

Electronic Supplementary Information

Oxidative dehalogenation of trichlorophenol catalyzed by a promiscuous artificial heme-enzyme

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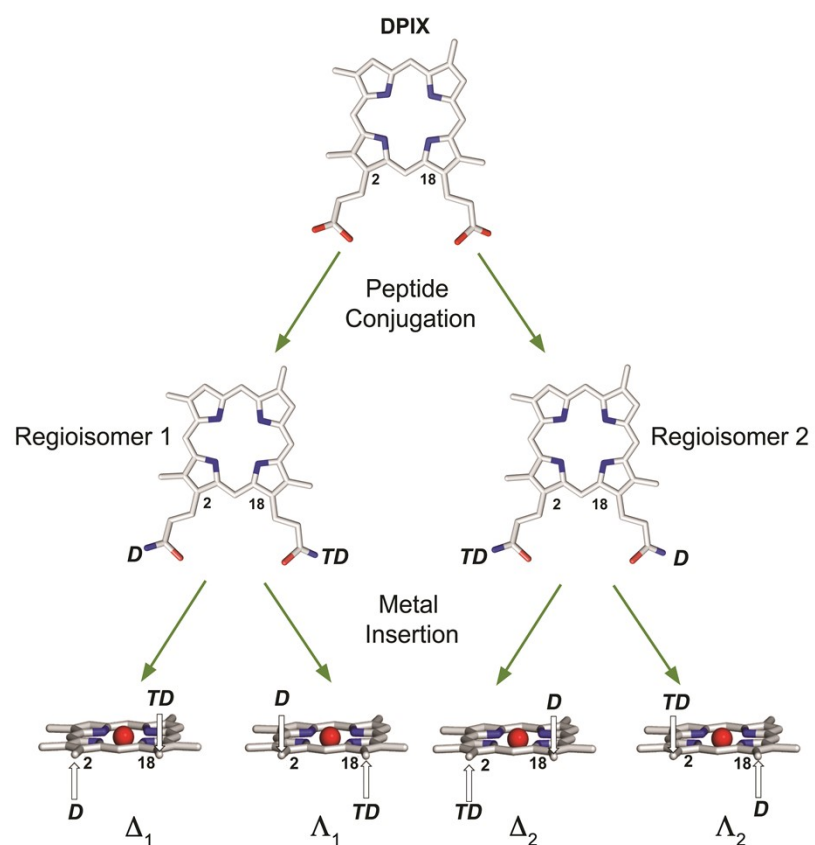


Figure S1. Schematic representation of MC6*a regioisomers and diastereoisomers formation. The decapetide chain and the tetradecapetide chain are indicated as D and TD, respectively. The metal ion is shown as a red sphere. Reproduced from ref. 52 with permission from the Royal Society of Chemistry.

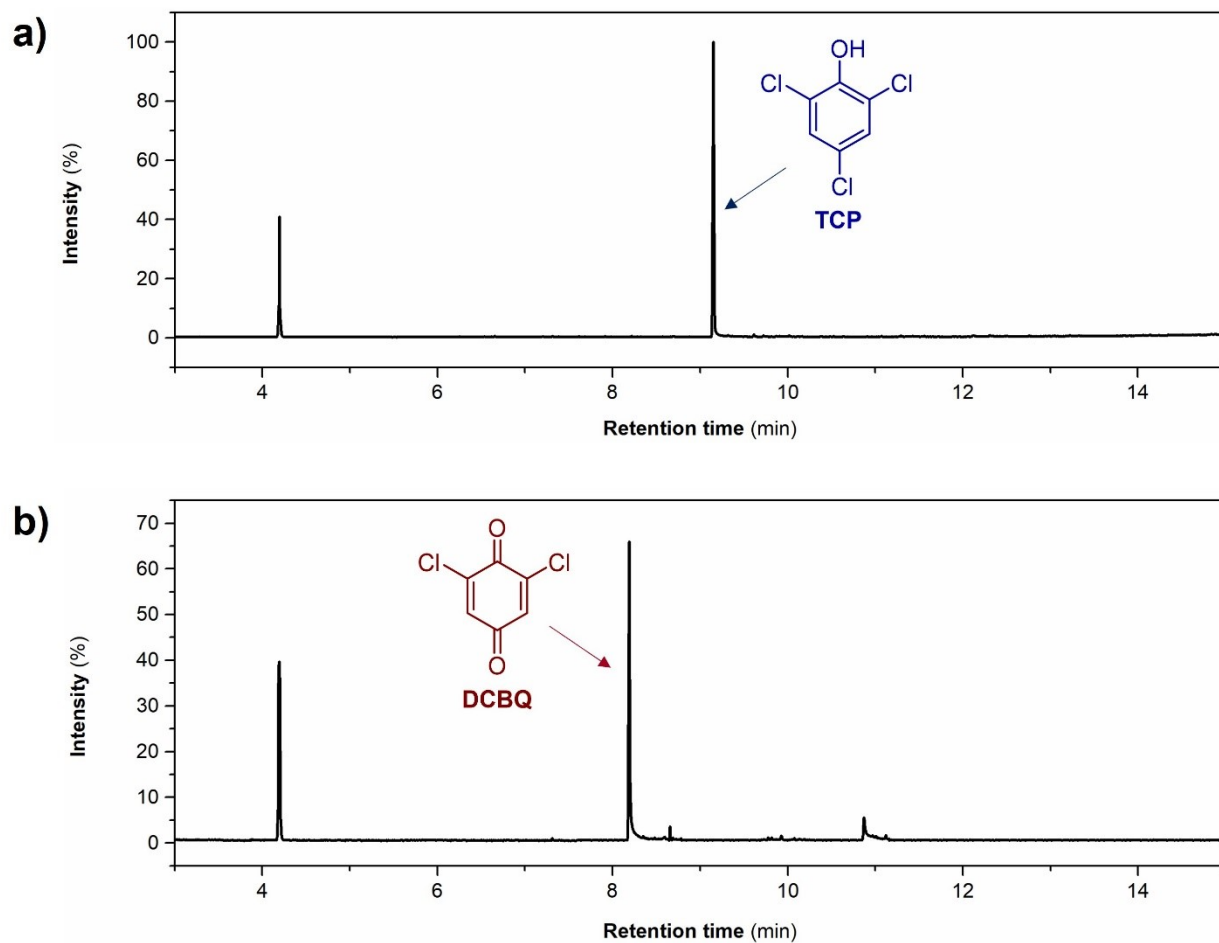


Figure S2. GC-MS profile of the FeMC6*a-catalyzed TCP dehalogenation reaction. Total Ion Current (TIC) chromatograms were acquired (a) before H₂O₂ addition or (b) 5 min after H₂O₂ addition. CLB (R_t 4.152 min) was used as internal standard.

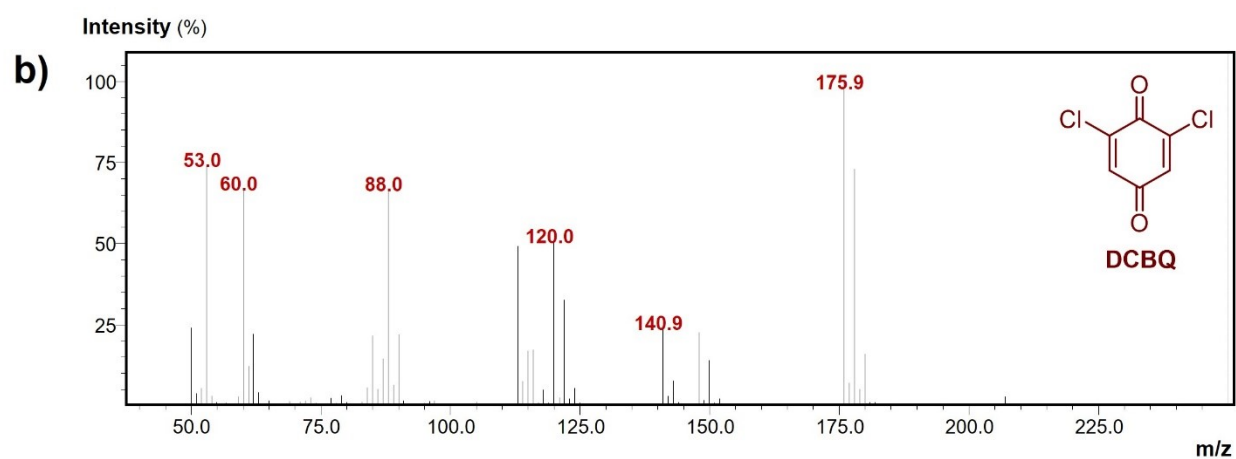
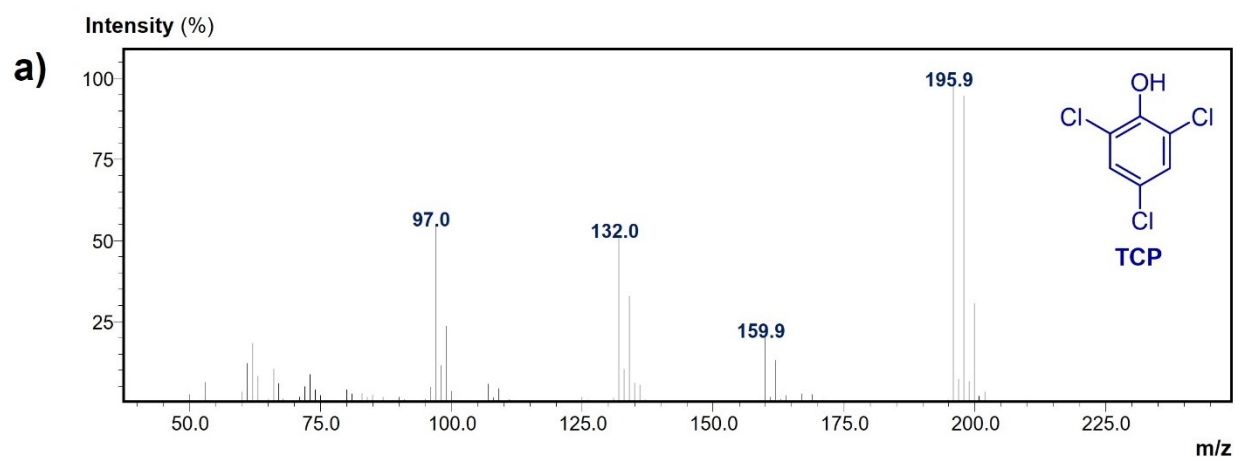


Figure S3. a) Mass spectrum of the peak at 9.120 min corresponding to TCP ($[M]^{++} = 195.9$ amu); b) mass spectrum of the peak at 8.153 min corresponding to DCBQ ($[M]^{++} = 175.9$ amu).

Table S1. Areas of TCP (compared with those of CLB) obtained from GC-MS analysis of the reaction mixture. TIC chromatograms were acquired before ($t = 0$) and after ($t = 5$ and 15 min) H_2O_2 addition.

Reaction time (min)	CLB (Area)	TCP (Area)
$t = 0$	338627	1824512
$t = 5$	386522	505314
$t = 15$	354266	439018

Conditions: [TCP] = 340 μ M; [CLB] = 340 μ M; [H_2O_2] = 410 μ M; [FeMC6*a] = $6.7 \cdot 10^{-8}$ M; buffer solution: 50 mM sodium phosphate (pH 6.5) with 50% TFE (v/v).