Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

Dual Emission of a Bis(Pyrene)-Functionalized, Perbenzylated β-Cyclodextrin

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Table of Contents

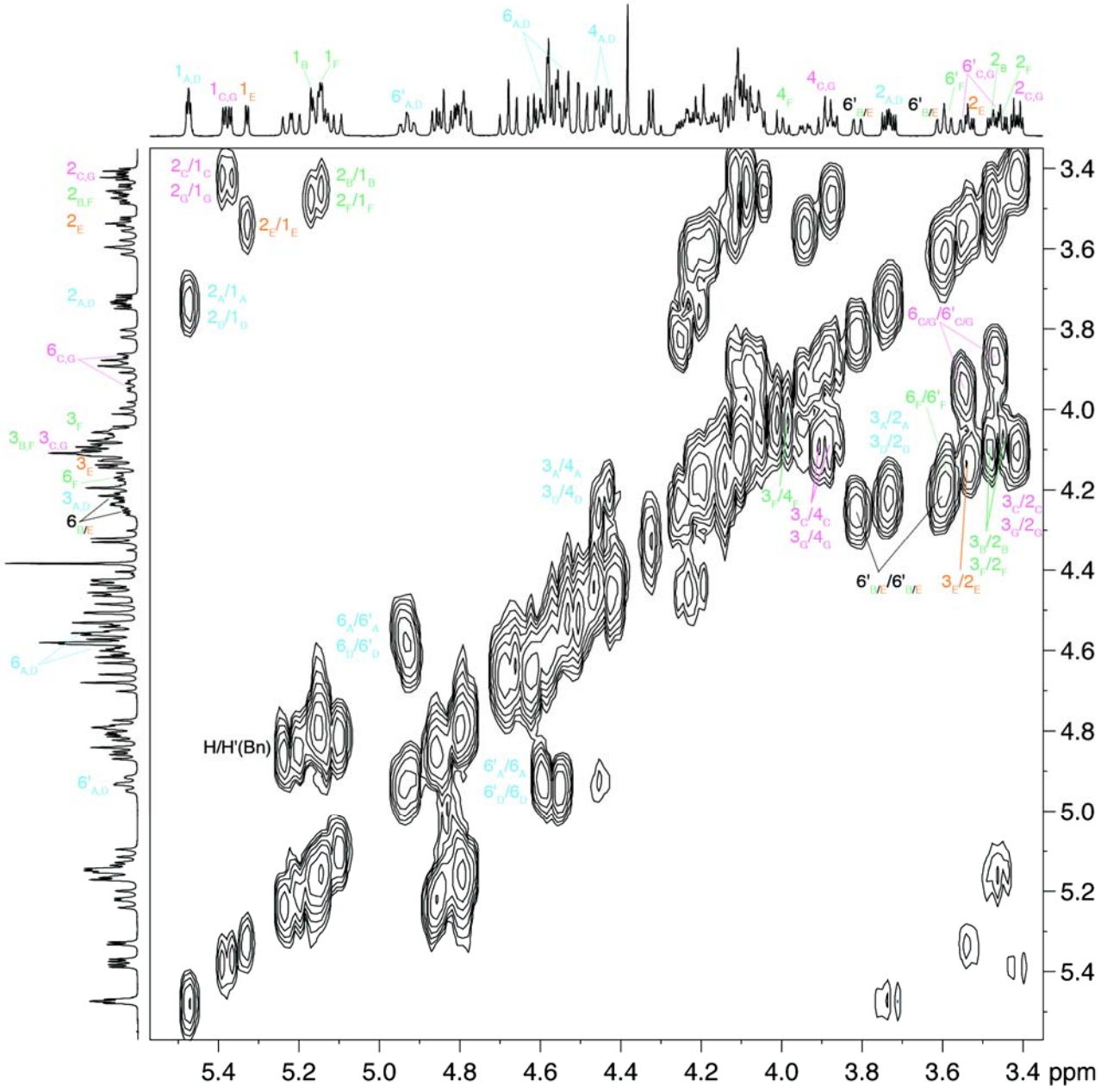


Figure S 1: Detail (aliphatic region) of the $^{1}H/^{1}H$ COSY map of **1** (600 MHz, d^{6}-acetone).

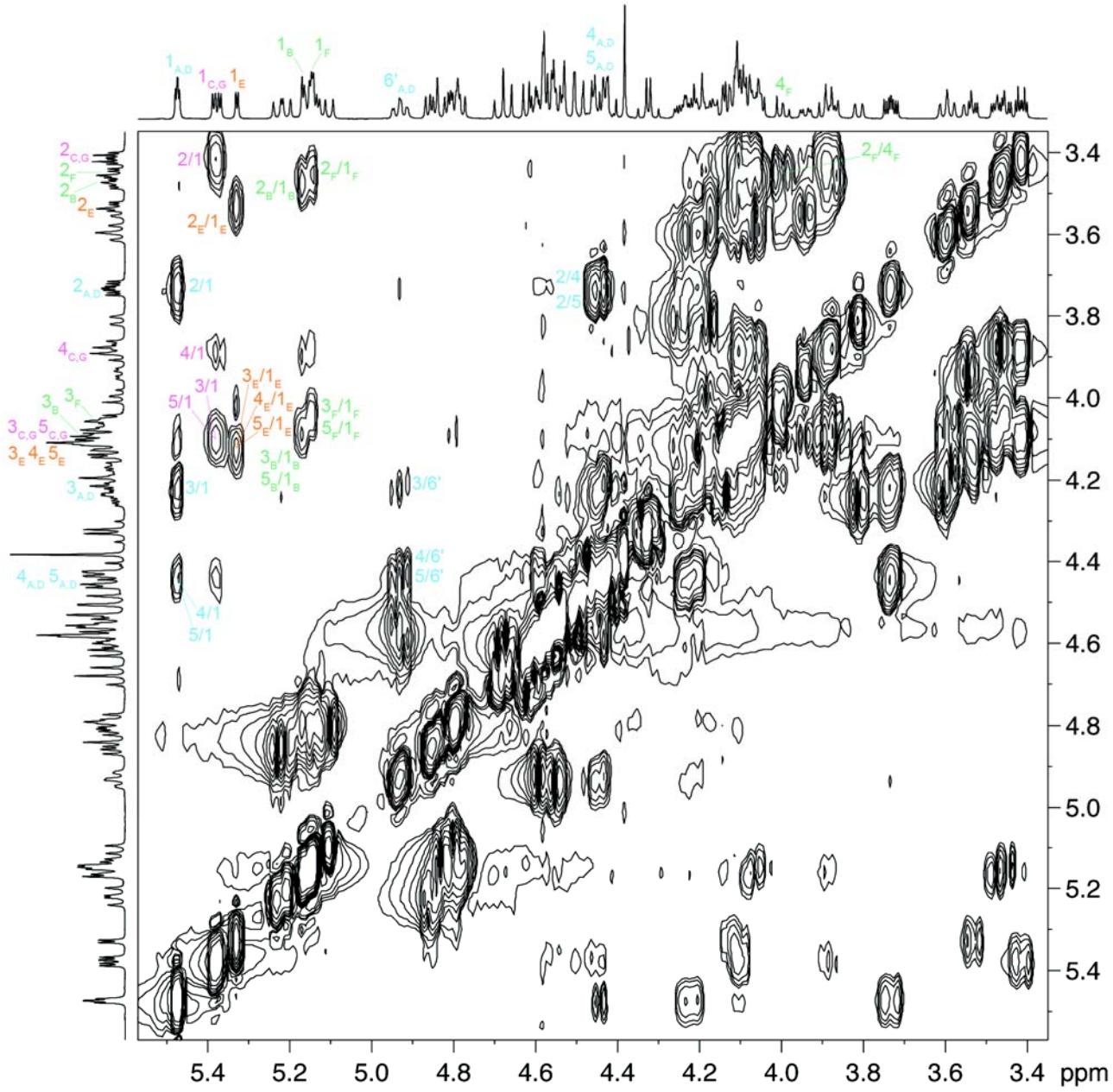


Figure S 2: Detail (aliphatic region) of the TOCSY map of **1** (600 MHz, d^6-acetone).

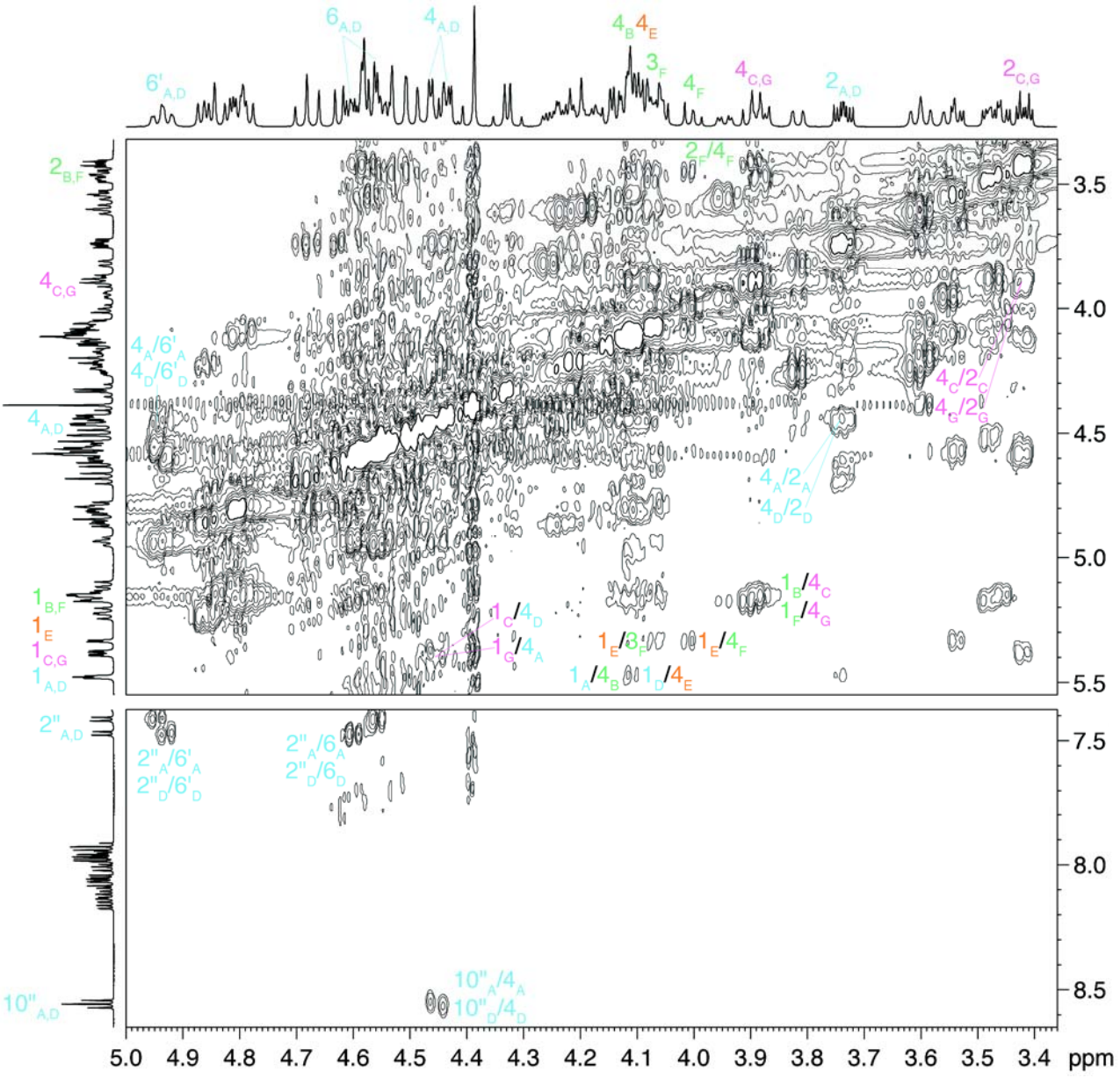


Figure S 3: Selected regions of the $^{1}H/^{1}H$ ROESY map of **1** (600 MHz, d^{6}-acetone, mixing time: 300 ms).

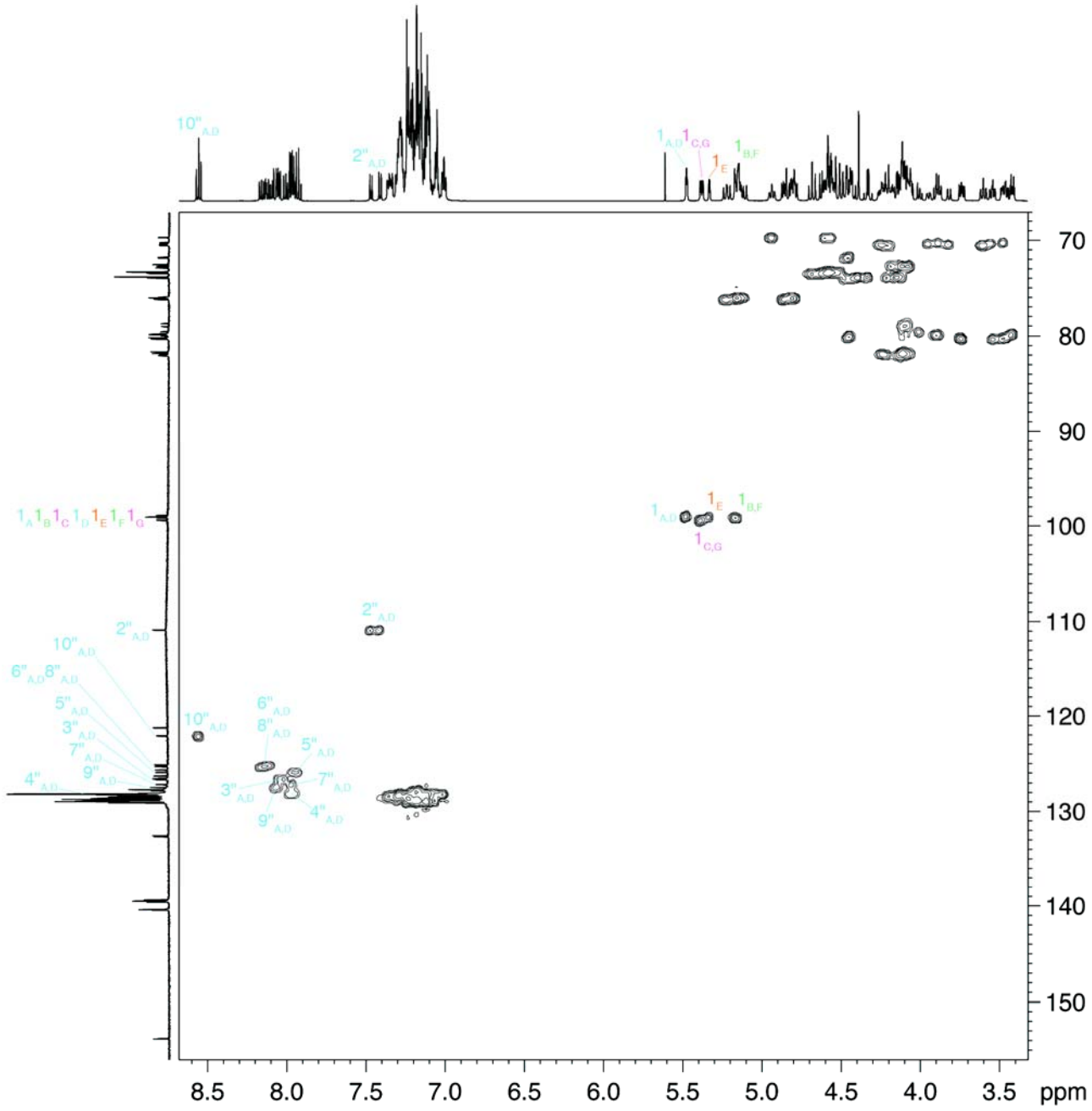


Figure S 4: $^{13}C/^{1}H$ HSQC map of **1** (600 MHz, d^6-acetone).

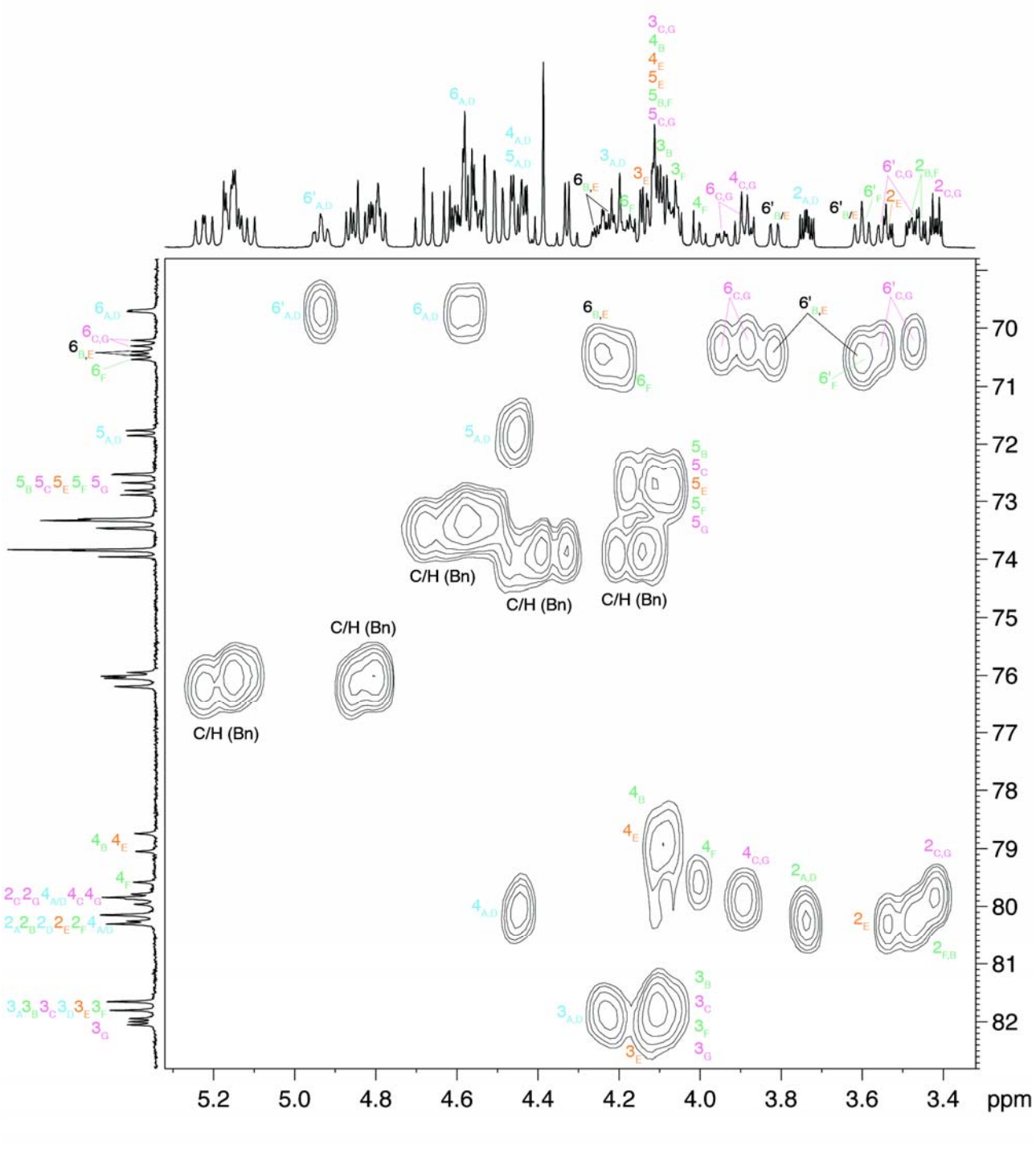


Figure S 5: Detail (aliphatic region) of the $^{13}C/^{1}H$ HSQC map of **1** (600 MHz, d^6-acetone).

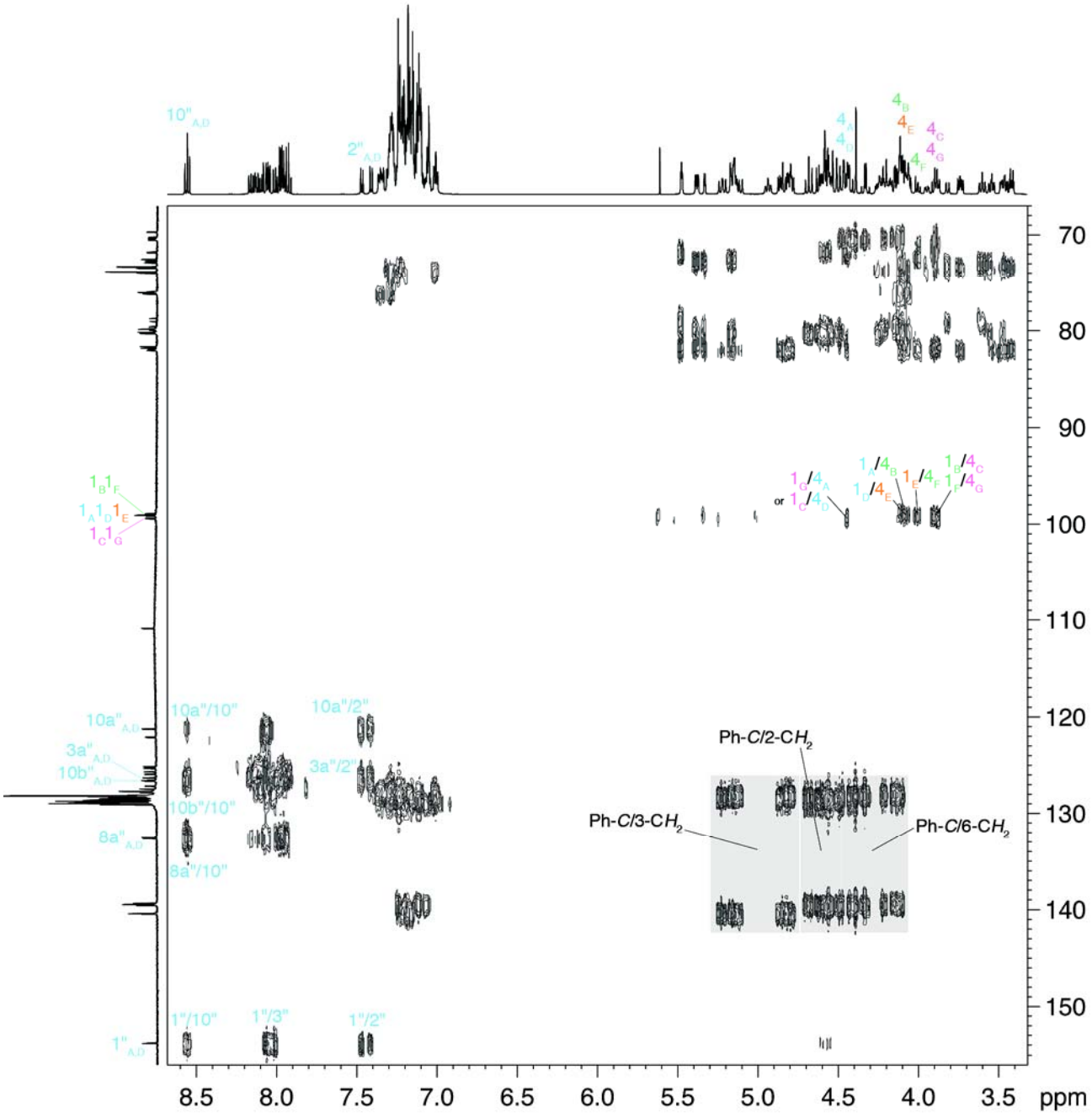


Figure S 6: $^{13}C/^{1}H$ HMBC map of **1** (600 MHz, d^6-acetone).

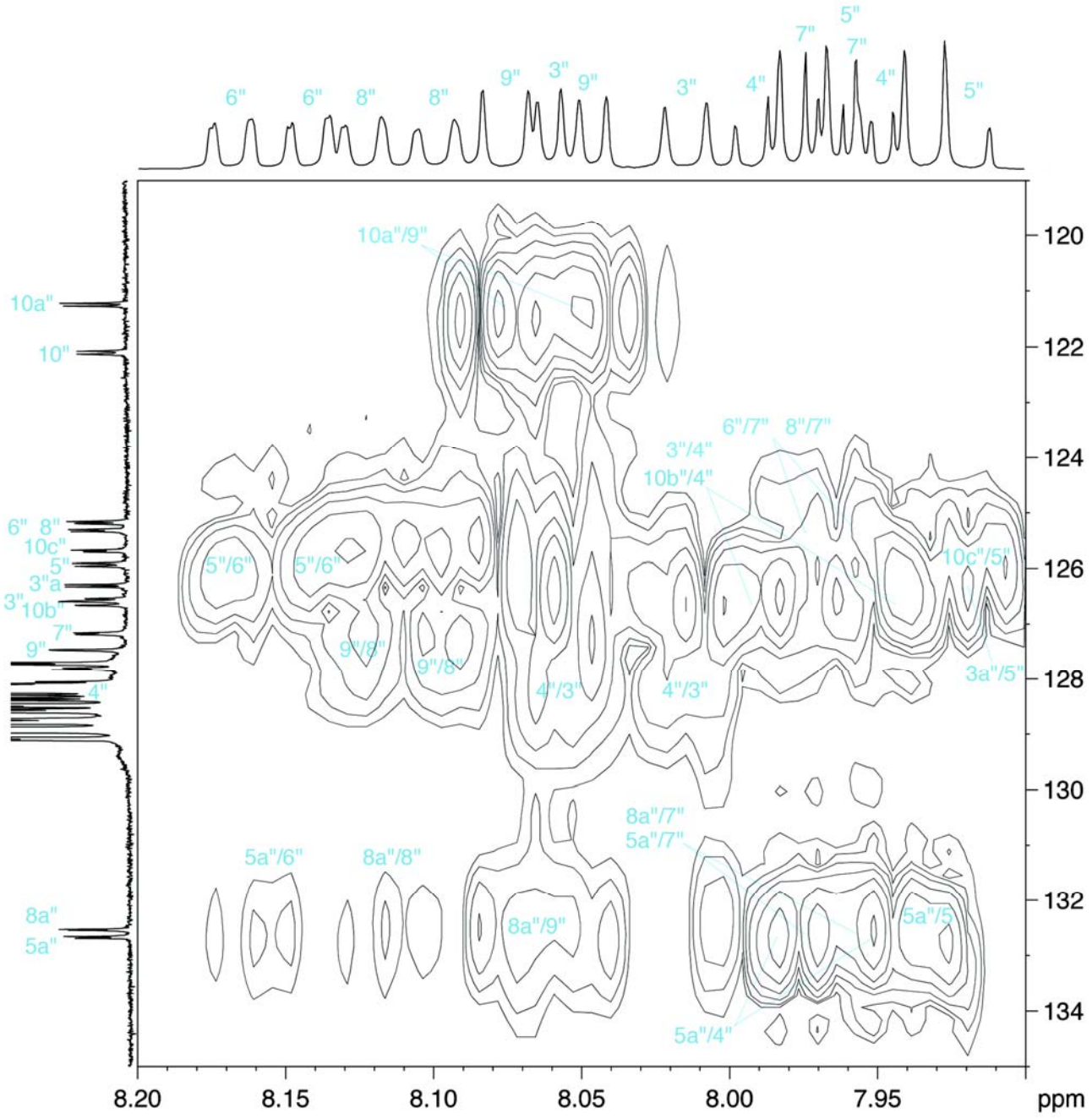


Figure S 7: Detail (aromatic region) of the $^{13}C/^{1}H$ HMBC map of **1** (600 MHz, d^6-acetone).

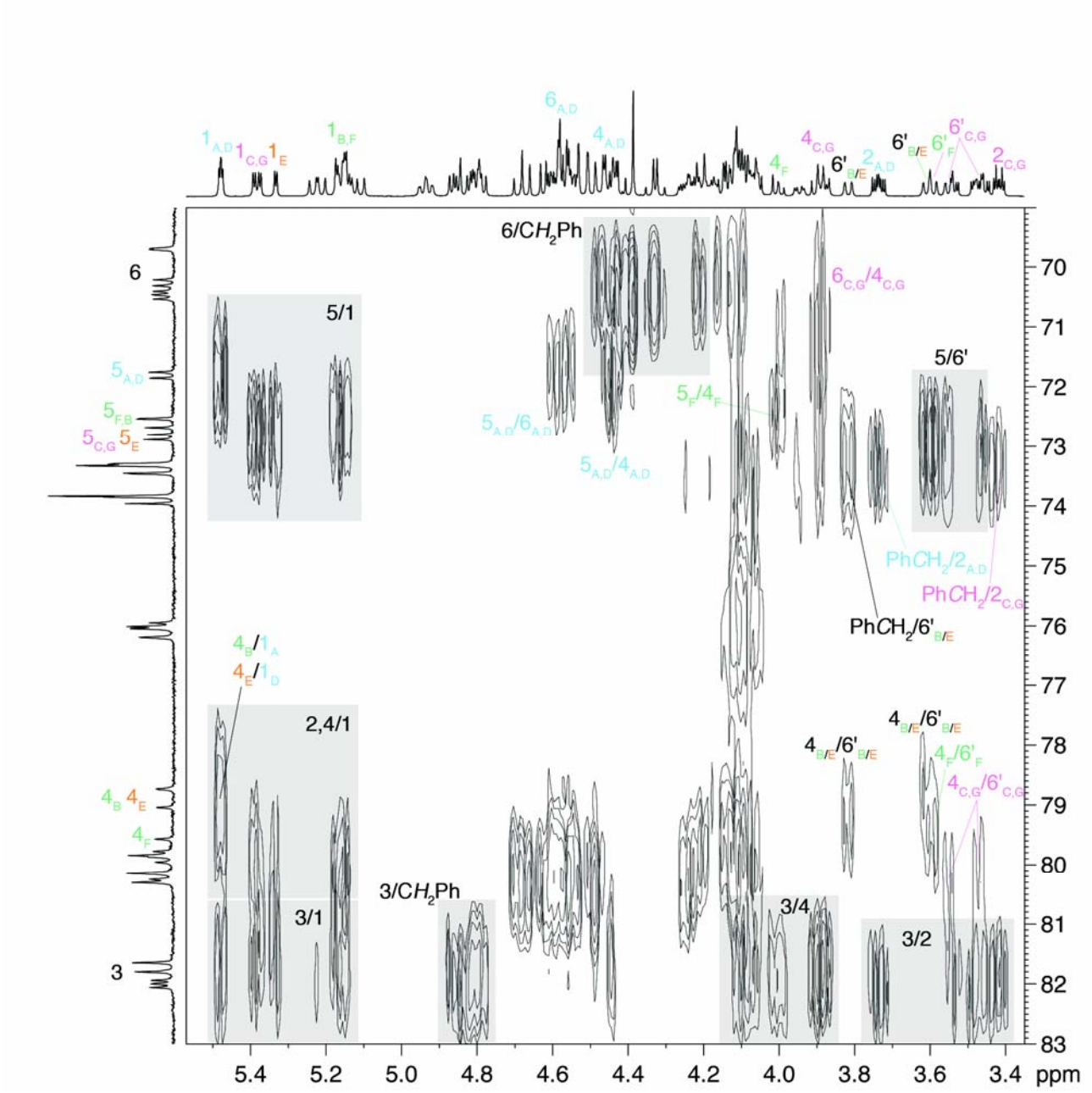


Figure S 8: Detail (aliphatic region) of the $^{13}C/^{1}H$ HMBC map of **1** (600 MHz, d^6-acetone).

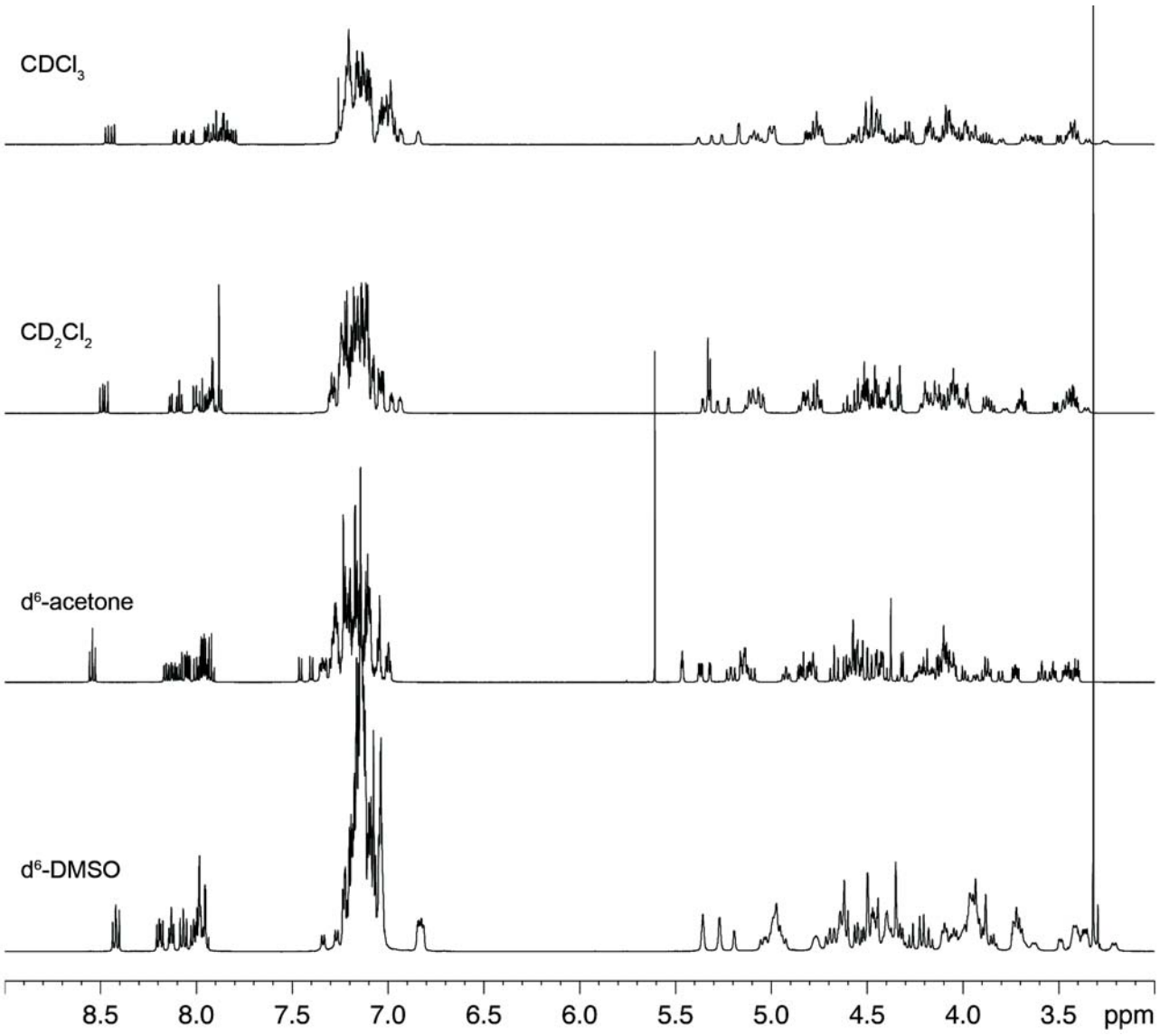


Figure S 9: ^{1}H NMR (600 MHz) spectrum of **1** in various solvents.

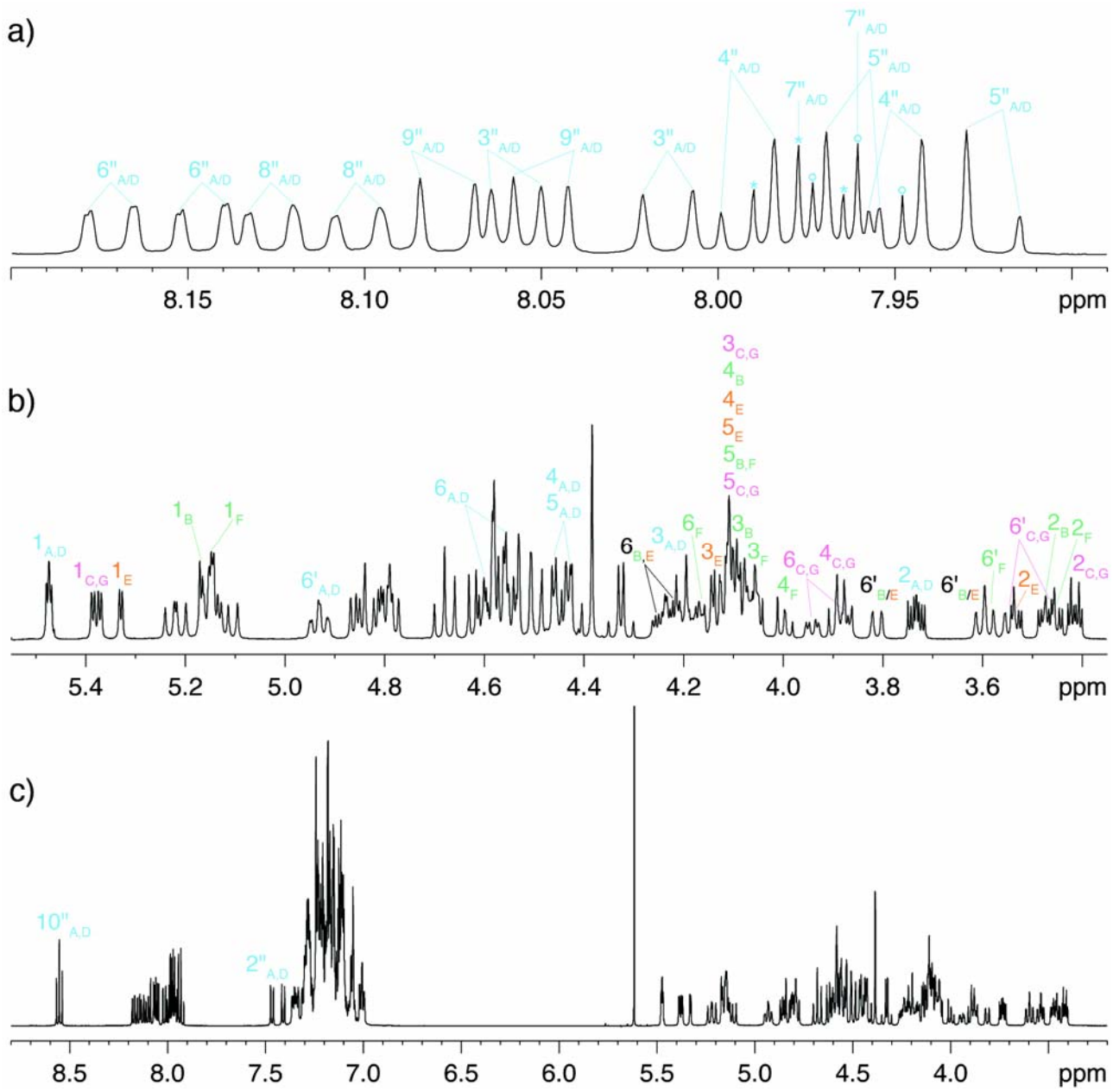


Figure S 10: ^{1}H NMR spectrum of **1** (600 MHz, d^{6}-acetone). a) Aromatic region (∗ and o show the triplets of 7”$_{A/D}$). b) Aliphatic region. c) Full spectrum.

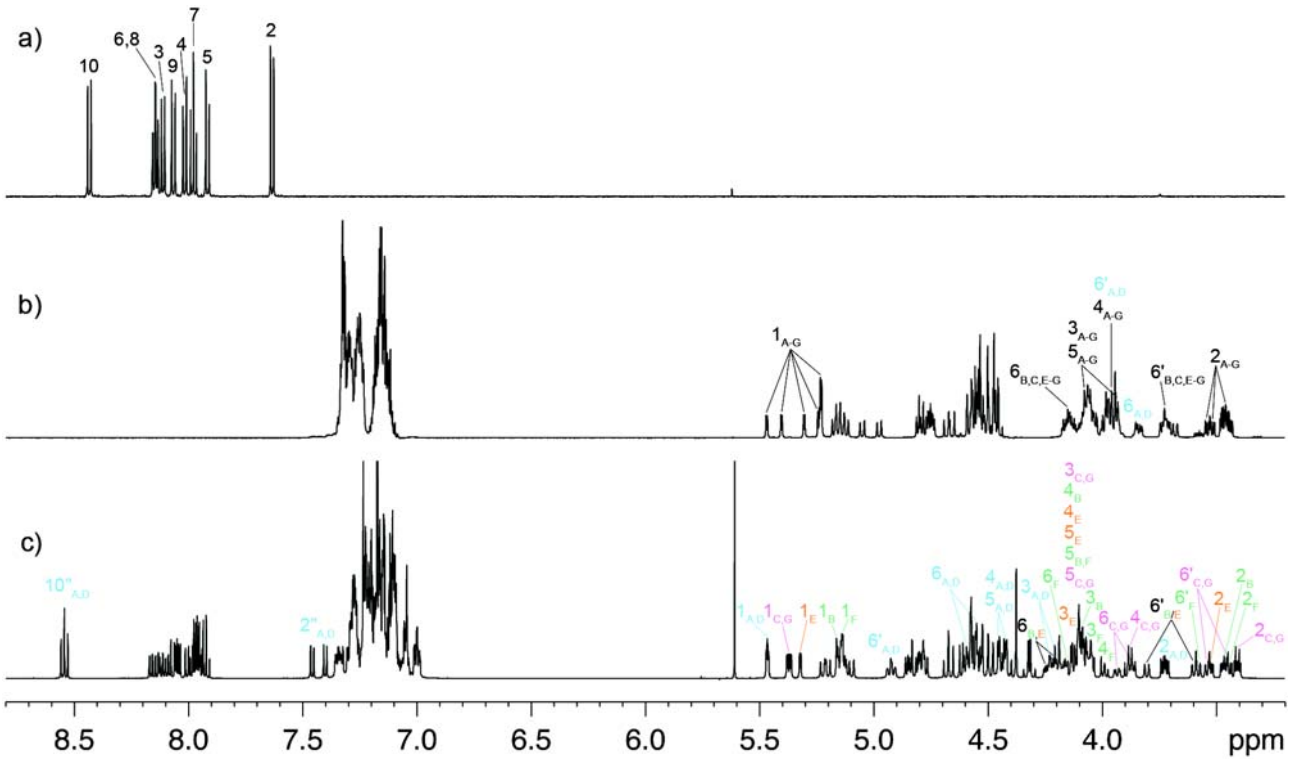


Figure S 11: Comparison of the ^{1}H NMR spectra of 1-hydroxypyrene (a) and **3** (b) with the spectrum of **1** (600 MHz, d^{6}-acetone).

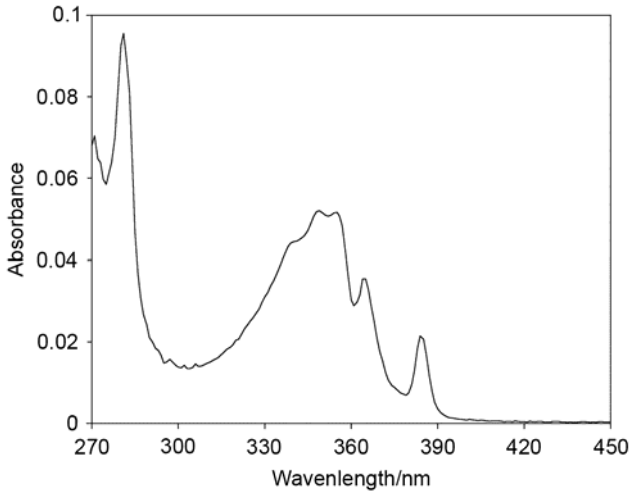


Figure S 12: Electronic absorption spectrum of **1** (1.0×10^{-6} mol dm^{-3}) in DMSO.

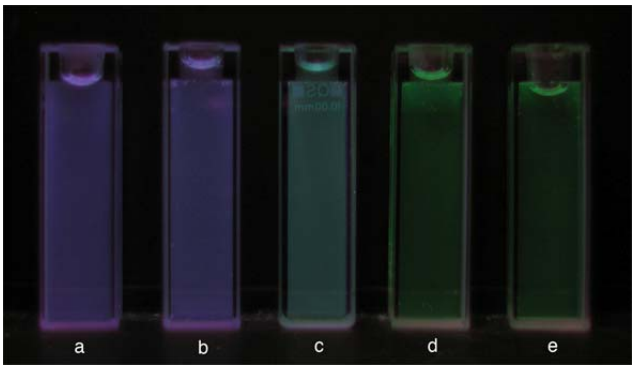


Figure S 13: Fluorescence emission from a solution of **1** (1.0×10^{-6} mol dm^{-3}) in H_2O/DMSO mixtures with increasing water concentration (a: pure DMSO, b: 15%, c: 18%, d: 20%, e: 40%) under a UV lamp (365 nm).

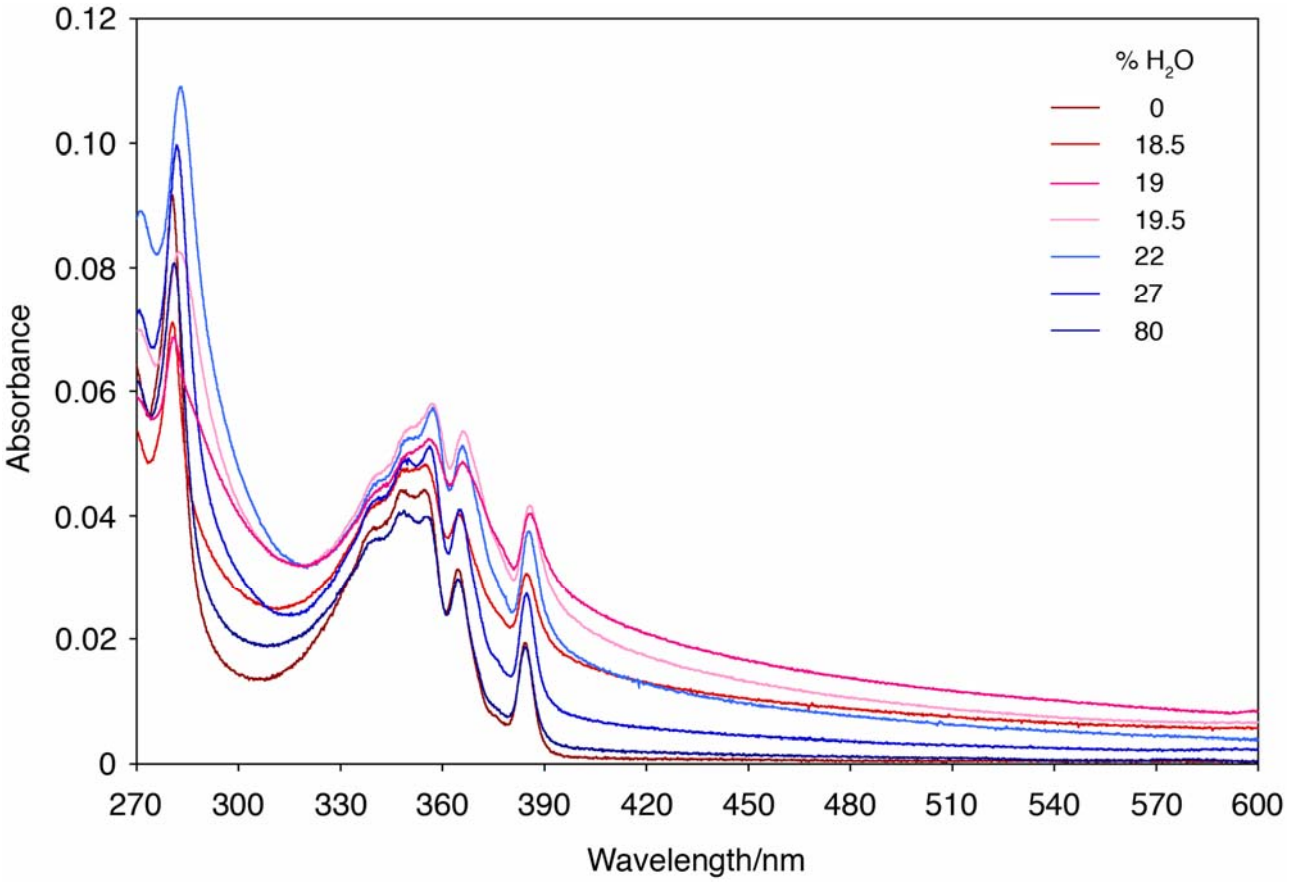


Figure S 14: Electronic absorption spectra of solutions of **1** (~ 1.0×10^{-6} mol dm^{-3}) in selected H_2O/DMSO mixtures.

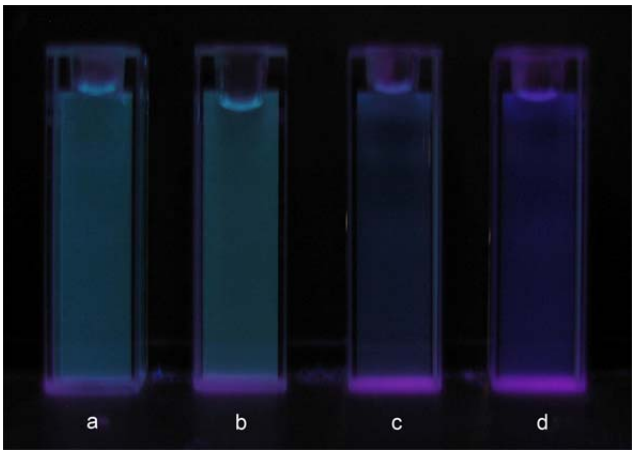


Figure S 15: Fluorescence emission of **1** (1.0×10^{-6} mol dm^{-3}) in H_2O/DMSO 80:20 v/v upon addition of 1-heptanoic acid (a: 0, b: 1.0×10^{-2}, c: 2.0×10^{-2}, d: 3.0×10^{-2} mol dm^{-3}) under a UV lamp (365 nm).

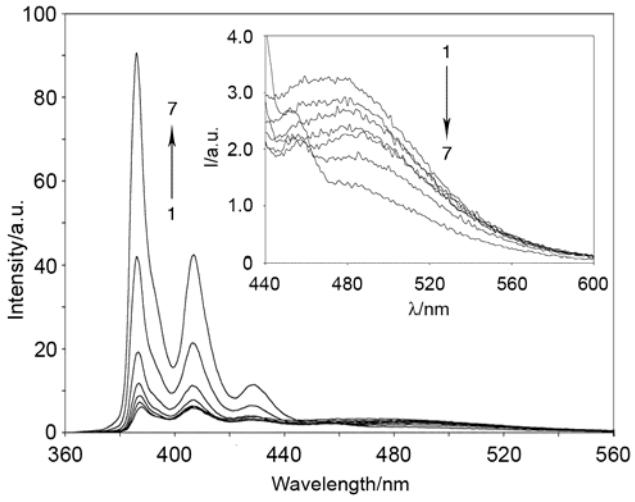


Figure S 16: Fluorescence spectra of **1** (1.0×10^{-6} mol dm^{-3}, 25 °C) upon addition of 1-decanoic acid (1: 0, 2: 2.0×10^{-4}, 3: 4.0×10^{-4}, 4: 6×10^{-4}, 5: 8.0×10^{-4}, 6: 1×10^{-3}, 7: 1.2×10^{-3} mol dm^{-3}) in H_2O/DMSO 80:20 v/v containing 0.04% aqueous HCl. The inset shows the excimer emission band.

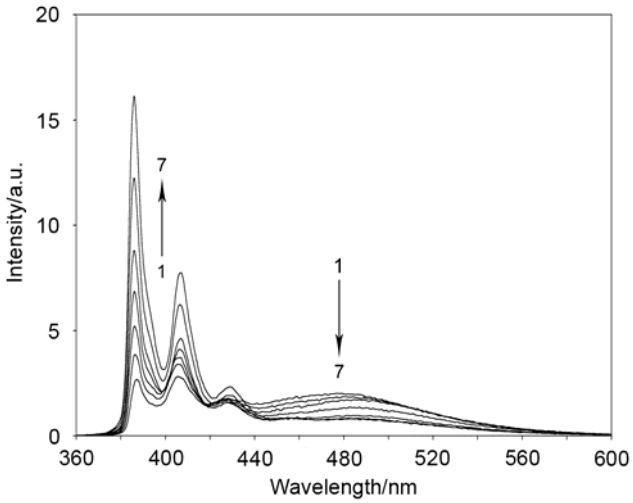


Figure S 17: Fluorescence spectra of **1** (1.0×10^{-6} mol dm^{-3}, 25 °C) upon addition of 6-chloro-1-hexanol (1: 0, 2: 5.0×10^{-3}, 3: 1.0×10^{-2}, 4: 1.5×10^{-2}, 5: 2.0×10^{-2}, 6: 2.5×10^{-2}, 7: 3.0×10^{-2} mol dm^{-3}) in H_2O/DMSO 80:20 v/v.

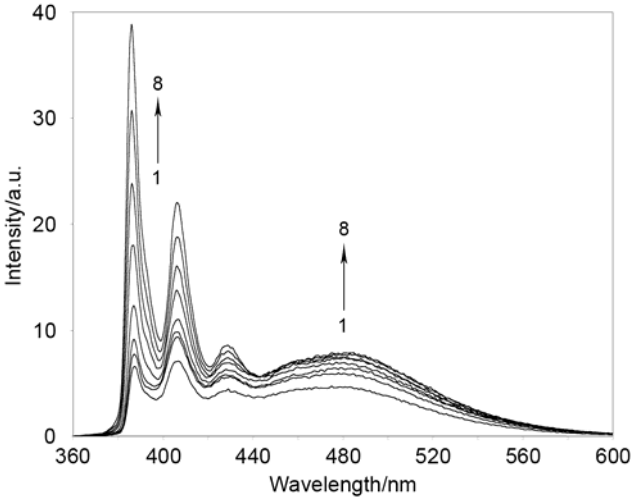
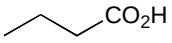
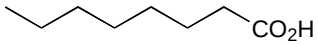


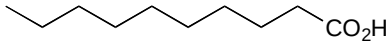
Figure S 18: Fluorescence spectra of **1** (1.0×10^{-6} mol dm^{-3}, 25 °C) upon addition of 1-decanol (1: 0, 2: 2.0×10^{-4}, 3: 4.0×10^{-4}, 4: 6.0×10^{-4}, 5: 8.0×10^{-4}, 6: 1.0×10^{-3}, 7: 1.2×10^{-3}, 8: 1.4×10^{-3} mol dm^{-3}) in H_2O/DMSO 80:20 v/v.



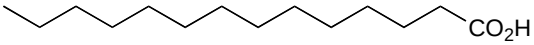
1-butanoic acid



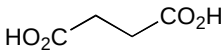
1-heptanoic acid



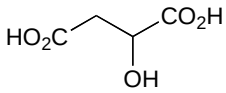
1-decanoic acid



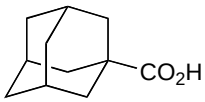
myristic acid



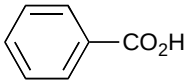
1,4-butanedioic acid



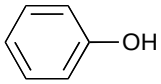
2-hydroxy-1,4-butanedioic acid



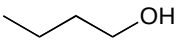
1-adamantylcarboxylic acid



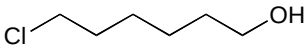
benzoic acid



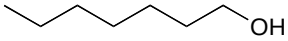
phenol



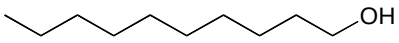
1-butanol



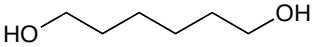
6-chloro-1-hexanol



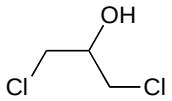
1-heptanol



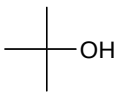
1-decanol



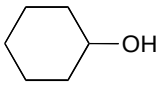
1,6-hexanediol



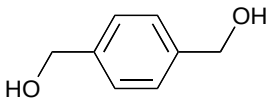
1,3-dichloro-2-propanol



tert-butanol



cyclohexanol



1,4-benzenedimethanol

Chart S 1: The various substrates investigated.

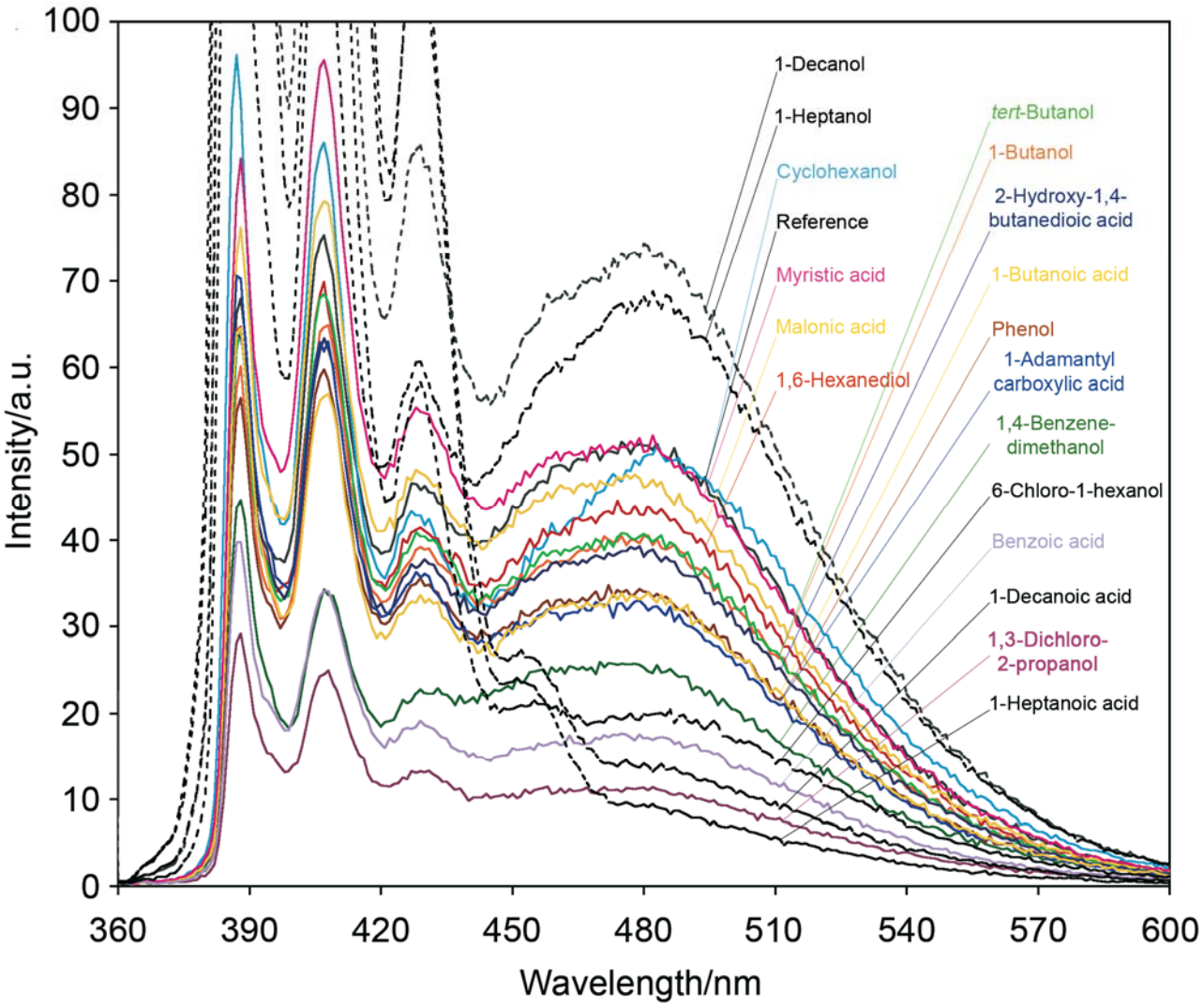


Figure S 19: Detail of the stacked plot of the fluorescence spectra of **1** (1×10^{-6} mol dm^{-3}, 25 °C) in the presence of the compounds of Chart S 1 in H_2O/DMSO 80:20 v/v. All compounds 0.1 mol dm^{-3}, excepted 1,4-benzenedimethanol diol (5.0×10^{-2} mol dm^{-3}), adamantyl carboxylic acid (2.0×10^{-3} mol dm^{-3}), and myristic (tetradecanoic) acid (5.0×10^{-4} mol dm^{-3}).