Supporting Information

Selective Formation of a Stable \( \mu \)-Peroxo Ferric Heme-Cu\( ^{II} \) Complex from the Corresponding \( \mu \)-Oxo Fe\( ^{III} \)-Cu\( ^{II} \) Species with Hydrogen Peroxide

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Fig. S1. ORTEP view of \([(TMP)Fe^{III}-(O)-(5MeTPA)Cu^{II}]^+\) in crystals of 2 drawn with the thermal ellipsoids at the 50 % probability level. All hydrogen atoms were omitted for clarity. Selected bond length [Å] and angles [deg]: Cu(1)-O(2) 1.856(3), Fe(1)-O(2) 1.758(3), Cu(1)-N(1) 2.069(4), Cu(1)-N(2) 2.079(4), Cu(1)-N(3) 2.144(4), Cu(1)-N(4) 2.095(4), Fe(1)-N(5) 2.121(4), Fe(1)-N(6) 2.113(4), Fe(1)-N(7) 2.106(4), Fe(1)-N(8) 2.119(4), Cu(1)-O(2)-Fe(1) 172.8(2).
Fig. S2. ESI-mass spectra (CH$_3$CN, room temperature): (A) 2, (B) 2 + H$_2^{16}$O$_2$ and (C) 2 + H$_2^{18}$O$_2$. The magnified ones are shown in the right side with their simulated isotope patterns in bars.