Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

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

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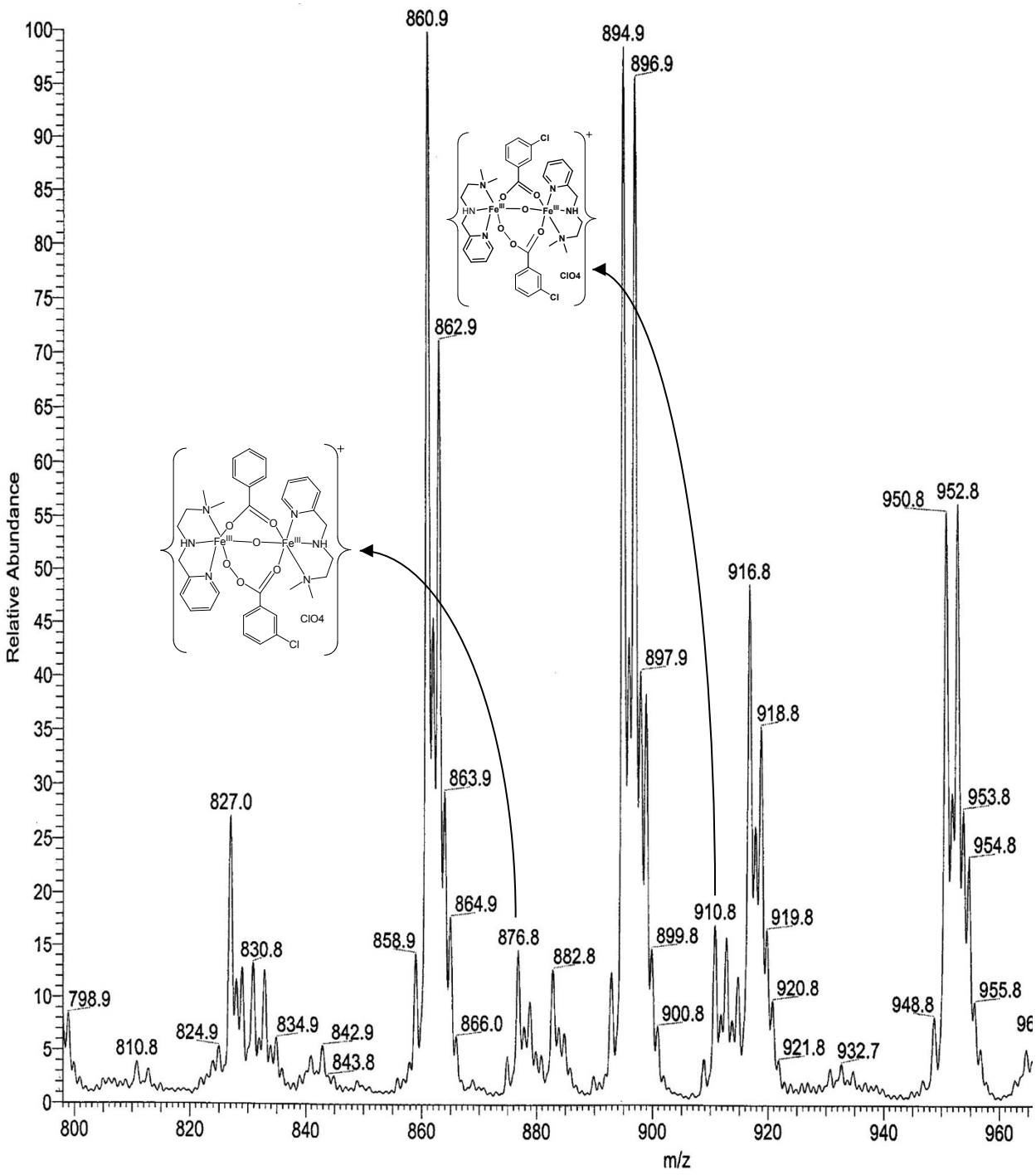

Figure S1. ESI-MS spectrum of the reaction of **4** with 5 eq. of *m*-CPBA and 1 eq. of TEA. Intense peak in the spectrum at m/z = 860.9, 894.8, 916.8 and 950.7 corresponding to $\{[Fe_2^{III}(O)(L)_2(OBz)_2]ClO_4\}^+$, $\{[Fe_2^{III}(O)(L)_2(OBz)_2](OBzCl)\}^+$, $\{[Fe_2^{III}(O)(L)_2(OBz)(OBzCl)](OBzCl)\}^+$ and $\{[Fe_2^{III}(O)(L)_2(OBzCl)_2](OBzCl)\}^+$. Less intense peaks in the spectrum are assigned to the *m*-CPBA adducts $\{[Fe_2^{III}(O)(L)_2(OBz)(OOCOC_6H_4Cl)]ClO_4\}^+$ (m/z = 876.8) and $\{[Fe_2^{III}(O)(L)_2(OBzCl)(OOCOC_6H_4Cl)]ClO_4\}^+$.

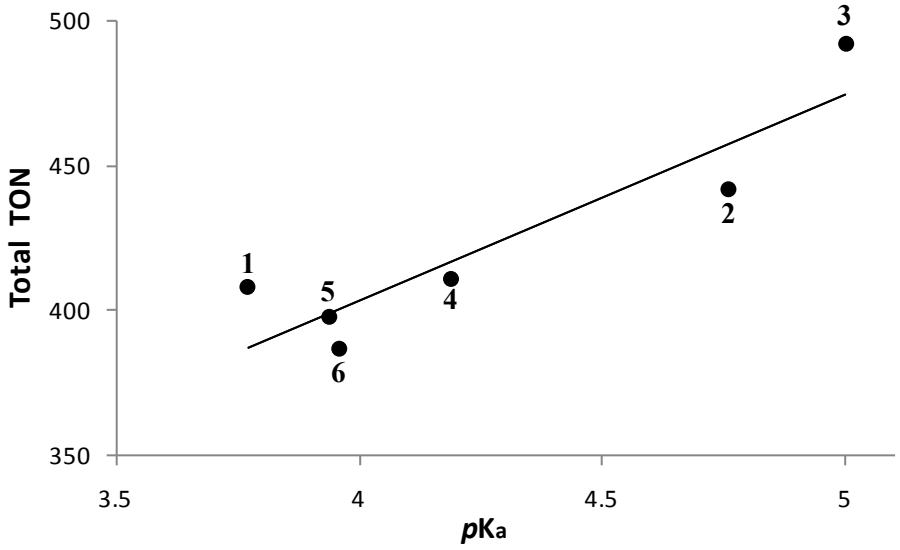

Figure S2. A linear correlation (R^2, 0.84) between pK_a value of bridging carboxylates and total TON of diiron(III) complexes for cyclohexane oxidation

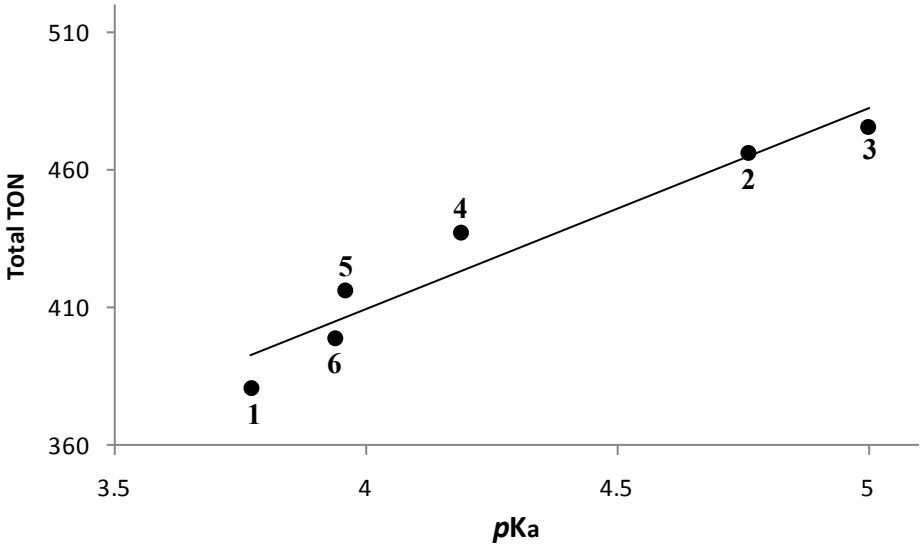

Figure S3.A linear correlation (R^2, 0.93) between pK_a value of bridging carboxylates and total TON of diiron(III) complexes for adamantane oxidation

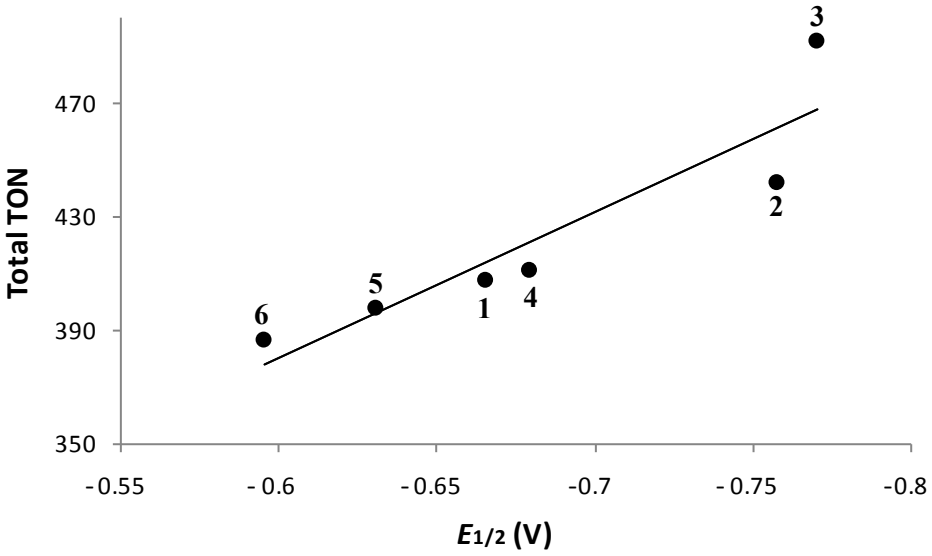

Figure S4. A linear correlation (R^2, 0.84) between $E_{1/2}$ value and total TON of diiron(III) complexes for cyclohexane oxidation.

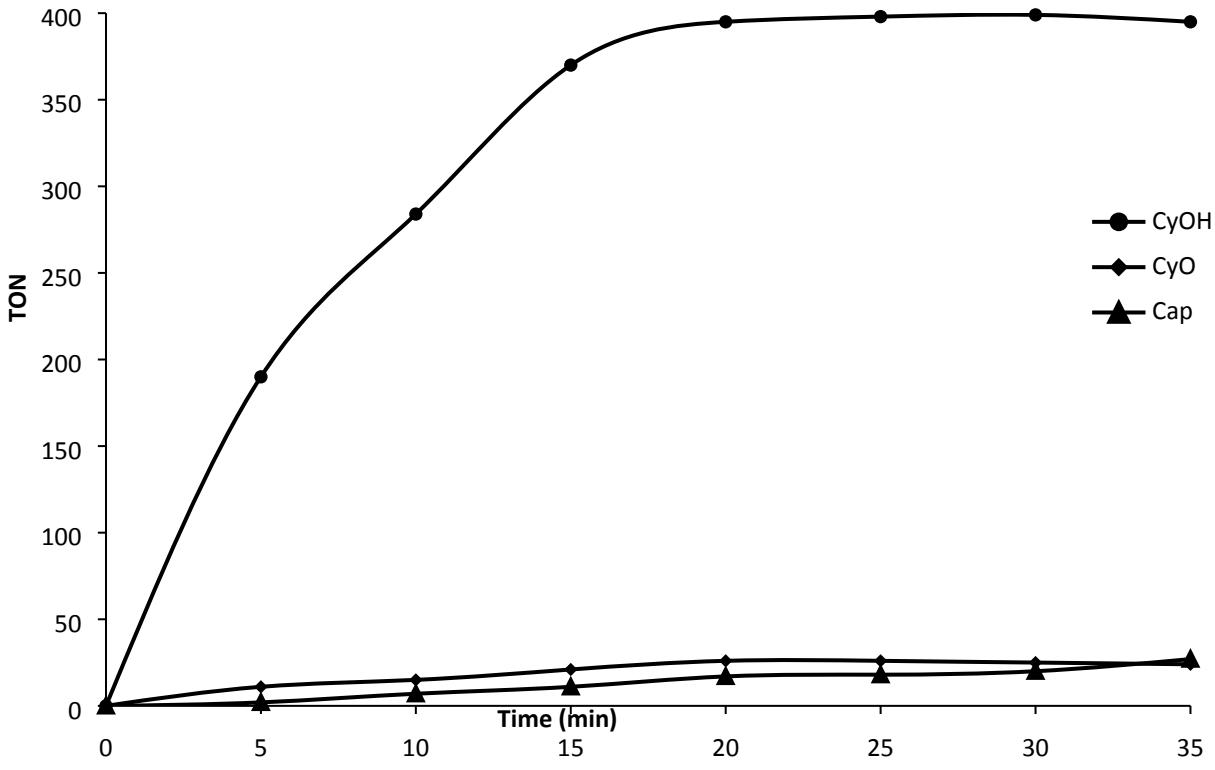

Figure S5. Time dependent oxidation of cyclohexane catalyzed by **2** with *m*-CPBA