

**SUPPORTING INFORMATION**

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**Title:** Connecting [4Fe–4S] Clusters and Hemes – Towards Modeling the Active Site of Sulfite Reductase

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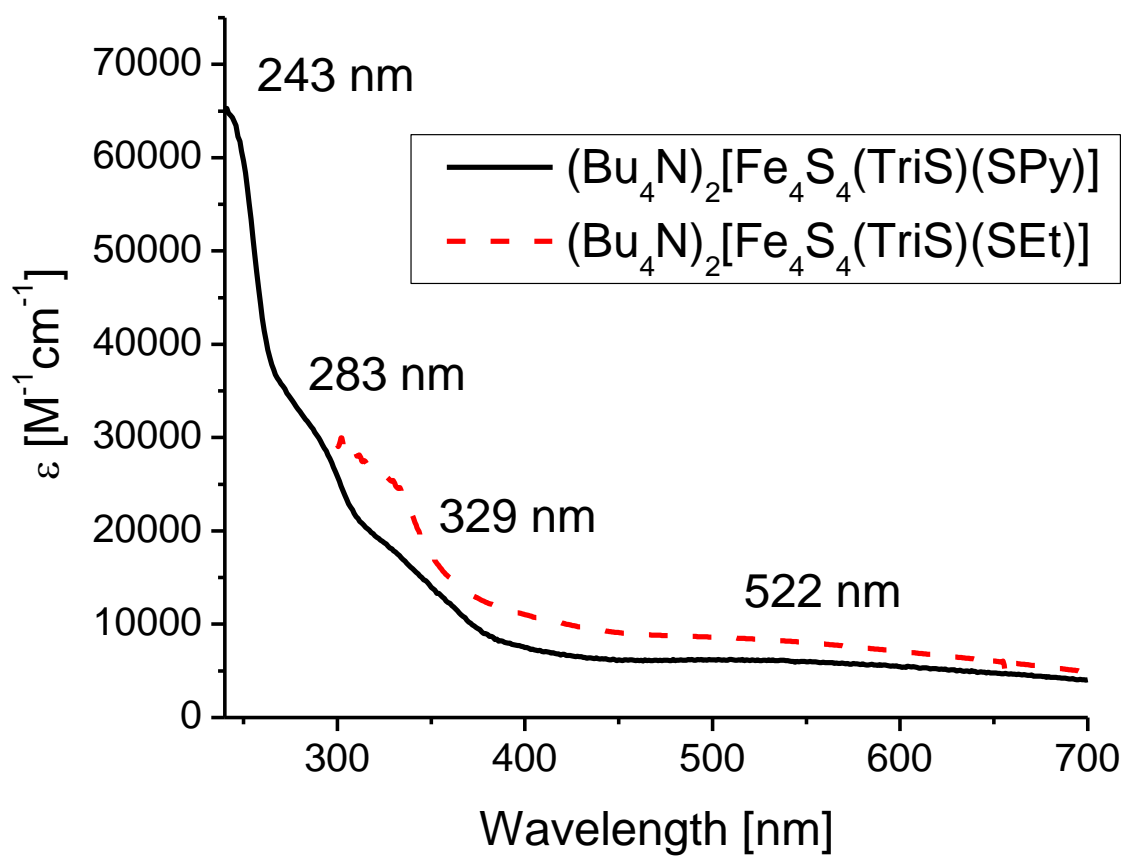


Figure S1. UV-Vis absorption spectrum of  $(Bu_4N)_2[Fe_4S_4(TriS)(SPy)]$ .

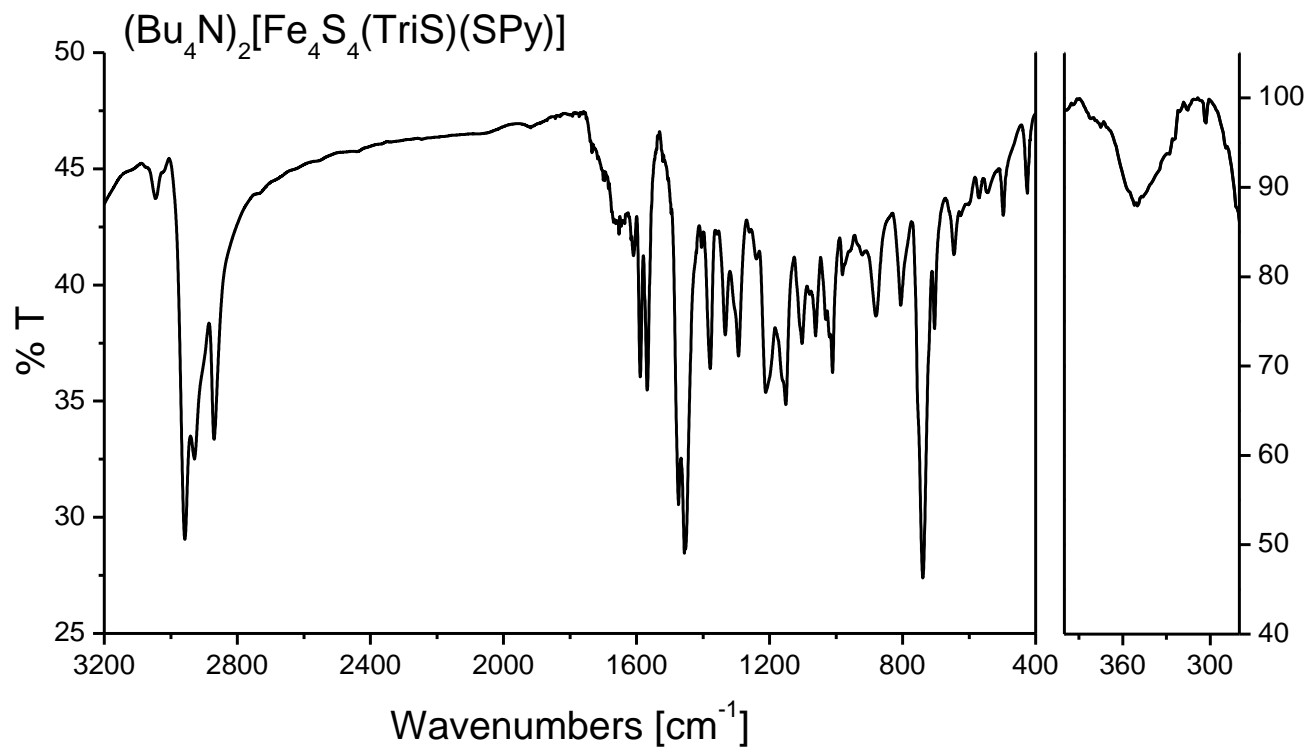


Figure S2. Mid- (left) and Far-IR (right) spectra of  $(\text{Bu}_4\text{N})_2[\text{Fe}_4\text{S}_4(\text{TriS})(\text{SPy})]$ .

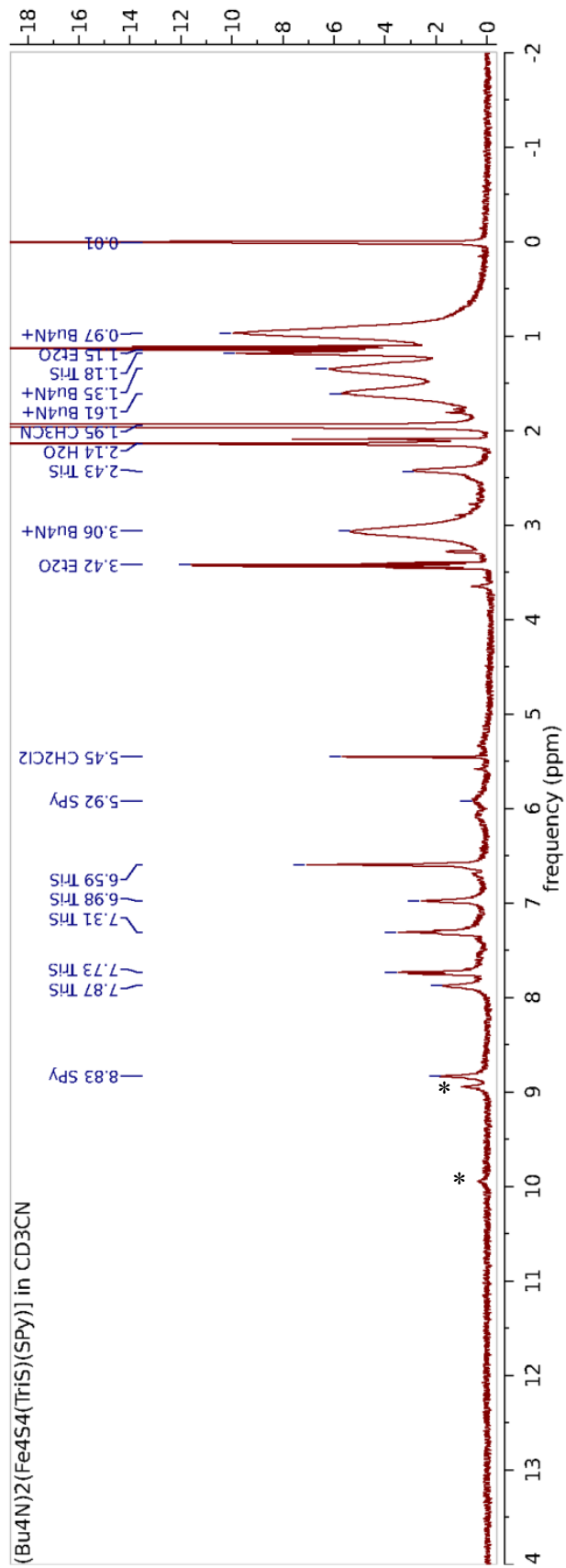


Figure S3. <sup>1</sup>H-NMR spectrum of (Bu<sub>4</sub>N)<sub>2</sub>[Fe<sub>4</sub>S<sub>4</sub>(Tris)(SPy)] (impurities labeled by \*).

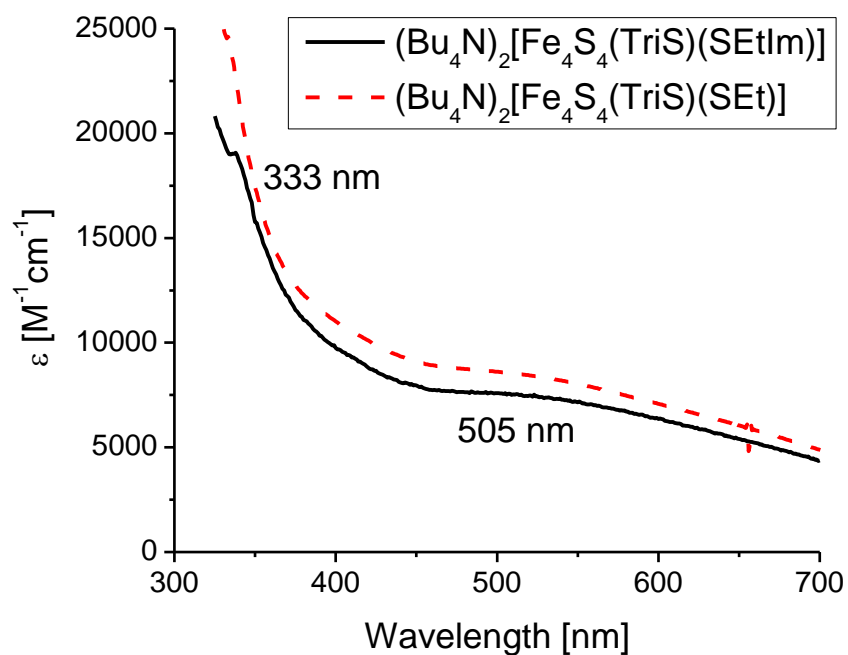


Figure S4. UV-Vis absorption spectrum of  $(\text{Bu}_4\text{N})_2[\text{Fe}_4\text{S}_4(\text{TriS})(\text{SEtIm})]$ .

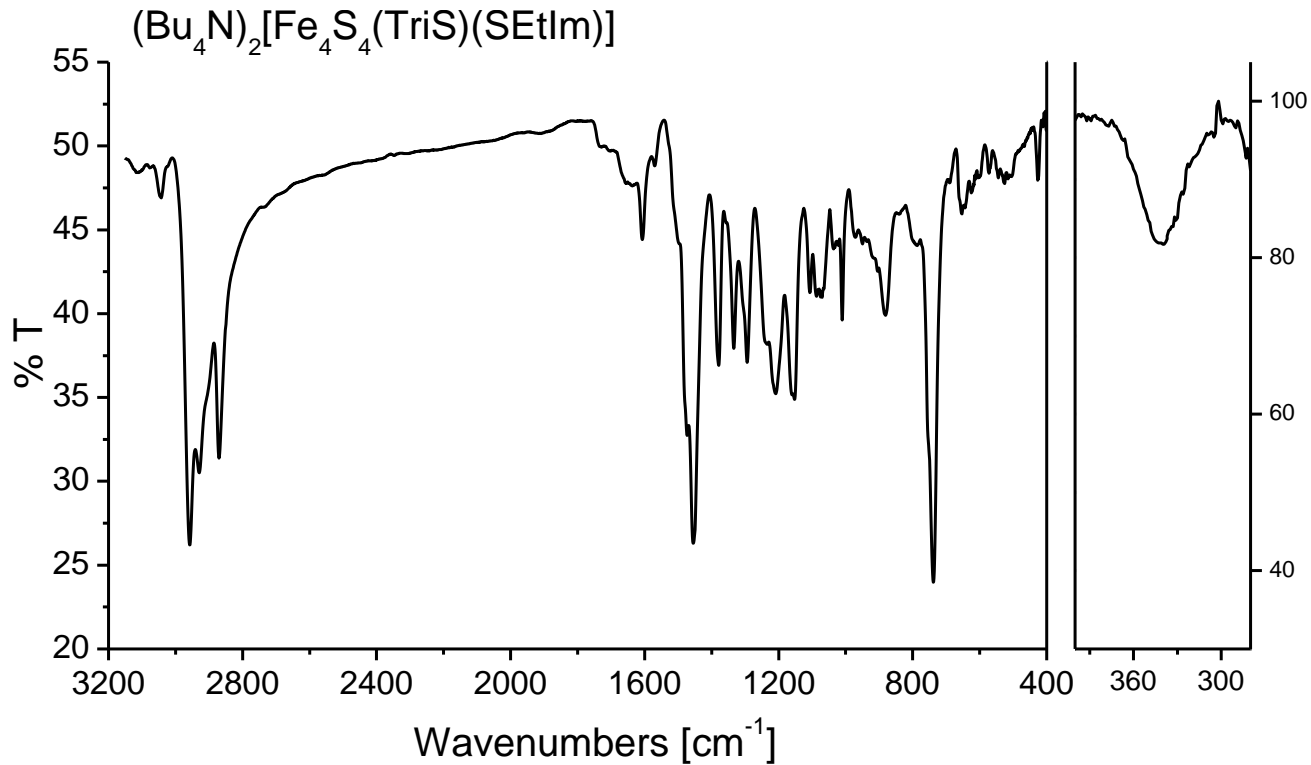


Figure S5. Mid- (left) and Far-IR (right) spectra of  $(\text{Bu}_4\text{N})_2[\text{Fe}_4\text{S}_4(\text{TriS})(\text{SEtIm})]$ .

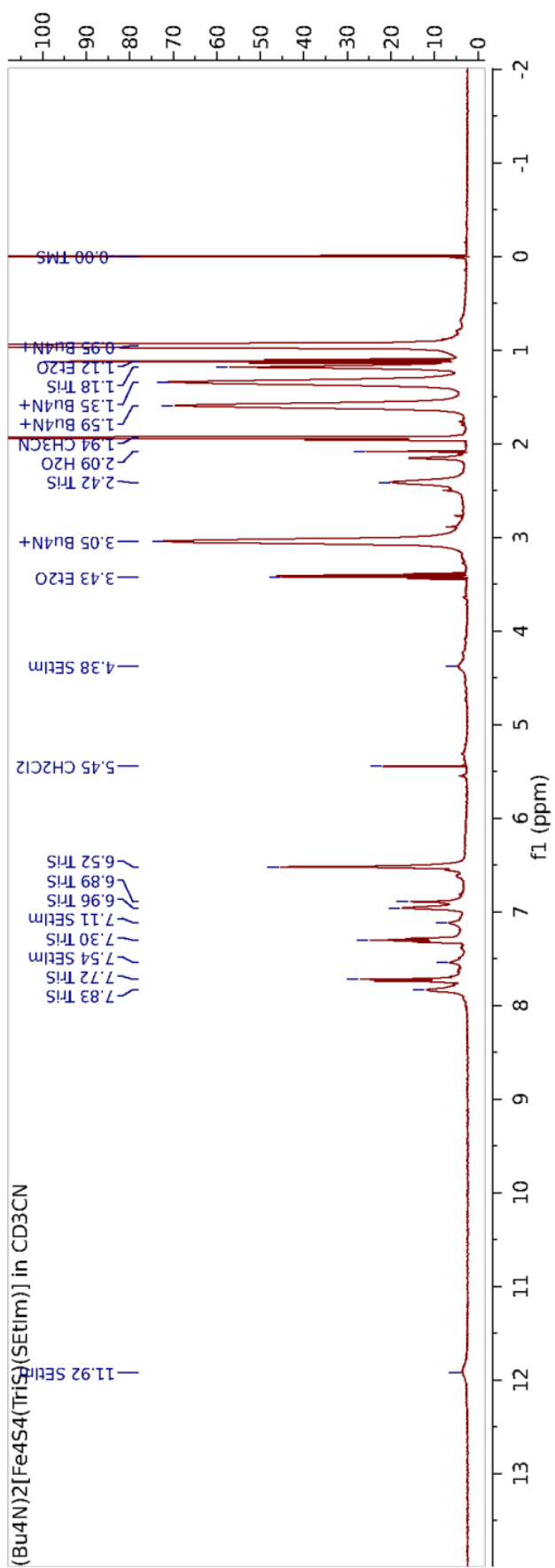


Figure S6. <sup>1</sup>H-NMR spectrum of (Bu<sub>4</sub>N)<sub>2</sub>[Fe<sub>4</sub>S<sub>4</sub>(TriS)(SEtIm)].

Table S1. Titration conditions for determination of binding constants.

Zinc porphyrin, Stock concentration	Cuvette volume, [Zn(P)] volume	Base, Stock concentration	Volume addition, Molar equivalent
[Zn(TPP)]			
4.91 mM	3 mL, 10 $\mu$ L	pyridine, 12.4 mM	10 $\mu$ L, 2.5 eq
4.91 mM	3 mL, 10 $\mu$ L	1-methylimidazole, 12.5 mM	2 $\mu$ L, 0.51 eq
4.91 mM	3 mL, 10 $\mu$ L	(Bu <sub>4</sub> N) <sub>2</sub> [Fe <sub>4</sub> S <sub>4</sub> (TriS)(SEtIm)], 7.55 $\mu$ L	3 $\mu$ L, 0.46 eq
[Zn( <i>To</i> -F <sub>2</sub> PP)]			
4.90 mM	3 mL, 30 $\mu$ L	pyridine, 12.4 mM	3 $\mu$ L, 0.25 eq
4.90 mM	3 mL, 30 $\mu$ L	1-methylimidazole, 12.5 mM	1 $\mu$ L, 0.085 eq
4.96 mM	3 mL, 30 $\mu$ L	(Bu <sub>4</sub> N) <sub>2</sub> [Fe <sub>4</sub> S <sub>4</sub> (TriS)(SPy)], 7.51 mM	5 $\mu$ L, 0.25 eq
4.90 mM	3 mL, 30 $\mu$ L	(Bu <sub>4</sub> N) <sub>2</sub> [Fe <sub>4</sub> S <sub>4</sub> (TriS)(SEtIm)], 7.55 mM	3 $\mu$ L, 0.15 eq
[Zn( <i>Tper</i> -F <sub>3</sub> PP)]			
4.82 mM	3 mL, 30 $\mu$ L	pyridine, 12.4 mM	2 $\mu$ L, 0.17 eq
4.82 mM	3 mL, 30 $\mu$ L	1-methylimidazole, 12.5 mM	1 $\mu$ L, 0.086 eq
4.86 mM	3 mL, 30 $\mu$ L	(Bu <sub>4</sub> N) <sub>2</sub> [Fe <sub>4</sub> S <sub>4</sub> (TriS)(SPy)], 7.37 mM	5 $\mu$ L, 0.25 eq
4.82 mM	3 mL, 30 $\mu$ L	(Bu <sub>4</sub> N) <sub>2</sub> [Fe <sub>4</sub> S <sub>4</sub> (TriS)(SEtIm)], 7.55 mM	3 $\mu$ L, 0.16 eq

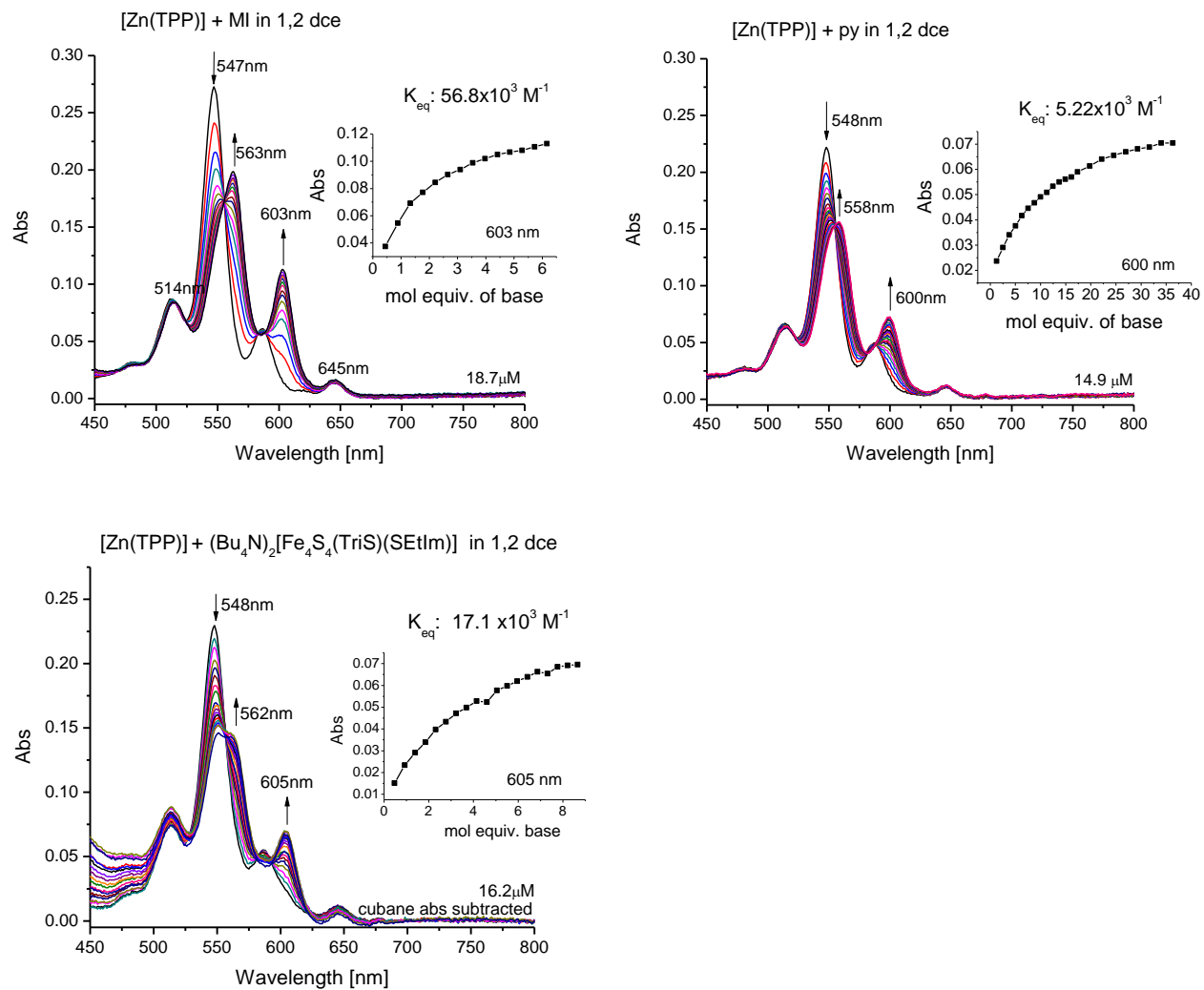


Figure S7. Titration plots for [Zn(TPP)] with 1-methylimidazole (top, left), pyridine (top, right), and (Bu<sub>4</sub>N)<sub>2</sub>[Fe<sub>4</sub>S<sub>4</sub>(Tris)(SEIm)] (bottom, left) for the determination of binding constants.



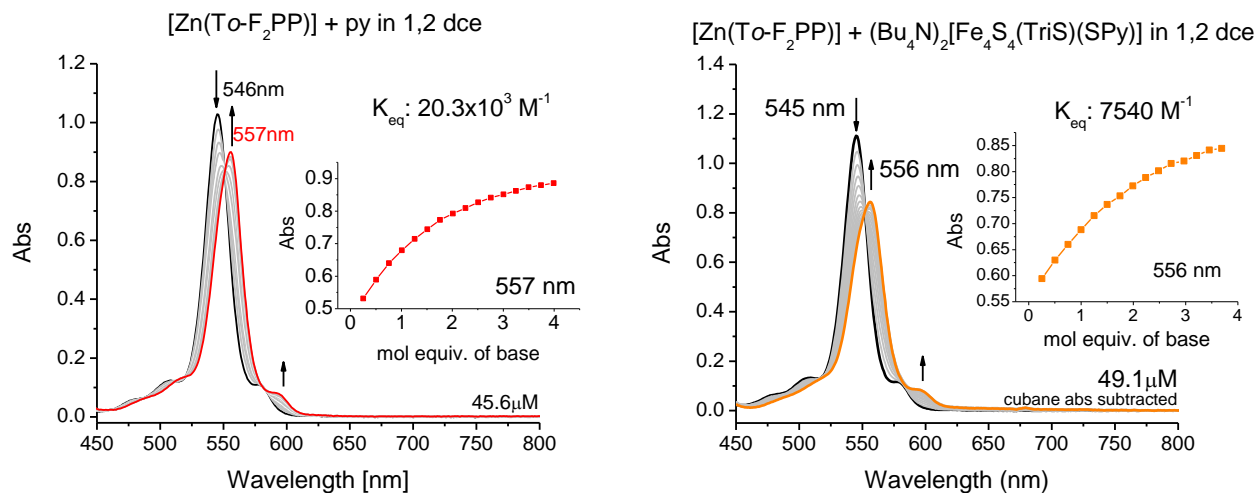


Figure S8. Titration plots for [Zn(To-F<sub>2</sub>PP)] with pyridine (left), and (Bu<sub>4</sub>N)<sub>2</sub>[Fe<sub>4</sub>S<sub>4</sub>(TriS)(SPy)] (right) for the determination of binding constants.

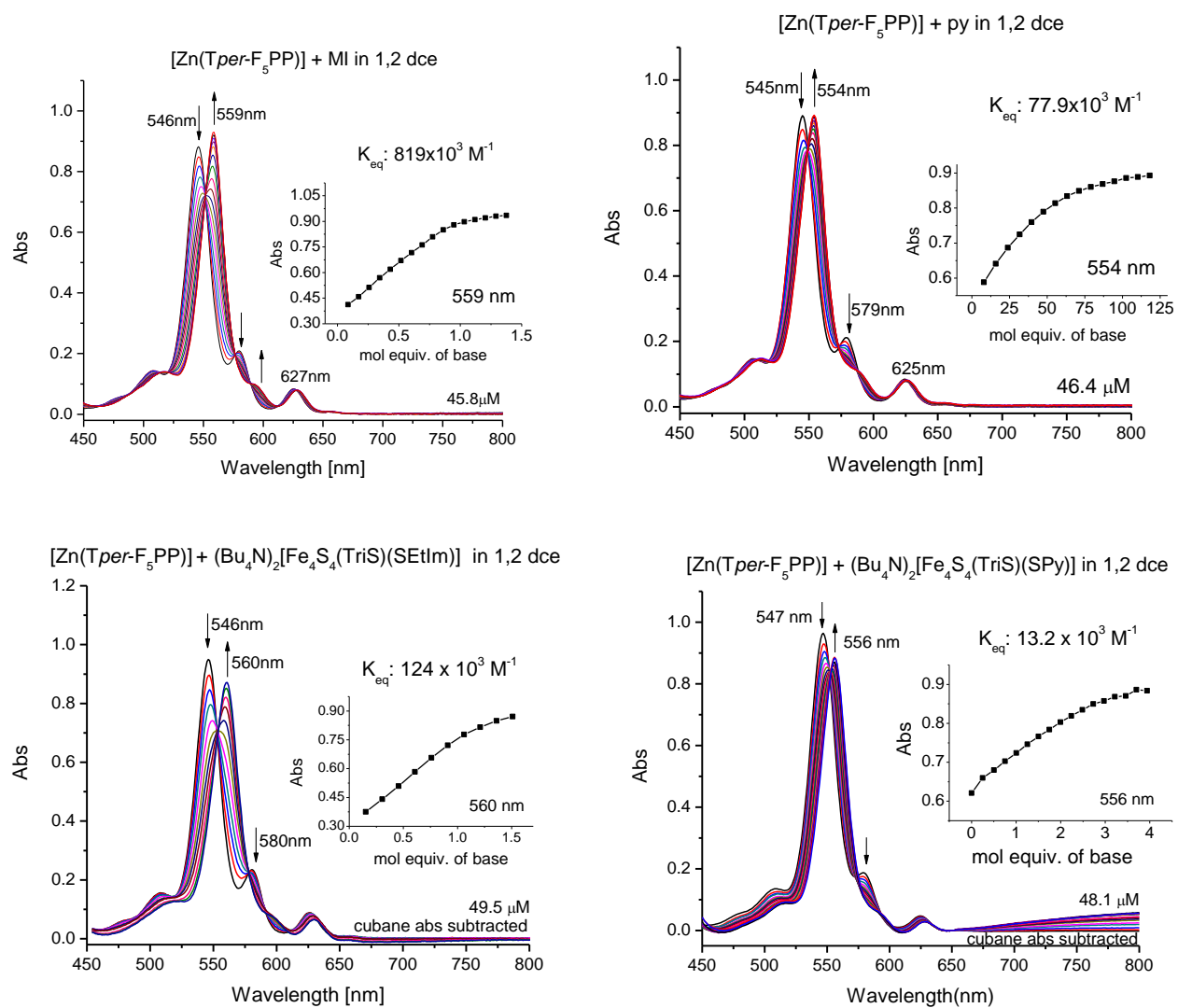


Figure S9. Titration plots for  $[Zn(Tper-F_5PP)]$  with 1-methylimidazole (top, left), pyridine (top, right),  $(Bu_4N)_2[Fe_4S_4(Tris)(SEtIm)]$  (bottom, left), and  $(Bu_4N)_2[Fe_4S_4(Tris)(SPy)]$  (bottom, right) for the determination of binding constants.