

Electronic Supplementary Information for

An aza-Diels–Alder approach to nitrogen-containing tetrabenzoacene derivatives

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Table of Contents:

I.	¹ H NMR and ¹³ C NMR Spectroscopy Data	S-2
II.	UV-Vis Spectroscopy Data	S-40

I. ^1H NMR and ^{13}C NMR Spectroscopy Data

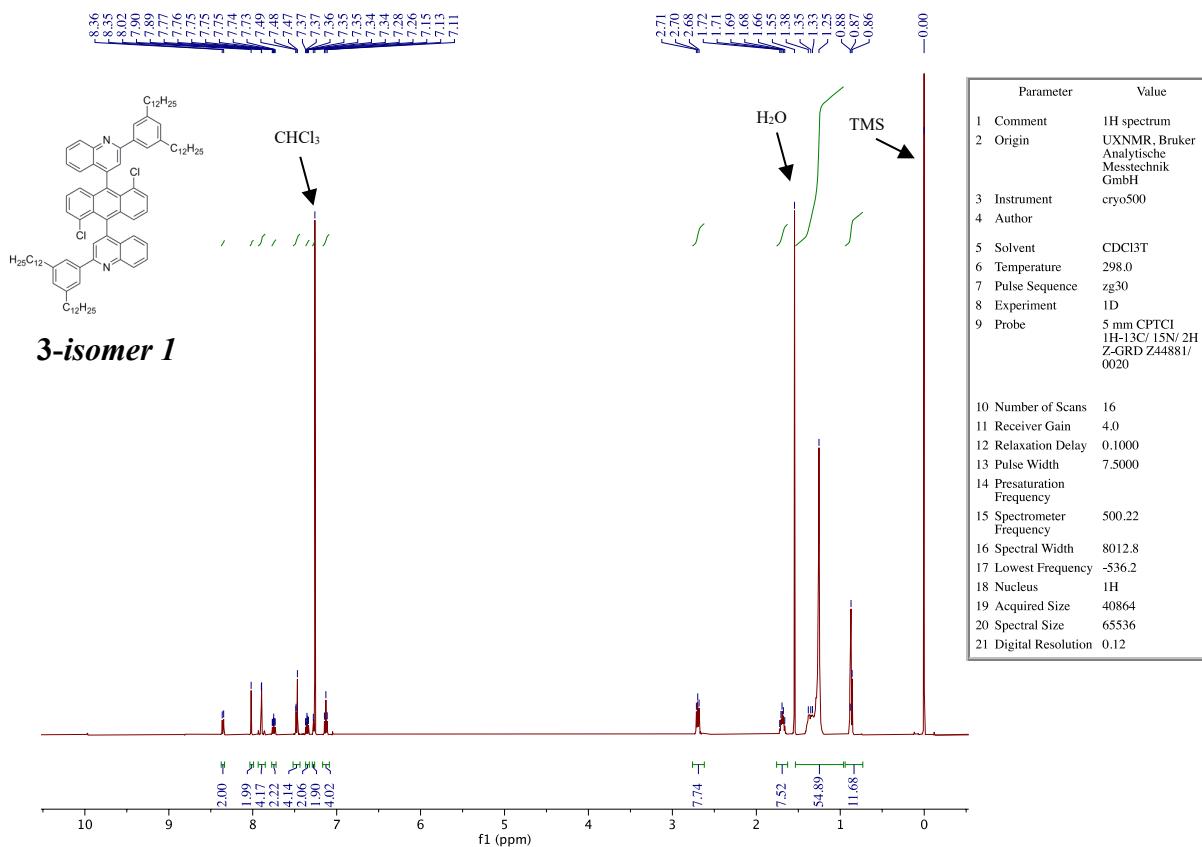


Figure S1. The ^1H NMR spectrum obtained for **3-isomer 1**.

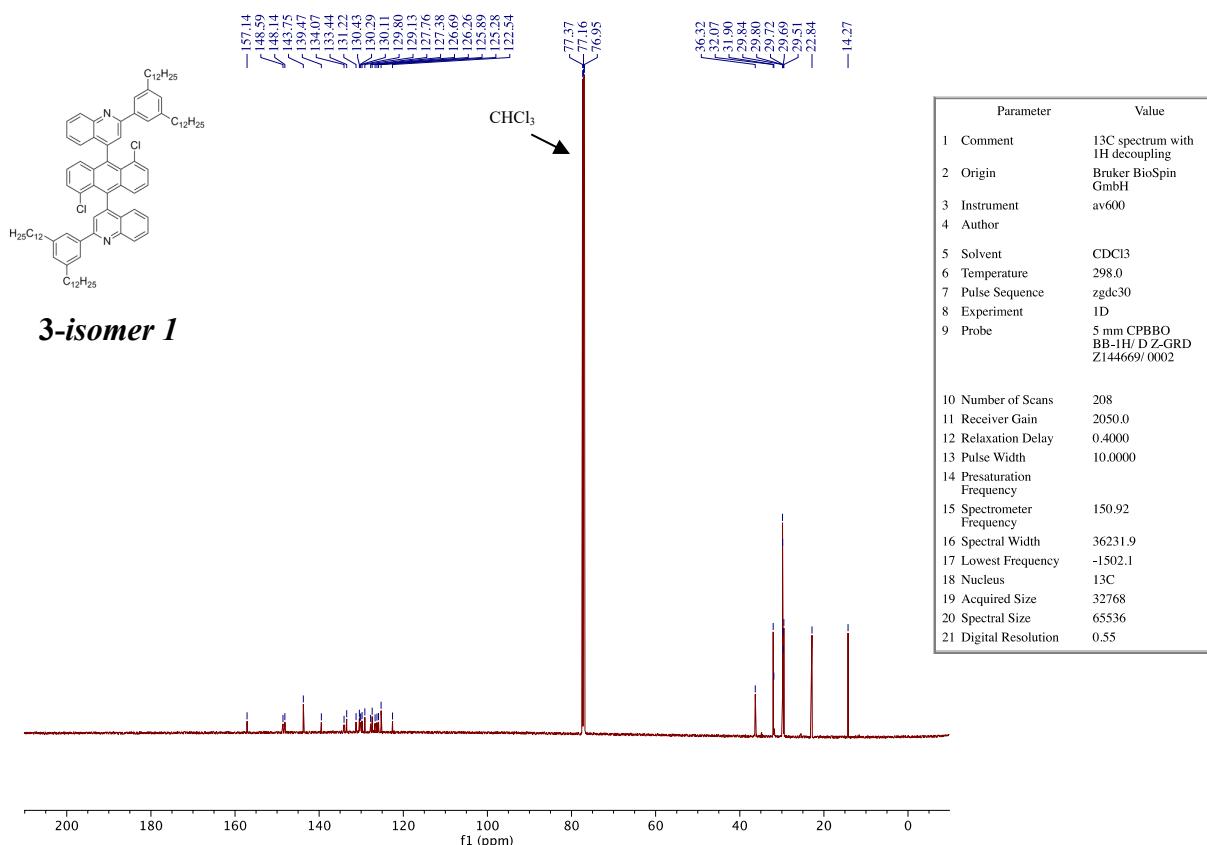


Figure S2. The ¹³C NMR spectrum obtained for **3-isomer 1**.

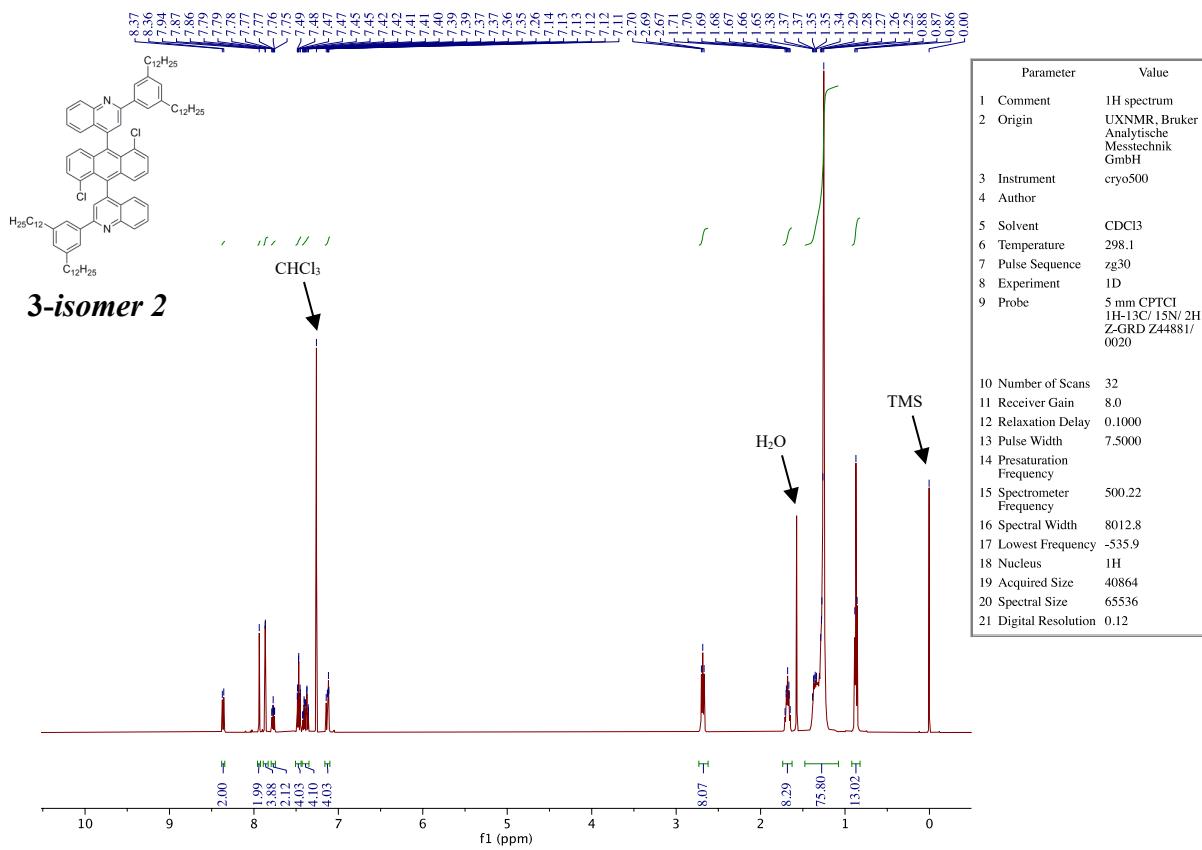


Figure S3. The ¹H NMR spectrum obtained for 3-isomer 2.

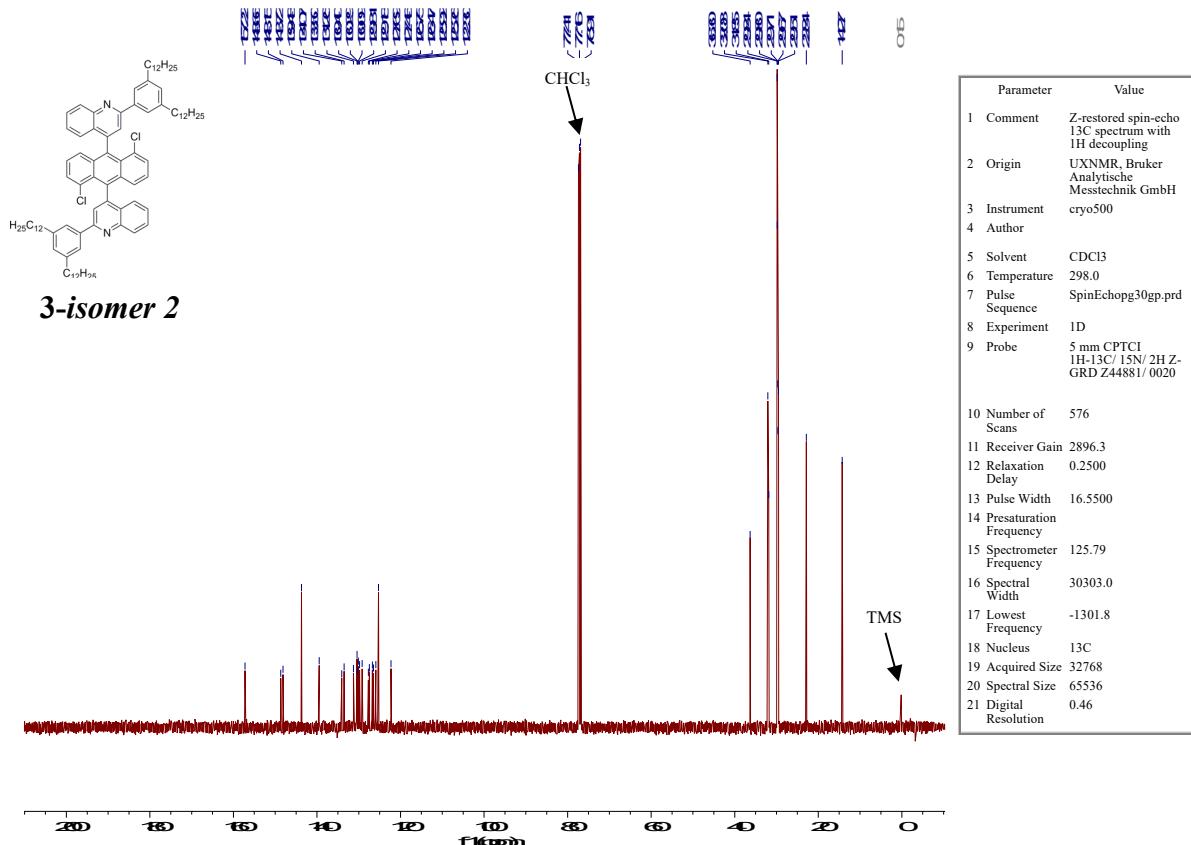


Figure S4. The ^{13}C NMR spectrum obtained for **3-isomer 2**.

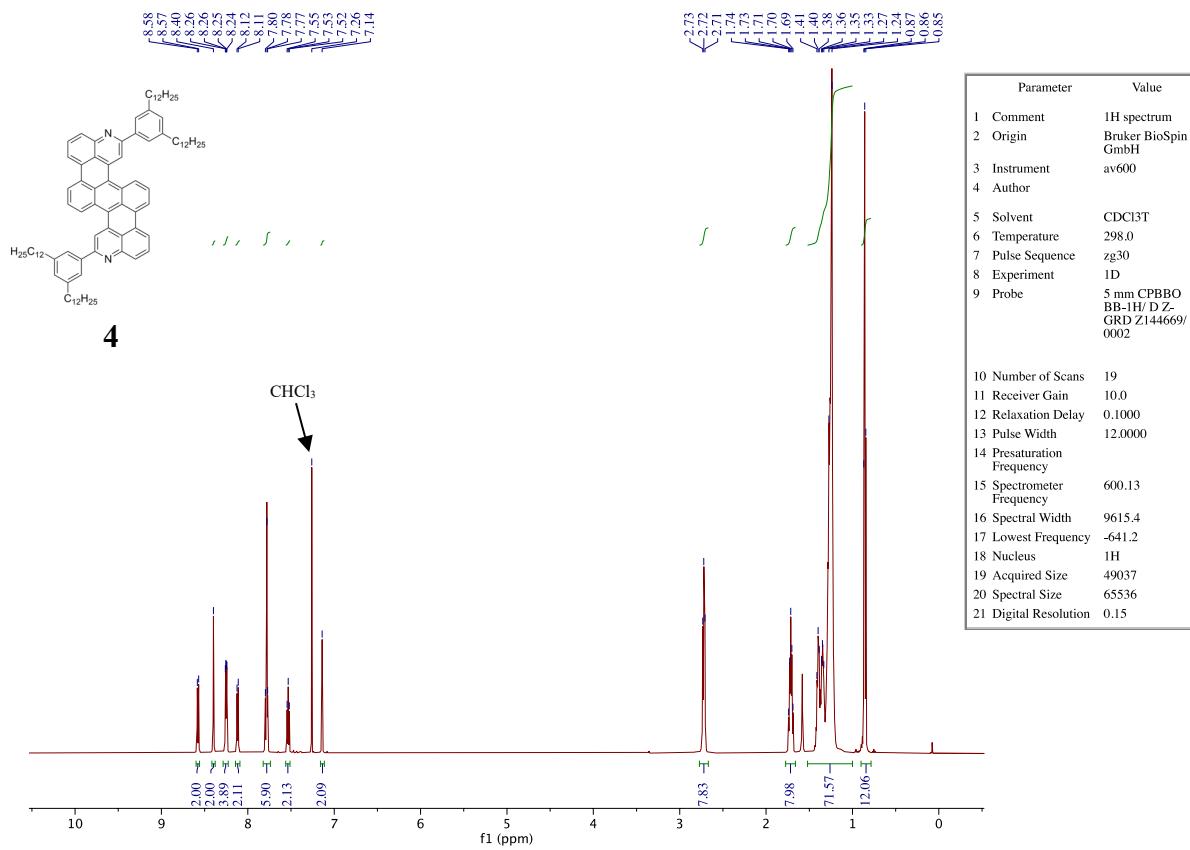


Figure S5. The ^1H NMR spectrum obtained for **4**.

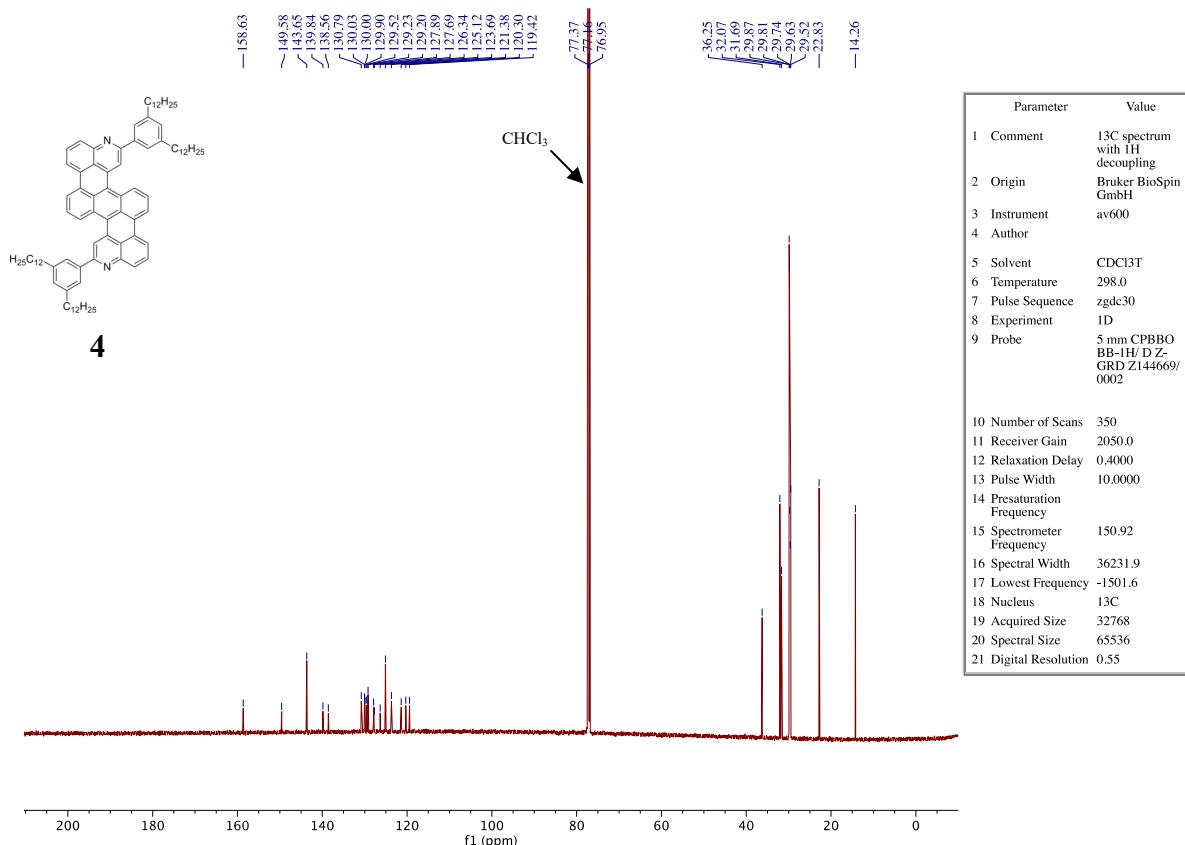


Figure S6. The ¹³C NMR spectrum obtained for 4.

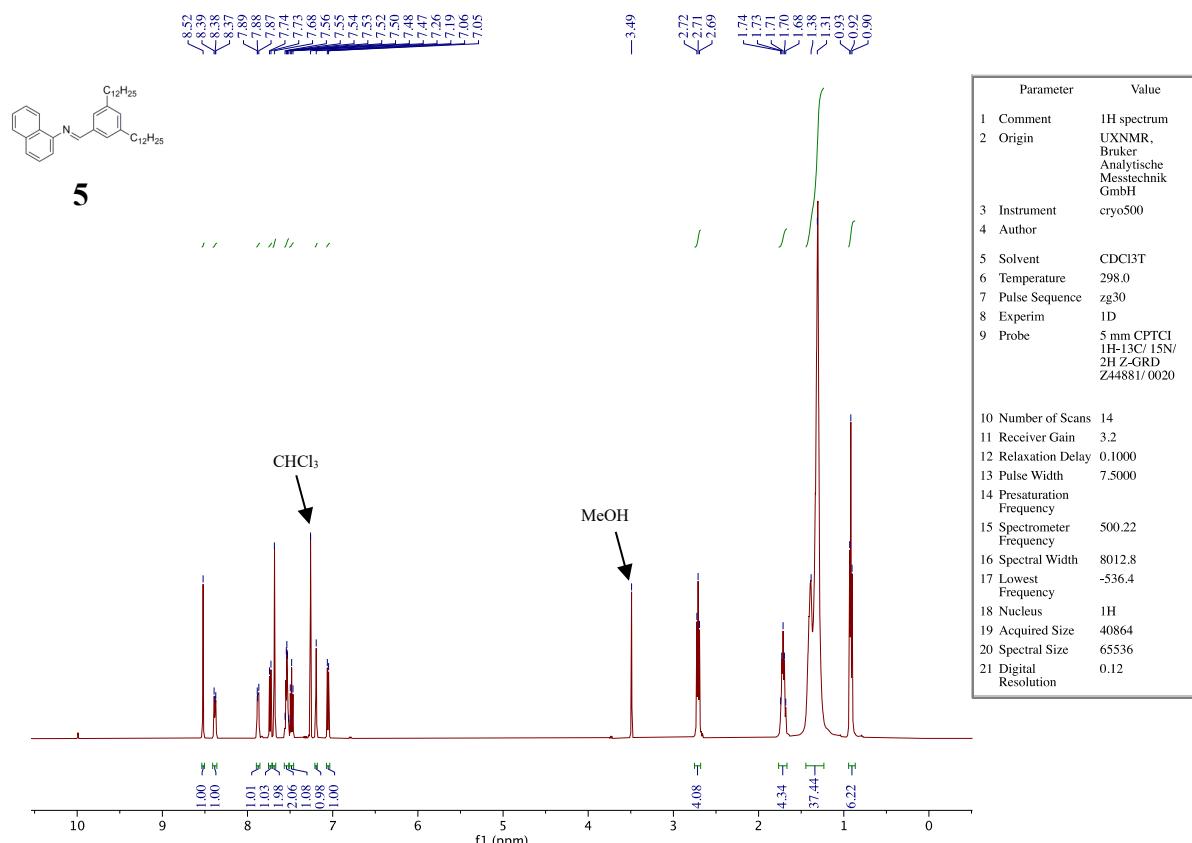


Figure S7. The ¹H NMR spectrum obtained for **5**.

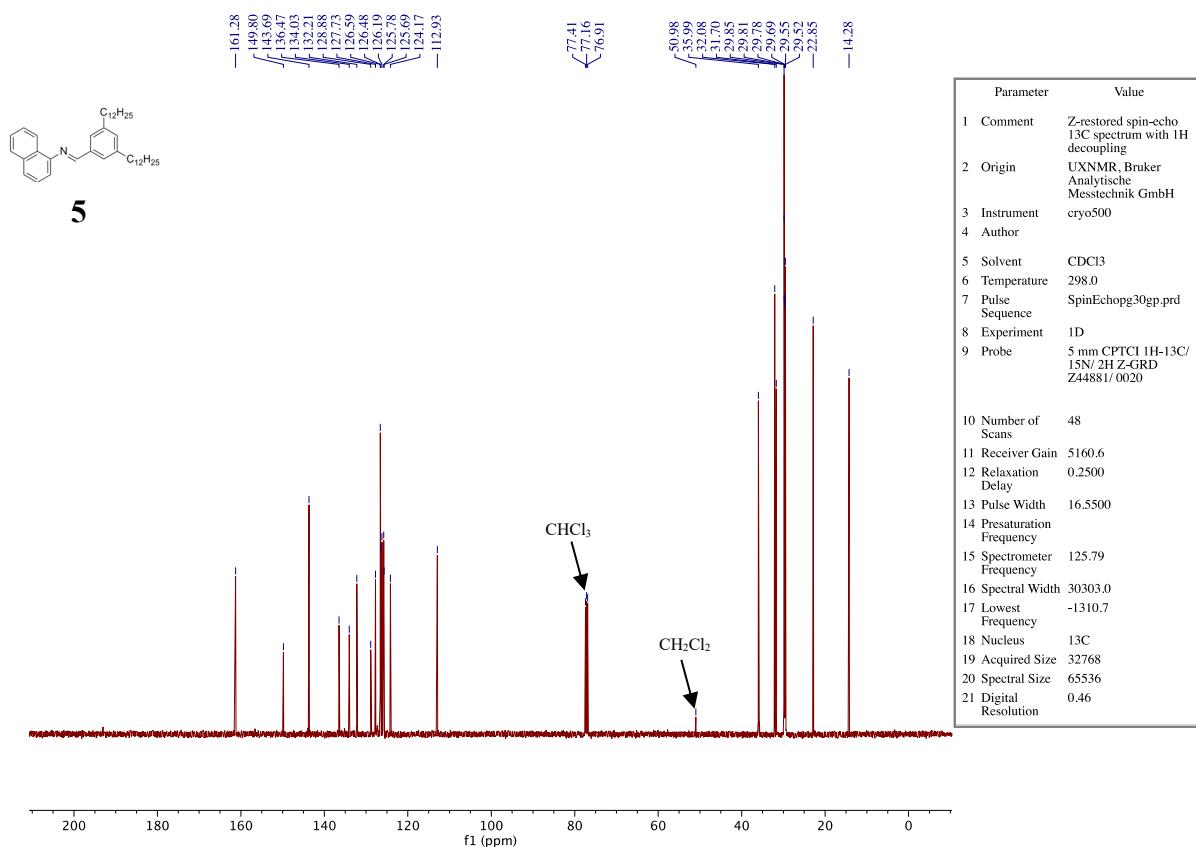


Figure S8. The ^{13}C NMR spectrum obtained for **5**.

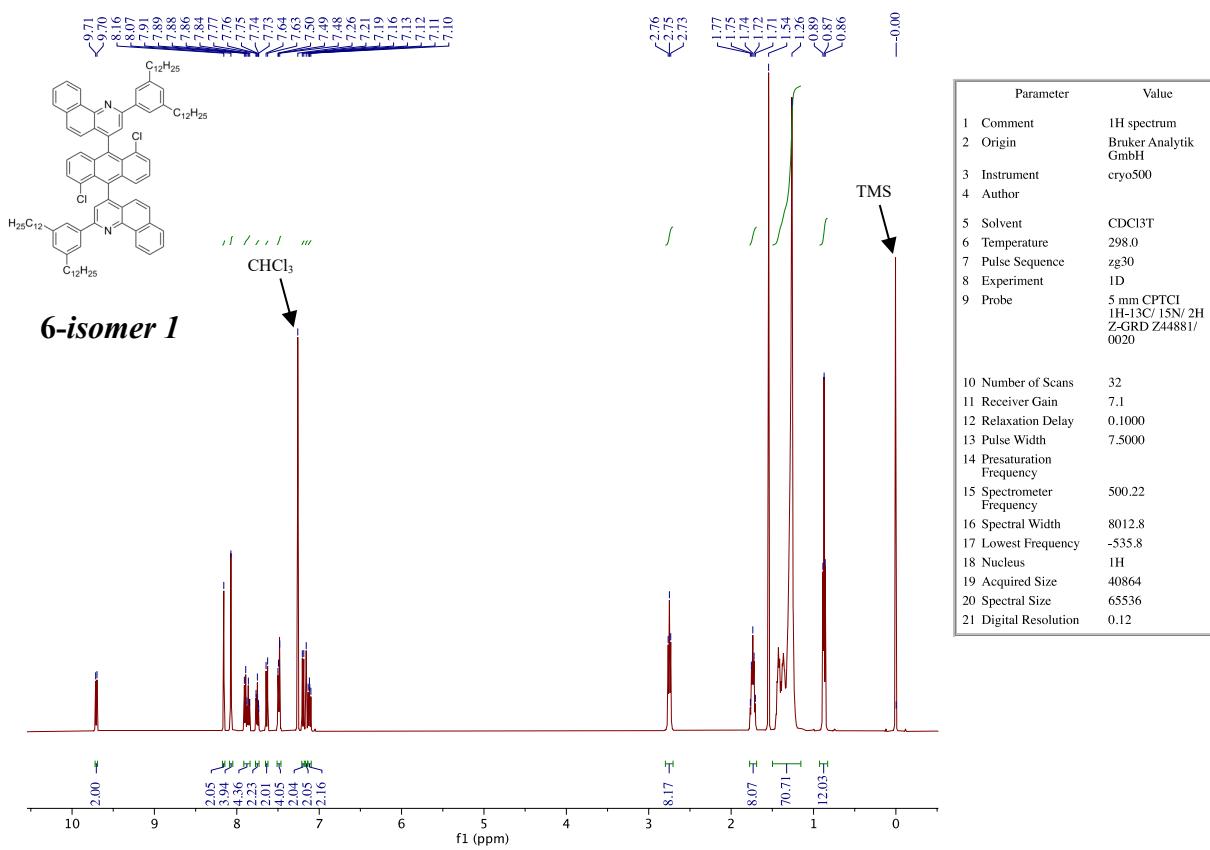


Figure S9. The ^1H NMR spectrum obtained for **6-isomer 1**.

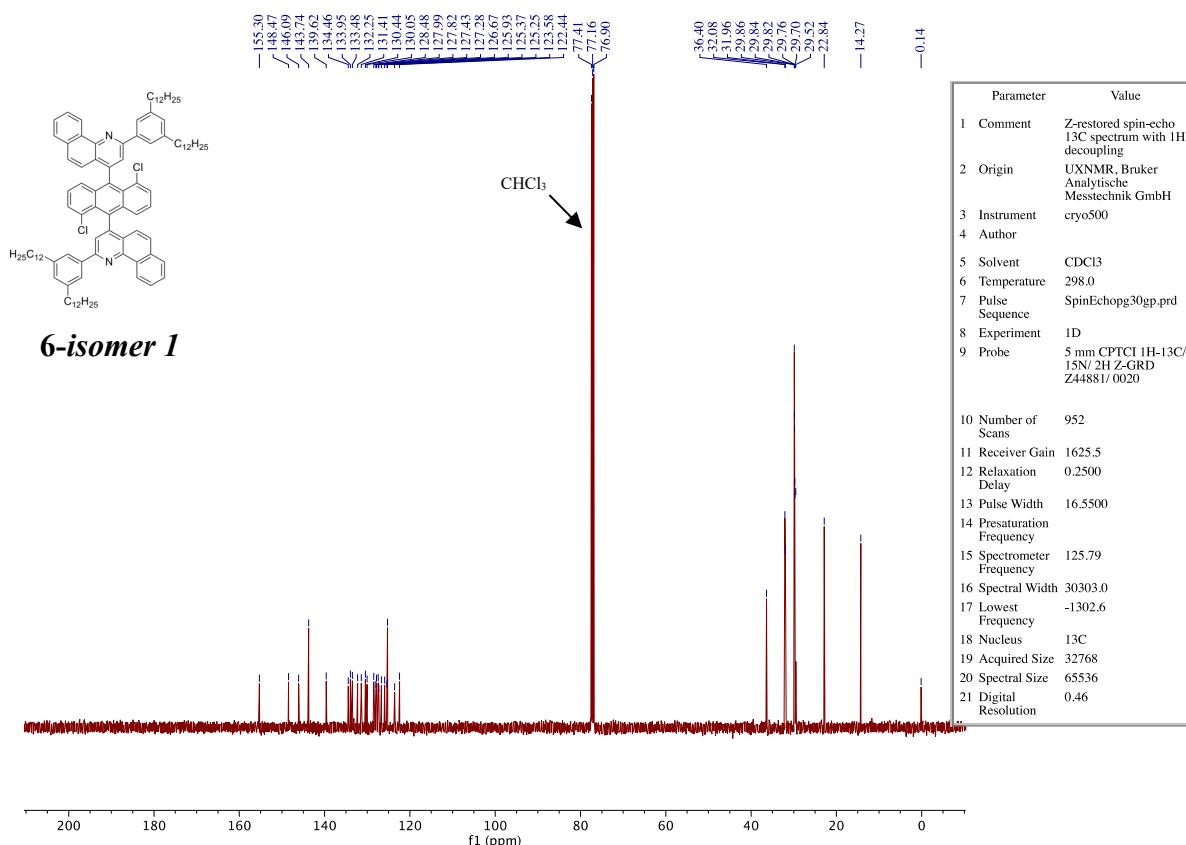


Figure S10. The ^{13}C NMR spectrum obtained for **6-isomer 1**.

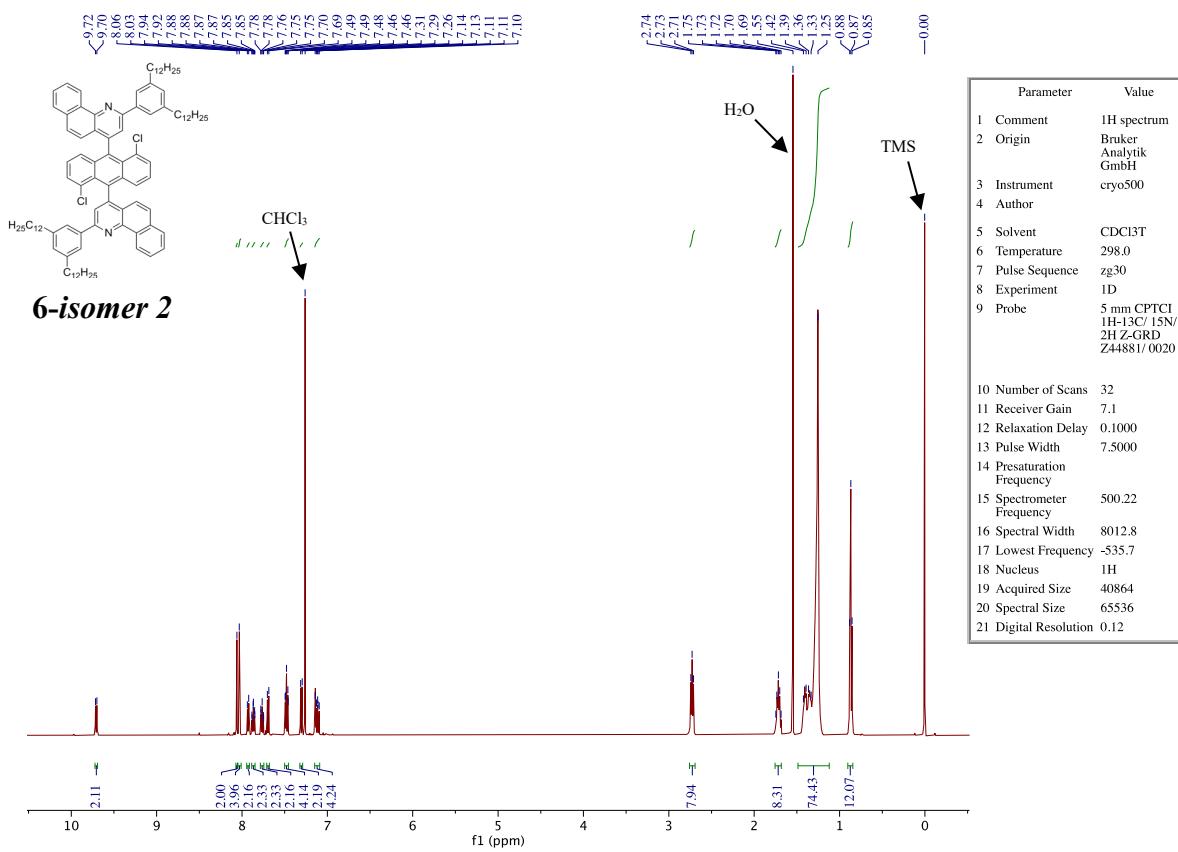


Figure S11. The ¹H NMR spectrum obtained for **6-isomer 2**.

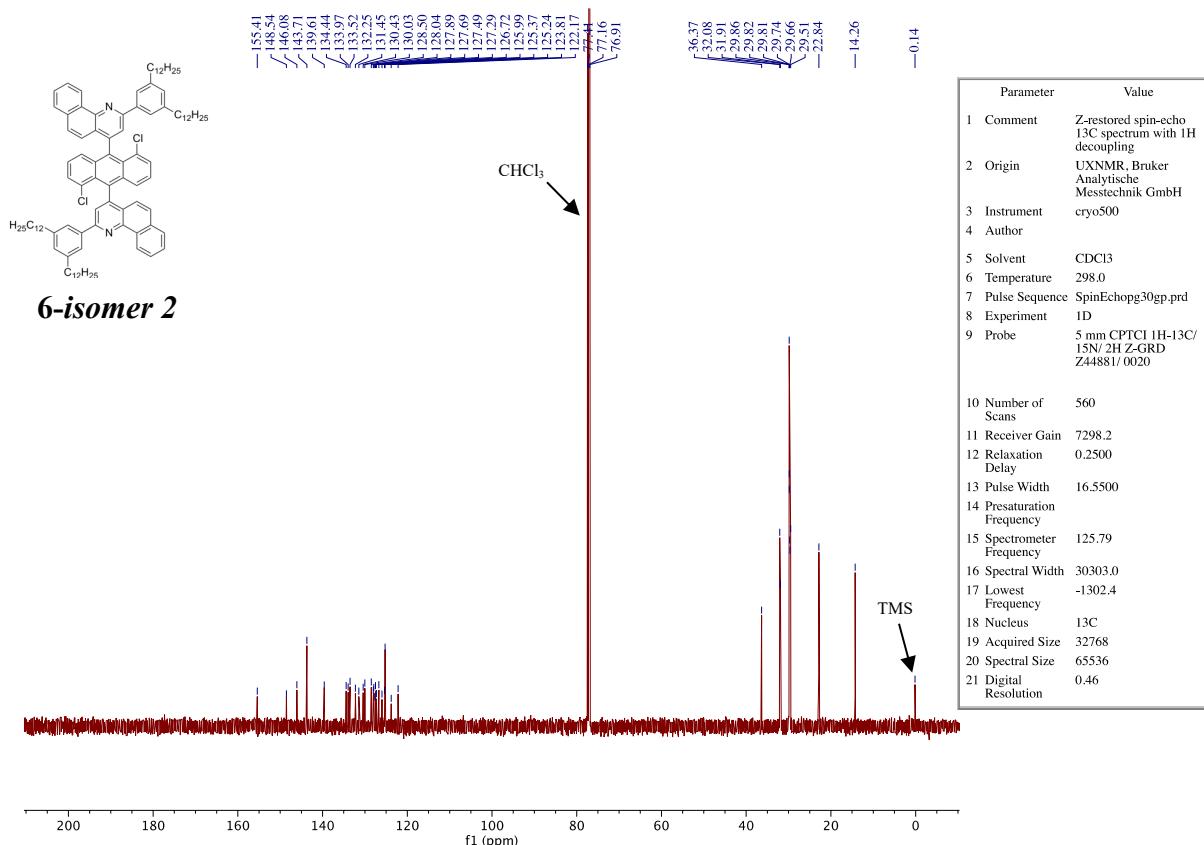


Figure S12. The ¹³C NMR spectrum obtained for **6-isomer 2**.

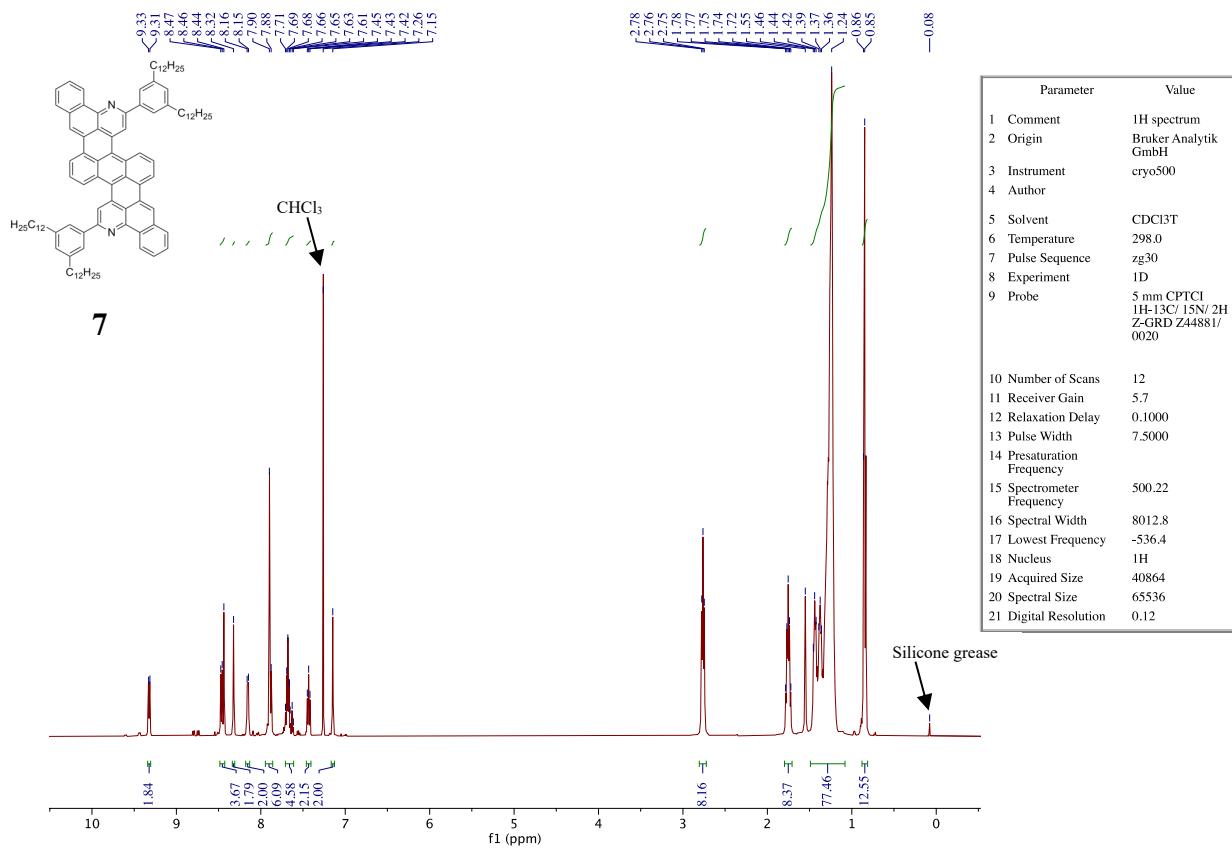


Figure S13. The ^1H NMR spectrum obtained for 7.

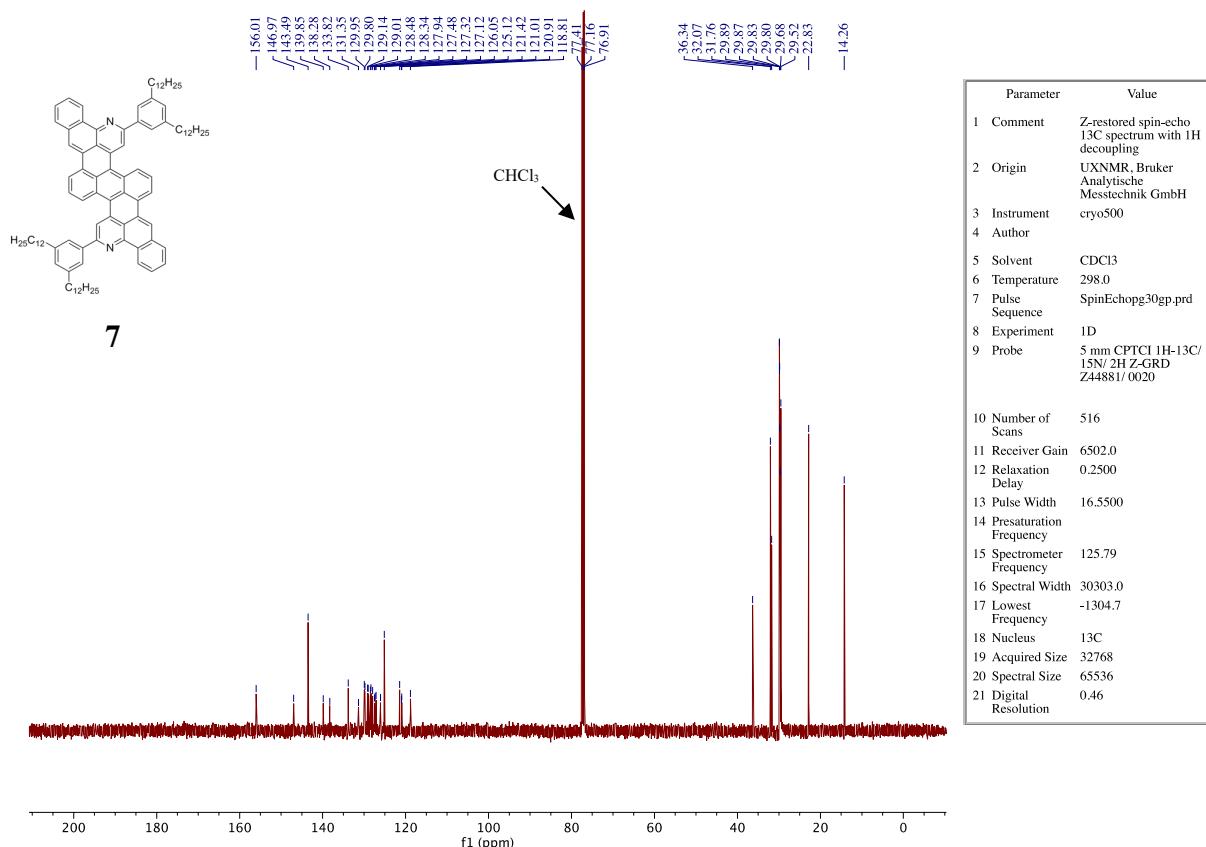


Figure S14. The ¹³C NMR spectrum obtained for 7.

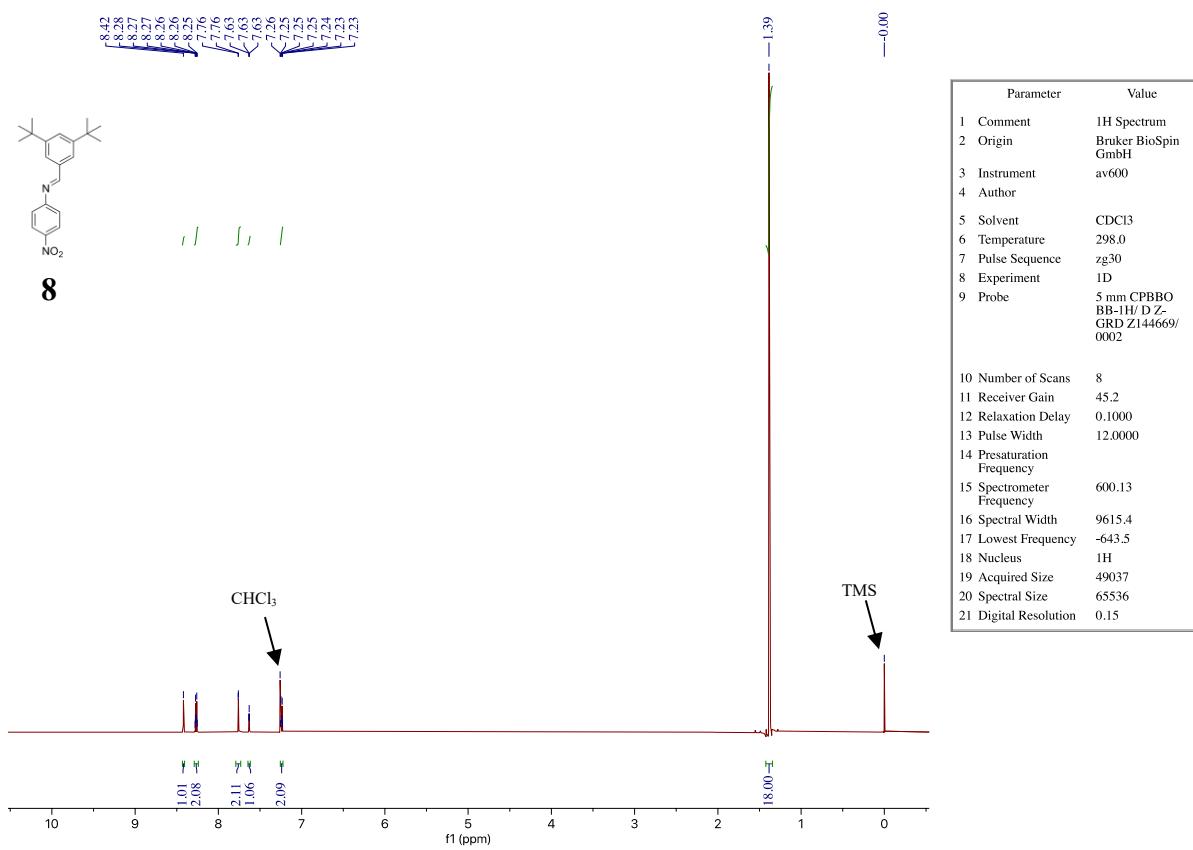
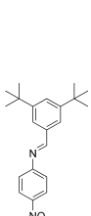


Figure S15. The ¹H NMR spectrum obtained for **8**.



8

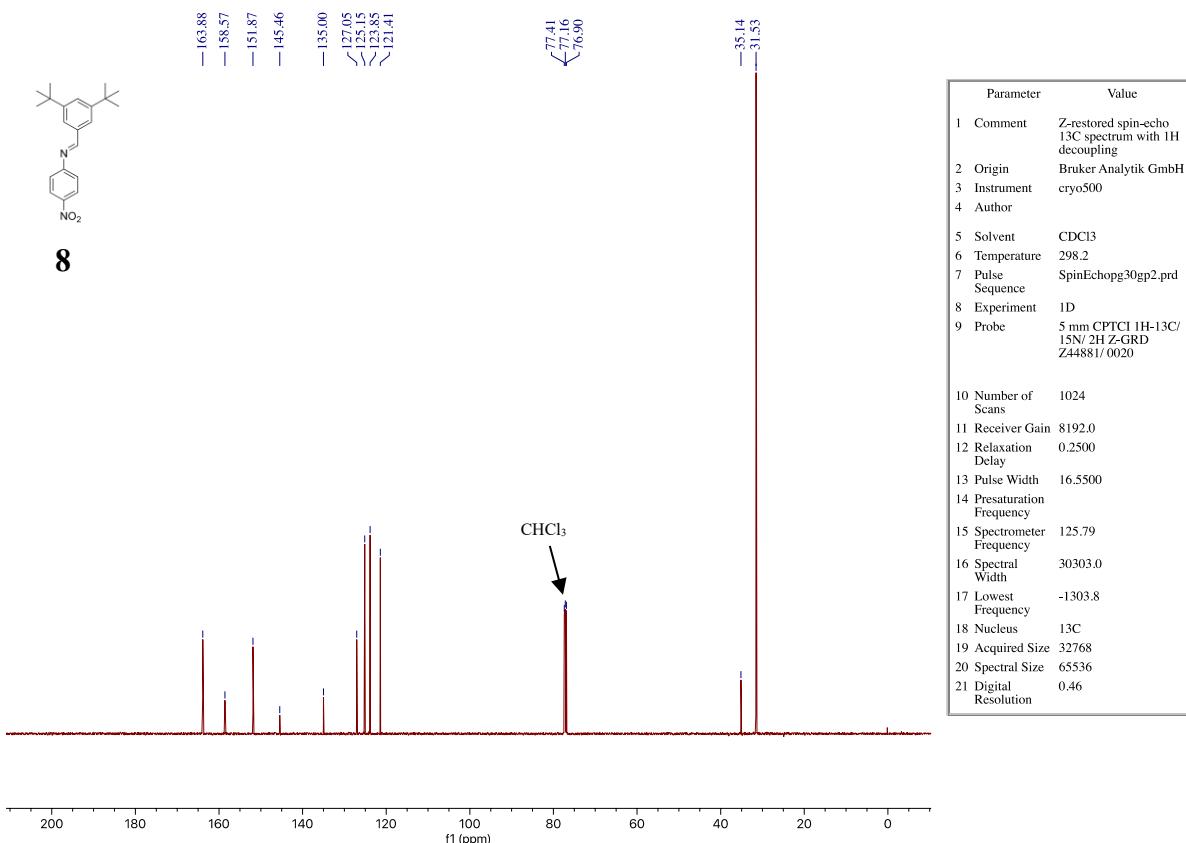


Figure S16. The ¹³C NMR spectrum obtained for **8**.

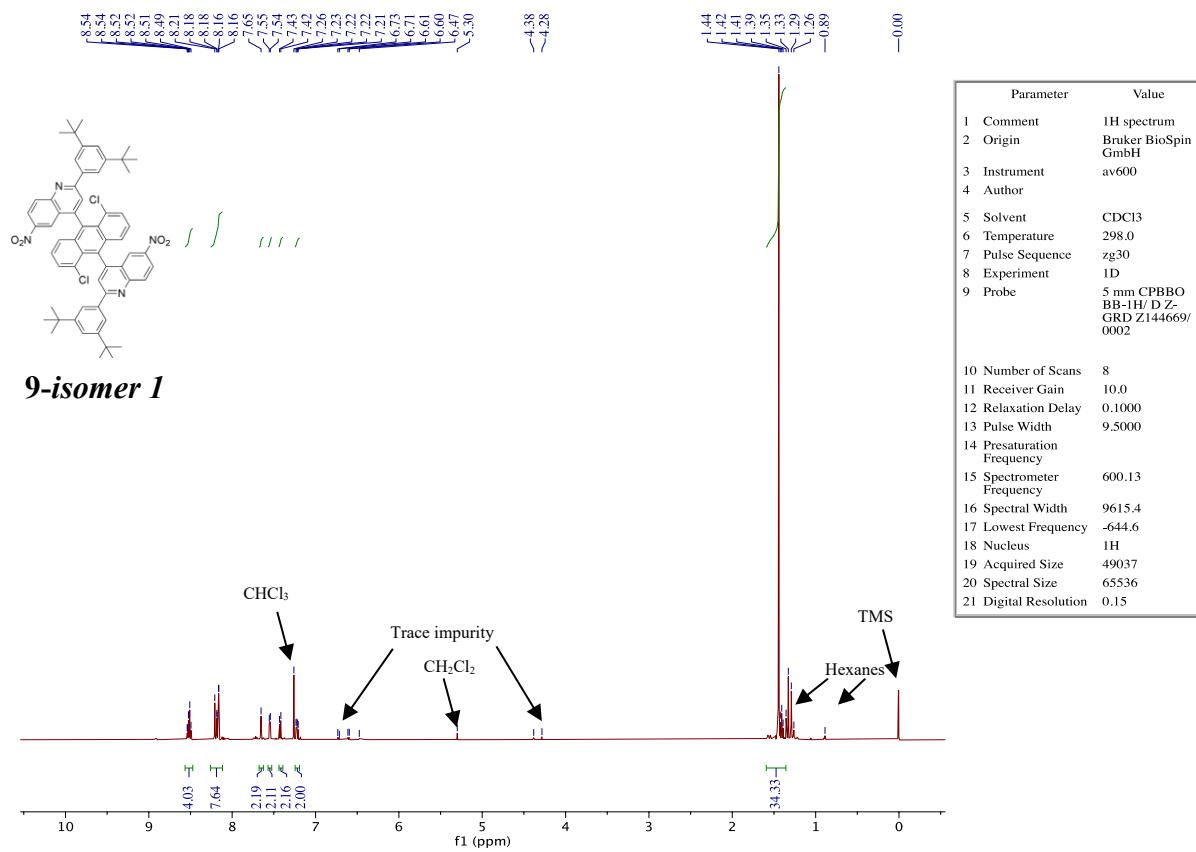


Figure S17. The ¹H NMR spectrum obtained for **9-isomer 1**.

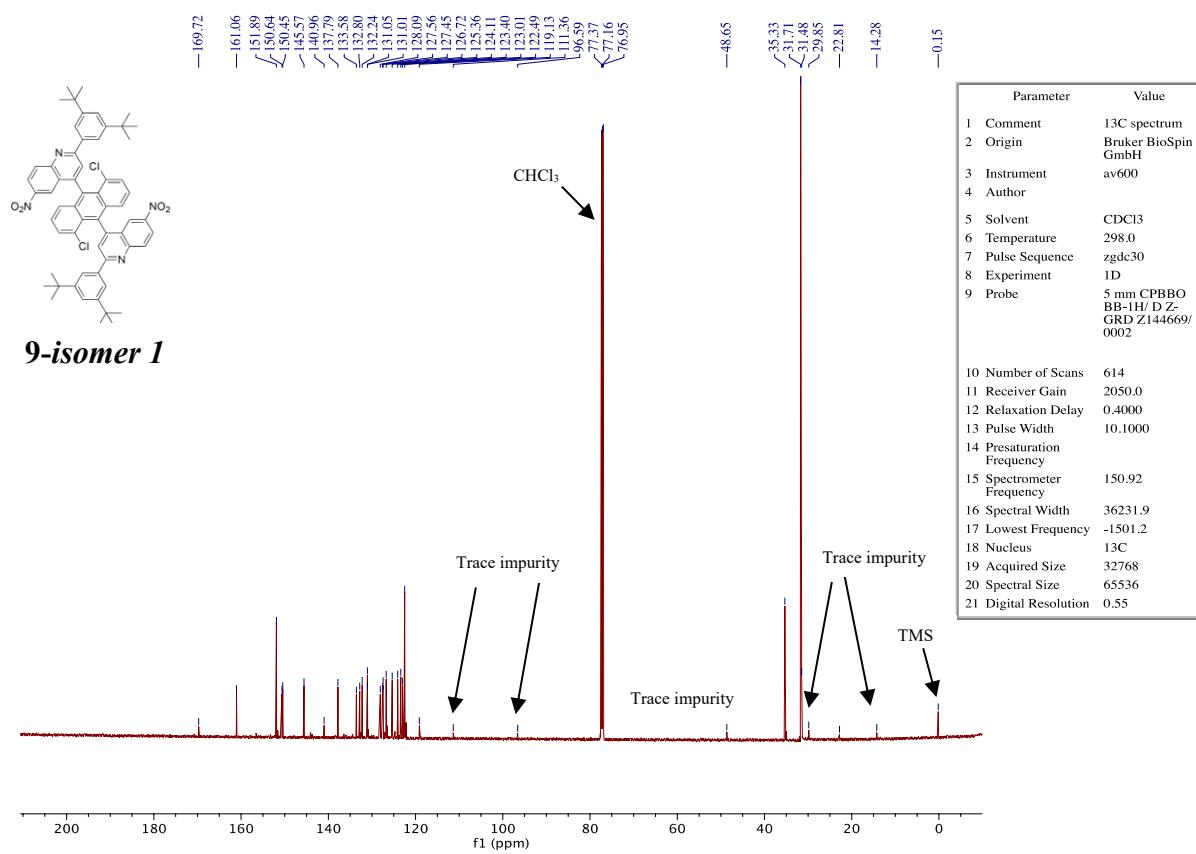


Figure S18. The ¹³C NMR spectrum obtained for **9-isomer 1**.

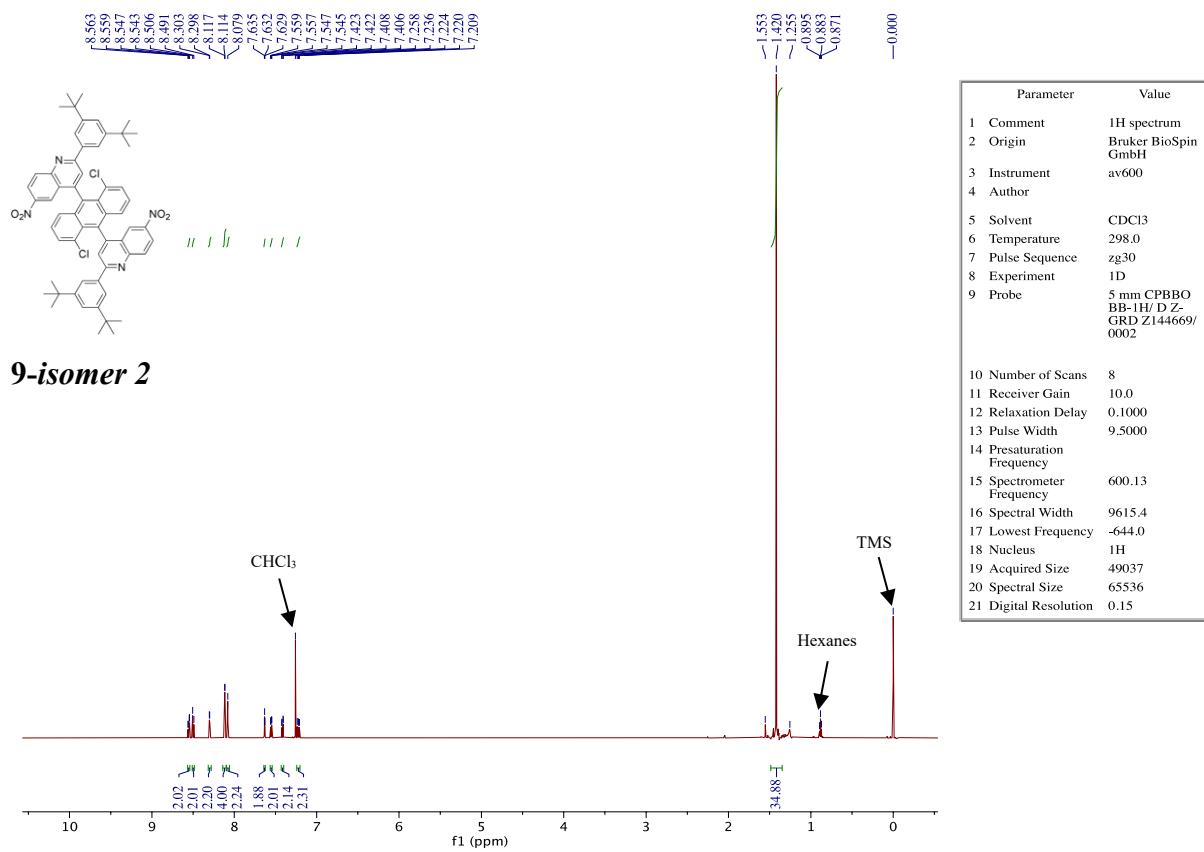


Figure S19. The ¹H NMR spectrum obtained for **9-isomer 2**.

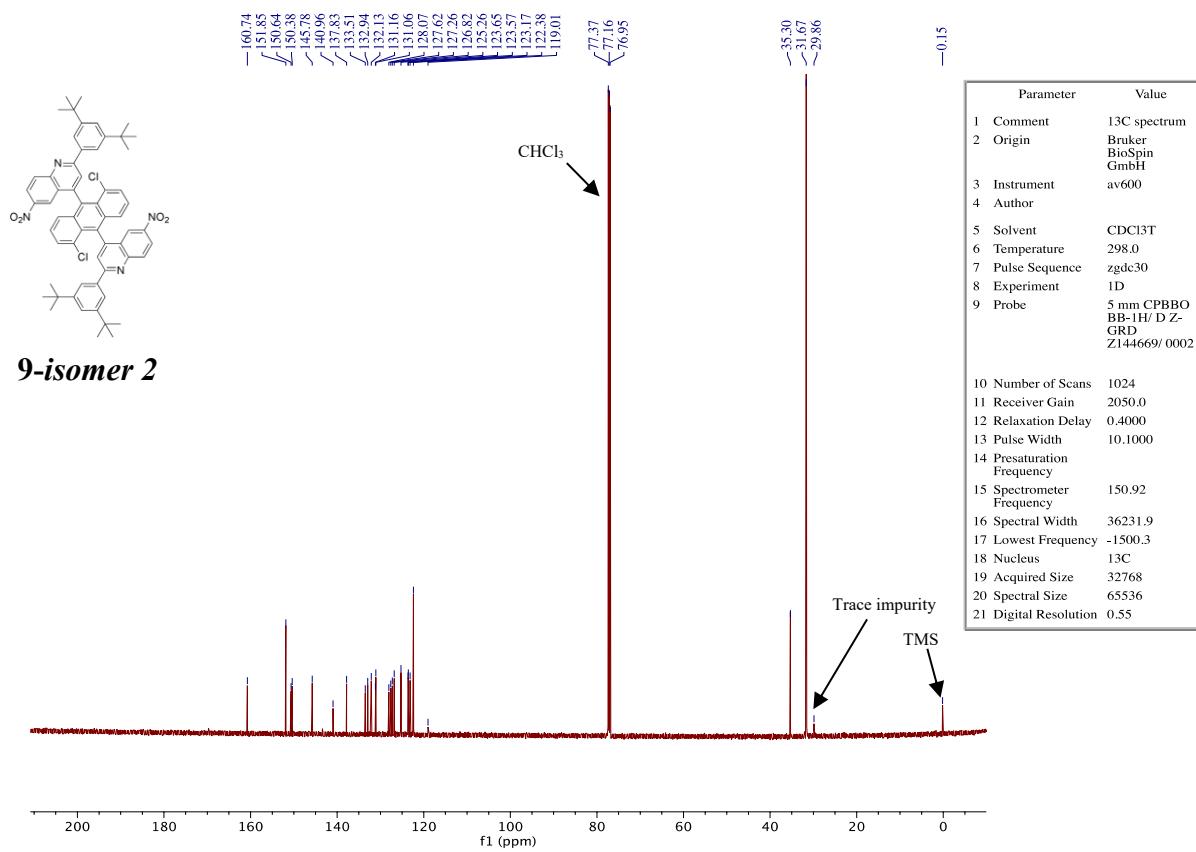


Figure S20. The ¹³C NMR spectrum obtained for **9-isomer 2**.

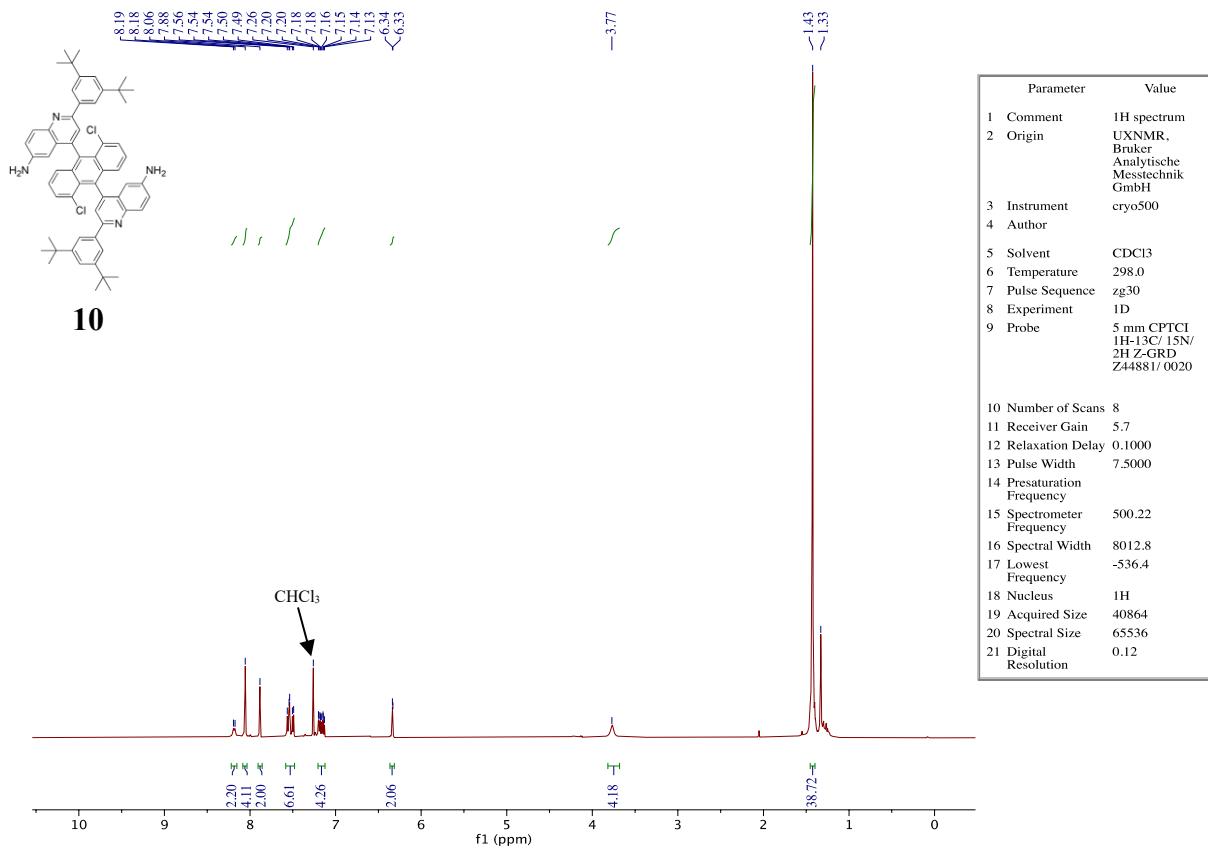


Figure S21. The ¹H NMR spectrum obtained for **10**.

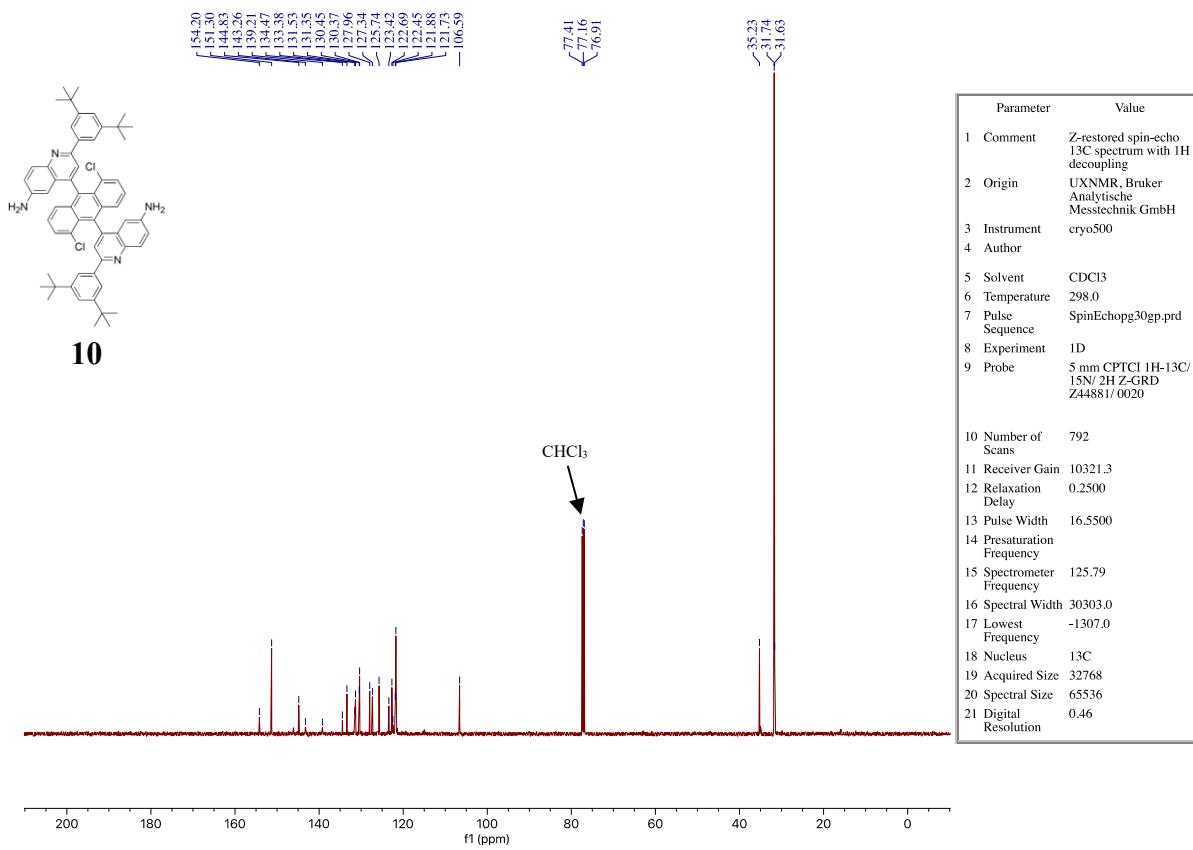


Figure S22. The ¹³C NMR spectrum obtained for **10**.

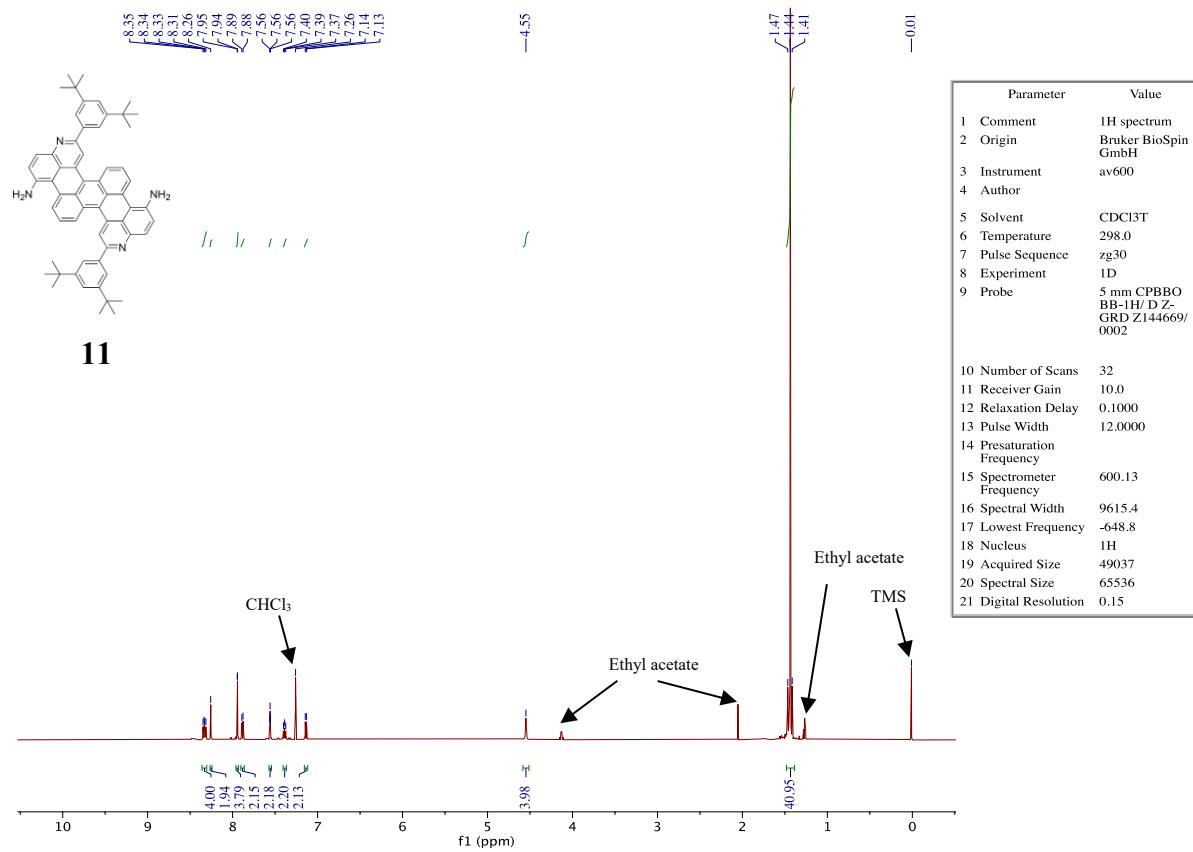


Figure S23. The ¹H NMR spectrum obtained for **11**.

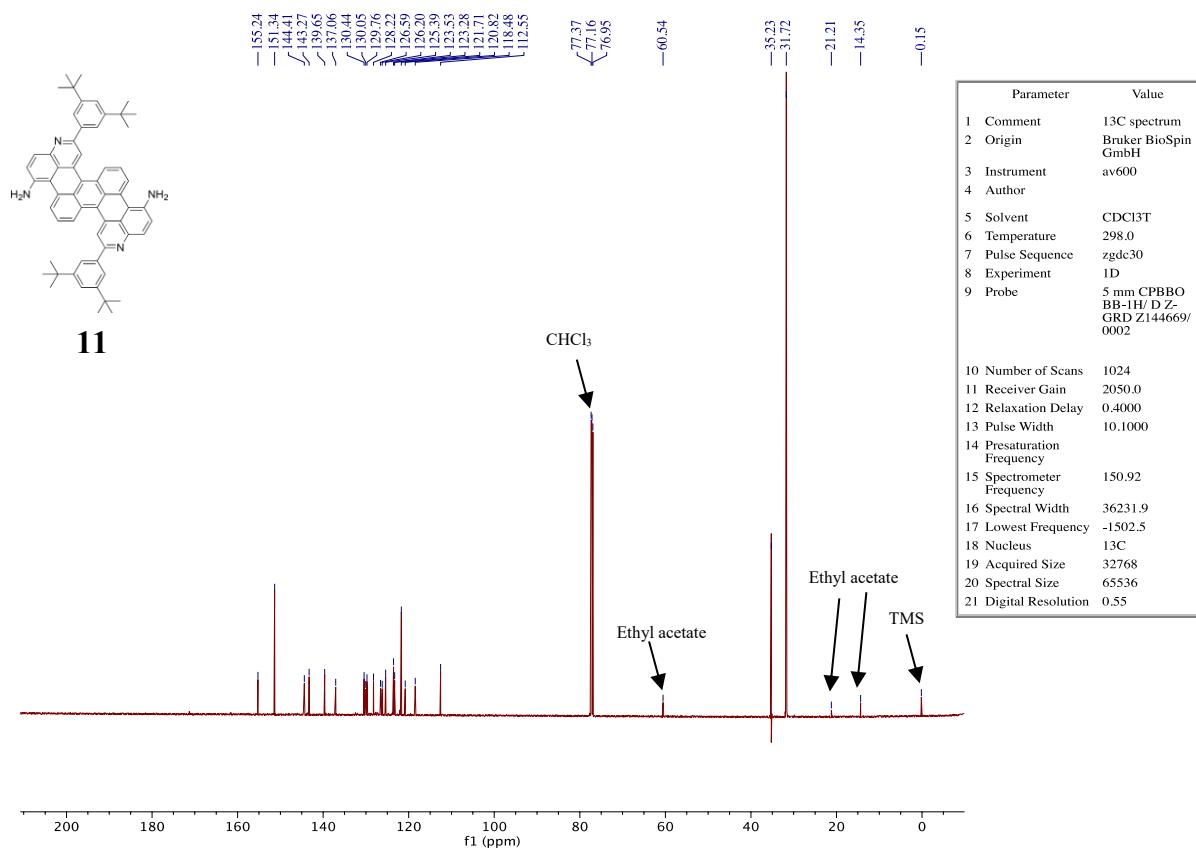


Figure S24. The ¹³C NMR spectrum obtained for **11**.

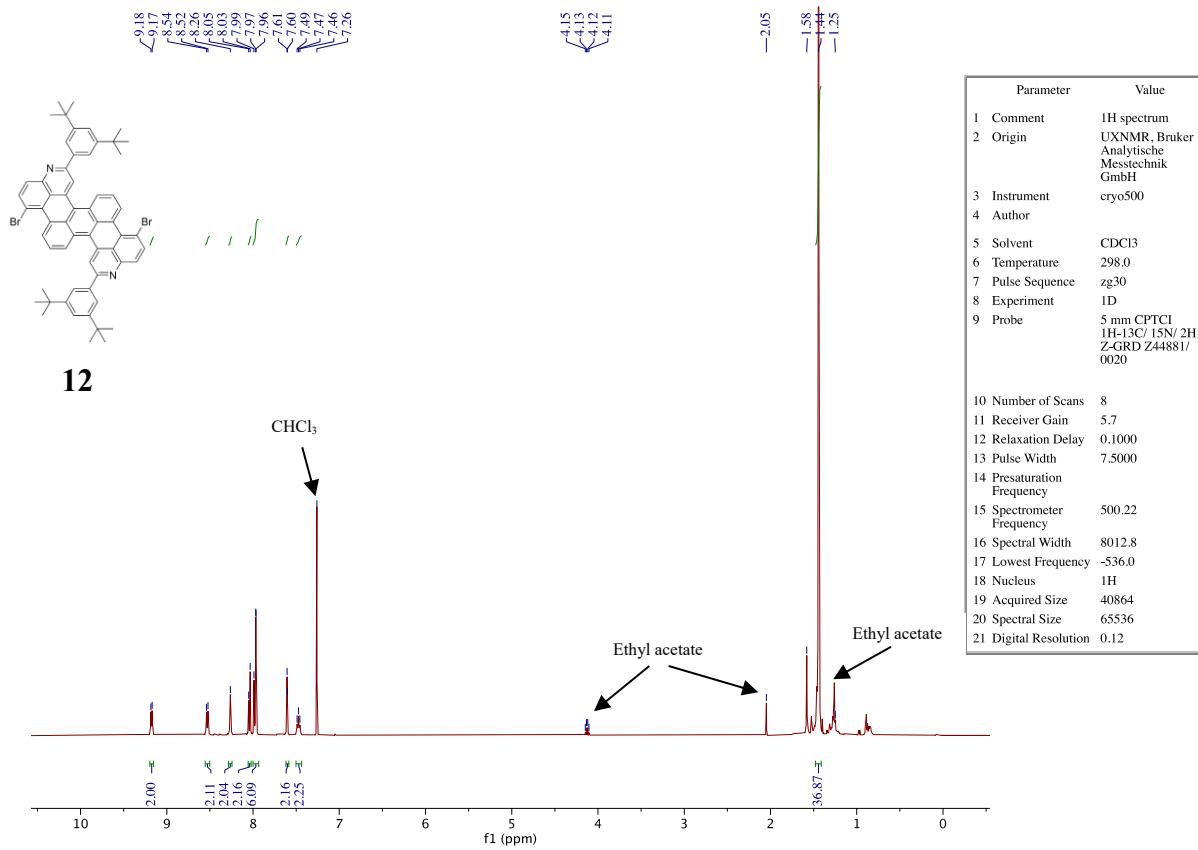


Figure S25. The ¹H NMR spectrum obtained for **12**.

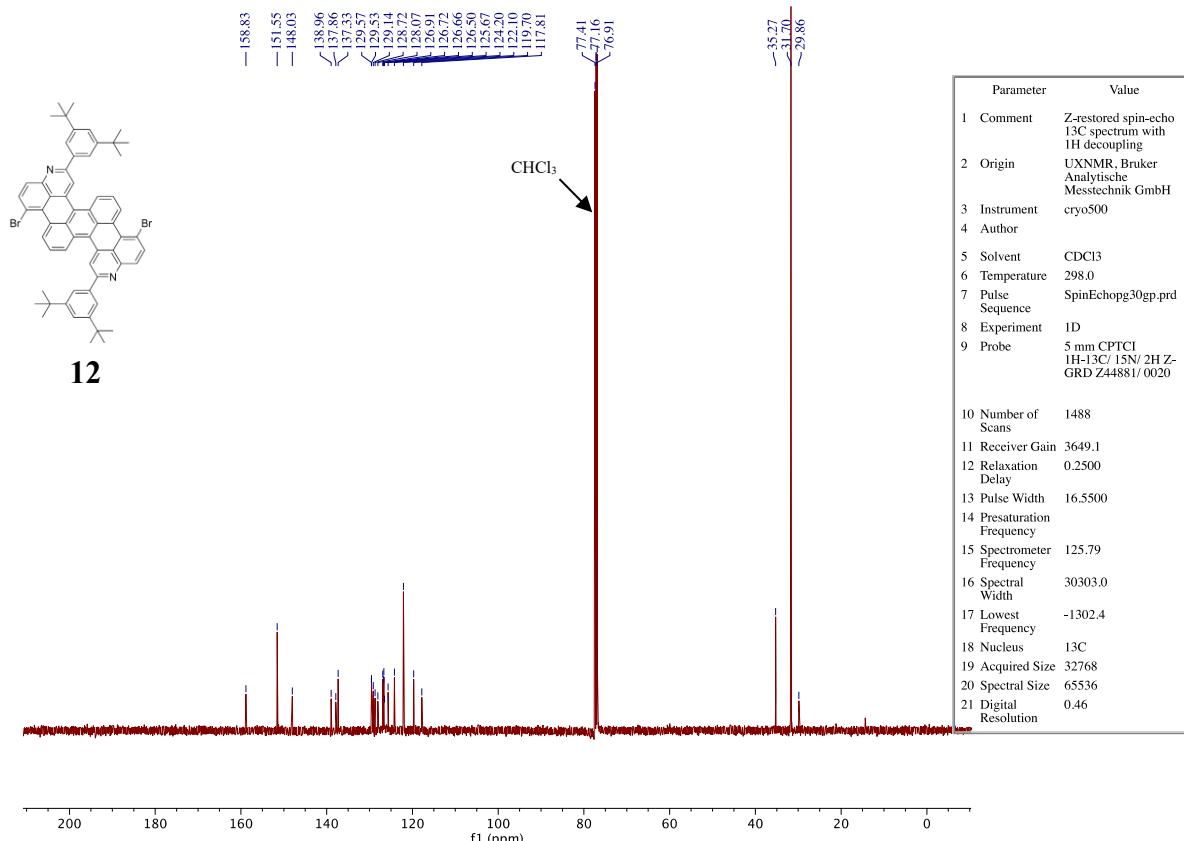


Figure S26. The ¹³C NMR spectrum obtained for **12**.

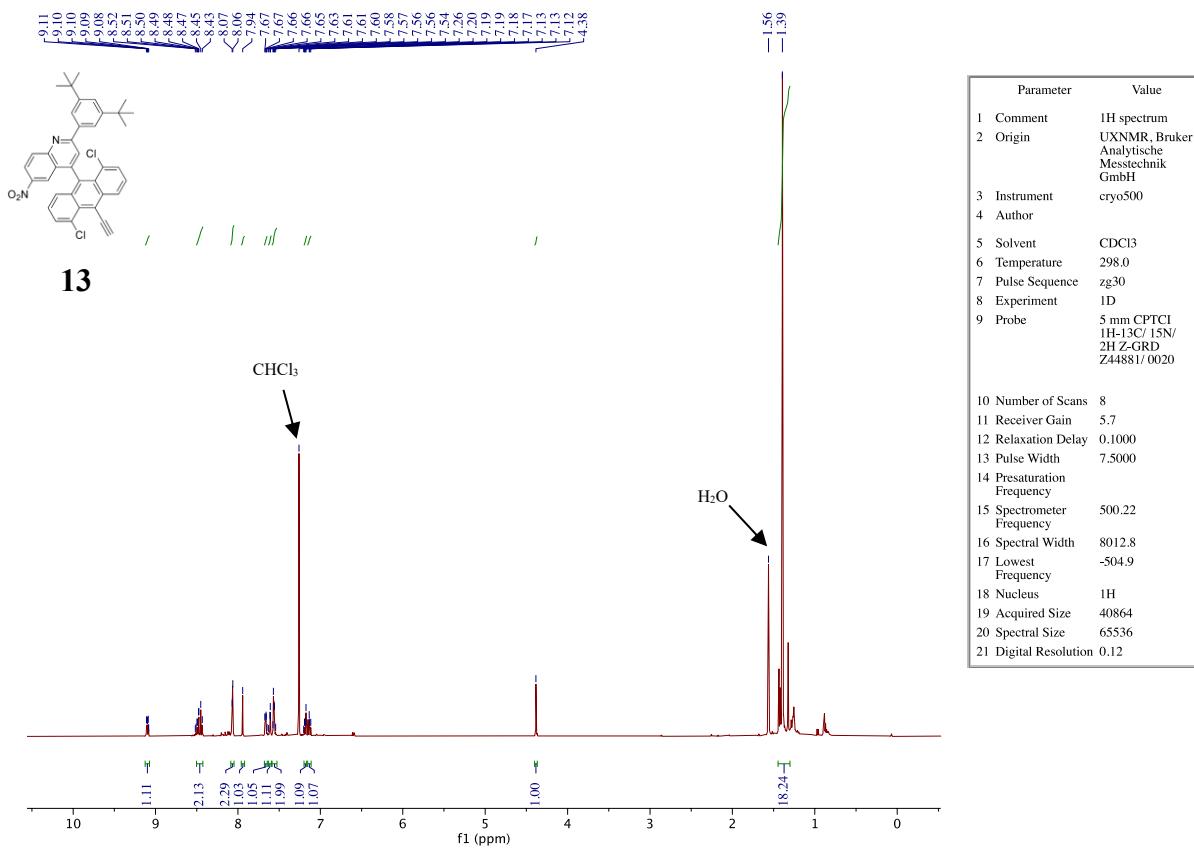


Figure S27. The ¹H NMR spectrum obtained for **13**.

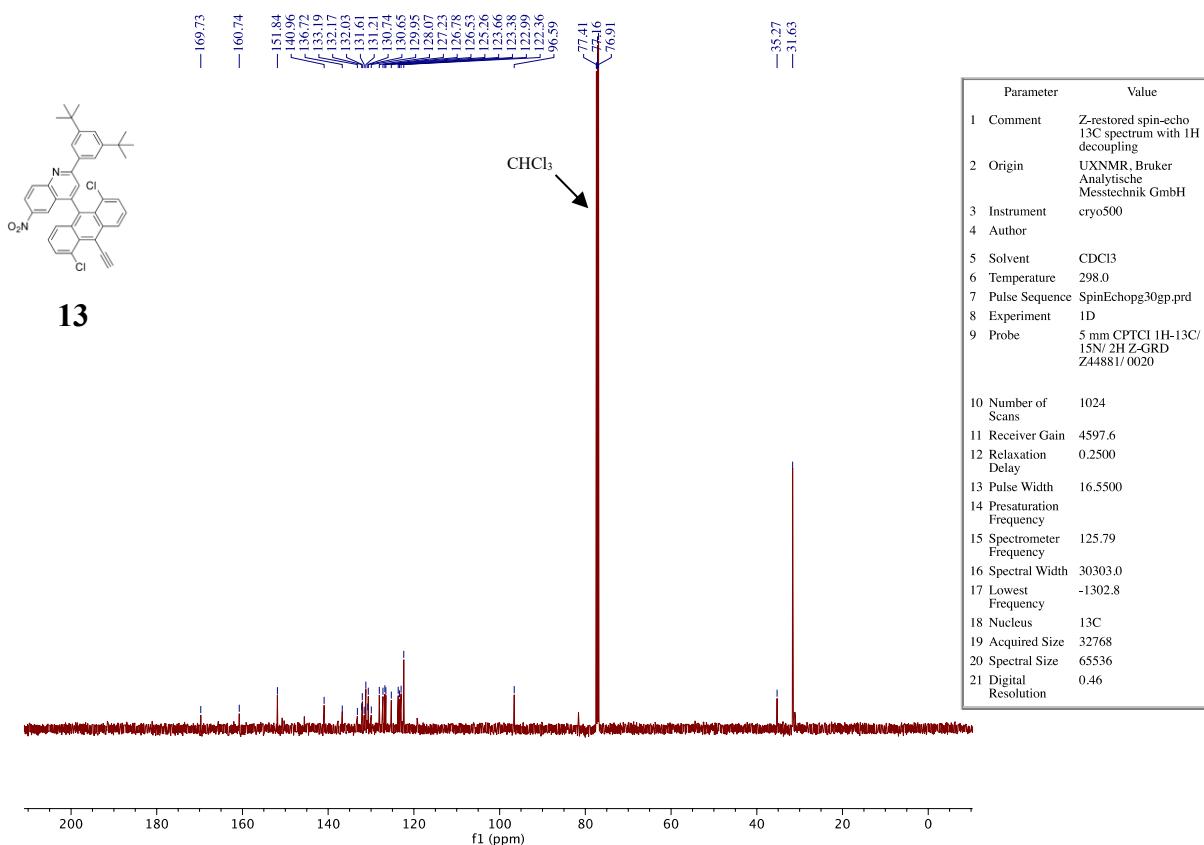


Figure S28. The ¹³C NMR spectrum obtained for **13**.

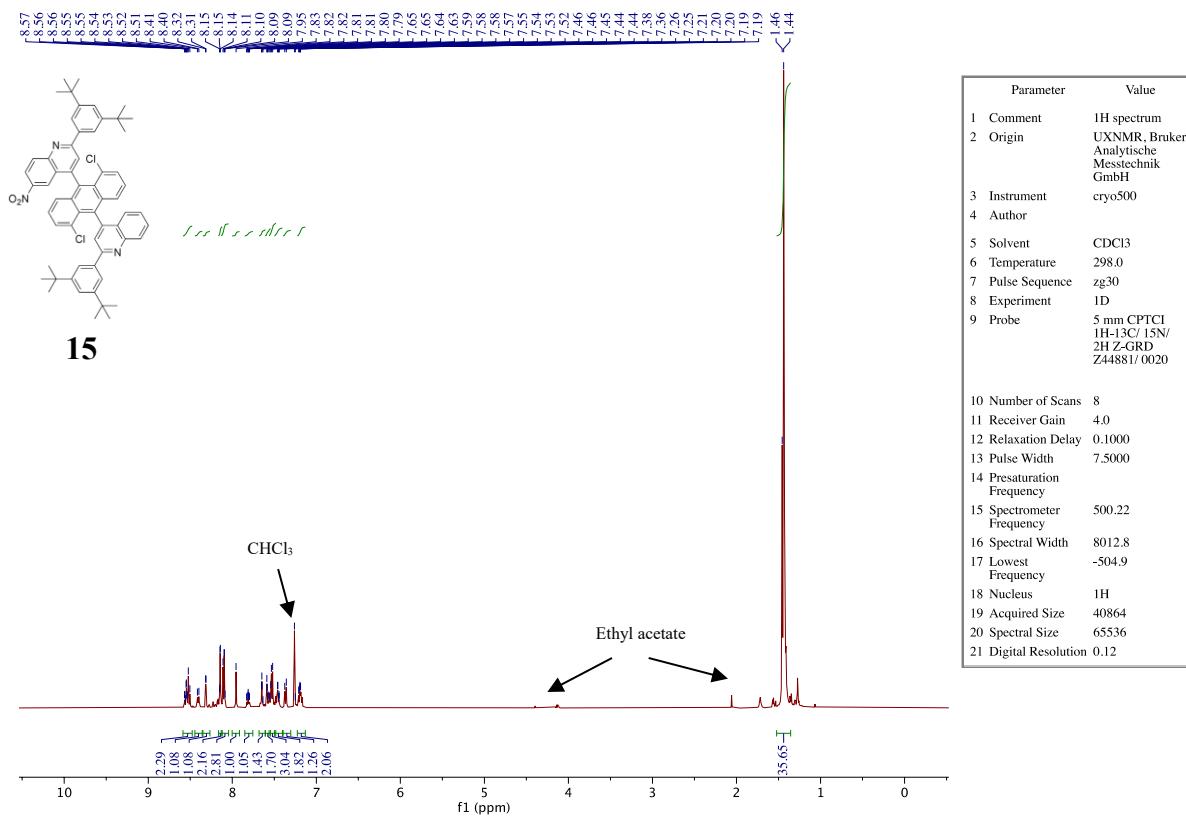


Figure S29. The ¹H NMR spectrum obtained for **15**.

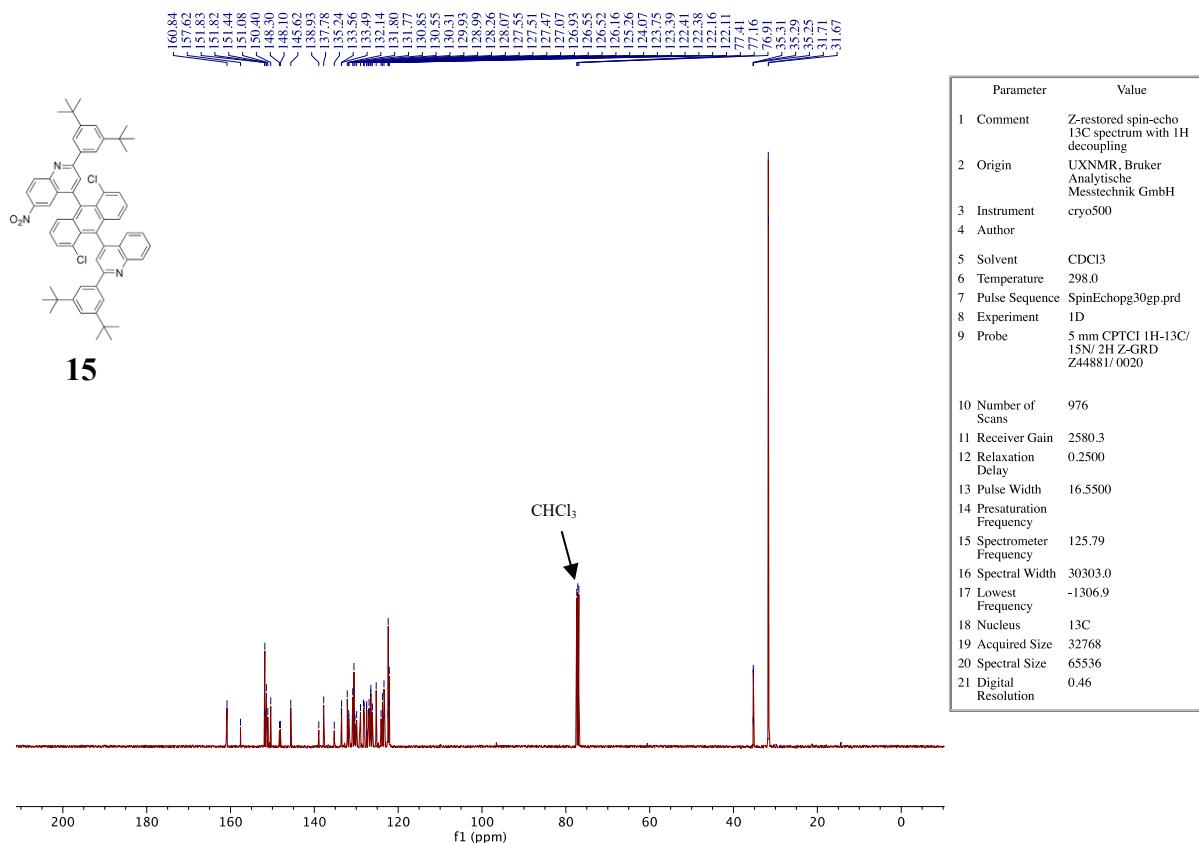


Figure S30. The ^{13}C NMR spectrum obtained for **15**.

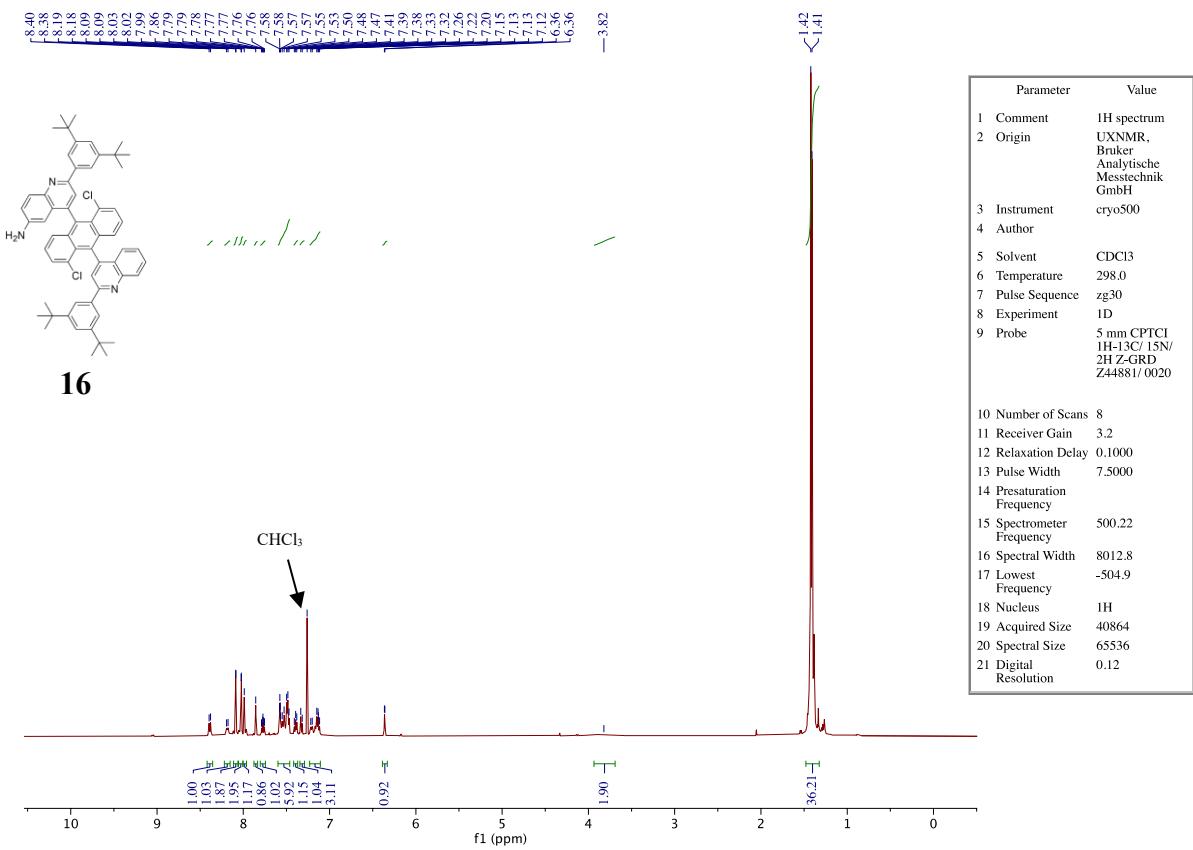


Figure S31. The ¹H NMR spectrum obtained for **16**.

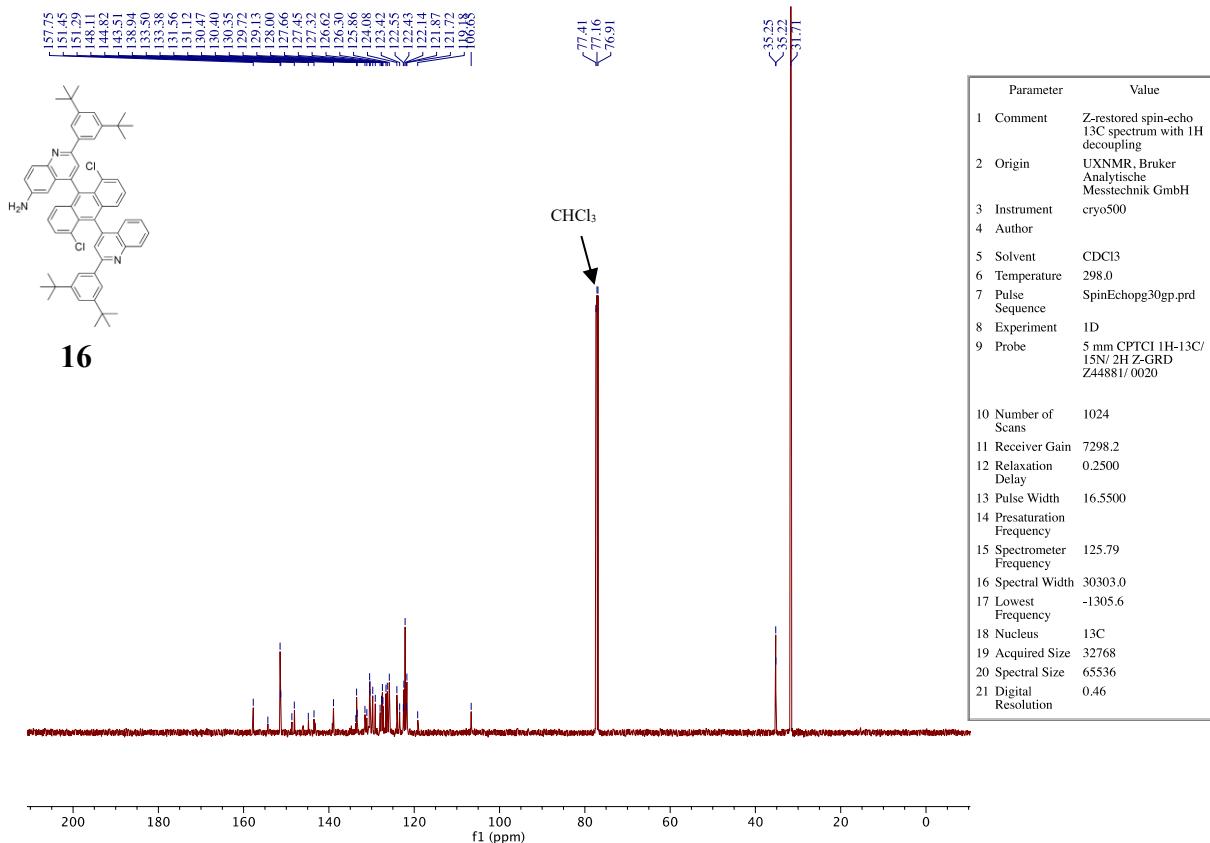


Figure S32. The ¹³C NMR spectrum obtained for **16**.

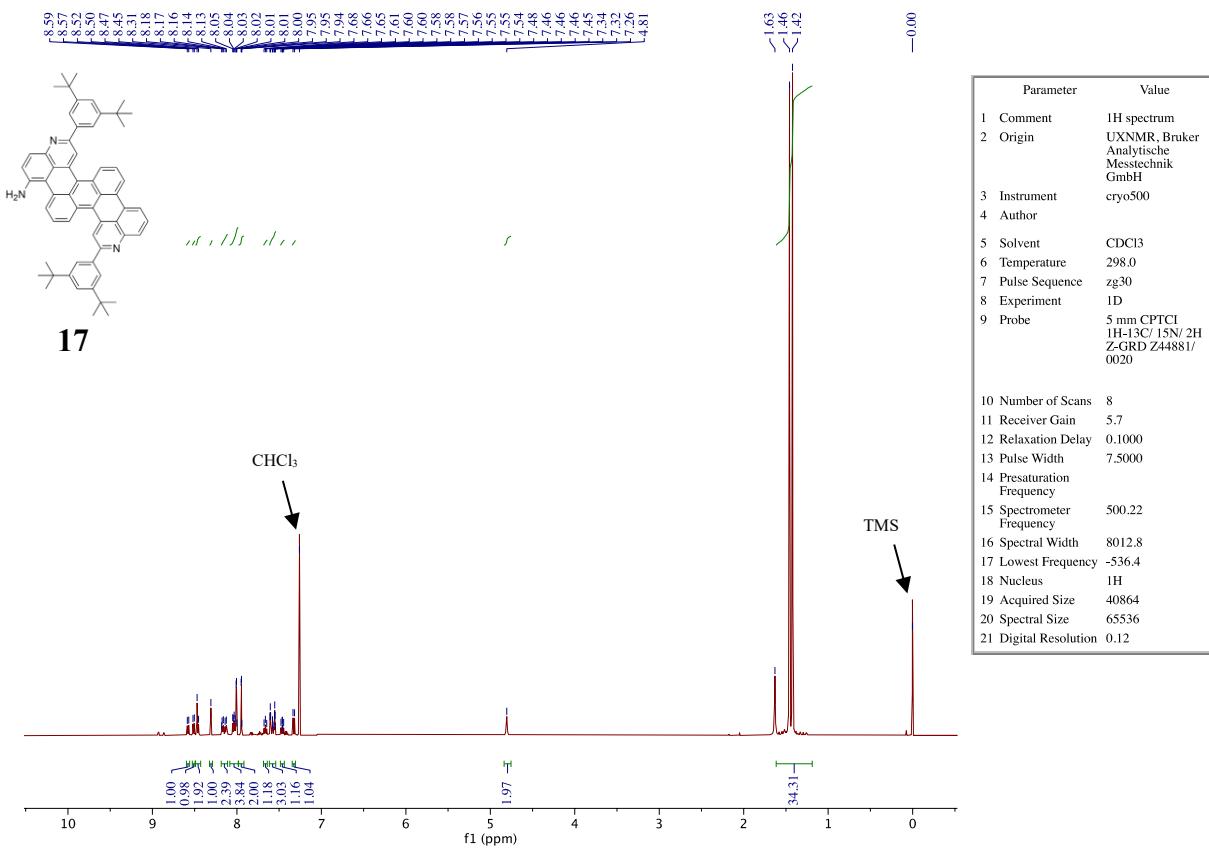


Figure S33. The ¹H NMR spectrum obtained for **17**.

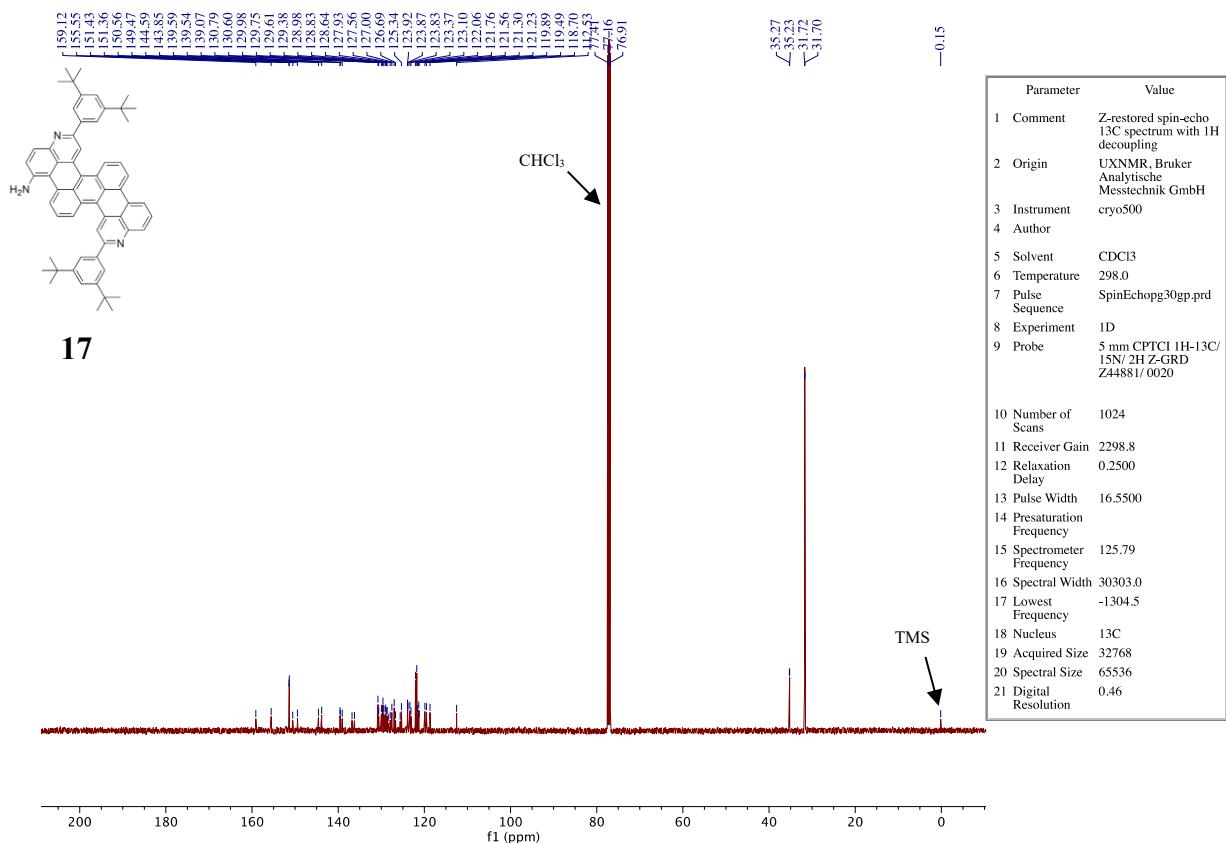


Figure S34. The ¹³C NMR spectrum obtained for **17**.

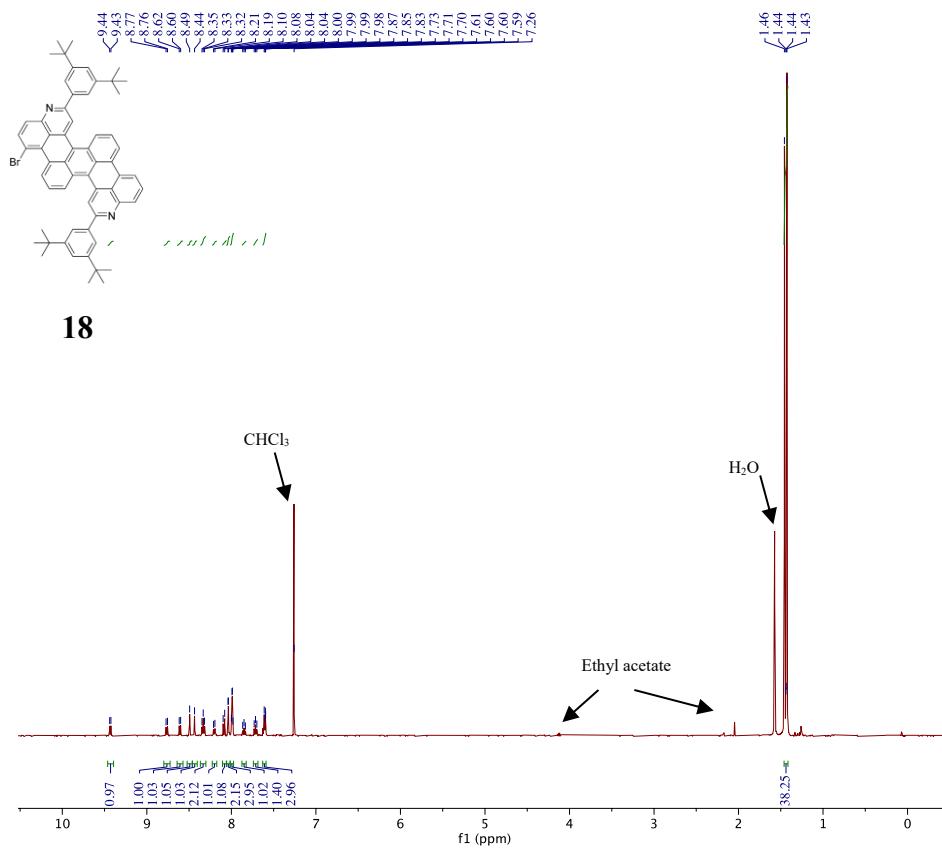


Figure S35. The ¹H NMR spectrum obtained for **18**.

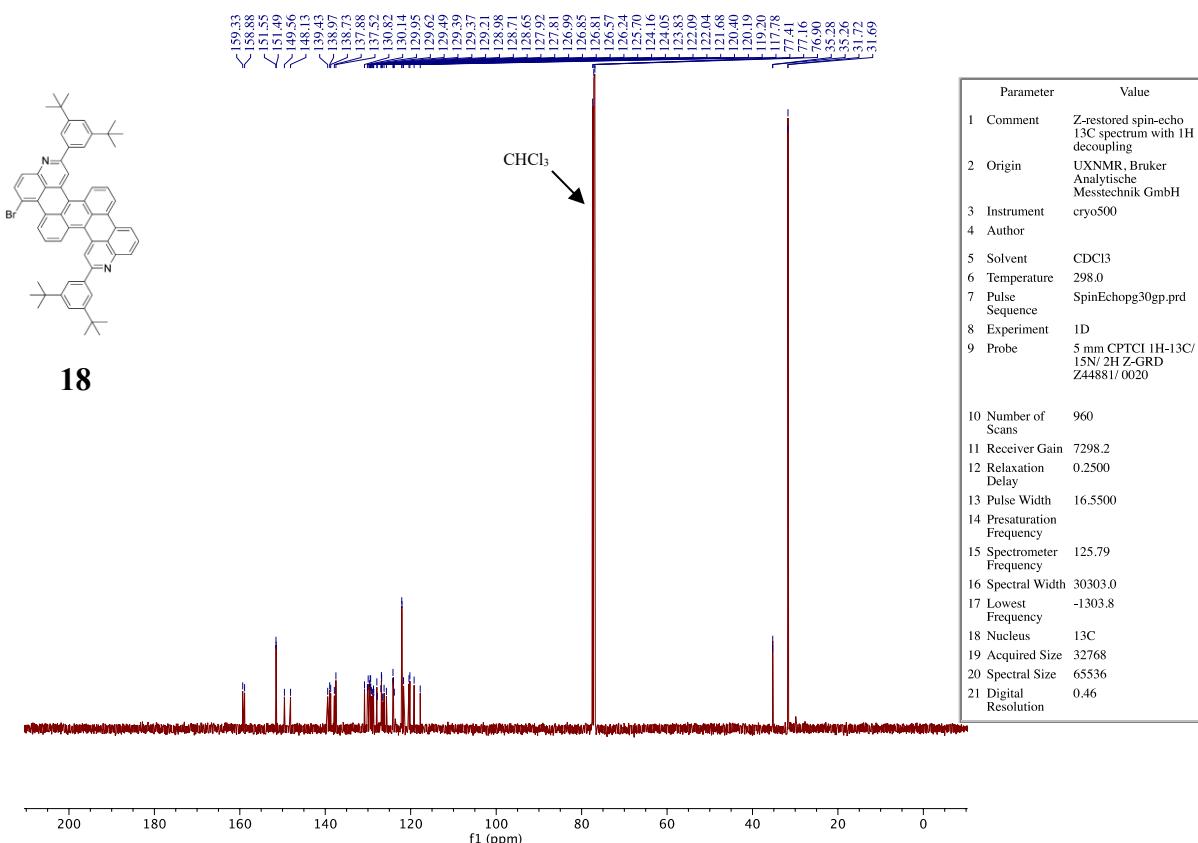


Figure S36. The ¹³C NMR spectrum obtained for **18**.

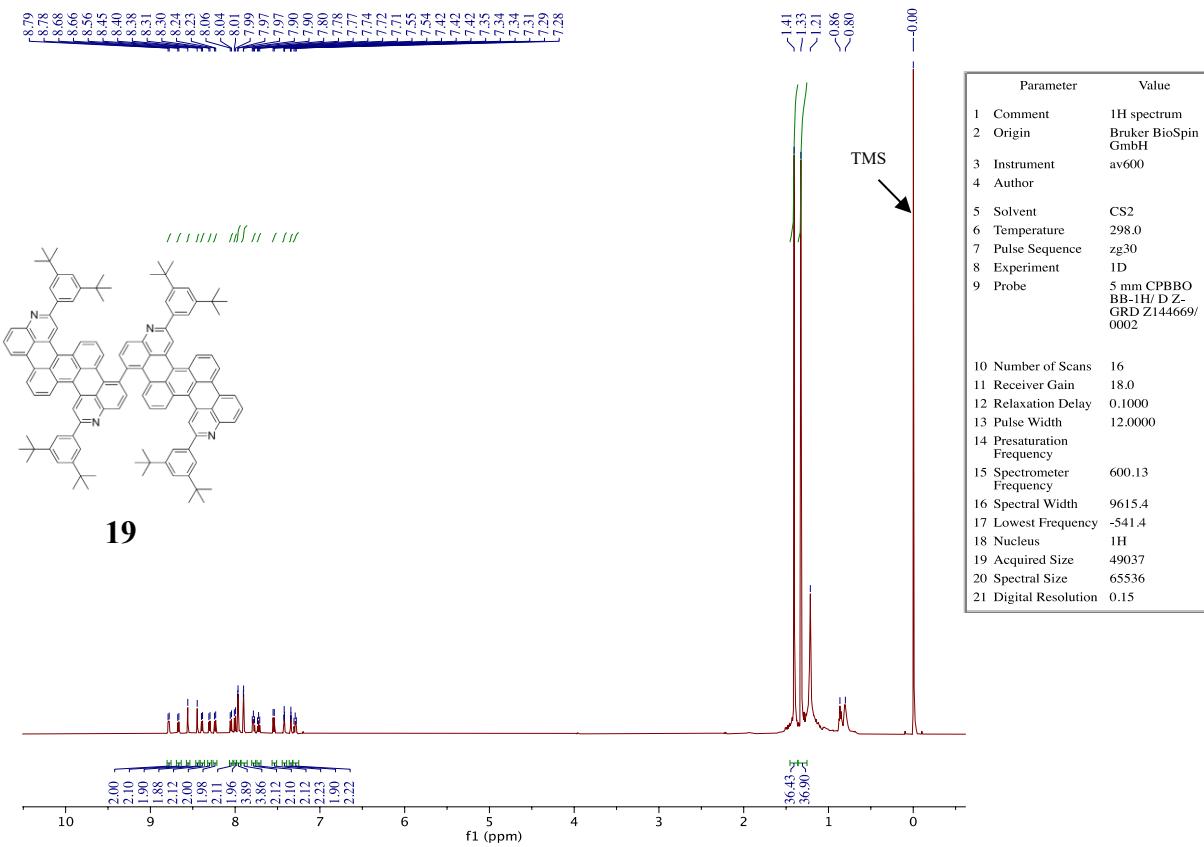


Figure S37. The ^1H NMR spectrum obtained for **19**.

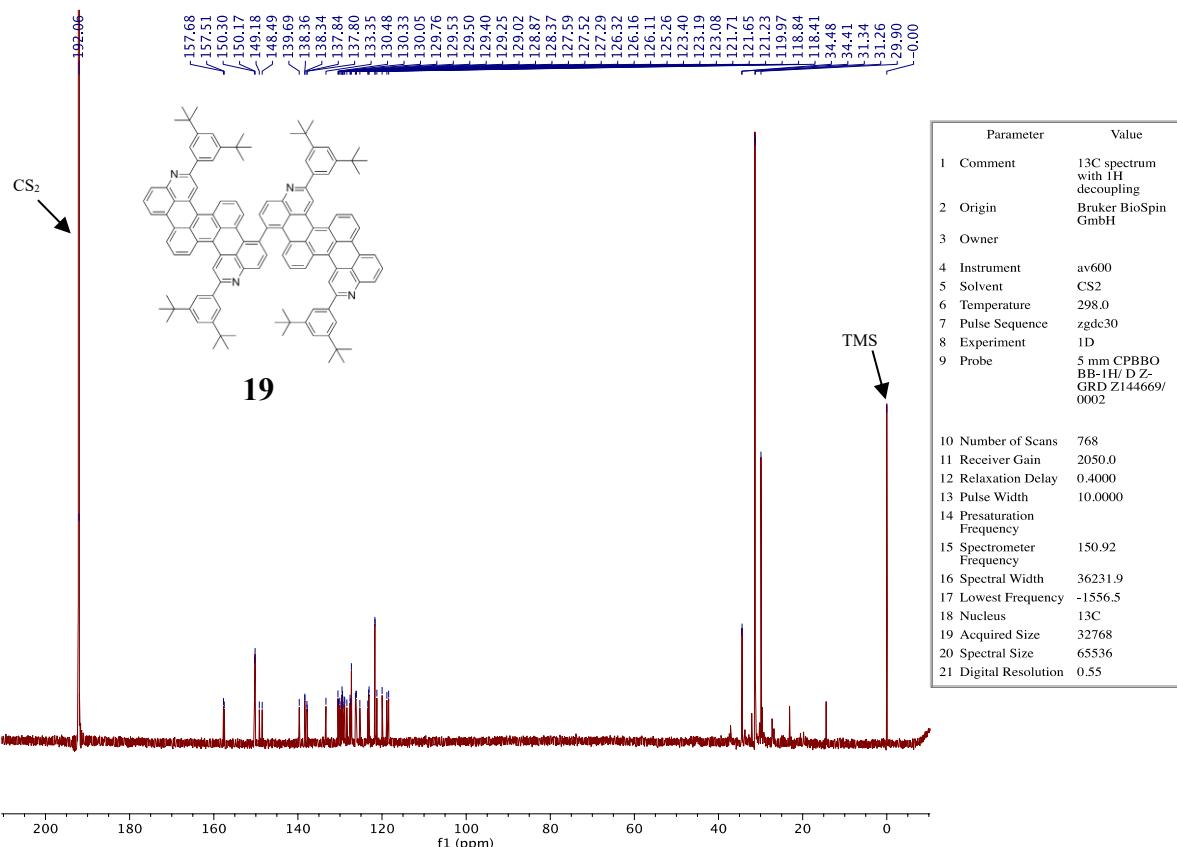


Figure S38. The ¹³C NMR spectrum obtained for **19**.

II. UV-Vis Spectroscopy Data

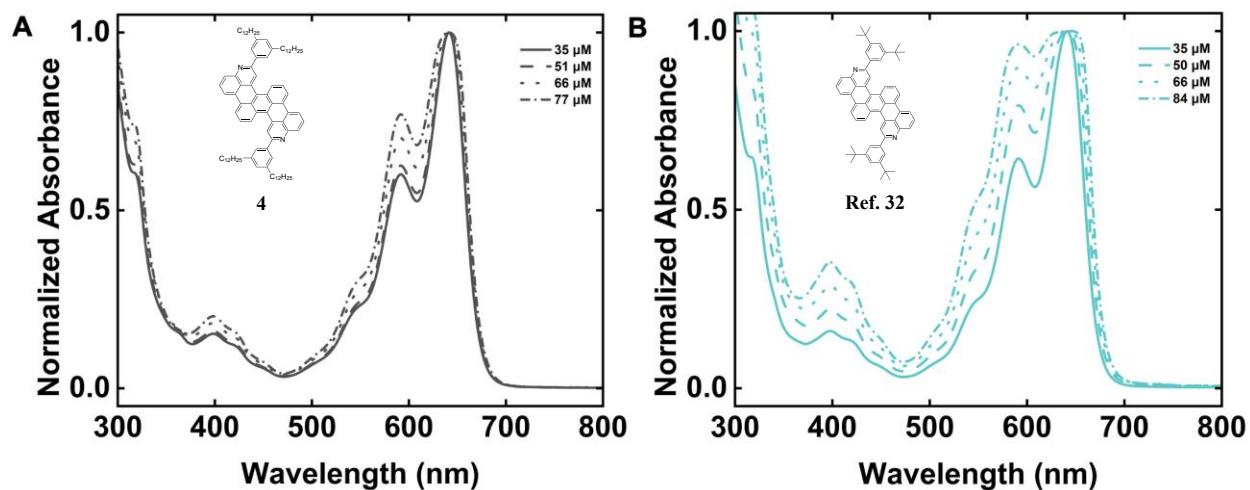


Figure S39. (A) The UV-Vis absorption spectra obtained for dodecyl-substituted tetrabenzopentacene **4** at different concentrations. (B) The UV-Vis absorption spectra measured for a previously-reported tert-butyl-substituted tetrabenzopentacene at different concentrations (see reference 32). Note that the absorption spectra were normalized by using their maximum absorbance peak within the 600 nm to 700 nm wavelength range in order to facilitate direct comparisons.