Preparation and characterization of persistent maltose-conjugated triphenylmethyl radicals

Juan Antonio Mesa,[†] Amado Velázquez-Palenzuela,[‡] Enric Brillas,[‡] Josep Coll,[†] Josep Lluís Torres,[†] Luis Juliá[†*]

[†]*Departament de Química Biològica i Modelització Molecular, Institut de Química Avançada de Catalunya (CSIC), Jordi Girona 18-26, 08034 Barcelona, Spain.*
[‡]*Departament de Química Física, Universitat de Barcelona, Martí i Franquès 1-11, 08028 Barcelona, Spain.*

SUPPLEMENTARY MATERIAL

Table of contents **page**

Bis(2,4,6-trichlorophenyl){2,6-dichloro-4-[2,3,4,6-tetra-*O*-acetyl-α-D-glucopyranosyl-(1→4)-2,3,6-tri-*O*-acetyl-β-D-glucopyranosyloxy]phenyl}methyl radical (1)

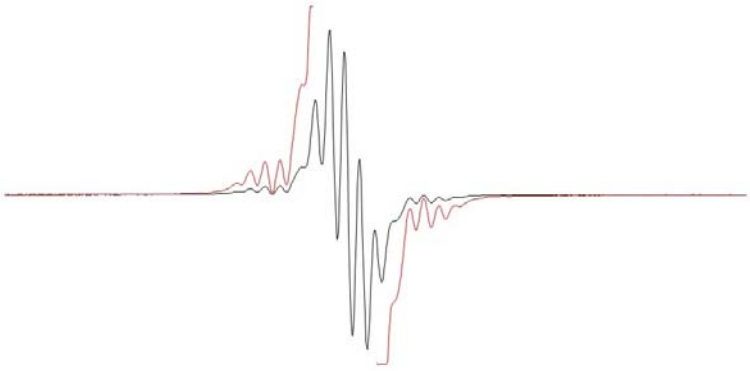

Figure S1. Experimental EPR of radical **1** in CH_2Cl_2 at 180 K. The red lines are y-axis expanded spectra.

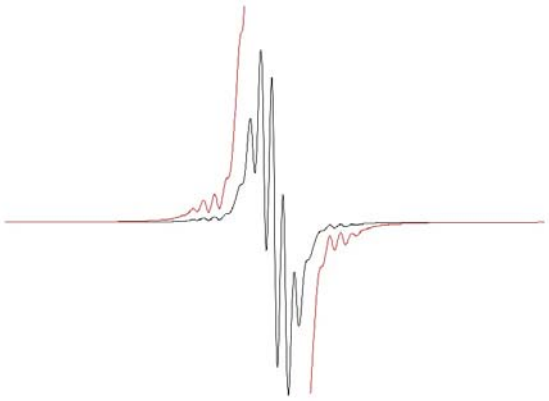

Figure S2. Simulated EPR of radical **1** in CH_2Cl_2 at 180 K. The red lines are y-axis expanded spectra.

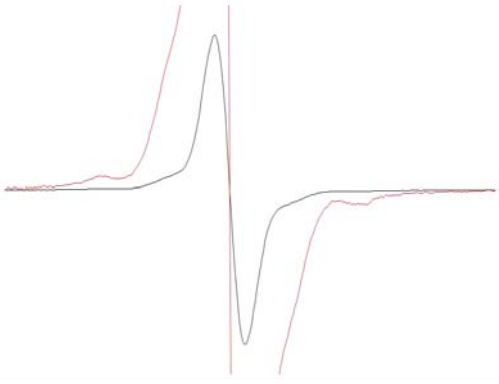

Figure S3. Experimental EPR of radical **1** in CH_2Cl_2 at room temperature. The red lines are y-axis expanded spectra.

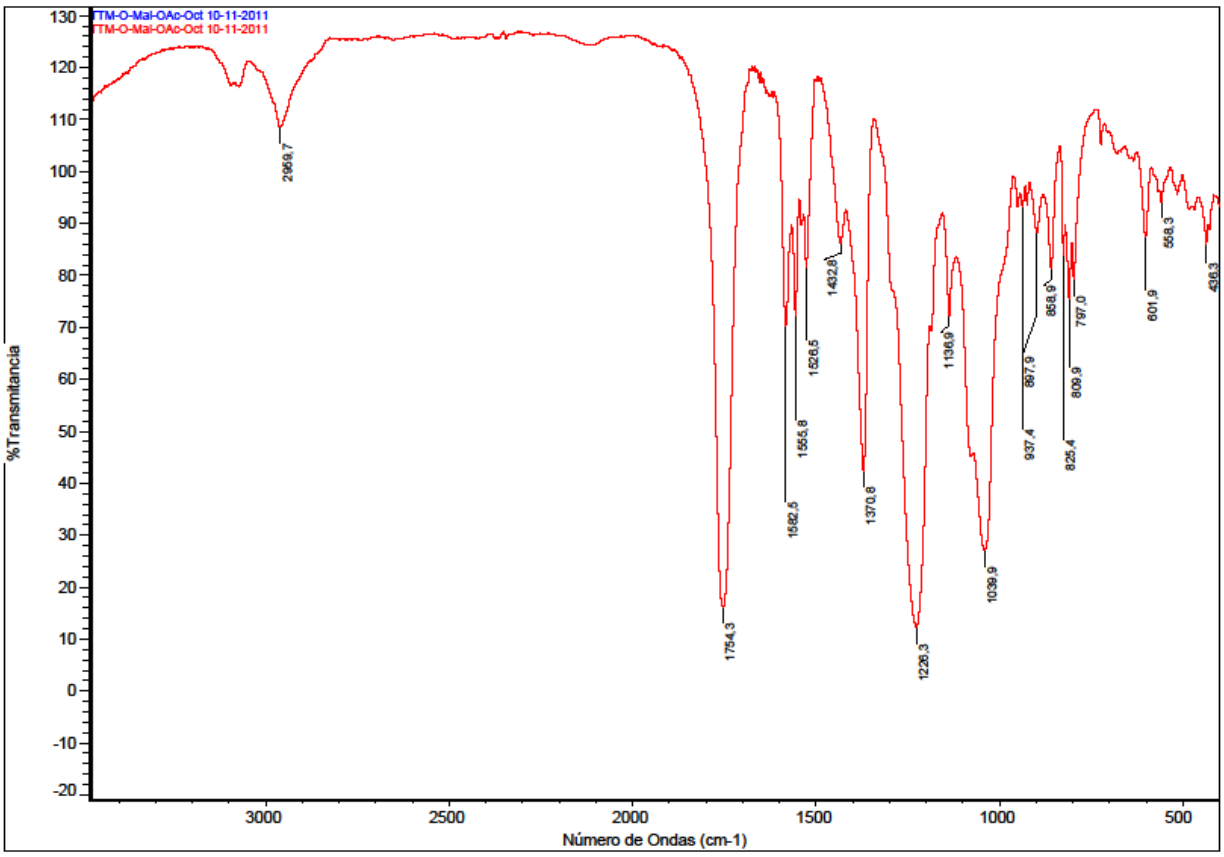

Figure S4. Infrared spectrum of r**adical 1**

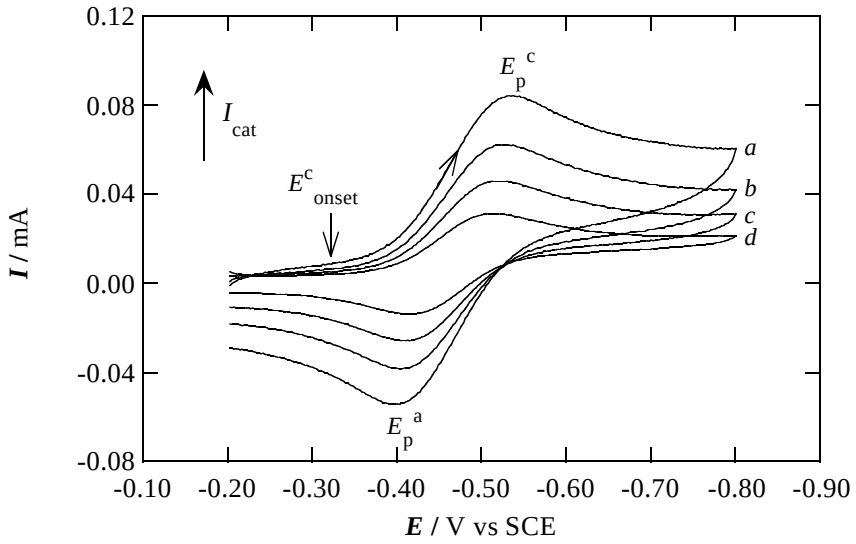

Figure S5. Cyclic voltammograms obtained for the reduction of radical **1 (**10^{-3} M) in THF/water 10:1 (v/v) with TBPA (0.1 M) on a Pt electrode at 25 ºC under N_2 atmosphere. Initial and final potential: -0.20 V, reversal potential: -0.80 V. Scan rate: (a) 200, (b) 100, (c) 50 y (d) 20 mV s^{-1}.

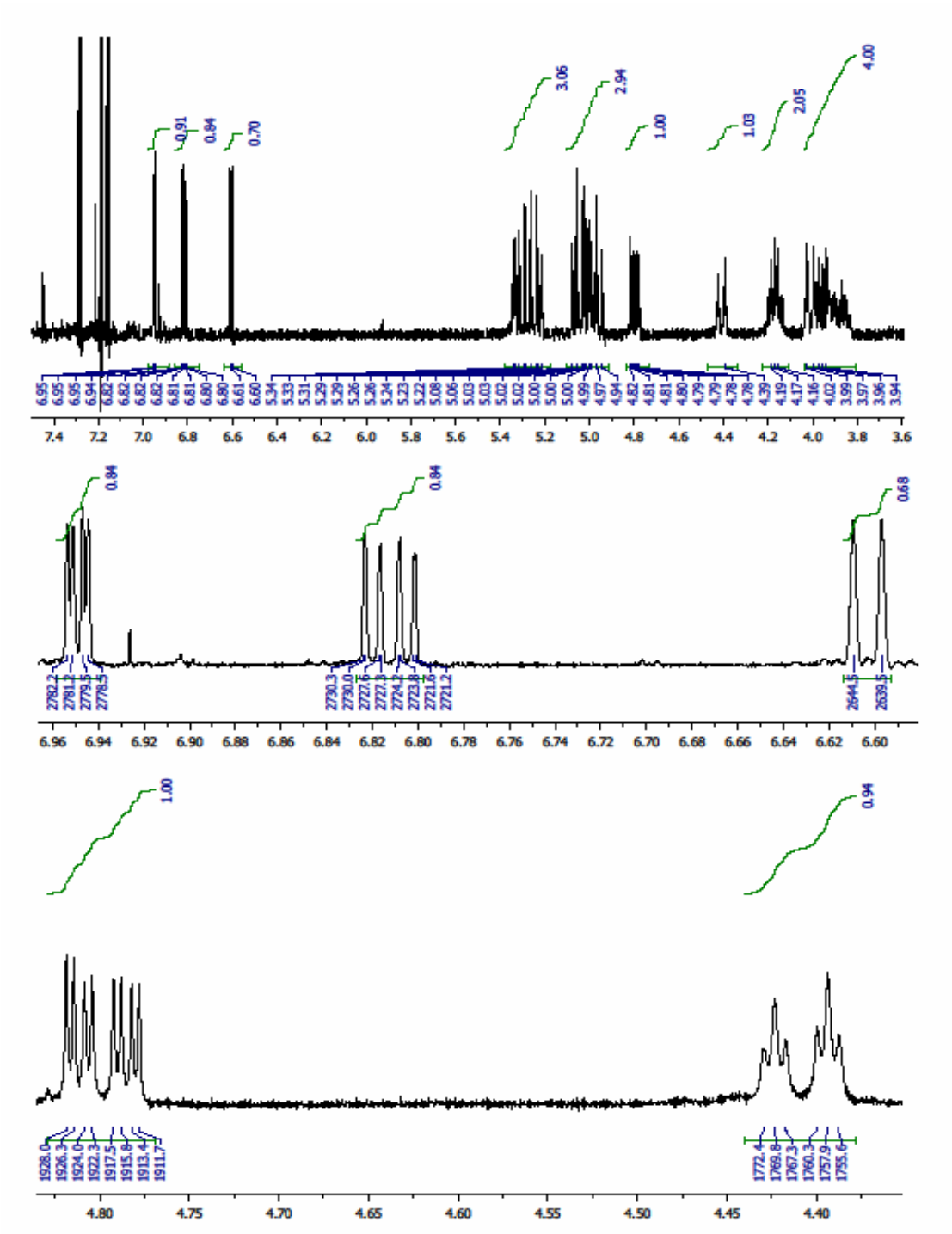

Figure S6. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum and expansions of the same of compound **1H**

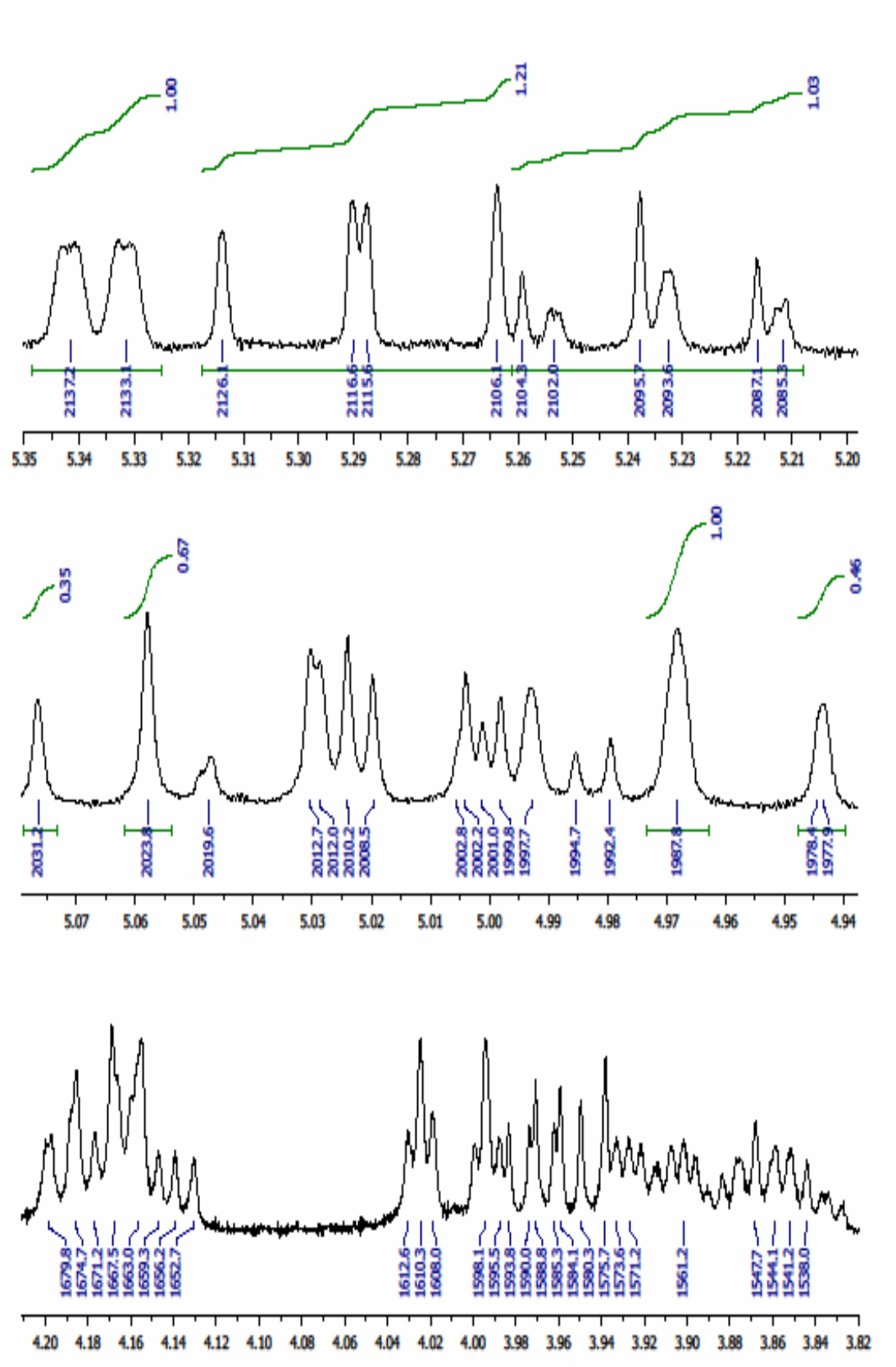

Figure S7. Expansions of the ^{1}H NMR ($CDCl_3$, 400 MHz) of compound **1H**

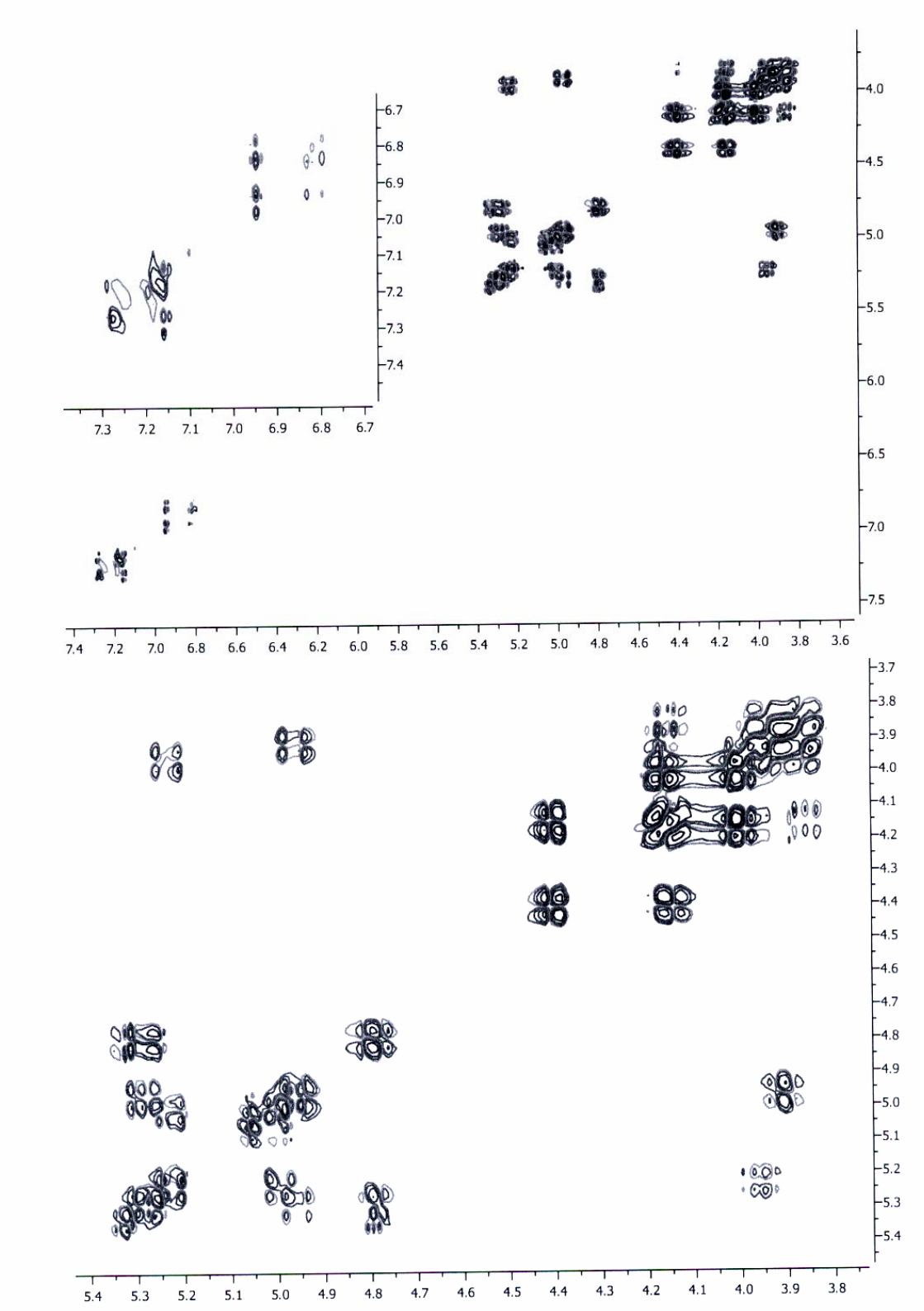

Figure S8. Details of the DQ-COSY NMR ($CDCl_3$, 400 MHz) spectrum of **1H**

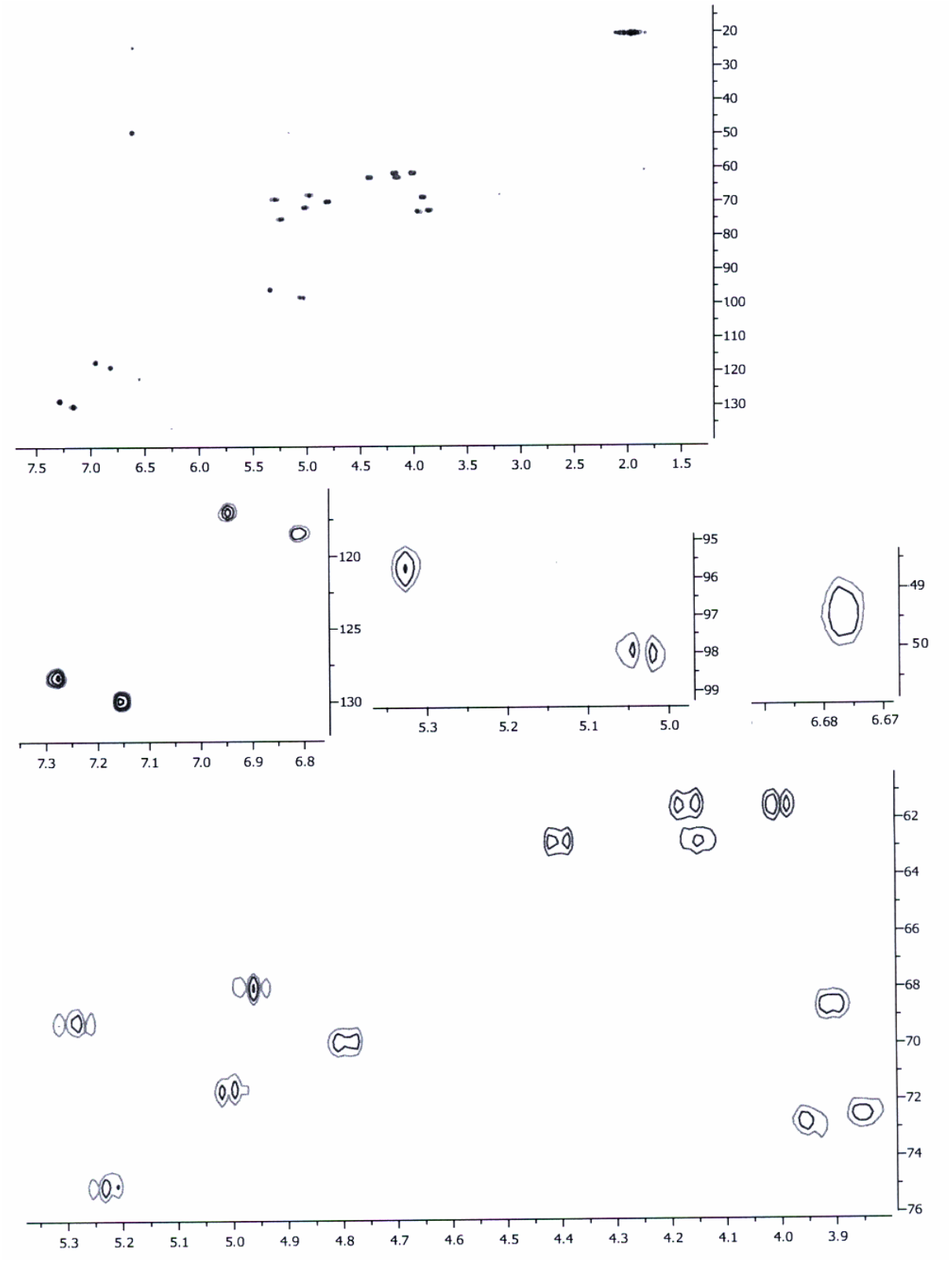

Figure S9. Details of the HSQC NMR ($CDCl_3$, 400 MHz) spectrum of **1H**

Bis(2,3,4,5,6-pentachlorophenyl){2,3,5,6-tetrachloro-4-[2,3,4,6-tetra-*O*-acetyl-α-D-glucopyranosyl-(1→4)-2,3,6-tri-*O*-acetyl-β-D-glucopyranosyloxy]phenyl}methyl radical (2)

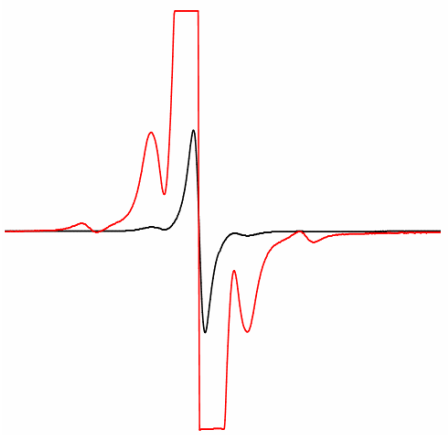

Figure S10. Experimental EPR of radical **2** in CH_2Cl_2 at room temperature. The red lines are y-axis expanded spectra.

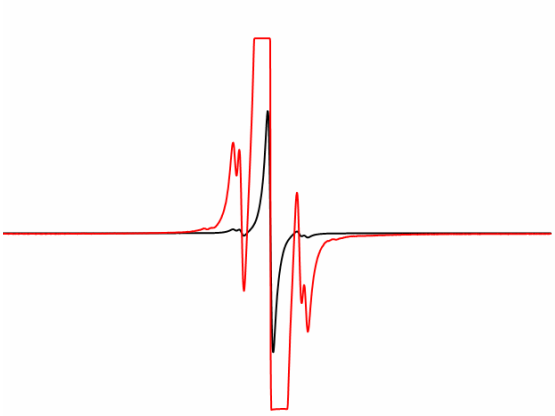

Figure S11. Experimental EPR of radical **2** in CH_2Cl_2 at 193 K. The red lines are y-axis expanded spectra.

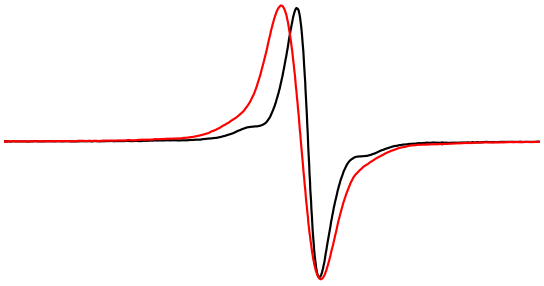

Figure S12. Experimental EPR of radical **1** (black) (g = 2.0025 ± 0.0001) and **2** (red) (g = 2.0030 ± 0.0001) in EtOH solution (~ 10^{-3} M) at room temperature

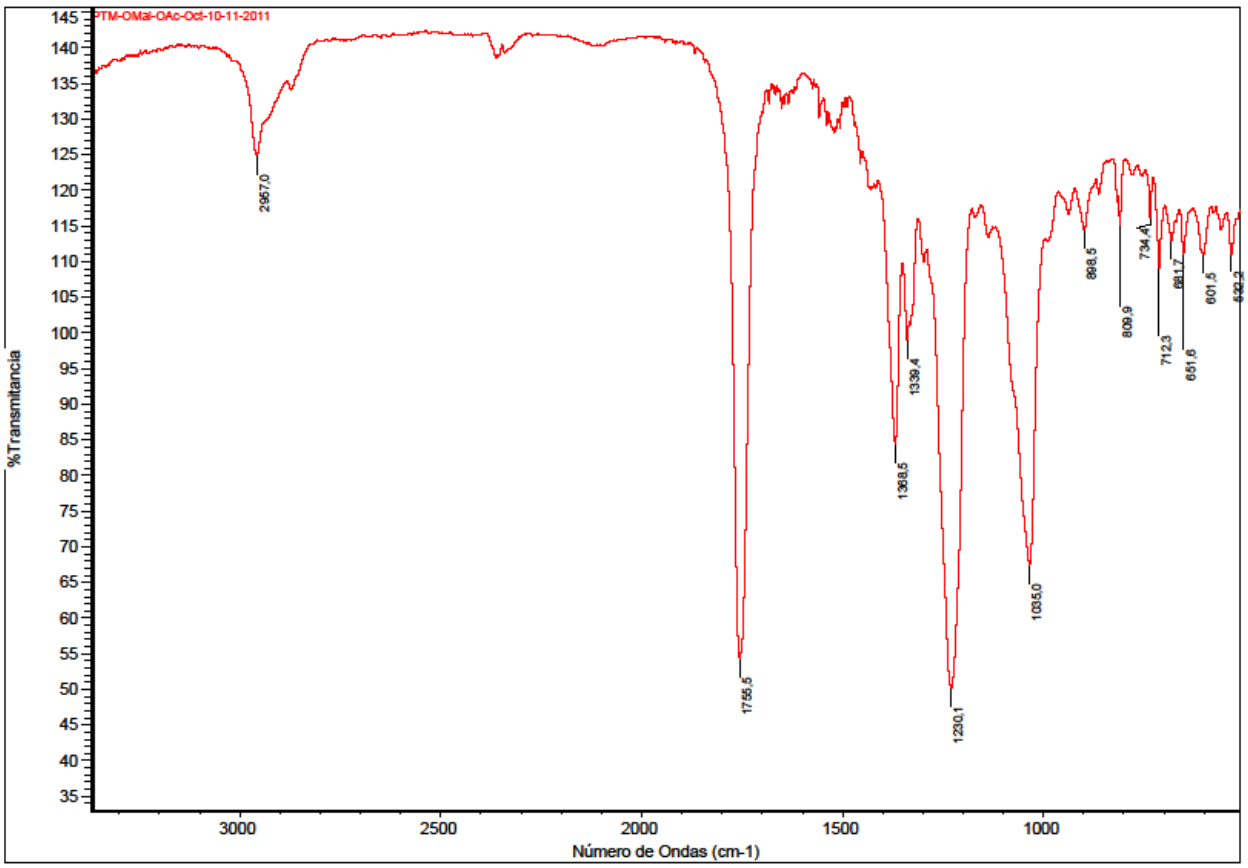

Figure S13. Infrared spectrum of r**adical 2**

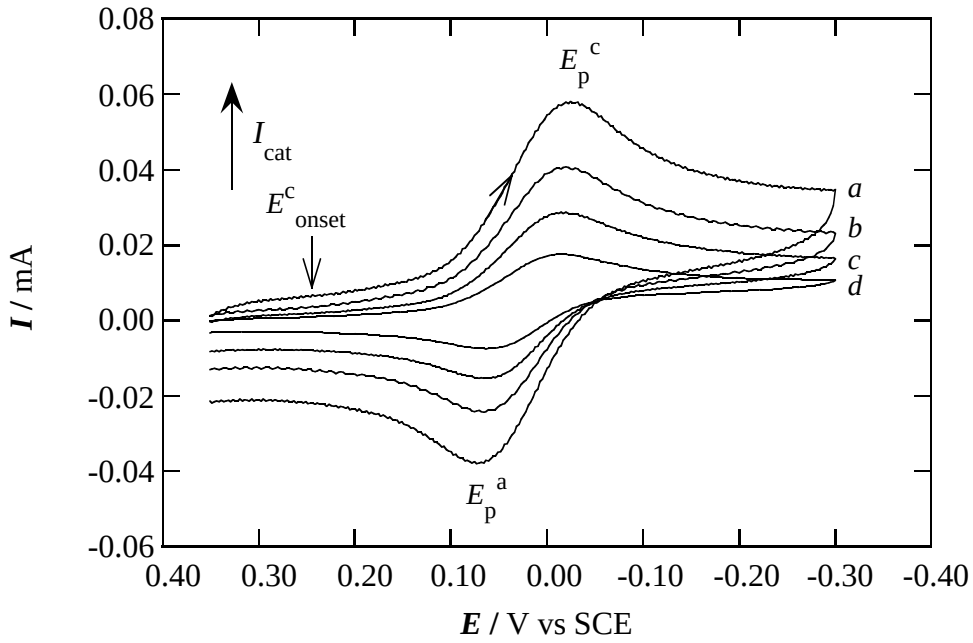

Figure S14. Cyclic voltammograms obtained for the reduction of radical **2 (**10^{-3} M) in THF/water 10:1 (v/v) with TBPA (0.1 M) on a Pt electrode at 25 ºC under N_2 atmosphere. Initial and final potential: 0.35 V, reversal potential: -0.30 V. Scan rate: (a) 200, (b) 100, (c) 50 y (d) 20 mV s^{-1}.

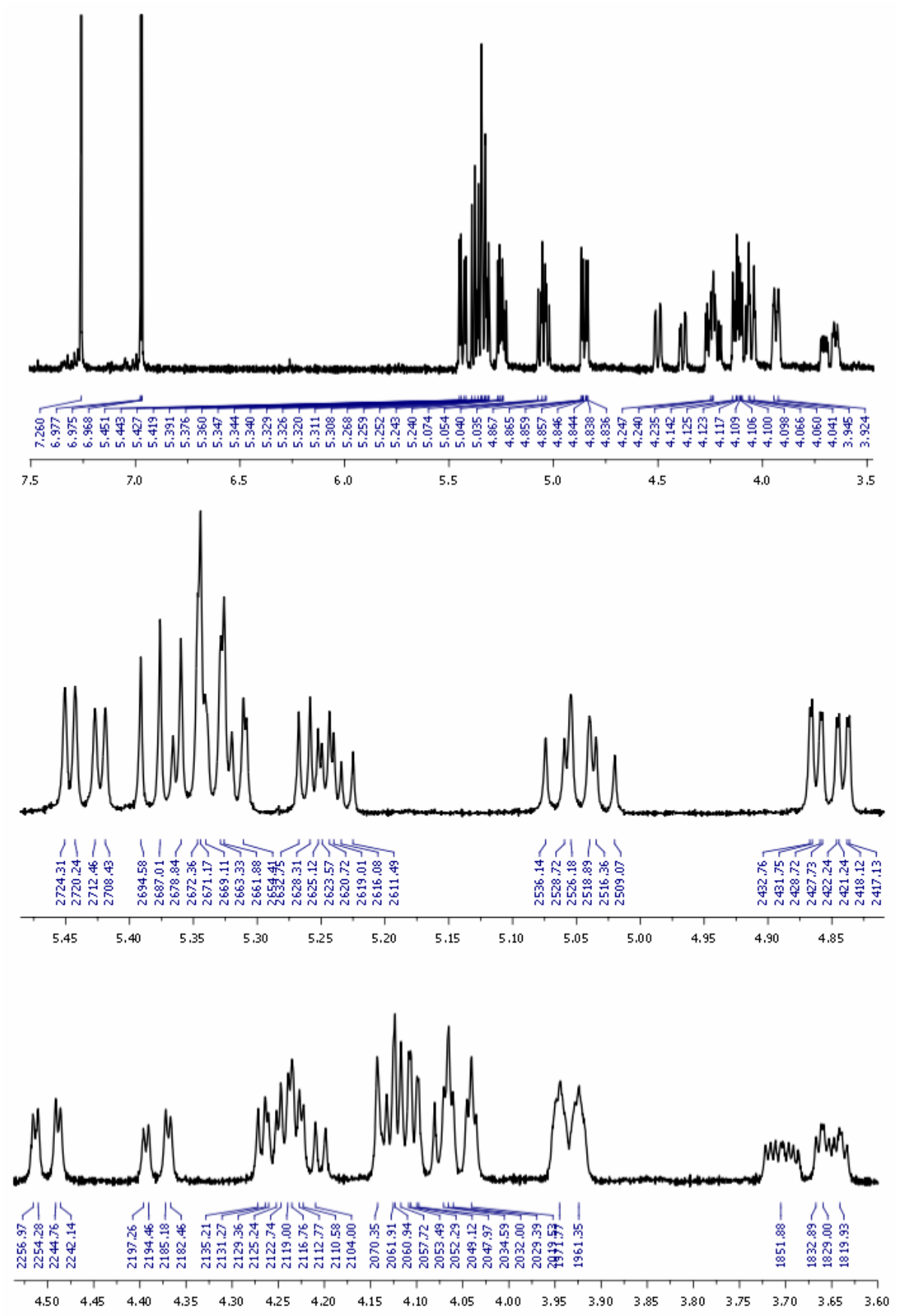

Figure S15. ^{1}H NMR spectrum and expansions ($CDCl_3$, 400 MHz) of compound **2H**

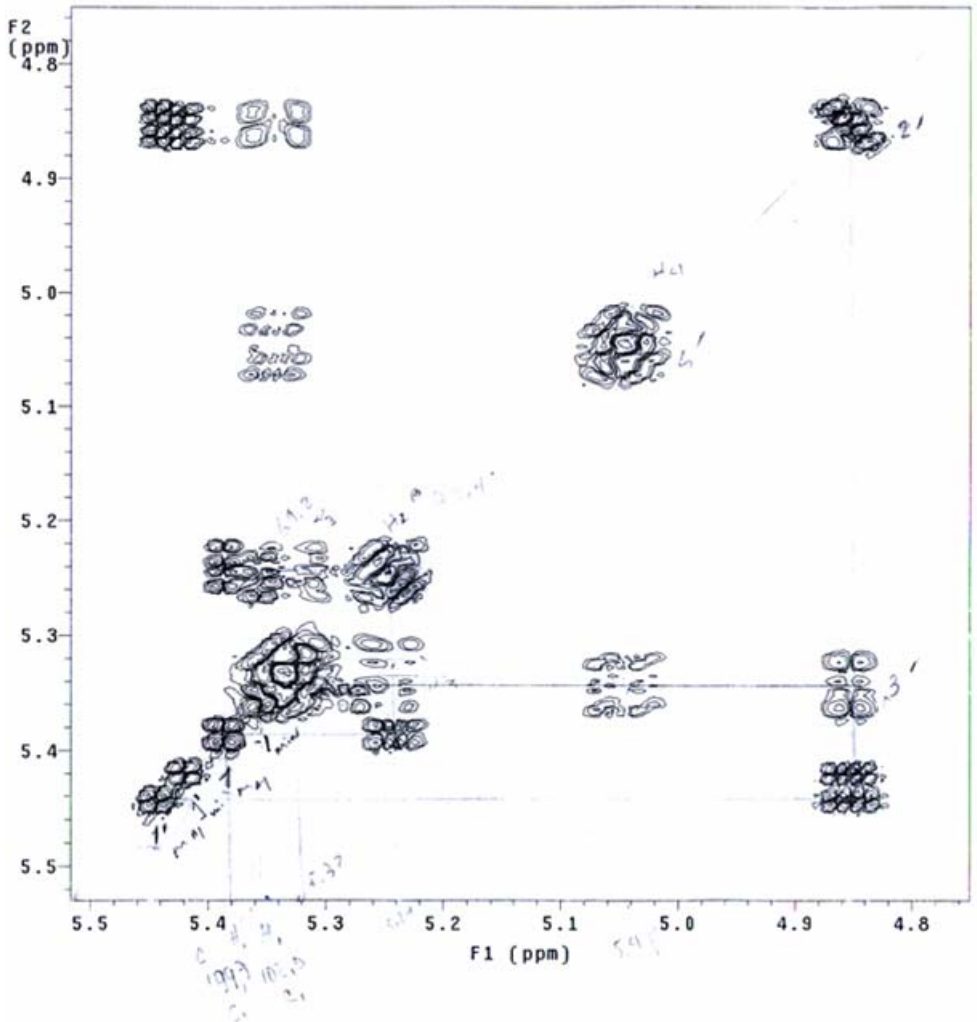

Figure S16. Details of the DQ-COSY NMR ($CDCl_3$, 400 MHz) spectrum of **2H**

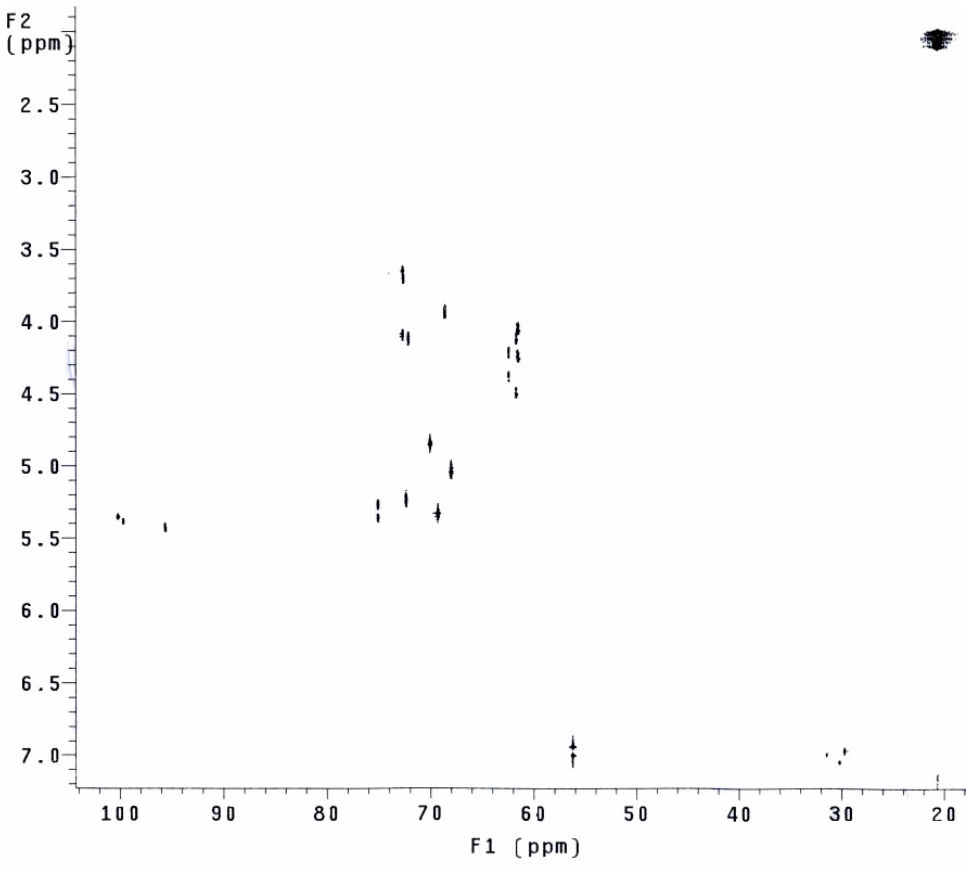

Figure S17. HSQC ($CDCl_3$, 400 MHz) spectrum of **2H**

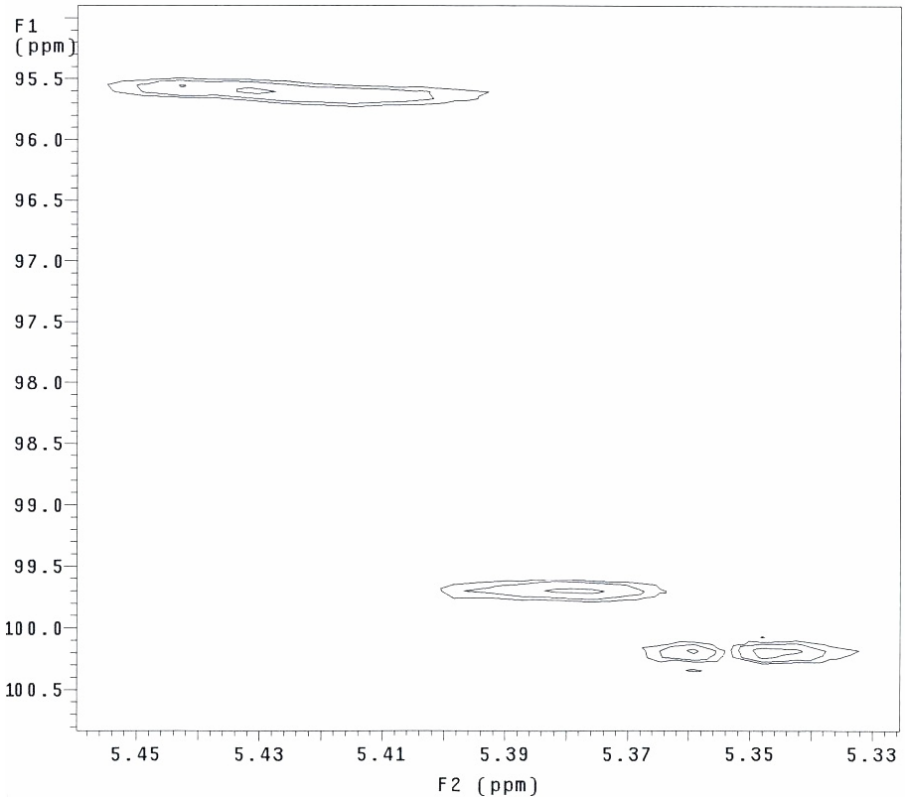

Figure S18. Details of the HSQC NMR ($CDCl_3$, 400 MHz) spectrum of **2H**

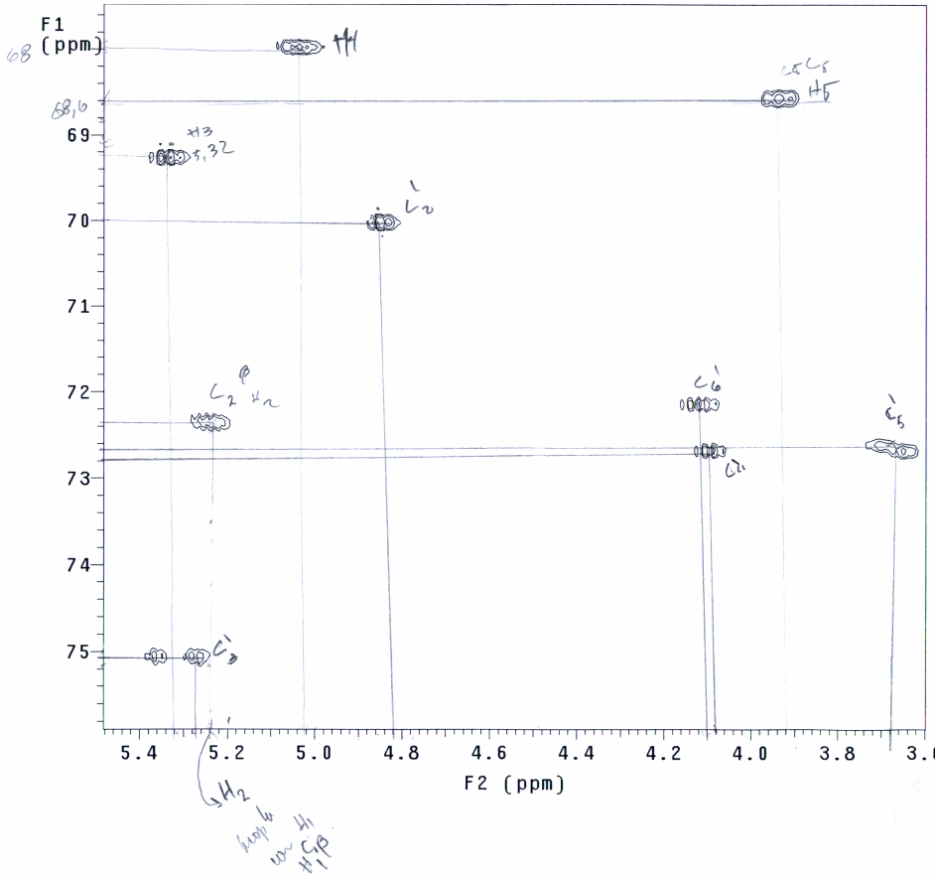

Figure S19. Details of the HSQC NMR ($CDCl_3$, 400 MHz) spectrum of **2H**

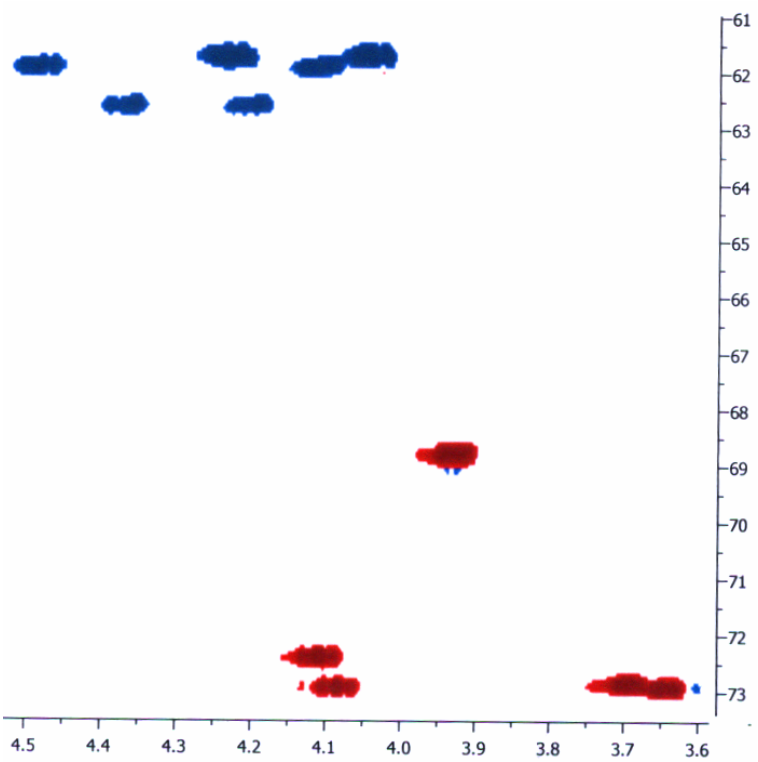

Figure S20. Details of the HSQC NMR ($CDCl_3$, 400 MHz) spectrum of **2H**

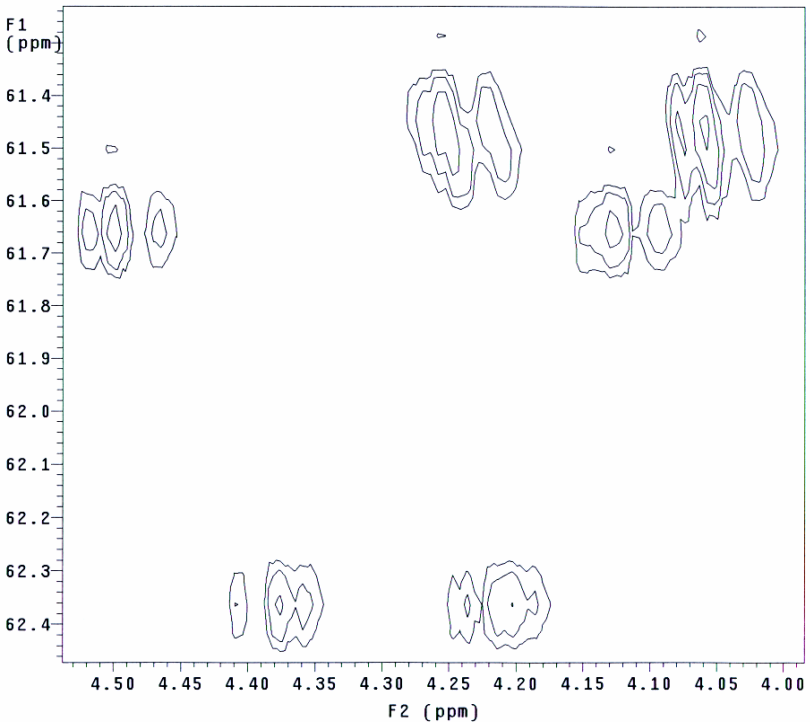

Figure S21. Details of the HSQC NMR ($CDCl_3$, 400 MHz) spectrum of **2H**

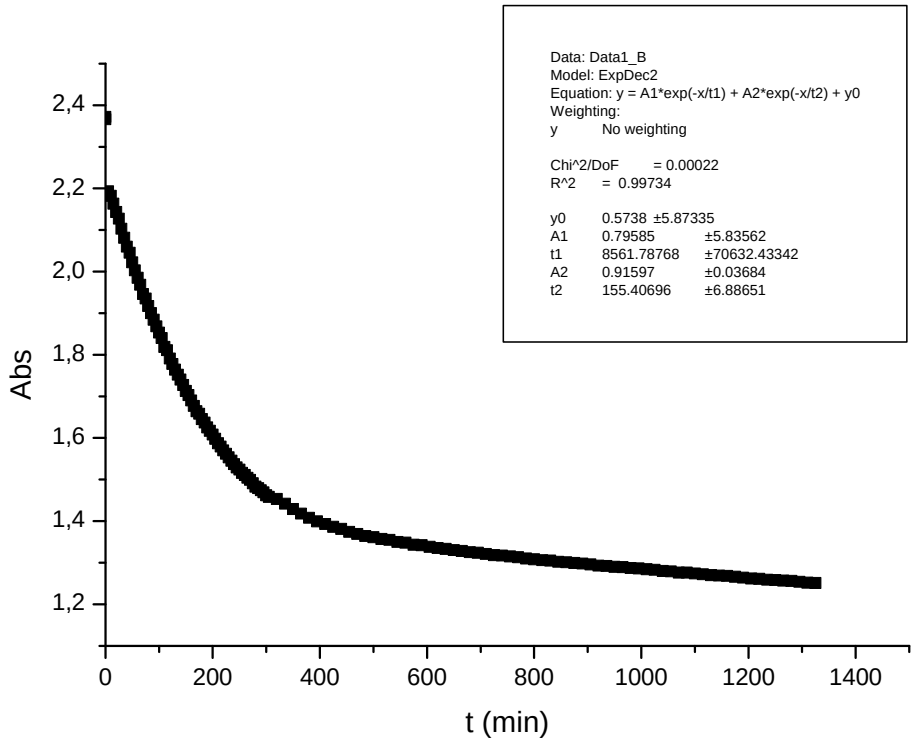

Figure S22. Decay of the UV absorbance (384 nm) of 2 (86 µM) solution in THF/H2O 10:1 v/v (rt) following addition of ascorbic acid (19 µM)

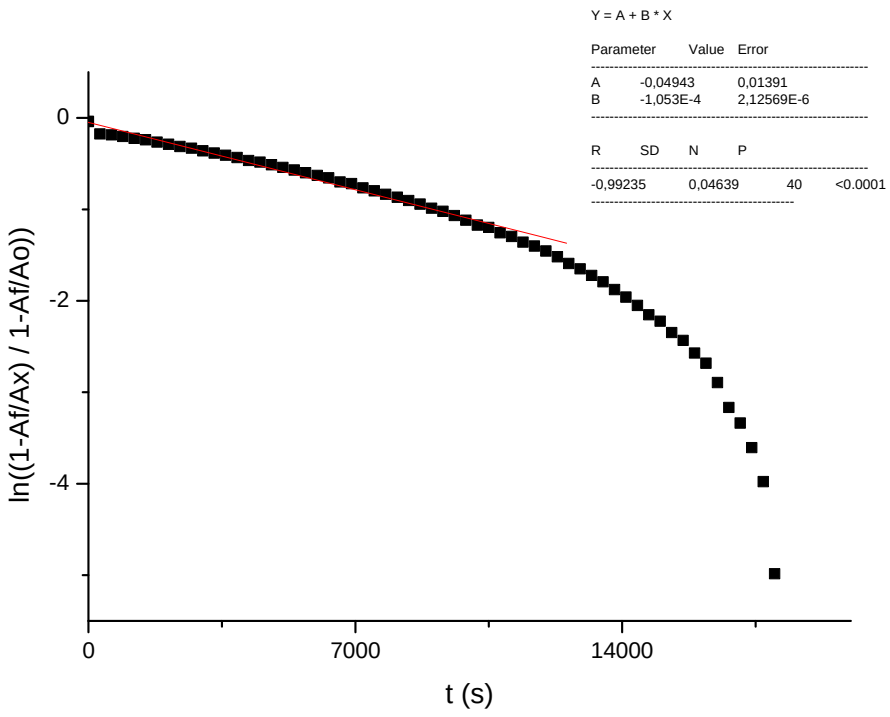

Figure S23. Estimation of the rate constant (k_1) using equation 2 in the manuscript.