

*Supplementary Materials*

# Catalytic, Theoretical, and Biological Investigations of Ternary Metal (II) Complexes Derived from L-Valine-Based Schiff Bases and Heterocyclic Bases

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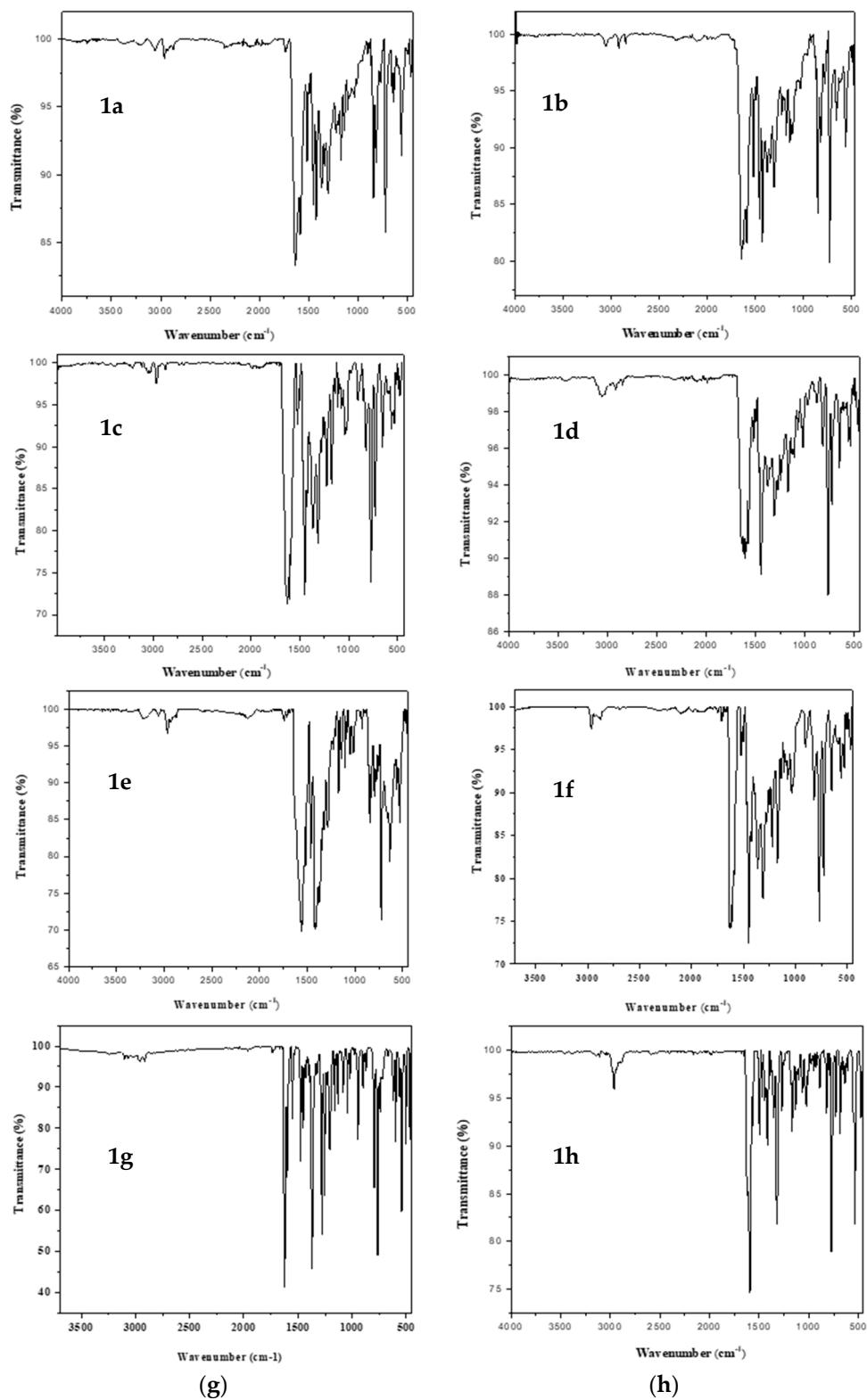
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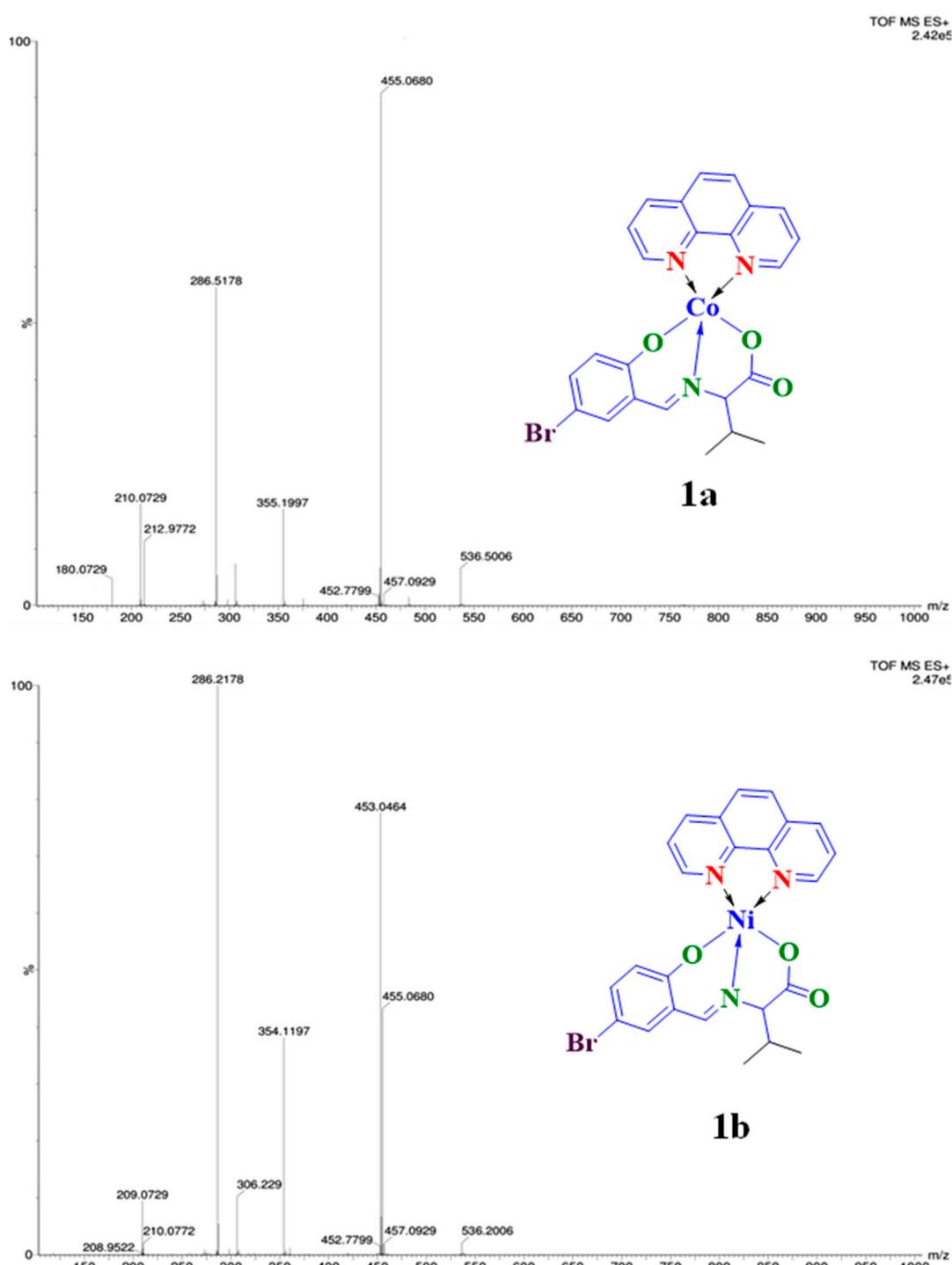
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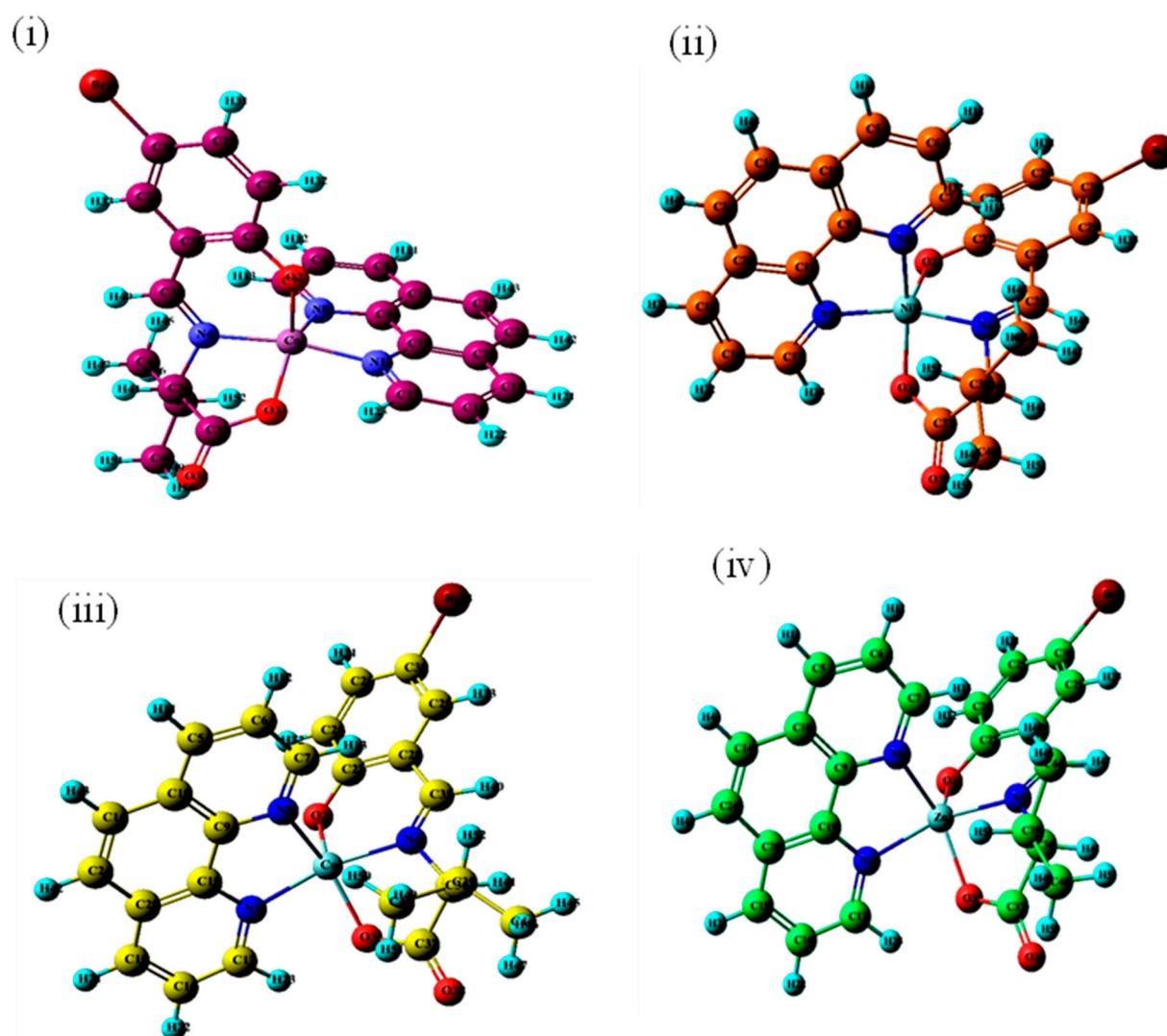
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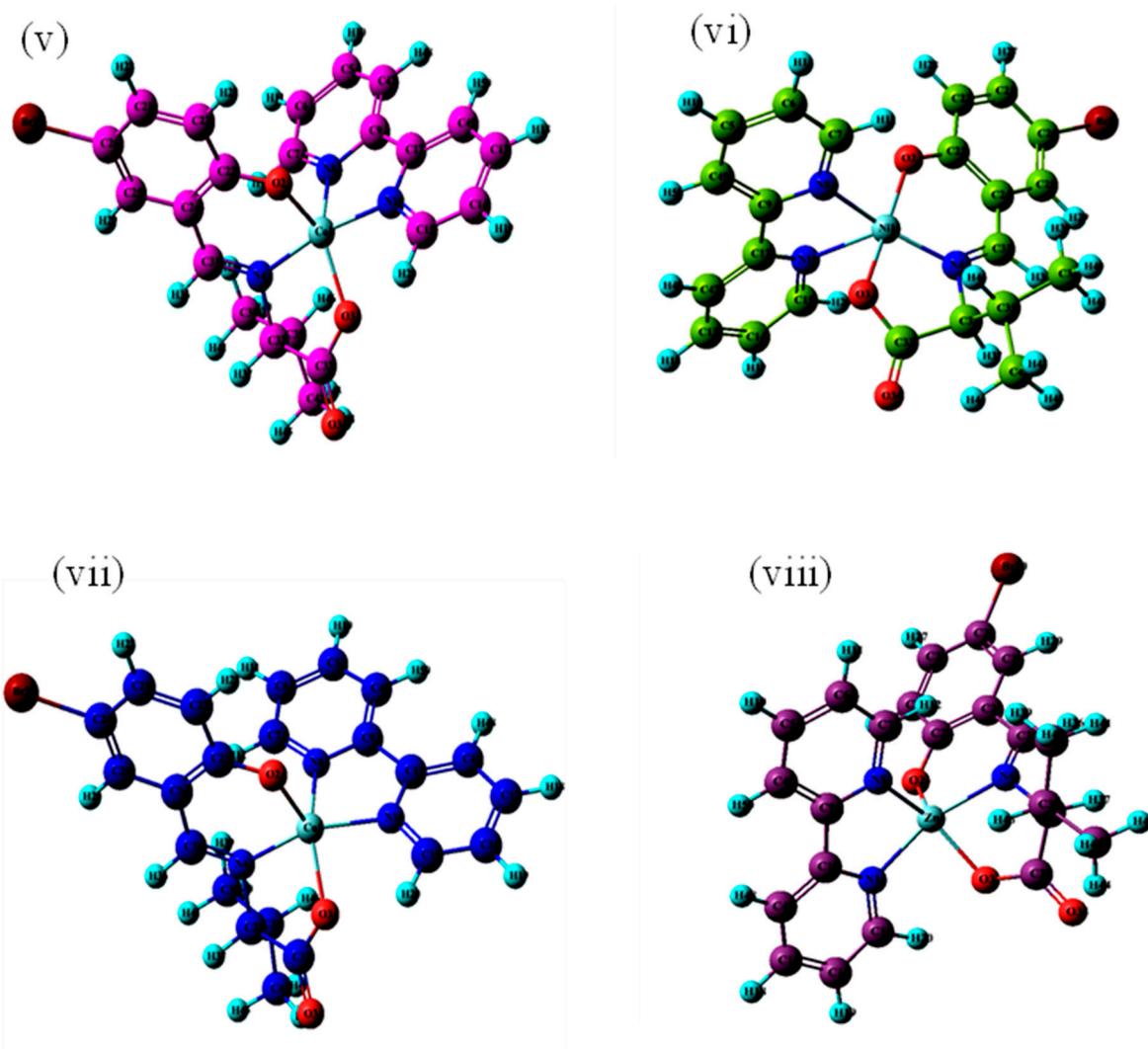
**Figure S1.** FT-IR spectra of metal(II) complexes **1a–1h**.



**Figure S2.** ESI-Mass spectra of metal(II) complexes  $[\text{Co}(\text{L})(\text{phen})]$  **1a** and  $[\text{Ni}(\text{L})(\text{phen})]$  **1b**.



**Figure S3.** Optimized molecular structure of (i) cobalt(II) complex 1a, (ii) nickel(II) complex 1b, (iii) copper(II) complex 1c and (iv) zinc(II) complex 1d using B3LYP/LACVP++ basis set.



**Figure S4.** Optimized molecular structure of (v) cobalt(II) complex 1e, (vi) nickel(II) complex 1f, (vii) copper(II) complex 1g and (viii) zinc(II) complex 1h using B3LYP/LACVP++ basis set.