

Supporting Information

Binuclear nickel complexes of a new di(hydroxyphenyl)imidazolate

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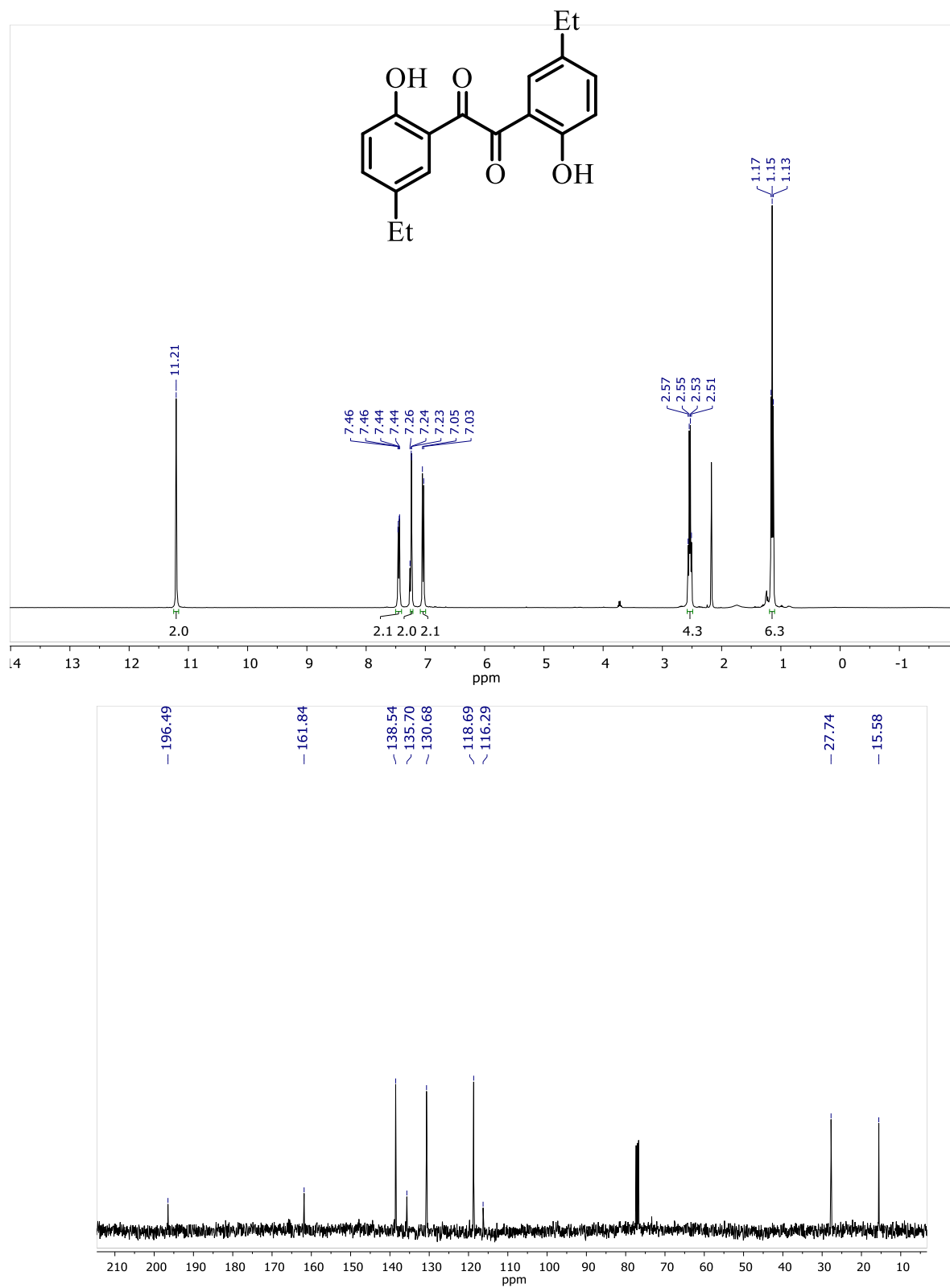
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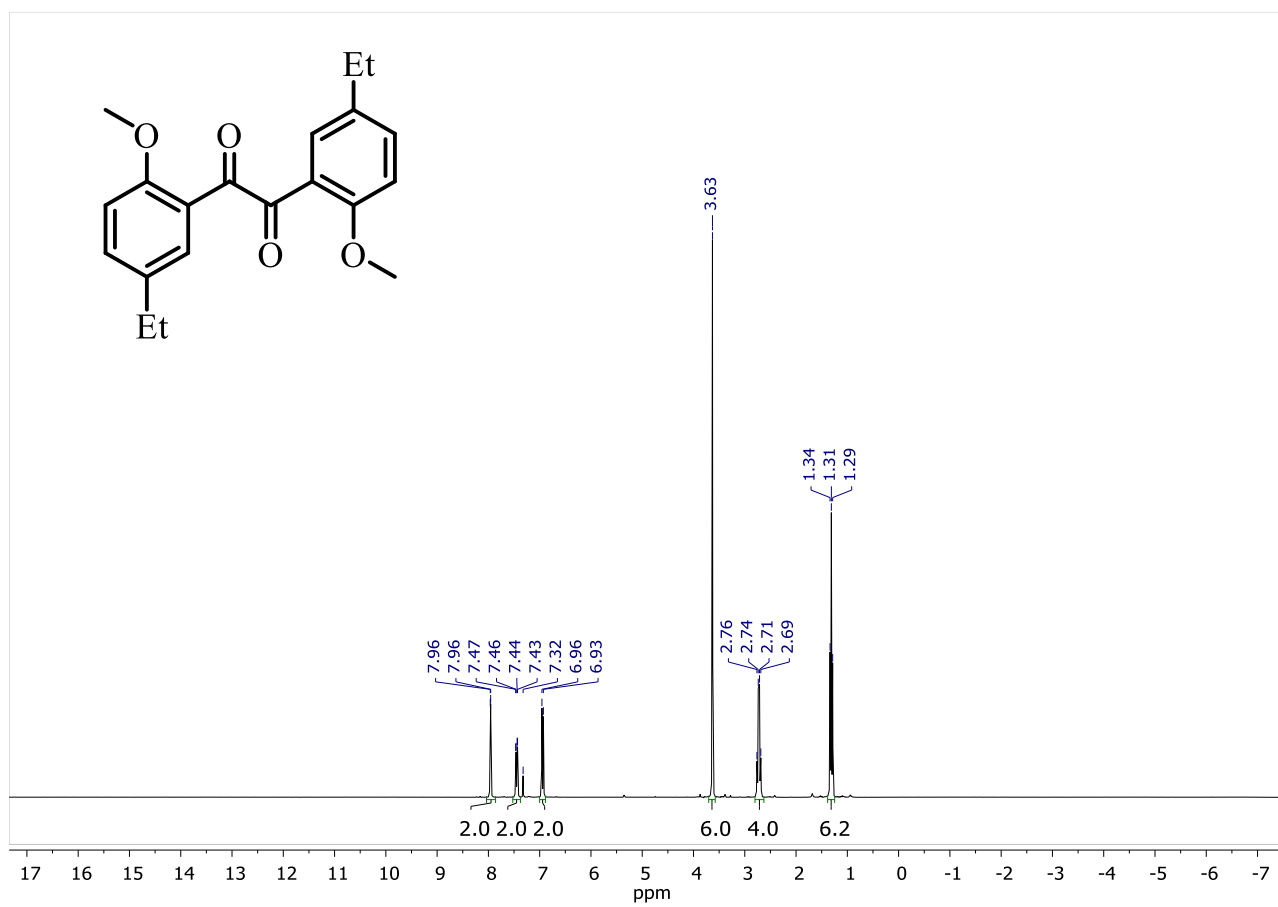
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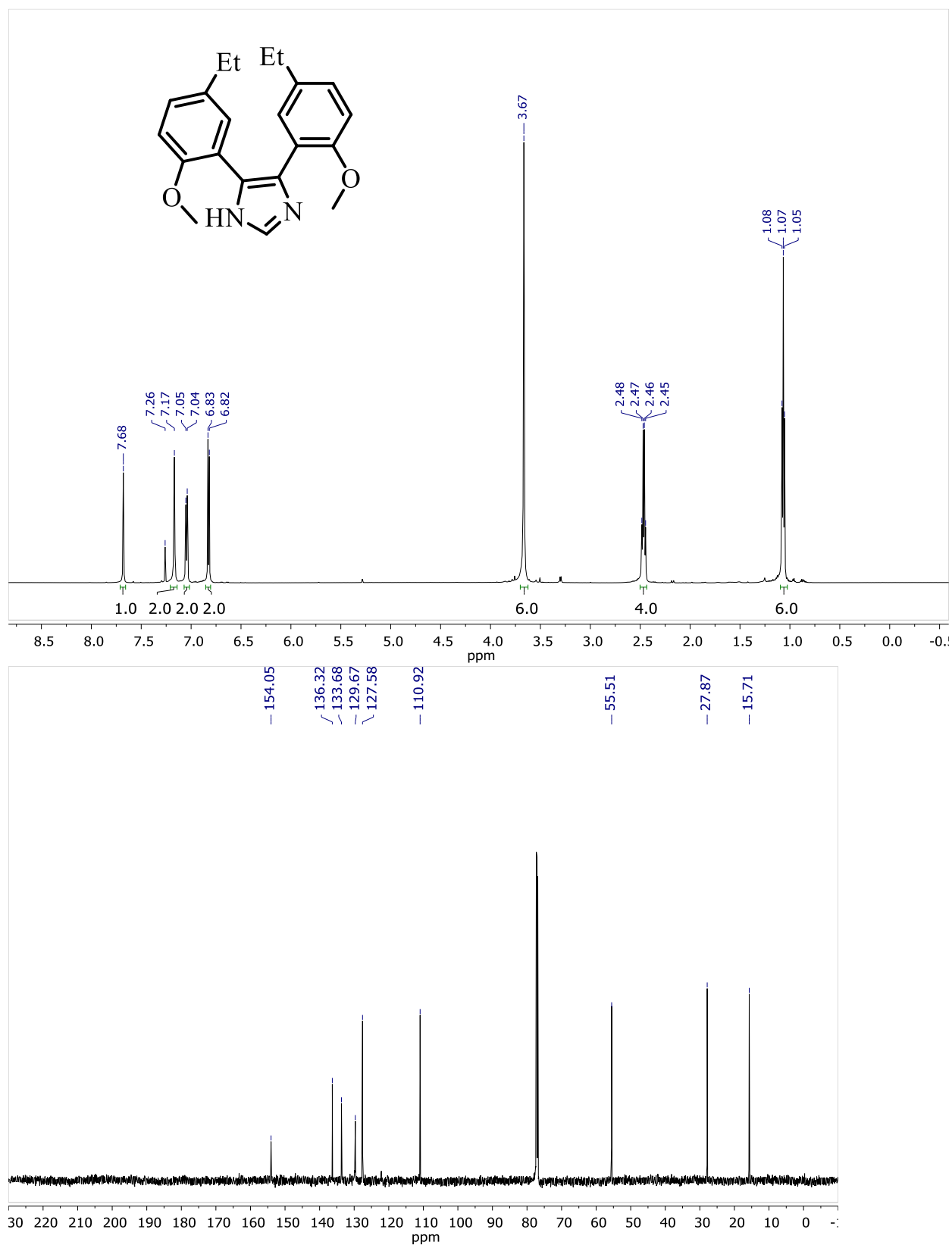
S1. ^1H (top) and ^{13}C NMR (bottom) spectra of 1,2-bis(5-ethyl-2-hydroxyphenyl)ethane-1,2-dione.



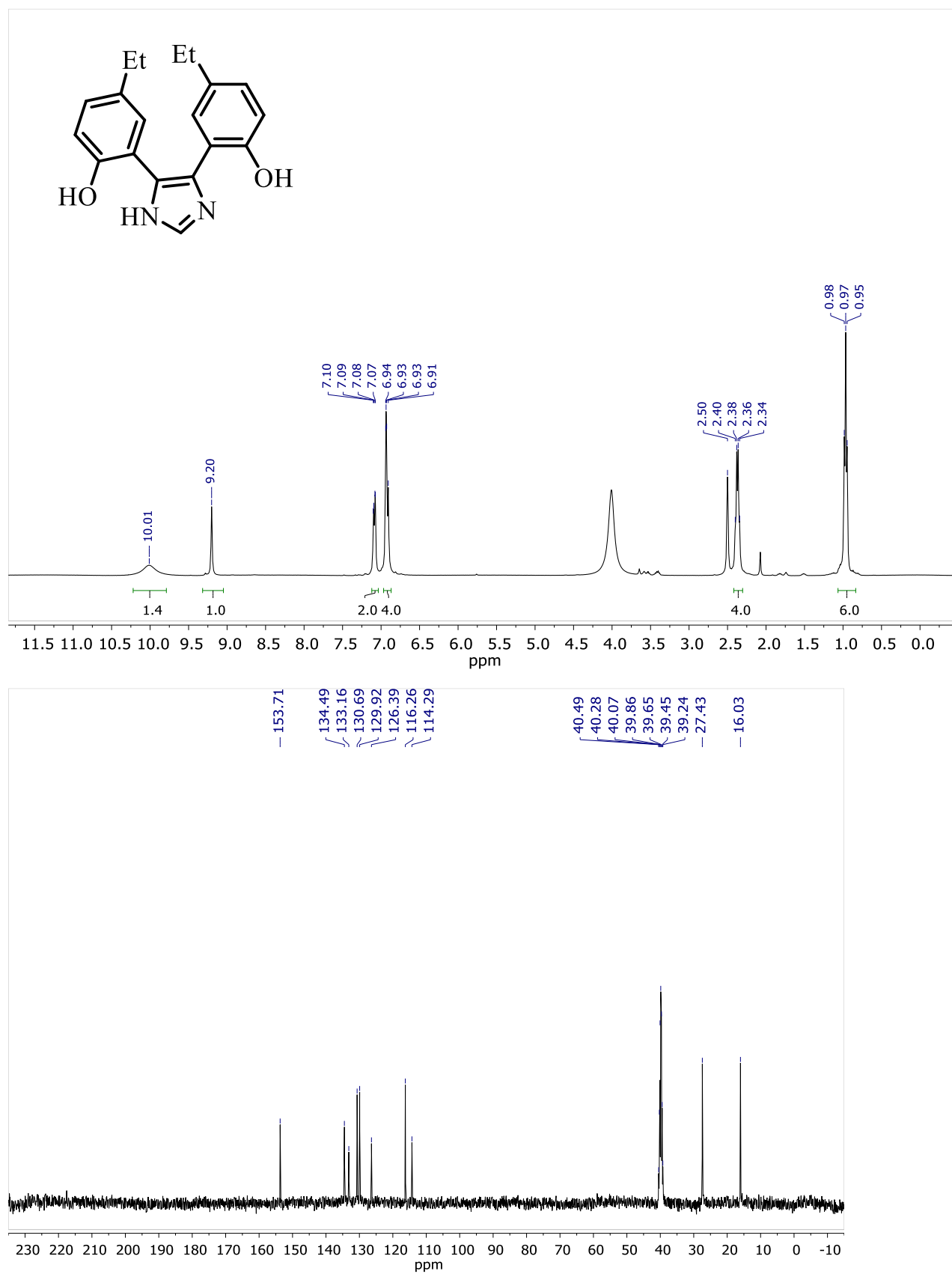
S2. ^1H spectra of 1,2-bis(5-ethyl-2-methoxyphenyl)ethane-1,2-dione.



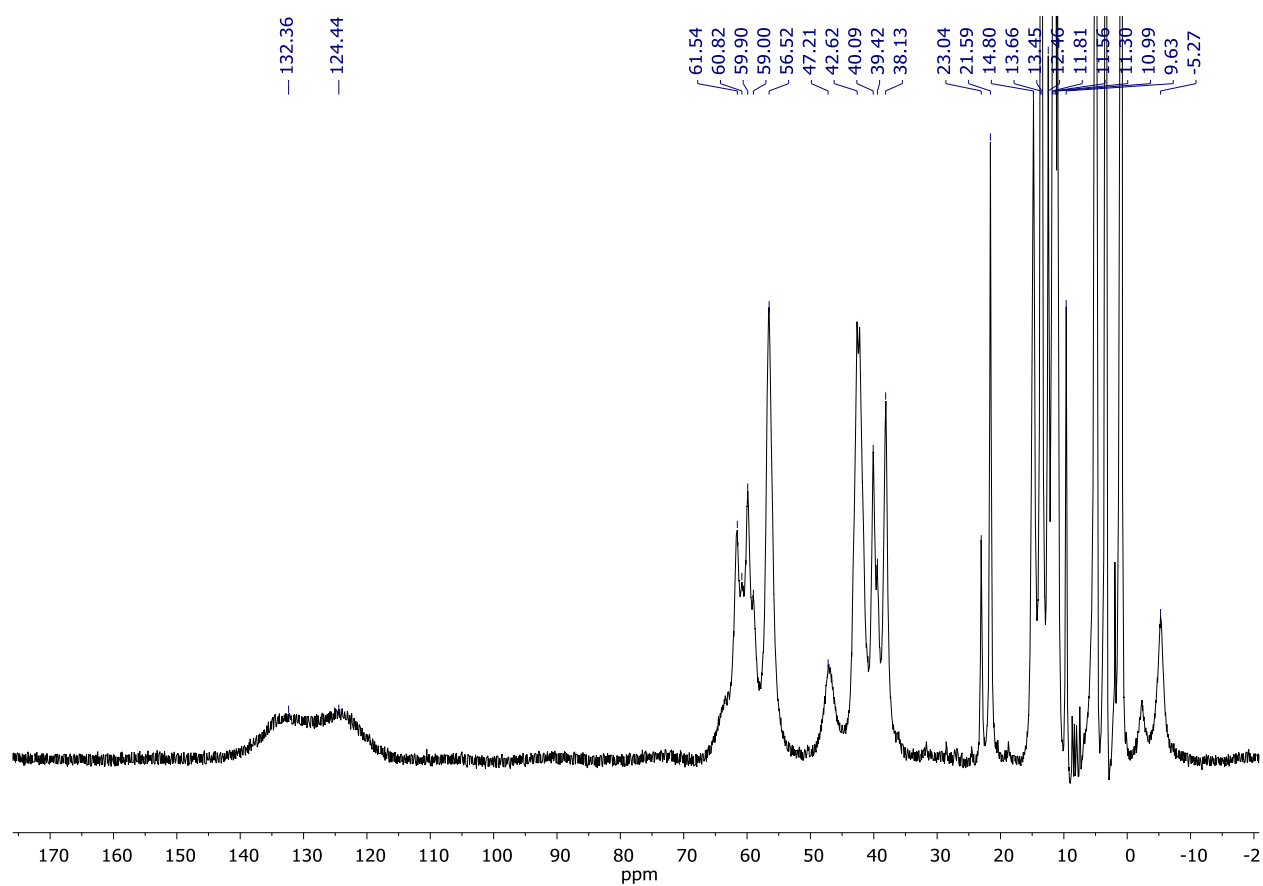
S3. ^1H (top) and ^{13}C NMR (bottom) spectra of 4,5-bis(5-ethyl-2-methoxyphenyl)-1H-imidazole.



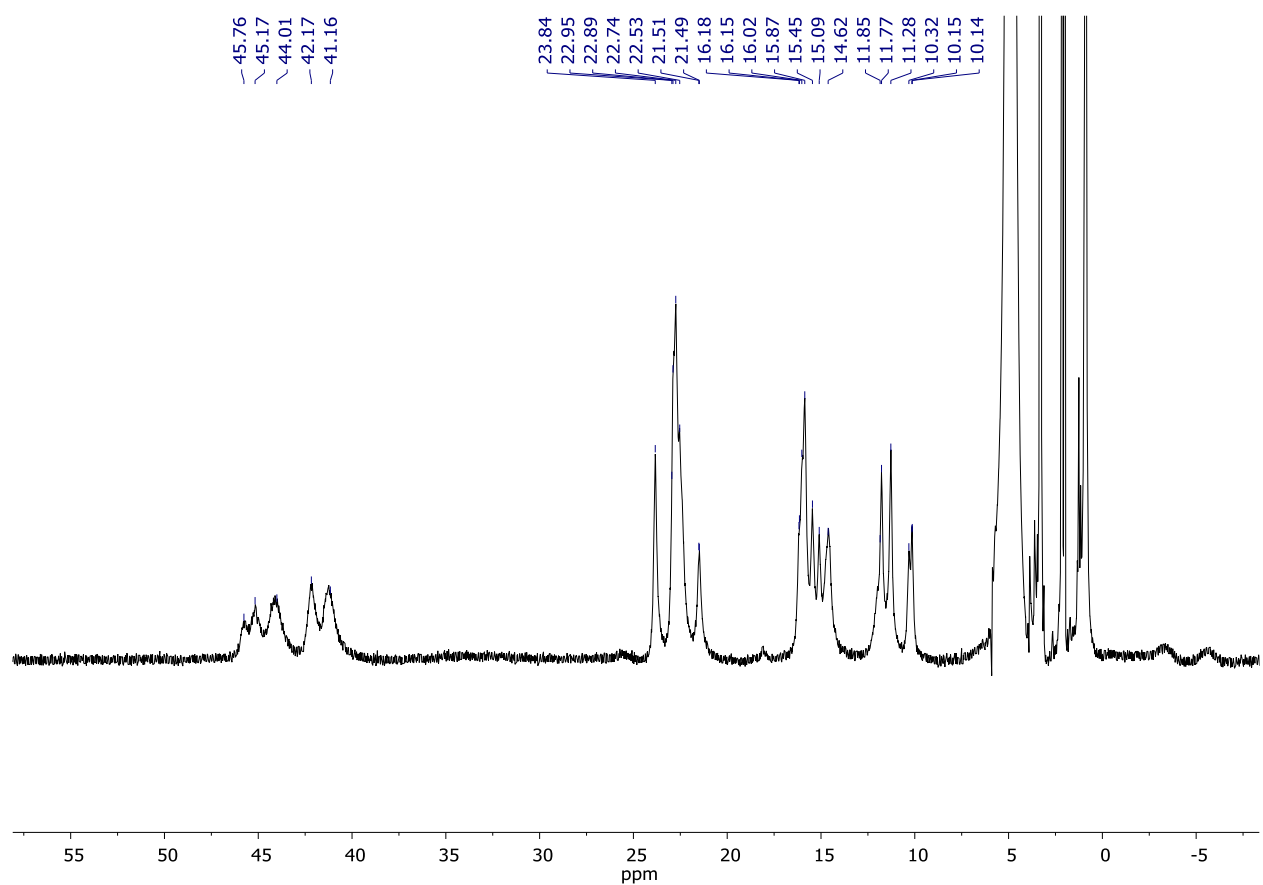
S4. ^1H (top) and ^{13}C NMR (bottom) spectra of 2,2'-(1H-imidazole-4,5-diyl)bis(4-ethylphenol)(L).



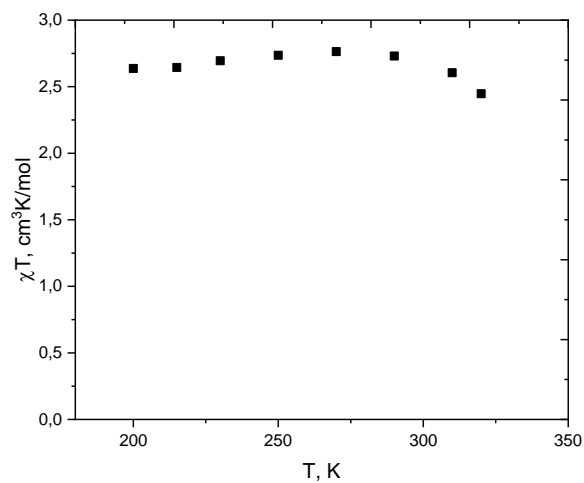
S5. ^1H NMR spectra of $[(\text{bipy})_4\text{Ni}_2(\text{L})](\text{Cl})$.



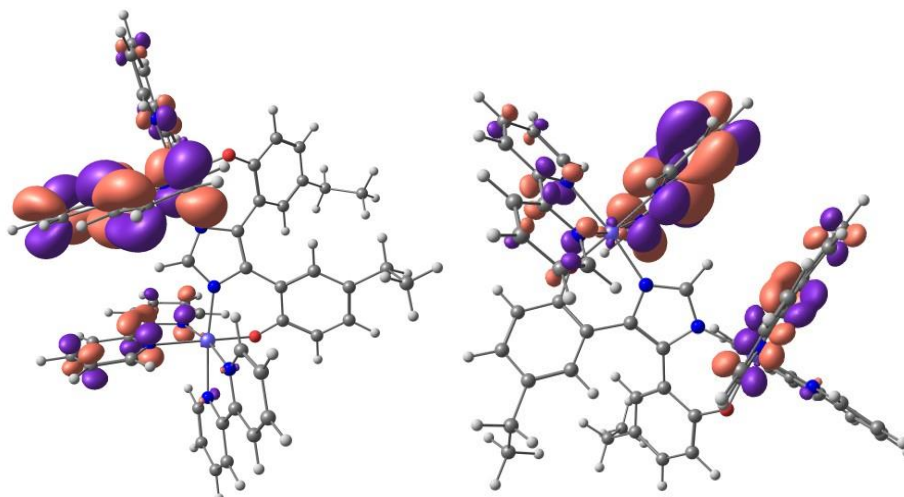
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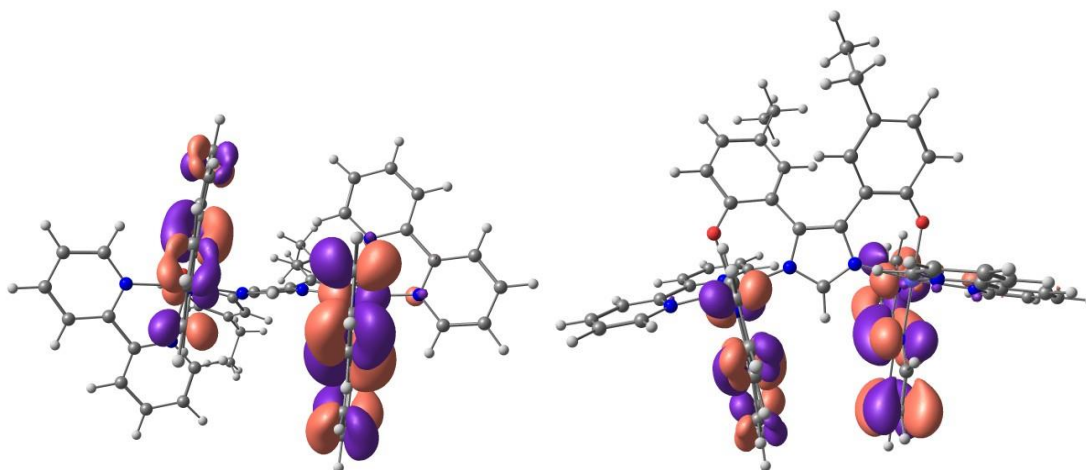
S7. Variable-temperature magnetic susceptibility for a methanol solution of **[(phen)₄Ni₂(L)](Cl)** from the Evans technique.



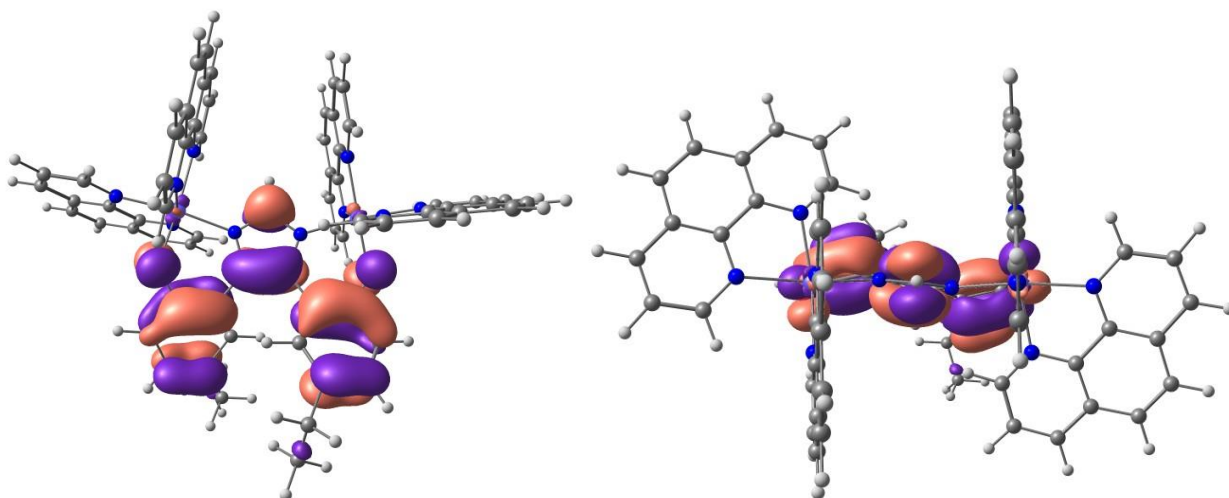
S8. α -LUMO orbital (0.03 isosurface level) for [(bipy)₄Ni₂(L)]⁺ ($E^{\text{LUMO}} = -0.0887$ a.u.)



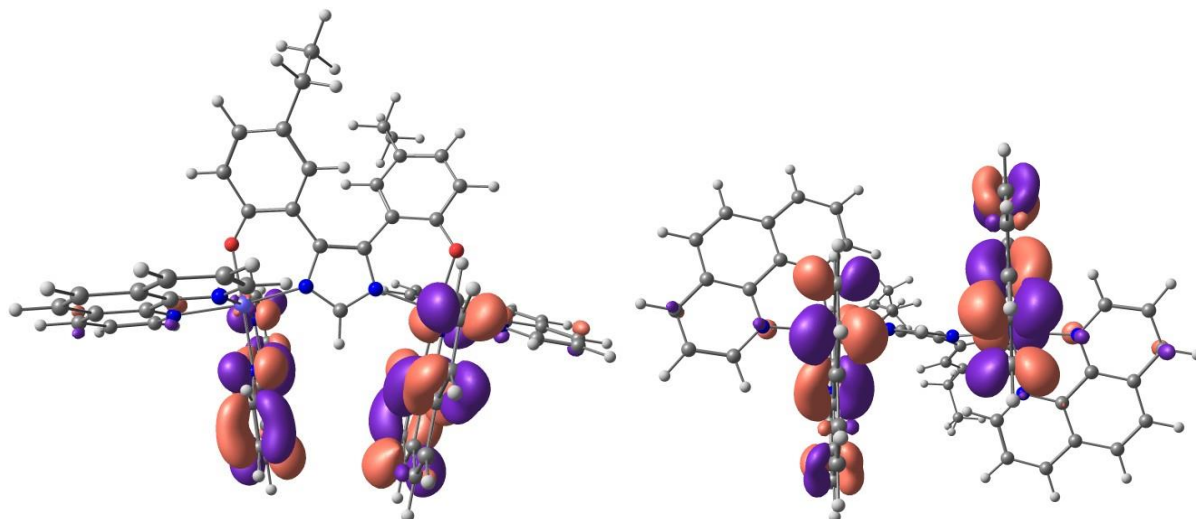
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S10. α -HOMO orbital (0.03 isosurface level) for $[(\text{phen})_4\text{Ni}_2(\text{L})]^{2+}$ ($E^{\text{HOMO}} = -0.1976$ a.u.)



S11. α -LUMO orbital (0.03 isosurface level) for $[(\text{phen})_4\text{Ni}_2(\text{L})]^{2+}$ ($E^{\text{LUMO}} = -0.1008$ a.u.)



S12. Spin density (0.0065 isosurface level) for $[(\text{phen})_4\text{Ni}_2(\text{L})]^{2+}$

