Electronic Supplementary Information (ESI)

for

Oxidative Degradation of Toxic Organic Pollutants by Water Soluble Nonheme Iron(IV)-Oxo Complexes of Polydentate Nitrogen Donor Ligands

*Sandip Munshi, Rahul Dev Jana and Tapan Kanti Paine**

School of Chemical Sciences, Indian Association for the Cultivation of Science,
2A & 2B Raja S. C. Mullick Road, Jadavpur, Kolkata-700032, India

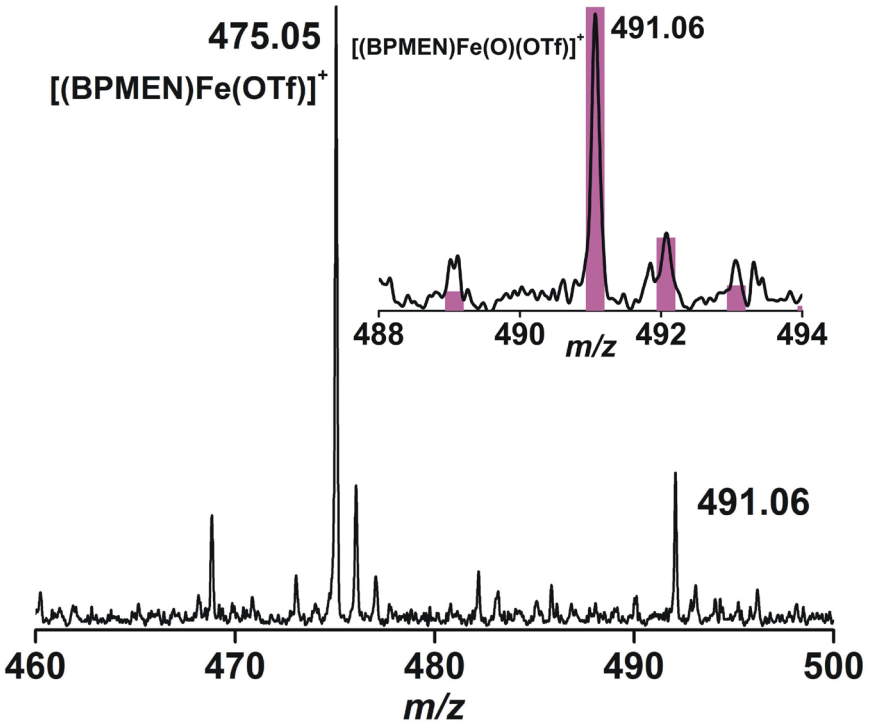

Fig. S1 ESI-mass spectrum (positive ion mode in water) of **1**.

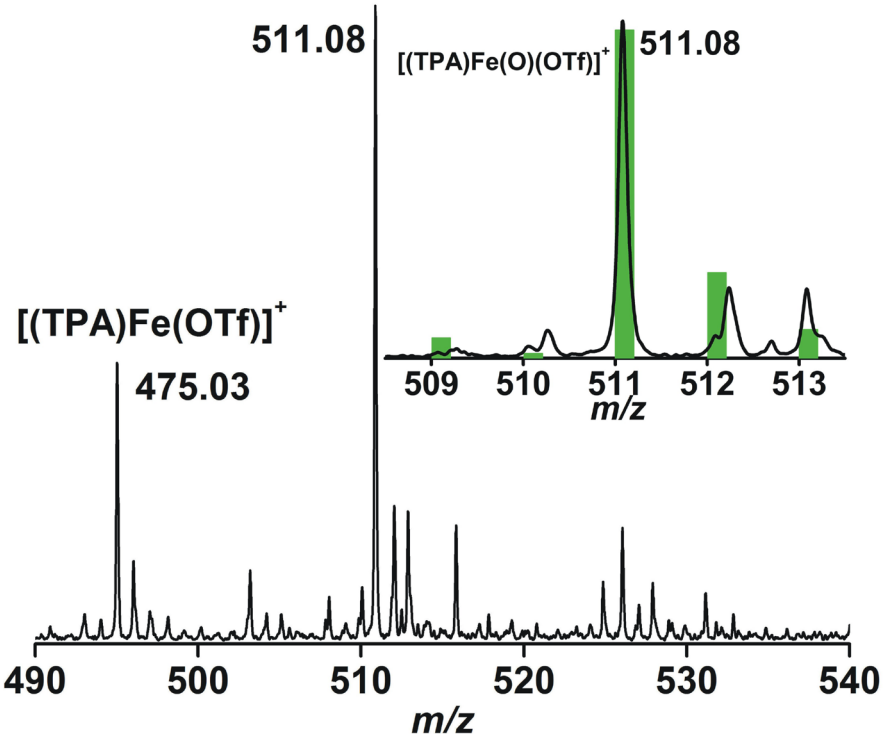

Fig. S2 ESI-mass spectrum (positive ion mode in water) of **2**.

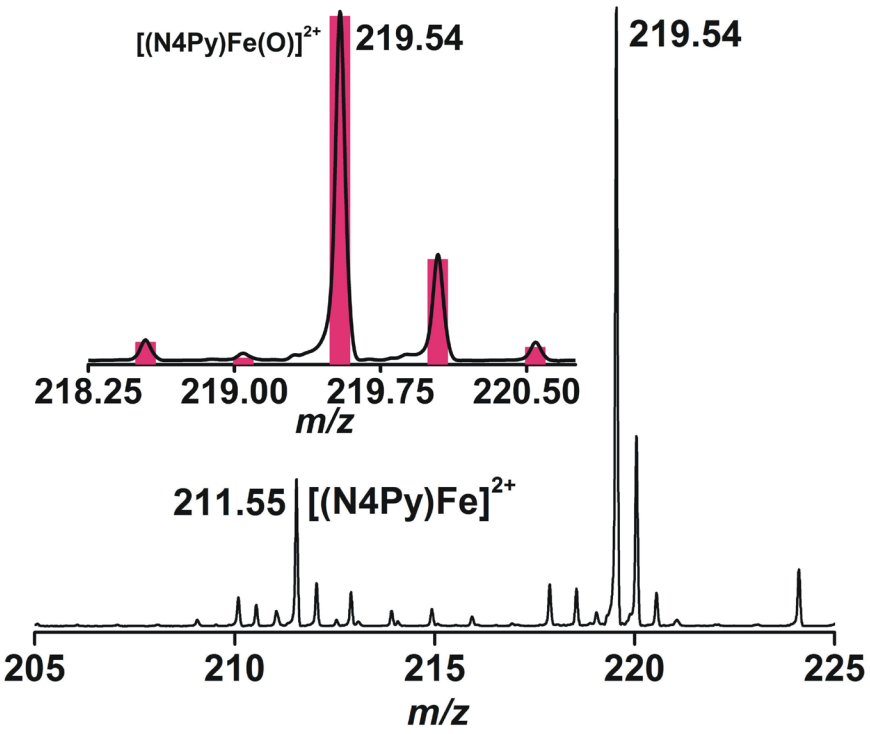

Fig. S3 ESI-mass spectrum (positive ion mode in water) of **3**.

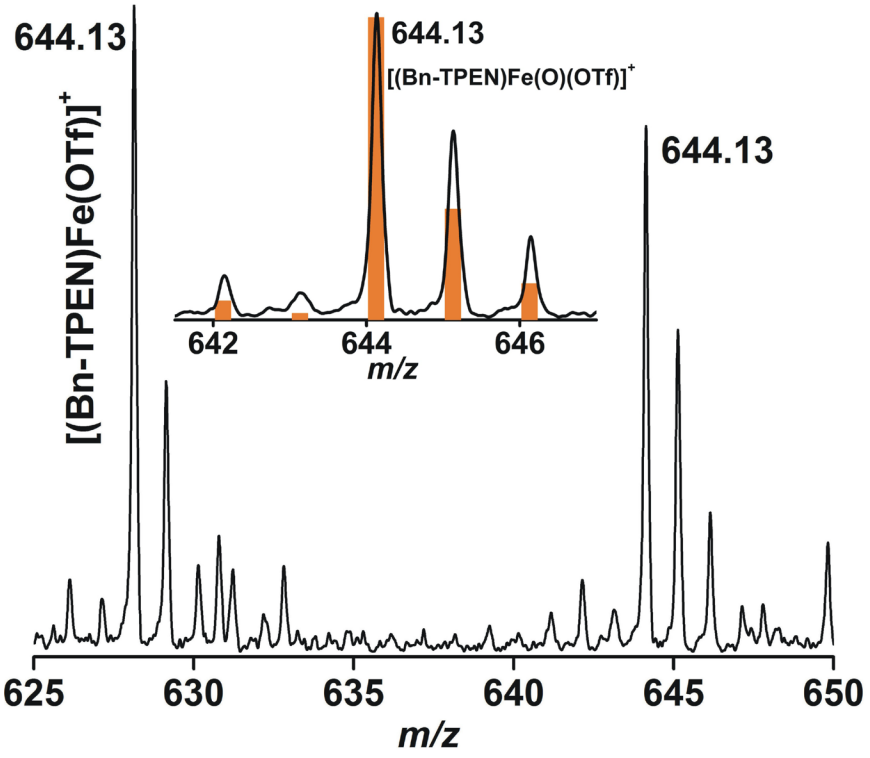

Fig. S4 ESI-mass spectrum (positive ion mode in water) of **4**.

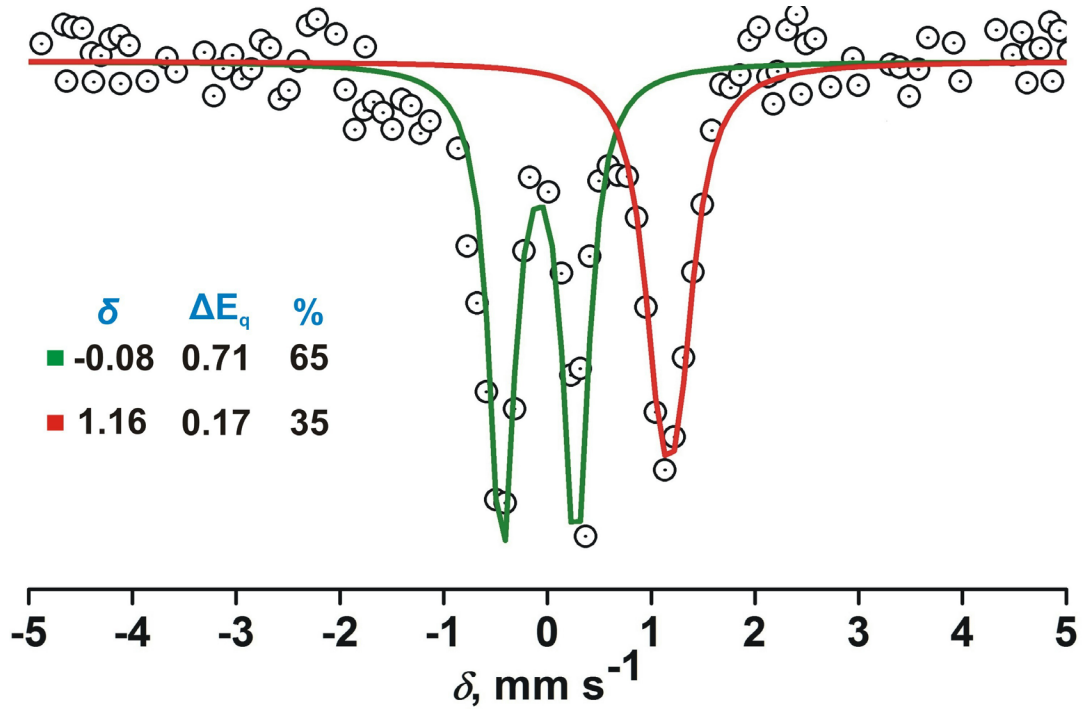

Fig. S5 Zero-field ^{57}Fe Mössbauer spectrum of the frozen sample of complex **4** at 77 K. Simulation shows the presence of an iron(IV)-oxo species (65%) and the starting iron (II) complex (35%) in the sample used for data collection.

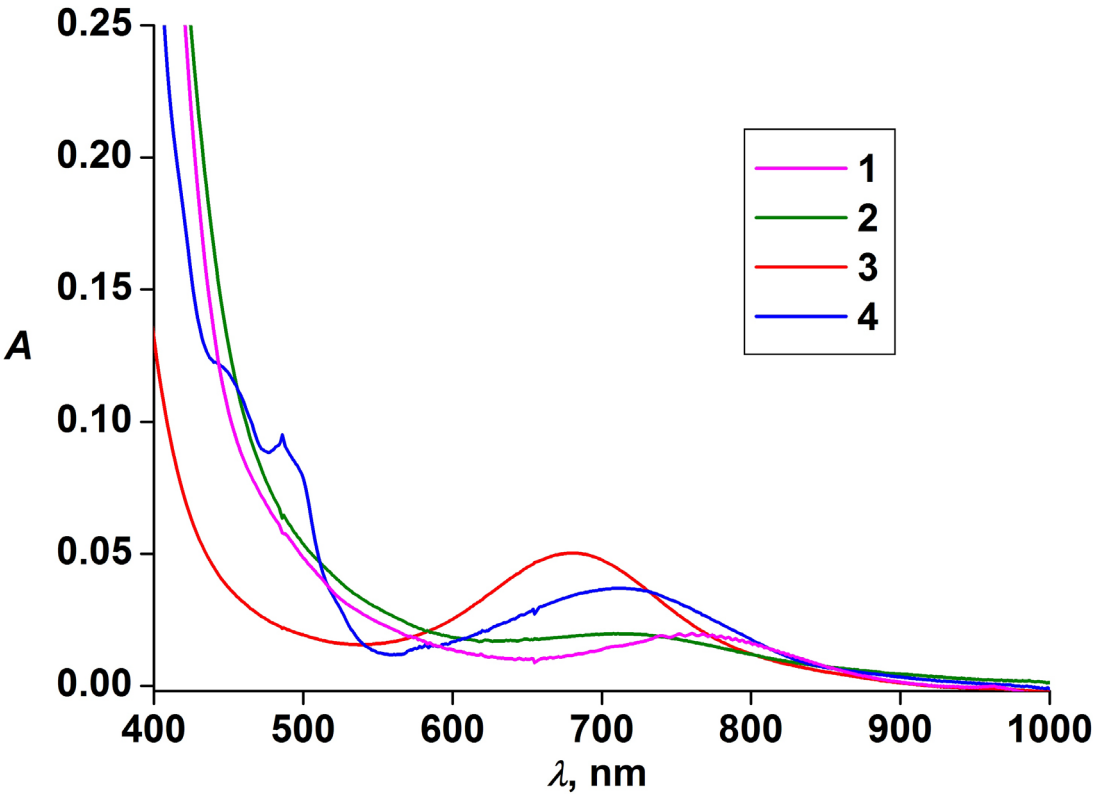

Fig. S6 Optical spectra of the iron(IV)-oxo species (**1**-**4**) generated by oxone (0.25 mM in water at 298 K).

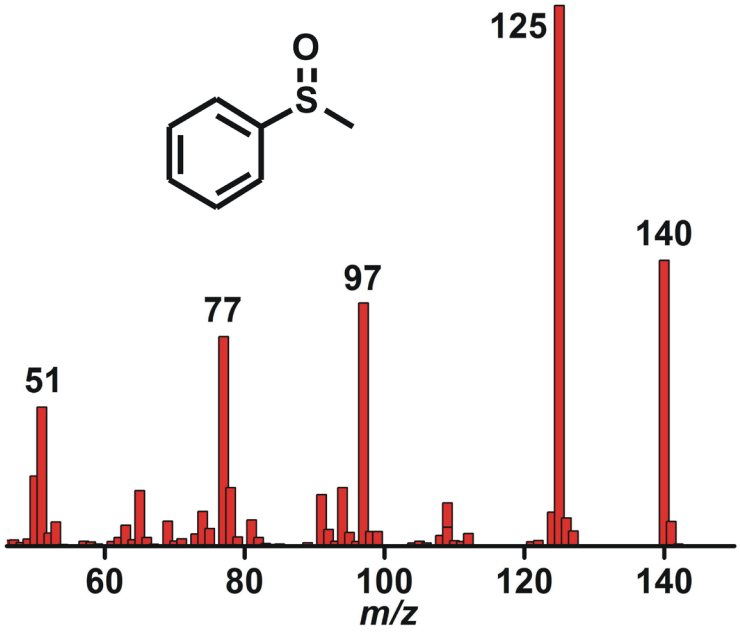

Fig. S7 GC-mass spectrum of thioanisole oxide formed in the reaction of iron(IV)-oxo species (**1**) with thioanisole (10 equiv.).

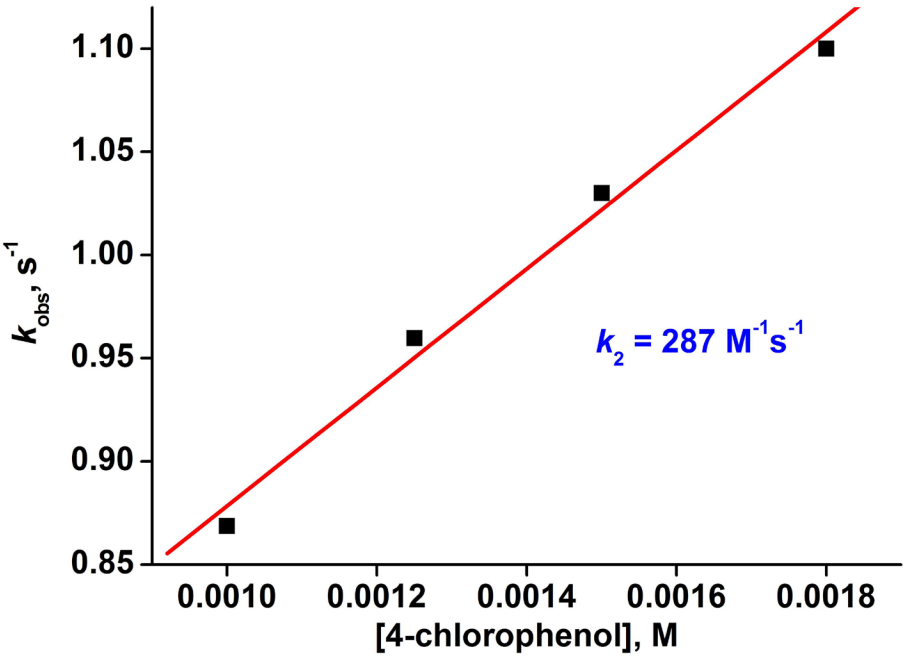

Fig. S8 Second order rate constant for 4-chlorophenol oxidation by **2**.

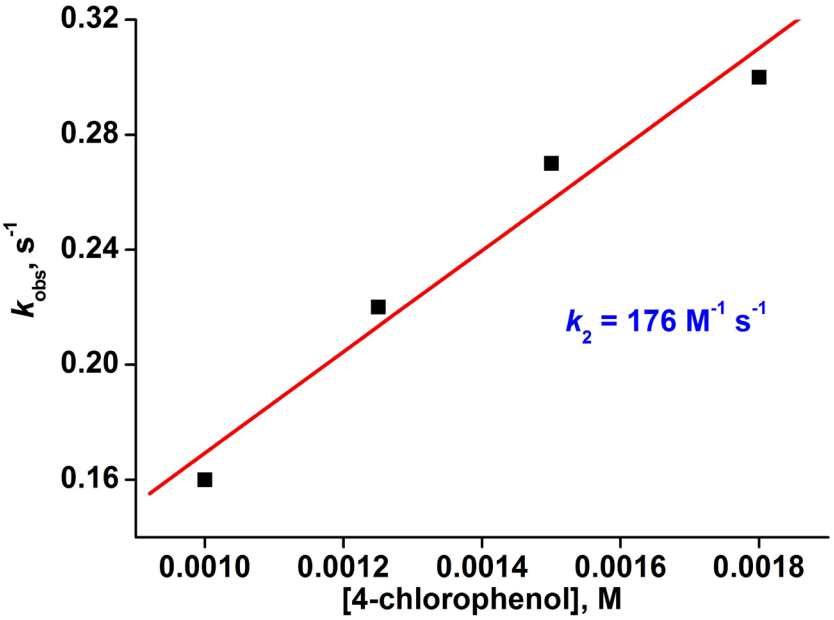

Fig. S9 Second order rate constant for 4-chlorophenol oxidation by **3**.

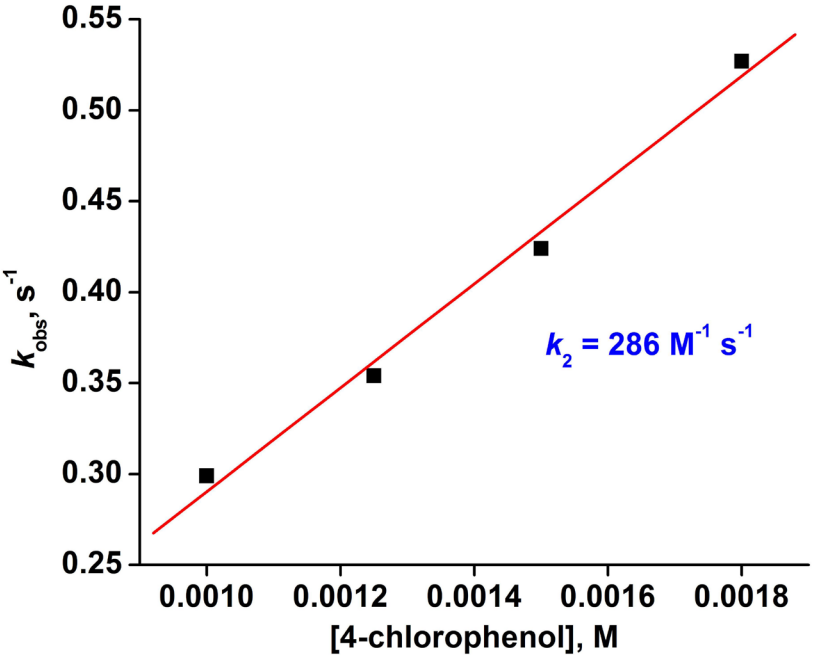

Fig. S10 Second order rate constant for 4-chlorophenol oxidation by **4**.

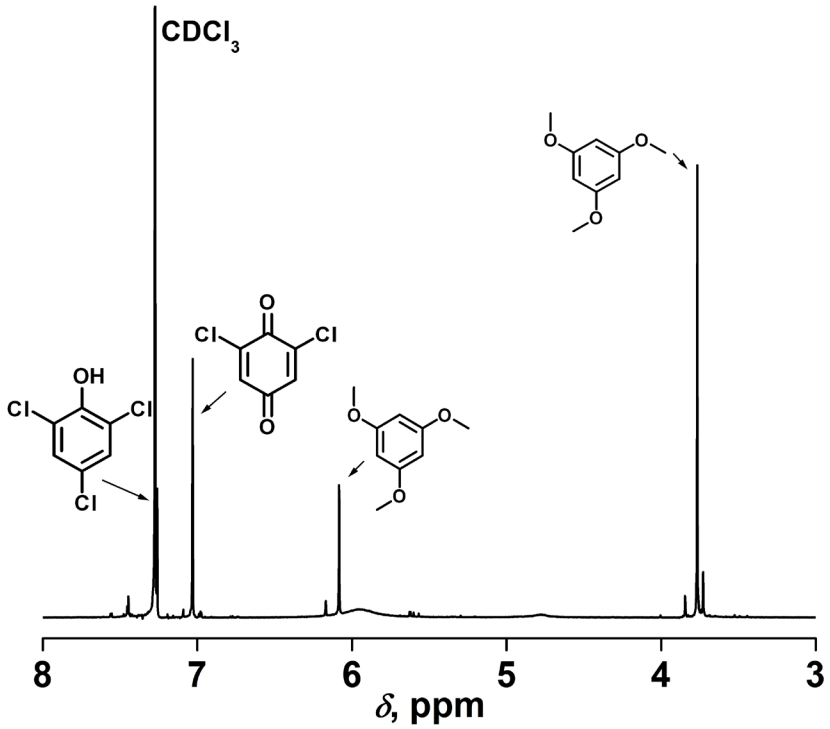

Fig. S11 ^{1}H NMR (300 MHz, $CDCl_3$, 298 K) spectrum of organic product formed in the reaction of 2,4,6-trichlorophenol (10 equiv.) with **1**.

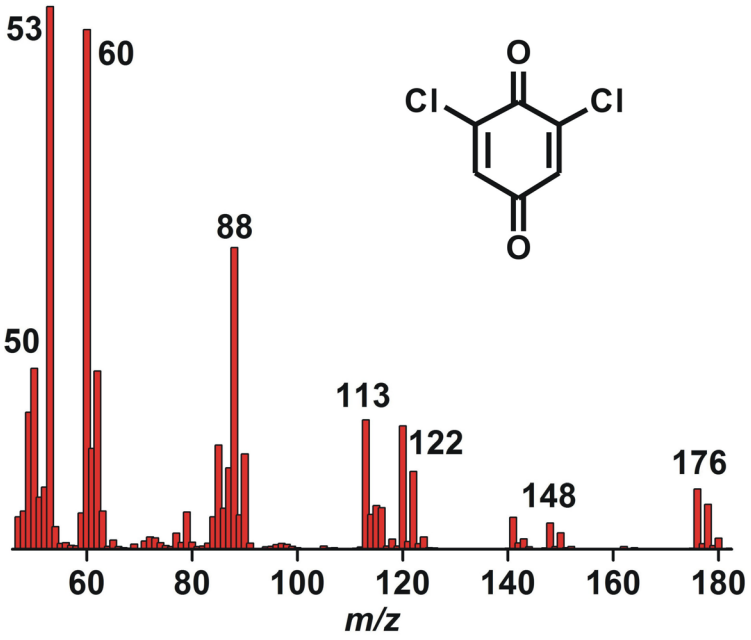

Fig. S12 GC-mass spectrum of 2,6-dichloro-*p*-benzoquinone formed in the reaction of **3** with 2,4,6-trichlorophenol (10 equiv.).

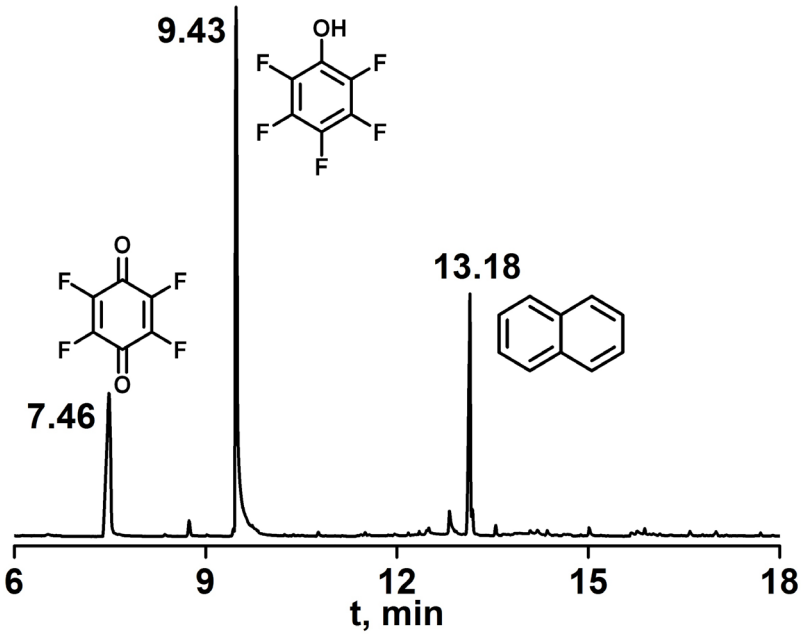

Fig. S13 GC chromatogram of 2,3,5,6-tetrafluoro-*p*-benzoquinone obtained in the reaction of **4** with pentafluorophenol (10 equiv.).

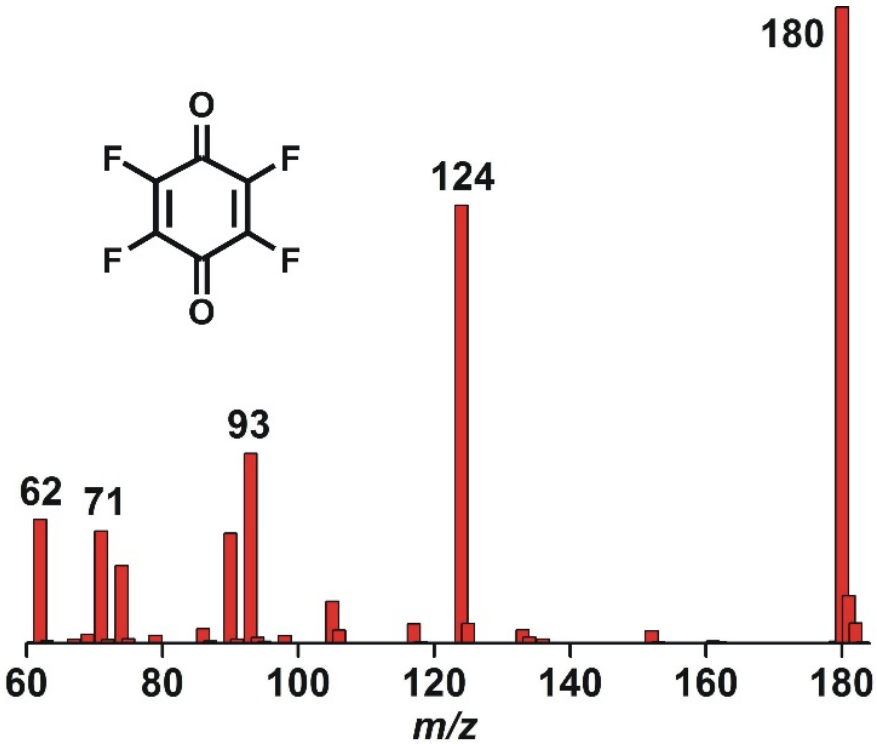

Fig. S14 GC-mass spectrum of 2,3,5,6-tetrafluoro-*p*-benzoquinone formed in the reaction of **4** with pentafluorophenol (10 equiv.).

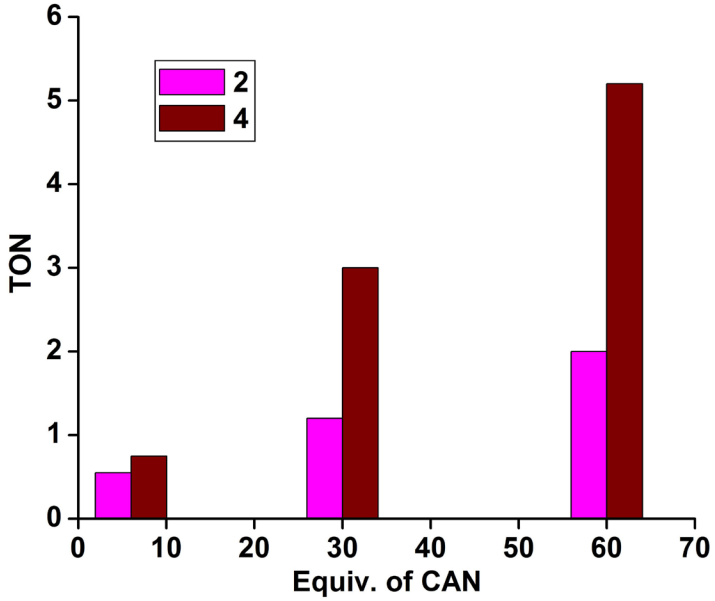

Fig. S15 TON of 2,3,5,6-tetrafluoro-*p*-benzoquinone derived from pentafluorophenol oxidation by **2** and **4** in the presence of CAN (60 equiv).

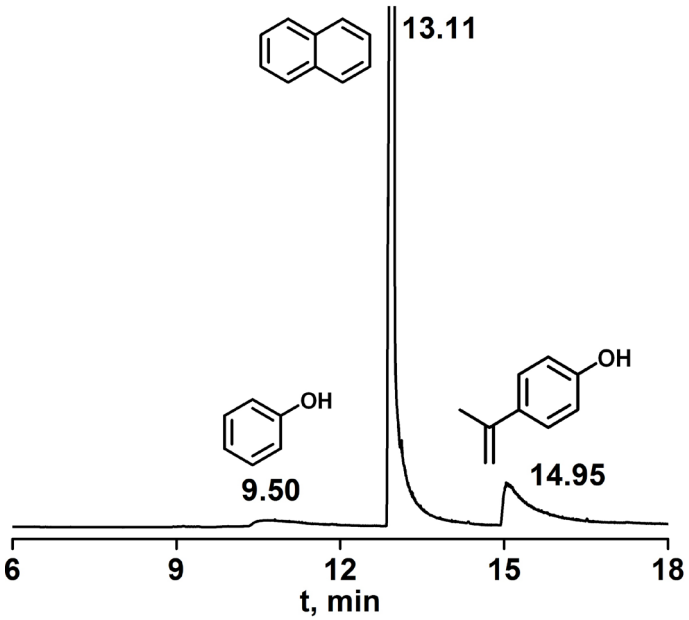

Fig. S16 GC chromatogram of phenols obtained in the oxidation of Bisphenol A (10 equiv.) by **3**.

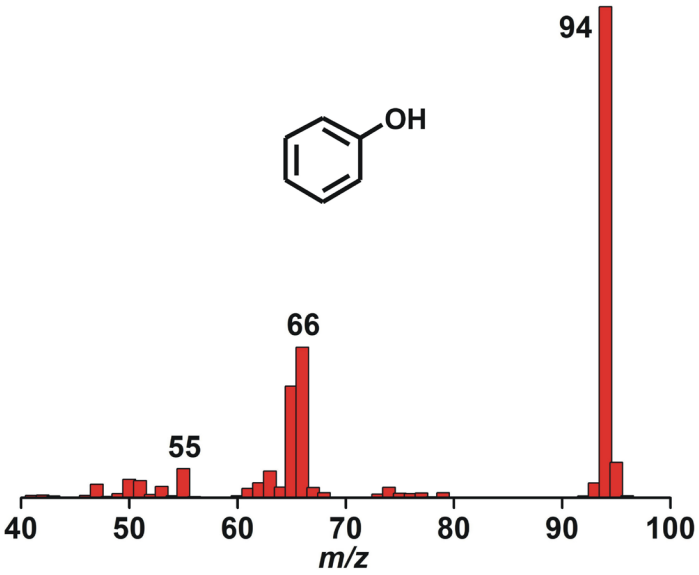

Fig. S17 GC-mass spectrum of phenol formed in the reaction of **3** with Bisphenol A (10 equiv.).

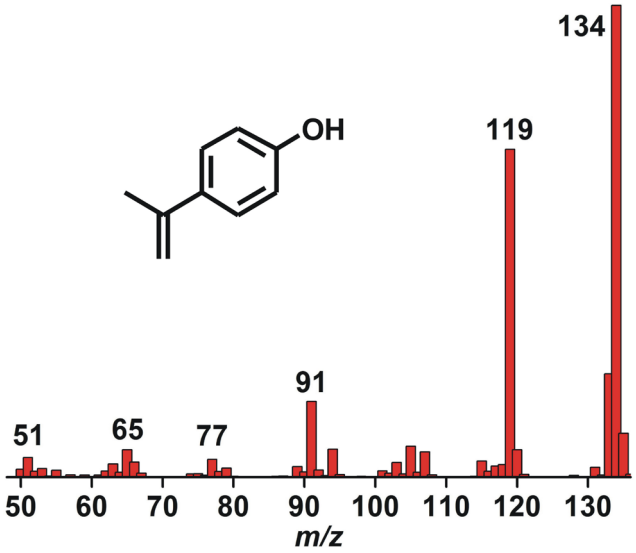

Fig. S18 GC-mass spectrum of *p*-isopropenylphenol formed in the reaction of **3** with Bisphenol A (10 equiv.).

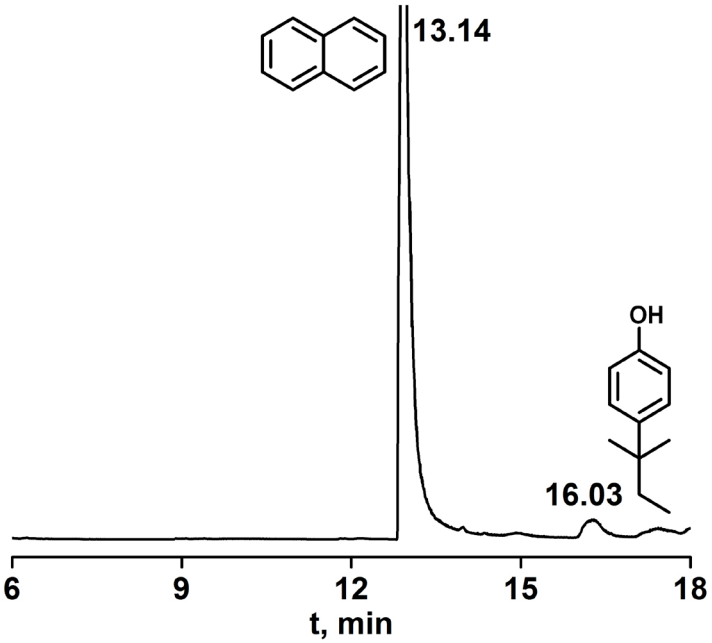

Fig. S19 GC chromatogram of products obtained in the oxidation of nonylphenol (10 equiv.) by **2**.

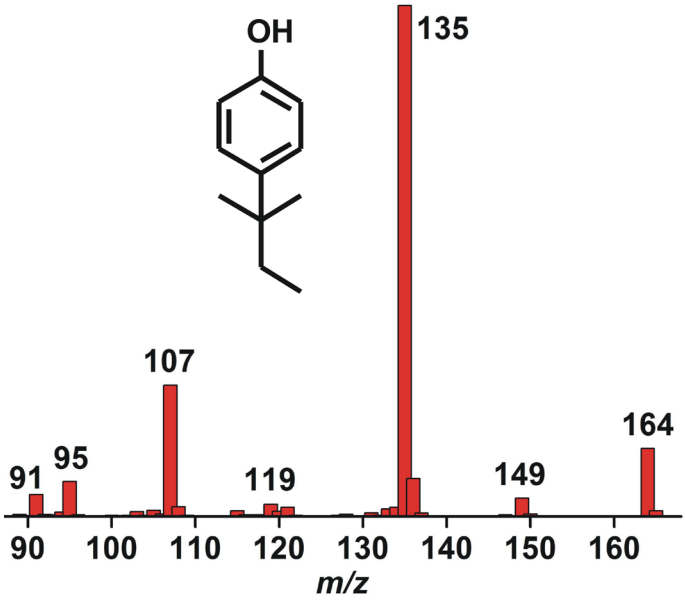

Fig. S20 GC-mass spectrum of *p*-dimethylpropylphenol formed in the reaction of **2** with nonylphenol (10 equiv.).

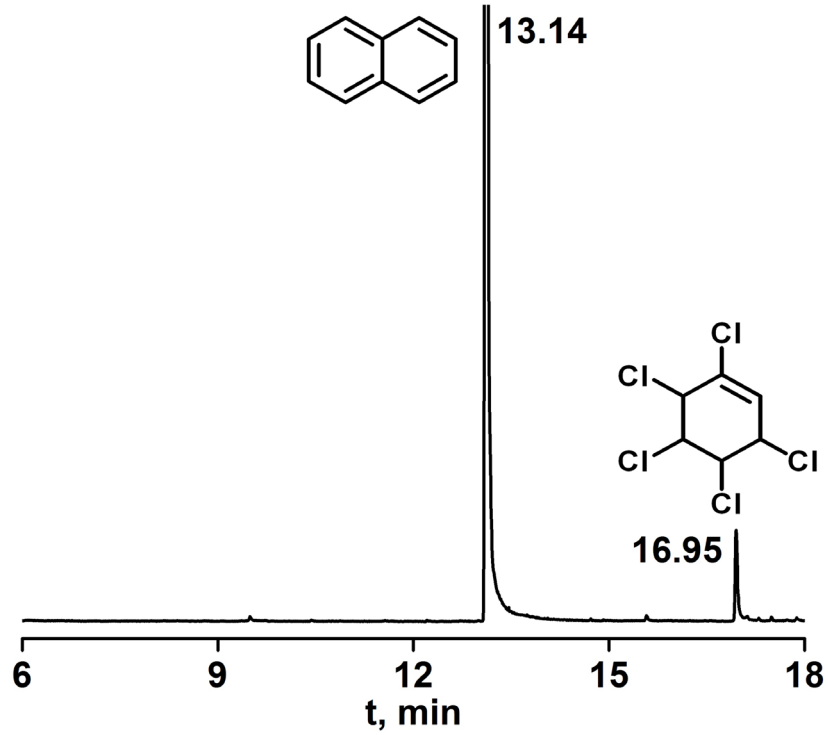

Fig. S21 GC chromatogram of pentachlorocyclohexene obtained in the oxidation of lindane (10 equiv.) by **1**.

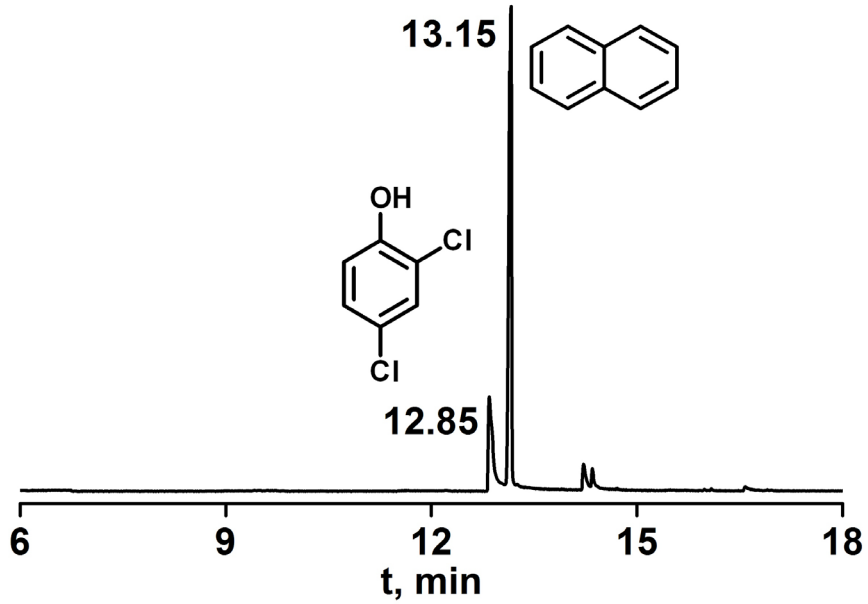

Fig. S22 GC chromatogram of 2,4-dichlorophenol obtained in the oxidation of 2,4-dichlorophenoxyacetic acid (10 equiv.) by **1**.

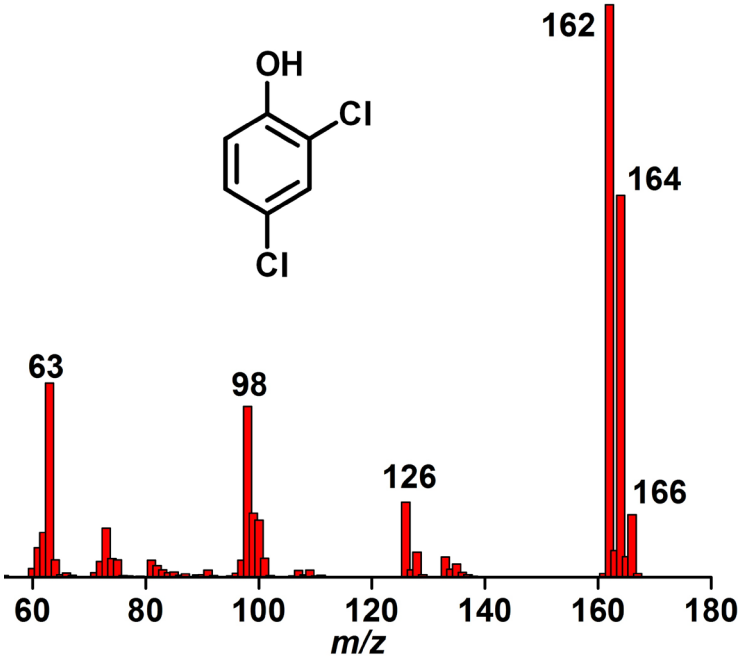

Fig. S23 GC-mass spectrum of 2,4-dichlorophenol formed in the reaction of **1** with 2,4-dichlorophenoxyacetic acid (10 equiv.).

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