Modulated Photochemical Reactivities of O-Acetylated (3’,5’-Dimethoxyphenyl)heteroaryl Acyloin Derivatives Under Direct Irradiation And Photo-induced Electron Transfer Conditions

Rajesh Bisht[†, §], *Saumya Singh*[¶,§] *Kothandam Krishnamoorthy*[¶,§,*] *and Jayaraj Nithyanandhan*[†,§,*]

† *Physical and Material Chemistry Division, CSIR-National Chemical Laboratory, CSIR-Network of Institutes for Solar Energy, Dr. Homi Bhaba Road, Pune, India-411008.*

¶*Polymer Science Engineering Division, CSIR-National Chemical Laboratory, CSIR-Network of Institutes for Solar Energy, Dr. Homi Bhaba Road, Pune, India-411008.*

§ *Academy of Scientific and Innovative Research (AcSIR), New Delhi 110025, India*

Supporting Information

List of contents

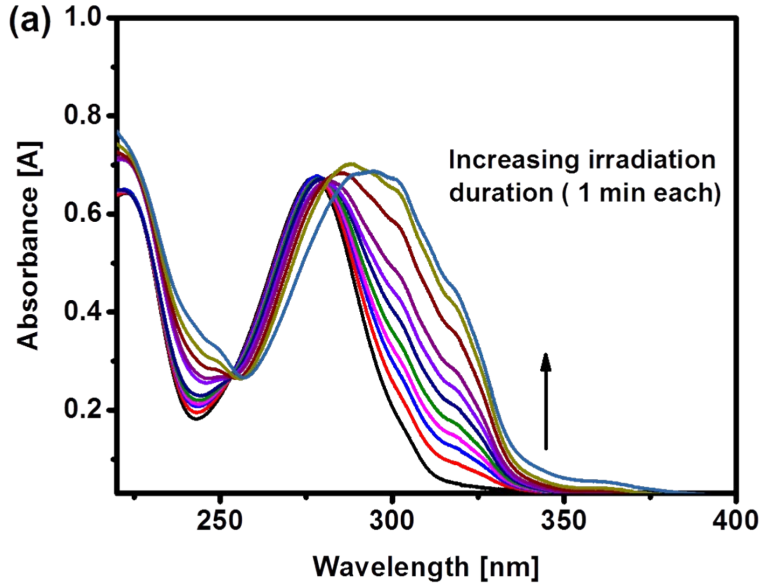


Figure S1. Change in UV-visible absorption spectra of furan derivative (4b) with increasing photolysis at 365 nm under 100 watt UV lamp in MeCN recorded at interval of 1 min each.

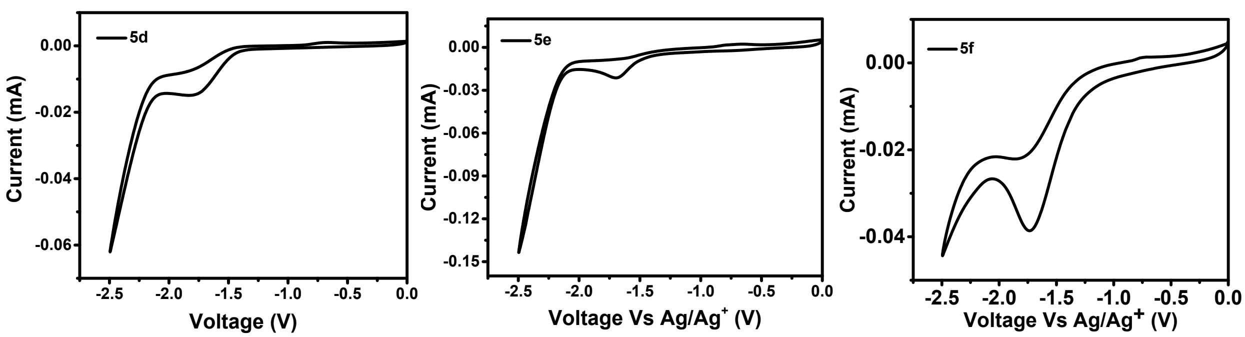


Figure S2. Cyclic Voltammogram (reduction scan) of 5d, 5e and 5f measured in CH_2Cl_2 (platinum wire as working electrode, non-aqueous Ag/Ag^+ (0.01M) as reference electrode and platinum foil as counter electrode) with $TBAClO_4$ (0.1 M) as electrolyte at the scan rate of 50 mV s^{-1}.

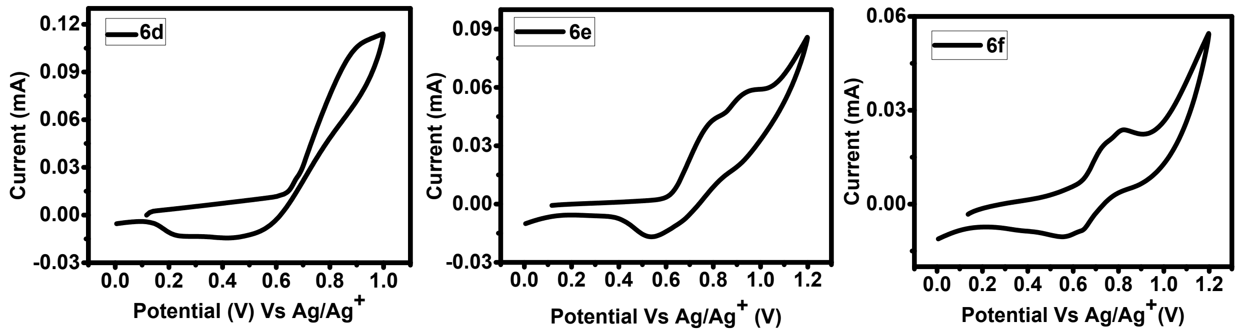
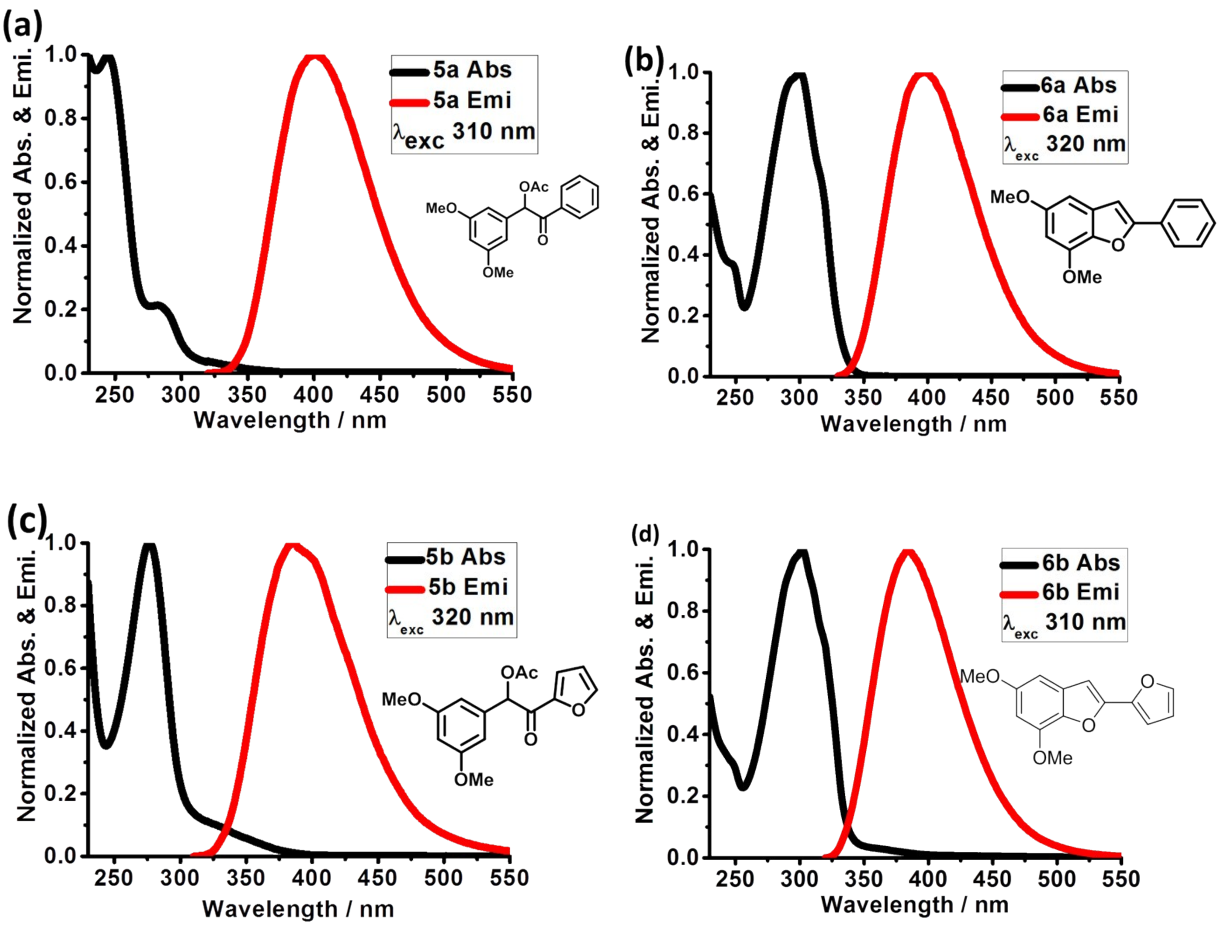


Figure S3. Cyclic Voltammogram (oxidation scan) of 6d, 6e and 6f measured in CH_2Cl_2 (platinum wire as working electrode, non-aqueous Ag/Ag^+ (0.01M) as reference electrode and platinum foil as counter electrode) with $TBAClO_4$ (0.1 M) as electrolyte at the scan rate of 50 mV $s^{-1.}$



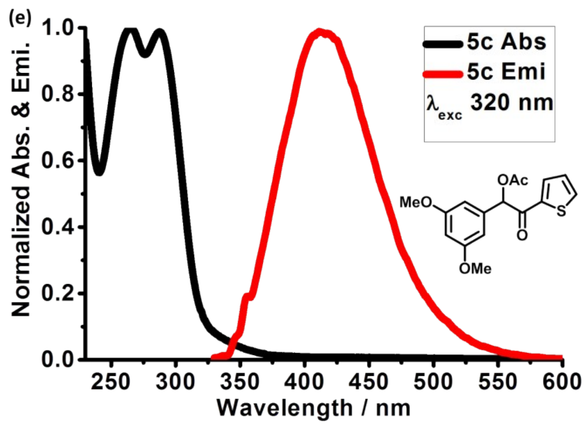
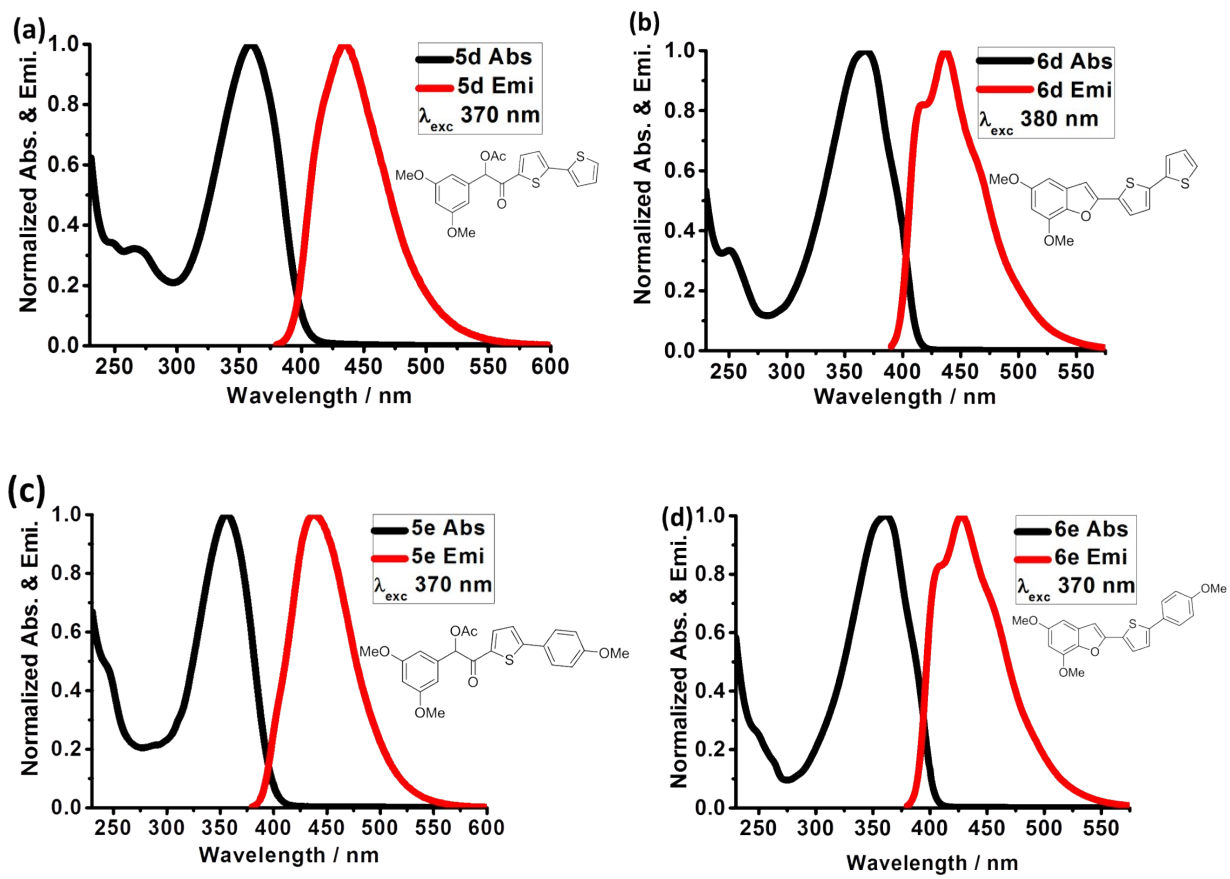


Figure S4. Absorption and emission curves of phtototriggers and cyclized products



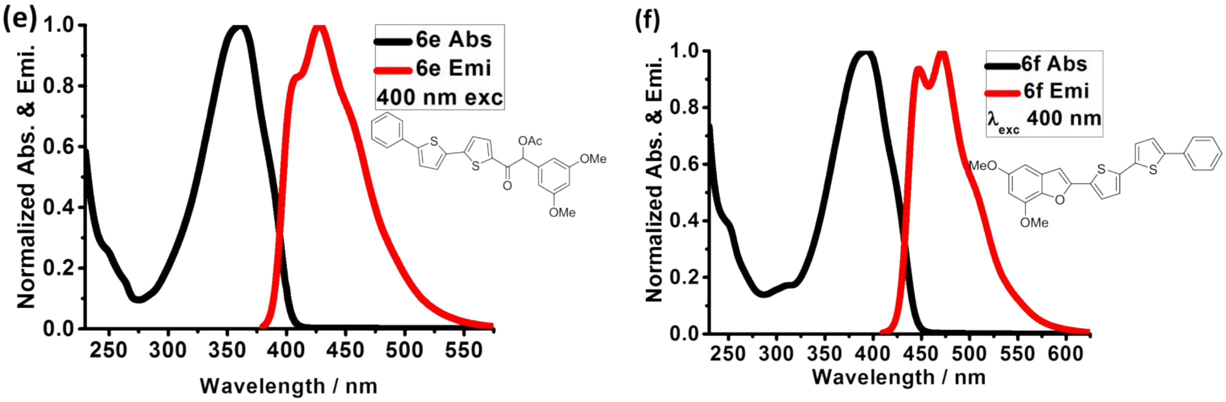


Figure S5. UV absorption and emission curves of extended phtototriggers and cyclized products

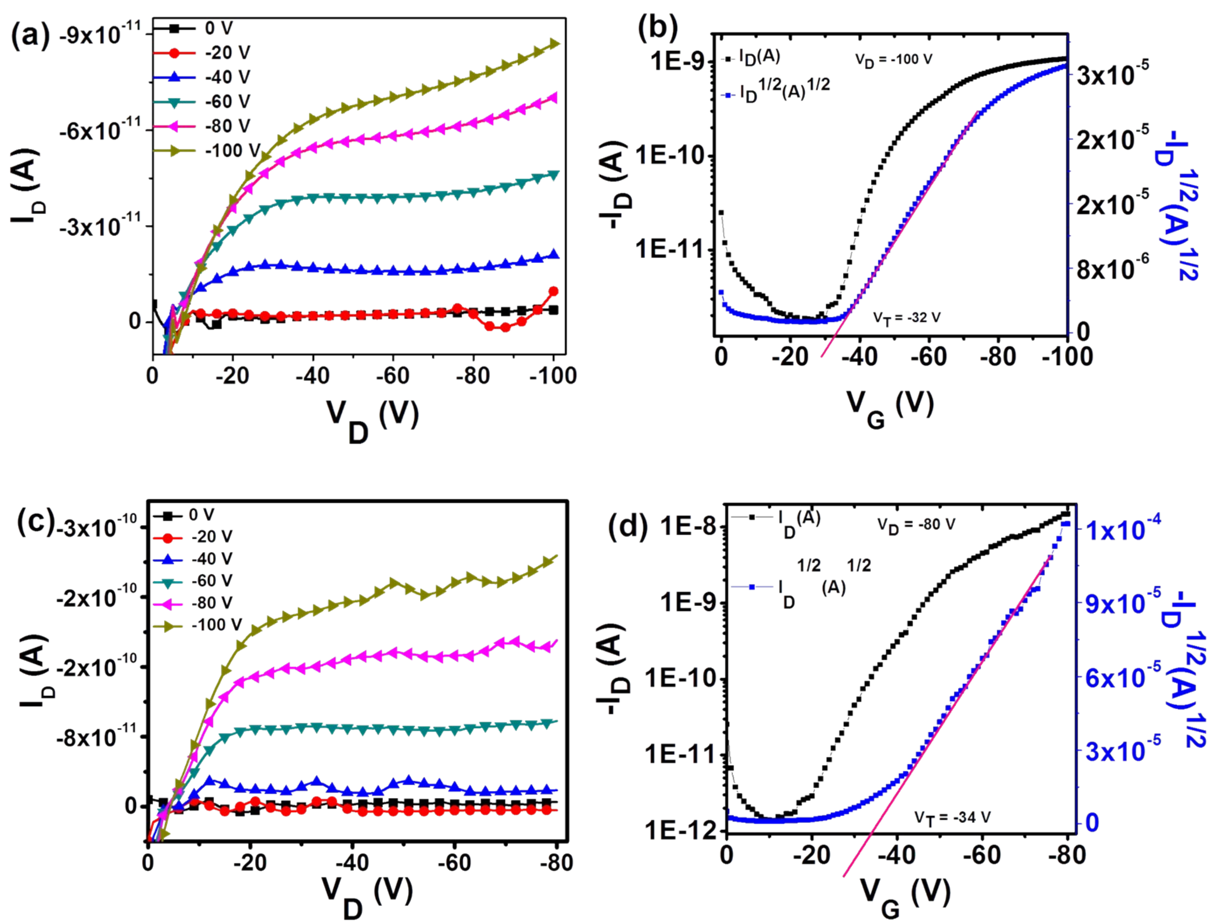


Figure S6. Output and transfer characteristics of 6d, without annealing (a) and (b), with annealing at 50^{o}C for 10 min (c) and (d). Channel length is 5 µm

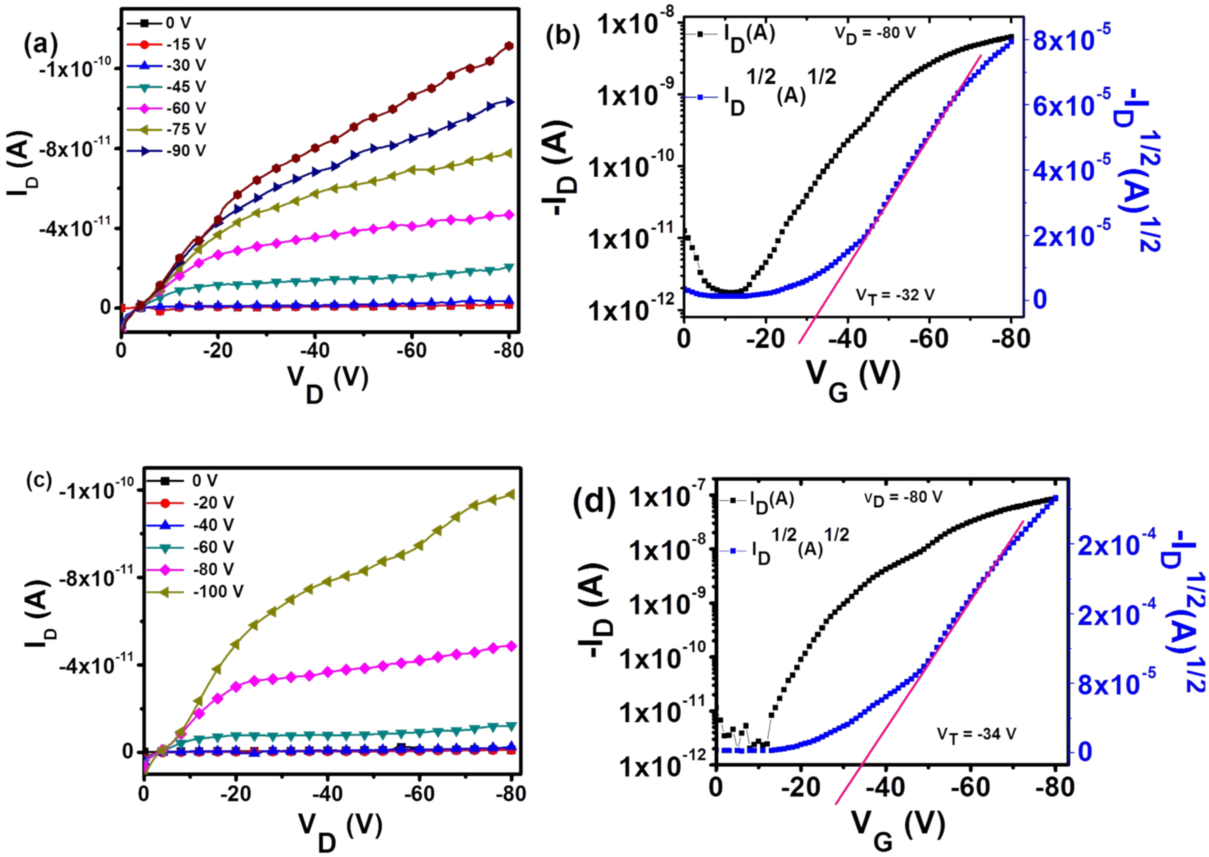


Figure S7. Output and transfer characteristics of **6e**, without annealing (a) and (b), with annealing at 50°C for 10 min (c) and (d). Channel length is 2.5 μm.

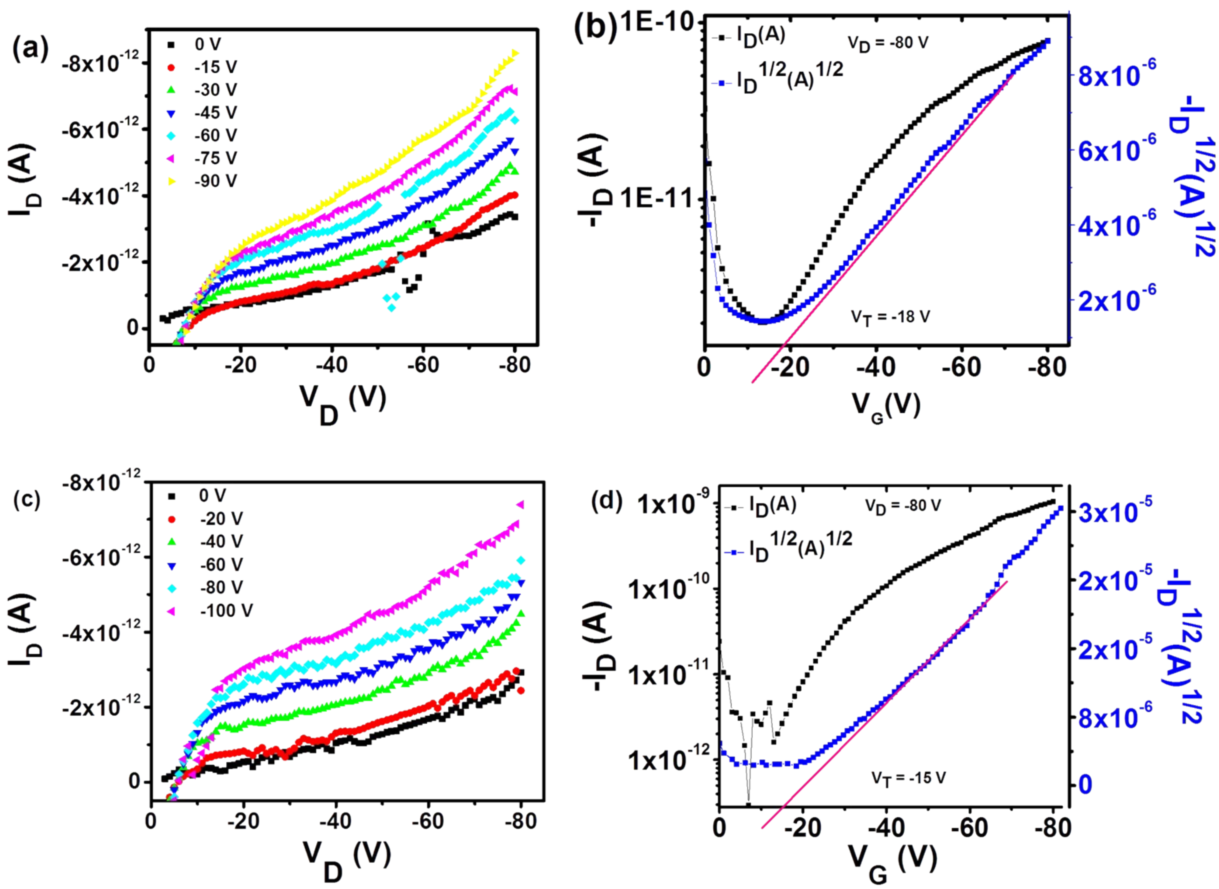


Figure S8. Output and transfer characteristics of **6f**, without annealing (a) and (b), with annealing at 50^{o}C for 10 min (c) and (d). Channel length is 2.5 μm.

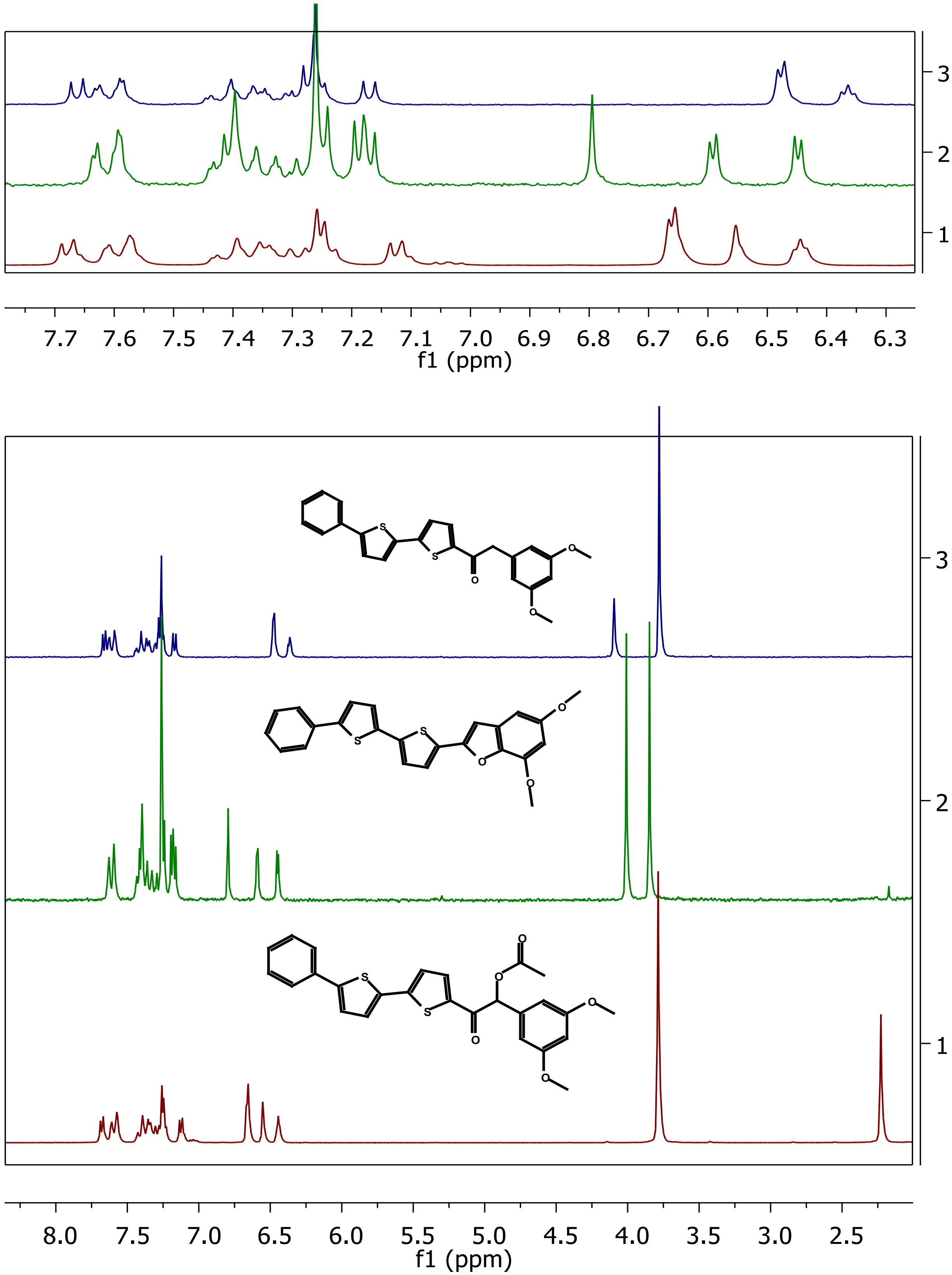


Figure S9. Stacked ^{1}H NMR spectra of **5f** (bottom), **6f** (middle) and **7f** (top)

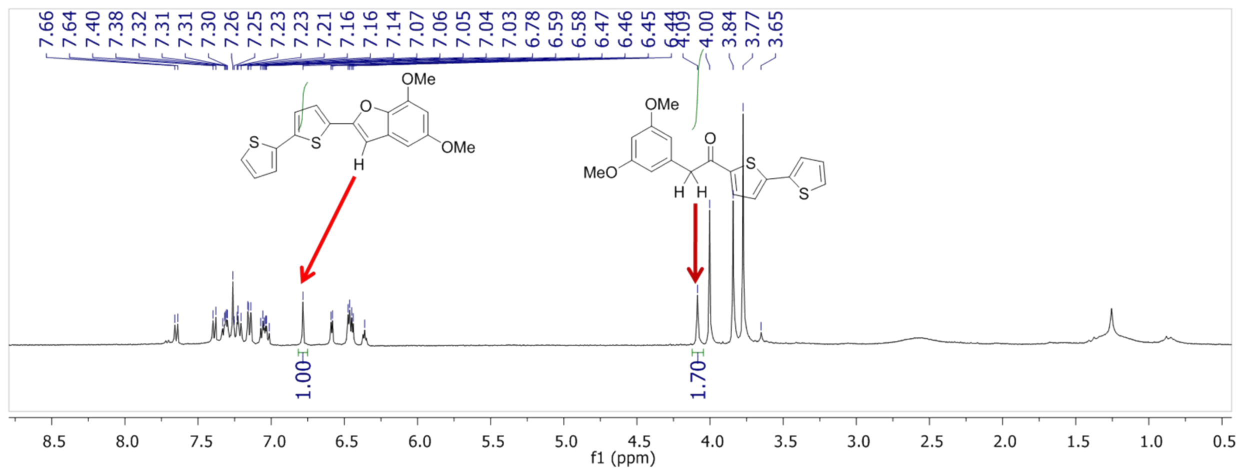


Figure S10. [1]H-NMR spectrum for the mixture of **6d** and **7d** obtained by the photochemical reaction of 5d in MeCN in the presence of Et_3N (1 equiv.) for 1 h and evaporated the solvent (Entry 8, Table 2 in the manuscript).

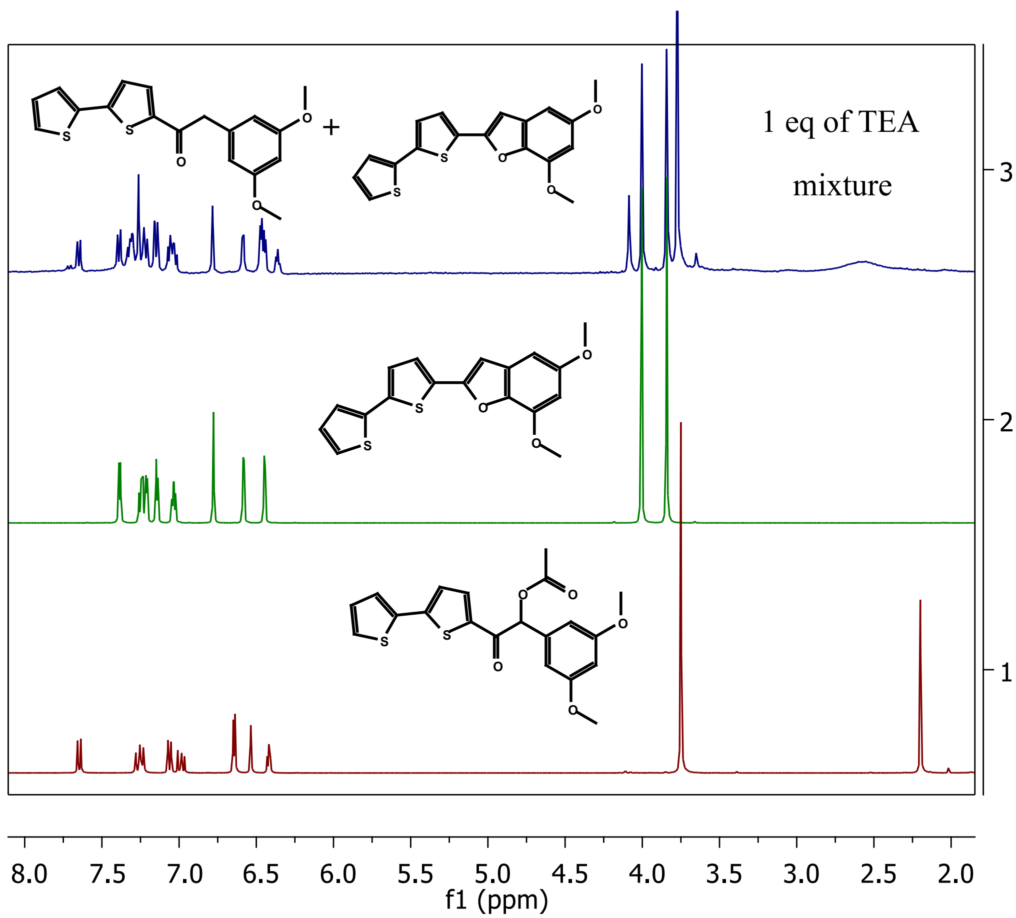


Figure S11. Stacked [1]H NMR spectra of **5d** (bottom), **6d** (middle) and **6d** + **7d** mixture (top)

Figure S12. ^{1}H- and ^{13}C-NMR spectra of 2-phenyl-1,3-dithiane (**2a**)

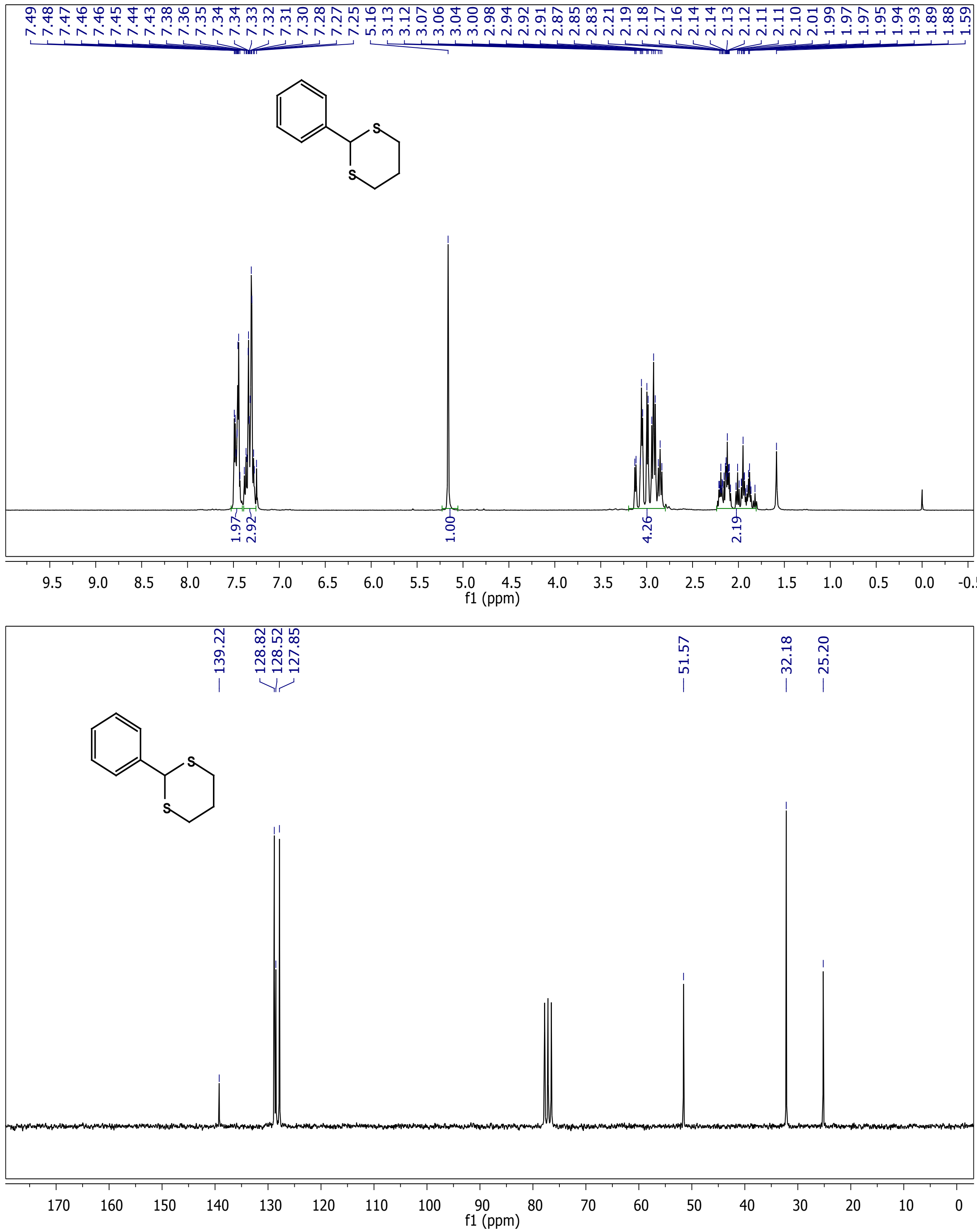
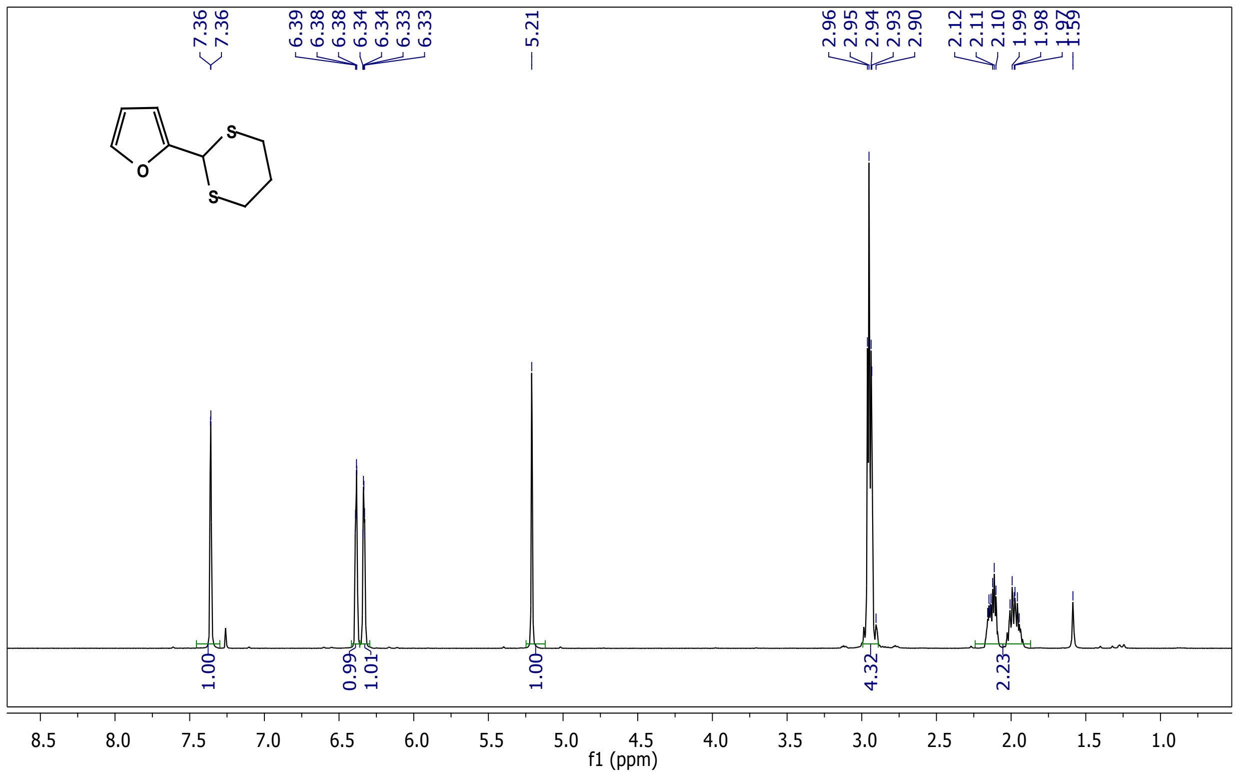


Figure S13. ^{1}H and ^{13}C NMR spectra of 2-(1,3-dithian-2-yl)furan (**2b**)



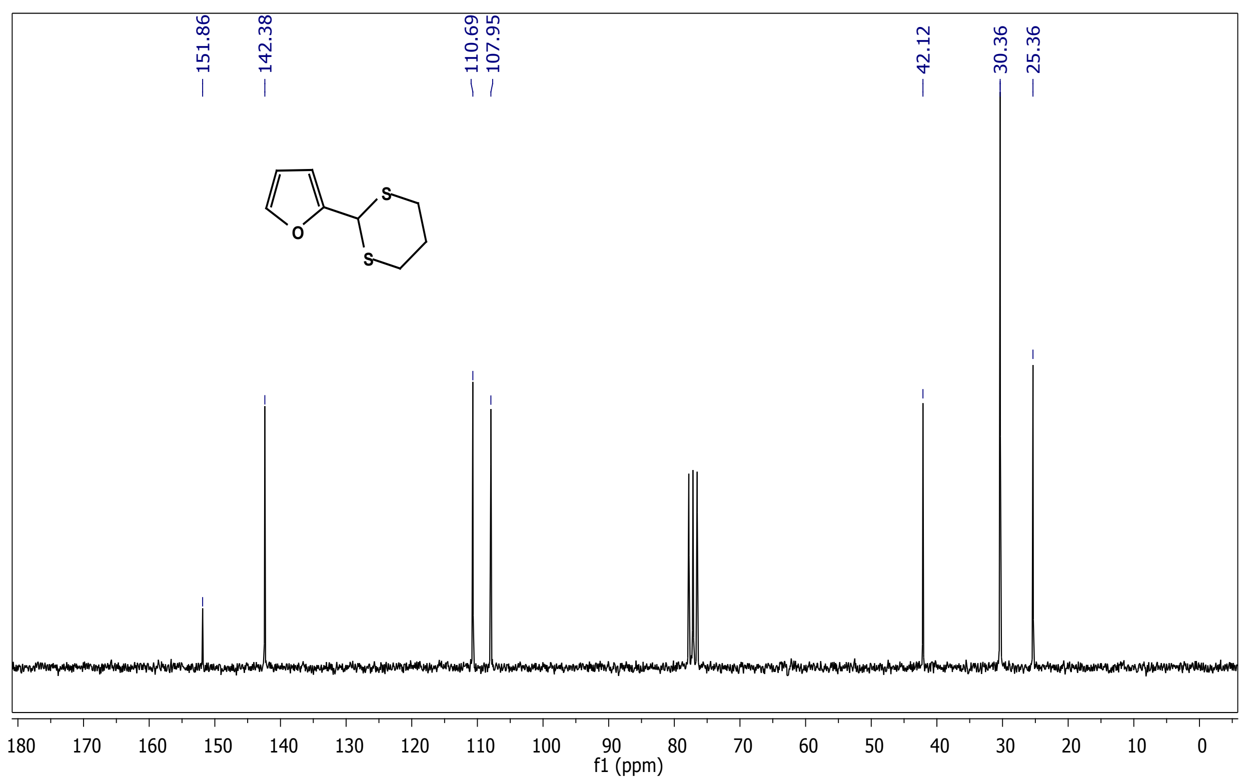
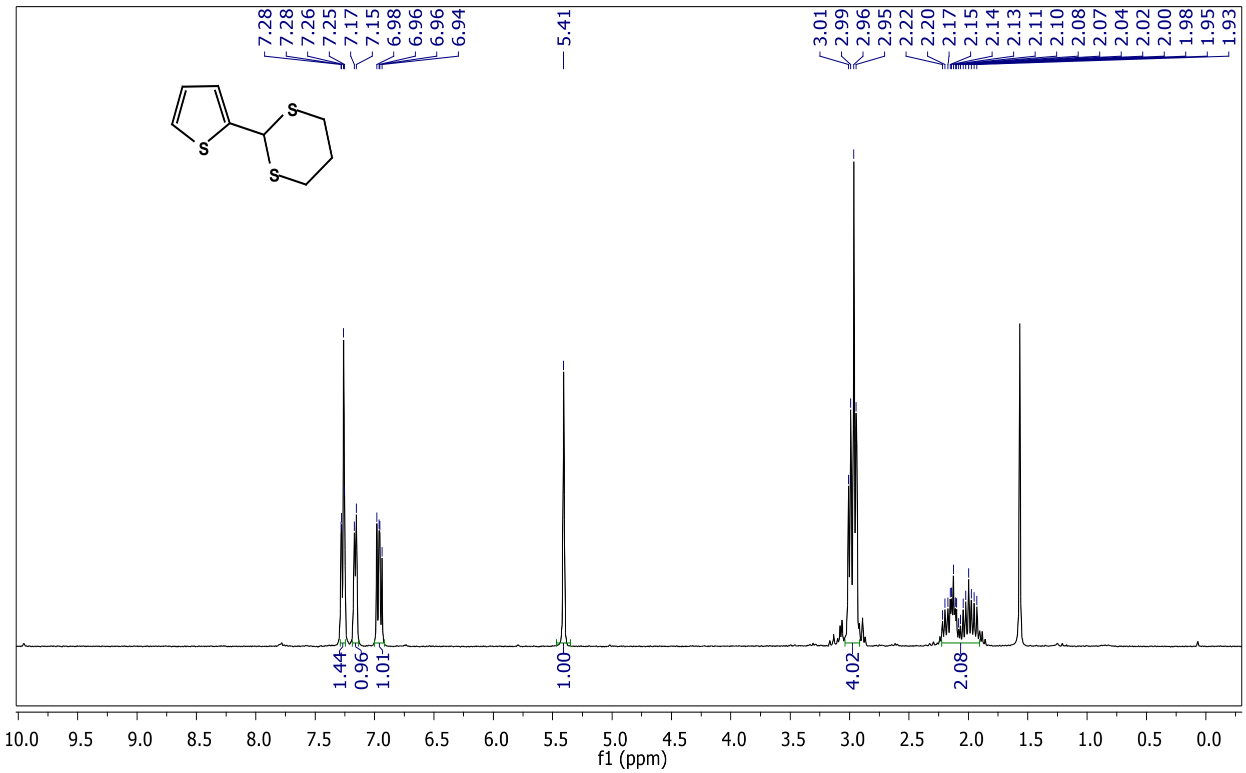


Figure S14. ^{1}H and ^{13}C NMR spectra of 2-(thiophen-2-yl)-1,3-dithiane (**2c**)



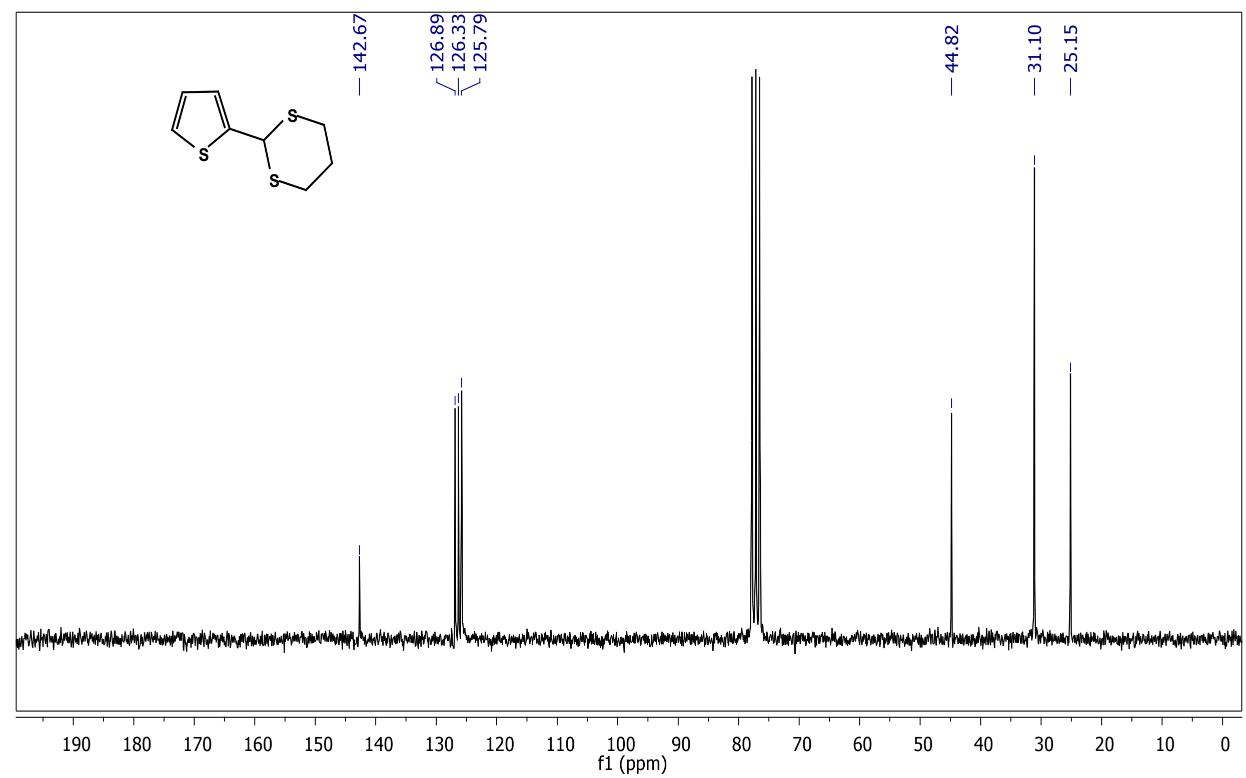
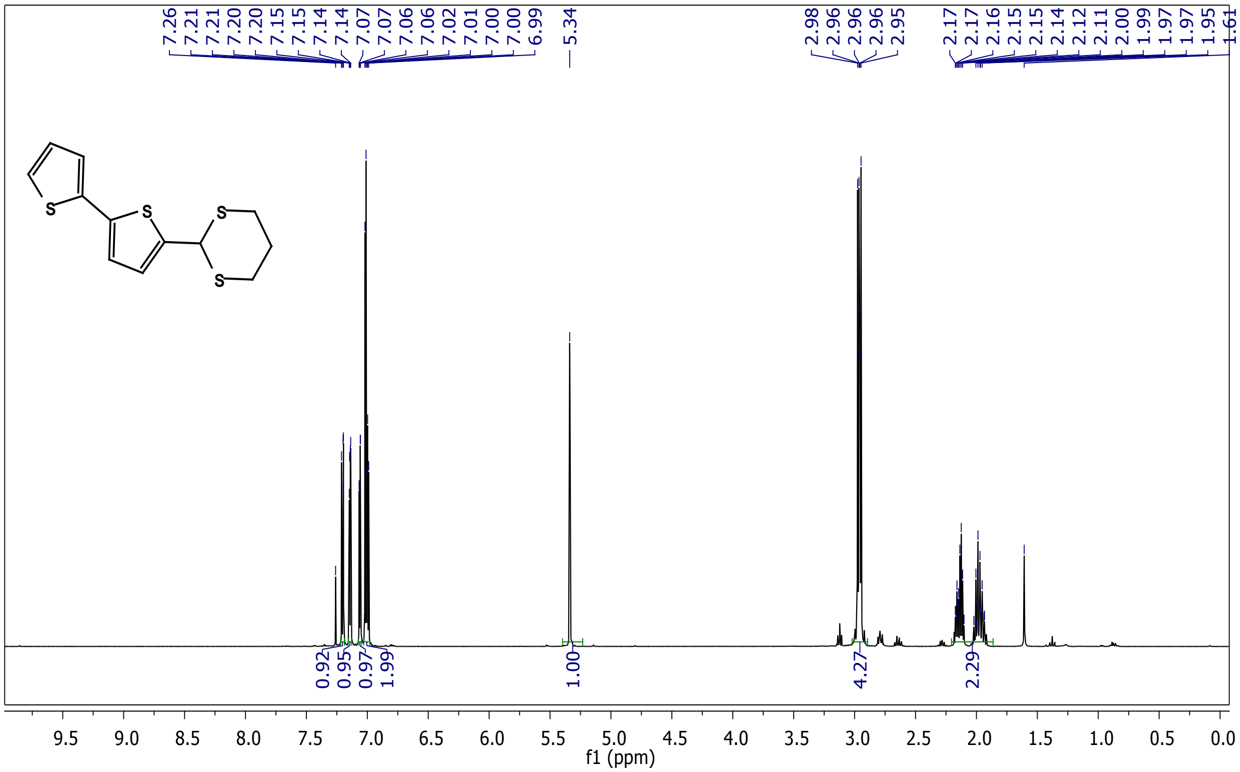


Figure S15. ^{1}H and ^{13}C NMR of 5-(1,3-dithian-2-yl)-2,2'-bithiophene (**2d**)



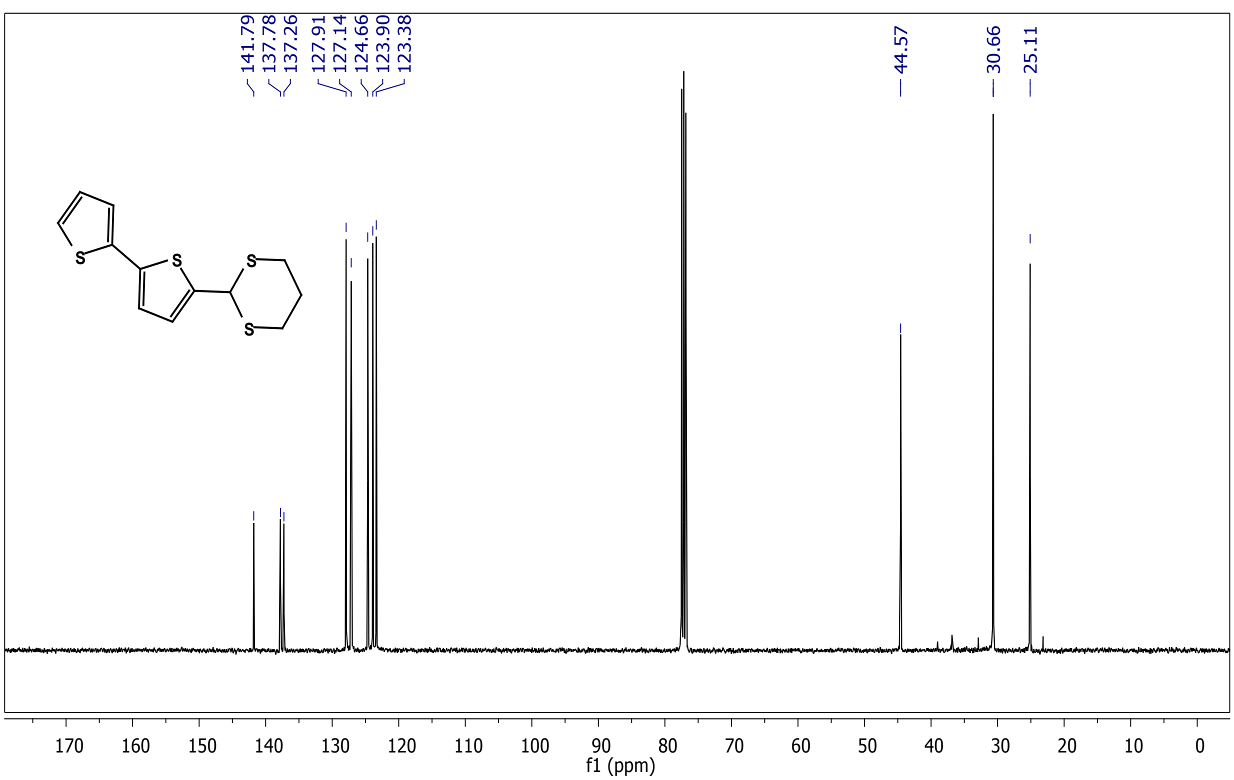


Figure S16. ^{1}H and ^{13}C NMR of (3,5-dimethoxyphenyl)(2-phenyl-1,3-dithian-2-yl)methanol **(3a)**

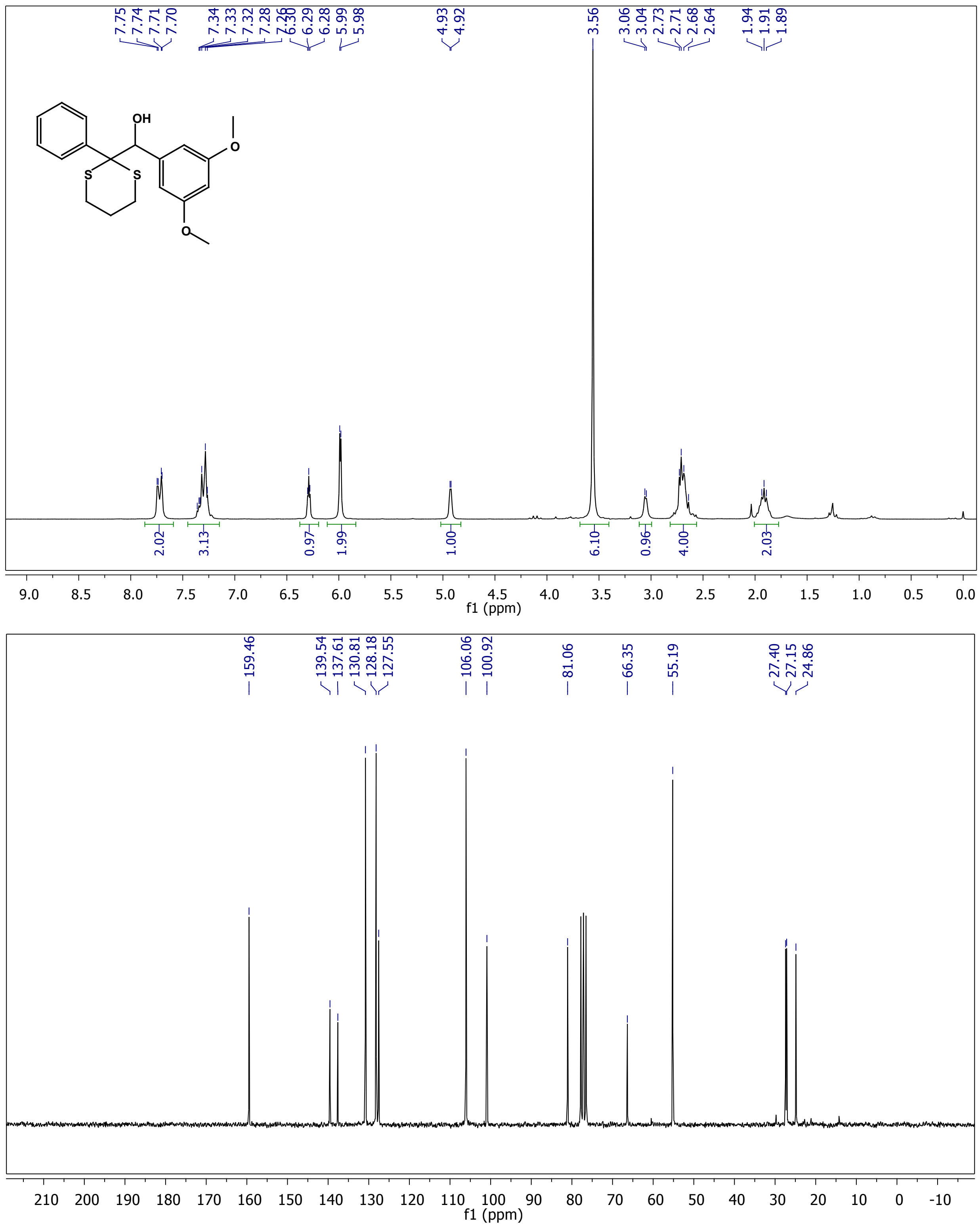
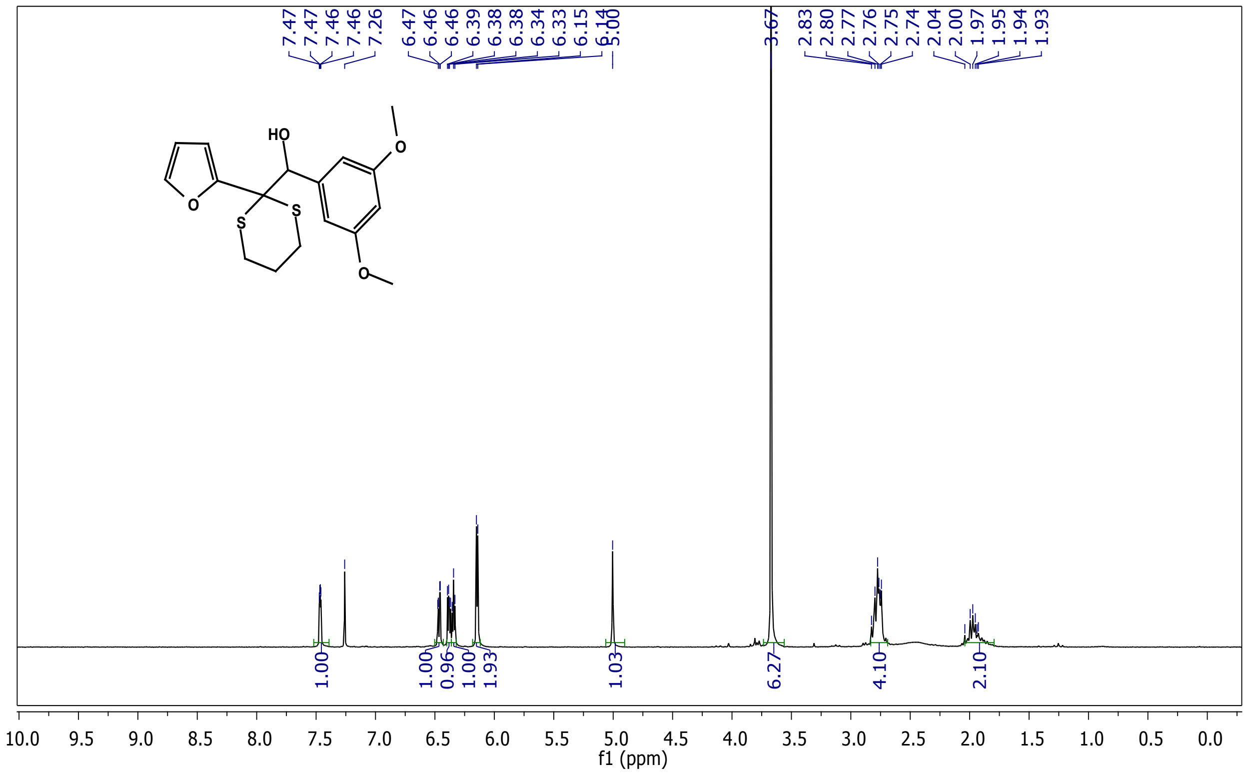


Figure S17. ^{1}H and ^{13}C NMR spectra of 3,5-dimethoxyphenyl)(2-(furan-2-yl)-1,3-dithian-2-yl)methanol (3b)



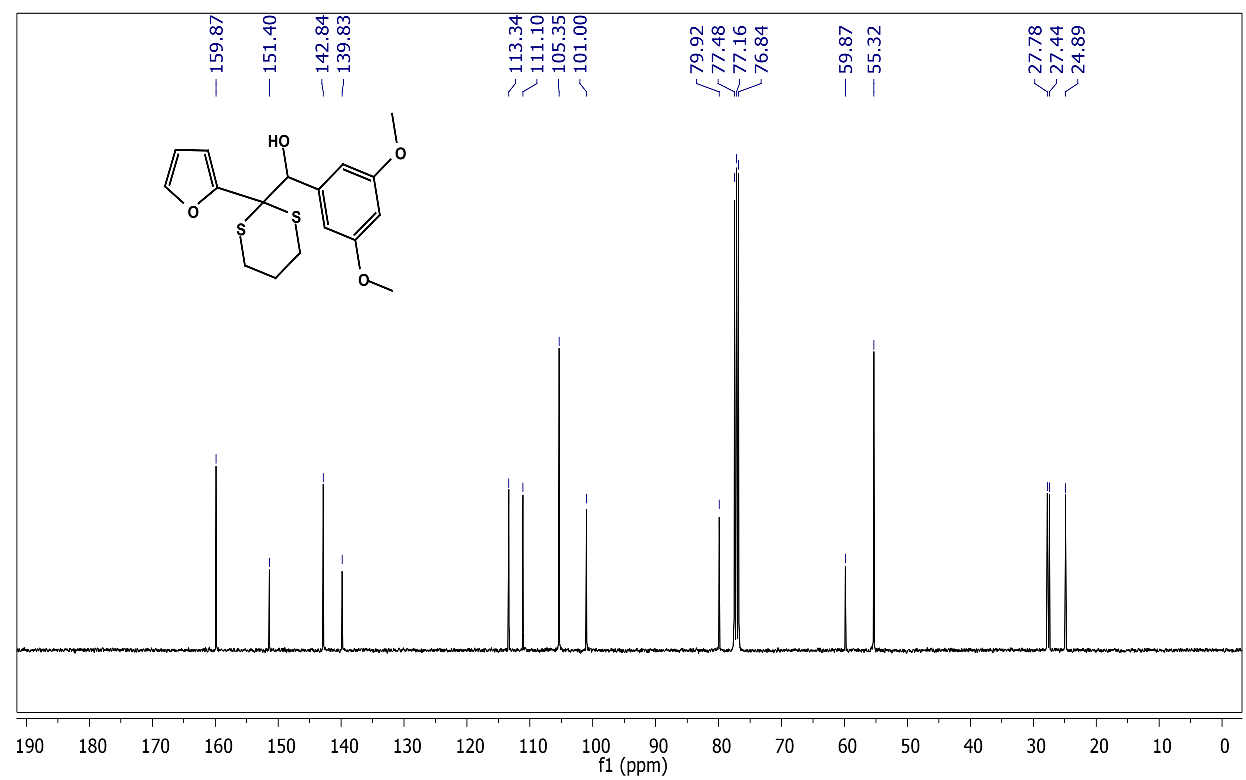
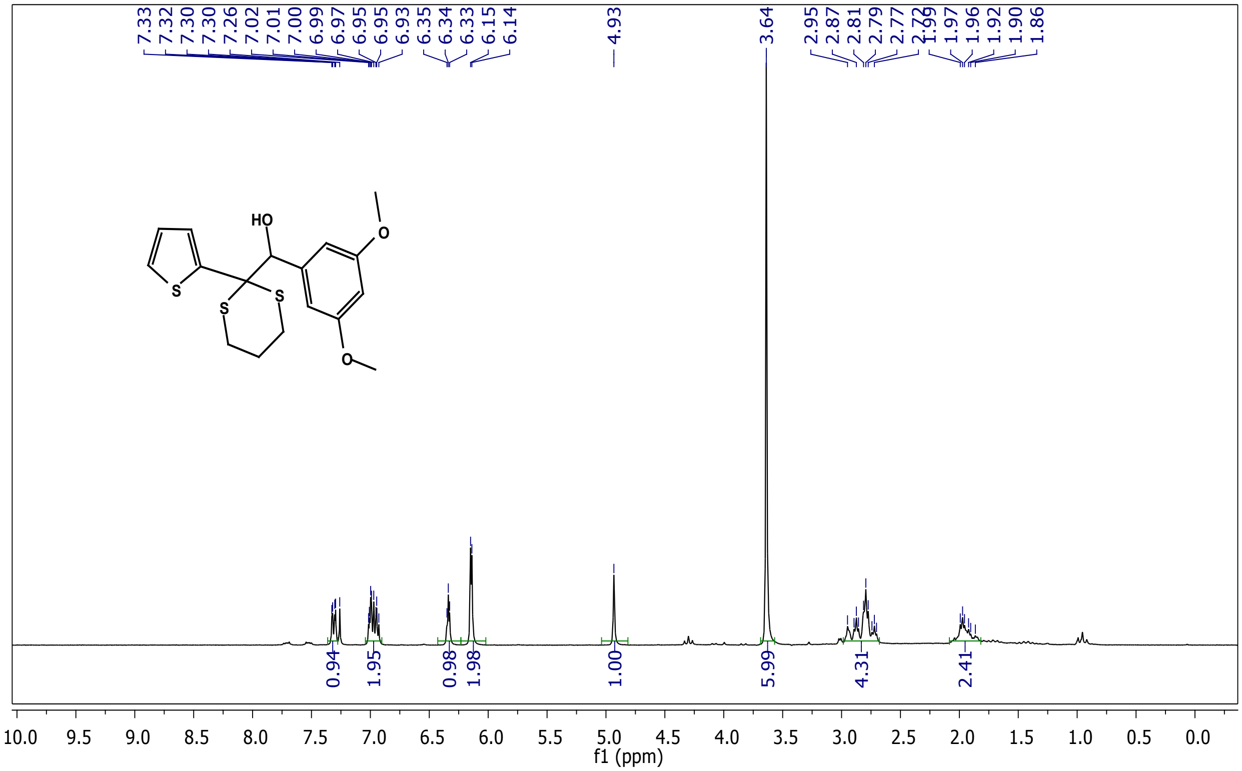


Figure S18. ^{1}H and ^{13}C NMR spectra of 3,5-dimethoxyphenyl)(2-(thiophen-2-yl)-1,3-dithian-2-yl)methanol (**3c**)



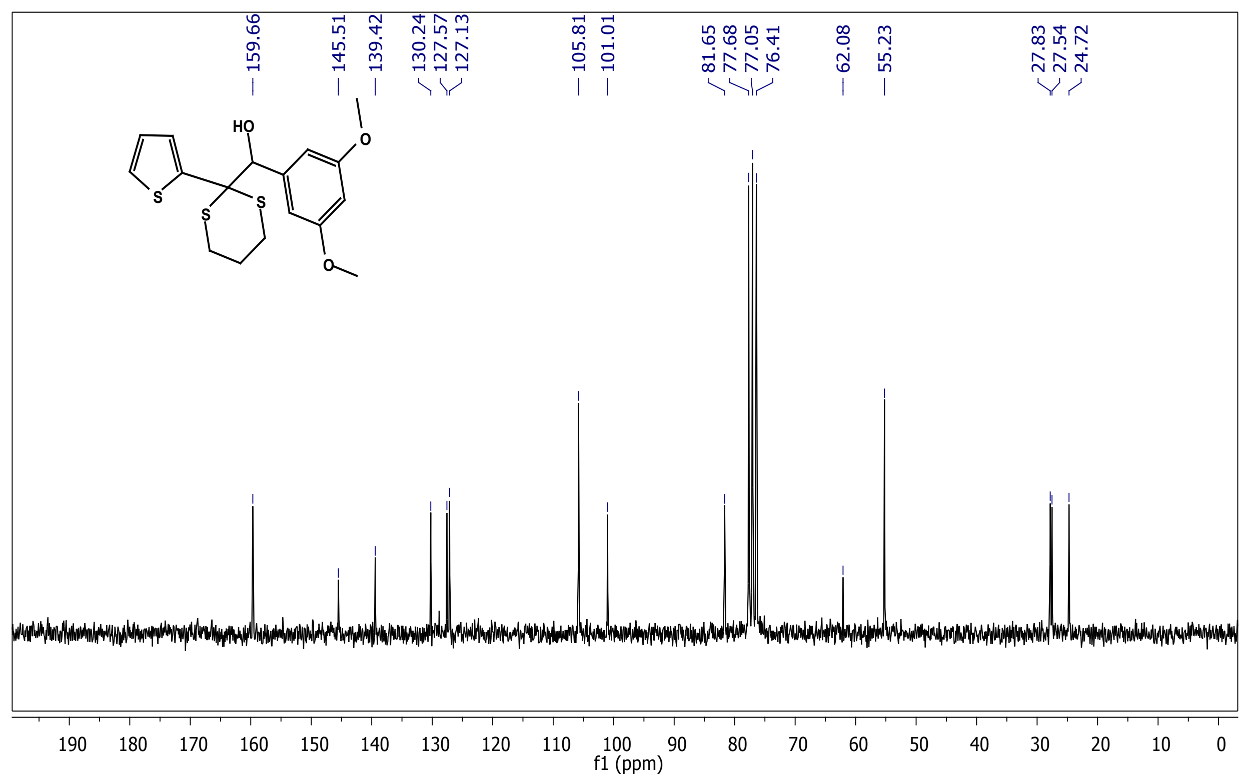
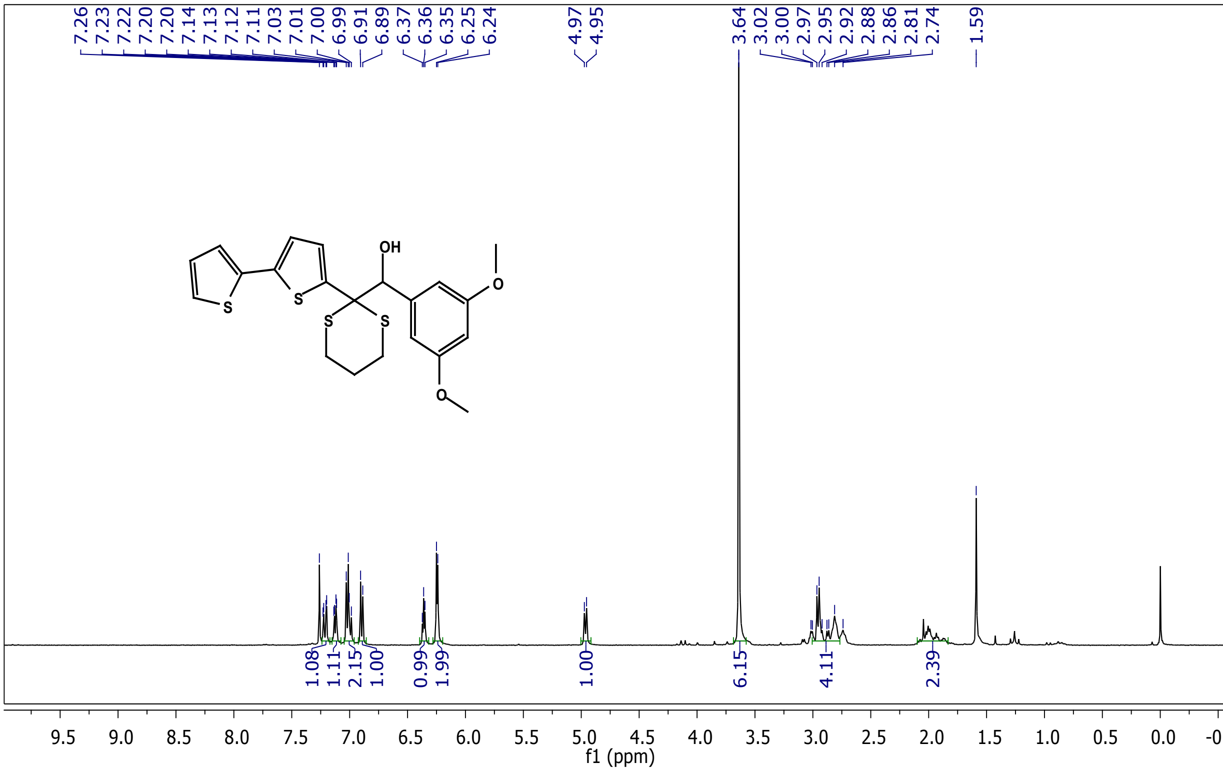


Figure S19. ^{1}H and ^{13}C NMR spectra of 2-([2,2'-bithiophen]-5-yl)-1,3-dithian-2-yl)(3,5-dimethoxyphenyl)methanol (**3d**)



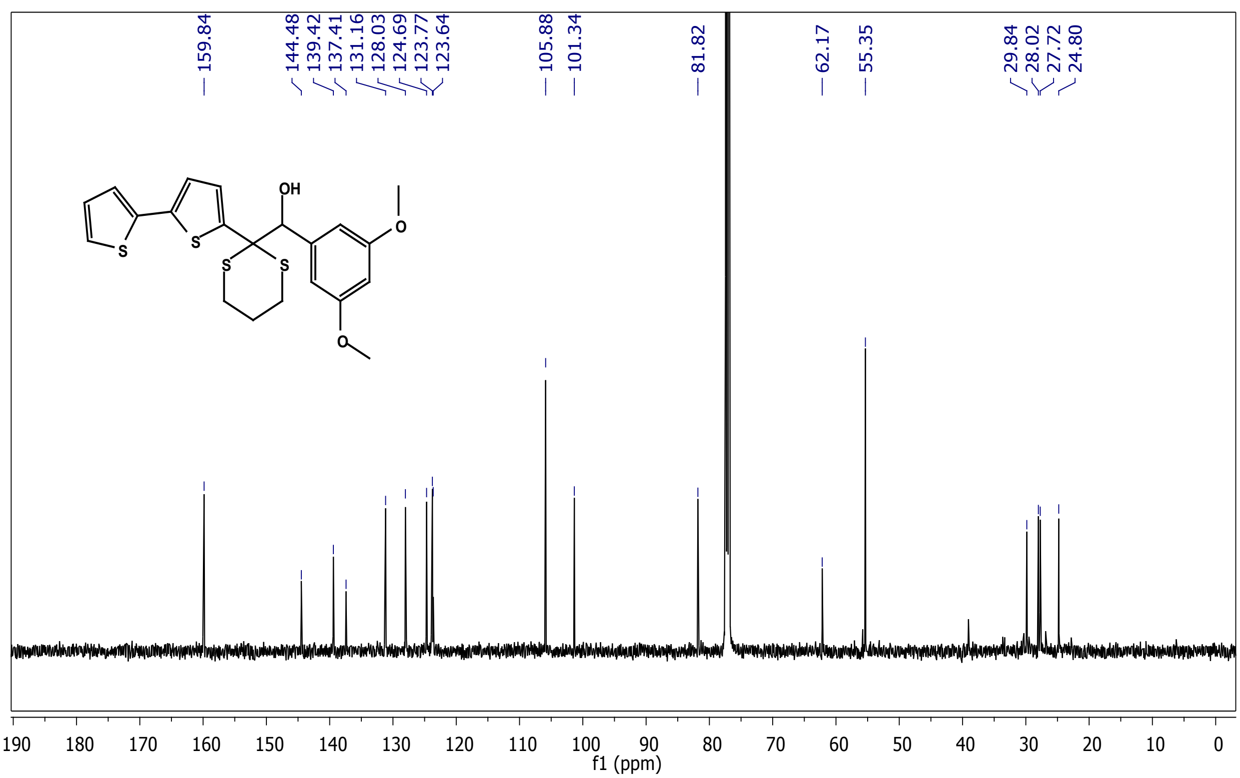
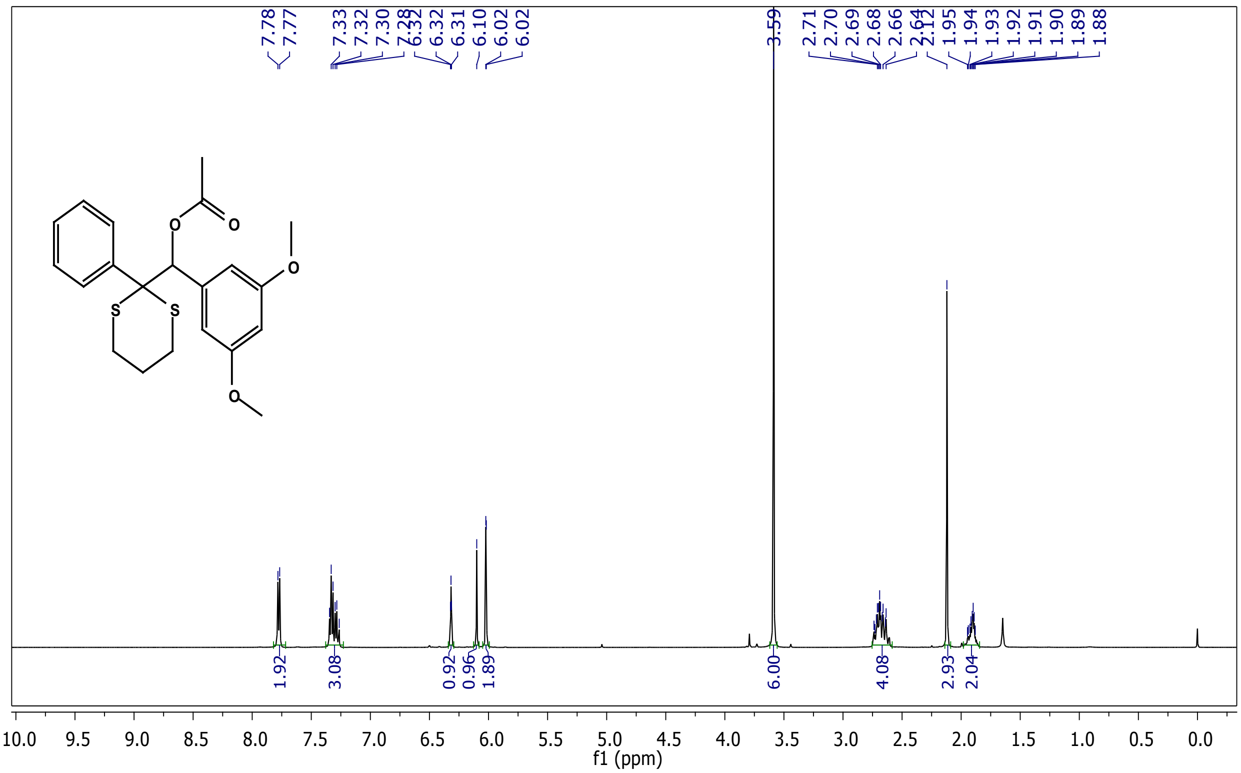


Figure S20. ^{1}H and ^{13}C NMR spectra of 3,5-dimethoxyphenyl)(2-phenyl-1,3-dithian-2-yl)methyl acetate (**4a**)



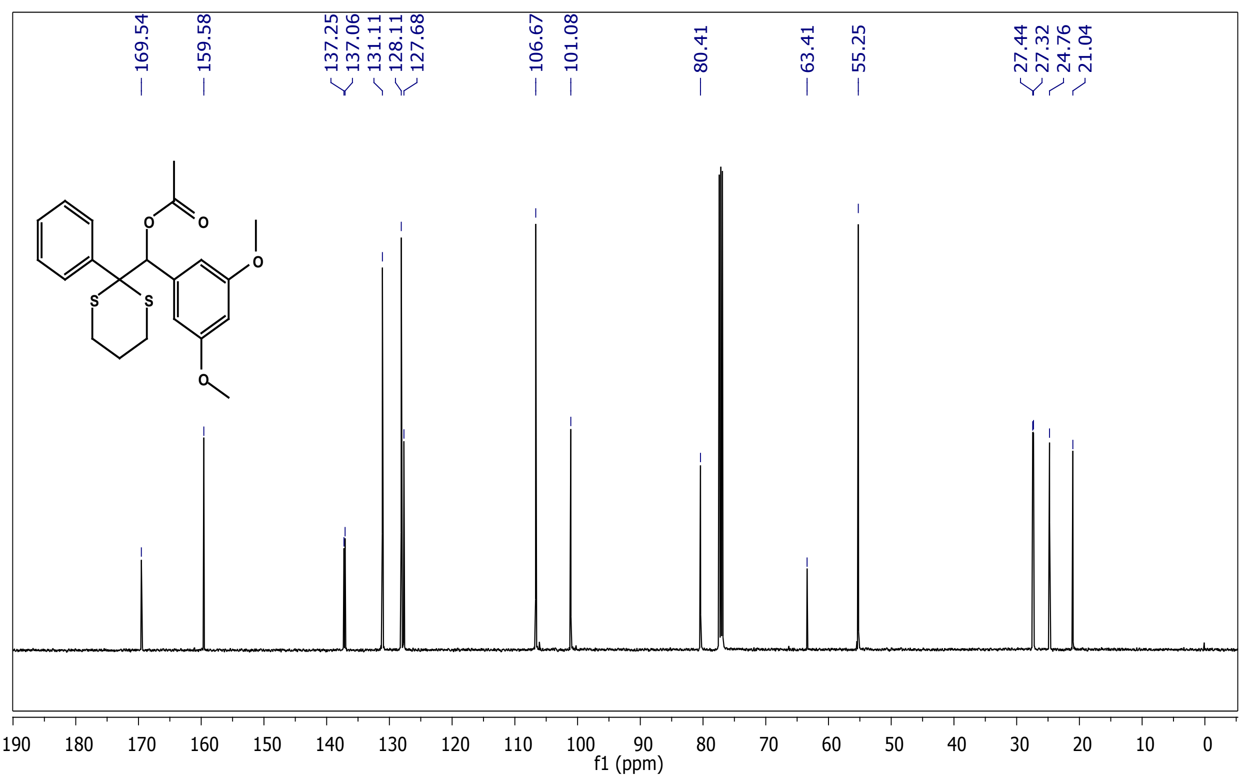
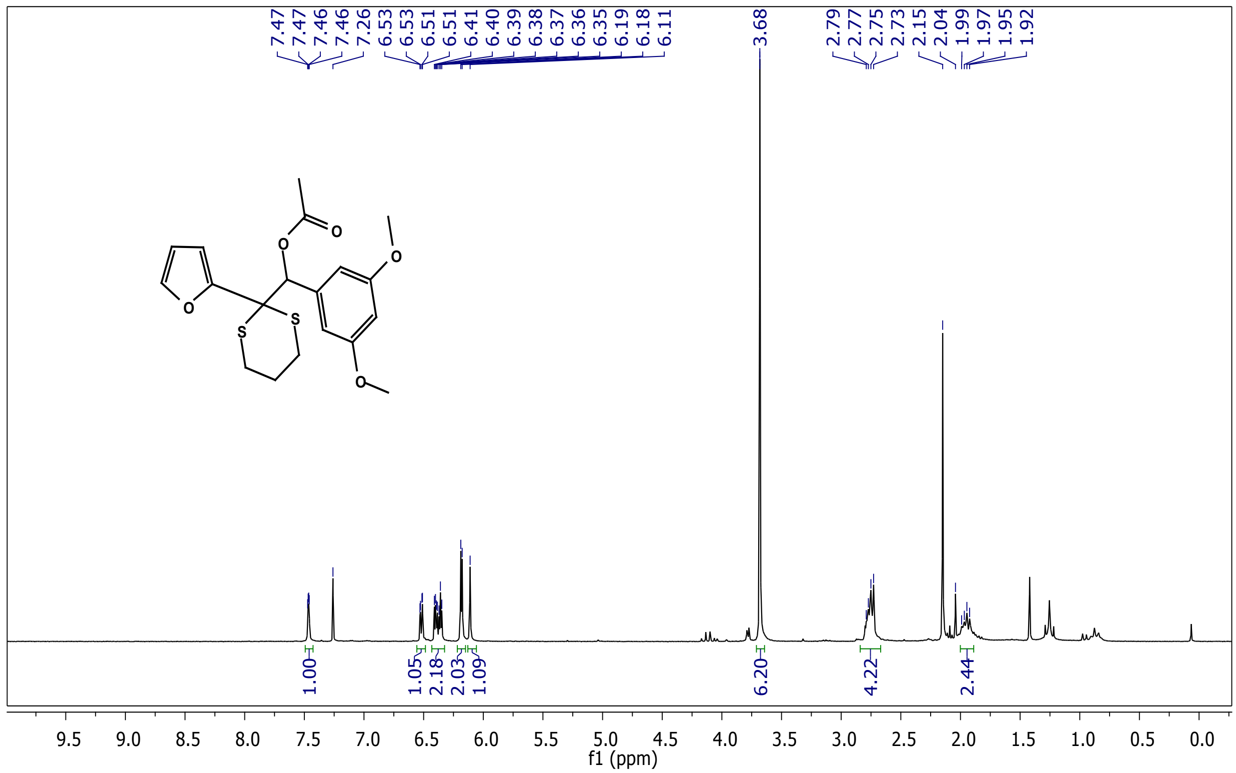


Figure S21. ^{1}H and ^{13}C NMR spectra of 3,5-dimethoxyphenyl)(2-(furan-2-yl)-1,3-dithian-2-yl)methyl acetate (**4b**)



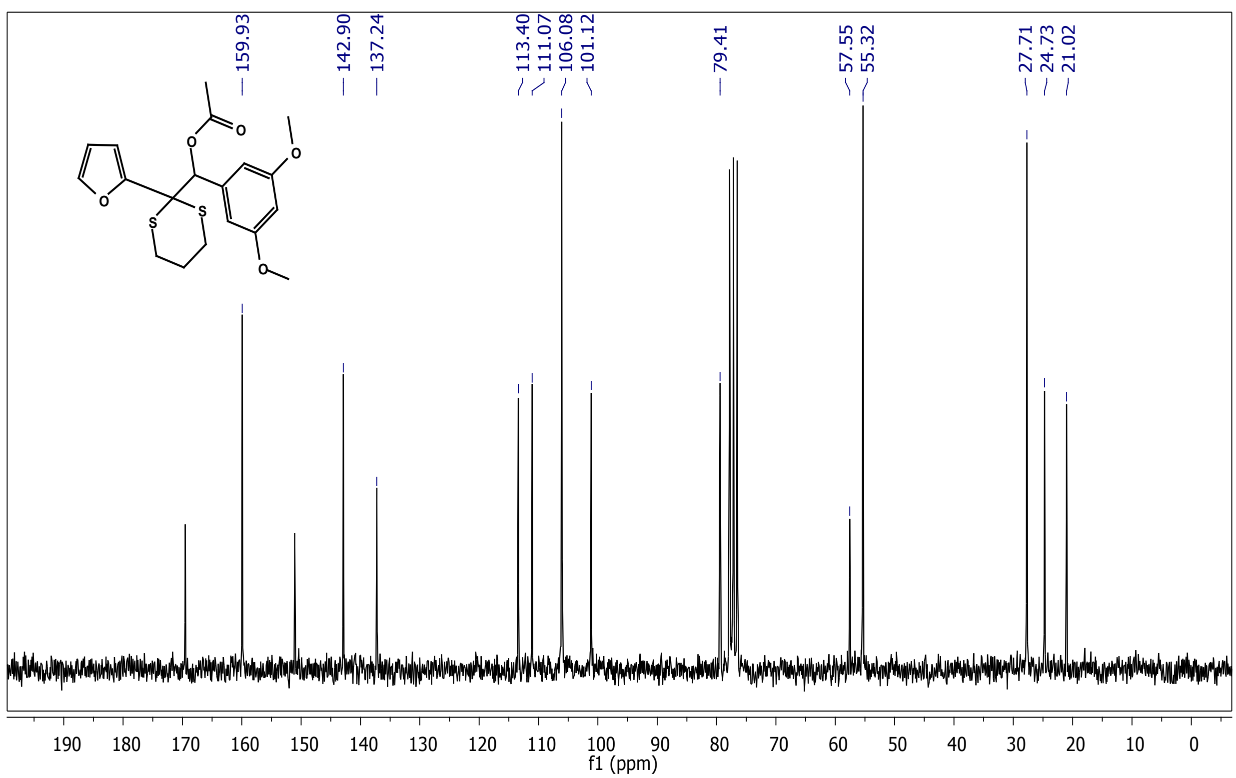
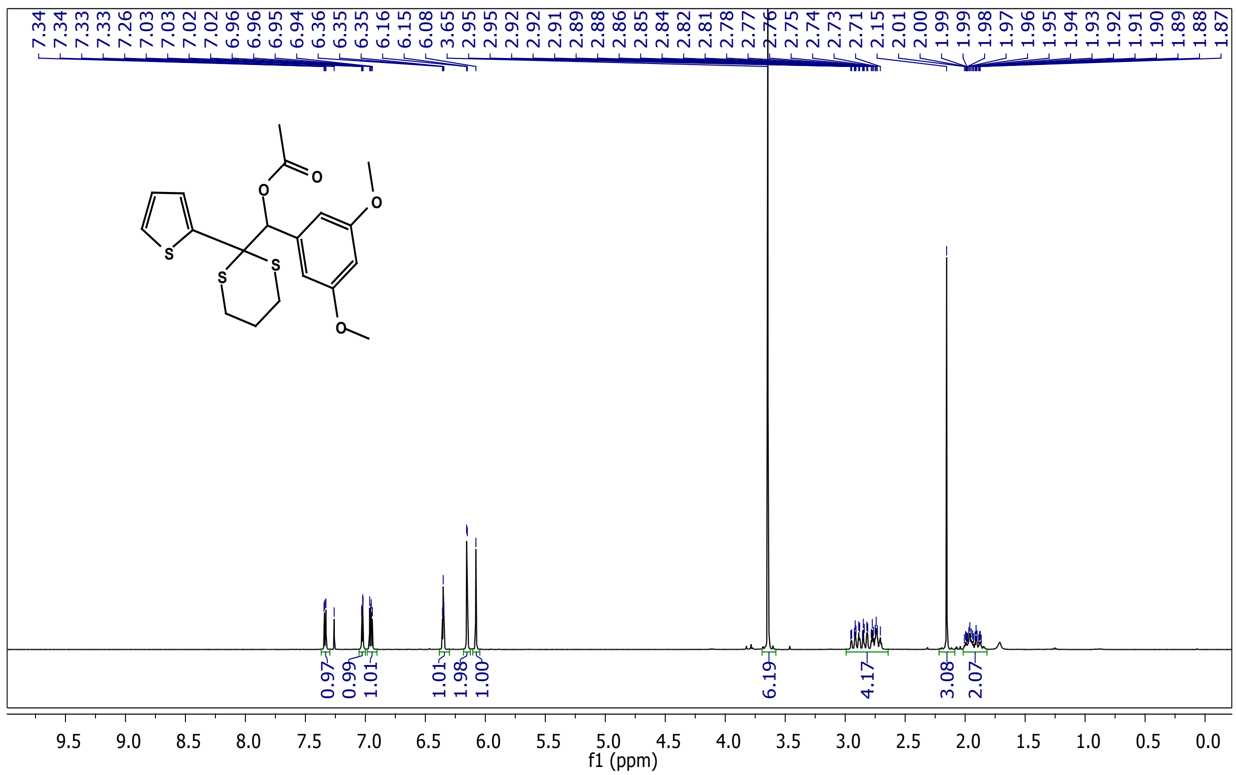


Figure S22. ^{1}H and ^{13}C NMR spectra of 3,5-dimethoxyphenyl)(2-(thiophen-2-yl)-1,3-dithian-2-yl)methyl acetate (**4c**)



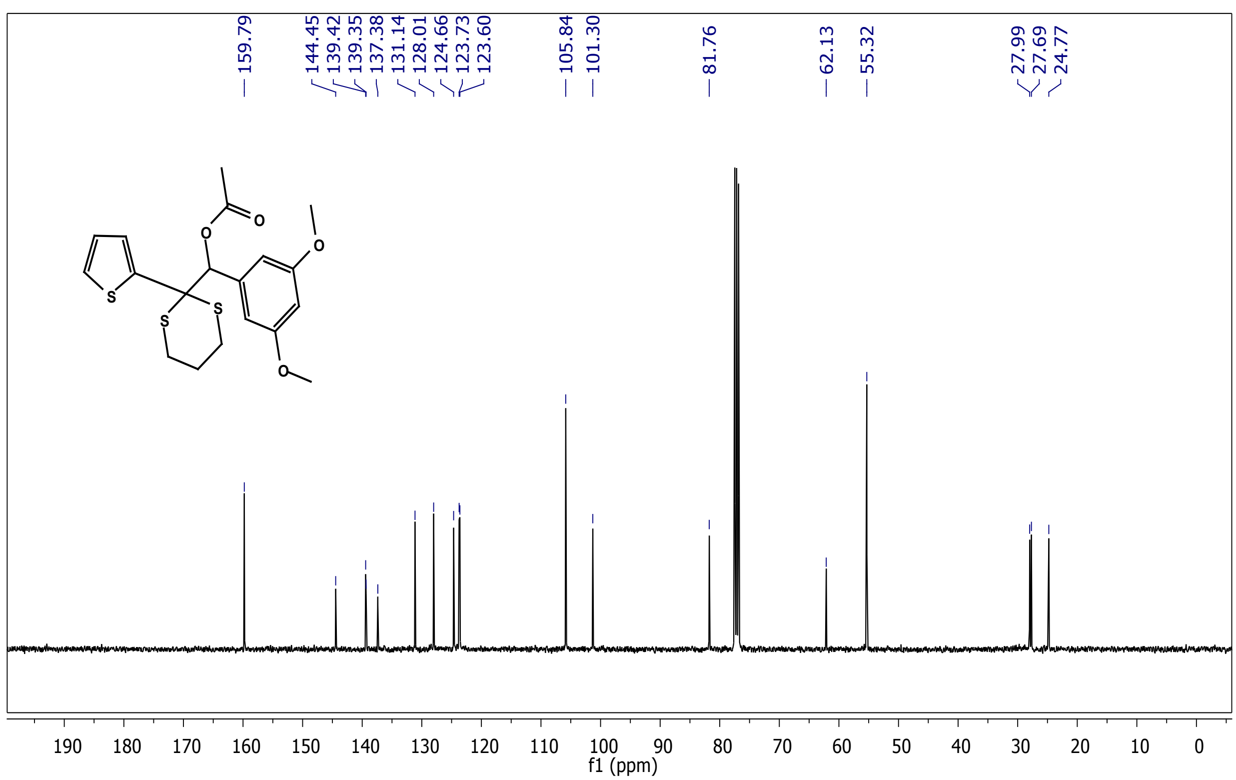
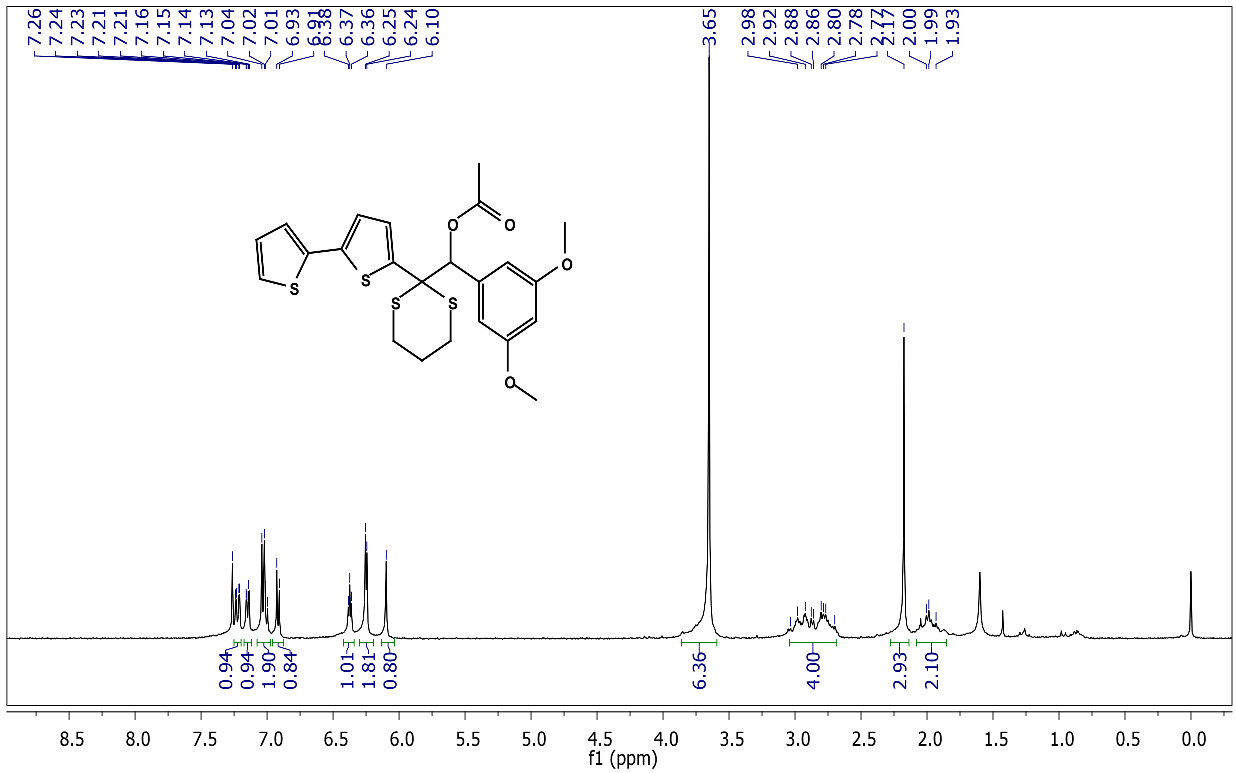


Figure S23. ^{1}H and ^{13}C NMR spectra of 2-([2,2'-bithiophen]-5-yl)-1,3-dithian-2-yl)(3,5-dimethoxyphenyl)methyl acetate (**4d**)



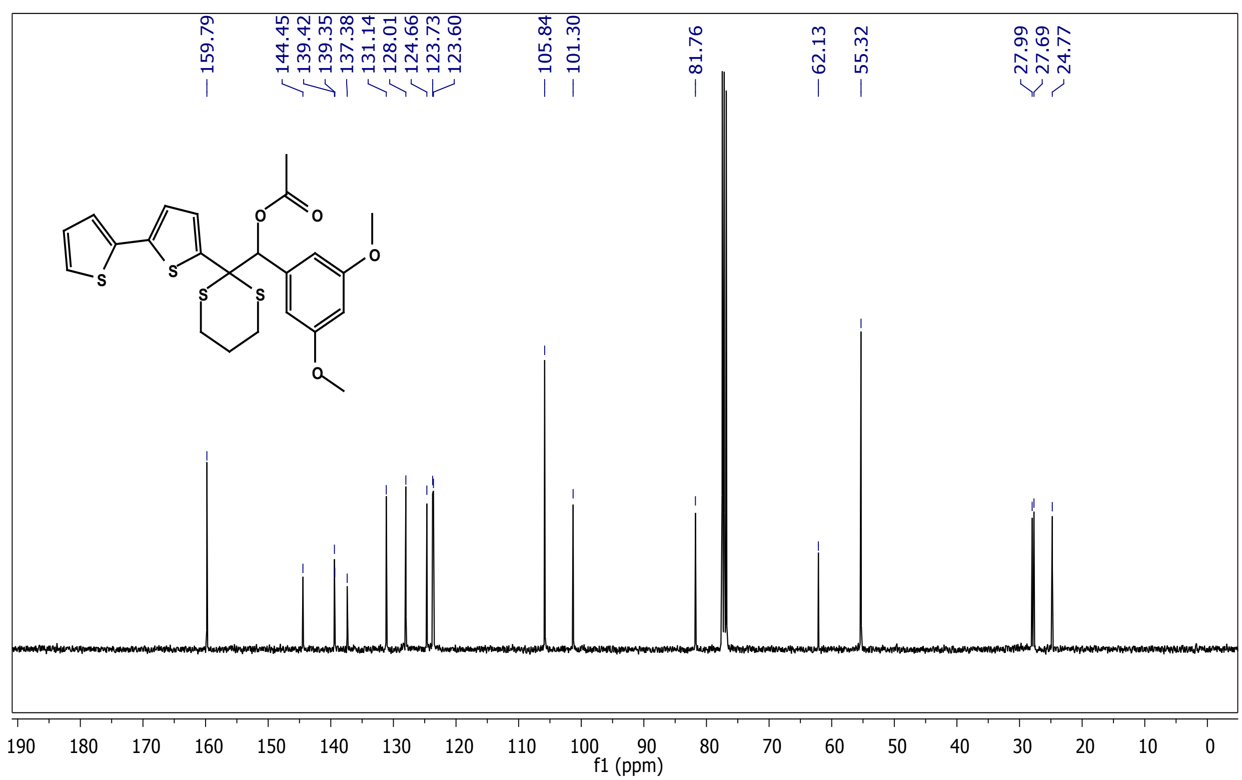
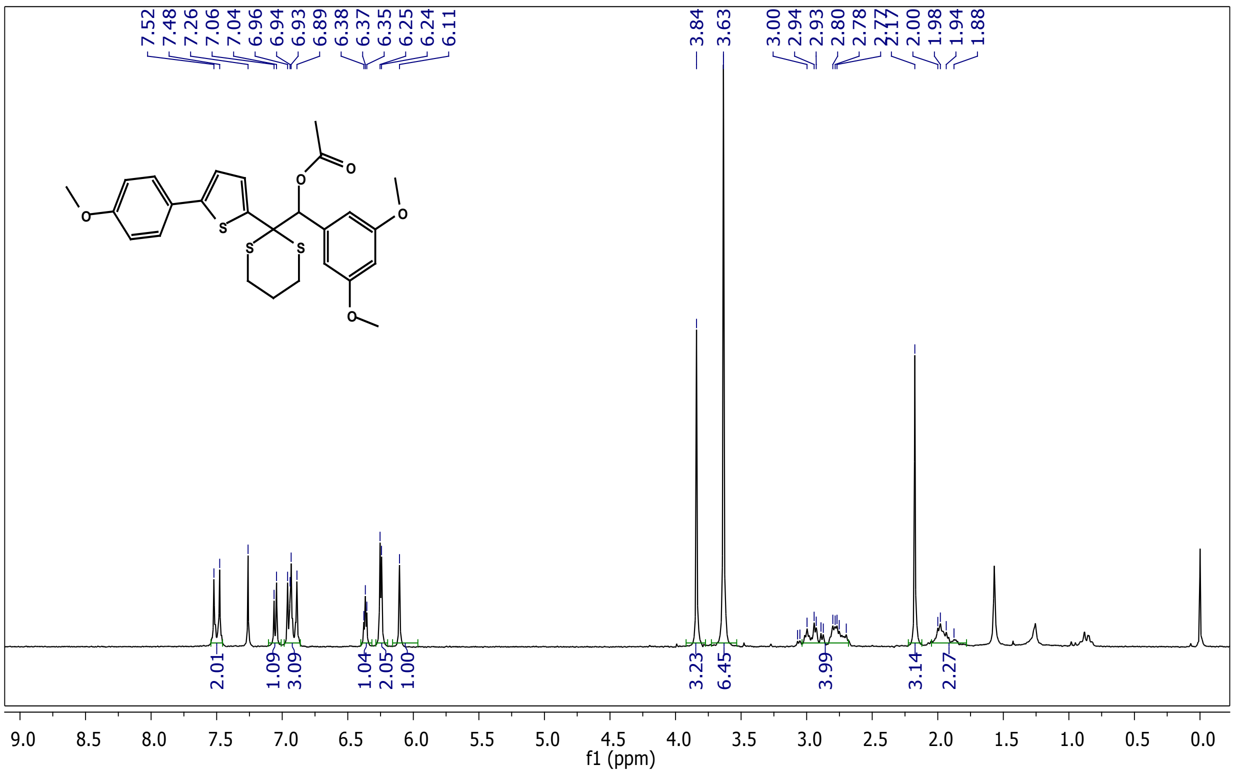


Figure S24. ^{1}H and ^{13}C NMR spectra of 3,5-dimethoxyphenyl)(2-(5-(4-methoxyphenyl)thiophen-2-yl)-1,3-dithian-2-yl)methyl acetate (**4e**)



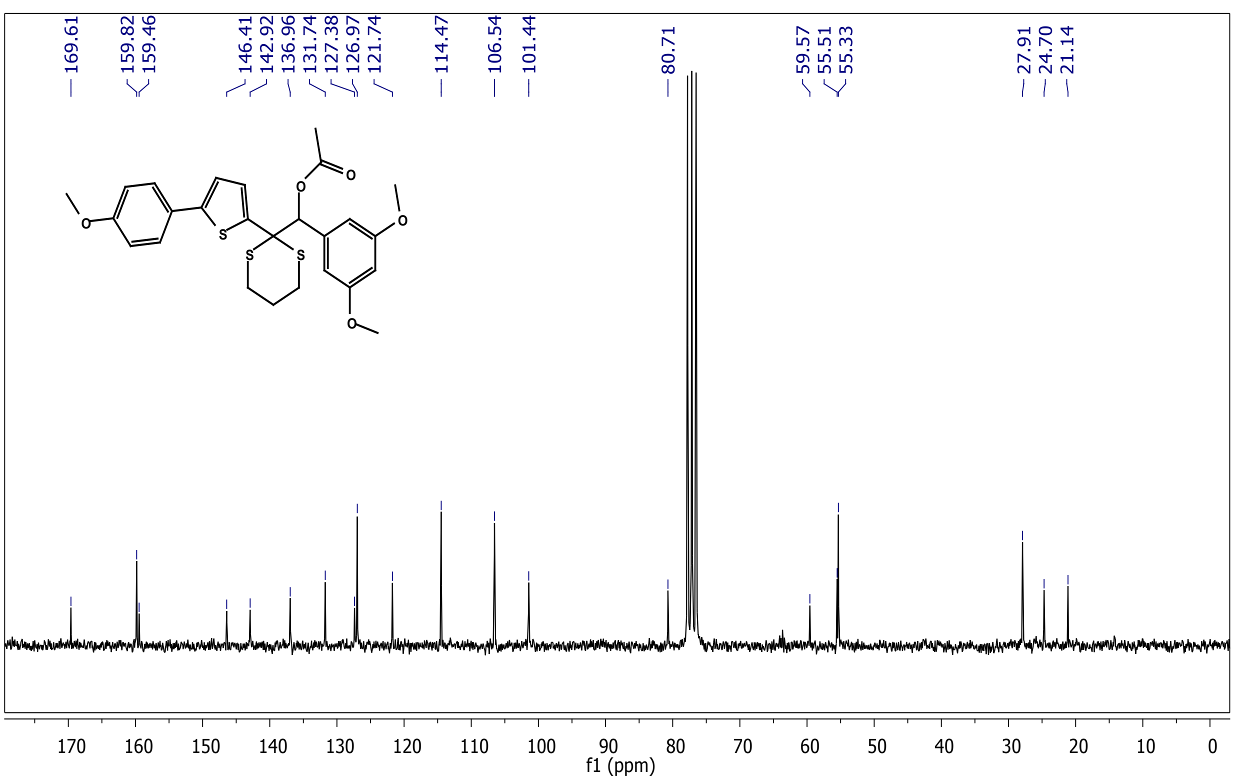
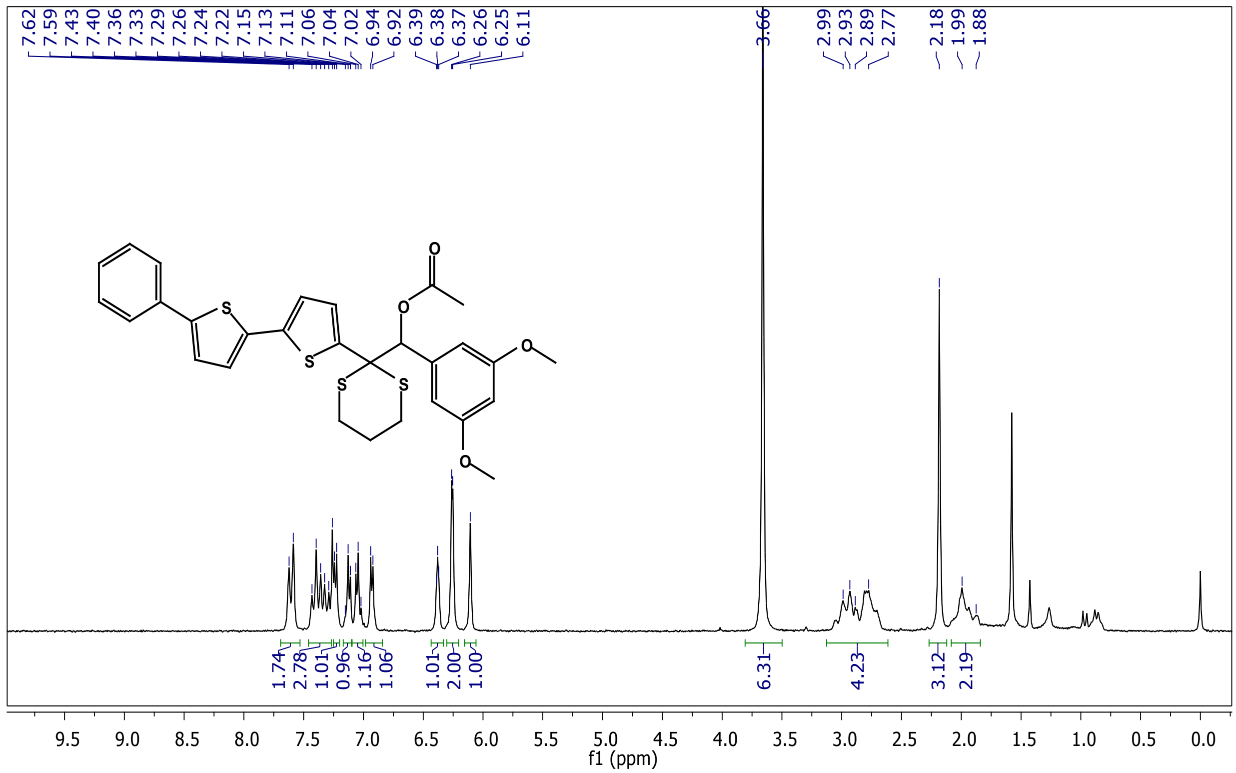


Figure S25. ^{1}H and ^{13}C NMR spectra of 3,5-dimethoxyphenyl)(2-(5'-phenyl-[2,2'-bithiophen]-5-yl)-1,3-dithian-2-yl)methyl acetate (**4f**)



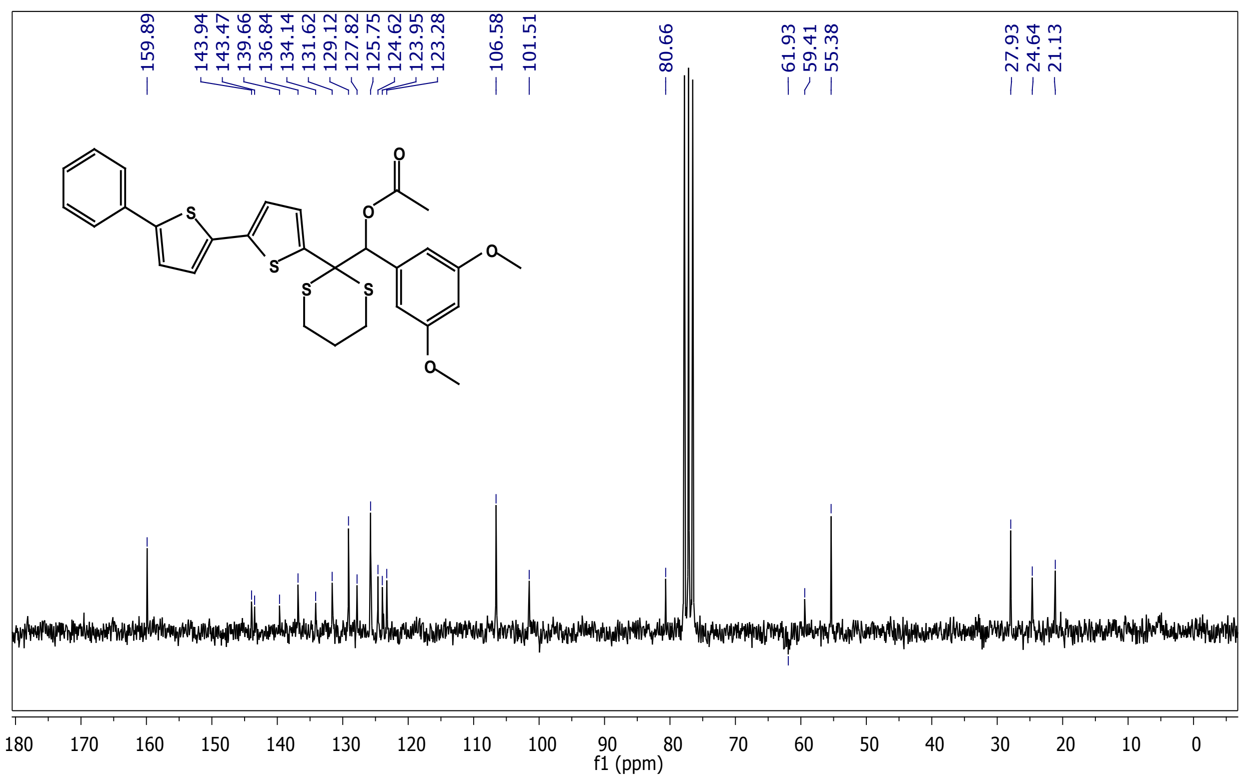
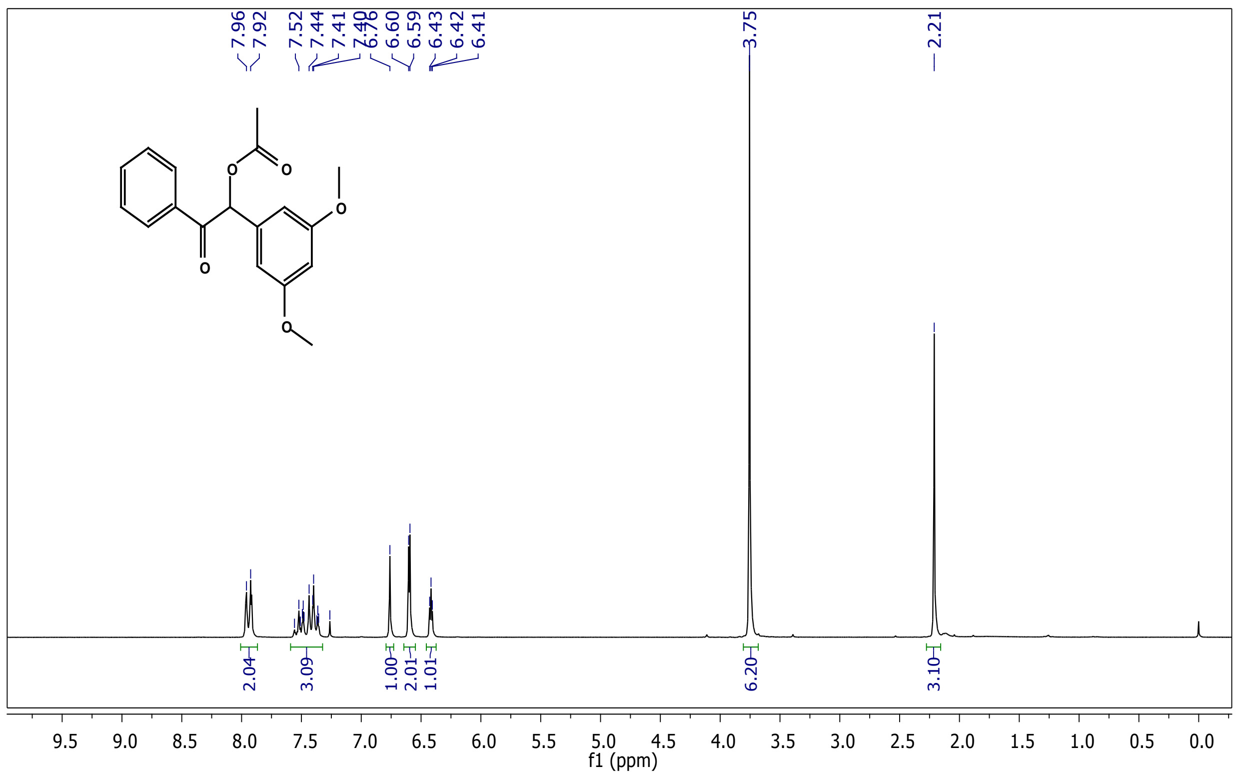


Figure S26. ^{1}H and ^{13}C NMR spectra of 1-(3,5-dimethoxyphenyl)-2-oxo-2-phenylethyl acetate (**5a**)



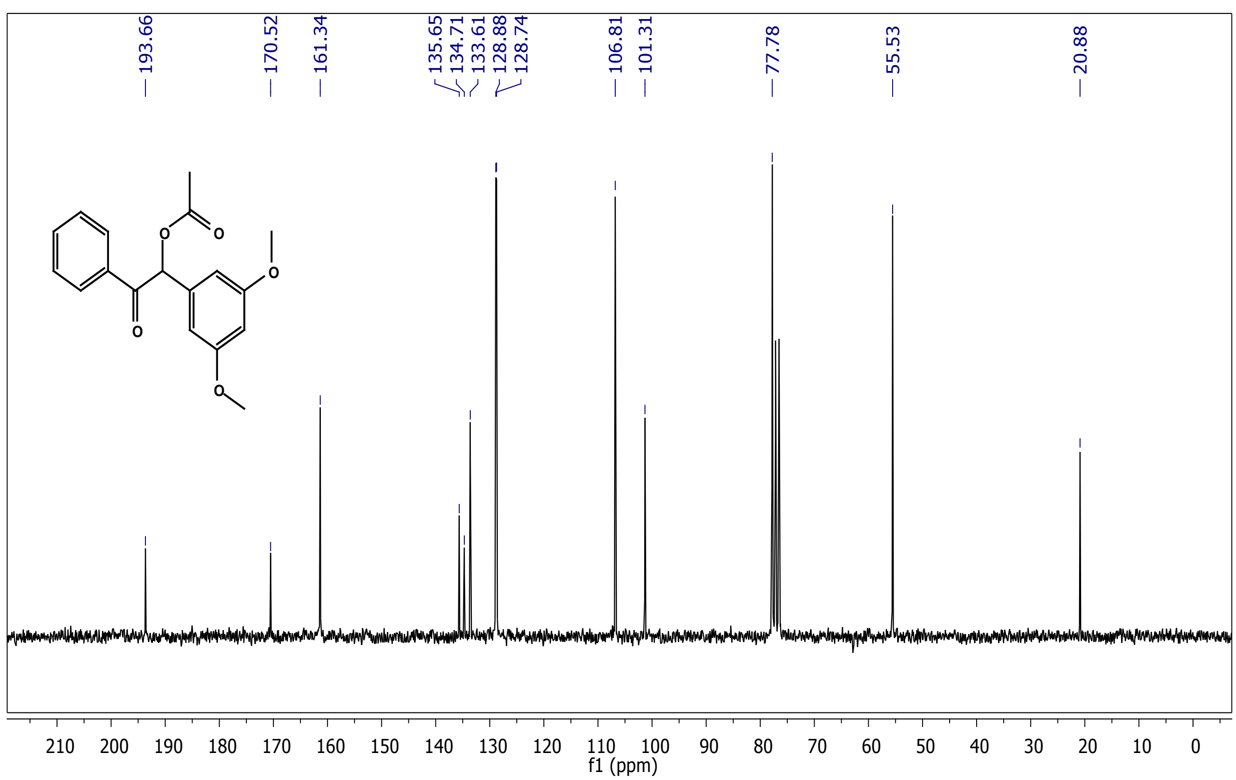
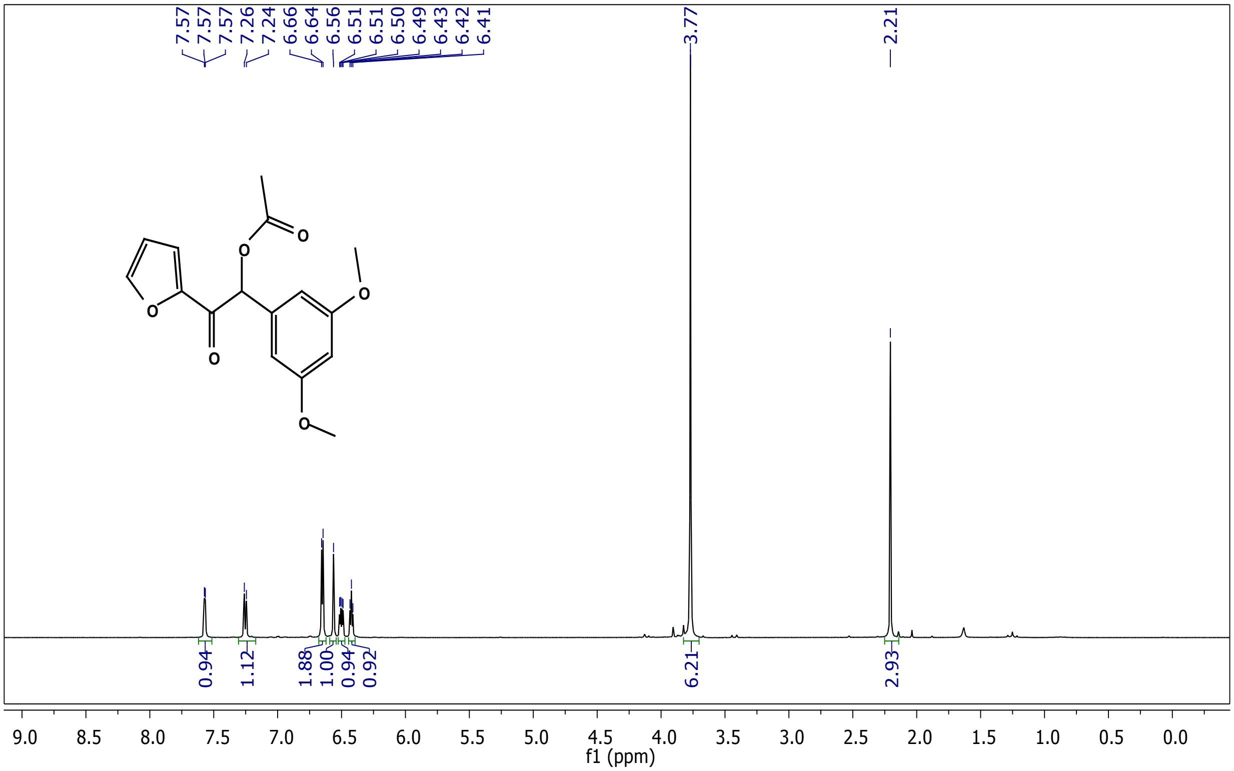


Figure S27. ^{1}H and ^{13}C NMR spectra of of 1-(3,5-dimethoxyphenyl)-2-(furan-2-yl)-2-oxoethyl acetate (**5b**)



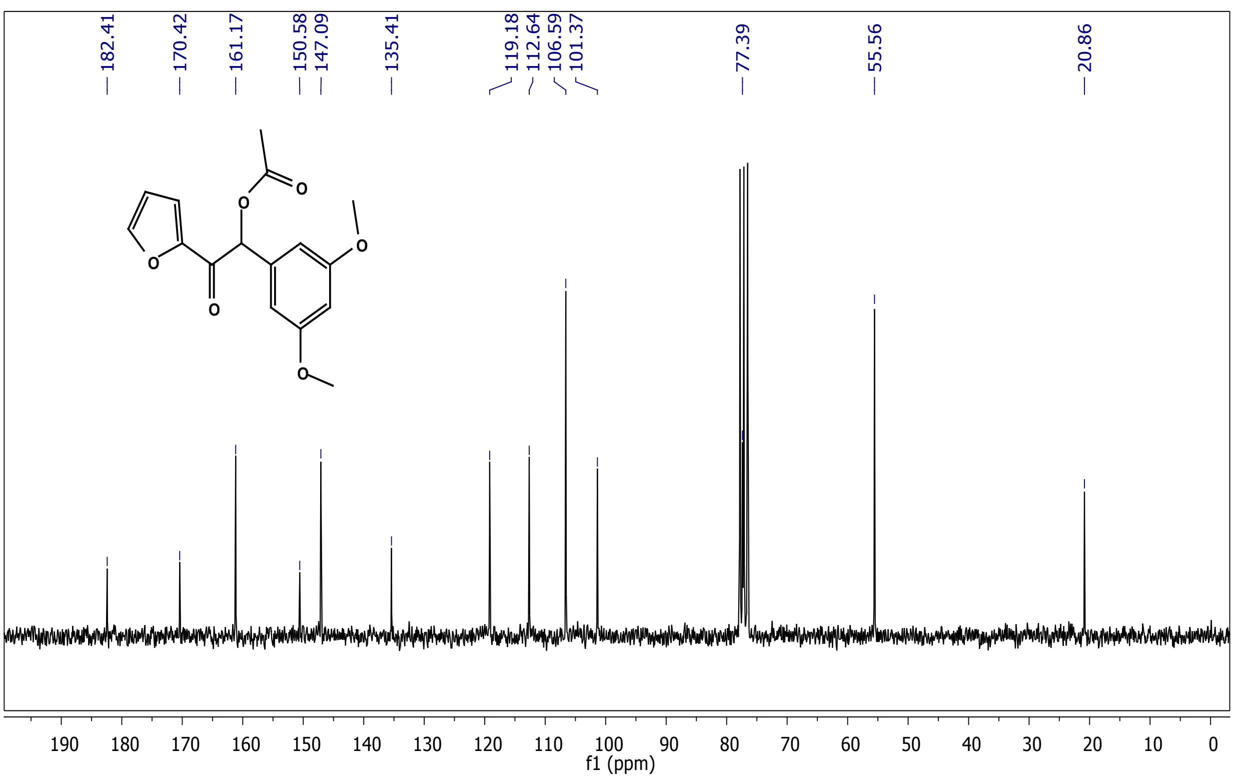
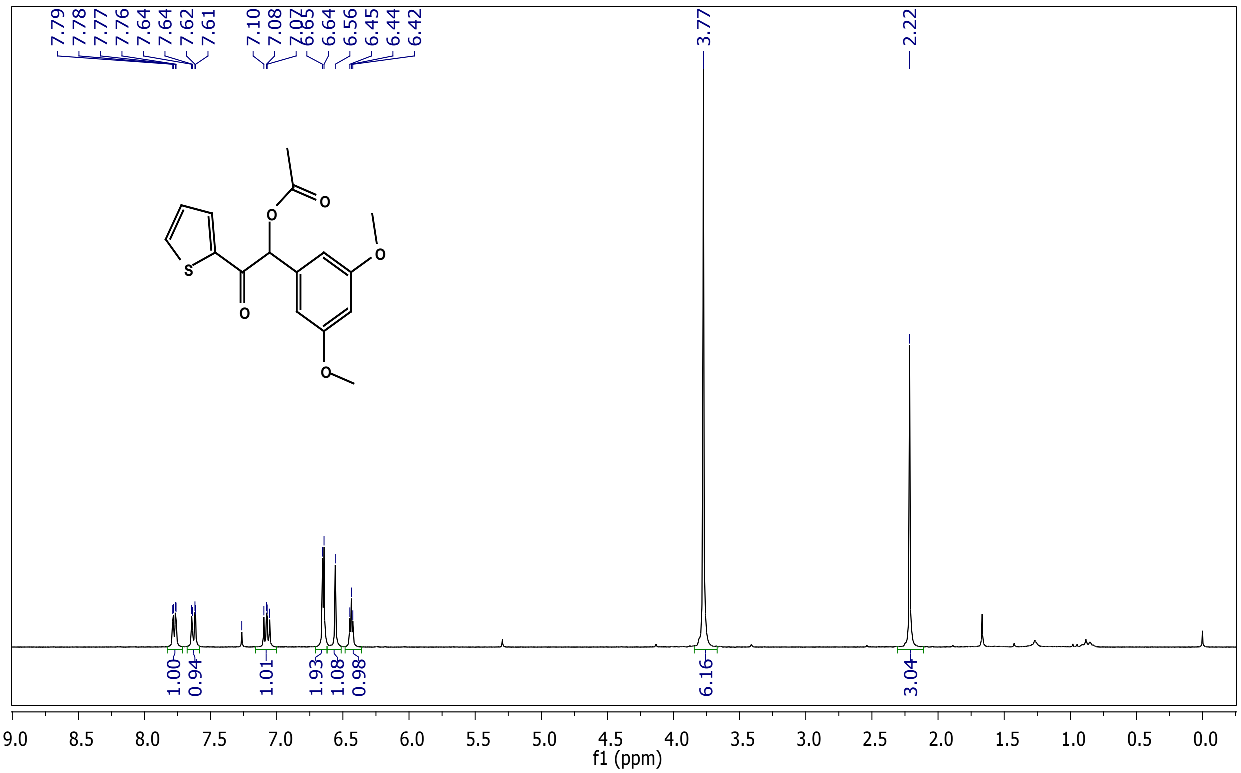


Figure S28. ^{1}H and ^{13}C NMR spectra of 1-(3,5-dimethoxyphenyl)-2-oxo-2-(thiophen-2-yl)ethyl acetate (**5c**)



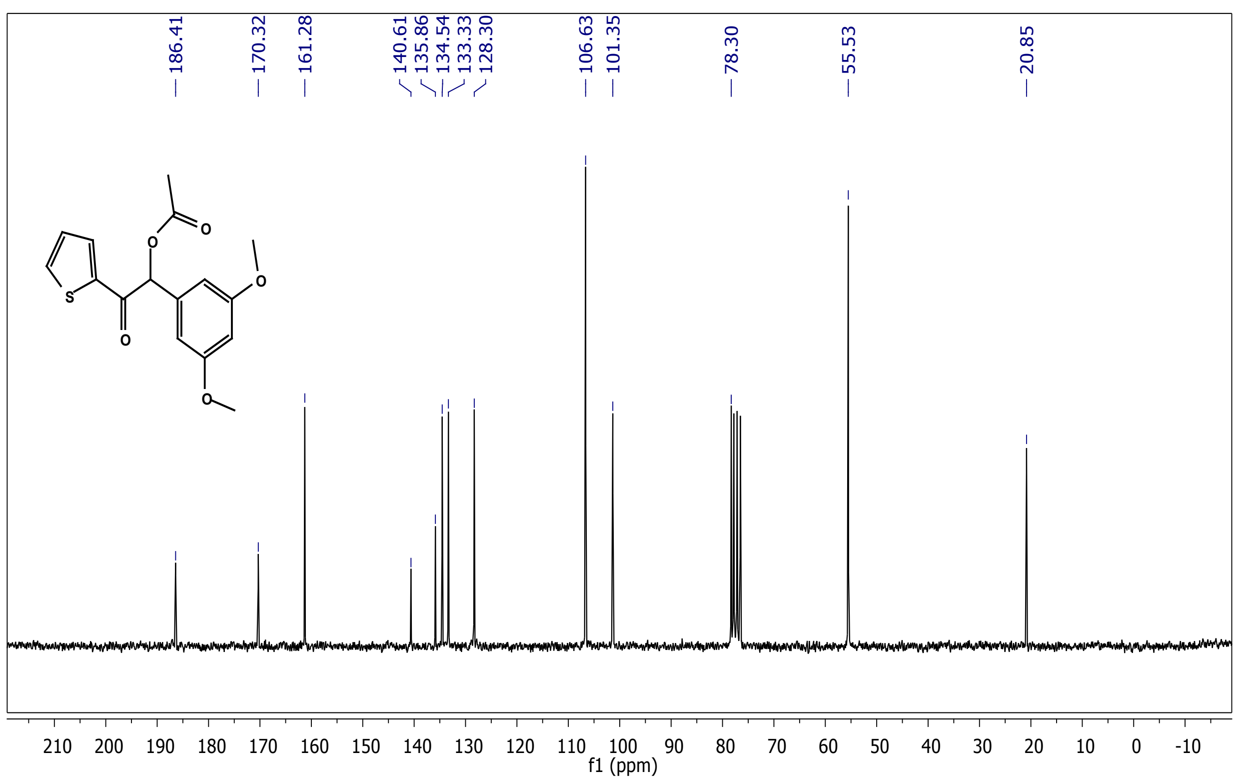
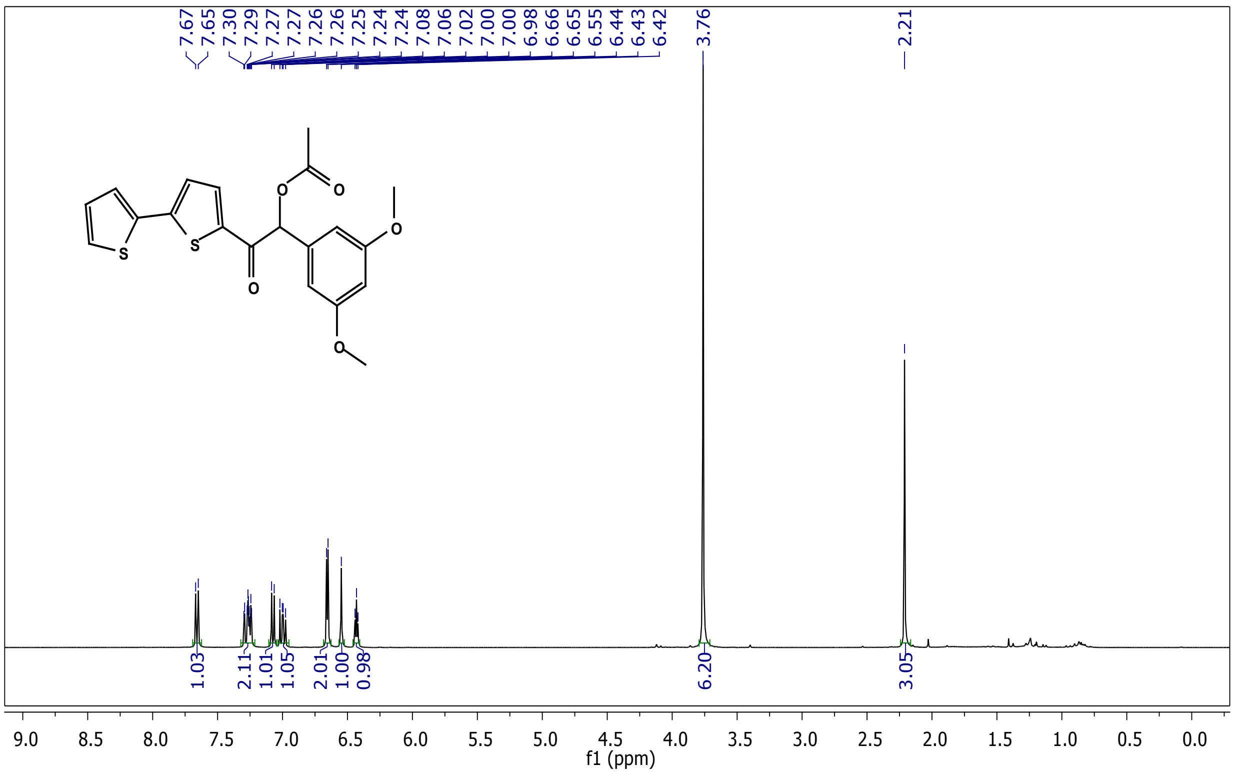


Figure S29. ^{1}H and ^{13}C NMR spectra of 2-([2,2'-bithiophen]-5-yl)-1-(3,5-dimethoxyphenyl)-2-oxoethyl acetate (**5d**)



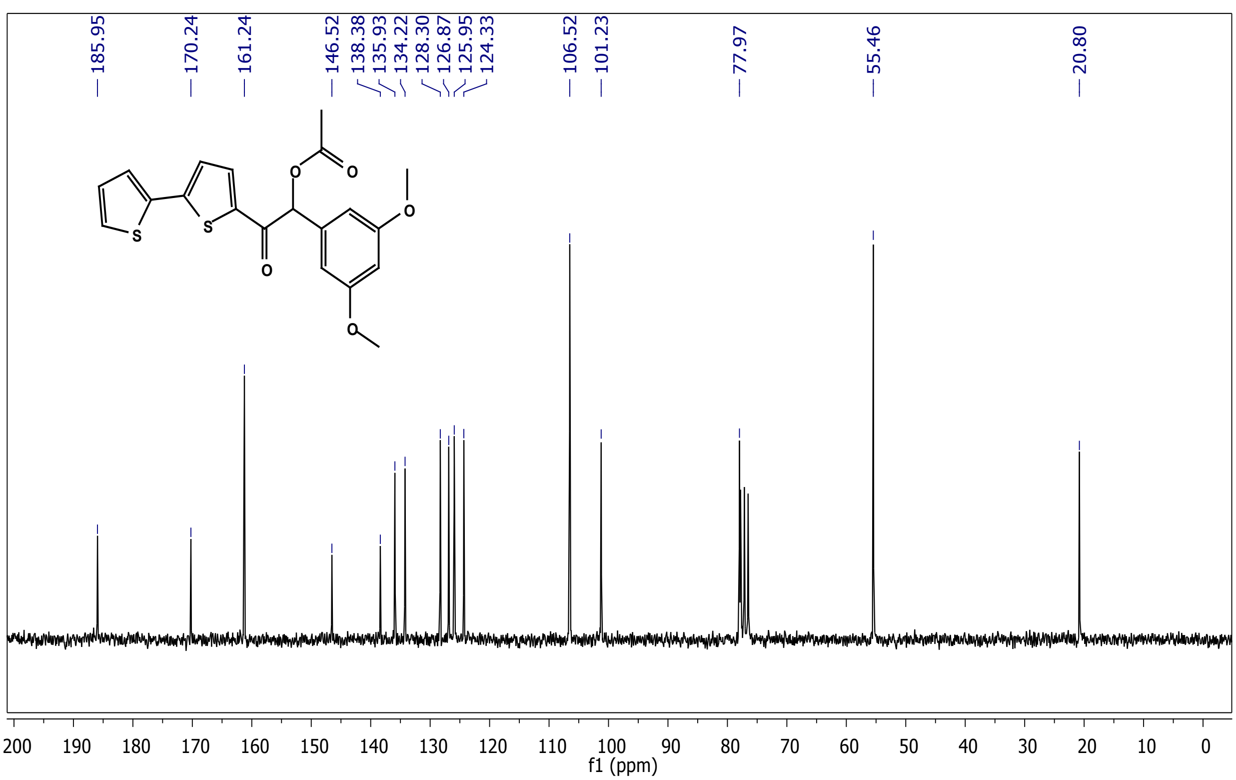
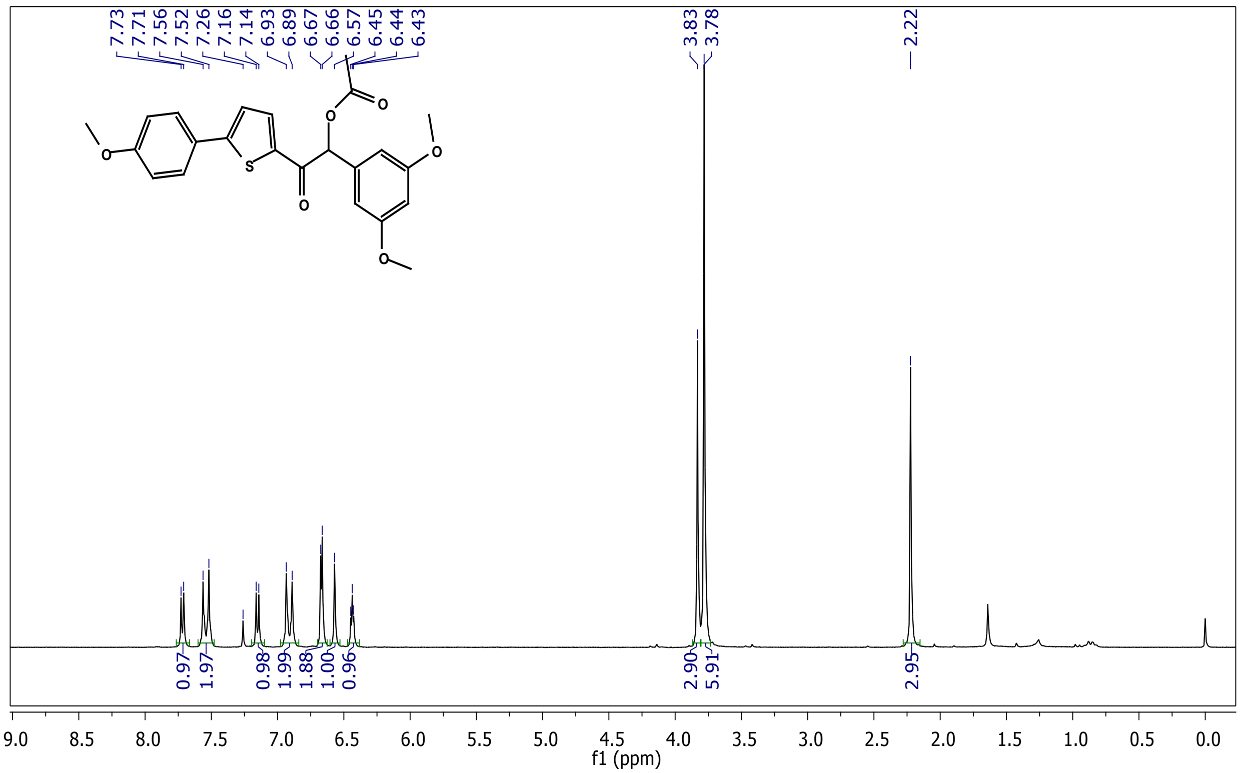


Figure S30. ^{1}H and ^{13}C NMR spectra of 1-(3,5-dimethoxyphenyl)-2-(5-(4-methoxyphenyl)thiophen-2-yl)-2-oxoethyl acetate (**5e**)



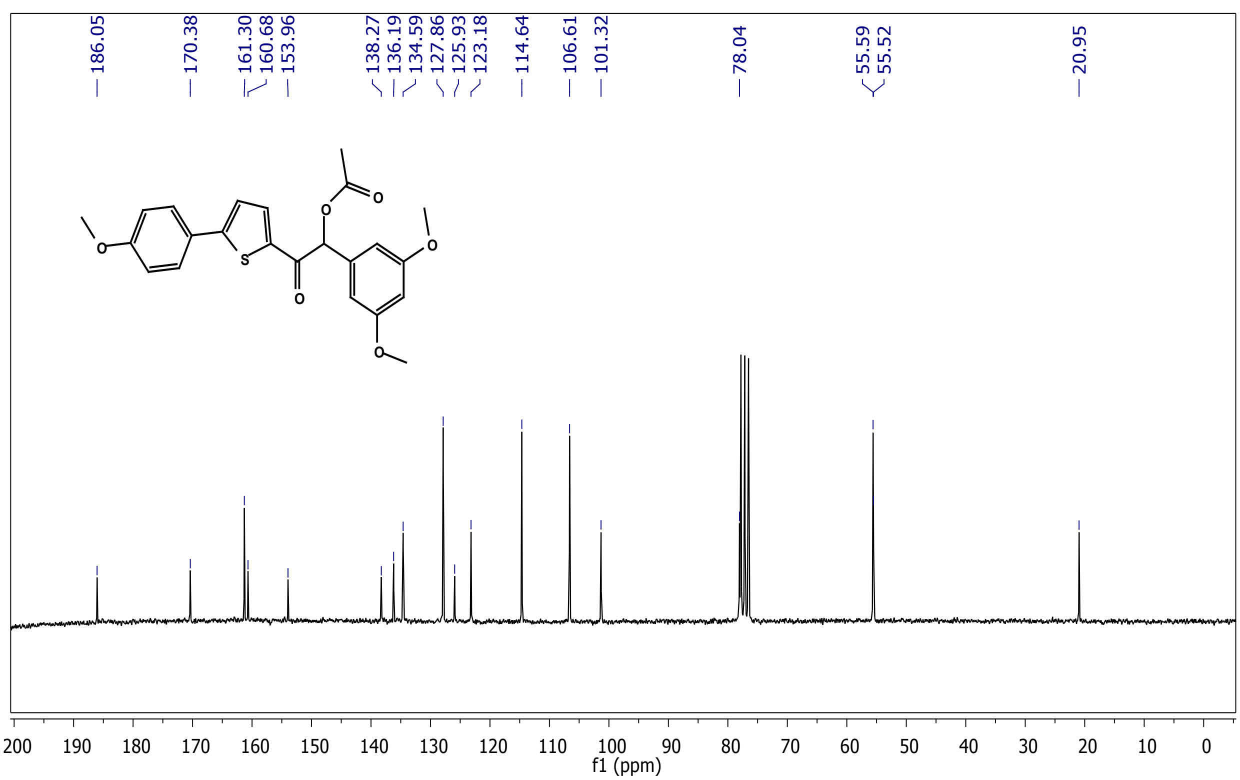
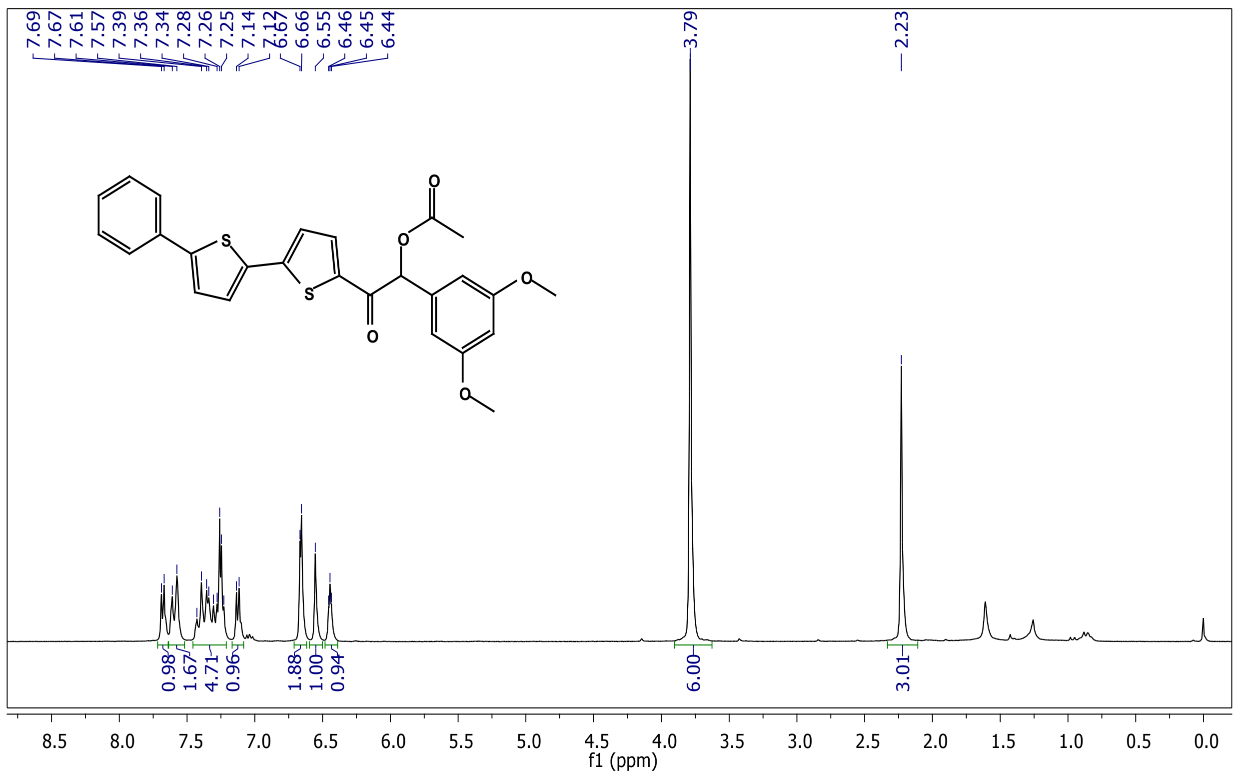


Figure S31. [1]H and [13]C NMR spectra of 1-(3,5-dimethoxyphenyl)-2-oxo-2-(5'-phenyl-[2,2'-bithiophen]-5-yl)ethyl acetate (**5f**)



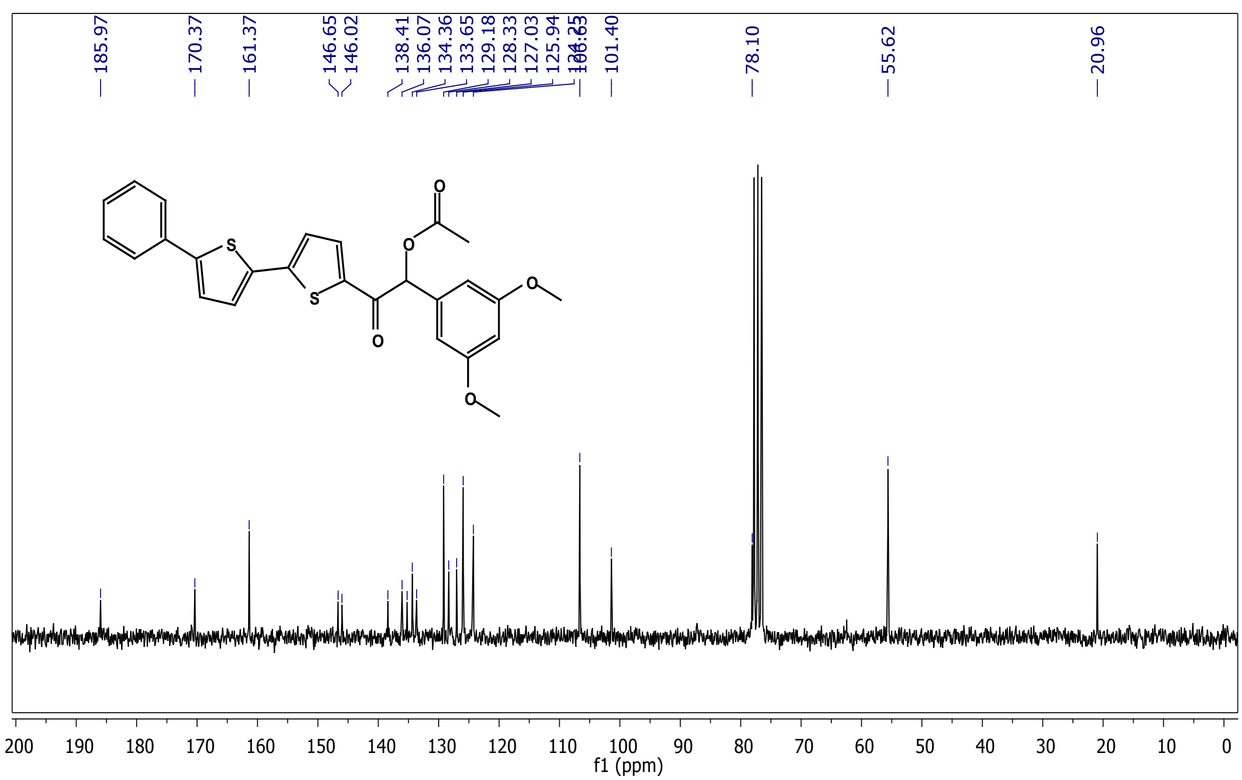
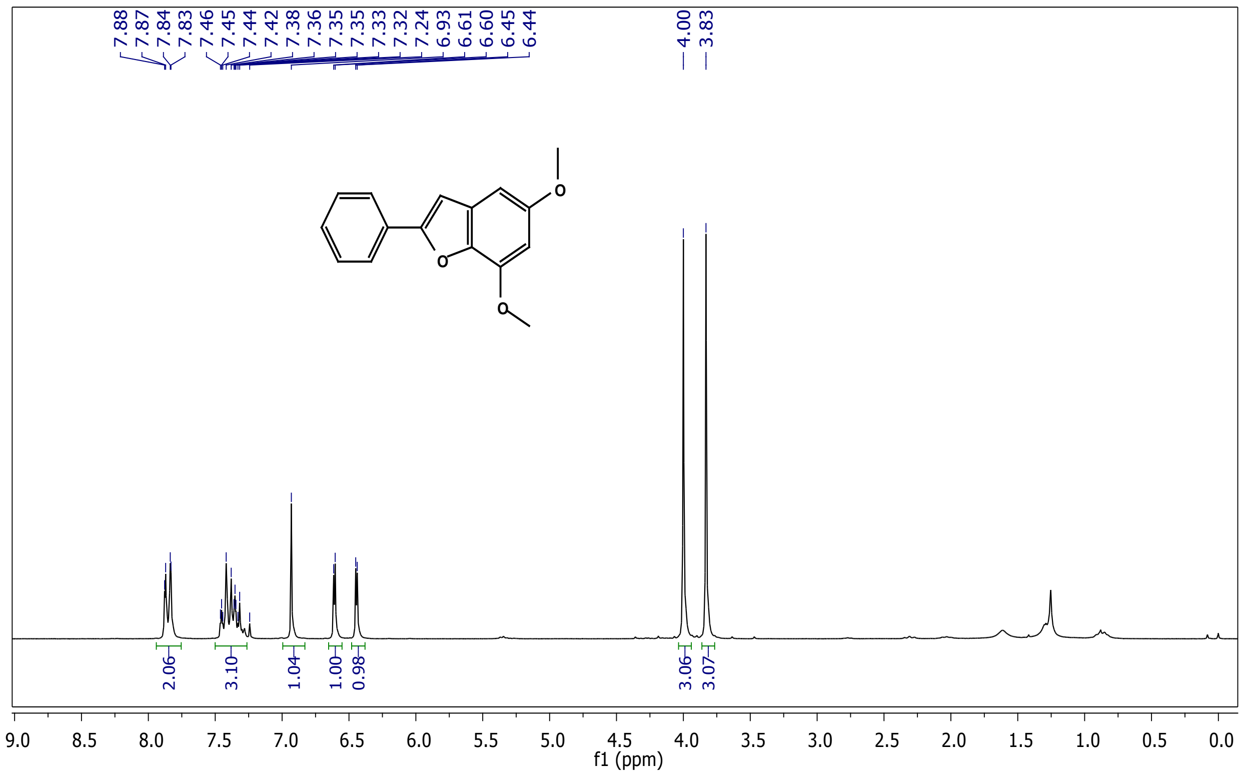


Figure S32. ^{1}H and ^{13}C NMR spectra of 5,7-dimethoxy-2-phenylbenzofuran (**6a**)



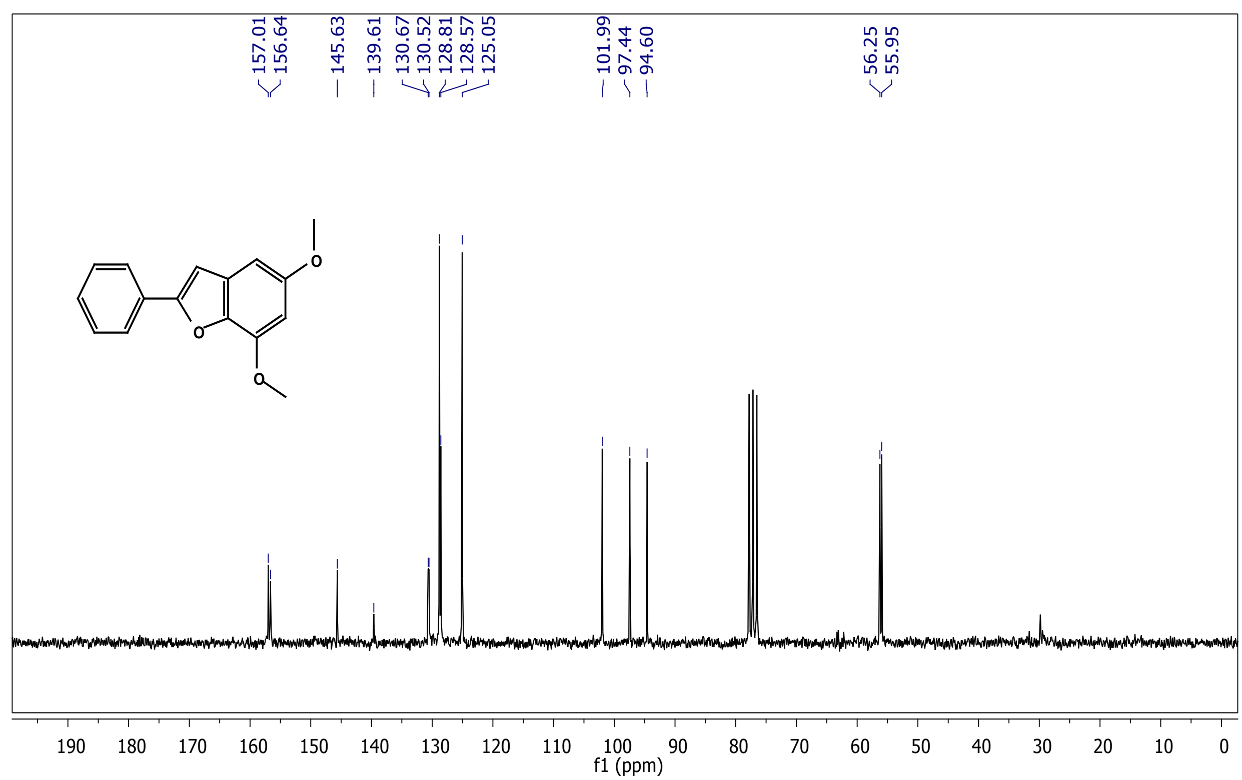
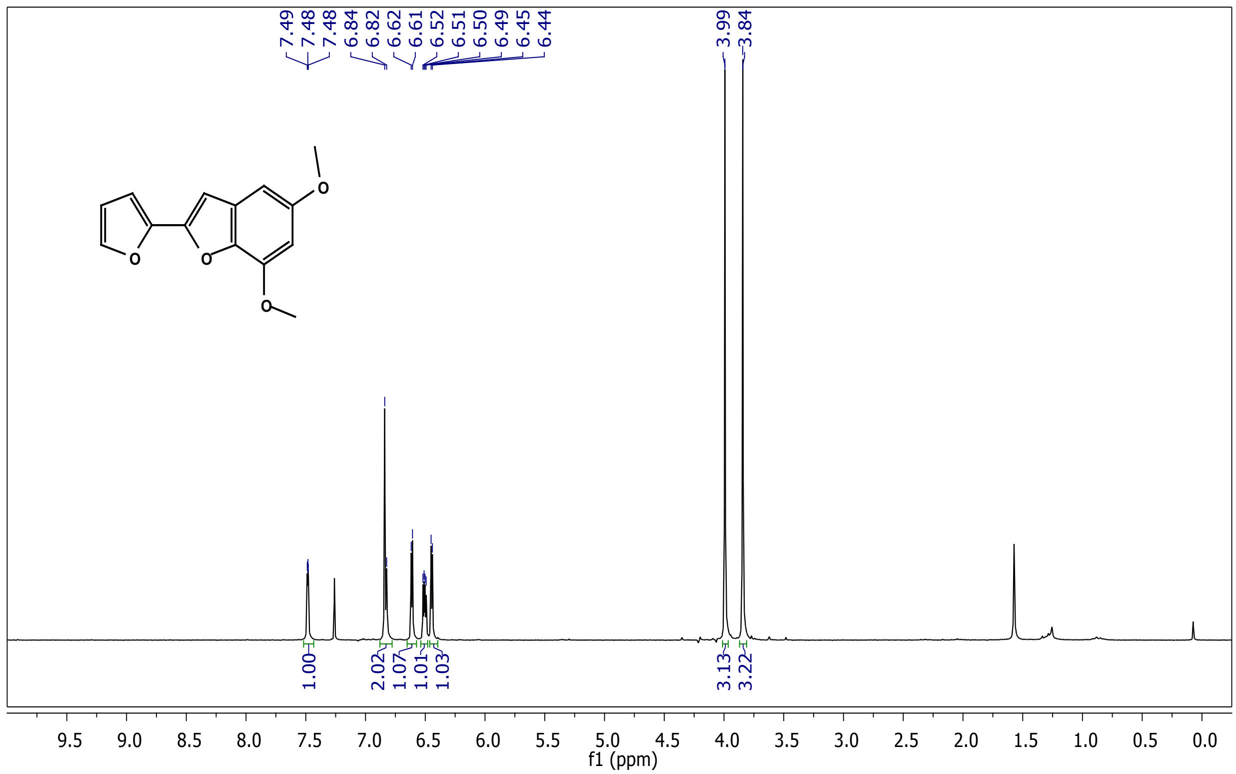


Figure S33. ^1H and ^{13}C NMR spectra of 2-(furan-2-yl)-5,7-dimethoxybenzofuran (**6b**)



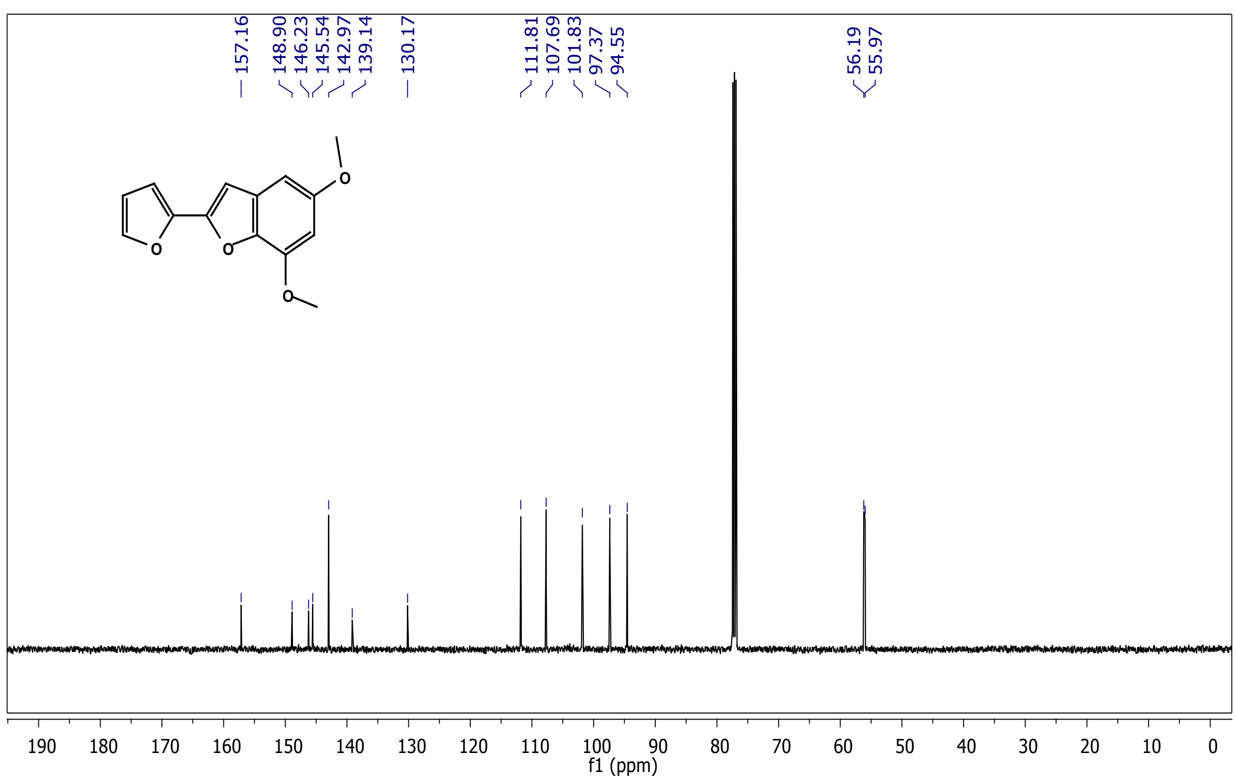
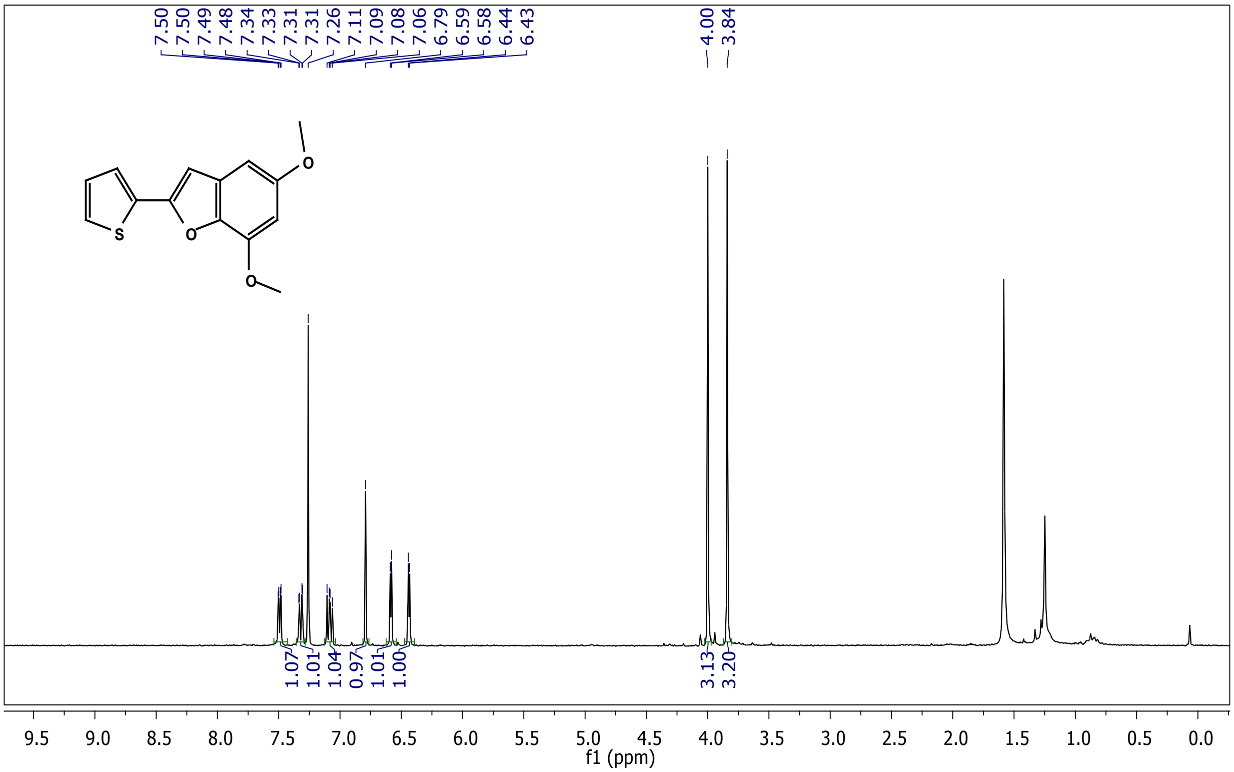


Figure S34. ^{1}H and ^{13}C NMR spectra of 5,7-dimethoxy-2-(thiophen-2-yl)benzofuran (6c)



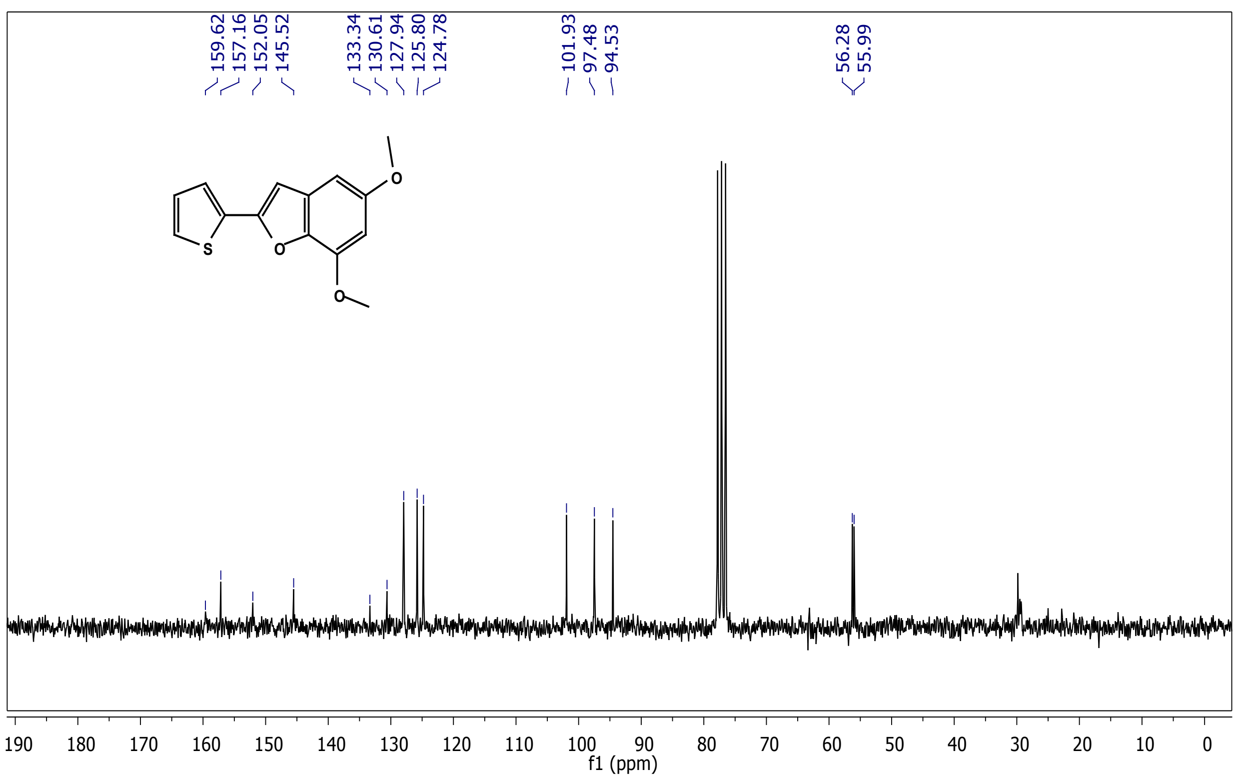
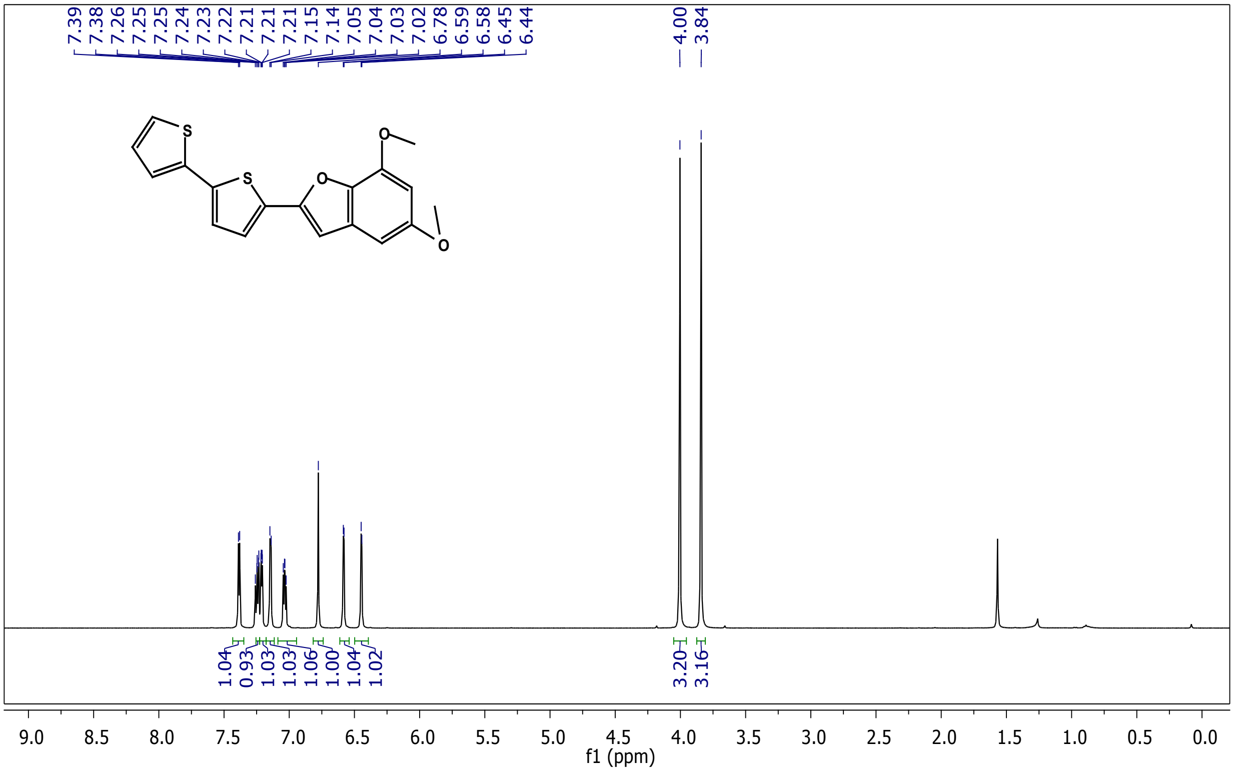


Figure S35. ^{1}H and ^{13}C NMR spectra of 2-([2,2'-bithiophen]-5-yl)-5,7-dimethoxybenzofuran (**6d**)



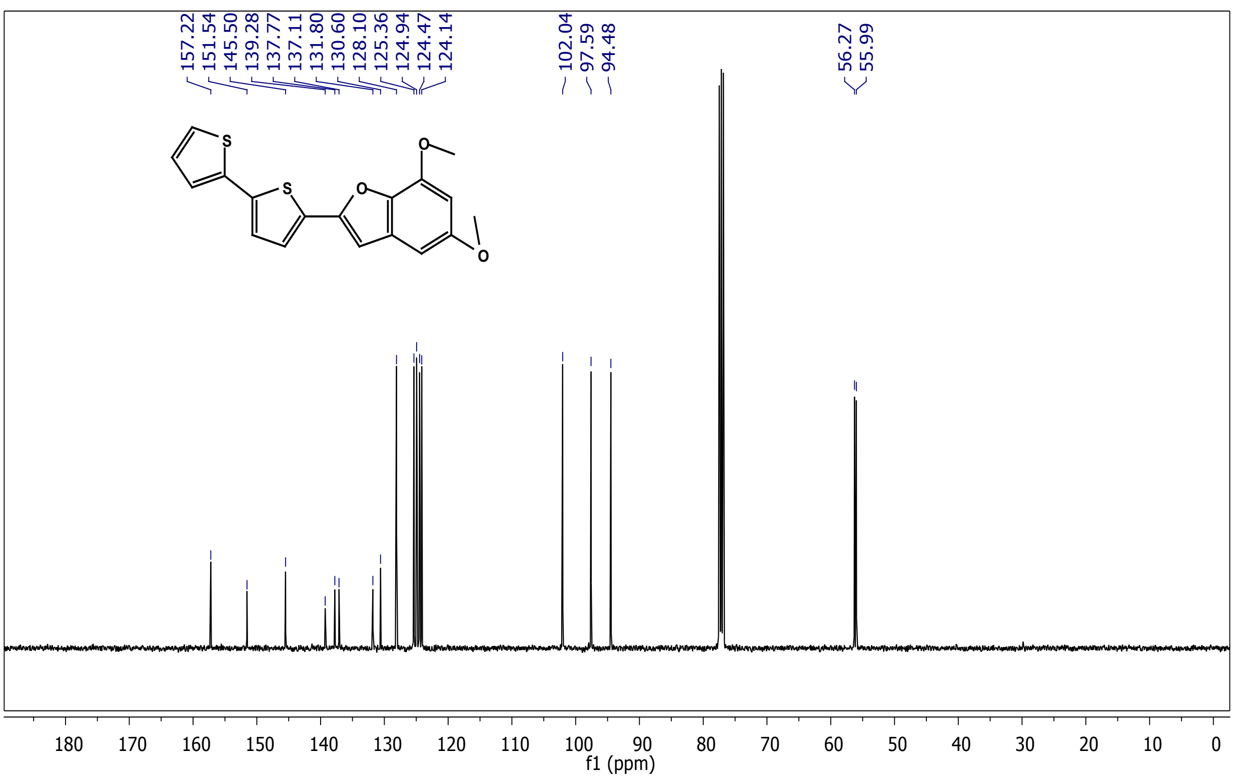
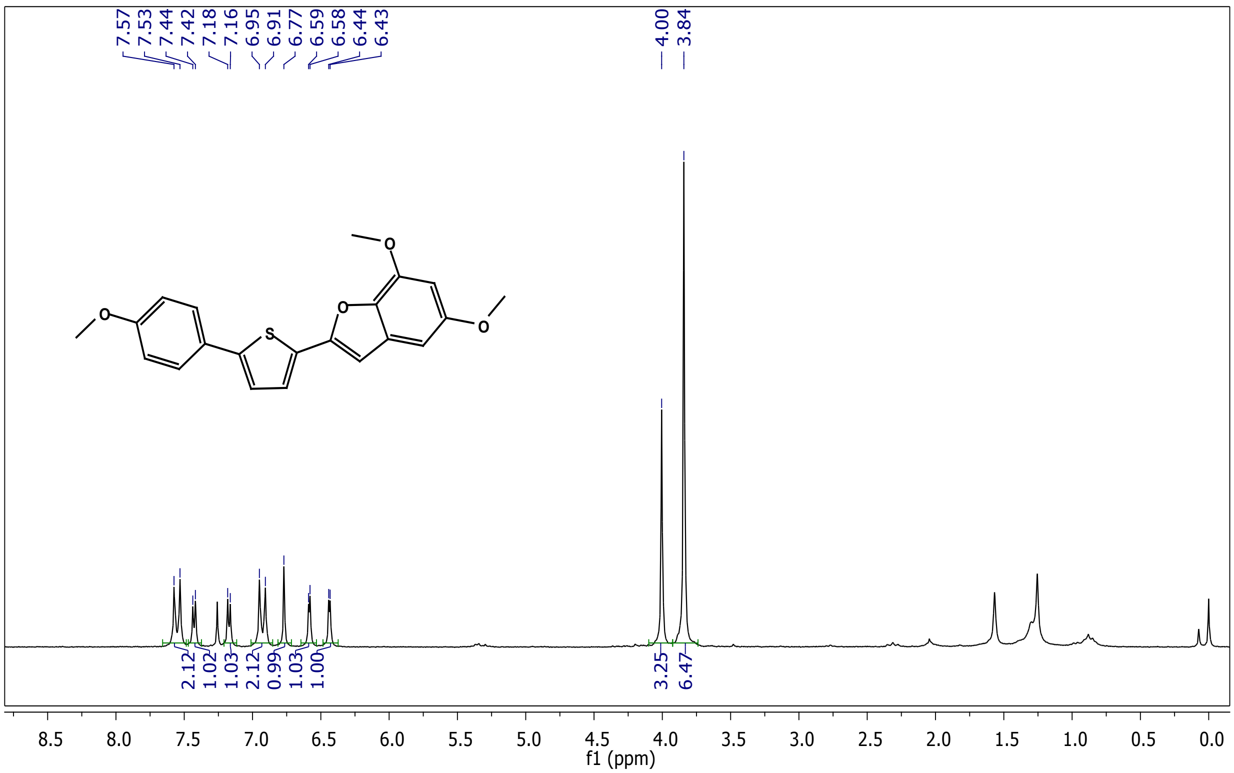


Figure S36. ^{1}H and ^{13}C NMR spectra of 5,7-dimethoxy-2-(5-(4-methoxyphenyl)thiophen-2-yl)benzofuran (**6e**)



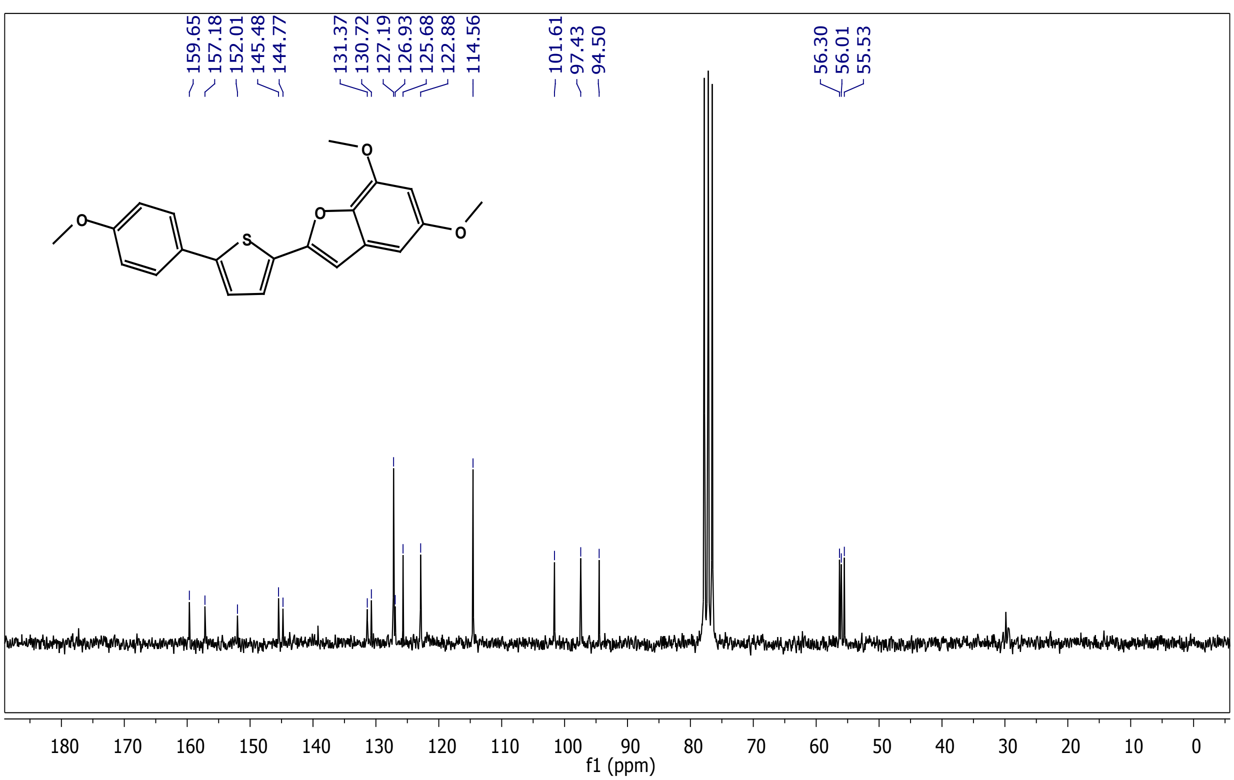
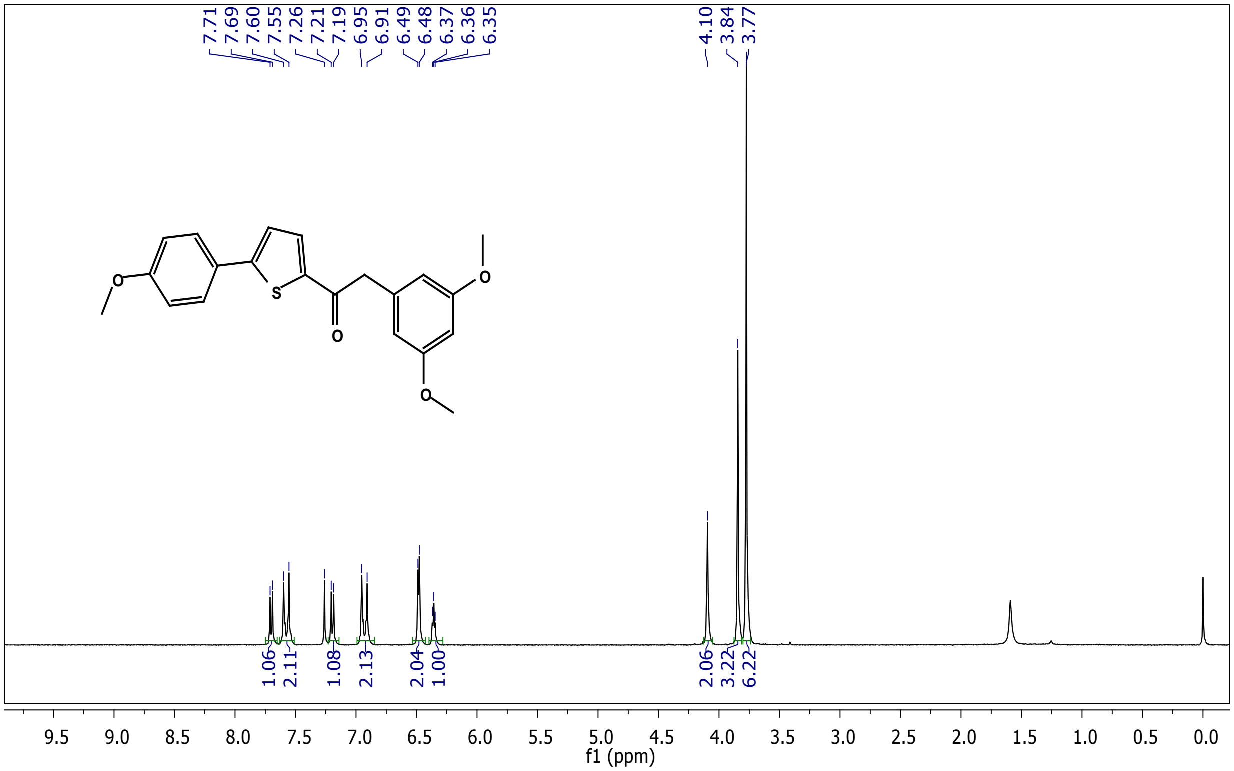


Figure S37. ^{1}H and ^{13}C NMR spectra of 2-(3,5-dimethoxyphenyl)-1-(5-(4-methoxyphenyl)thiophen-2-yl)ethan-1-one (**7e**)



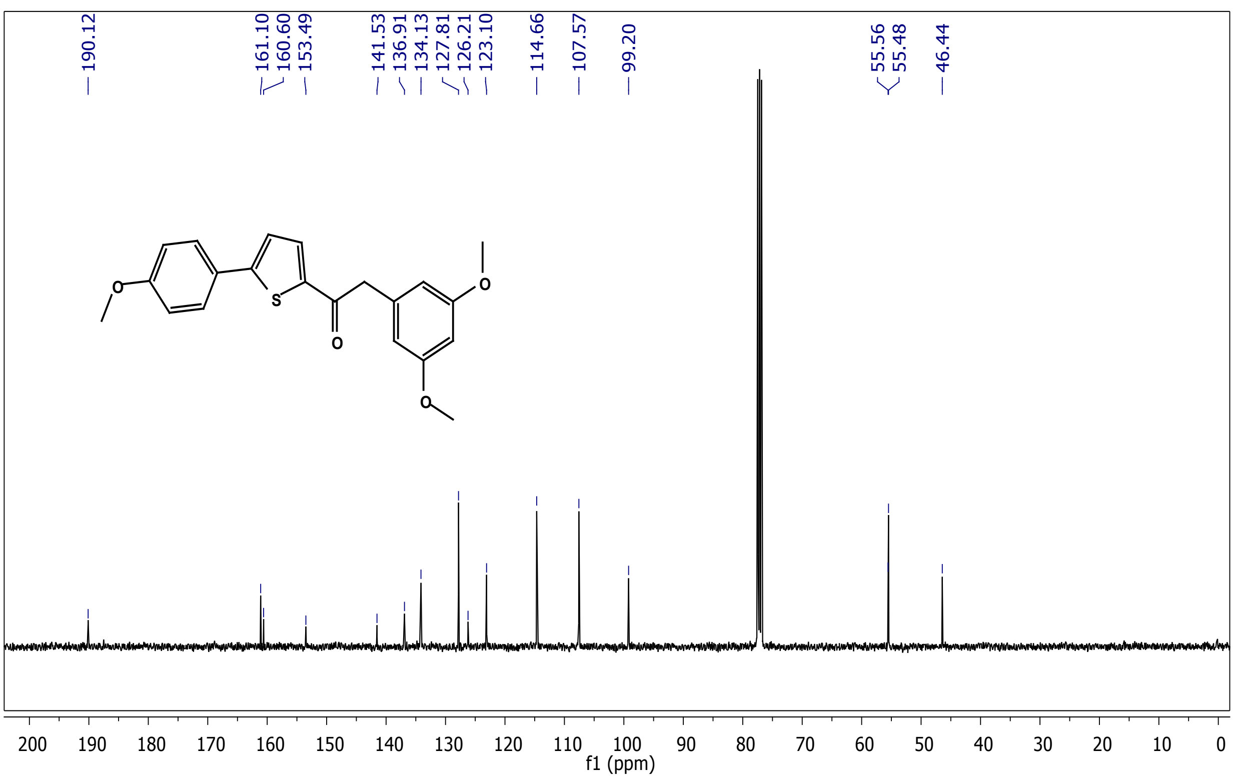
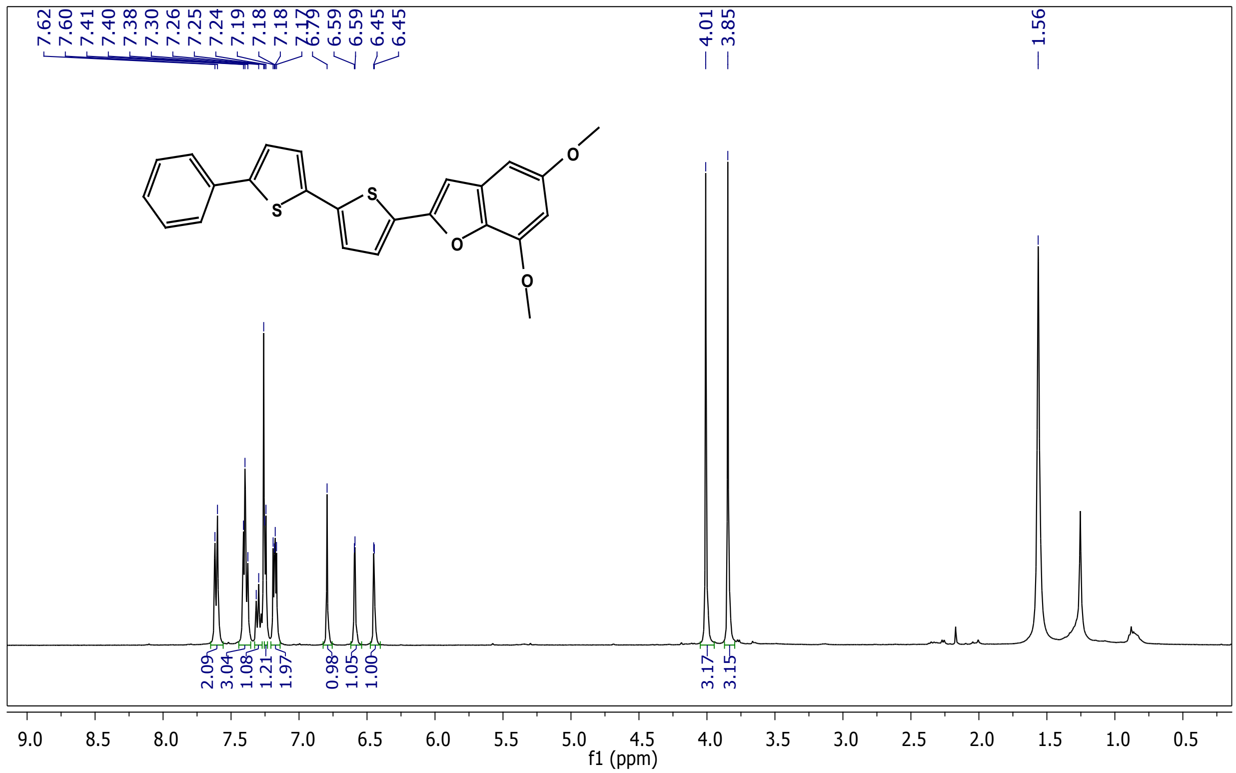


Figure S38. ¹H and ¹³C NMR spectra of 5,7-dimethoxy-2-(5'-phenyl-[2,2'-bithiophen]-5-yl)benzofuran (**6f**)



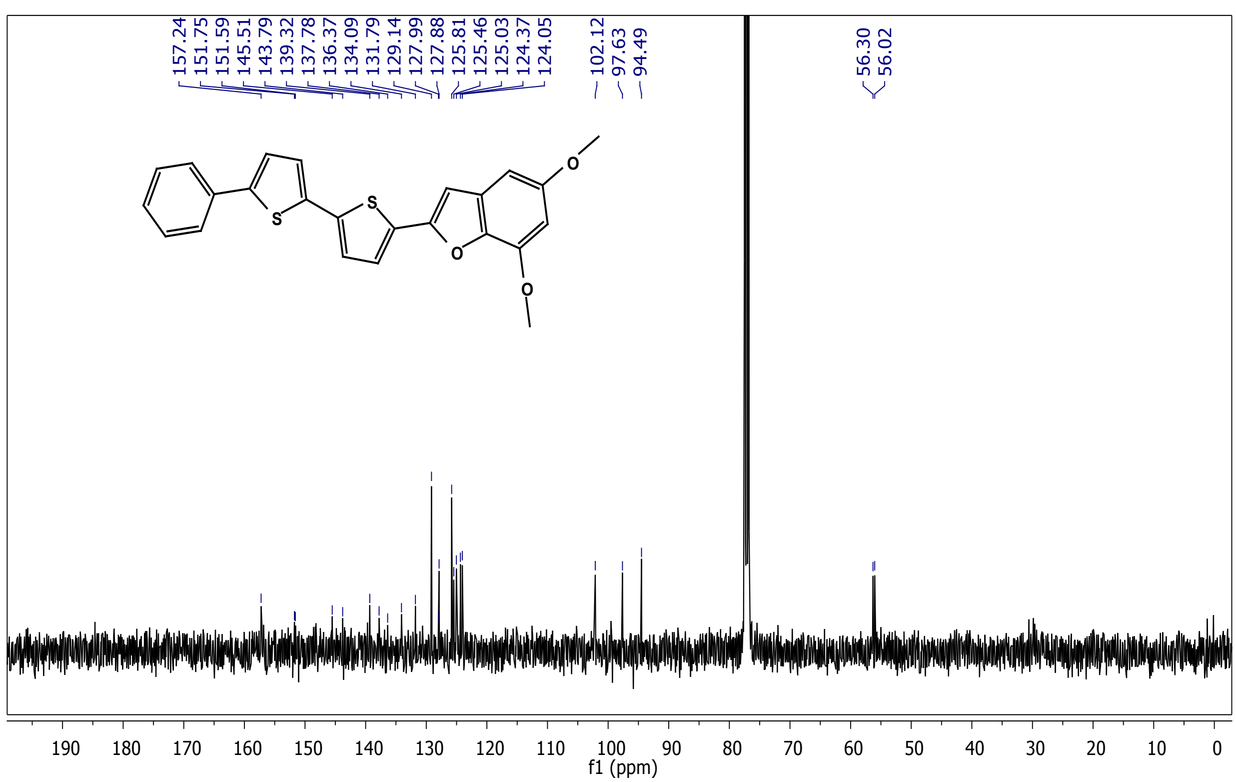


Figure S39. ^{1}H and ^{13}C NMR spectra of 2-(3,5-dimethoxyphenyl)-1-(5'-phenyl-[2,2'-bithiophen]-5-yl)ethan-1-one (**7f**)