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Supplementary Information for:

Solvent Dependent Spin-State Behavior via Hydrogen Bonding in Neutral Fe(II) Diimine Complexes

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Figures S1 and S2: ^{1}H NMR spectra collected for **1** in deuterated methanol and acetonitrile, respectively. The top spectra are obtained under "normal" conditions; the bottom spectra are obtained under "paramagnetic" conditions (increased number of scans, no time between excitation and measurement).

Figures S3 – S5: ^{1}H NMR spectra collected for **2** in deuterated methanol, acetonitrile and dichloromethane, respectively. The top spectra are obtained under "normal" conditions; the bottom spectra are obtained under "paramagnetic" conditions (increased number of scans, no time between excitation and measurement).

Figures S6 and S7: Electronic absorption spectra for **1** and **2**, respectively, obtained in methanol.

Figures S8 and S9: π-π stacking plots for **1** and **2**, respectively.

Figure S1. NMR of $[Fe(pizH)_2(NCS)_2]$ in CD_3OD at 273 K:

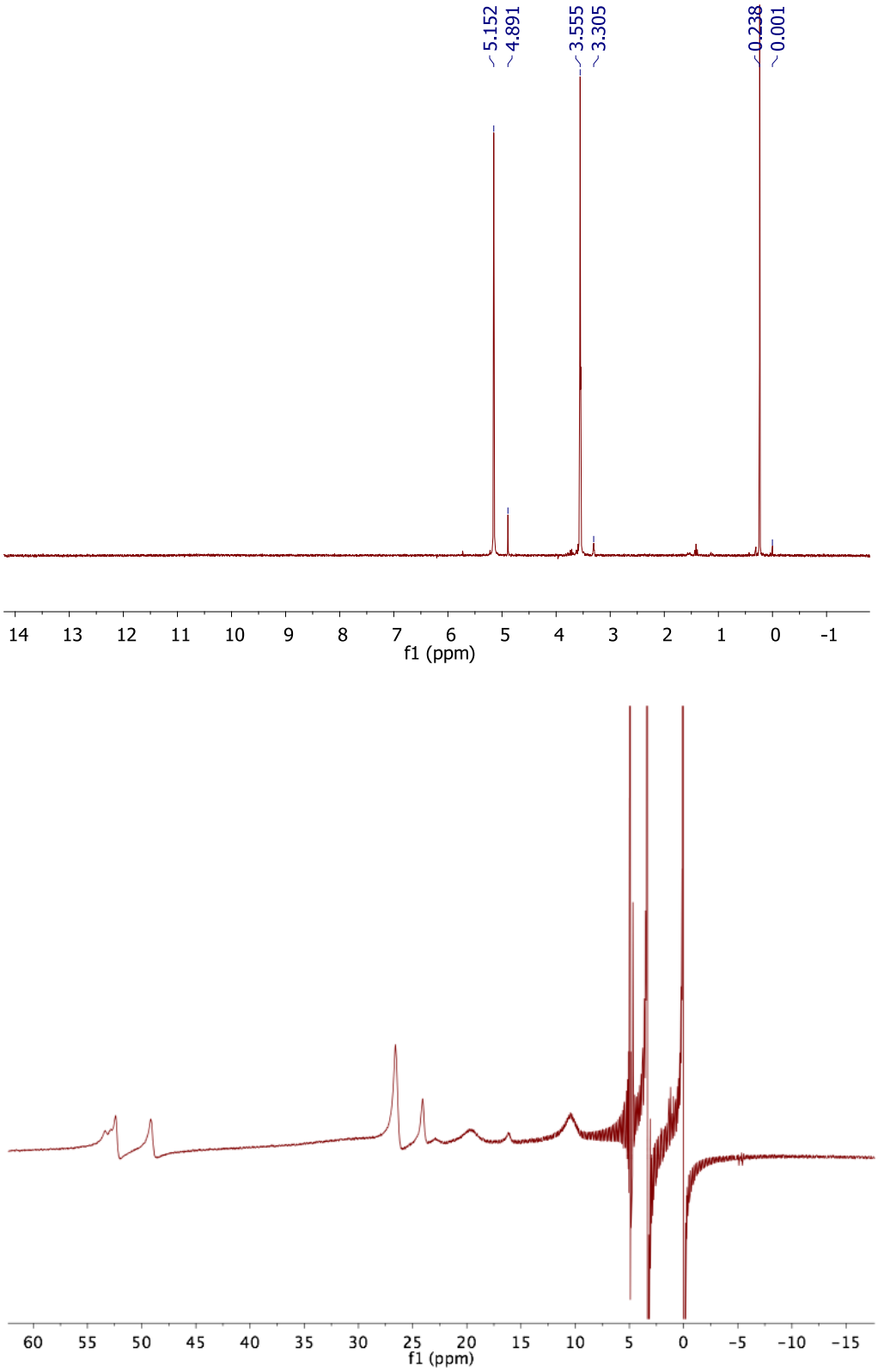


Figure S2. NMR of $[Fe(pizH)_2(NCS)_2]$ in CD_3CN at 293 K:

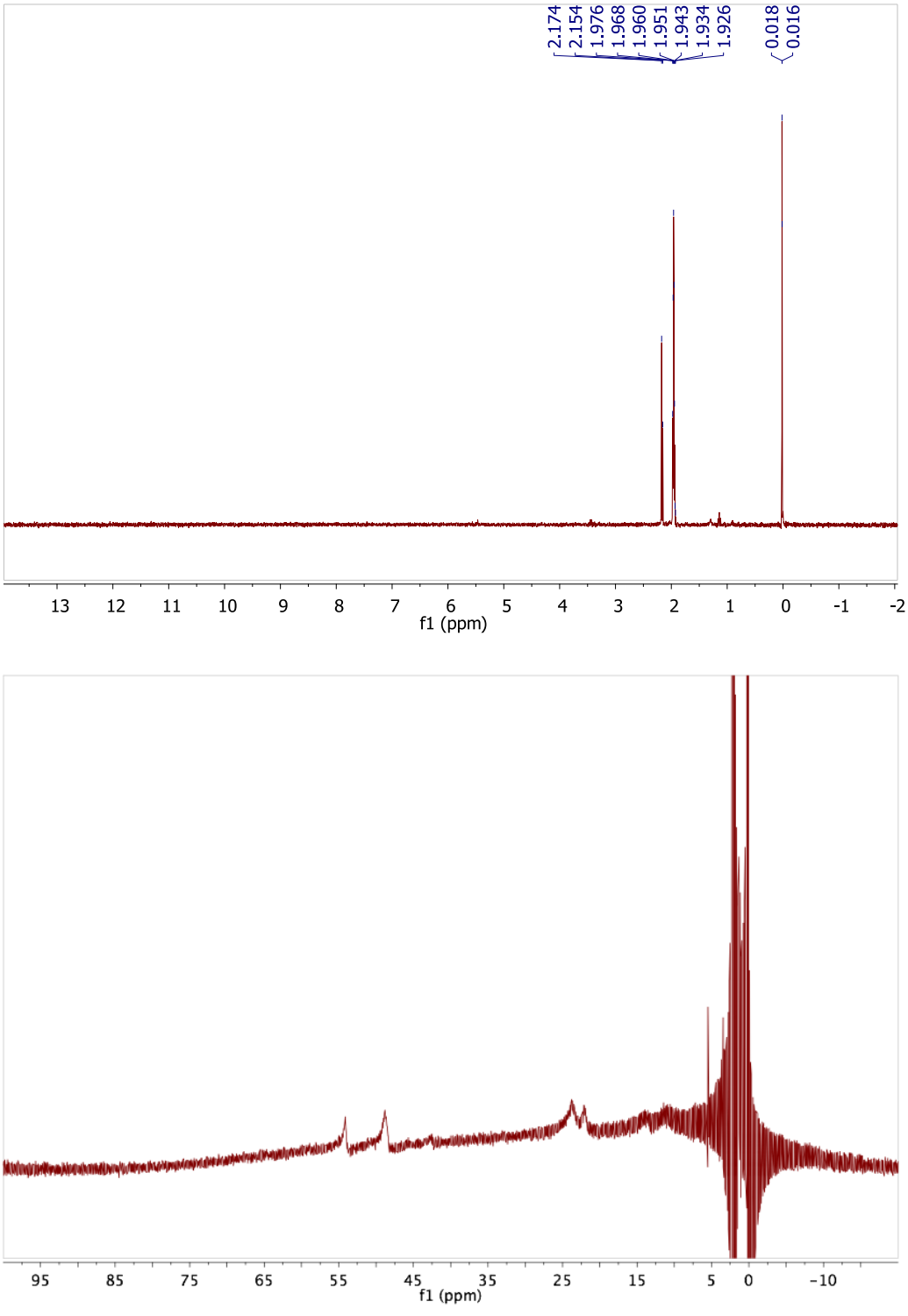


Figure S3. NMR of $[Fe(pizMe)_2(NCS)_2]$ in CD_3OD at 293 K:

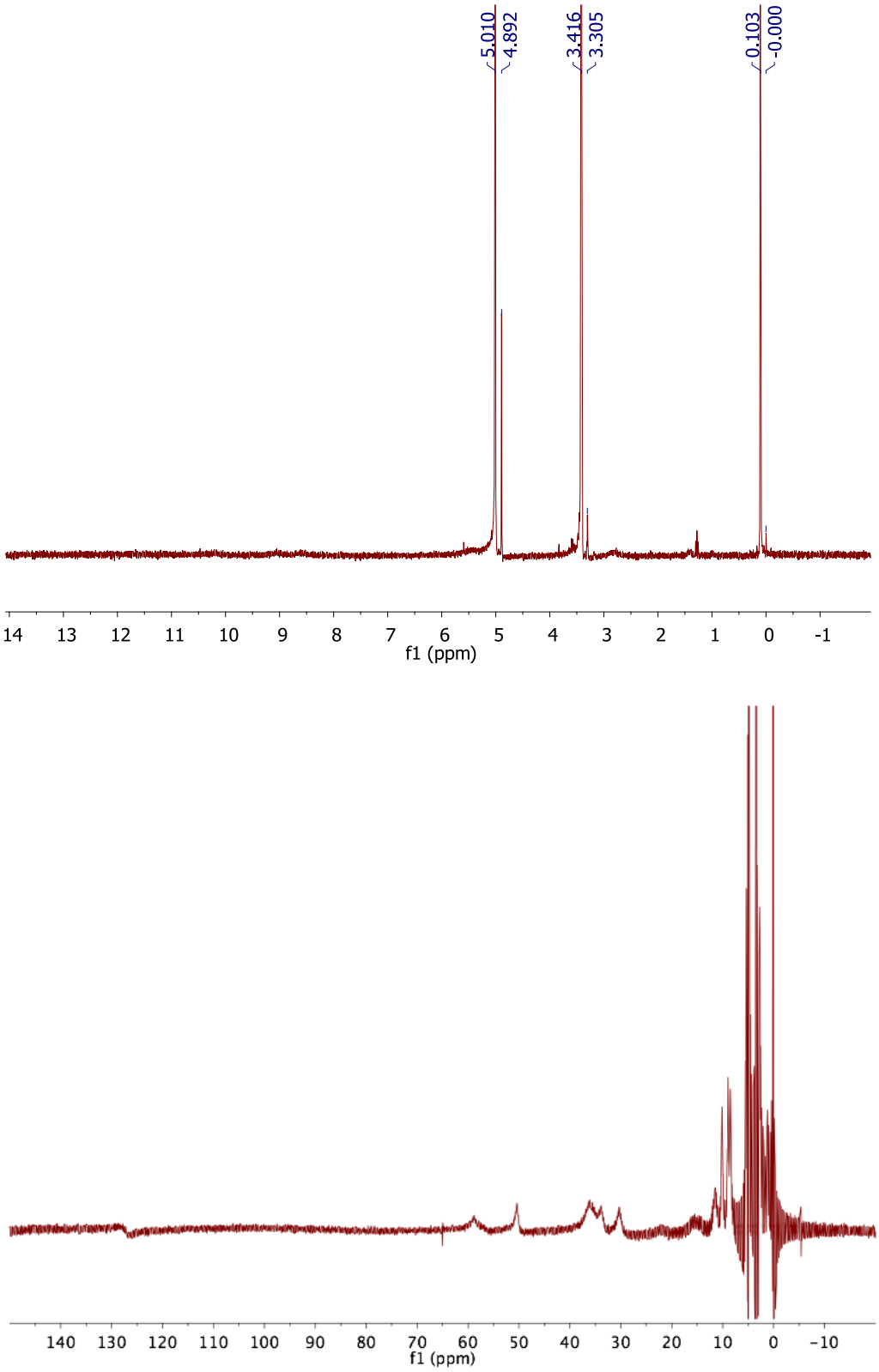
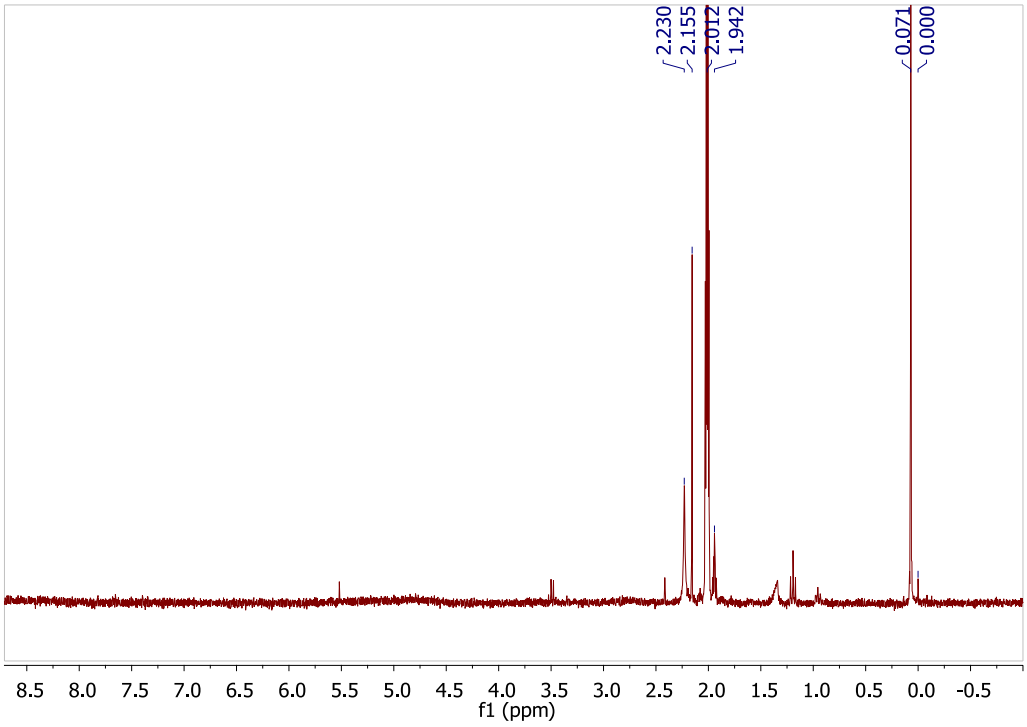


Figure S4. NMR of $[Fe(pizMe)_2(NCS)_2]$ in CD_3CN at 293 K:



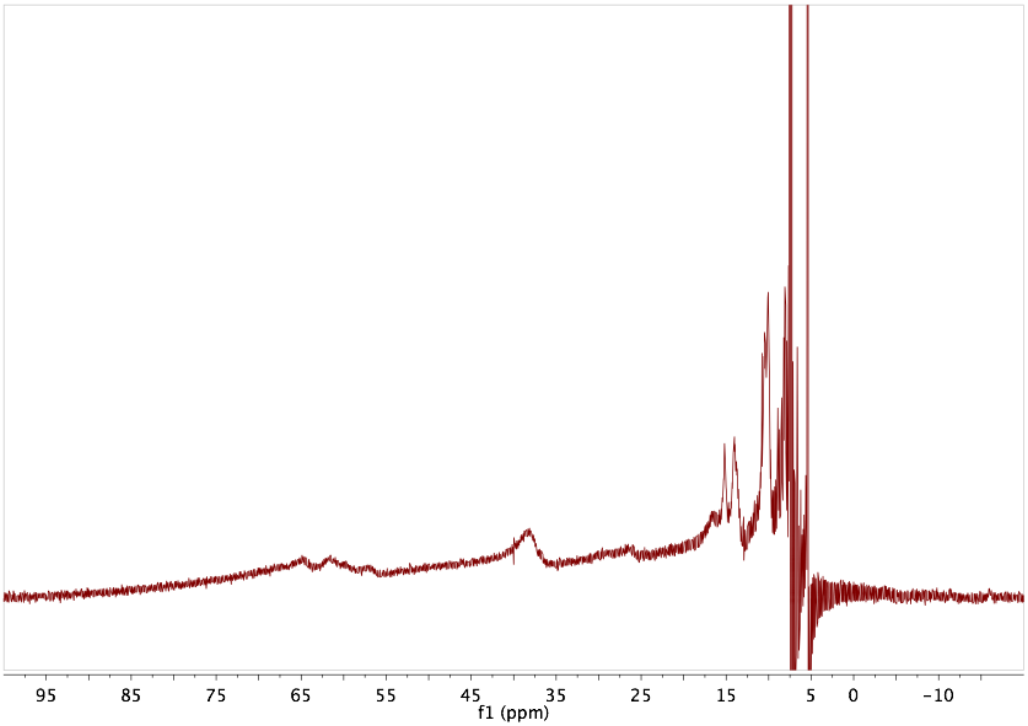


Figure S5. NMR of $[Fe(pizMe)_2(NCS)_2]$ in CD_2Cl_2 at 293 K:

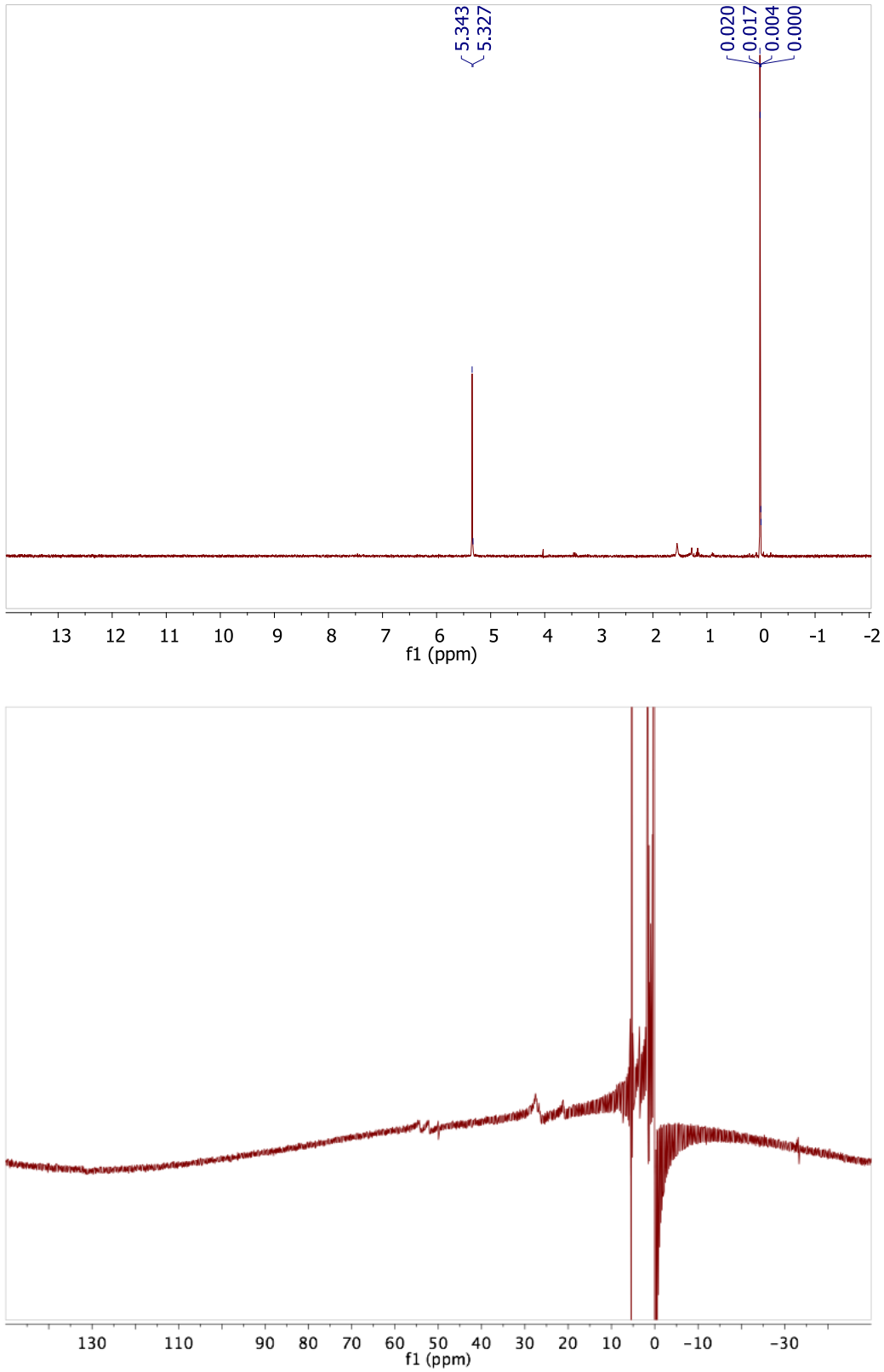


Figure S6. UV-vis of $[Fe(pizH)_2(NCS)_2]$ in CH_3OH:

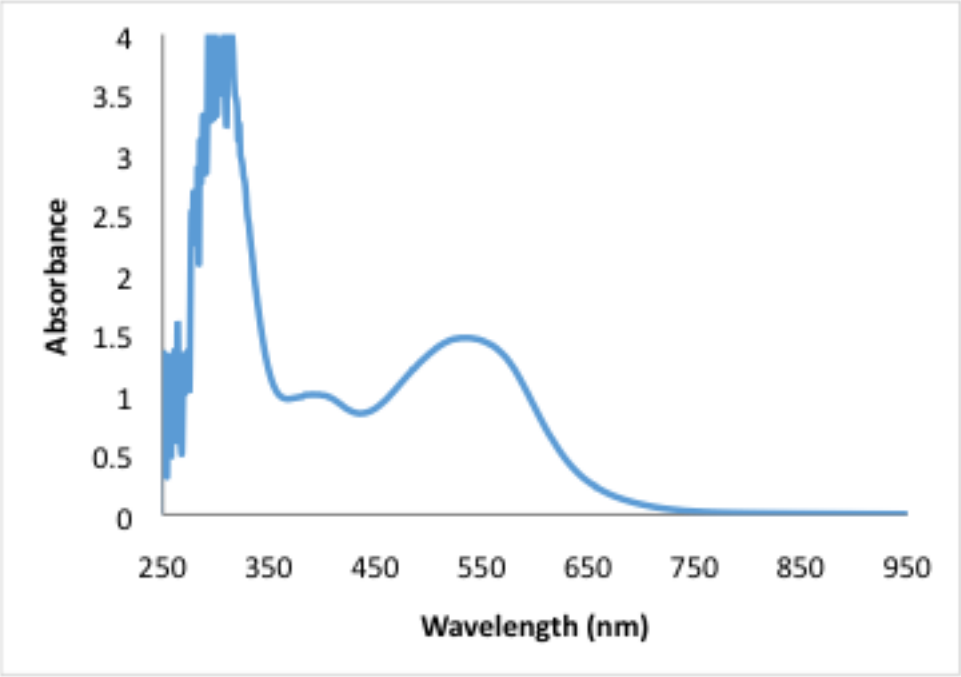


Figure S7. UV-vis of $[Fe(pizMe)_2(NCS)_2]$ in CH_3OH:

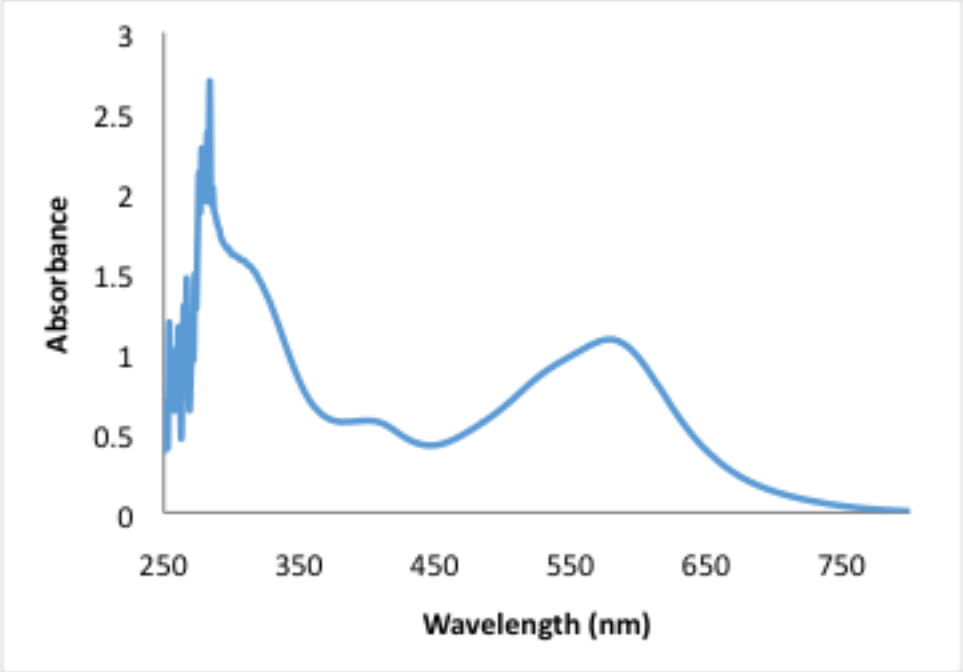


Figure S8. π-π stacking plot of $[Fe(pizH)_2(NCS)_2]$ (**1**). The pyridine–imidazoline overlap centroid–centroid distances (Å) are shown in green. The rings are offset by ~1.4 Å from direct overlap. The mean planes of each pizH ligand are *not* parallel, with the angle between planes = 3.55°.

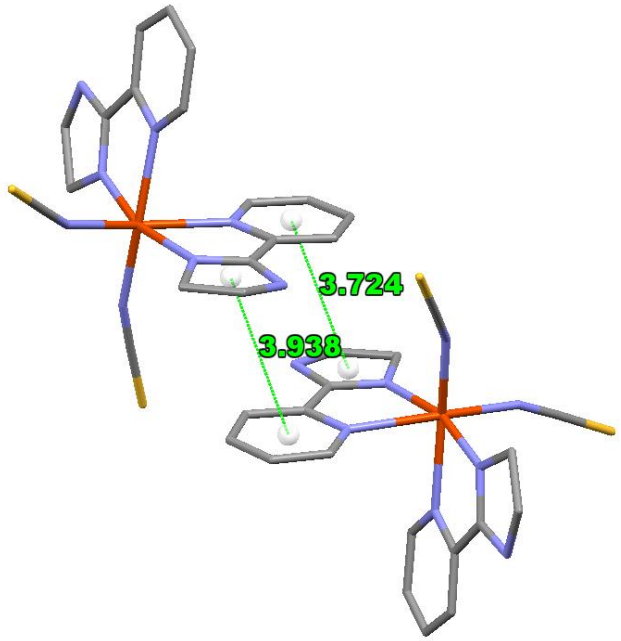


Figure S9. π-π stacking plot of $[Fe(pizMe)_2(NCS)_2]$ (**2**). The pyridine–imidazoline overlap centroid–centroid distances (Å) are shown in green. The rings are offset by ~1.9 Å from direct overlap. The mean planes of each pizMe ligand are parallel to one another (i.e. angle between planes = 0°) and an interplanar distance of 3.339 Å.