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Electronic Supporting Information

Aromatic Hydroxylation by an Oxo-bridged Diiron(III) Complex: A Bio-inspired Functional Model of *Toluene Monooxygenases*

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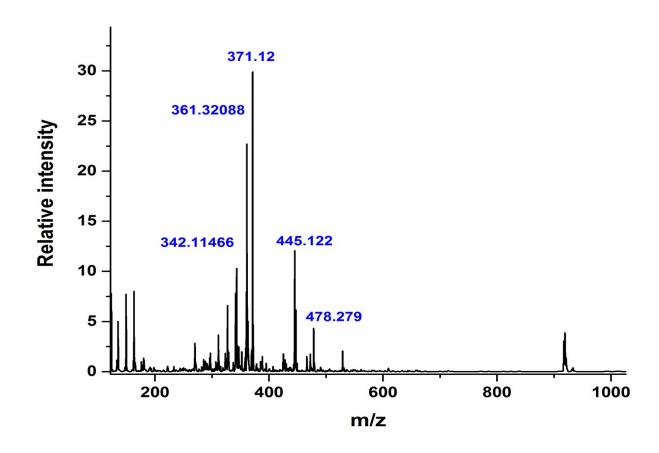


Figure S1a. ESIMS spectrum obtained during the course of benzene hydroxylation by 2/H₂O₂.

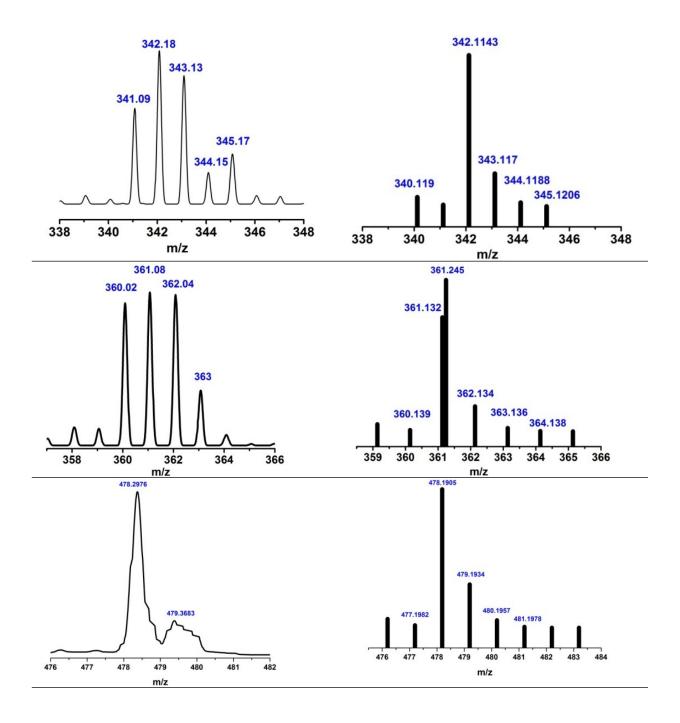


Figure S1b. Experimental and theoretical isotope distribution patterns. The peak at m/z = 342 has been assigned to $[(bpmen)Fe^{III}(O)]^+$ whereas the peak at m/z = 361 can be assigned to the species $[\{(bpmen)Fe^{III}(O)(OH_2)\}+H]^+$. The peak at m/z = 478 can be assigned to $[(bpmen)Fe^{III}(OPh)(OH)(MeCN)+H]^+$.

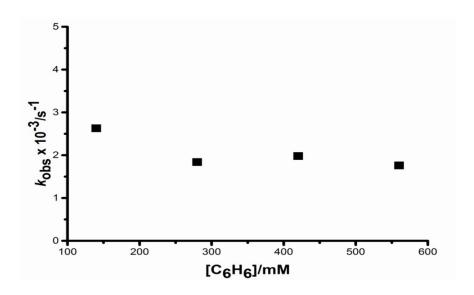


Figure S2. Rate of formation of phenolate as a function of benzene concentration.

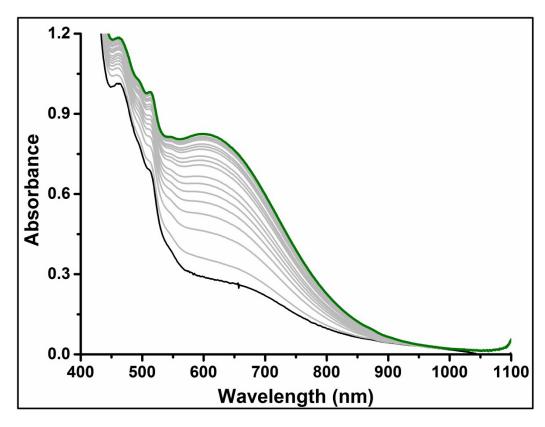


Figure S3. Electronic changes observed after the addition of additional H_2O_2 (10 mM) to the final diiron(III) complex (black line). The final spectrum corresponding to the phenolate bound iron(III) species is shown in green.

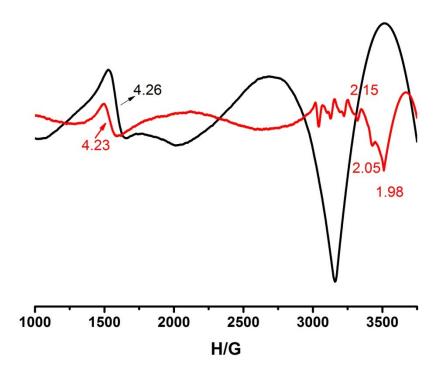


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