molecules

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*Supplementary Material*

# Green Aromatic Epoxidation with an Iron Porphyrin Catalyst for One-Pot Functionalization of Renewable Xylene, Quinoline, and Acridine

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# 1. Additional characterization of *o*-Xylene products

## 1.1. Compound **1a**

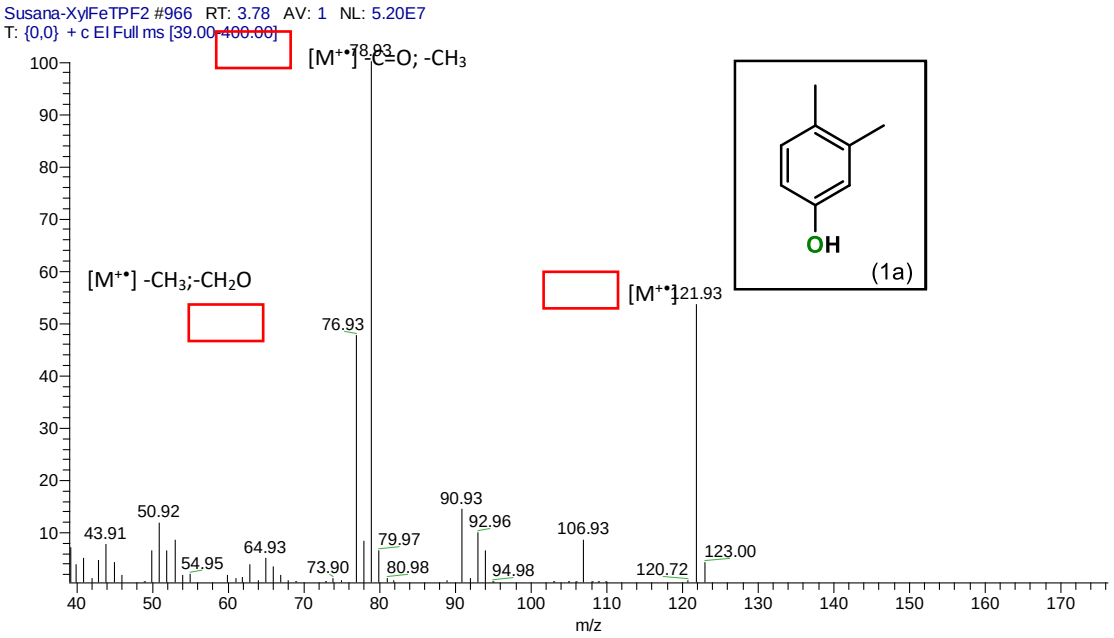


**Figure S1.** MS spectrum (EI) of product **1a** obtained from GC-MS analysis of *o*-Xylene oxidation reaction.

## 1.2 Compound 1b

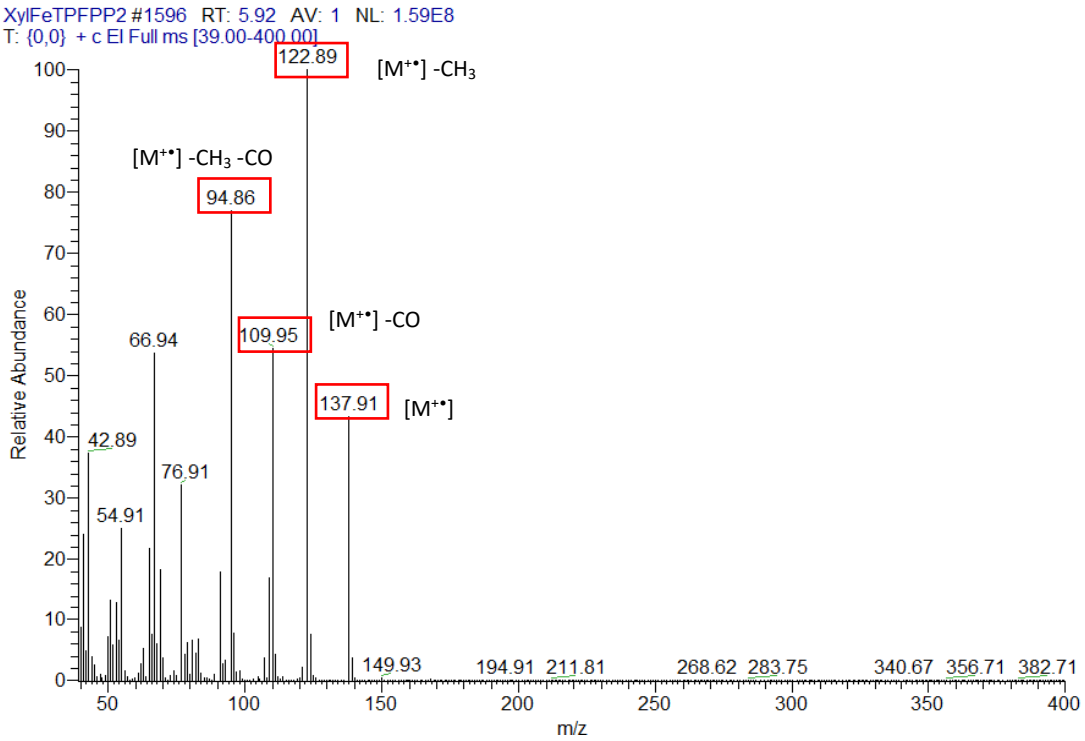


**Figure S2.** MS spectrum (EI) of product **1b** obtained from GC-MS analysis of *o*-Xylene oxidation reaction.

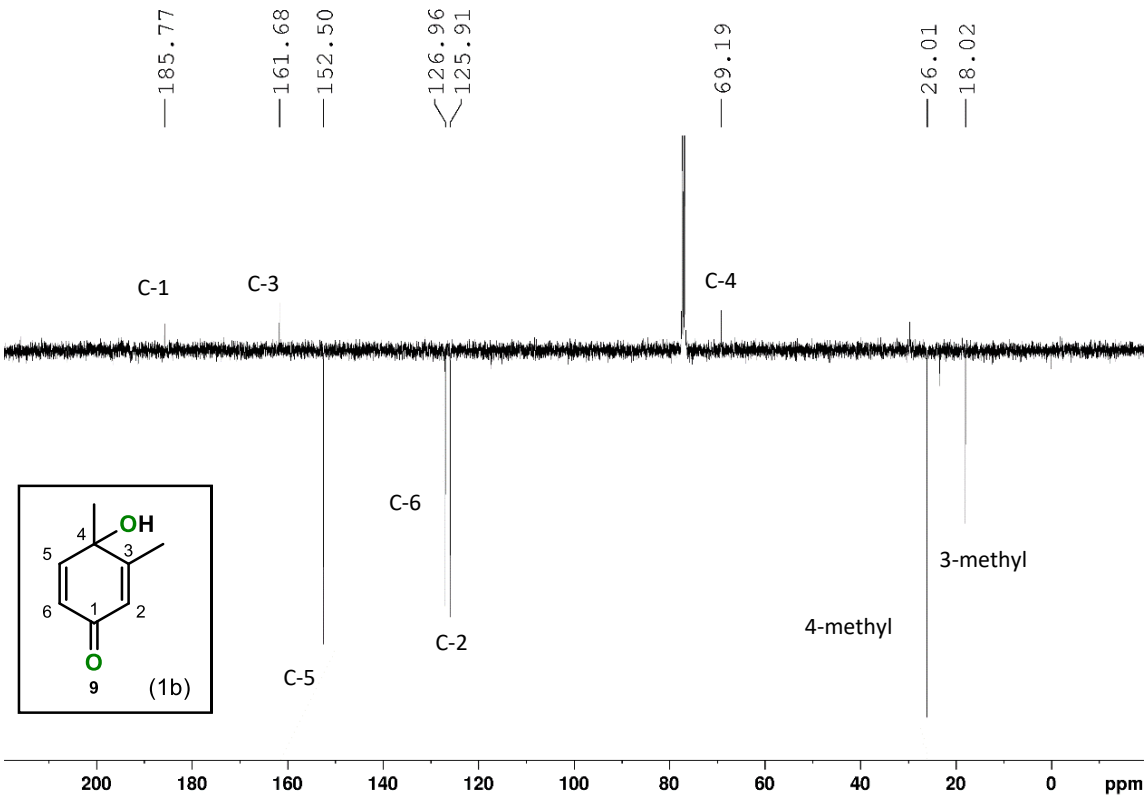


**Figure S3.** APT spectrum for product **1b** in $CDCl_3$.

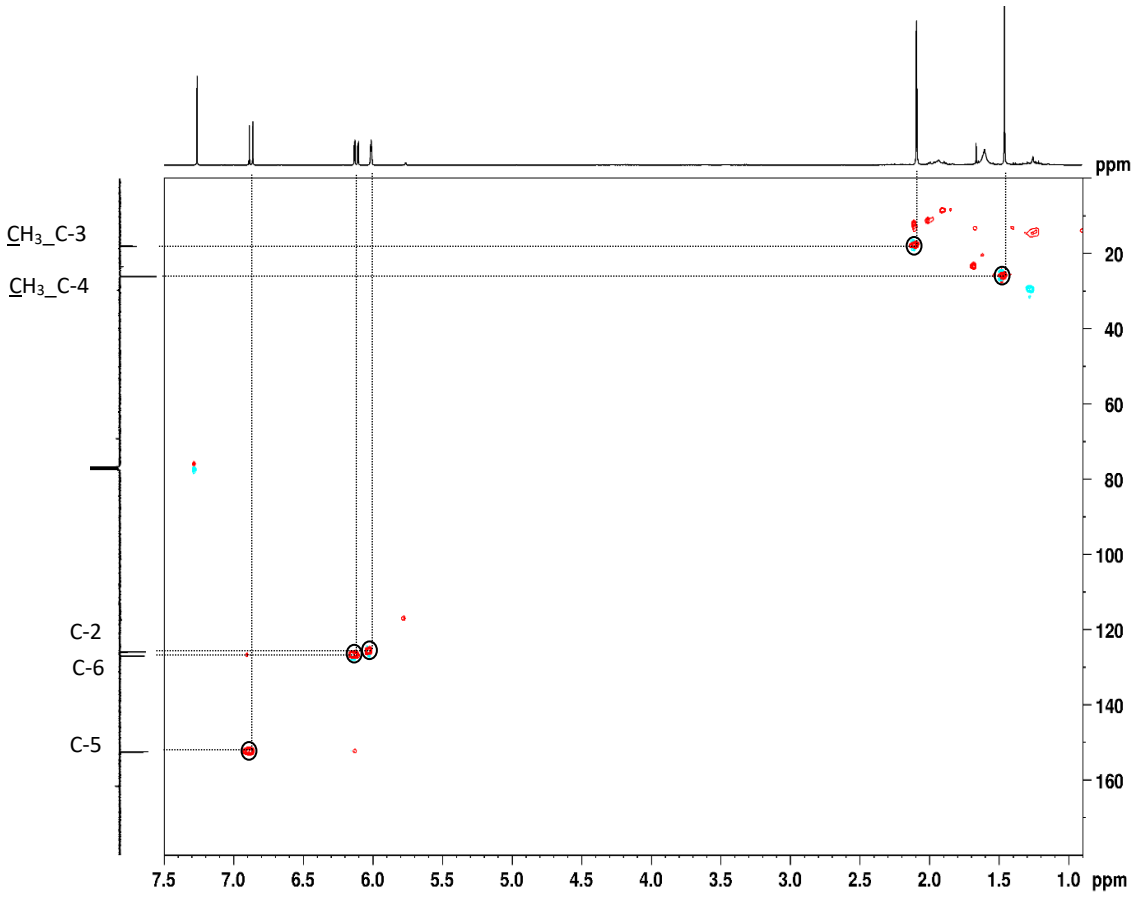


**Figure S4.** HSQC spectrum for product **1b** in $CDCl_3$.

# 2. Additional characterization of quinoline products

## 2.1. Compounds 2a

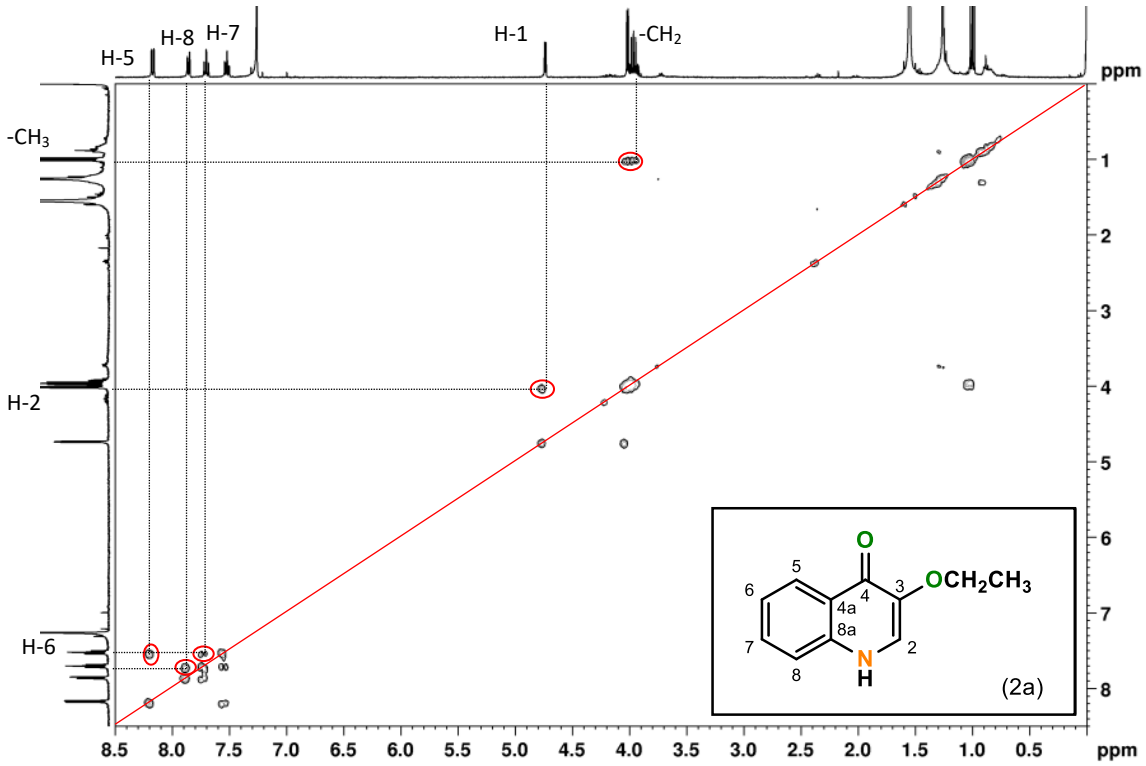


**Figure S5.** COSY spectrum from product **2a** in $CDCl_3$.

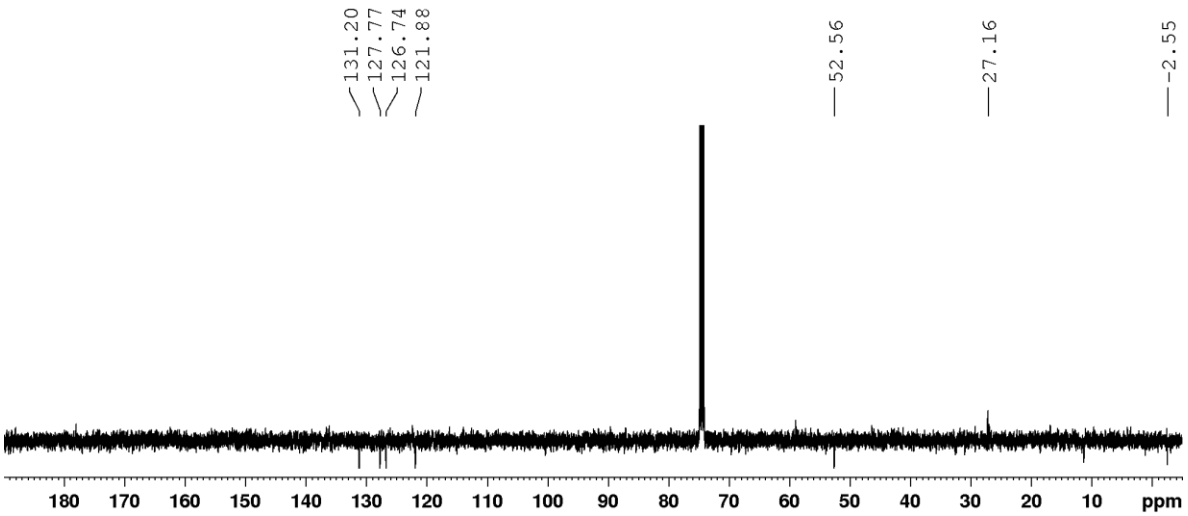


**Figure S6.** APT spectrum from product **2a** in $CDCl_3$. Mesomerism present in the aza-ring justifies the low intensity of related signals relatively to the signals of the phenyl ring.

## 2.2. Compounds **2b** and **2c**

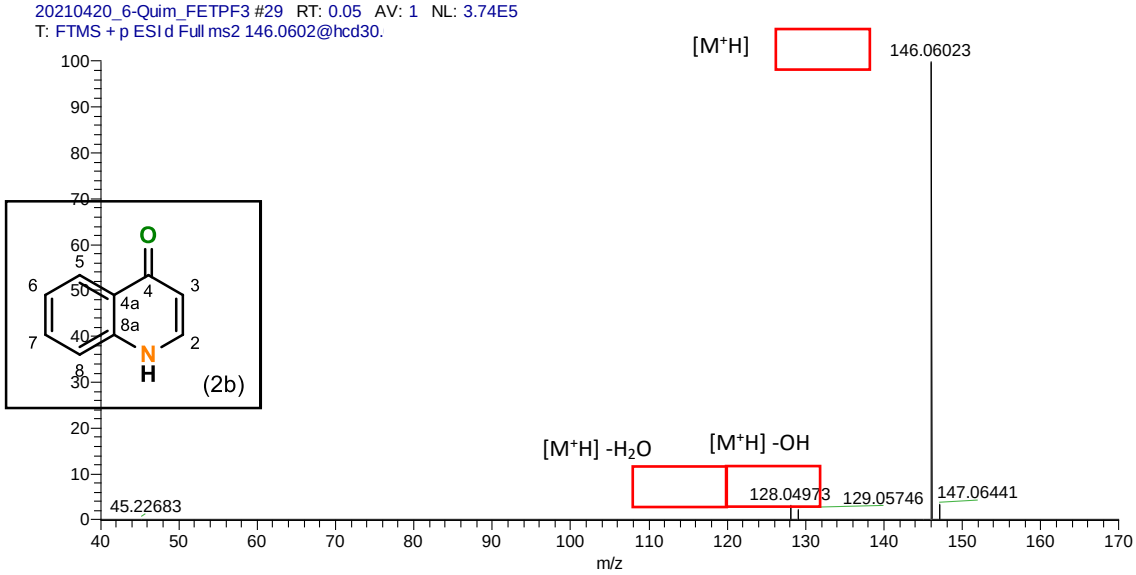


**Figure S7.** HR-MS$^2$ (ESI) spectrum from molecular ion corresponding to product **2b** at *m/z* 146.

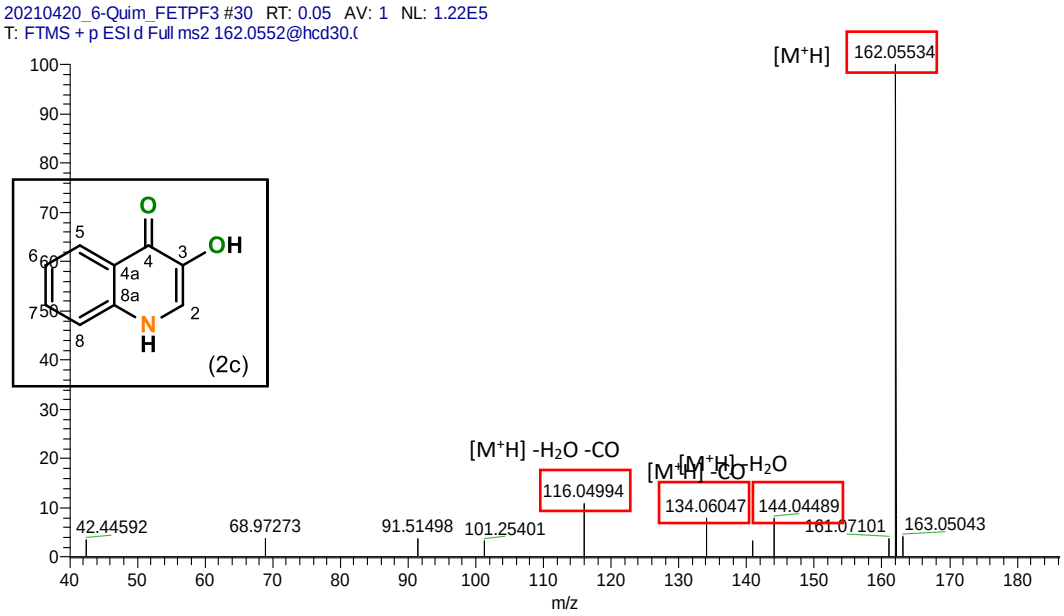


**Figure S8.** HR-MS$^2$ (ESI) spectrum from molecular ion corresponding to product **2c** at *m/z* 162.

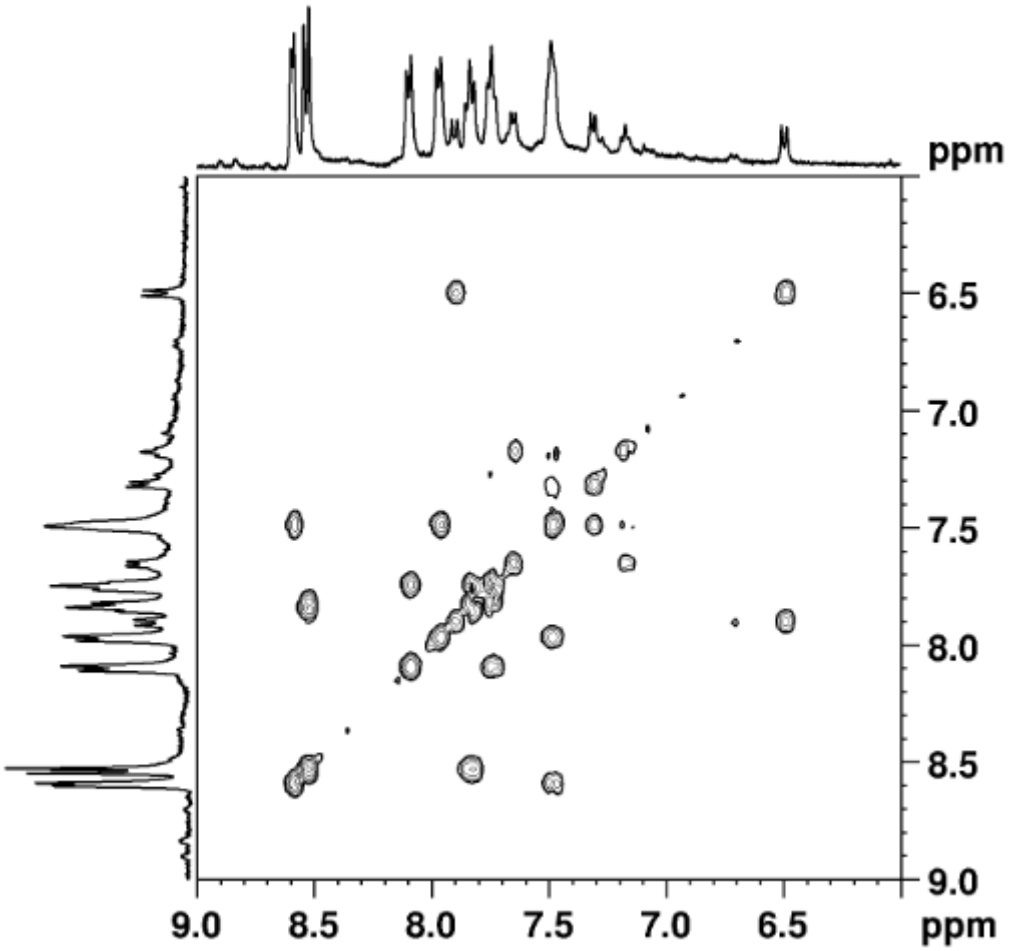


**Figure S9.** Amplified COSY spectrum in DMSO-d6 of a TLC fraction from a quinoline oxidation reaction under Path II. Compounds **2b**, **2b*** and **2c*** were identified.

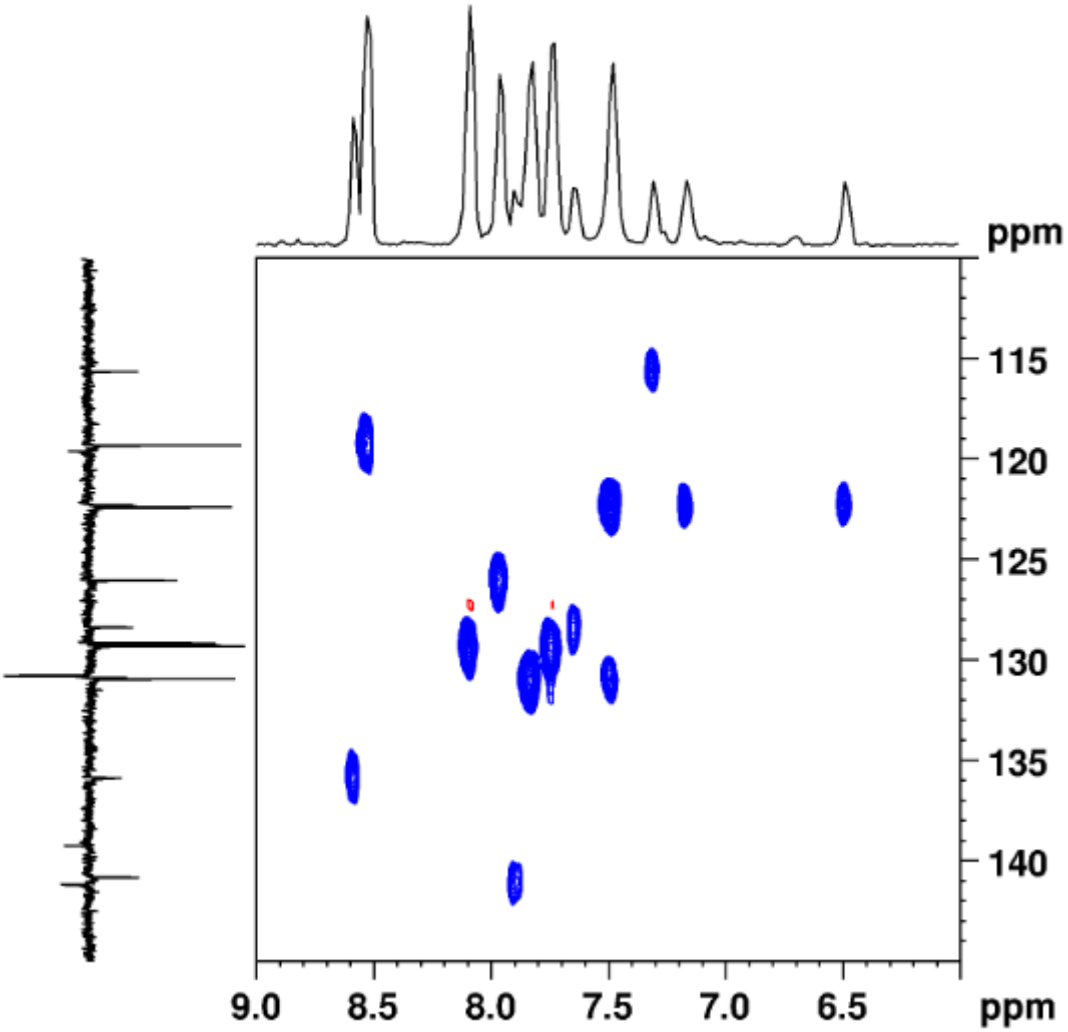


**Figure S10.** Amplified HSQC spectrum DMSO-d6 of a TLC fraction from a quinoline oxidation reaction under Path II. Compounds **2b**, **2b*** and **2c*** were identified.

# 3. NMR spectra of a quinoline total reaction mixture

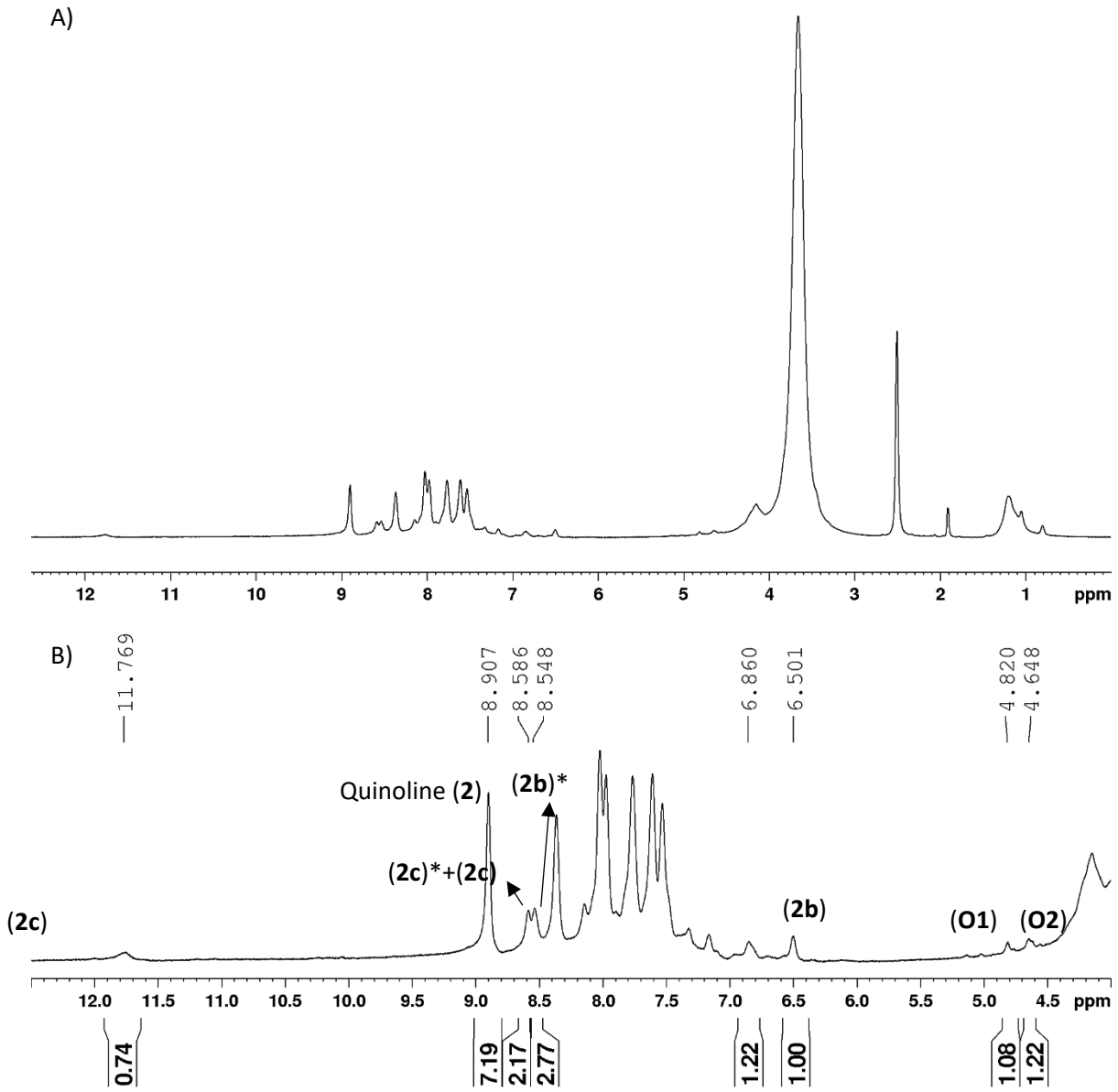


**Figure S11.** A) Full and B) amplified $^{1}$H spectrum of quinoline total reaction mixture in DMSO-d6. The peaks used to quantify the individual products in the reaction mixture are marked: Quinoline (**2**) at δ **8.90** ppm (H-2); compound **2b** at δ **6.50** ppm (H-3, doublet with *J*=9.4 Hz typical of H-*cis* from double bonds, coupling with peak at δ 7.91 ppm); Compound **2b*** at δ **8.55** ppm (H-8); Compound **2c** at δ **11.7** ppm (OH); Compound **2c*** at δ **8.60** ppm (H-2, doublet with *J*=4.8 Hz coupling with OH, minus the area of compound **2c**); Others (**O**) include δ 6.85 ppm ascribed to an intermediate product and δ 4.82 ppm (coupling with peak at δ 4.19 ppm, similarly to compound **2a**);.

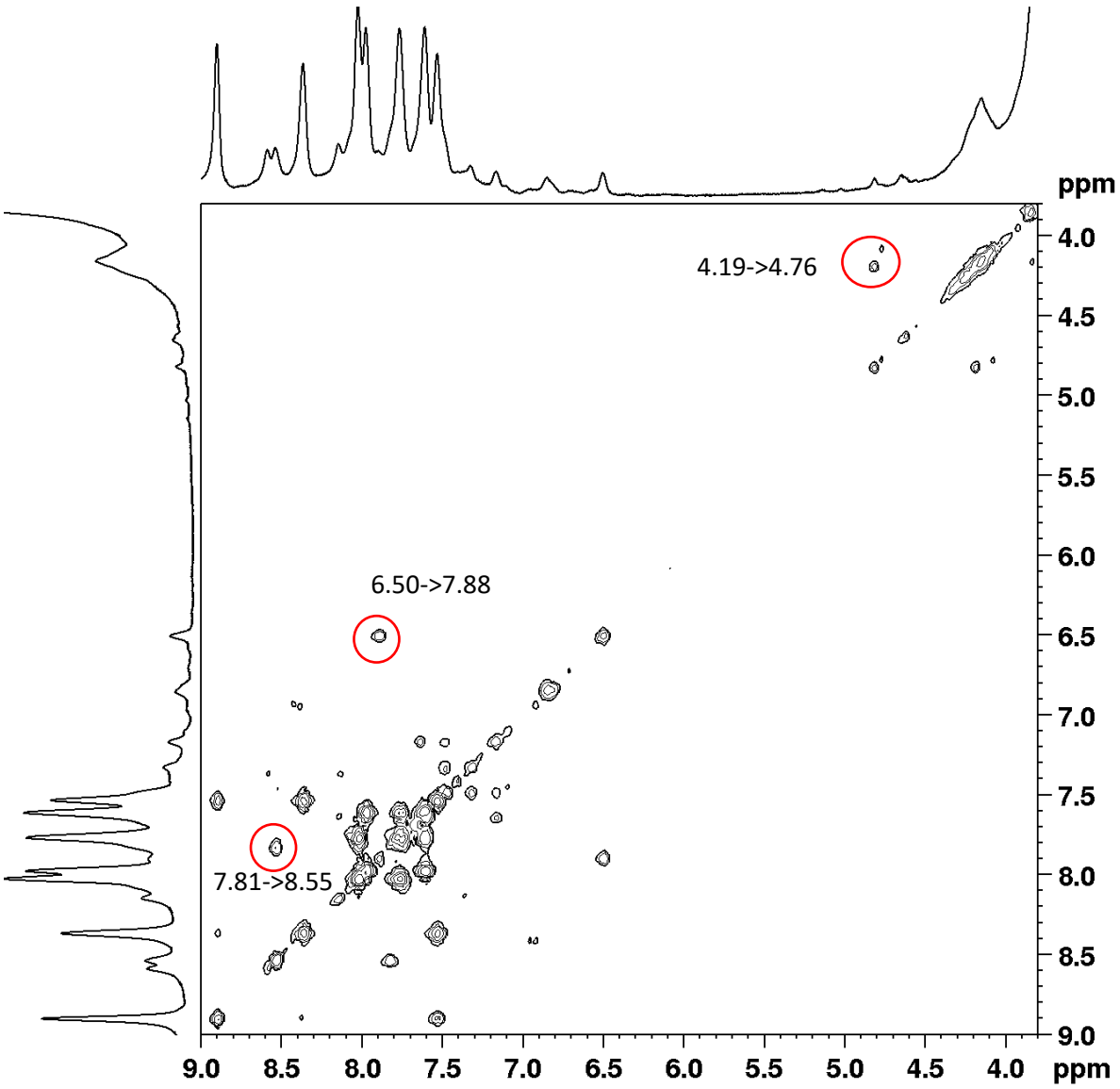


**Figure S12.** Amplified COSY spectrum in DMSO-d6 of reaction mixture from a quinoline oxidation reaction under Path II.

# 4. Additional characterization of acridine products

## 4.1. Compound **3a** and **3b**

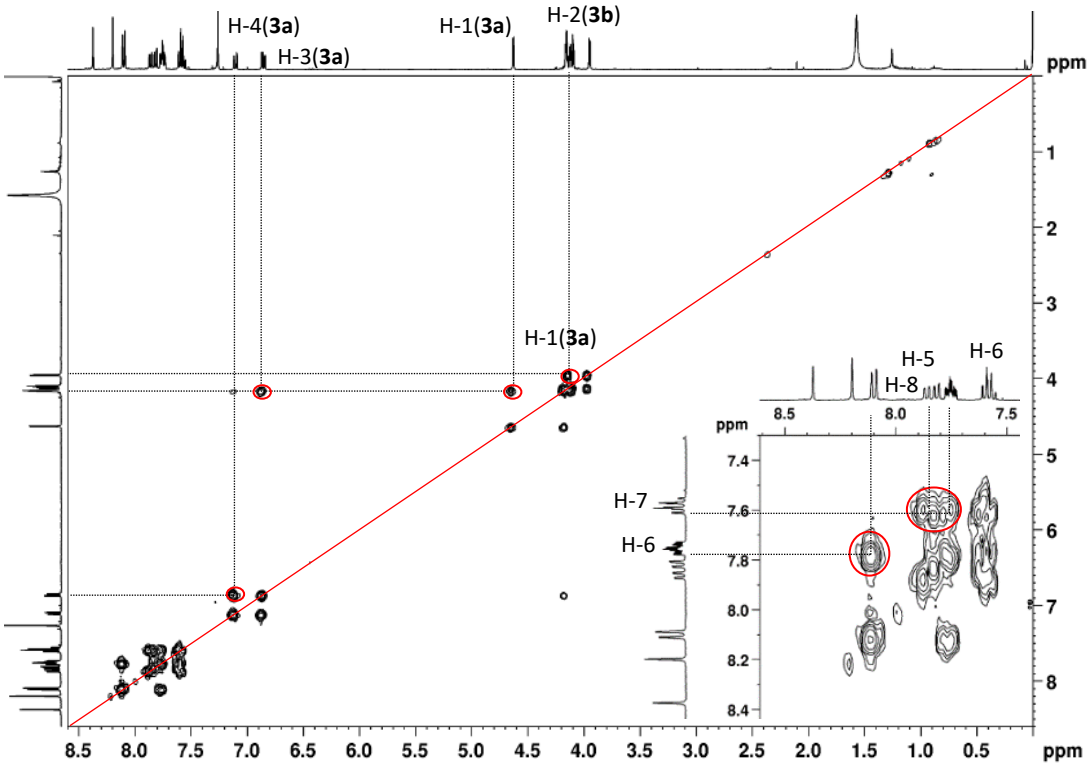


**Figure S13.** COSY spectrum from a fraction containing a mixture of products **3a** and **3b** in $CDCl_3$.

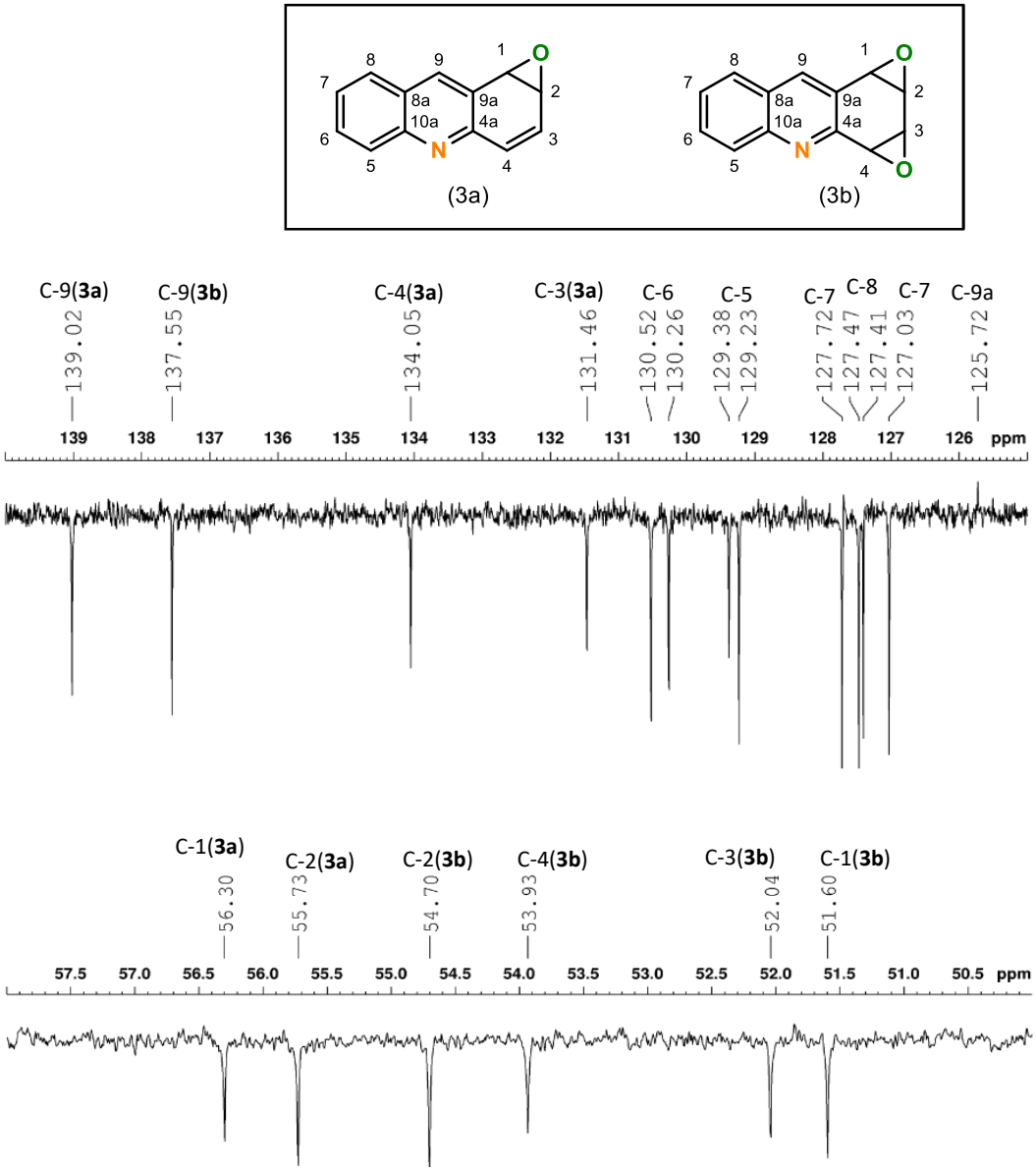


**Figure S14.** APT spectrum from a fraction containing a mixture of products **3a** and **3b** in $CDCl_3$.

## 5. Catalyst stability studies

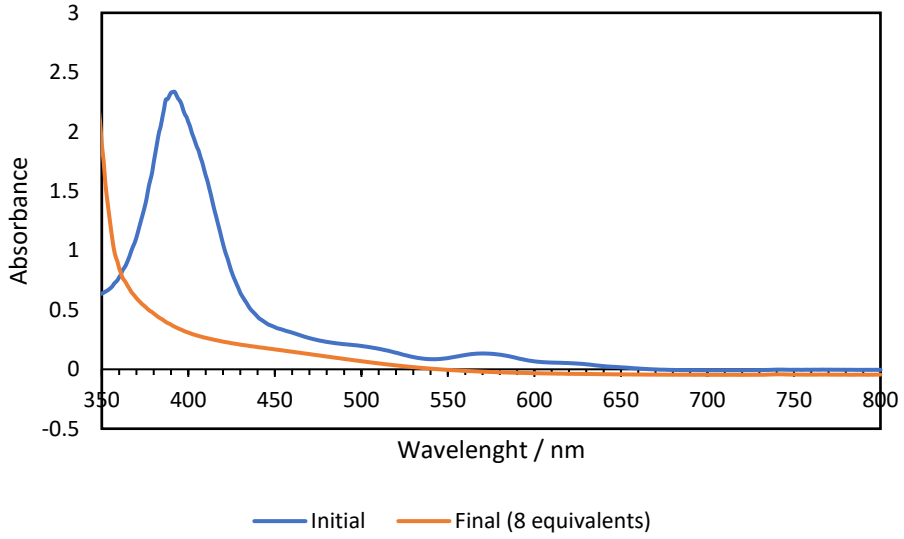


**Figure S15.** UV-vis of quinoline reaction mixture in $CHCl_3$. The bands observed in the initial spectrum are from the catalyst [Fe(TPFPP)Cl]. The Soret band is observed at ~400 nm.

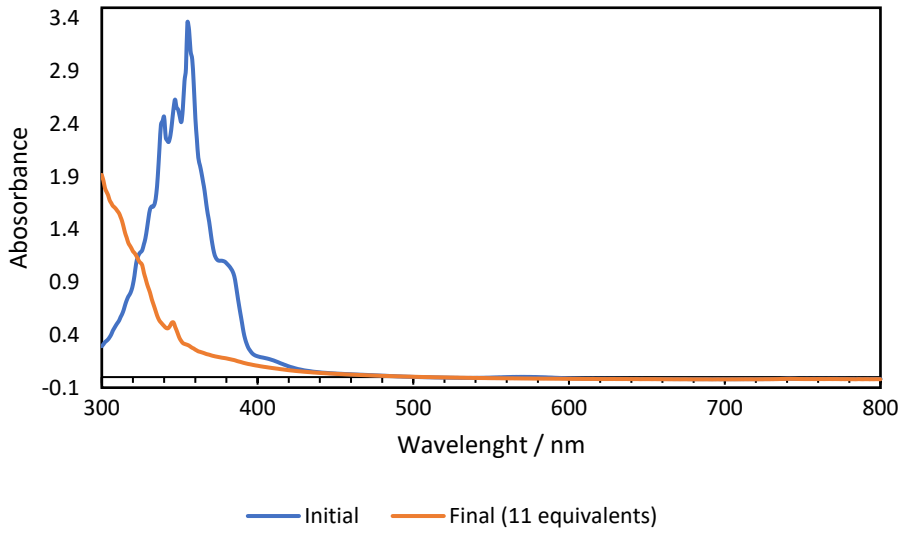


**Figure S16.** UV-vis of acridine reaction mixture in $CHCl_3$. The bands observed in the initial spectrum are from acridine (more intense bands) and the catalyst [Fe(TPFPP)Cl] (Soret band at 410 nm).