Supplementary Material

New V-shaped push-pull systems on the basis of 4,5-di(hetero)aryl substituted pyrimidines: synthesis and application for detection of nitroaromatic explosives

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Dedicated to Professor Oleg G. Sinyashin on the occasion of his 60th anniversary

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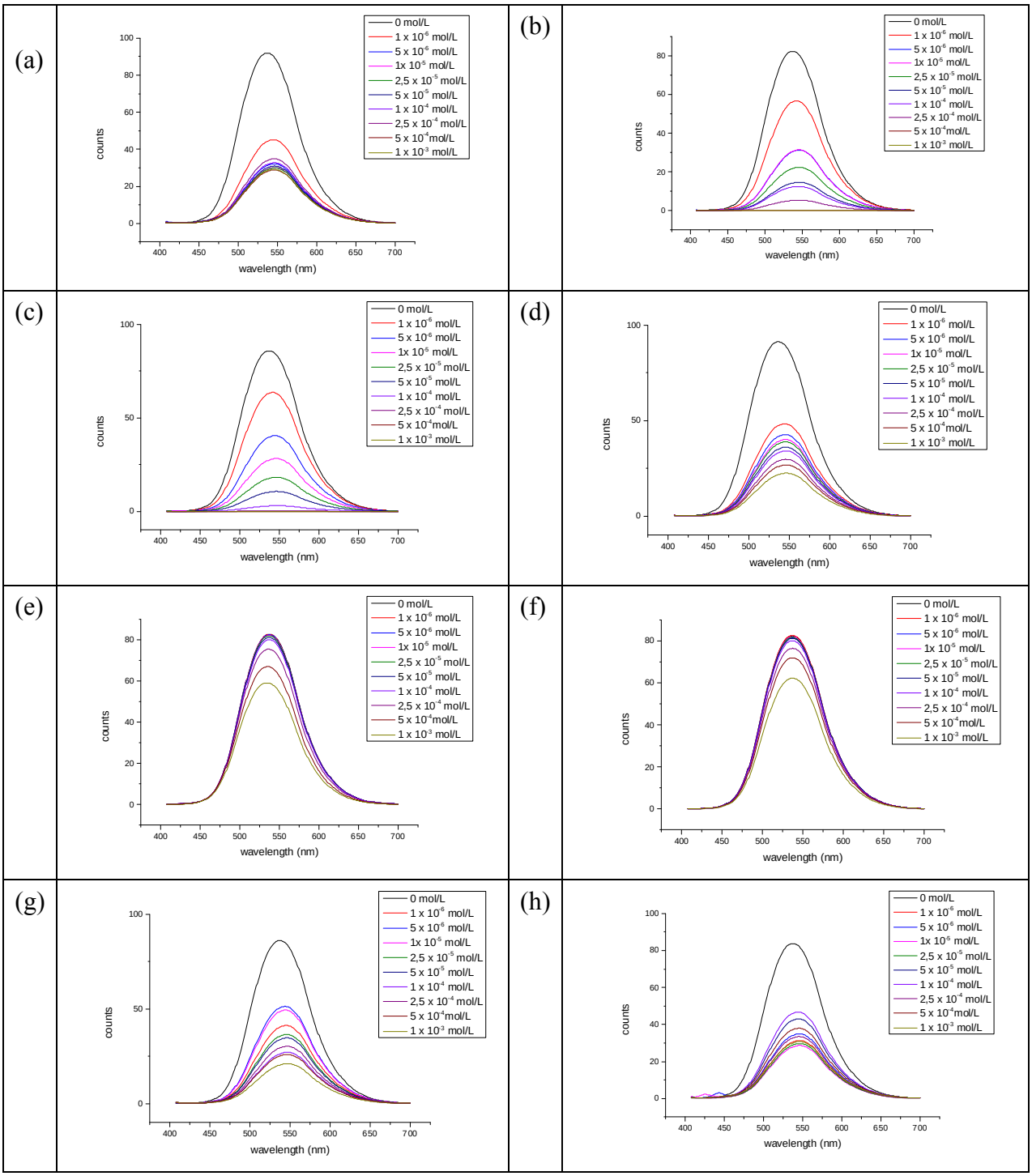


Figure S1. Fluorescence quenching studies of **6b** (1.0×10^{-5} mol/L) recorded in the presence of various amounts of DNAN (a), PA (b), SA (c), TETNB (d), DNT (e), TNT (f), NB (g) and Tol (h), of which 385 nm was taken as the excitation wavelength.

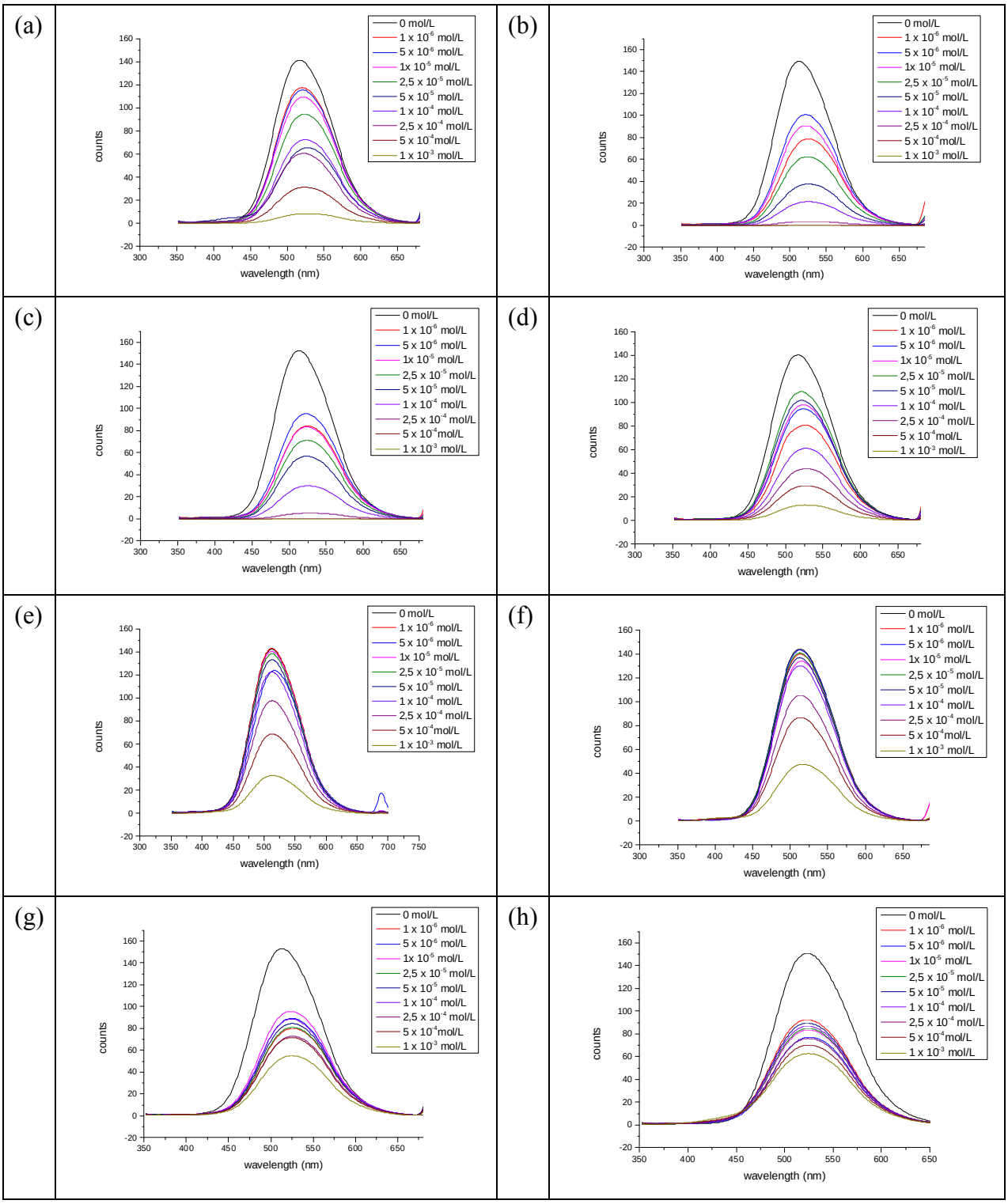


Figure S2. Fluorescence quenching studies of **6c** (1.0×10^{-5} mol/L) recorded in the presence of various amounts of DNAN (a), PA (b), SA (c), TETNB (d), DNT (e), TNT (f), NB (g) and Tol (h), of which 385 nm was taken as the excitation wavelength.

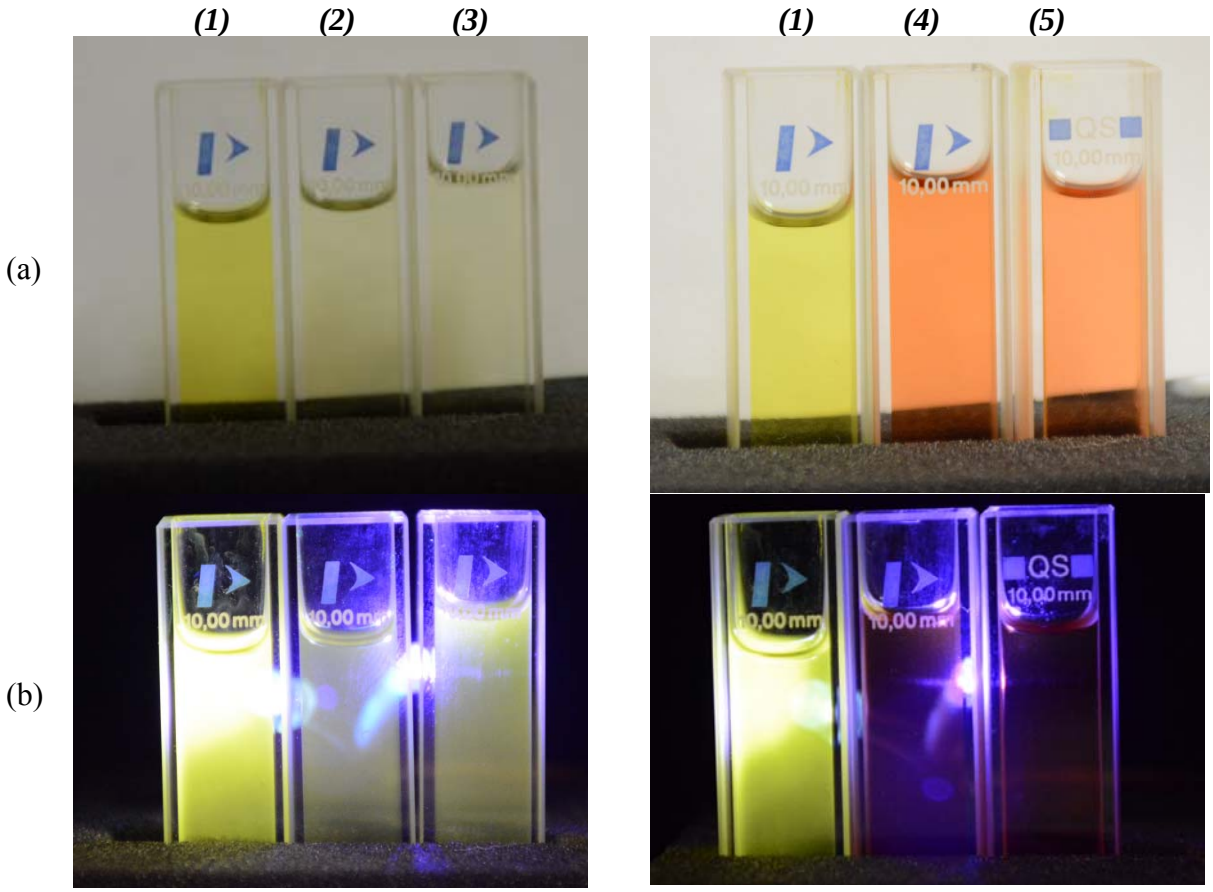


Figure S3. Solution photographs of compound **6b** (c = 1.0×10^{-5} M) in acetonitrile (*1*), solution **6a** with the presence of solution TETNB (c = 1.0×10^{-5} M) in acetonitrile (*2*), solution **6b** with the presence of solution DNAN (c = 1.0×10^{-5} M) in acetonitrile (*3*), solution **6b** with the presence of solution PA (c = 1.0×10^{-5} M) in acetonitrile (4), solution **6b** with the presence of solution SA (c = 1.0×10^{-5} M) in acetonitrile (5): before radiation (a – no emission) and during radiation (b – emission, λ_{ex}= 375 nm) at room temperature.

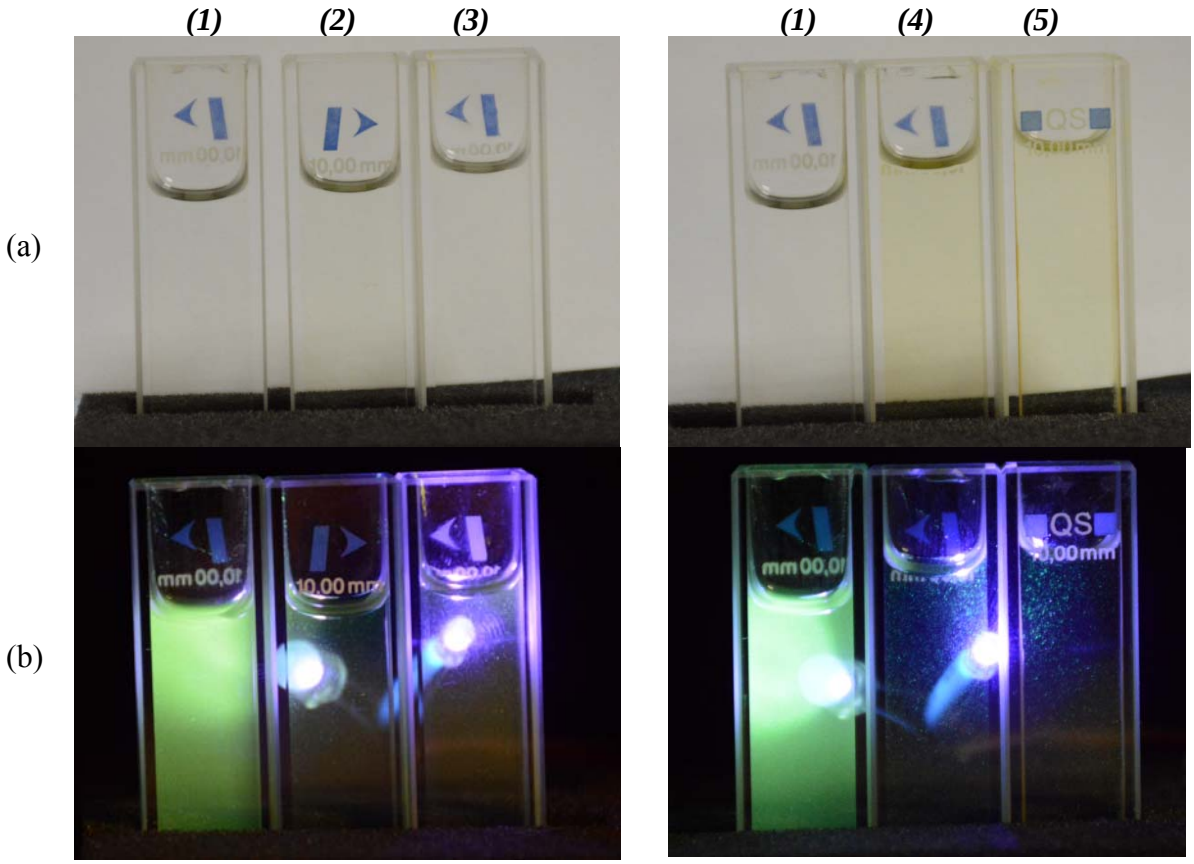


Figure S4. Solution photographs of compound **6c** (c = 1.0×10^{-5} M) in acetonitrile (*1*), solution **6a** with the presence of solution TETNB (c = 1.0×10^{-5} M) in acetonitrile (*2*), solution **6c** with the presence of solution DNAN (c = 1.0×10^{-5} M) in acetonitrile (*3*), solution **6c** with the presence of solution PA (c = 1.0×10^{-5} M) in acetonitrile (4), solution **6c** with the presence of solution SA (c = 1.0×10^{-5} M) in acetonitrile (5): before radiation (a – no emission) and during radiation (b – emission, λ_{ex}= 375 nm) at room temperature.

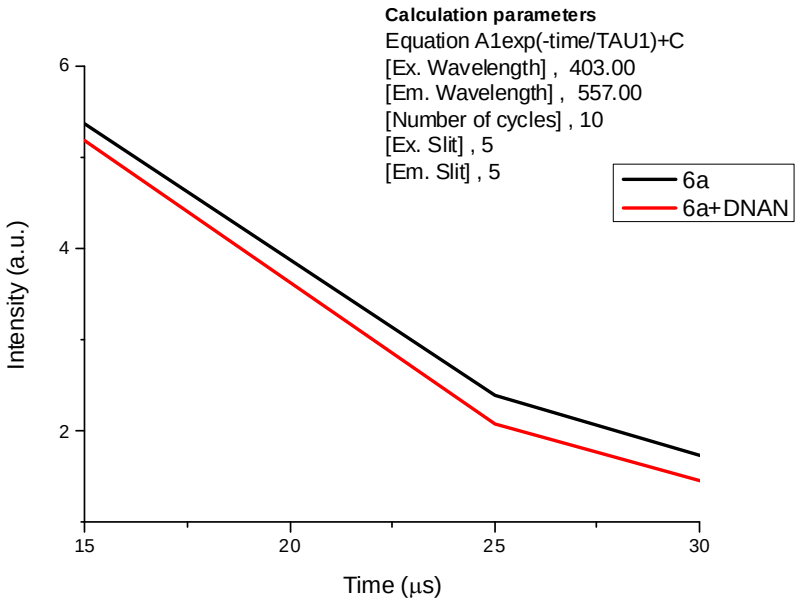


Figure S5. Time-resolved fluorescence emission of **6a** and adduct with DNAN at different mole ratios of the analyte.

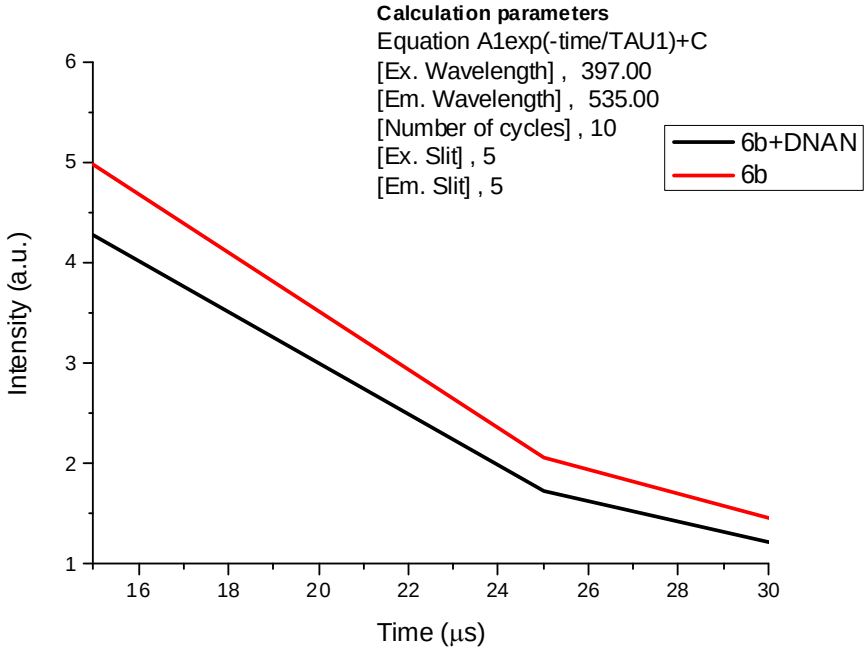


Figure S6. Time-resolved fluorescence emission of **6b** and adduct with DNAN at different mole ratios of the analyte.

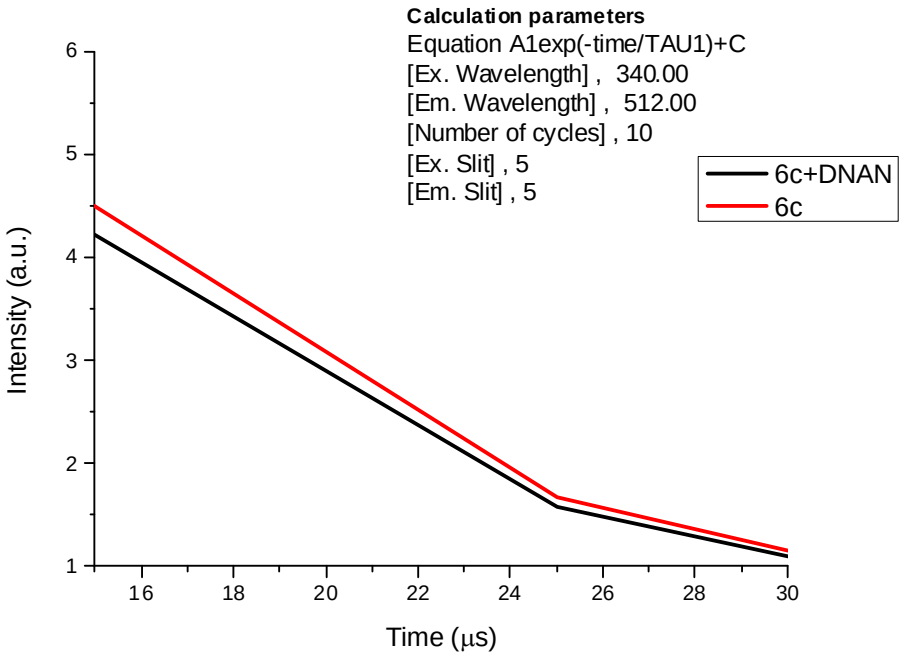


Figure S7. Time-resolved fluorescence emission of **6c** and adduct with DNAN at different mole ratios of the analyte.

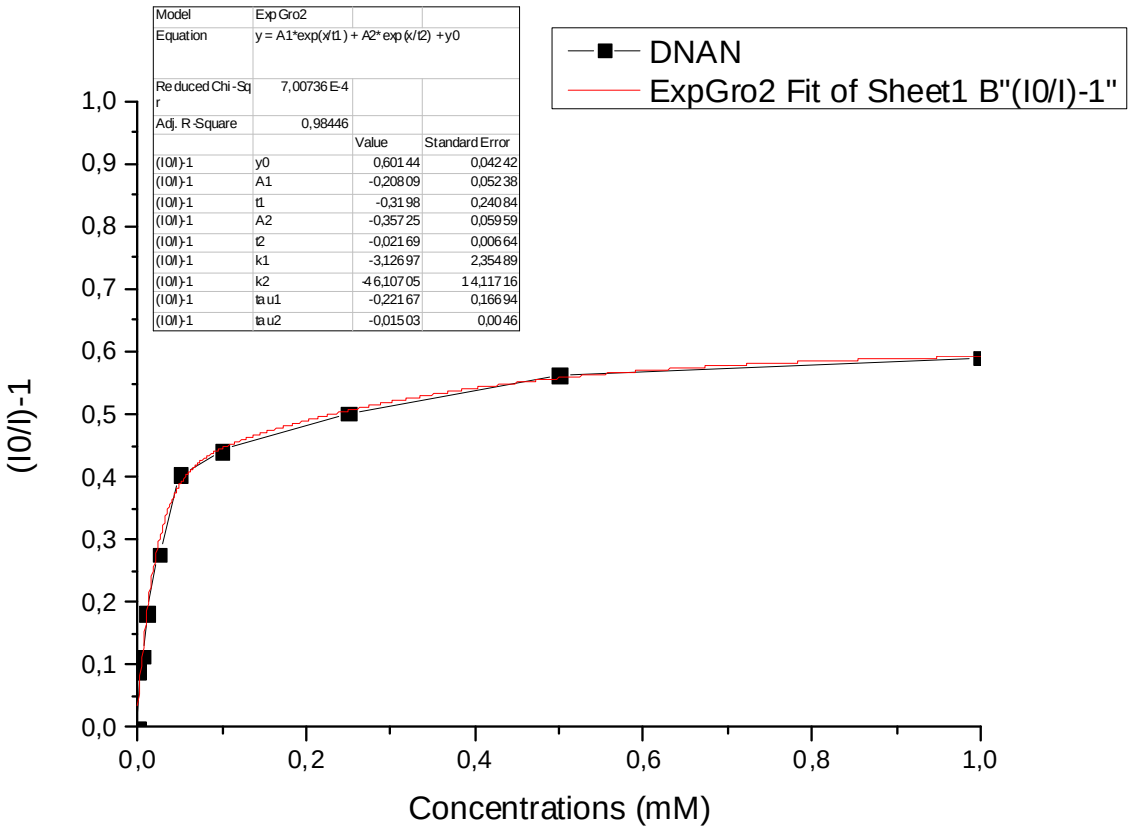


Figure S8. The Stern–Volmer plots as function of DNAN concentration in CH_3CN, with an excitation wavelength of 403 nm for **6a** solution.

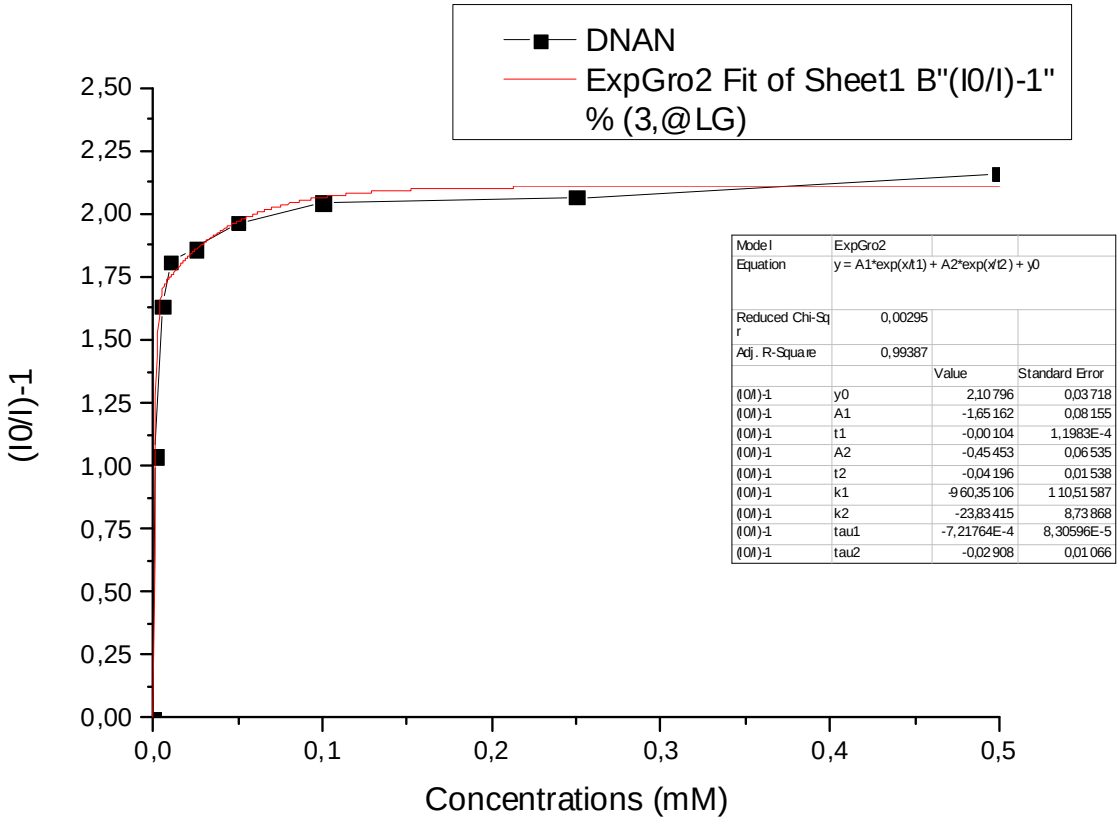


Figure S9. The Stern–Volmer plots as function of DNAN concentration in CH_3CN, with an excitation wavelength of 397 nm for **6b** solution.

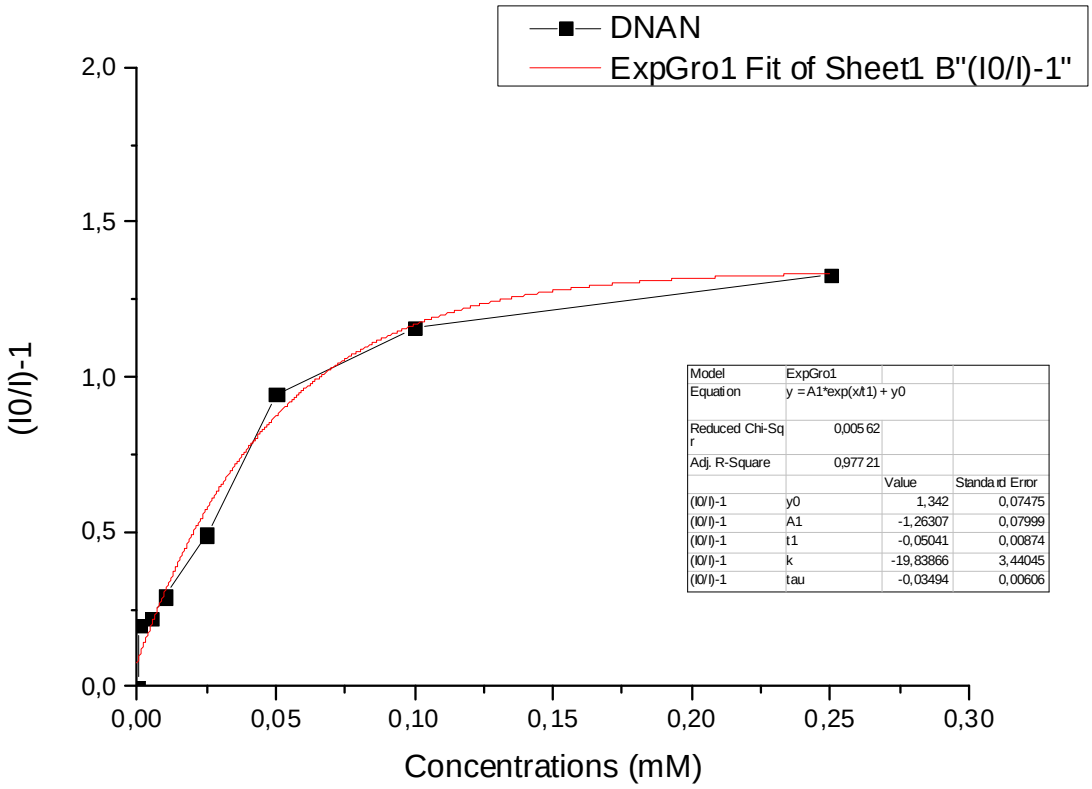
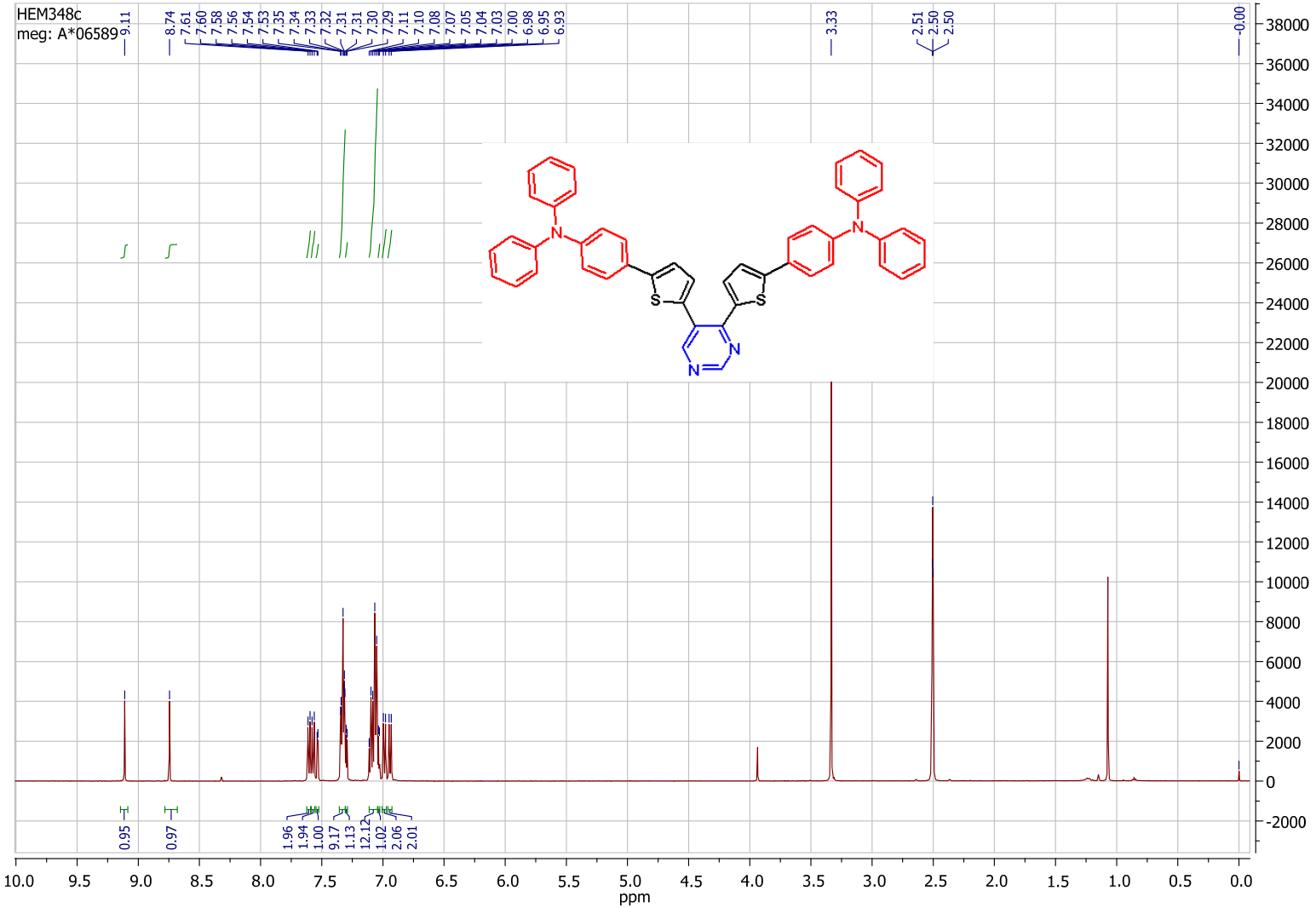


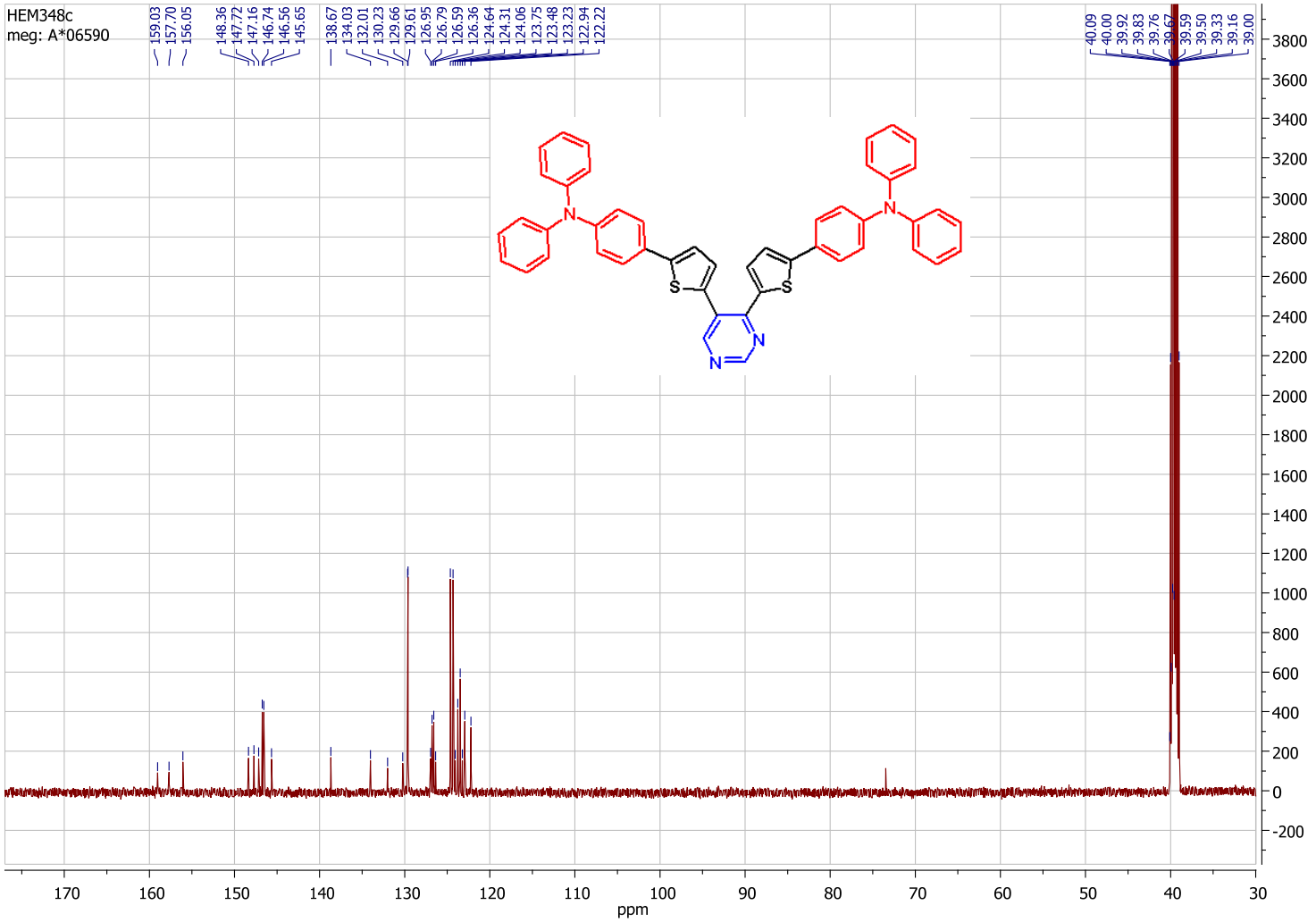
Figure S10. The Stern–Volmer plots as function of DNAN concentration in CH_3CN, with an excitation wavelength of 340 nm for **6c** solution.

Table S1. Fluorescence life time data of pure **6a-c** fluorophores at different mole ratios of DNAN

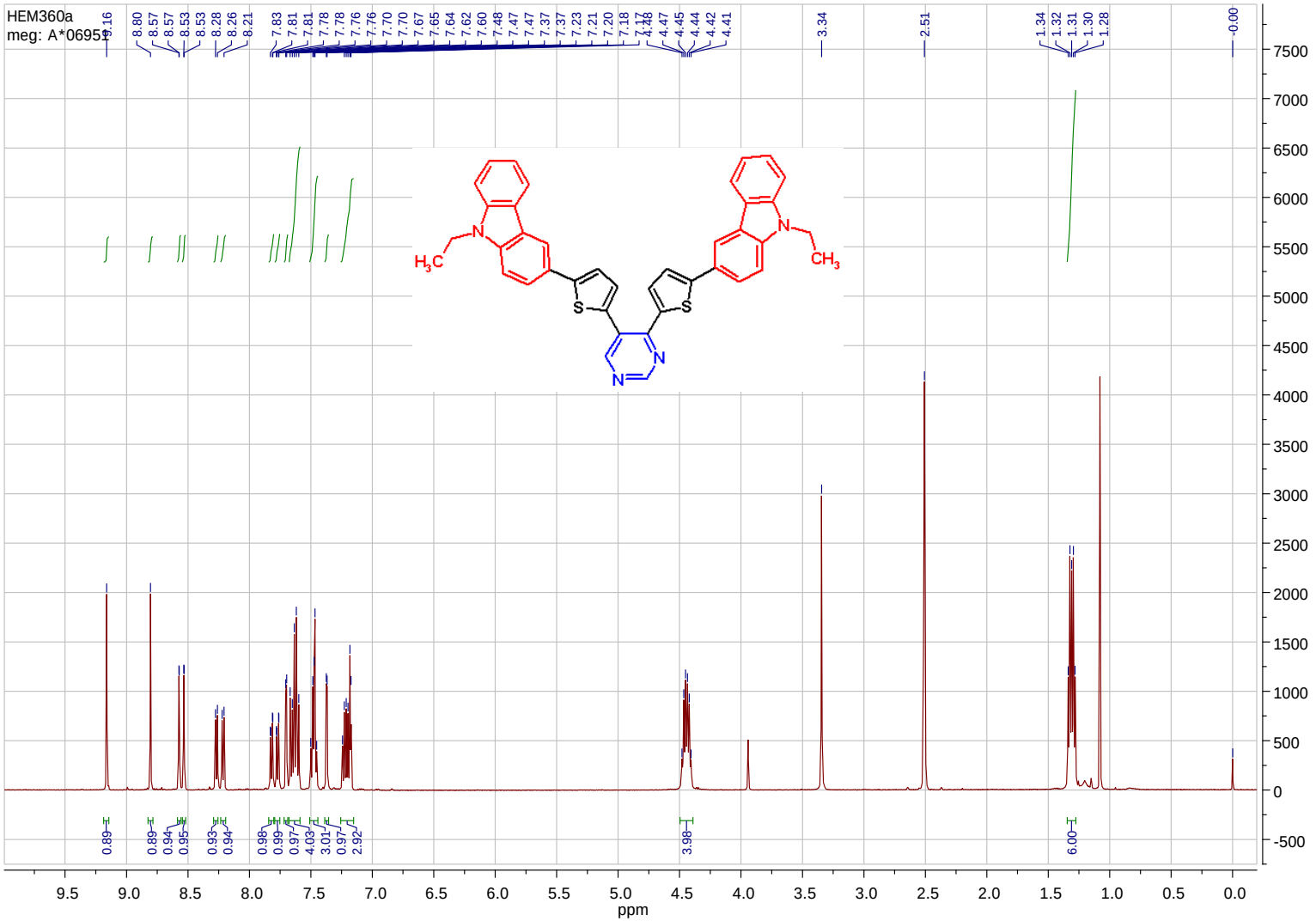
Mole ratio *vs* DNAN	Fluorophore 6a (µs)	Fluorophore 6b (µs)	Fluorophore 6c (µs)
0	0.011	0.011	0.010
1:1	0.011	0.011	0.010



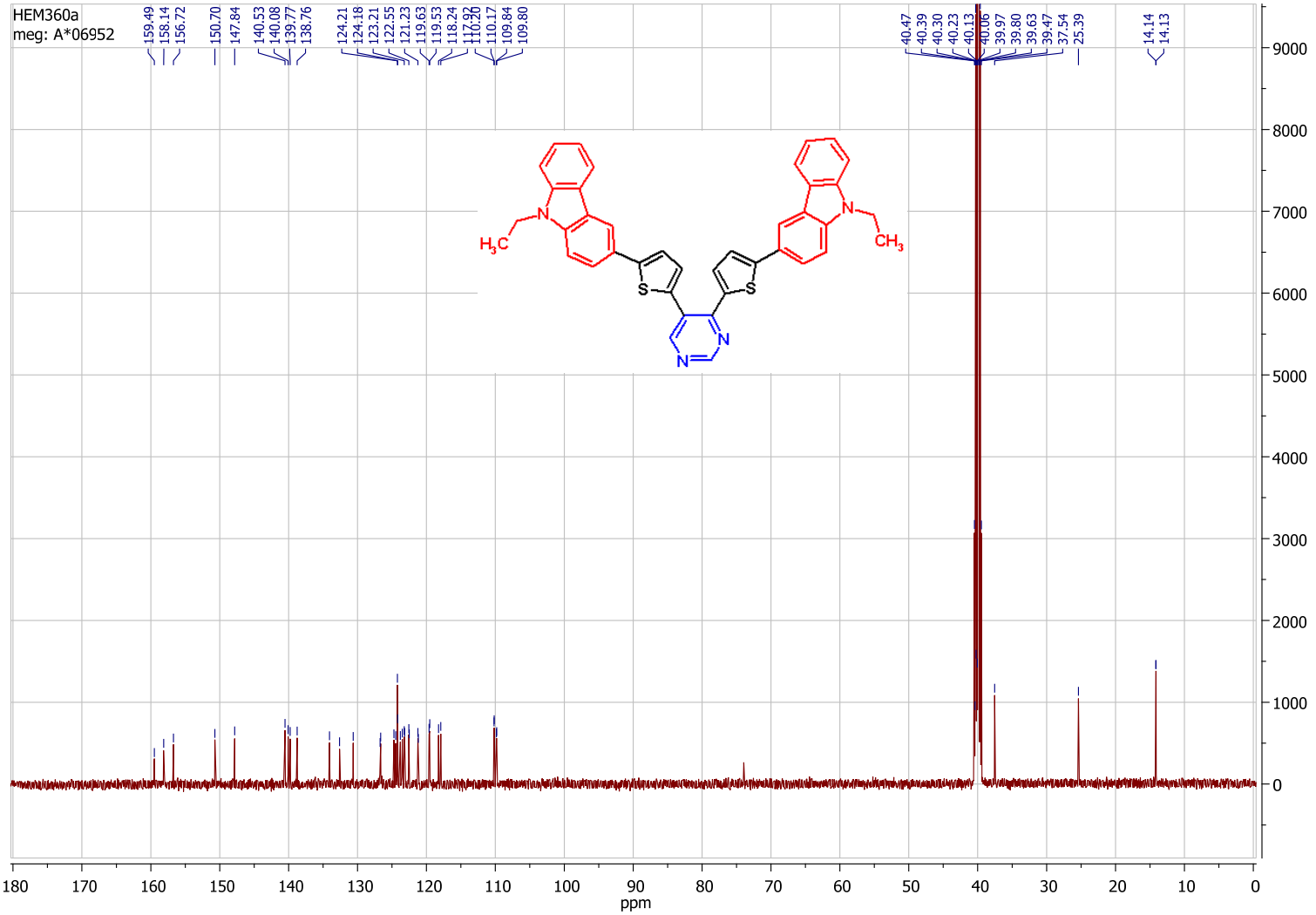
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **6a**.



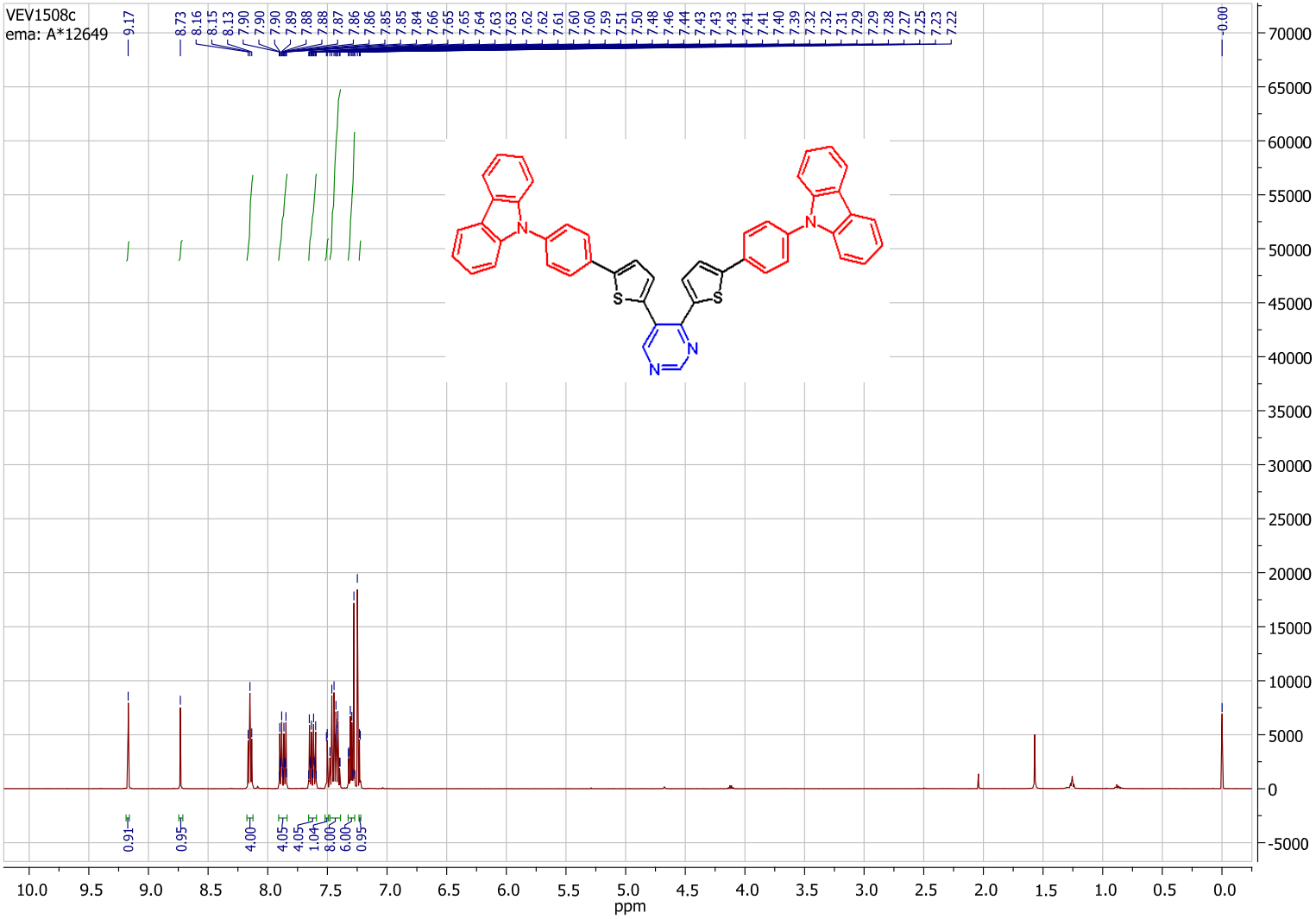
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **6a**.



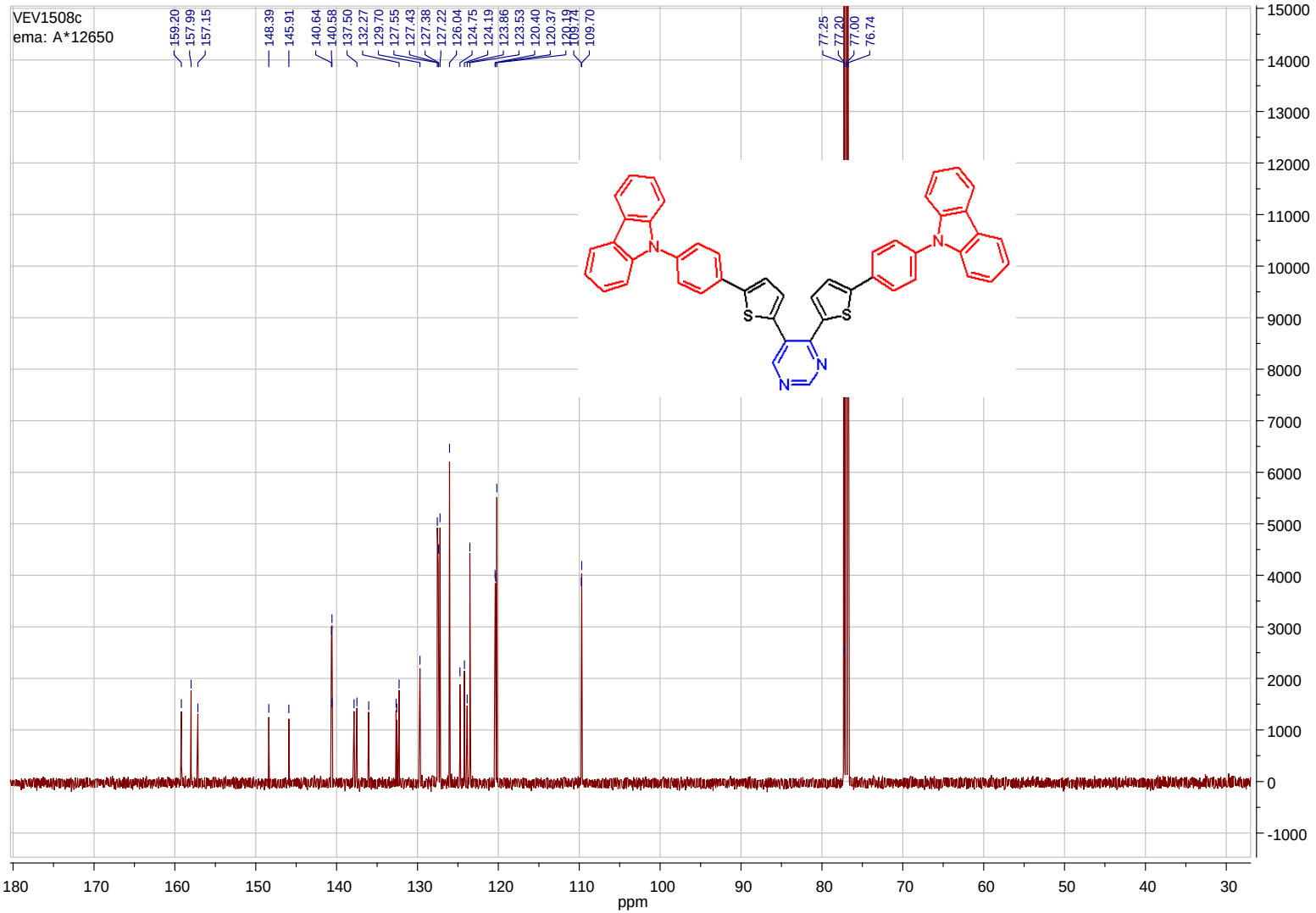
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **6b**.



^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **6b**.



^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **6c**.



^{13}C NMR (126 MHz, $CDCl_3$) spectrum of **6c**.