

Tuning the Through-Space Charge Transfer Emission in Triarylborane and Triarylamine Functionalized Dipeptide Organogels

Supporting Information

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Table of Contents

S1. Gel and Photophysical Properties

S2. NMR and HRMS Spectra

S1. Gelation Properties

Table S1. Results of the gelation studies with **B1** and **N1** in aliphatic and aromatic solvents.^a (All compounds were heated to completely dissolve and then cooled to room temperature.)

Solvent	Status	
	N1 (MGC) ^b	B1 (MGC) ^b
Benzene	G (20%)	S
Toluene	G (20%)	S
o-xylene	G (20%)	S
m-xylene	G (20%)	S
p-xylene	G (20%)	S
Mesitylene	G (20%)	S
Trichloromethane	G (20%)	S
Ether	G (20%)	I
acetone	G (20%)	S

^a G : gel; S : solution; I : insoluble; ^b MGC : minimum gelation concentration

Table S2. Results of the gelation studies with **B2** and **N2** in aliphatic and aromatic solvents.^a (All compounds were heated to completely dissolve and then cooled to room temperature.

Solvent	Status	
	N2 (MGC) ^b	B2 (MGC) ^b
Trichloromethane	S	S
Ether	I	I
Acetone	S	S
Benzene	G (1.5 %)	S
Toluene	G (1.5 %)	S
o-xylene	G (1.5 %)	G (1.5 %)
m-xylene	G (1.0 %)	G (2.0 %)
p-xylene	G (1.0 %)	G (1.0 %)
Mesitylene	G (1.0 %)	G (0.5 %)

^a G : gel; S : solution; I : insoluble; ^b MGC : minimum gelation concentration

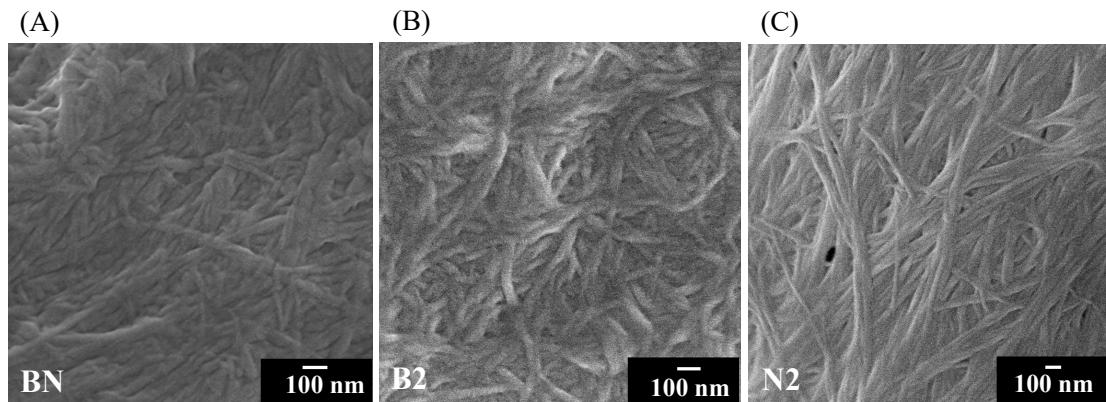


Figure S1. SEM images of the single gels in mesitylene (wt.% = 2%): (A) BN, (B) B2 and (C) N2.

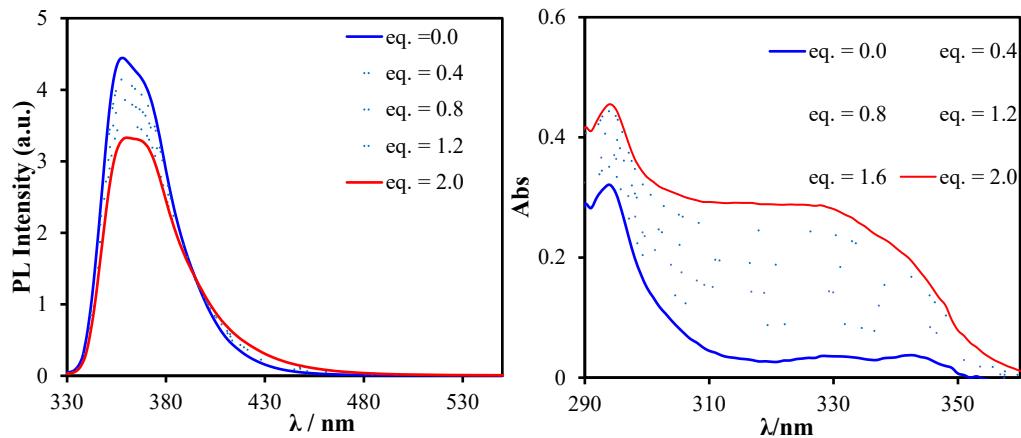


Figure S2. Emission (left) and Absorption (right) spectral change of N2 with the addition of B2 in mesitylene ($1.0 \times 10^{-5} \text{ M}$).

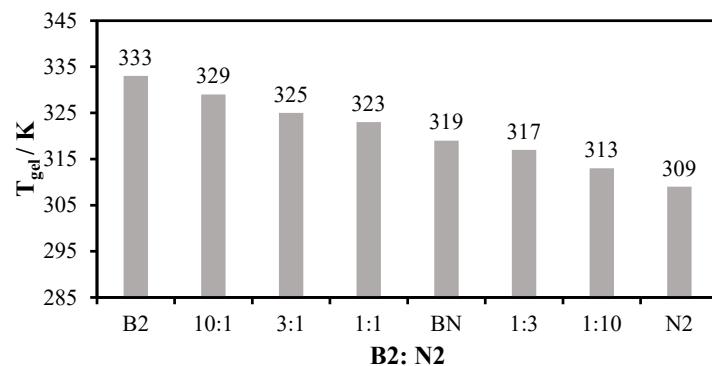


Figure S3. Sol-gel transition temperature (T_{gel}) of binary gels with different B2 to N2 ratios in mesitylene (wt.% = 2%) (Single component $\mathbf{B2}_{(\text{gel})}$, $\mathbf{N2}_{(\text{gel})}$ and $\mathbf{BN}_{(\text{gel})}$ are included as controls).

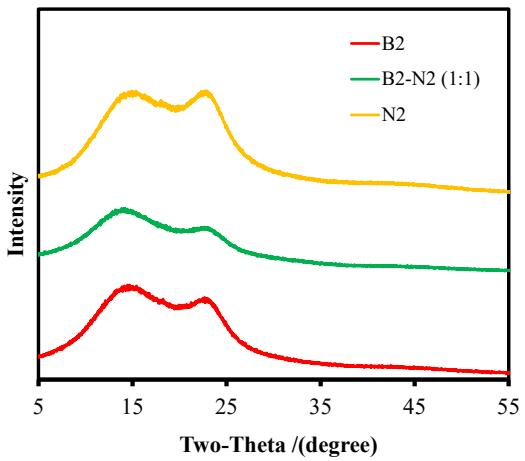


Figure S4. XRD patterns of xerogels in the region of 1-55°.

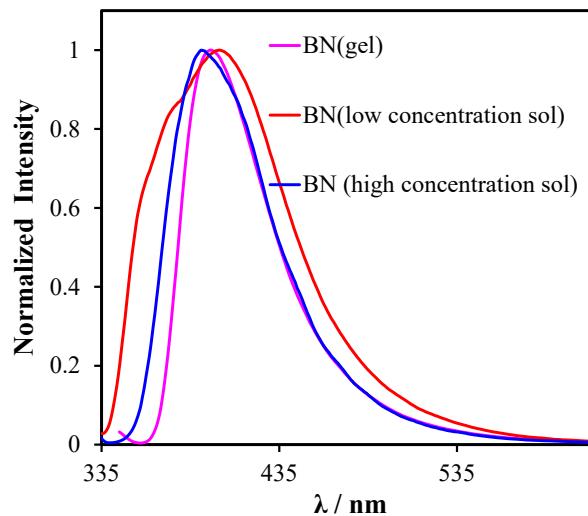


Figure S5. Emission spectra of BN in mesitylene at different concentrations (pink: gel state; red: $C = 10^{-5} \text{ M}$; blue: $c = 10^{-3} \text{ M}$).

S2. NMR and HRMS Spectra

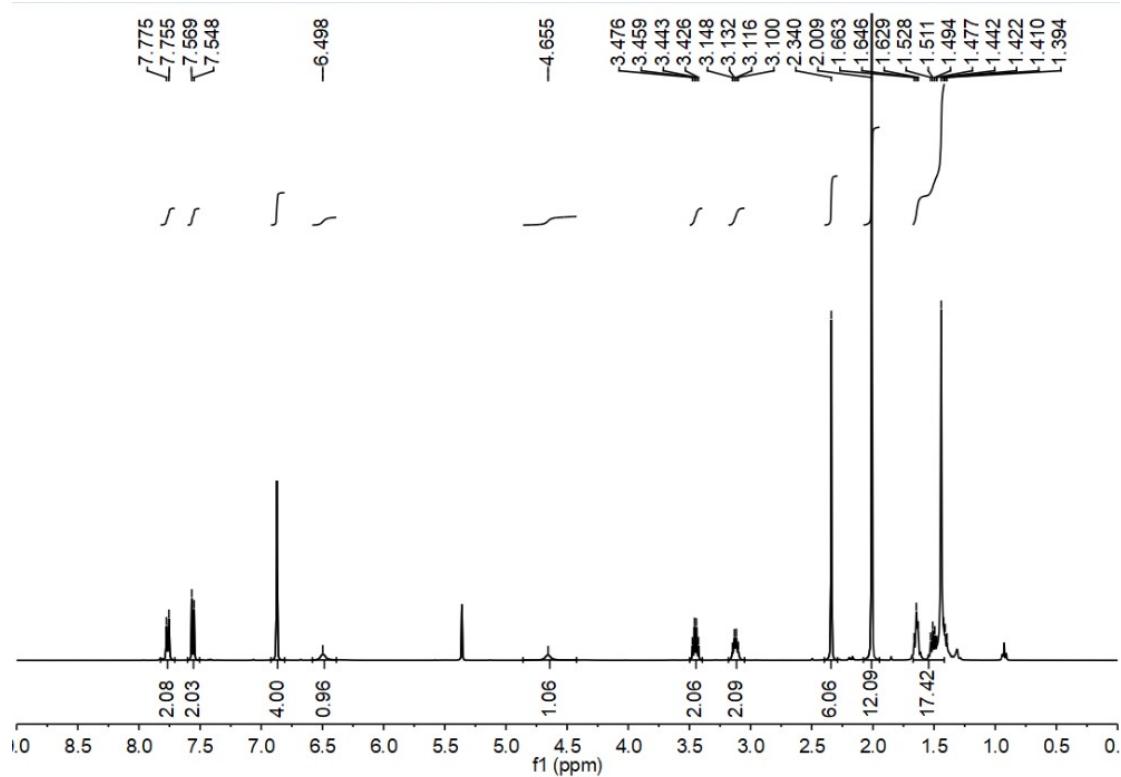


Figure S6. ^1H NMR (400 MHz, CD_2Cl_2) spectrum of **1-2**.

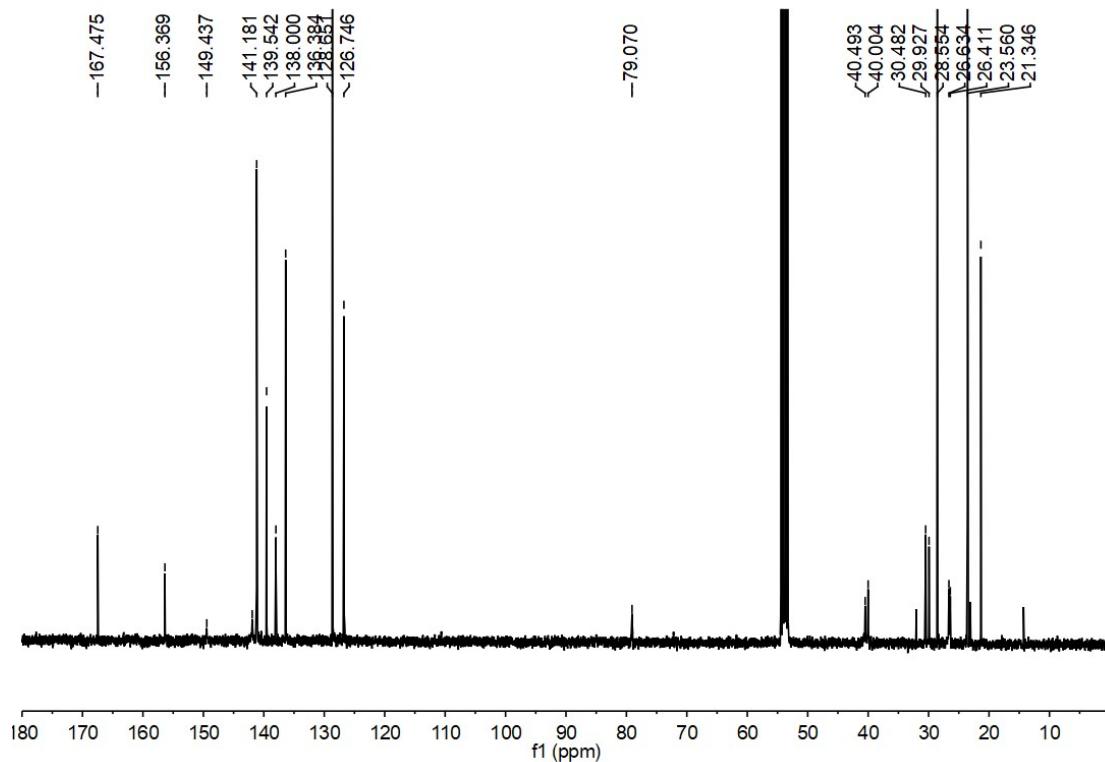


Figure S7. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of **1-2**.

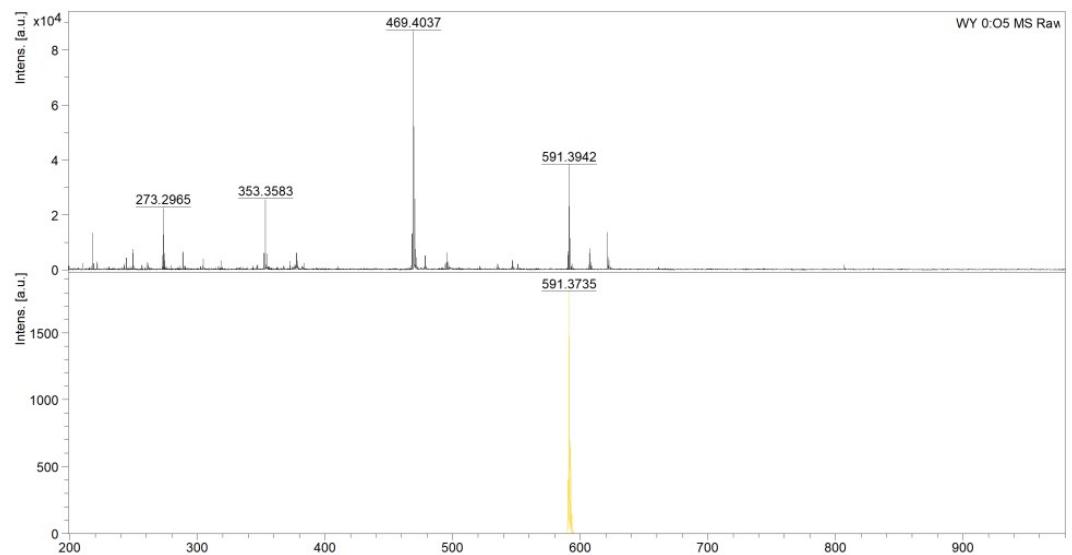


Figure S8. HRMS spectrum for **1-2**.

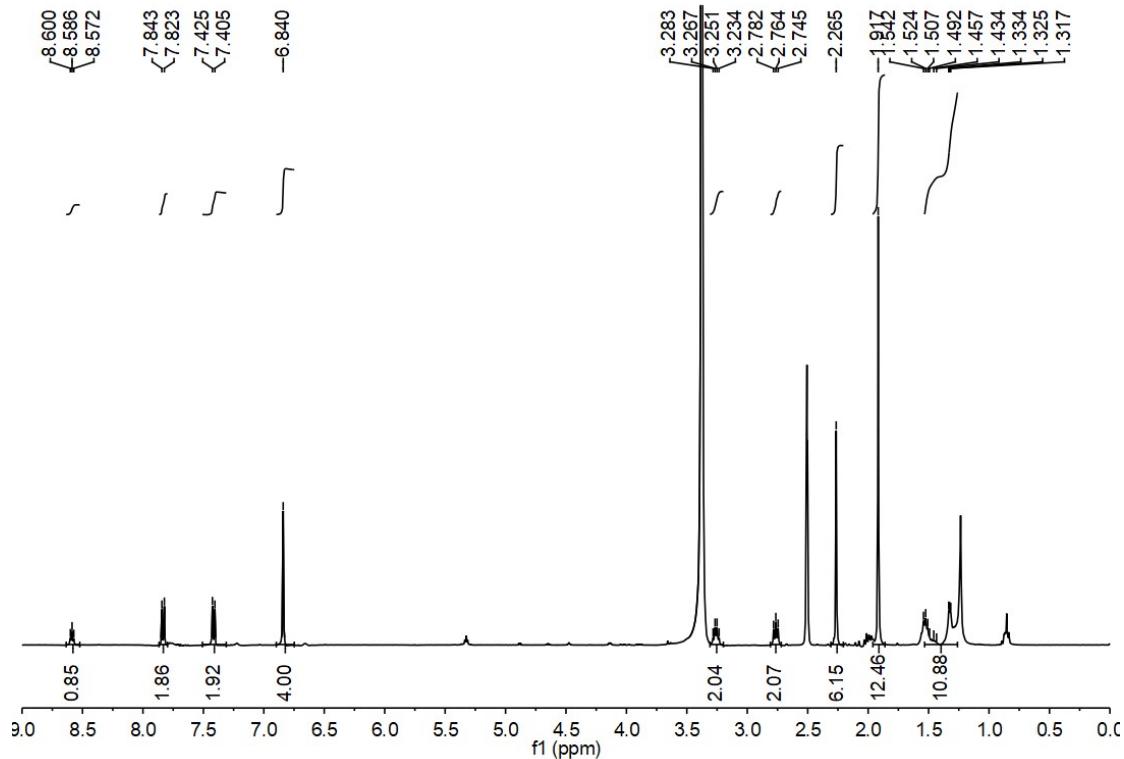


Figure S9. ^1H NMR (400 MHz, DMSO) spectrum of **C6B**.

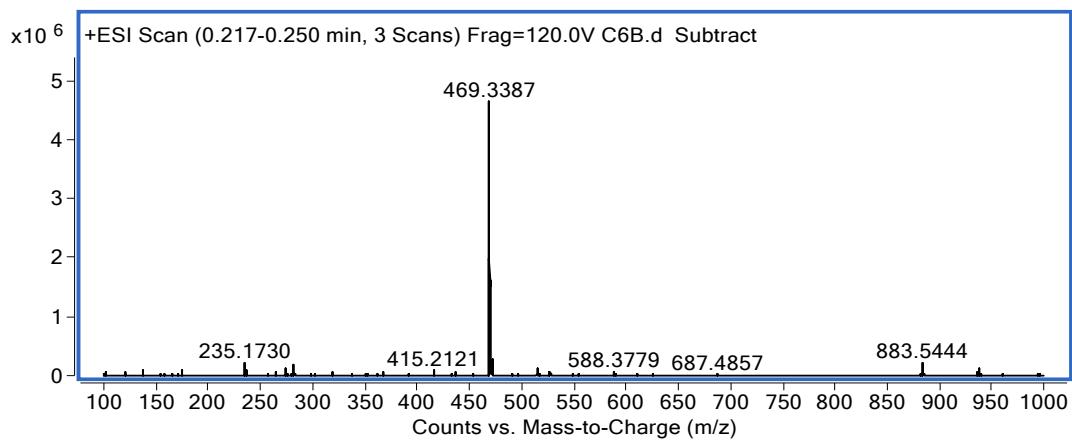


Figure S10. HRMS spectrum for **C6B**.

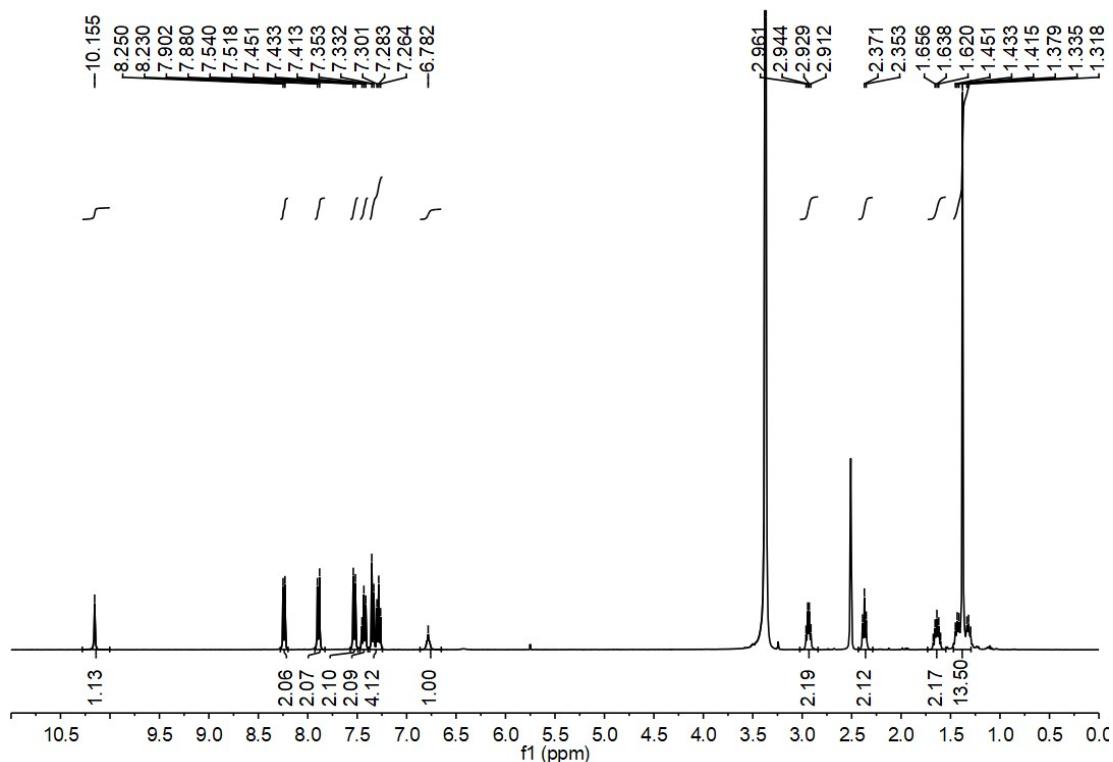


Figure S11. ^1H NMR (400 MHz, DMSO) spectrum of **2-2**.

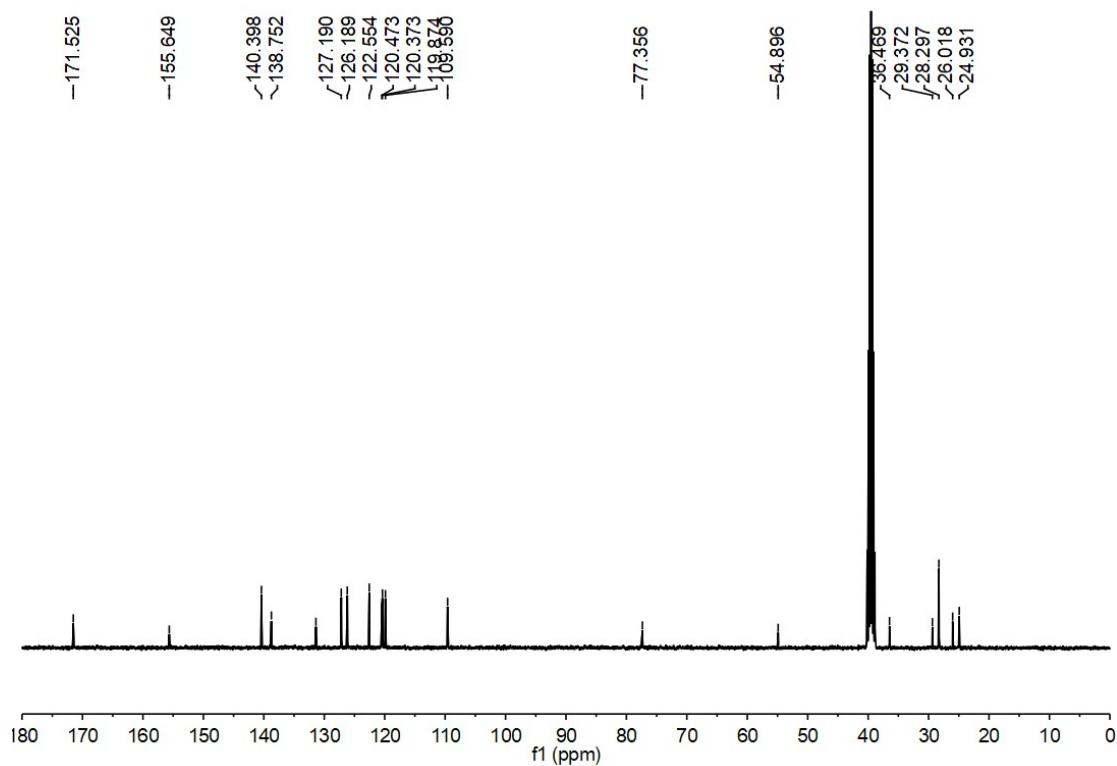


Figure S12. ¹³C NMR (101 MHz, DMSO) spectrum of 2-2.

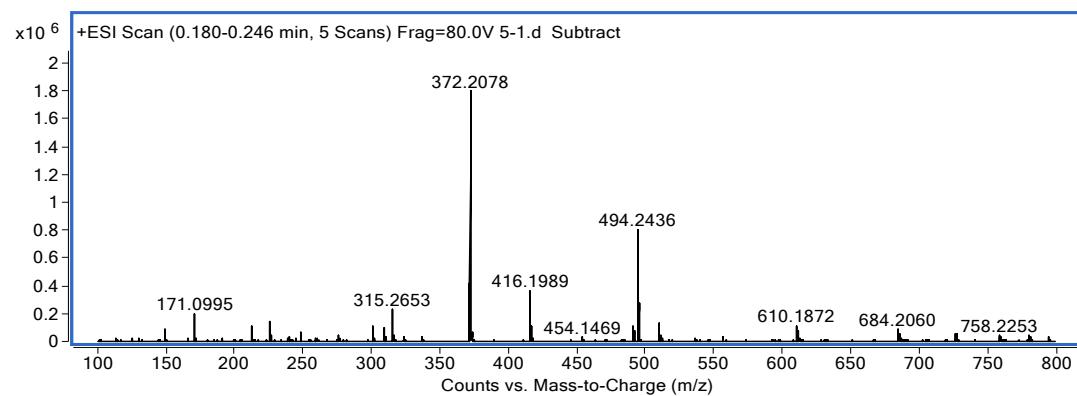


Figure S13. HRMS spectrum for 2-2.

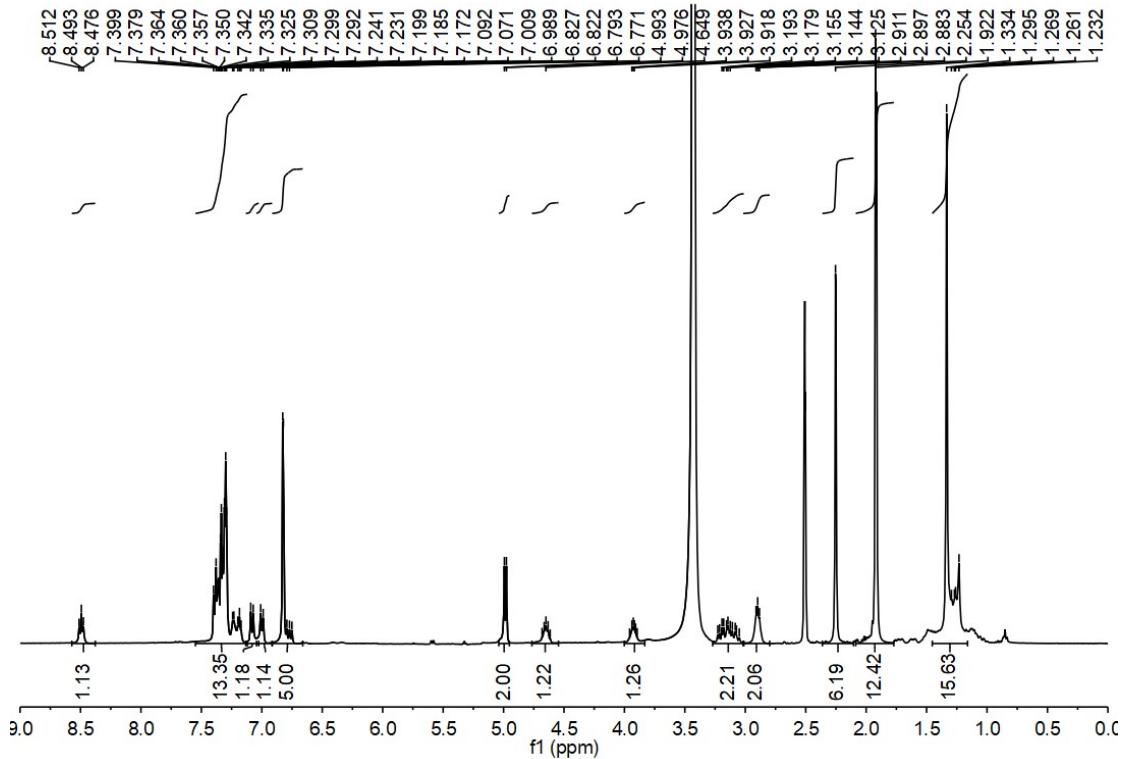


Figure S14. ^1H NMR (400 MHz, DMSO) spectrum of **B1**.

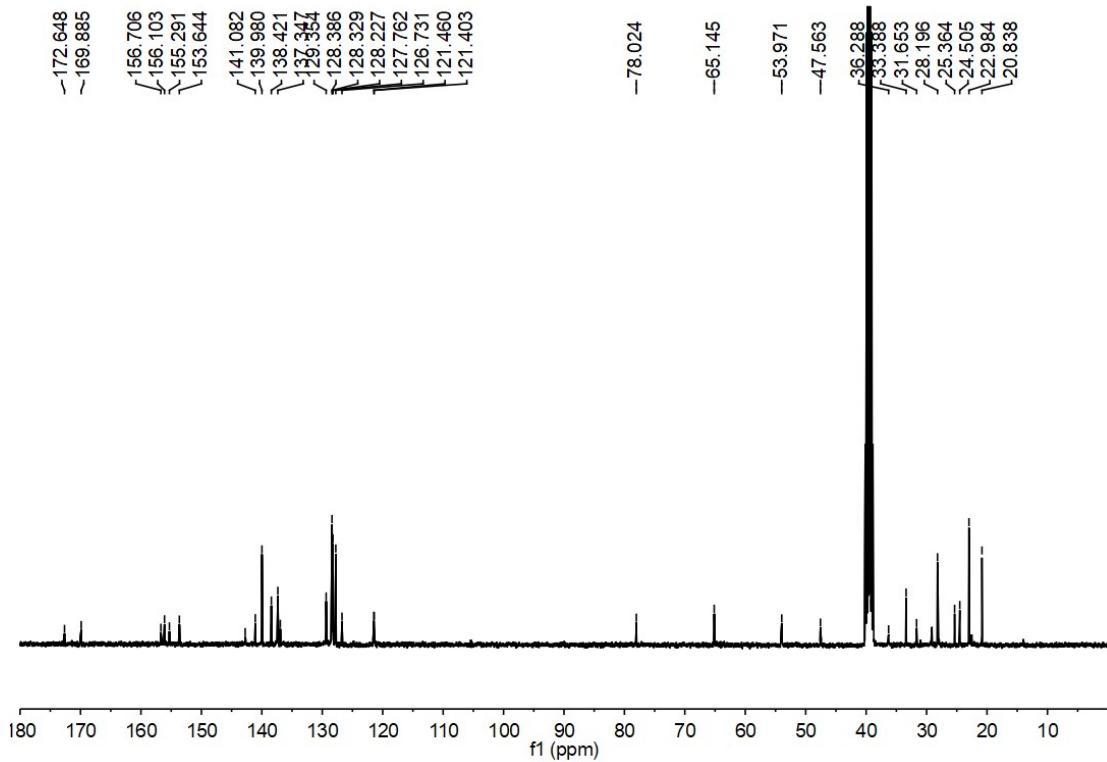


Figure S15. ^{13}C NMR (101 MHz, DMSO) spectrum of **B1**.

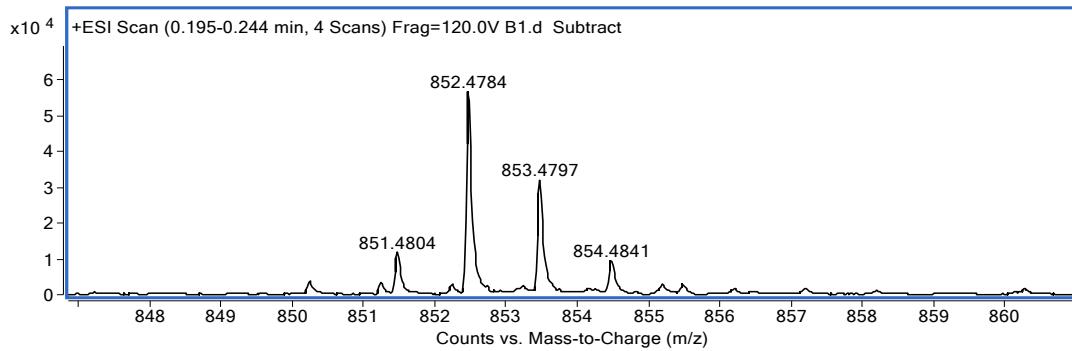


Figure S16. HRMS spectrum for **B1**.

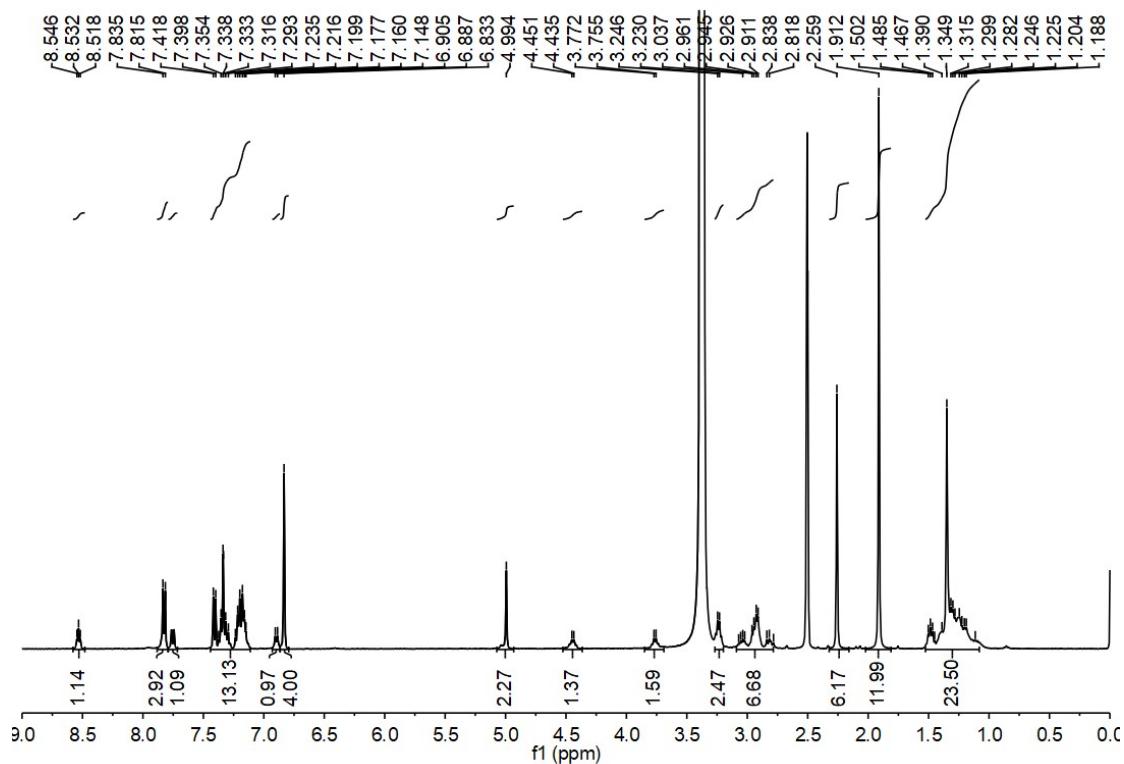


Figure S17. ^1H NMR (400 MHz, DMSO) spectrum of **B2**.

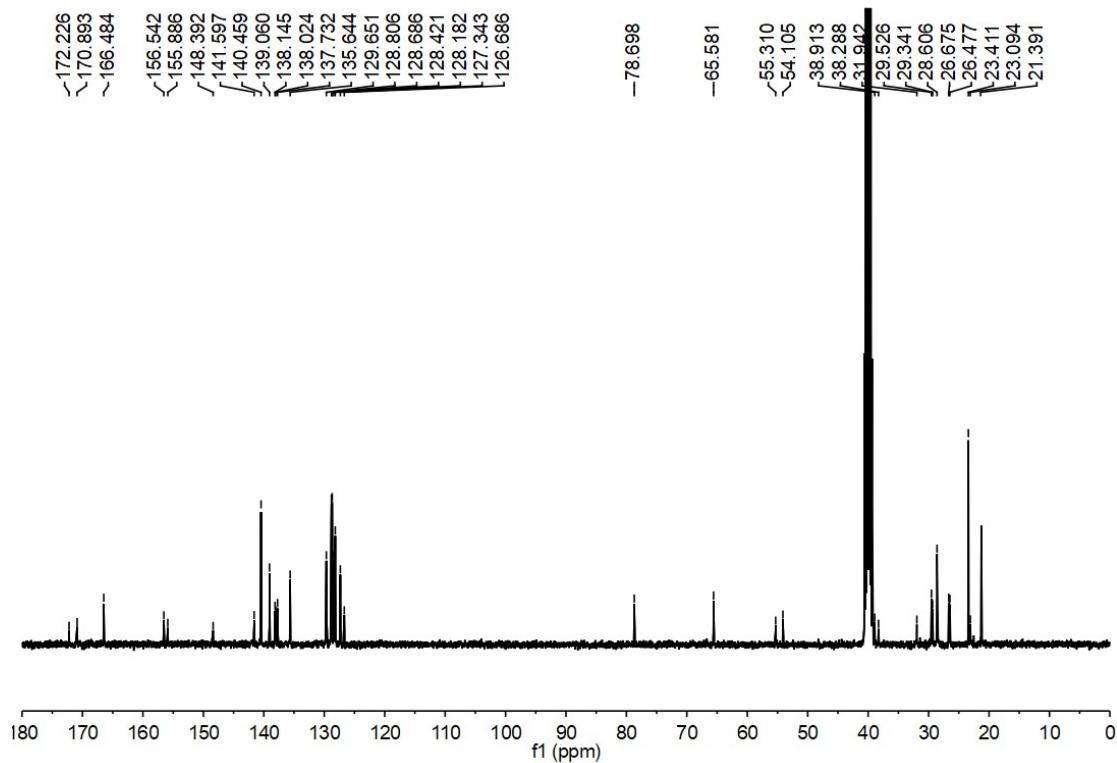


Figure S18. ^{13}C NMR (101 MHz, DMSO) spectrum of **B2**.

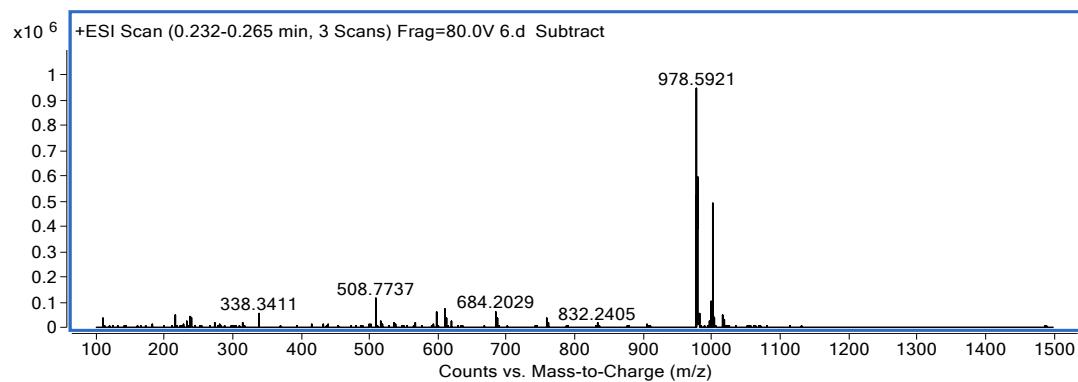


Figure S19. HRMS spectrum of **B2**.

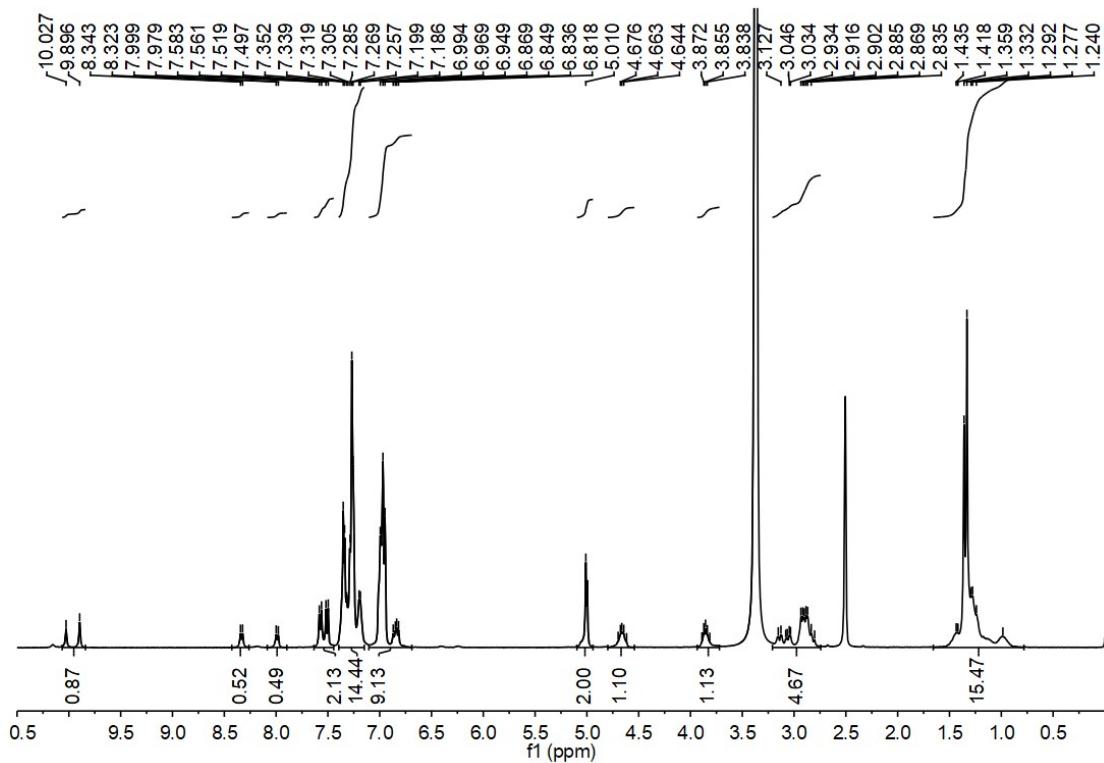


Figure S20. ^1H NMR (400 MHz, DMSO) spectrum of **N1**.

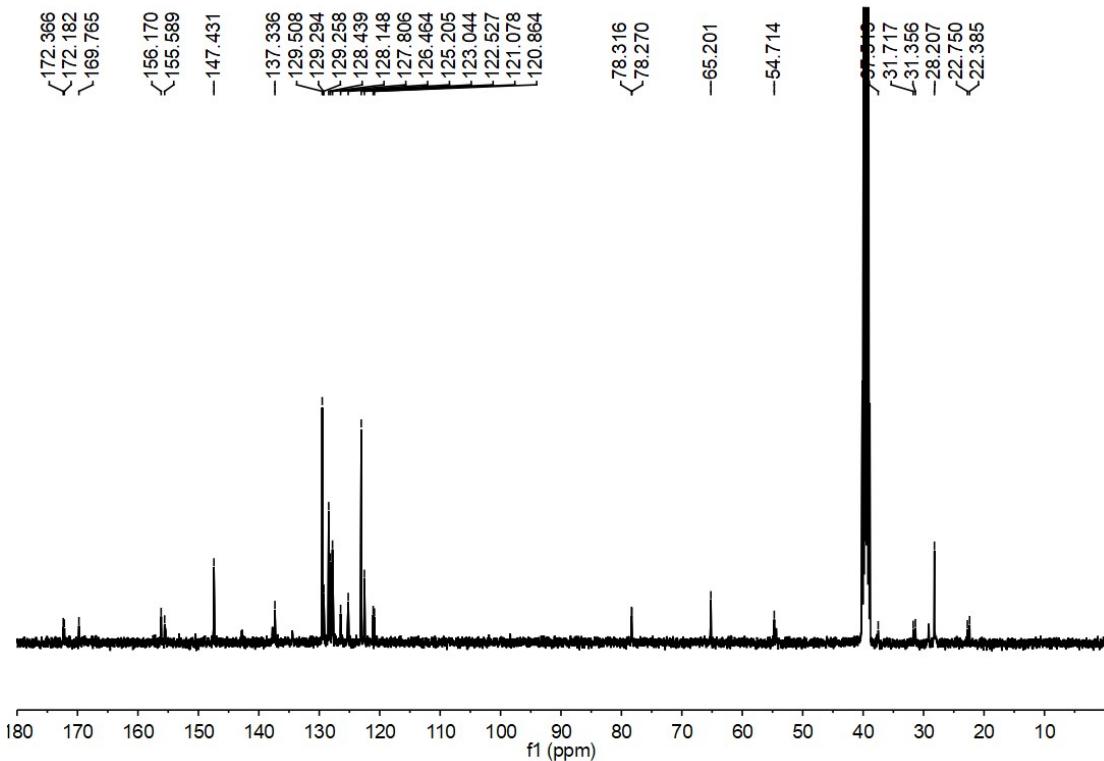


Figure S21. ^{13}C NMR (101 MHz, DMSO) spectrum of **N1**.

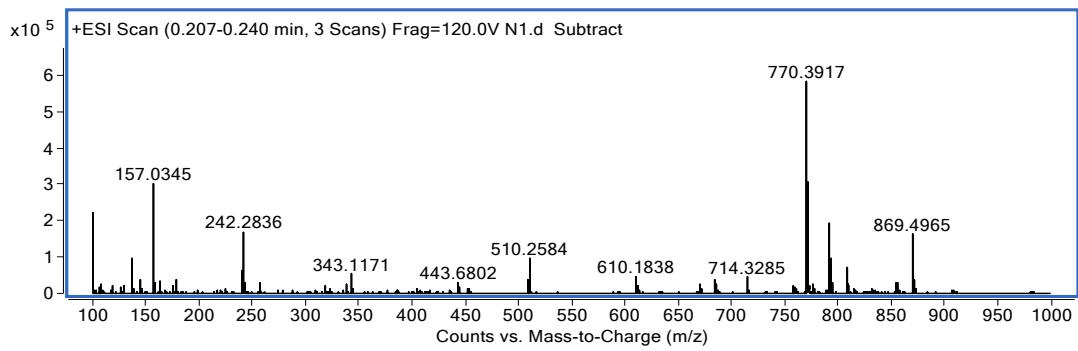


Figure S22. HRMS spectrum of N1.

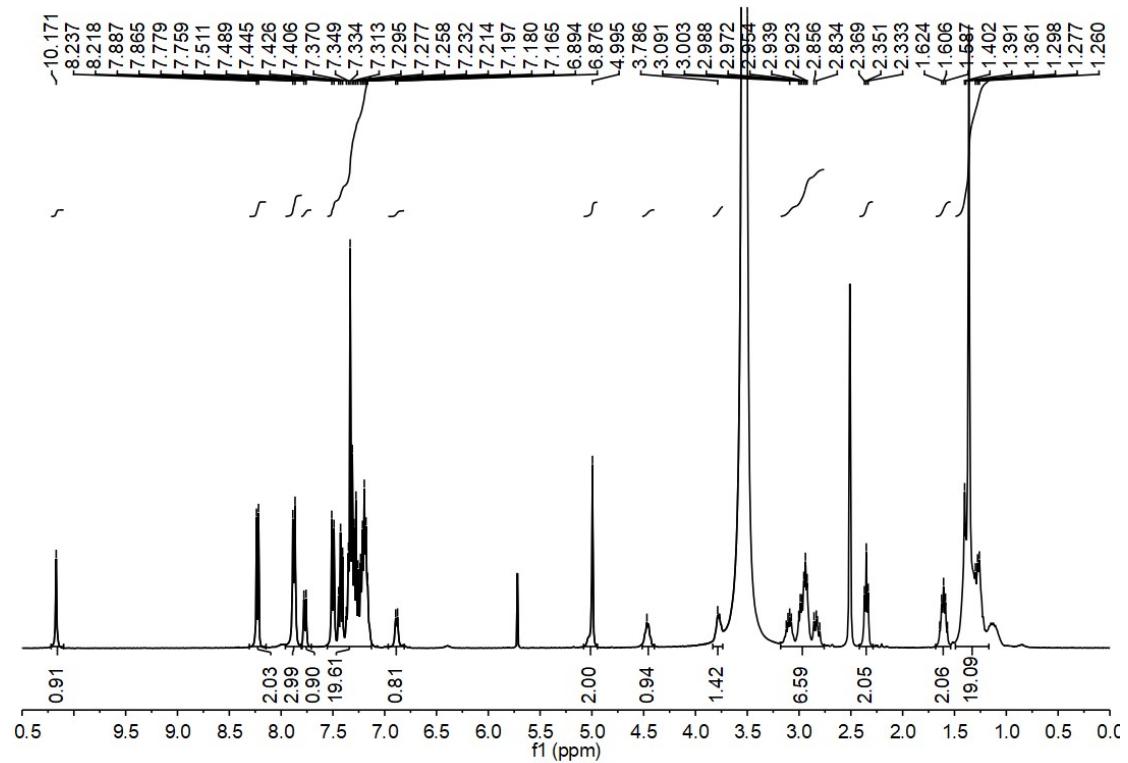


Figure S23. ^1H NMR (400 MHz, DMSO) spectrum of N2

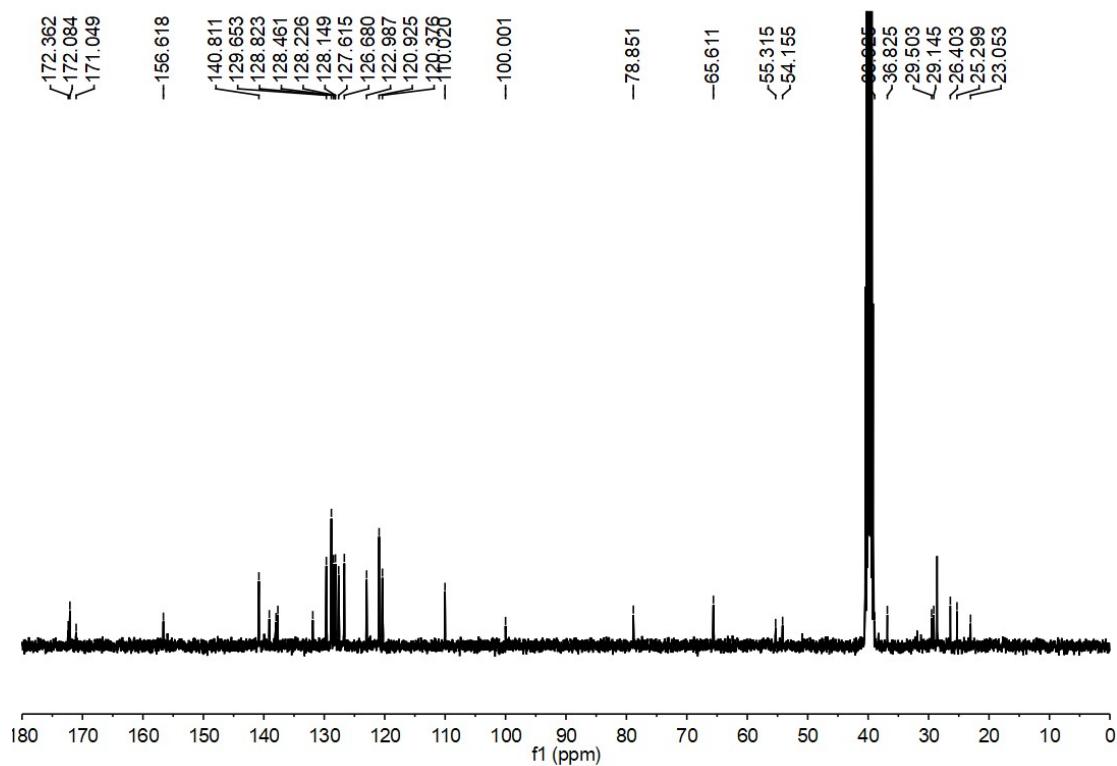


Figure S24. ^{13}C NMR (101 MHz, DMSO) spectrum of **N2**.

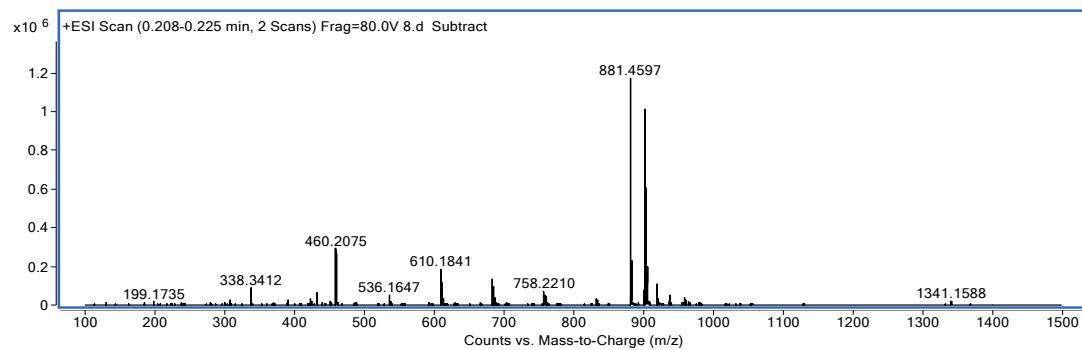


Figure S25. HRMS spectrum of **N2**.

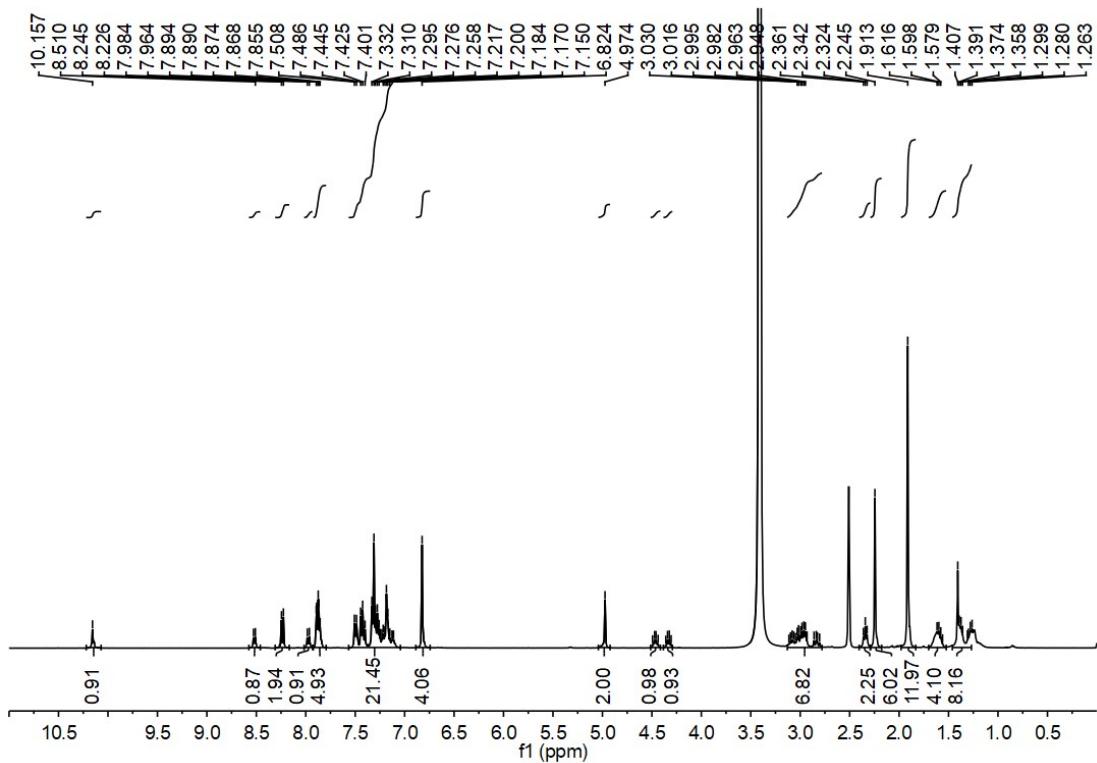


Figure S26. ^1H NMR (400 MHz, DMSO) spectrum of **BN**.

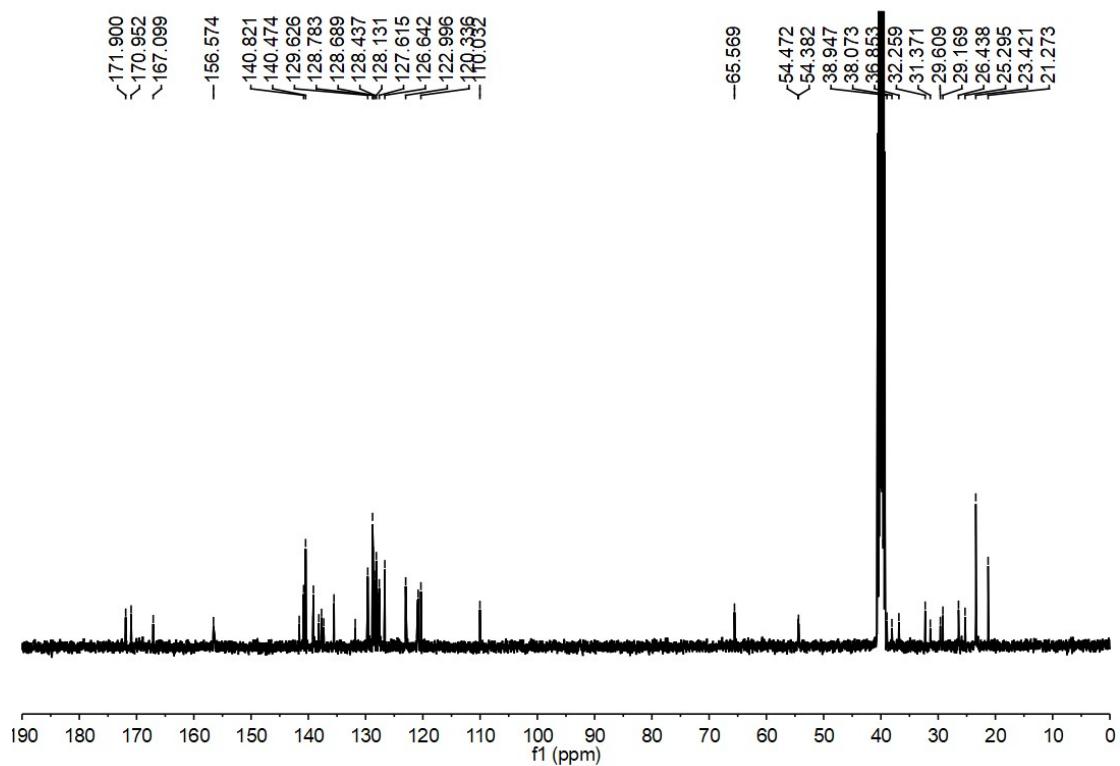


Figure S27. ^{13}C NMR (101 MHz, DMSO) spectrum of BN.

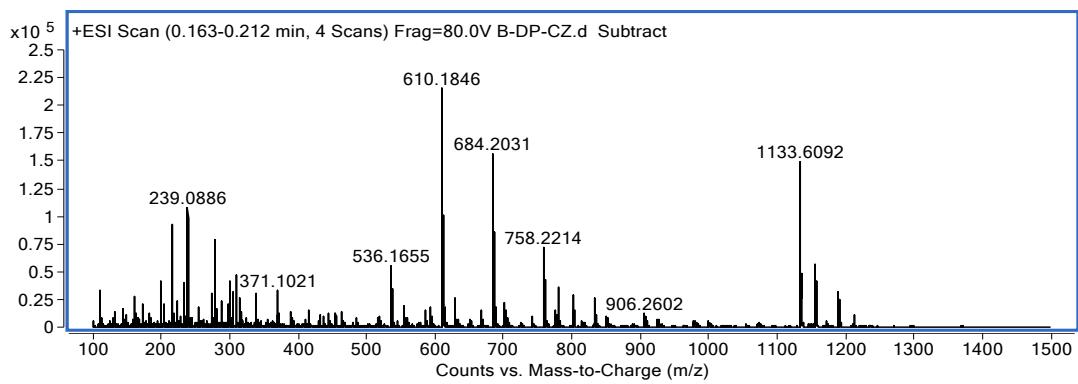


Figure S28. HRMS spectrum for BN.