Alkyl Tail Variation on Chalcone-based Quaternary Pyridinium Salts as Rule-of-Thumb for Antimicrobial Activity

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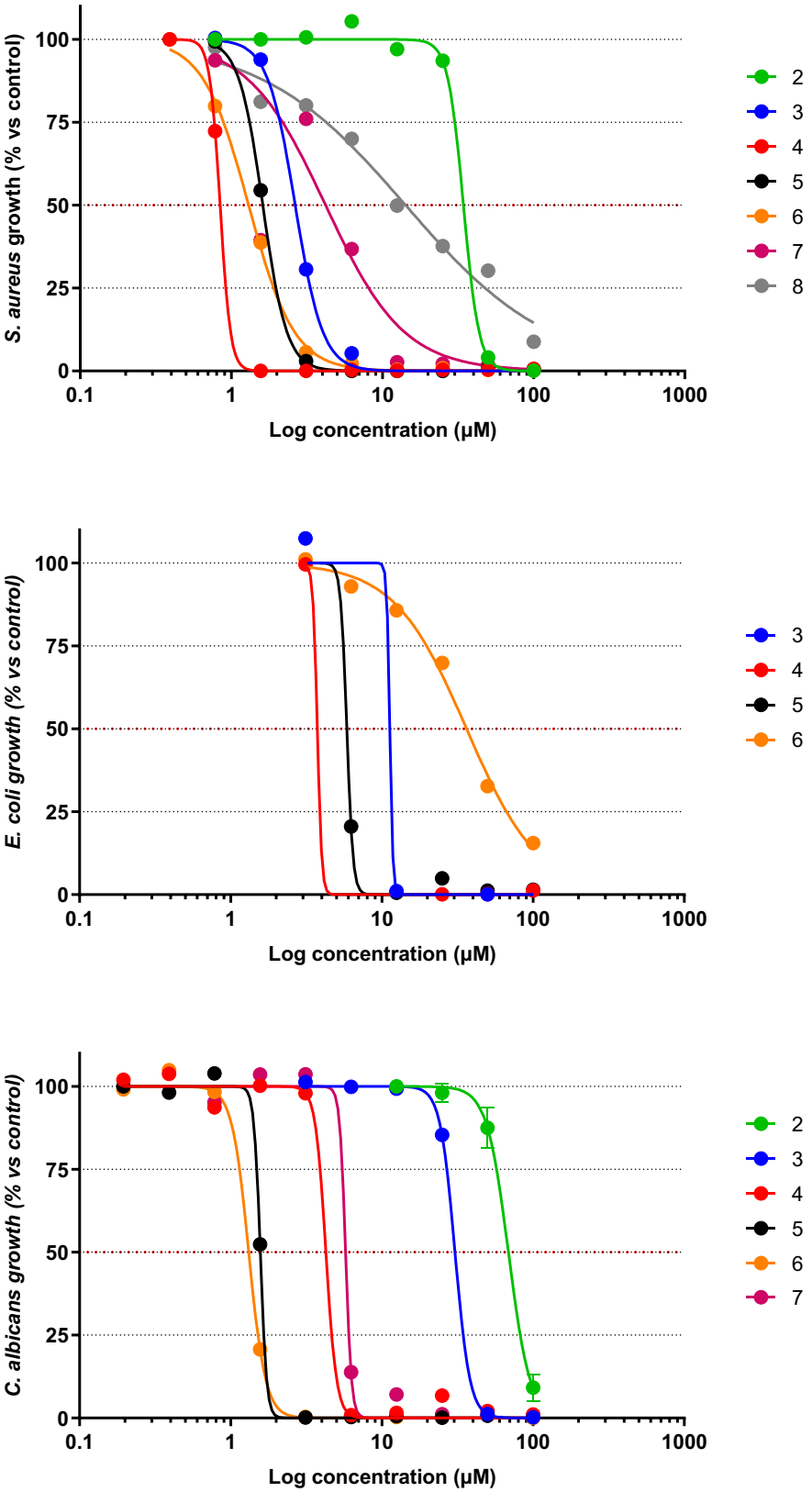


Figure S1. Dose-response curves of the active chalcone-based QPySs on the tested reference strains. Curves are obtained by using a nonlinear regression equation and a variable slope model (log(inhibitor) vs. normalised response -- Variable slope (GraphPad Prism version 9.4.1 for Windows).

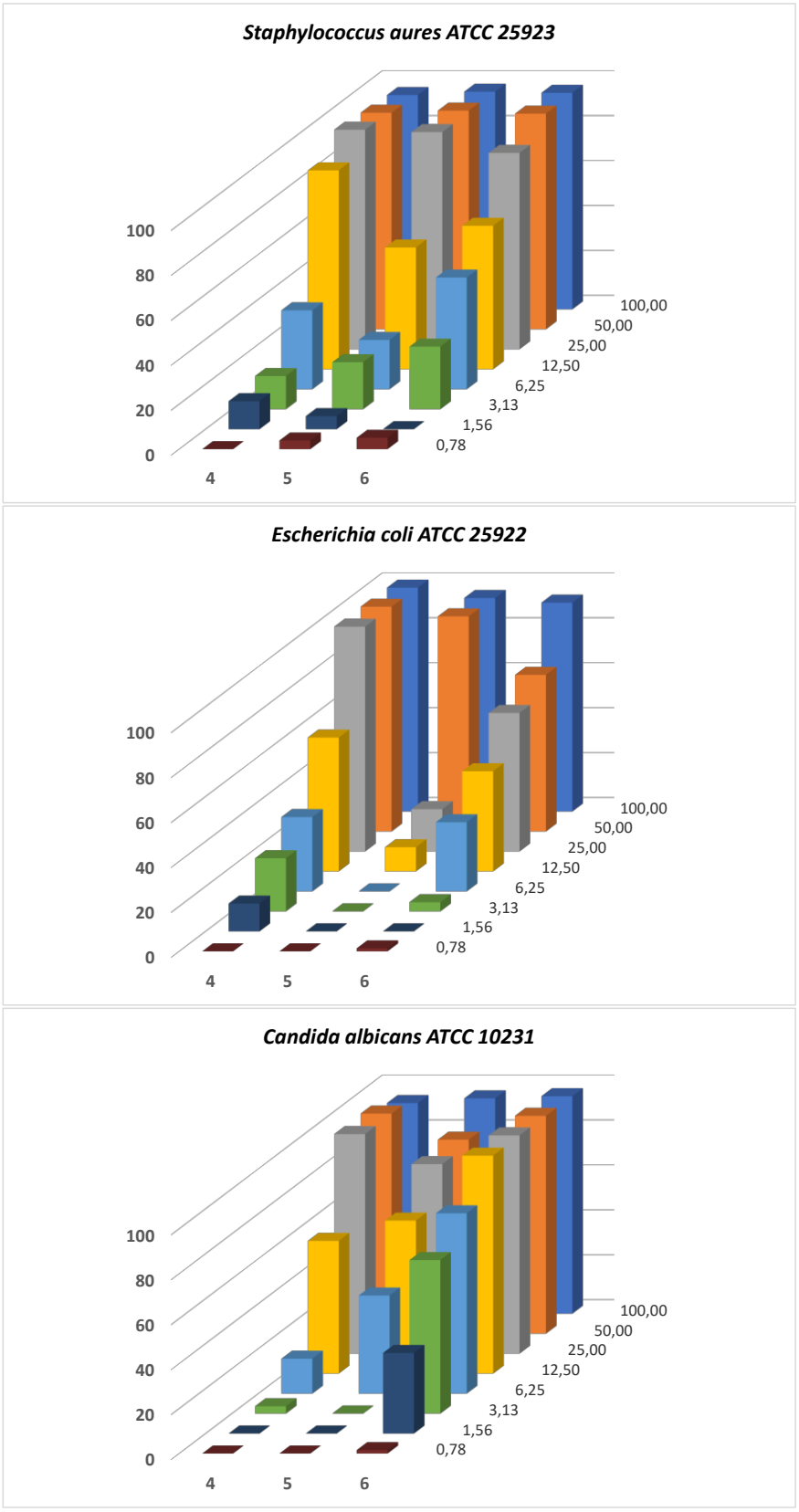
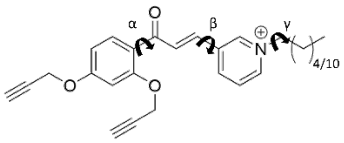


Figure S2. Antibiofilm activity of the chalcone-based QPySs (4-6) on the tested reference strains. Data are the mean percentage values of the biofilm biomass determined by CV staining of the compounds at the different concentrations relative to the untreated biofilms.



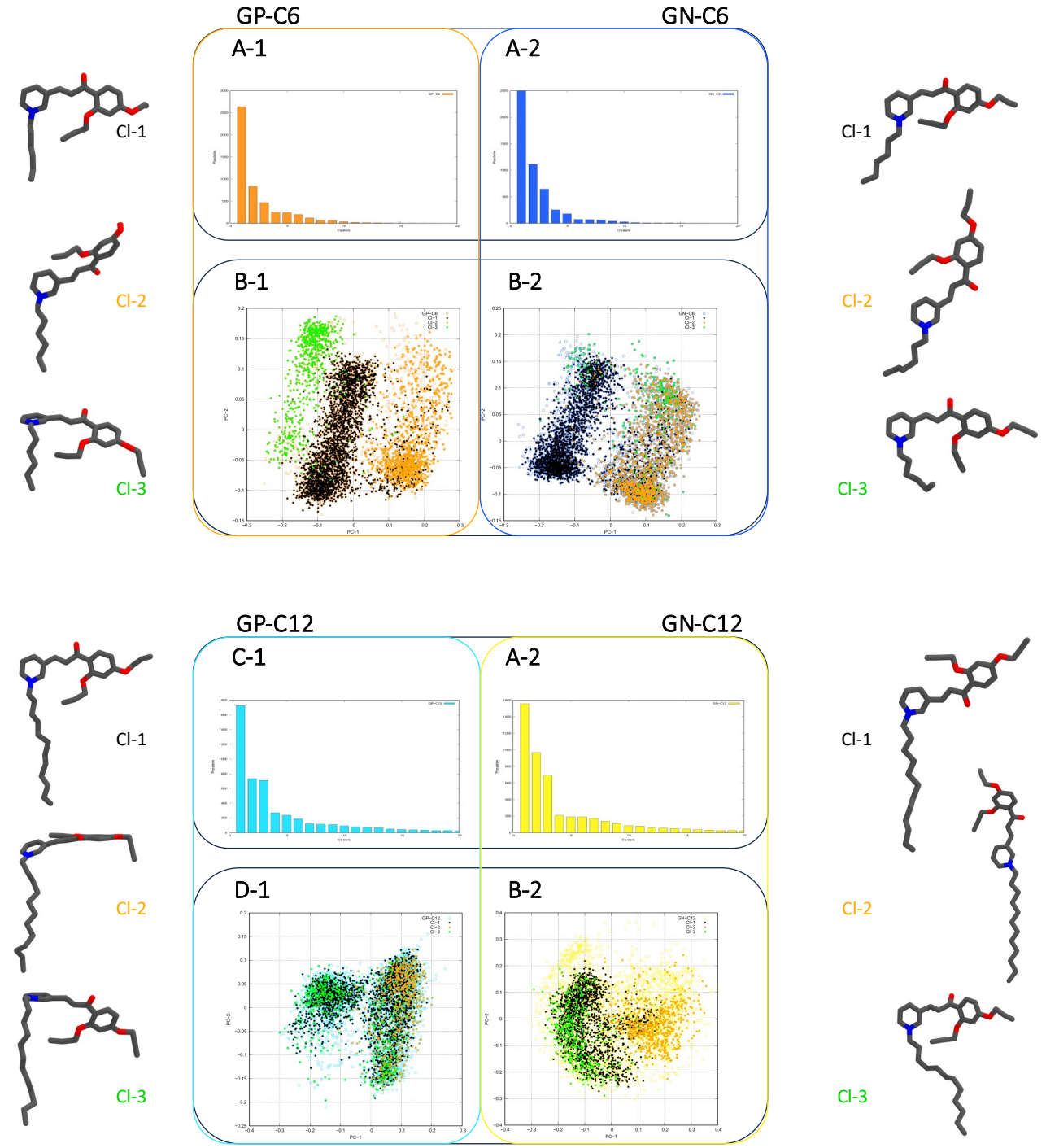
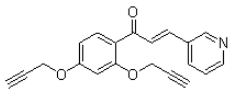


Figure S3. Cluster Analysis of QPySs 2 and 5. All dihedral angles were considered to cluster the ligands. The Gromos method was used adopting a 1.25 Å for the RMSD cut-off. QPySs structures corresponding to the three main clusters are represented for comparison. Each structure belonging to the three main clusters is also projected on the first two components obtained from a Principal Component Analysis performed considering α,β,γ dihedral angles.

NMR spectra



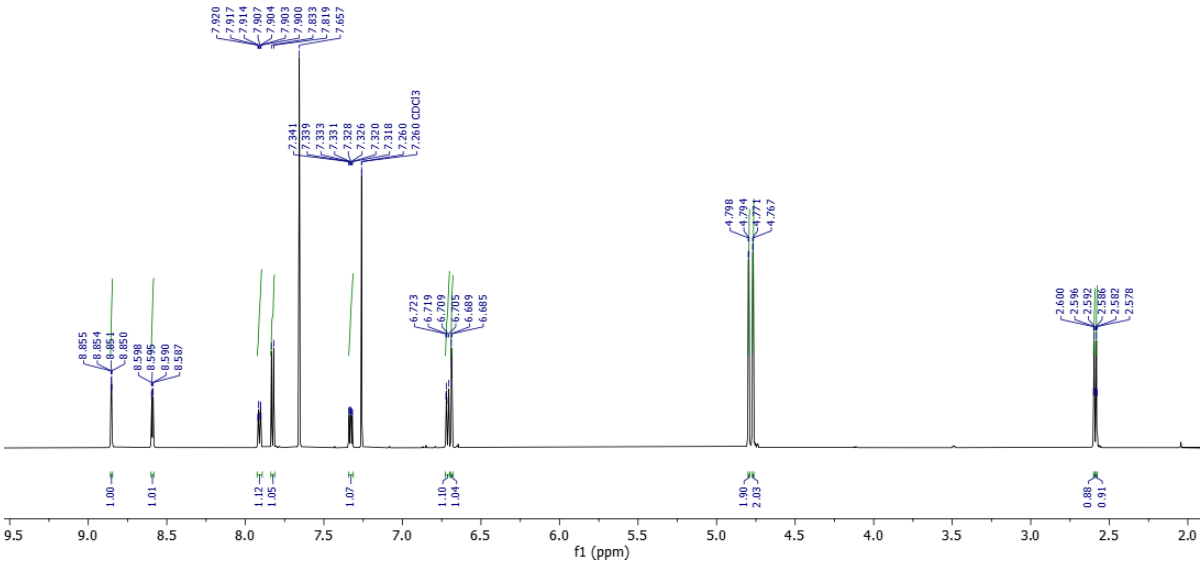


Figure S4. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **1**.

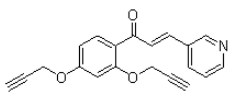


Figure S5. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **1**.

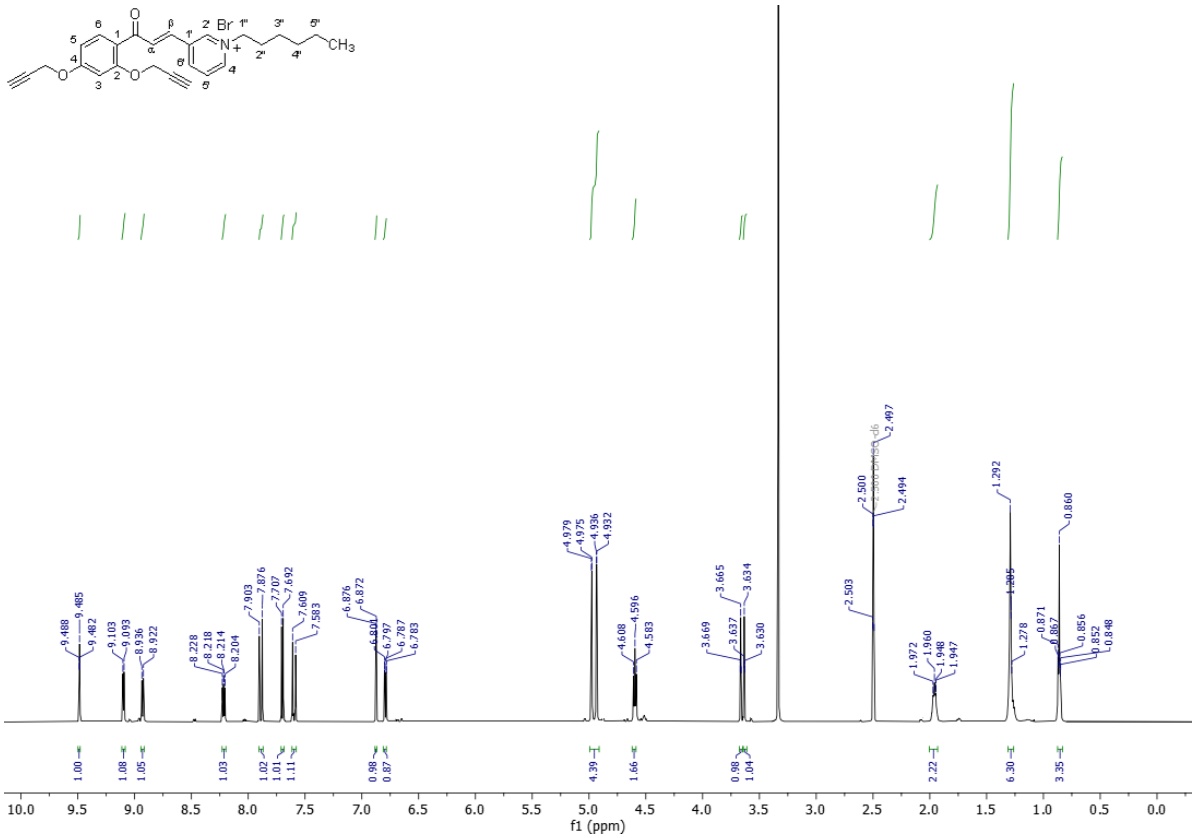


Figure S6. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **2**.

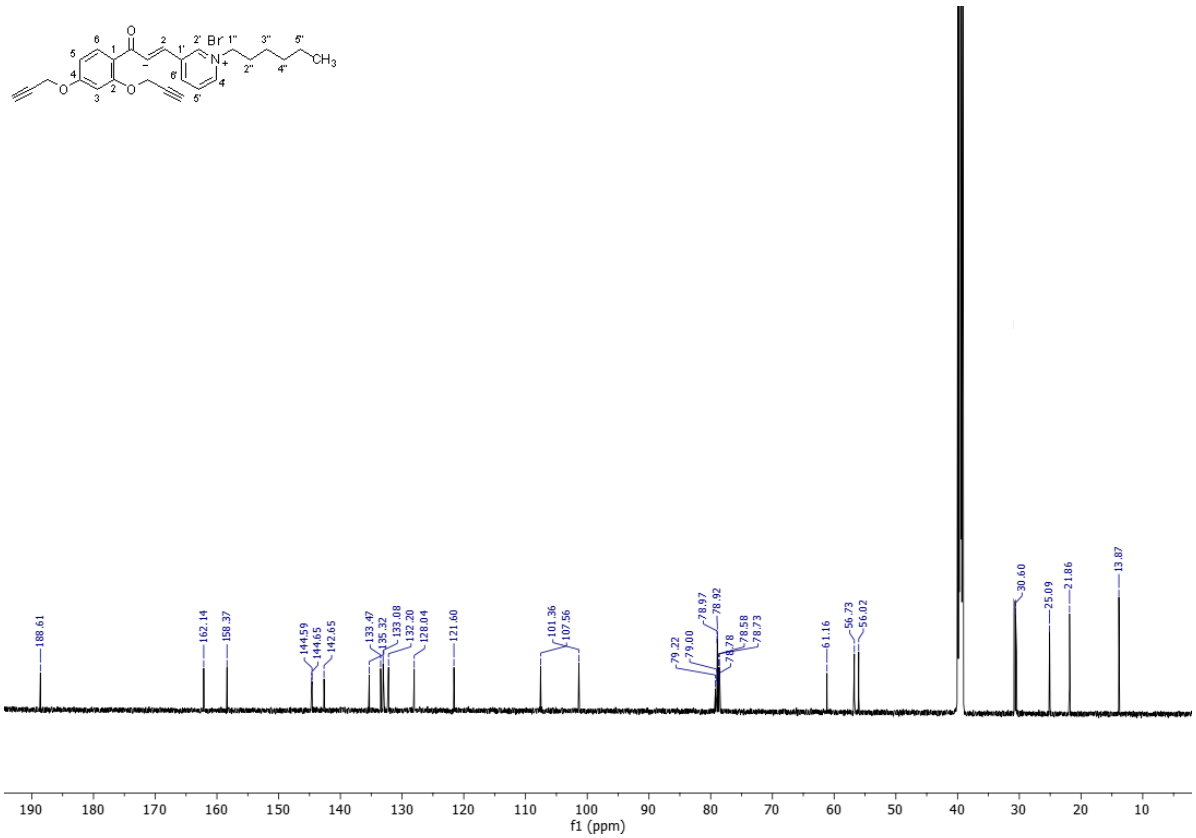


Figure S7. ^{13}C NMR spectrum (151 MHz, DMSO-d_6) of compound **2**.

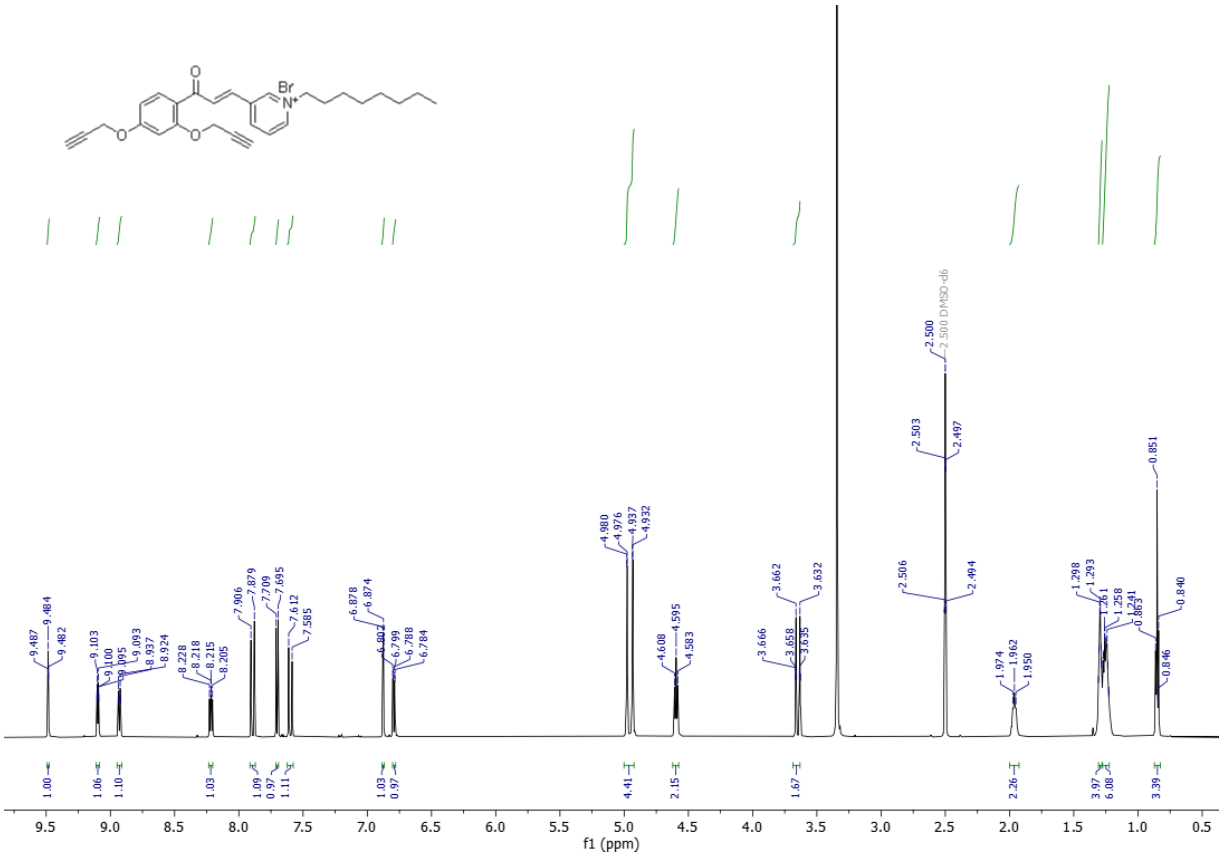


Figure S8. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **3**.

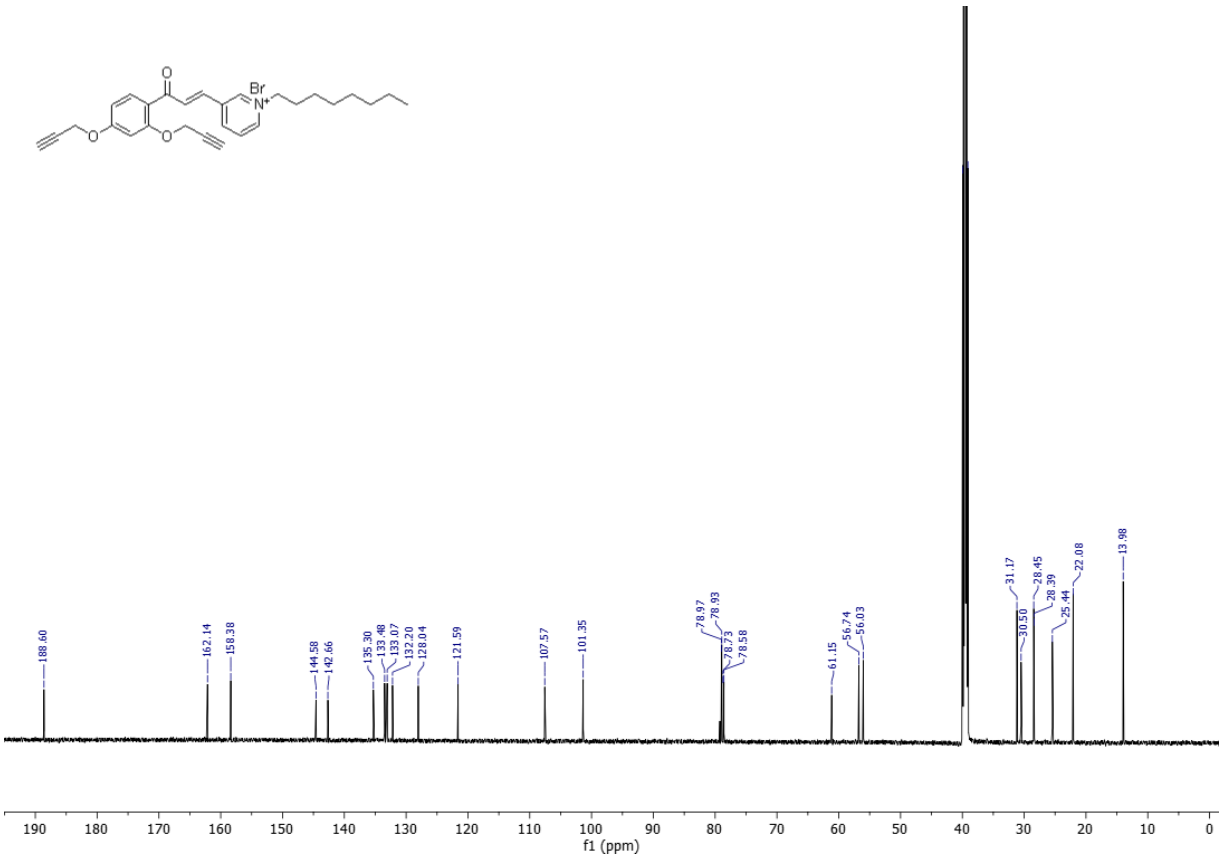


Figure S9. ^{13}C NMR spectr*um* (151 MHz, DMSO-d_6) of compound **3**.

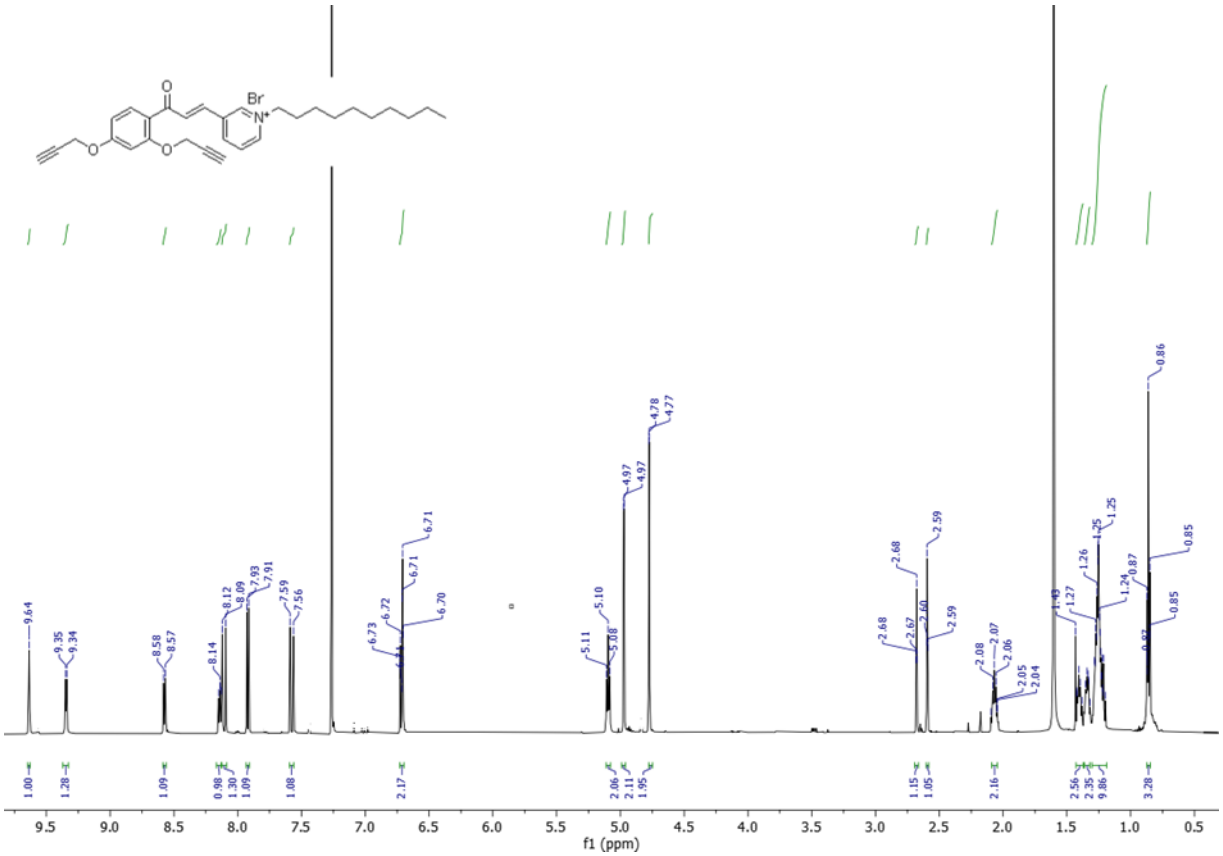


Figure S10. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **4**

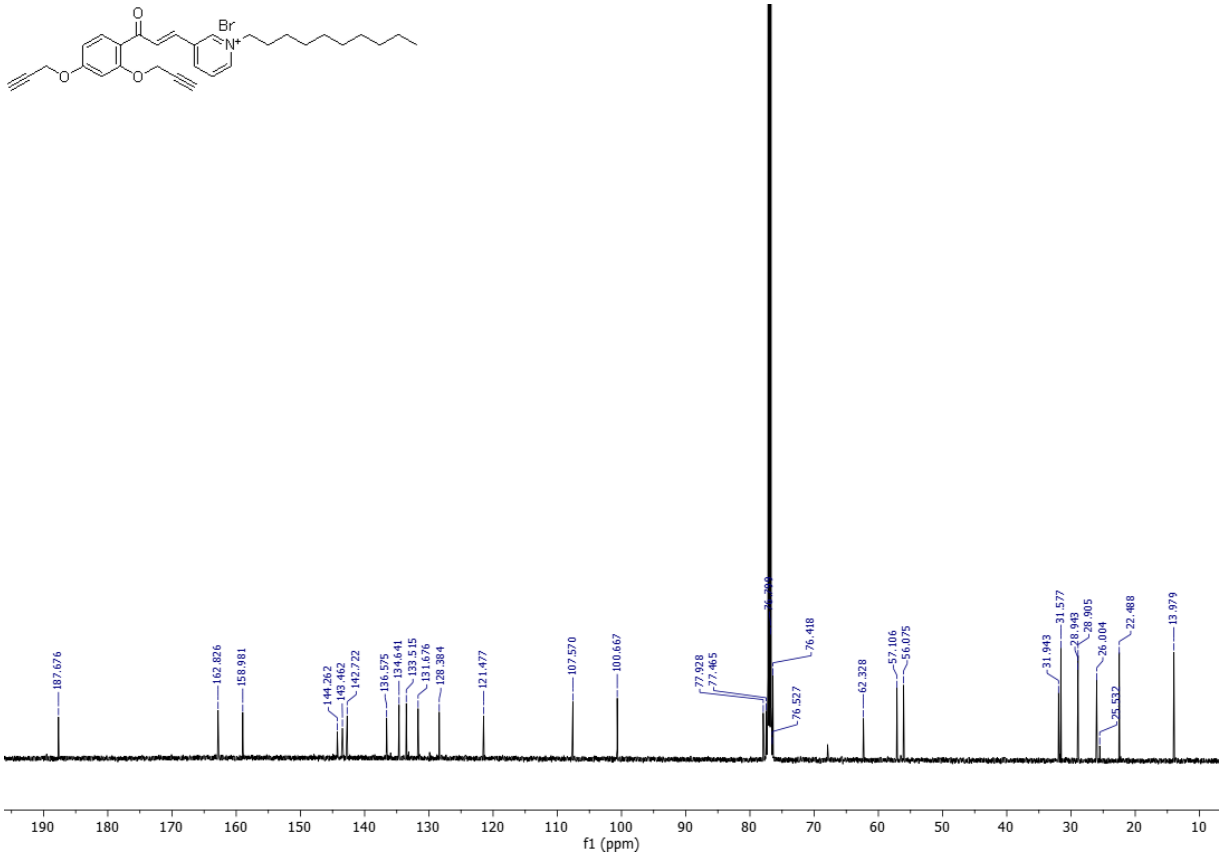


Figure S11. ^{13}C NMR spectrum (151 MHz, $CDCl_3$) of compound **4**

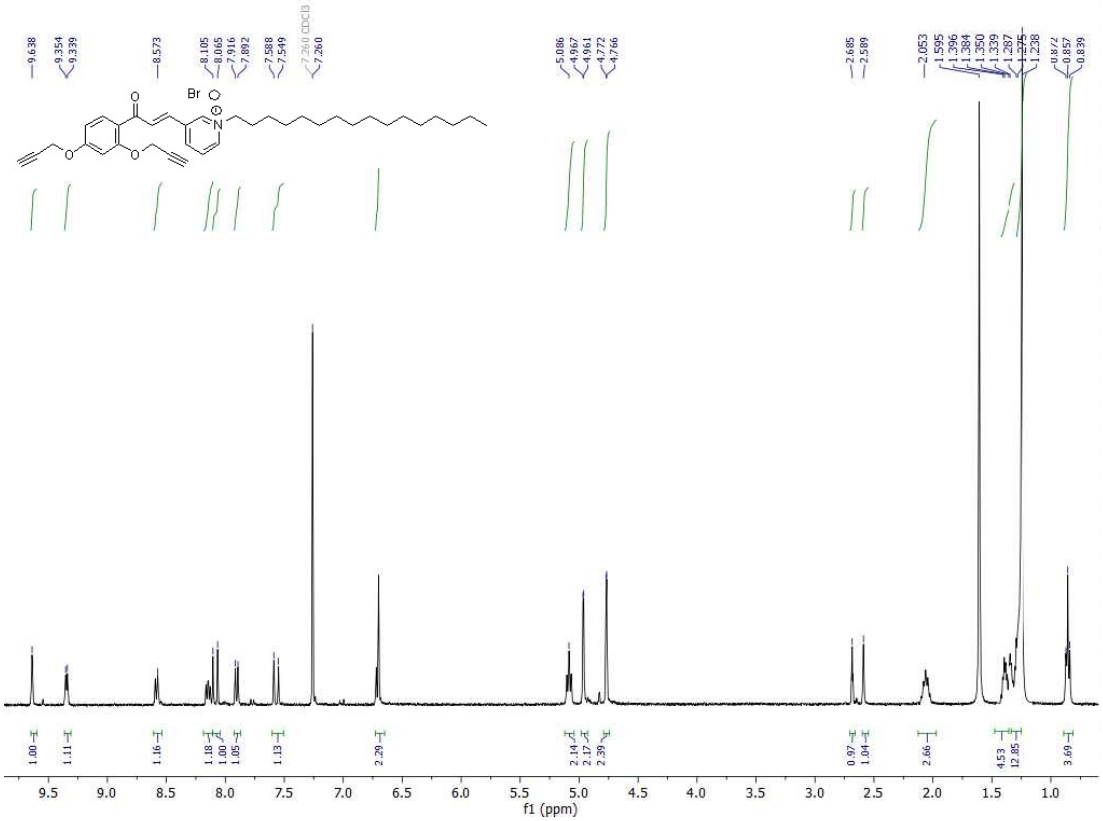


Figure S12. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **5**.

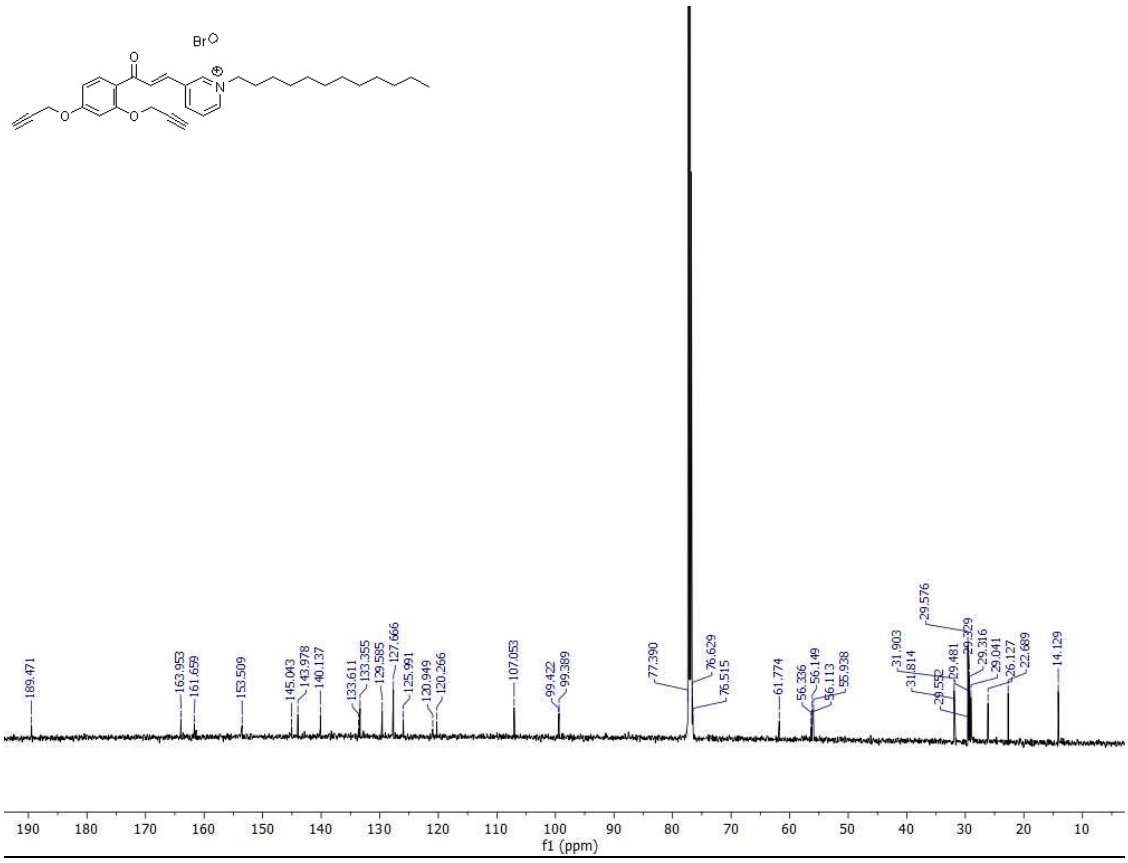


Figure S13. ^{13}C NMR spectrum (400 MHz, $CDCl_3$) of compound **5**.

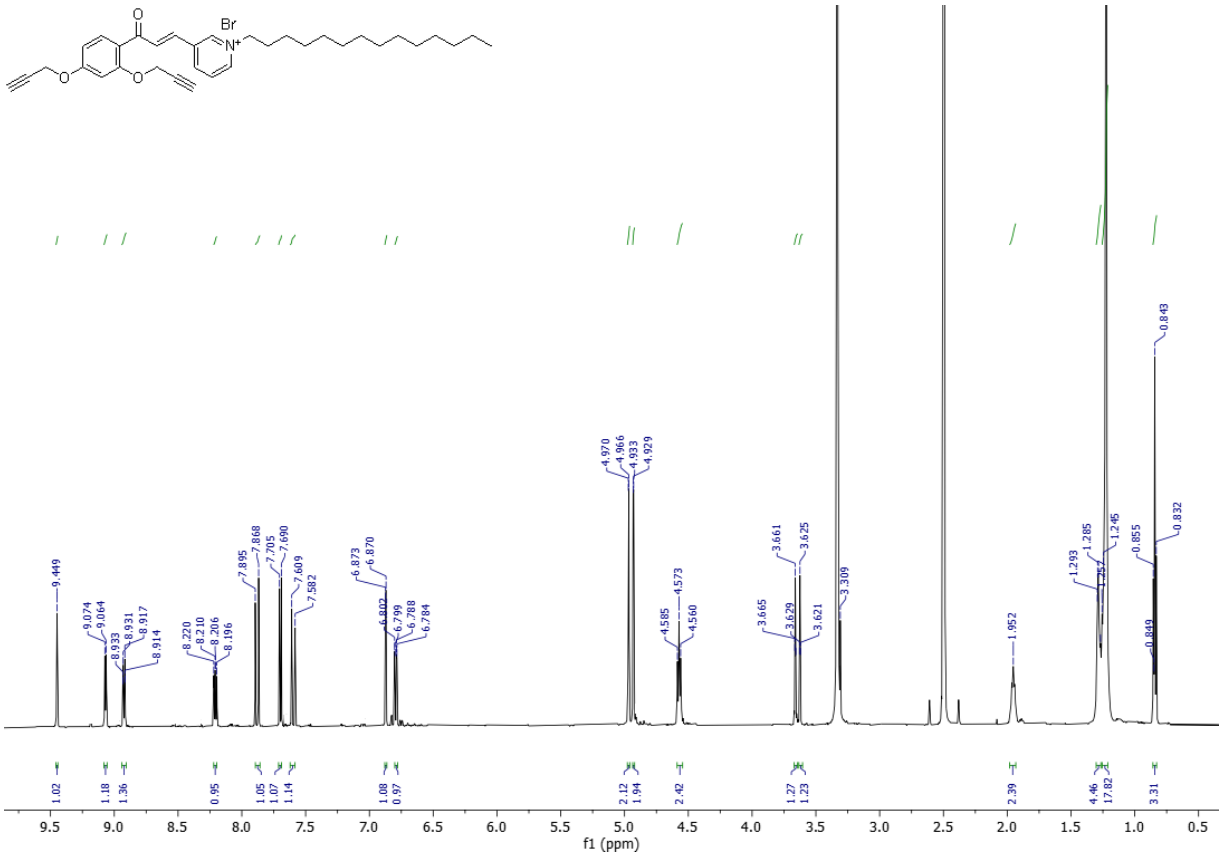


Figure S14. ^{1}H NMR spectr*um* (600 MHz, $CDCl_3$) of compound **6.**

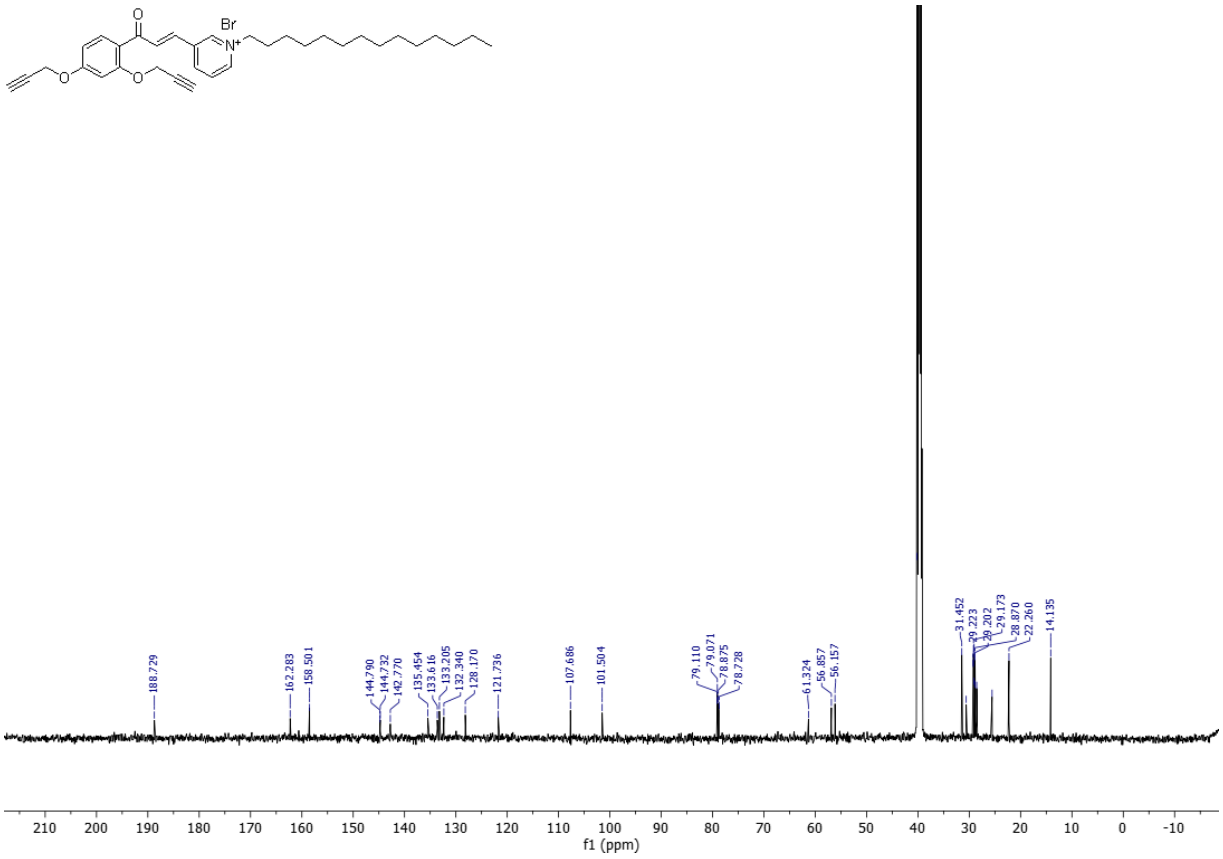


Figure S15. ^{13}C NMR spectr*um* (151 MHz, $CDCl_3$) of compound **6.**

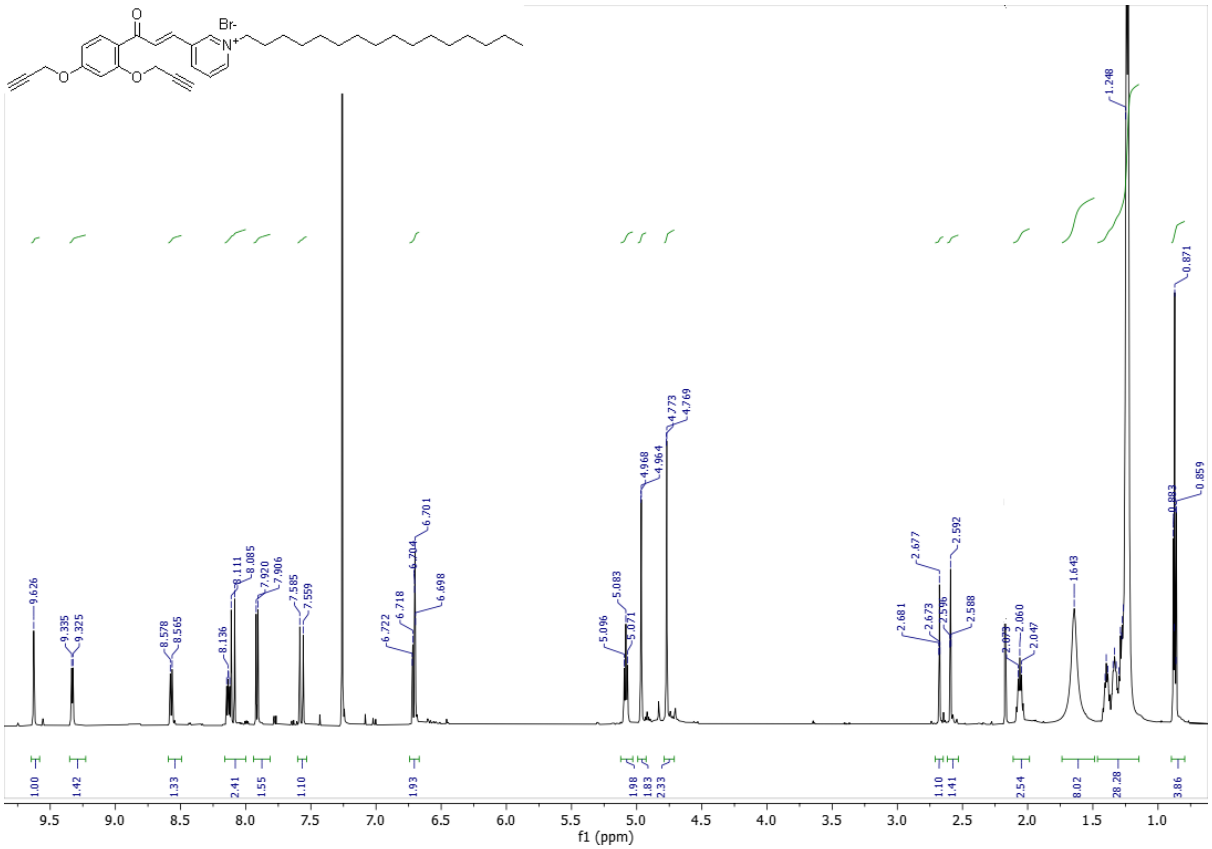


Figure S16. ^{1}H NMR spectr*um* (600 MHz, $CDCl_3$) of compound **7.**

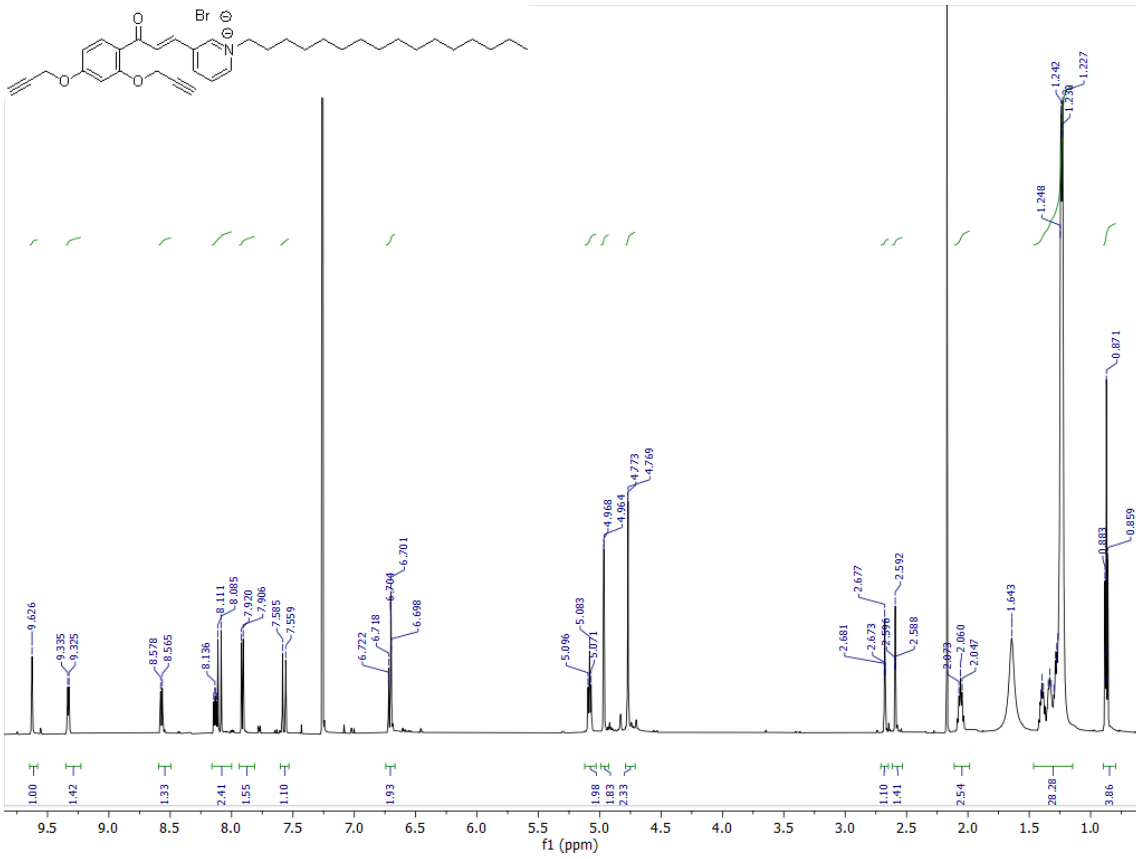
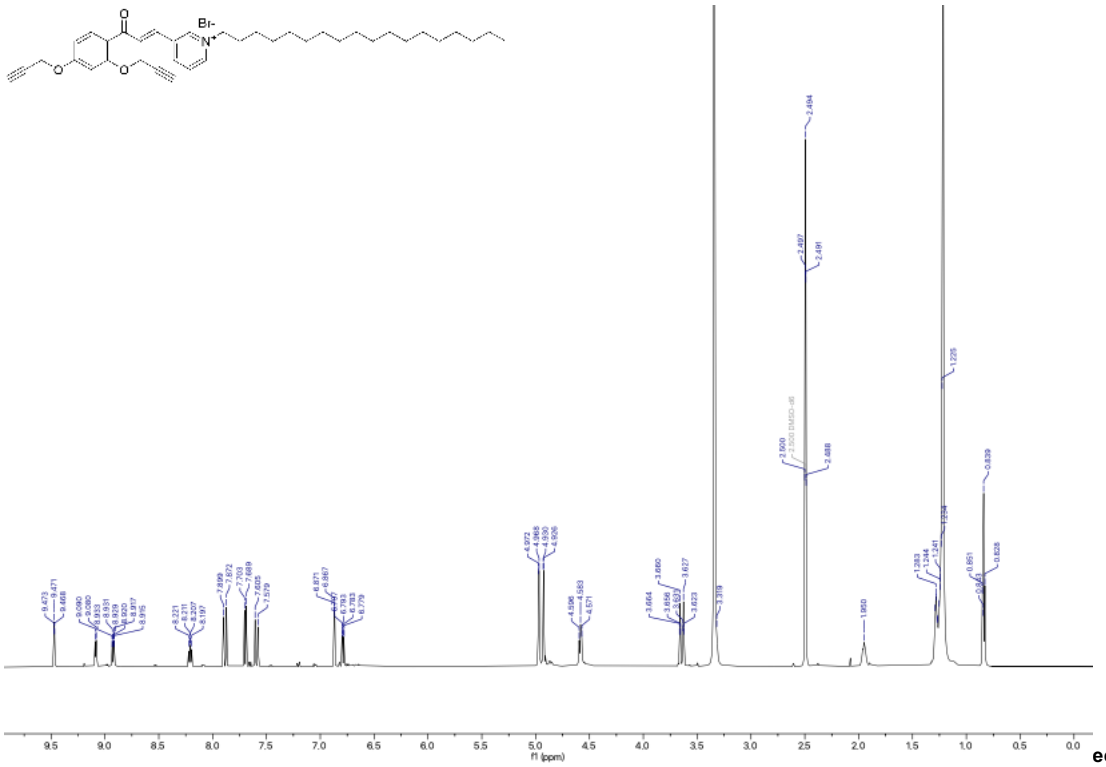


Figure S17. ^{13}C NMR spectr*um* (151 MHz, $CDCl_3$) of compound **7**



ectra (600 MHz,

Figure S18. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **8**

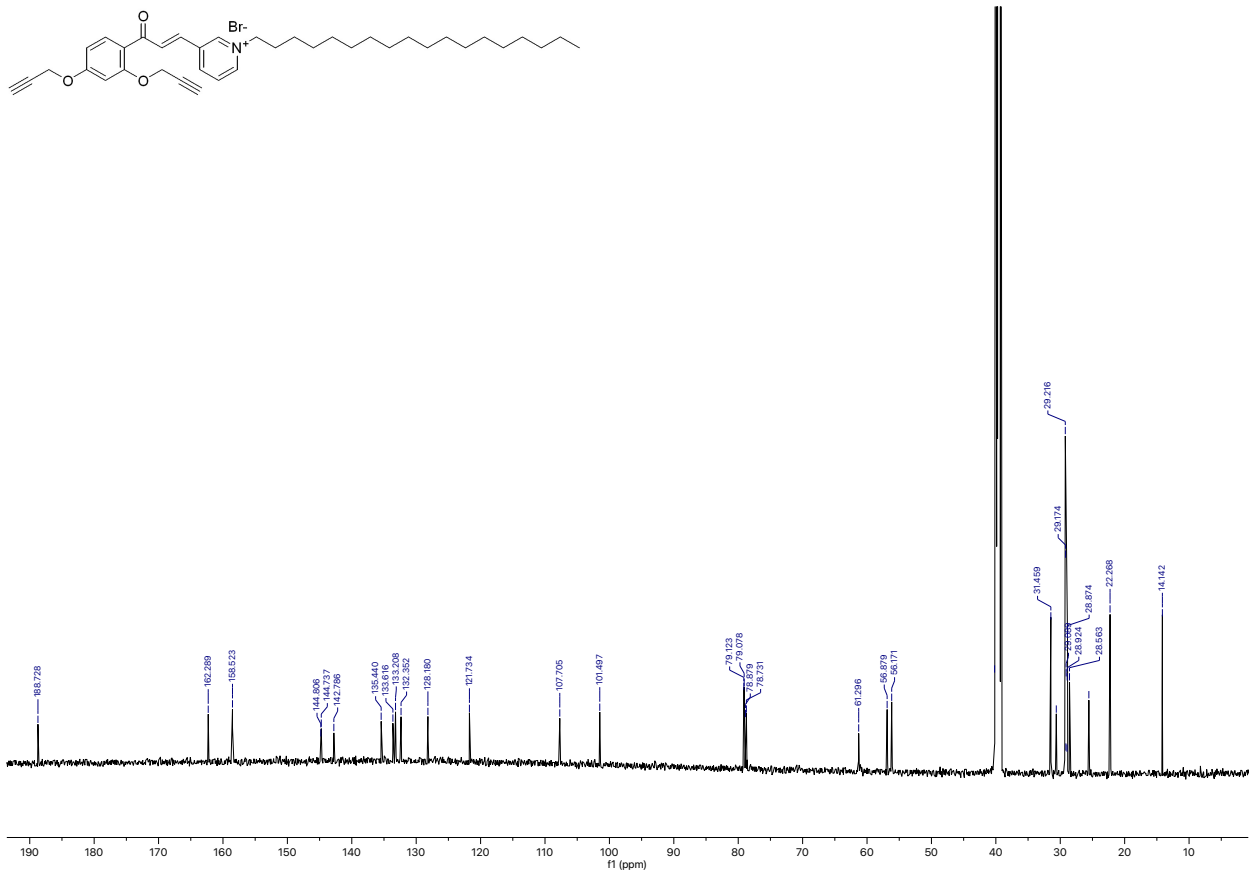


Figure S19. ^{13}C NMR spectr*um* (151 MHz, DMSO-d_6) of compound **8**

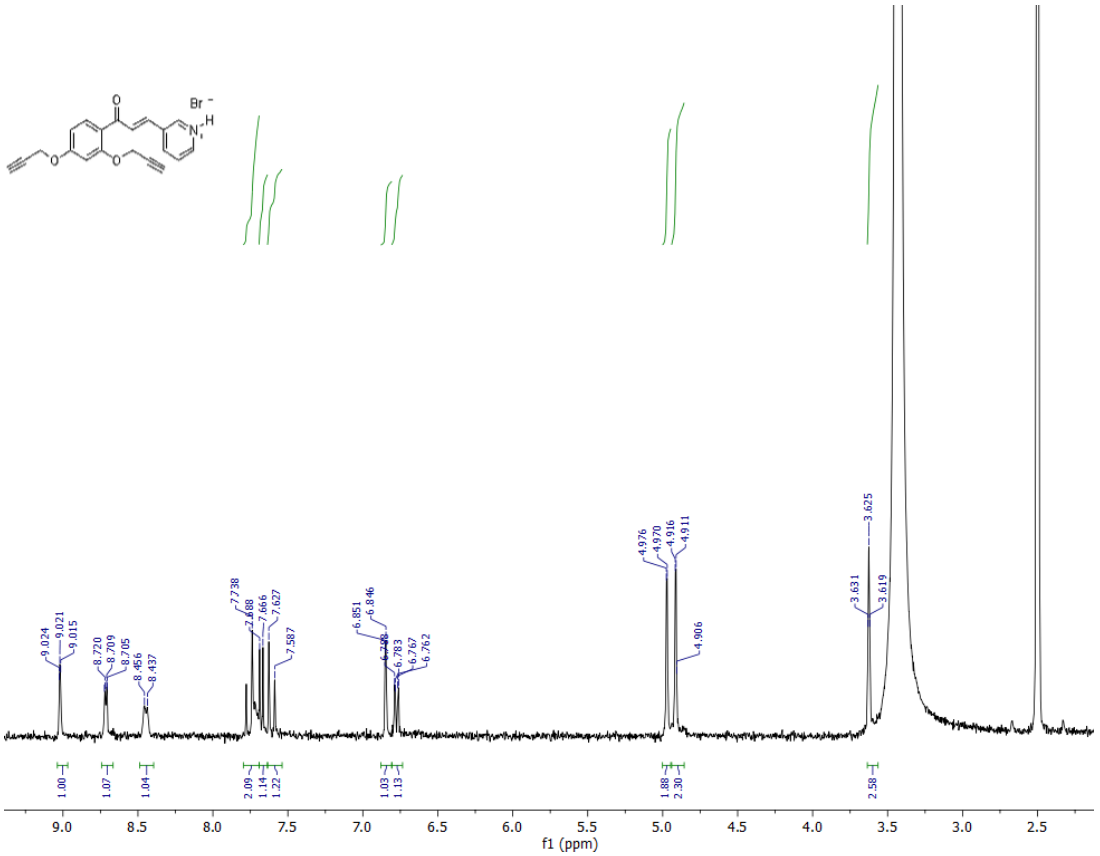


Figure S20. ^{1}H NMR spectr*um* (400 MHz, DMSO-d_6) of compound **9**

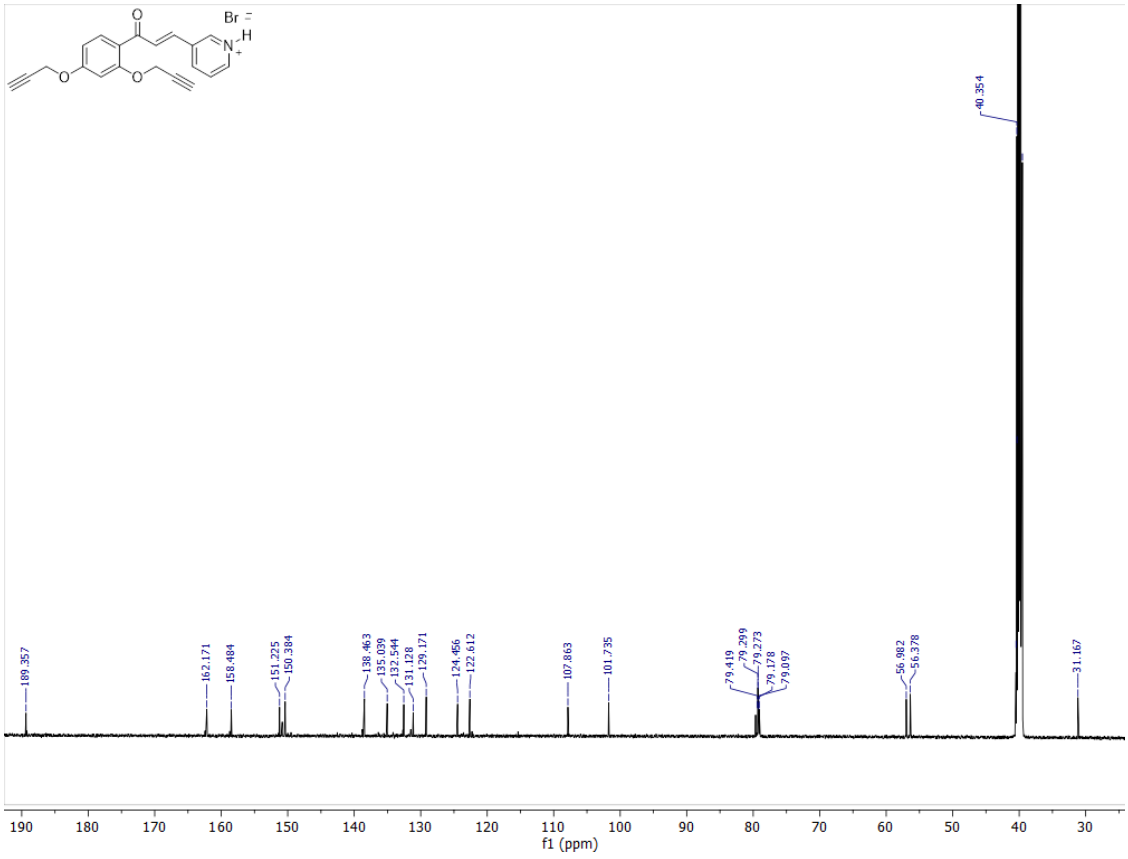


Figure S21. ^{13}C NMR spectr*um* (151 MHz, $CDCl_3$) of compound **9**

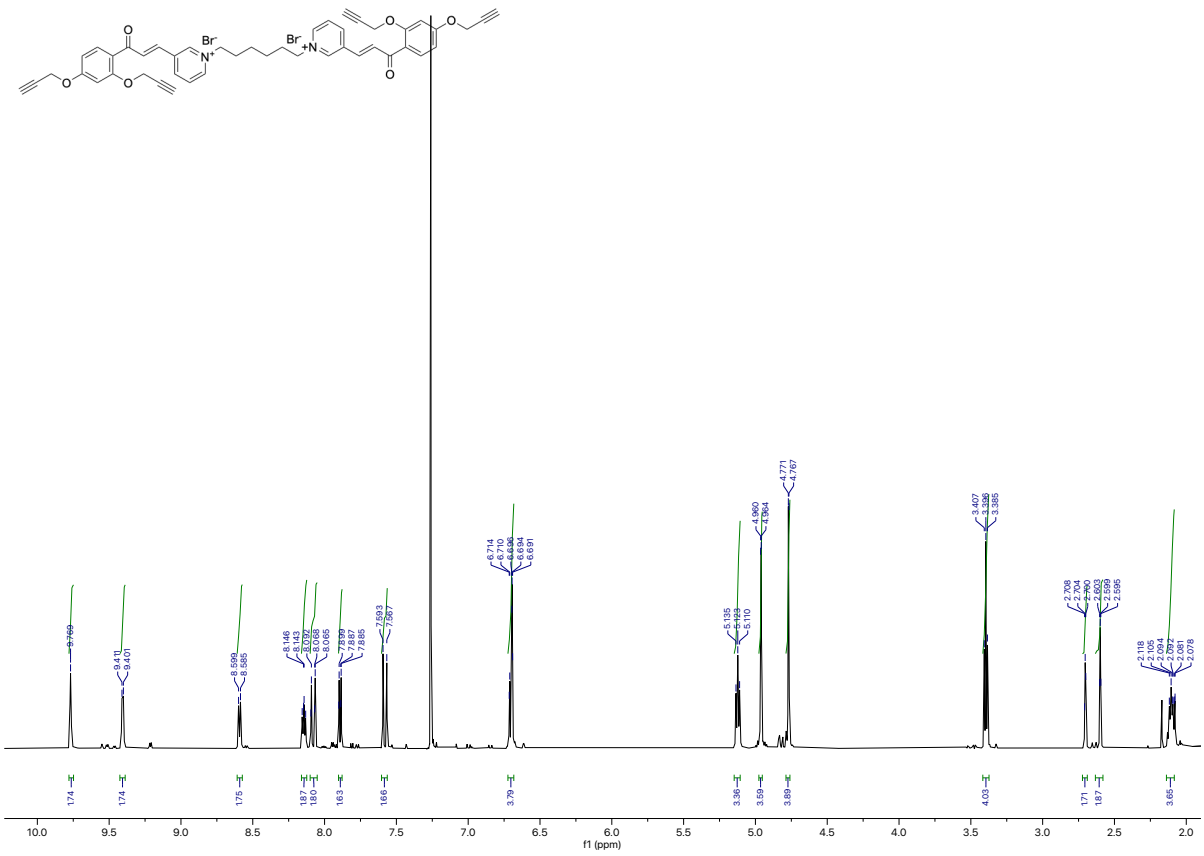


Figure S22. ^{1}H NMR spectr*um* (600 MHz, $CDCl_3$) of compound **10.**

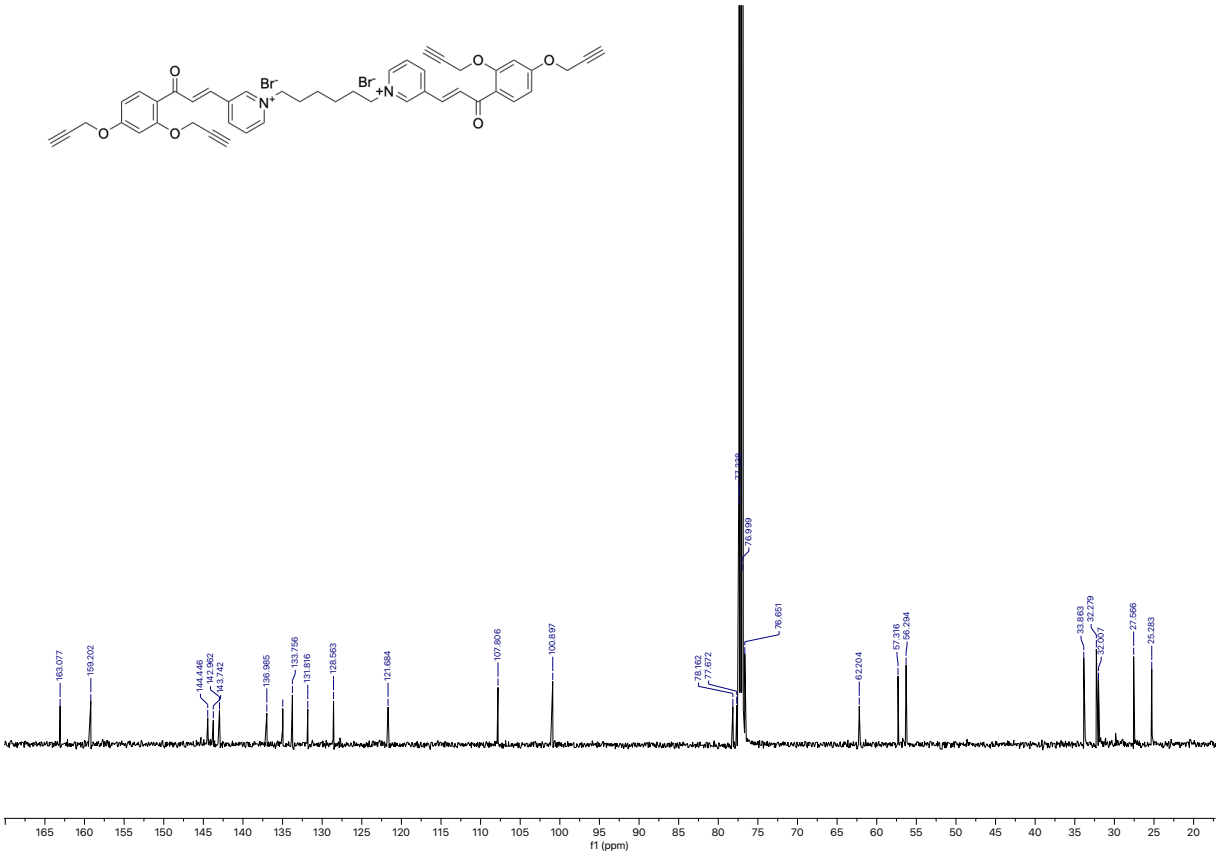
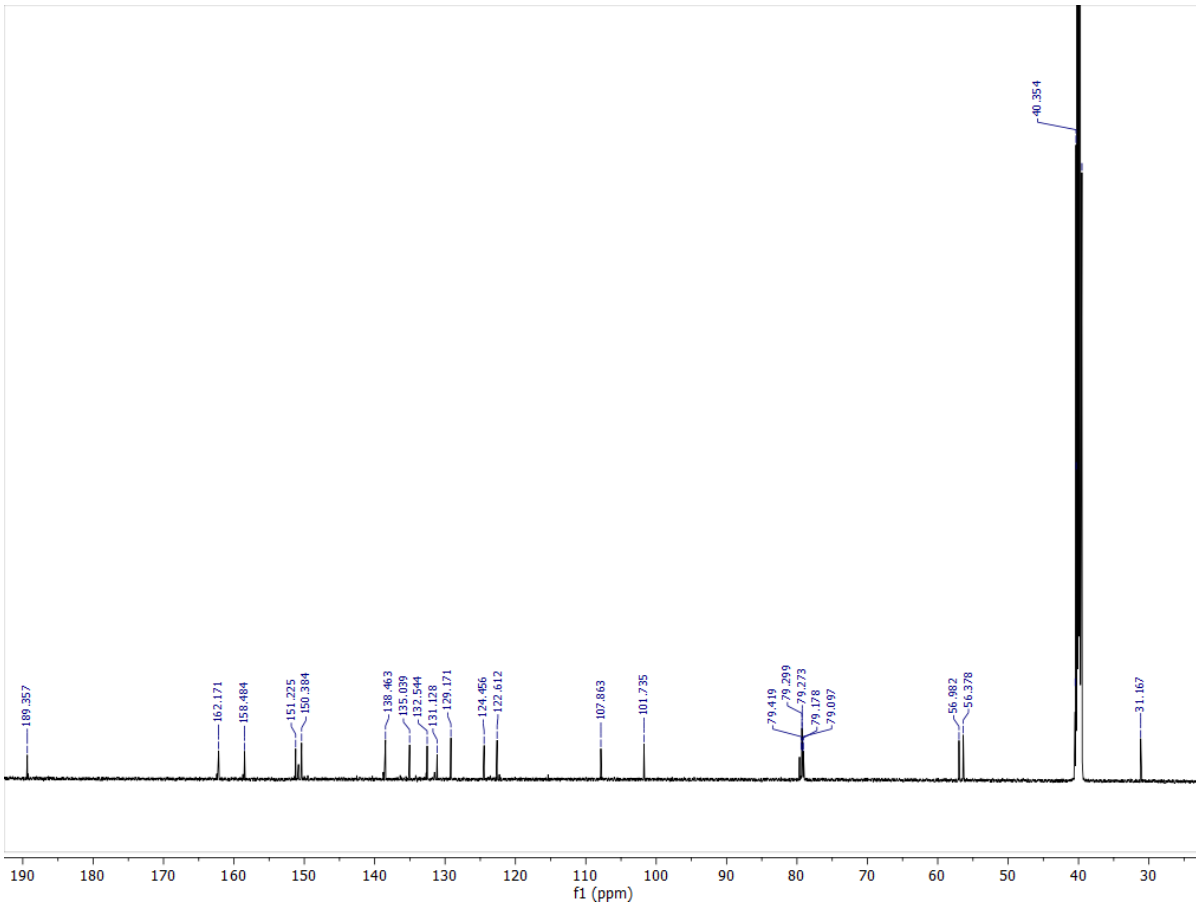


Figure S23. ^{13}C NMR spectr*um* (151 MHz, $CDCl_3$) of compound **1**



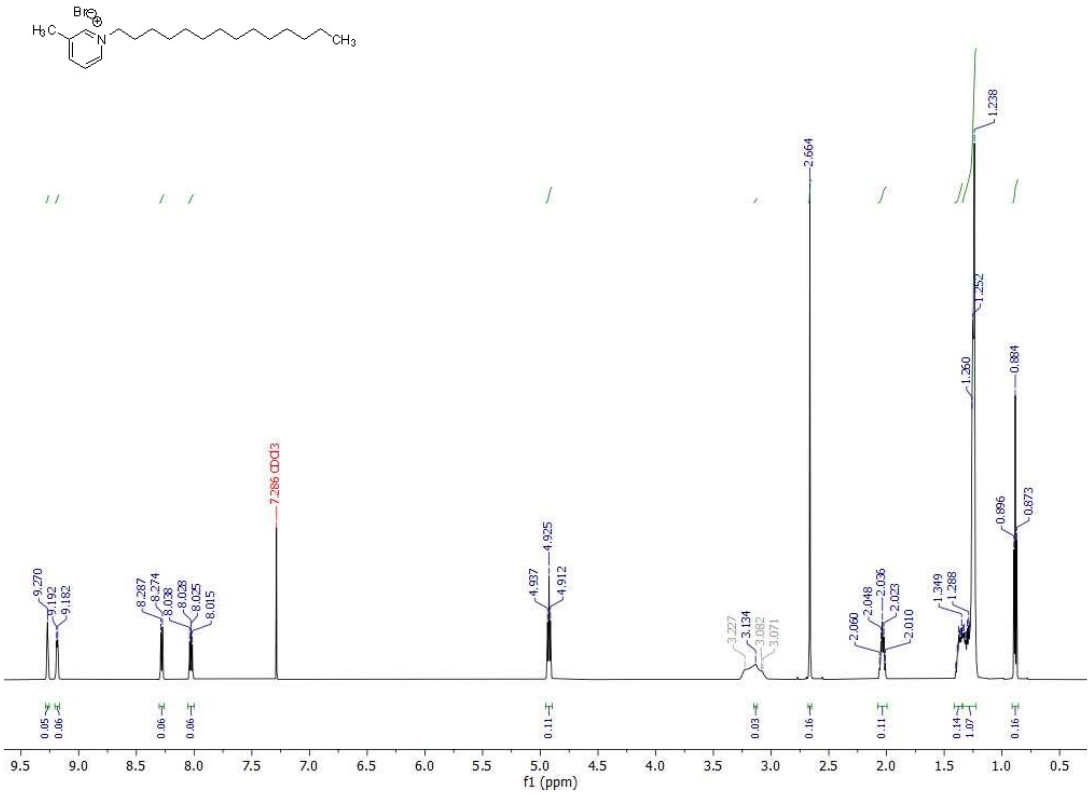


Figure S24. ^{1}H NMR (600 MHz, $CDCl_3$) of compound **11**.

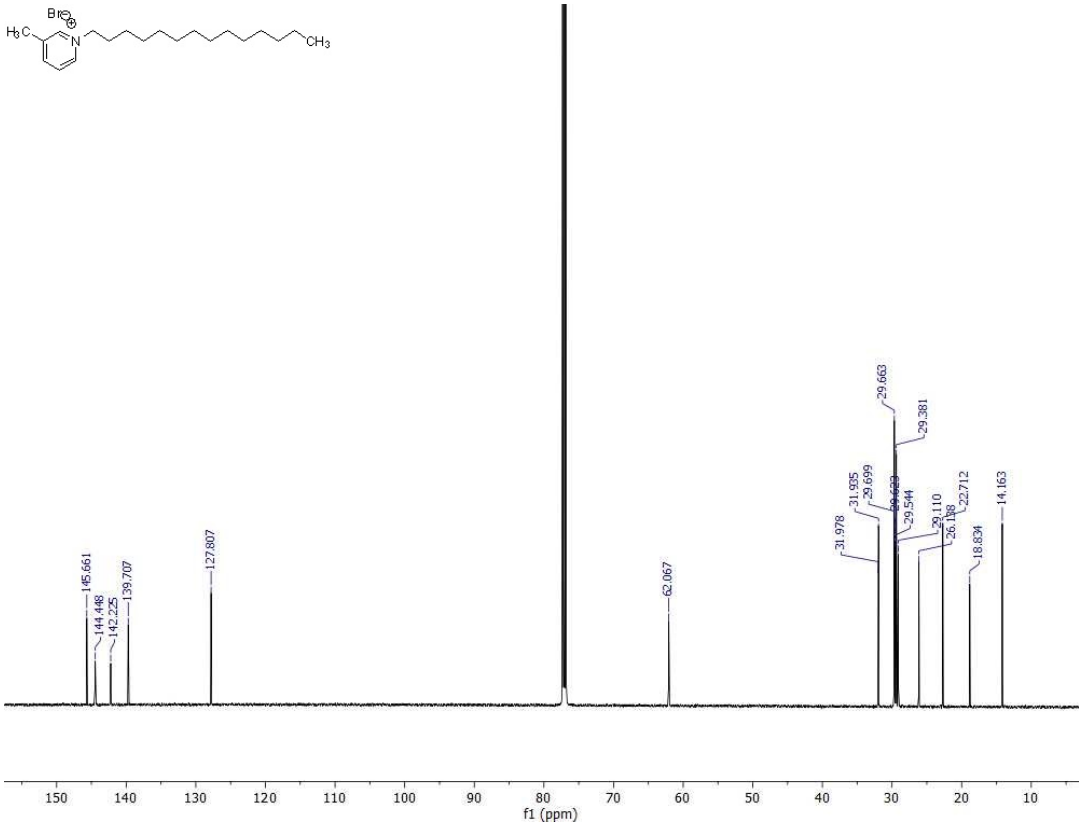


Figure S25. ^{13}C NMR (151 MHz, $CDCl_3$) of compound **11**