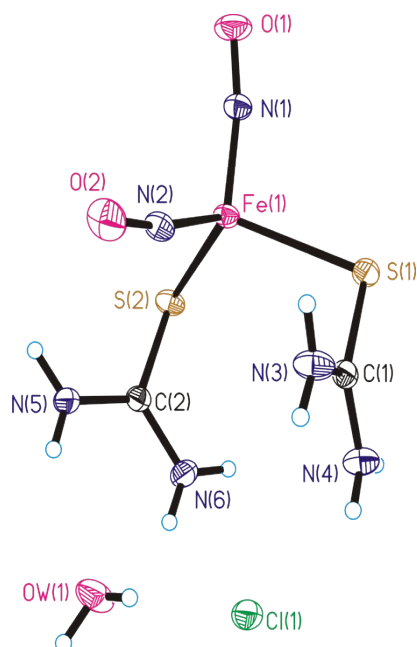


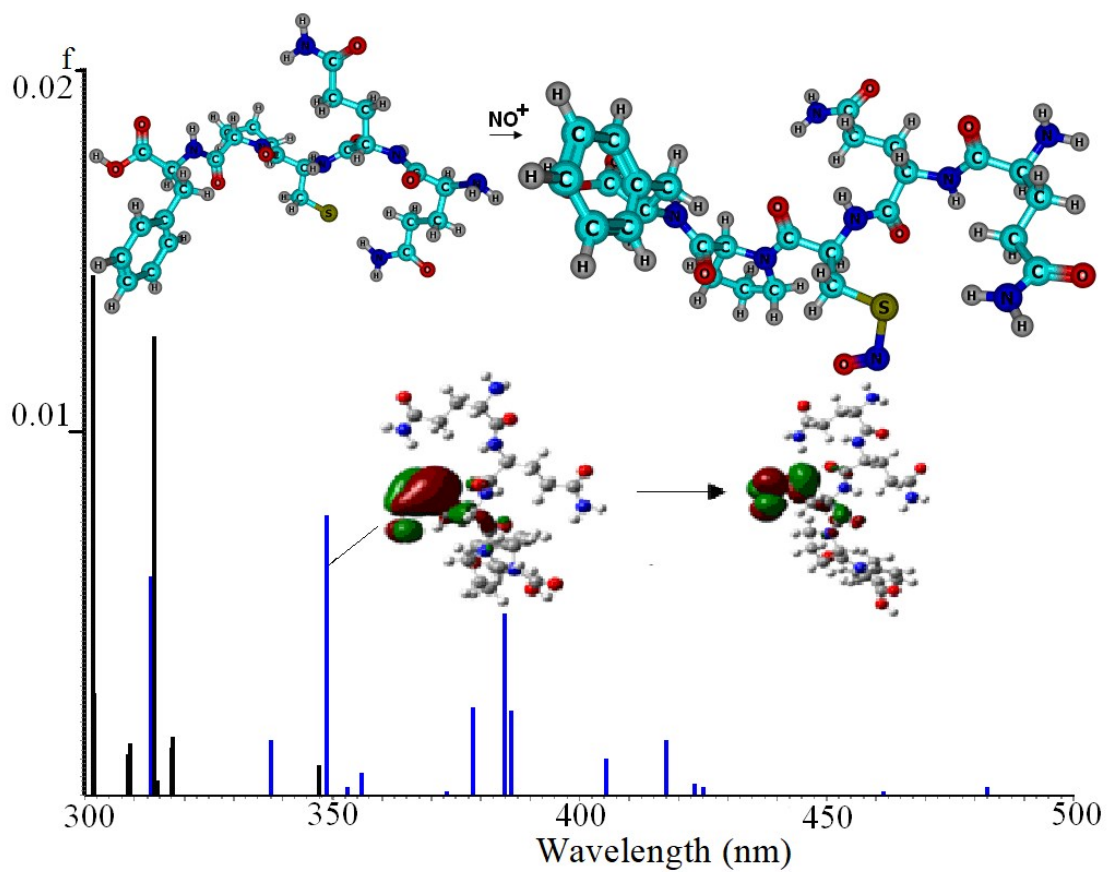
Supplementary materials to

Effect of albumin on the transformation of dinitrosyl iron complexes with thiourea ligands.

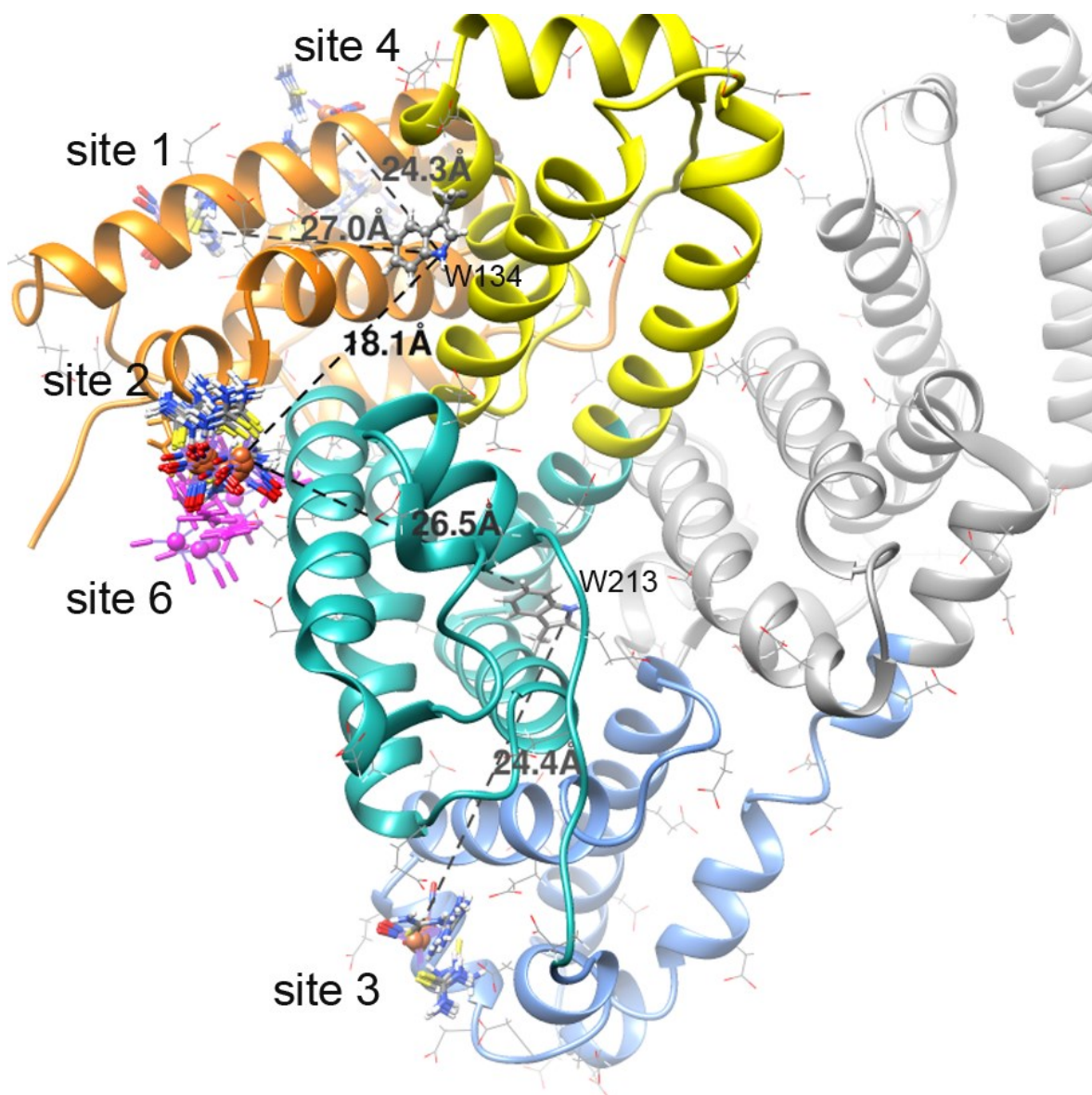
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Alexander I. Kotelnikov, Natalia A. Sanina, Sergey M. Aldoshin



**Fig. S1** Molecular structure of cationic mononuclear complex [Fe(SC(NH<sub>2</sub>)<sub>2</sub>)<sub>2</sub>(NO)<sub>2</sub>]<sup>+</sup>Cl<sup>-</sup>·H<sub>2</sub>O (X-ray data published previously<sup>14</sup>).



**Fig. S2** TDDFT spectrum of the segment of the initial protein containing Cys (black) and TDDFT spectrum of this segment with nitrosylated Cys (blue). The orbitals, which participate in the electron transitions corresponding to the absorption maximum (348.52 nm) are shown.



**Fig. S3** The docked positions of the lowest energy conformer of complex 1 at BSA and the effective distances to nitrogens of Trp 134 and Trp 213. The color scheme is explained in Fig. 4.