

Supporting information

Tetrahydroindazolone substituted 2-aminobenzamides as fluorescent probes: switching metal ion selectivity from zinc to cadmium by interchanging the amino and carbamoyl groups on the fluorophore

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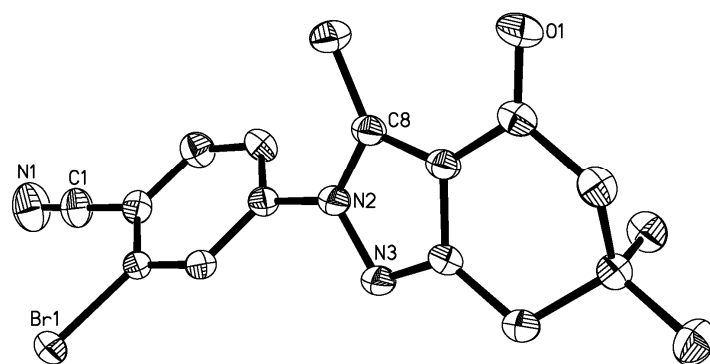


Figure S1. X-ray crystallographic structure of **8b**.

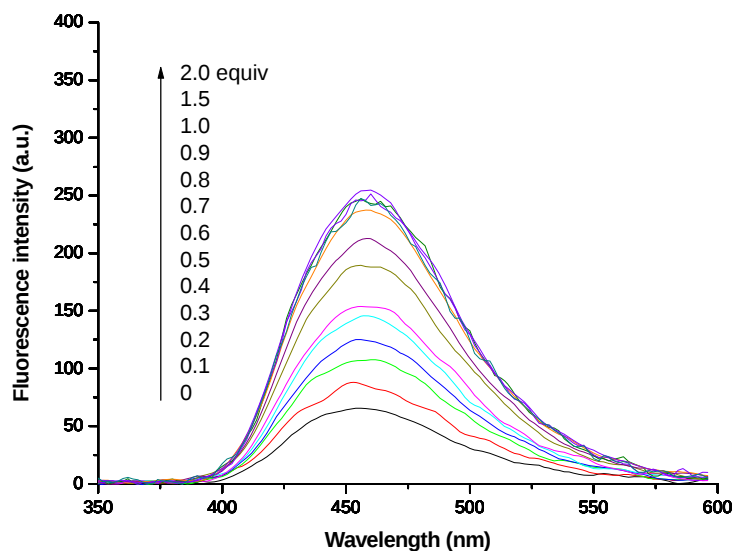


Figure S2. Fluorescence emission spectra ($\lambda_{\text{ex}} = 260$ nm) of CdABA (10 μM , 25mM HEPES buffer, 0.1 M NaClO_4 , pH = 7.4, $I = 0.1$) upon addition of Cd^{2+} [added as $\text{Cd}(\text{ClO}_4)_2$, 0-20 μM].

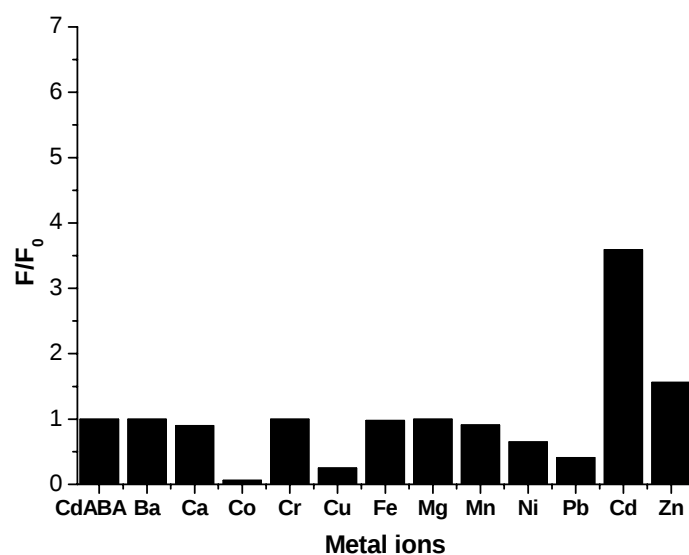


Figure S3. Selectivity of CdABA towards various metal ions. Experimental conditions: CdABA (10 μM , 25mM HEPES buffer, 0.1 M NaClO_4 , pH = 7.4, $I = 0.1$), 10 μM Ba^{2+} , Ca^{2+} , Co^{2+} , Cr^{3+} , Cu^{2+} , Fe^{3+} , Mg^{2+} , Mn^{2+} , Ni^{2+} , Pb^{2+} , Cd^{2+} and Zn^{2+} , $\lambda_{\text{ex}} = 260$ nm, $\lambda_{\text{em}} = 454$ nm.

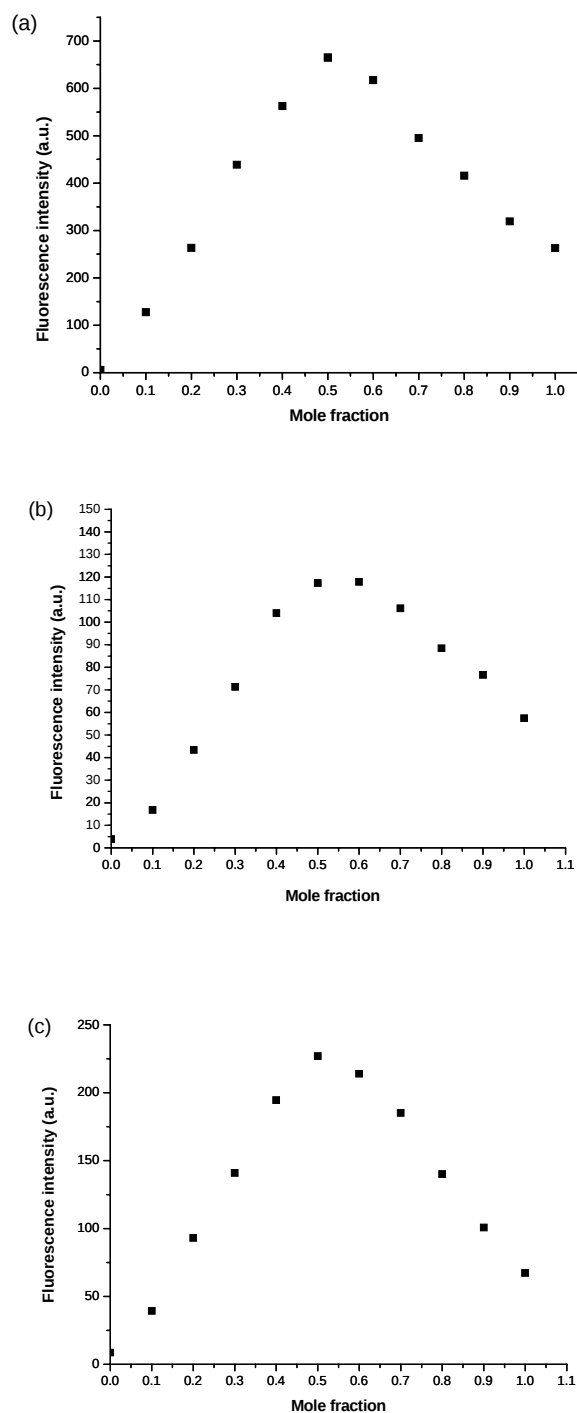


Figure S4. A Job's plot of (a) CdABA' and Cd²⁺, (b) CdABA and Cd²⁺, and (c) ZnABA' and Zn²⁺. The total concentrations of sensors and Zn²⁺/Cd²⁺ are 10 μ M. The experiments were measured at room temperature in buffer solution (HEPES buffer, 25 mM, 0.1 M NaClO₄, pH = 7.4, I = 0.1).

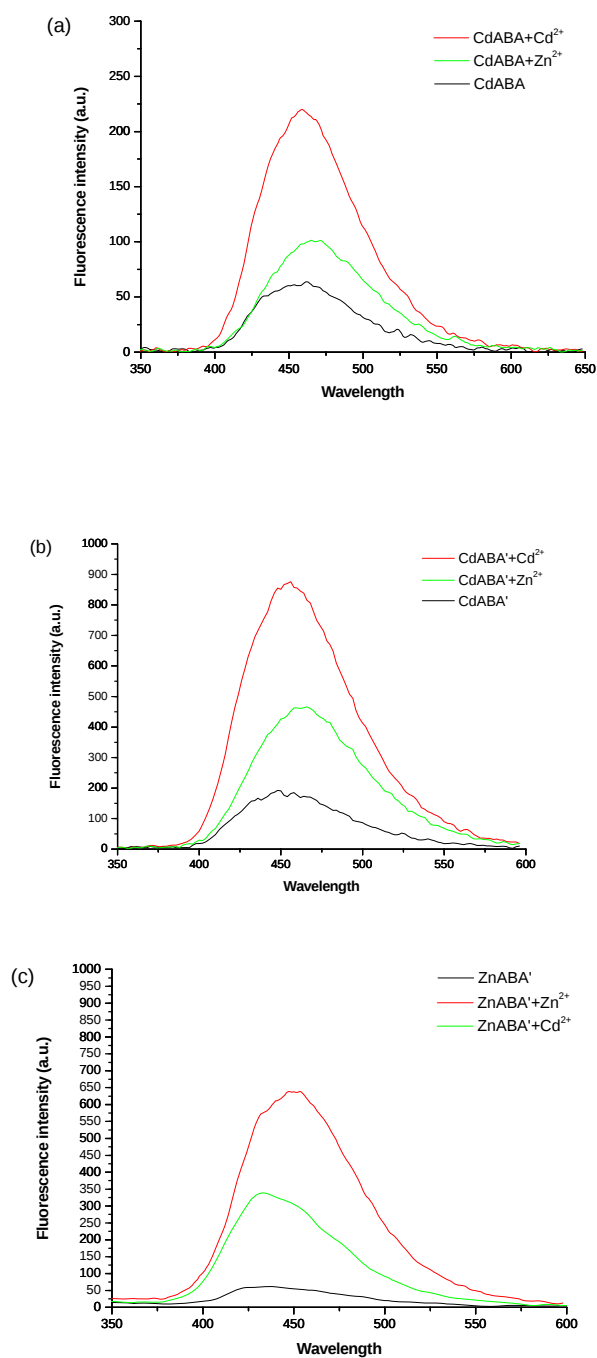


Figure S5. Fluorescence emission spectra of (a) CdABA, CdABA with Zn^{2+} and CdABA with Cd^{2+} , (b) CdABA', CdABA' with Zn^{2+} and CdABA' with Cd^{2+} , (c) ZnABA', ZnABA' with Zn^{2+} and ZnABA' with Cd^{2+} in aqueous solution (10 μM , 25mM HEPES buffer, 0.1 M NaClO_4 , pH = 7.4, $I = 0.1$). All the metal ions are 1 equiv., and the excitation wavelengths are at 260nm.

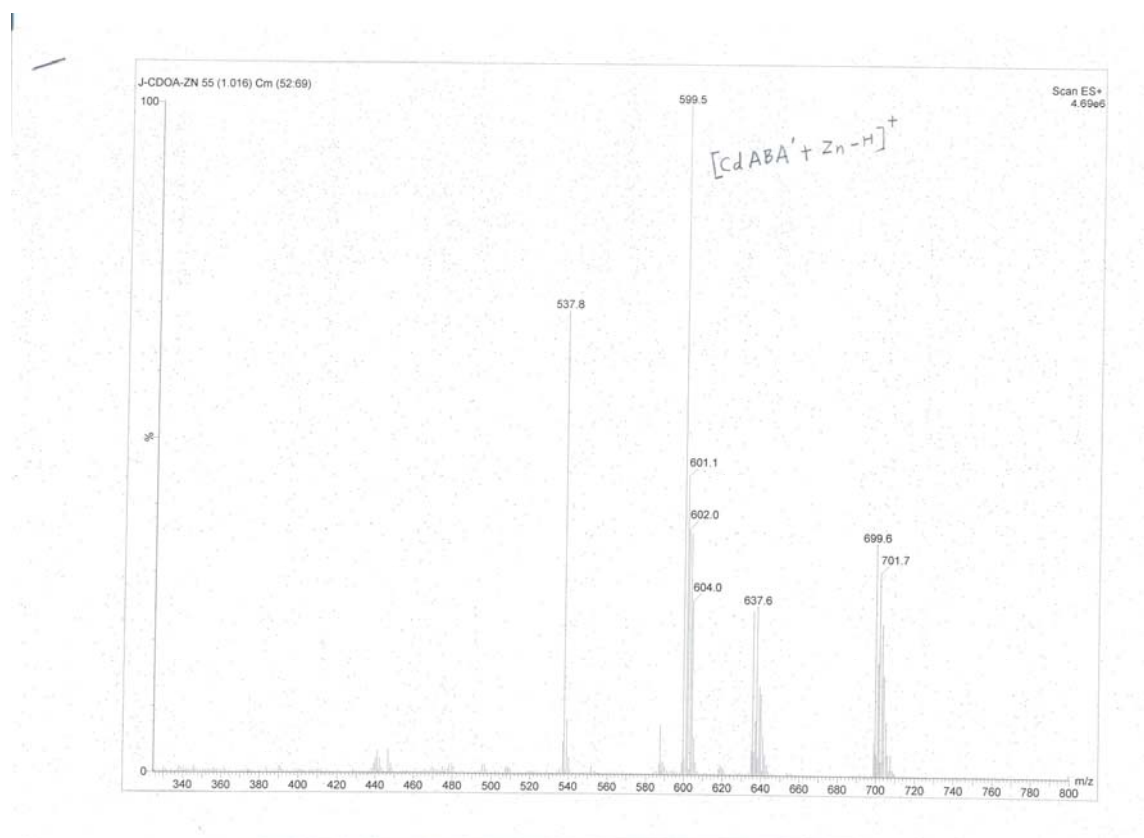
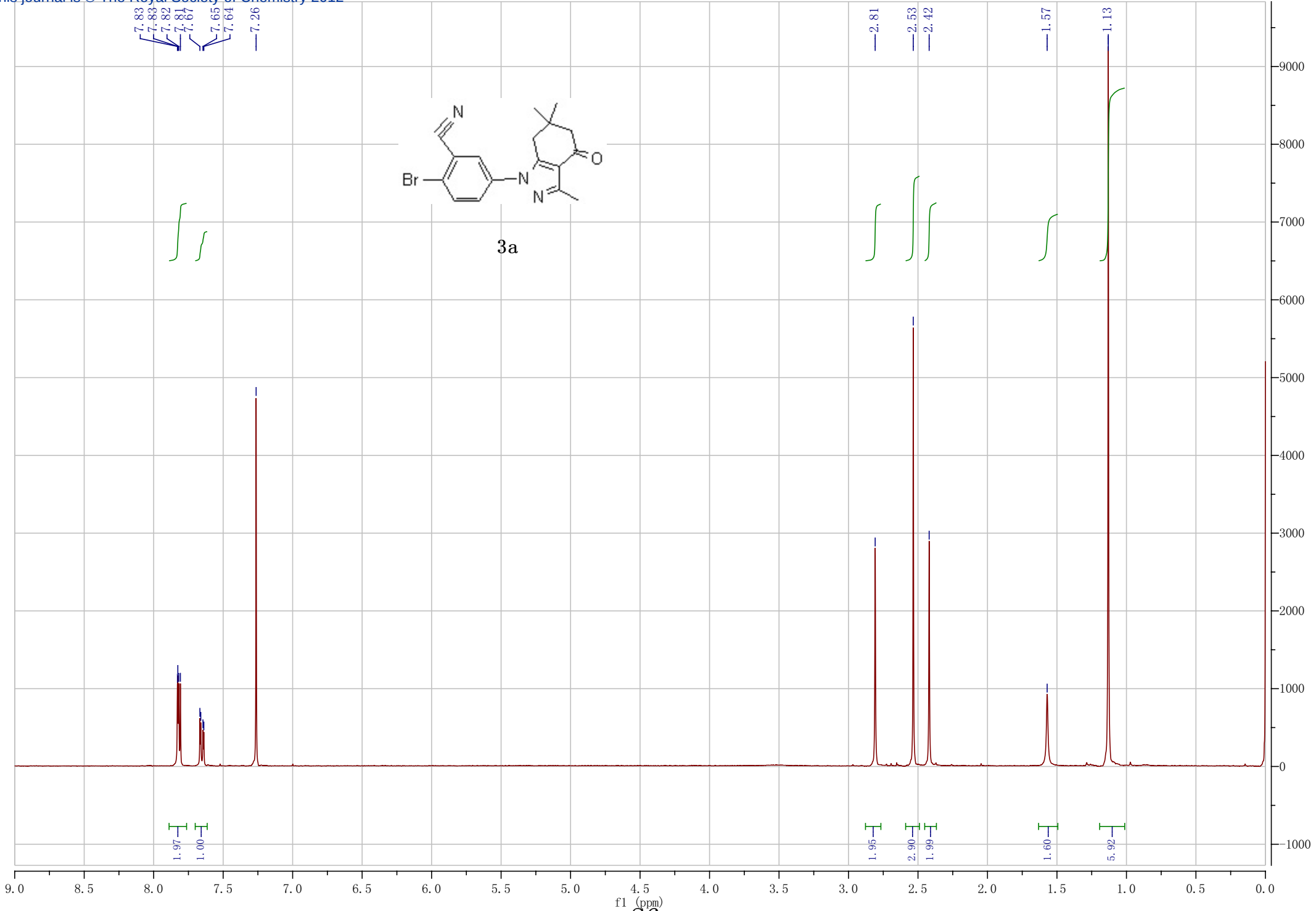
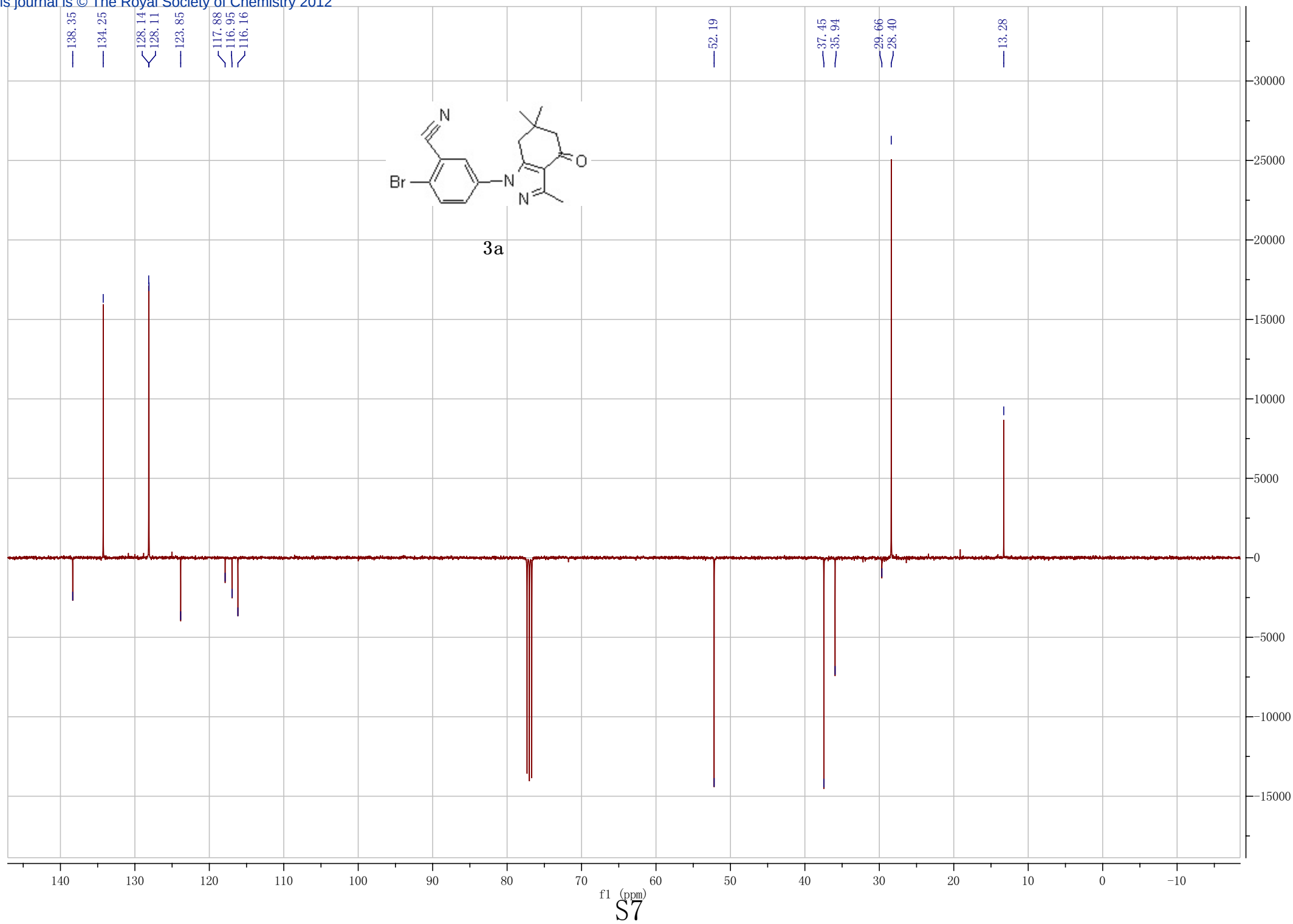
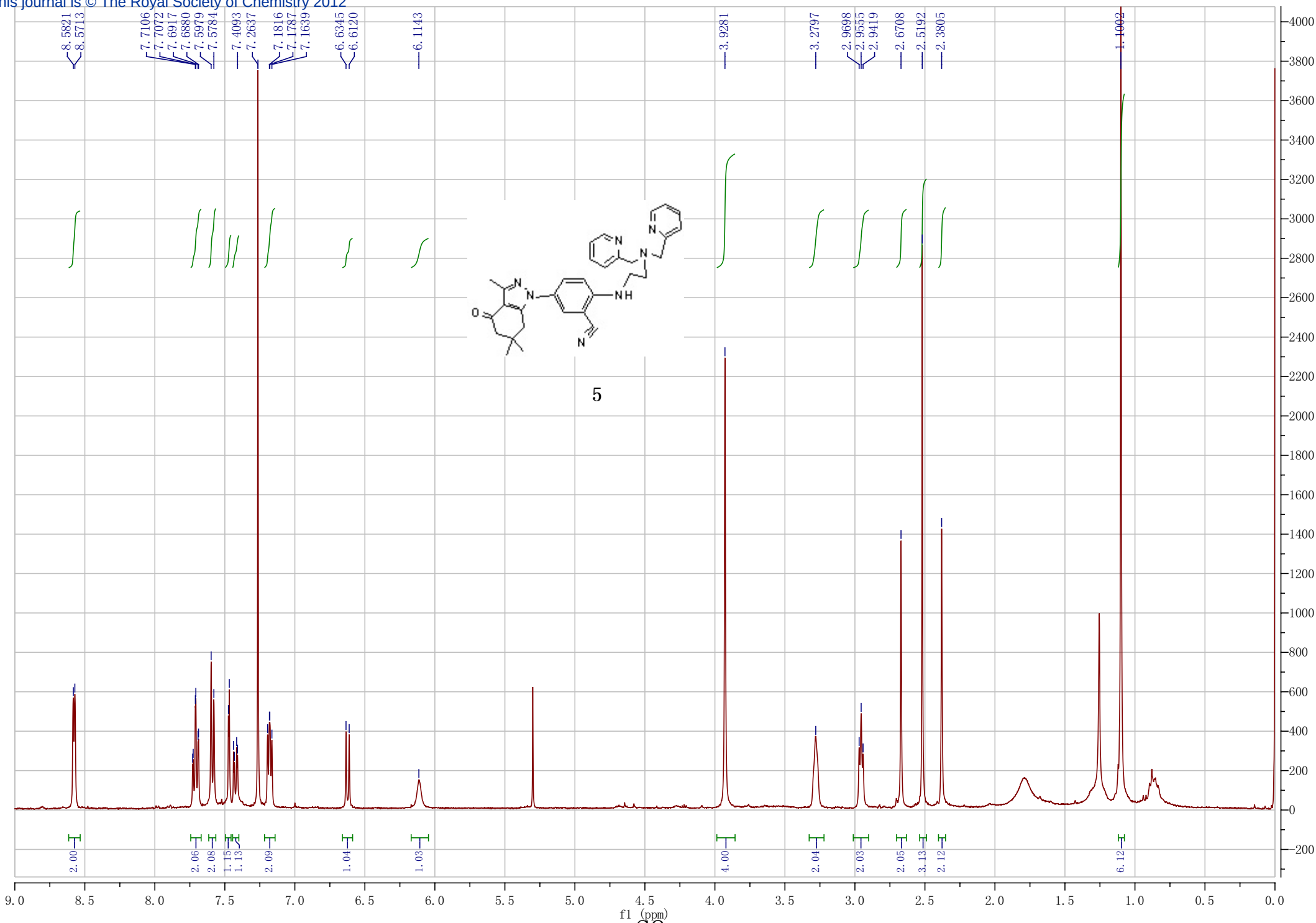
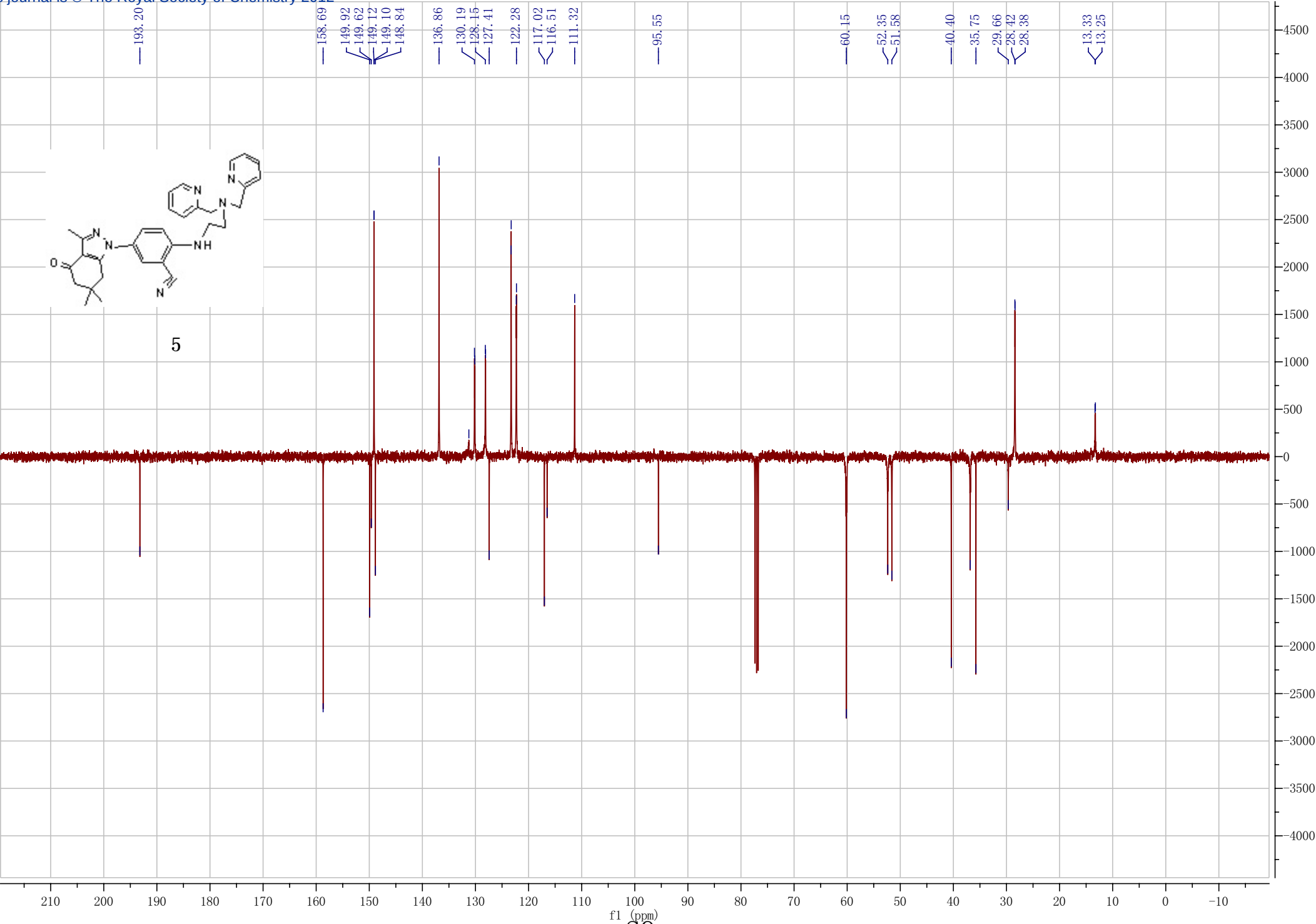


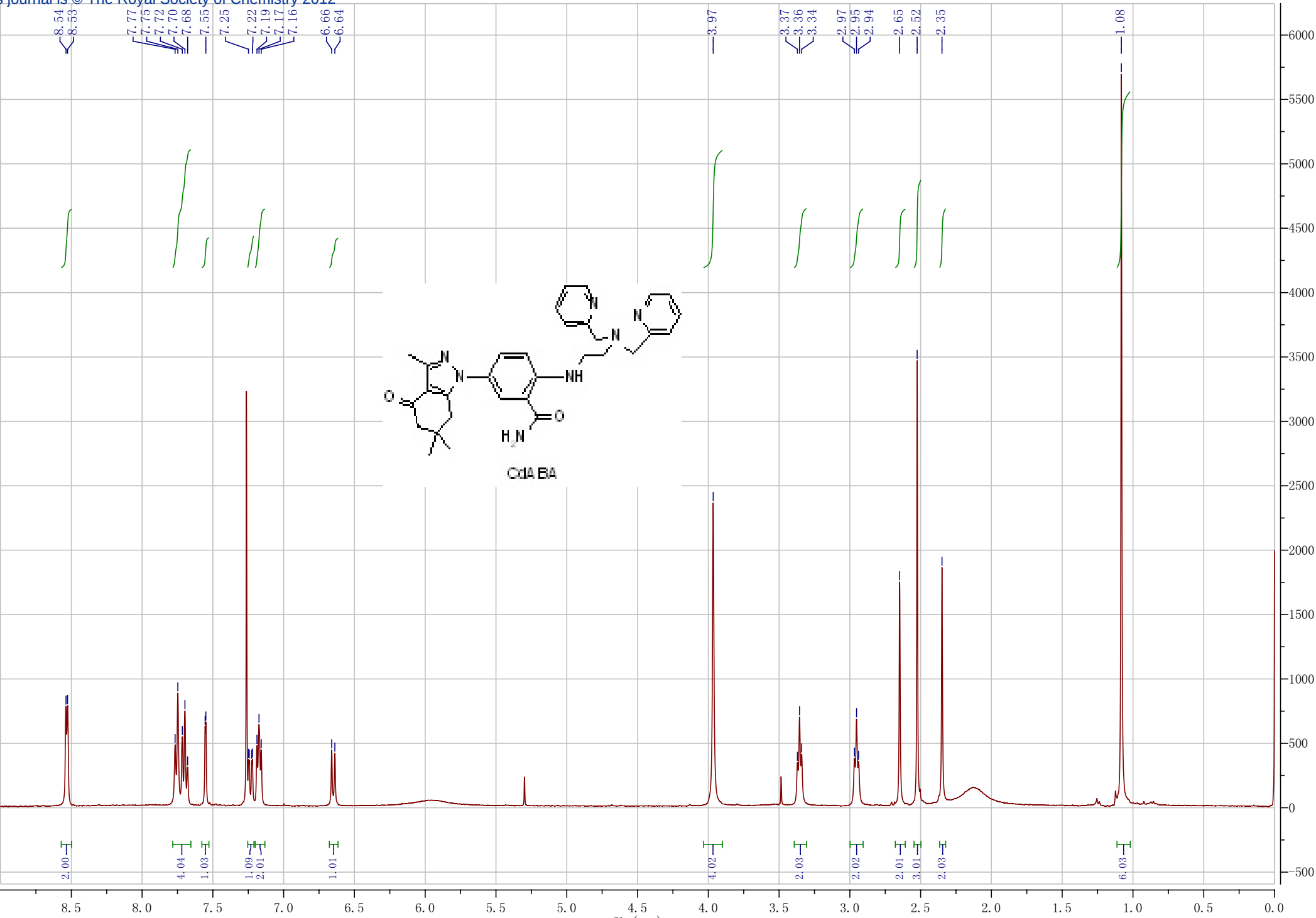
Figure S6. ESI-Mass spectrum of CdABA' + 1.0 equiv Zn²⁺ in methanol.

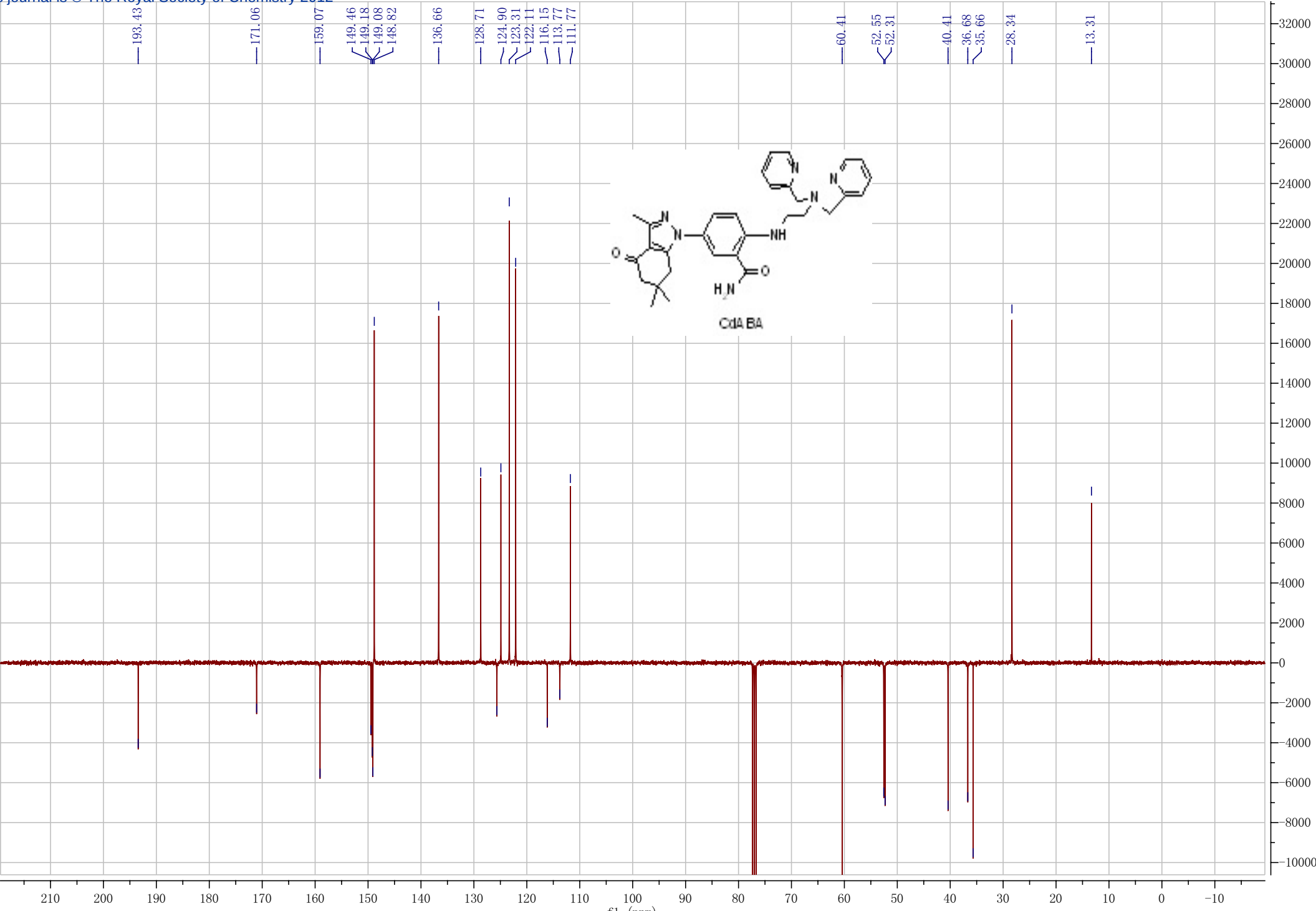


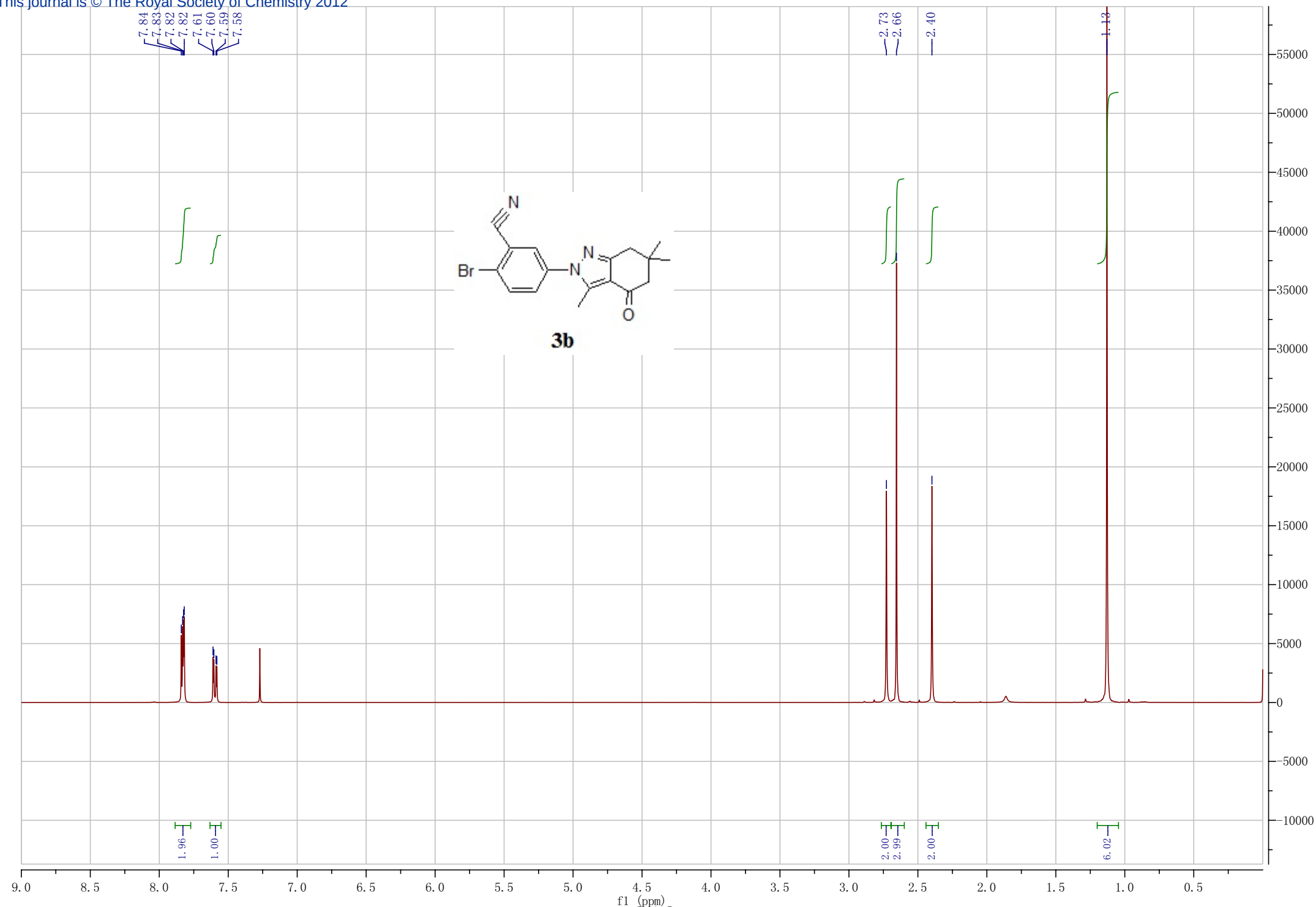


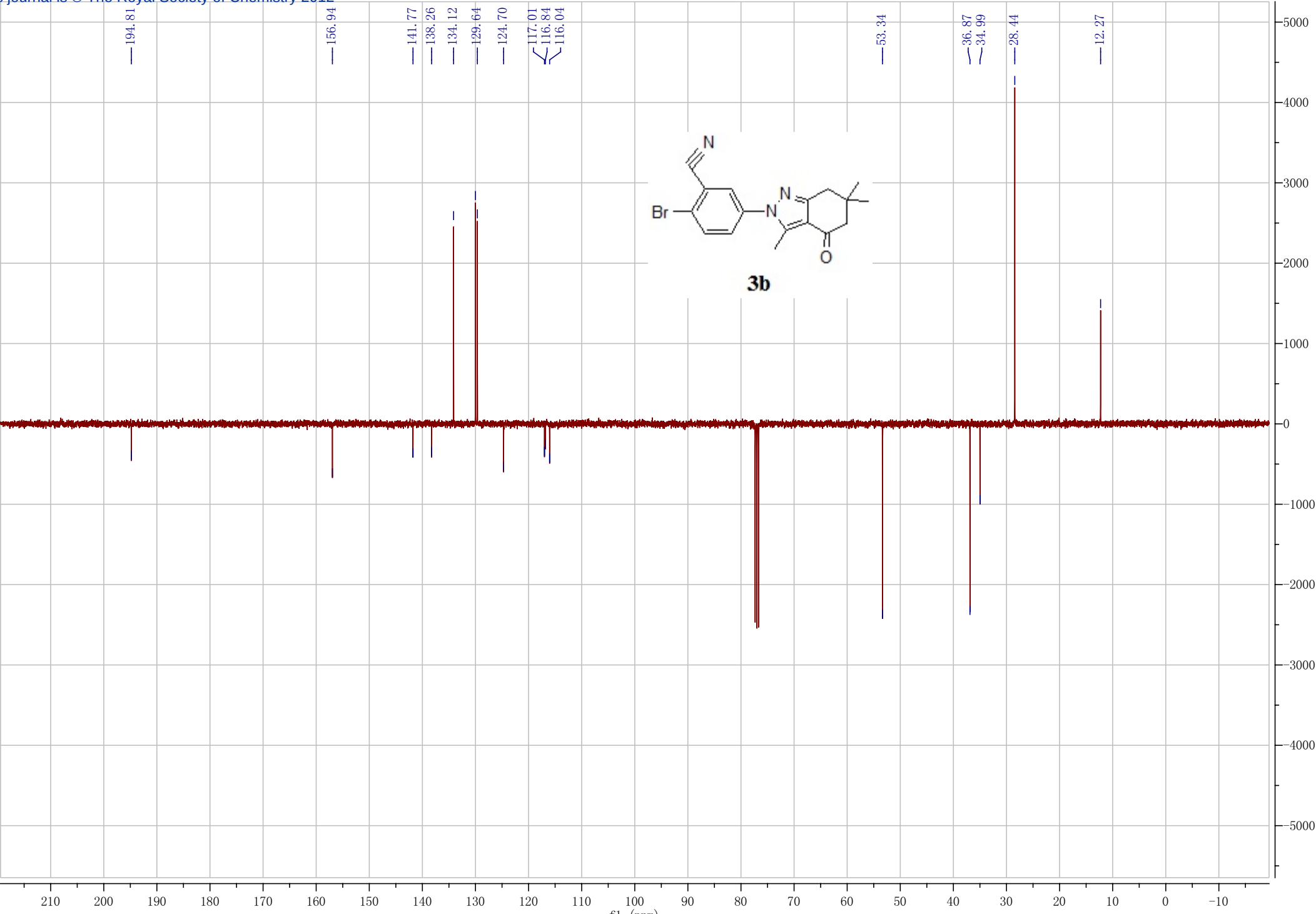


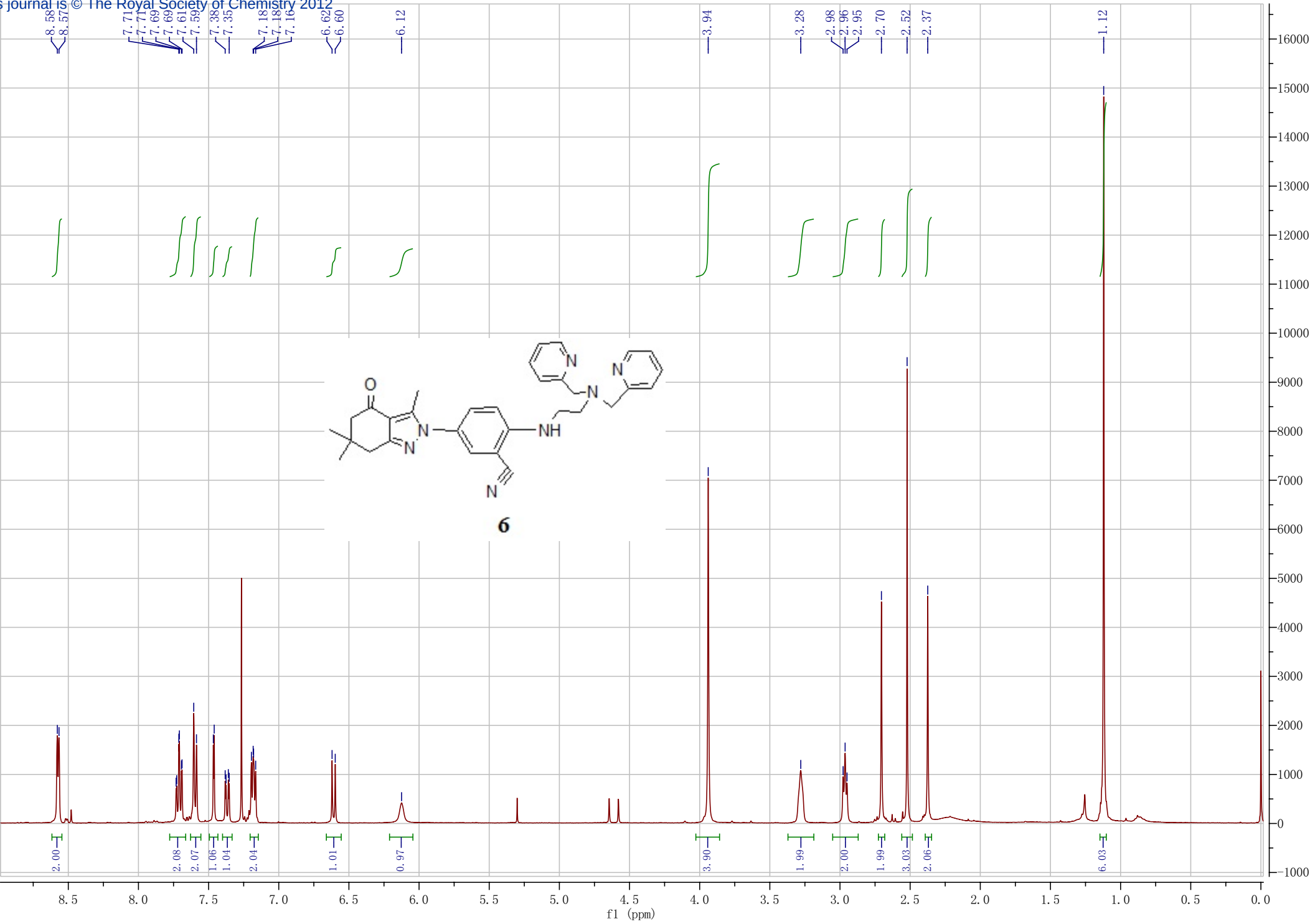


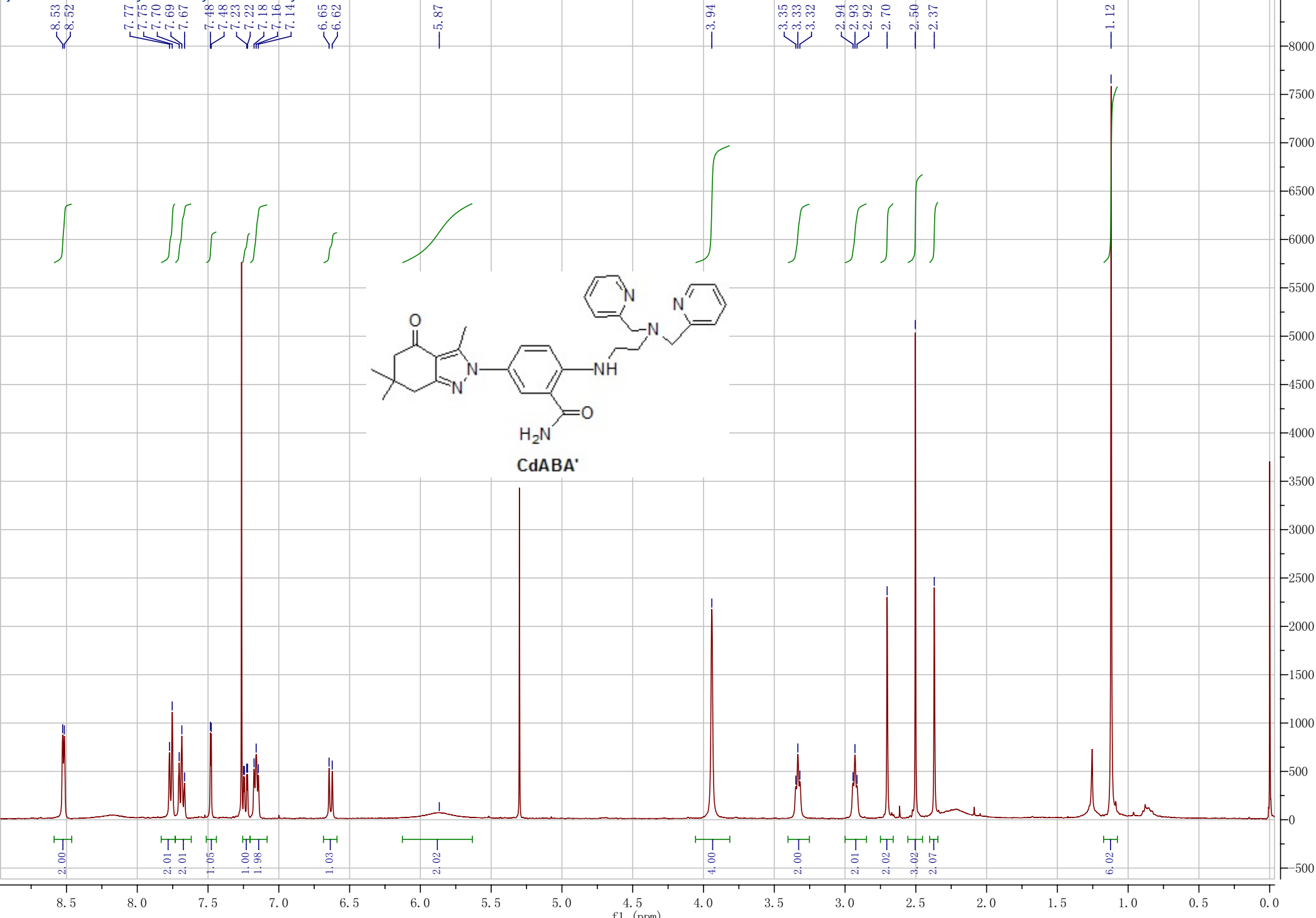


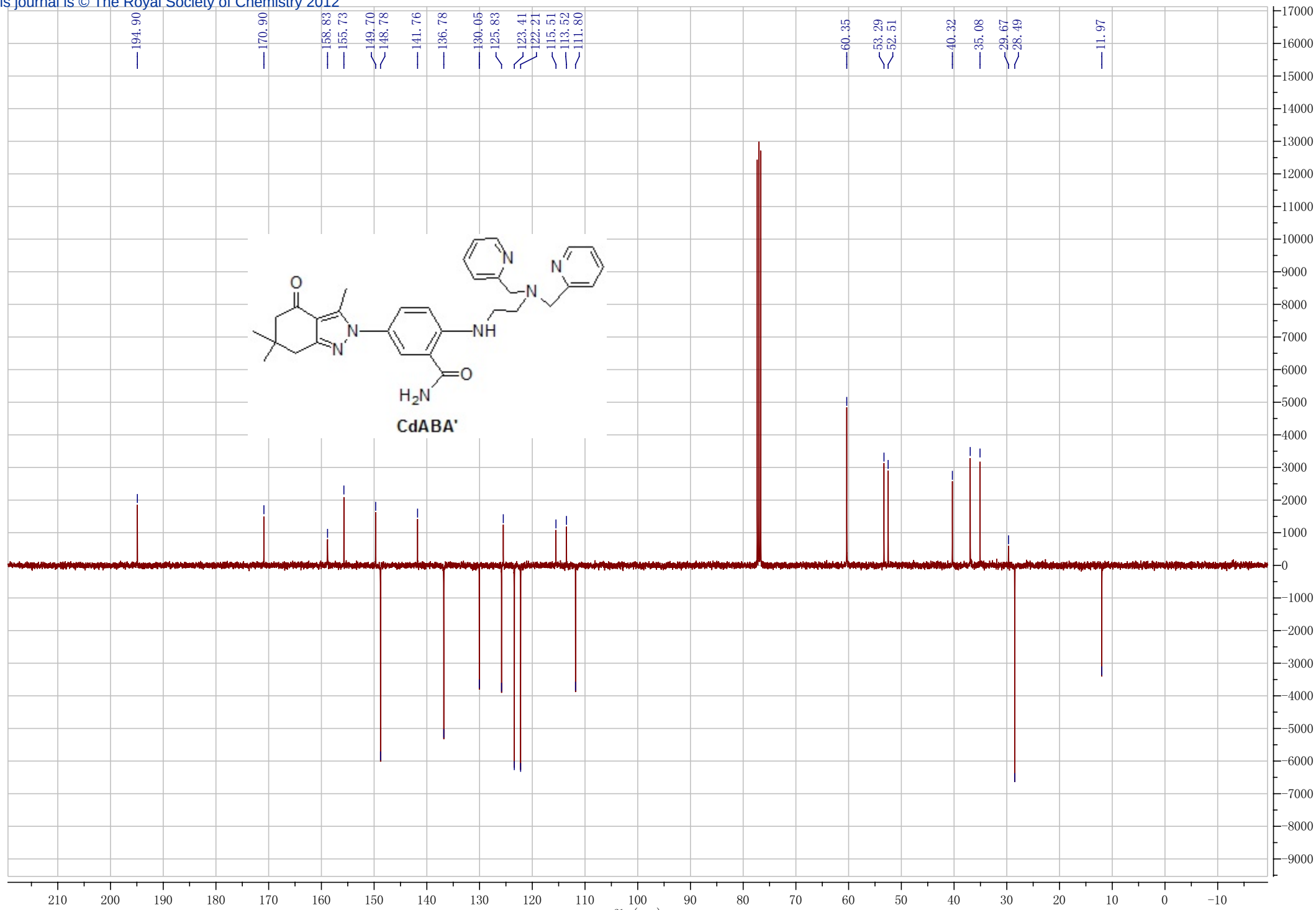


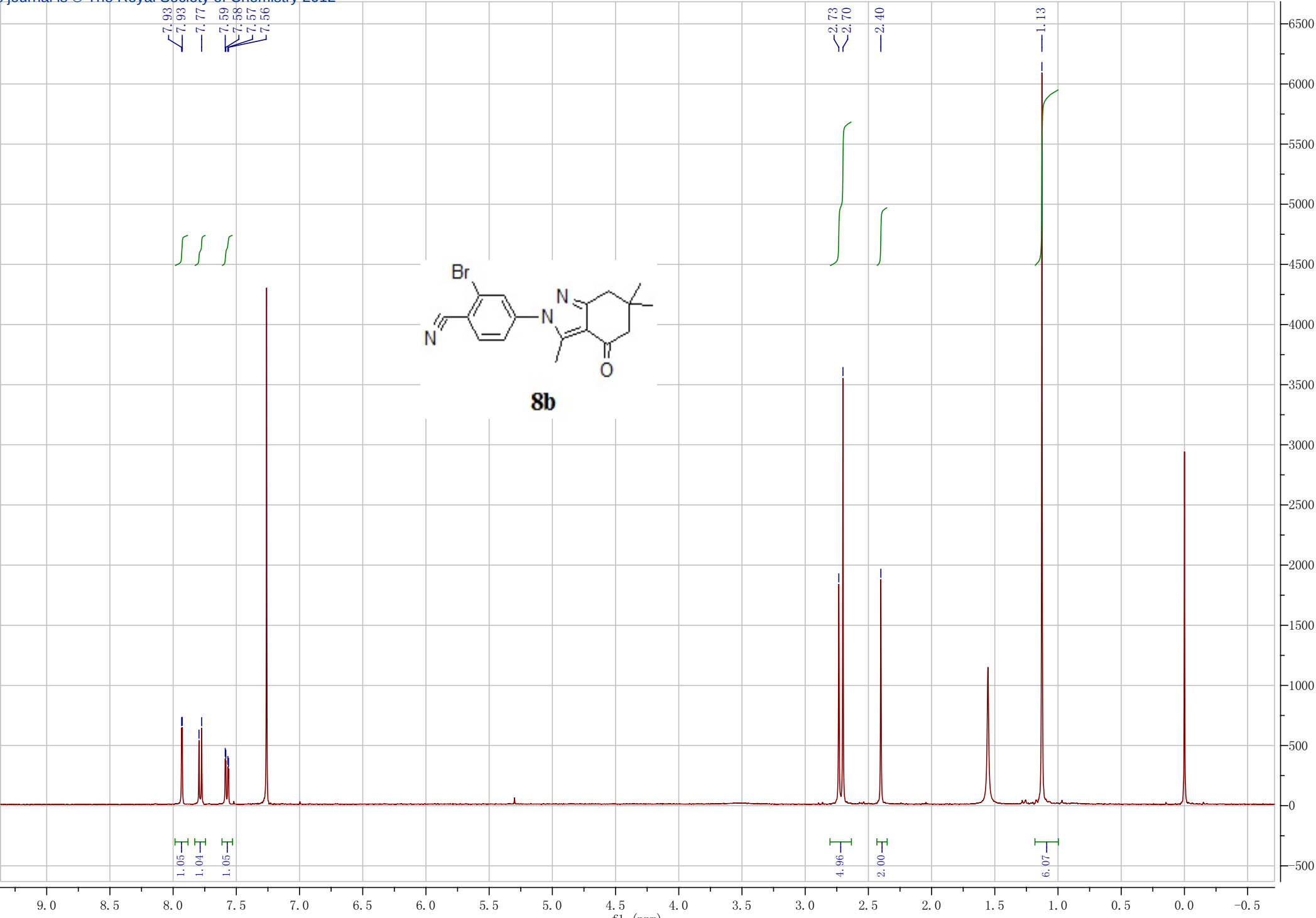


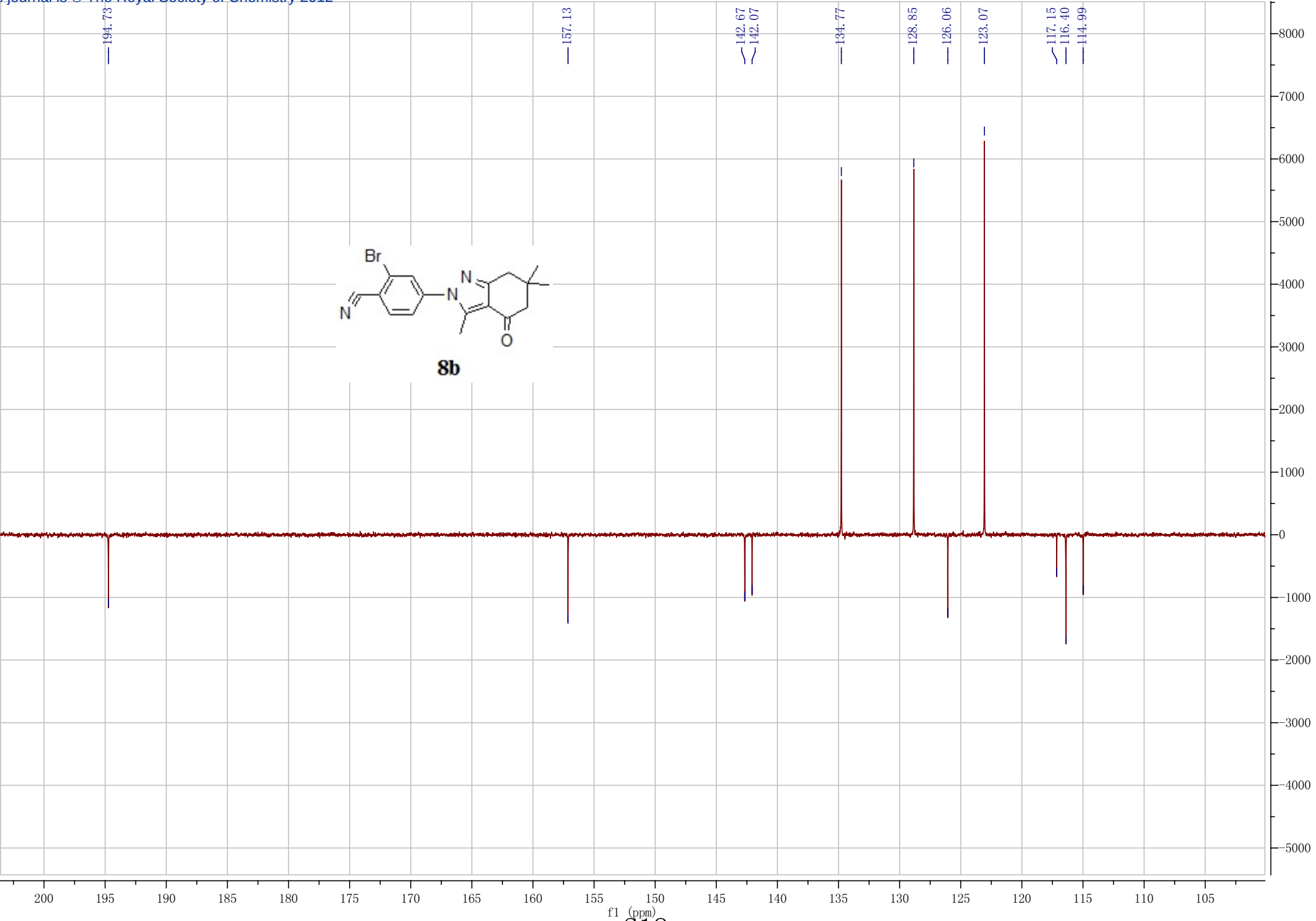
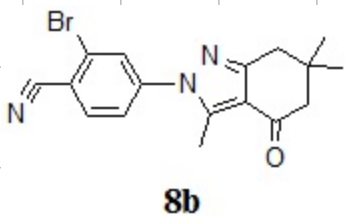


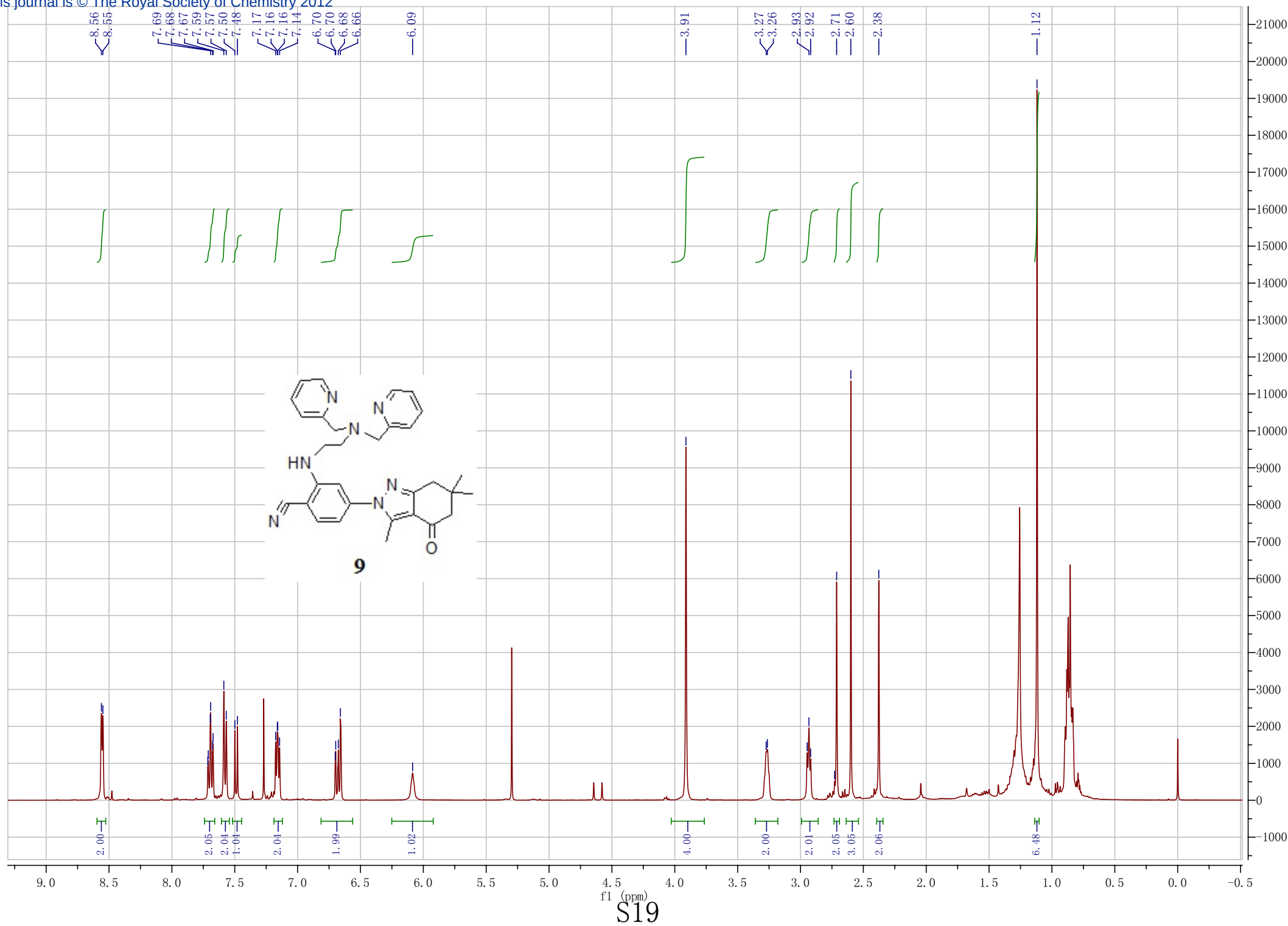


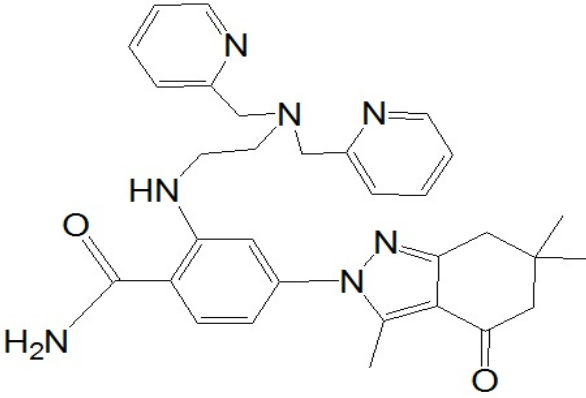












ZnABA'

