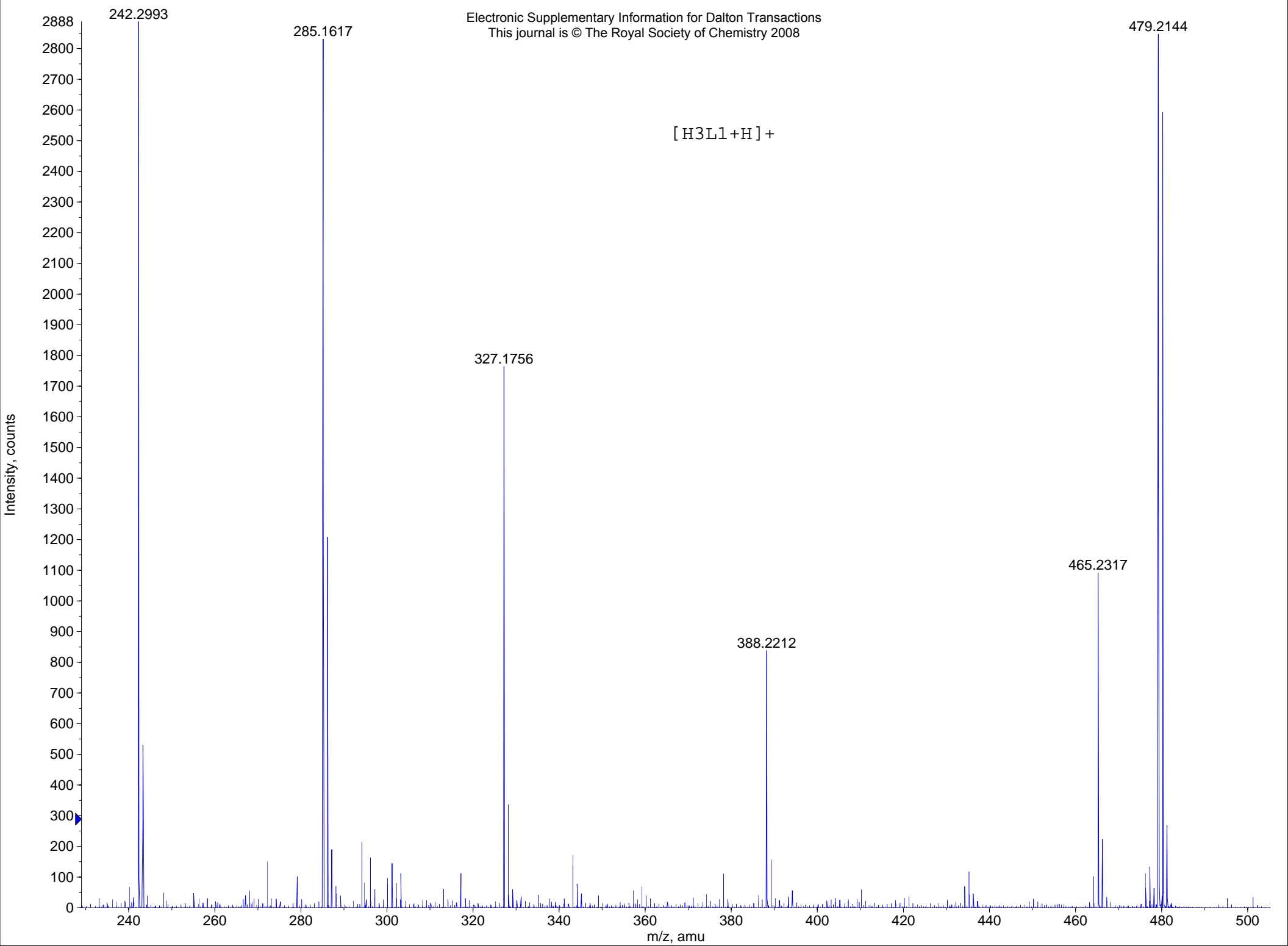


**Supplementary Material for the manuscript**

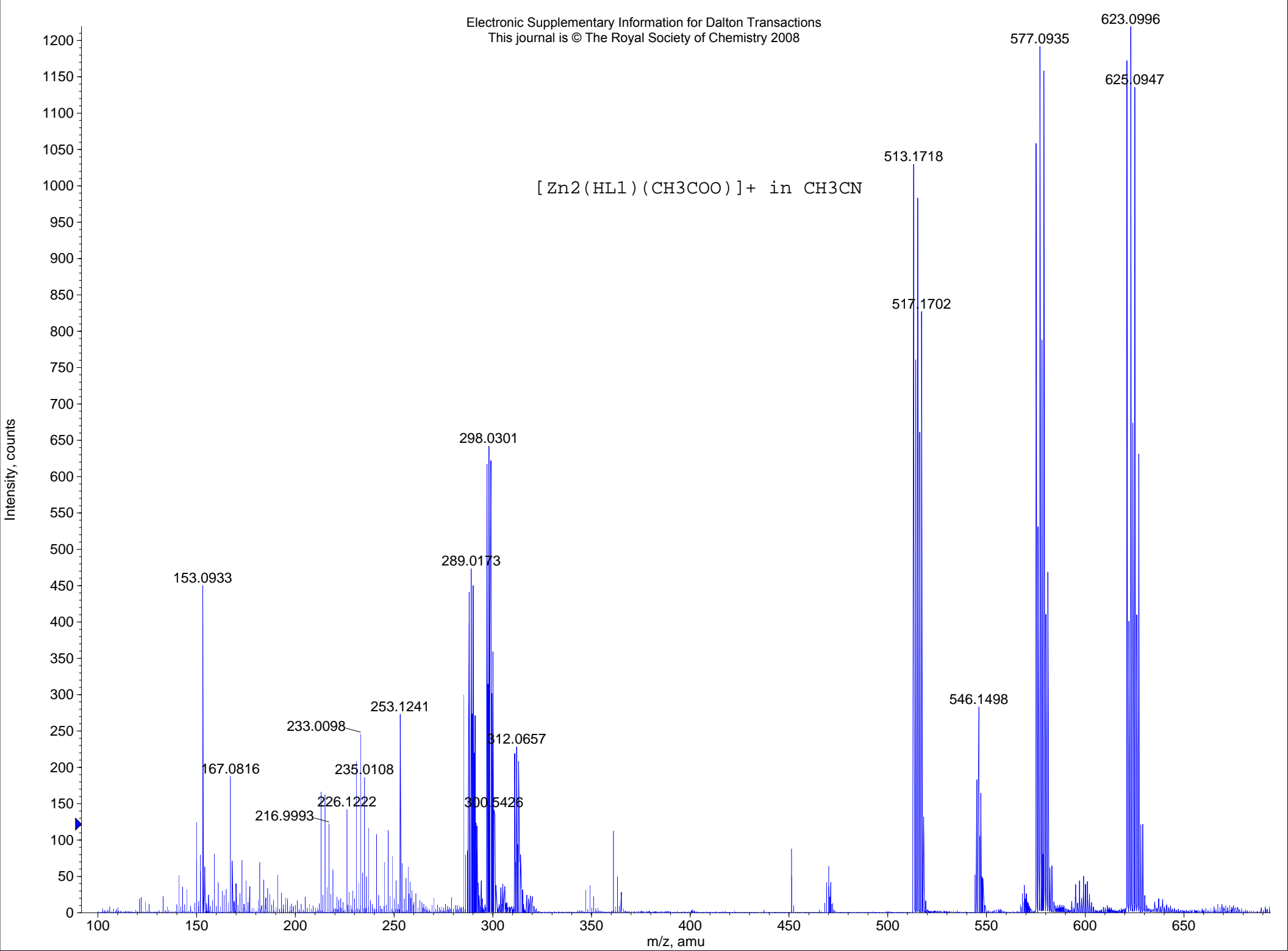
**A Structural and catalytic model for zinc phosphoesterases**

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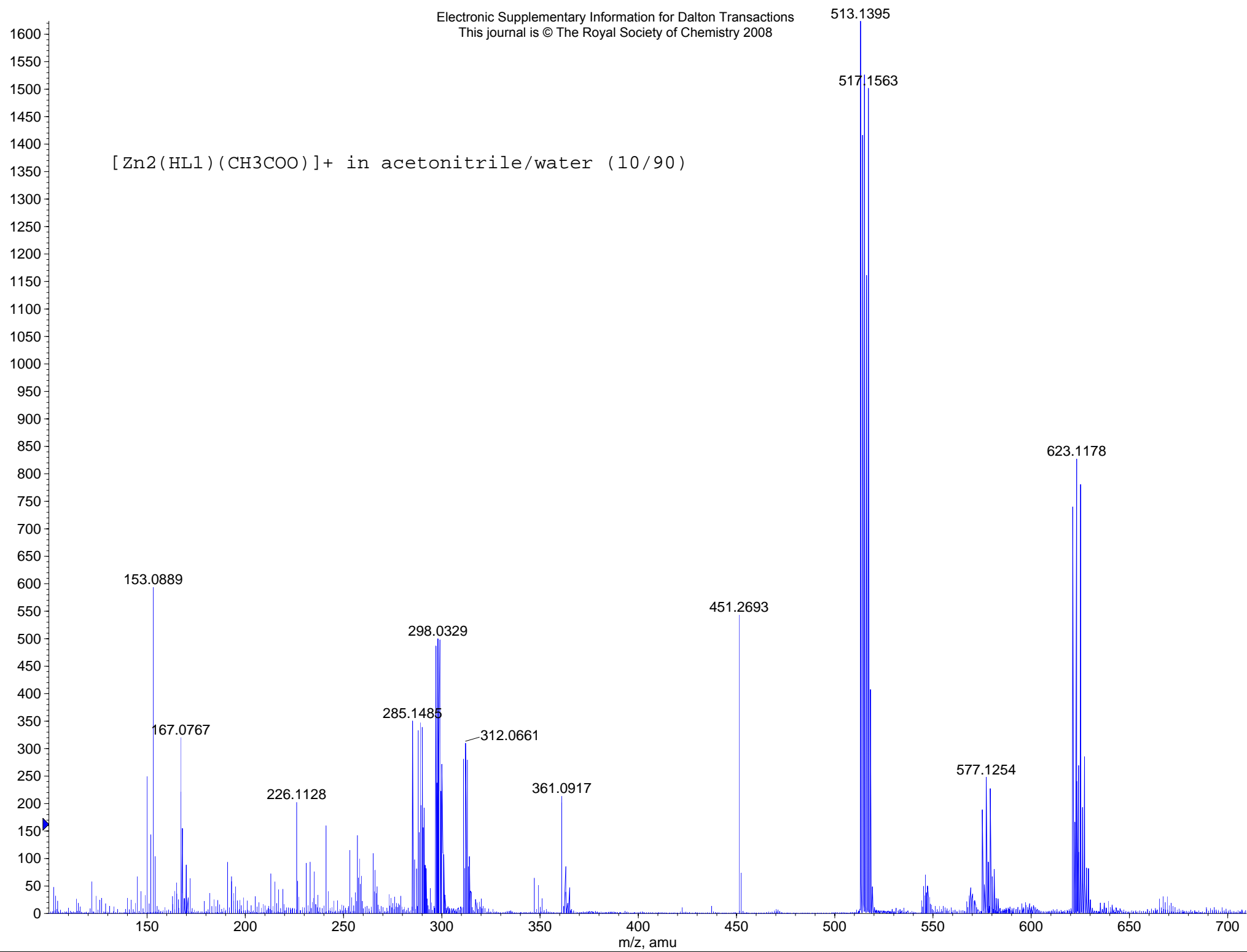
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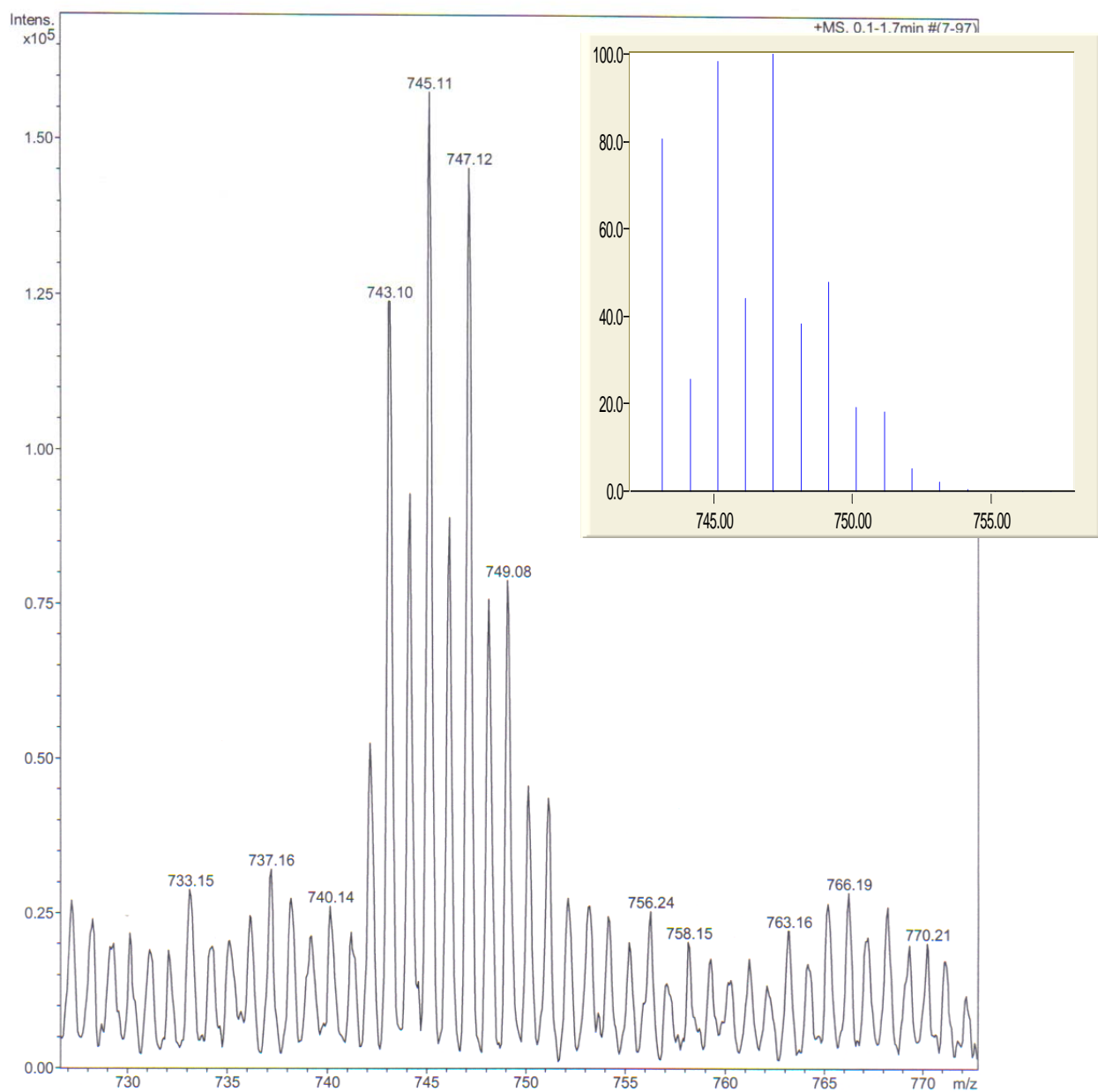
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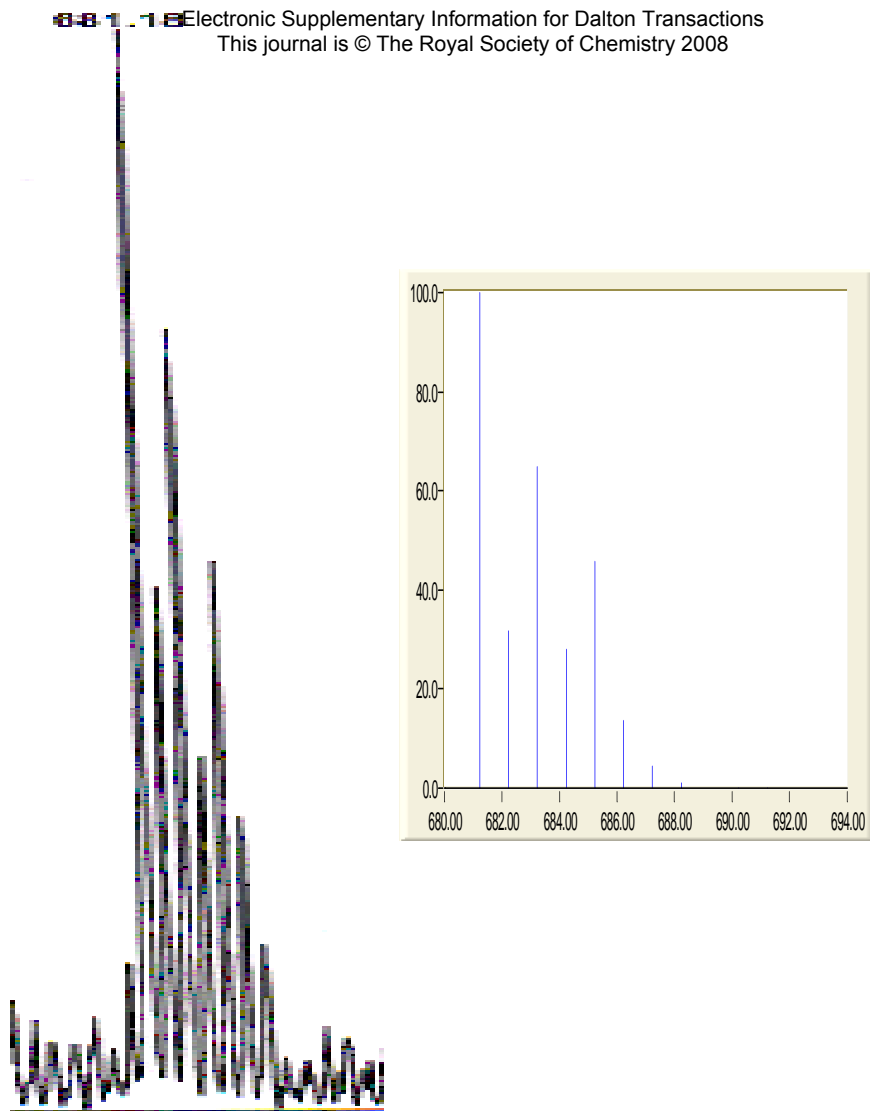
[Zn<sub>2</sub>(HL1)(CH<sub>3</sub>COO)]<sup>+</sup> in acetonitrile/water (10/90)

Intensity, counts



Calculated mass spectrum for  $[\text{Zn}_2(\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4)(\text{CH}_3\text{COO})(\text{H}_2\text{O})_6]^+$   
(743.14, 80.64; 745.14, 98.46; 747.14, 100.00; 748.14, 38.19%)





Calculated mass spectrum for  $[\text{Zn}(\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_4)(\text{CH}_3\text{COO})(\text{H}_2\text{O})_6+2\text{H}]^+$  (681.23, 100.00; 682.23, 31.81; 683.23, 64.74%)