

Supporting Information

μ -Oxo- and Bis(μ -carboxylato)-bridged Diiron(III) Complexes of a 3N Ligand as Catalysts for Alkane Hydroxylation: Stereoelectronic Factors of Carboxylate Bridge Determine the Catalytic Efficiency

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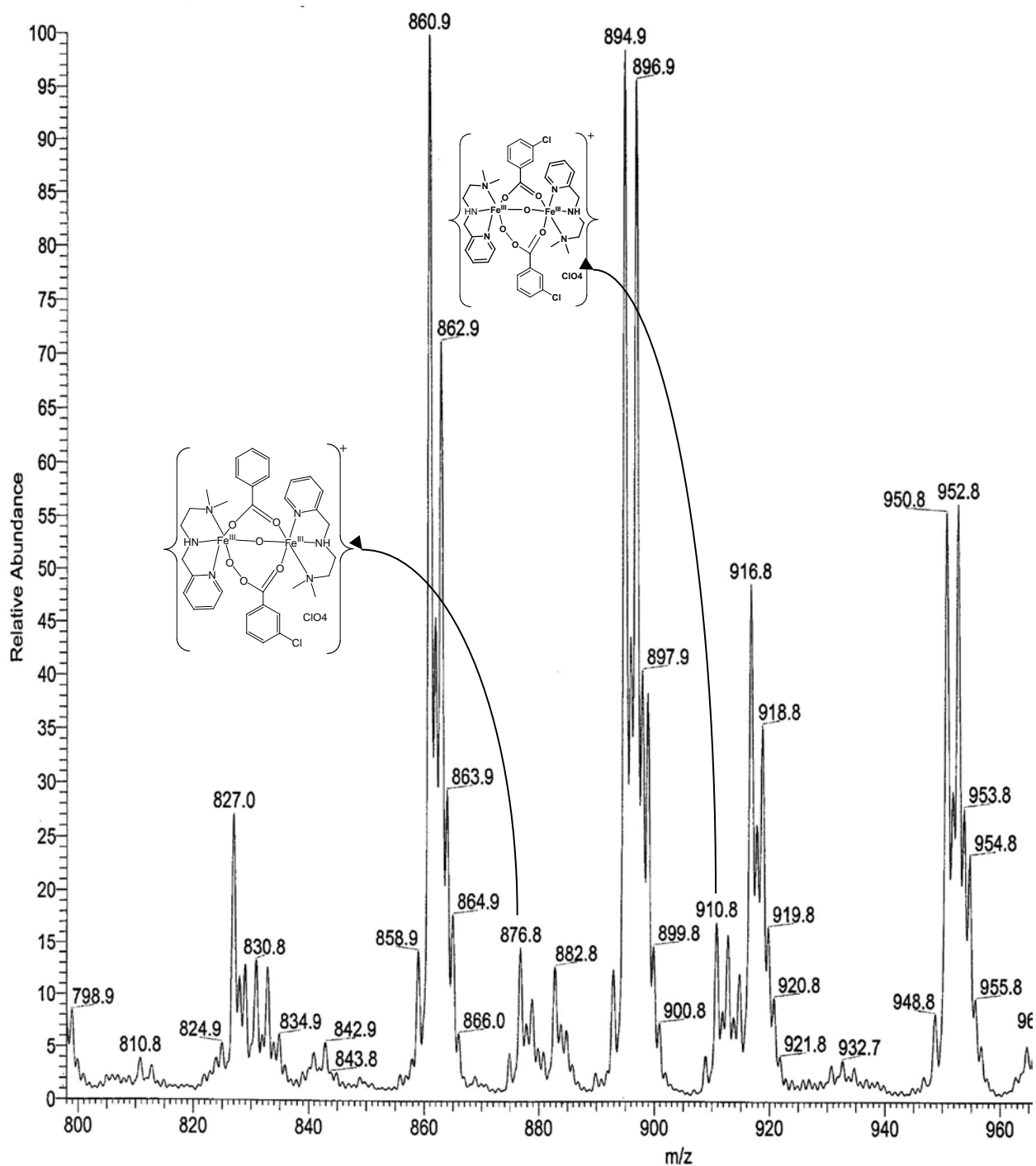


Figure S1. ESI-MS spectrum of the reaction of **4** with 5 eq. of *m*-CPBA and 1 eq. of TEA. Intense peak in the spectrum at $m/z = 860.9, 894.8, 916.8$ and 950.7 corresponding to $\{[\text{Fe}_2^{\text{III}}(\text{O})(\text{L})_2(\text{OBz})_2]\text{ClO}_4\}^+$, $\{[\text{Fe}_2^{\text{III}}(\text{O})(\text{L})_2(\text{OBz})_2](\text{OBzCl})\}^+$, $\{[\text{Fe}_2^{\text{III}}(\text{O})(\text{L})_2(\text{OBz})(\text{OBzCl})](\text{OBzCl})\}^+$ and $\{[\text{Fe}_2^{\text{III}}(\text{O})(\text{L})_2(\text{OBzCl})_2](\text{OBzCl})\}^+$. Less intense peaks in the spectrum are assigned to the *m*-CPBA adducts $\{[\text{Fe}_2^{\text{III}}(\text{O})(\text{L})_2(\text{OBz})(\text{OOCOC}_6\text{H}_4\text{Cl})]\text{ClO}_4\}^+$ ($m/z = 876.8$) and $\{[\text{Fe}_2^{\text{III}}(\text{O})(\text{L})_2(\text{OBzCl})(\text{OOCOC}_6\text{H}_4\text{Cl})]\text{ClO}_4\}^+$.

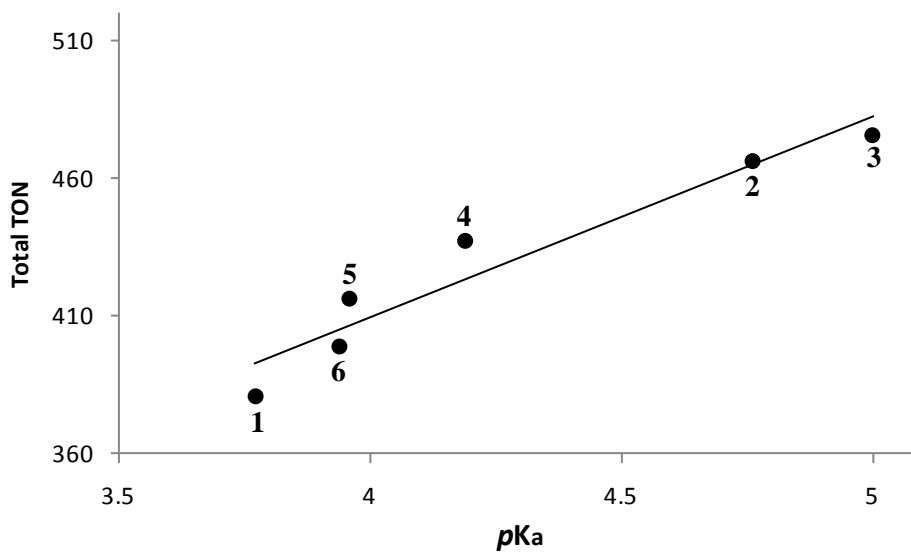


Figure S2. A linear correlation (R^2 , 0.93) between pK_a value of bridging carboxylates and total TON of diiron(III) complexes for adamantane oxidation

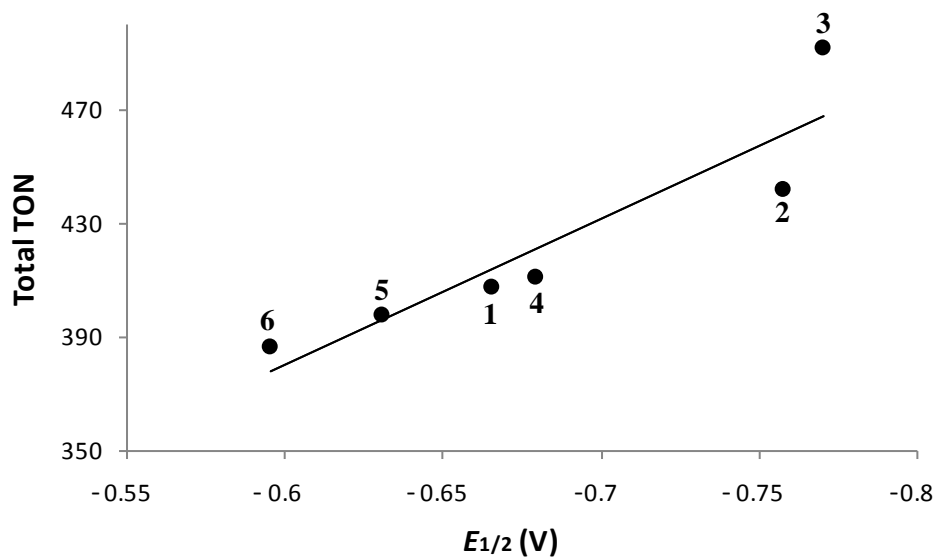


Figure S3. A linear correlation (R^2 , 0.84) between $E_{1/2}$ value and total TON of diiron(III) complexes for cyclohexane oxidation.

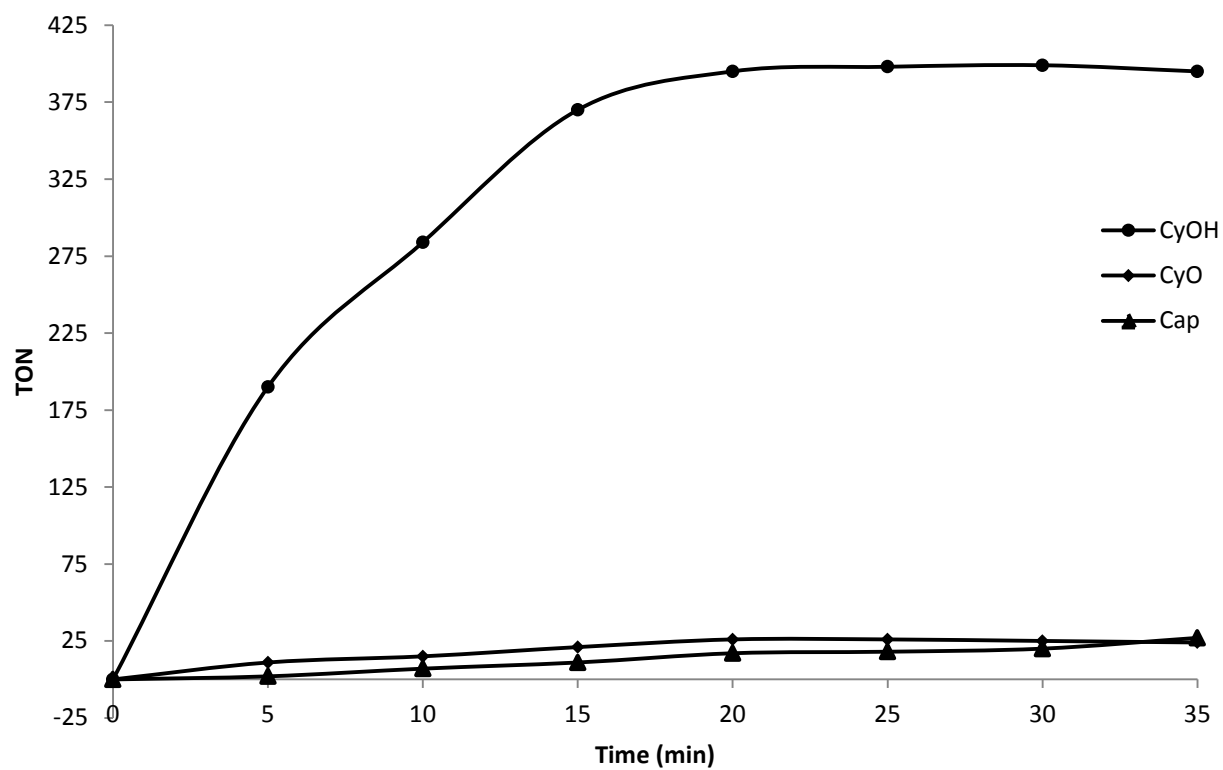


Figure S4. Time dependent oxidation of cyclohexane catalyzed by **2** with *m*-CPBA