

Supplementary Information

Pairing Multicomponent Stators with Aromatic Rotators for New Emissive Molecular Rotors

Ma. Carmen García-González, Jorge Espinosa-Rocha, Lizbeth A. Rodríguez-Cortés, Yoarhy
A. Amador-Sánchez, Luis D. Miranda* and Braulio Rodríguez-Molina*

brodriguez@iquimica.unam.mx

CONTENTS

<u>Photophysical properties</u>	S2-S11
<u>Solution NMR spectra</u>	S12-S25
<u>MS spectra</u>	S26-S28

Aggregation-Induced Enhanced Emission (AIEE) Experiments.

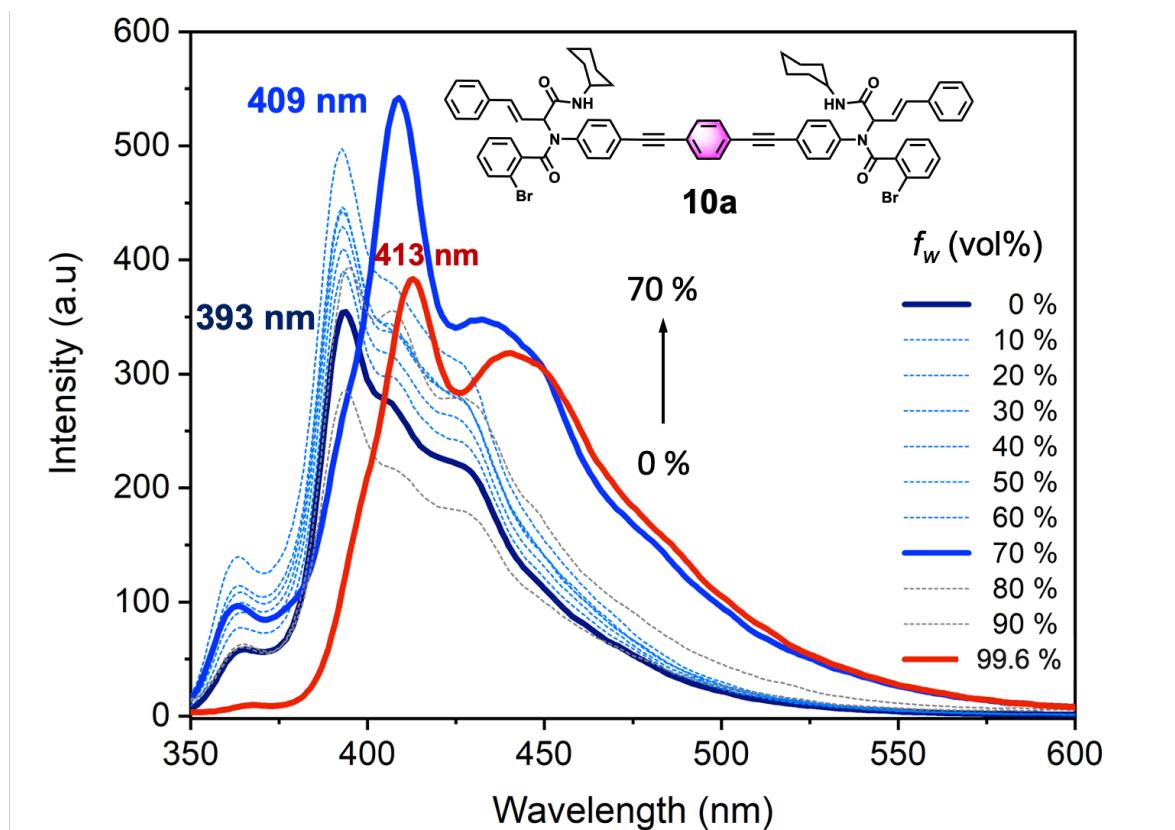


Figure S 1. Fluorescence experiments of **10a** (4×10^{-6} M) performed on different THF/water fractions (f_w).

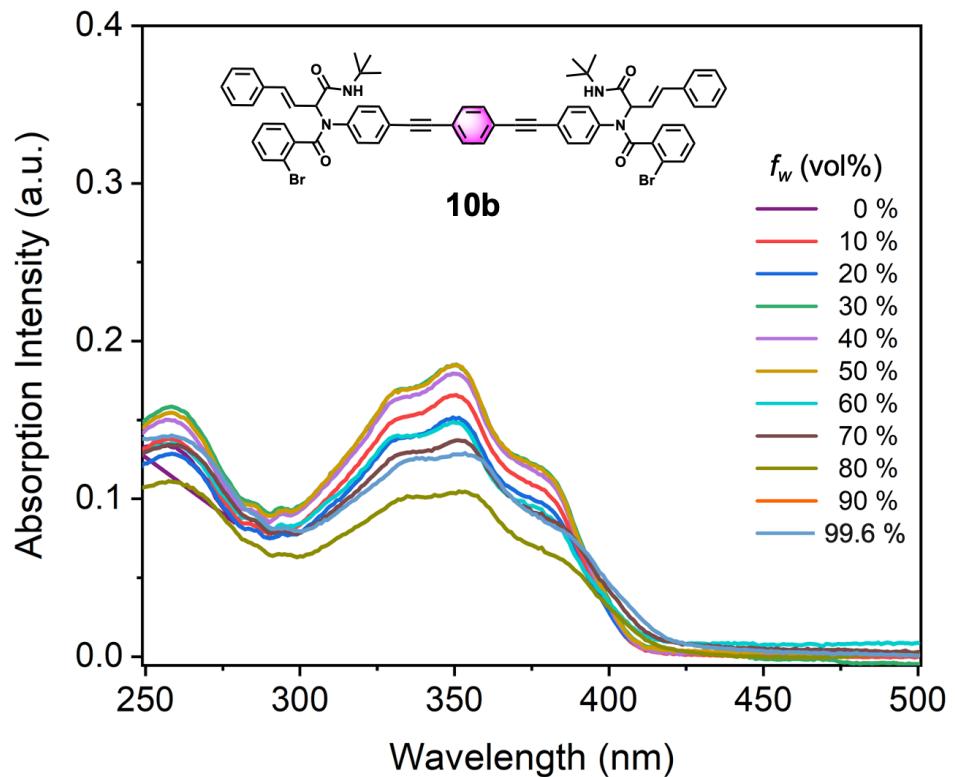


Figure S 2. Absorption spectra of **10b** in different THF/water mixtures (4×10^{-6} M).

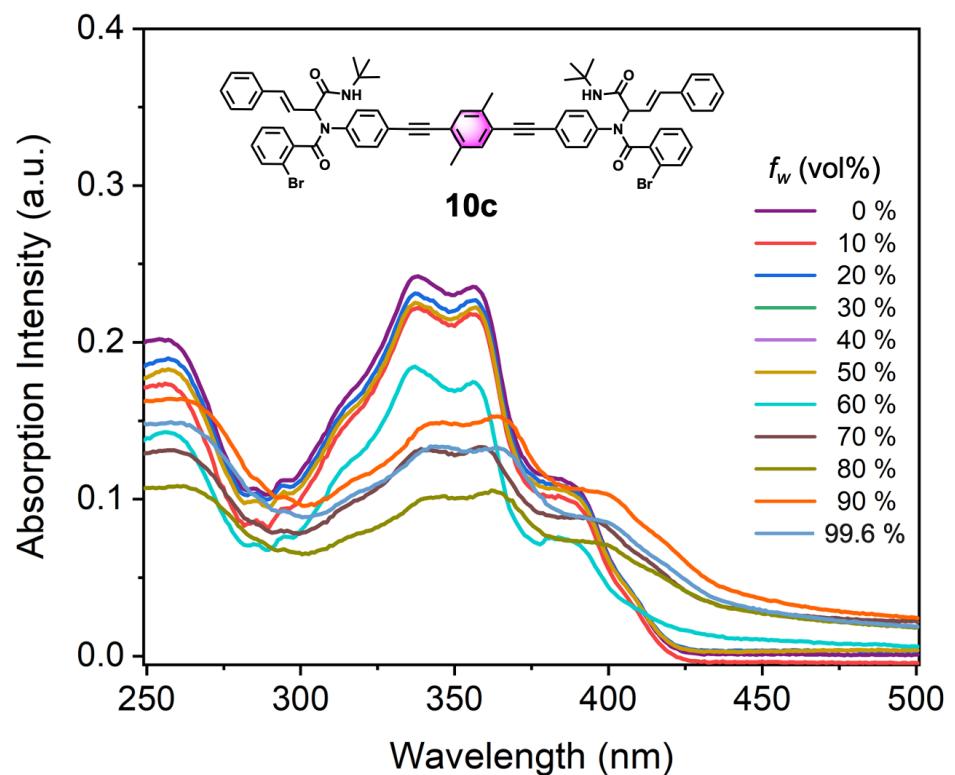


Figure S 3. Absorption spectra of **10c** with different THF/water mixtures (4×10^{-6} M).

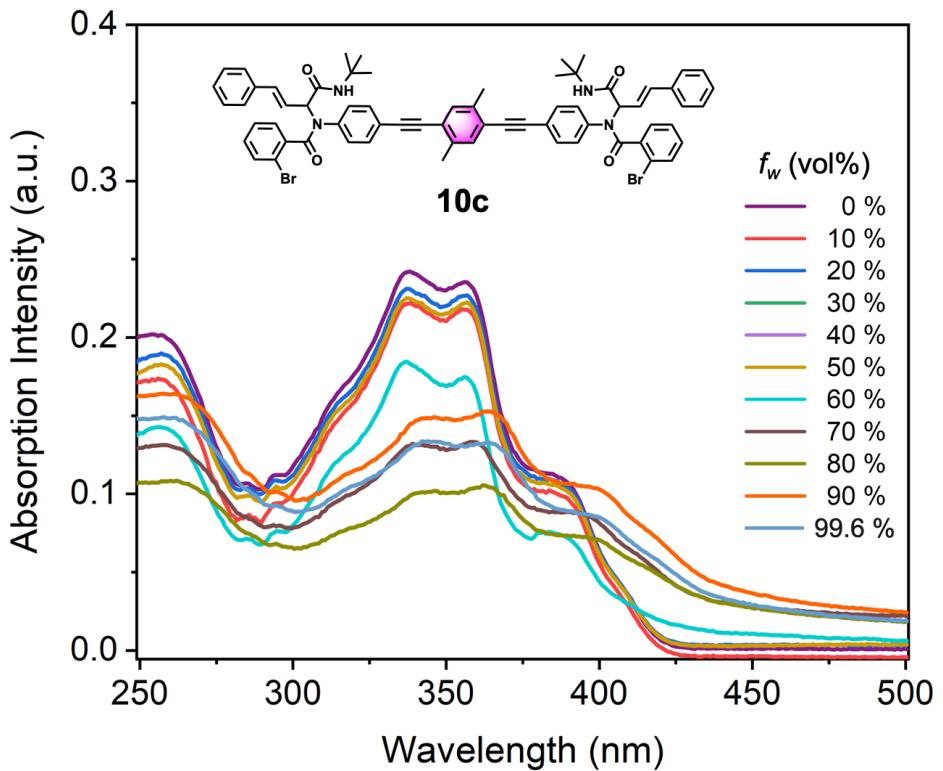


Figure S 4. Absorption spectra of **10d** with different THF/water mixtures (4×10^{-6} M).

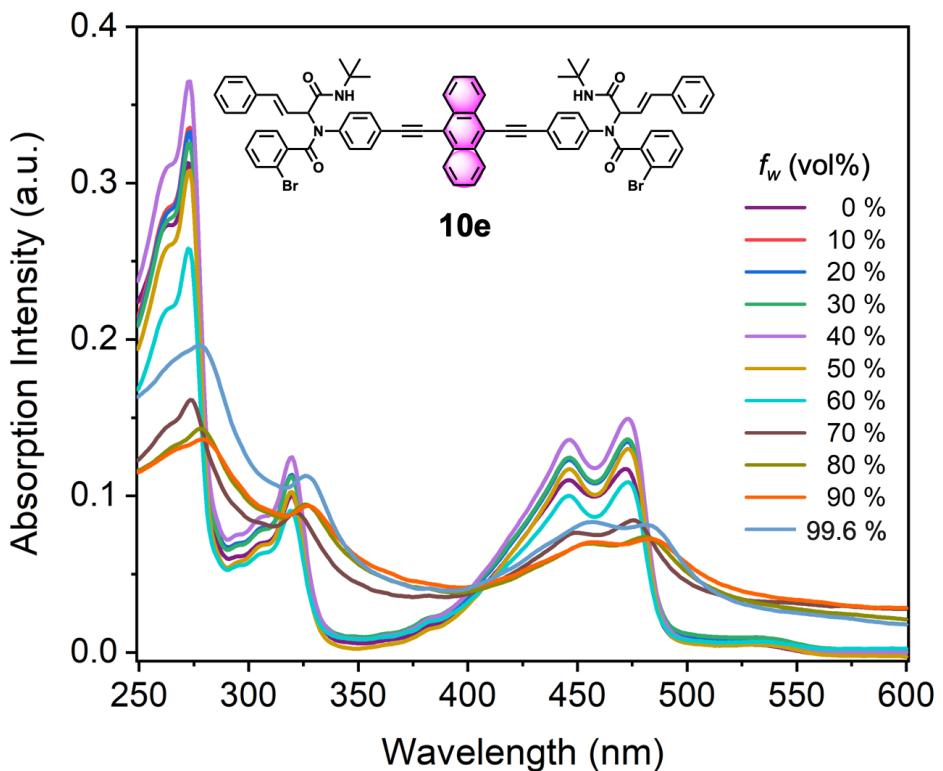


Figure S 5. Absorption spectra of **10e** with different THF/water mixtures (4×10^{-6} M).

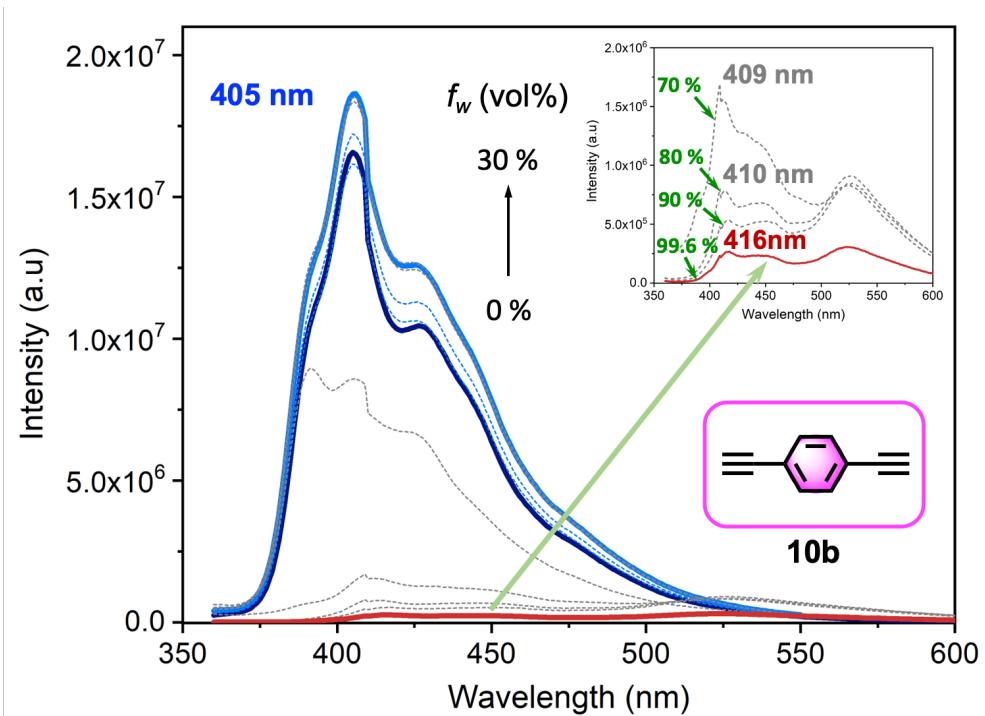


Figure S 6. Fluorescence experiments of **10b** carried out in different THF/water mixtures (4×10^{-6} M). Insert: Emission spectra corresponding to the addition of large fractions of water (f_w); 70% ($\lambda_{\text{em}} = 409$ nm), 80% ($\lambda_{\text{em}} = 410$ nm) 90% and 99.6% ($\lambda_{\text{em}} = 416$ nm).

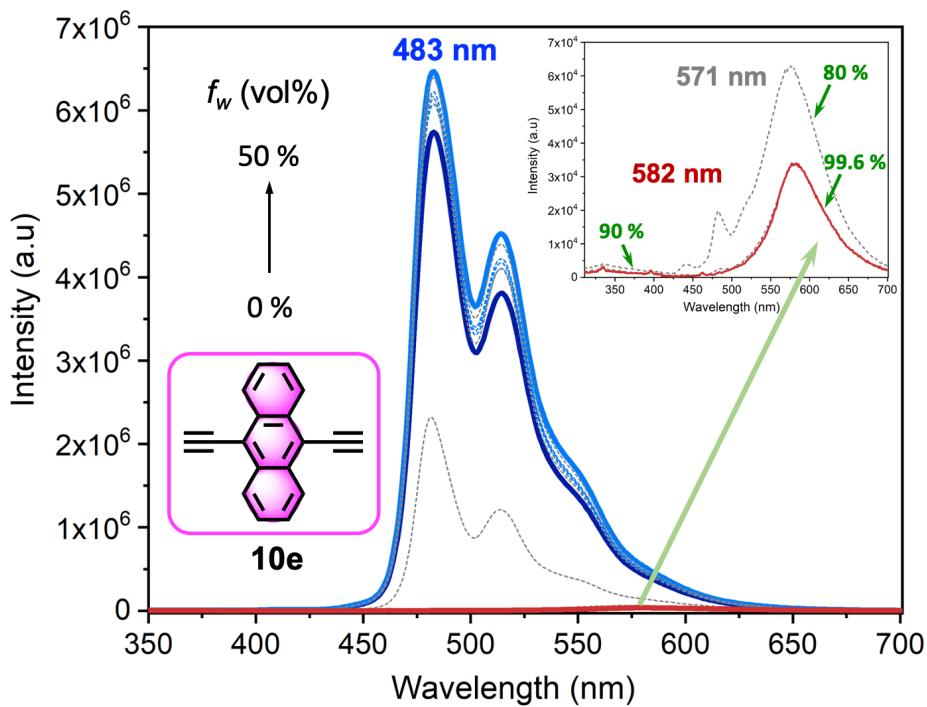


Figure S 7. Fluorescence experiments of **10e** carried out in different THF/water mixtures (4×10^{-6} M). Insert: Emission spectra corresponding to the addition of large fractions of water (f_w); 80% ($\lambda_{\text{em}} = 571$ nm), 90% and 99.6% ($\lambda_{\text{em}} = 582$ nm).

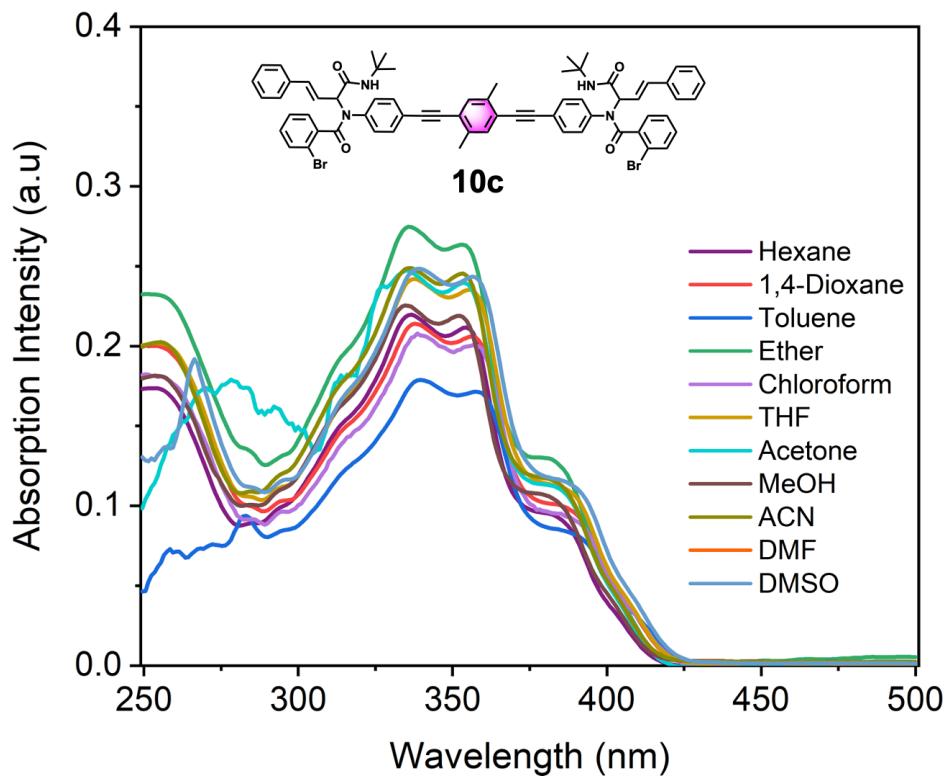


Figure S 8. Solvent effect on the absorption of **10c** (4×10^{-6} M): hexane, 1,4-dioxane, toluene, ether, chloroform, tetrahydrofuran (THF), acetone, methanol (MeOH), acetonitrile (ACN), dimethyl formamide (DMF) and dimethyl sulfoxide (DMSO).

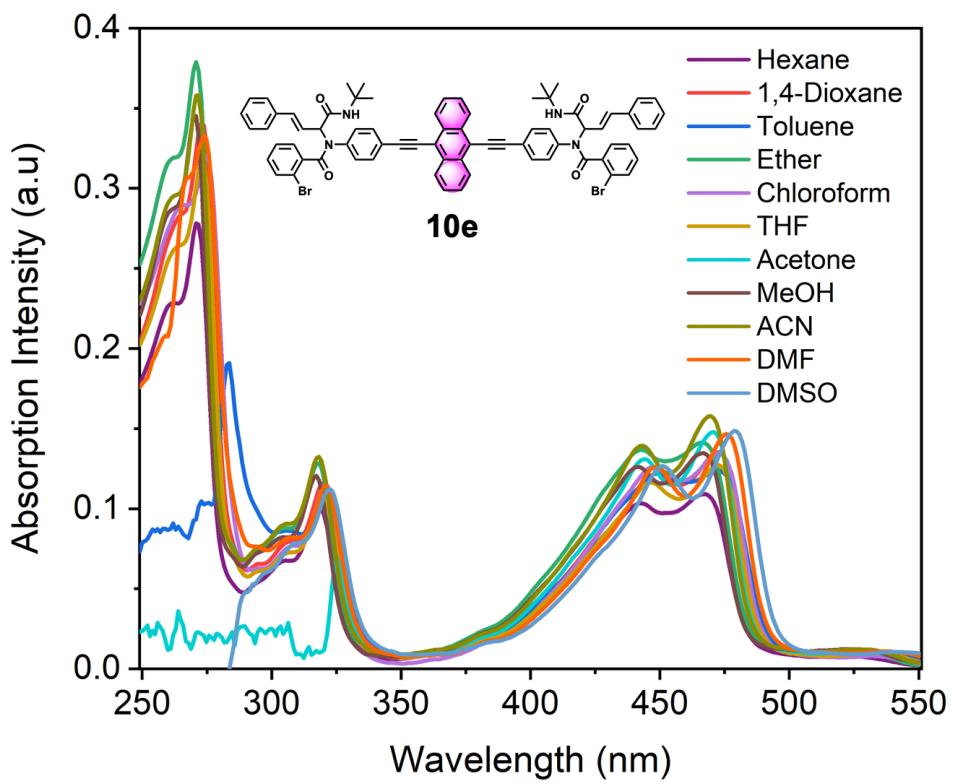


Figure S 9. Solvent effect on the absorption of **10e** (4×10^{-6} M): hexane, 1,4-dioxane, toluene, ether, chloroform, tetrahydrofuran (THF), acetone, methanol (MeOH), acetonitrile (ACN), dimethyl formamide (DMF) and dimethyl sulfoxide (DMSO).

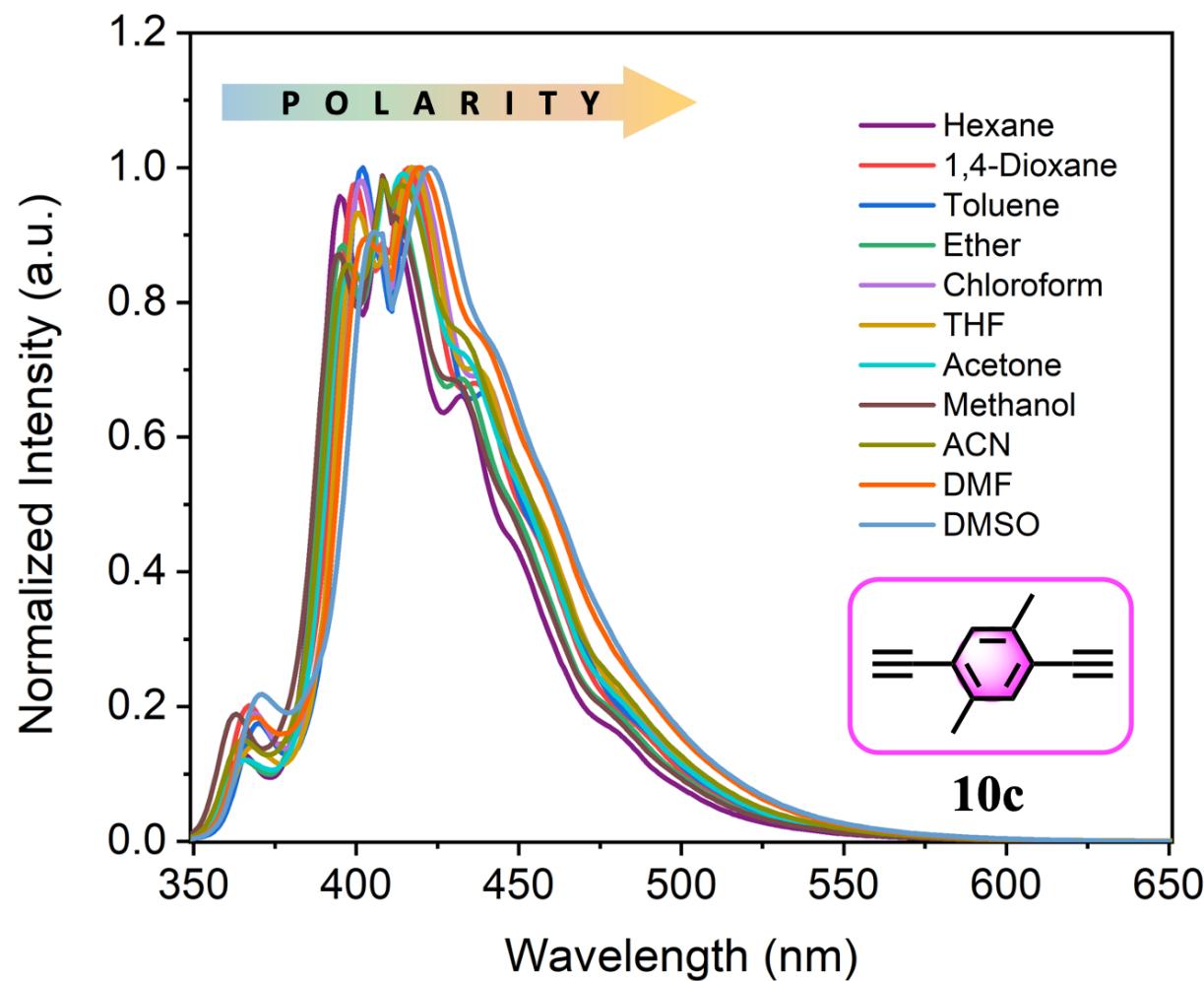


Figure S 10. Photophysical properties of **10c** (4×10^{-6} M): hexane, 1,4-dioxane, toluene, ether, chloroform, tetrahydrofuran (THF), acetone, methanol (MeOH), acetonitrile (ACN), dimethyl formamide (DMF) and dimethyl sulfoxide (DMSO).

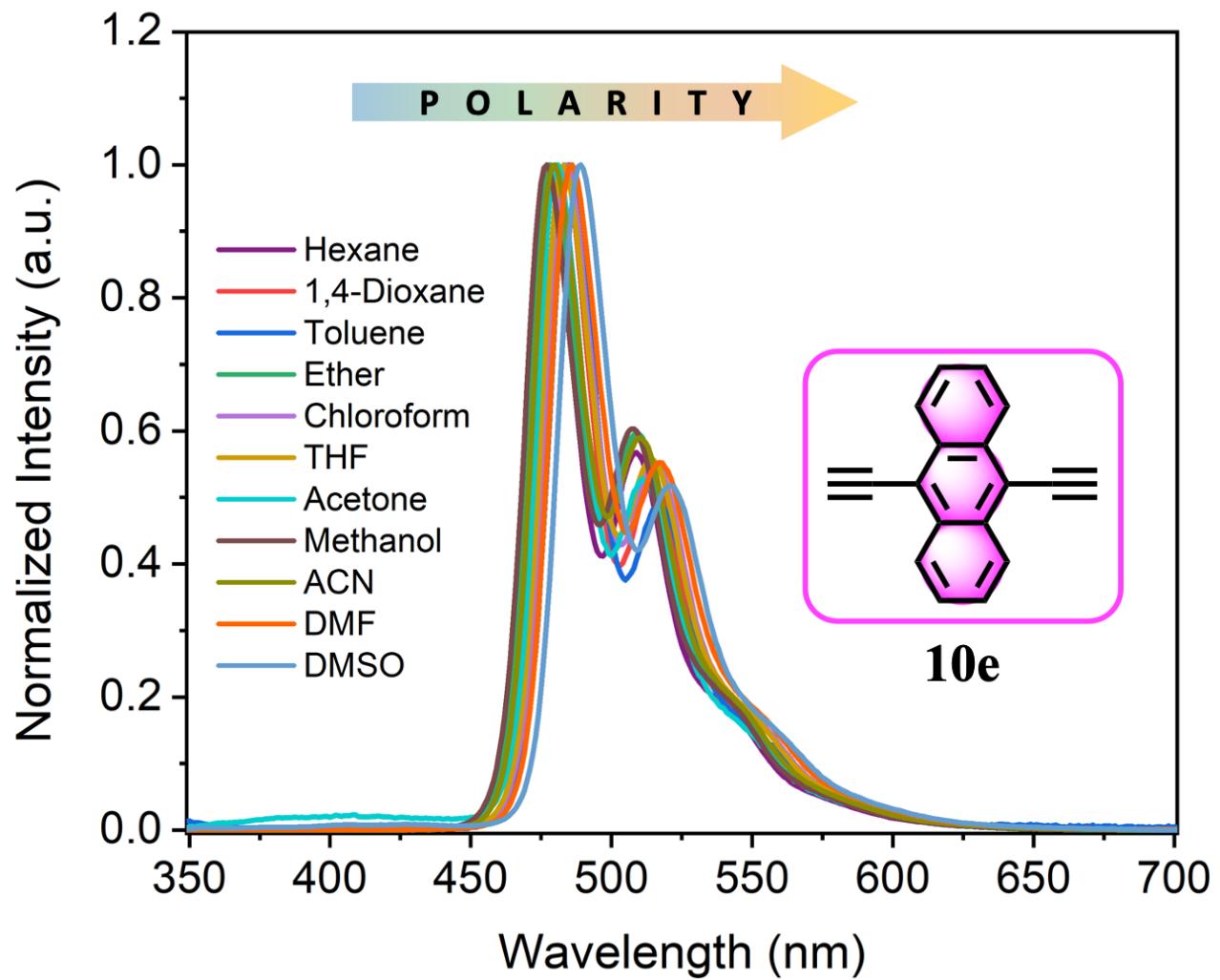


Figure S 11. Photophysical properties of **10e** (4×10^{-6} M): hexane, 1,4-dioxane, toluene, ether, chloroform, tetrahydrofuran (THF), acetone, methanol (MeOH), acetonitrile (ACN), dimethyl formamide (DMF) and dimethyl sulfoxide (DMSO).

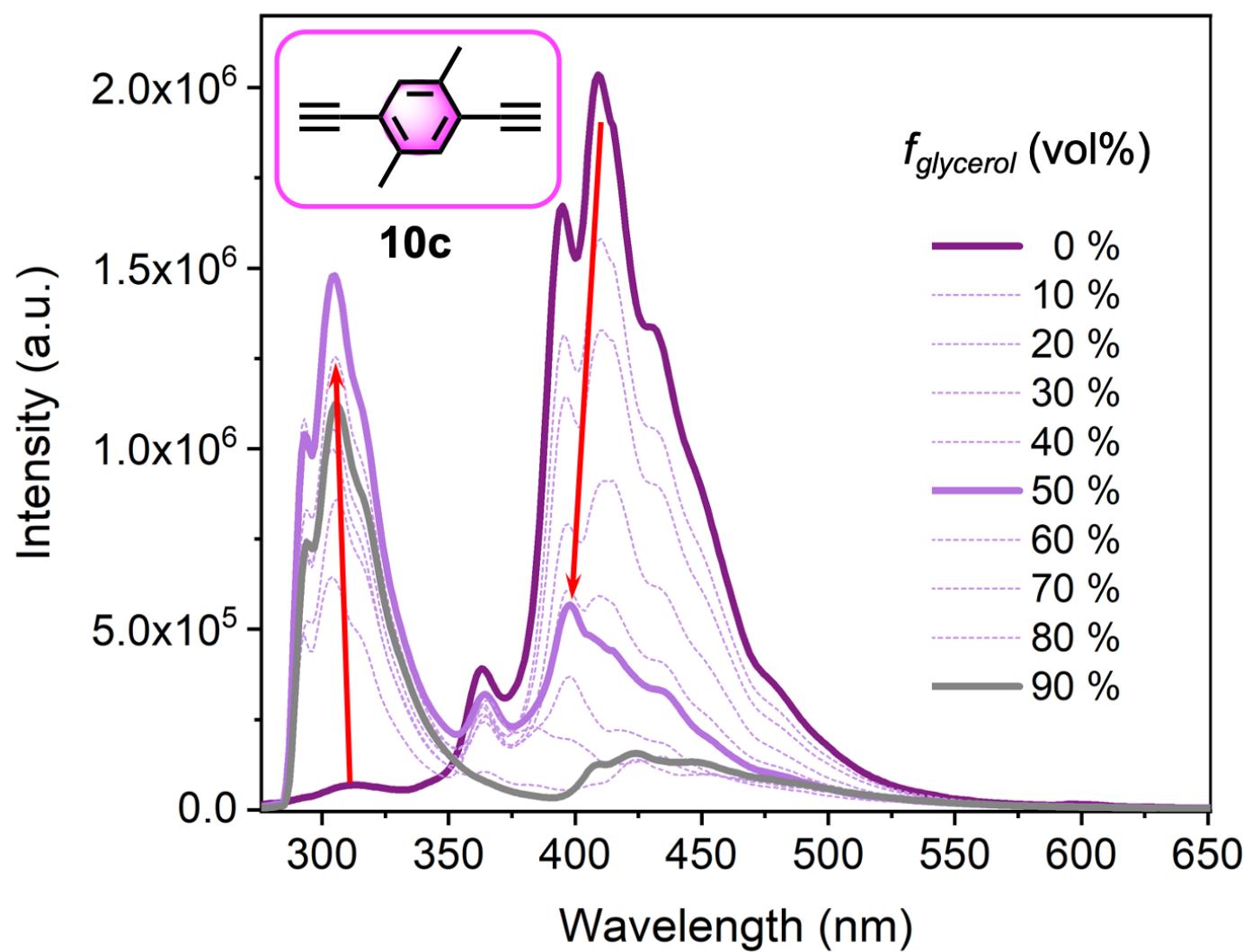


Figure S 12. Emission spectra of **10c** (4 \times 10⁻⁶ M), in mixed solvents of methanol/glycerol.

Solution NMR spectra

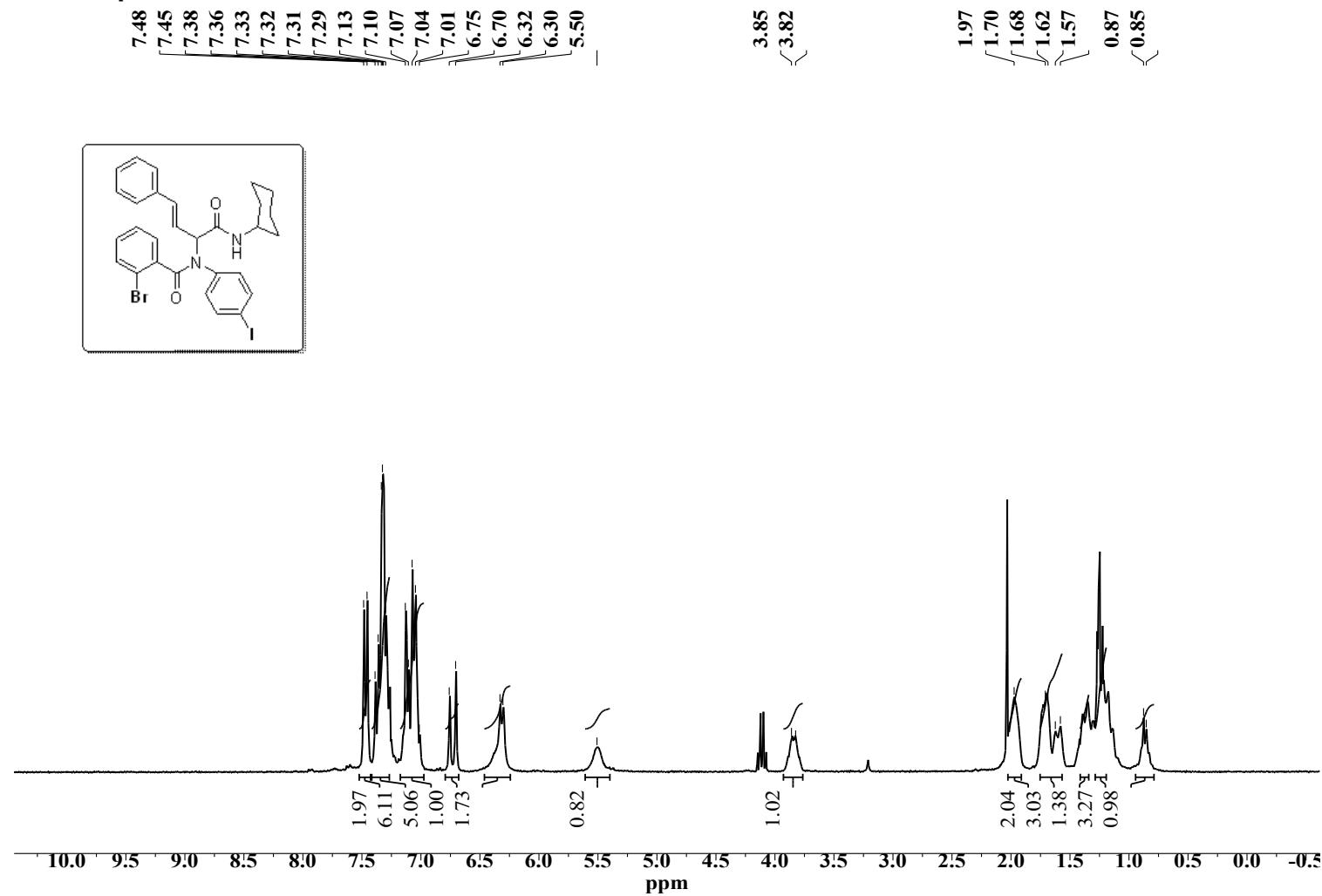


Figure S 13. ^1H NMR of compound **9a** in CDCl_3 at 300 MHz.

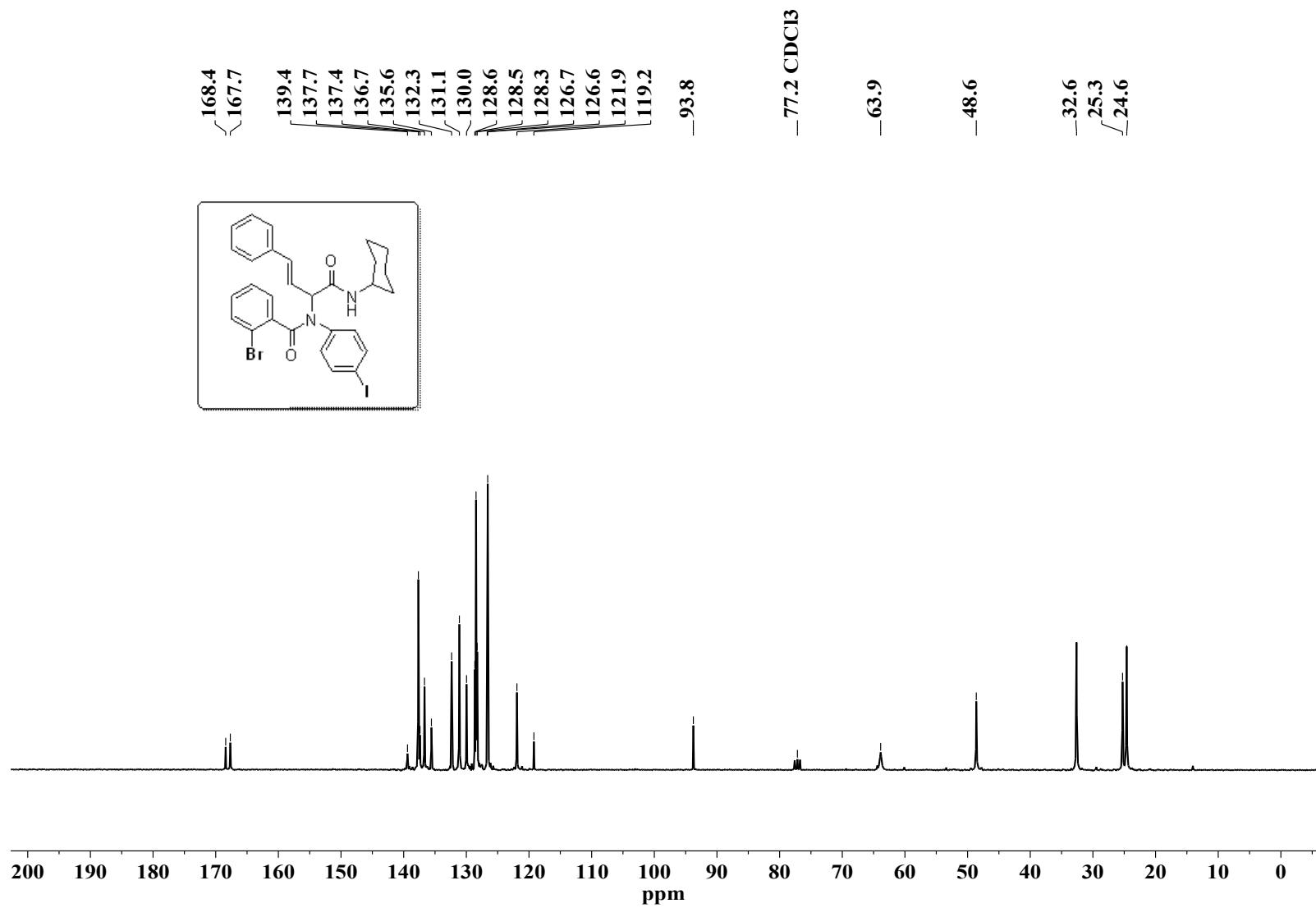


Figure S 14. ^{13}C NMR of compound **9a** in CDCl_3 at 75 MHz.

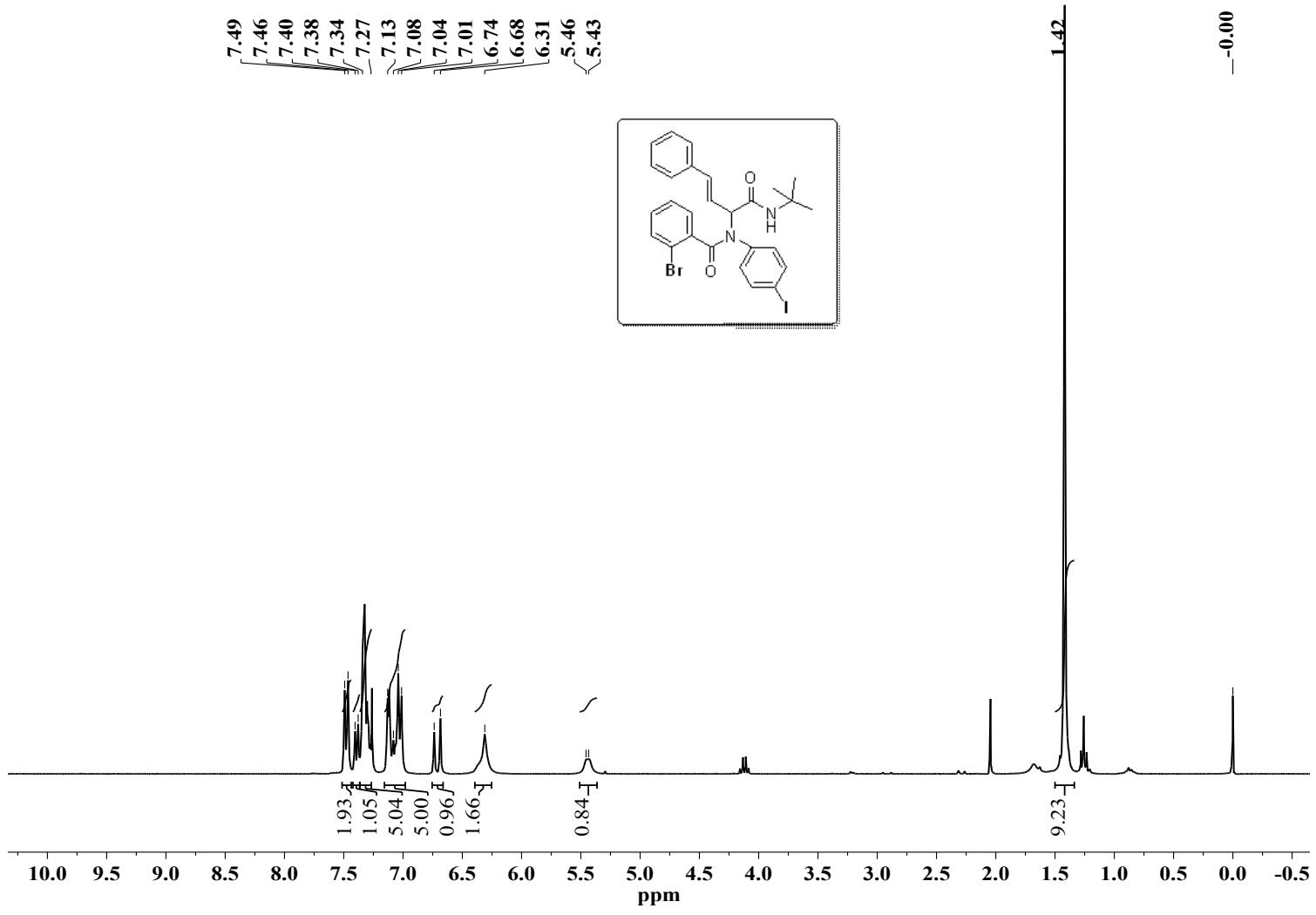


Figure S 15. ^1H NMR of compound **9b** in CDCl_3 at 300 MHz.

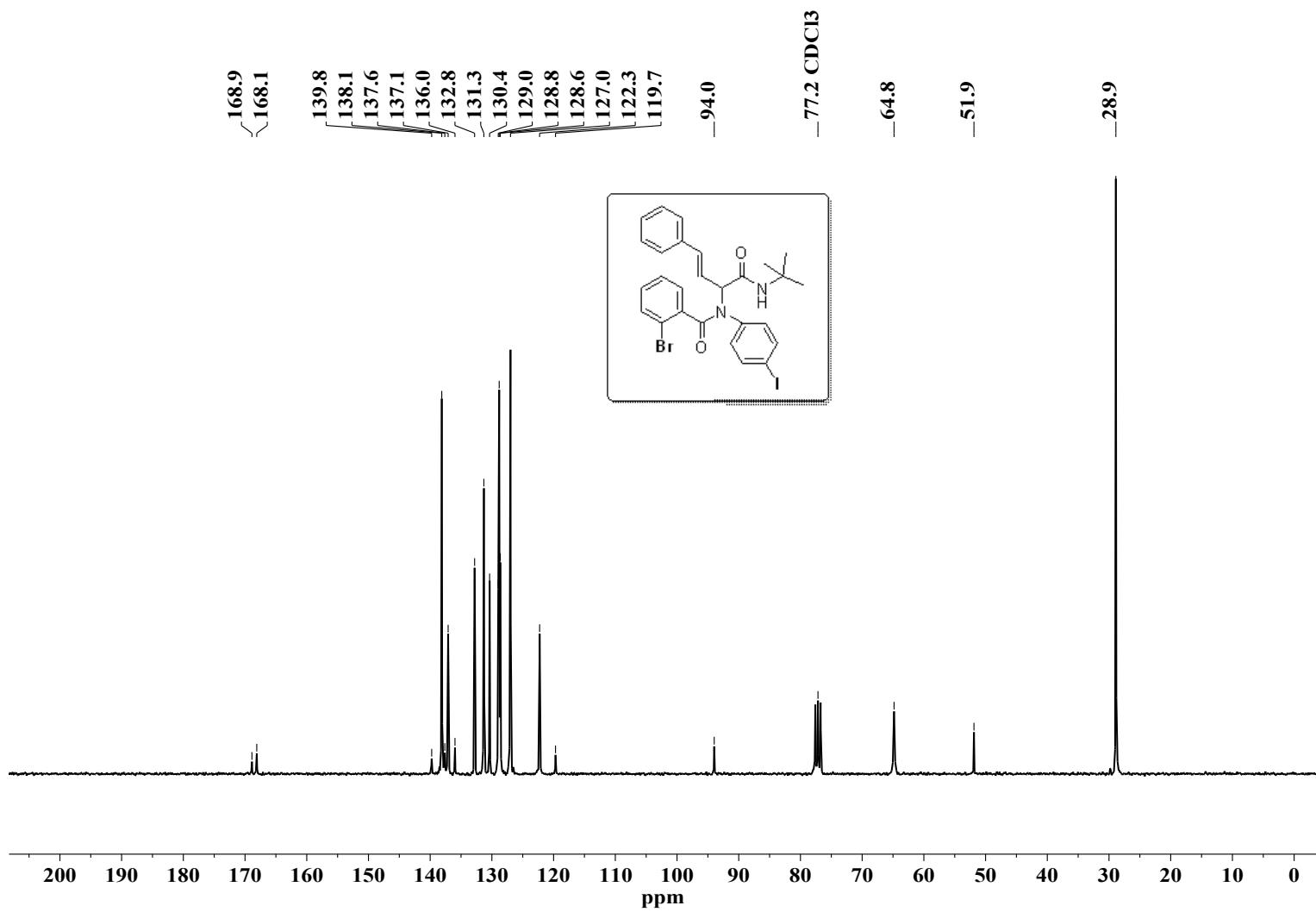


Figure S 16. ^{13}C NMR of compound **9b** in CDCl_3 at 75 MHz

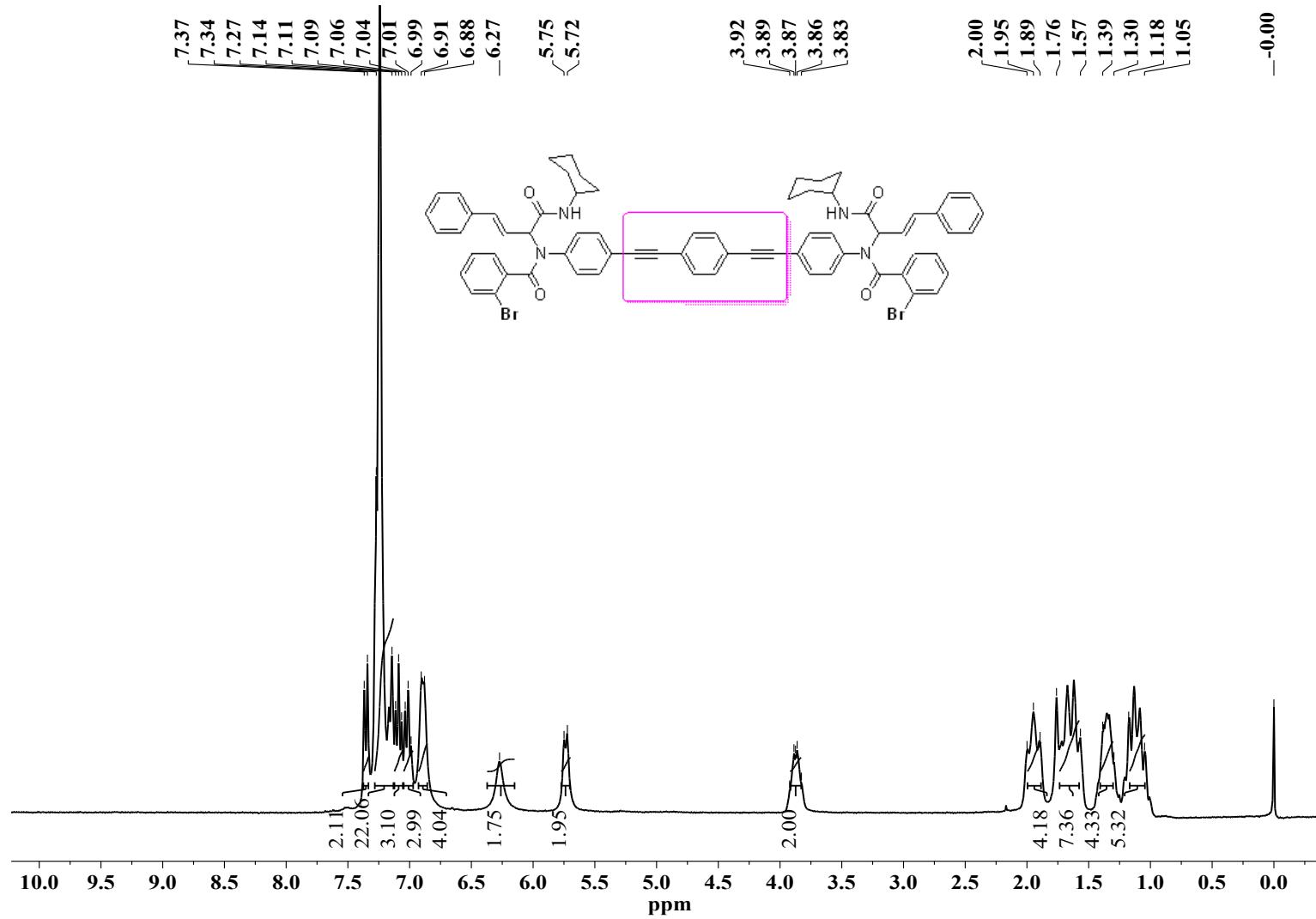


Figure S 17. ^1H NMR of rotor **10a** in CDCl_3 at 300 MHz

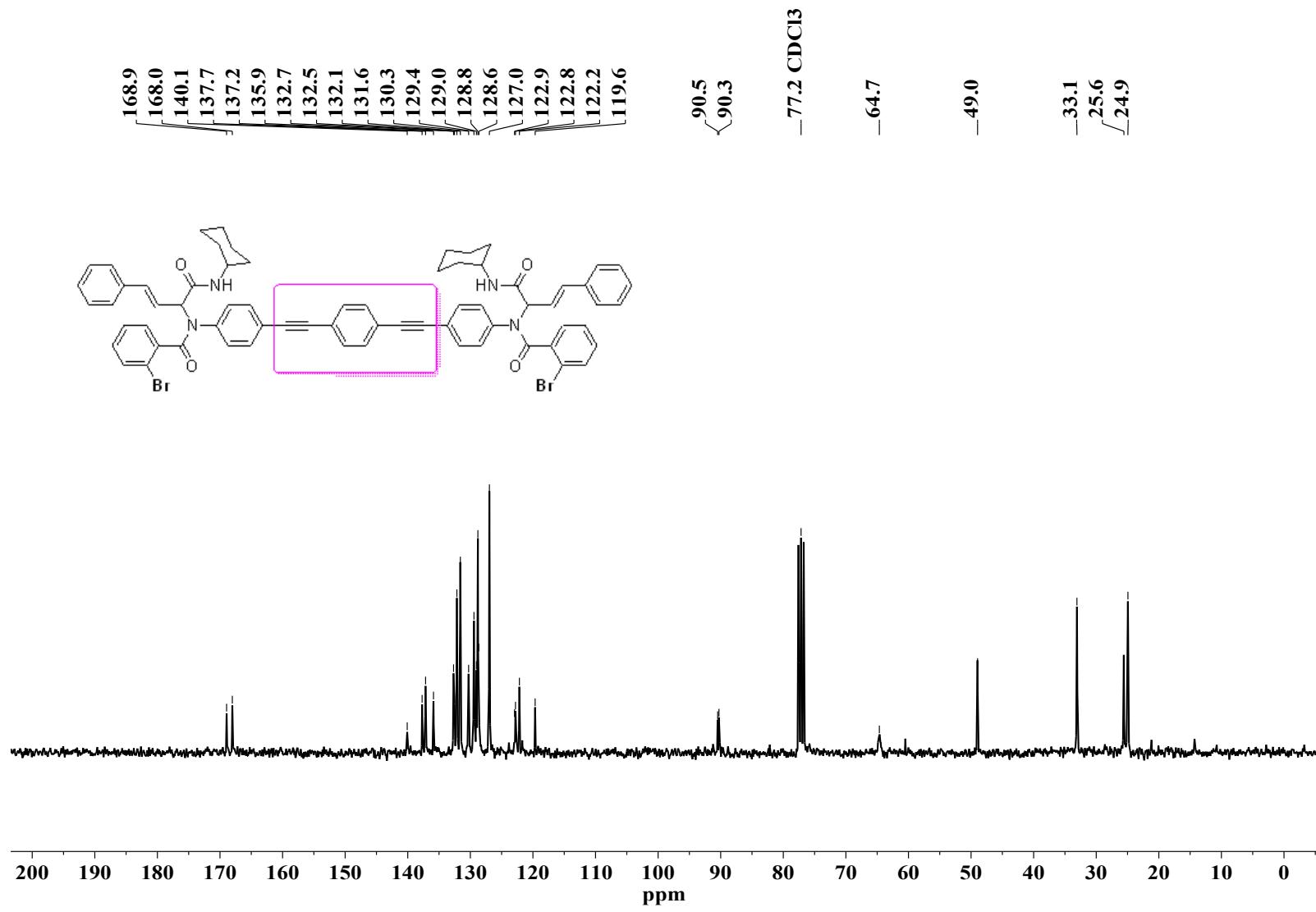


Figure S 18. ^{13}C NMR of rotor 10a in CDCl_3 at 75 MHz.

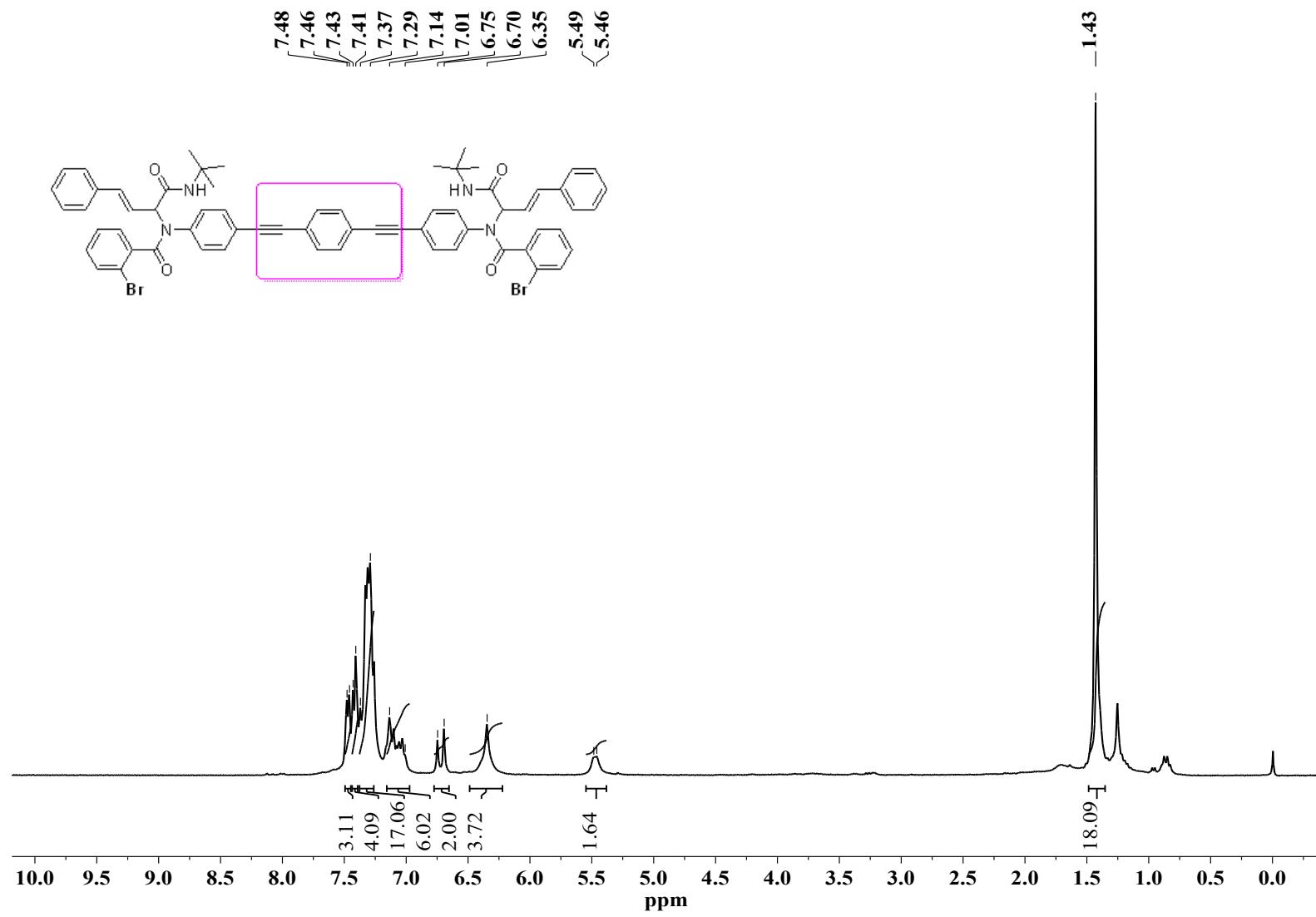


Figure S 19. ^1H NMR of rotor **10b** in CDCl_3 at 300 MHz.

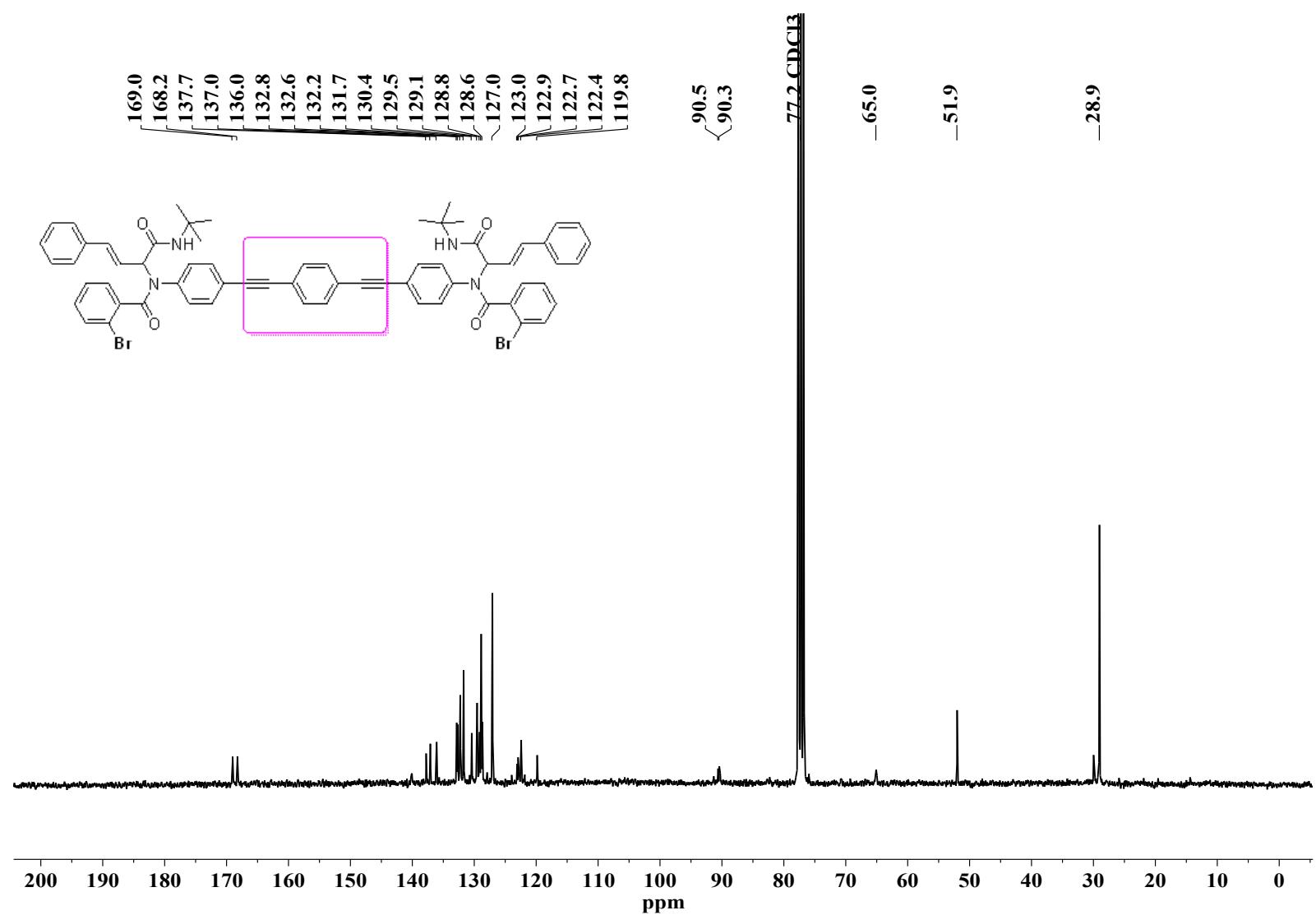


Figure S 20. ^{13}C NMR of **10b** in CDCl_3 at 75 MHz.

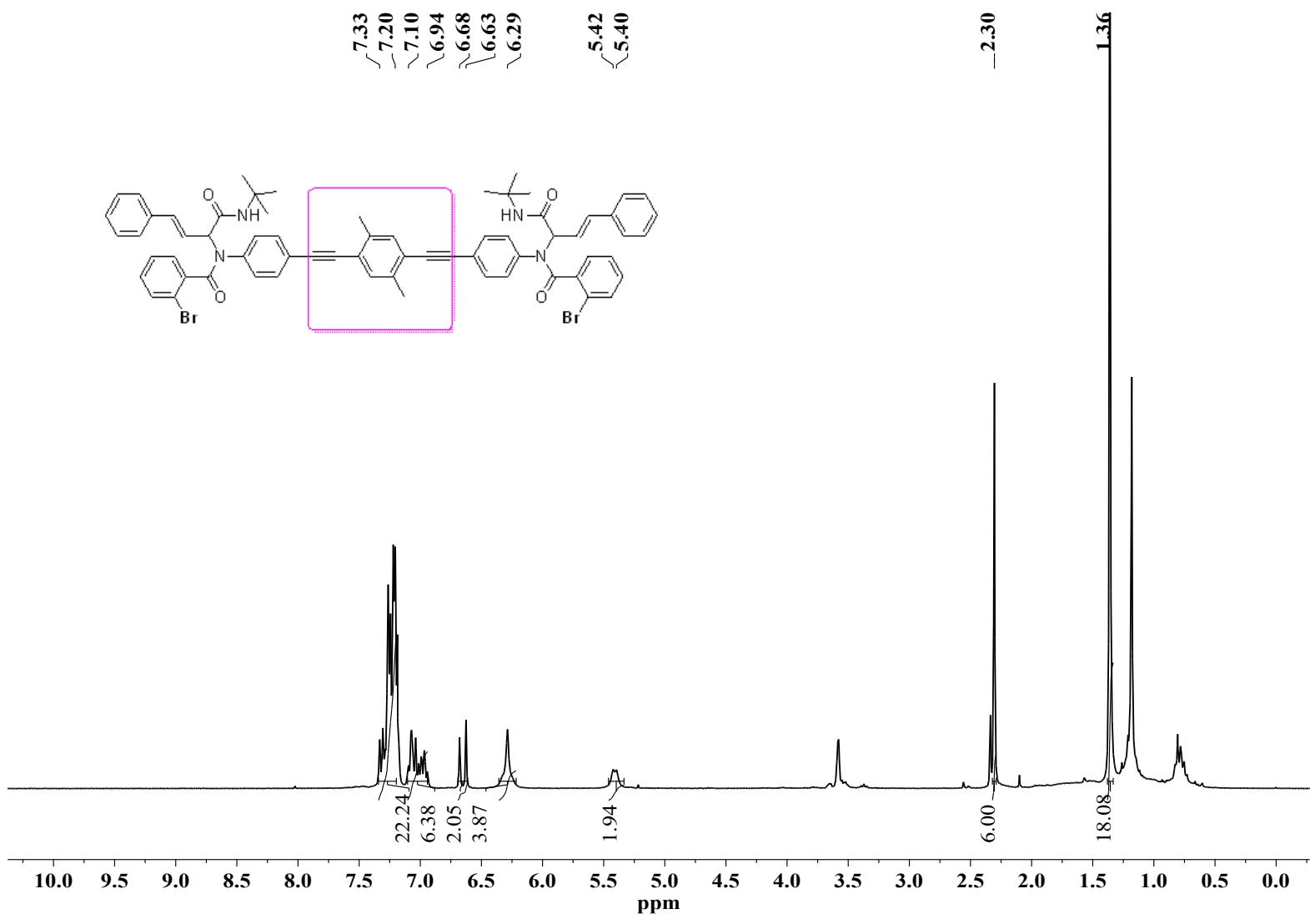


Figure S 21. ^1H NMR of rotor **10c** in CDCl_3 at 300 MHz.

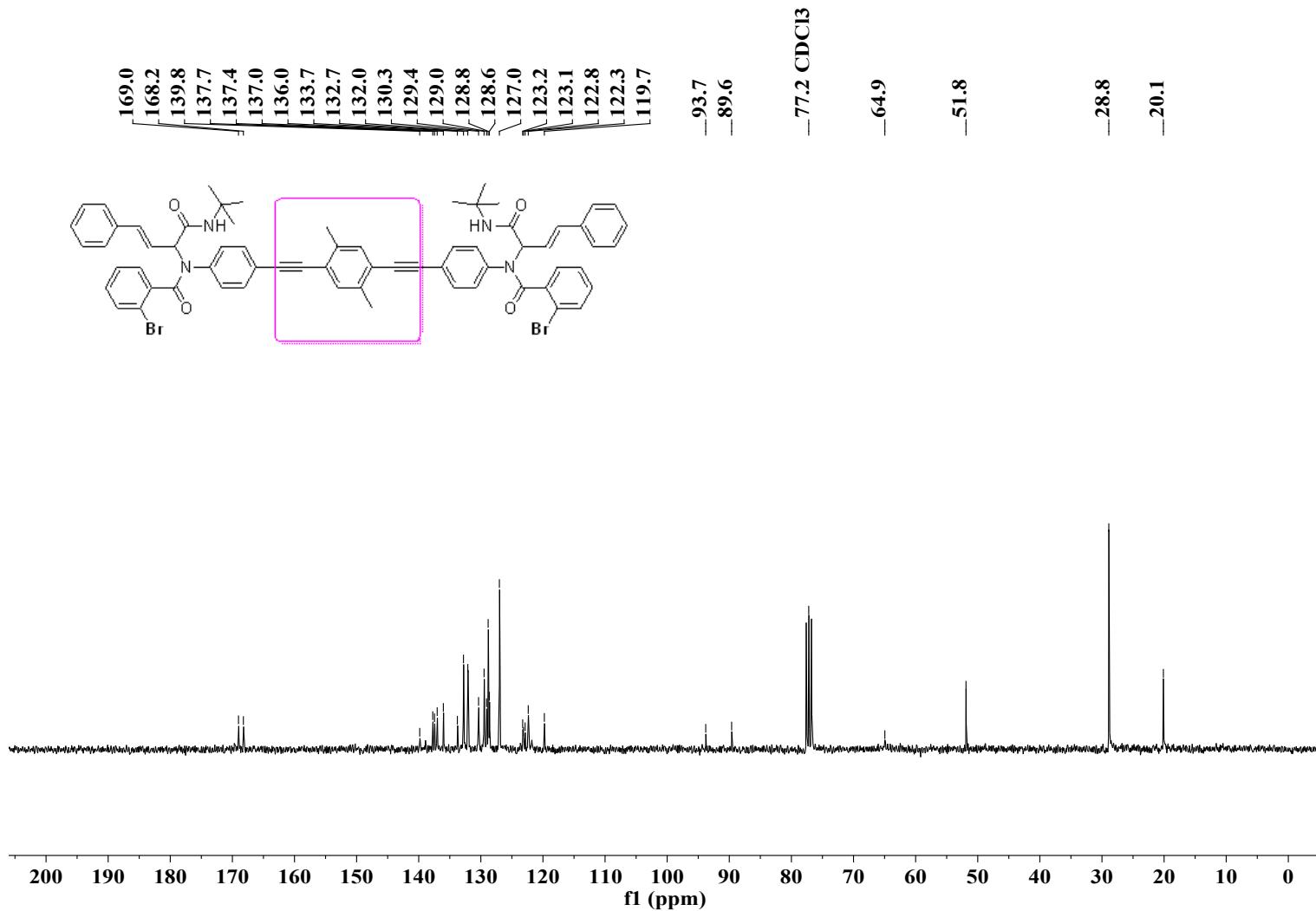


Figure S 22. ^{13}C NMR of rotor **10c** in CDCl_3 at 75 MHz.

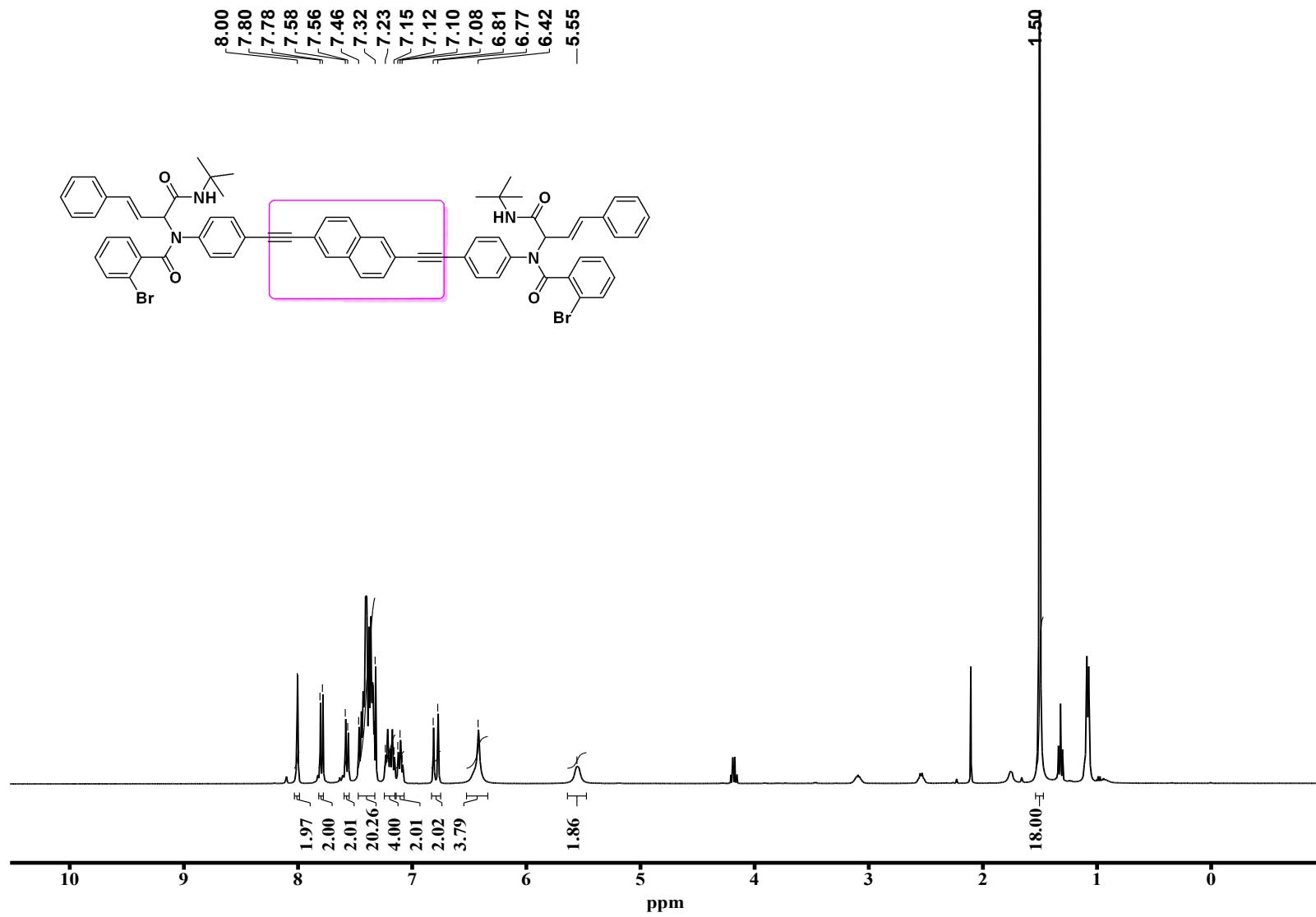


Figure S 23. ^1H NMR of rotor **10d** in CDCl_3 at 400 MHz.

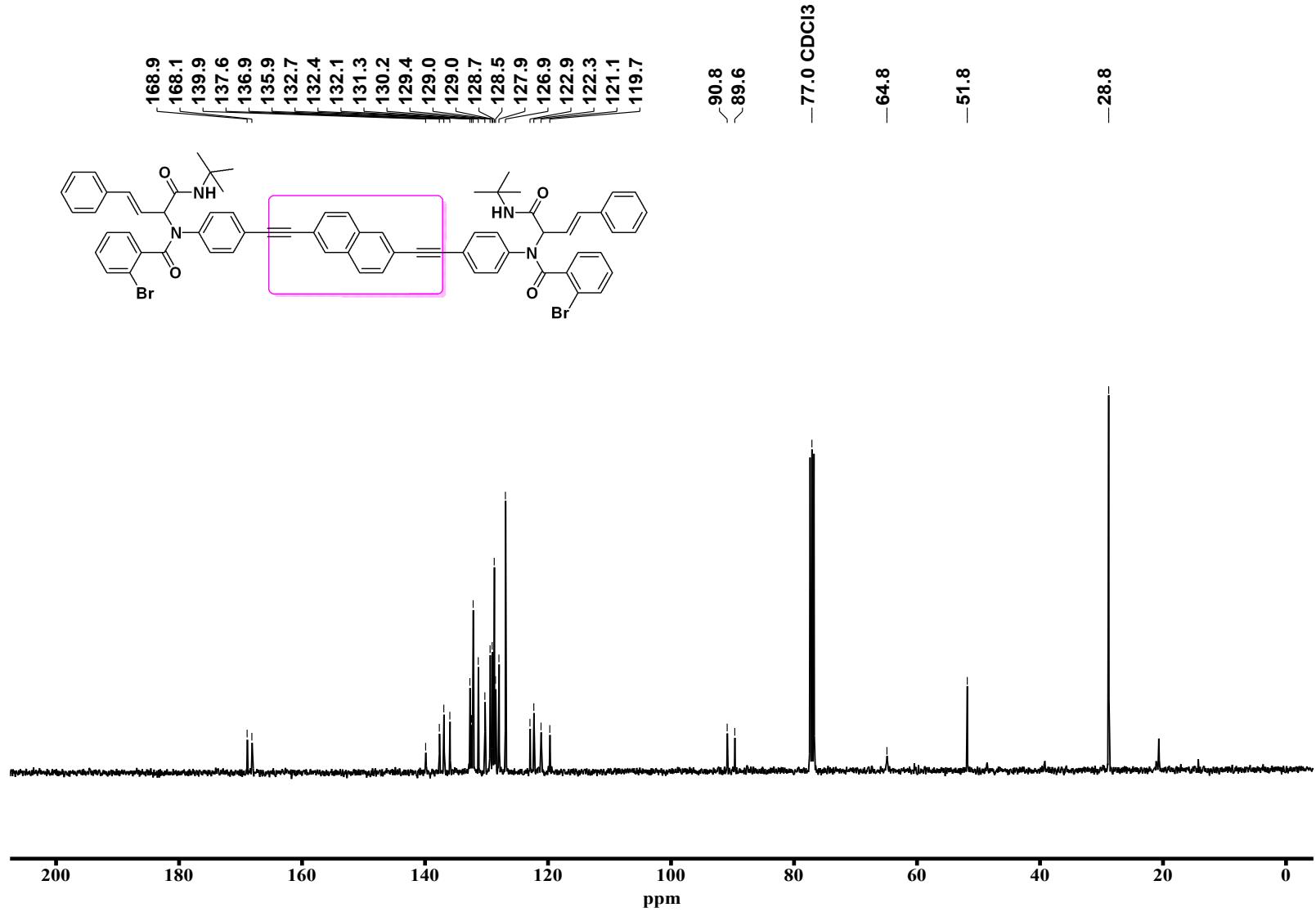


Figure S 24. ^{13}C NMR of rotor **10d** in CDCl_3 at 100 MHz.

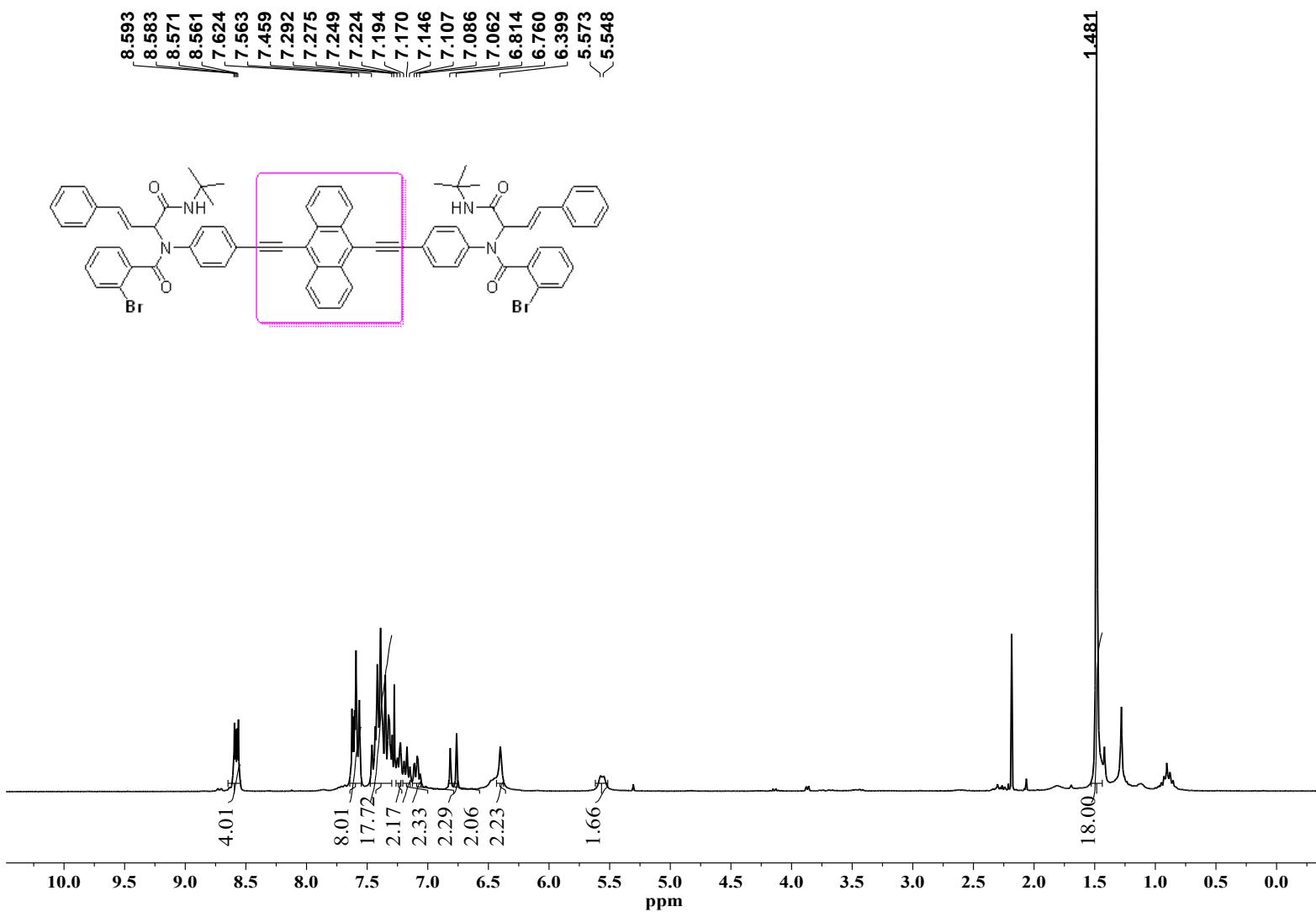


Figure S 25. ^1H NMR of rotor **10e** in CDCl_3 at 300 MHz.

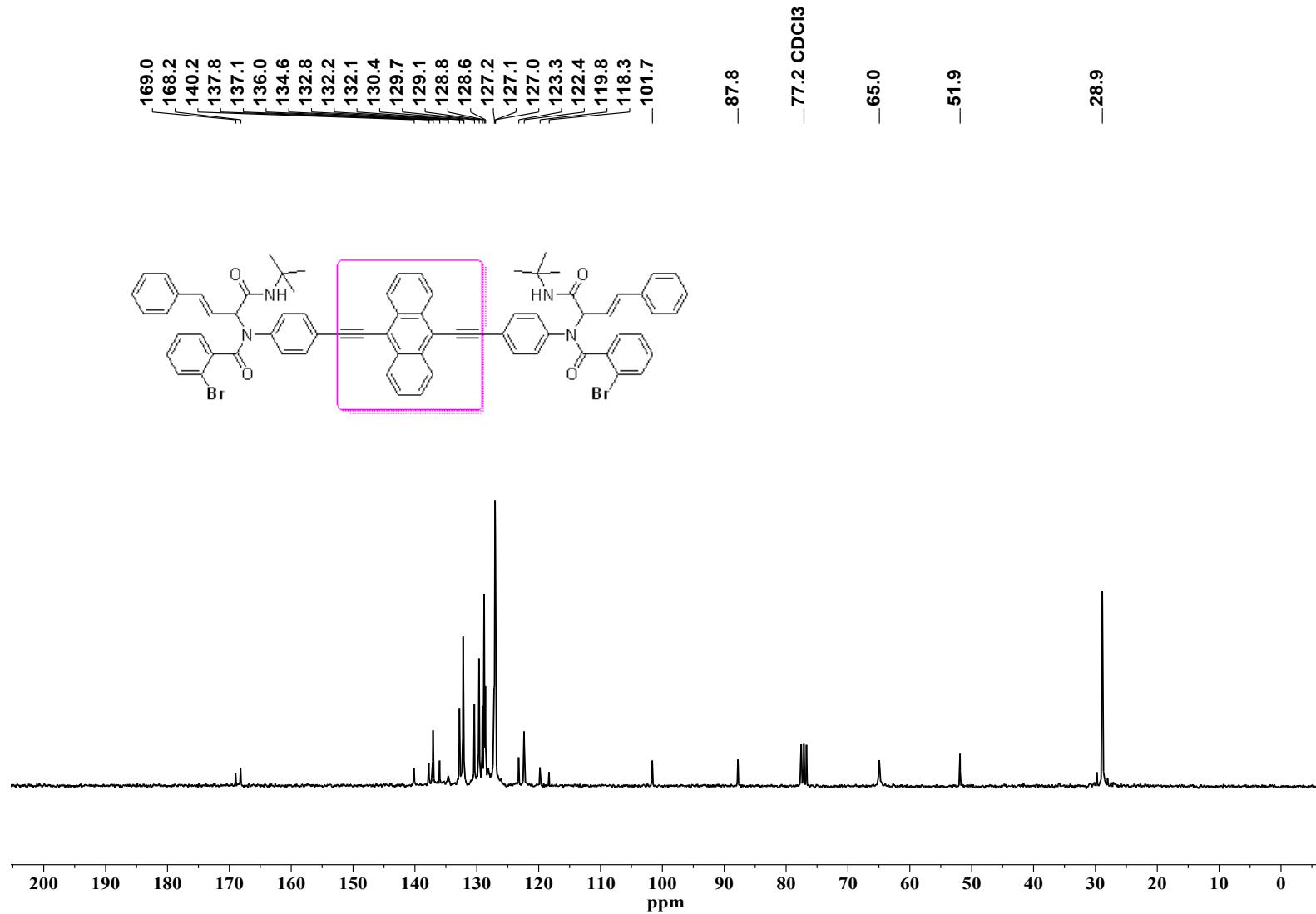


Figure S 26. ^{13}C NMR of rotor **10e** in CDCl_3 at 75 MHz.

MS spectra

In all cases, the experimental isotopic distributions are consistent with the calculated ones.

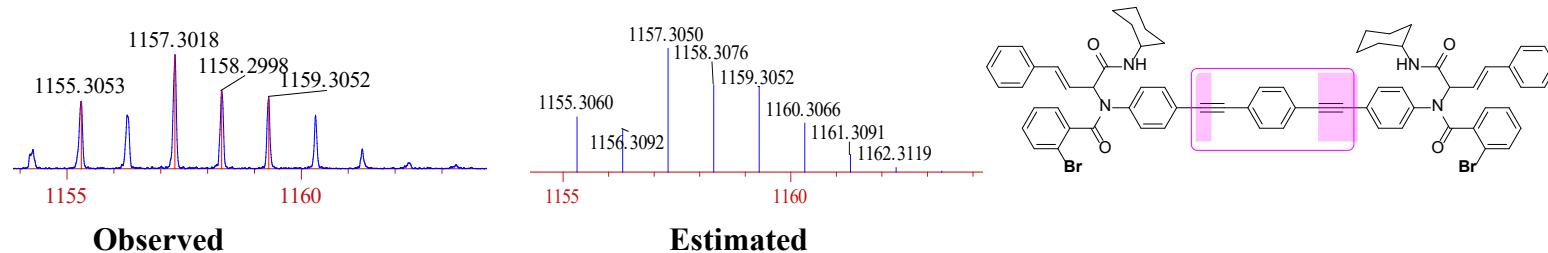


Figure S 27. High resolution FAB-MS spectra of **rotor 10a**.

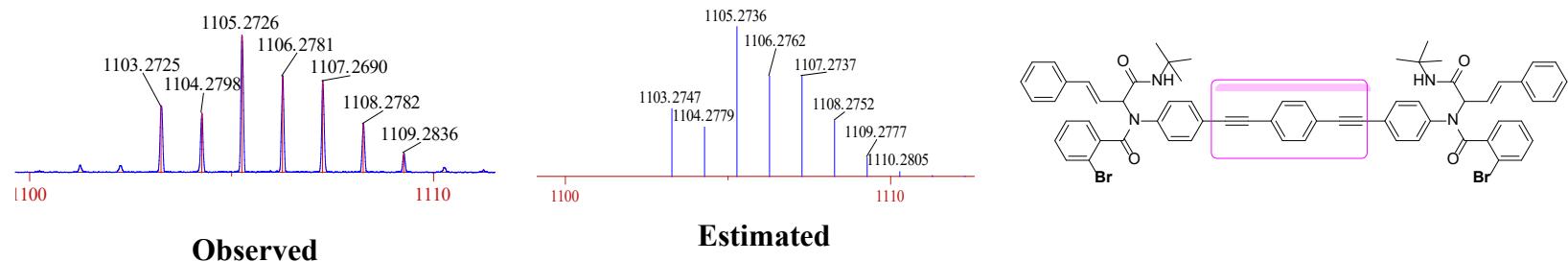


Figure S 28. High resolution FAB-MS spectra of **rotor 10b**.

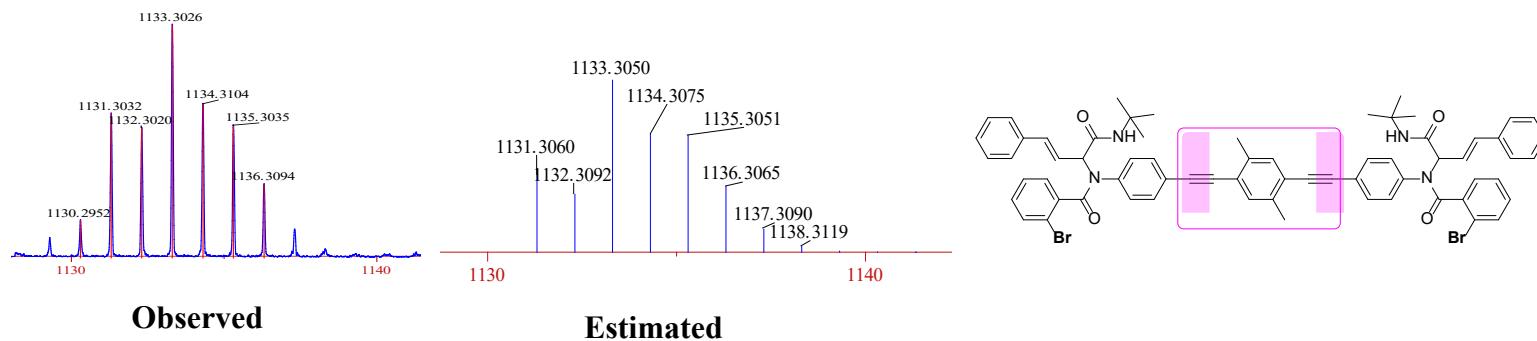


Figure S 29. High resolution FAB-MS spectra of **rotor 10c**.

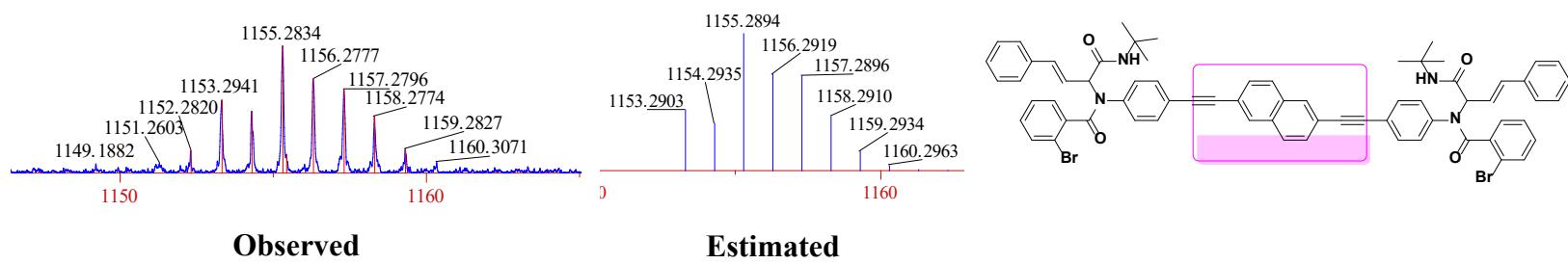


Figure S 30. High resolution FAB-MS spectra of **rotor 10d**.

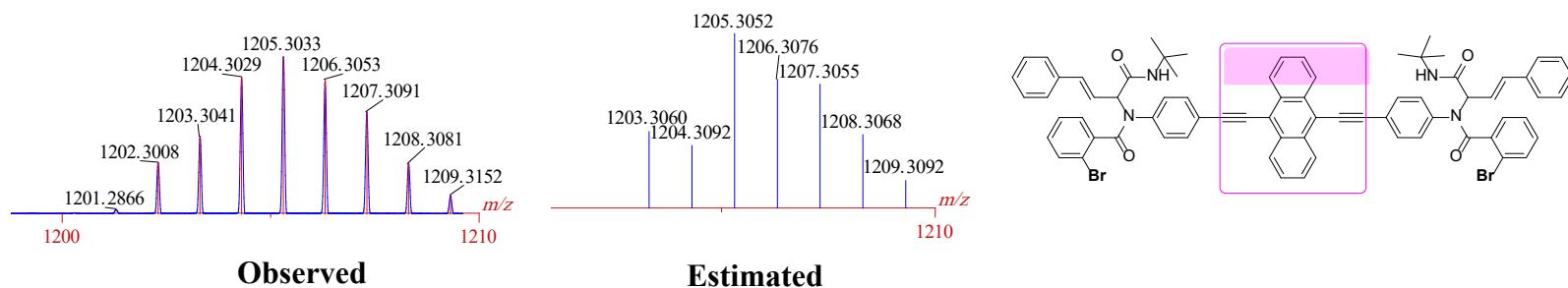


Figure S 31. High resolution FAB-MS spectra of **rotor 10e**.