Electronic Supplementary Information

Lophine and pyrimidine based photoactive molecular hybrids. Synthesis, photophysics, BSA interaction and DFT study

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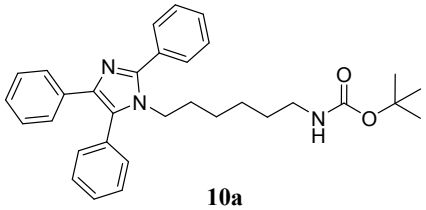
Summary

Spectroscopic characterization



10a

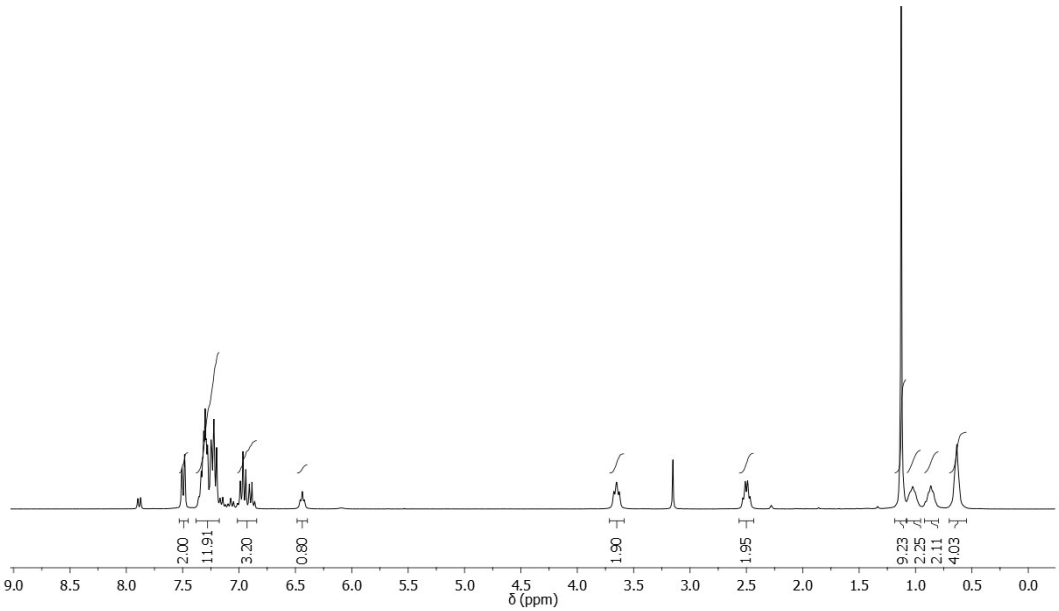


Figure ESI1. ^{1}H NMR Spectrum (DMSO-d_6, 300 MHz) of compound **10a**.

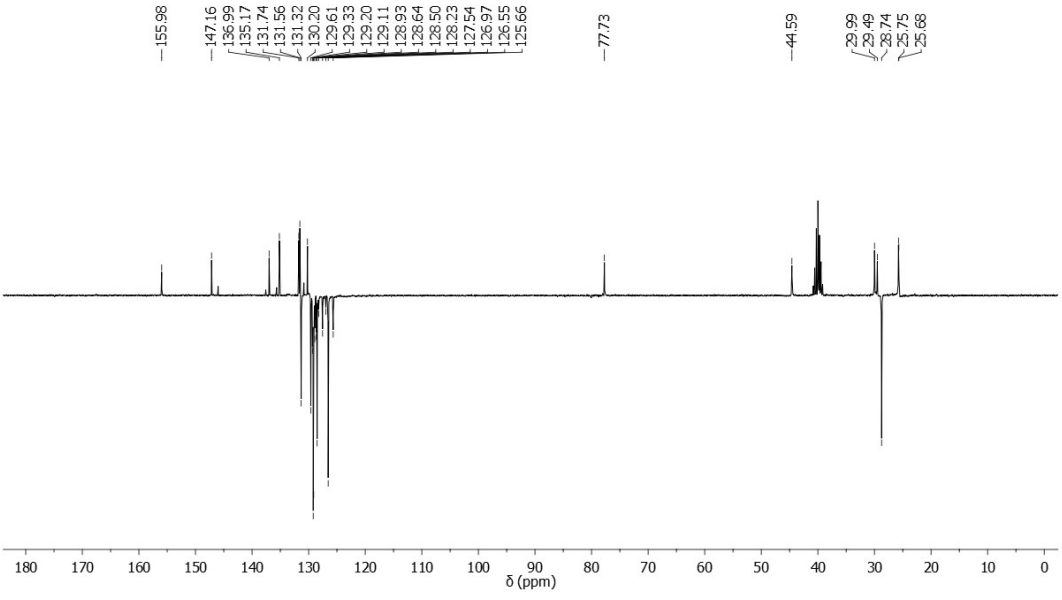


Figure ESI2. ^{13}C NMR Spectrum, APT (DMSO-d_6, 75 MHz) of compound **10a**.

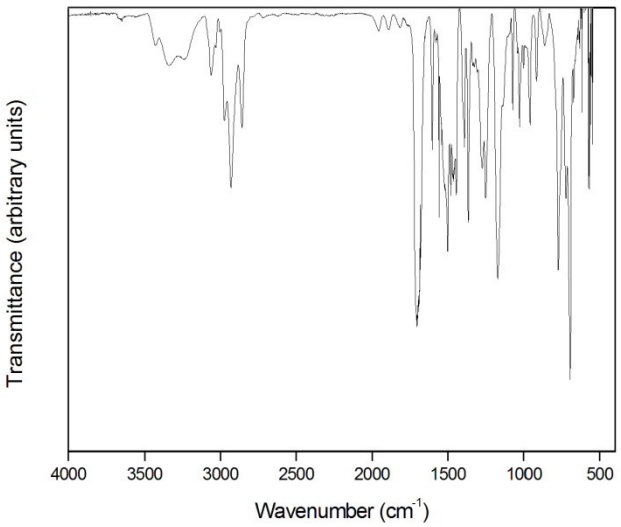
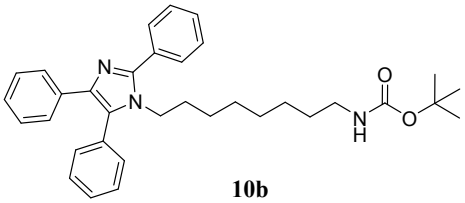


Figure ESI3. FTIR spectrum (KBr pellet) of compound **10a**.



10b

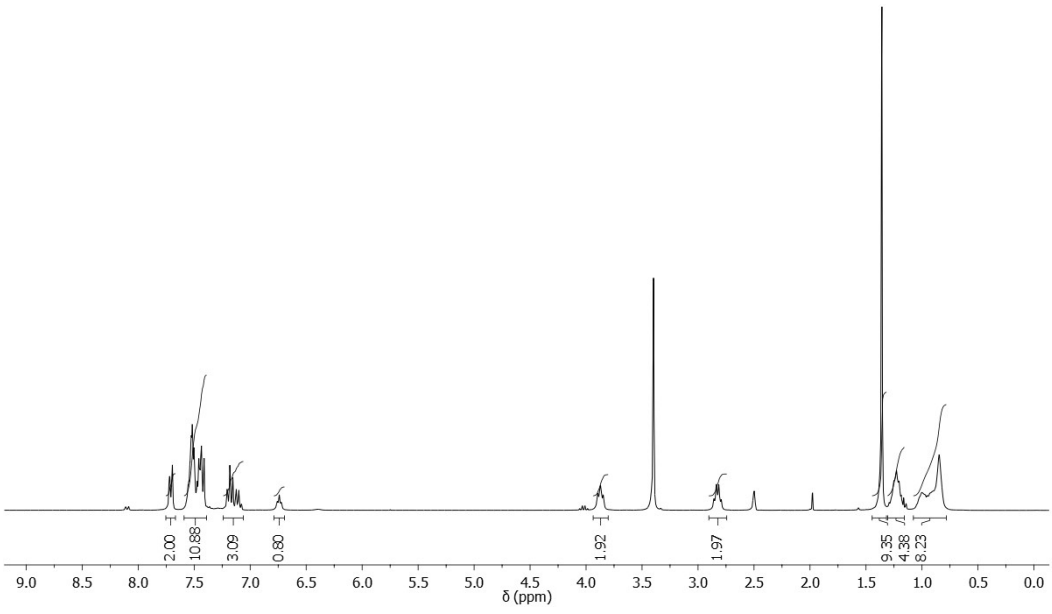


Figure ESI4. ^{1}H NMR Spectrum (DMSO-d_6, 300 MHz) of compound **10b**.

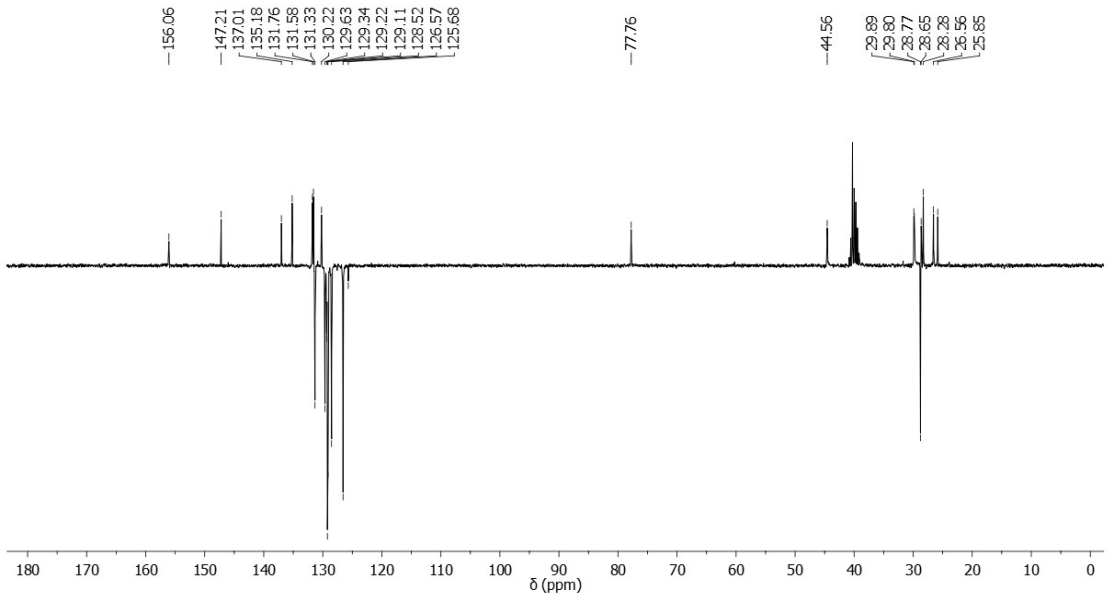


Figure ESI5. ^{13}C NMR Spectrum, APT (DMSO-d_6, 75 MHz) of compound **10b.**

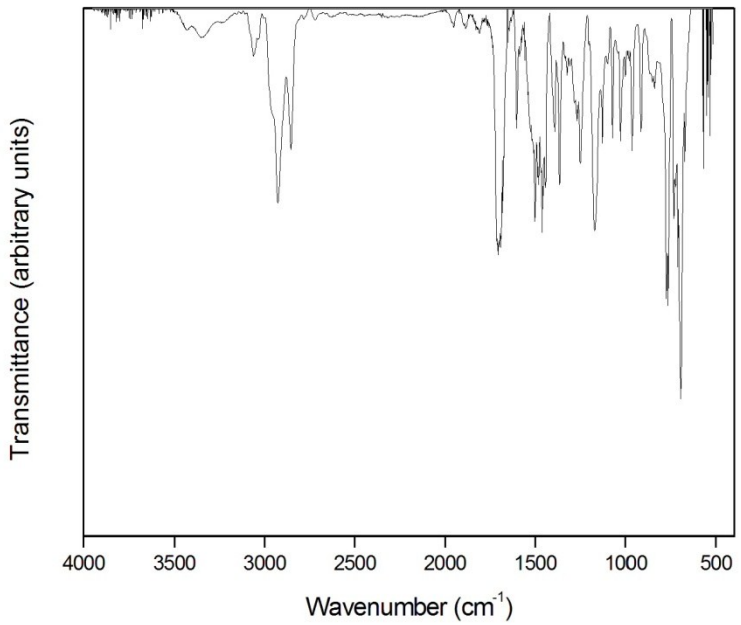


Figure ESI6. FTIR spectrum (KBr pellet) of compound **10b**.

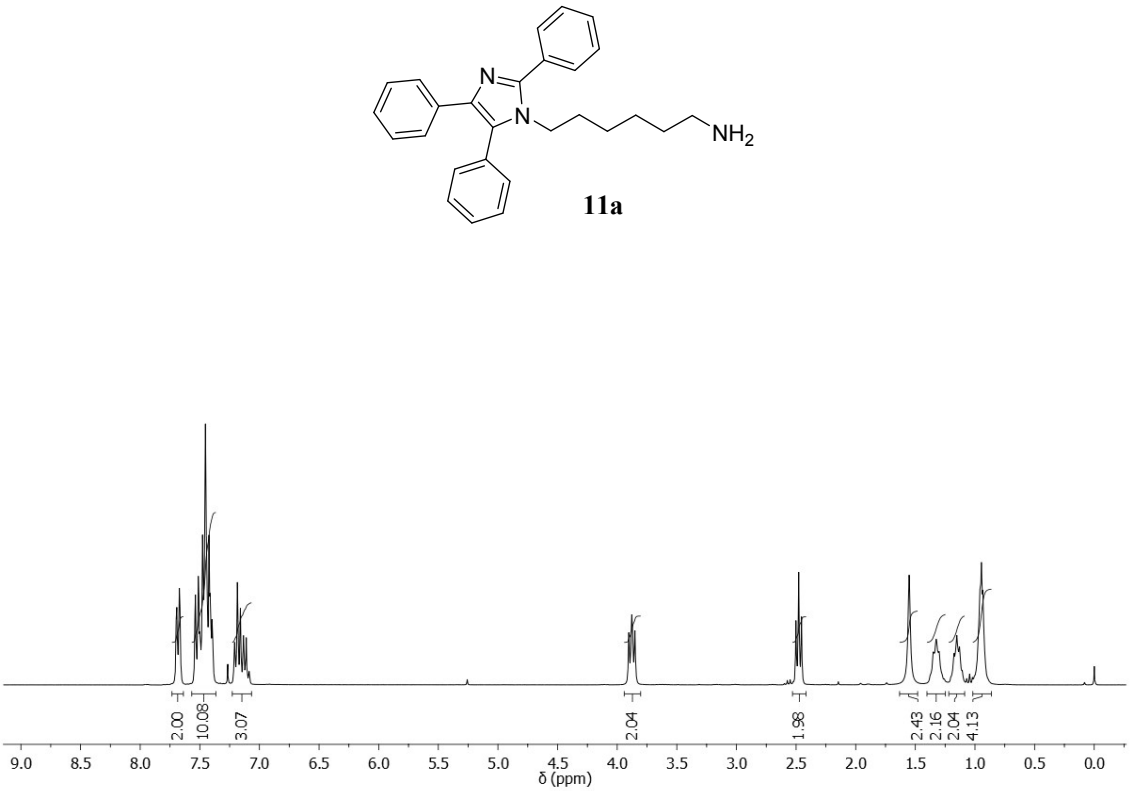


Figure ESI7. ^{1}H NMR Spectrum ($CDCl_3$, 300 MHz) of compound **11a**.

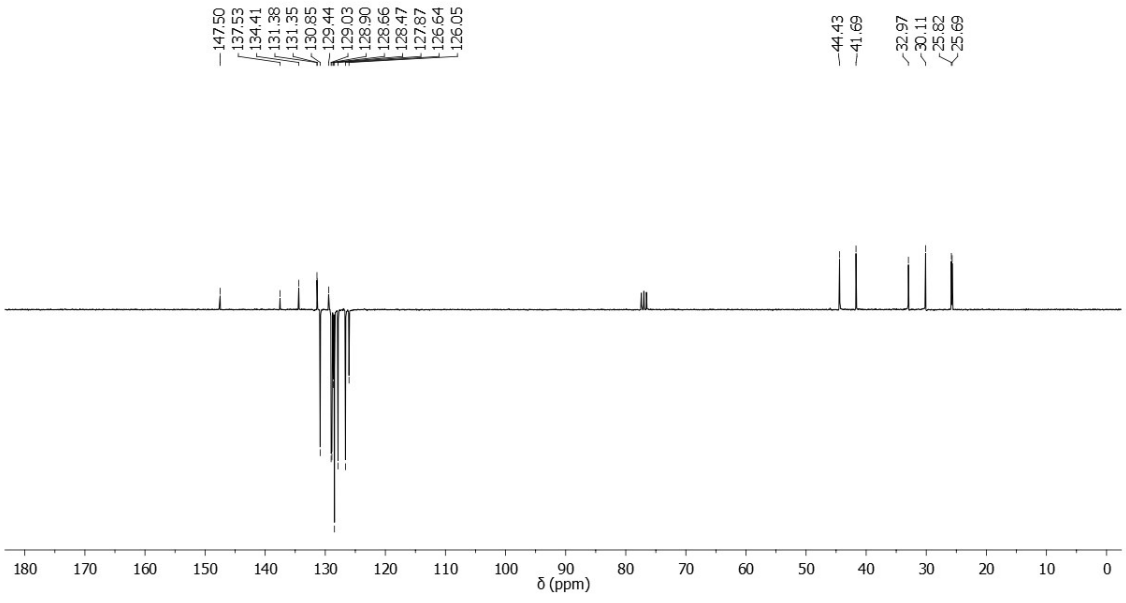


Figure ESI8. ^{13}C NMR Spectrum, APT ($CDCl_3$, 75 MHz) of compound **11a.**

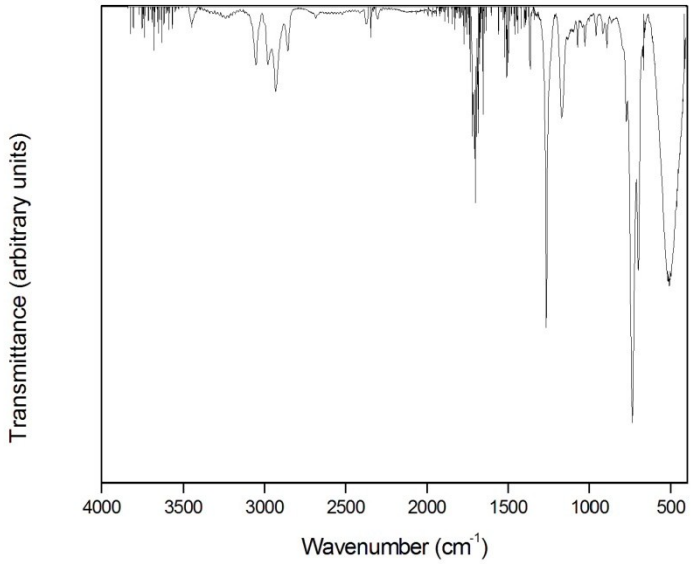
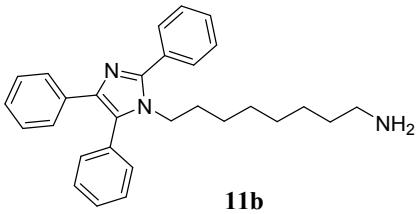


Figure ESI9. IR spectrum (KBr pellet) of compound **11a**.



11b

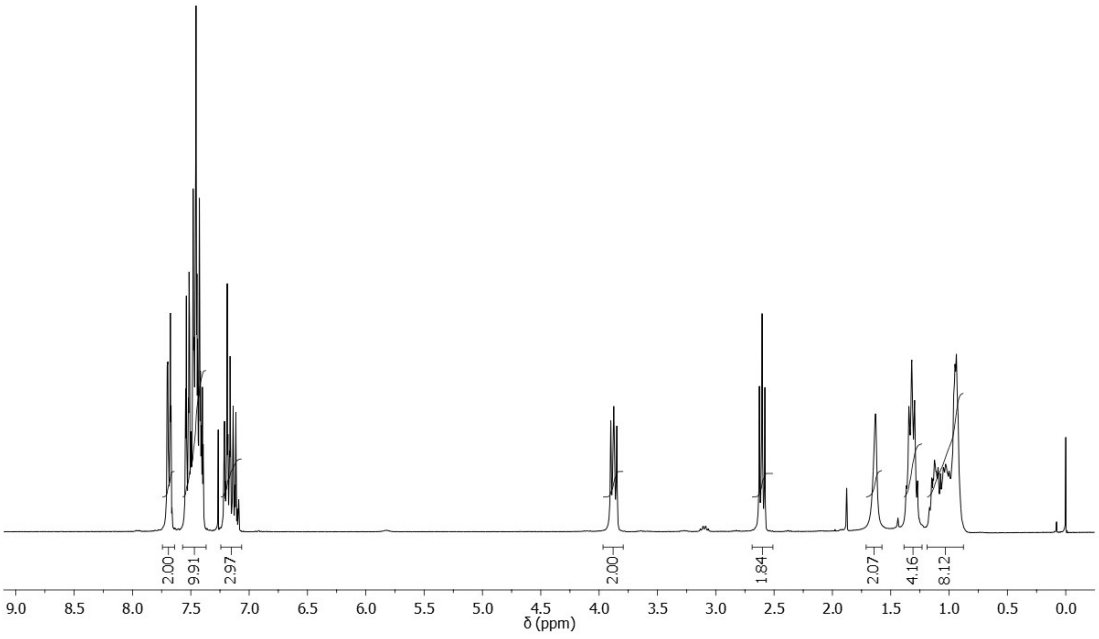


Figure ESI10. ^{1}H NMR Spectrum ($CDCl_3$, 300 MHz) of compound **11b**.

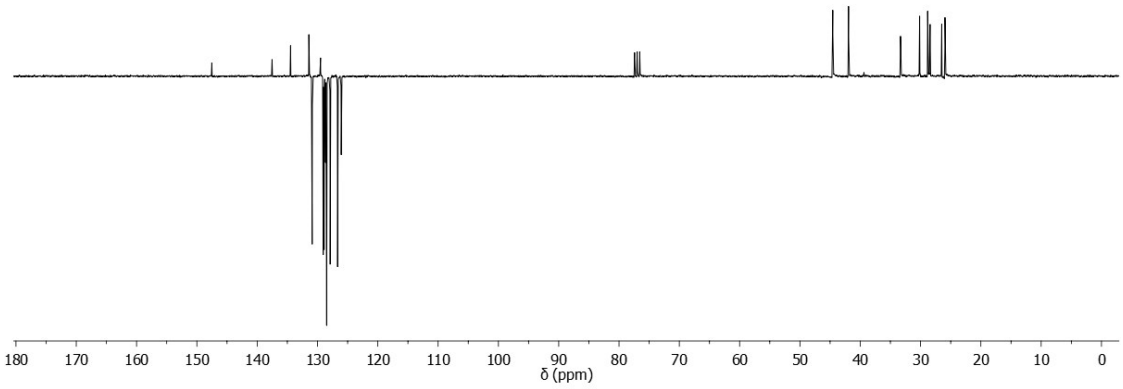


Figure ESI11. ^{13}C NMR Spectrum, APT ($CDCl_3$, 75 MHz) of compound **11b**.

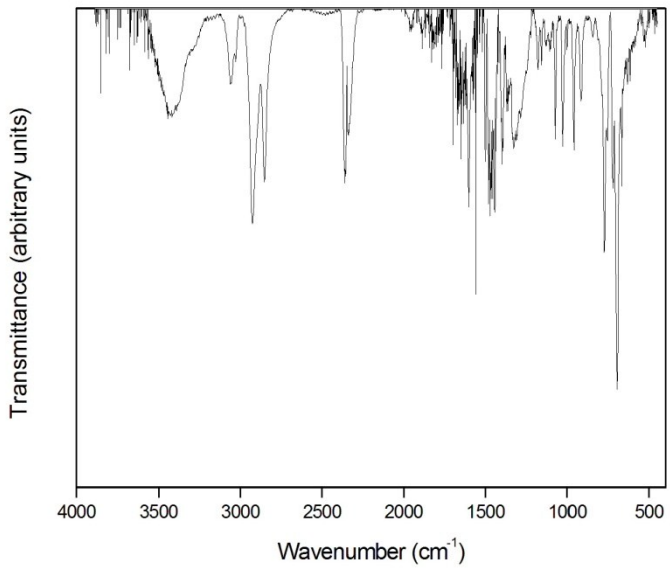


Figure ESI12. FTIR spectrum (KBr pellet) of compound **11b**.

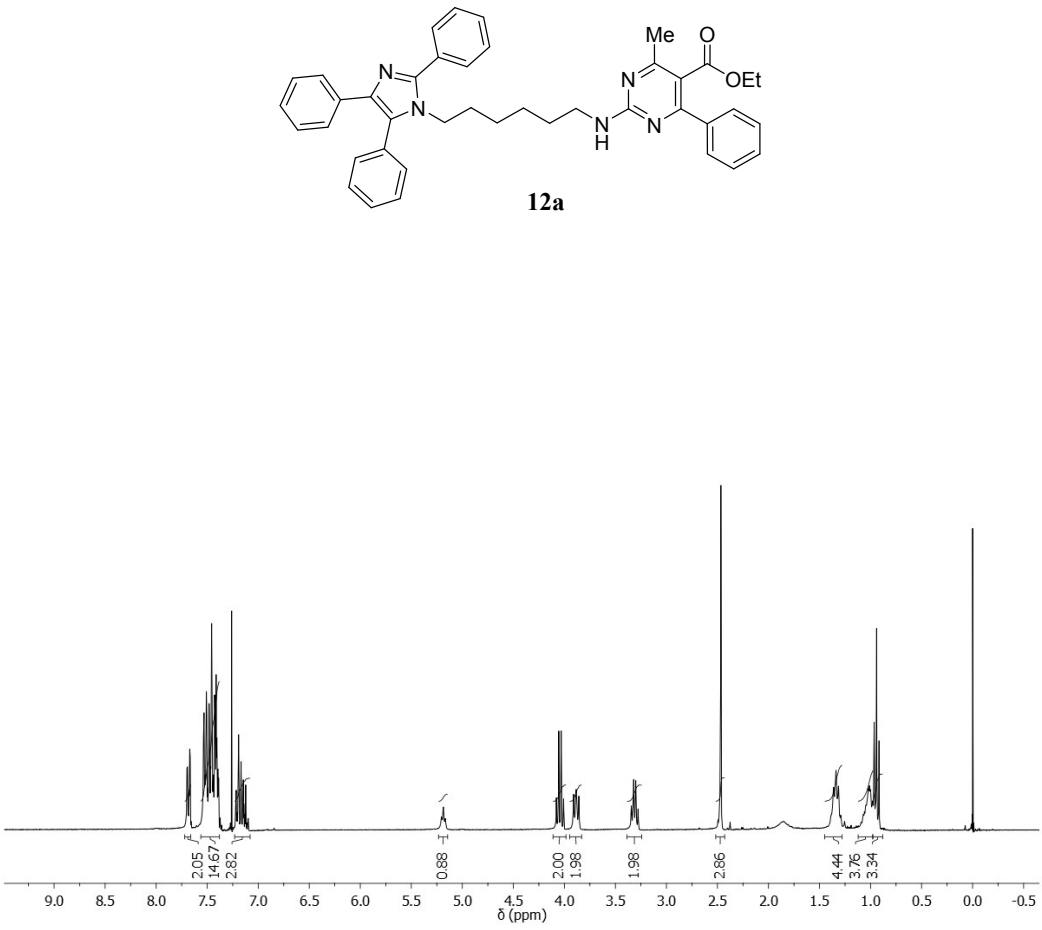


Figure ESI13. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **12a**.

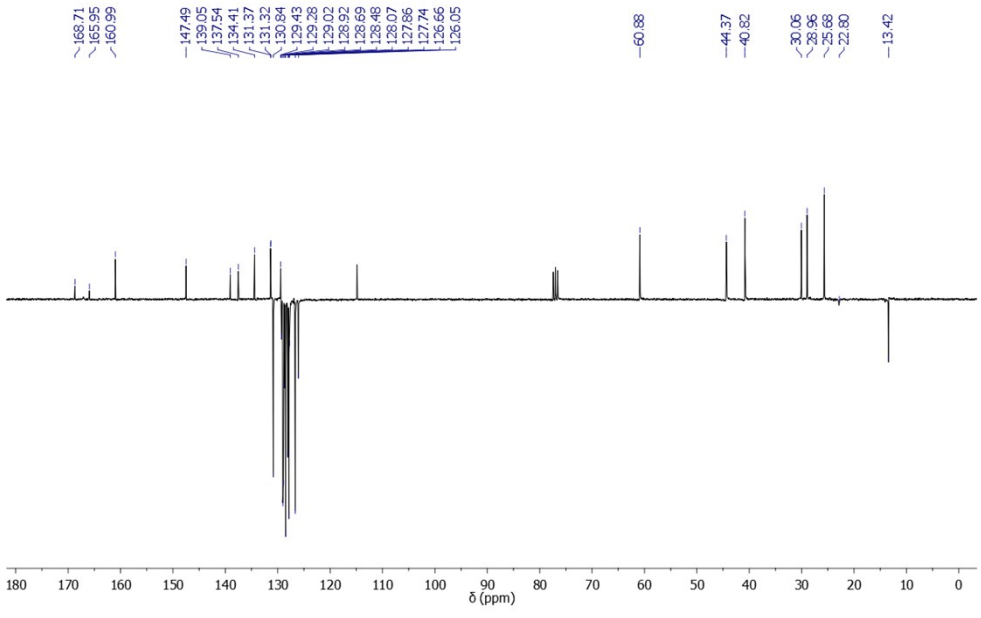


Figure ESI14. ^{13}C NMR spectrum APT (75 MHz, $CDCl_3$) of compound **12a**.

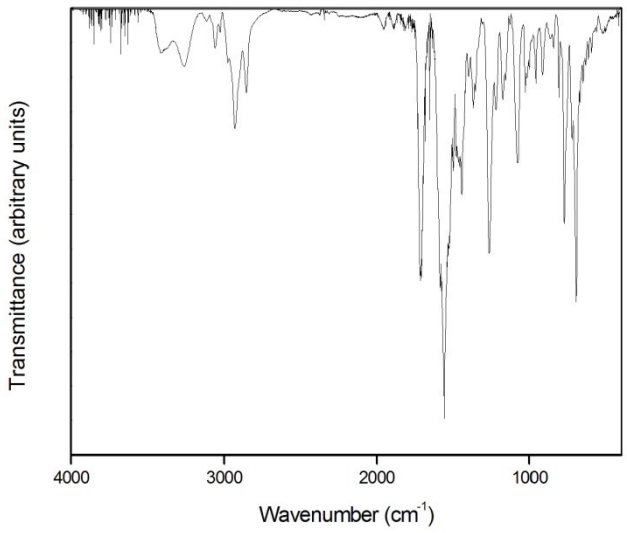
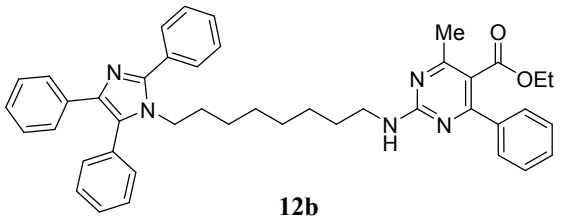


Figure ESI15. FTIR spectrum (KBr pellet) of compound **12a**.



12b

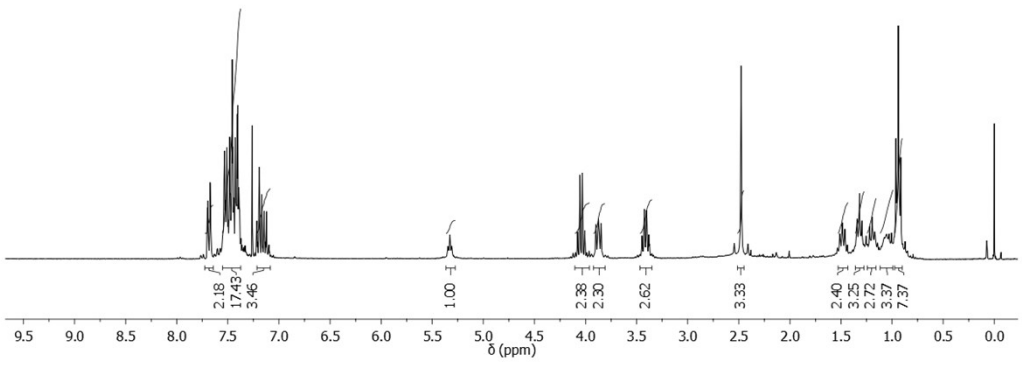


Figure ESI16. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **12b**.

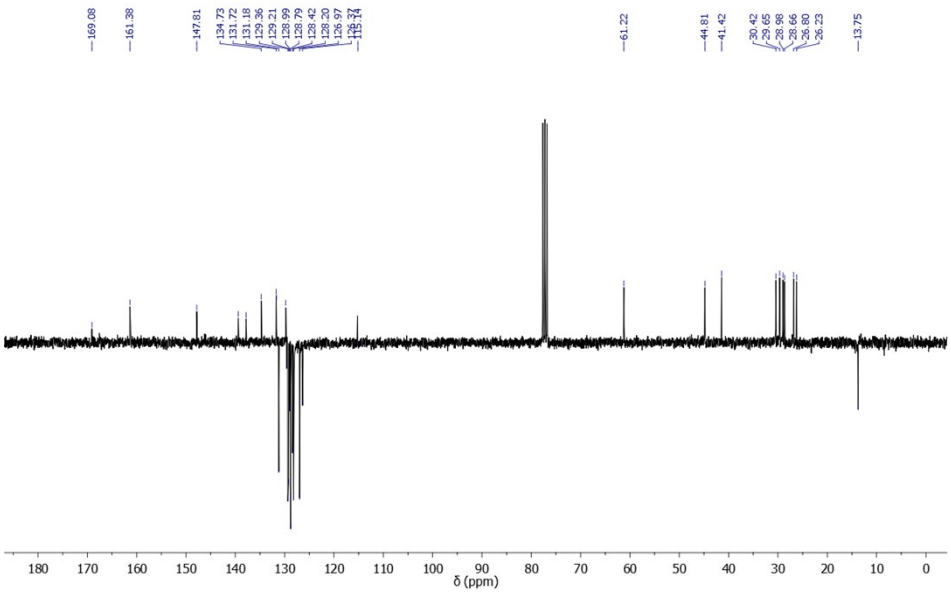


Figure ESI17. ^{13}C NMR spectrum APT (75 MHz, $CDCl_3$) of compound **12b**.

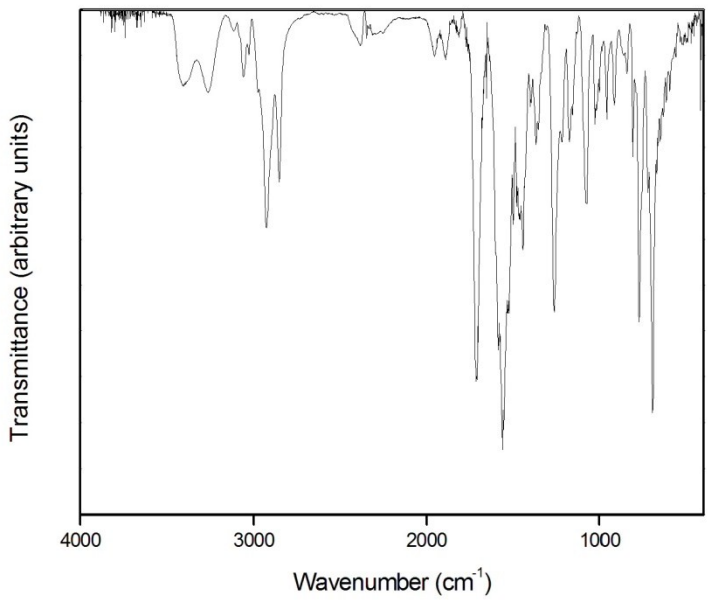


Figure ESI18. FTIR spectrum (KBr pellet) of compound **12b**.

Additional theoretical data

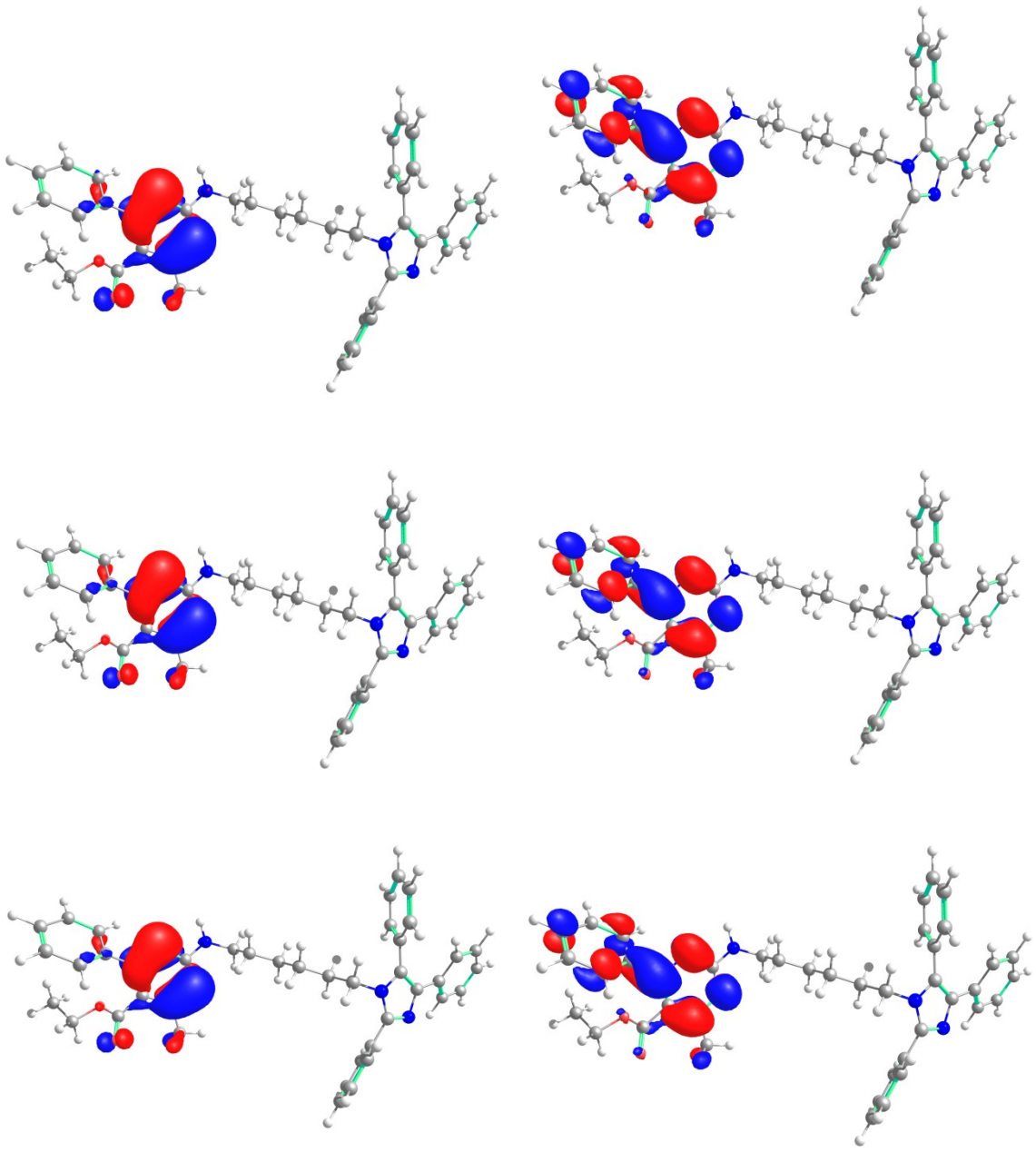


Figure ESI19. HOMO-1/LUMO pair is assigned to the NTOs for the $S_0 \rightarrow S_1$ transitions, for the 1,4-dioxane, MeCN and EtOH solvents (top to bottom, respectively).

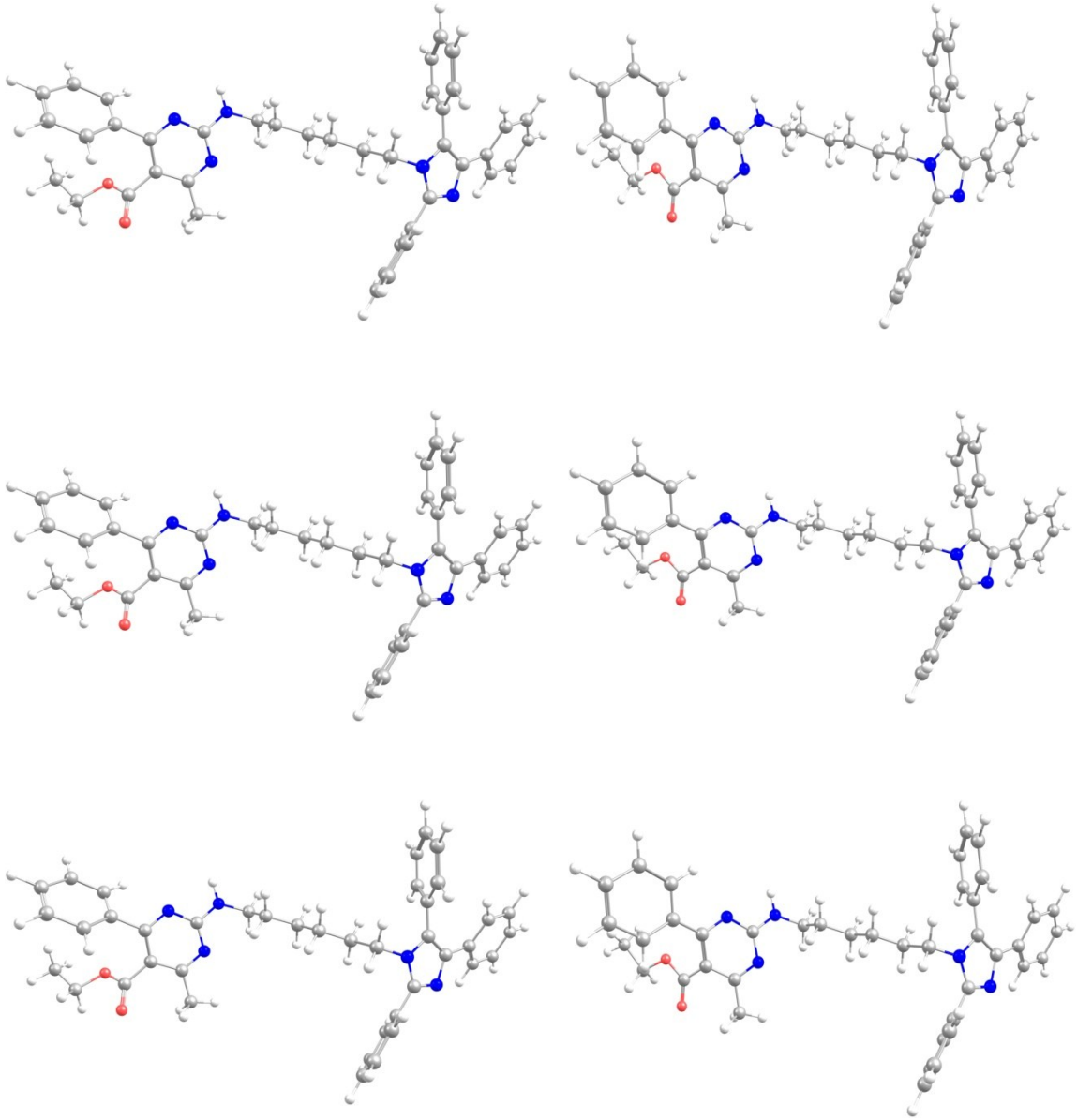


Figure ESI20. Geometries S_0 and S_1, for the solvents 1,4-dioxane, MeCN and EtOH (top to bottom, respectively).

Additional photophysical data

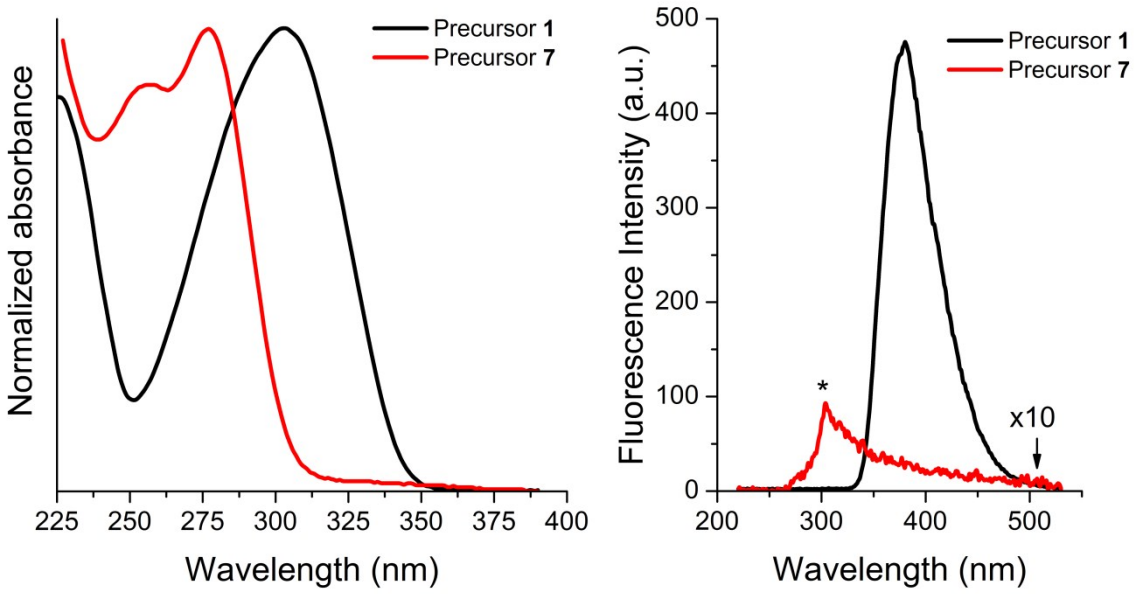


Figure ESI21 (Left) Normalized UV-Vis and (right) fluorescence emission spectra of lophine **(1)** and pyrimidine **(7)** precursors in ethanol.

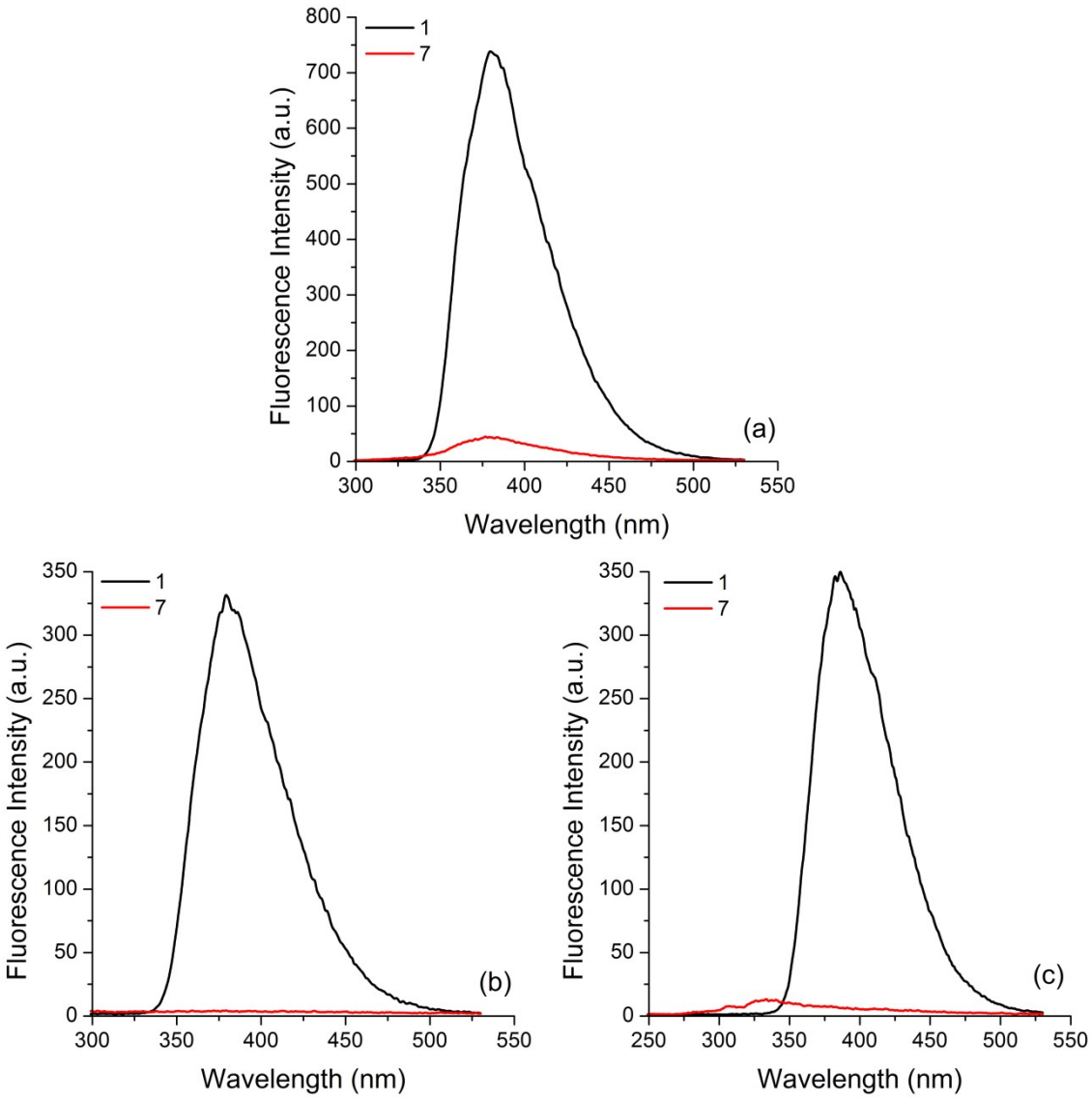


Figure ESI22 Fluorescence emission spectra in solution of lophine **(1)** and pyrimidine **(7)** precursors in (a) 1,4-dioxane, (b) acetonitrile and (c) DMSO at the same concentration.

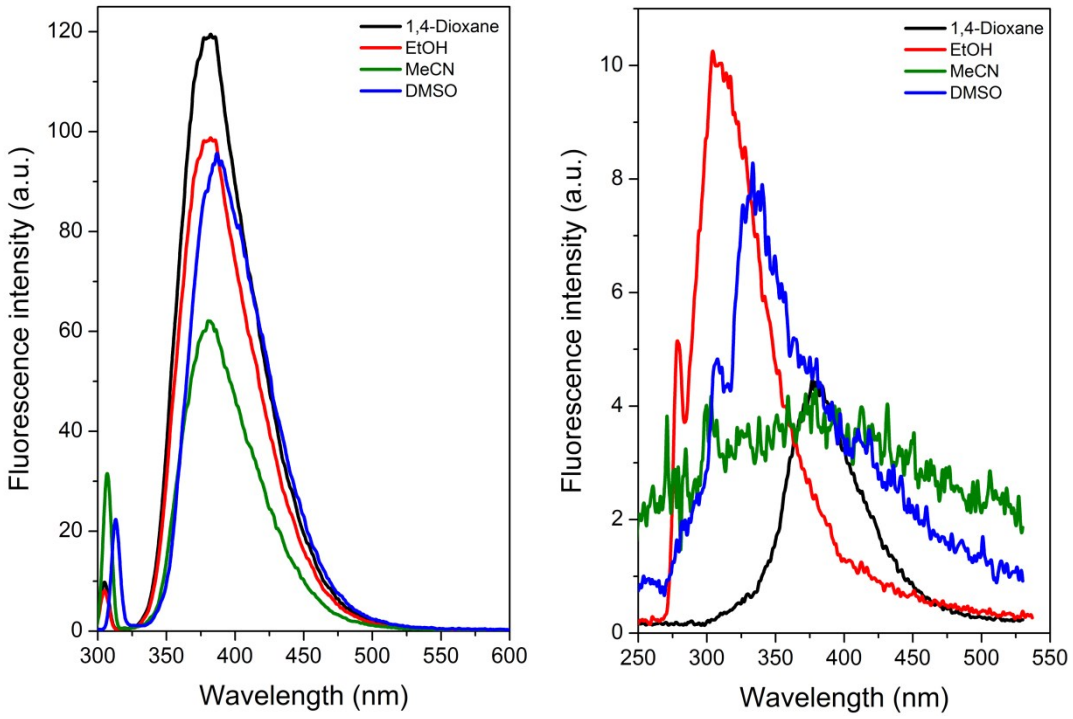


Figure ESI23 Fluorescence emission spectra in solution of lophine **(1)** and pyrimidine **(7)** precursors at the same concentration of the molecular hybrids.

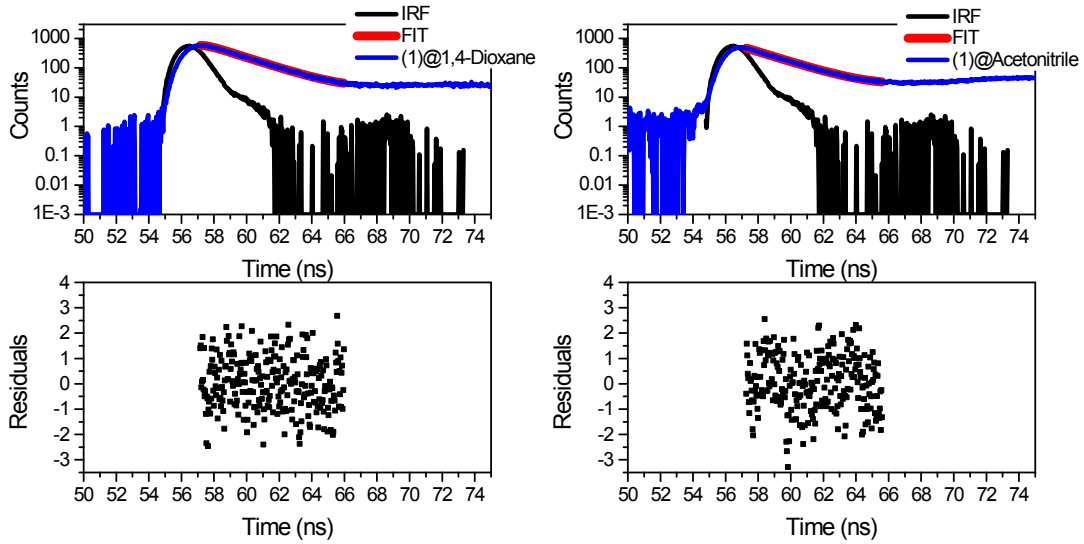


Figure ESI24 Residuals from time resolved fluorescence emission spectra of precursor **1**.

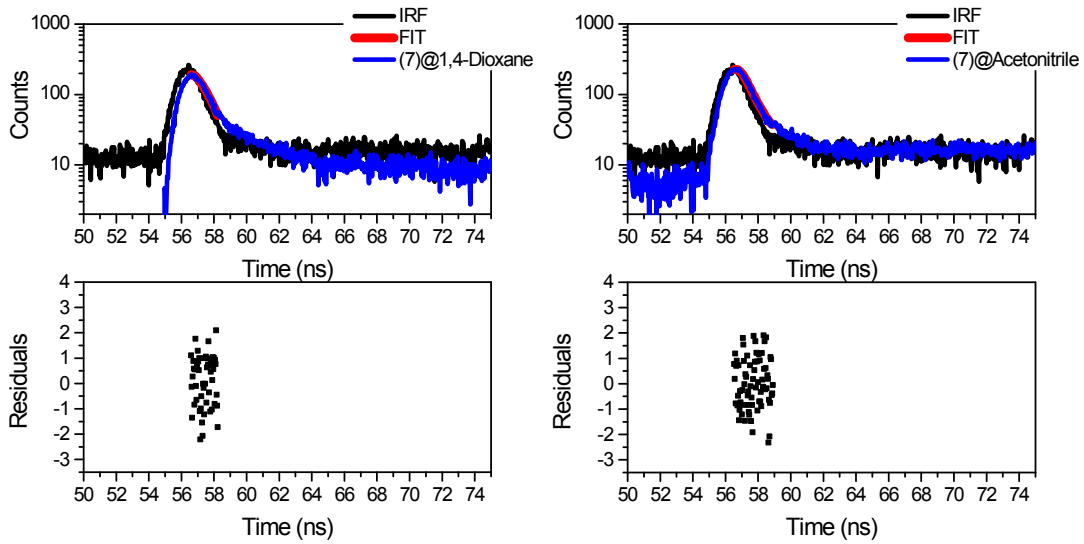


Figure ESI25 Residuals from time resolved fluorescence emission spectra of precursor **7**.

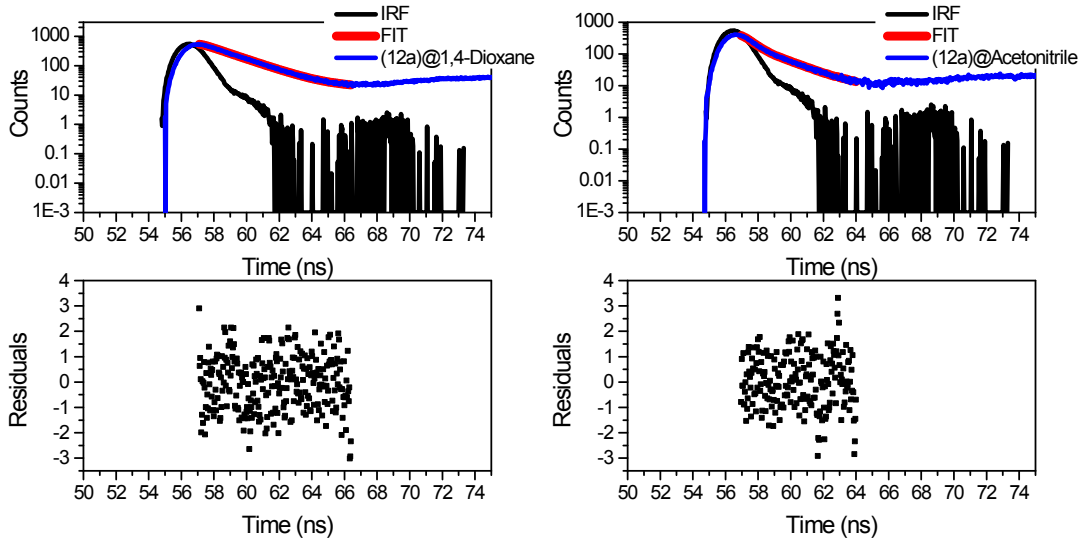


Figure ESI26 Residuals from time resolved fluorescence emission spectra of **12a**.

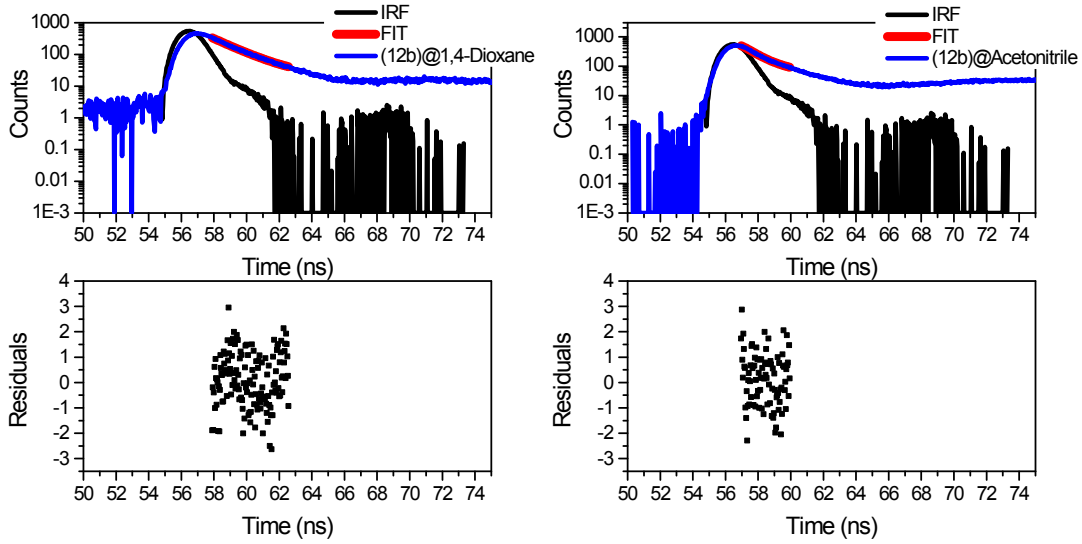


Figure ESI27 Residuals from time resolved fluorescence emission spectra of **12b**.