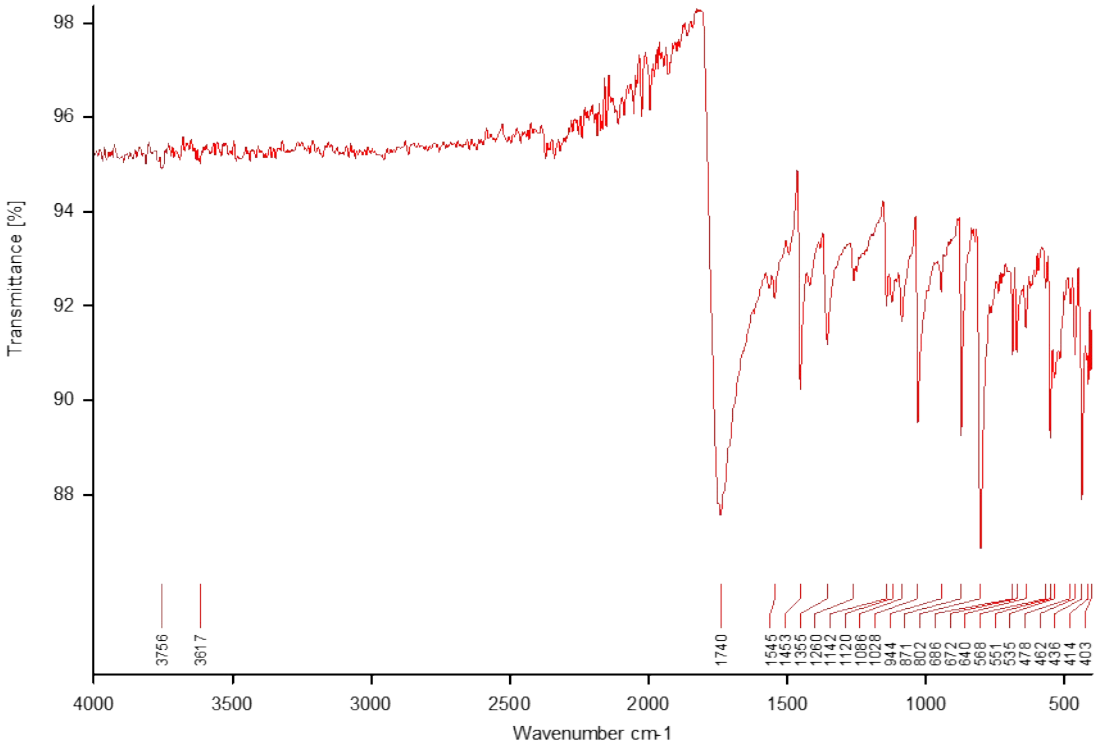


Fig. S1 IR spectrum of crystalline complex 1.

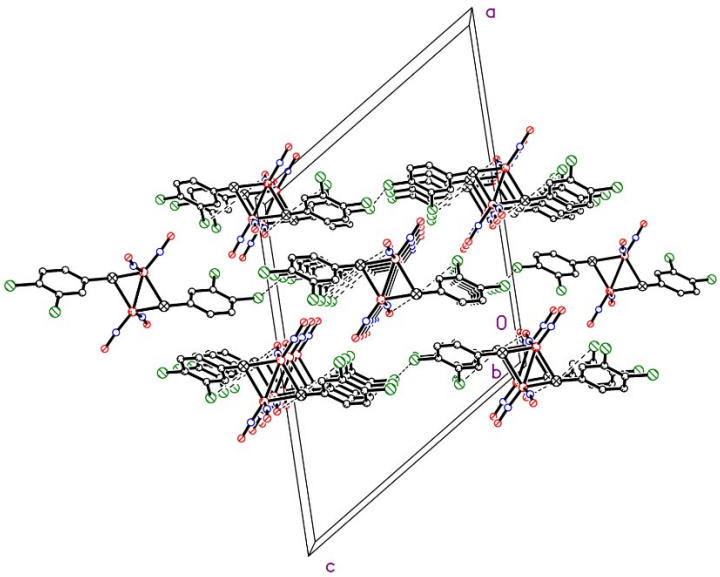


Fig. S2 Fragment of the crystalline structure of complex 1.

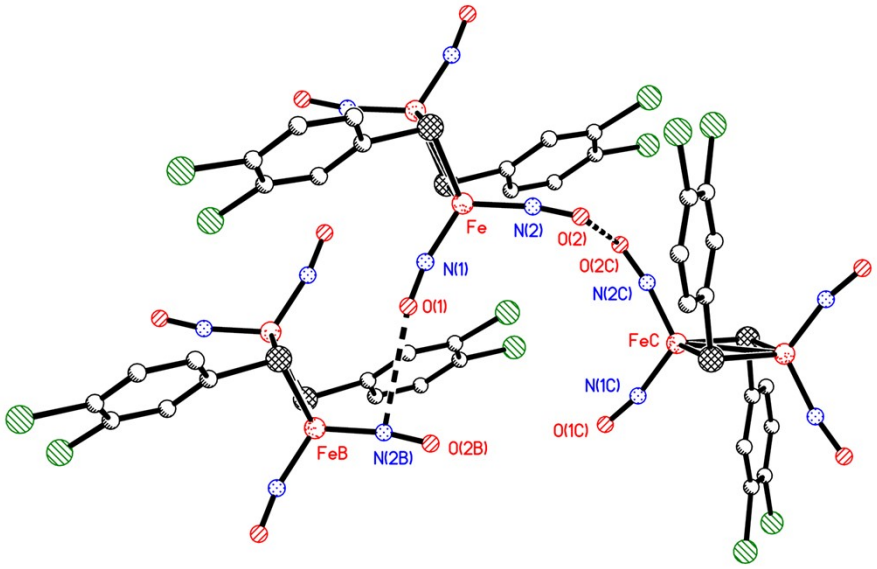


Fig. S3 Contacts between NO groups in crystal 1.

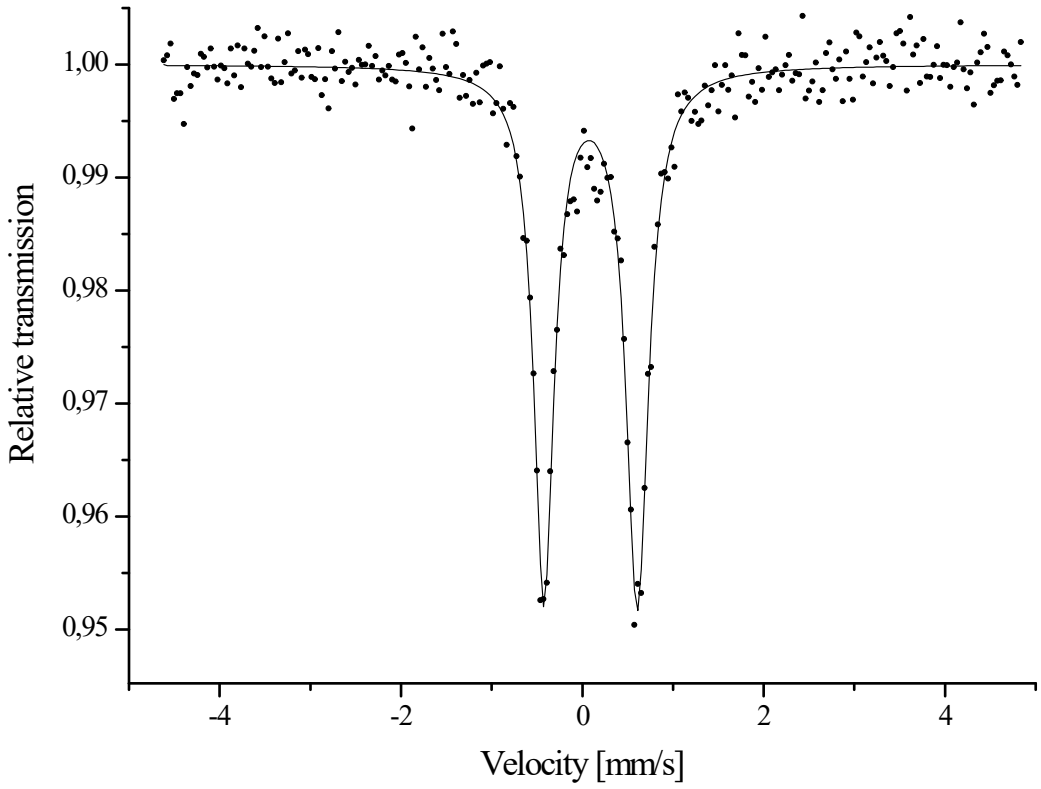


Fig. S4 Mossbauer spectrum of 1 polycrystals.

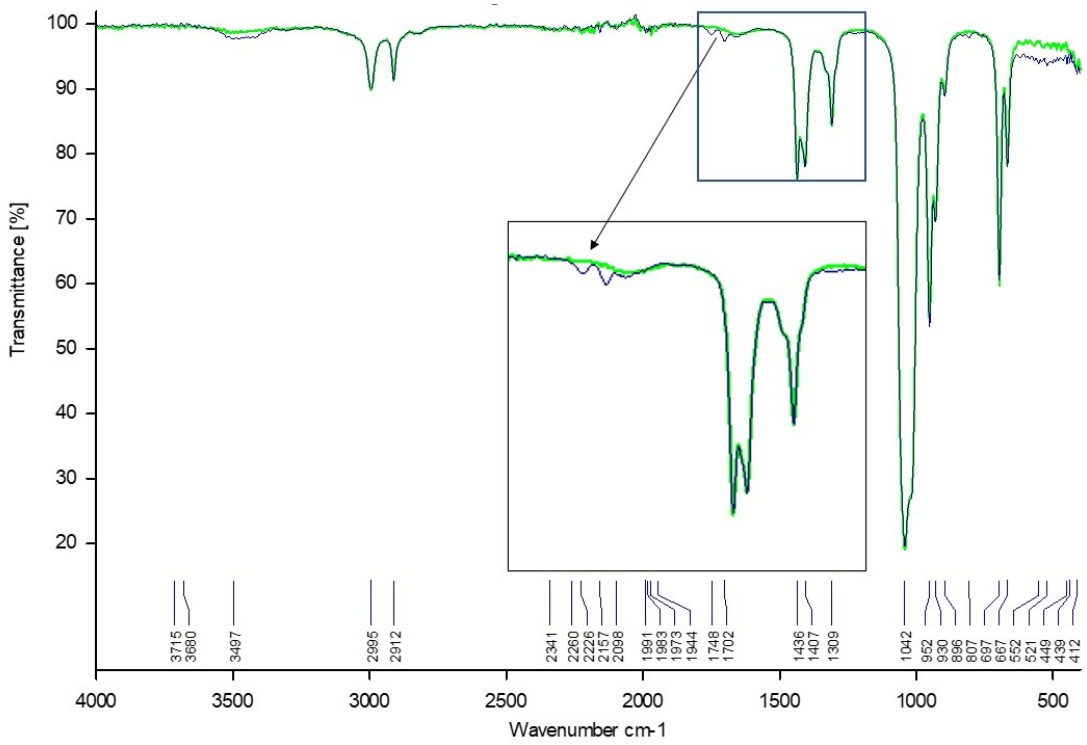


Fig. S5 Spectrum of complex 1 in DMSO (blue), and pure DMSO (green). Complex 1 concentration is $2.7 \cdot 10^{-2}$ M.

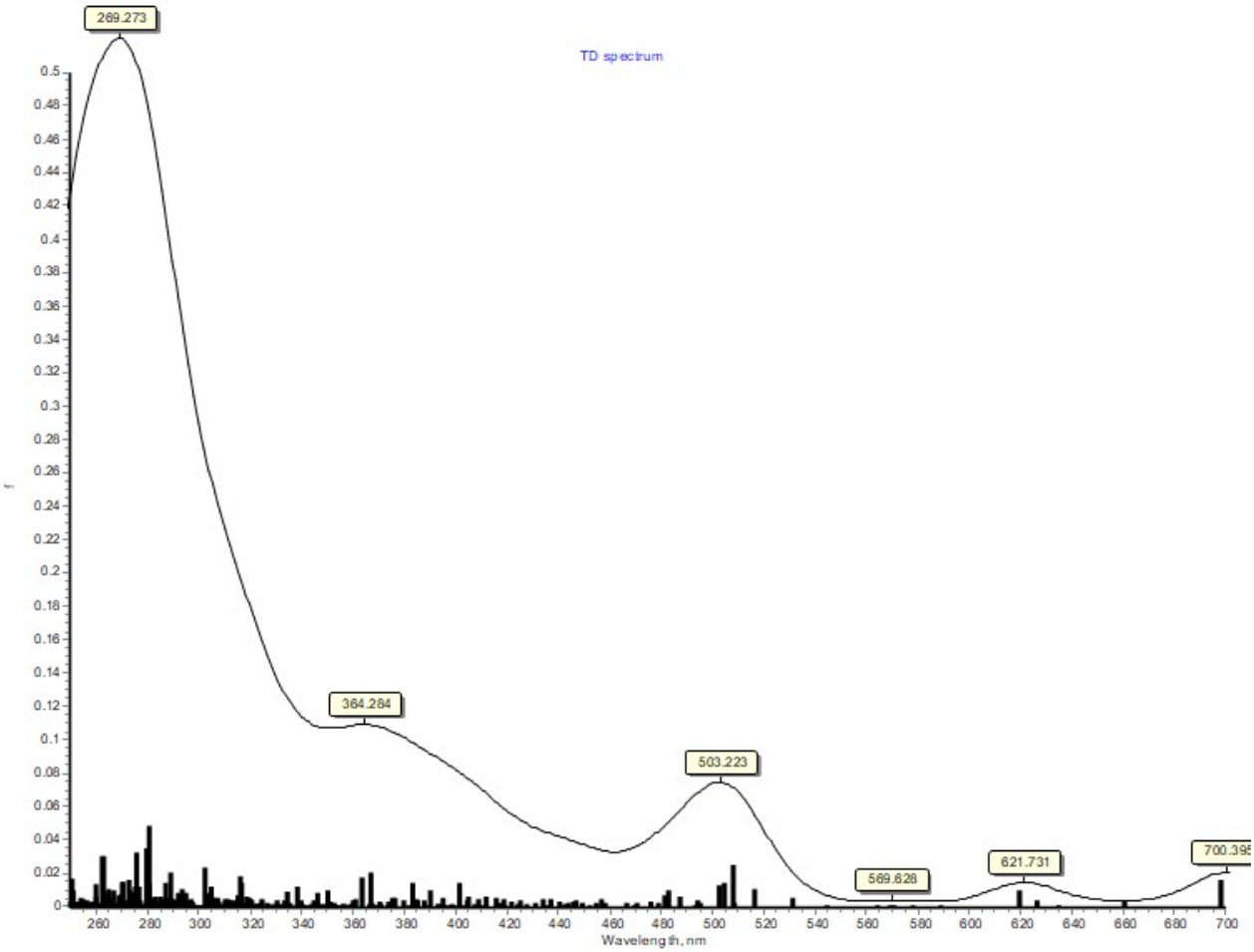


Fig. S6 Theoretical spectrum of intermediate complex 2

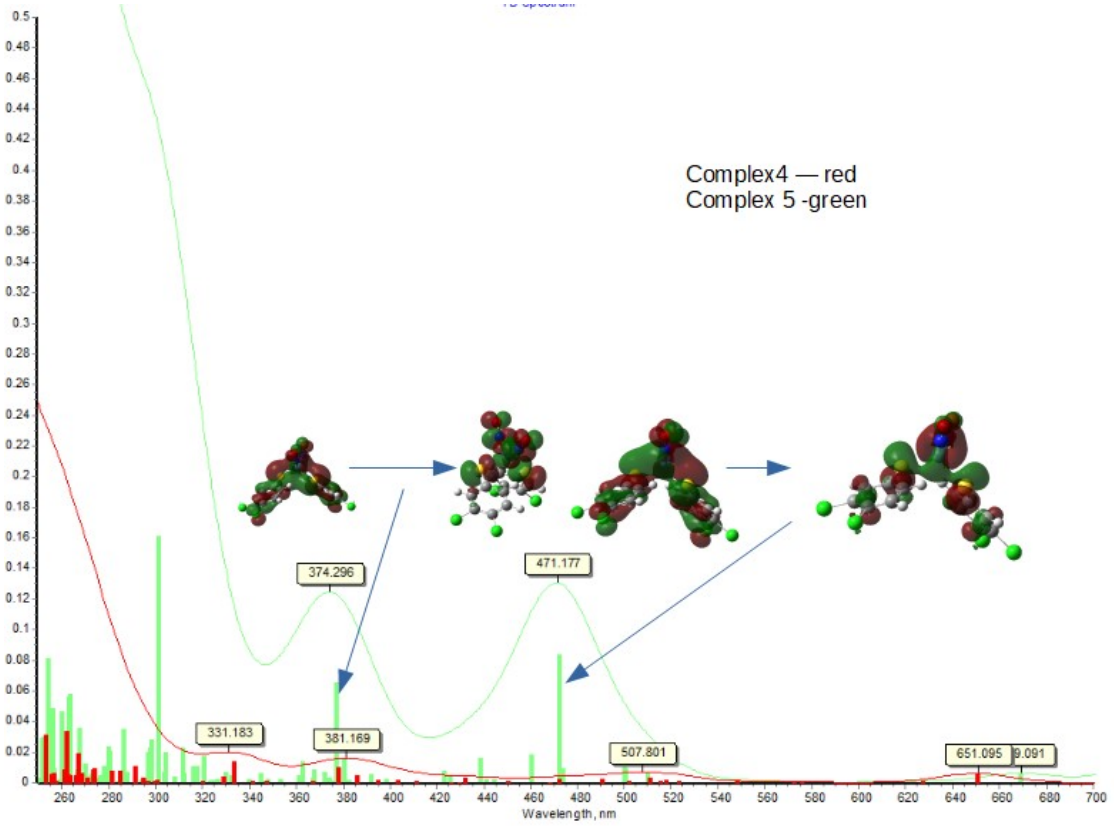


Fig. S7 Theoretical spectra of complexes 4 and 5.

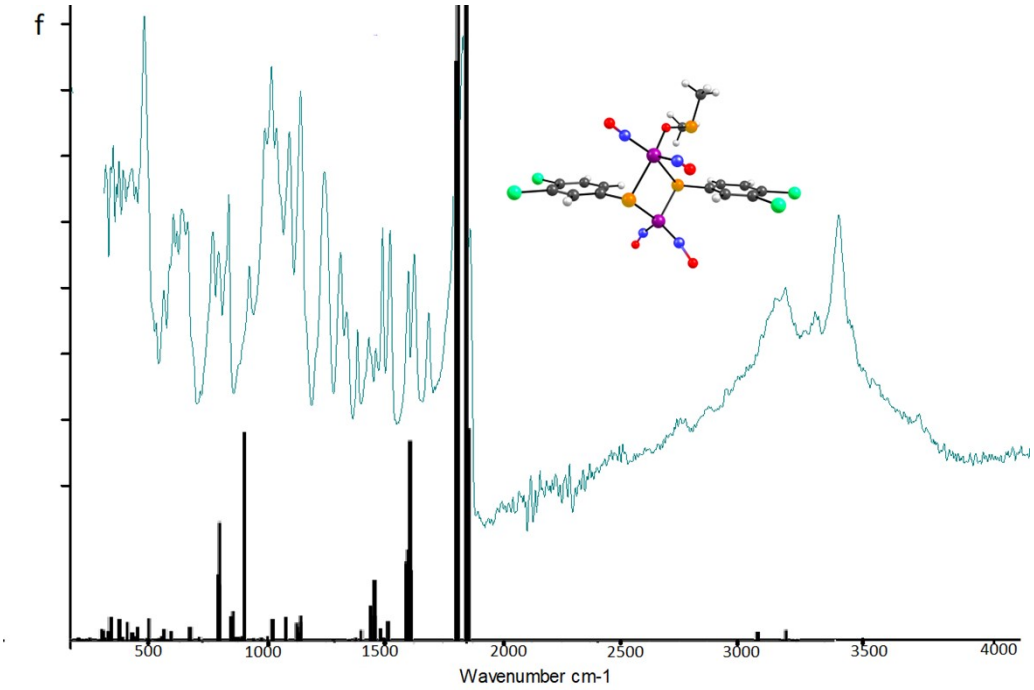


Fig. S8 IR spectrum of precipitate (blue) and theoretical spectrum of tetranitrosyl binuclear complex with four- and five-coordinated iron atoms (black).

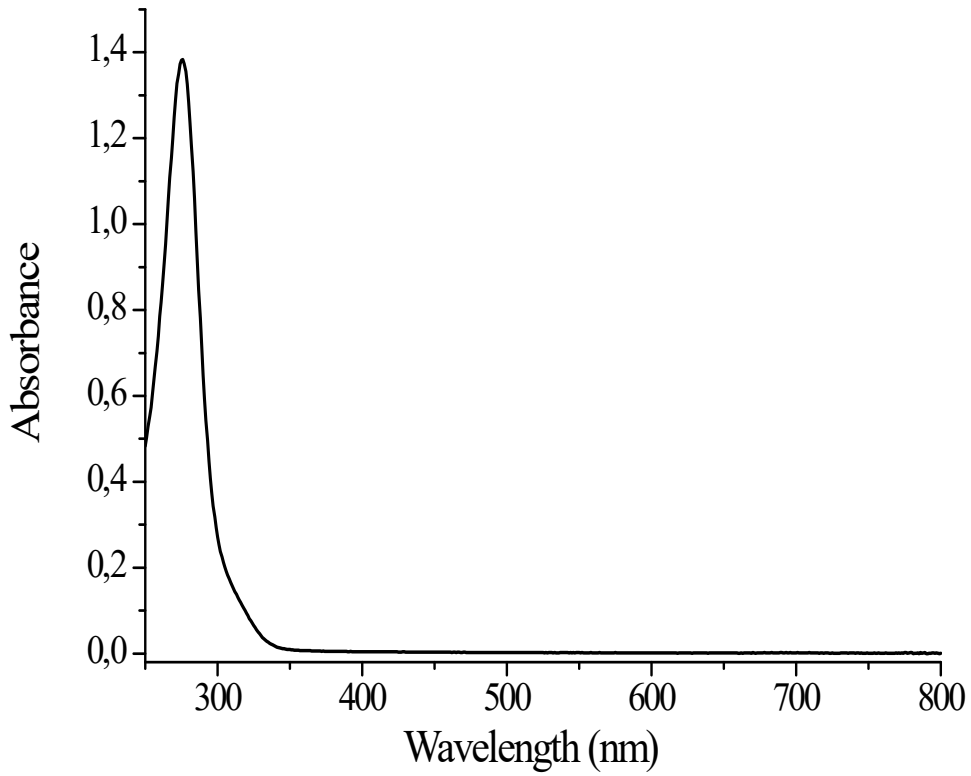


Fig. S9 UV-Vis spectrum of ligands in buffer. Concentration of ligands in buffer is $8.3 \cdot 10^{-5}$ M.

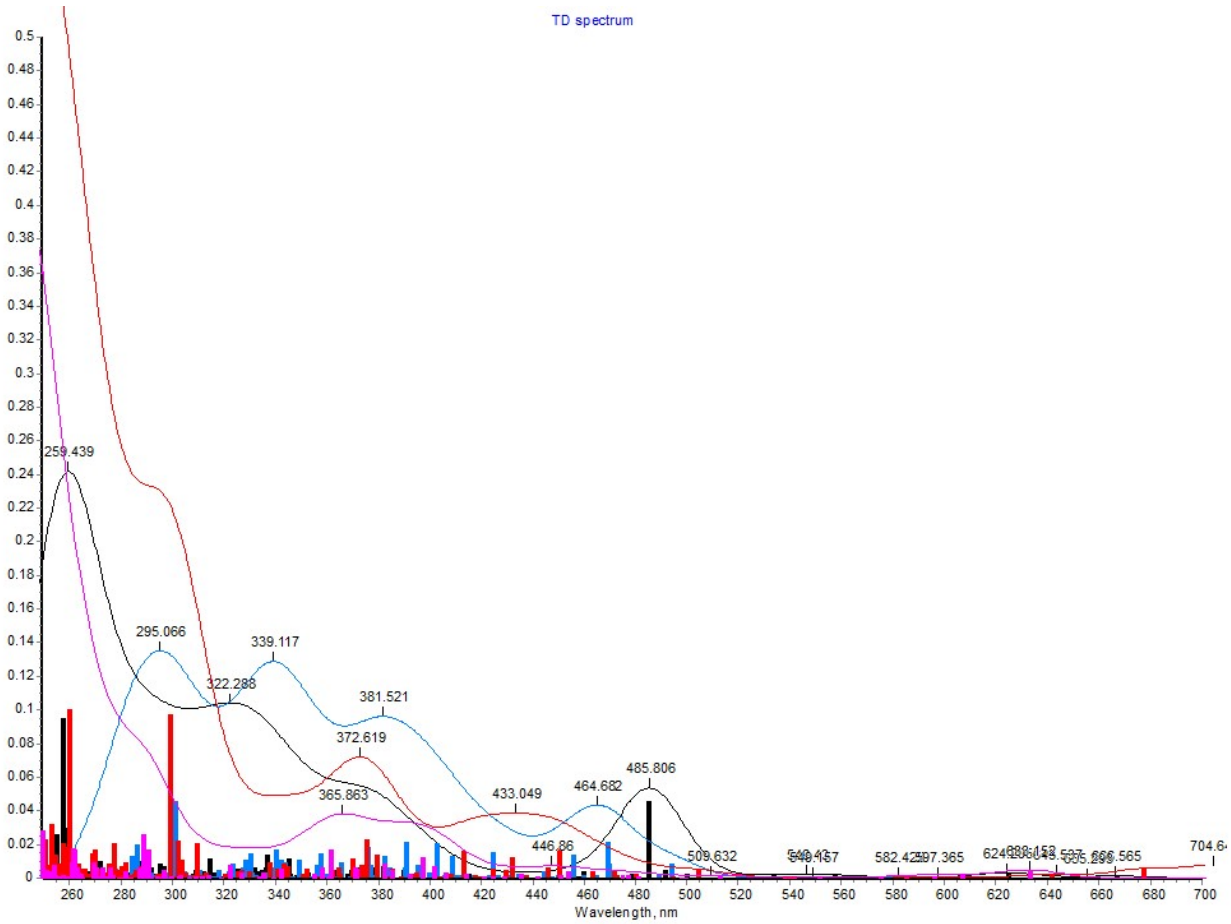


Fig. S10 Theoretical spectra of products with glutathione.

Table S1 Geometric deviation parameters calculated using the SHAPE program for various possible coordination geometries with four coordination numbers around iron ions for compound 1.

Compound 1	
T-4 (*Tetrahedron*)	vTBPY-4 (*Vacant trigonal bipyramid*)
1.280	3.589

Table S2 Structures of complexes 2, 3, and 3a.

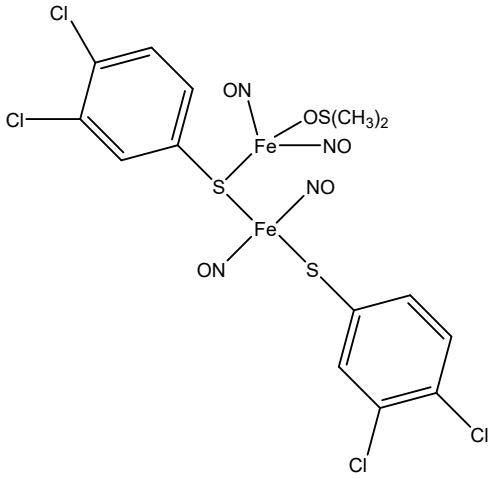
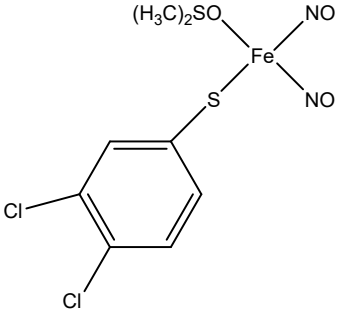
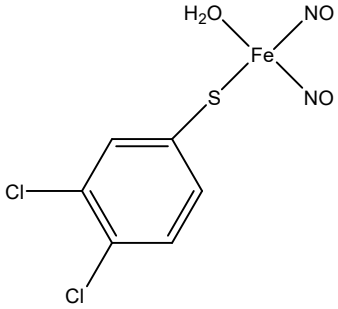
	Complex 2 $[Fe_2(SC_6H_3Cl_2)_2(NO)_4(OS(CH_3)_2)]$
	Complex 3 $[Fe(SC_6H_3Cl_2)(NO)_2(OS(CH_3)_2)]$
	Complex 3a $[Fe(SC_6H_3Cl_2)(NO)_2(H_2O)]$

Table S3 Comparison of NO-bonds parameters from NBO.

Complex	r		Wiberg index		Bond order	
3	1.699	1.699	1.244	1.236	1.606	1.588
6	1.792	1.723	1.098	1.215	1.308	1.429
7	1.829	1.744	1.086	1.199	1.247	1.371

Scheme S1 The reaction of formation of an insoluble binuclear complex