Electronic Supporting Information for:

Structural, Spectroscopic, and Electrochemical Properties of Nonheme Fe(II)-Hydroquinonate Complexes: Synthetic Models of Hydroquinone Dioxygenases

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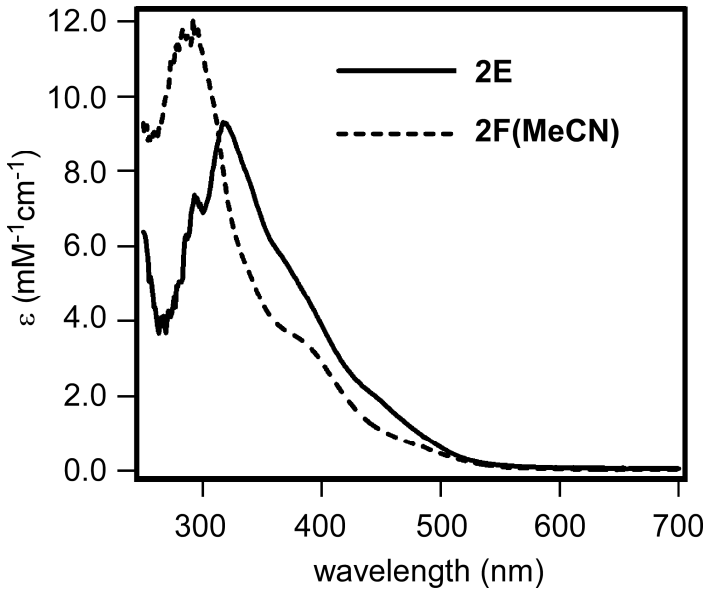

Figure S1. Electronic absorption spectra of **2E** and **2F(MeCN)** in CH_2Cl_2 at room temperature.

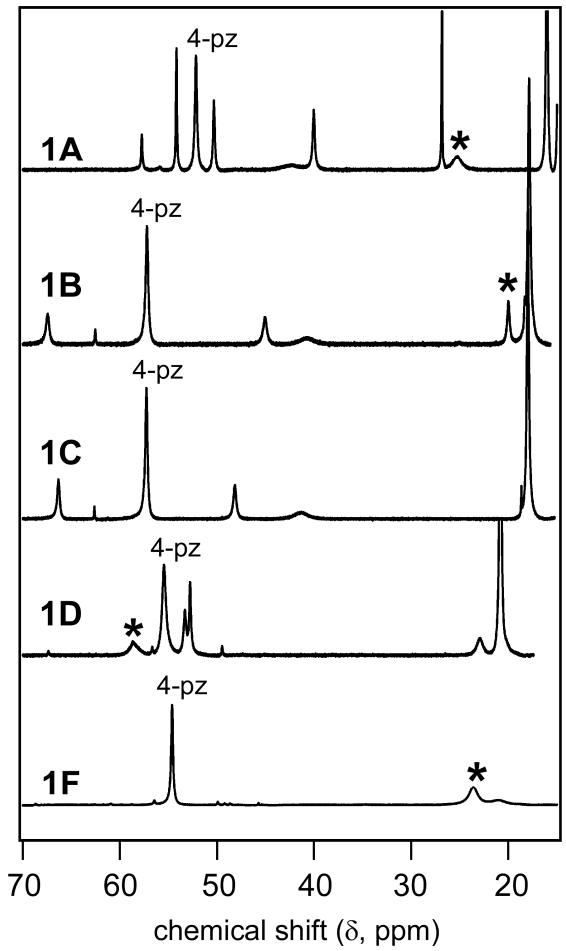

Figure S2. ^{1}H NMR spectra of **1A-1D,** and **1F** in CD_2Cl_2 at ambient temperature. Peaks marked with an asterisk (*) disappeared upon addition of a small amount of MeOH-d_4 and are therefore assigned to the exchangeable proton of the distal –OH moiety. Resonances arising from protons at the 4-positions of the ^{Ph2}Tp pyrazole rings (4-pz) were identified on the basis of peak integrations.

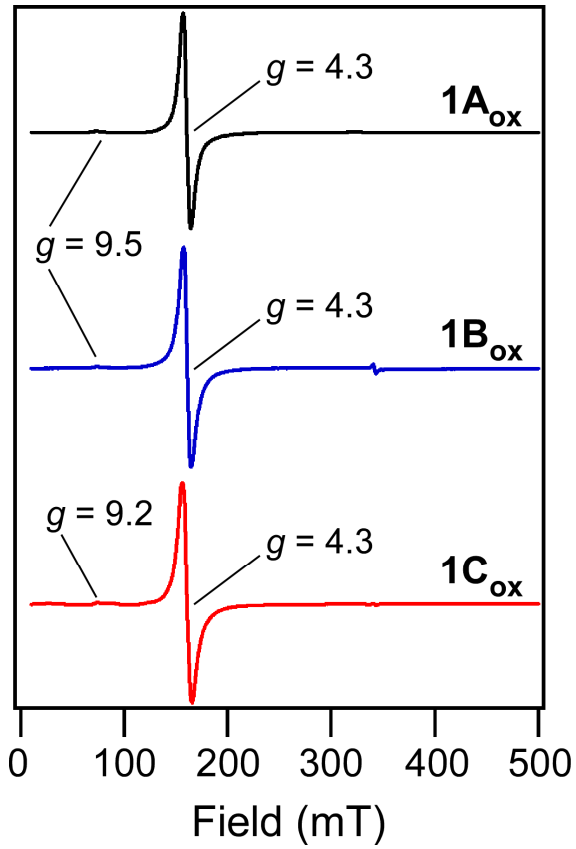

Figure S3. X-band EPR spectra of **1A$_{ox}$-1C$_{ox}$** in frozen CH_2Cl_2 solutions. The **1X$_{ox}$** species were obtained by treating the Fe(II) precursors with one equivalent of acetylferrocenuium (**1A$_{ox}$**) or $[N(C_6H_4Br\text{-}4)_3]^+$ (**1B$_{ox}$** and **1C$_{ox}$**). The spectra were collected under the following conditions: frequency = 9.63 GHz; power = 2.0 mW; modulation = 12 G; temperature = 10 K.

Computational Details.

Density functional theory (DFT) calculations of complex **1B** were performed using the ORCA 2.0 software package developed by Dr. F. Neese.[1] Atomic coordinates were obtained from the corresponding X-ray structure, although the 5-Ph groups of the ^{Ph2}Tp ligand were replaced by -CH_3 groups in the computational model. The DFT calculations employed the Becke-Perdew (BP86) functional[2] and Ahlrichs' valence triple-ζ basis set (TZV) for all atoms, in conjunction with the TZV/J auxiliary basis set.[3] Extra polarization functions were used on non-hydrogen atoms. Time-dependent DFT (TD-DFT) calculations[4] provided absorption energies and intensities within the Tamm-Dancoff approximation.[5] Forty excited states were calculated.

(1) Neese, F.; *ORCA - An ab initio, Density Functional and Semi-empirical Program Package,* version 2.8; University of Bonn: Bonn, Germany, 2010.

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