Supporting information for: Hypoxia-selective, enzymatic conversion of 6-nitroquinoline into a fluorescent helicene: pyrido[3,2-*f*]quinolino[6,5-*c*]cinnoline 3-oxide

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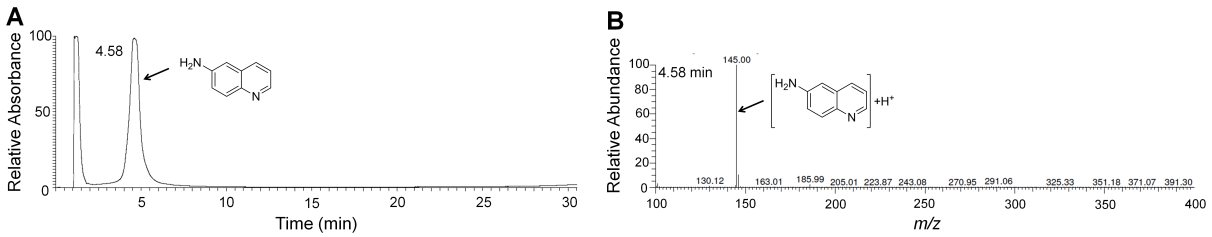

Figure S1. LC/MS analysis of 6-aminoquinoline (**2**). (A) UV chromatogram of **2**. (B) LC/MS analysis of the product eluting 4.6 min in the chromatogram.

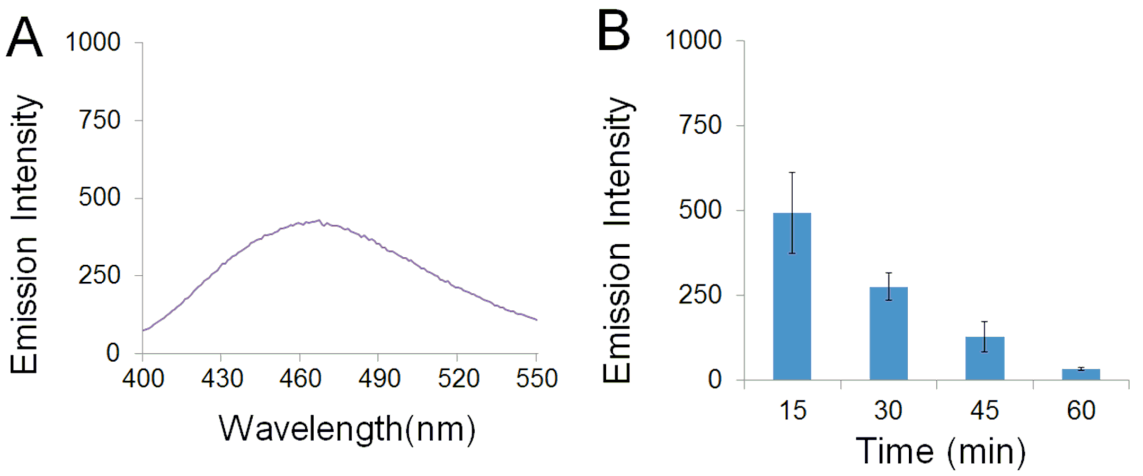

Figure S2. Fluorescence spectra of NADPH and evidence that residual NADPH is consumed during reaction workup. (A) Fluorescence spectrum of NADPH (50 μM, λ_{ex} 307 nm, in sodium phosphate buffer, 12 mM, pH 7.4). Note that the shape of the fluorescence emission peak generated by NADPH is different from that for **4** shown in the manuscript. (B) Control reactions showing that NADPH fluorescence diminishes over the course of 1 h under our typical workup conditions. Reactions containing **1** (0.8 mM), NADPH:cytochrome P450 reductase (1.1 U/mL), and NADPH (3 mM) in sodium phosphate buffer, 10 mM, pH 7.4 (λ_{ex} 307 nm, λ_{em} 460 nm) were incubated for various times before fluorescence analysis. This control experiment provides additional evidence that fluorescence detected in the metabolism of **1** is *not* due to residual NADPH.

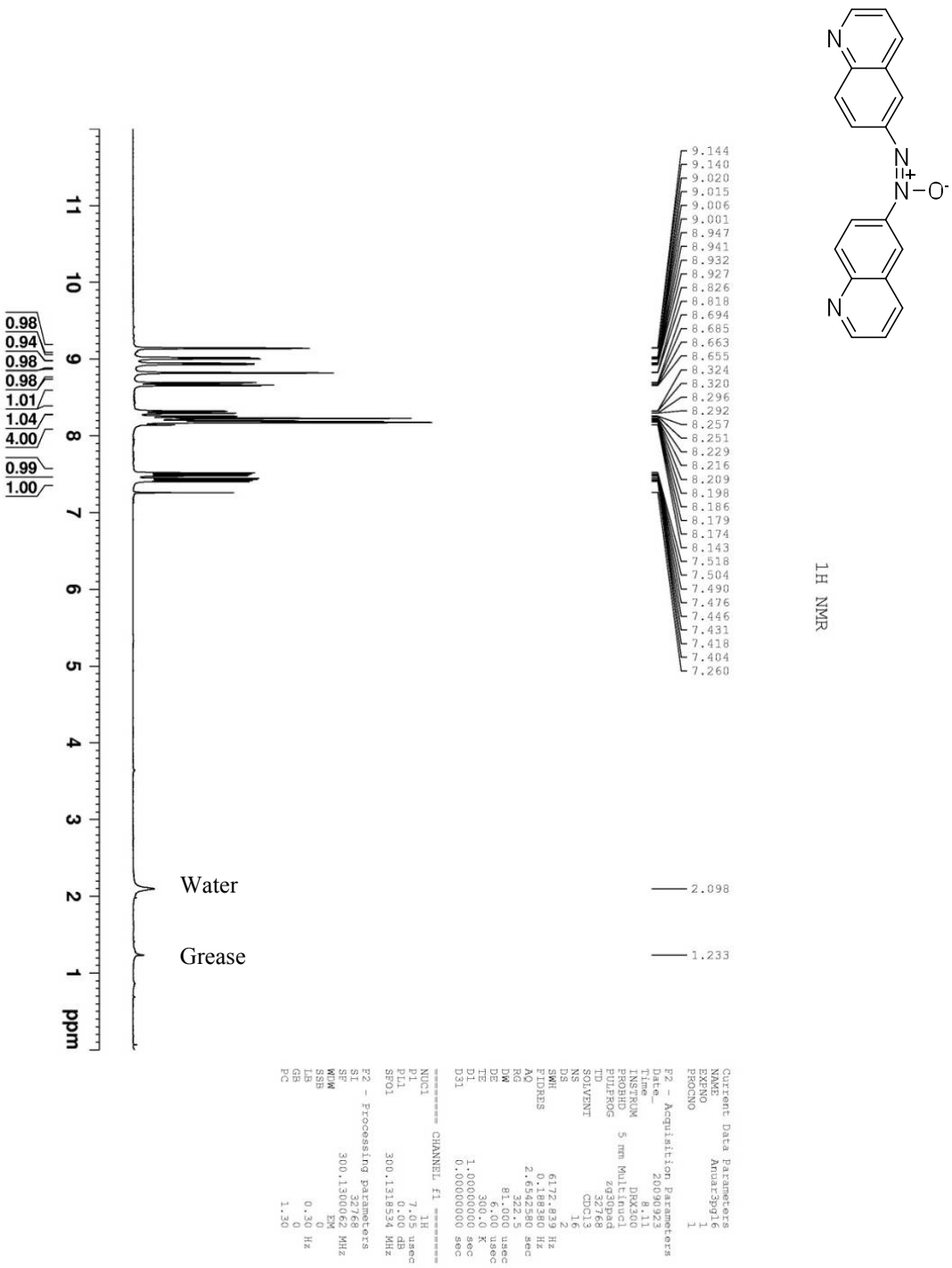

Figure S3. ^{1}H NMR of **3** ($CDCl_3$, 300 MHz).

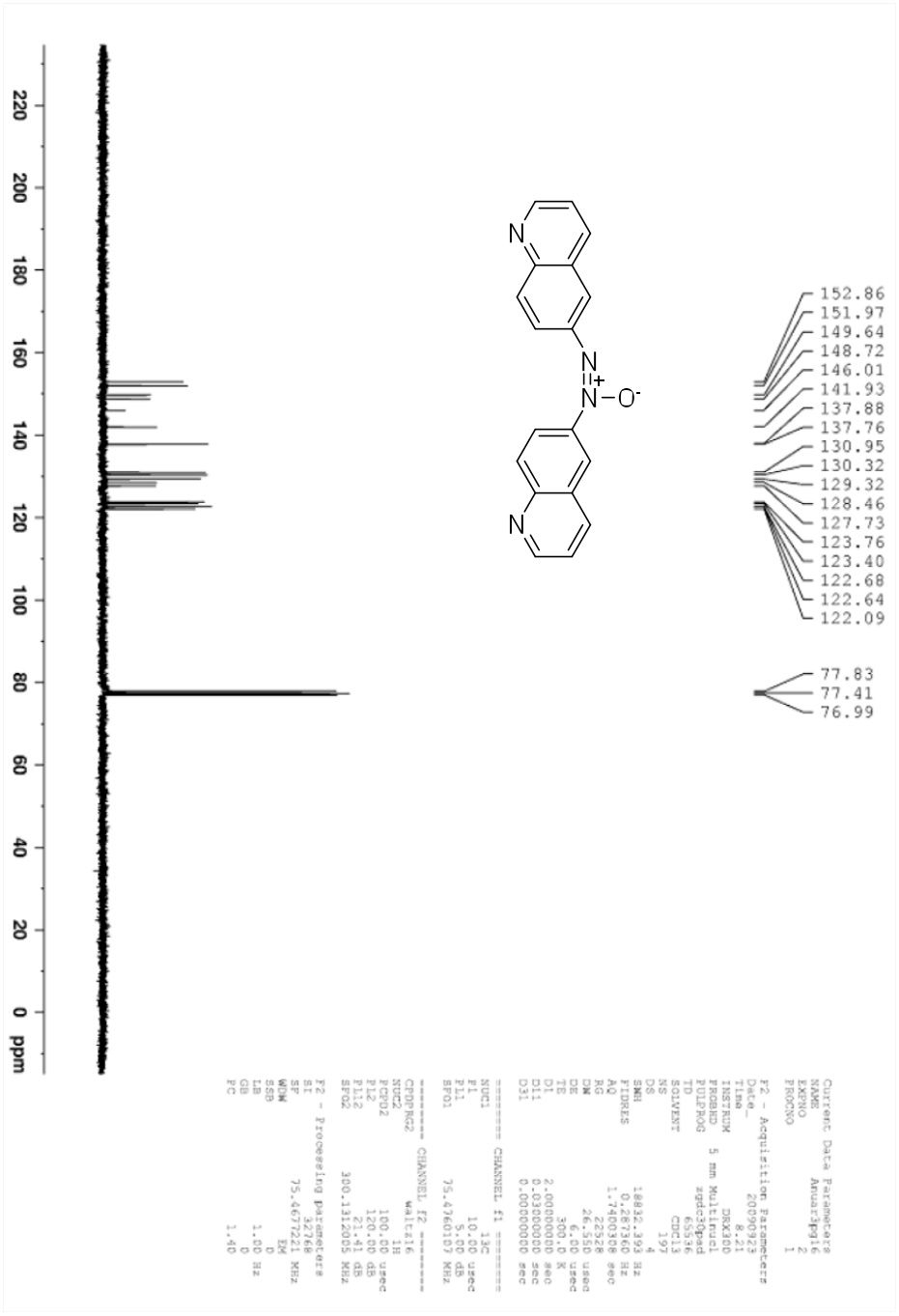

Figure S4. ^{13}C NMR of **3** ($CDCl_3$, 125 MHz).

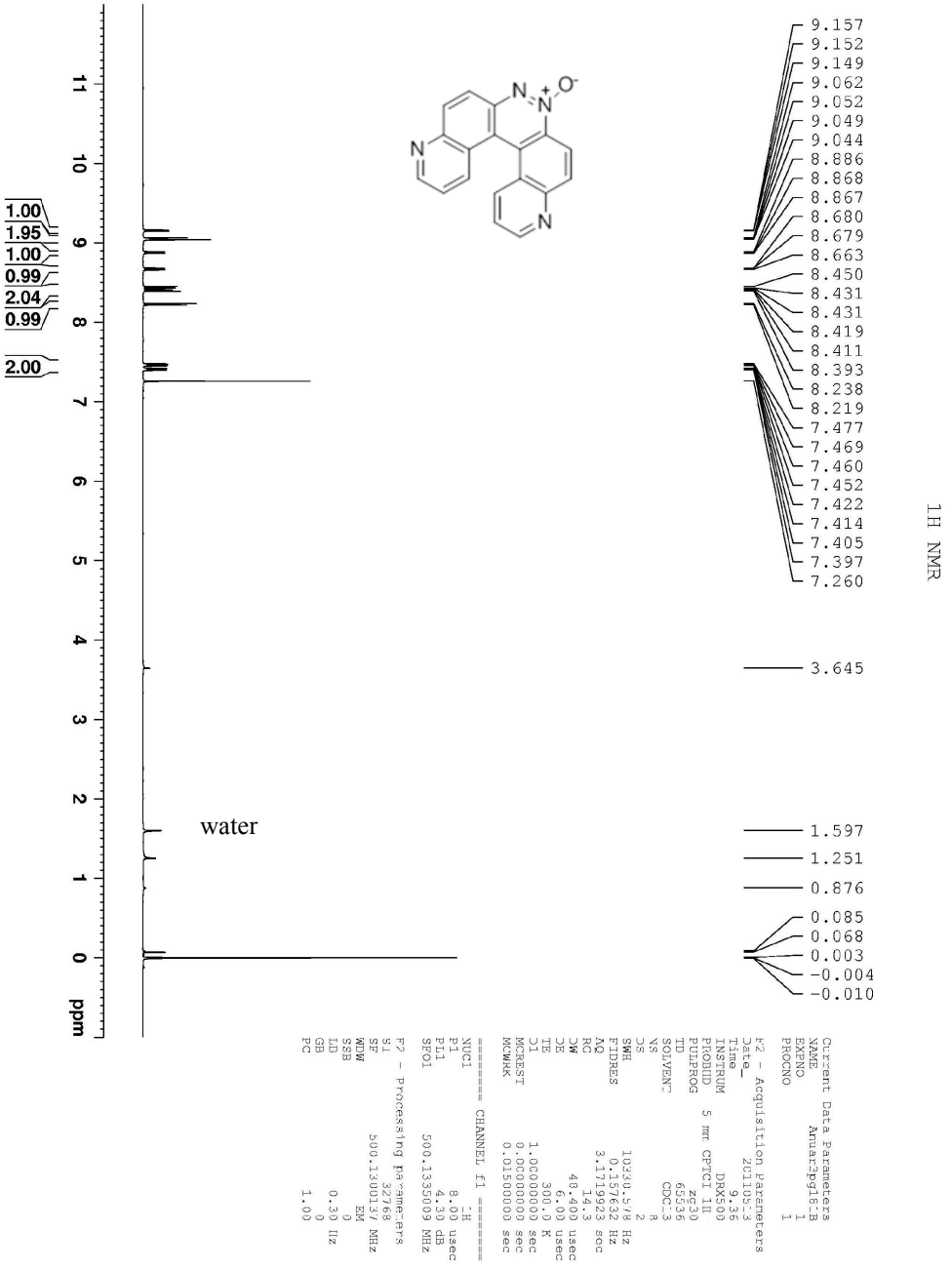

Figure S5. ^{1}H NMR of **4** ($CDCl_3$, 500 MHz).

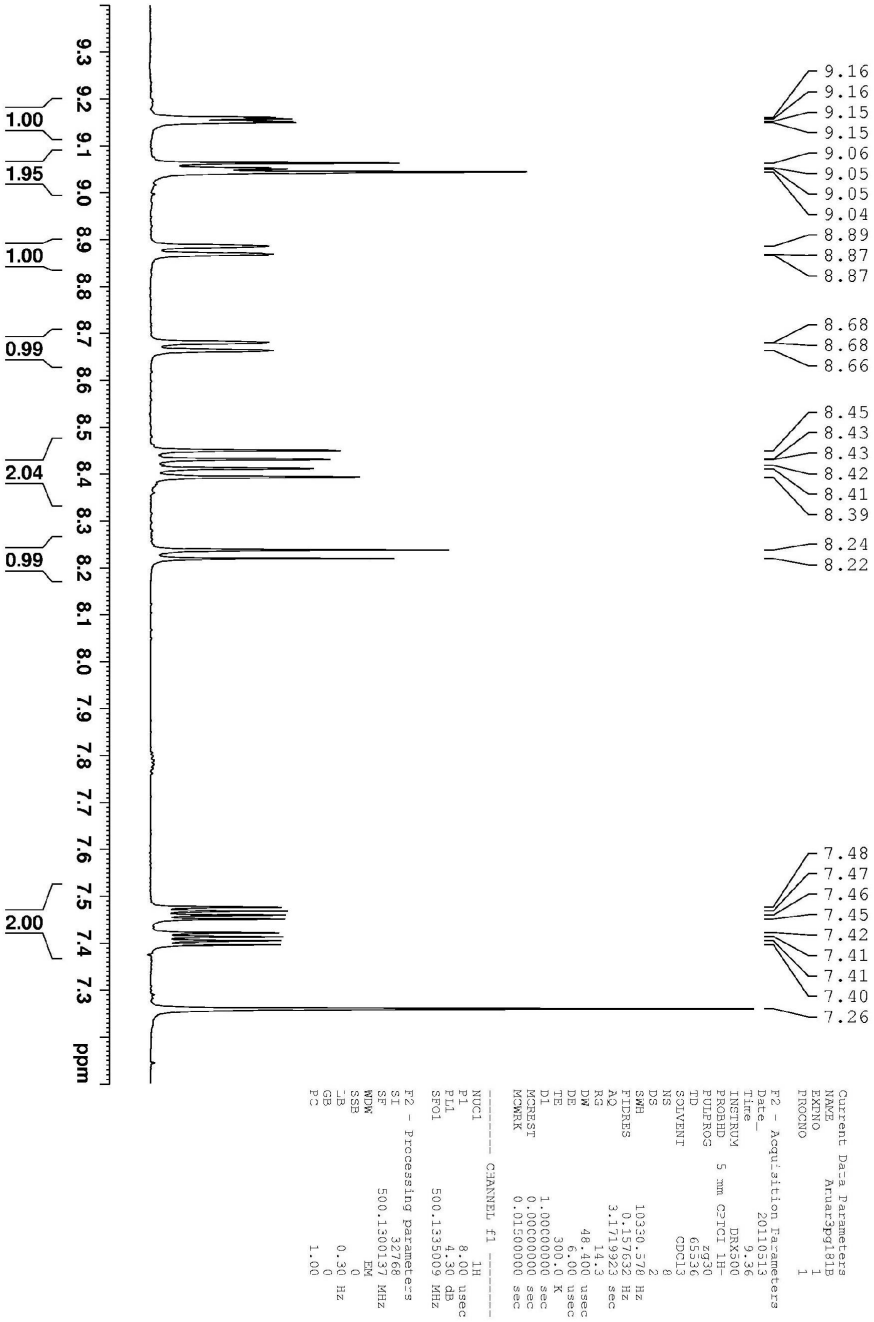

Figure S6. ^{1}H NMR of **4**, aromatic region ($CDCl_3$, 500 MHz).

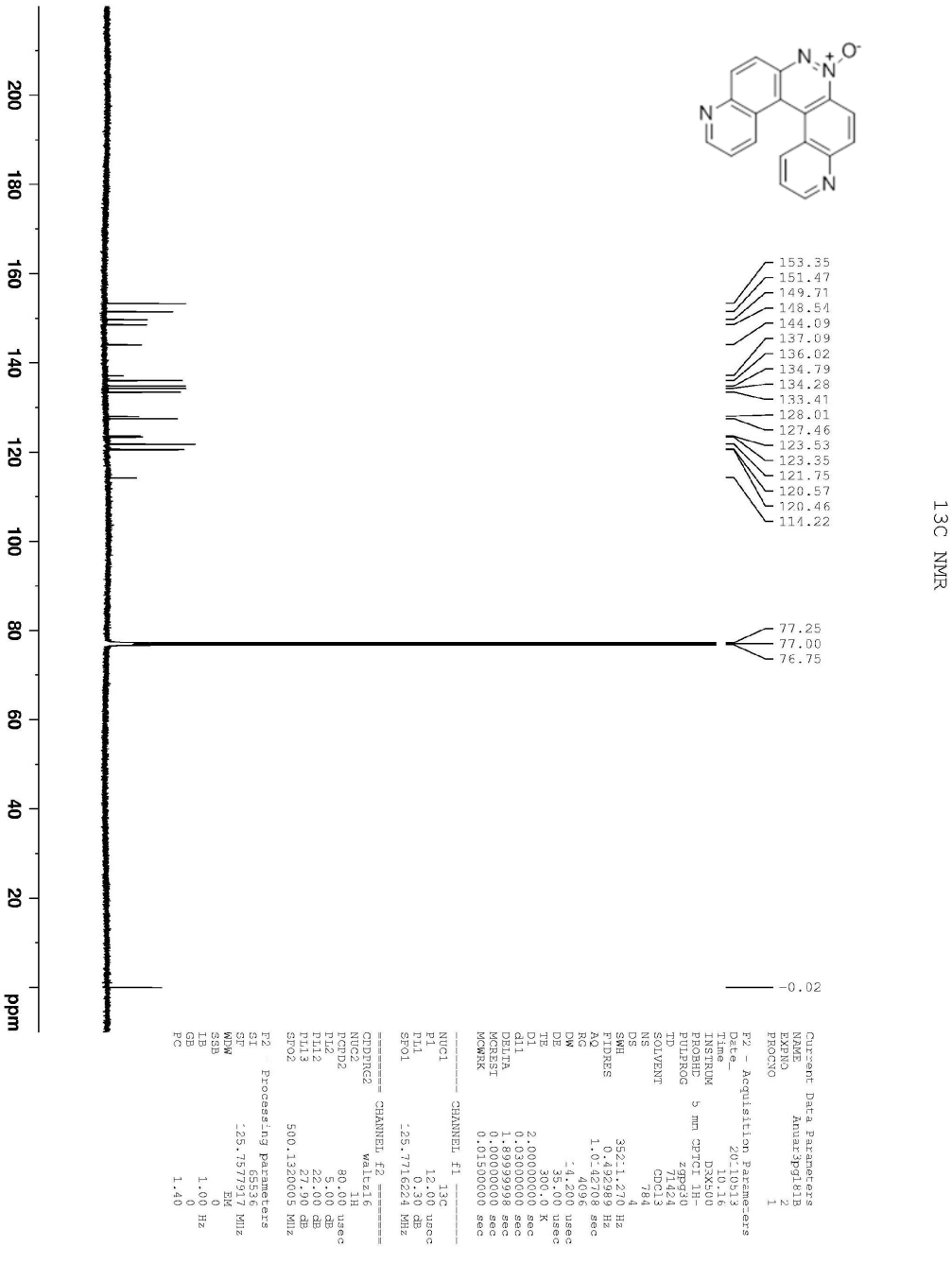

Figure S7. ^{13}C NMR of **4** ($CDCl_3$, 125 MHz).

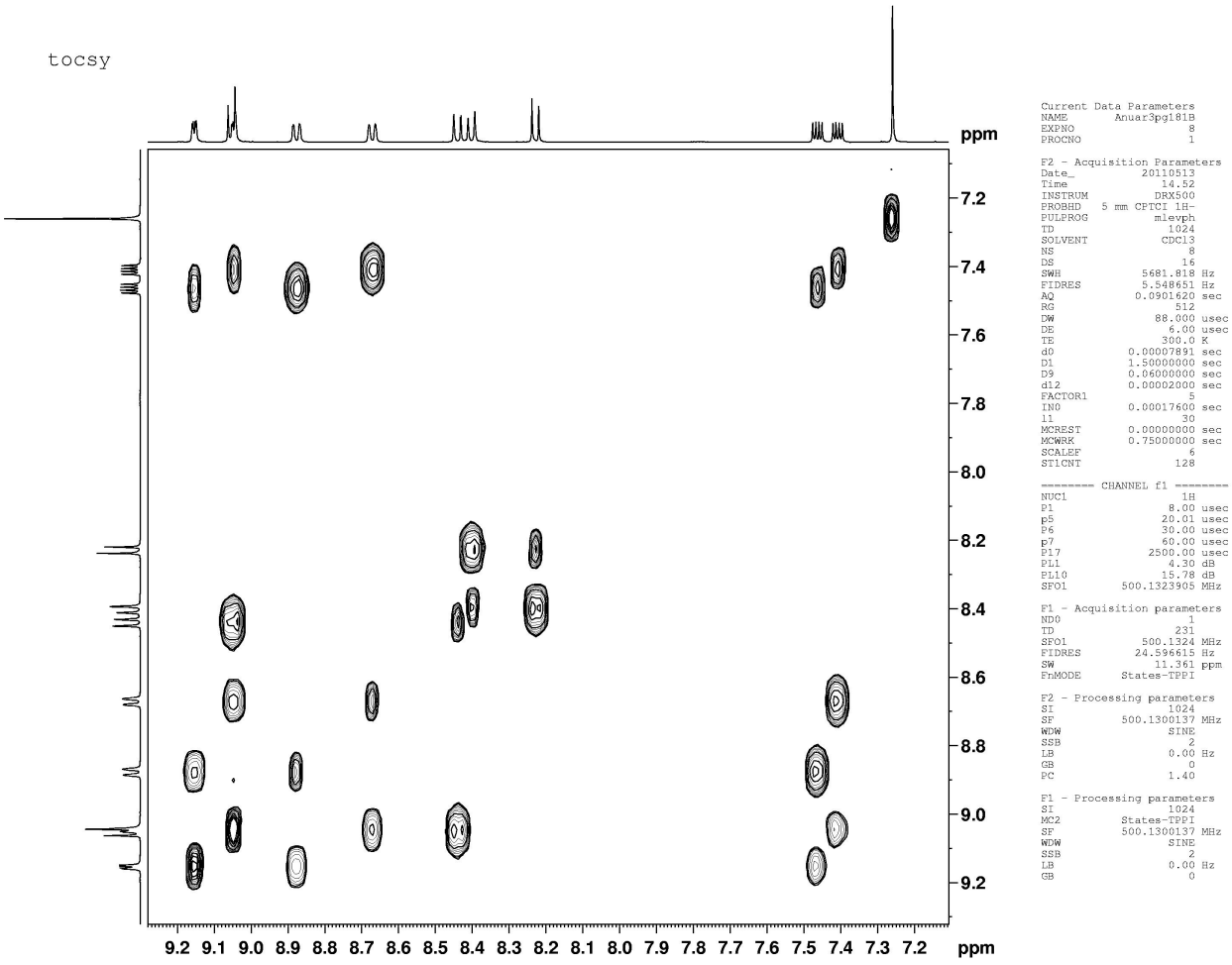

Figure S8. ^{1}H–^{1}H TOCSY of **4** ($CDCl_3$, 500 MHz).

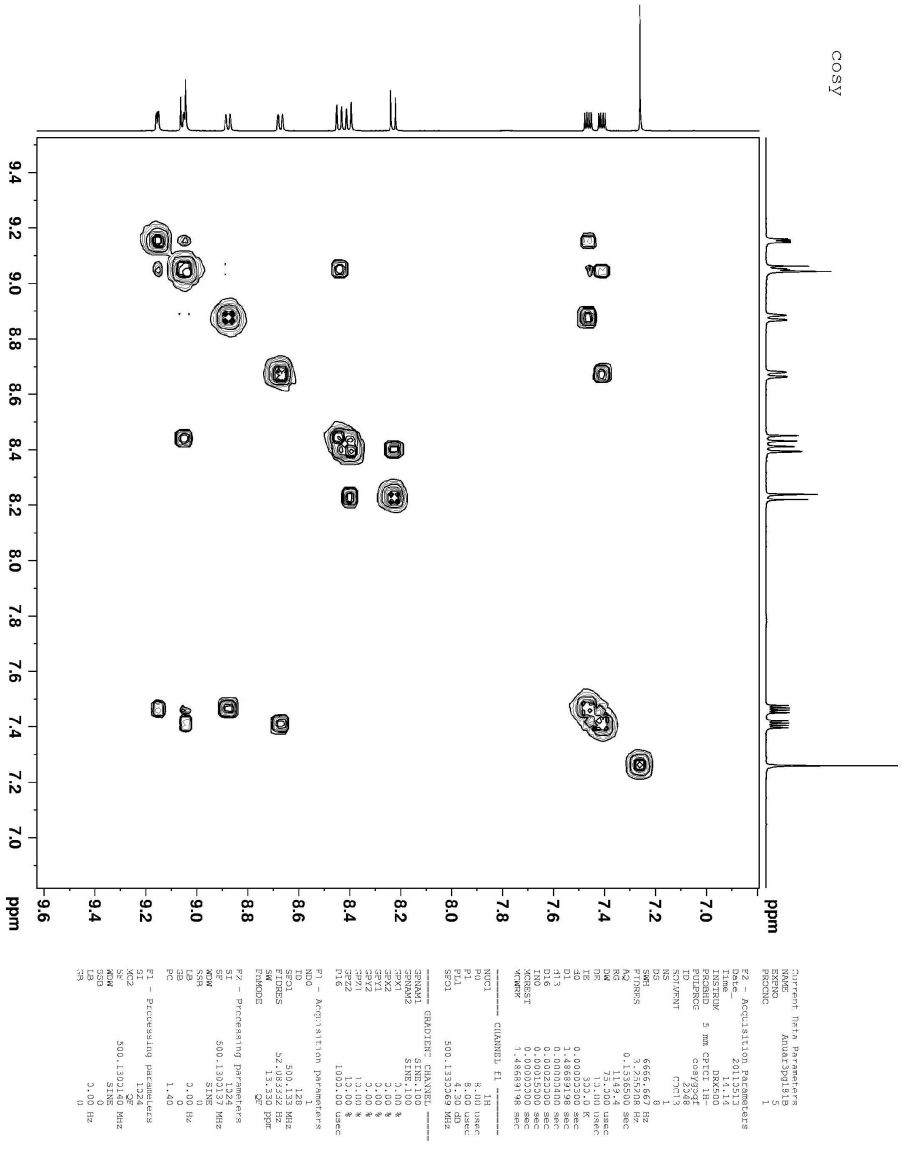

Figure S9. ^{1}H–^{1}H COSY of **4** ($CDCl_3$, 500 MHz).

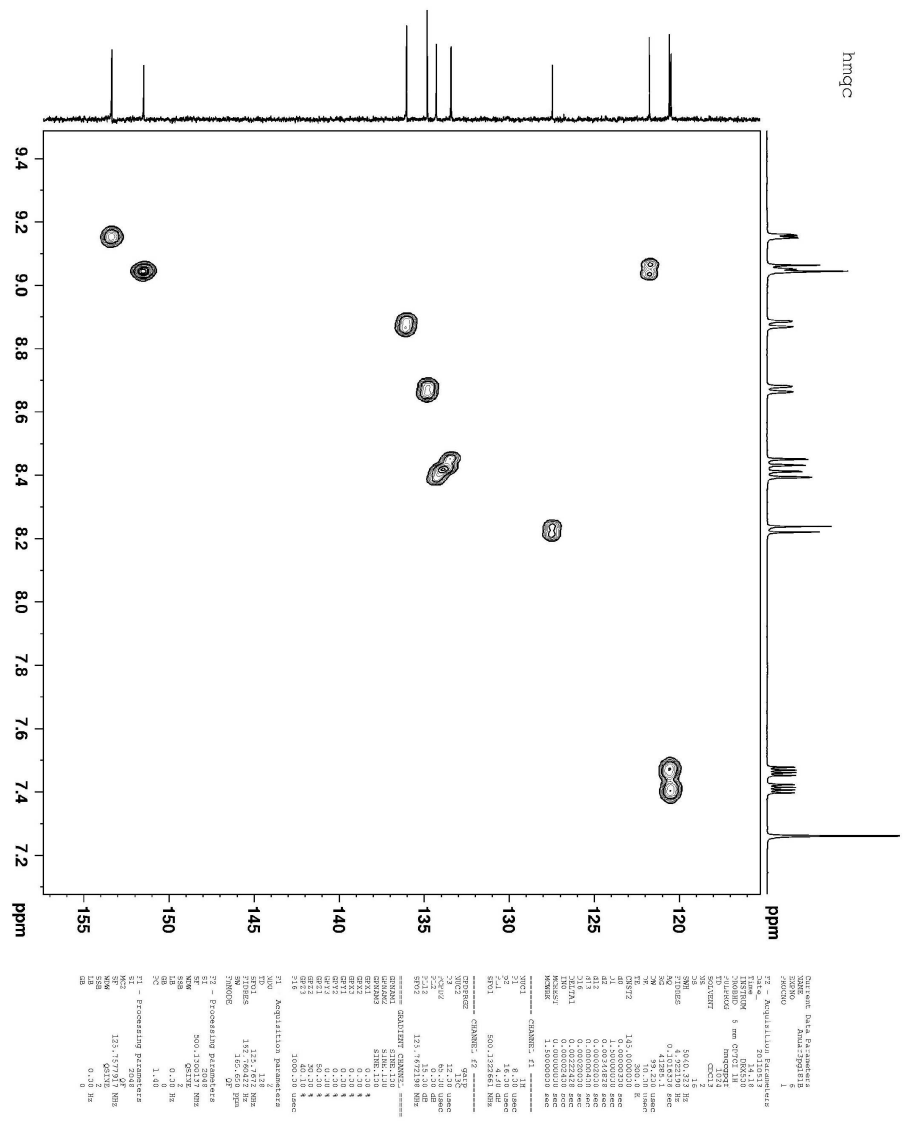

Figure S10. $^{1}H–^{13}C$ HMQC of **4** ($CDCl_3$).

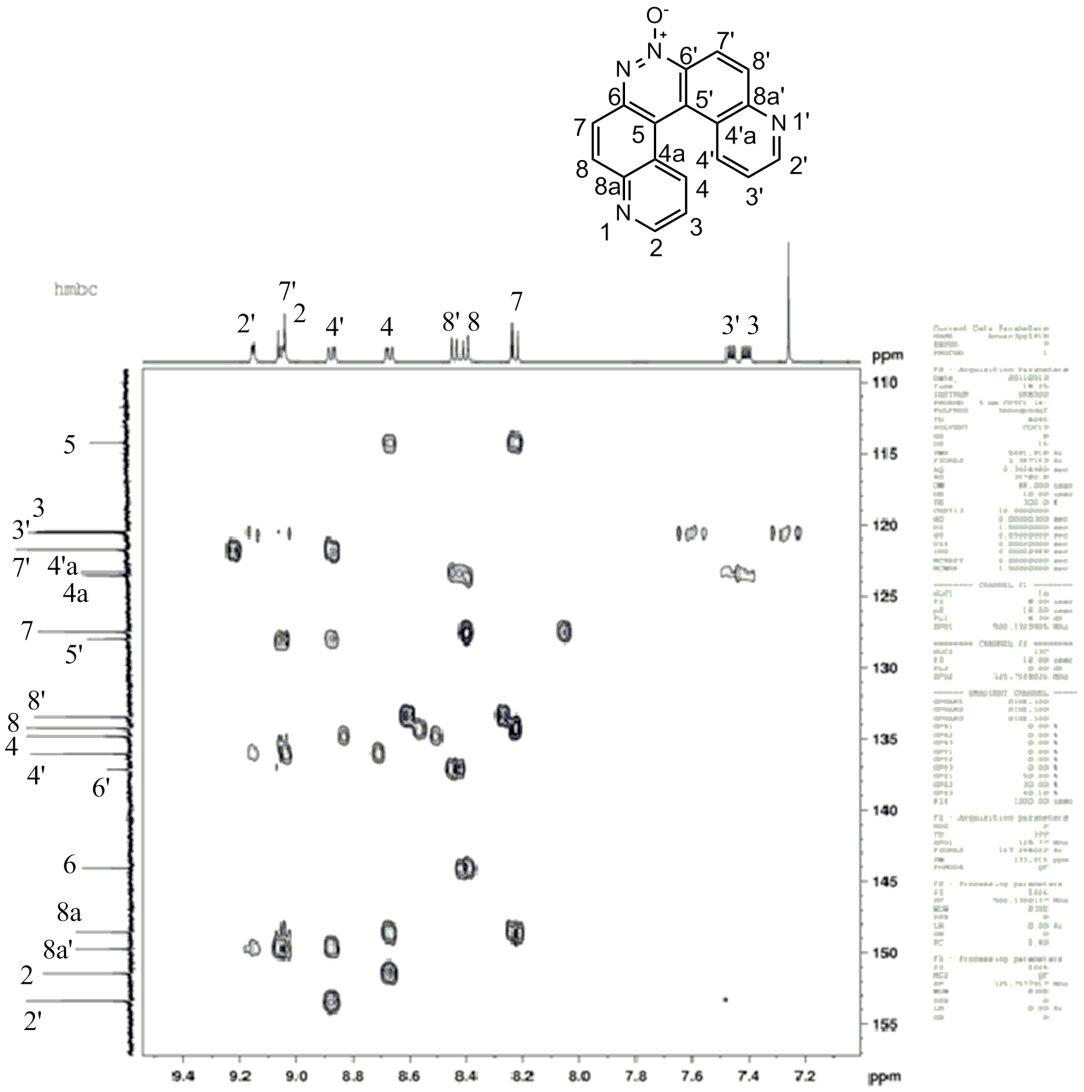

Figure S11. $^{1}H–^{13}C$ HMBC of **4** ($CDCl_3$).

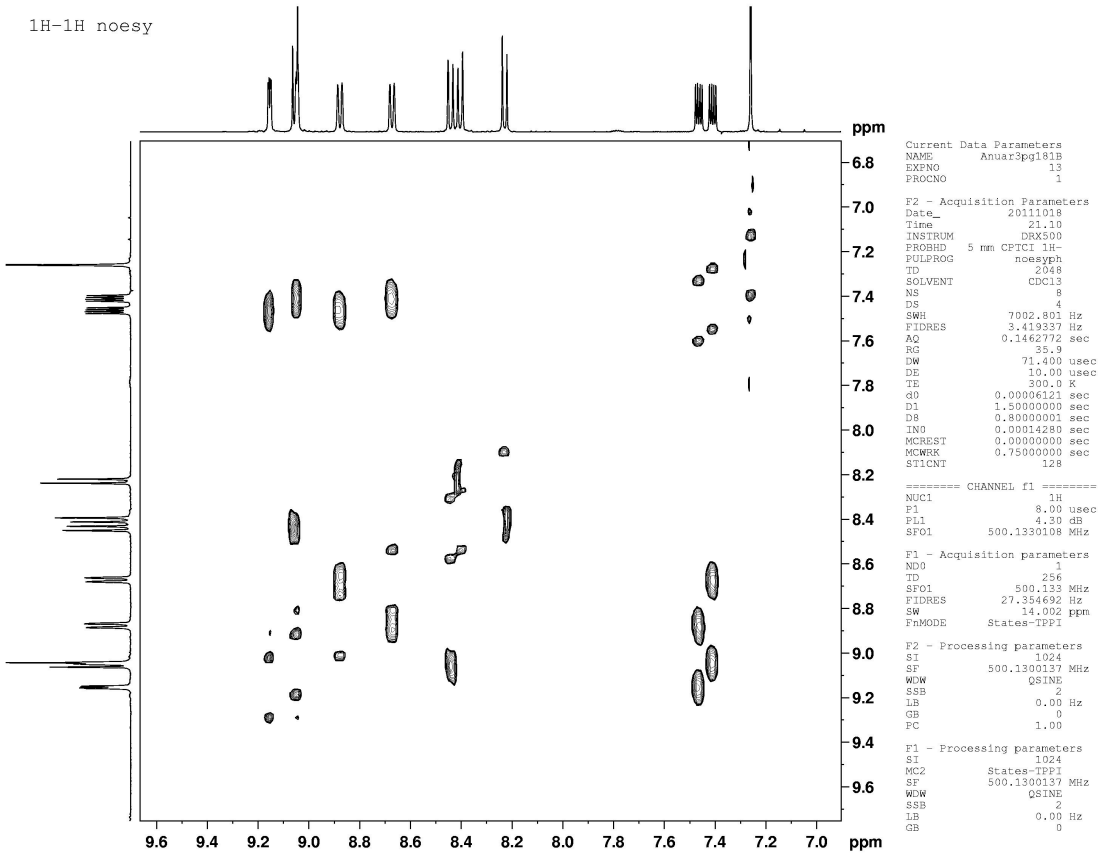

Figure S12. ^{1}H-^{1}H NOESY of **4** ($CDCl_3$, 500 MHz).

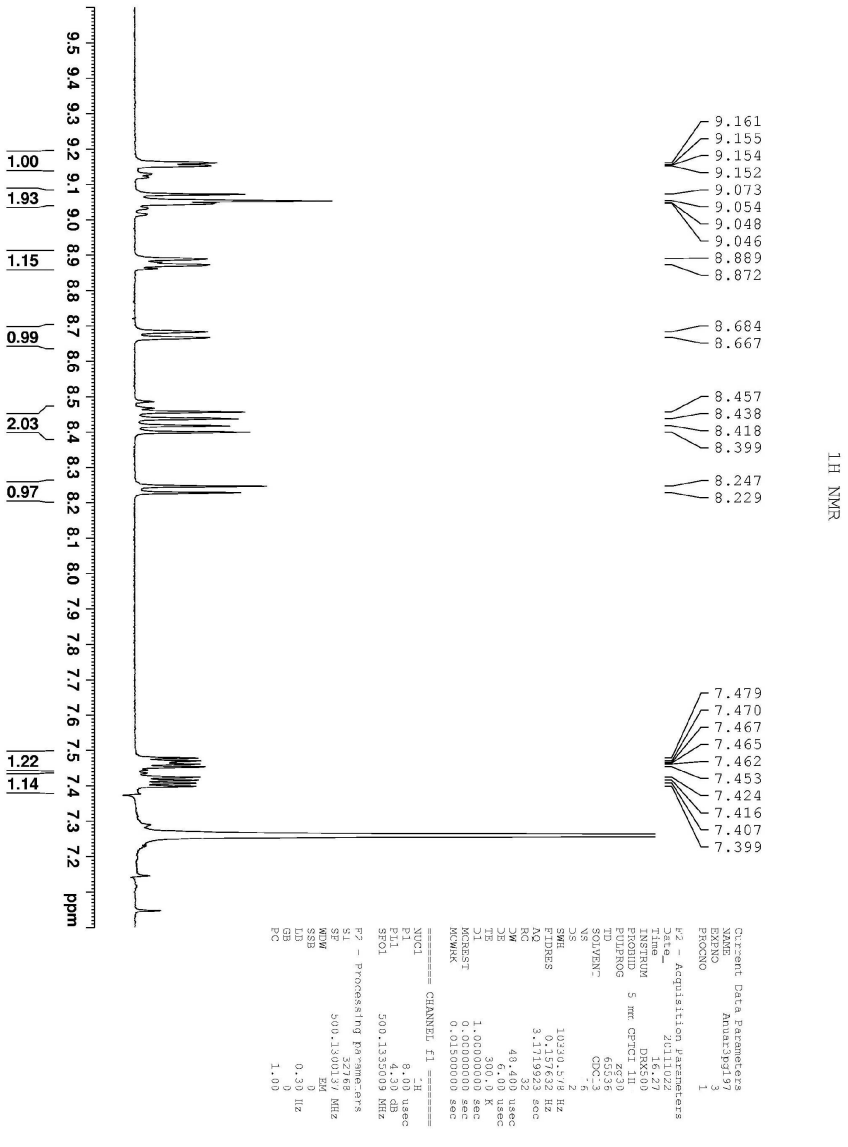

Figure S13. ^{1}H NMR of **4** ($CDCl_3$, 500 MHz), obtained from NADPH and NADPH:cytochrome P450 reductase-mediated synthesis.

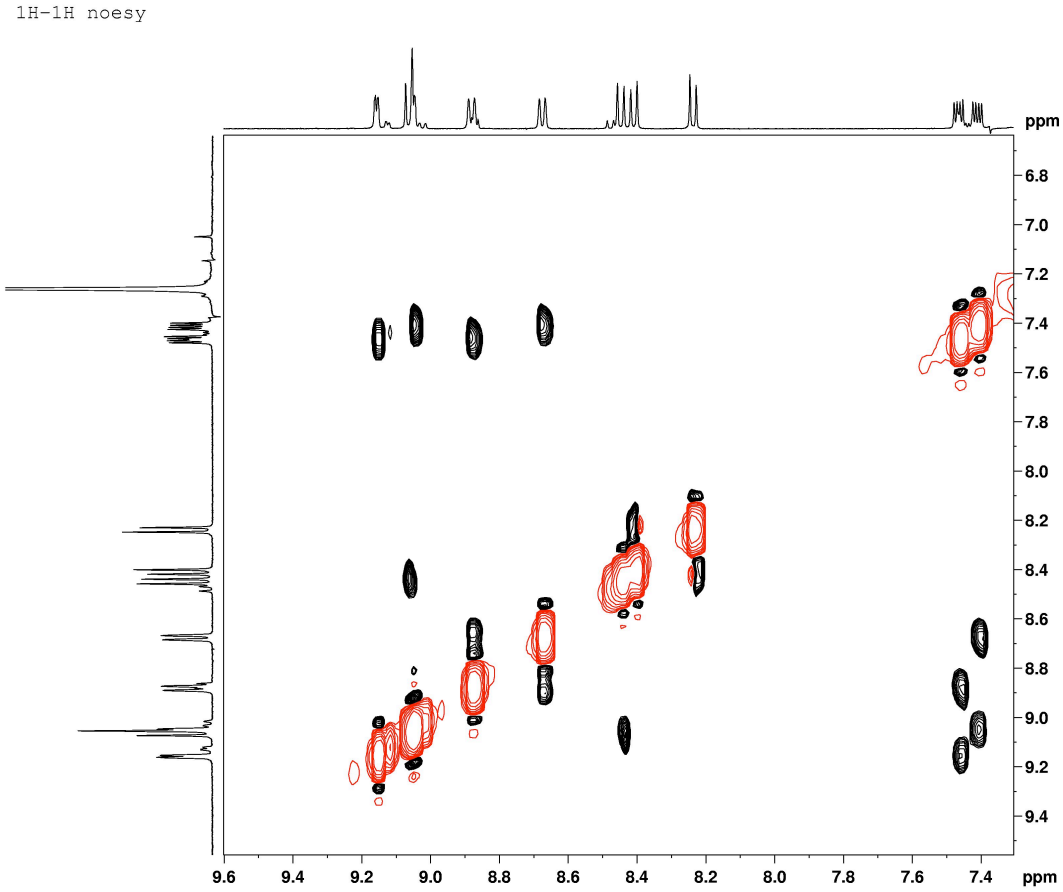

Figure S14. ^{1}H-^{1}H NOESY of **4** ($CDCl_3$, 500 MHz), obtained from NADPH and NADPH:cytochrome P450 reductase-mediated synthesis.