Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

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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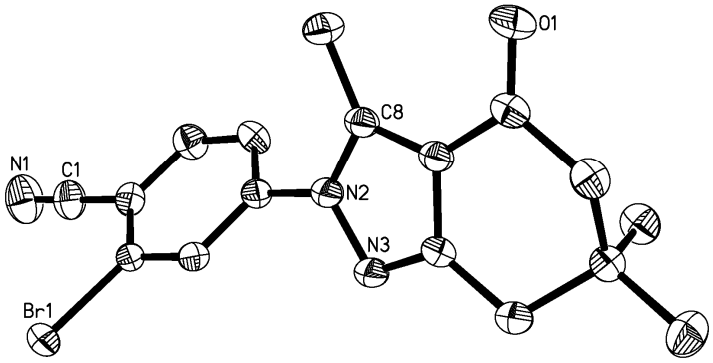


Figure S1. X-ray crystallographic structure of **8b**.

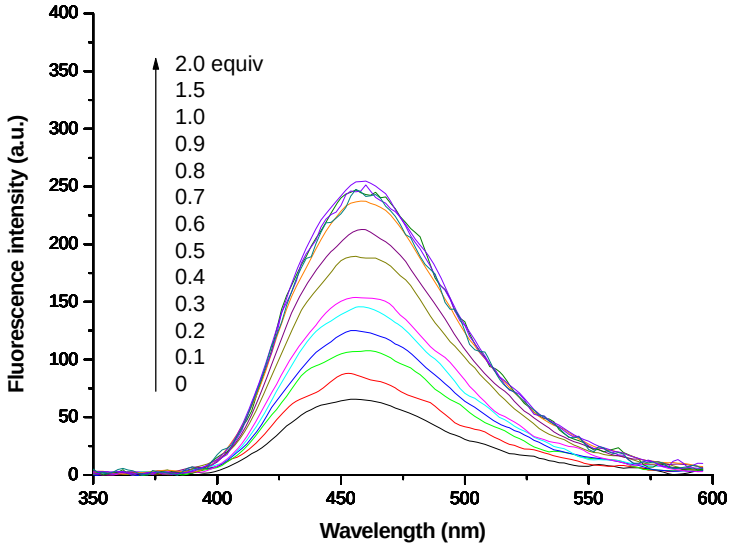


Figure S2. Fluorescence emission spectra (λ_{ex} = 260 nm) of CdABA (10 μM, 25mM HEPES buffer, 0.1 M $NaClO_4$, pH = 7.4, I = 0.1) upon addition of Cd^{2+} [added as $Cd(ClO_4)_2$, 0-20 μM].

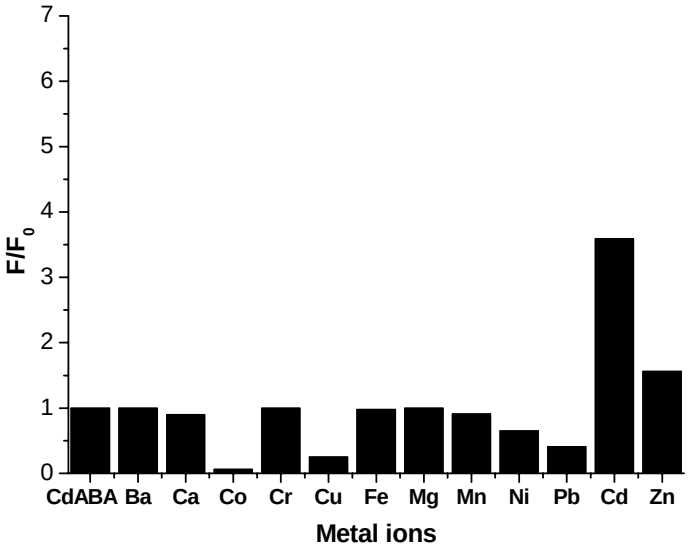


Figure S3. Selectivity of CdABA towards various metal ions. Experimental conditions: CdABA (10 μM, 25mM HEPES buffer, 0.1 M $NaClO_4$, pH = 7.4, I = 0.1), 10 μM Ba^{2+}, Ca^{2+}, Co^{2+}, Cr^{3+}, Cu^{2+}, Fe^{3+}, Mg^{2+}, Mn^{2+}, Ni^{2+}, Pb^{2+}, Cd^{2+} and Zn^{2+}, λ_{ex} = 260 nm, λ_{em} = 454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

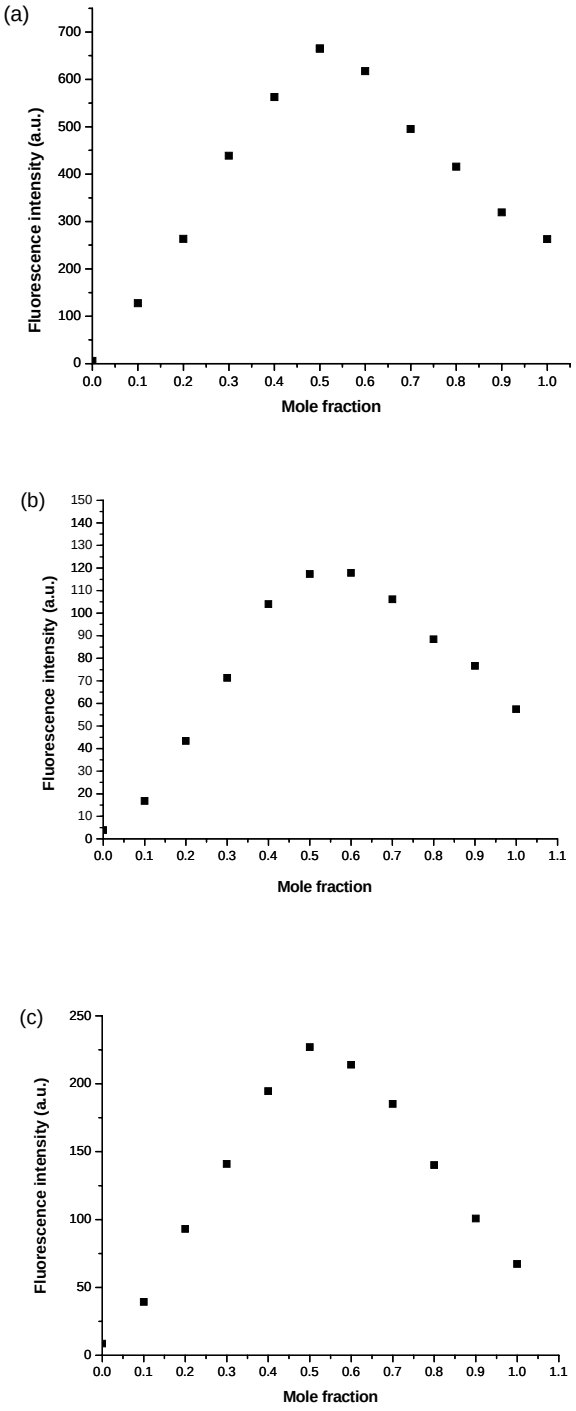


Figure S4. A Job's plot of (a) CdABA' and Cd^{2+}, (b) CdABA and Cd^{2+}, and (c) ZnABA' and Zn^{2+}. The total concentrations of sensors and Zn^{2+}/Cd^{2+} are 10 μM. The experiments were measured at room temperature in buffer solution (HEPES buffer, 25 mM, 0.1 M $NaClO_4$, pH = 7.4, I = 0.1).

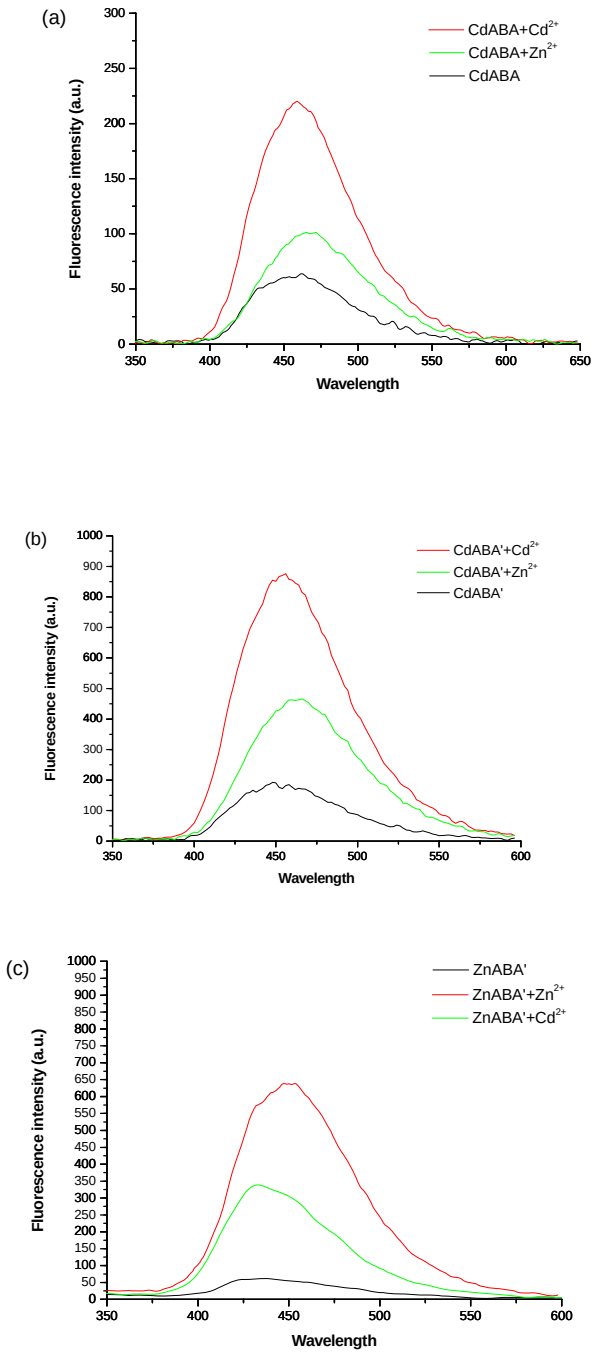


Figure S5. Fluorescence emission spectra of (a) CdABA, CdABA with Zn^{2+} and CdABA with Cd^{2+}, (b) CdABA', CdABA' with Zn^{2+} and CdABA' with Cd^{2+}, (c) ZnABA', ZnABA' with Zn^{2+} and ZnABA' with Cd^{2+} in aqueous solution (10 μM, 25mM HEPES buffer, 0.1 M $NaClO_4$, pH = 7.4, I = 0.1). All the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

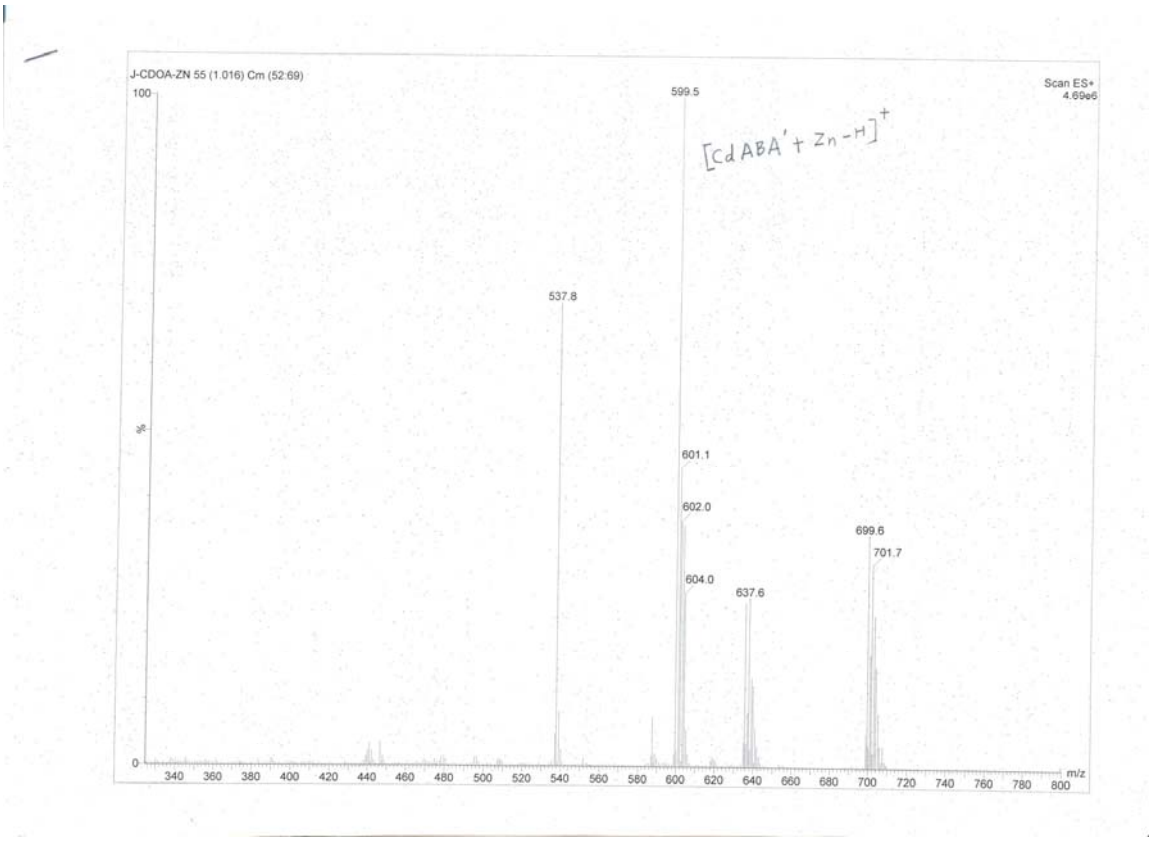
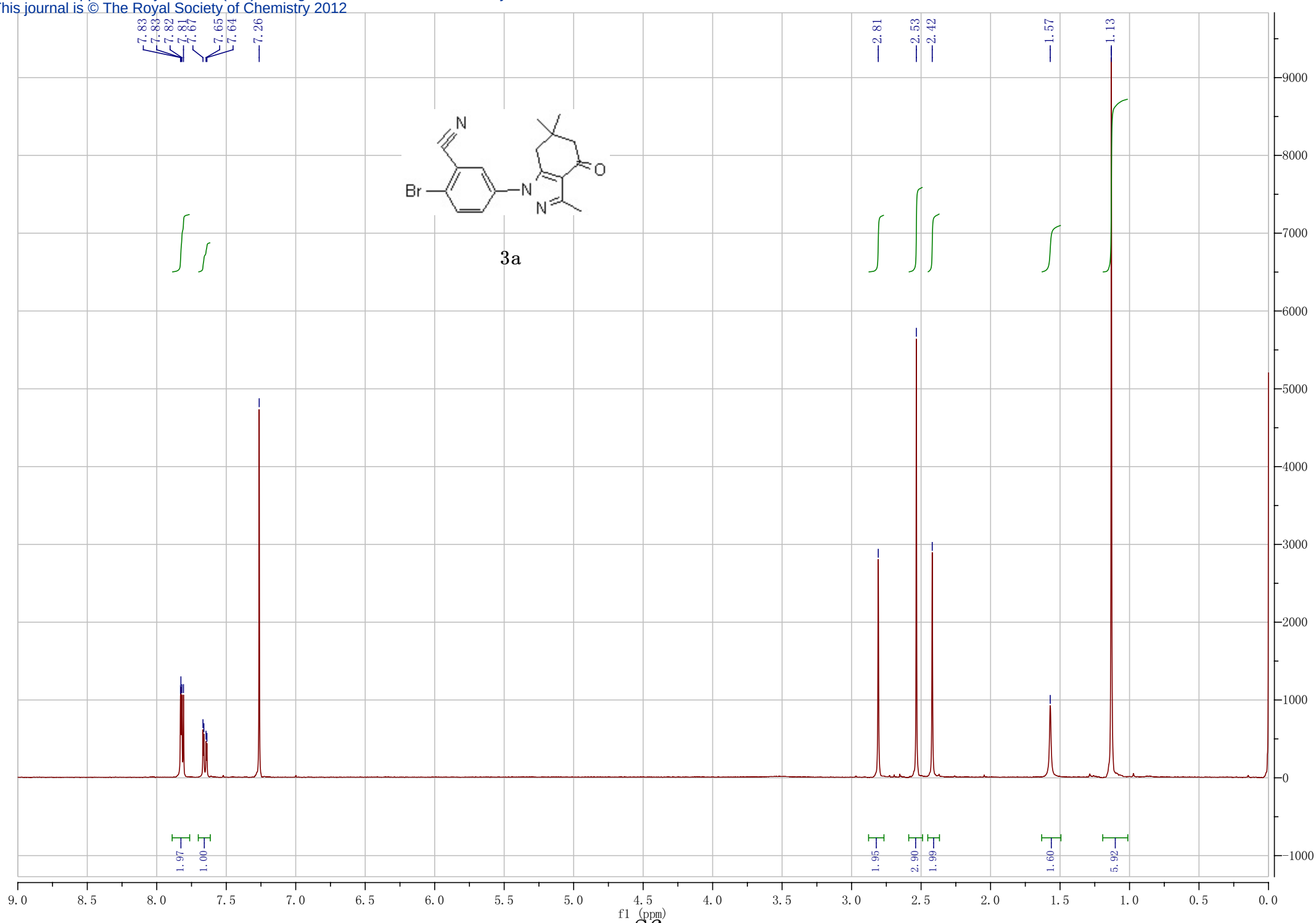
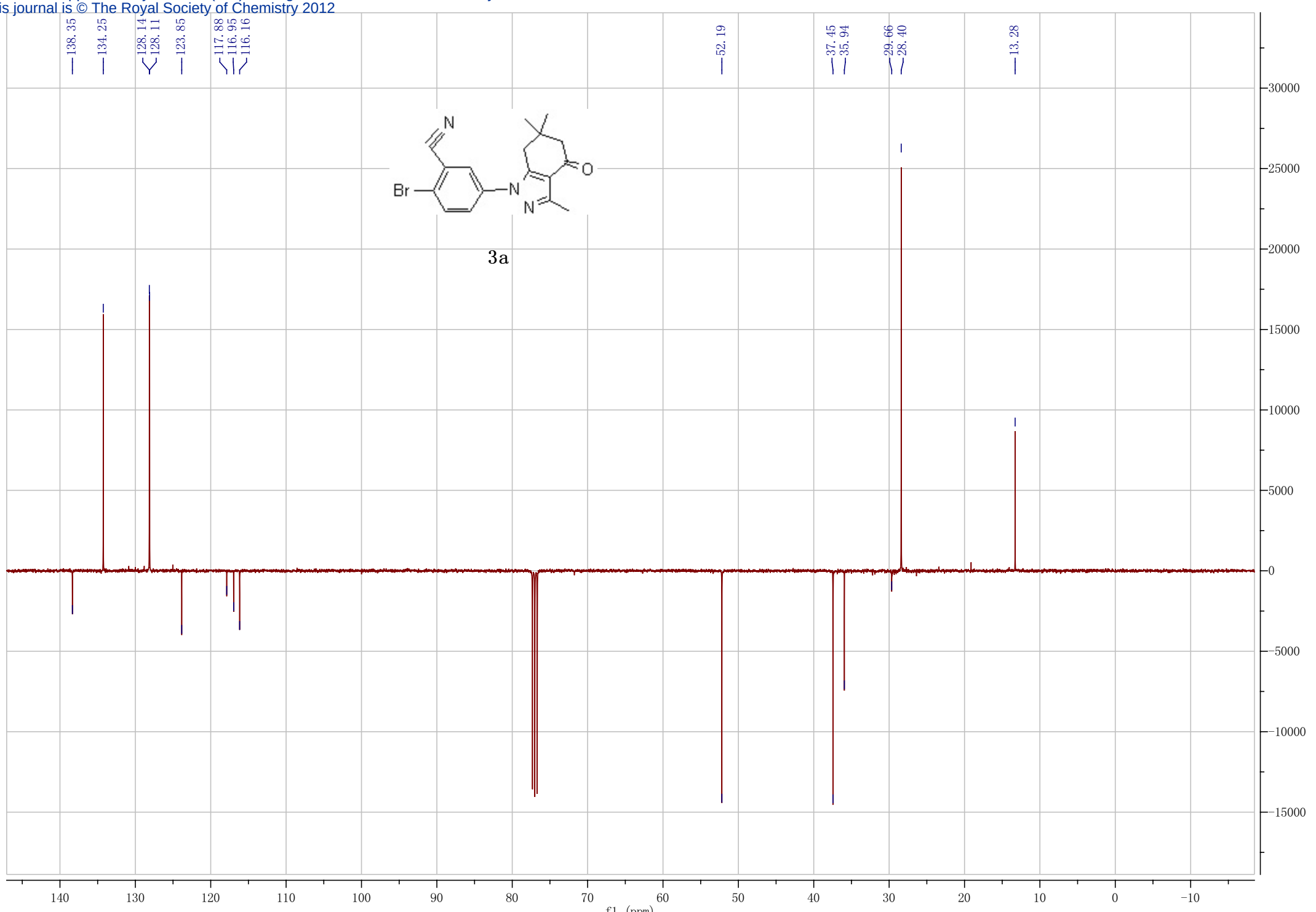


Figure S6. ESI-Mass spectrum of CdABA' + 1.0 equiv Zn^{2+} in methanol.





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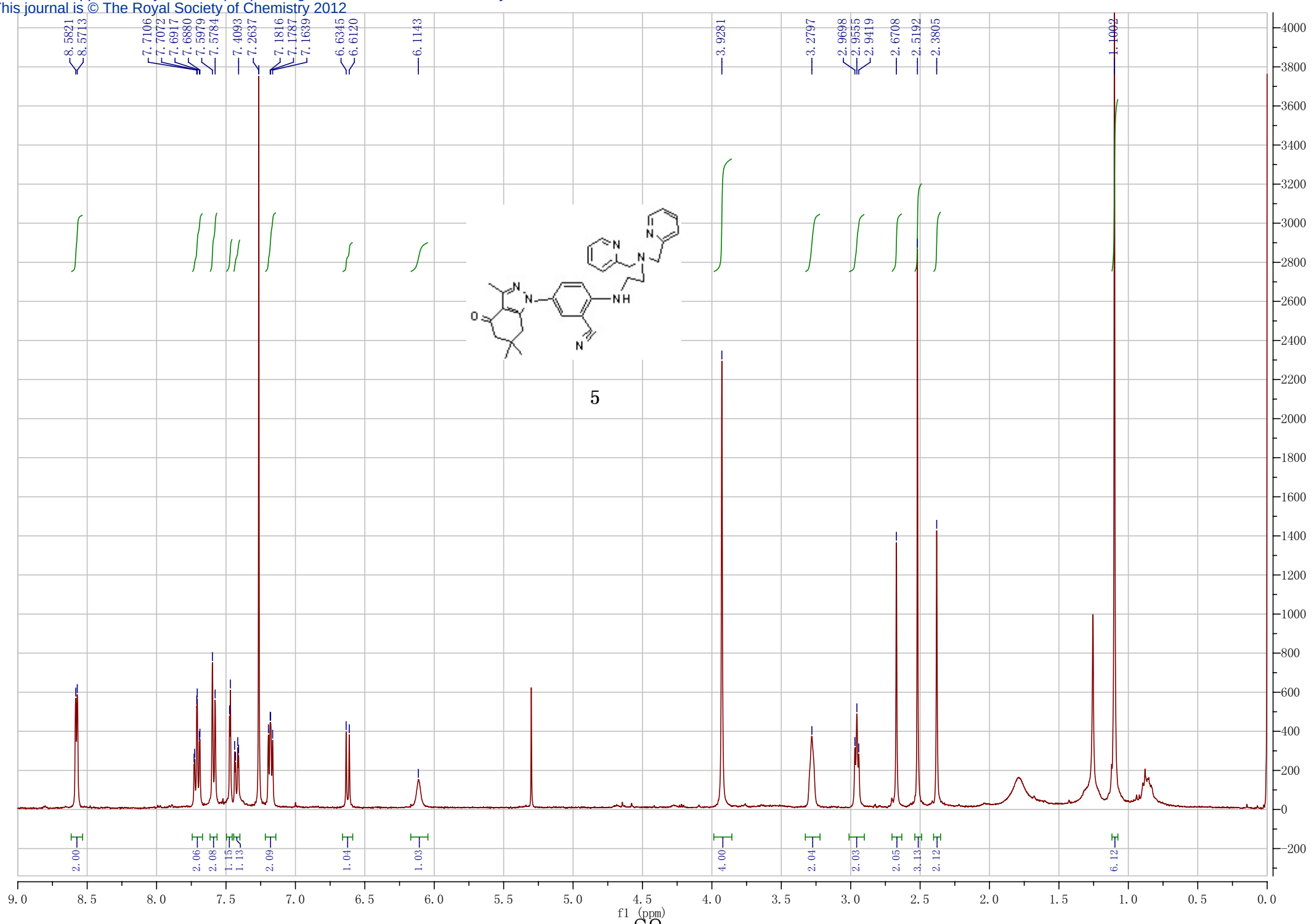

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