

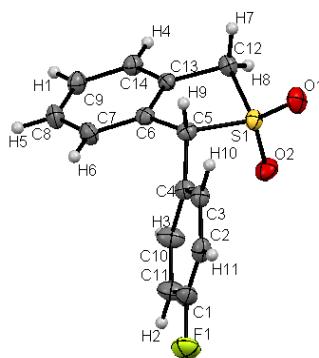
## Benzosulfones as Photochemically Activated Sulfur Dioxide (SO<sub>2</sub>) Donors

Satish R. Malwal and Harinath Chakrapani\*

Department of Chemistry, Indian Institute of Science Education and Research Pune, Dr. Homi Bhabha Road, Pashan Pune 411 008, Maharashtra, India.

E-mail: [harinath@iiserpune.ac.in](mailto:harinath@iiserpune.ac.in)

**X-ray data for 12h:** C<sub>14</sub>H<sub>11</sub>FO<sub>2</sub>S; Compound **12h** was crystallized from diethyl ether at room temperature. A colorless rectangular shaped crystal with approximate dimensions 0.302 x 0.210 x 0.052 mm gave monoclinic crystal with space group P21/c;  $a = 11.4383(13)$   $b = 11.6596(15)$   $c = 9.4849(12)$  Å,  $\alpha = 90^\circ$   $\beta = 104.523(3)^\circ$   $\gamma = 90^\circ$ ;  $V = 1224.5(3)$  Å<sup>3</sup>;  $T = 296$  K;  $Z = 4$ ;  $\rho_{calc} = 1.423$  Mgm<sup>-3</sup>;  $2\theta_{max} = 56.70^\circ$ ;  $MoK\alpha\lambda = 0.71073$  Å. Fine-focus sealed tube



source with graphite monochromator.  $R = 0.0341$  (for 2601 reflection  $I > 2\sigma(I)$ ),  $wR = 0.1042$  which was refined against  $|F_2|$  and  $S = 1.491$  for 163 parameters and 3047 unique reflections. The structure was obtained by direct methods using SHELXS-97. All non-hydrogen atoms were refined isotropically. The hydrogen atoms were fixed geometrically in the idealized position and refined in the final cycle of refinement as riding over the atoms to which they are bonded.  $\mu = 0.267$  mm<sup>-1</sup>. **CCDC No.: 907013.**

Spectral Data:

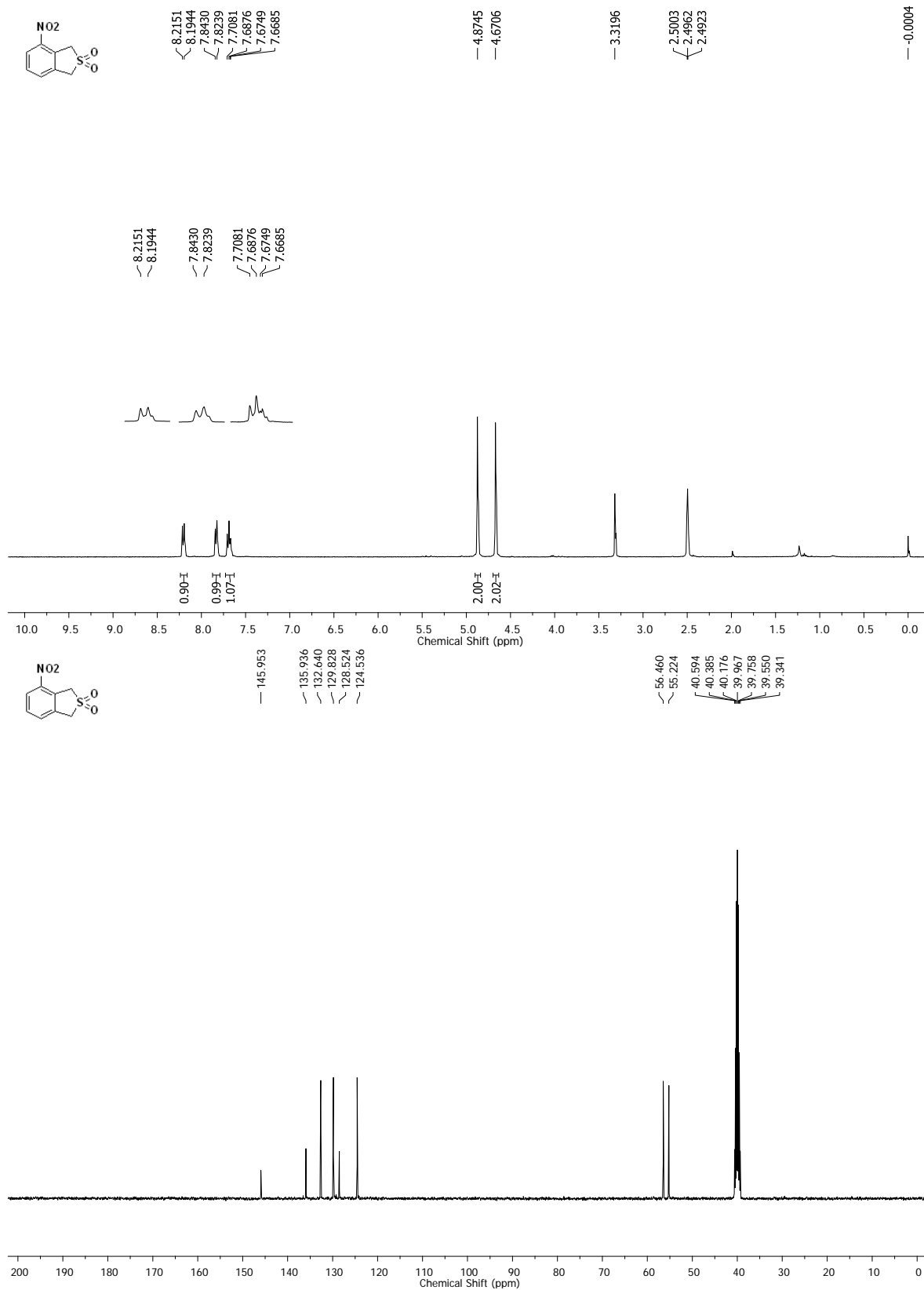
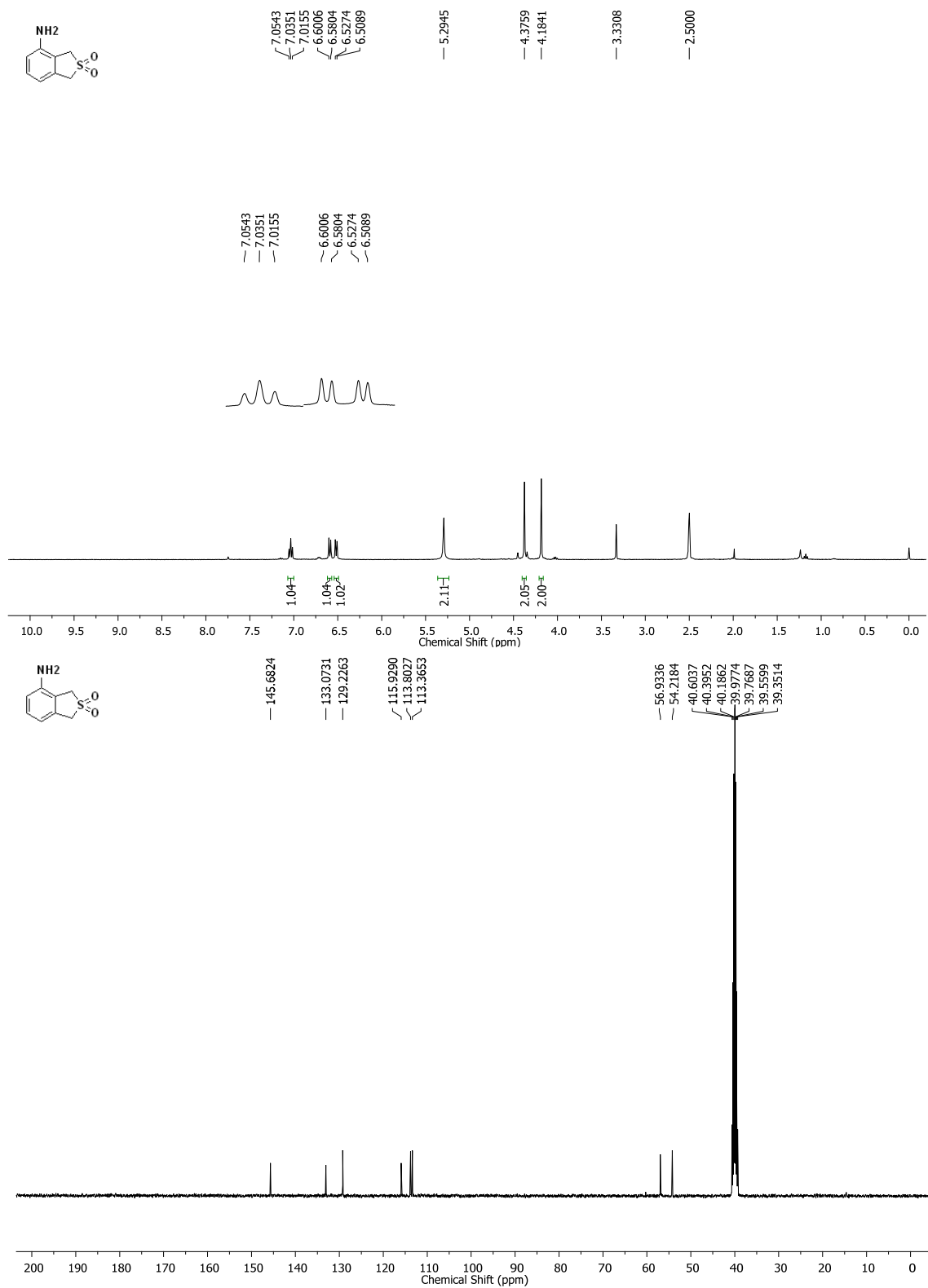
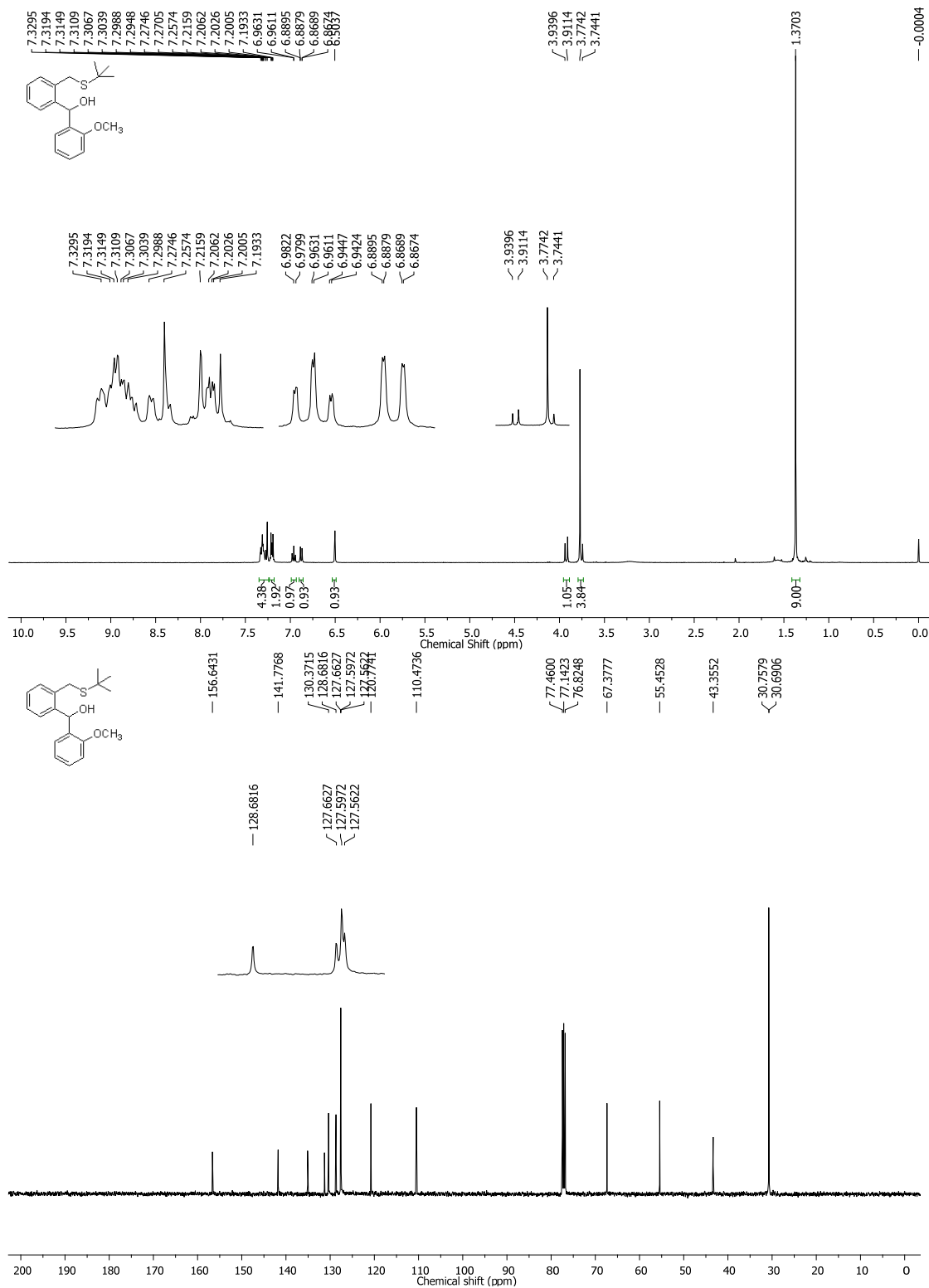


Figure S1. NMR spectra of **4b**



**Figure S2.** NMR spectra of **5a**



**Figure S3.** NMR spectra of **10b**

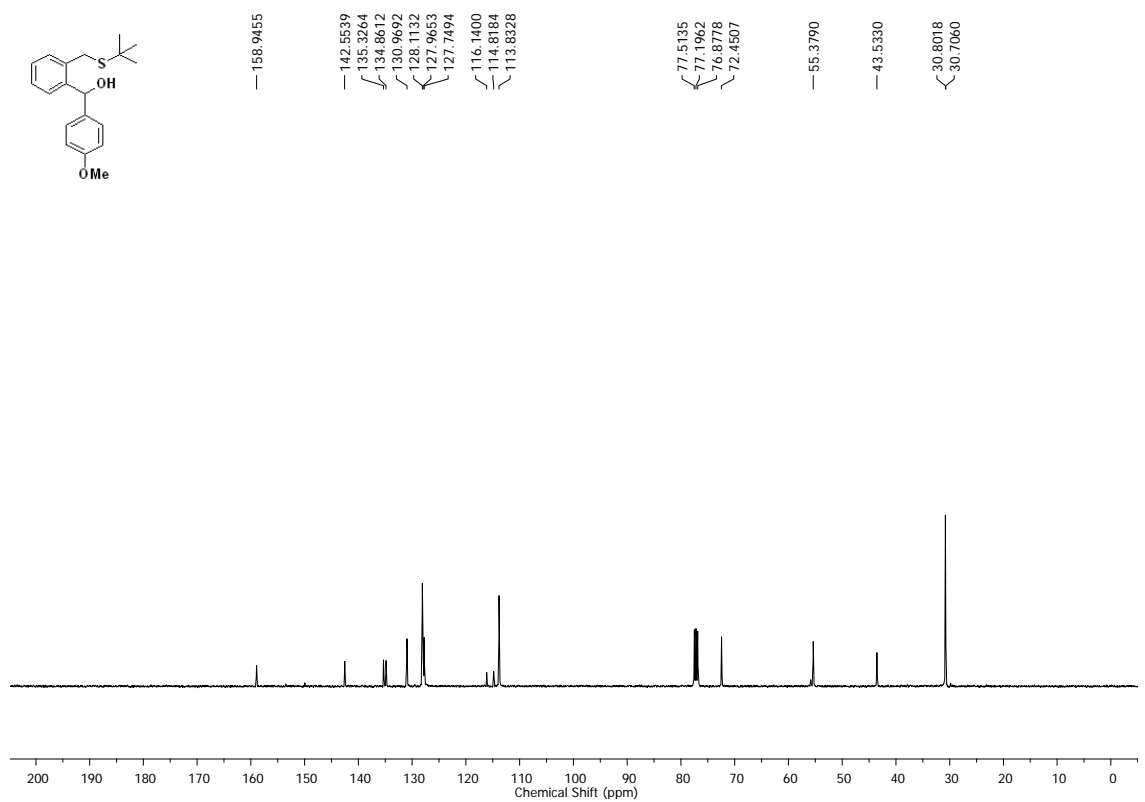
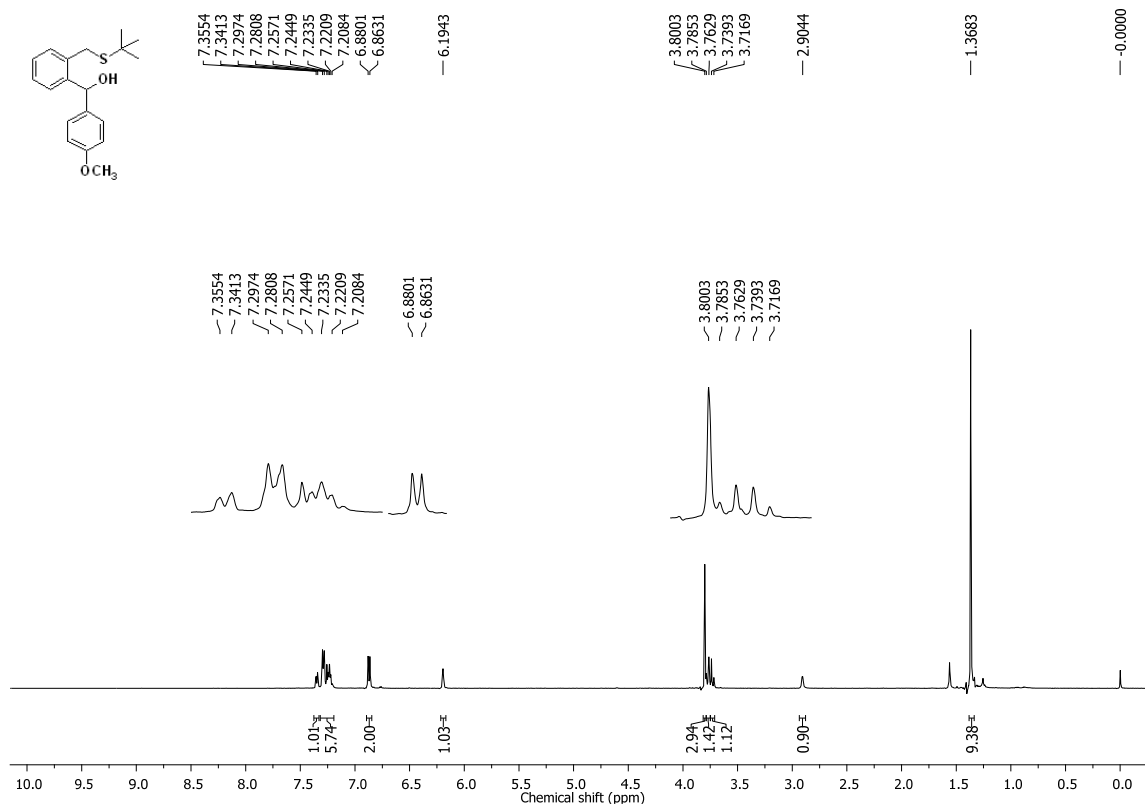


Figure S4. NMR spectra of **10f**

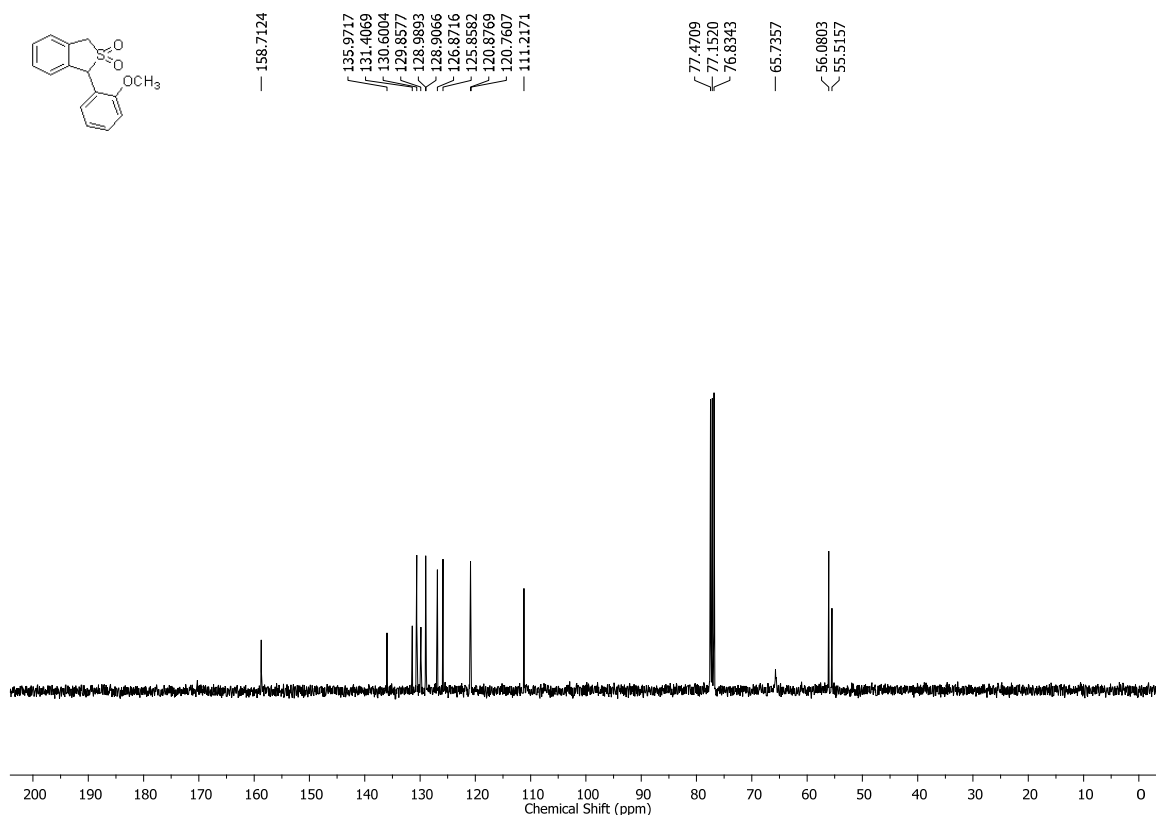
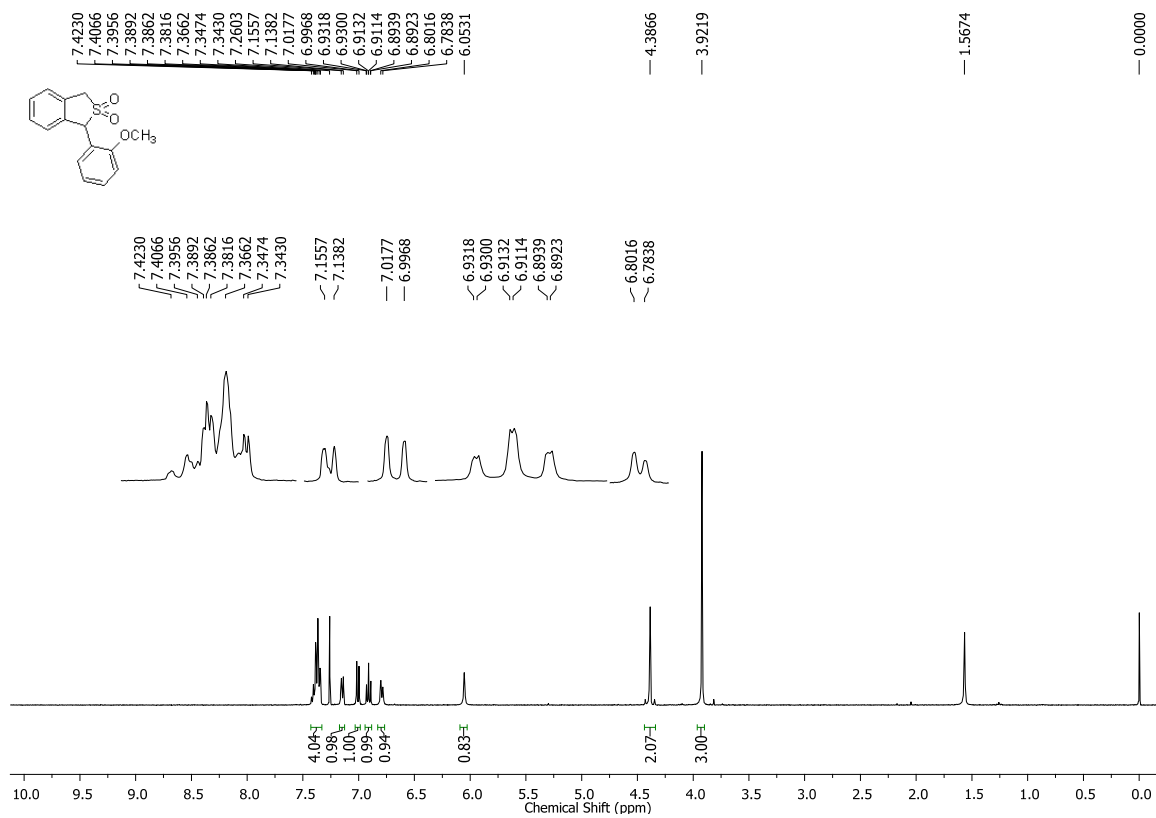


Figure S5. NMR spectra of **12b**

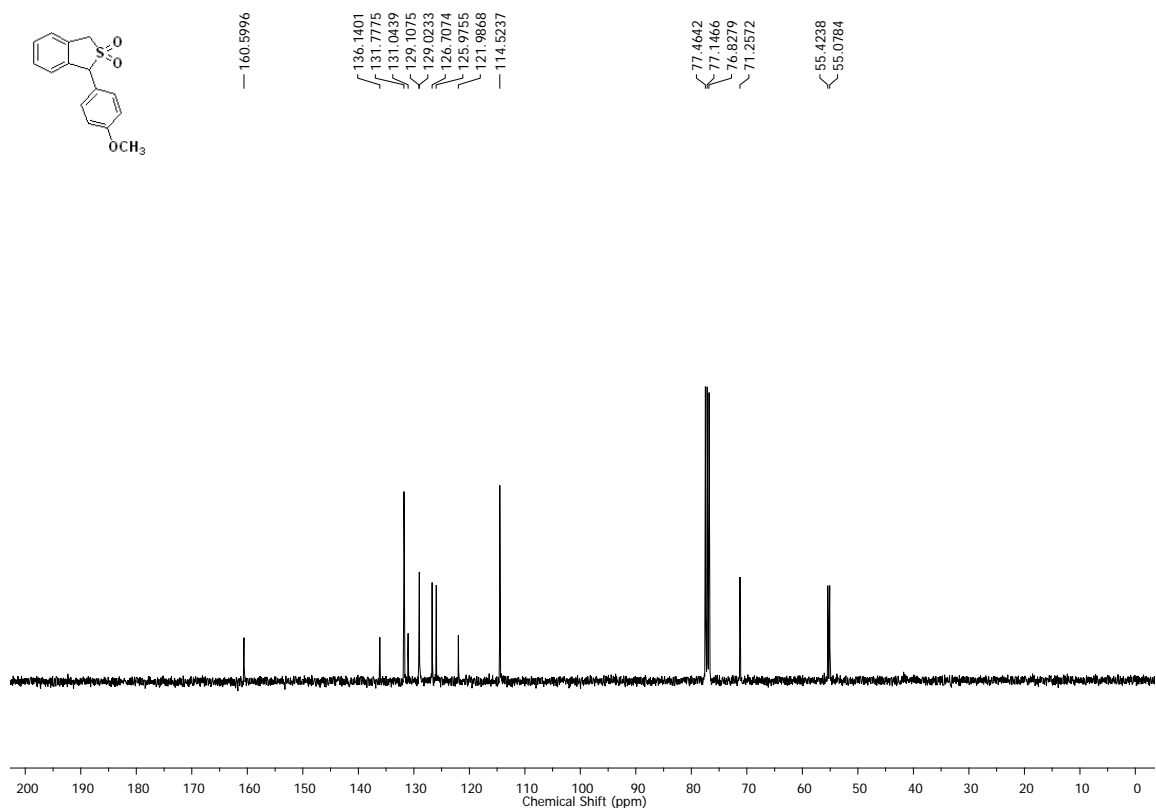
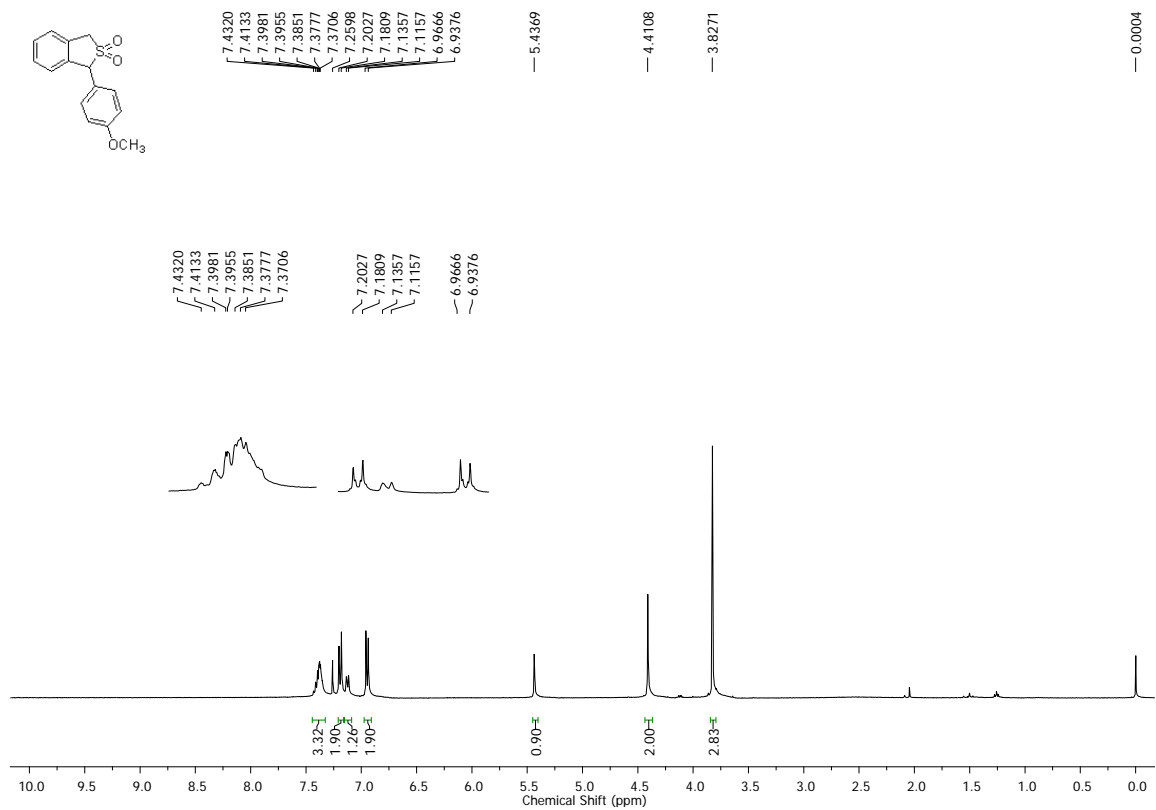


Figure S6. NMR spectra of **12f**

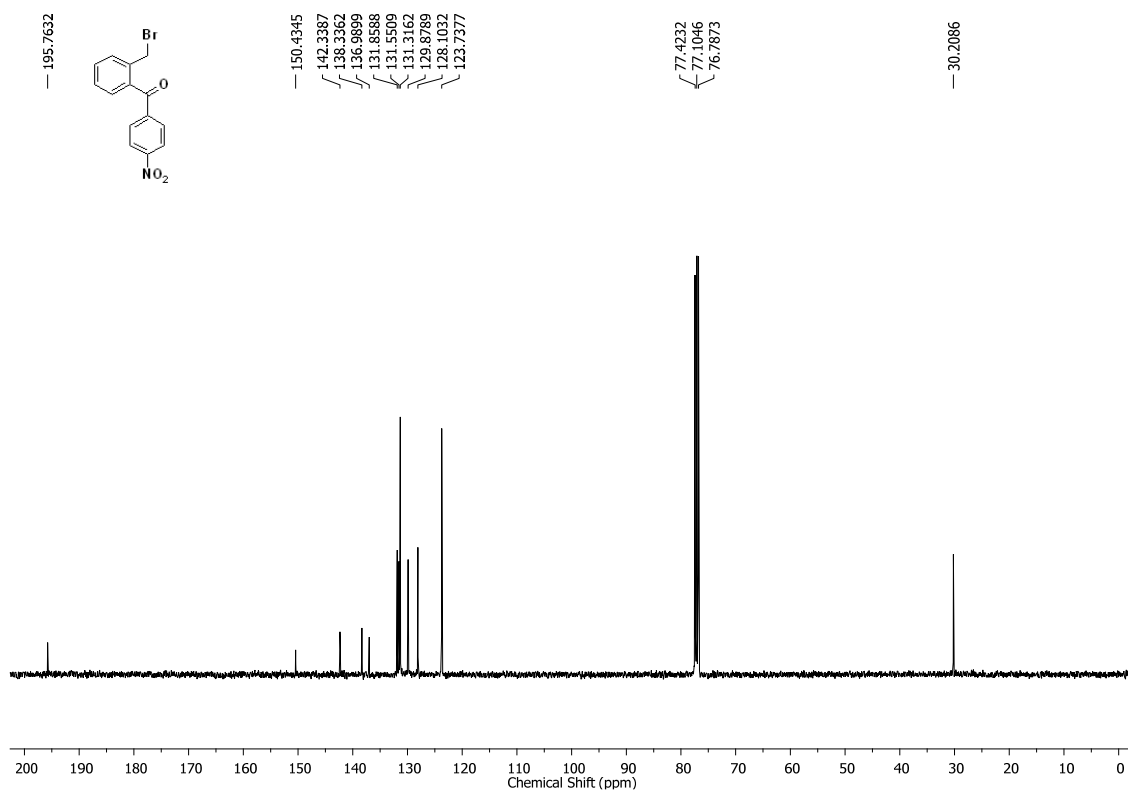
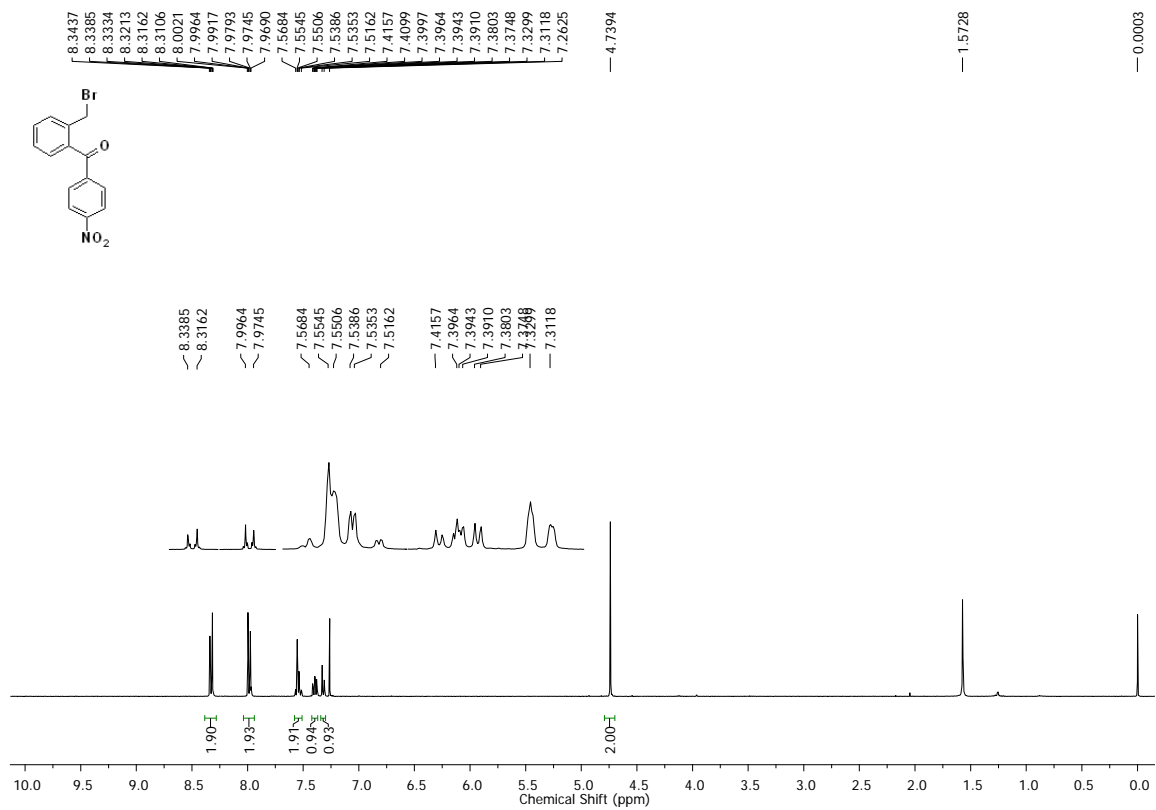


Figure S7. NMR spectra of **16**



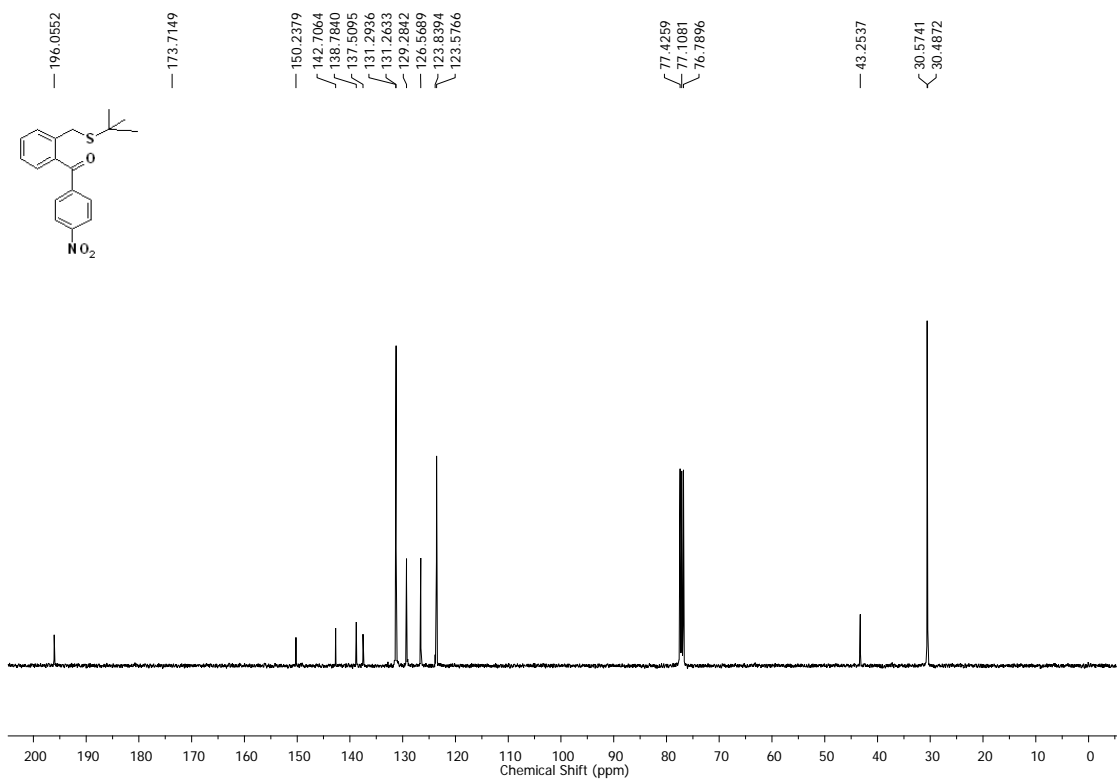
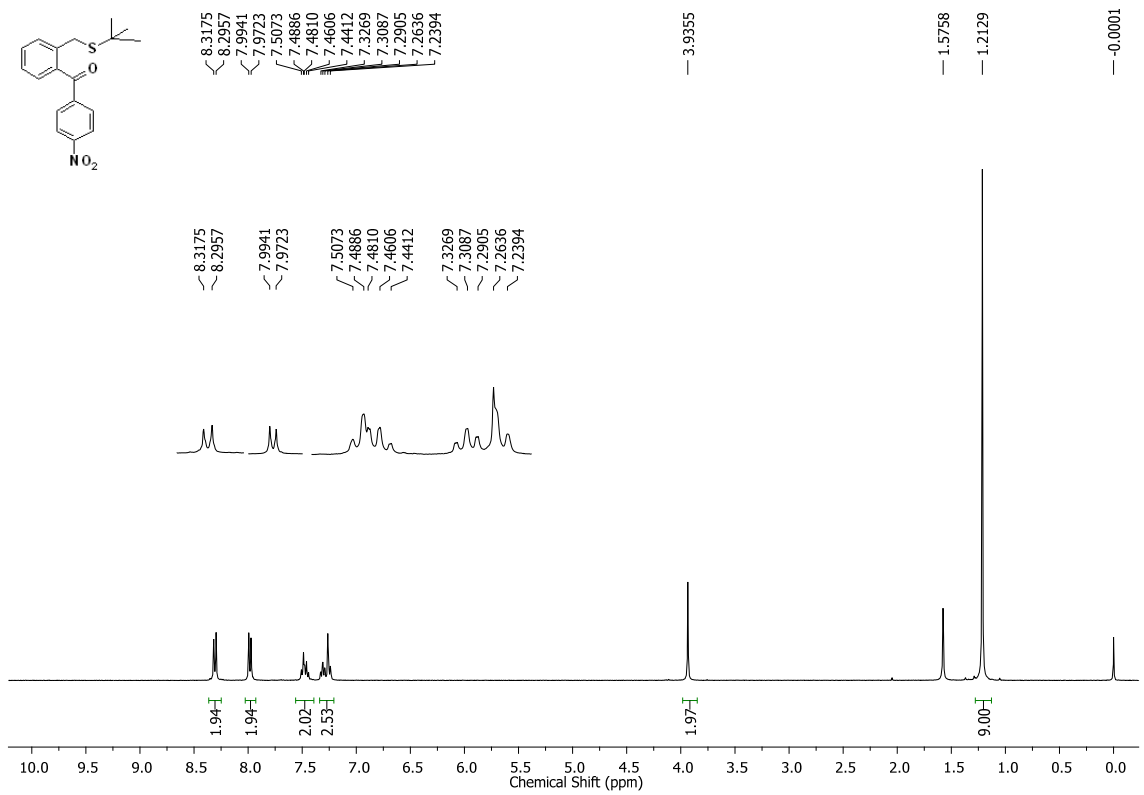


Figure S8. NMR spectra of **17**

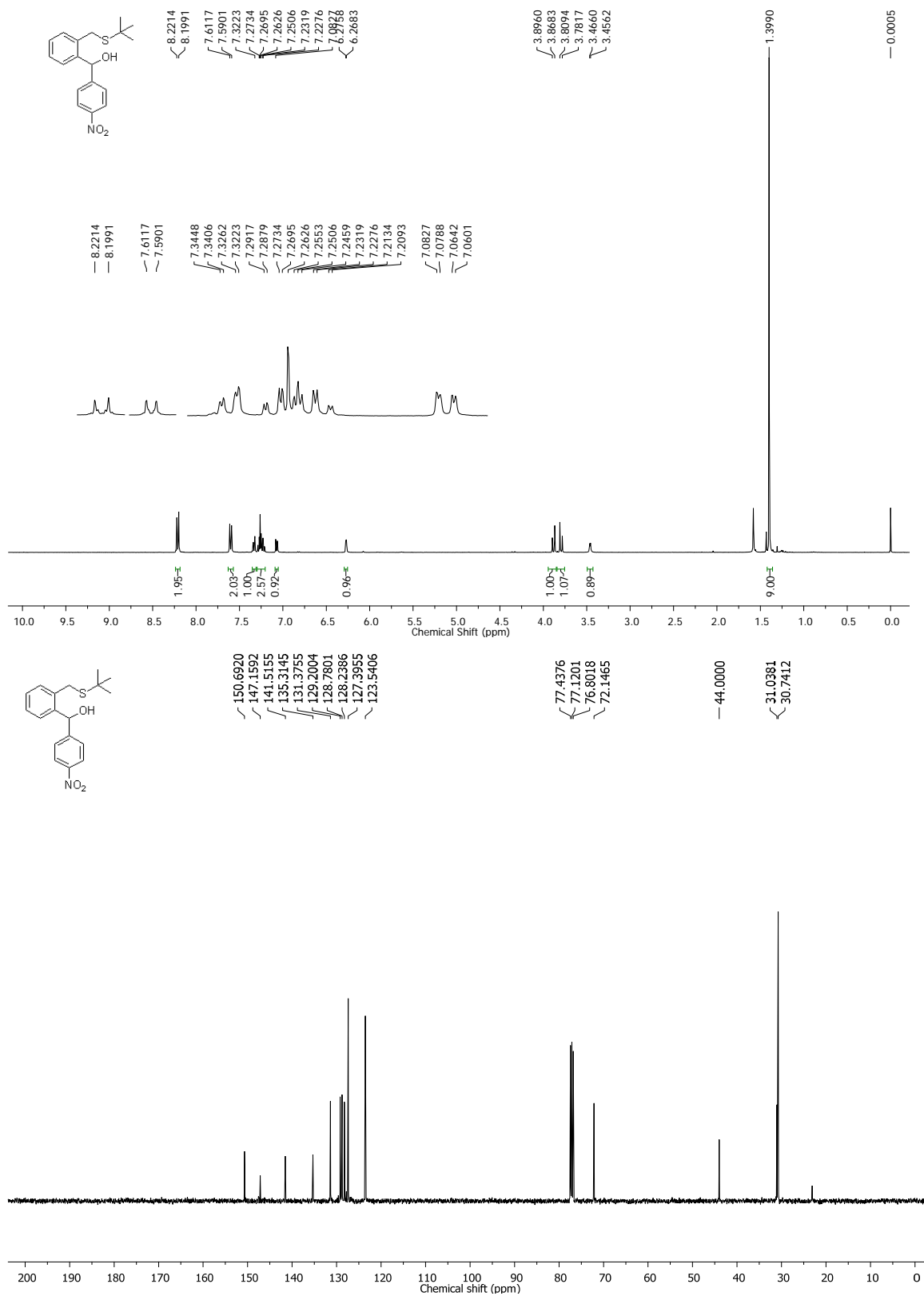


Figure S9. NMR spectra of **10j**

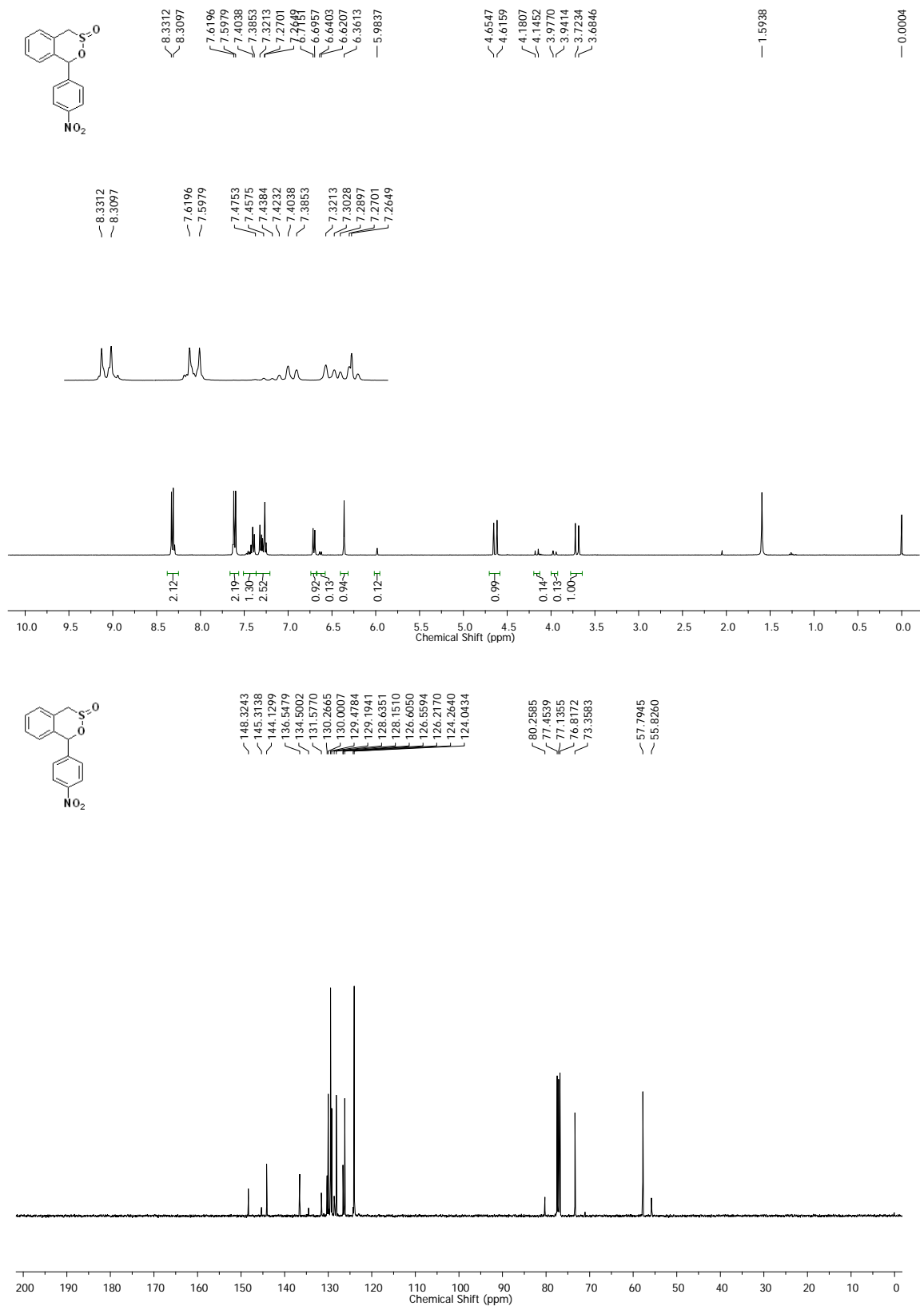


Figure S10. NMR spectra of 11j

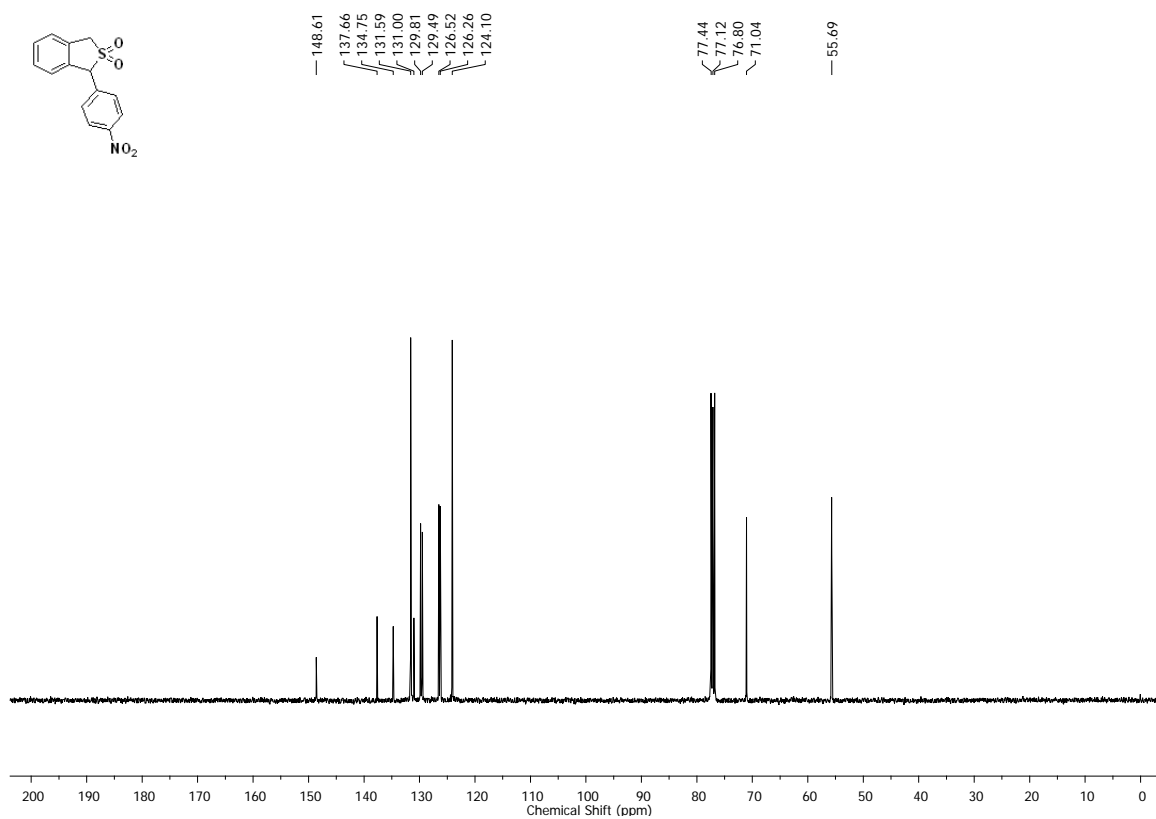
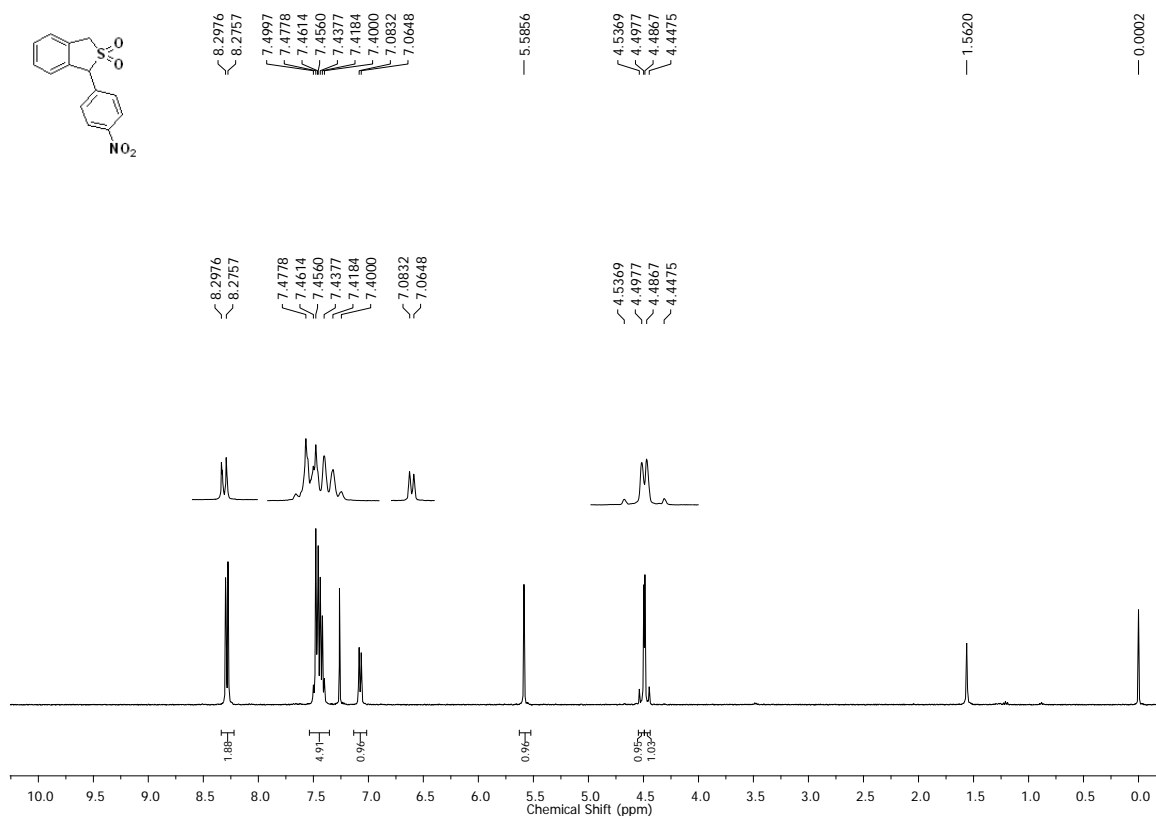


Figure S11. NMR spectra of 12j

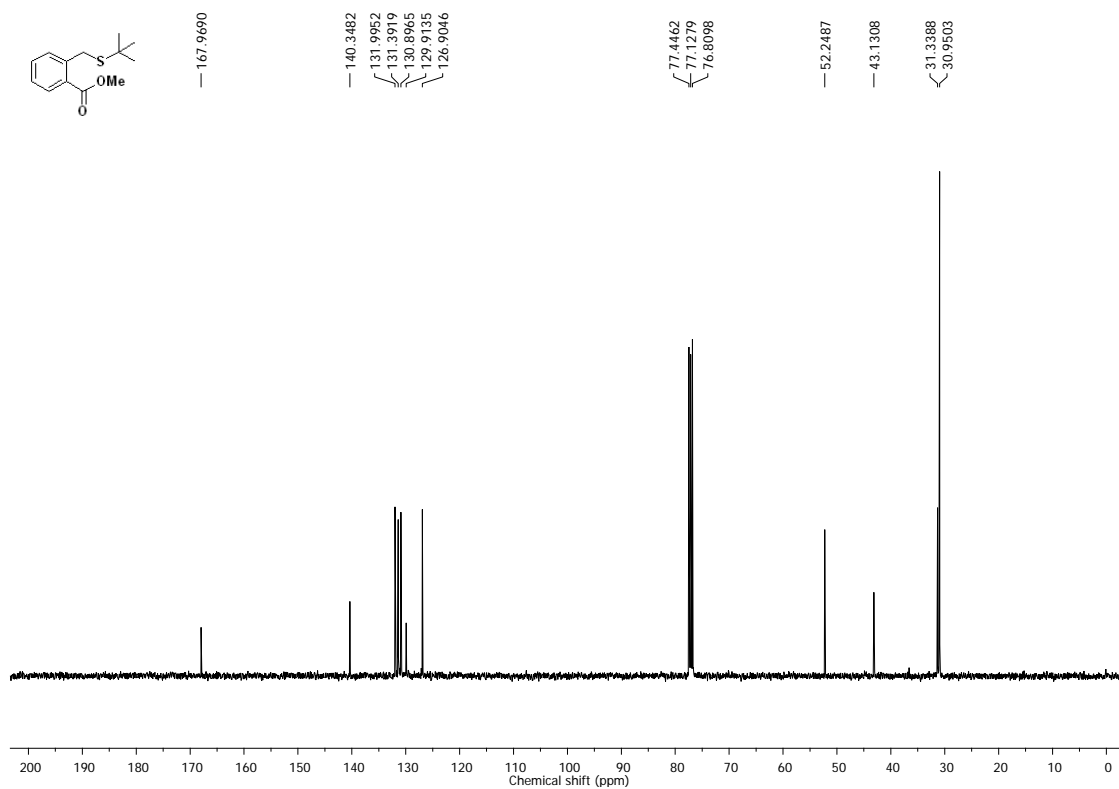
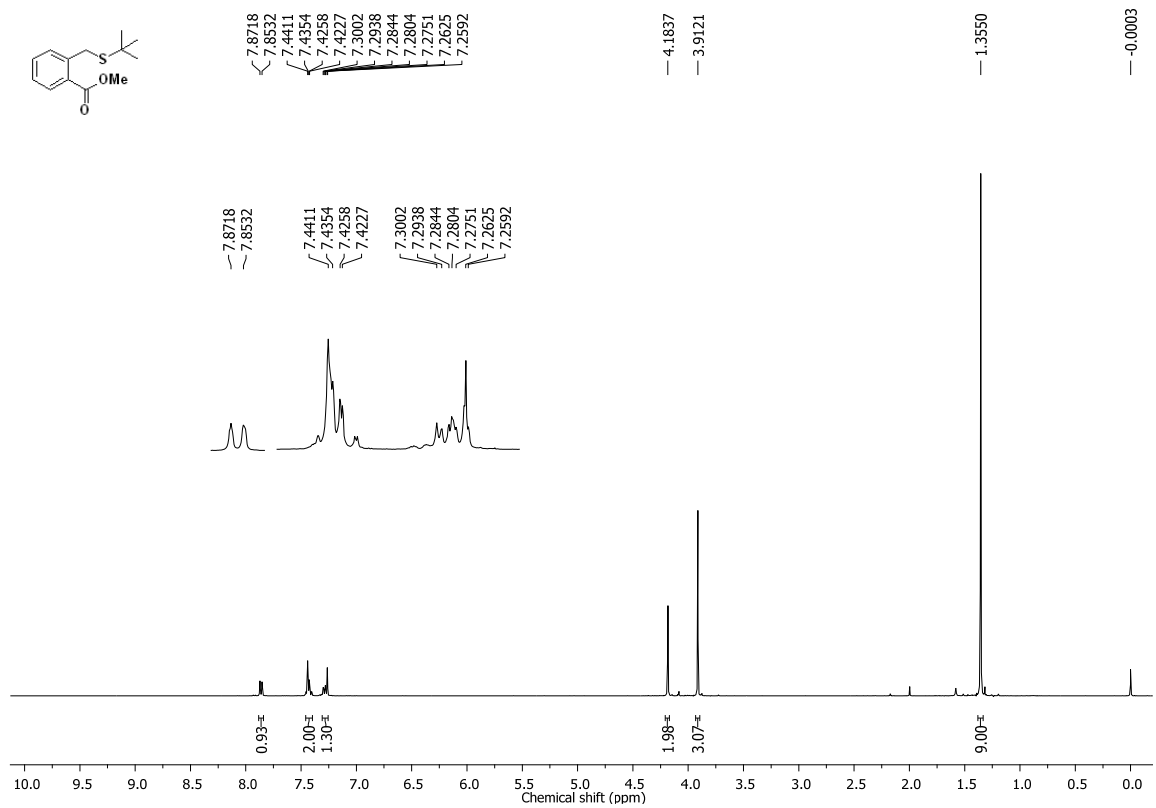


Figure S12. NMR spectra of **19**

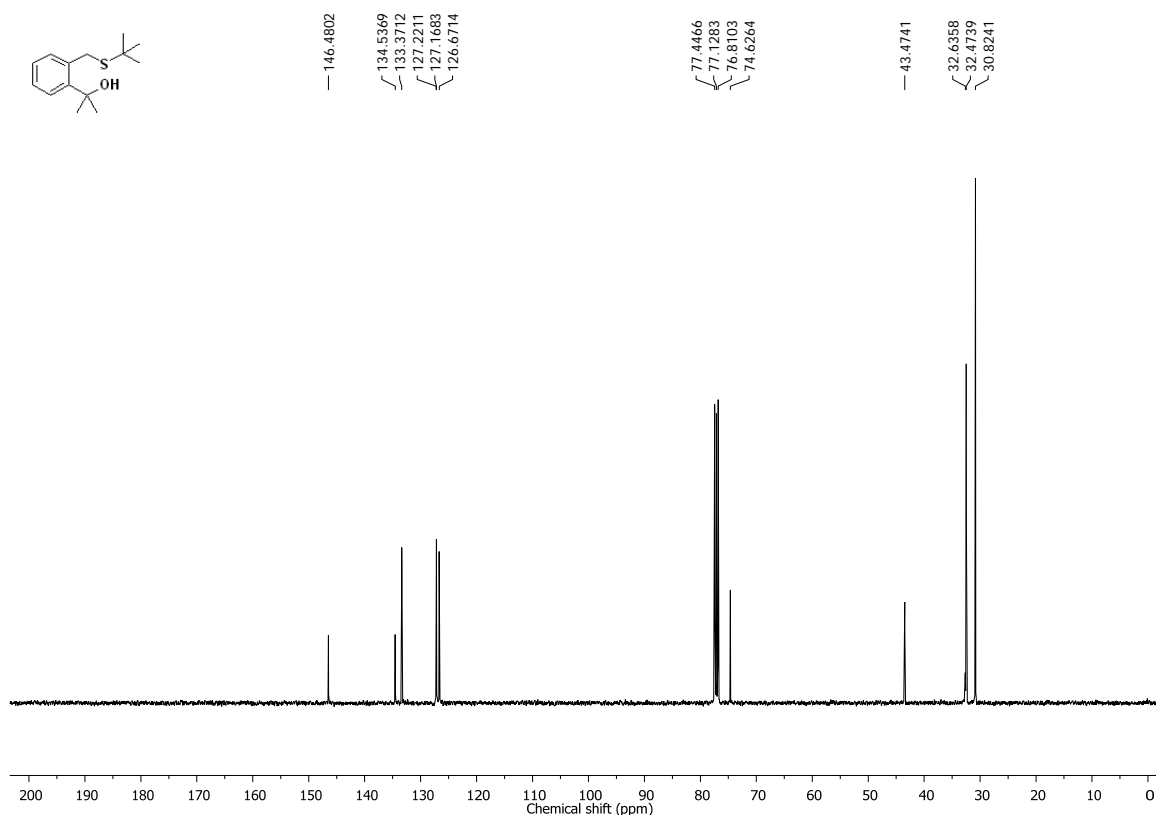
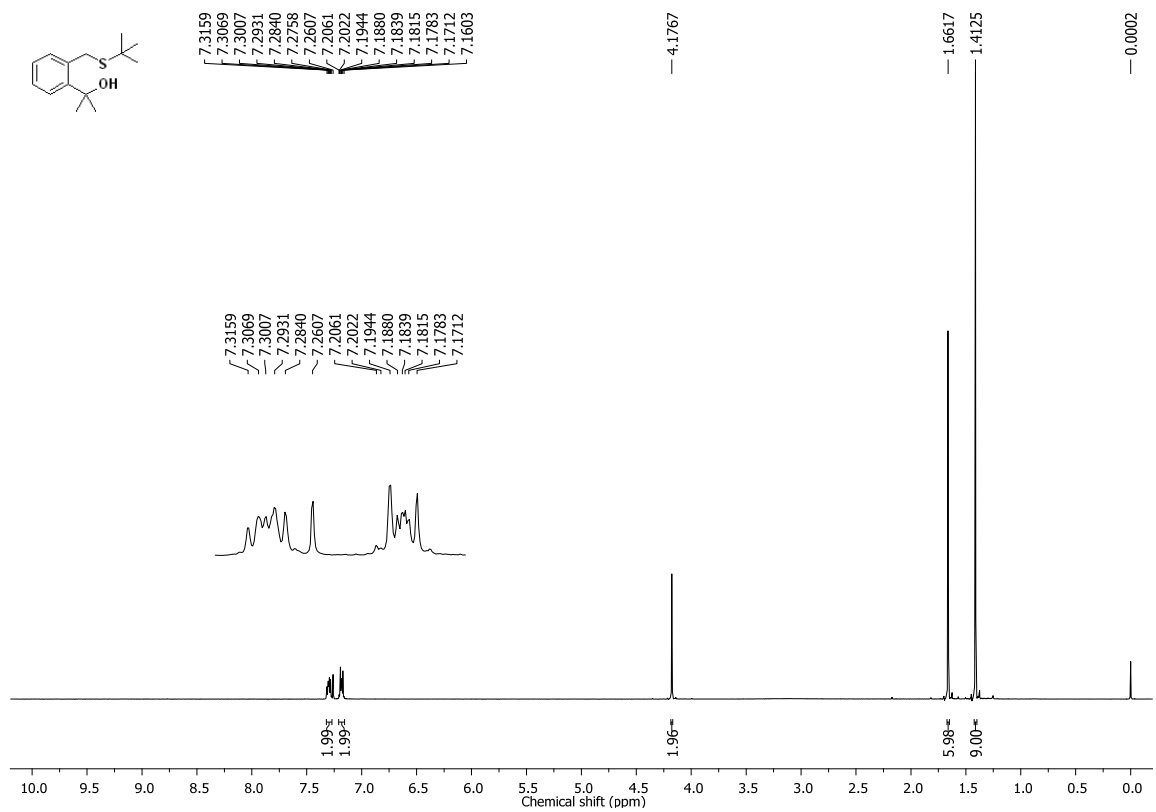
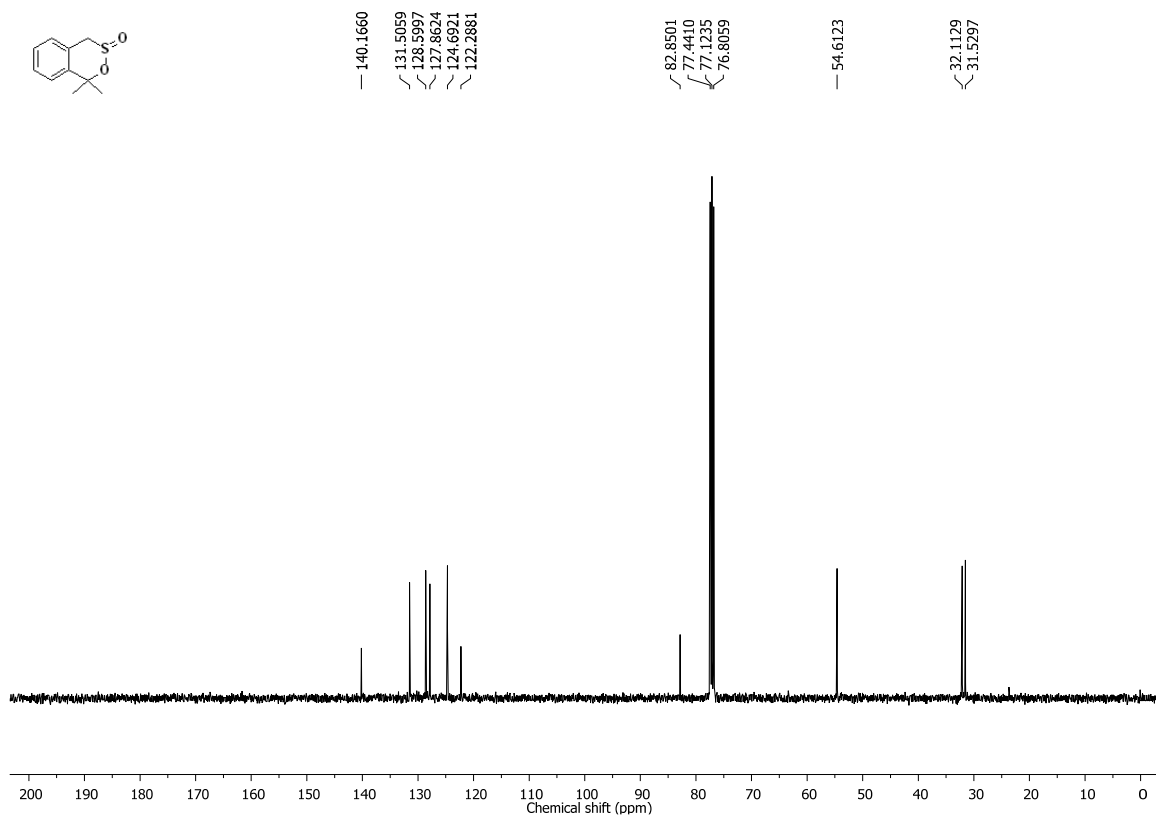
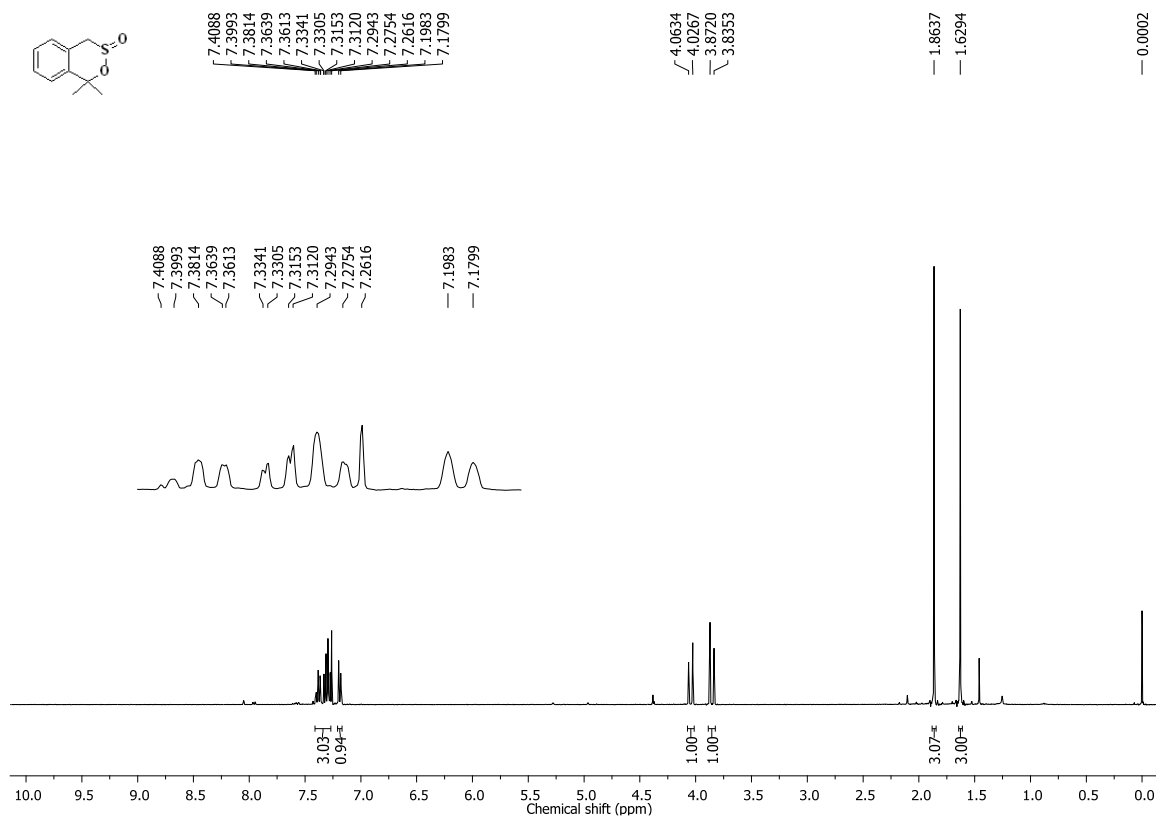


Figure S13. NMR spectra of **20**



**Figure S14.** NMR spectra of **21**

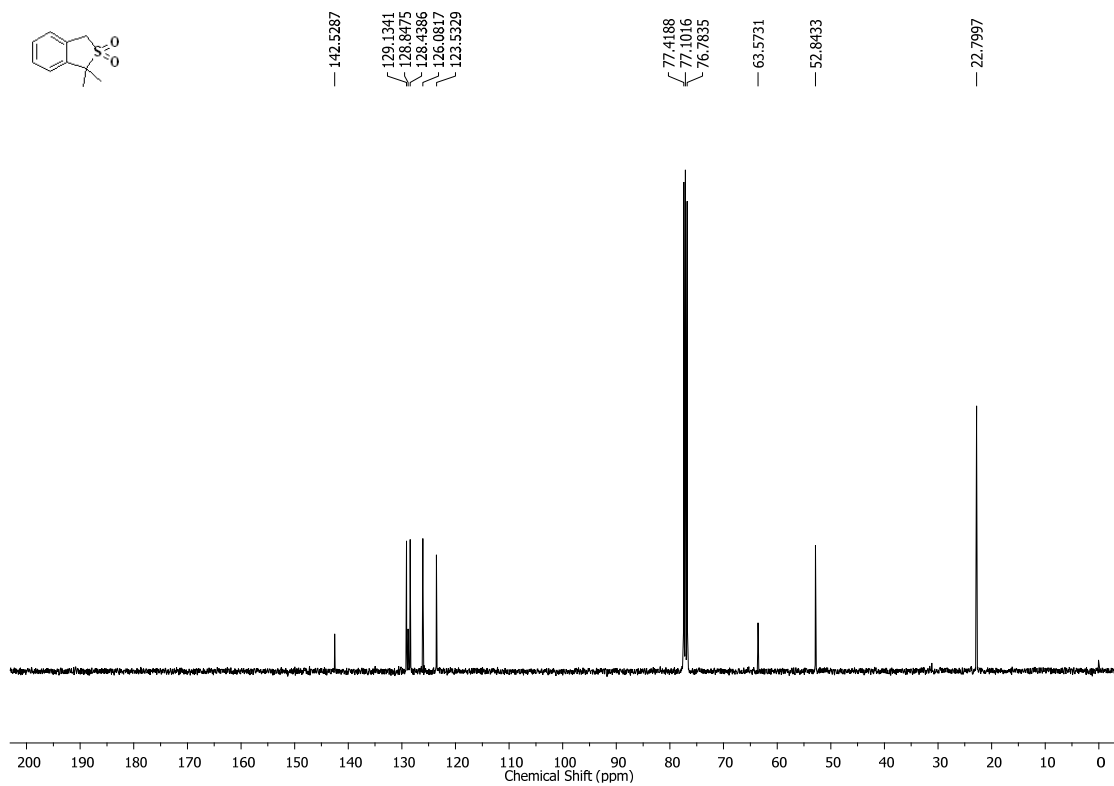
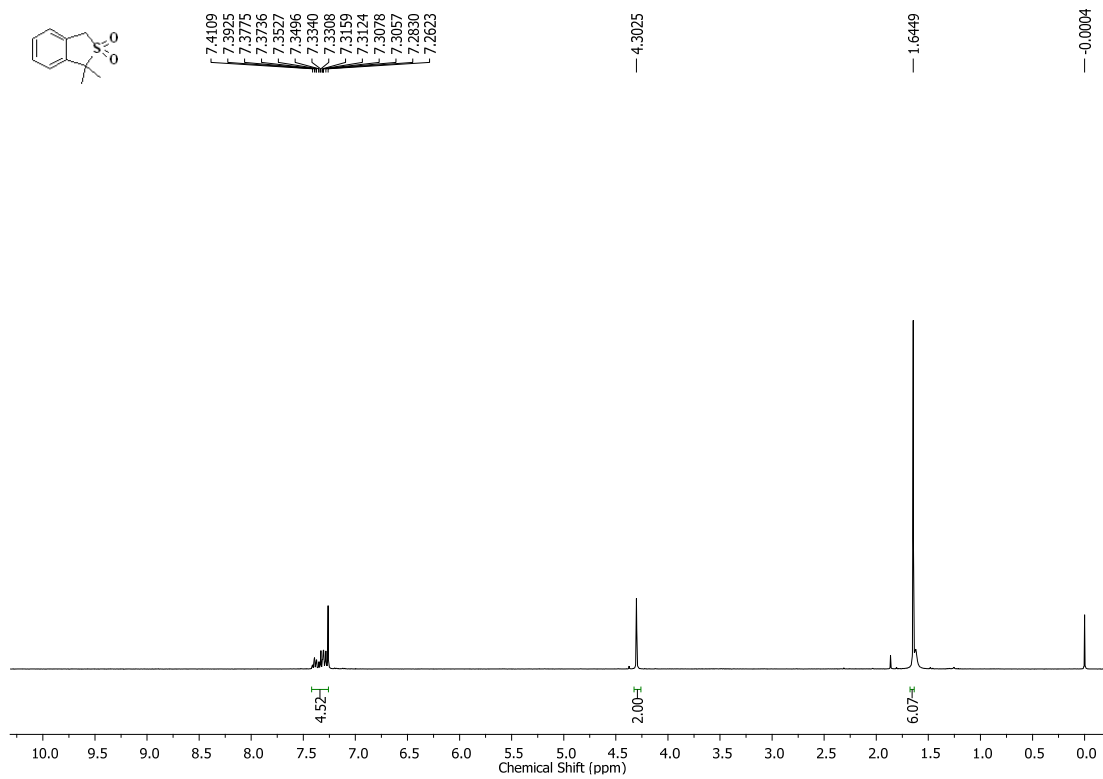


Figure S15. NMR spectra of 22