Electronic Supplementary Information

Chiral Photochemistry within a Confined Space: Diastereoselective Photorearrangements of a Tropolone and a Cyclohexadienone Included in a Synthetic Cavitand

Arun Kumar Sundaresan, Lakshmi S. Kaanumalle, Corinne L. D. Gibb, Bruce C. Gibb, and V. Ramamurthy

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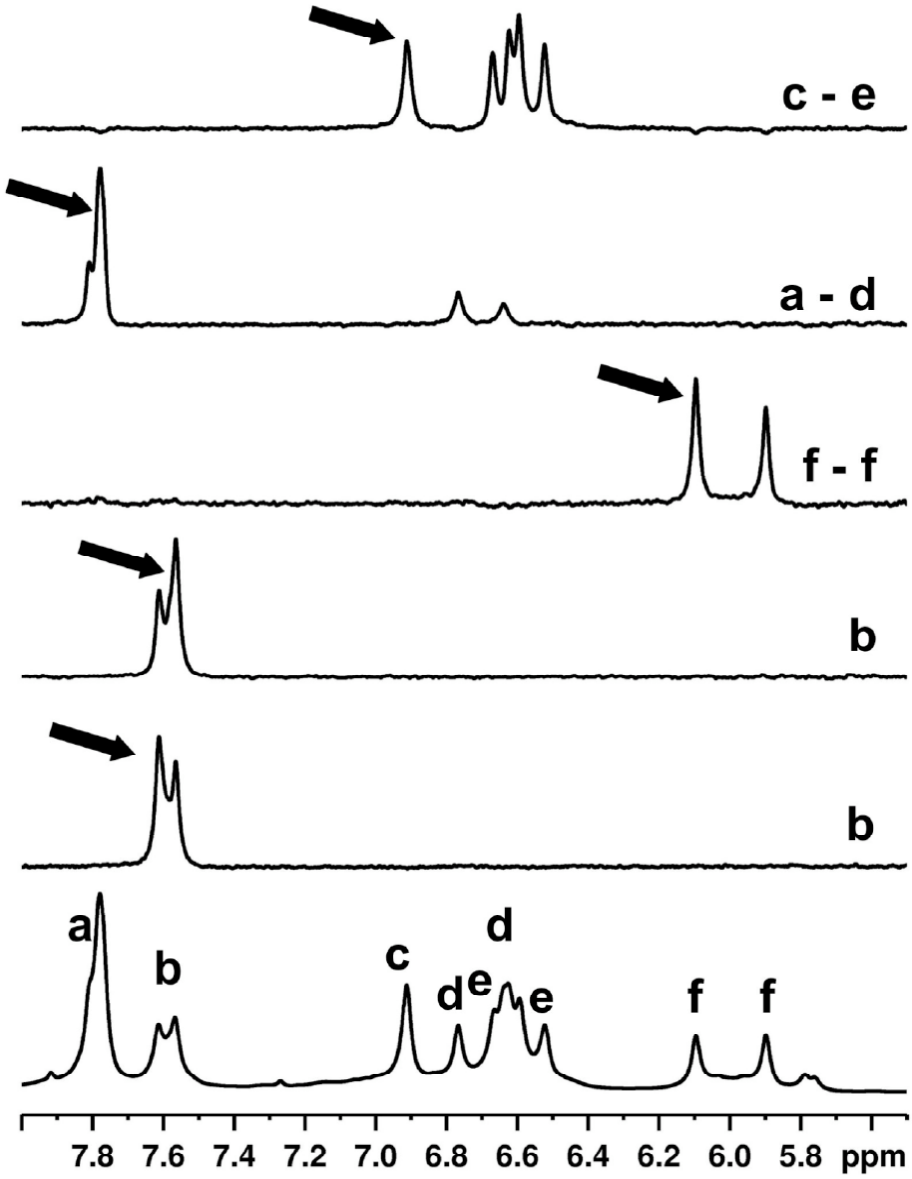

Figure ESI-1: 1D selective TOCSY NMR spectra (500 MHz, D_2O, 5×10^{-3} M OA, 5×10^{-2} M Na_2BO_4, 0.12 s mixing time), of **2**@OA_2 complex. Irradiated signals are marked with an arrow.

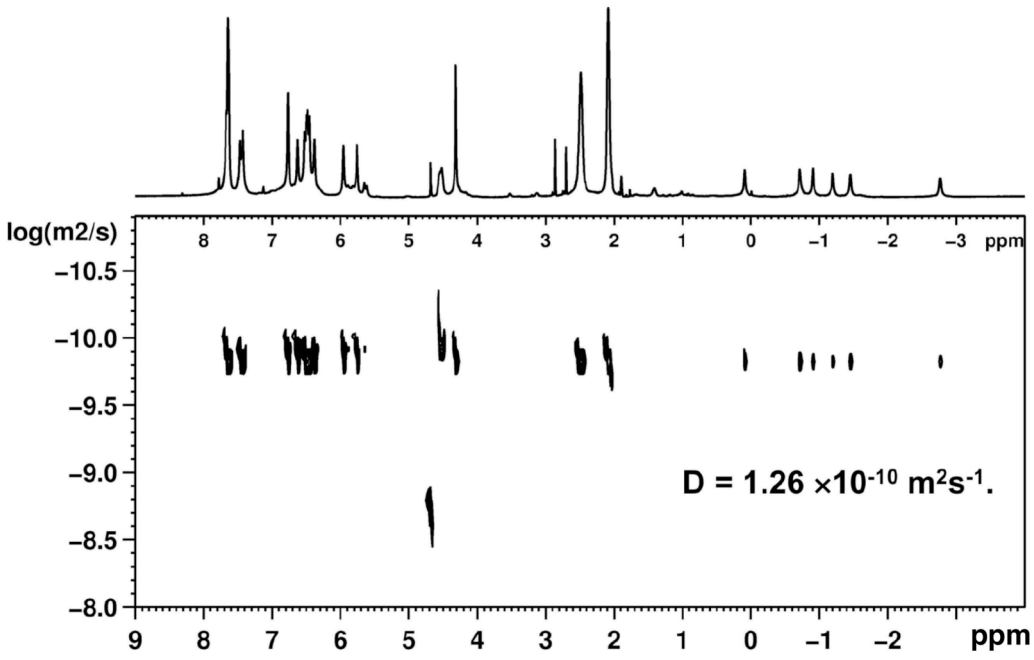

Figure ESI-2: DOSY NMR (500 MHz, 298 K, D_2O, 5×10^{-3} M OA, 5×10^{-2} M Na_2BO_4) of **2**@OA_2 complex. The diffusion coefficient was calculated to be 1.26×10^{-10} m^2s^{-1}.

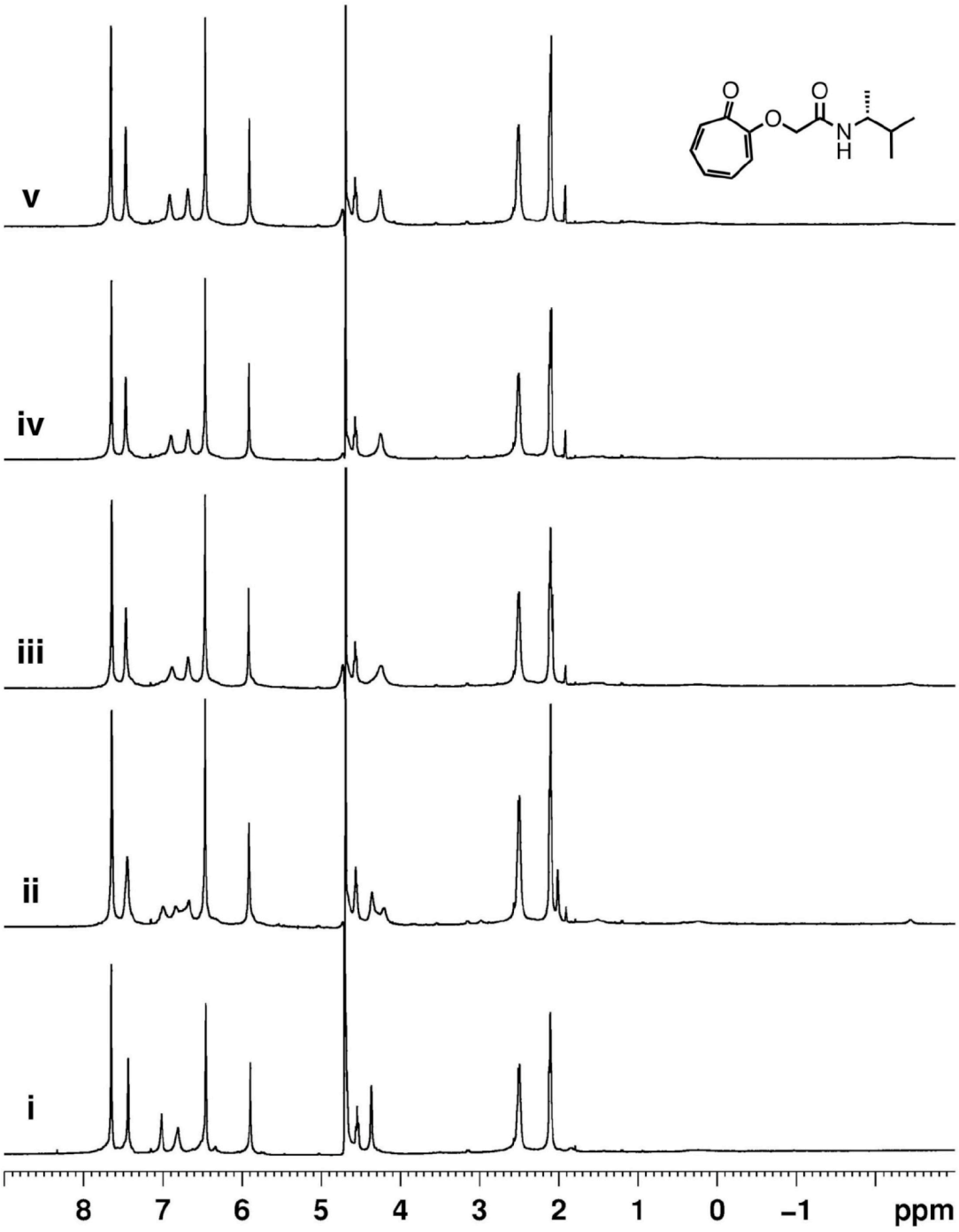

Figure ESI-3: ^{1}H NMR titration spectra (500 MHz, 298 K, D_2O, 10^{-3} M OA, 10^{-2} M Na_2BO_4) of (i) octa acid and octa acid containing (ii) 0.25 equiv, (iii) 0.5 equiv, (iv) 0.75 equiv and (v) 1 equiv **5** (each ratio with respect to 2 equiv octa acid, i.e., in spectrum (v) the ratio between octa acid and **5** is 2 : 1).

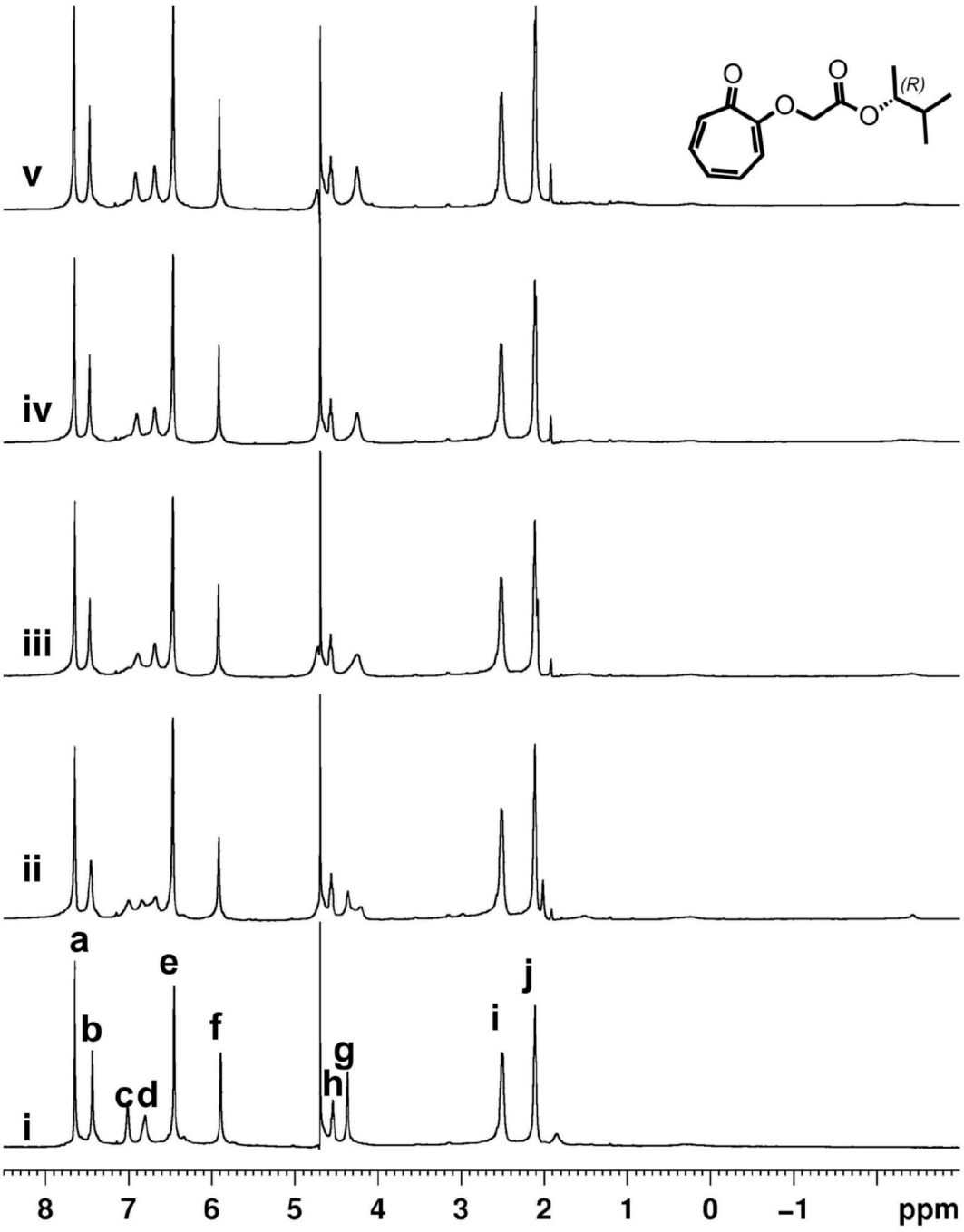

Figure ESI-4: ^{1}H NMR titration spectra (500 MHz, 298 K, D_2O, 10^{-3} M OA, 10^{-2} M $Na_2B_4O_7$) of (i) octa acid and octa acid containing (ii) 0.25 equiv, (iii) 0.5 equiv, (iv) 0.75 equiv and (v) 1 equiv **6** (each ratio with respect to 2 equiv octa acid, i.e., in spectrum (v) the ratio between octa acid and **6** is 2 : 1).

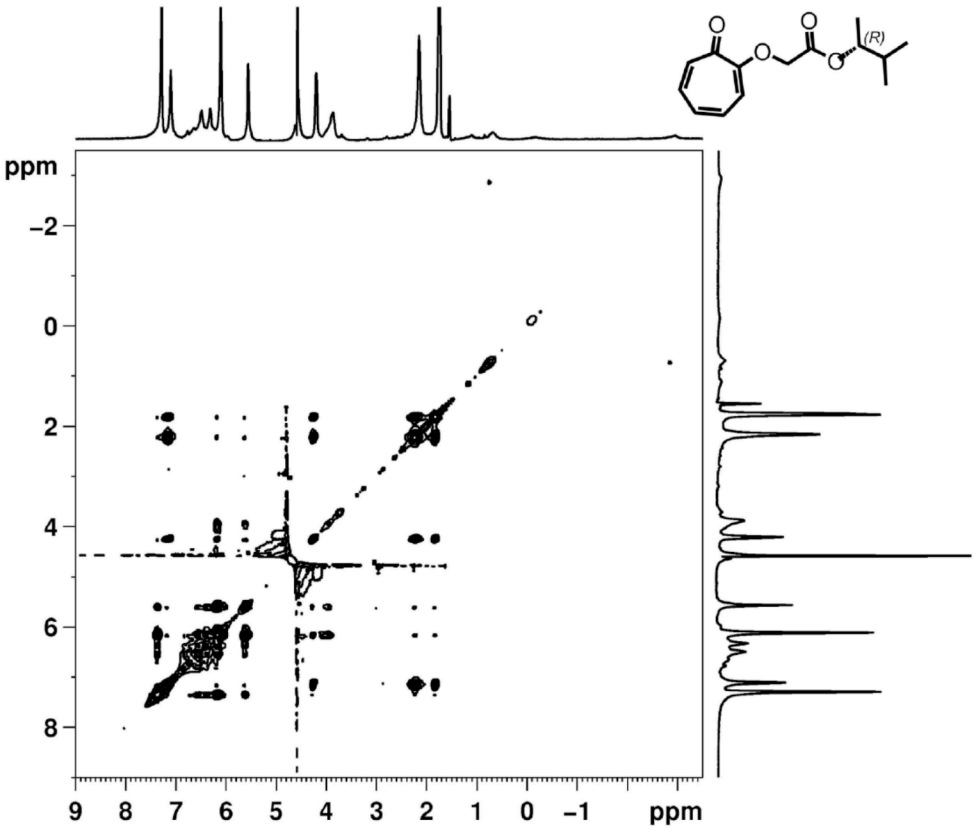

Figure ESI-5: NOESY NMR spectrum (500 MHz, D_2O, 278 K, 10^{-3} M OA, 10^{-2} M $Na_2B_4O_7$, 0.5 s mixing time) of **6** – octa acid complex. No intermolecular correlations were apparent even at 278 K.

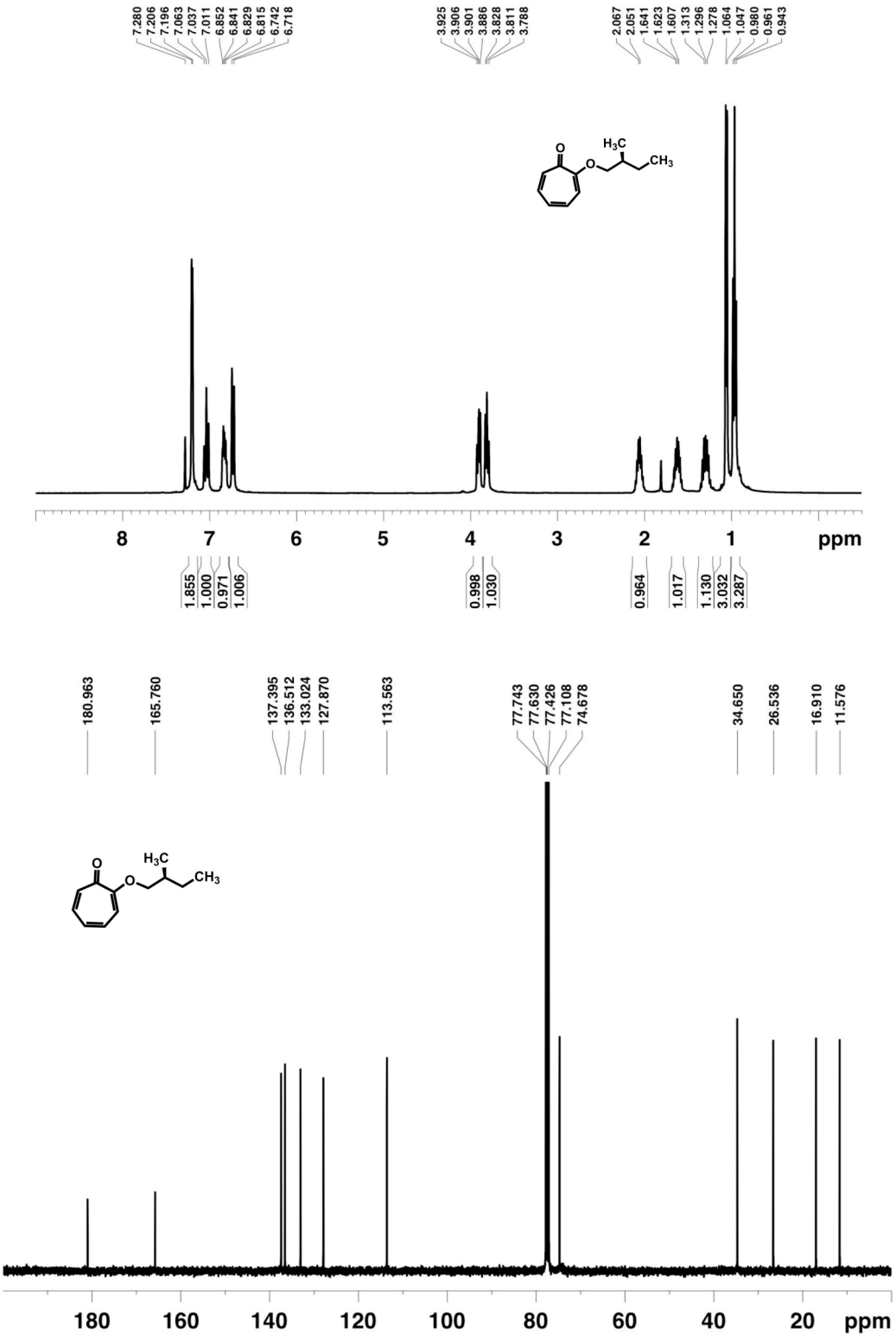

Figure ESI-6 ^{1}H (500 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz) spectra of **1**.

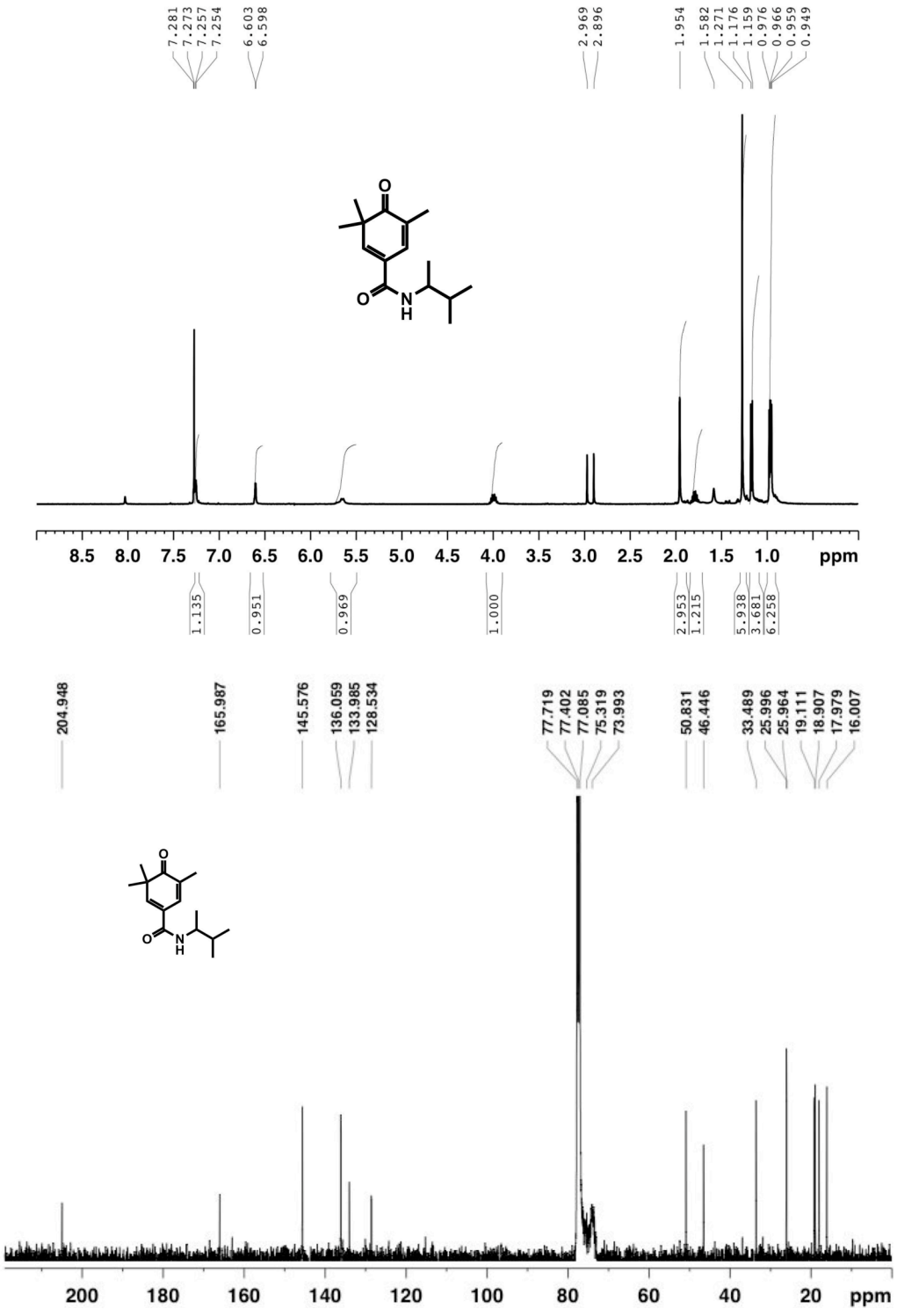

Figure ESI-7: ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz) spectra of **2**.