SUPPLEMENTARY MATERIALS

A norbornadiene-based molecular system for the storage of solar-thermal energy in aqueous solution: study of the heat-release process triggered by a Co(II)-complex

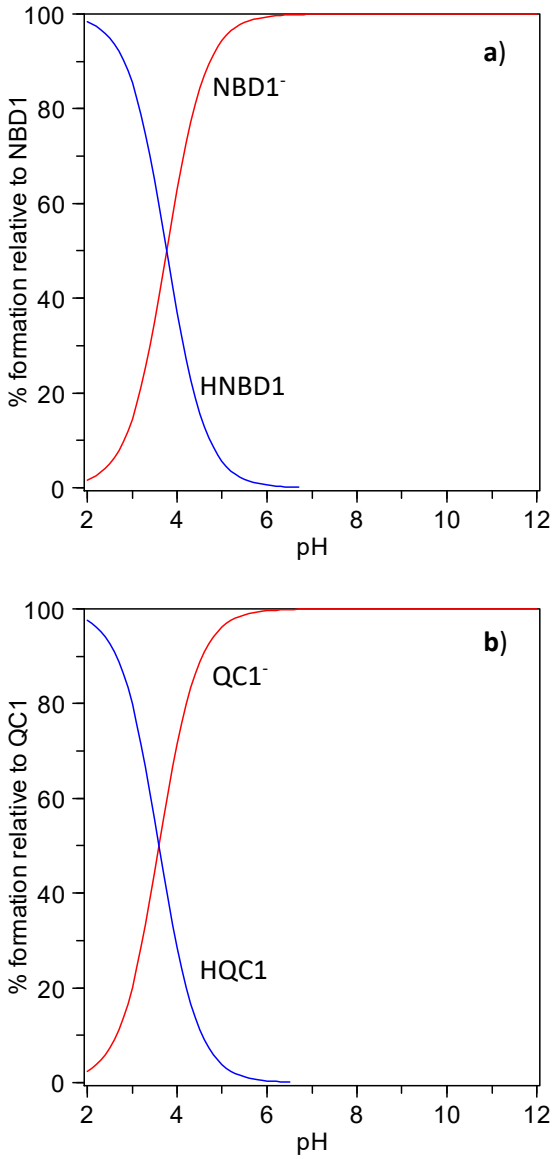
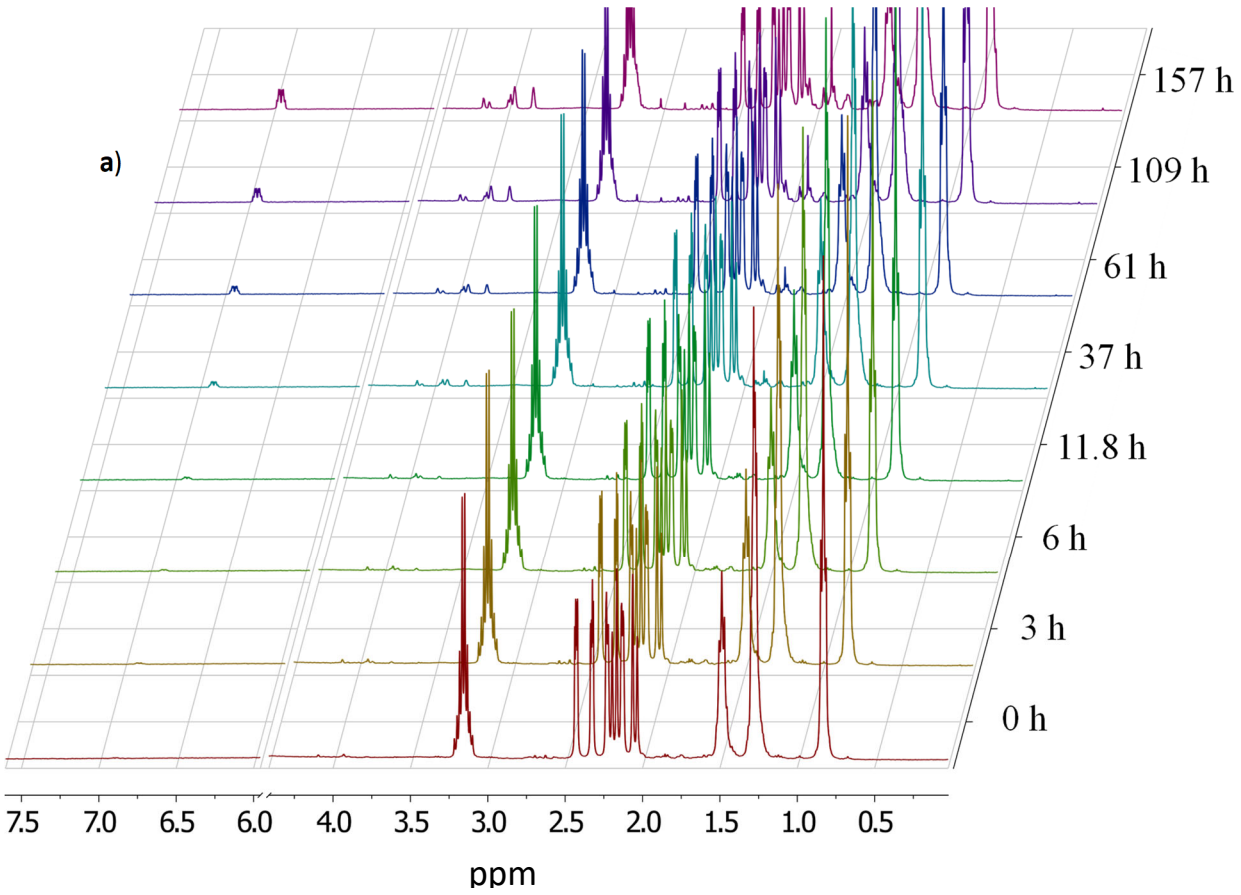


Figure S1. Distribution diagrams of the species formed by NBD1 (a) and QC1 (b) as a function of pH calculated by using the determined pK_a values.



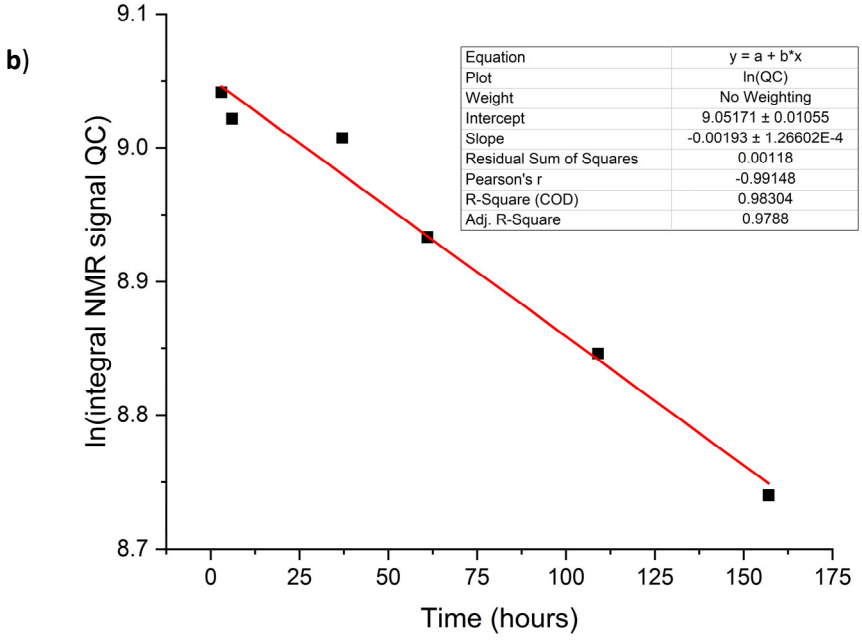


Figure S2. a) Evolution with time of the ^{1}H-NMR spectrum (D_2O, pH 11, 298 K, 400 MHz) of $QC1^-$ at 370 K. b) Logarithmic decay of the integral of the ^{1}H-NMR signal of $QD1^-$ at 2.5 ppm and corresponding fitting. Inset: Fitting details and parameters.

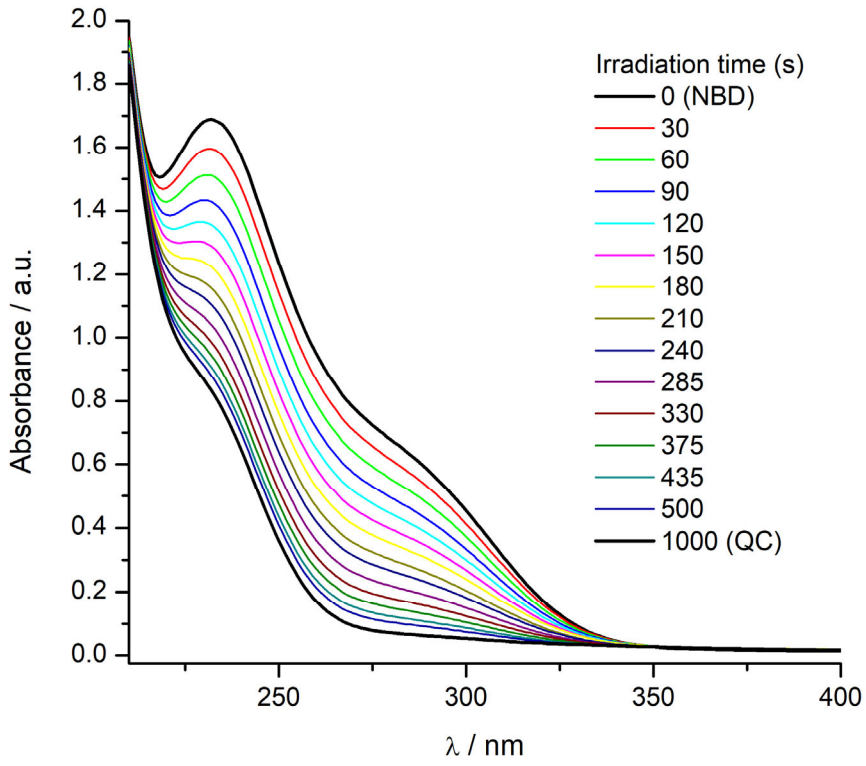


Figure S3: UV-Vis spectra measured after each irradiation time of a 1.524 mM D_2O solution of $NBD1^-$ at pH = 10.96.

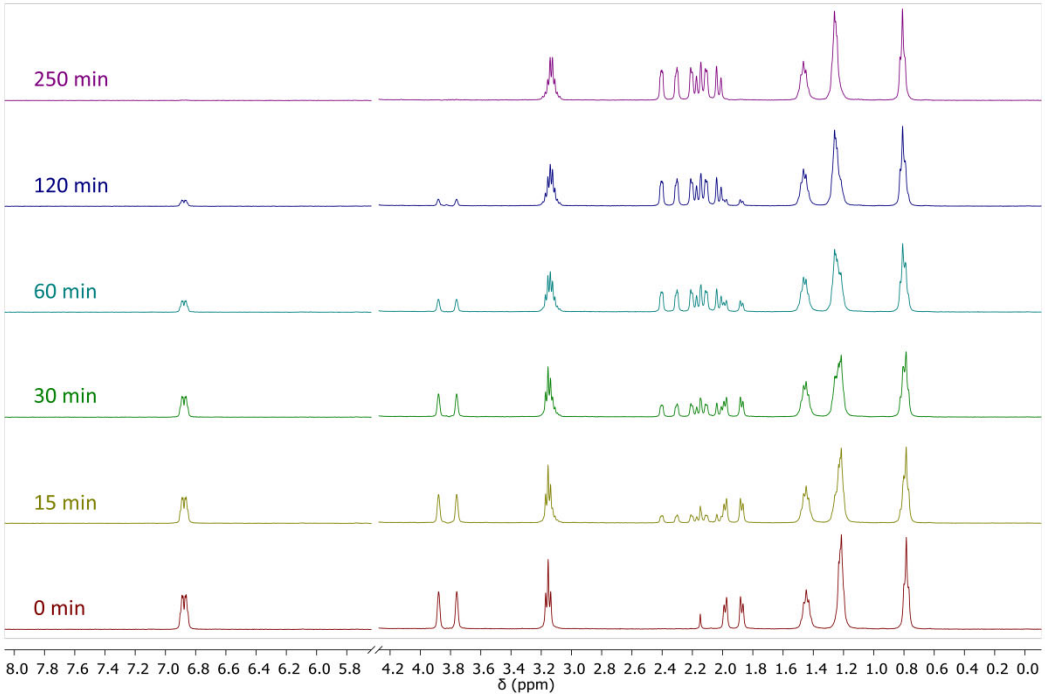


Figure S4. ^{1}H-NMR spectra measured after each irradiation period of a D_2O solution of $NBD1^-$ at pH = 10.67.

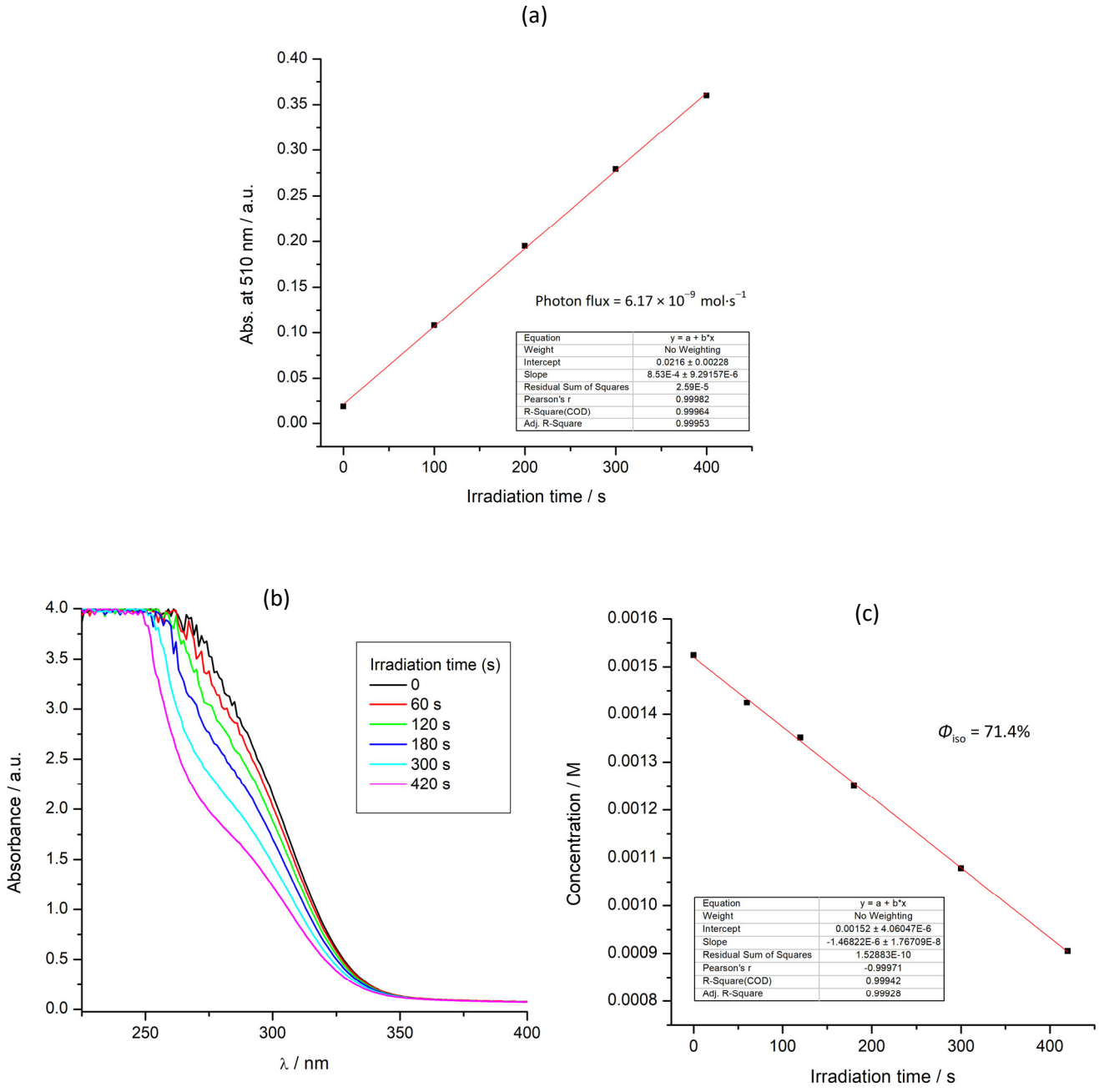


Figure S5. a) Photon flux determination of the 275 nm LED used in this work. b) UV-Vis absorption spectra recorded during the photoisomerization experiments performed for the determination of quantum yield. c) Linear fit of the concentration of NBD1$^-$ calculated using absorbance values at 300 nm. Initial concentration of NBD1$^-$ 1.524 mM, pH of 10.96.

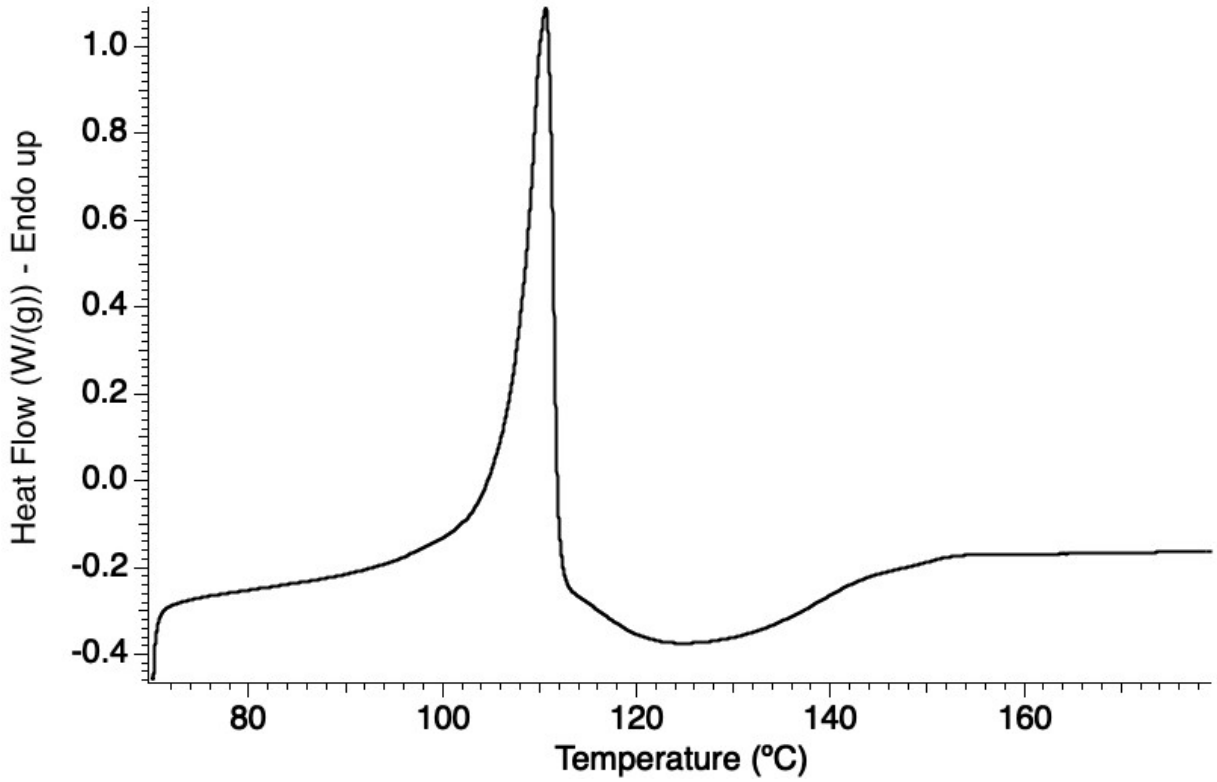


Figure S6. DSC thermograms for HNBD1. Scan rate 2 °C·min^{-1}.

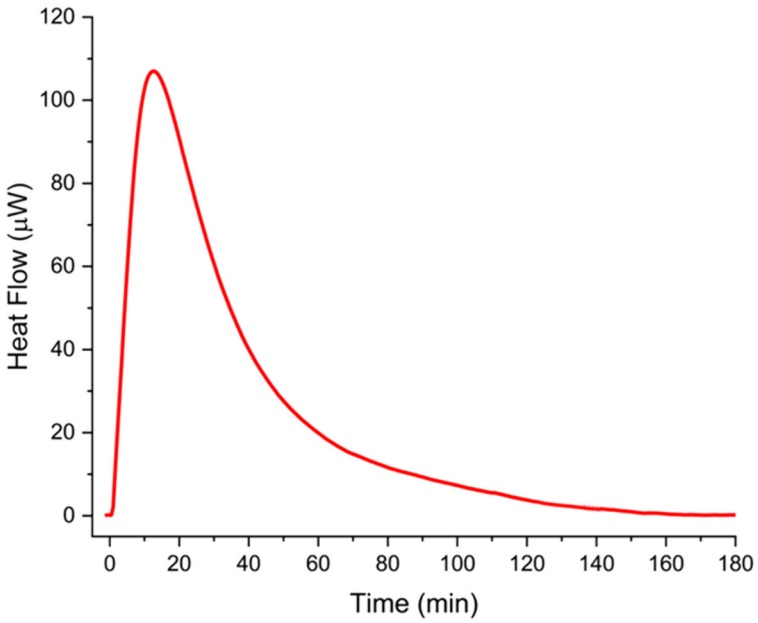


Figure S7. Example of ITC profile of the $QC1^-$ to $NBD1^-$ interconversion obtained upon addition of Co-TPPC (5% molar percentage relative to $QC1^-$) to an aqueous solution of $QC1^-$ (1.2 cm^3, 3.32 mM).

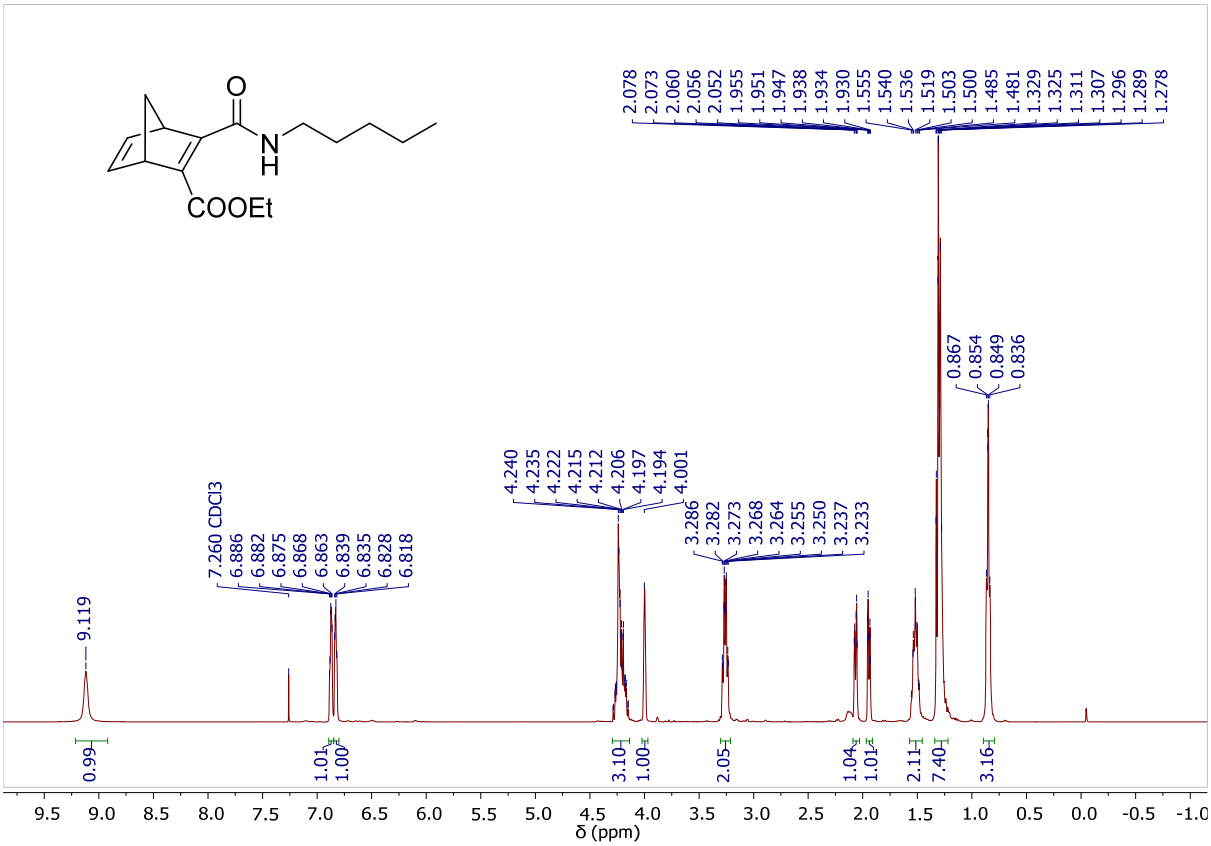


Figure S8. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of (**3**).

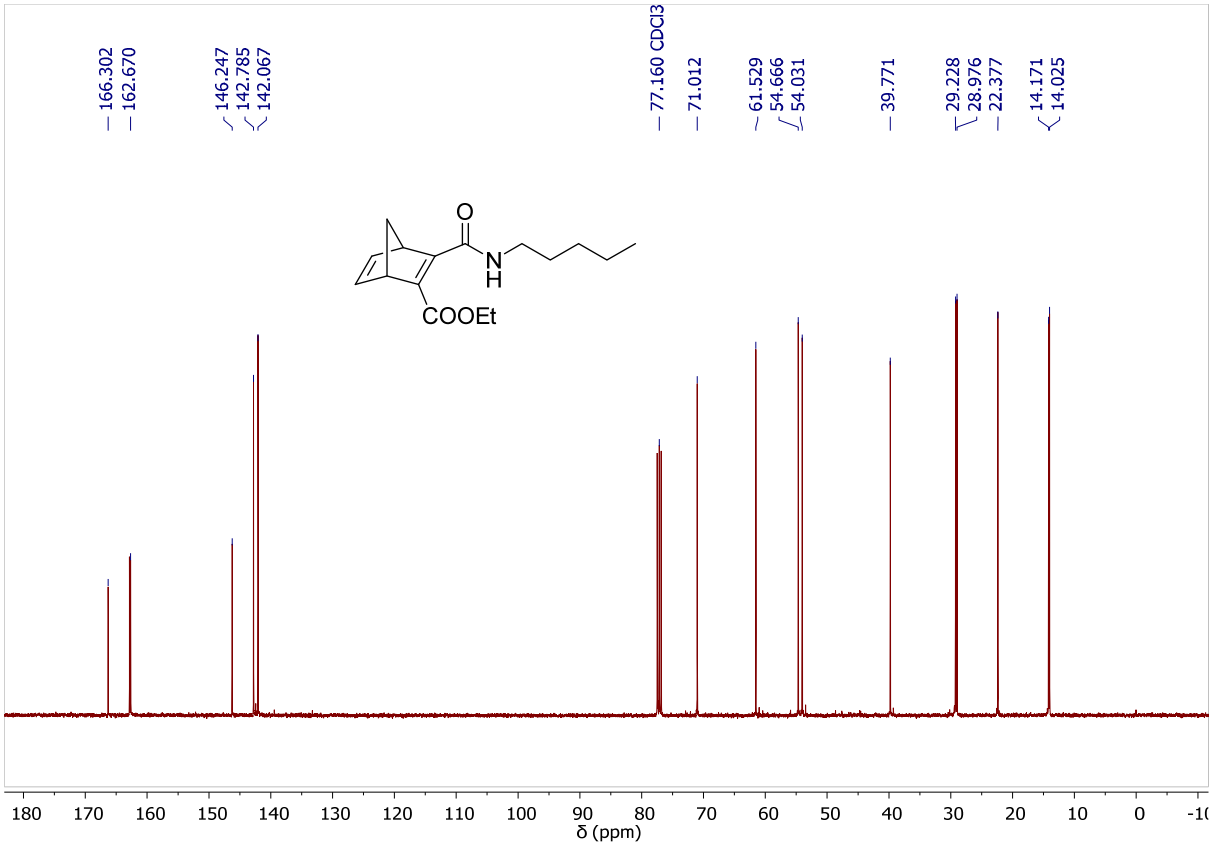


Figure S9. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$) of (**3**).

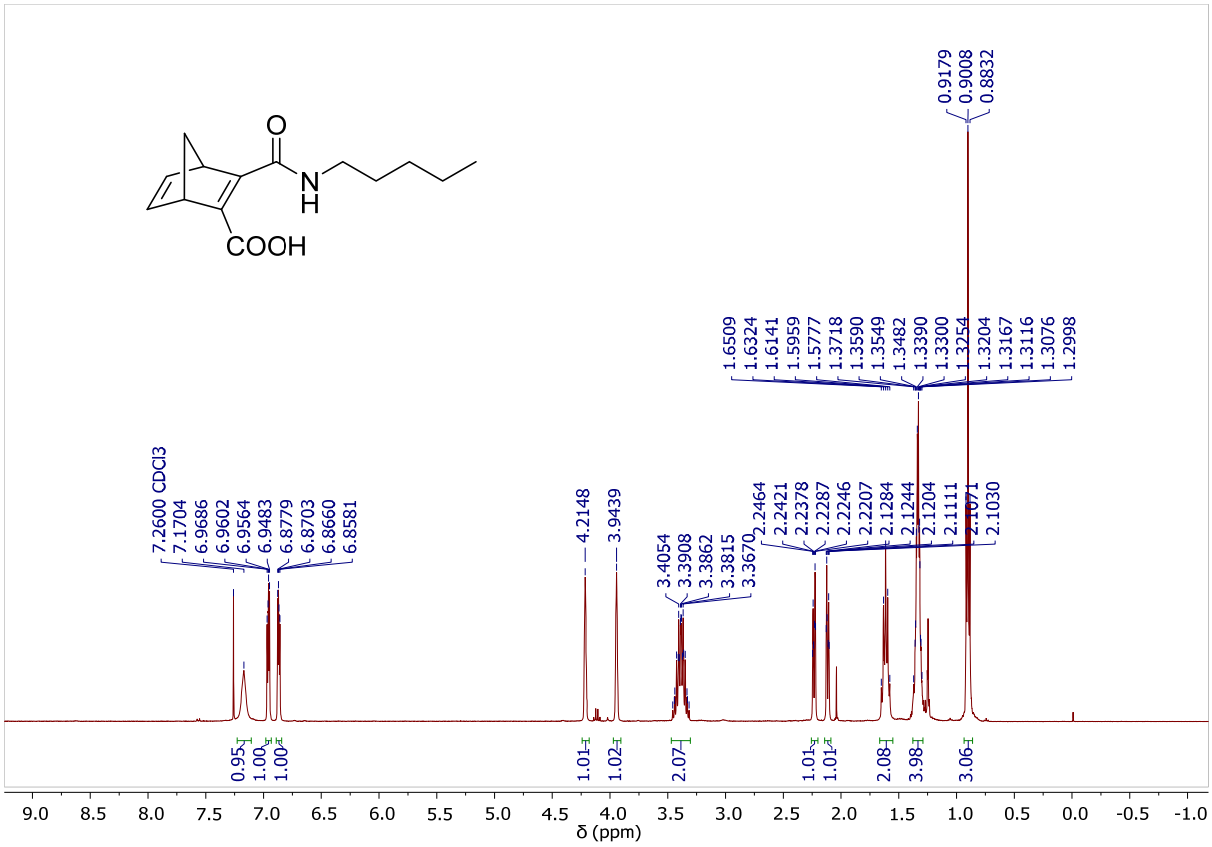


Figure S10. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of HNBD1.

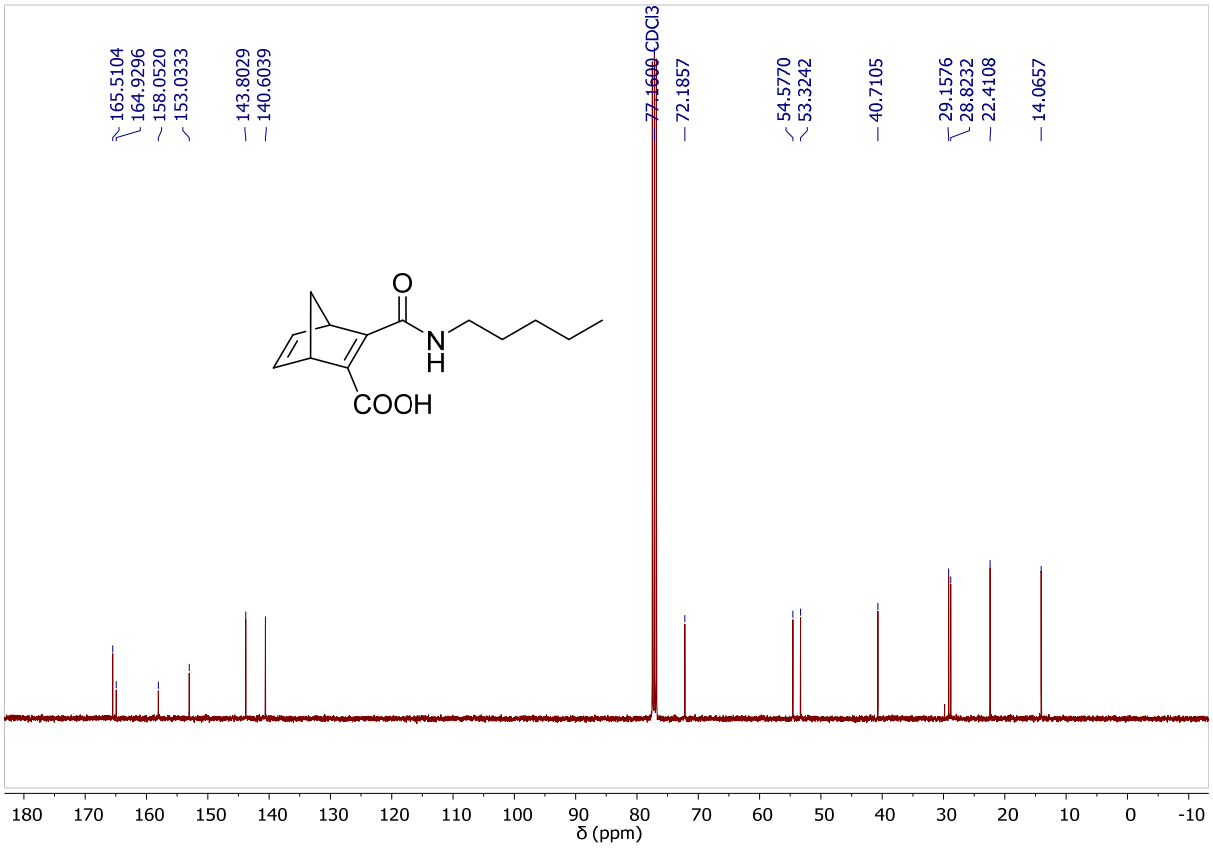


Figure S11. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$) of HNBD1.

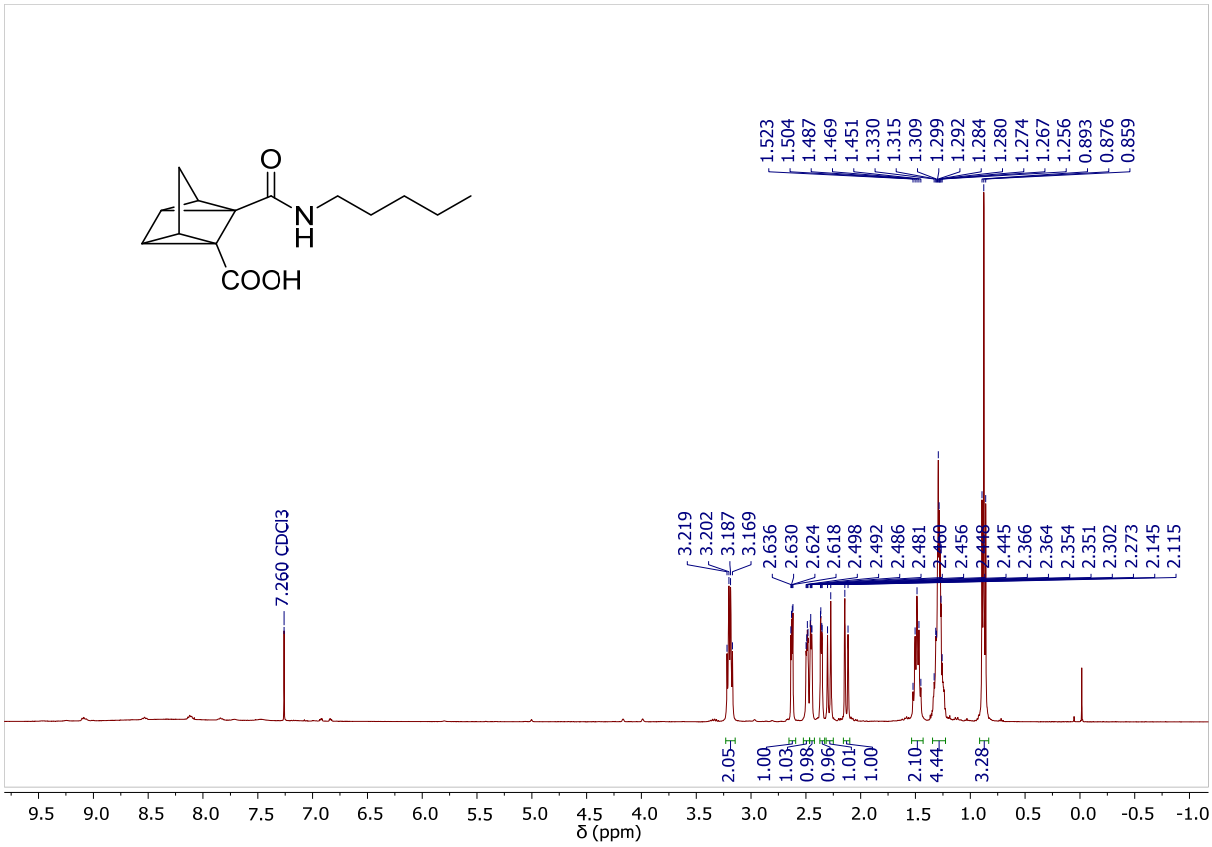


Figure S12. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of HQC1.

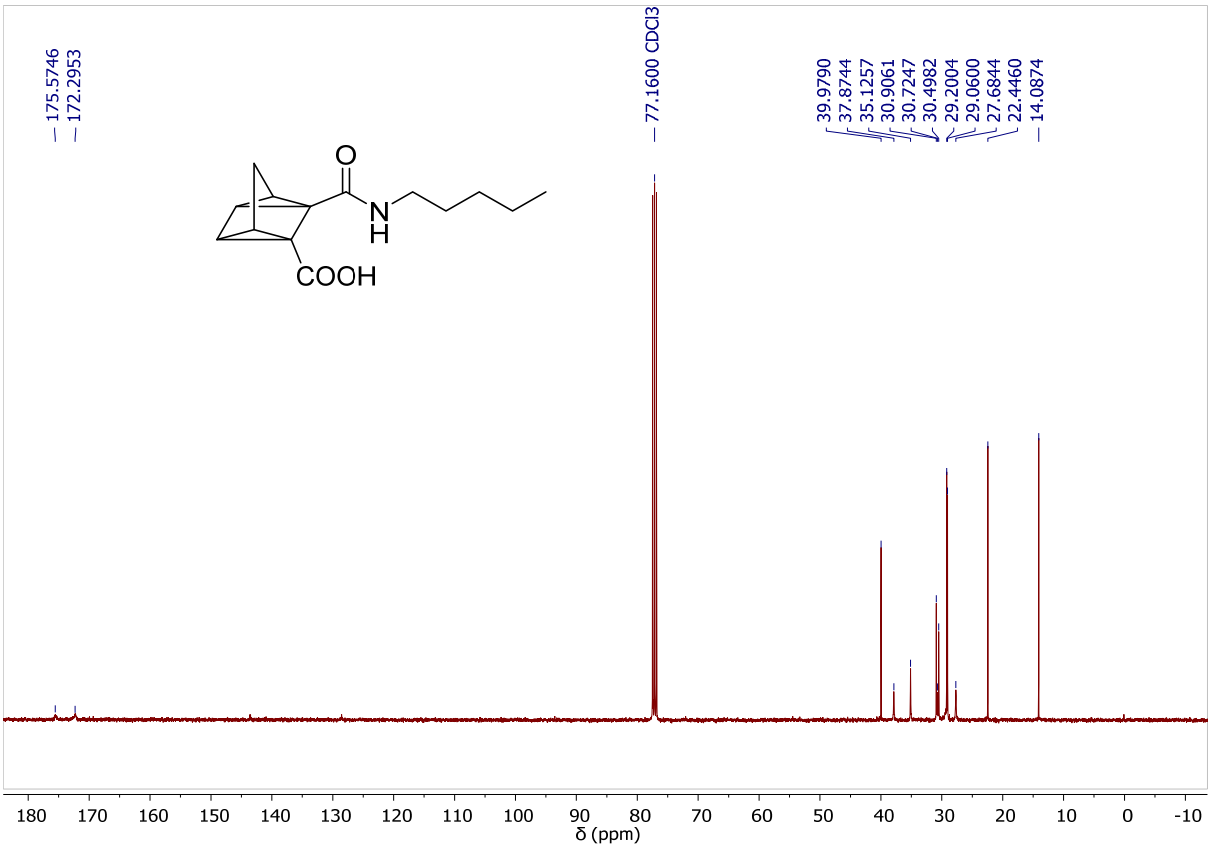


Figure S13. ^{13}C-NMR spectrum (100 MHz, $CDCl_3$) of HQC1.