

## Supporting Information for

# Oxidative Degradation of Decabromodiphenyl Ether (BDE 209) by Potassium Permanganate: Reaction Pathways, Kinetics, and Mechanisms Assisted with DFT Calculations

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Shaogui Yang<sup>\*</sup>, Zunyao Wang<sup>\*</sup>

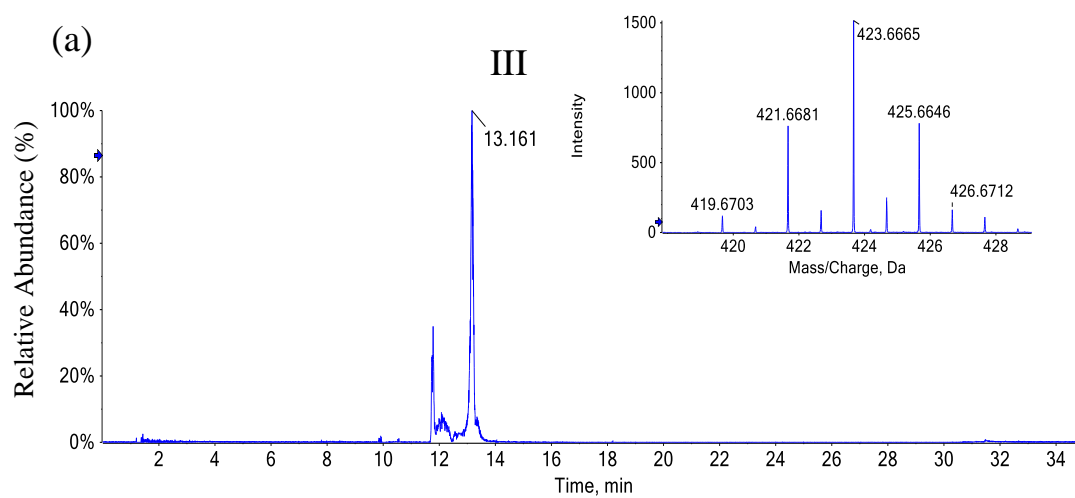
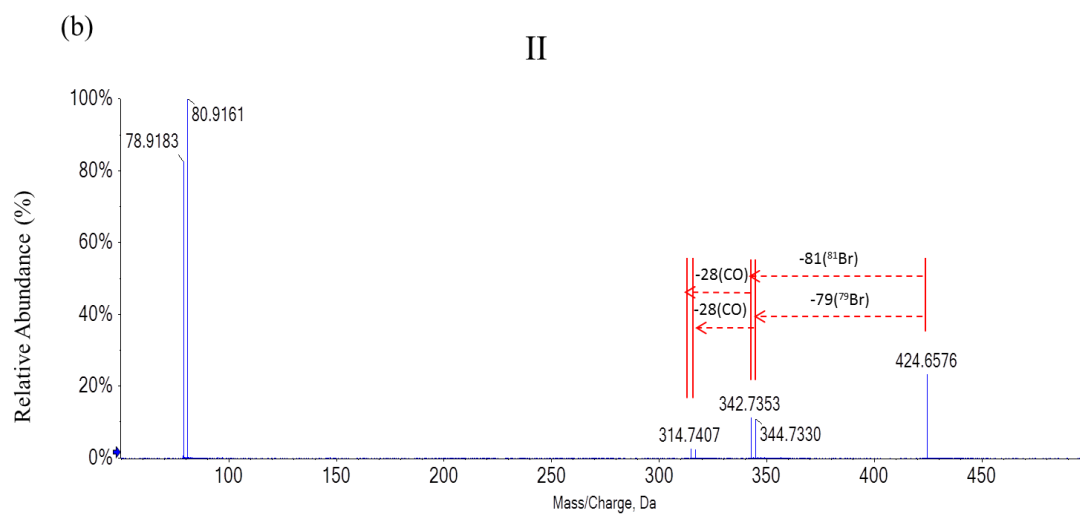
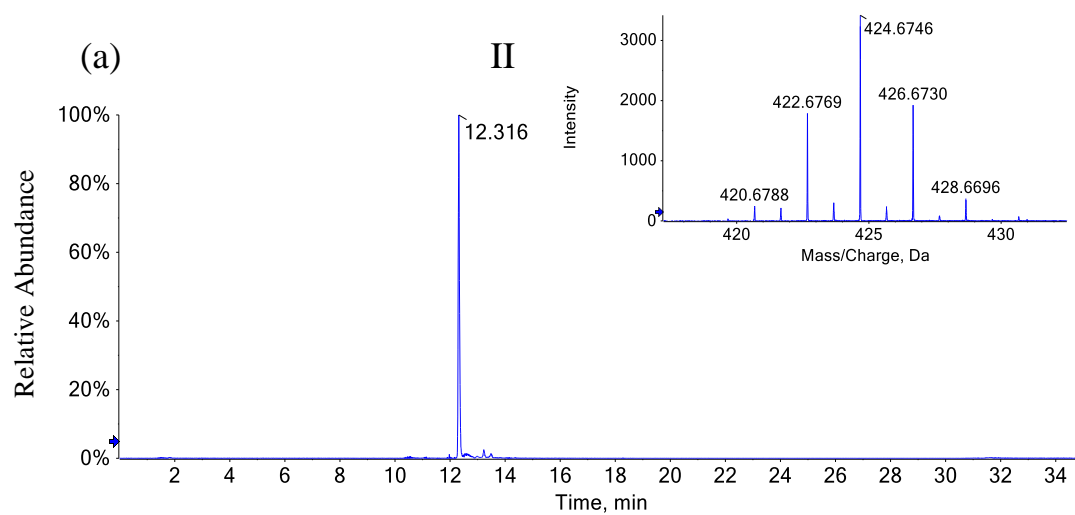
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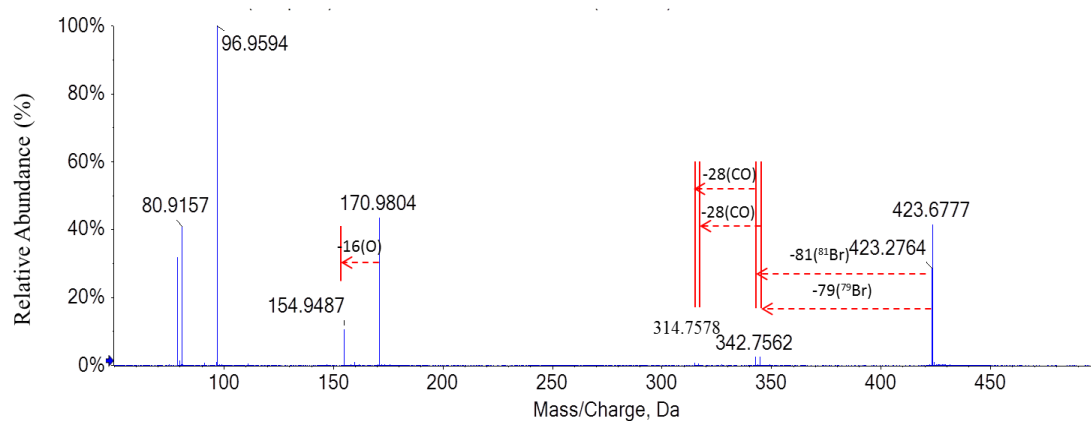
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This file of 17 pages contained 4 figures.



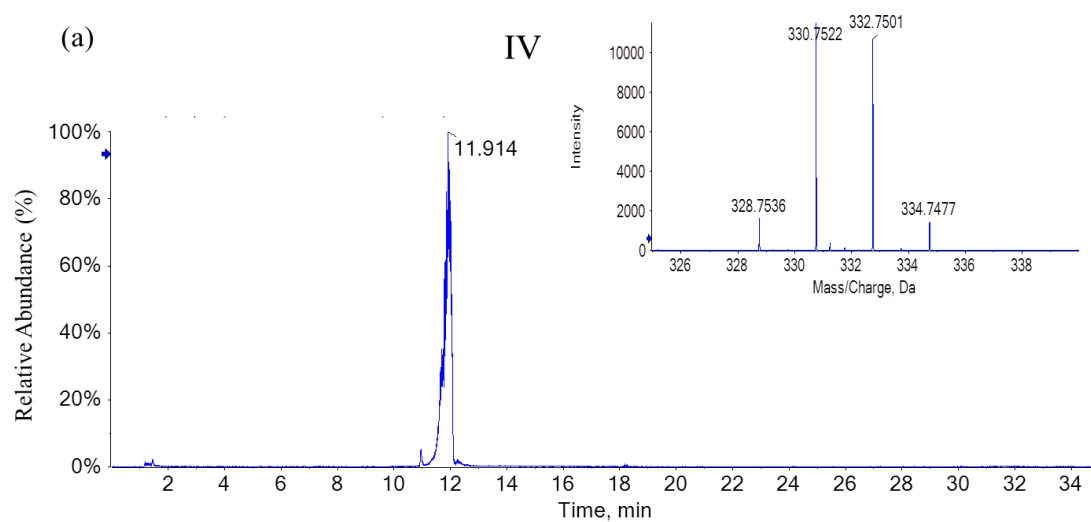
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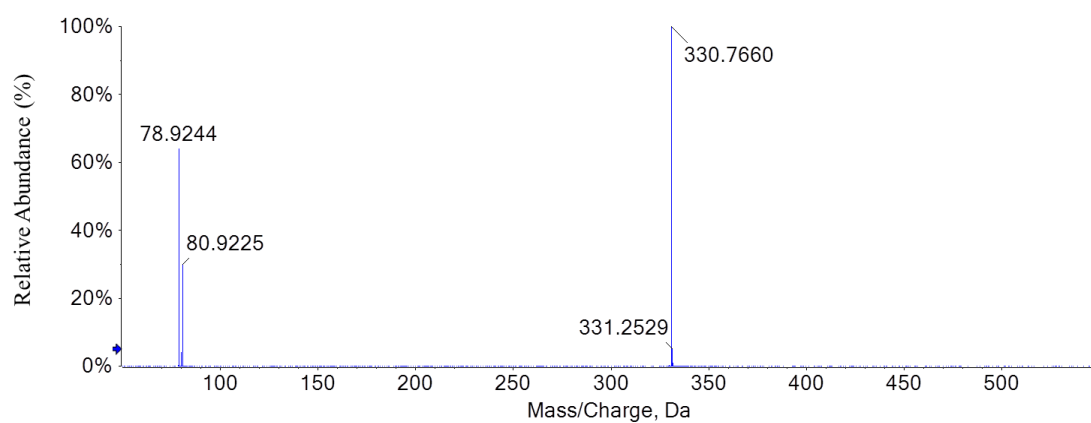
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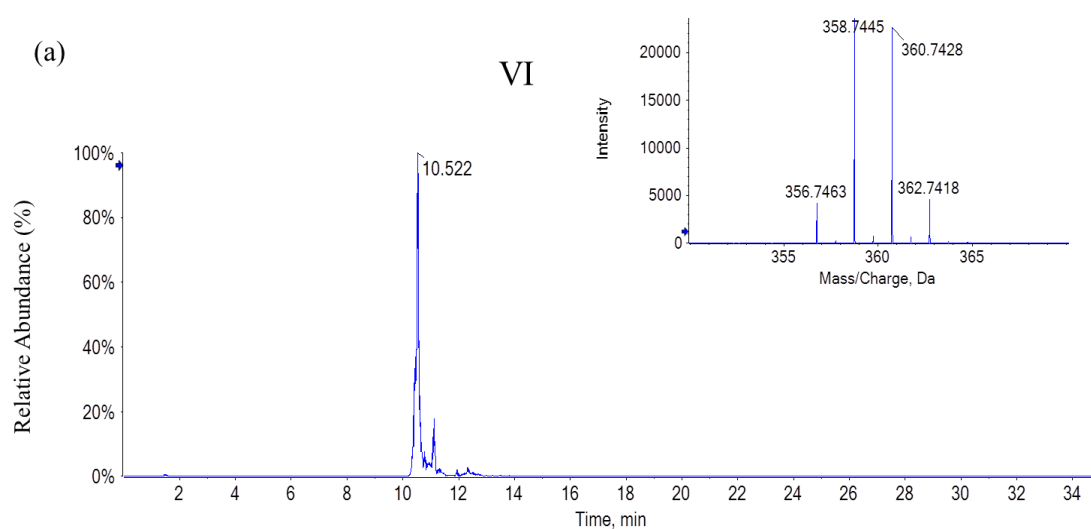
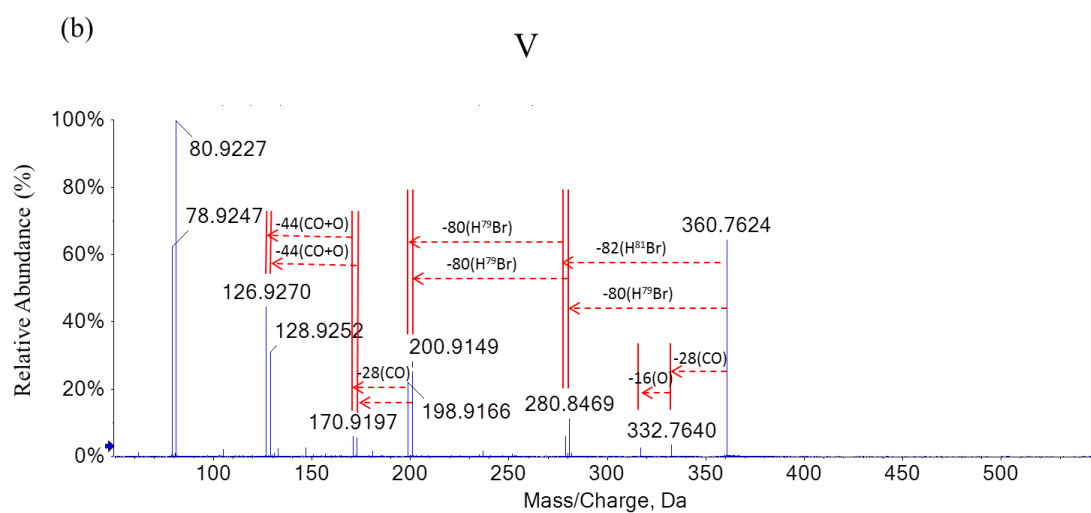
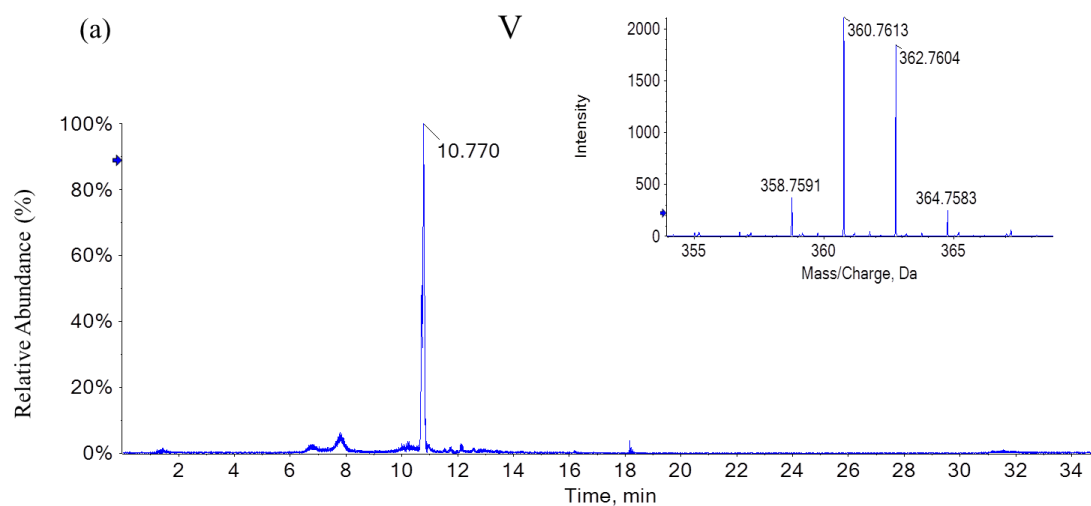
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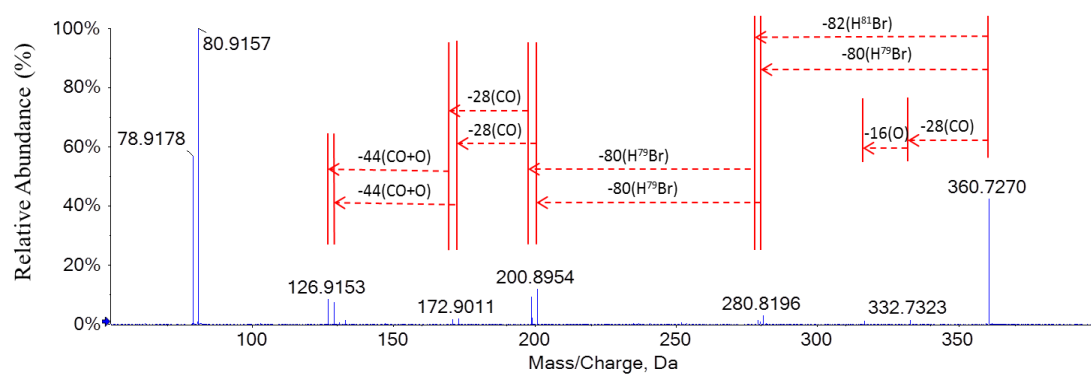
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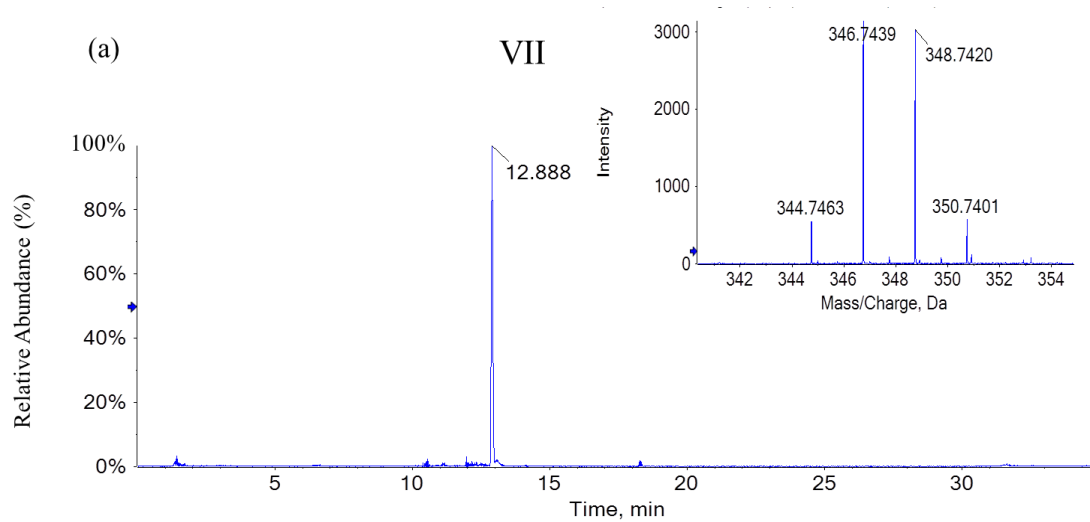
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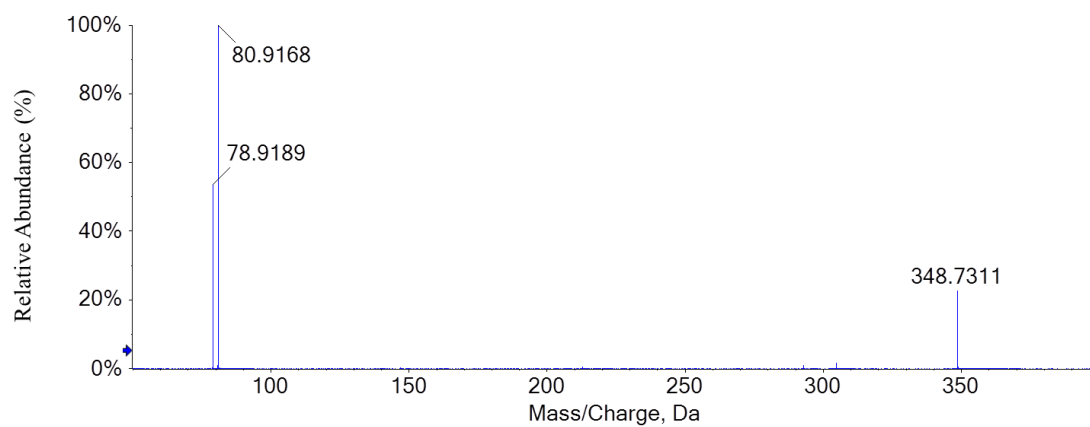
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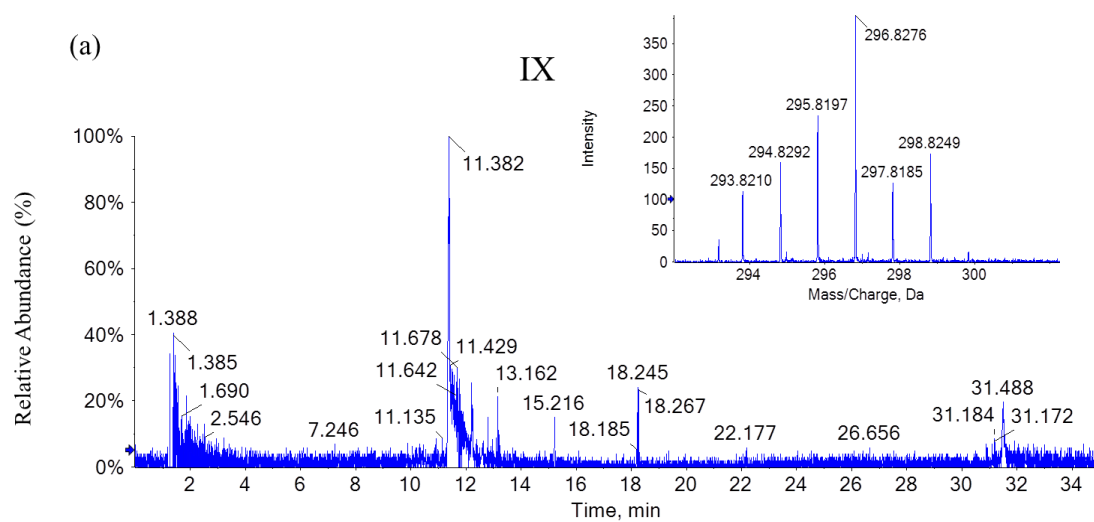
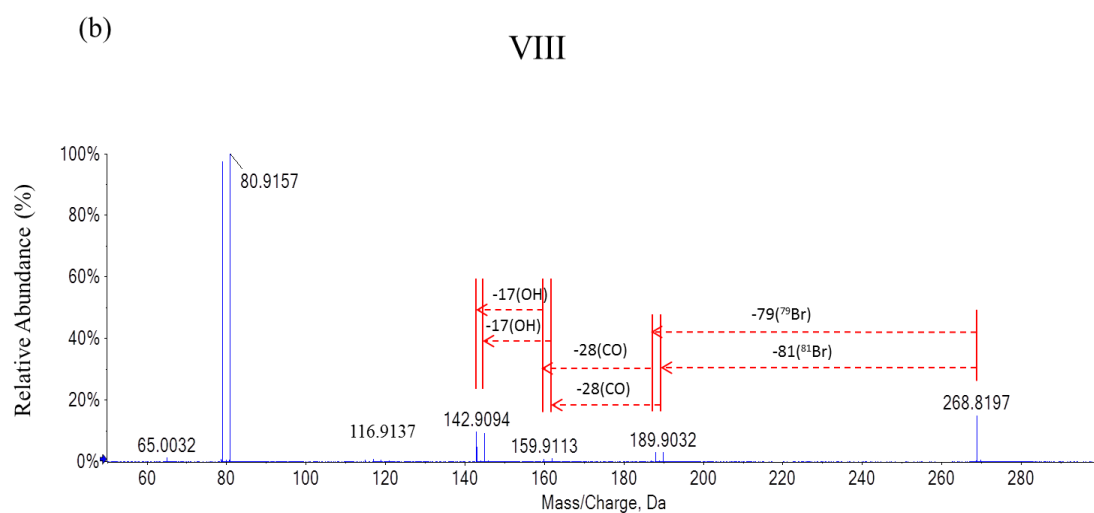
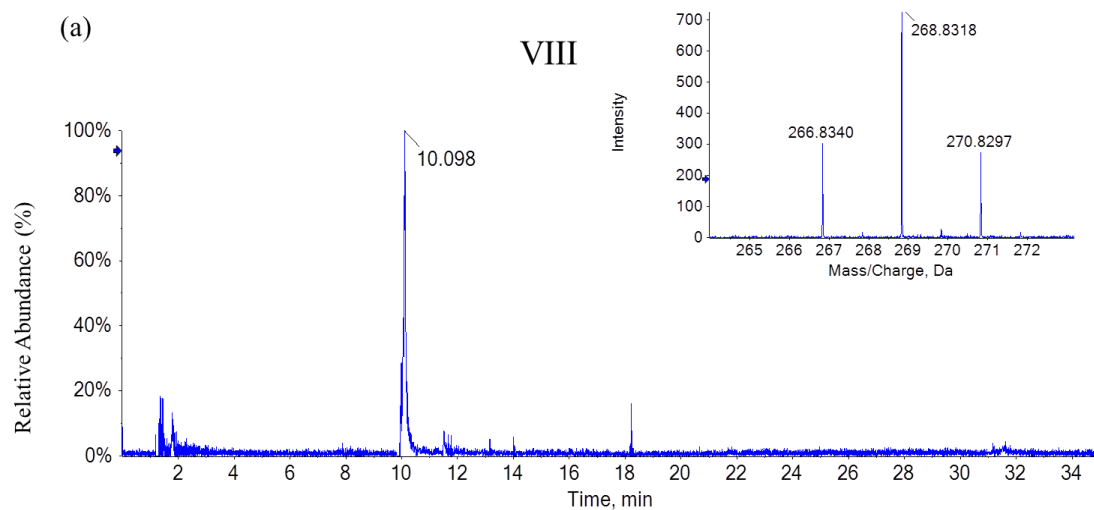
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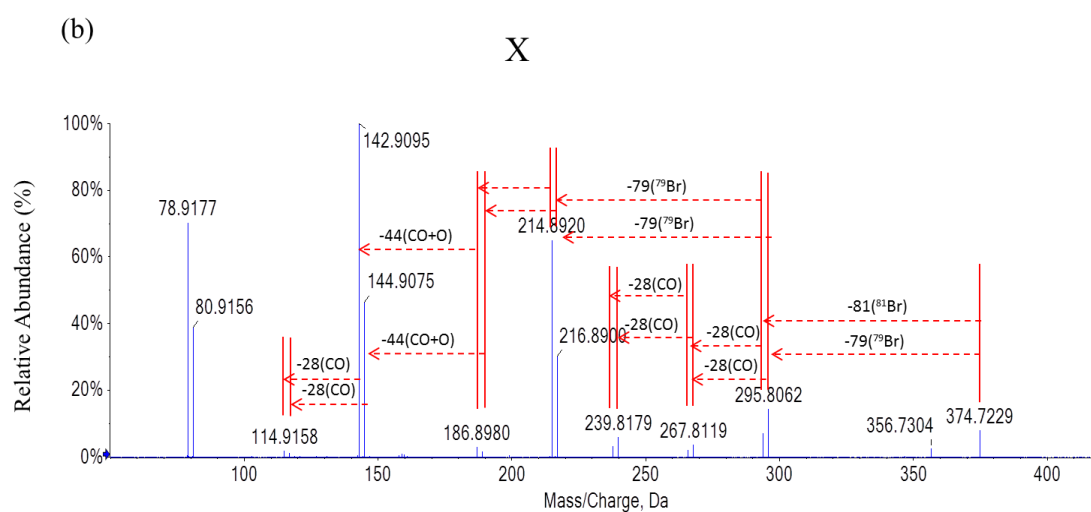
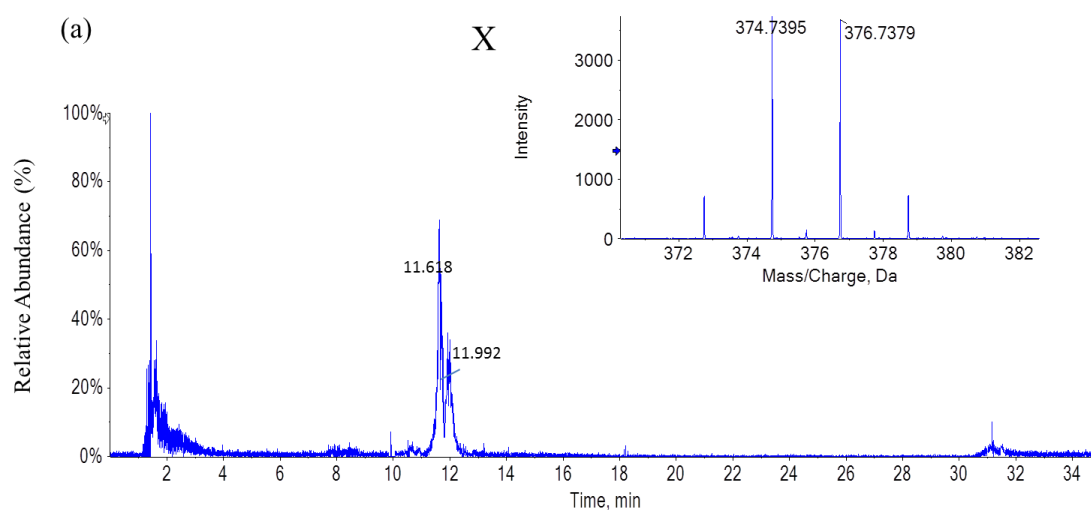
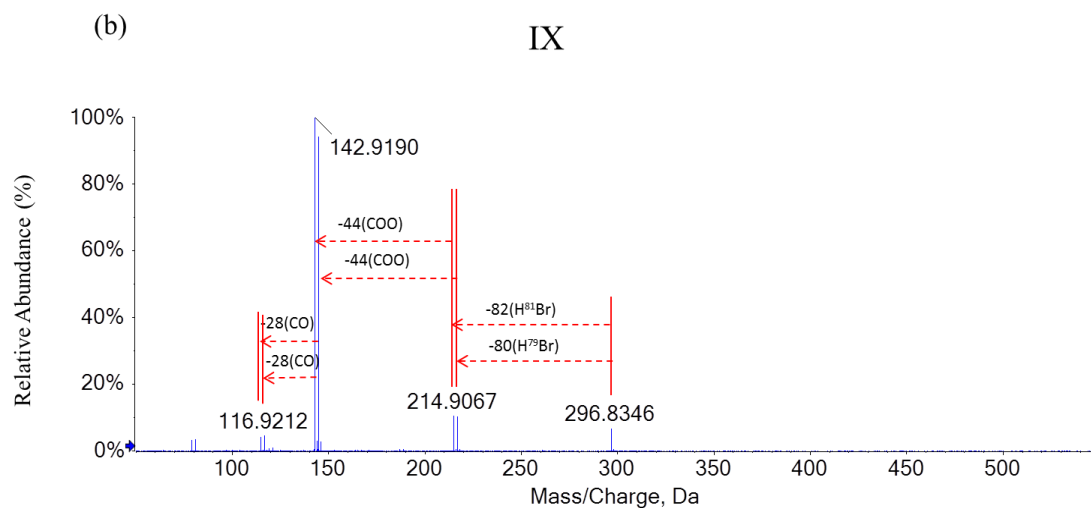


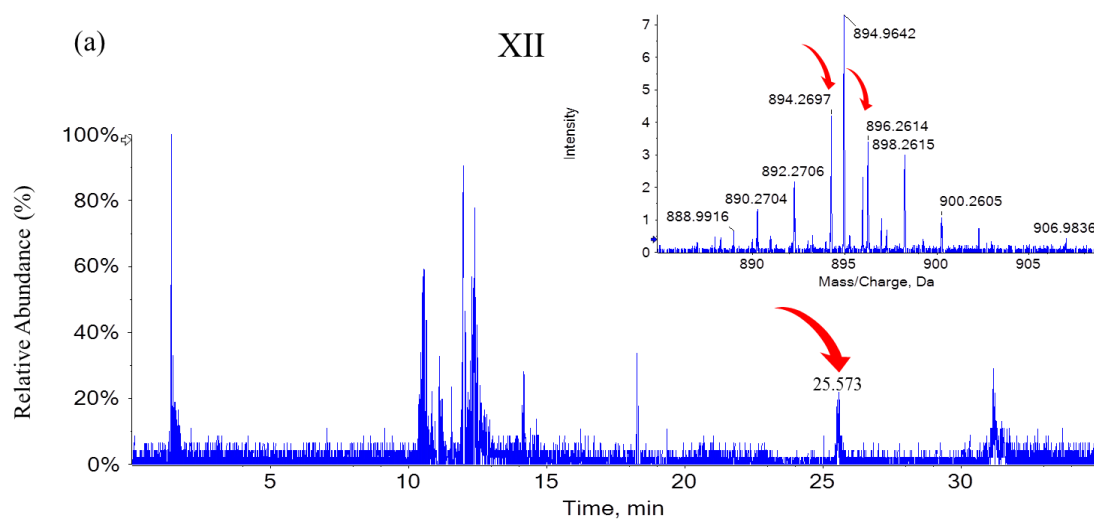
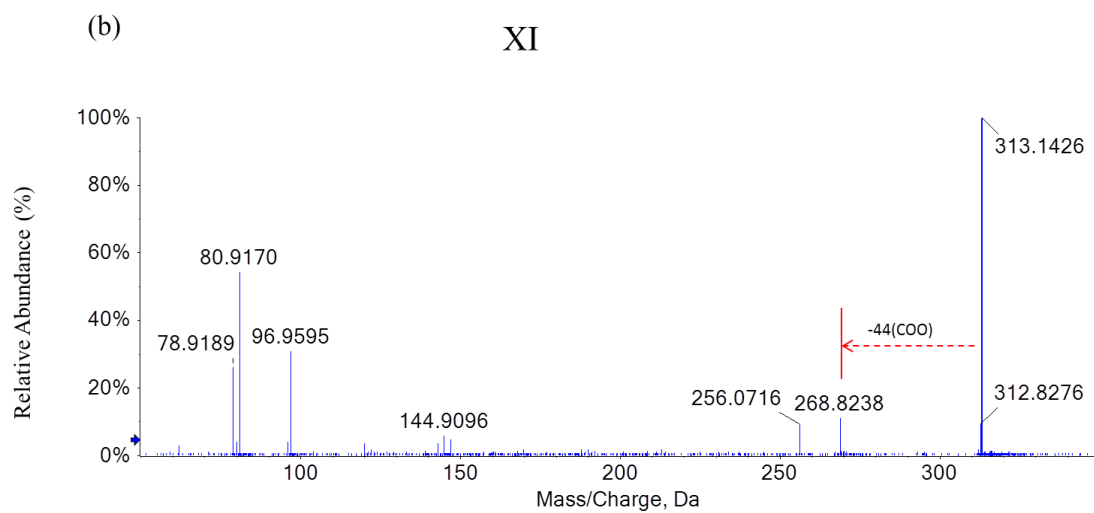
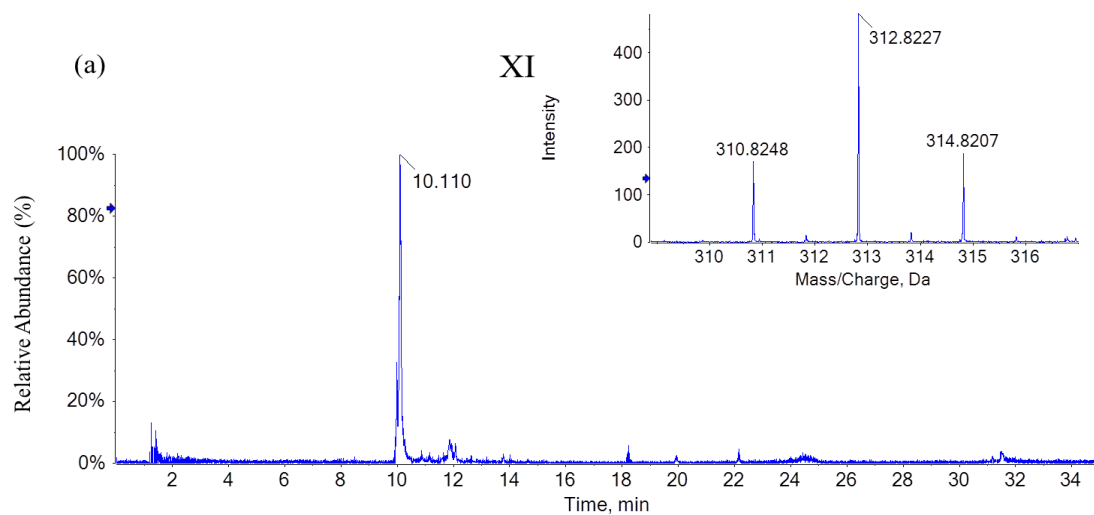
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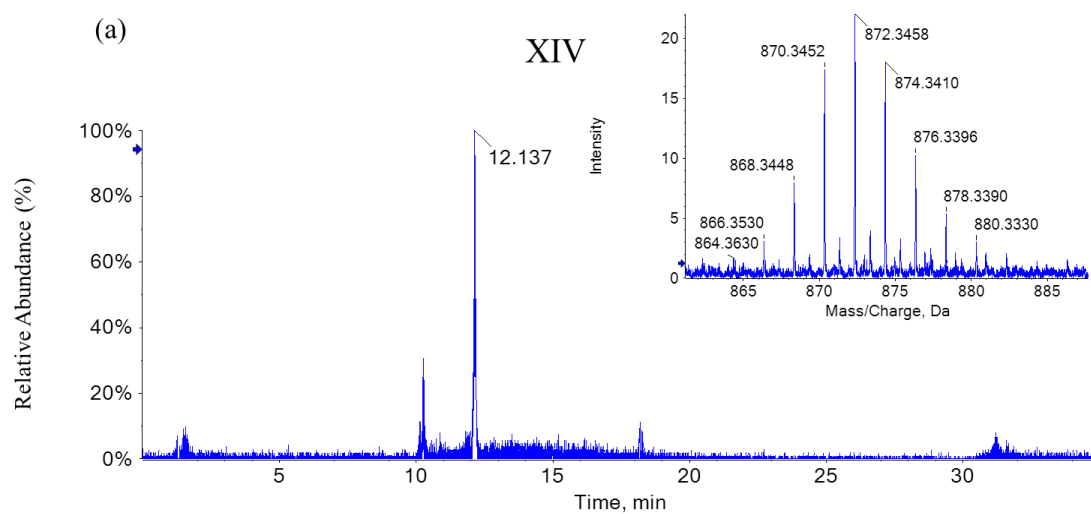
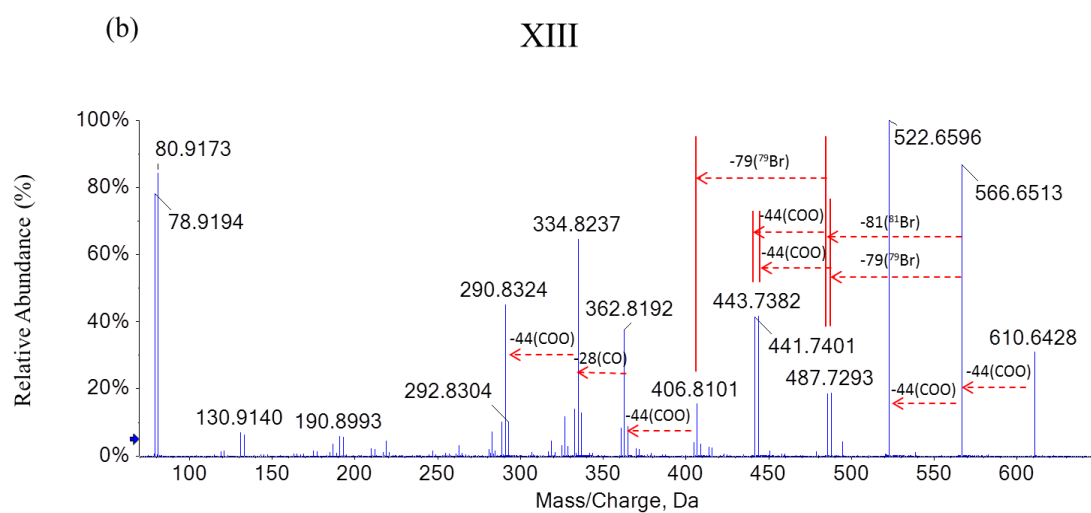
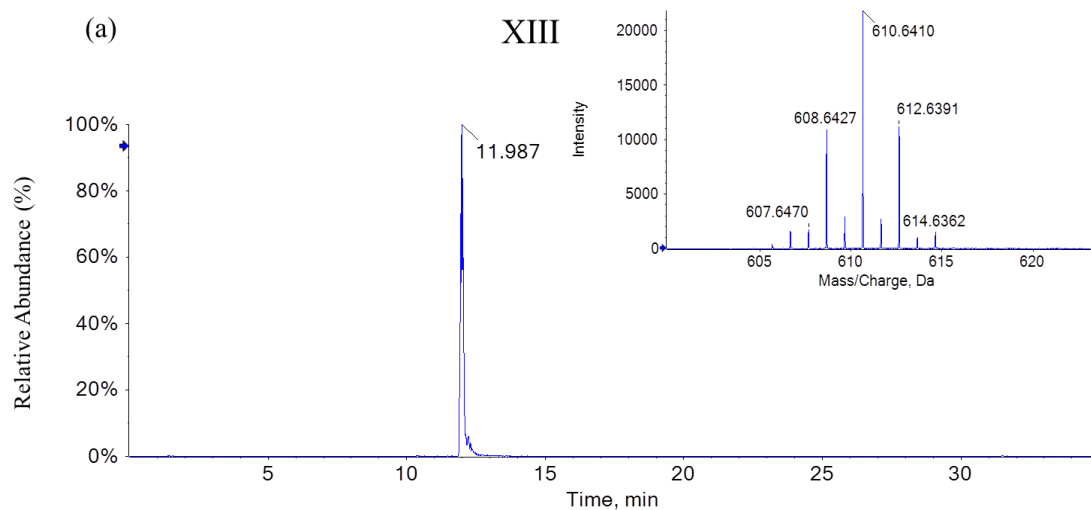












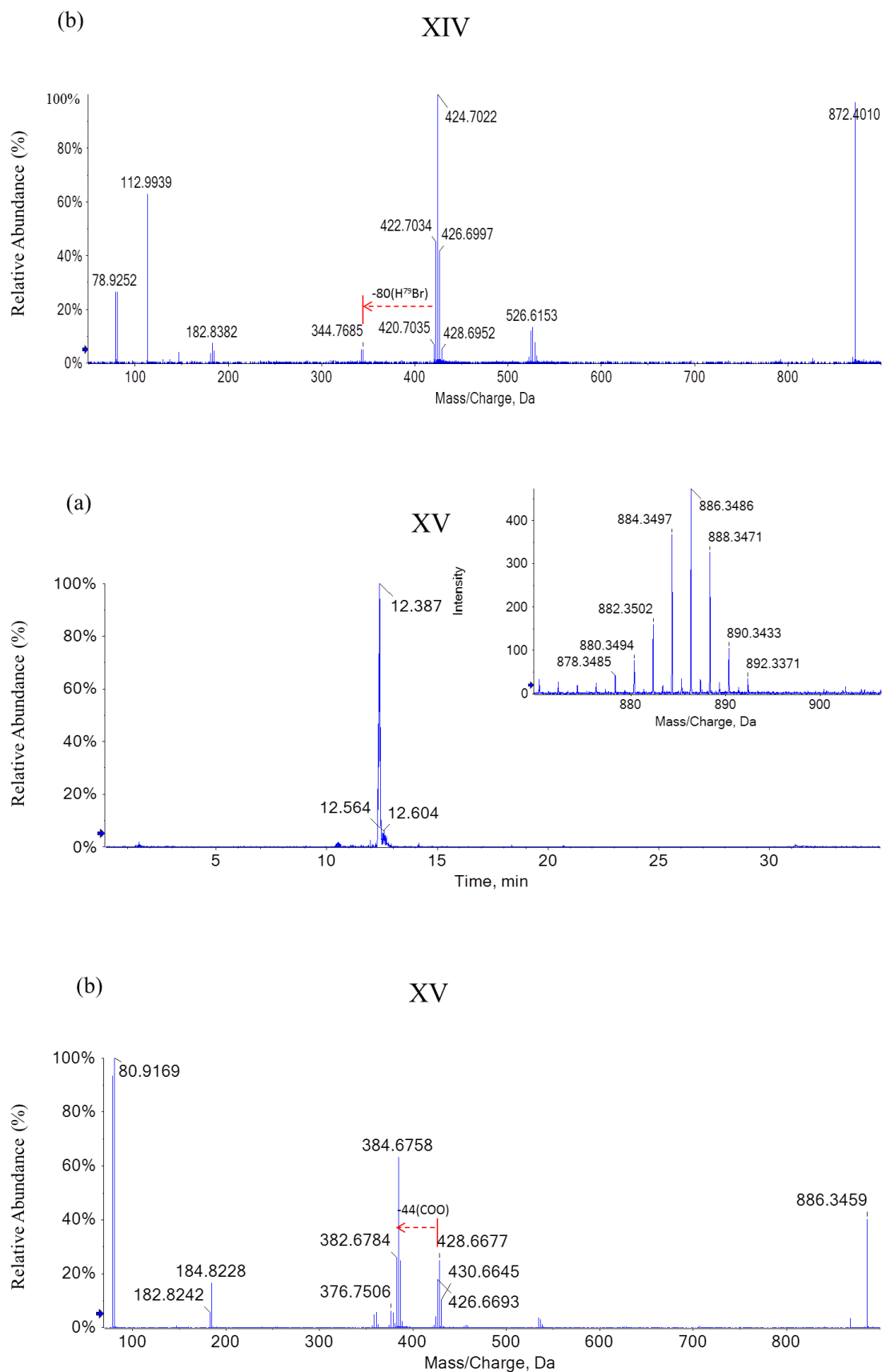
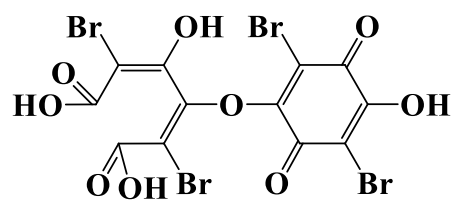
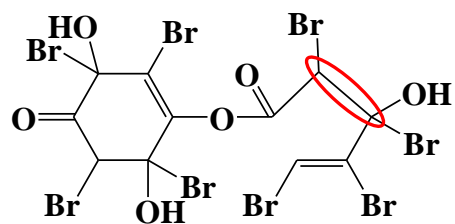


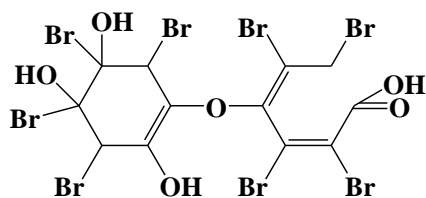
Figure S1. The HPLC/ESI chromatograms (a) and the product ion scan spectra (b) of products II–XV.



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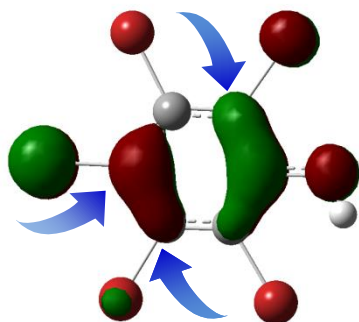
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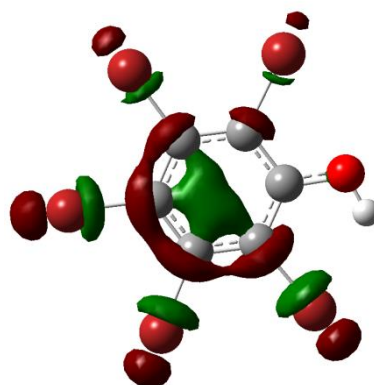
(XV)

Figure S2. The proposed structures of products XIII– XV. The red circle indicates one position where the water molecule addition occurs.

(I)

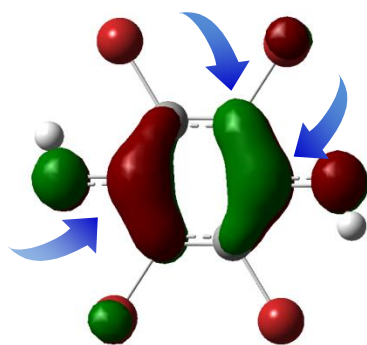


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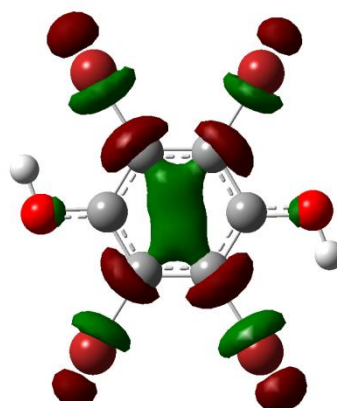


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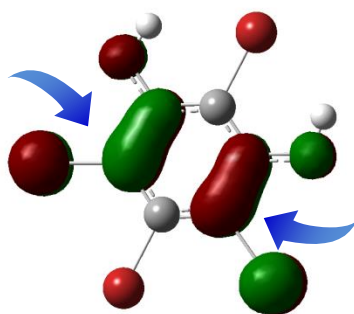


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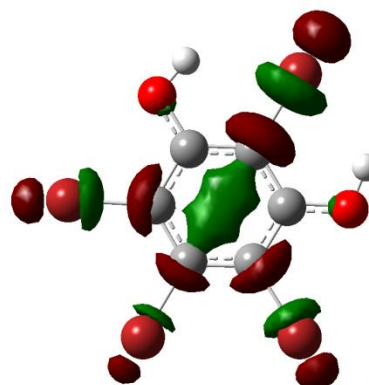


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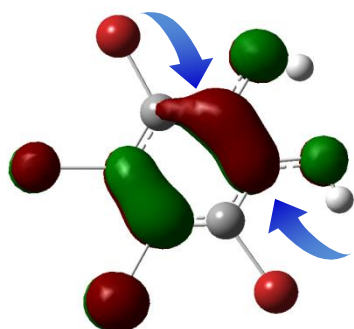


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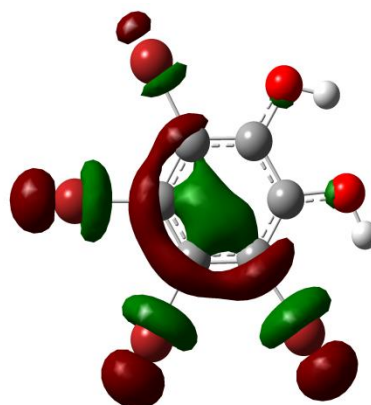


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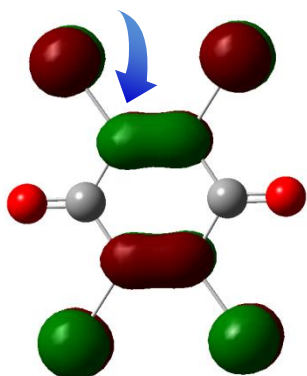


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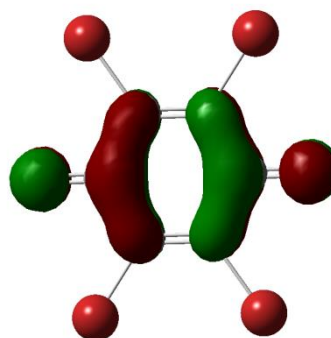


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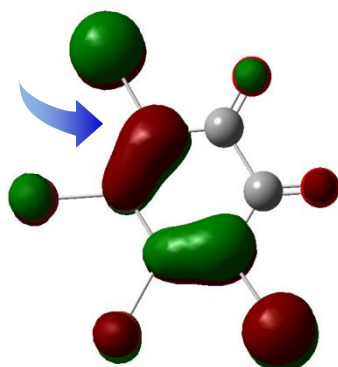


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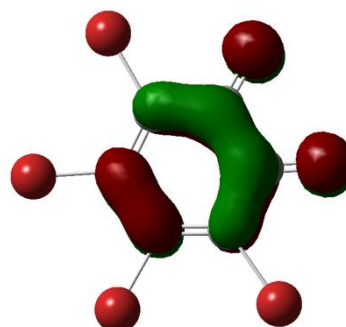


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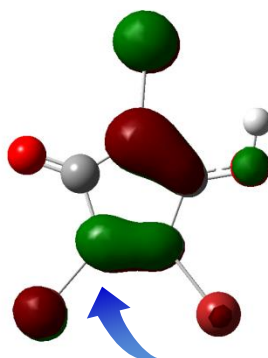


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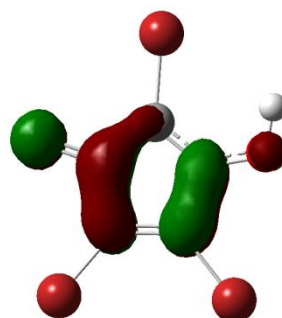


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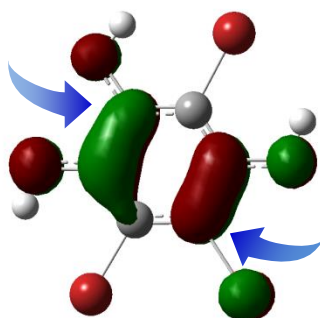


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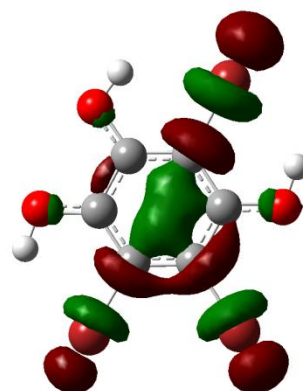


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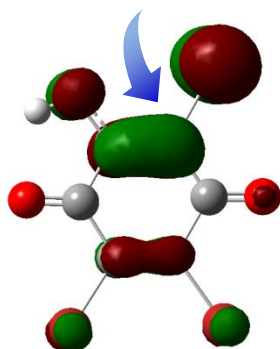


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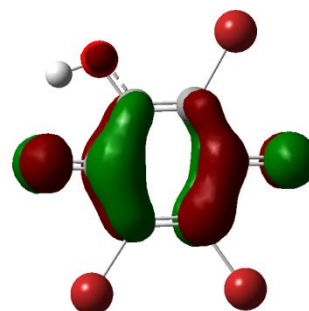


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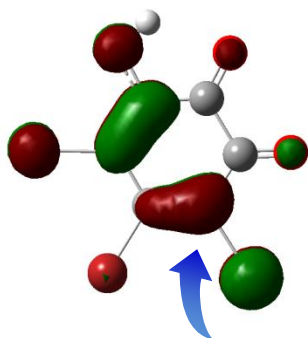


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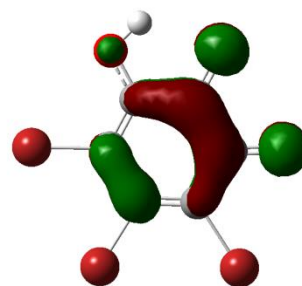


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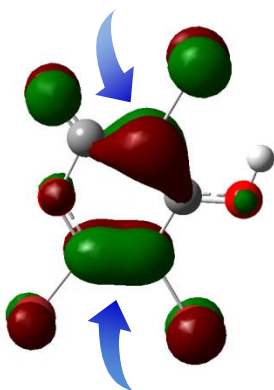


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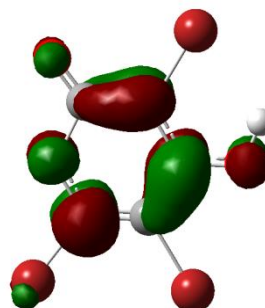


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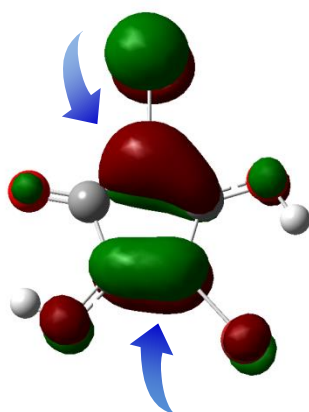


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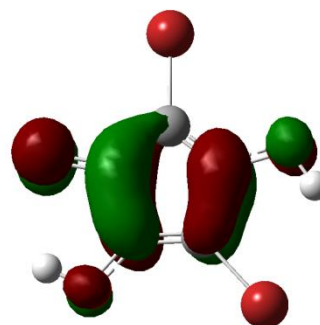


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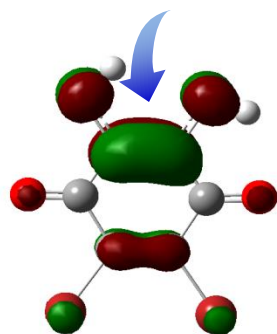


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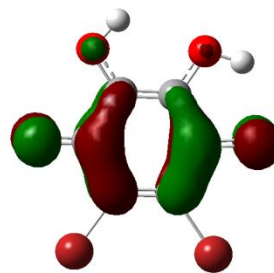


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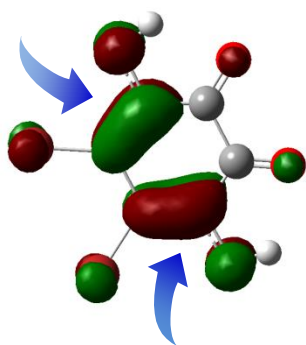


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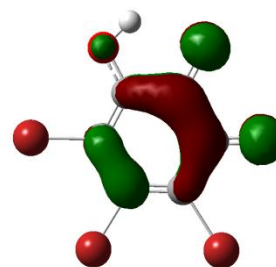


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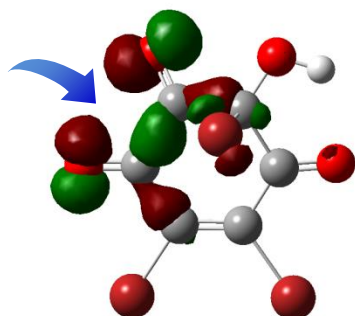


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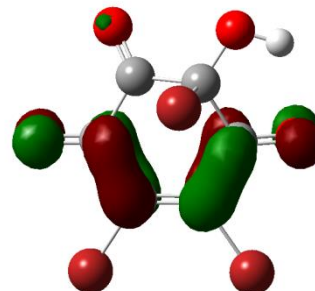


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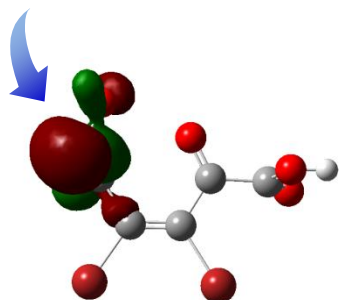
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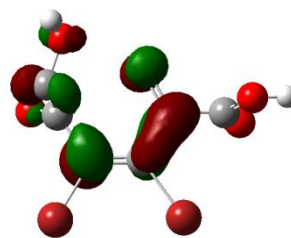
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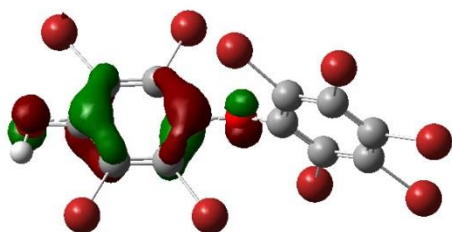


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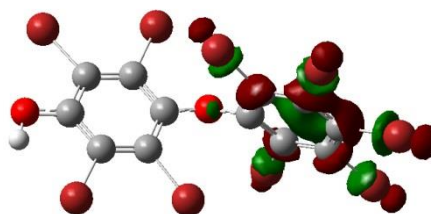


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Figure S3. Frontier molecular orbitals for the oxidant products. Arrows means the oxidation locations.

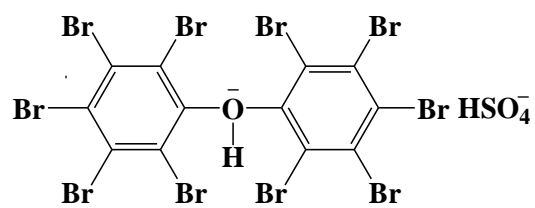


Figure S4. The structure of oxonium produced by reacting BDE 209 and concentrated sulphuric acid.