Supporting Information

Sensitized photochemistry of di(4-tetrazolouracil) dinucleoside monophosphate as a route to dicytosine cyclobutane photoproduct precursors

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NMR spectra and HPLC, HPLC/MS chromatograms:

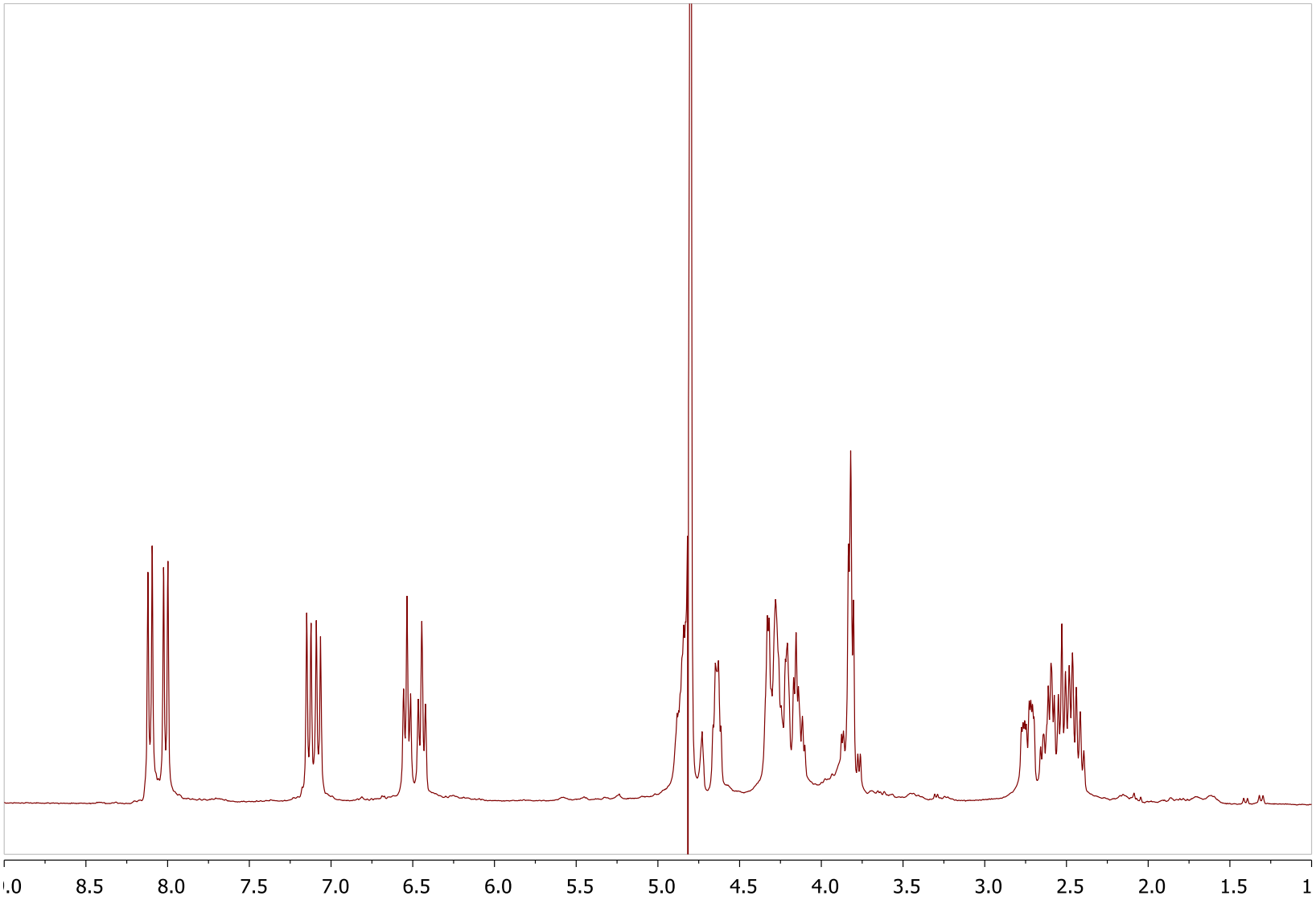


Figure S2: ^{1}H NMR spectrum of **2** (300 MHz, D_2O).

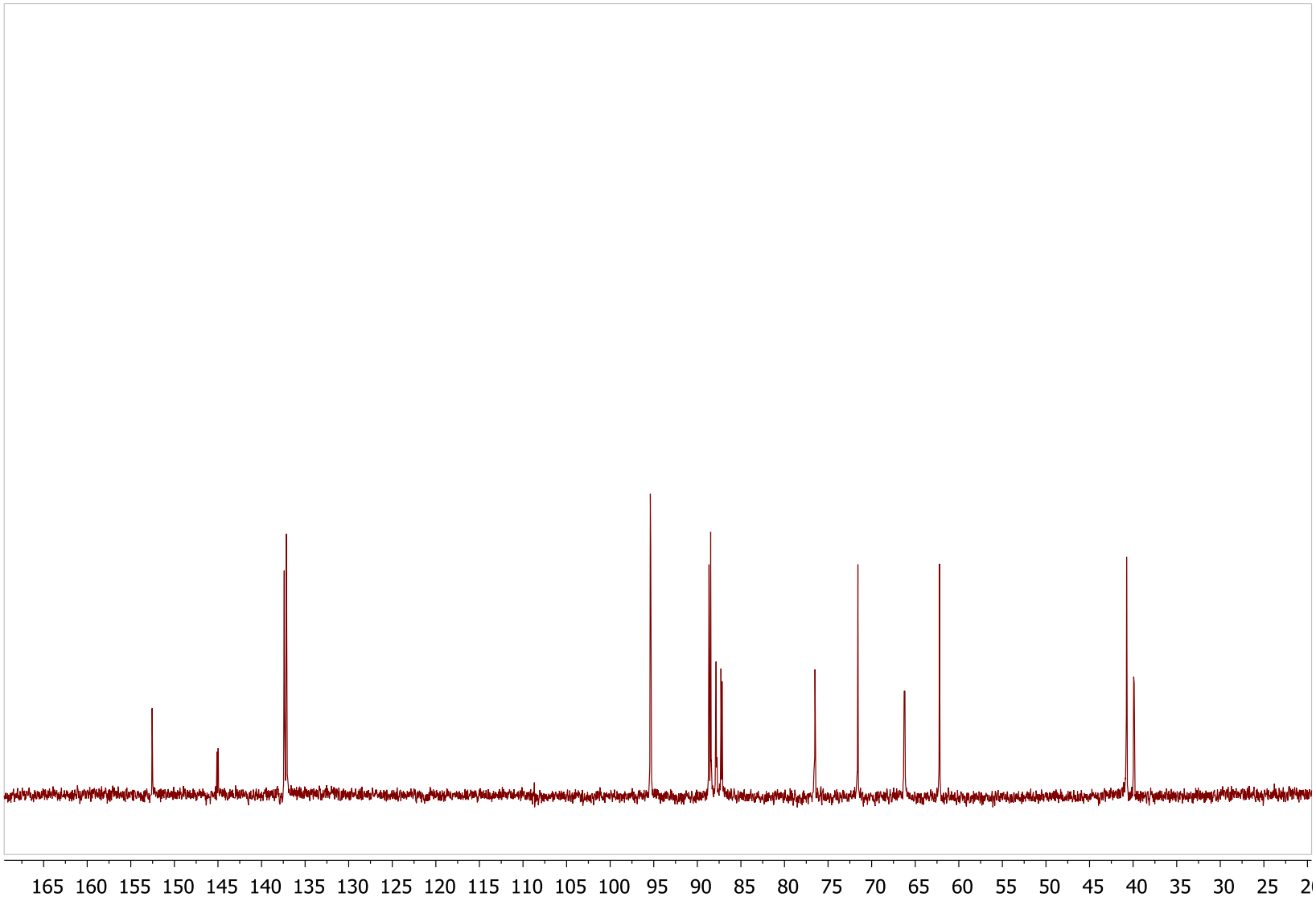


Figure S3: ^{13}C NMR spectrum of **2** (62.5 MHz, D_2O).

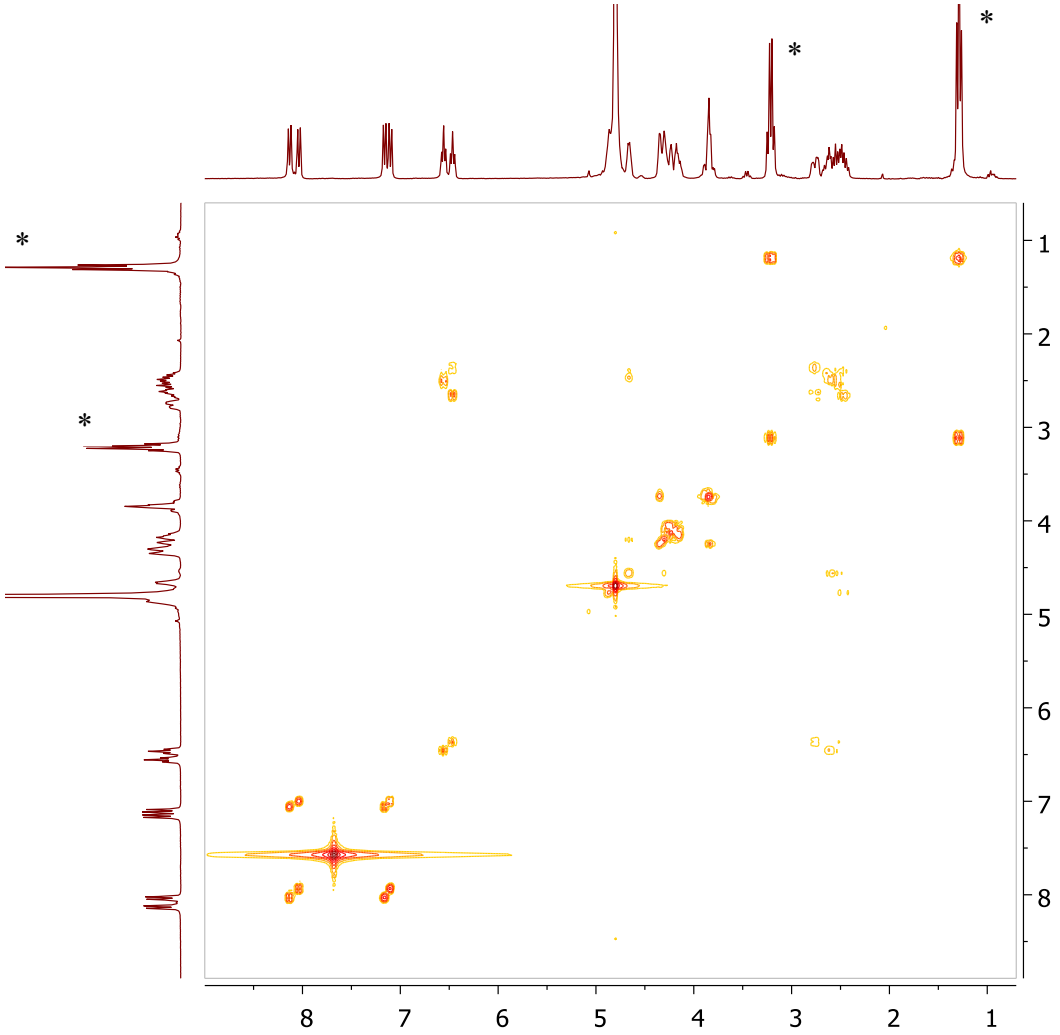


Figure S4: COSY spectrum of **2** (300 MHz, D_2O). *: Contaminated with Et_3N

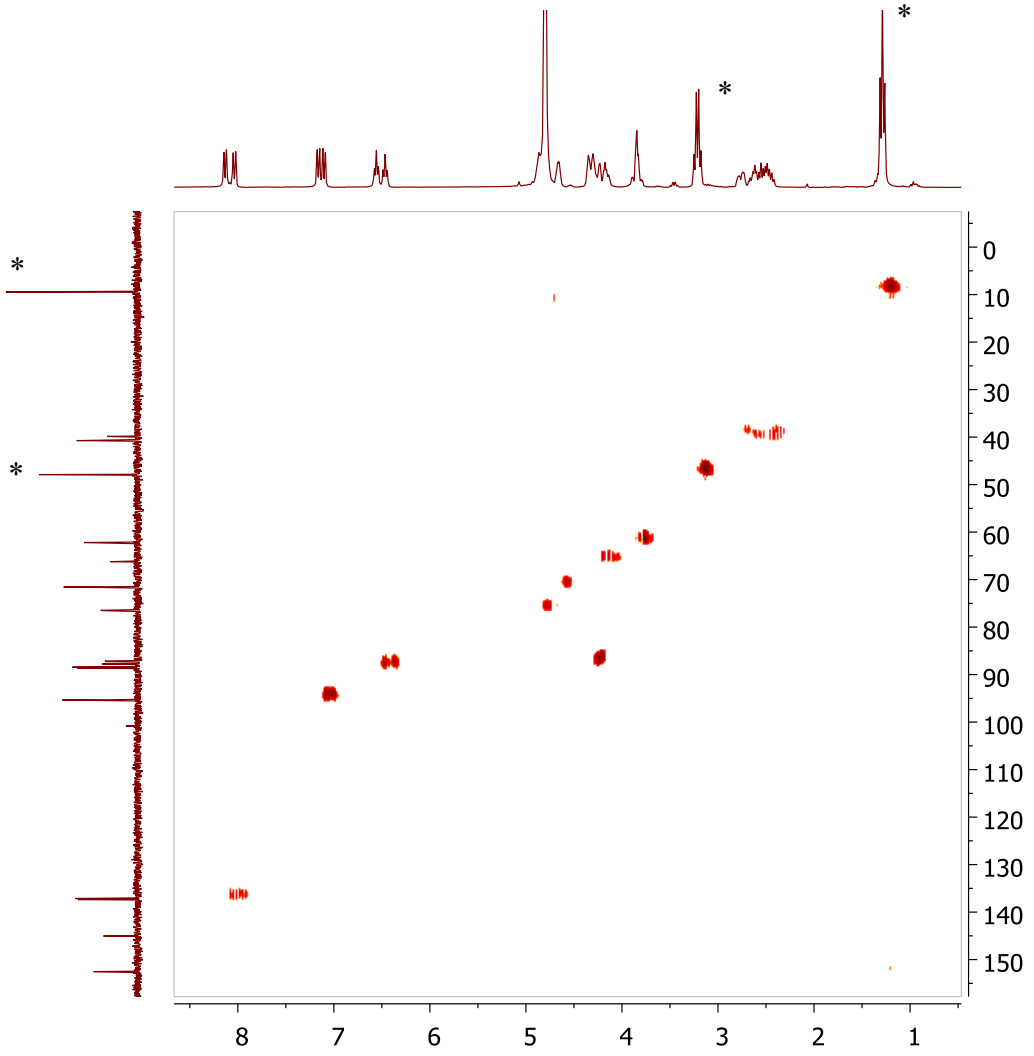


Figure S5: HMQC spectrum of **2** (300 MHz, D_2O). *: Contaminated with Et_3N

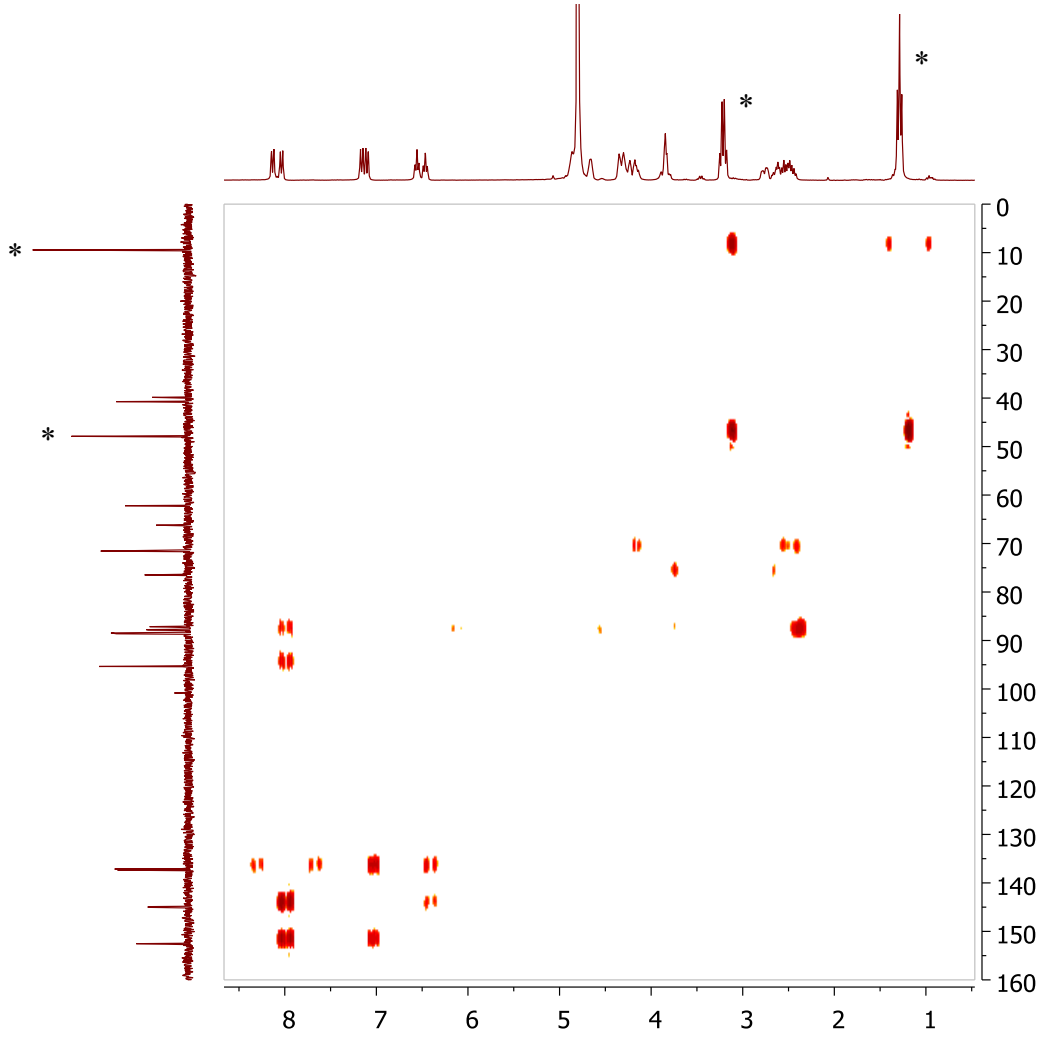


Figure S6: HMBC spectrum of **2** (300 MHz, D_2O). *: Contaminated with Et_3N

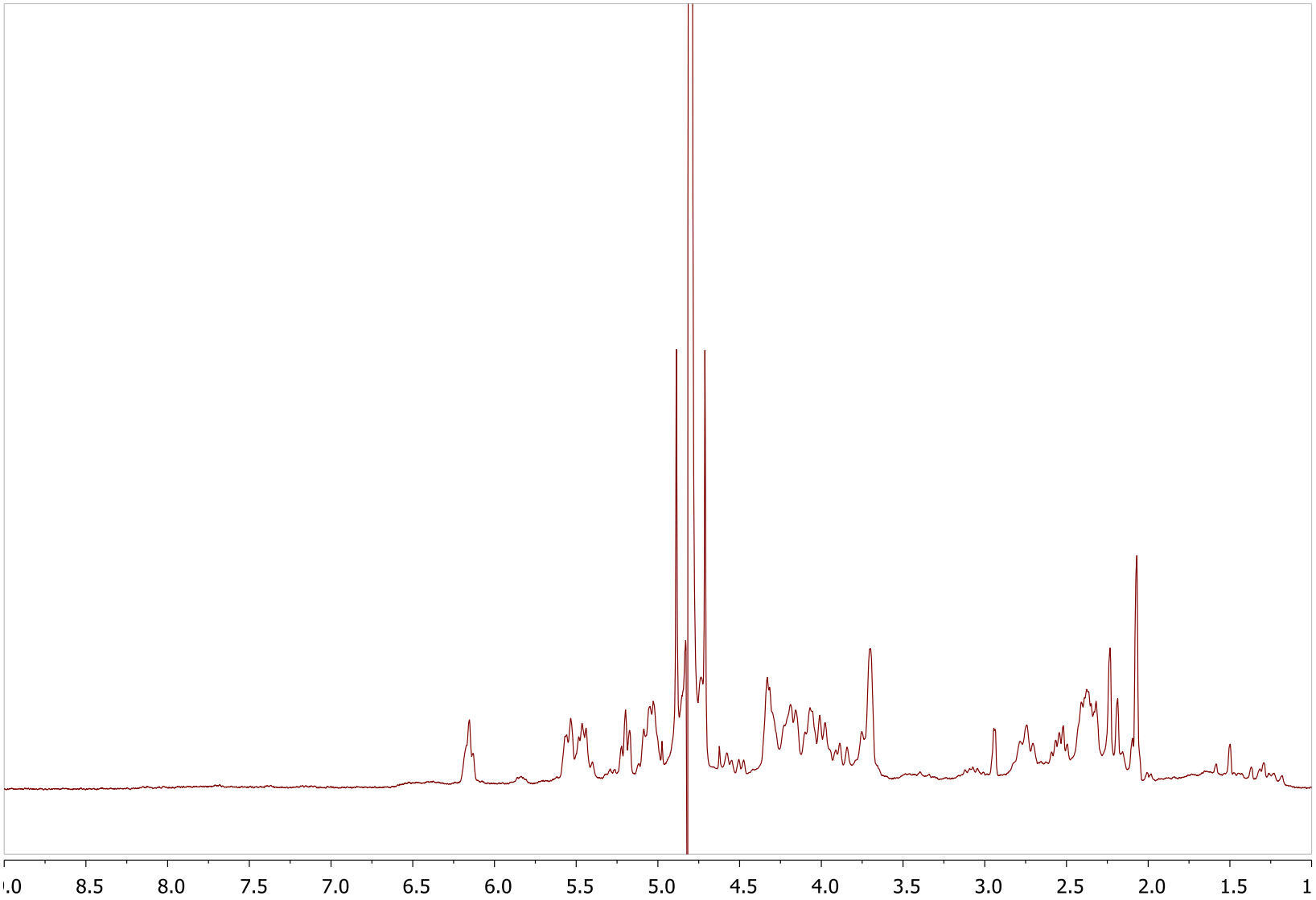
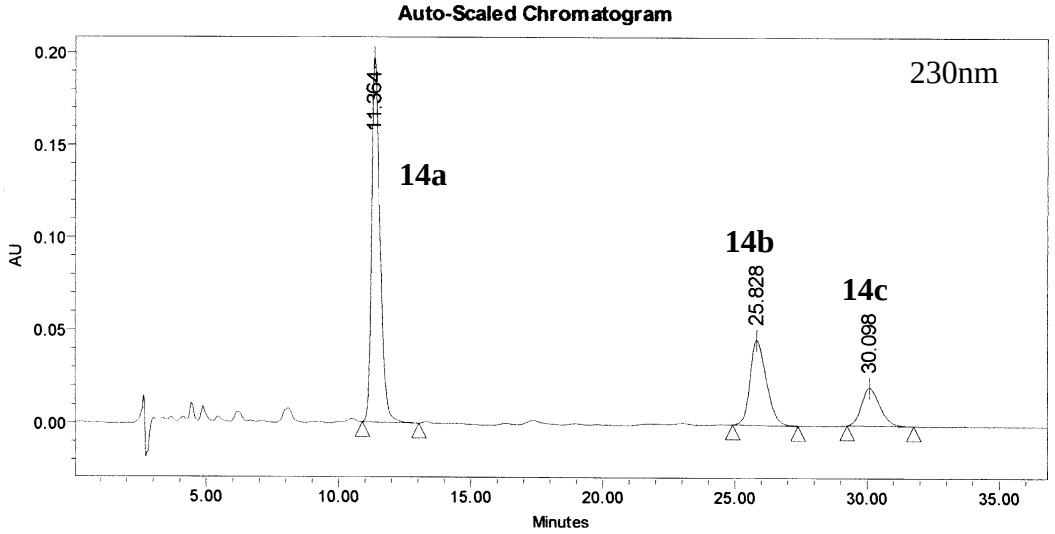


Figure S7: ^{1}H NMR spectrum of the photosensitized irradiation of **2** (300 MHz, D_2O).



Processed Channel: PDA 230.0 nm

	Processed Channel	Retention Time (min)	Area	% Area	Height
1	PDA 230.0 nm	11.364	4355764	59.74	197047
2	PDA 230.0 nm	25.828	1949602	26.74	45729
3	PDA 230.0 nm	30.098	985411	13.52	20260

Figure S8: HPLC chromatogram of the photosensitized irradiation of **2**.
(SYMMETRY C18 (5µm, 250x4.6 mm) column eluted with ammonium acetate 0.05 M at a flow rate of 1 mL/min)

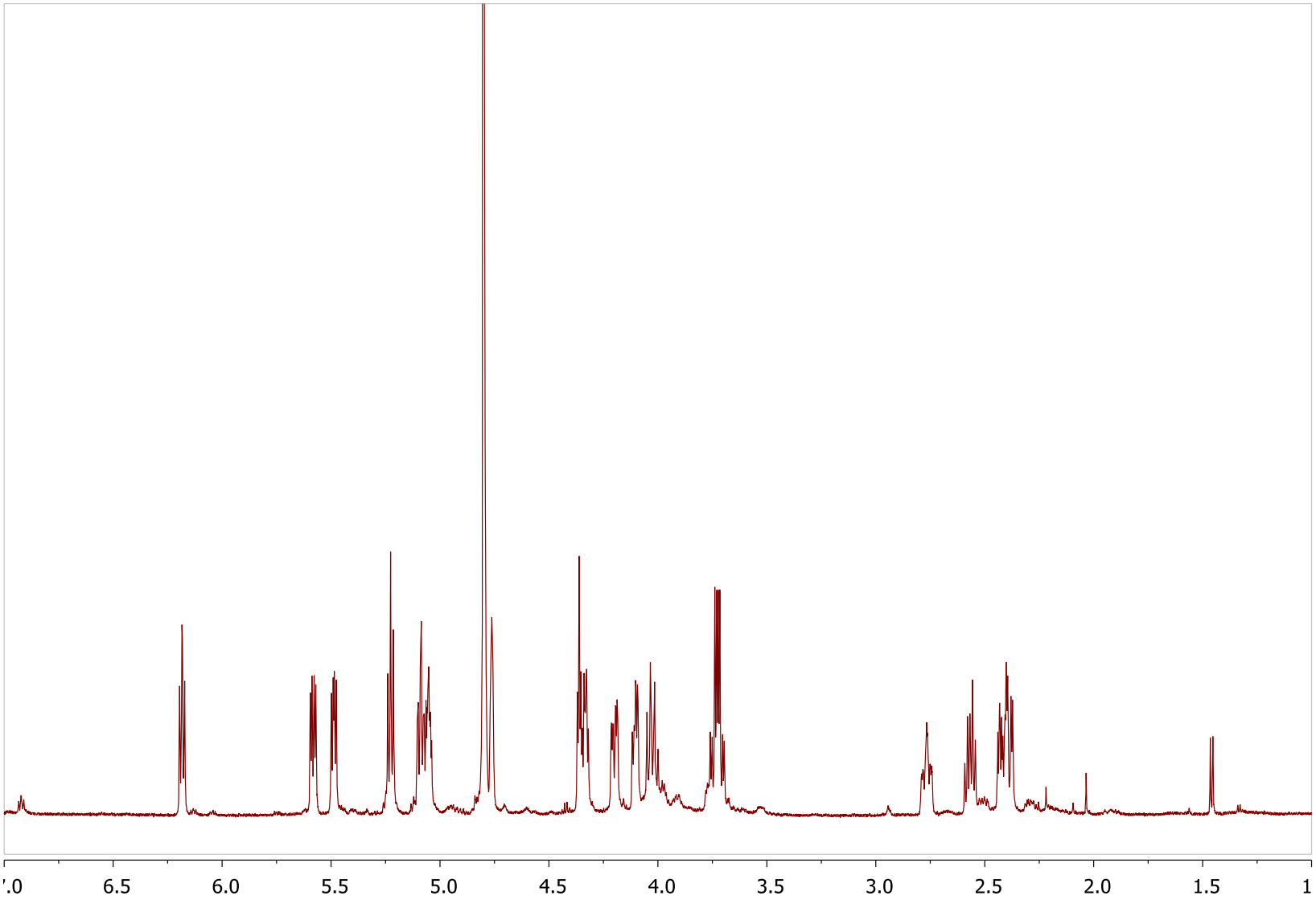


Figure S9: ^{1}H NMR spectrum of **14a** (600 MHz, D_2O).

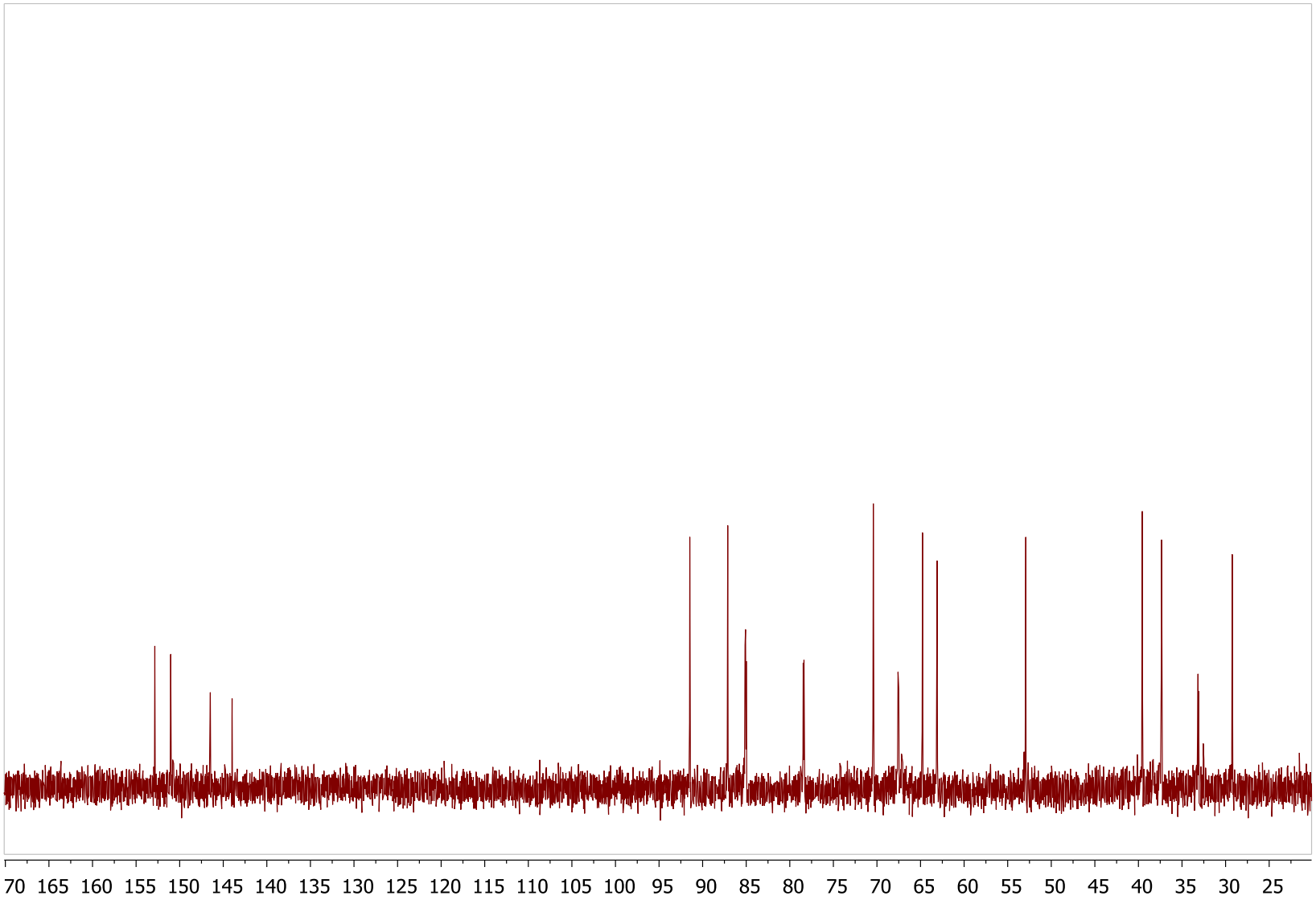


Figure S10: ^{13}C NMR spectrum of **14a** (62.5 MHz, D_2O).

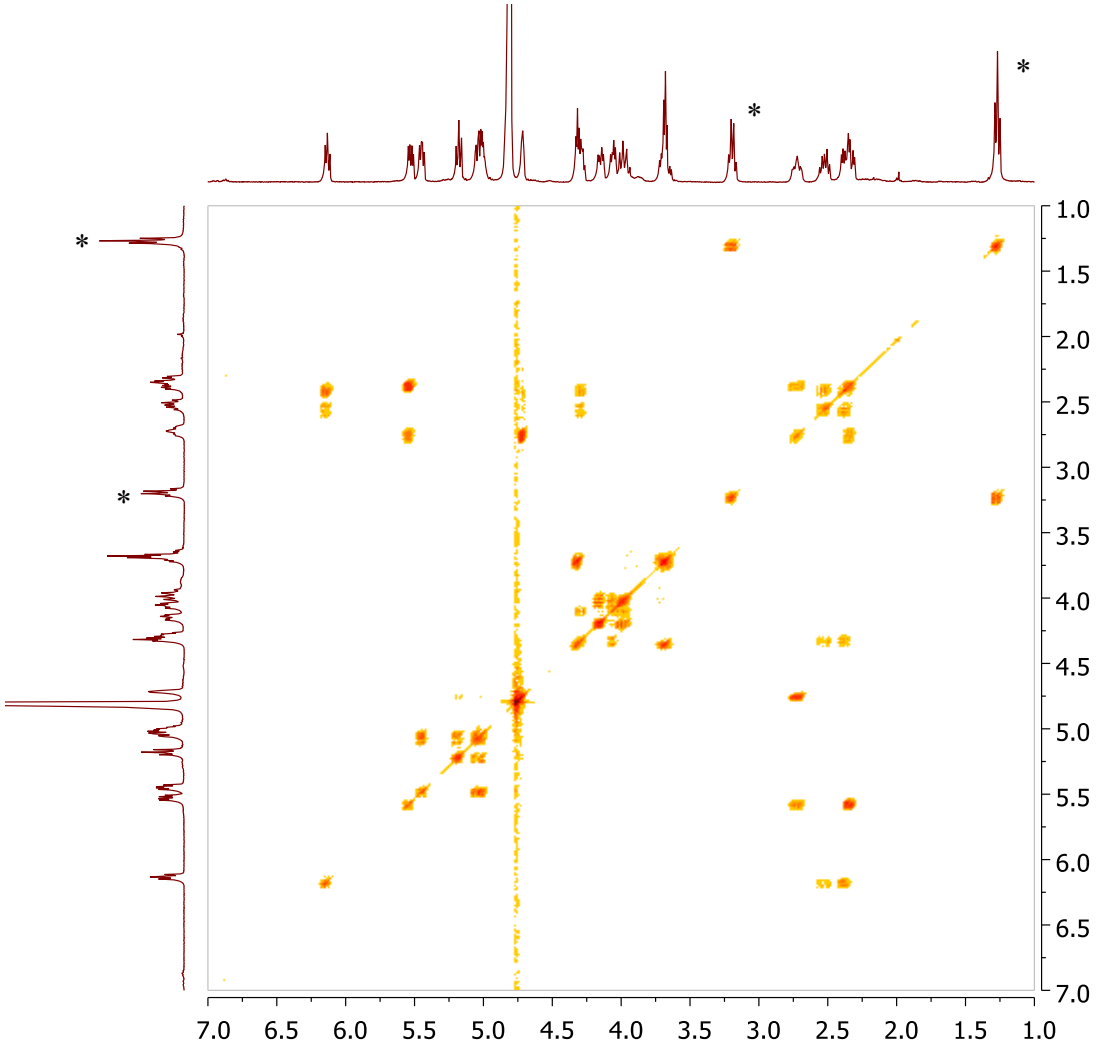


Figure S11: COSY spectrum of **14a** (400 MHz, D_2O). *: Contaminated with Et_3N

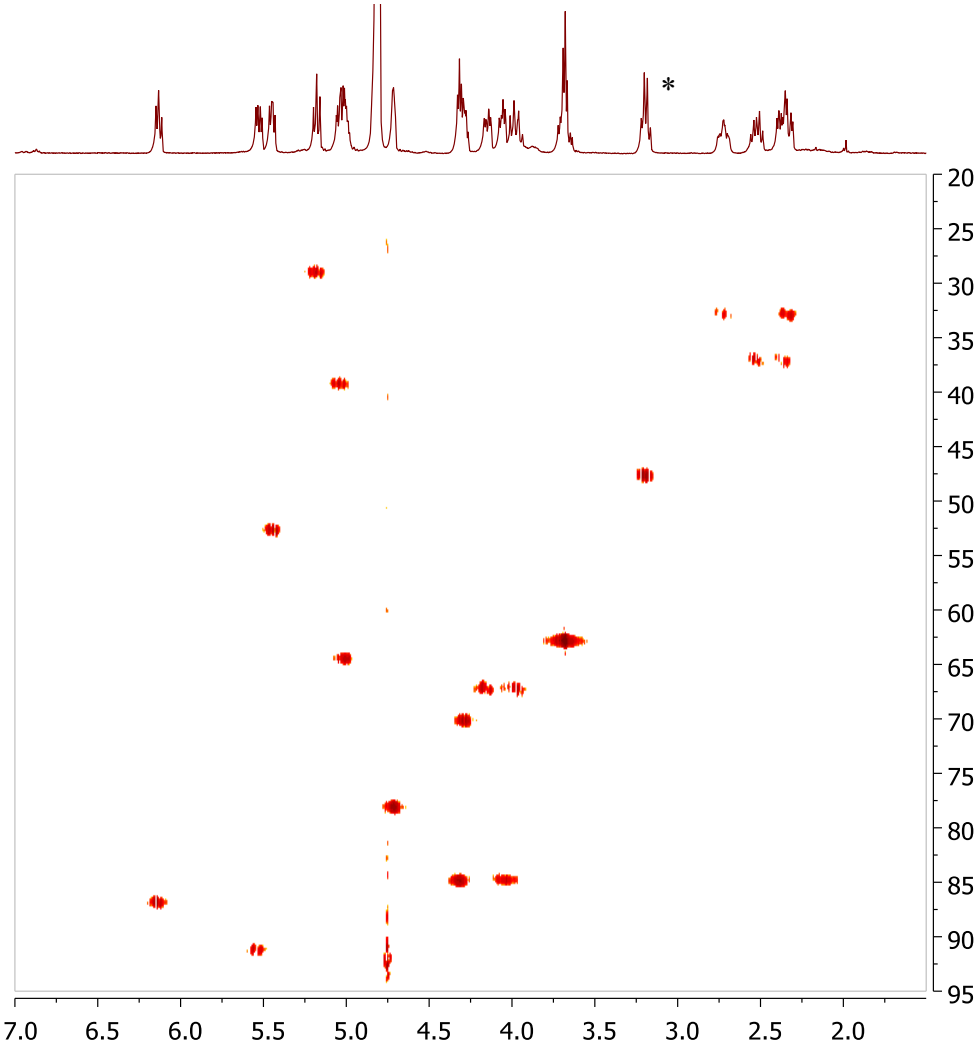


Figure S12: HMQC spectrum of **14a** (400 MHz, D_2O). *: Contaminated with Et_3N

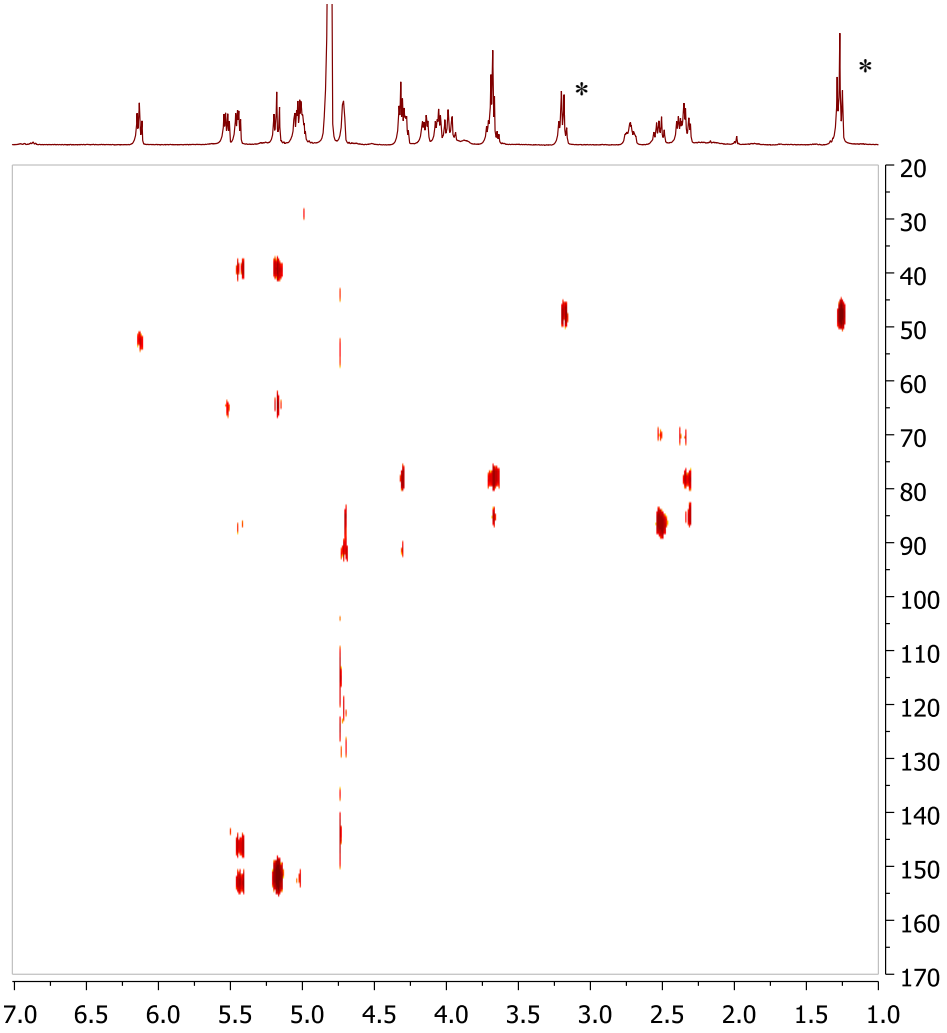


Figure S13: HMBC spectrum of **14a** (400 MHz, D_2O). *: Contaminated with Et_3N

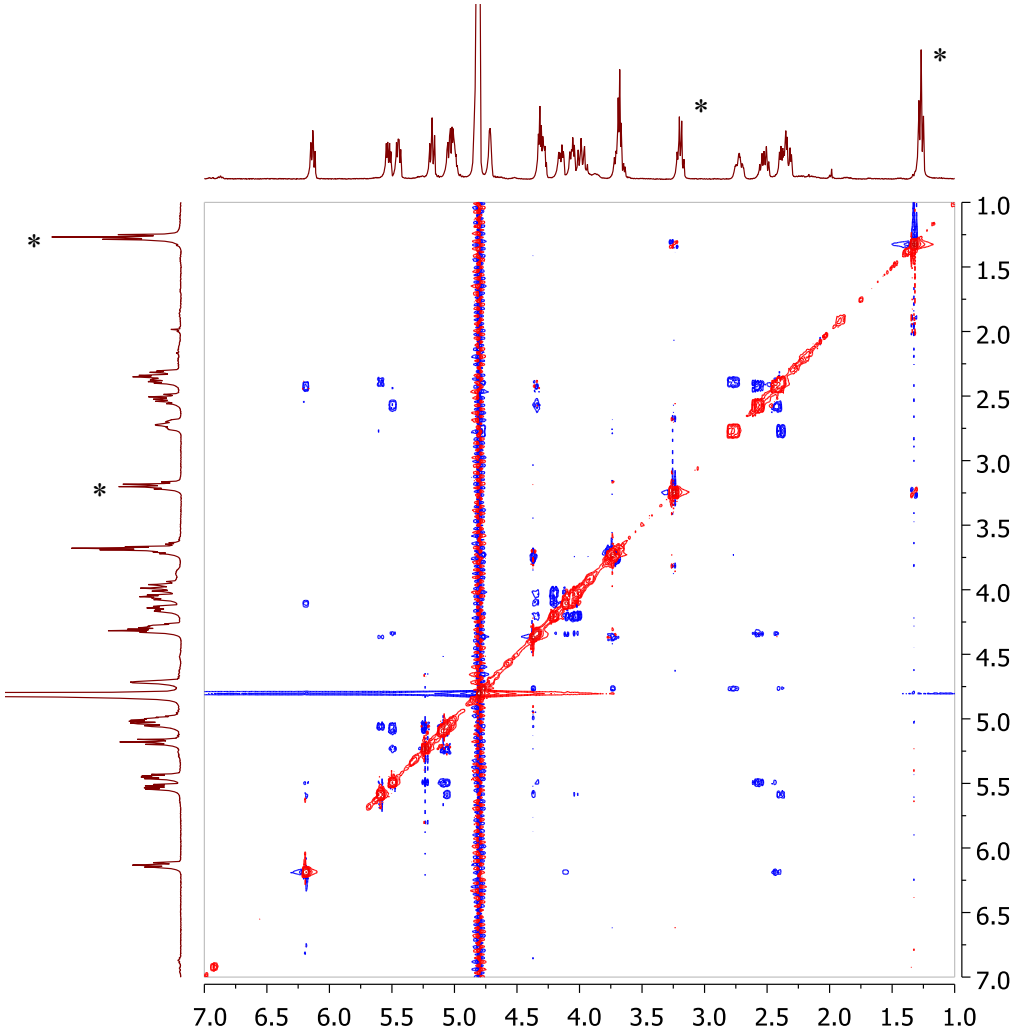


Figure S14: NOESY spectrum of **14a** (400 MHz, D_2O, mixing time 600 ms). *: Contaminated with Et_3N

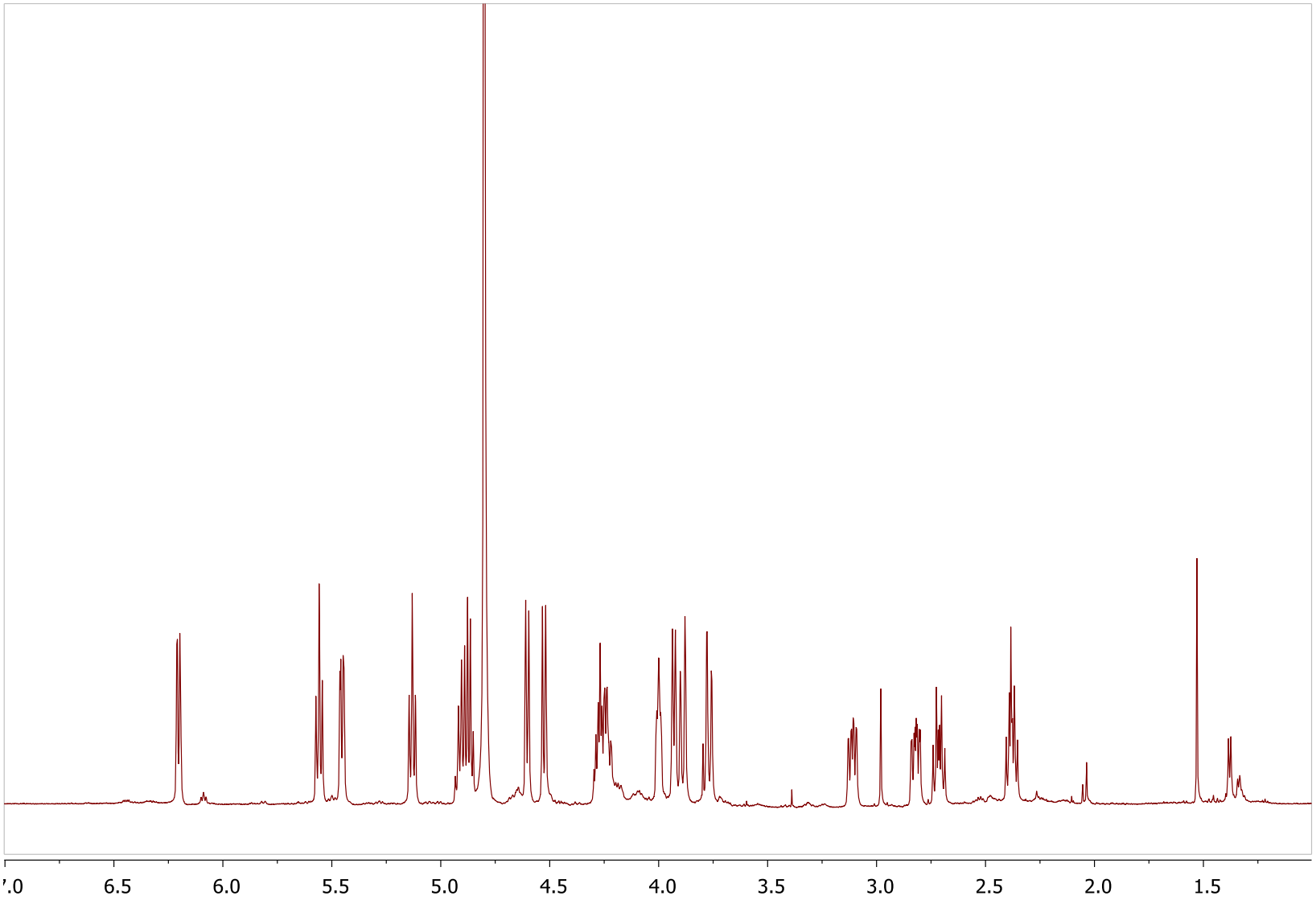


Figure S15: ^{1}H NMR spectrum of **14b** (600 MHz, D_2O).

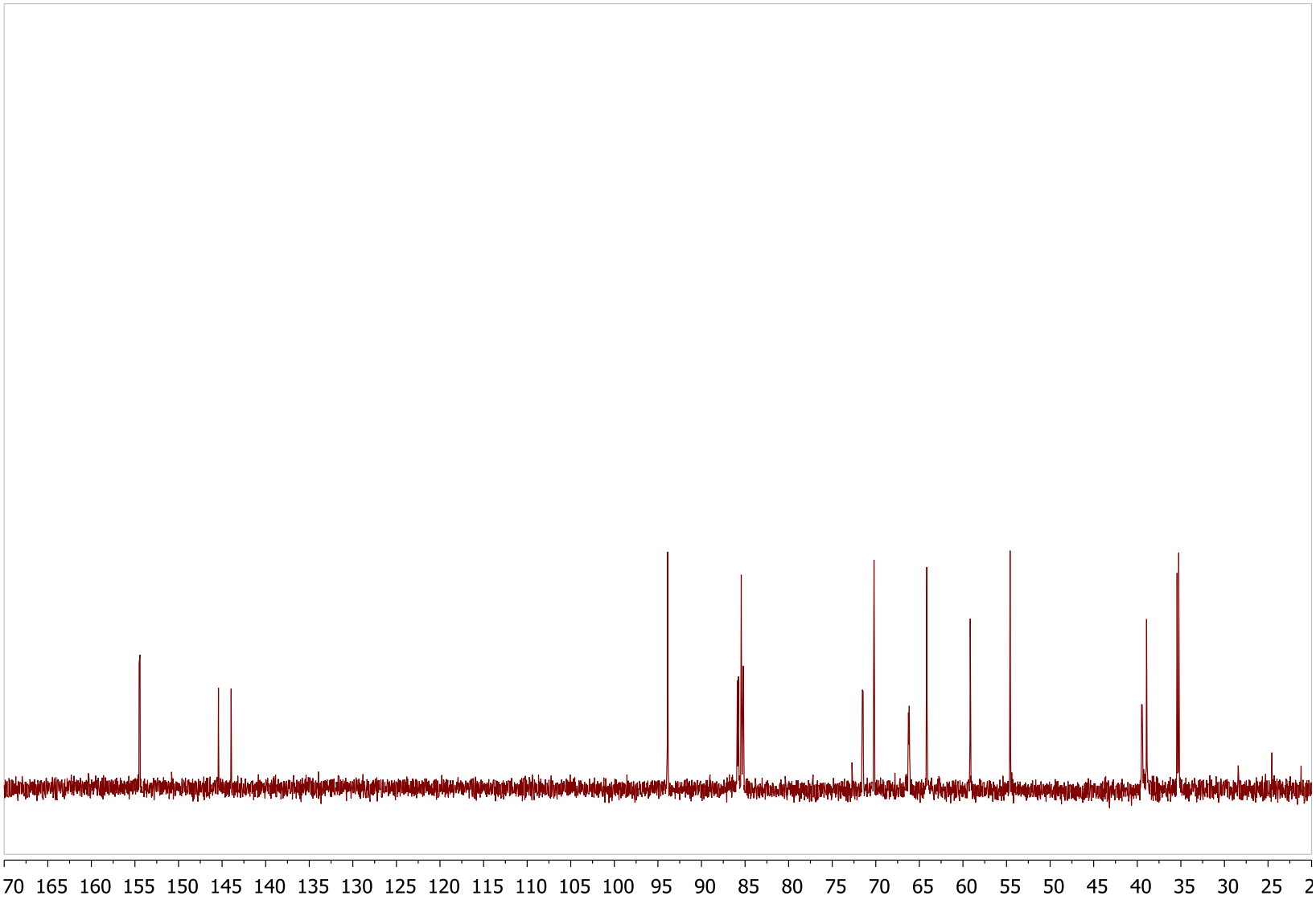


Figure S16: ^{13}C NMR spectrum of **14b** (75 MHz, D_2O).

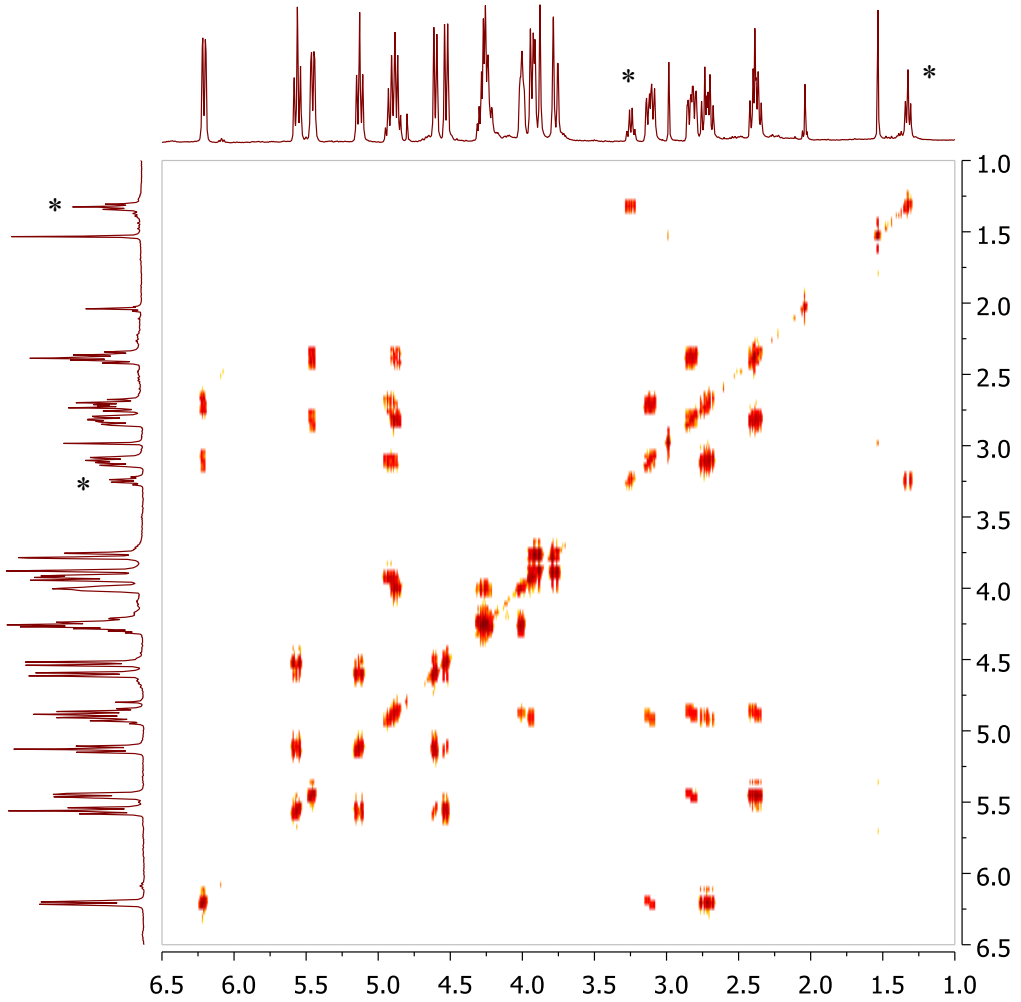


Figure S17: COSY spectrum of **14b** (400 MHz, D_2O). *: Contaminated with Et_3N

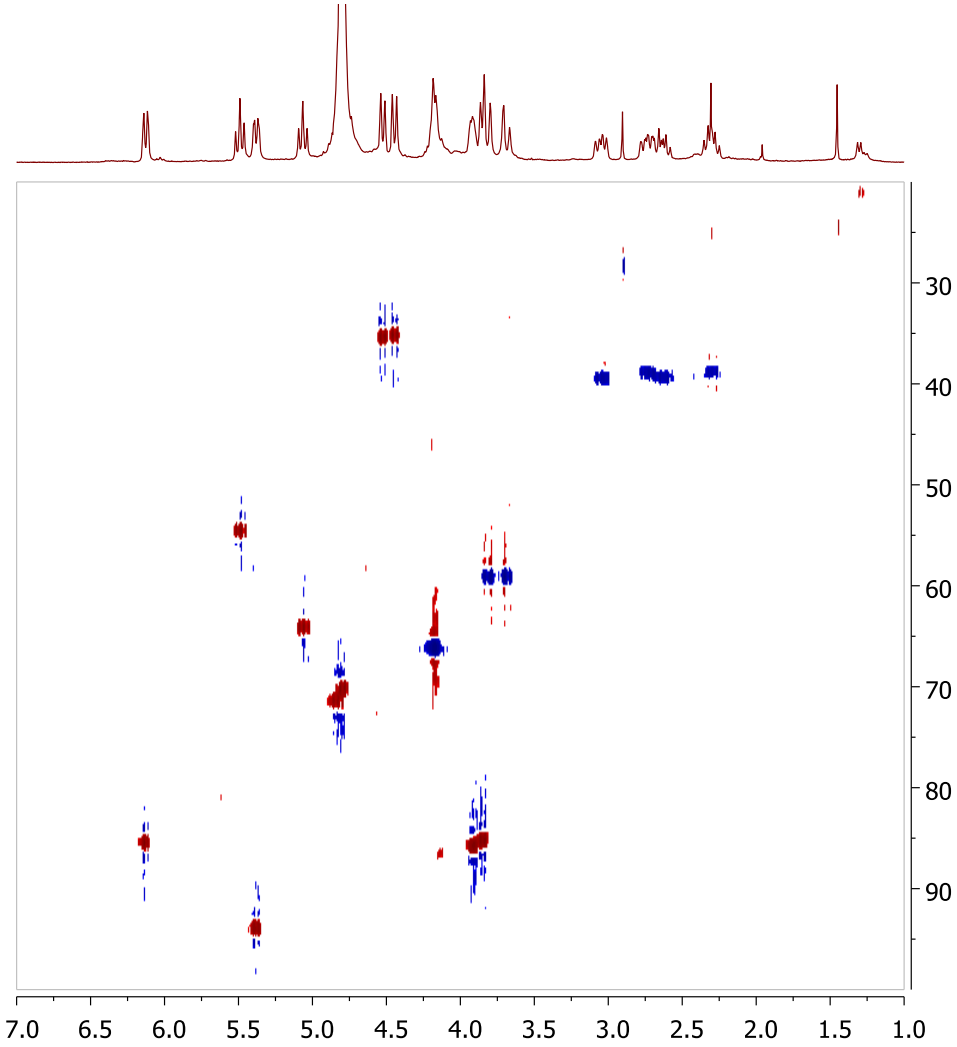


Figure S18: HMQC spectrum of **14b** (300 MHz, D_2O).

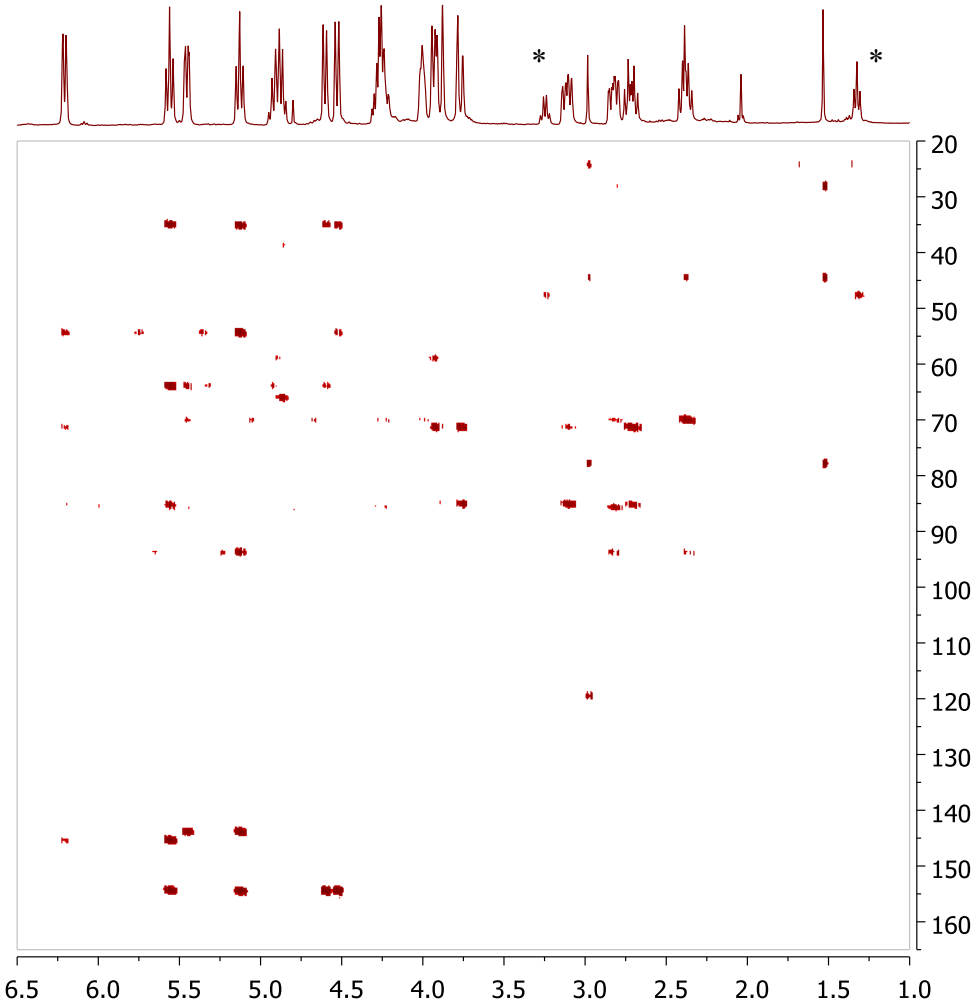


Figure S19: HMBC spectrum of **14b** (400 MHz, D_2O). *: Contaminated with Et_3N

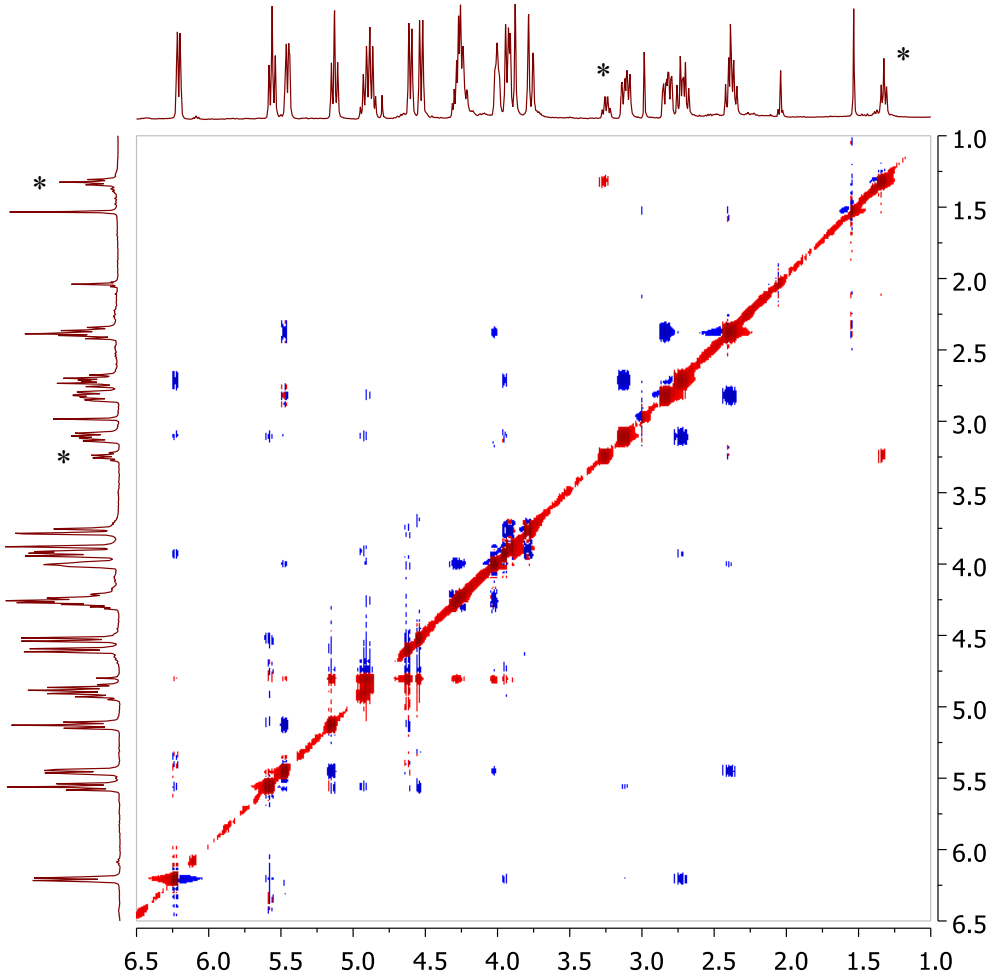


Figure S20: NOESY spectrum of **14b** (400 MHz, D_2O, mixing time 600 ms). *: Contaminated with Et_3N

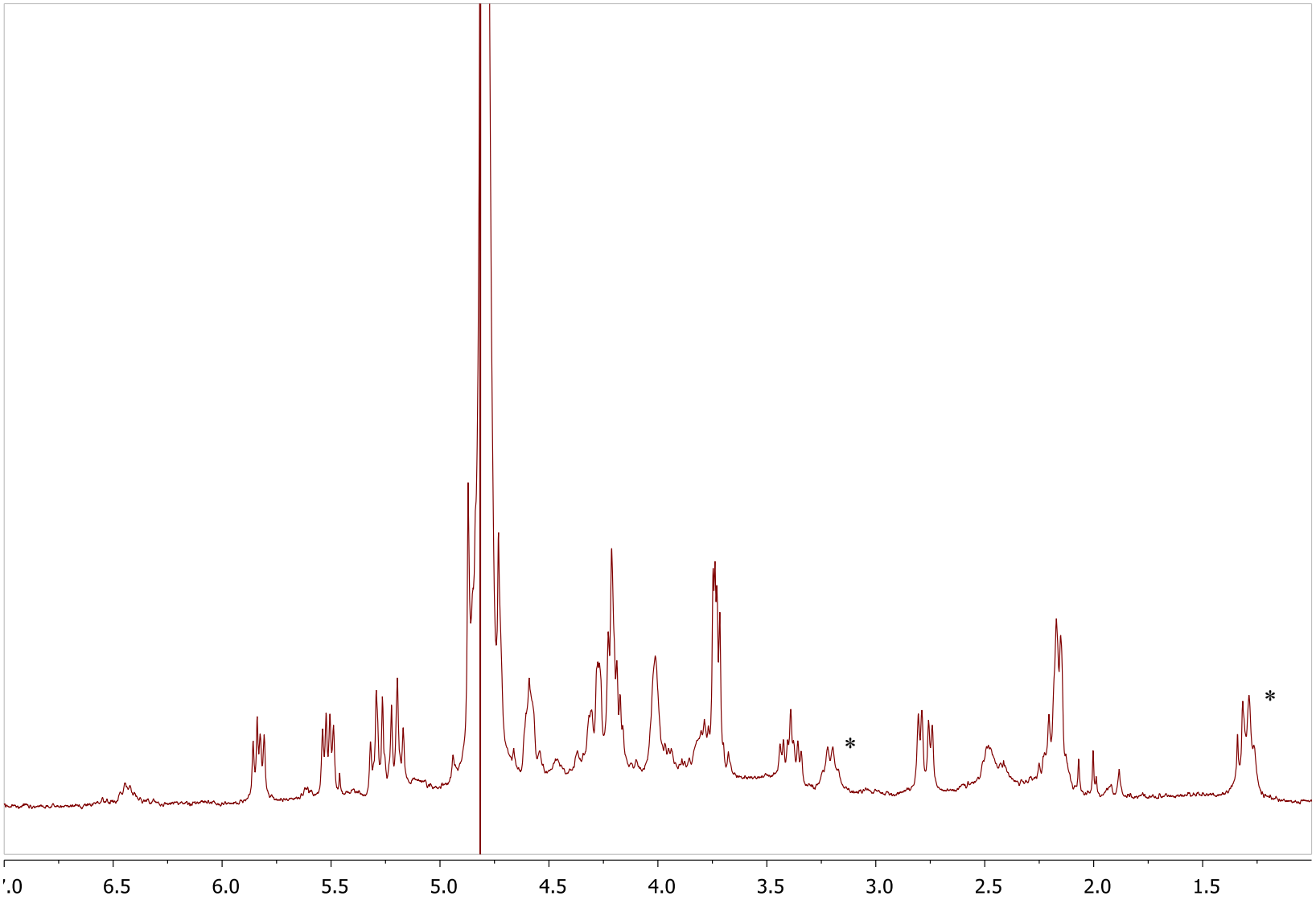
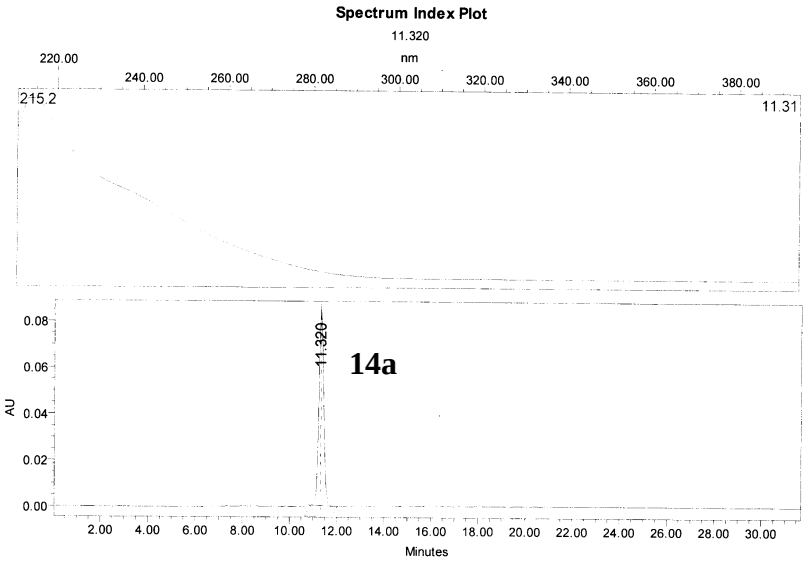


Figure S21: ^{1}H NMR spectrum of **14c** (300 MHz, D_2O). *: Contaminated with Et_3N

LC-MS analysis of the stability of 14a towards nucleophiles

Compound **14a** (1 mg) is solubilized in a 0.05M K_2CO_3/MeOH (1 mL) then evaporated and injected on to a SYMMETRY C18 (5µm, 250x4.6 mm) column eluted with ammonium acetate 0.05 M at a flow rate of 1 mL/min using a photodiode array detector and coupled to a an electrospray mass spectrometer (negative ion mode).

A



B

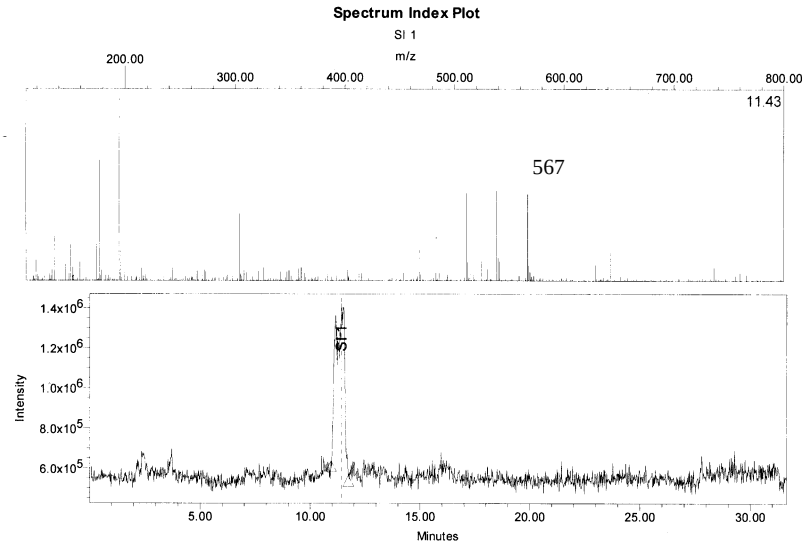
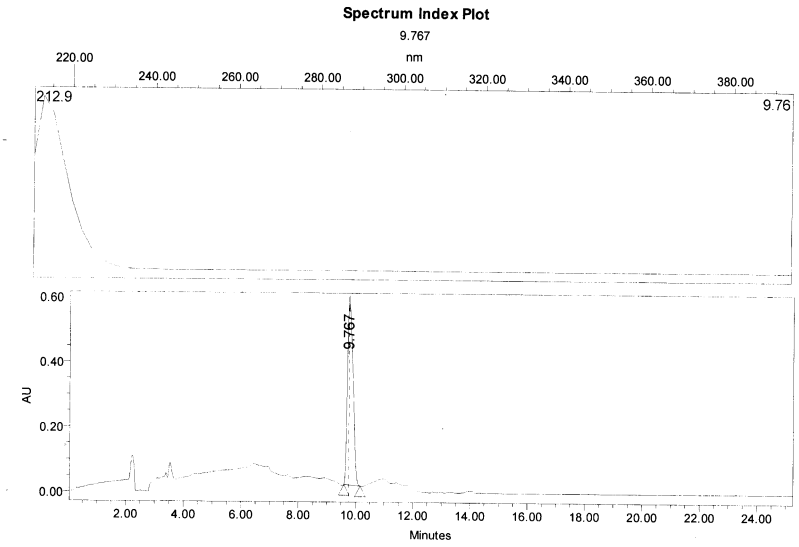


Figure S22: HPLC chromatogram (A) and HPLC/MS total ion current chromatogram (B) of **14a**.

A



B

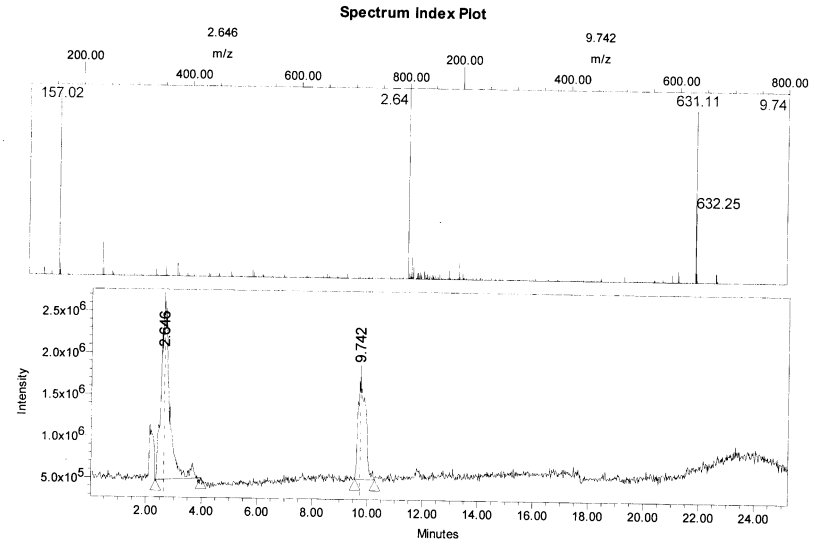


Figure S23: HPLC chromatogram (A) and HPLC/MS total ion current chromatogram (B) of the K_2CO_3/MeOH treatment of **14a**.