

Supporting Information

Synthesis, Characterization and Self-Assembly of a Tetrathiafulvalene (TTF)-Triglycyl Derivative

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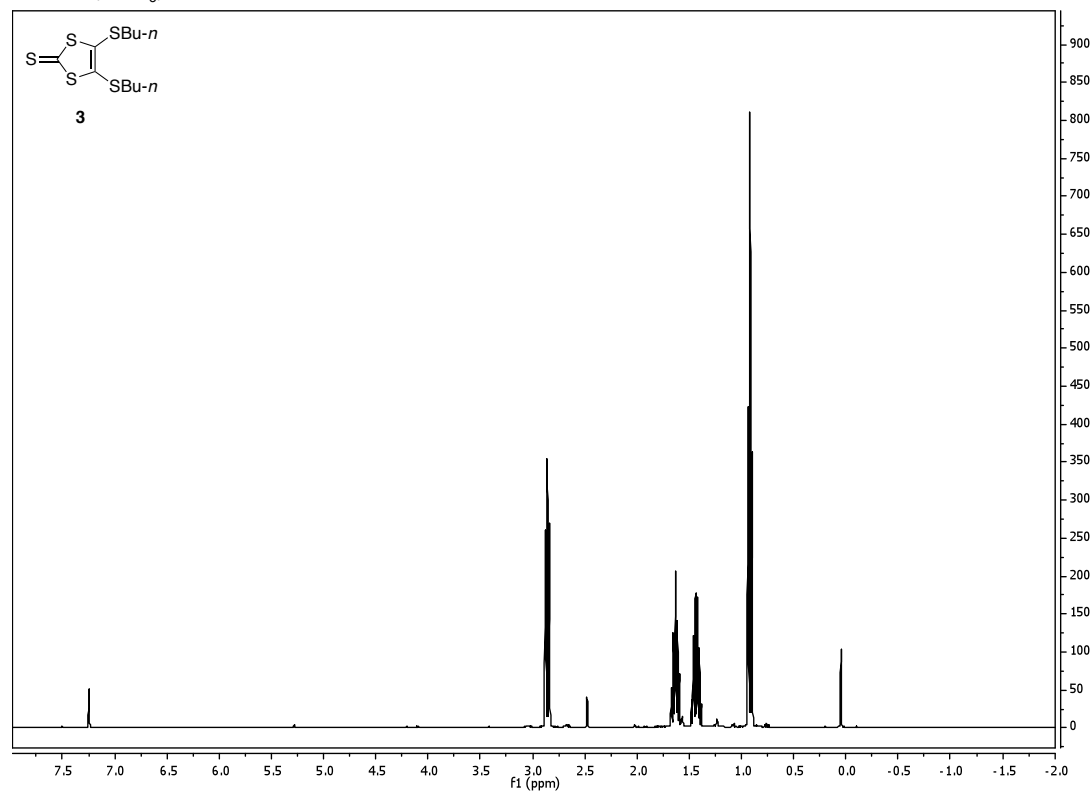
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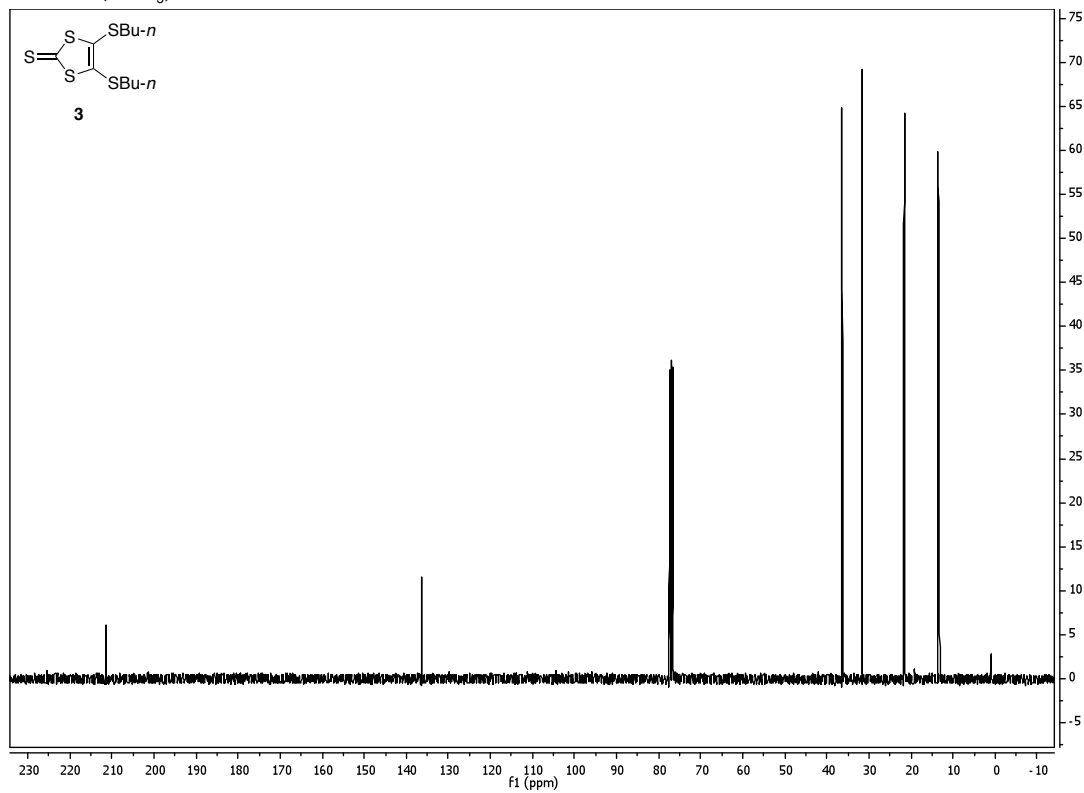
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1. NMR spectra of compounds

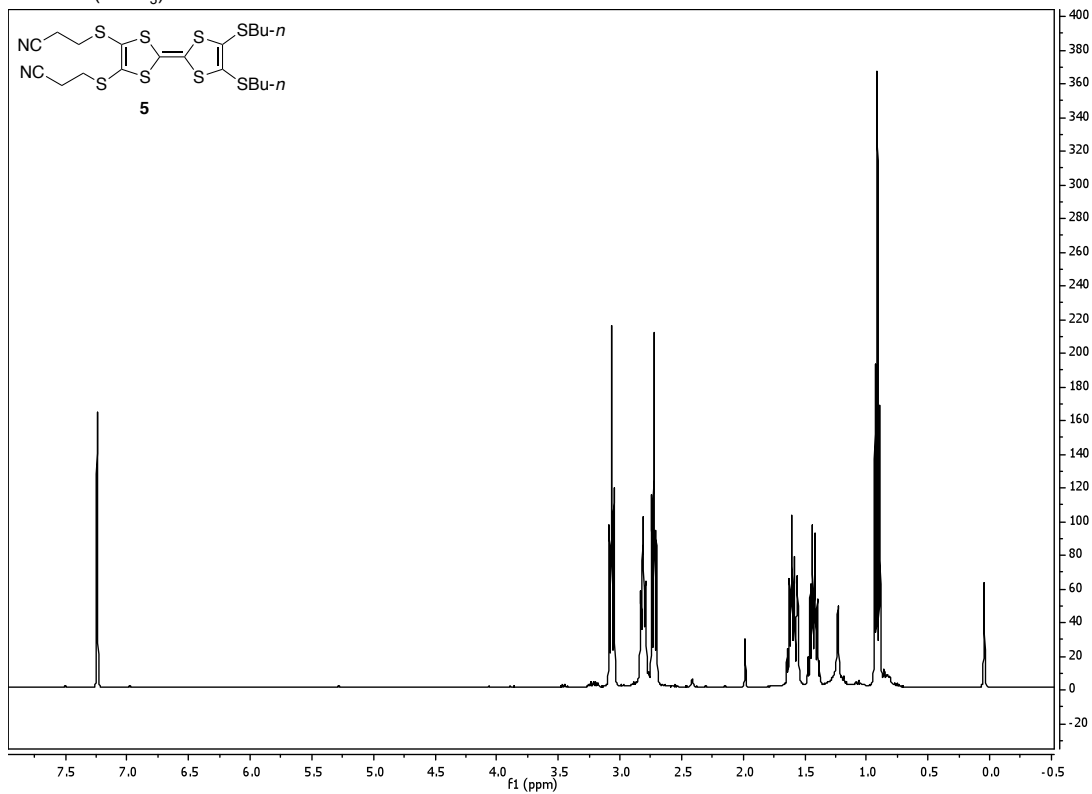
^1H NMR (CDCl_3)



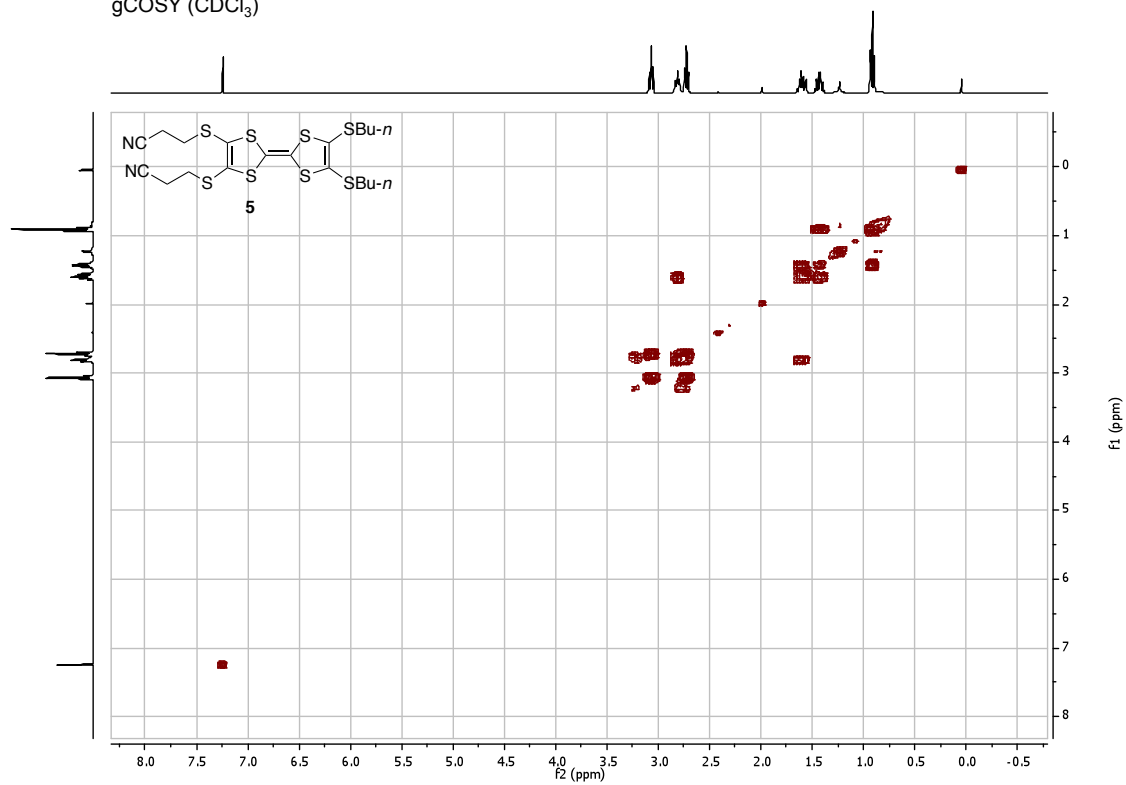
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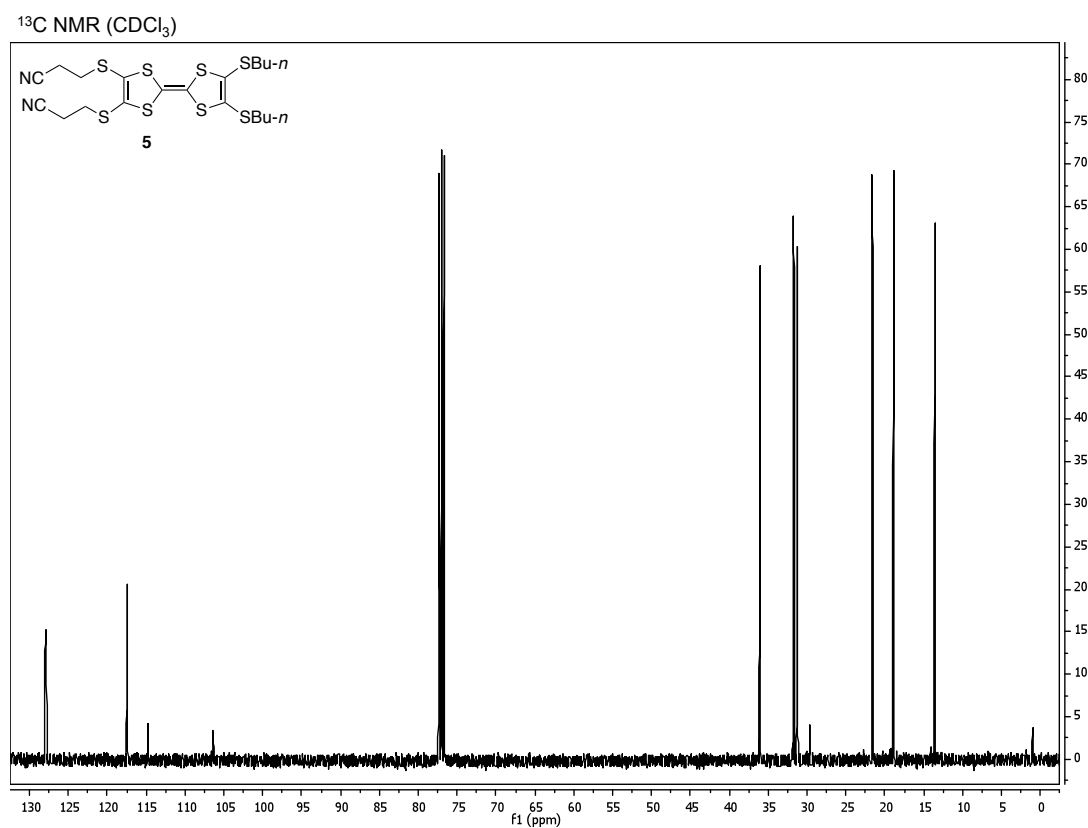
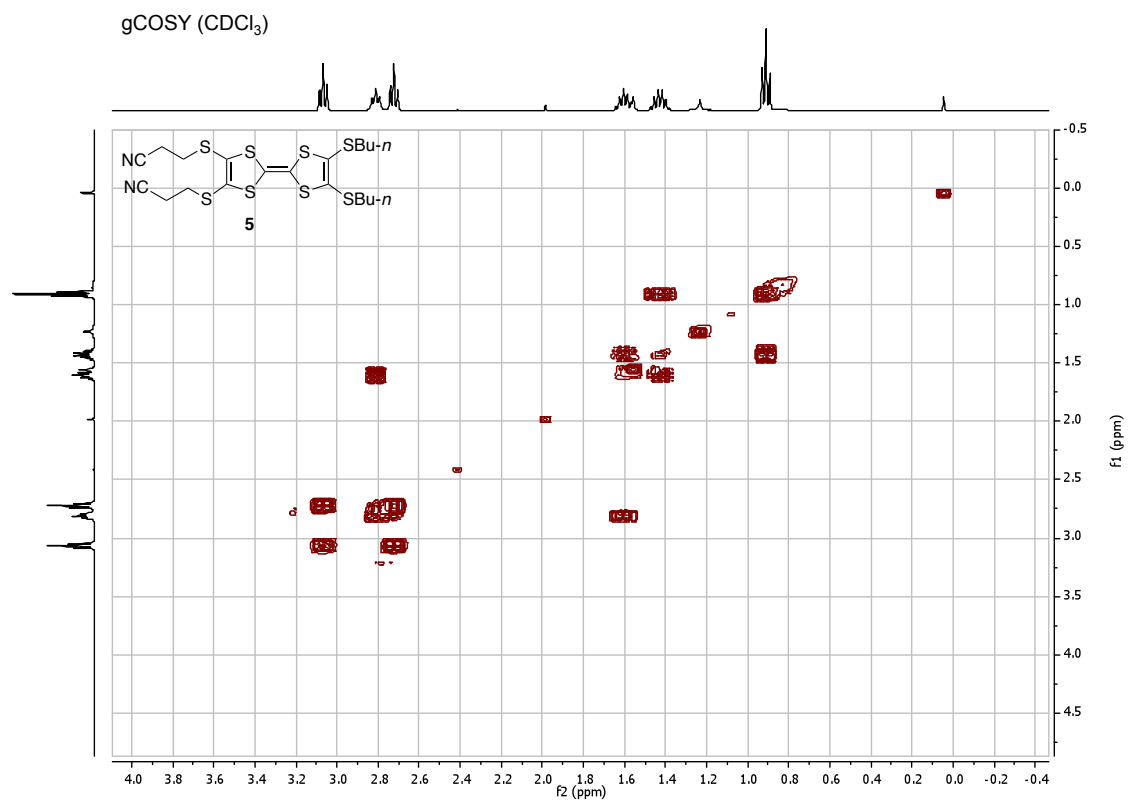


¹H NMR (CDCl₃)

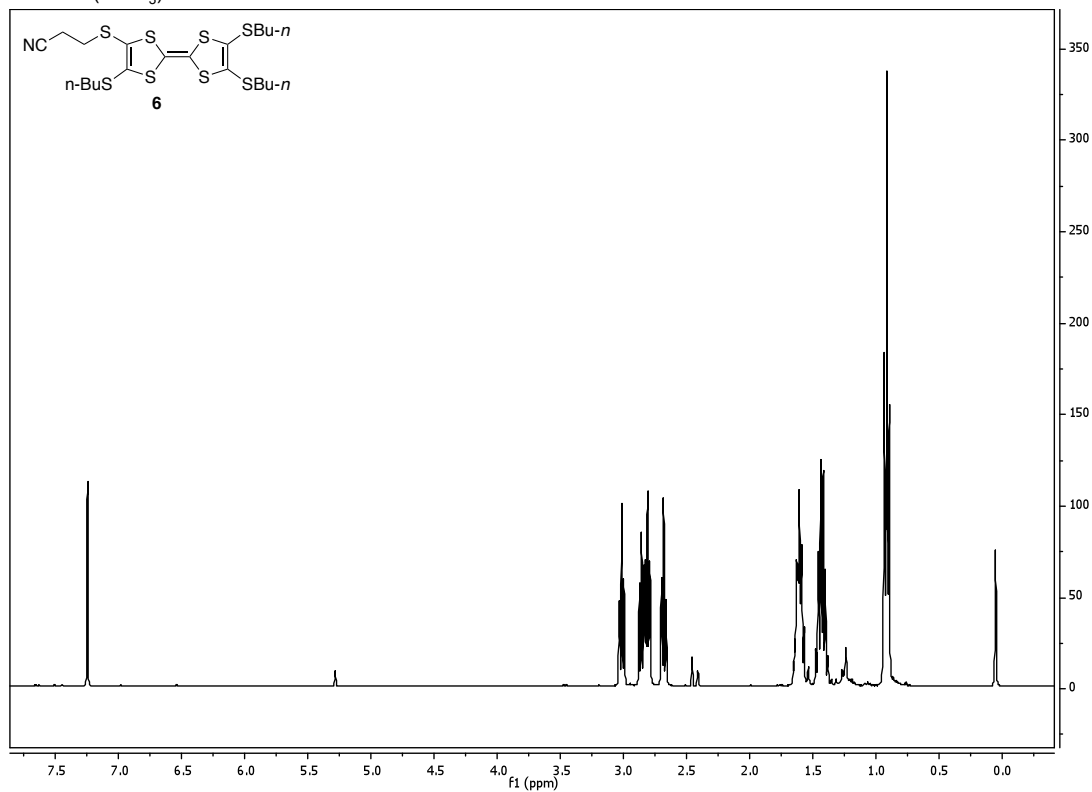


gCOSY (CDCl₃)

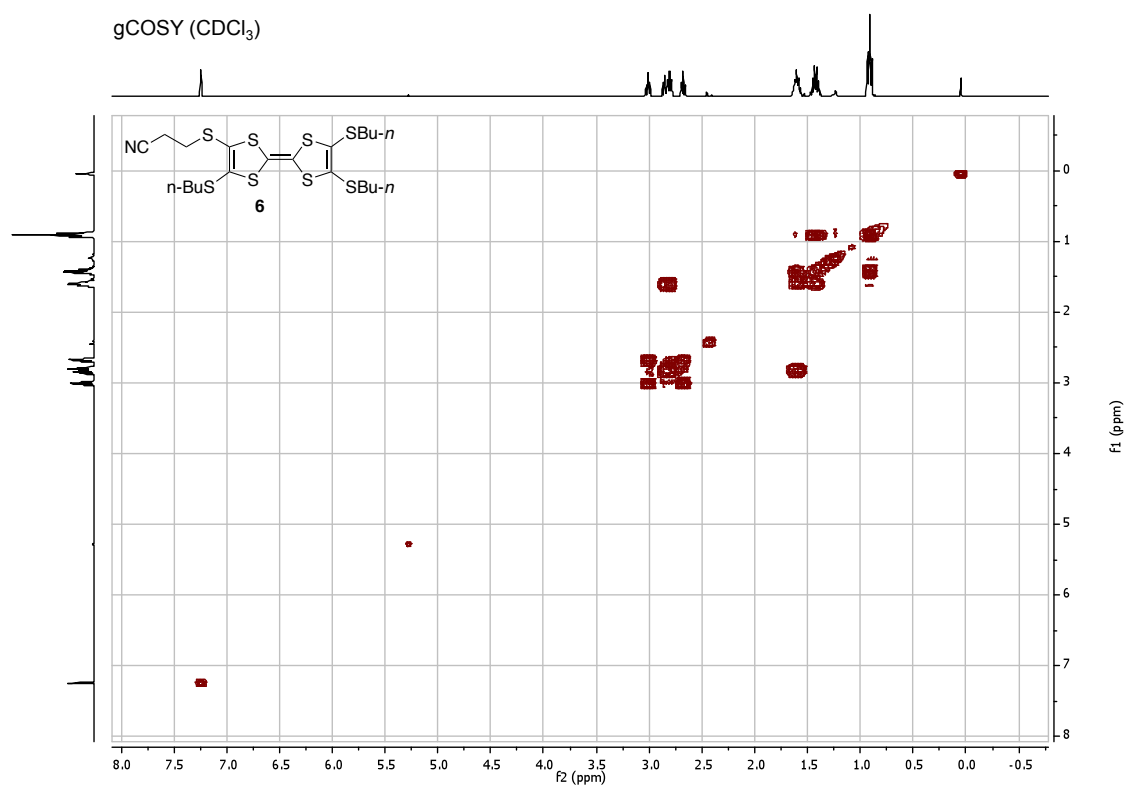




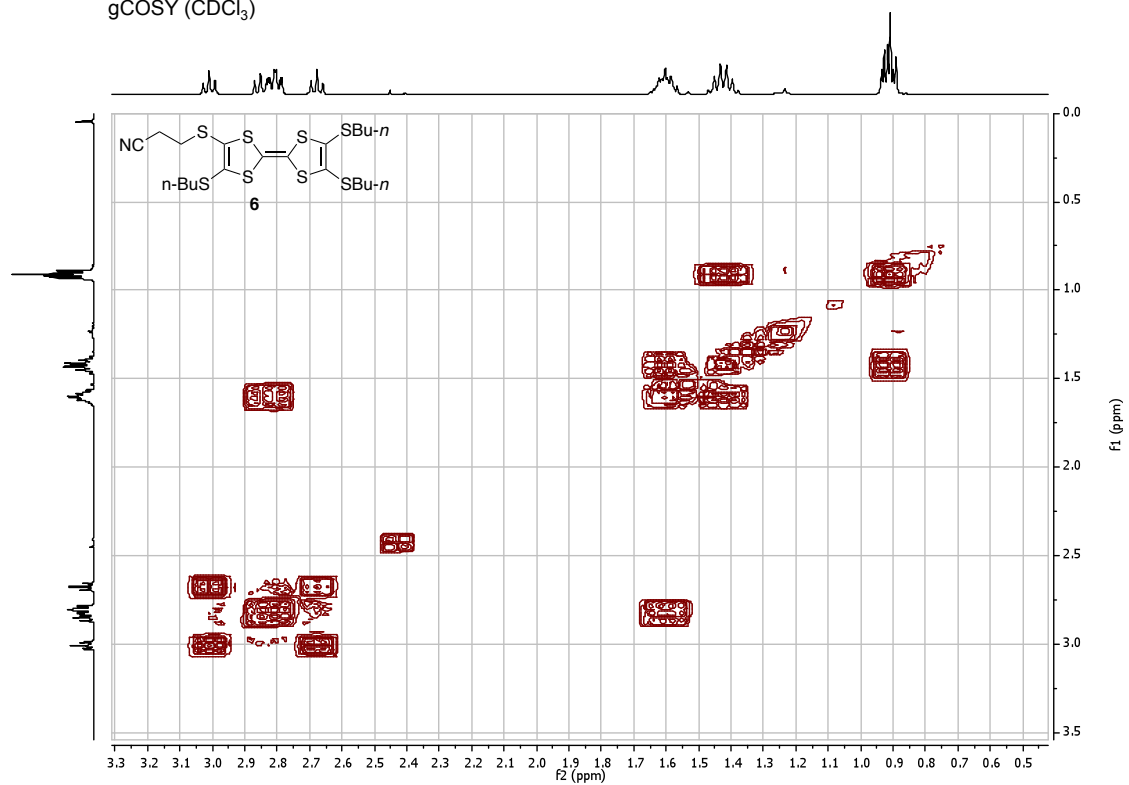
¹H NMR (CDCl₃)



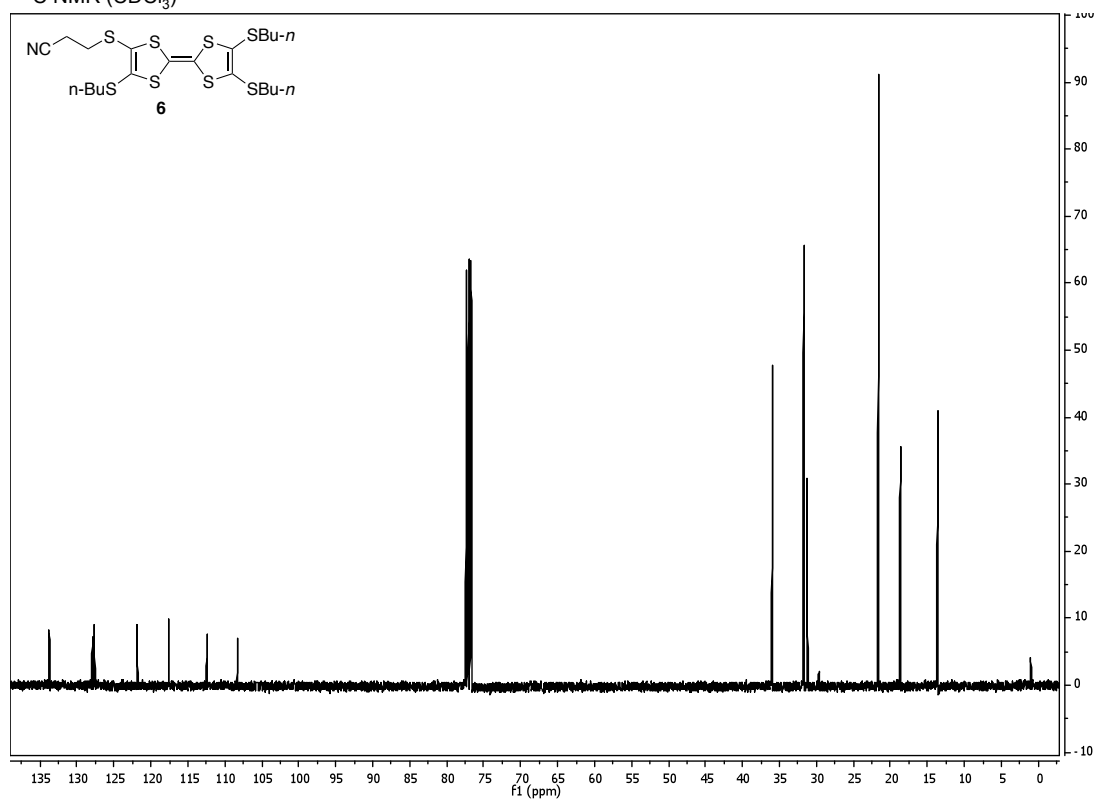
gCOSY (CDCl₃)



gCOSY (CDCl₃)

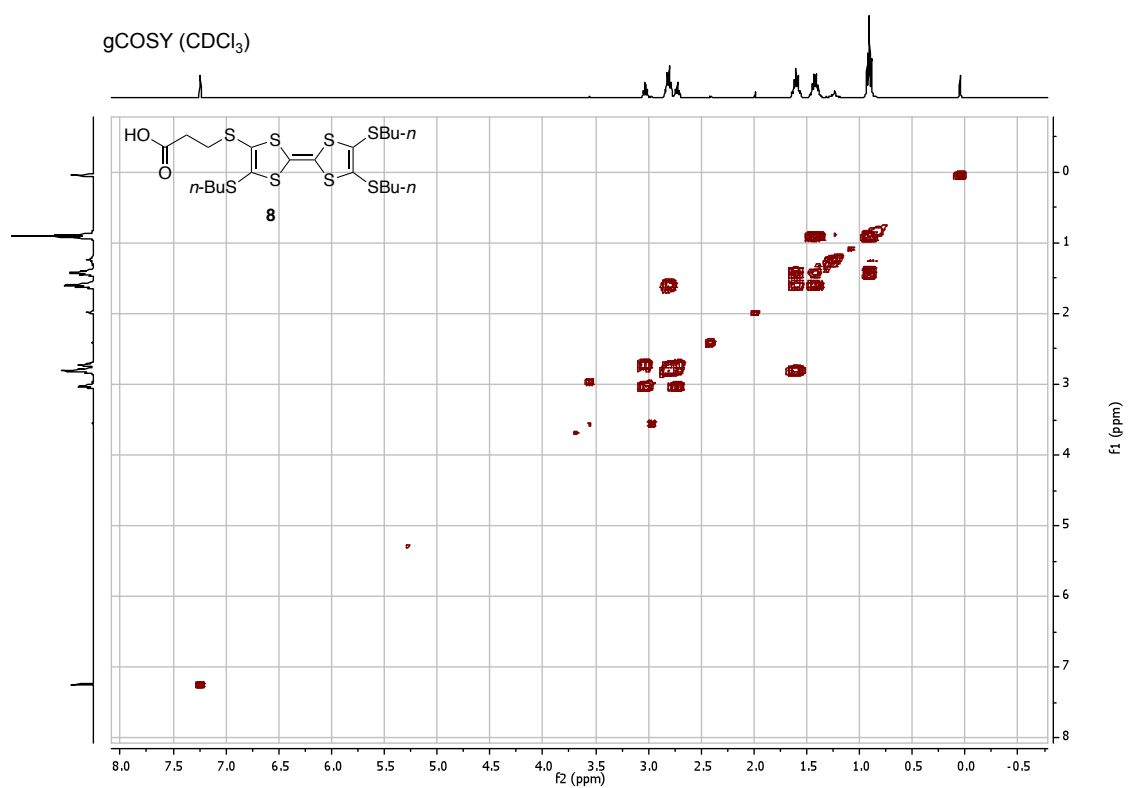


¹³C NMR (CDCl₃)

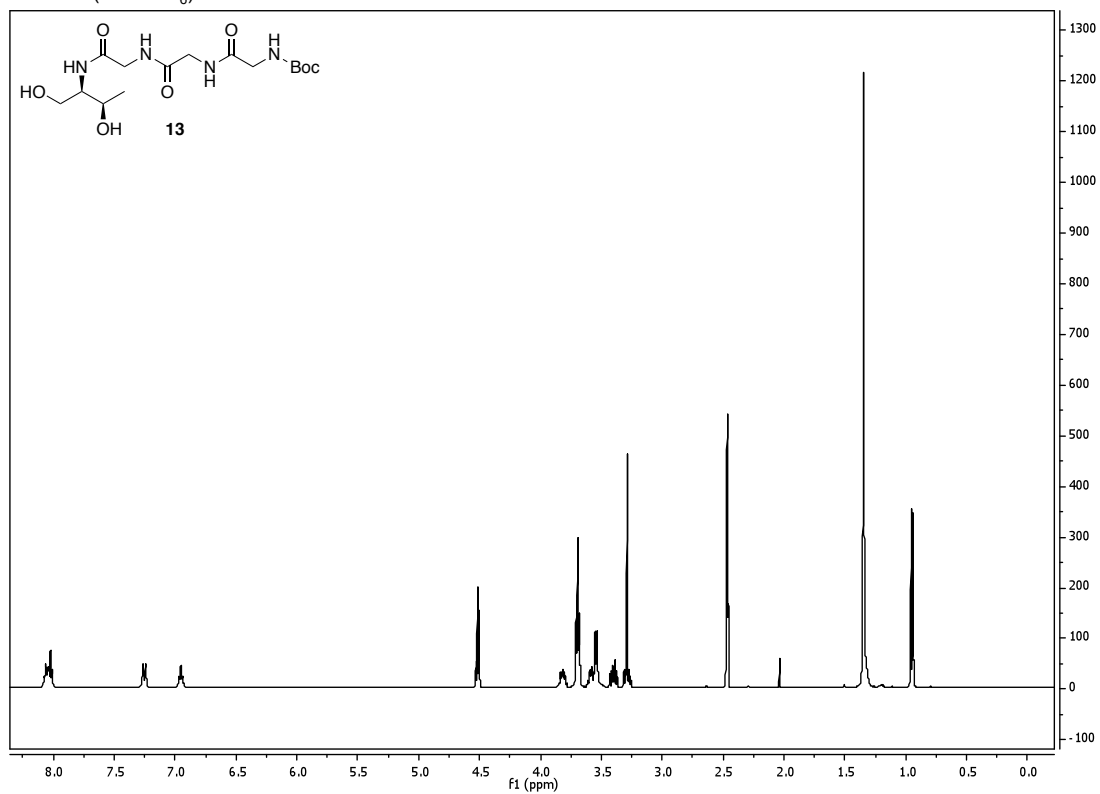


8

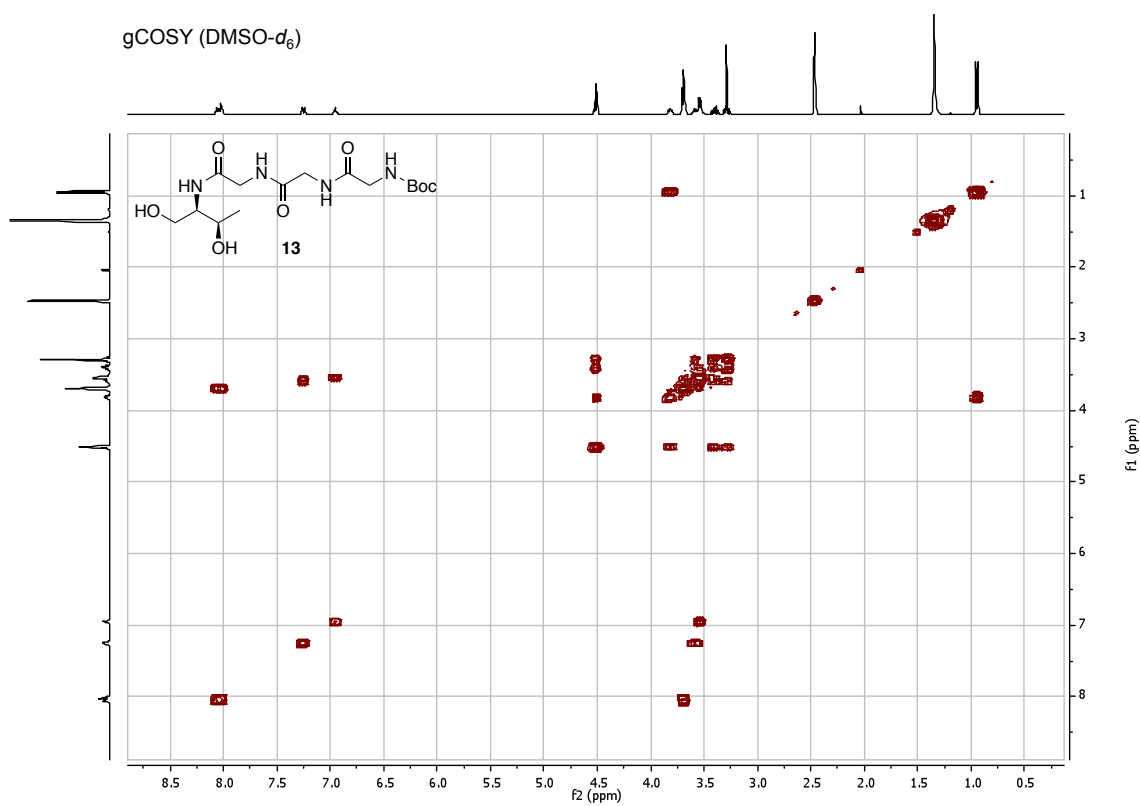
Chemical structure of compound **8** is shown above the spectrum. The structure is a bis-thiophene derivative with a central 1,3,5-trisubstituted thiophene ring. The substituents are a 3-oxopropyl group (HO-C(=O)-CH₂-CH₂-S-), an *n*-butyl group (S-Bu-*n*), and a 1,3,5-trisubstituted thiophene ring. The spectrum shows peaks corresponding to these groups: a sharp peak at ~7.2 ppm (aromatic protons), a small peak at ~4.3 ppm (aromatic protons), a small peak at ~3.5 ppm (aromatic protons), a multiplet between 2.8-3.2 ppm (aromatic protons), a small peak at ~2.5 ppm (aromatic protons), a multiplet between 1.4-1.8 ppm (aromatic protons), a large multiplet between 0.8-1.2 ppm (aromatic protons), and a sharp peak at ~0.0 ppm (aromatic protons).

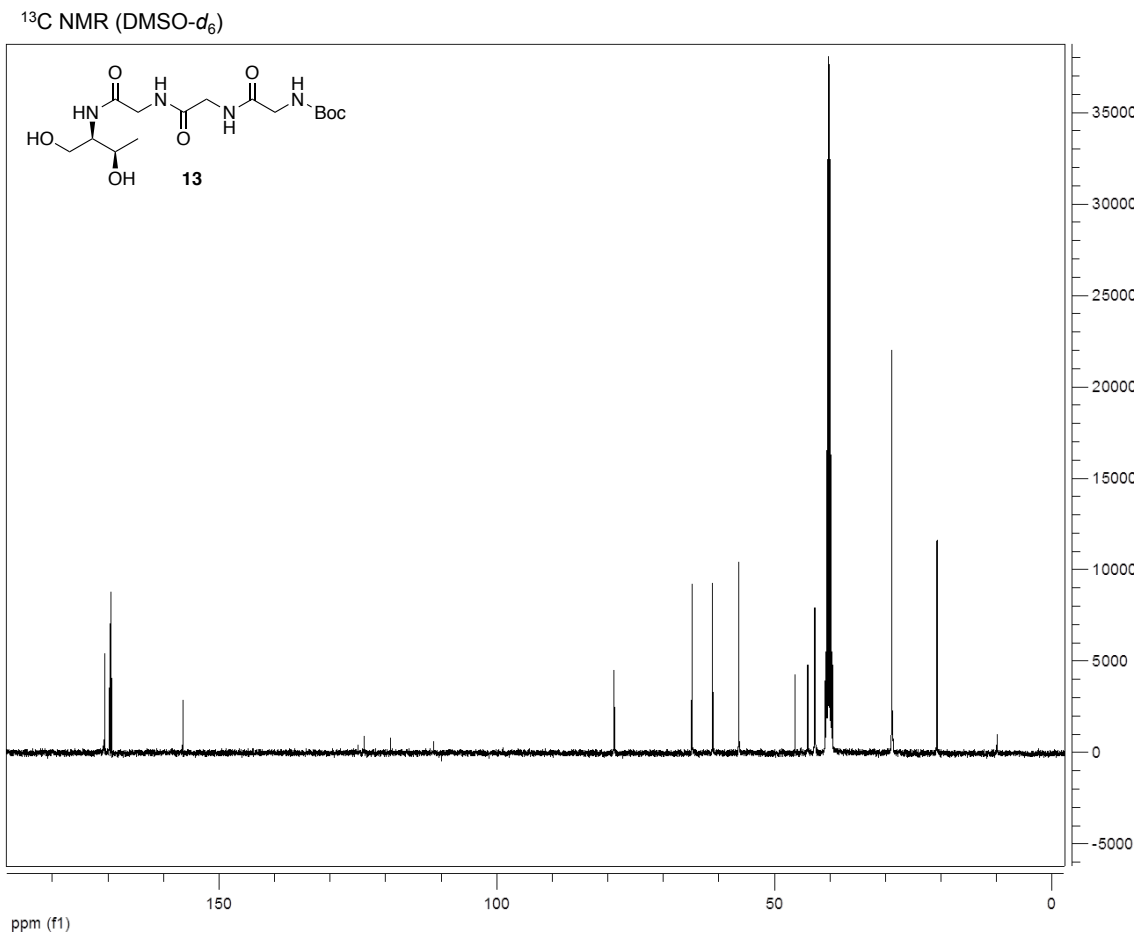
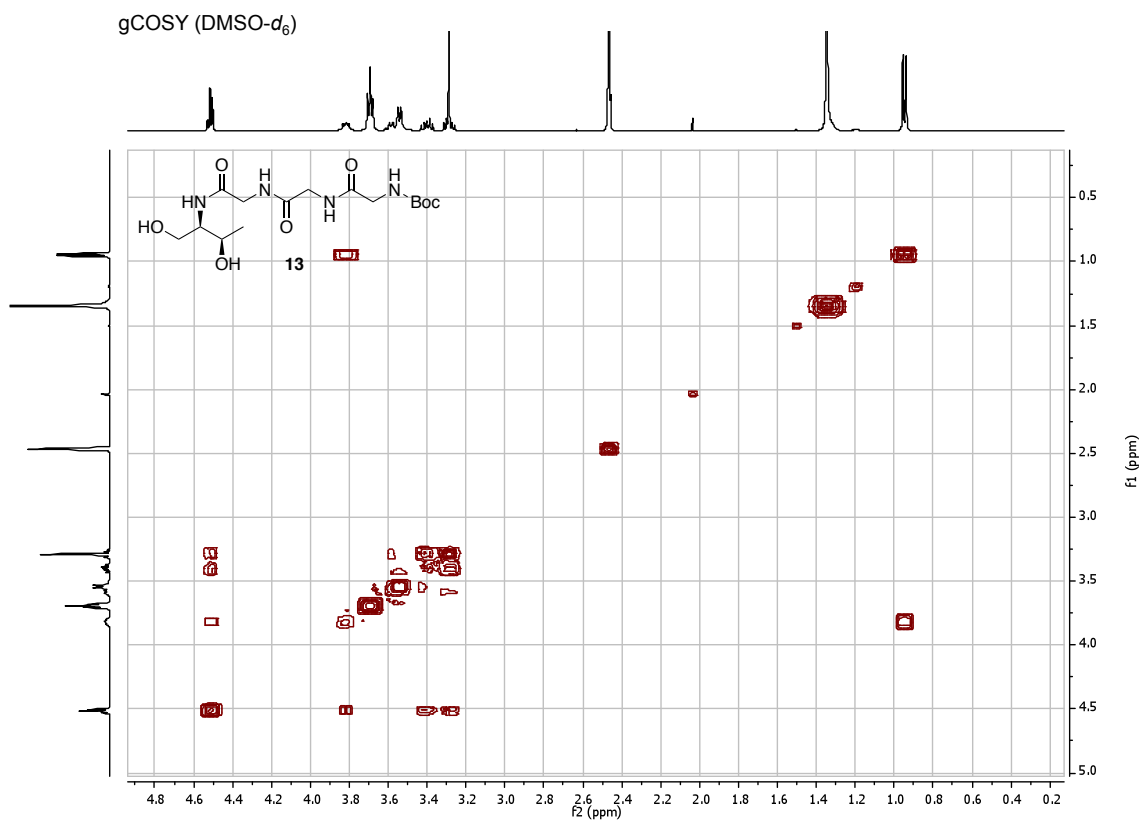


¹H NMR (DMSO-d₆)

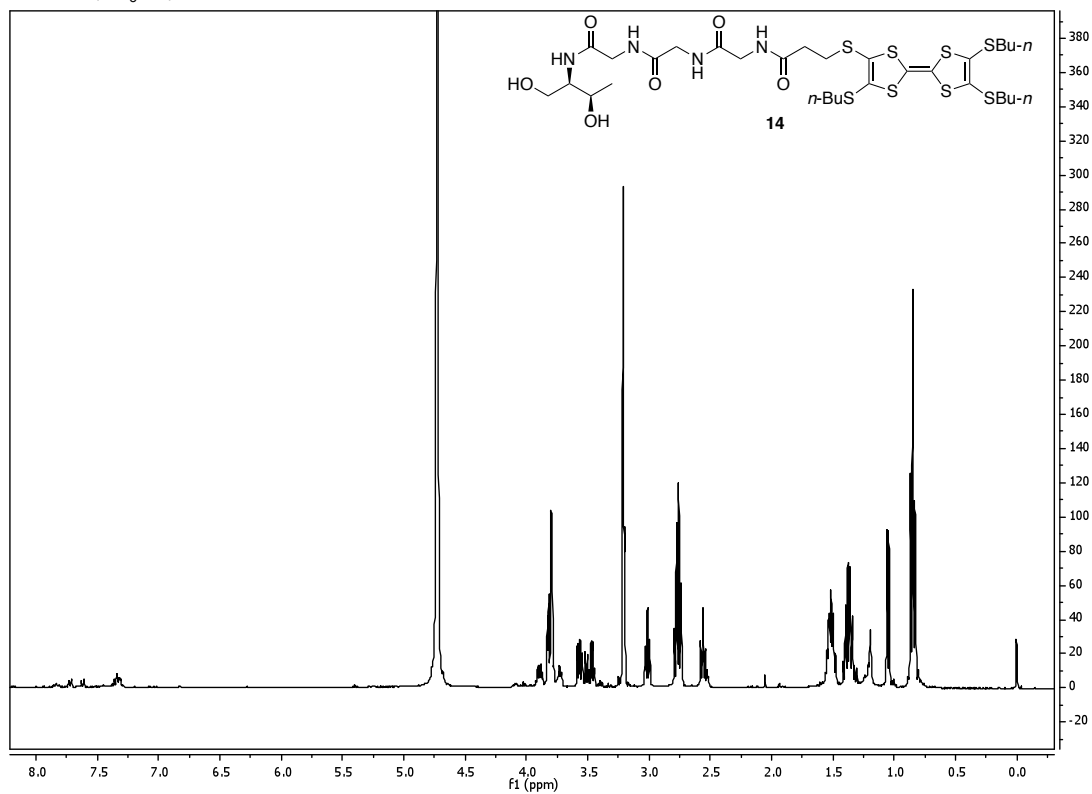


gCOSY (DMSO-d₆)

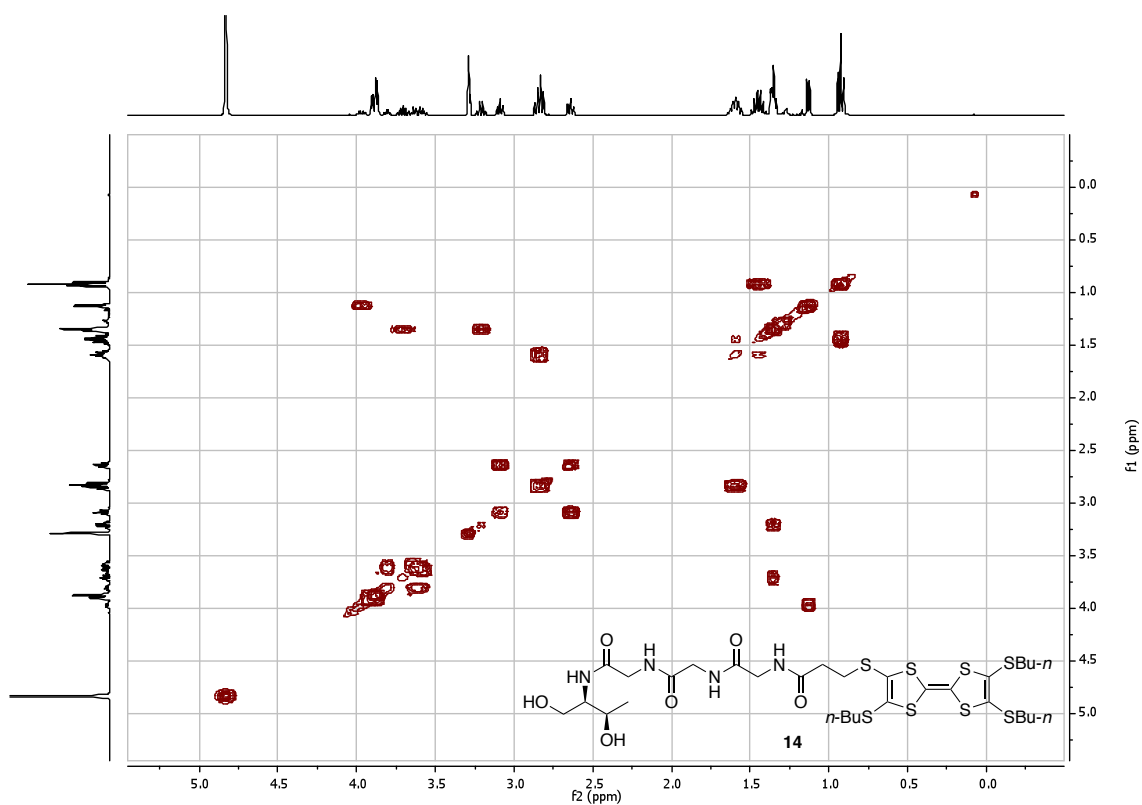




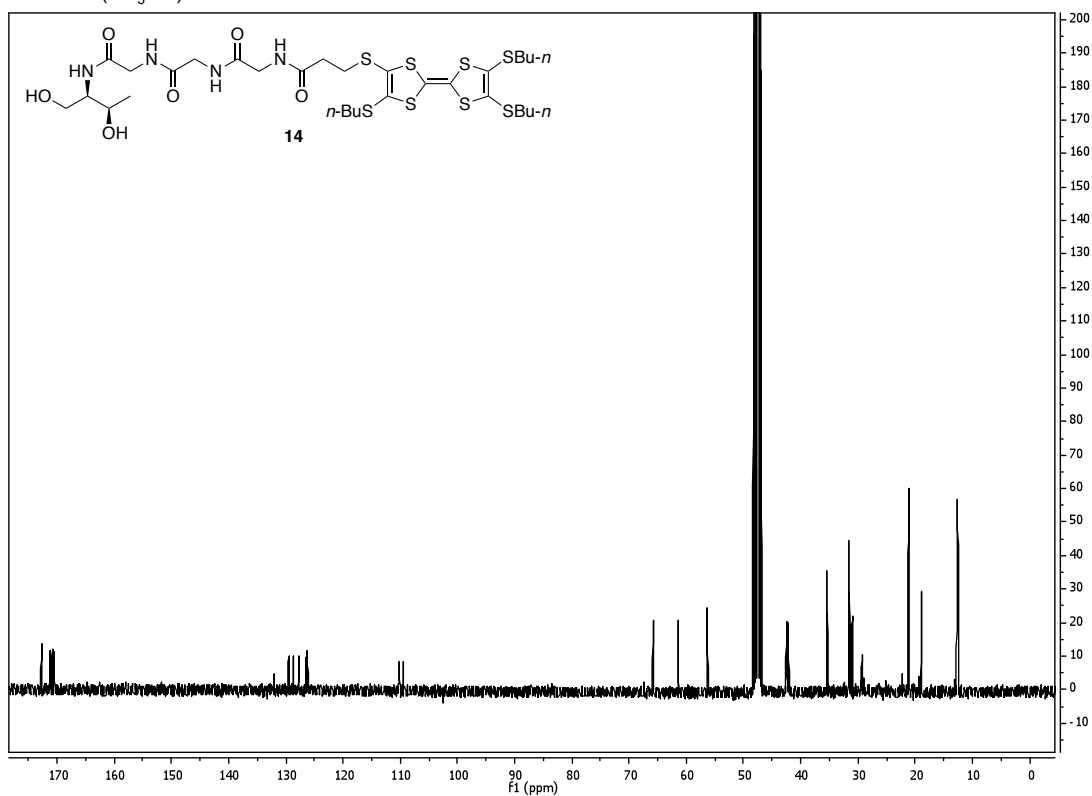
¹H NMR (CD₃OD)



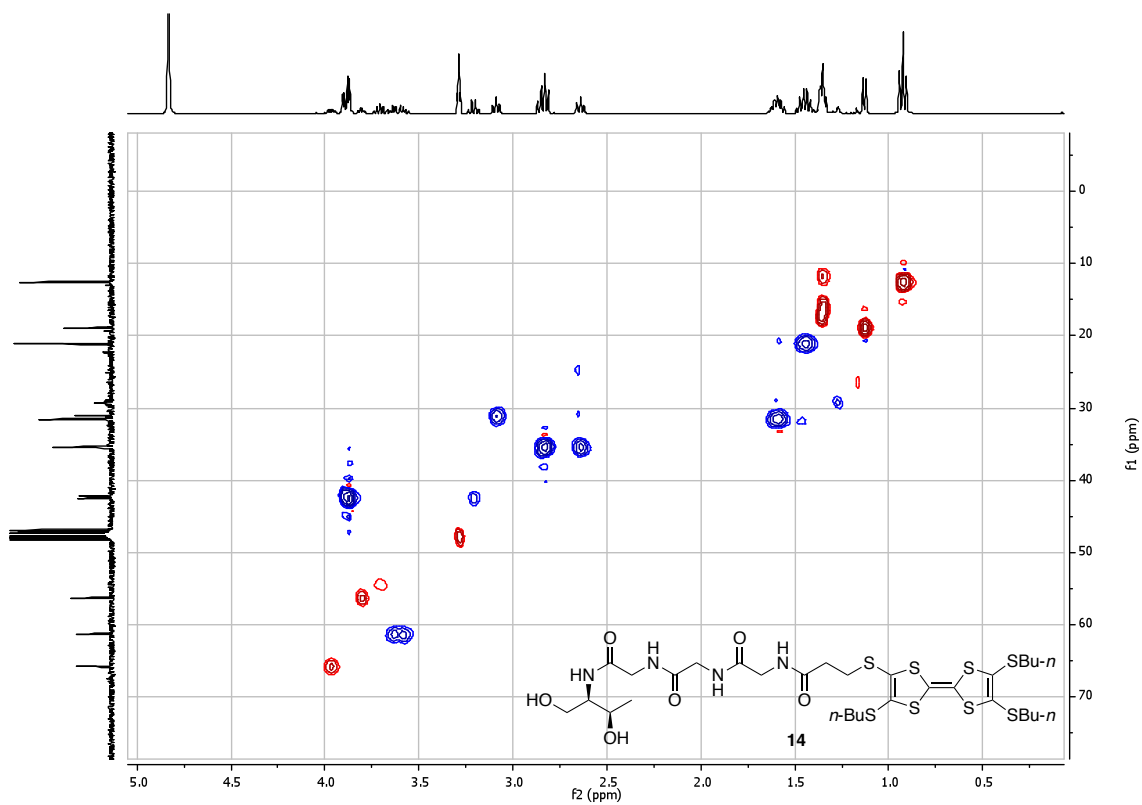
gCOSY (CD₃OD)



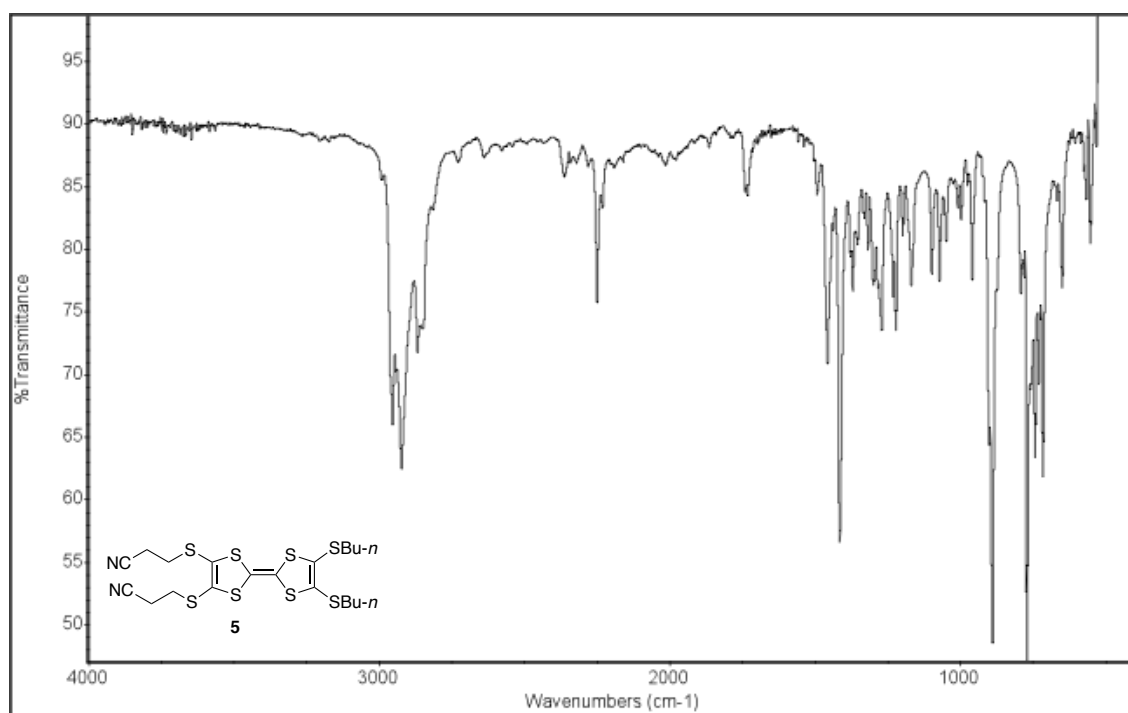
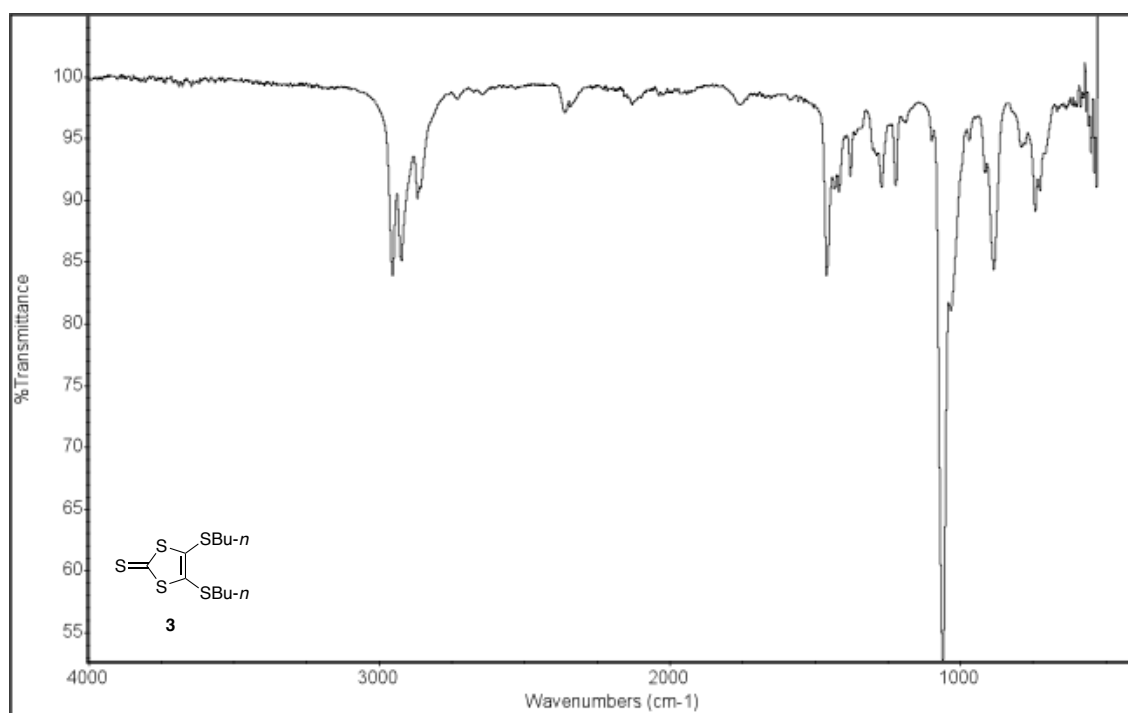
¹³C NMR (CD₃OD)

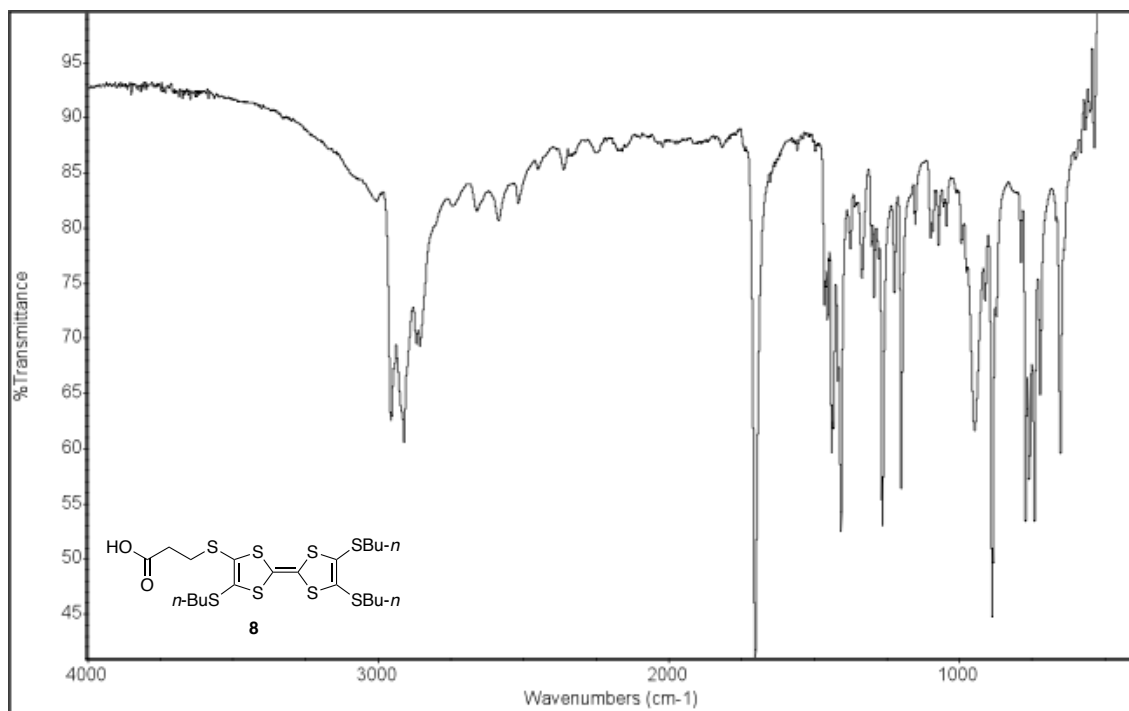
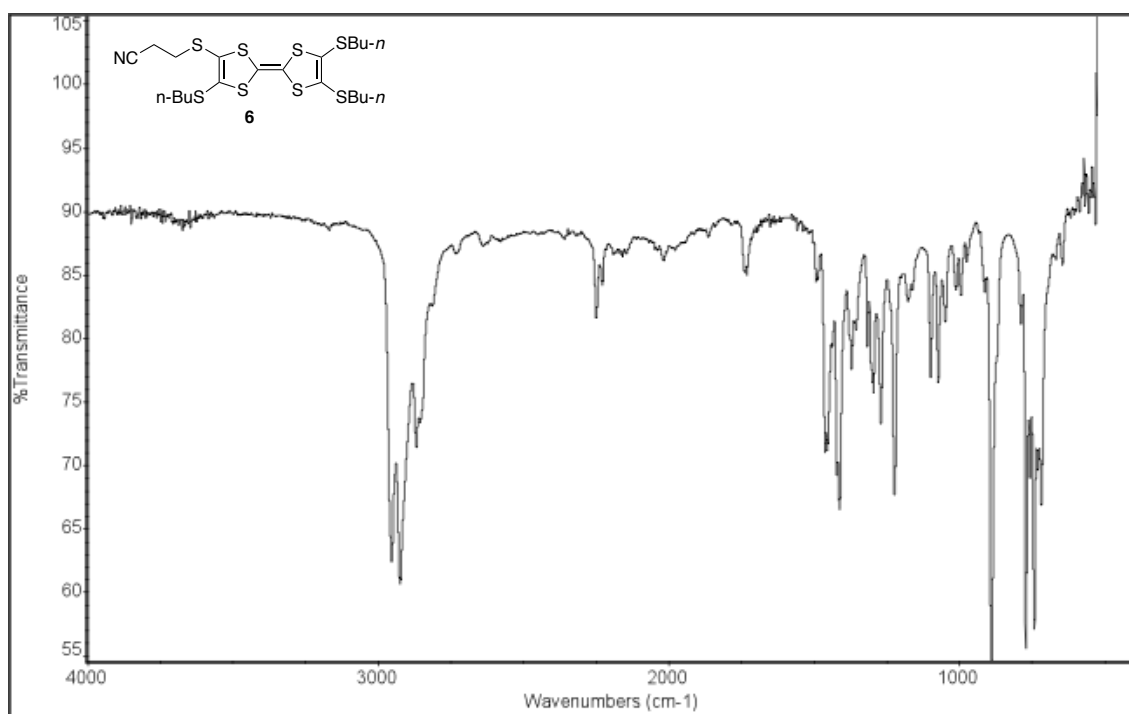


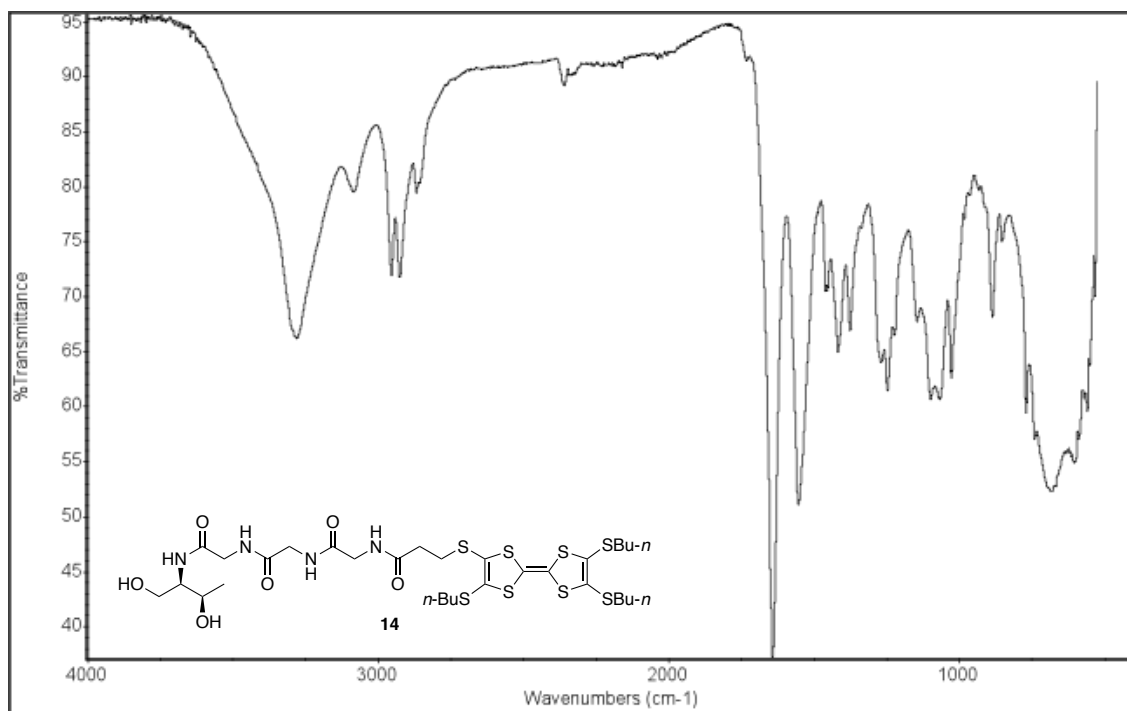
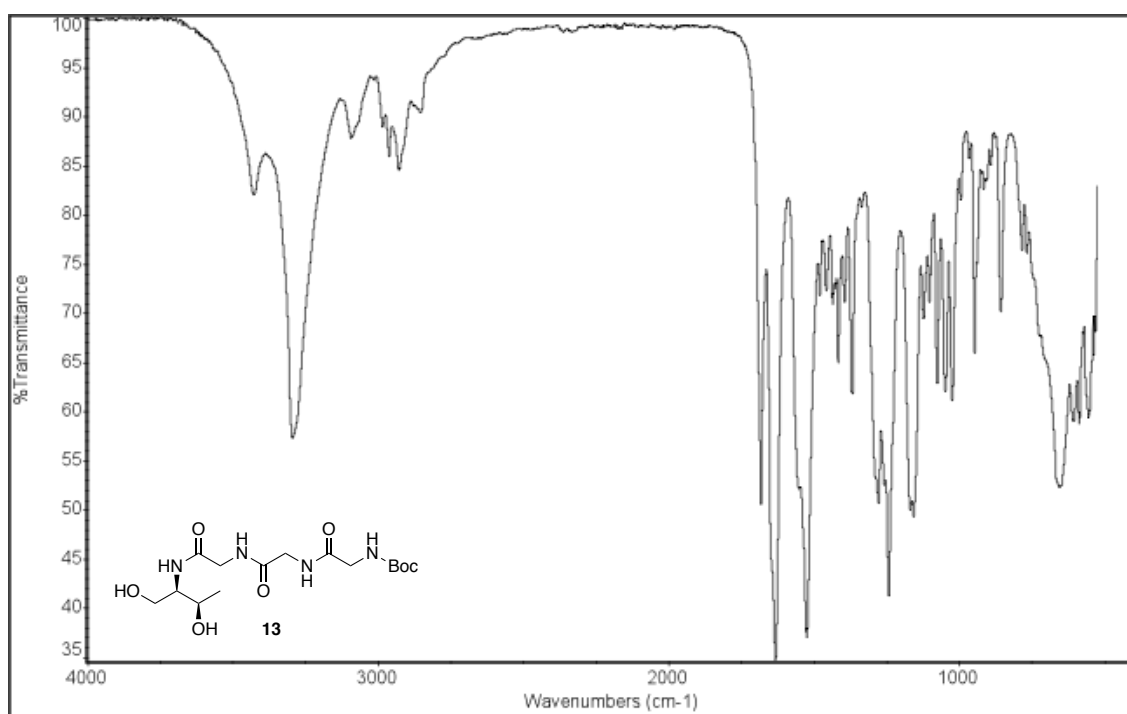
HCSQ (CD₃OD)



2. FT-IR spectra of compounds







3. Additional figures

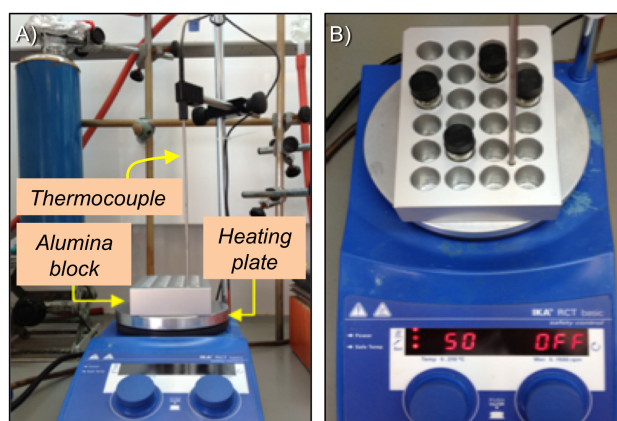


Figure S1. Thermoblock used for T_{gd} determinations. A) Front view of the set-up. B) Top view of the set-up during a typical experiment. The set-up was previously calibrated with literature data for known compounds.

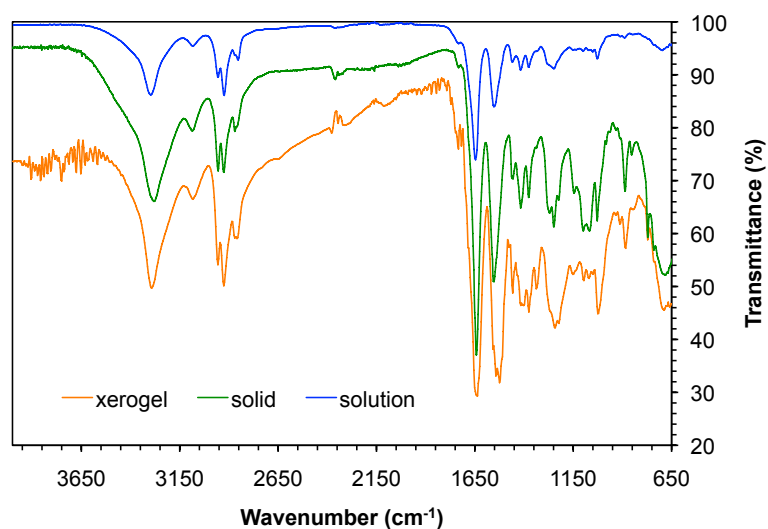


Figure S2. FT-IR spectra of solid **14**, **14** dissolved in DCM, and xerogel (i.e., prepared by freeze-drying the organogel made of **14** in DCM (29 g/L)).

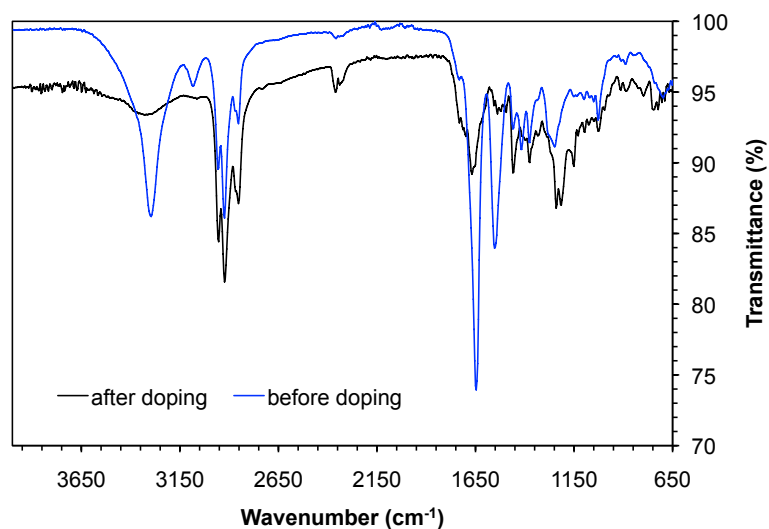


Figure S3. FT-IR spectra of the xerogel, obtained from the corresponding organogel made of **14** in DCM (29 g/L), before and after iodine-doping.