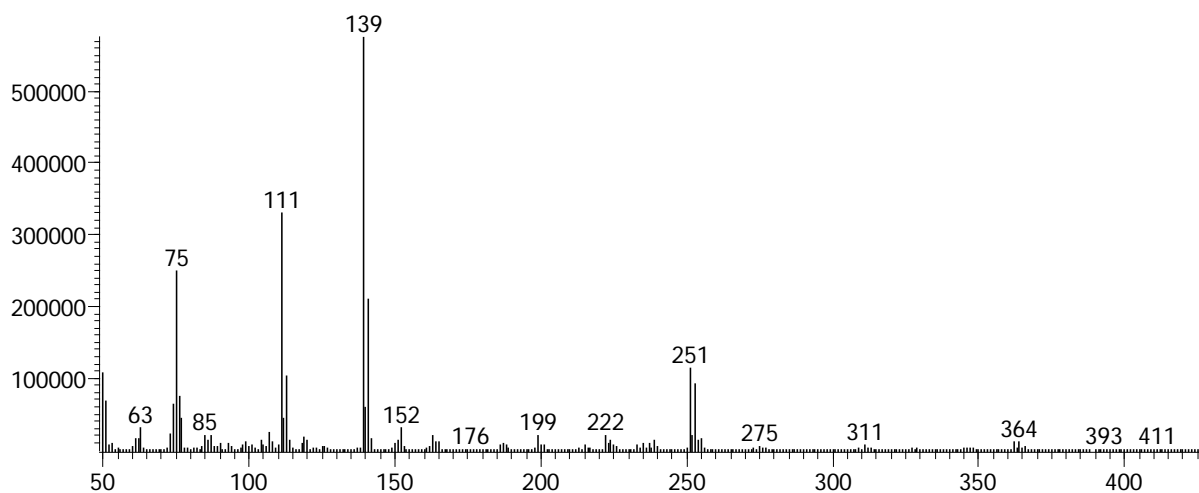
m/z 251: [M-C6H4Cl]<sup>+</sup>

m/z 362: M<sup>+</sup>

### 2. 1D RT, 2D RT (s): 1736.85, 2.099

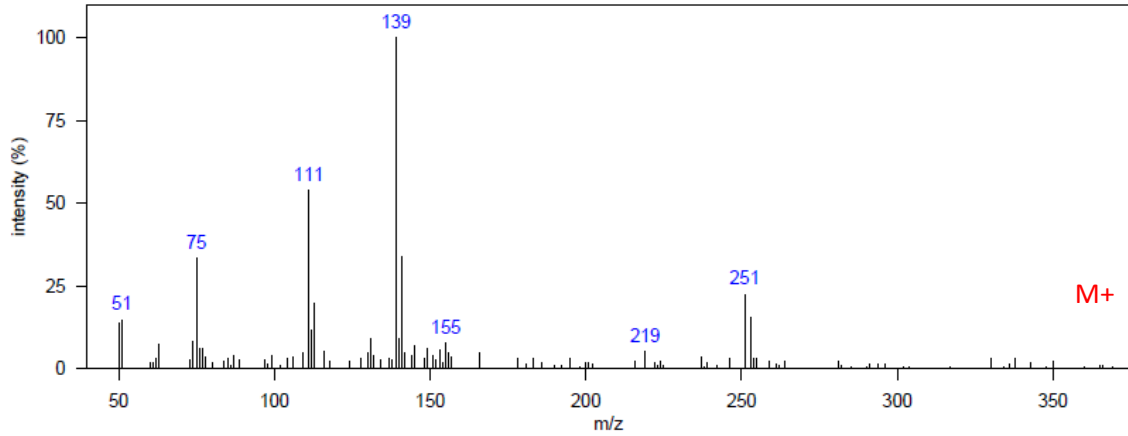
### 3. Identification: [2] Authentic MS (isomer)

### 4. Mass spectrum of 4,4',4''-TCPMOH standard



## TCPMOH 5

### 1. Mass Spectrum from SoCal dolphin blubber D6:



m/z 111:  $[M-C_6H_4Cl-C_6H_4Cl-COH]^+$  or  $C_6ClH_4^+$

m/z 139:  $[M-C_6H_4Cl-C_6H_4Cl-H]^+$  or  $C_7ClOH_4^+$

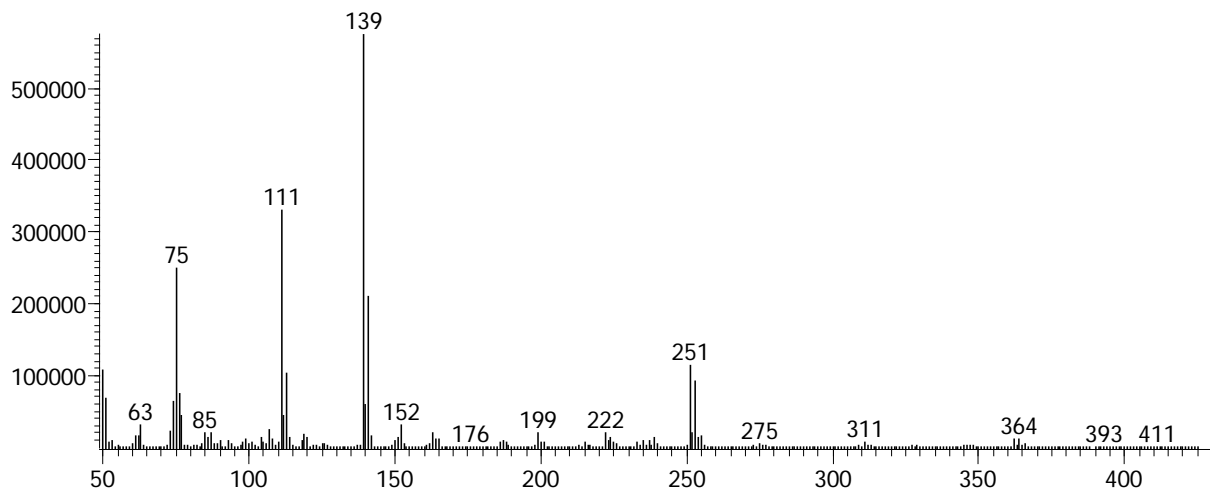
m/z 251:  $[M-C_6H_4Cl]^+$

m/z 362:  $M^+$

2. 1D RT, 2D RT (s): 1747.34, 1.987

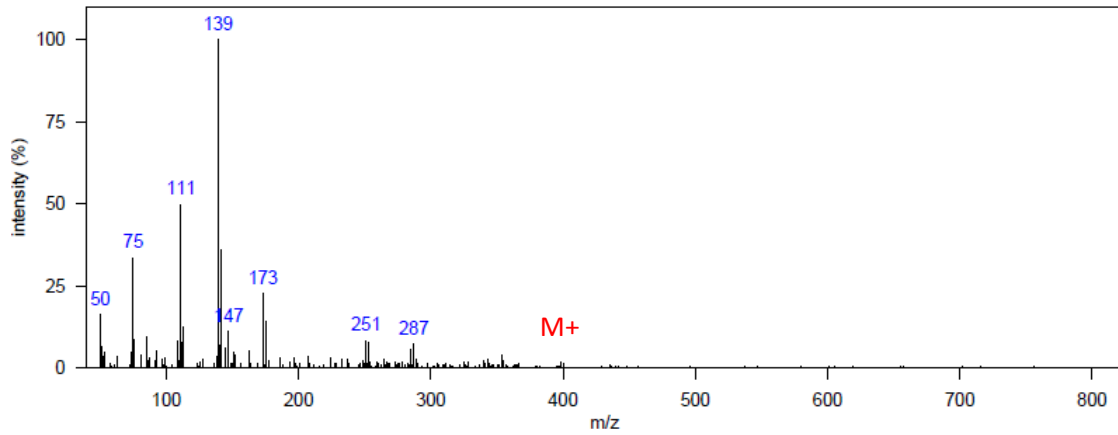
3. Identification: [2] Authentic MS (isomer)

4. Mass spectrum of 4,4',4''-TCPMOH standard



## TCPMOH 4Cl

### 1. Mass Spectrum from SoCal dolphin blubber D6:

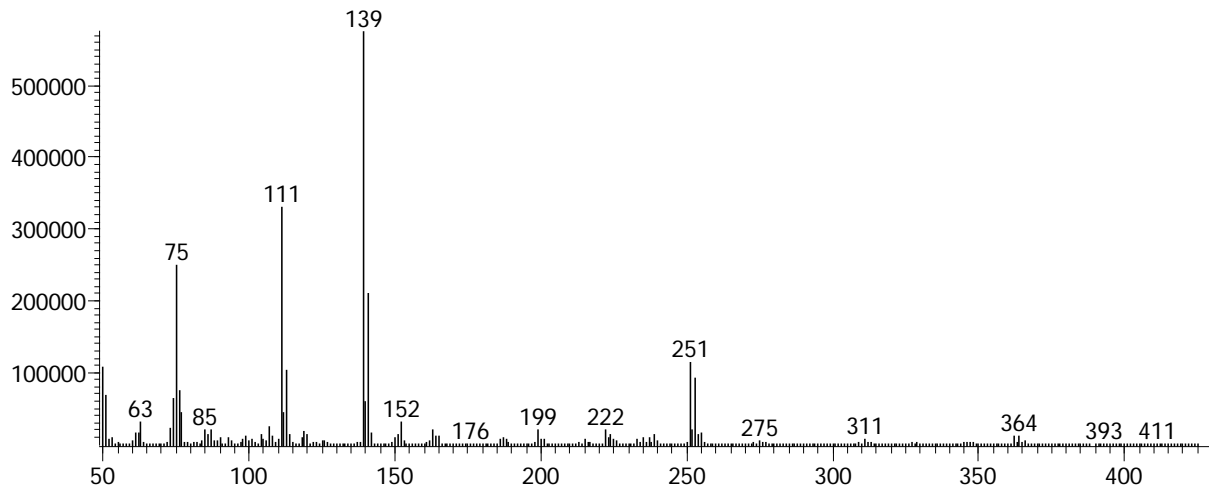


m/z 111: C<sub>6</sub>ClH<sub>4</sub><sup>+</sup>  
m/z 139: C<sub>7</sub>ClO<sub>4</sub>H<sup>+</sup>  
m/z 173: C<sub>7</sub>Cl<sub>2</sub>O<sub>3</sub>H<sup>+</sup>  
m/z 251: [M-C<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>]<sup>+</sup>  
m/z 285: [M-C<sub>6</sub>H<sub>4</sub>Cl]<sup>+</sup>  
m/z 396: M<sup>+</sup>

2. 1D RT, 2D RT (s): 1775.33, 2.066

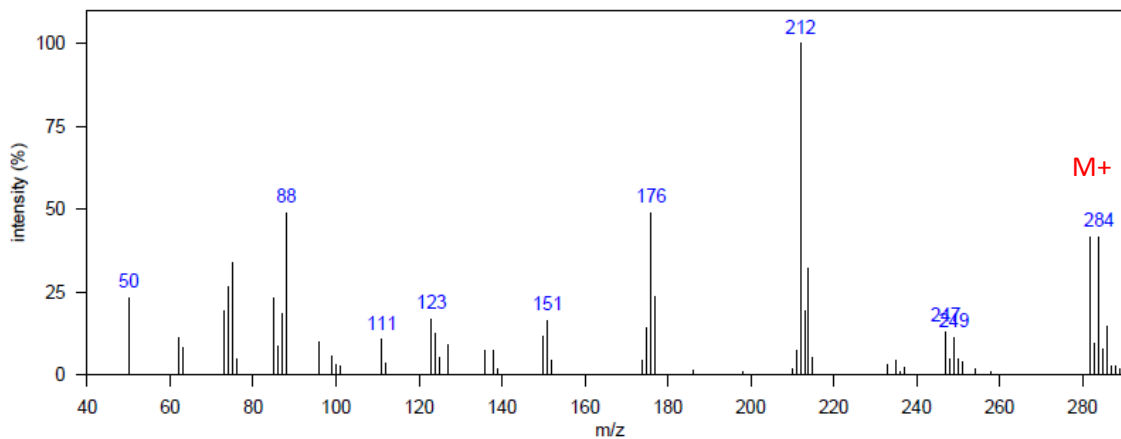
3. Identification: [4] Congener MS

4. Mass spectrum of 4,4',4''-TCPMOH standard



## DDT related 1

### 1. Mass Spectrum from SoCal dolphin blubber D4:

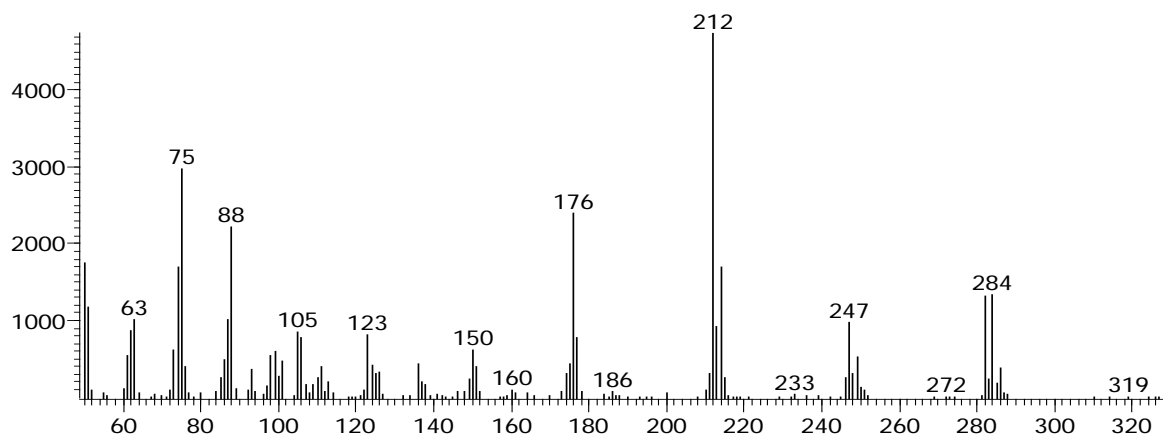


### 2. 1D RT, 2D RT (s): 1453.51, 1.069

Its RT deviated from the other DDE-like compounds so it was not identified as DDMU.

### 3. Identification: [3] Found in the DDT technical mixture/identical mass spectrum with p,p'-DDMU

### 4. Mass spectrum of the compound in the DDT technical mixture



### 5. Mass spectrum of p,p'-DDMU

