Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Reductive Dechlorination of Endosulfan Isomers and its Metabolites by Zero-Valent Metals: Reaction Mechanism and Degradation Products

by

Swatantra P. Singh [a†] and Purnendu Bose [a*]

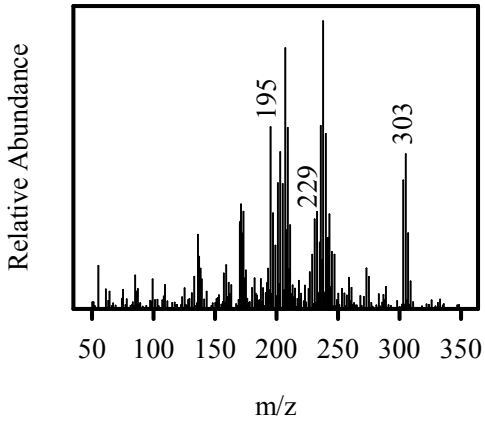
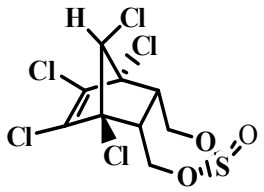
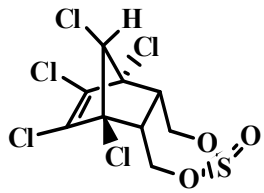
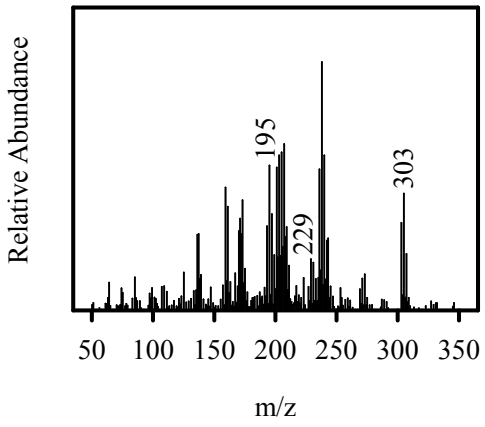
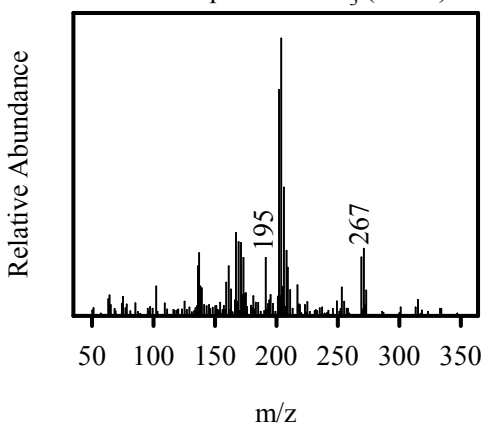
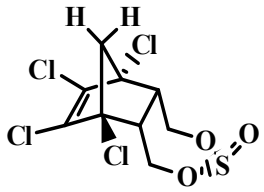
[a] Department of Civil Engineering, Indian Institute of Technology Kanpur-208016, India

[†Present Address] Department of Desalination and Water Treatment, Zuckerberg Institute of Water Research

Ben-Gurion University of Negev, Sede-Boqer-89990, Israel

Supplementary data has 17 pages (S1-S17), 7 Figures. (S1-S8), and 7 tables (S1-S7).

Table SI.1 Reductive dechlorination of ES-1 by NZVI: degradation products.

<table>
<tr>
<td>Mass Spectra: ES-1_1 (25.40)
 
</td>
<td rowspan="2">Proposed Chemical Structure of ES-1_1/ES-1_2
 
OR
  </td>
</tr>
<tr>
<td>Mass Spectra: ES-1_2 (26.65)
 
</td>
</tr>
<tr>
<td>Mass Spectra: ES-1_3 (23.95)
 
</td>
<td>Proposed Chemical Structure of ES-1_3
  </td>
</tr>
</table>

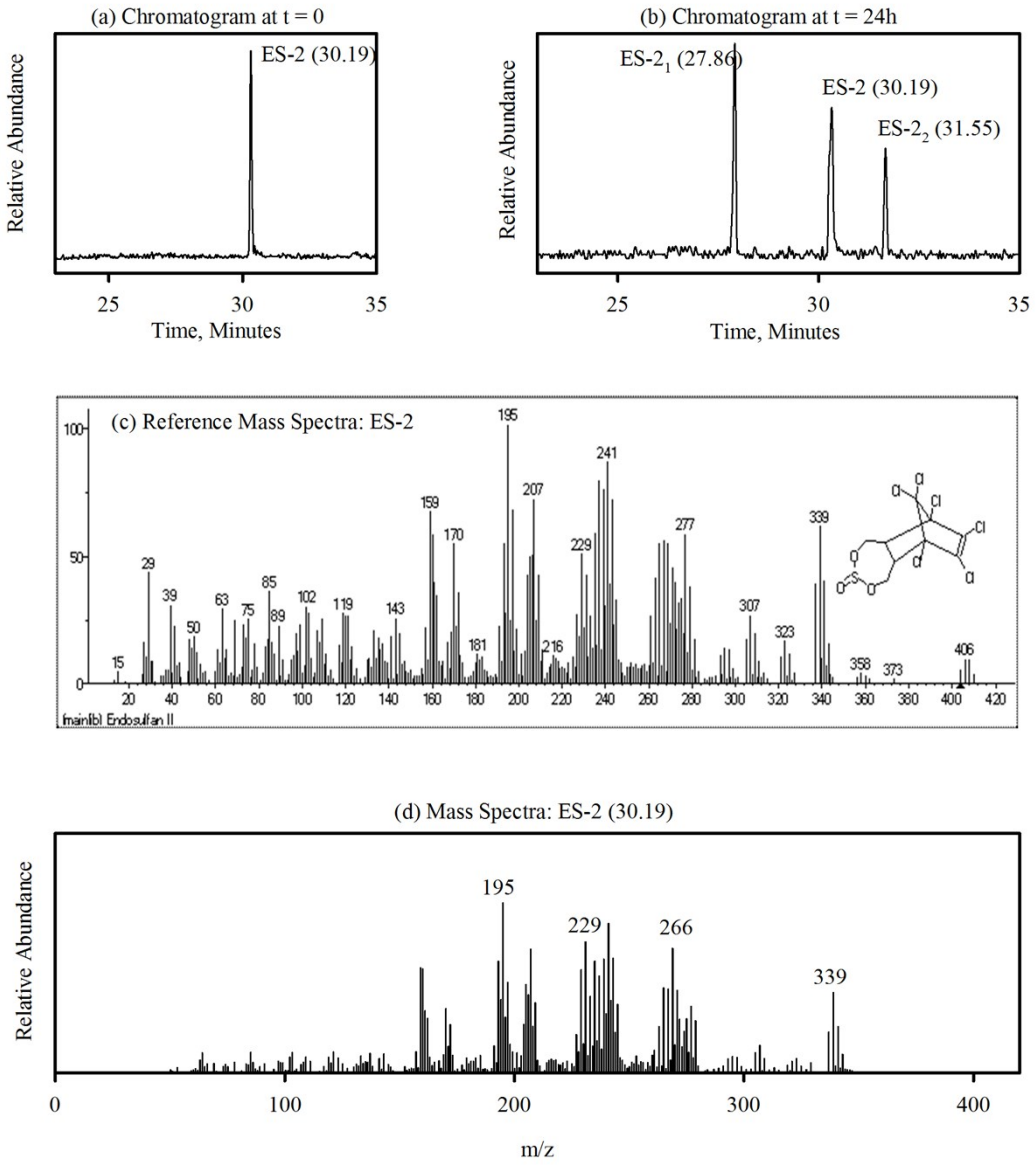
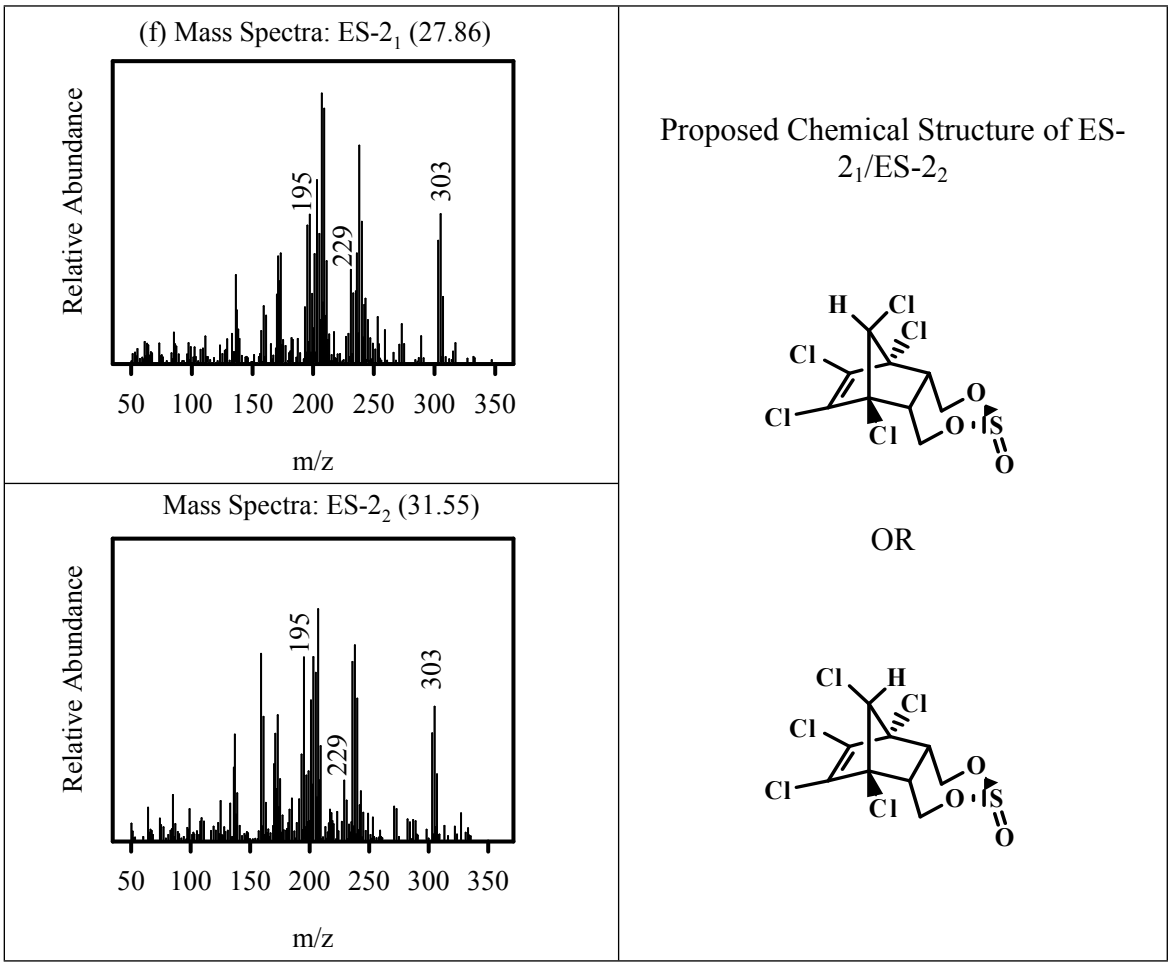


Fig. SI.1. Reductive dechlorination of ES-2 by NZVI.
a) Chromatogram at, t = 0; b) Chromatogram at, t = 24 h
c) Mass Spectra of ES-2 from NIST Library
d) Mass Spectra of ES-2 obtained in the Present Study

Table SI.2 Reductive dechlorination of ES-2 by NZVI: degradation products.



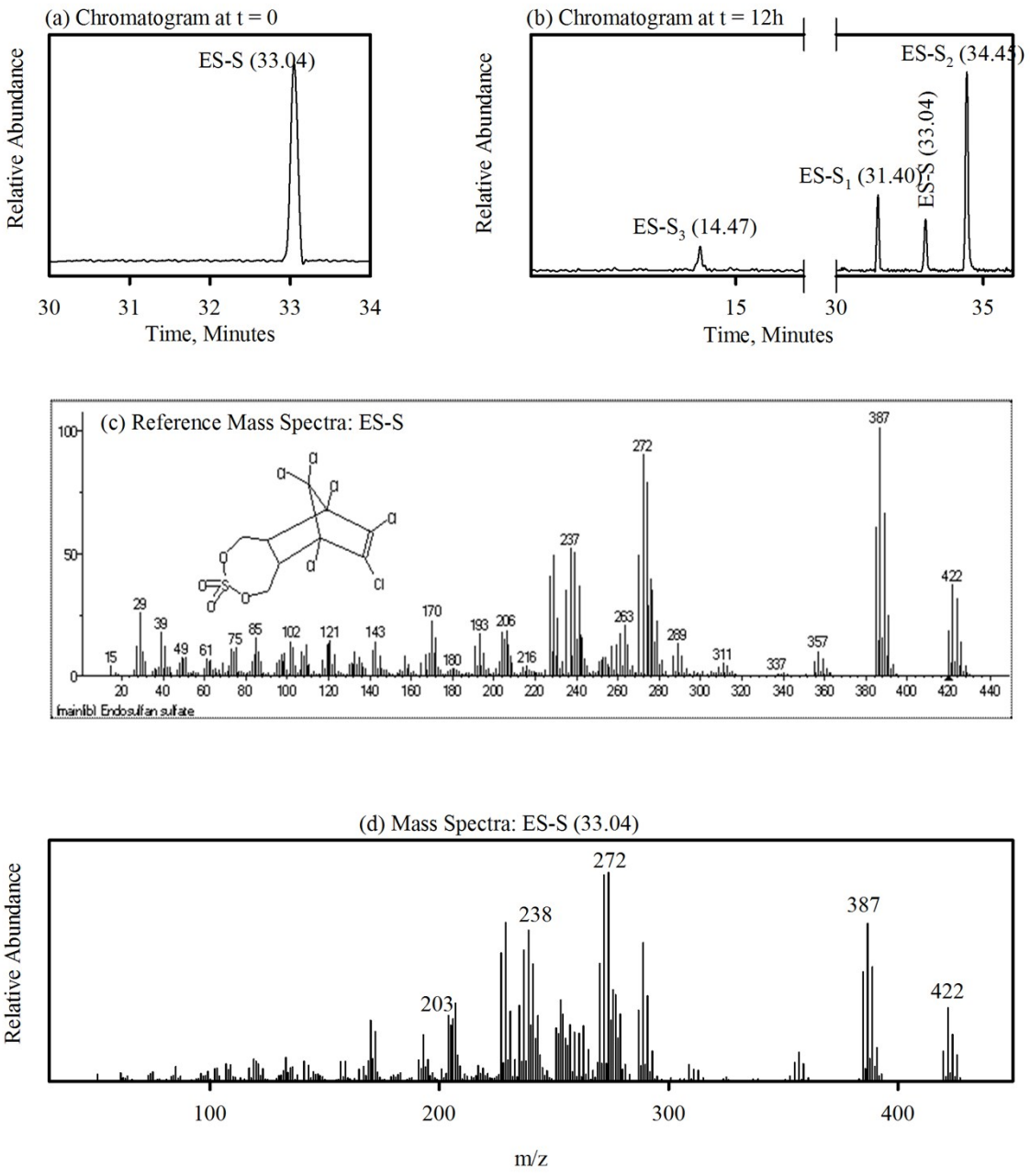
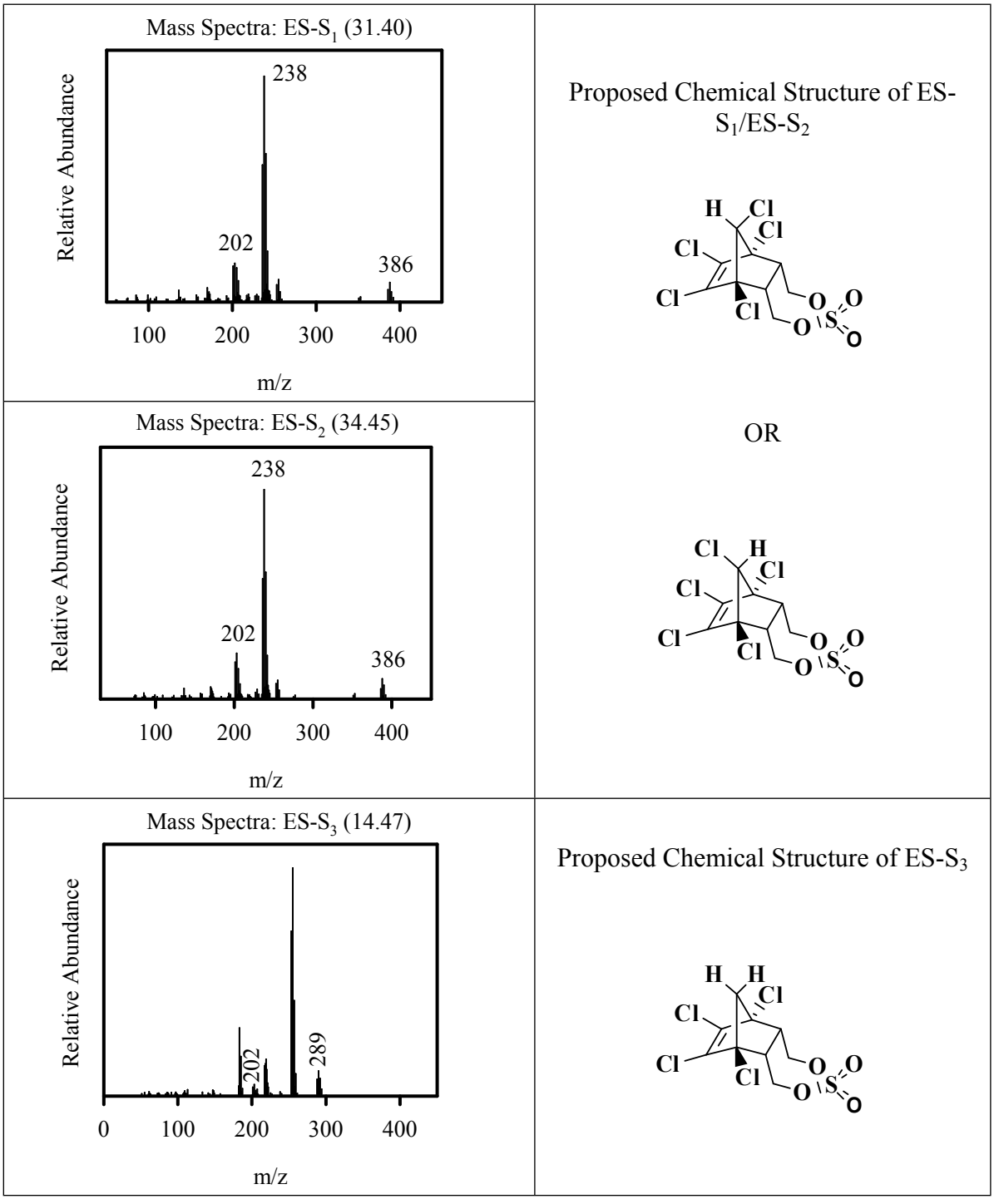


Fig. SI.2. Reductive dechlorination of ES-S by NZVI.
a) Chromatogram at, t = 0; b) Chromatogram at, t = 12 h
c) Mass Spectra of ES -S from NIST Library
d) Mass Spectra of ES -S obtained in the Present Study

Table SI.3 Reductive dechlorination of ES-S by NZVI: degradation products



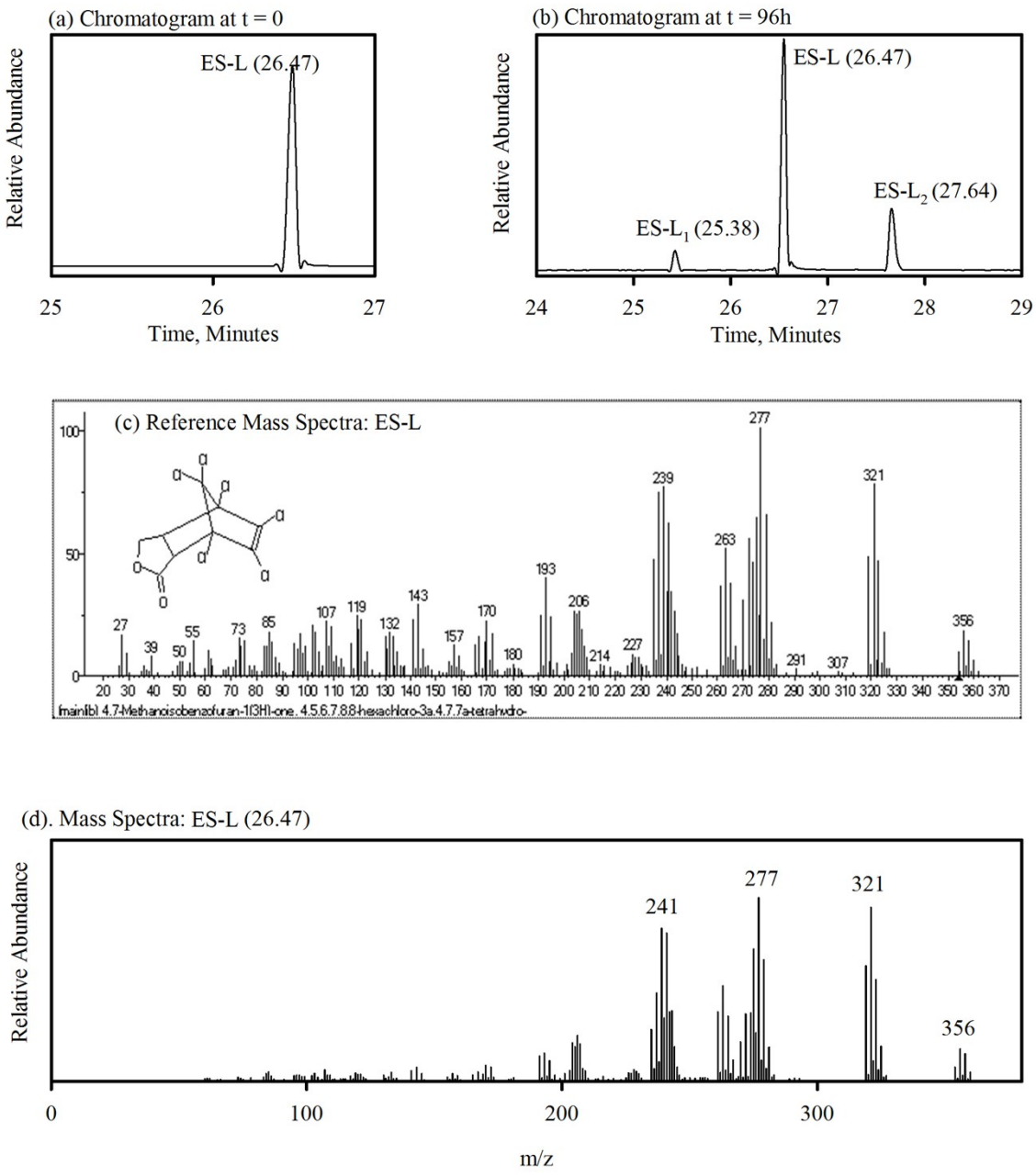
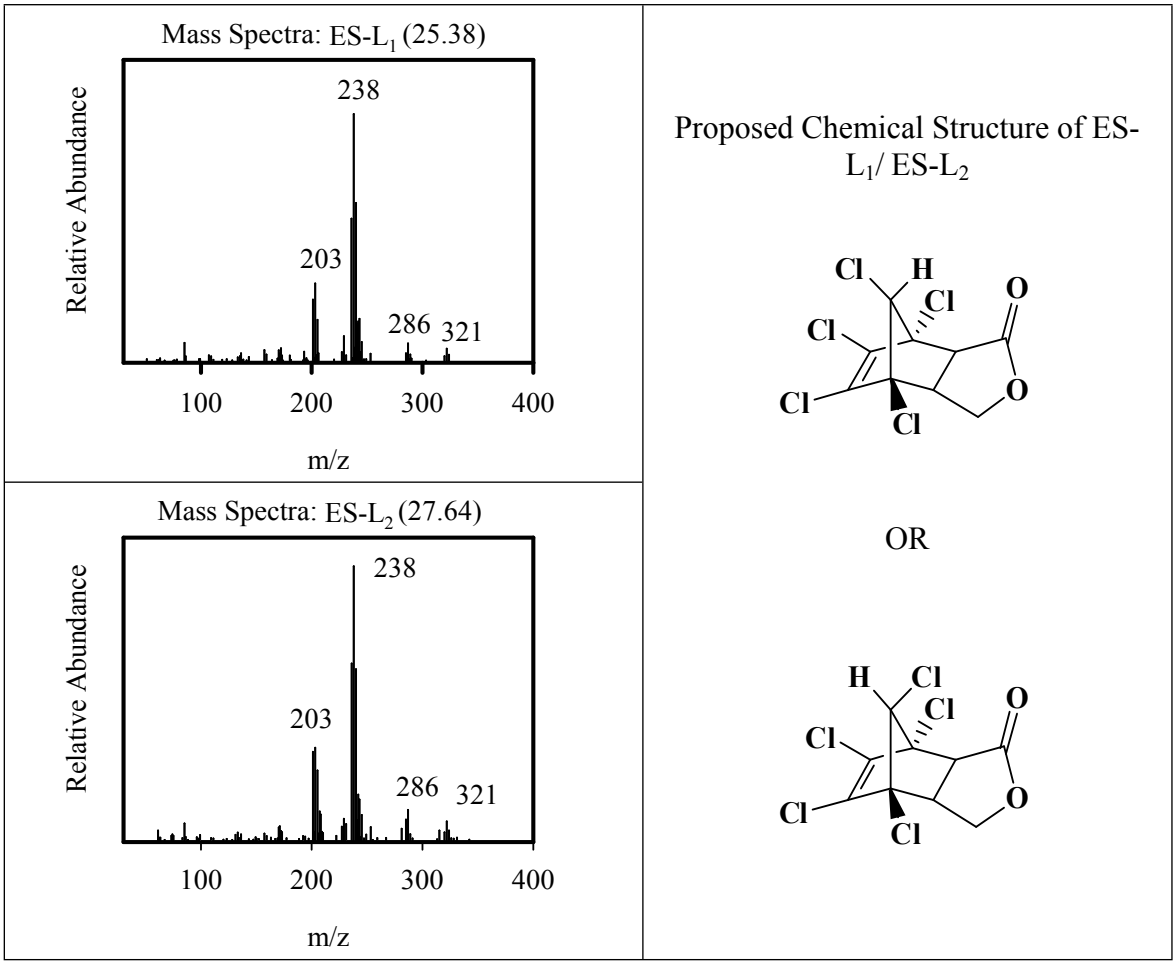


Fig. SI.3. Reductive dechlorination of ES-L by NZVI.
a) Chromatogram at, t = 0; b) Chromatogram at, t = 96 h
c) Mass Spectra of ES -L from NIST Library
d) Mass Spectra of ES -L obtained in the Present Study

Table SI.4 Reductive dechlorination of ES -L by NZVI: degradation products.



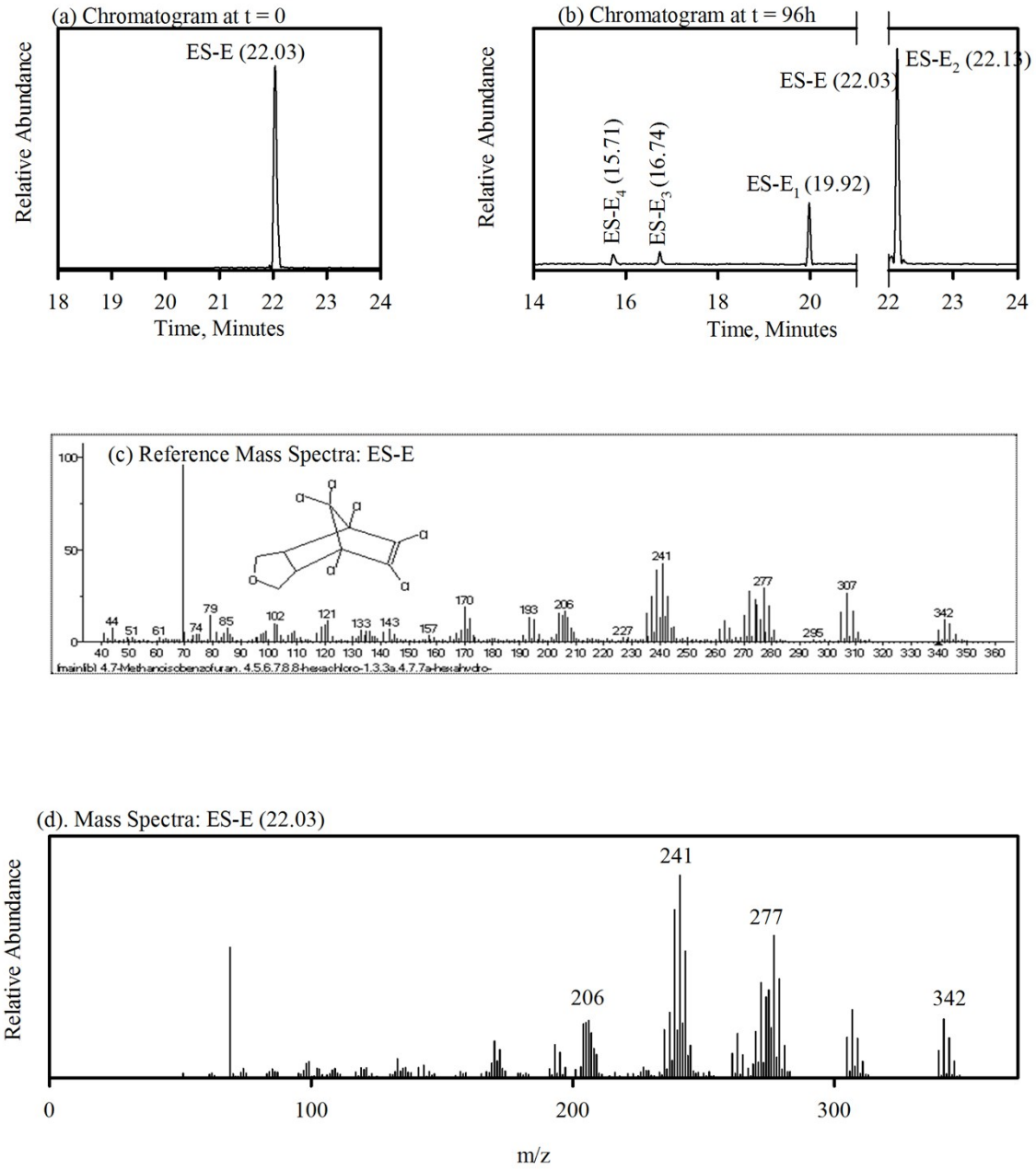
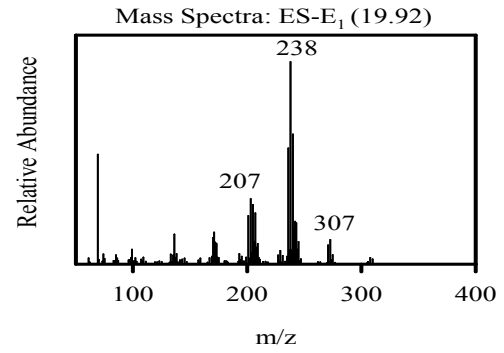
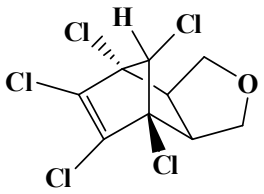
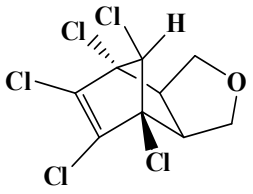
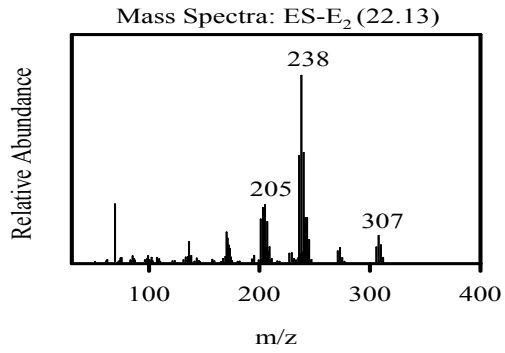
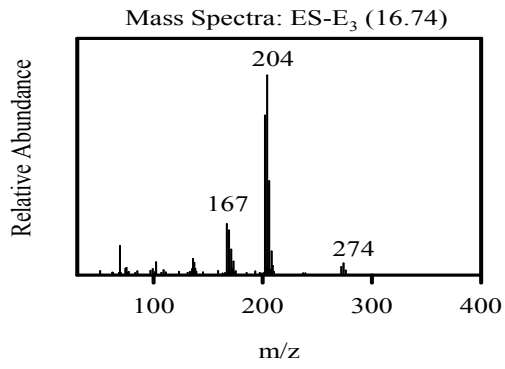
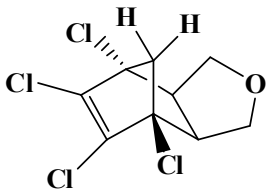
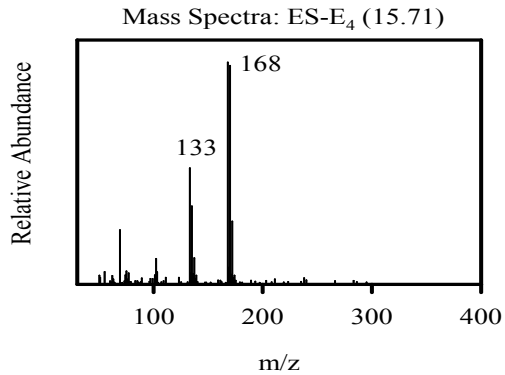
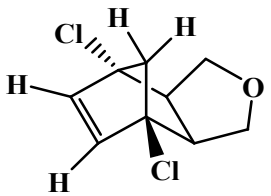


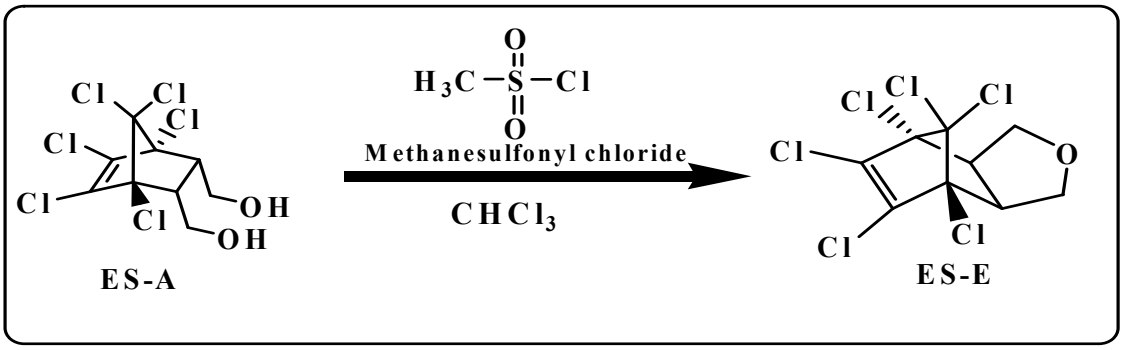
Fig. SI.4. Reductive dechlorination of ES-E by NZVI.
a) Chromatogram at, t = 0; b) Chromatogram at, t = 96 h
c) Mass Spectra of ES -E from NIST Library
d) Mass Spectra of ES -E obtained in the Present Study

Table SI.5 Reductive dechlorination of ES -E by NZVI: degradation products.

<table>
<tr>
<td> 
</td>
<td rowspan="2">Proposed Chemical Structure of ES-E1/ES-E2
 

OR
 
</td>
</tr>
<tr>
<td> 
</td>
</tr>
<tr>
<td> 
</td>
<td>Proposed Chemical Structure of ES-E3
 
</td>
</tr>
<tr>
<td> 
</td>
<td>Proposed Chemical Structure of ES-E4
 
</td>
</tr>
</table>

(a) Derivitization of ES-A



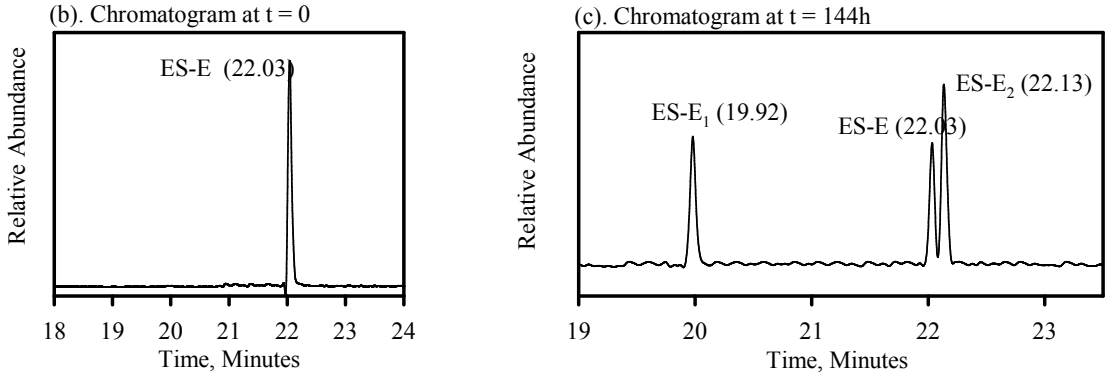


Fig. SI.5. Reductive dechlorination of ES-A by NZVI.
a) Derivatization procedure
b) Chromatogram at, t = 0; c) Chromatogram at, t = 144 h

Table SI.6 Reductive dechlorination of ES -E by Mg^0: degradation products.

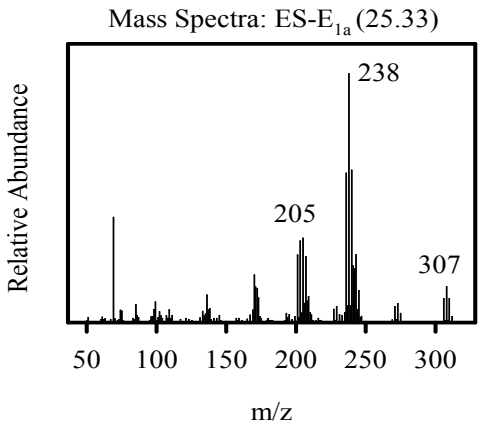
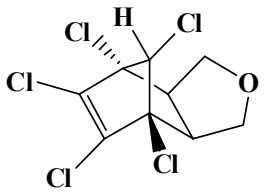
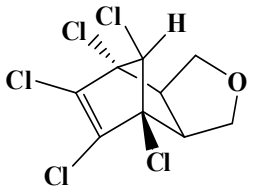
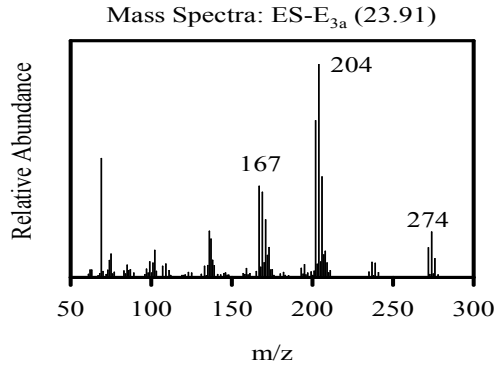
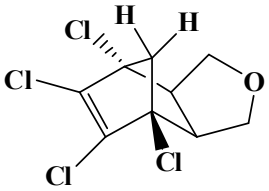
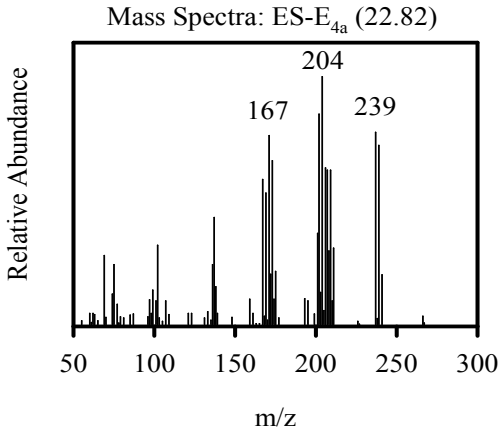
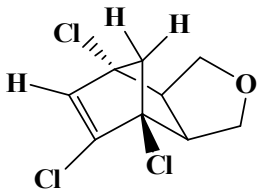
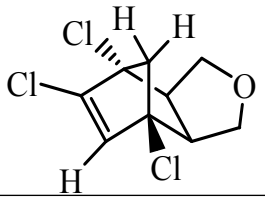
	Proposed Chemical Structure of ES-E_{1a}/ES-E_{2a}  OR 
	Proposed Chemical Structure of ES-E_{3a} 
	Proposed Chemical Structure of ES-E_{4a}  OR 

Table SI.6 (Cont.). Reductive dechlorination of ES-E by Mg^0: degradation products.

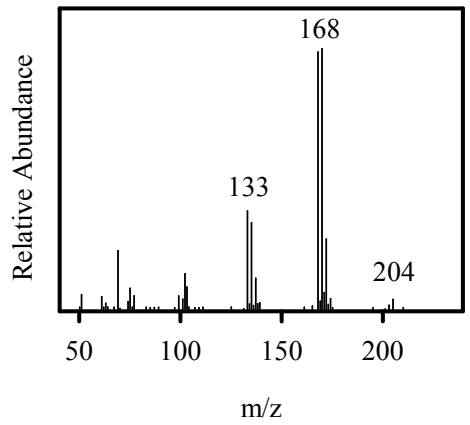
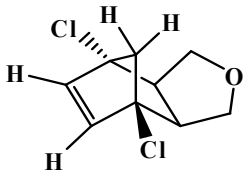
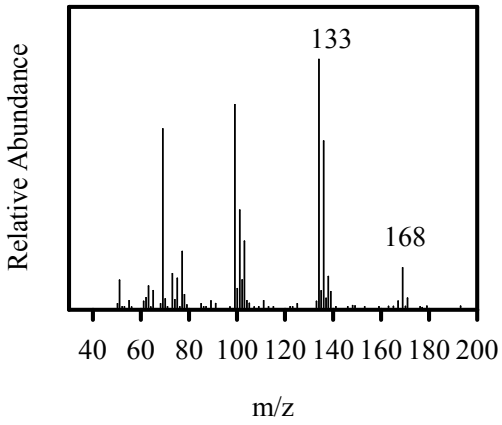
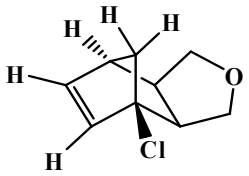
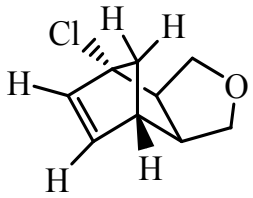
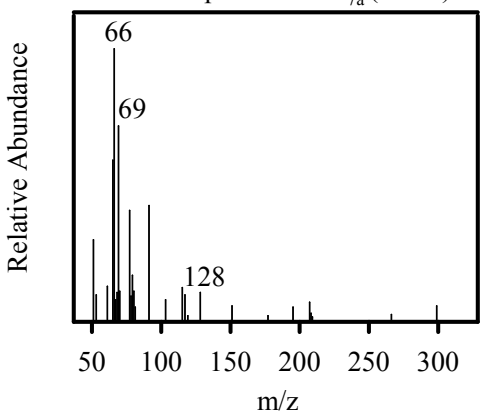
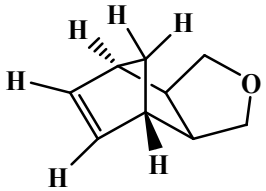
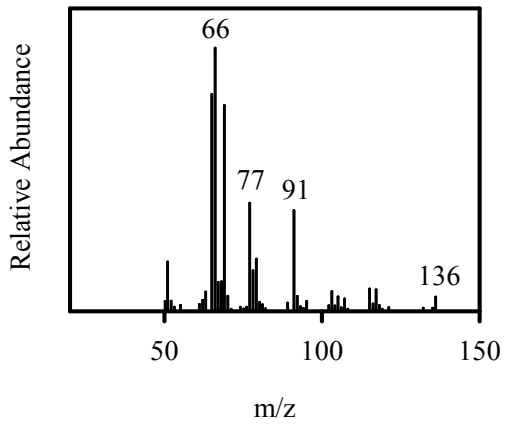
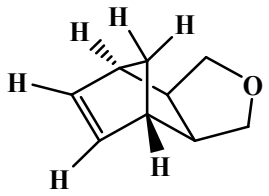
Mass Spectra: ES-E_{5a} (21.11)  	Proposed Chemical Structure for ES-E_{5a} 
Mass Spectra: ES-E_{6a} (19.84)  	Proposed Chemical Structure for ES-E_{6a}  **OR** 
Mass Spectra: ES-E_{7a} (16.08)  	Proposed Chemical Structure for ES-E_{7a} Endo-4-xoatricyclo[5.2.1.0(2.6)]dec-8-ene (confirmed by NIST library: (CAS No.: 1528-23-0 NIST No.: 105262 

Table SI.7. Reductive Dechlorination of ES -E by Na^0: Degradation Products

Mass Spectra: ES-E_7 (16.08)  	Chemical Structure for ES-E_{7b}  Endo-4-xoatricyclo[5.2.1.0(2.6)]dec-8-ene (confirmed by NIST library: (CAS No.: 1528-23-0 NIST No.: 105262)

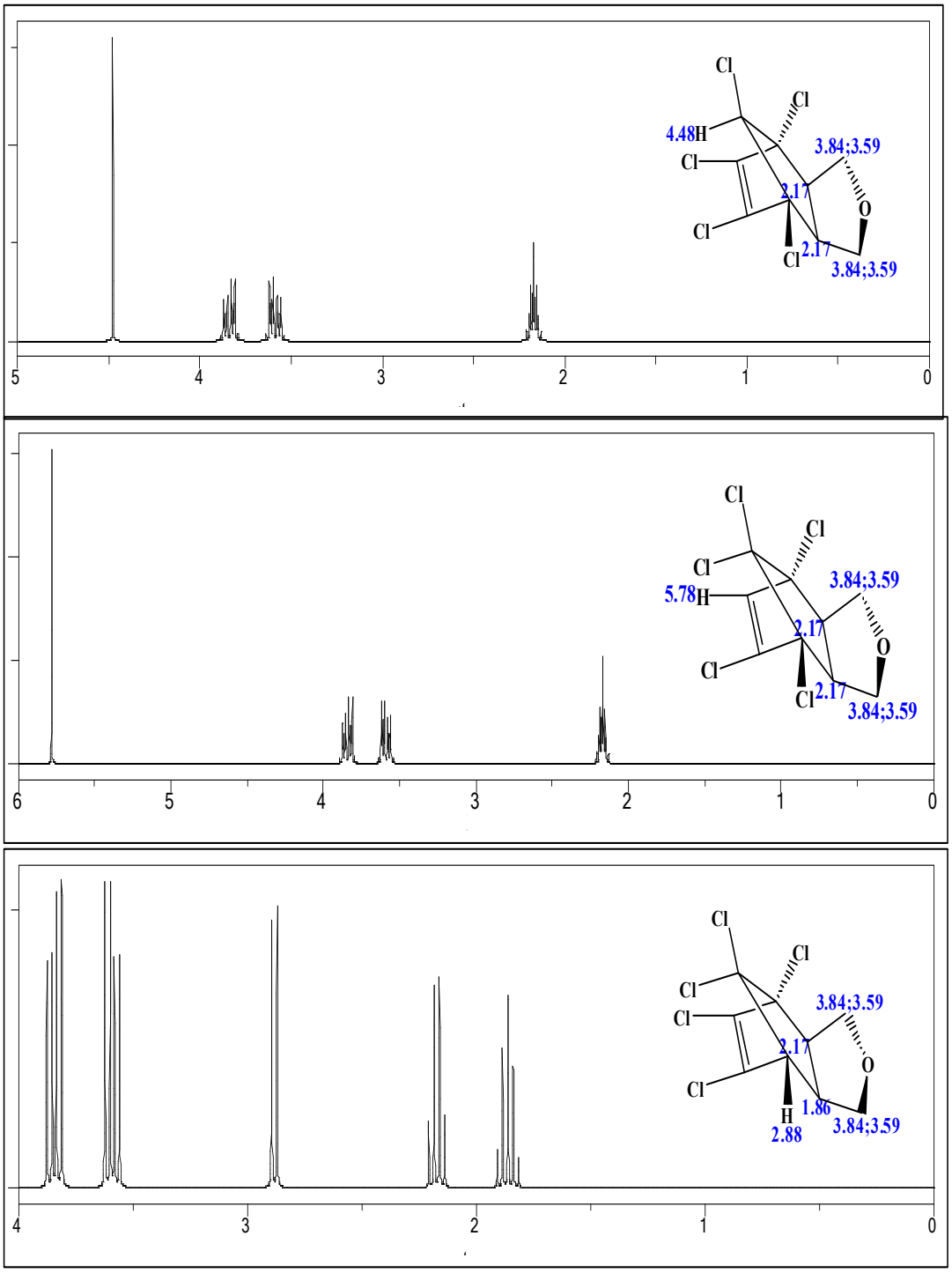


Fig. SI.6. Theoretical 1H-NMR of dechlorinated ES-E molecules.

(a) Dechlorination at position-1
(b) Dechlorination at position -2
(c) Dechlorination at position -3

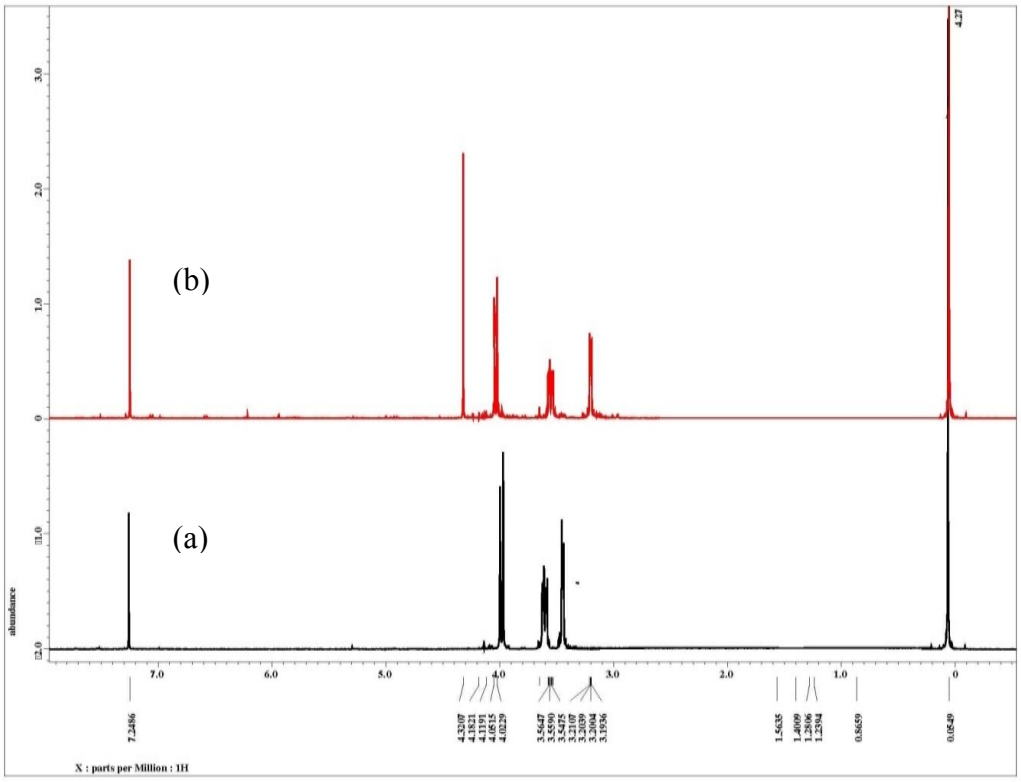


Fig. SI.7. Experimental ^{1}H-NMR for ES-E_{1a}
(a) ES –E; (b) Dechlorinated ES -E

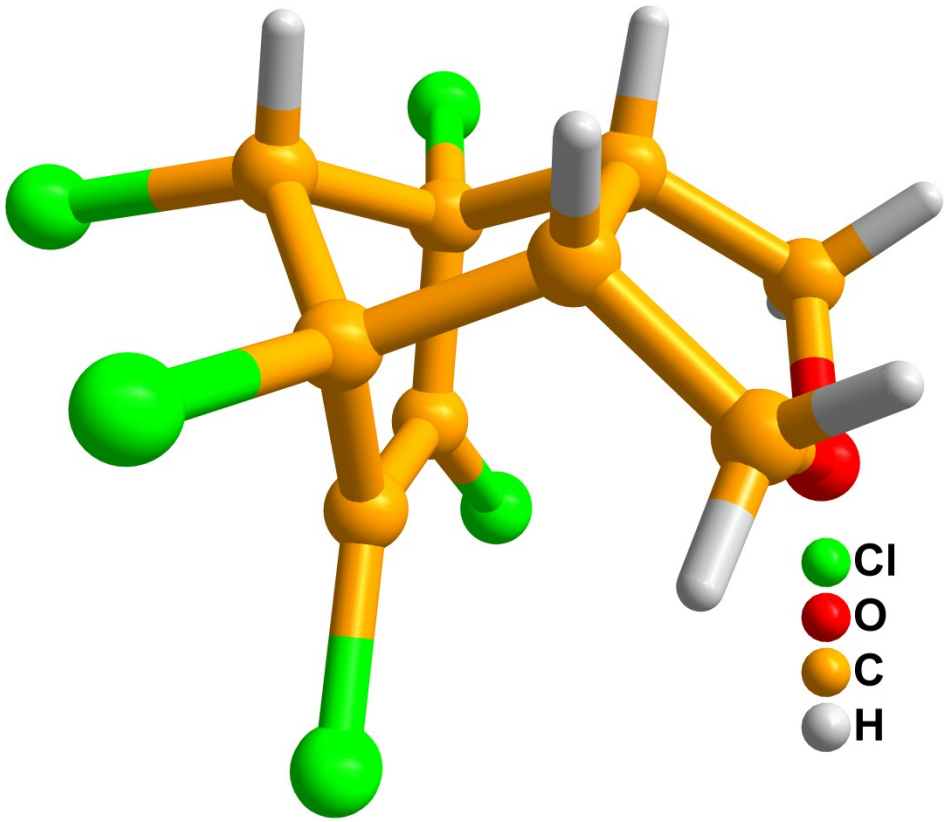


Fig. SI.8. X-ray crstalographic images (Diamond 3.2g) of dechlorinated ES-E_{1a} molecules.

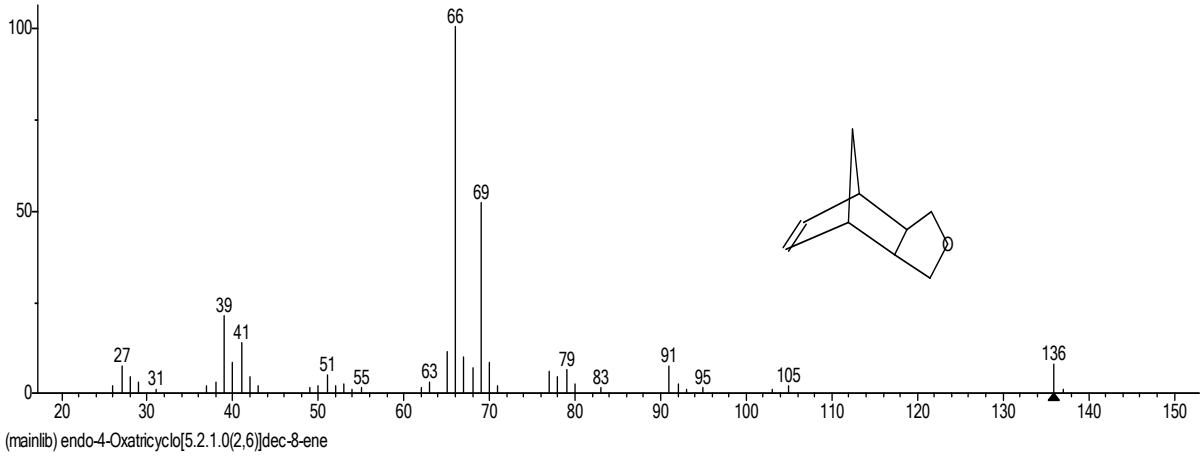


Fig. SI.9 Mass Spectra of Endo-4-xoatricyclo[5.2.1.0(2.6)]dec-8-ene from NIST Library.