

Supporting Information for

Binaphthyl-based Molecular Barrier Materials for Phosphoric Acid Poisoning in High-Temperature Proton Exchange Membrane Fuel Cells

*Dong-Cheol Jeong,^{1,#} Bohyun Mun,^{2,#} Hyekyung Lee,¹ Seung Jun Hwang,^{3,§}
Sung Jong Yoo,³ EunAe Cho,⁴ Yunmi Lee*² and Changsik Song*¹*

¹Department of Chemistry, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon, Gyeonggi 16419, Republic of Korea. ²Department of Chemistry, Kwangwoon University, 20 Kwangwoon-ro, Nowon-gu, Seoul 01897, Republic of Korea. ³Korea Institute of Science and Technology, 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea. ⁴Department of Materials Science & Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea.

Email: ymlee@kw.ac.kr and songcs@skku.edu

- ✓ **Figure S1.** Comparisons of cyclic voltammograms in an N₂-purged 0.1 M HClO₄ solution with 0.01 M H₃PO₄ at a scan rate of 50 mV s⁻¹.
- ✓ **Table S1.** ECSA and kinetic current densities at 0.8 V vs. RHE
- ✓ **Figure S2.** Comparisons of cyclic voltammograms with different dipping times in an N₂-purged 0.1 M HClO₄ solution with 0.01 M H₃PO₄ at a scan rate of 100 mV s⁻¹.
- ✓ **Figures S3 and S4.** ¹H and ¹³C NMR spectra of compound **2a**
- ✓ **Figures S5 and S6.** ¹H and ¹³C NMR spectra of compound **BNSH**
- ✓ **Figure S7 and S8.** ¹H and ¹³C NMR spectra of compound **2b**
- ✓ **Figure S9 and S10.** ¹H and ¹³C NMR spectra of compound **C2-BNSH**
- ✓ **Figure S11 and S12.** ¹H and ¹³C NMR spectra of compound **2c**
- ✓ **Figure S13 and S14.** ¹H and ¹³C NMR spectra of compound **C12-BNSH**
- ✓ **Figure S15 and S16.** ¹H and ¹³C NMR spectra of compound **2d**
- ✓ **Figure S17 and S18.** ¹H and ¹³C NMR spectra of compound **BN-1-SH**
- ✓ **Figure S19 and S20.** ¹H and ¹³C NMR spectra of compound **NASH**
- ✓ **Figure S21 and S22.** ¹H and ¹³C NMR spectra of compound **BNCN**

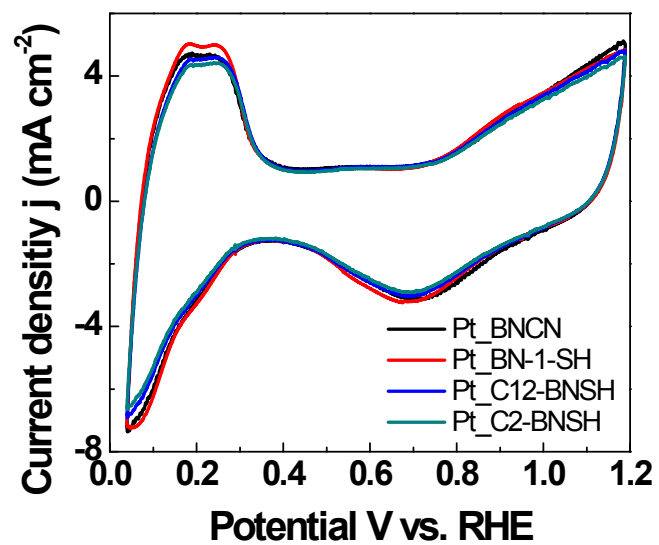


Figure S1. Comparisons of cyclic voltammograms in an N₂-purged 0.1 M HClO₄ solution with 0.01 M H₃PO₄ at a scan rate of 50 mV s⁻¹

Table S1. Electrochemically active surface area (ECSA) and kinetic current densities at 0.8 V vs. RHE^a

	specific ECSA (m ² g ⁻¹ Pt)	<i>j</i> (mA cm ⁻² at +0.80 V)	<i>j_k</i> (mA cm ⁻² at +0.80 V)
Pt	24.0	5.6	22.1
Pt_PA ^b	22.4	4.5	11.0
Pt_BNSH_PA	23.0	5.5	20.4
Pt_BN-CN_PA	22.8	5.3	17.0
Pt_BN-1-SH_PA	24.1	5.2	16.4
Pt_C12-BNSH_PA	21.9	5.0	14.9
Pt_C2-BNSH_PA	21.1	4.8	12.9
Pt_NSH_PA	20.1	3.6	6.9

^aThe ORR activities were measured in 0.1 M HClO₄ and 0.01 M H₃PO₄ solutions under O₂ using a glassy carbon rotating disk electrode (RDE) at a rotation and sweep rates of 1600 rpm and 10 mV s⁻¹, respectively.

^bPA: Phosphoric acid (0.01 M).

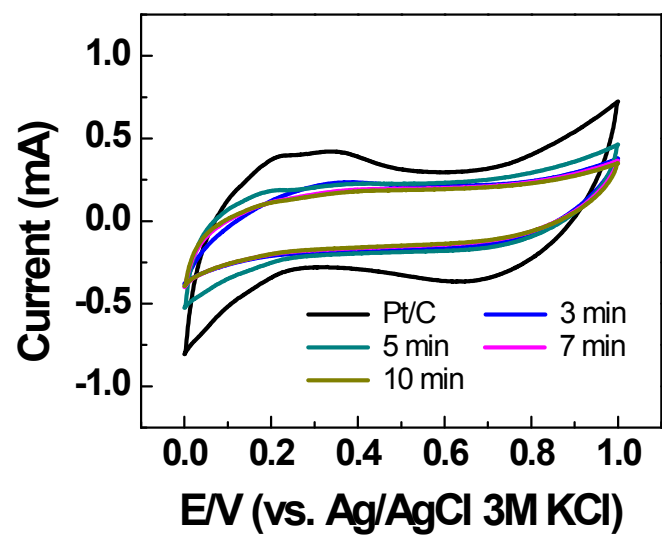


Figure S2. Comparisons of cyclic voltammograms with different dipping times in an N_2 -purged 0.1 M $HClO_4$ solution with 0.01 M H_3PO_4 at a scan rate of 100 mV s^{-1} .

■ ^1H NMR and ^{13}C NMR spectra for all products:

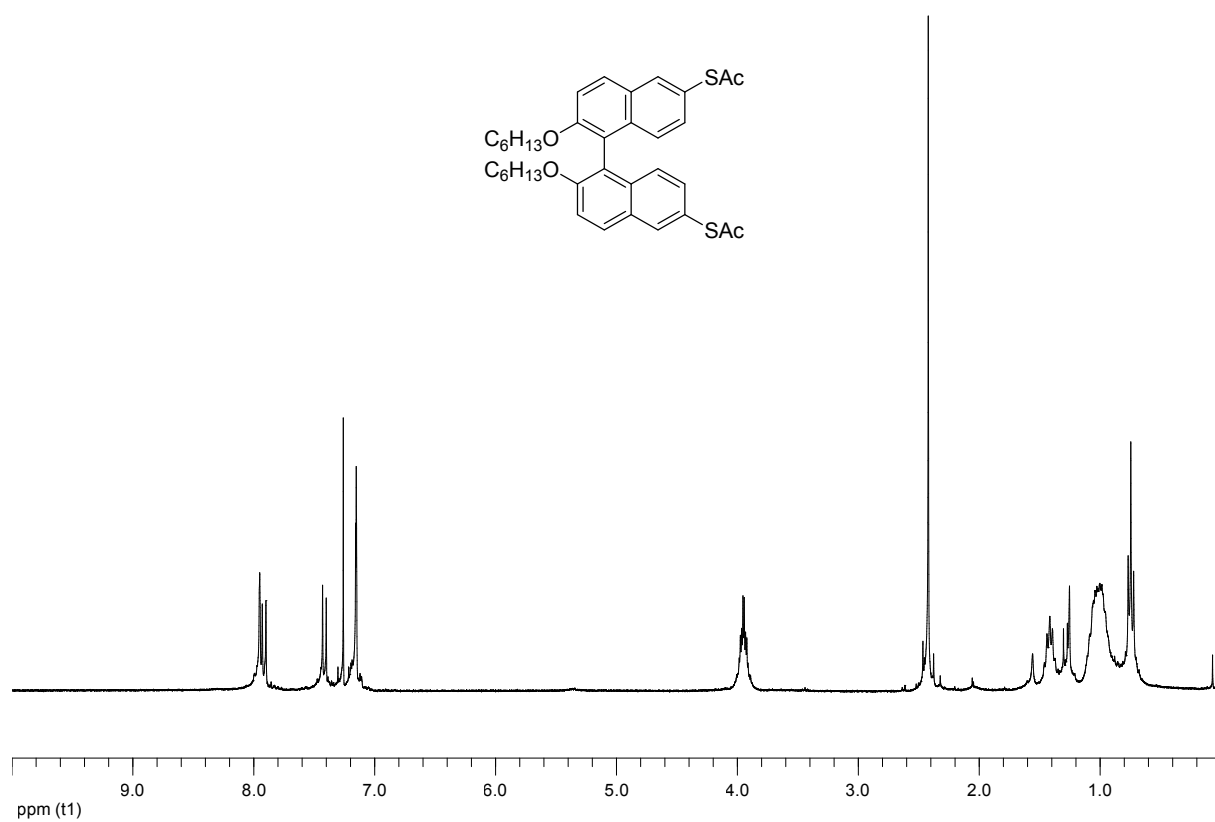


Figure S3. ^1H NMR spectrum of compound **2a**

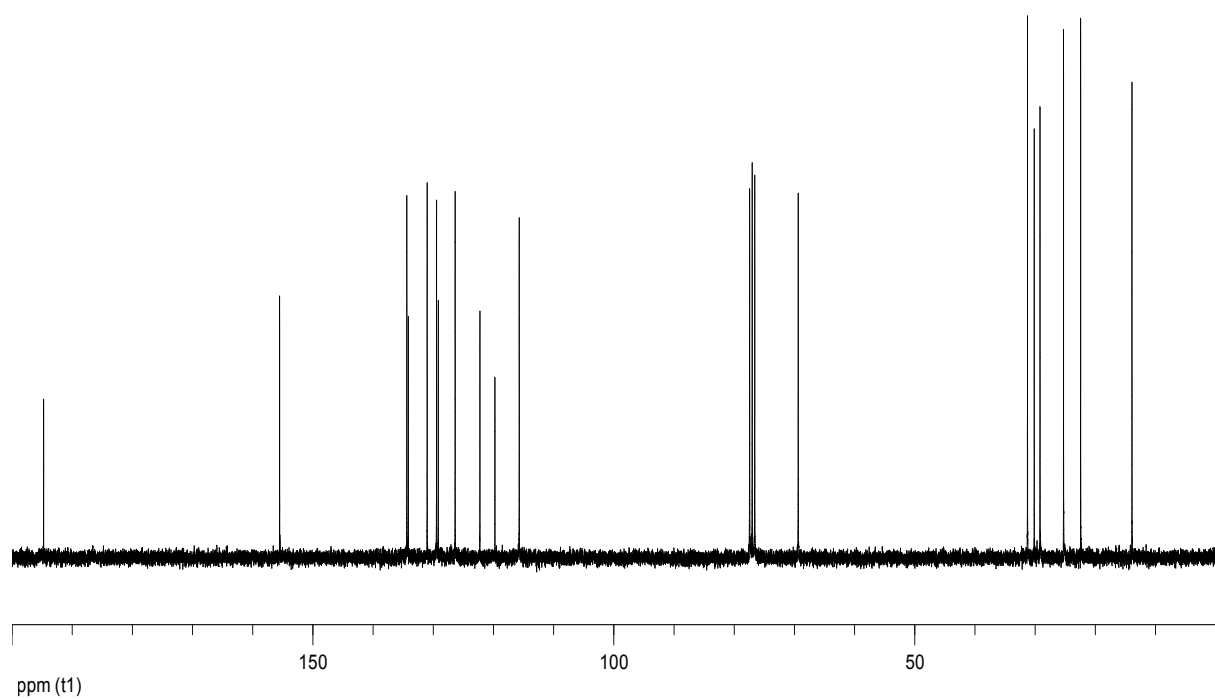


Figure S4. ^{13}C NMR spectrum of compound **2a**

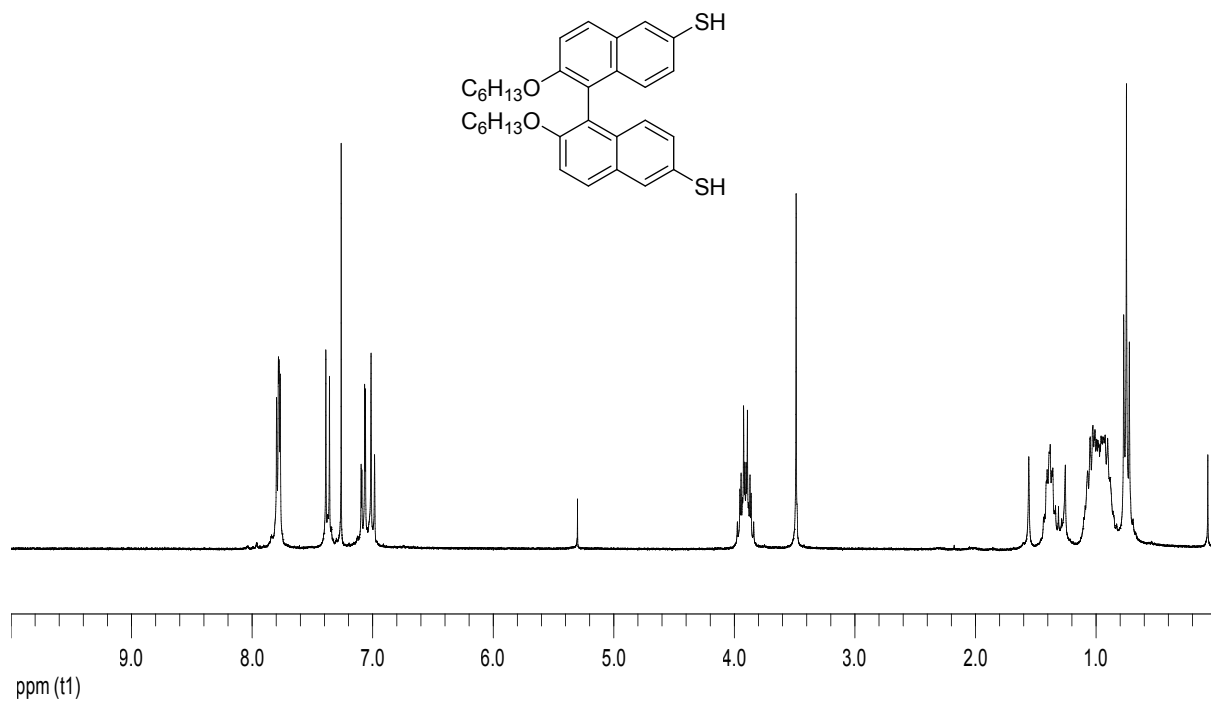


Figure S5. ¹H NMR spectrum of compound **BNSH**

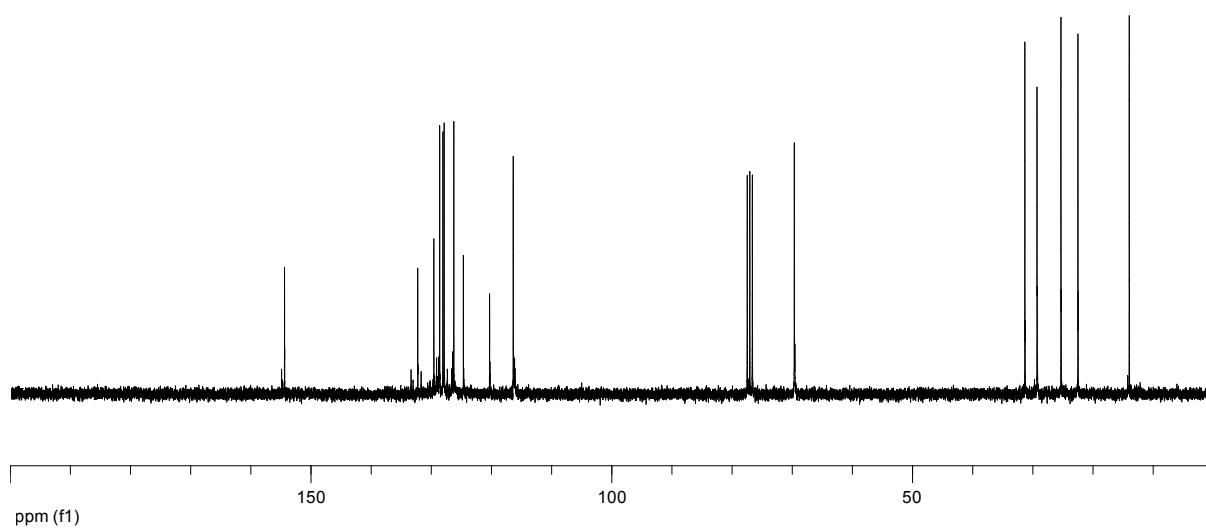


Figure S6. ¹³C NMR spectrum of compound **BNSH**

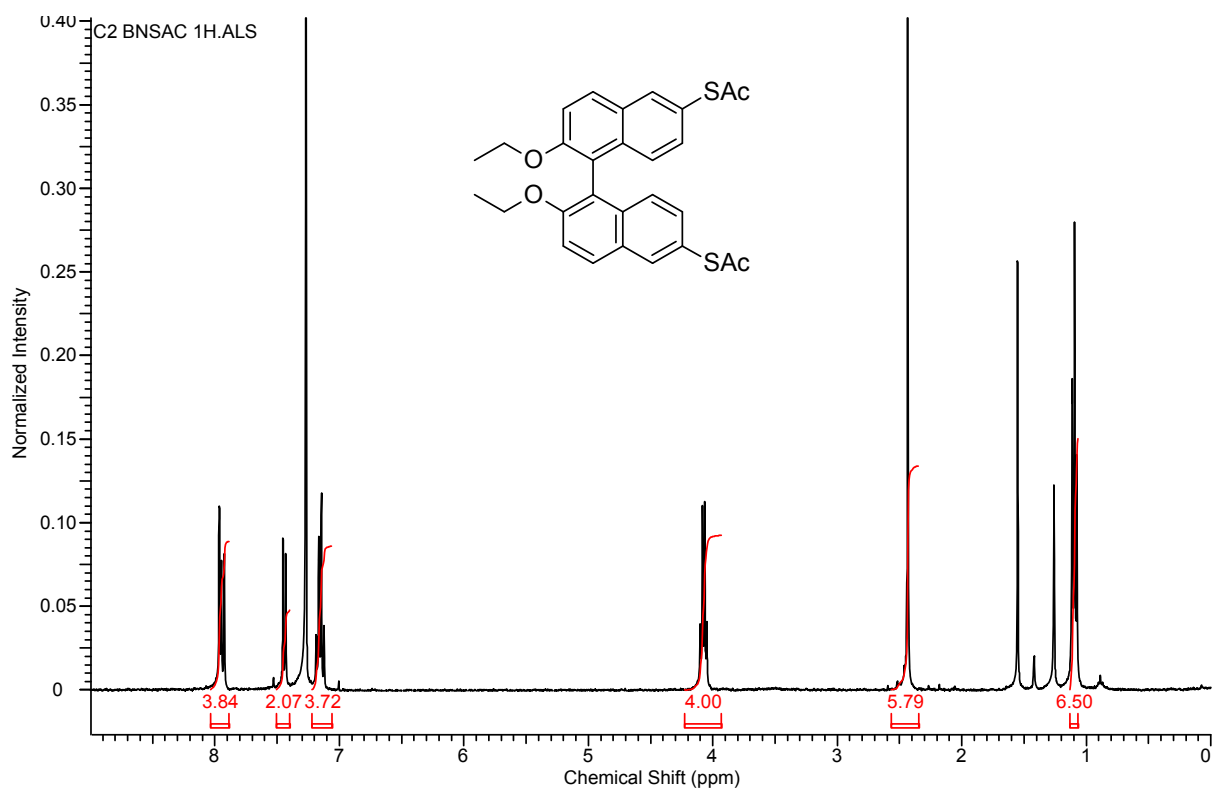


Figure S7. ^1H NMR spectrum of compound **2b**

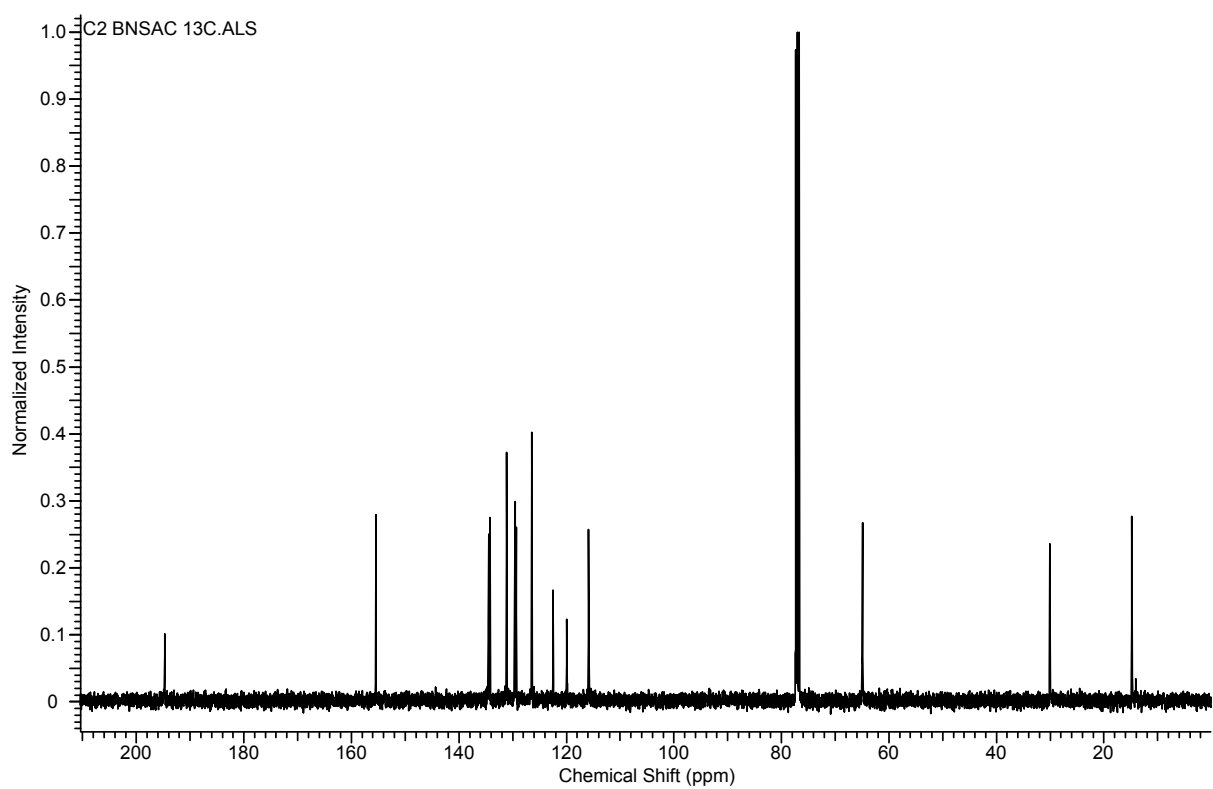


Figure S8. ^{13}C NMR spectrum of compound **2b**

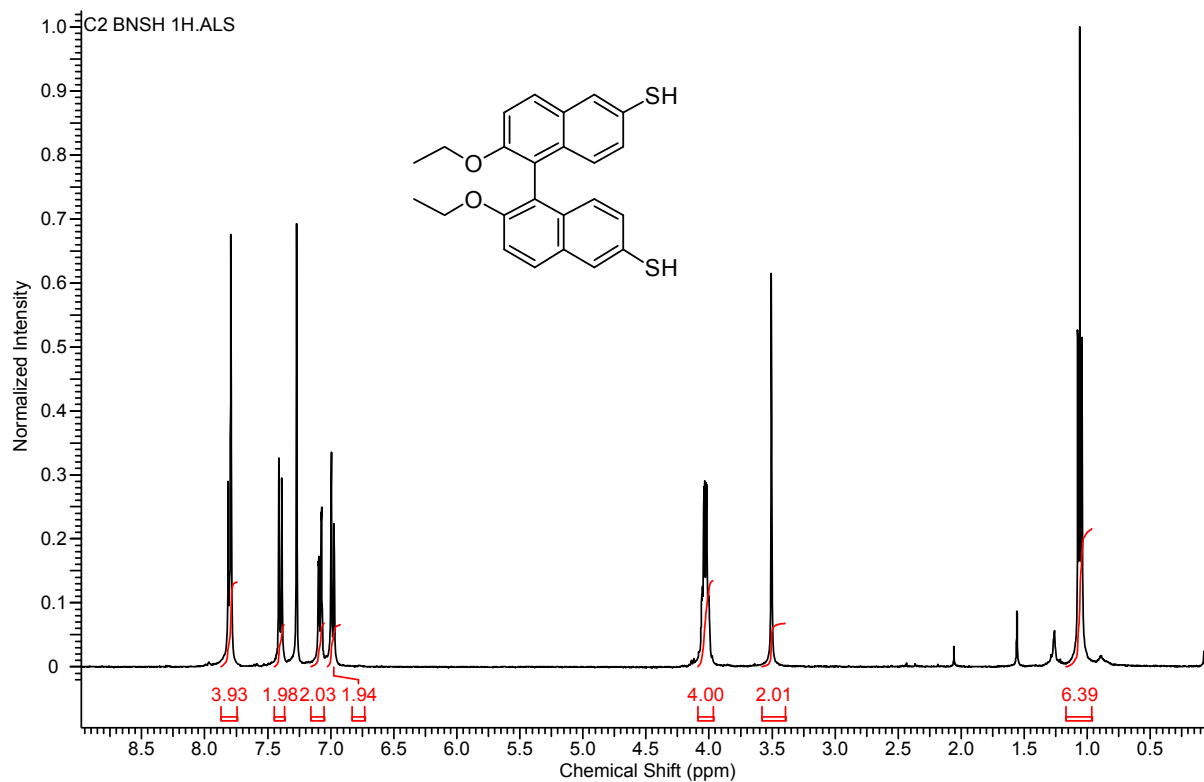


Figure S9. ^1H NMR spectrum of compound C2-BNSH

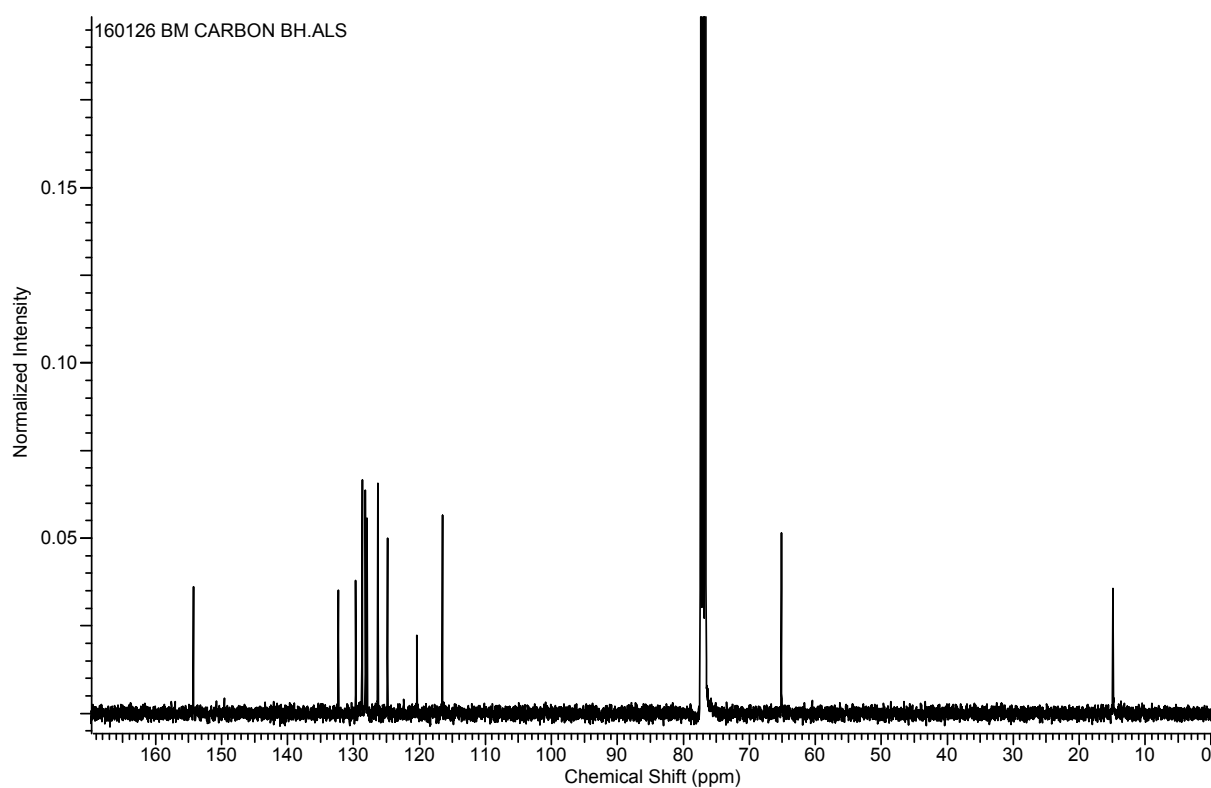


Figure S10. ^{13}C NMR spectrum of compound C2-BNSH

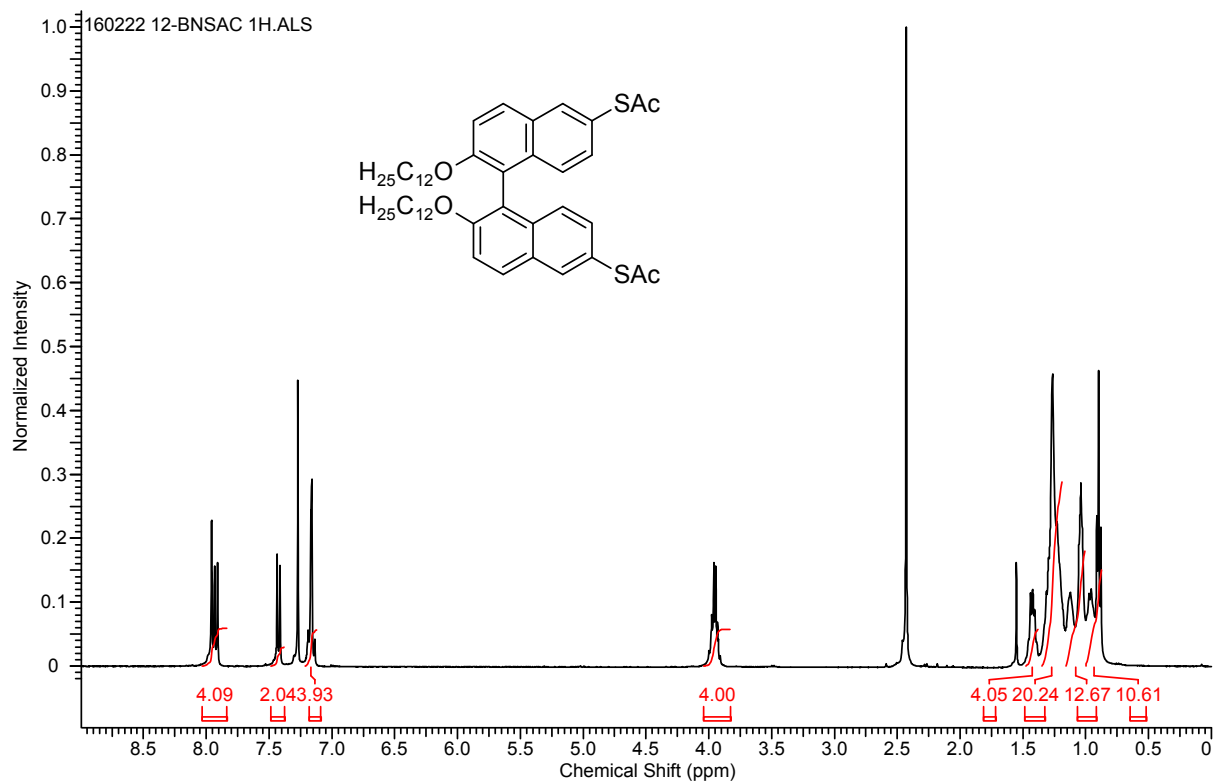


Figure S11. ^1H NMR spectrum of compound **2c**

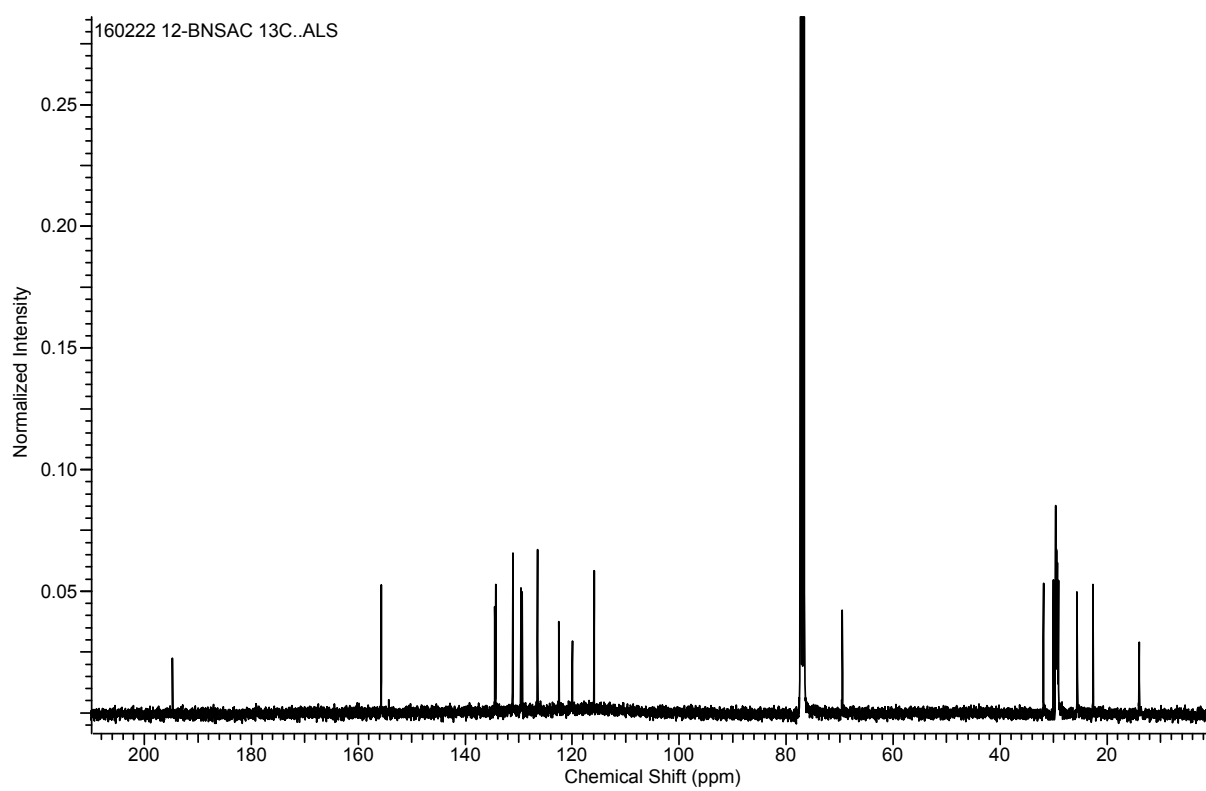


Figure S12. ^{13}C NMR spectrum of compound **2c**

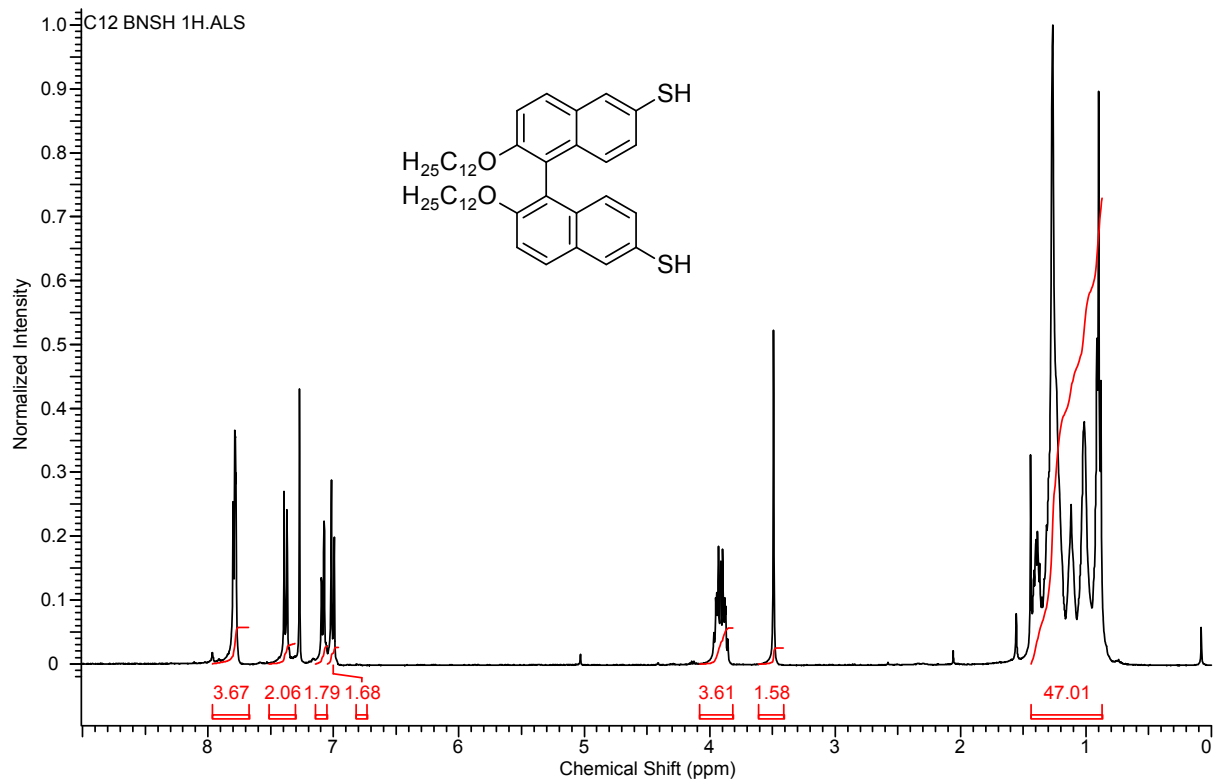


Figure S13. ^1H NMR spectrum of compound C12-BNSH

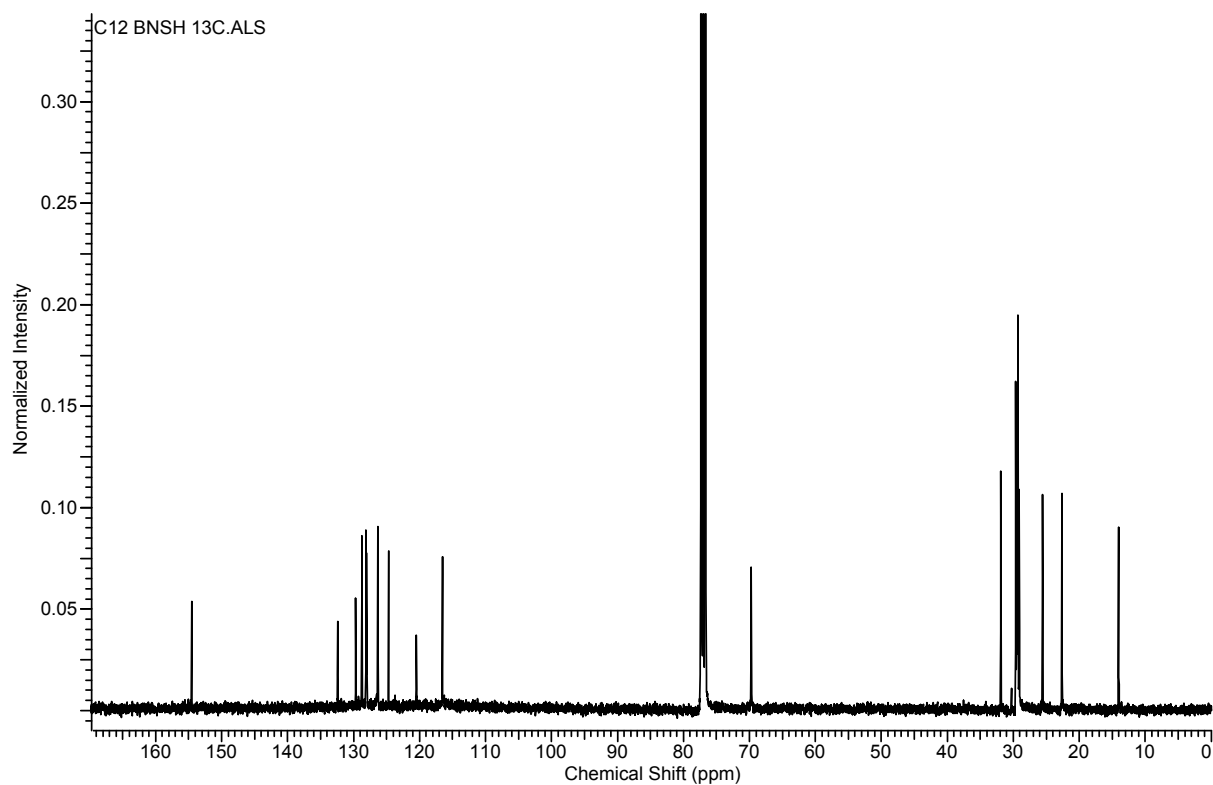


Figure S14. ^{13}C NMR spectrum of compound C12-BNSH

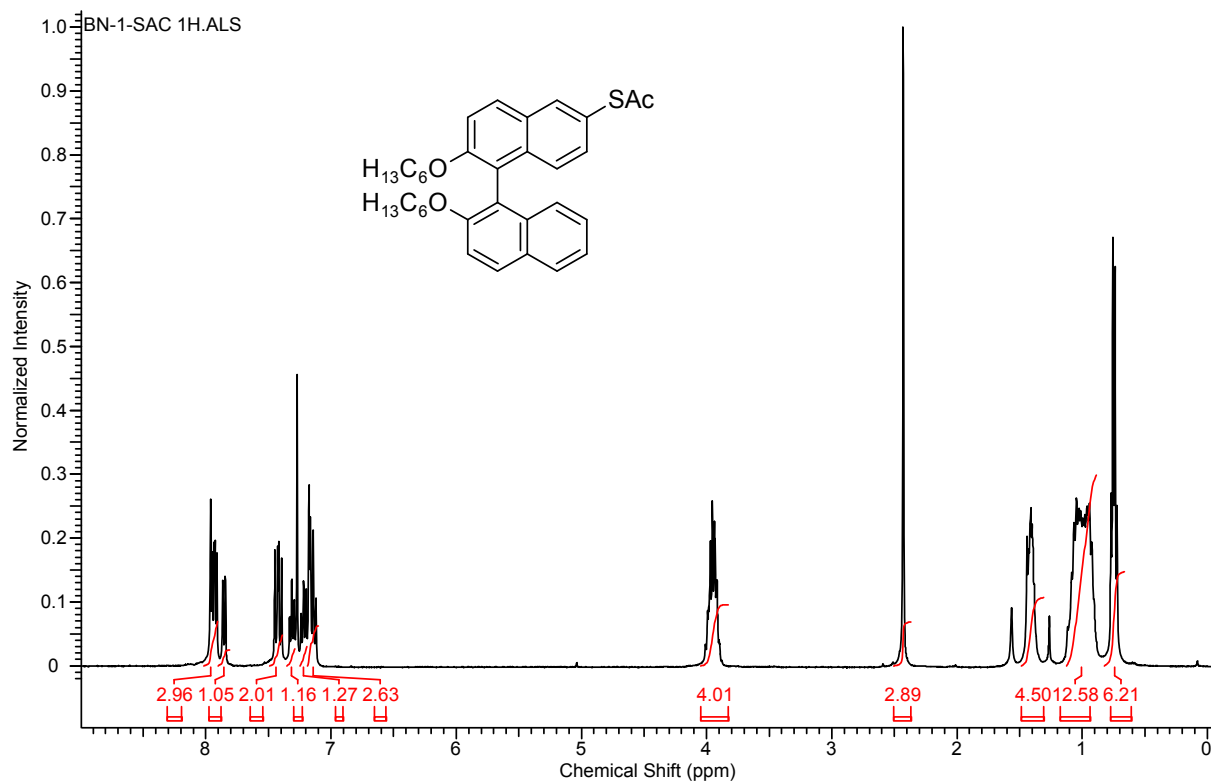


Figure S15. 1H NMR spectrum of compound **2d**

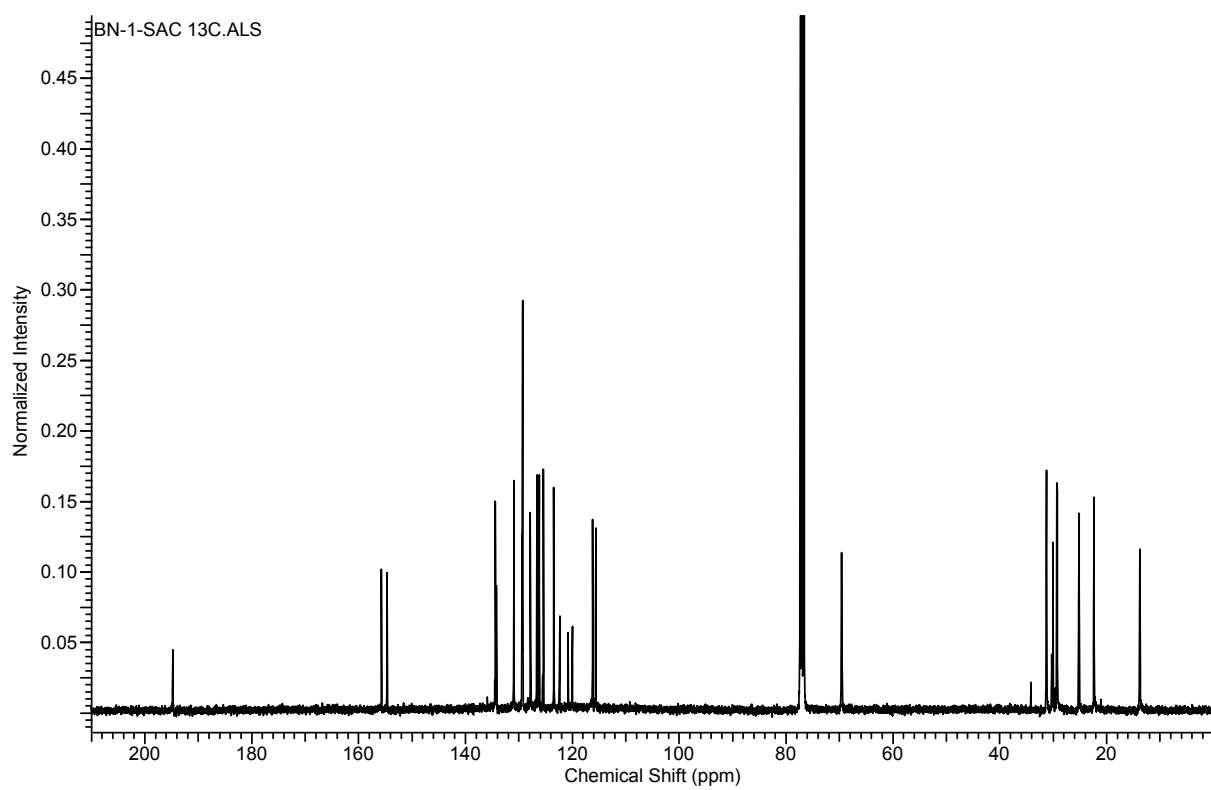


Figure S16. ^{13}C NMR spectrum of compound **2d**

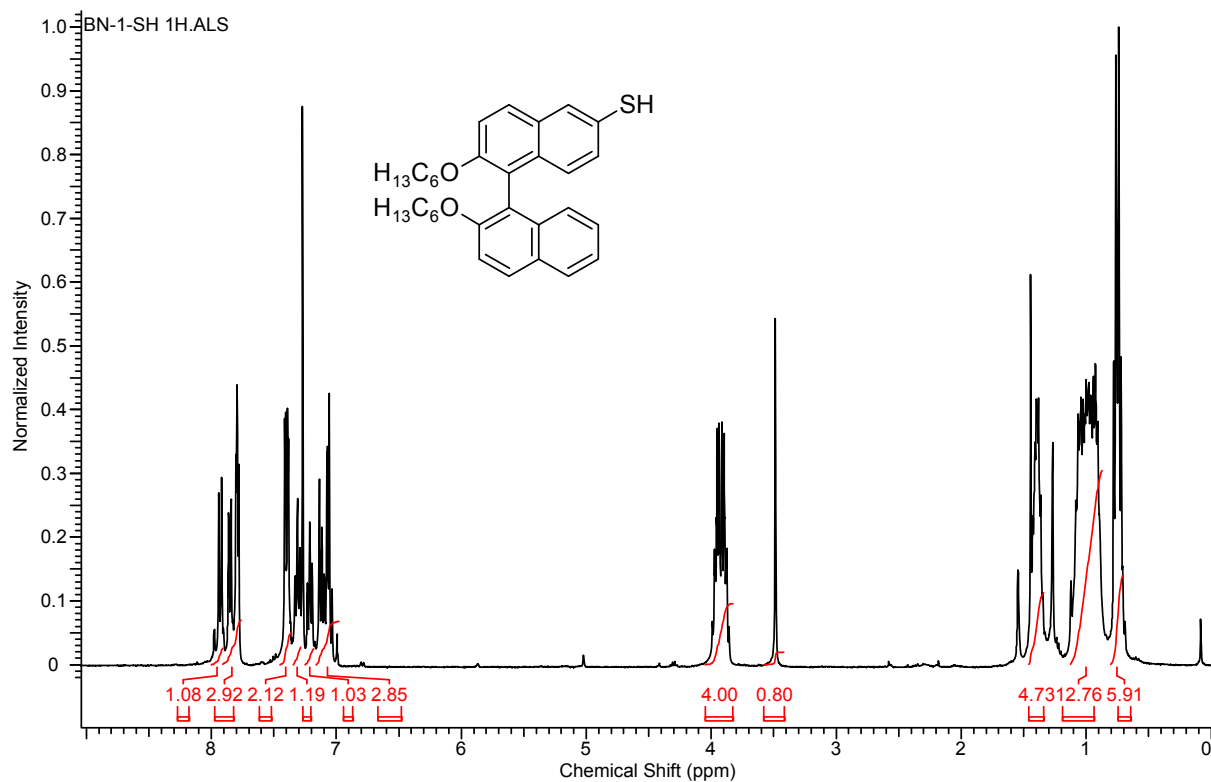


Figure S17. ^1H NMR spectrum of compound **BN-1-SH**

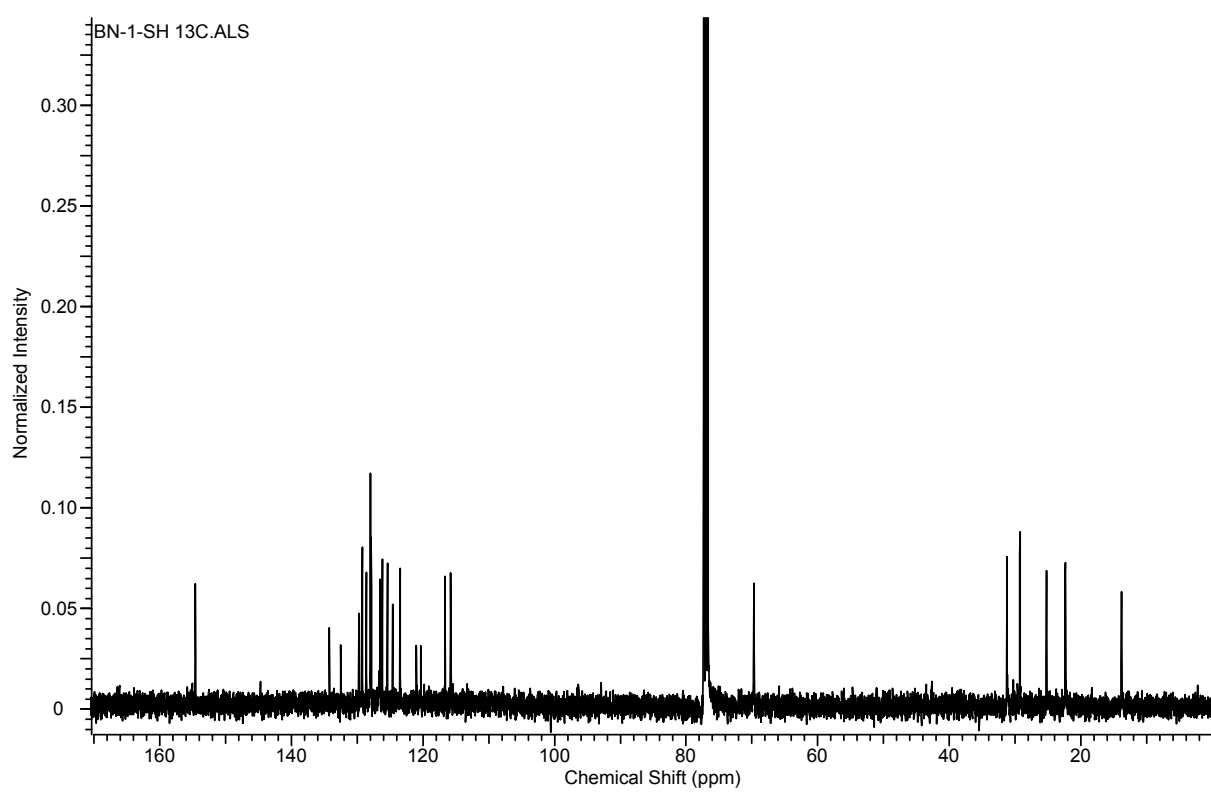


Figure S18. ^{13}C NMR spectrum of compound **BN-1-SH**

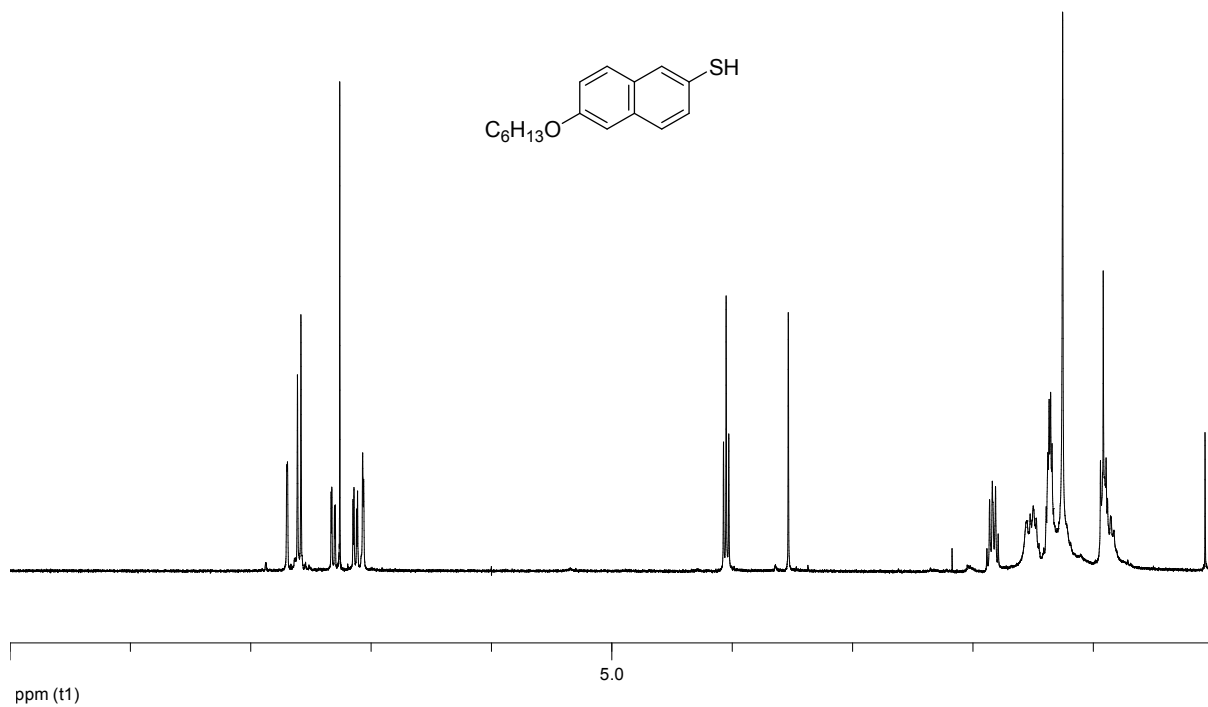


Figure S19. ¹H NMR spectrum of compound NASH

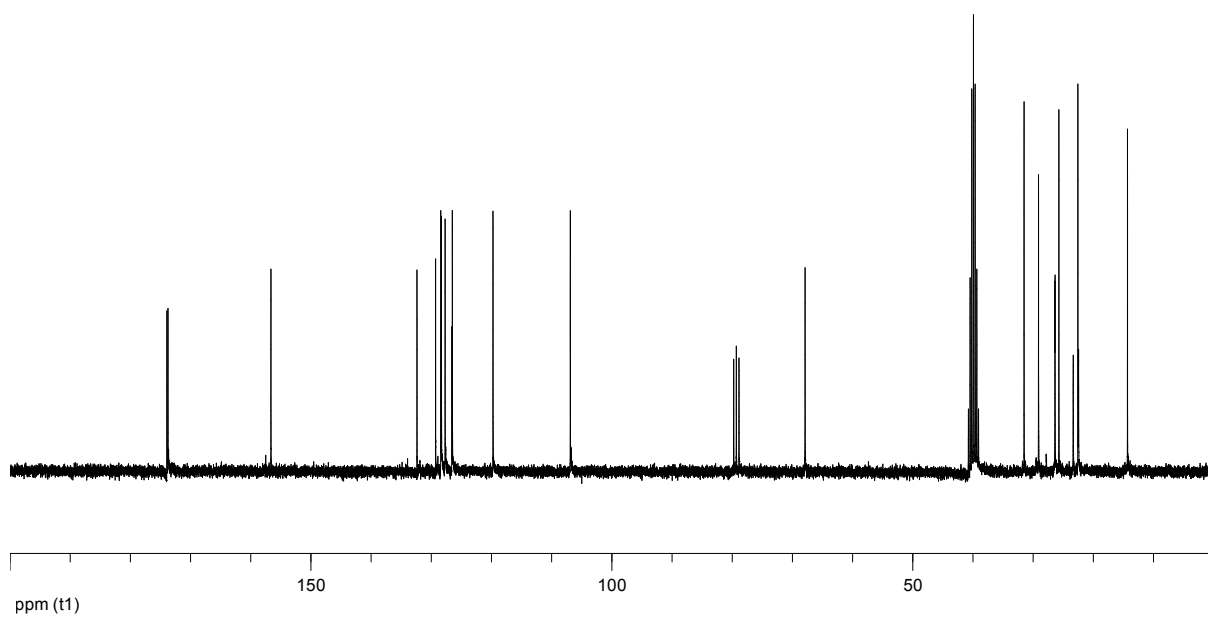


Figure S20. ¹³C NMR spectrum of compound NASH

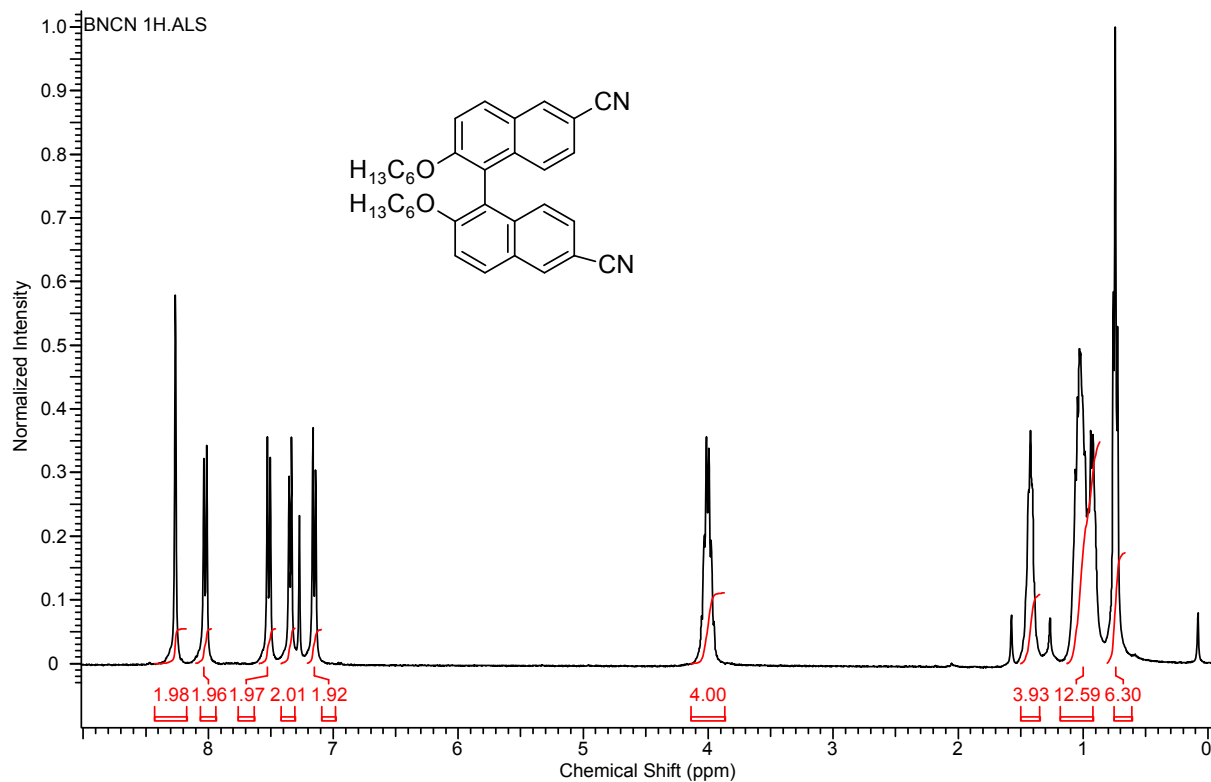


Figure S21. ^1H NMR spectrum of compound **BNCN**

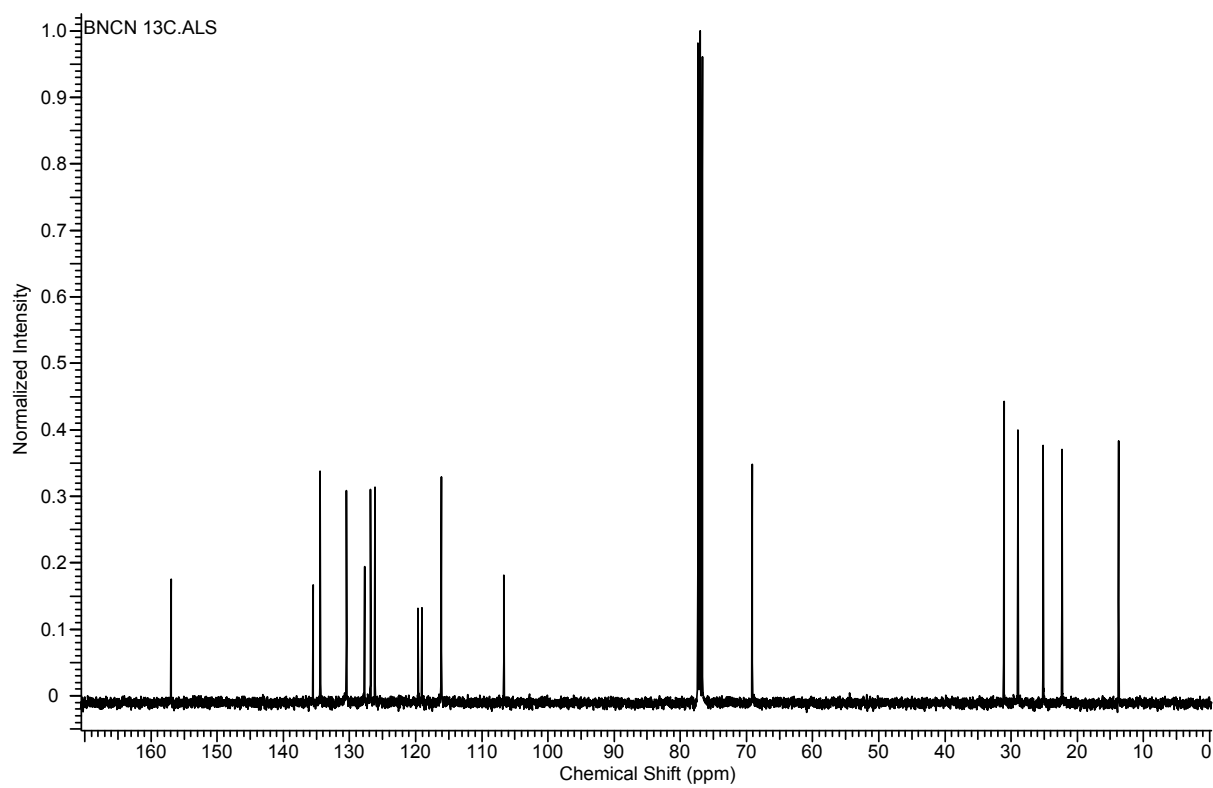


Figure S22. ^{13}C NMR spectrum of compound **BNCN**