Supporting information

Comparative studies on OLED performances of chloro and fluoro substituted Zn (II) 8-hydroxyquinolinates

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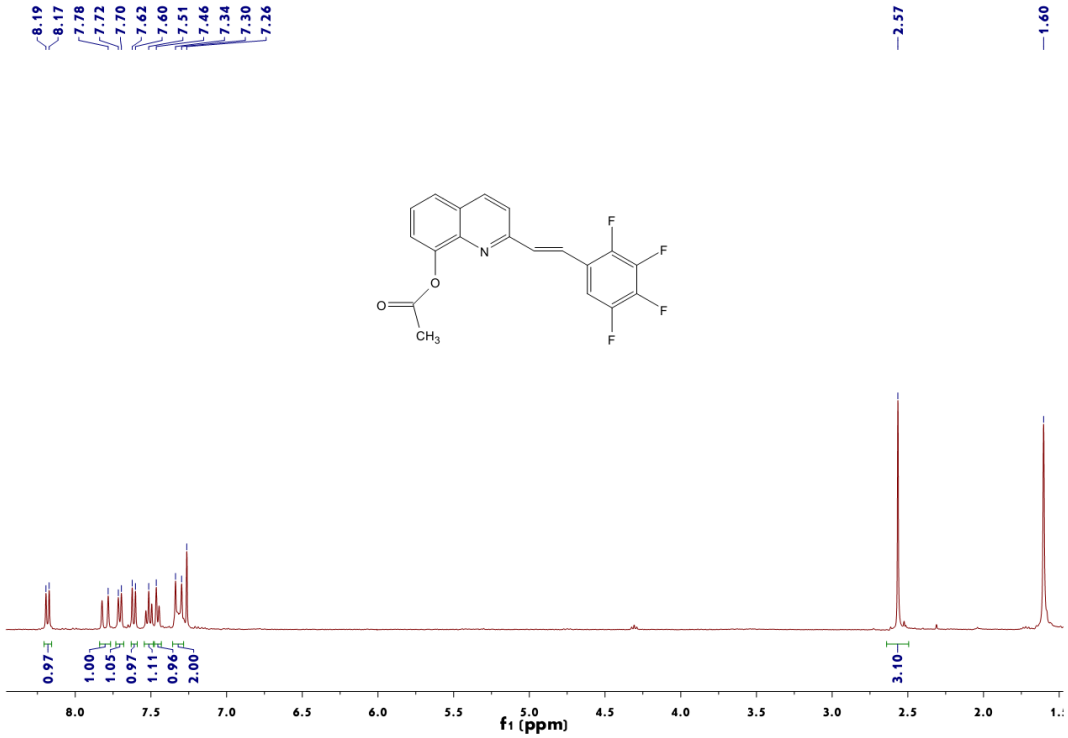
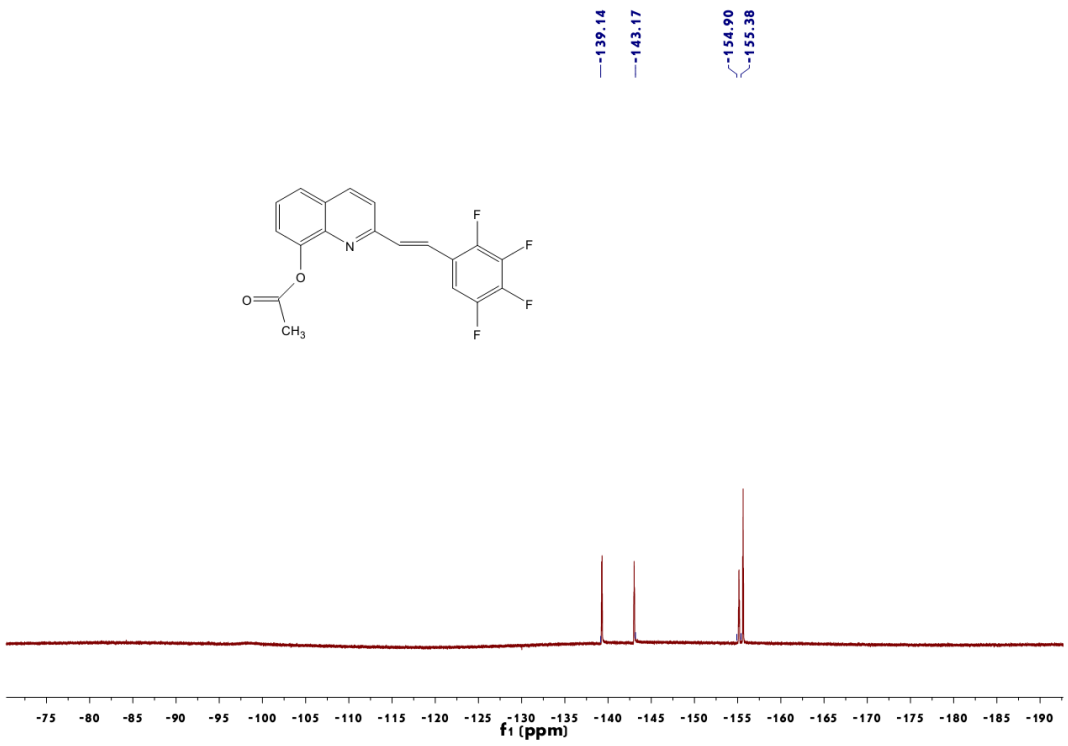
^{1}H NMR of **1**



^{19}F NMR of **1**



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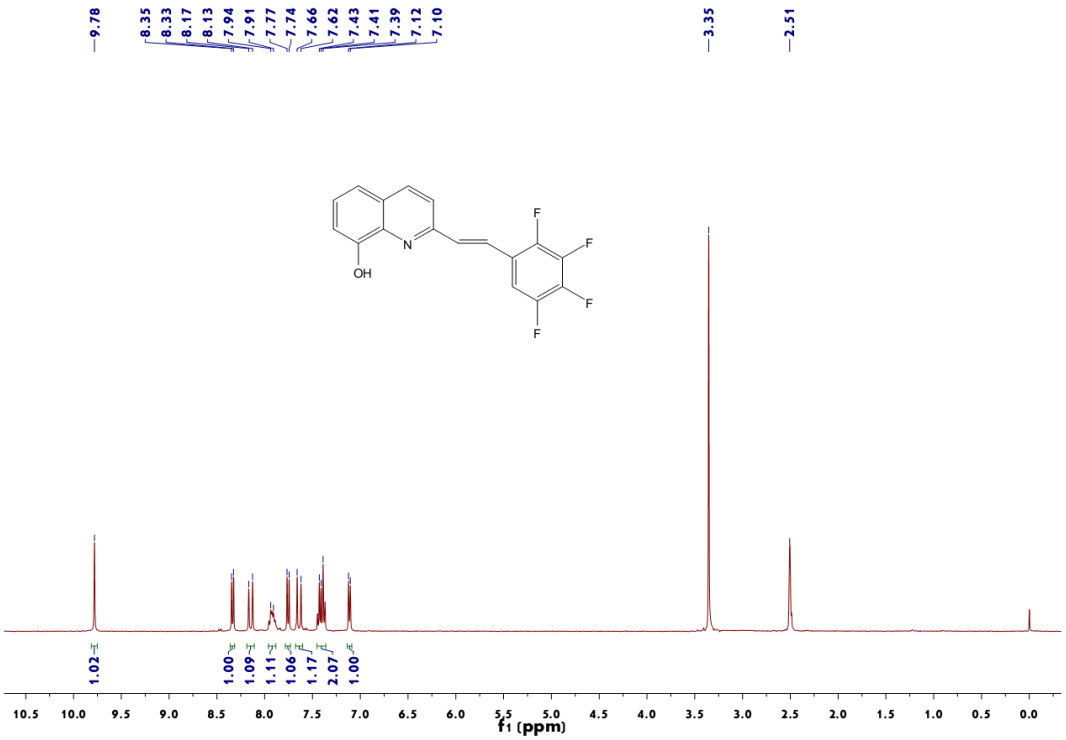

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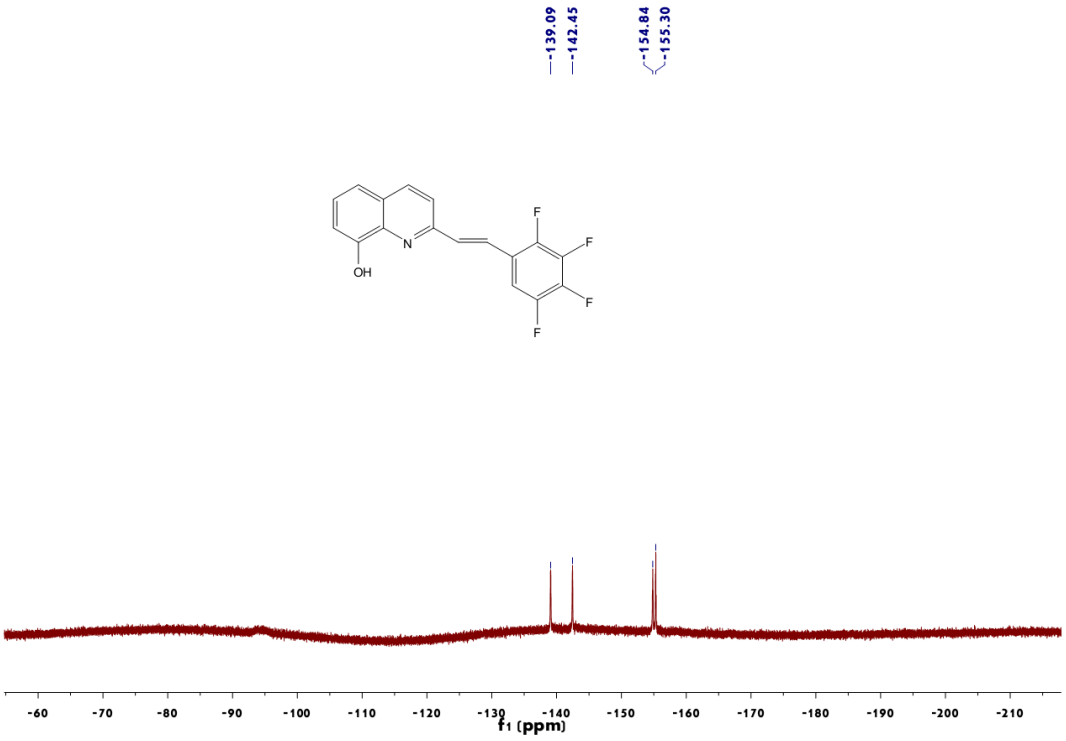

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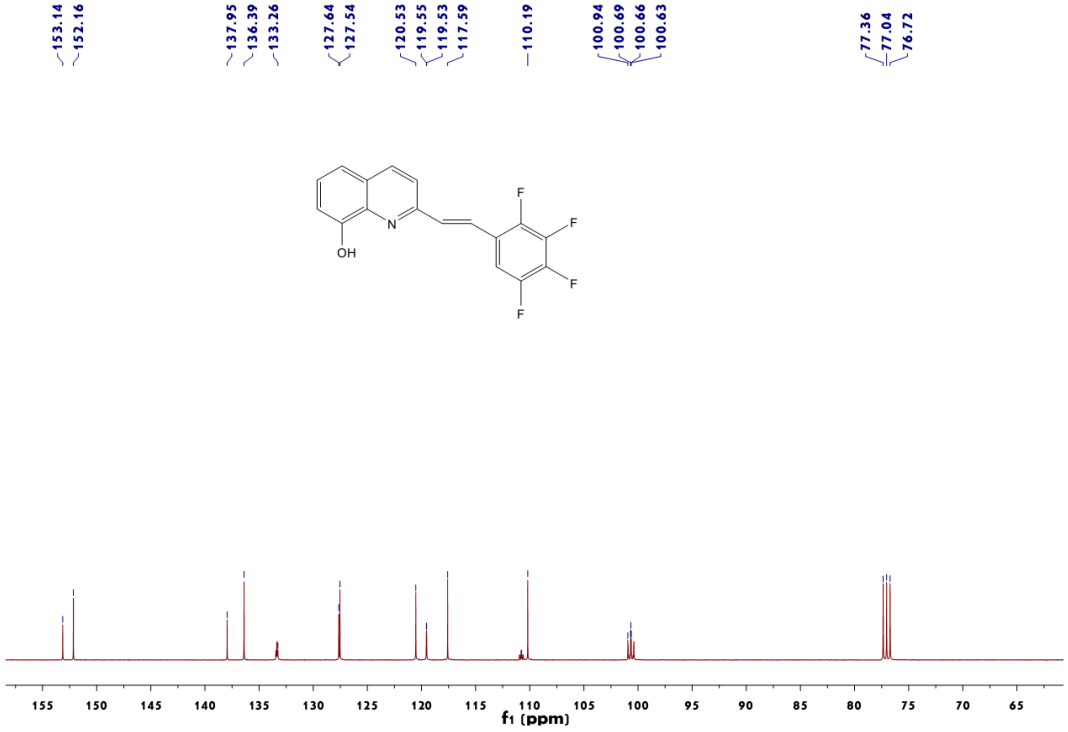

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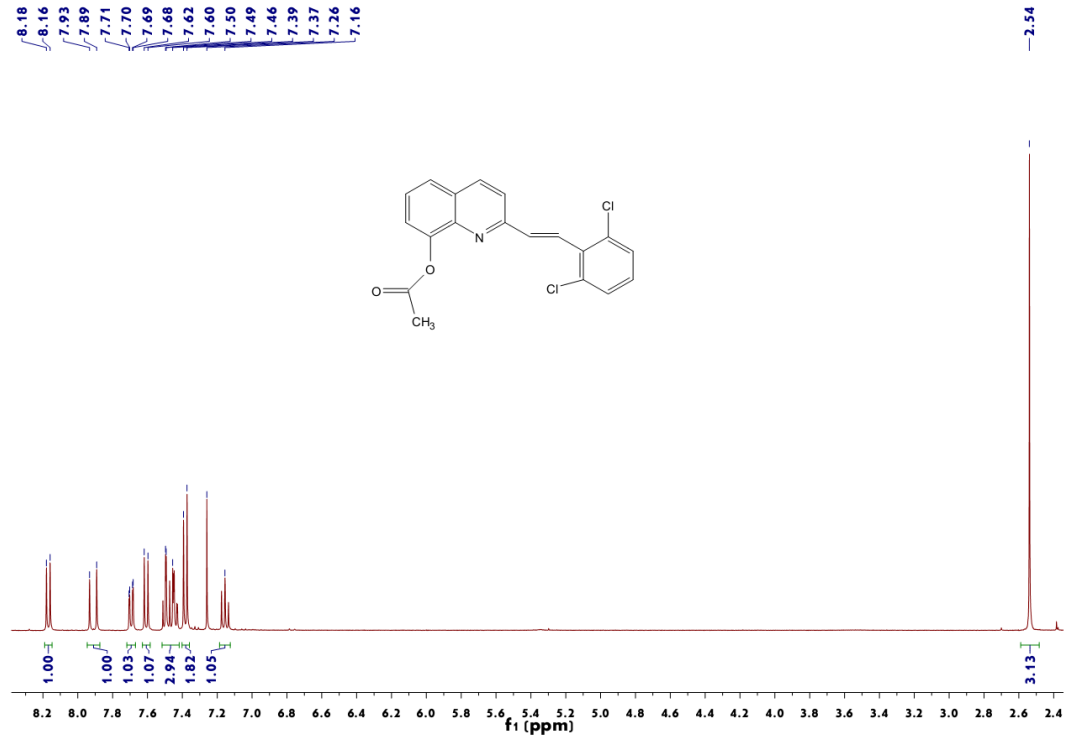

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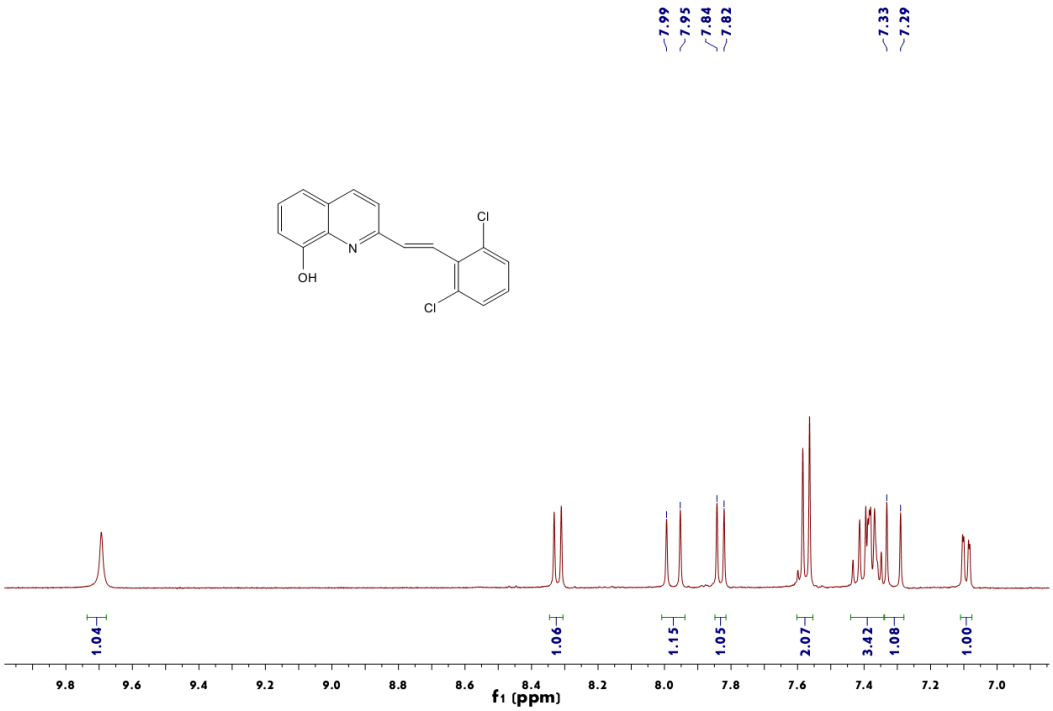

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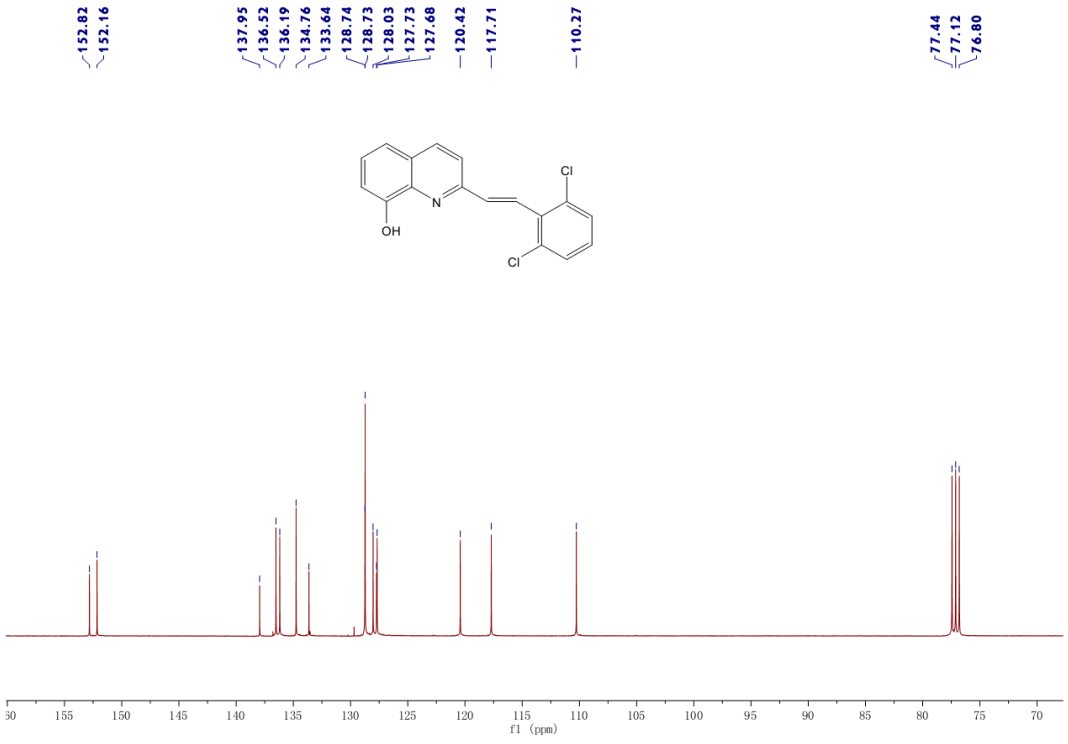

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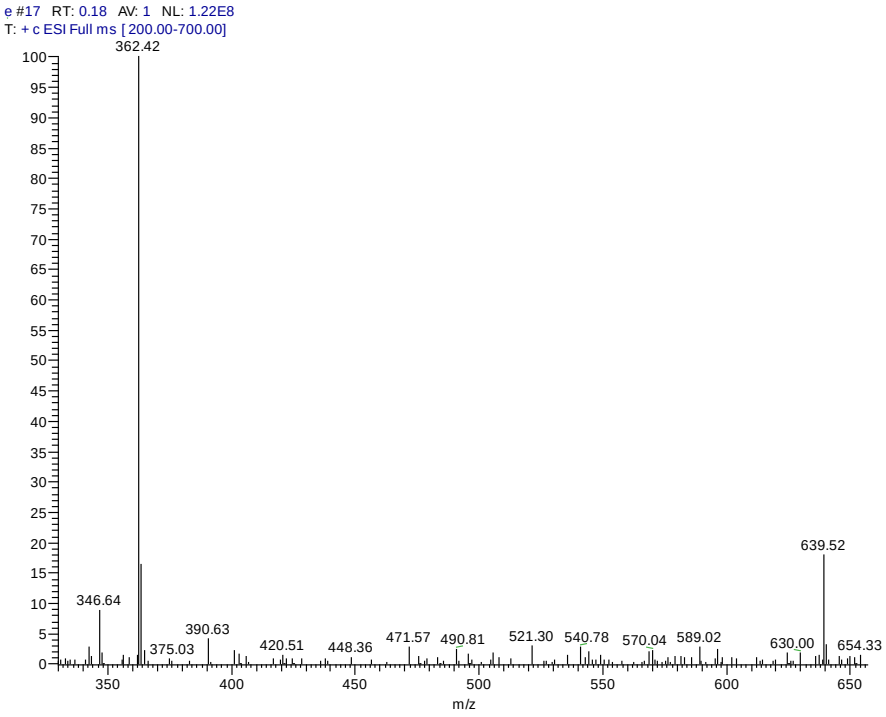

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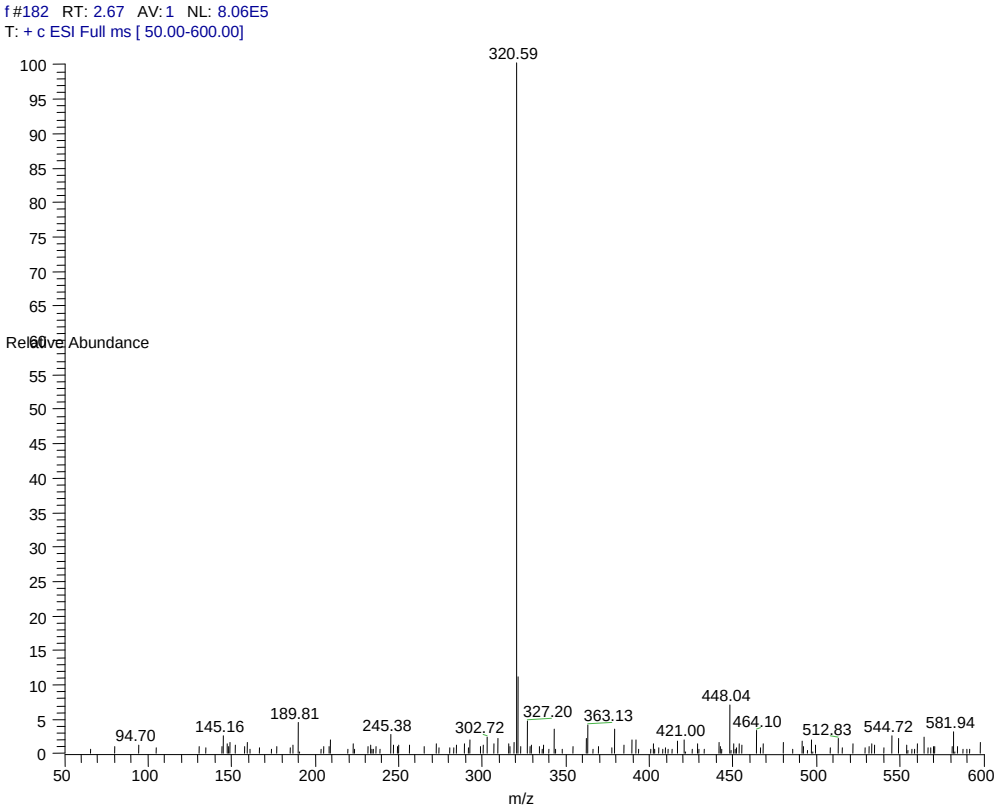
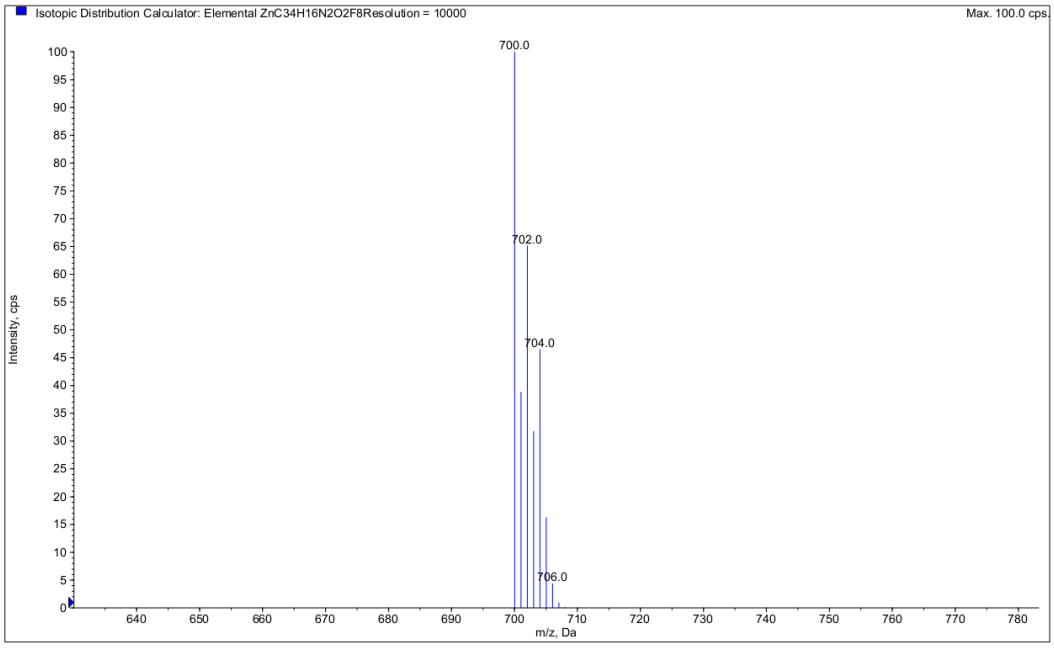


ESI-MS of **5**



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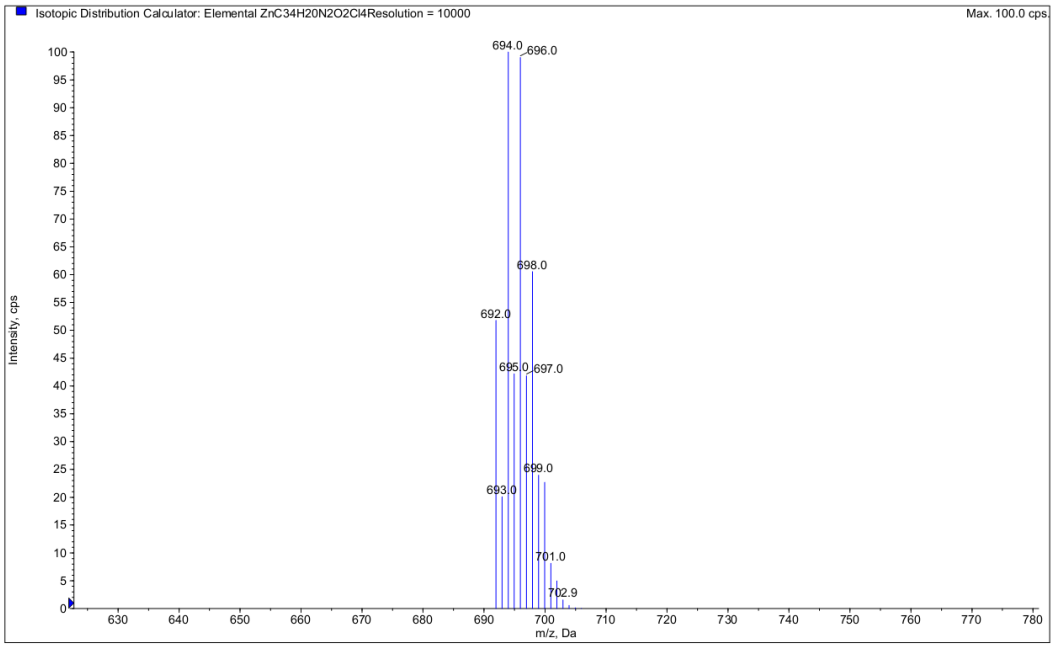
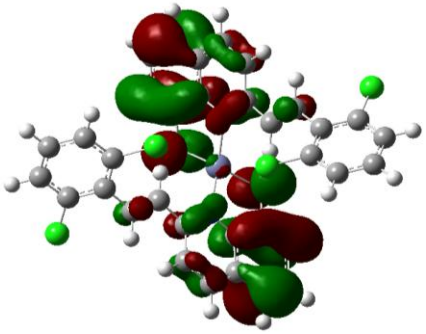
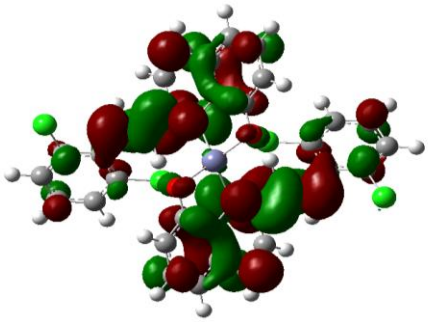


The energy levels of **5** and **6** have been calculated by TD-DFT in Gaussian 03.The results were similar to the energy levels of **5** and **6** calculated by using the DFT(density functional theory) model of a DMol3 package in Materials Studio

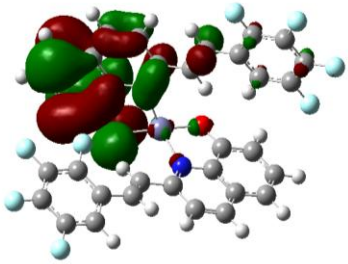
(version 5.5). The LUMO energy levels of the complexes **5** and **6** are calculated to be –3.095 and -3.312 eV, respectively. The HOMO energy levels of the complexes **5** and **6** are calculated to be –4.279 and -4.364 eV, respectively. The calculated HOMO–LUMO energy gaps (E_g) obtained from TD-DFT calculations were 1.184 and 1.052 eV, respectively, for complexes **5** and **6**.



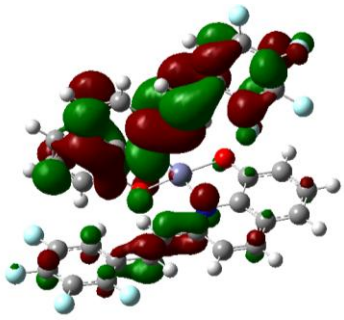
5 HOMO (-4.279 eV)



5 LUMO (-3.095 eV)



6 HOMO (-4.364 eV)



6 LUMO (-3.312 eV)