

Supplementary Material

Enhanced Activity in the Tosylation of Tolanophanes via Supramolecular HgCl₂ Recognition

Saeed Rastgar,^A Hossein Reza Darabi,^{A,B} Leila Sobhani,^A Kioumars Aghapoor,^A Rohoullah Firouzi,^A Farshid Mohsenzadeh,^A Hamed Yaghobi,^A and Farshad Jafary^A

^ANano and Organic Synthesis Lab, Chemistry and Chemical Engineering Research Center of Iran, Pajooresh Blvd, km 17, Karaj Highway, Tehran 14968-13151, Iran.

^BCorresponding author. Email: darabi@ccerci.ac.ir

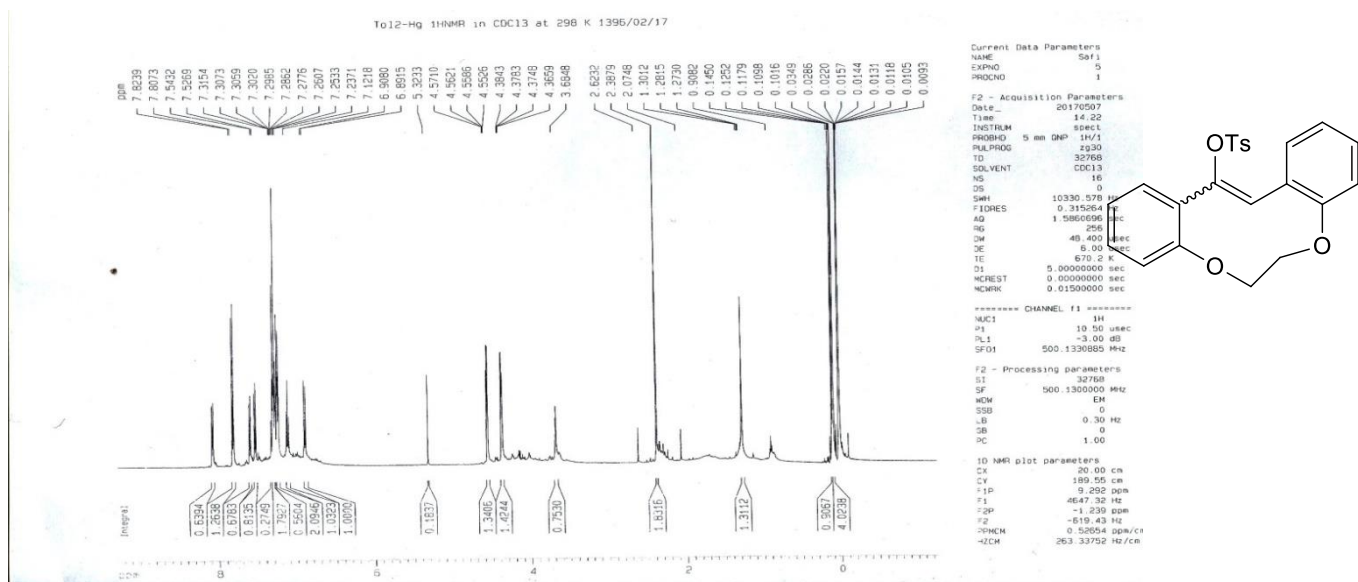


Fig S1. ¹H NMR spectrum of isomeric mixture of **5a** (E/Z = 95:5).

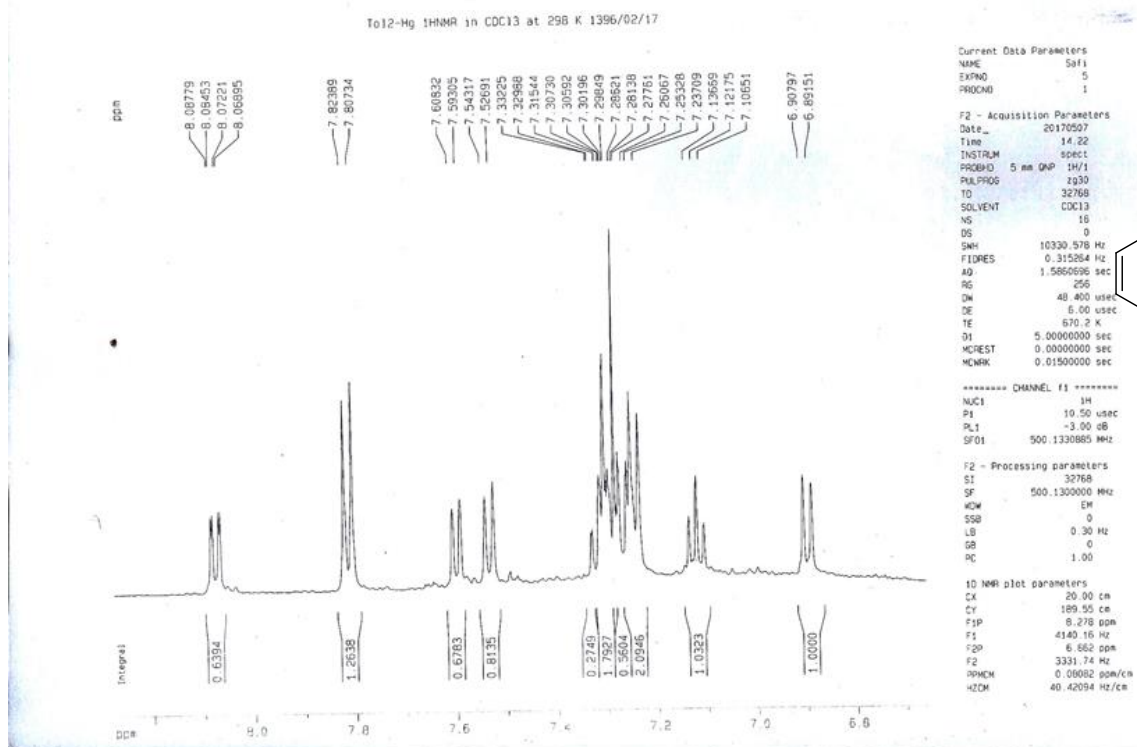


Fig S2. ¹H NMR spectrum of **5a** (E/Z = 95:5).

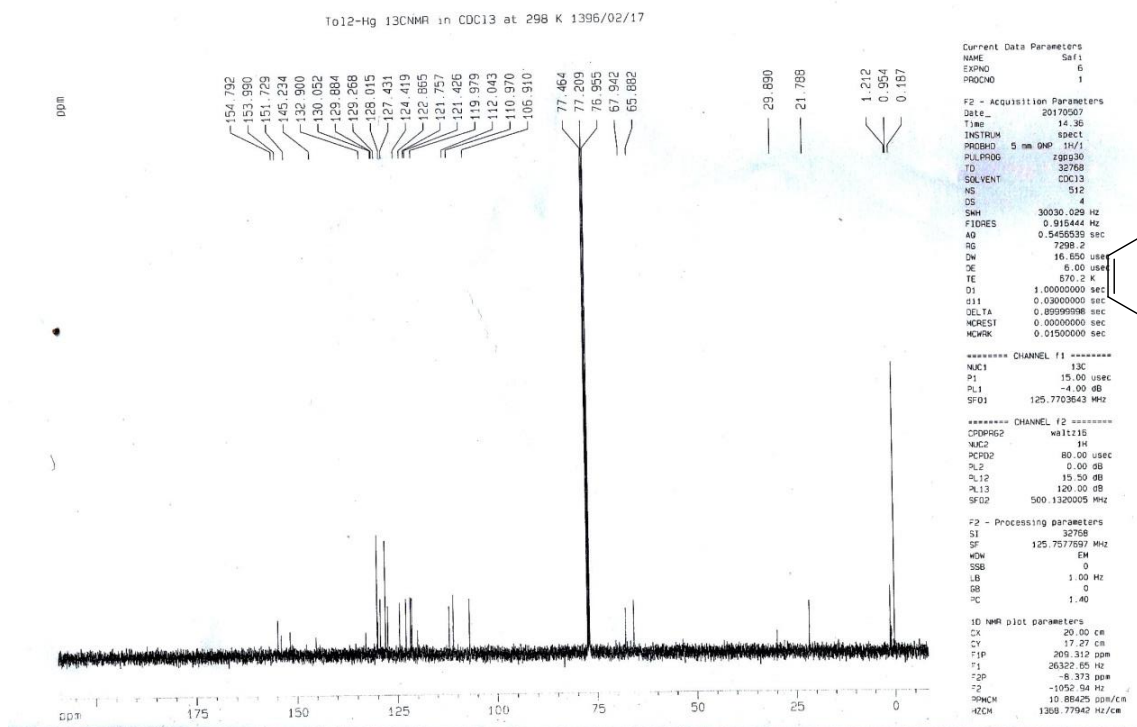


Fig S3. ¹³C NMR spectrum of **5a**

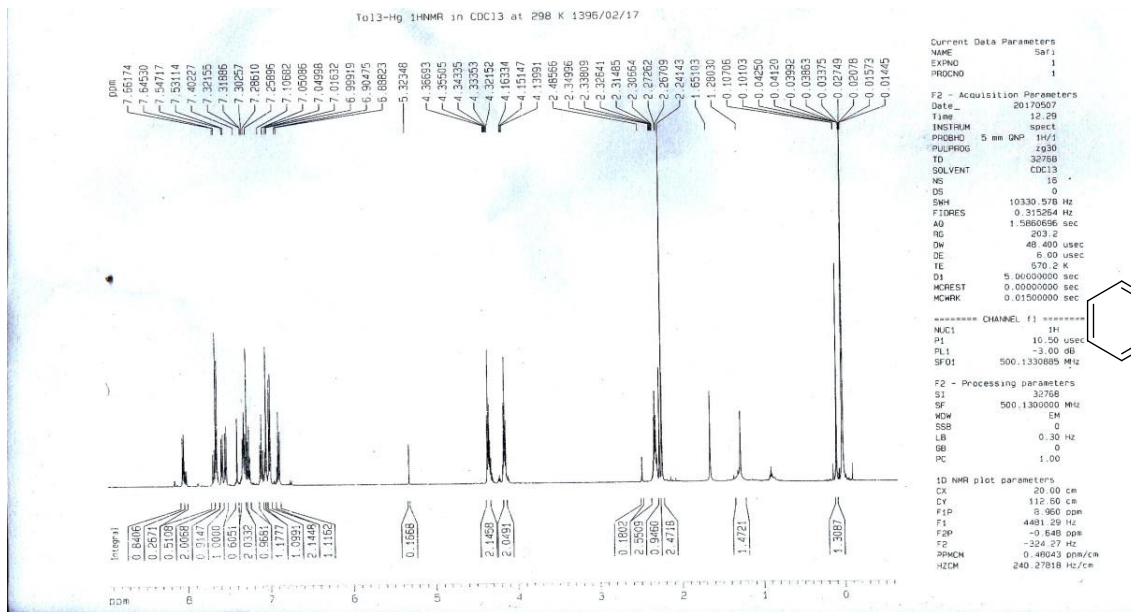


Fig S4. ¹H NMR spectrum of **5b** (E/Z = 75:25).

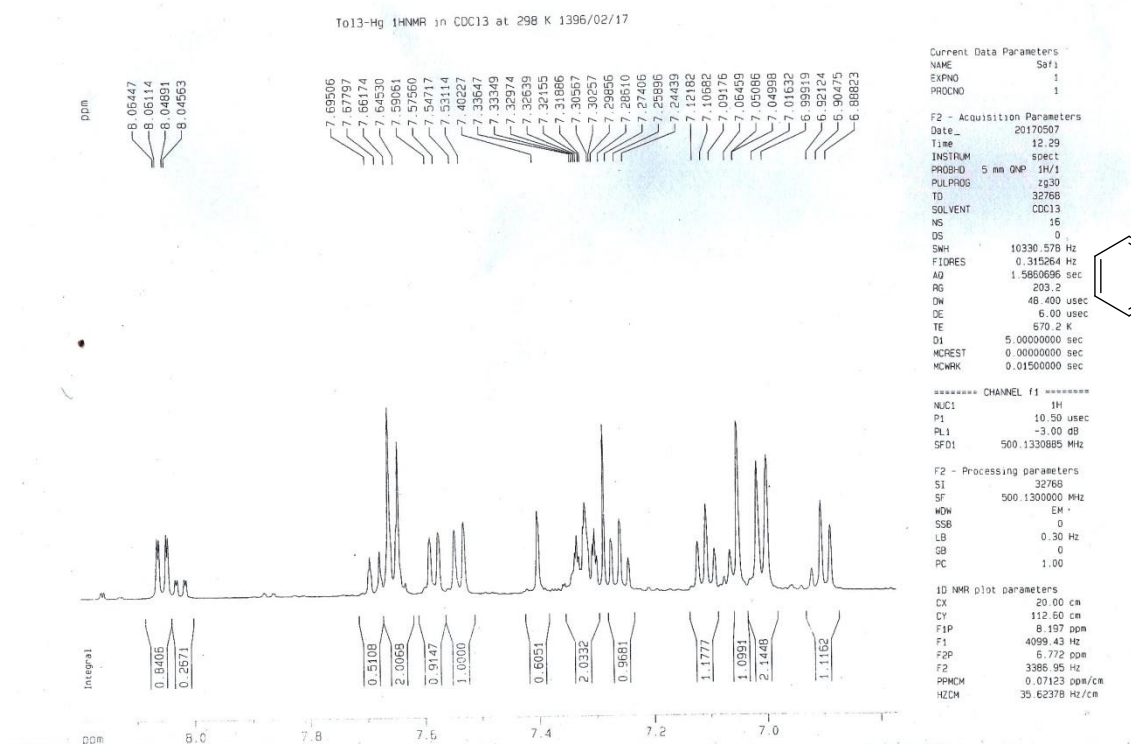


Fig S5. ¹H NMR spectrum of **5b** (E/Z = 75:25).

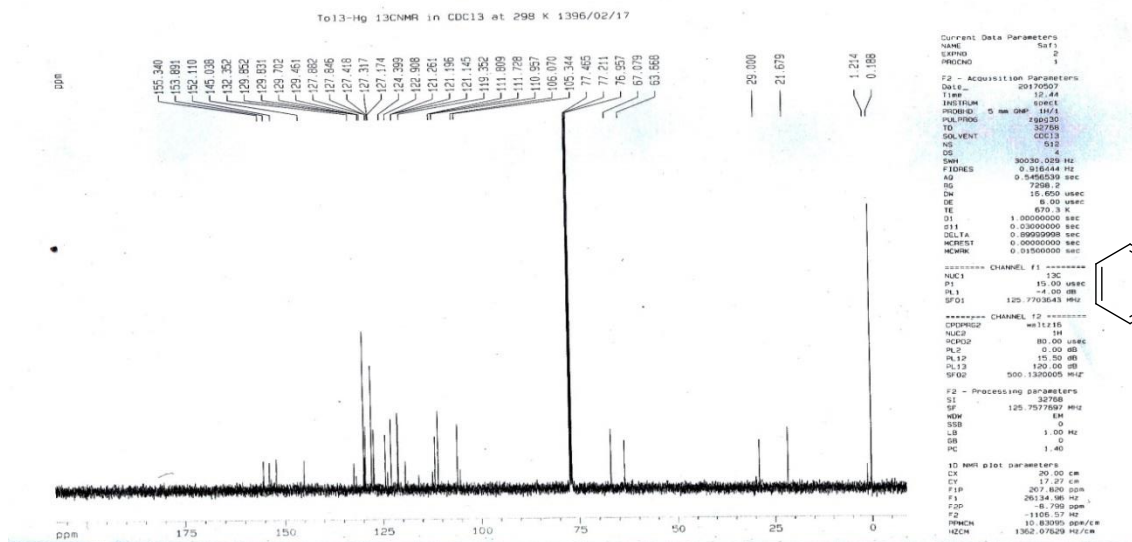


Fig S6. ¹³C NMR spectrum of **5b**

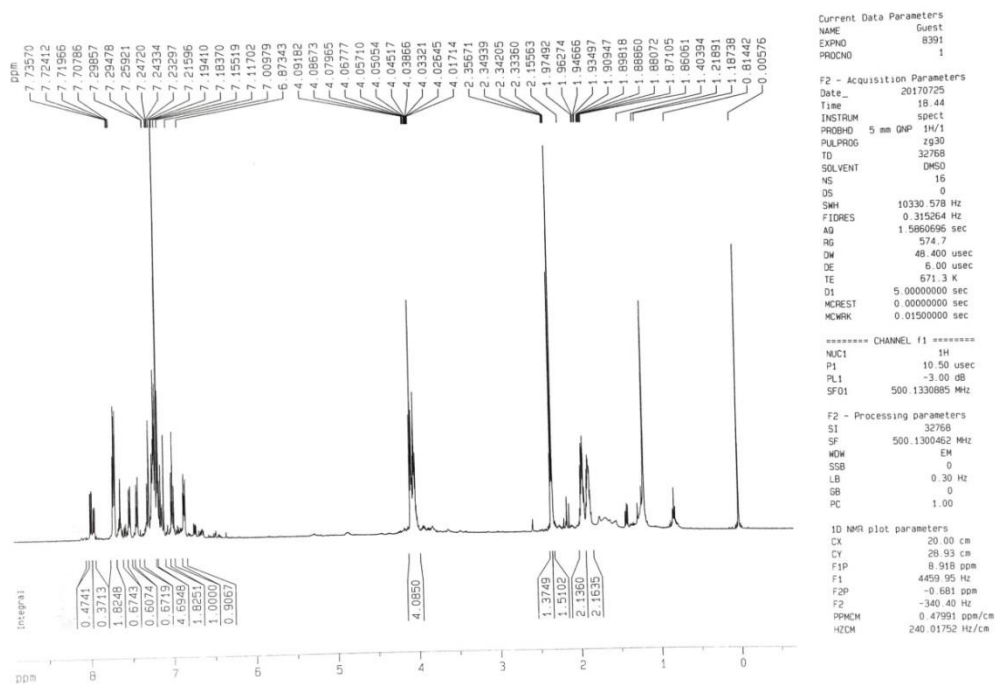


Fig S7. ¹H NMR spectrum of **5c** (E/Z = 40:60).

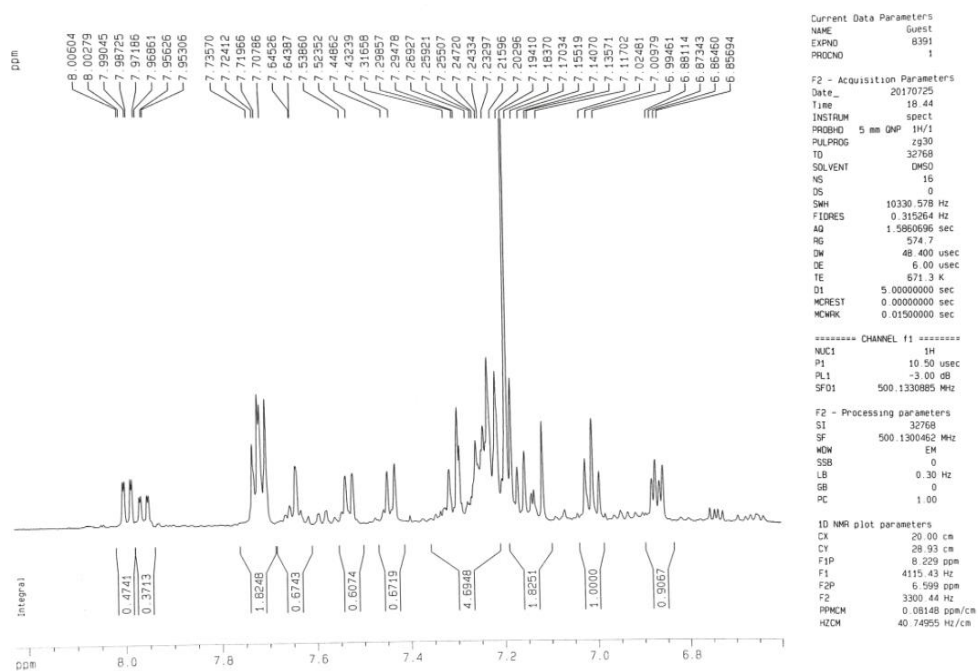
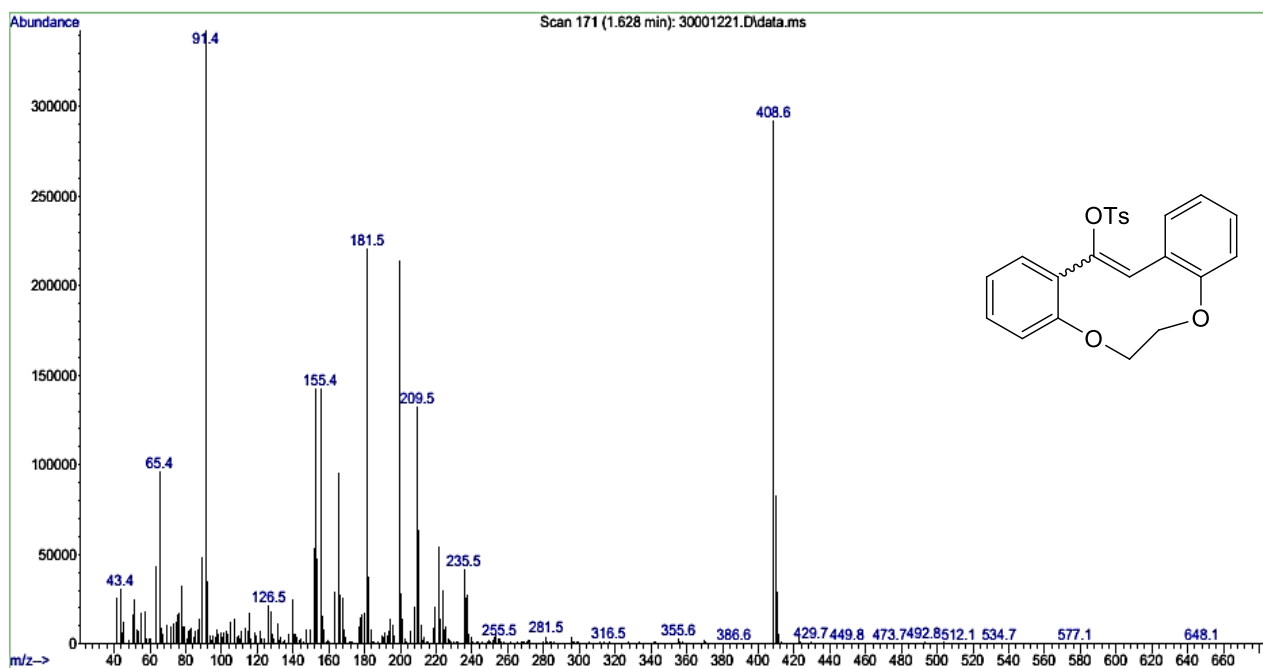


Fig S8. ¹H NMR spectrum of **5c** (E/Z = 40:60).



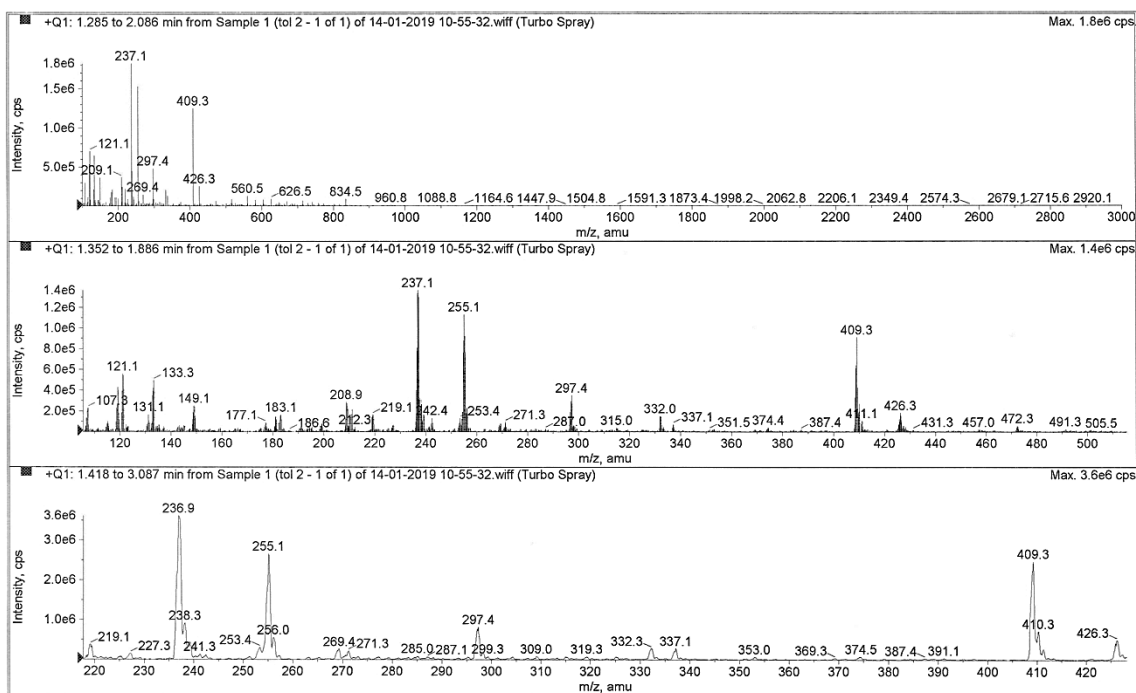
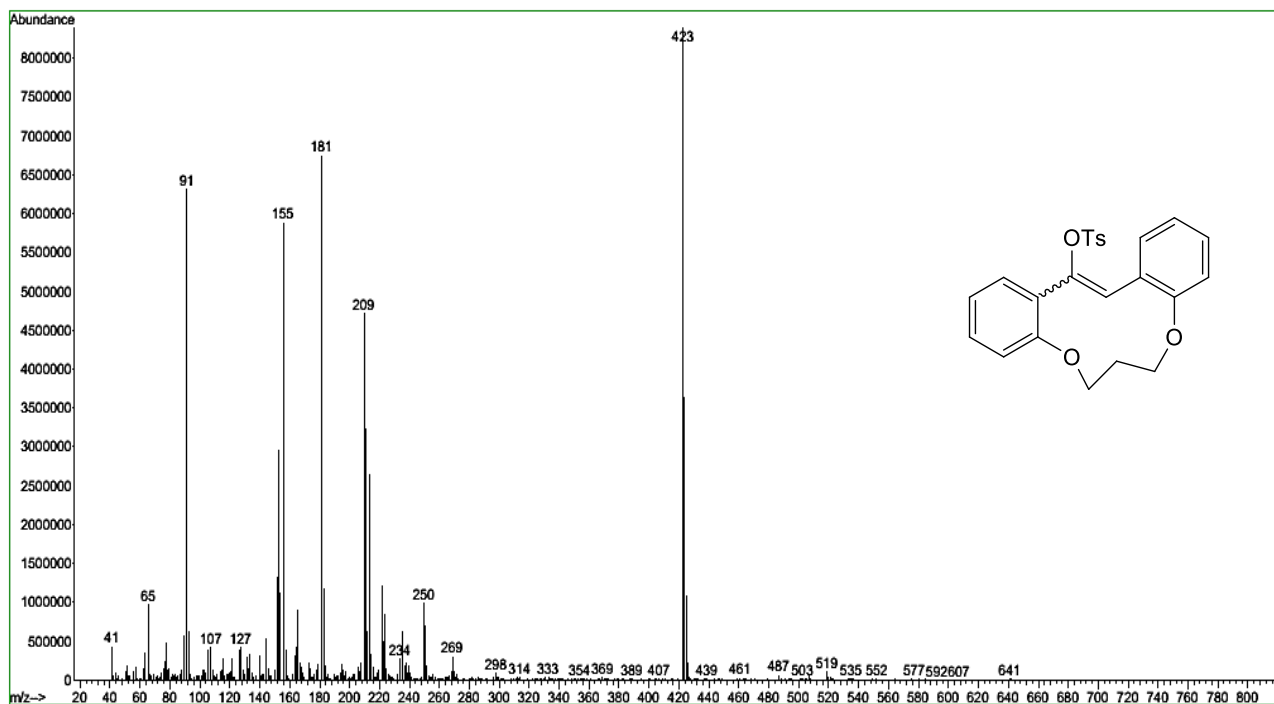


Fig S9. Mass spectrum and LC-Mass spectrum of **5a**



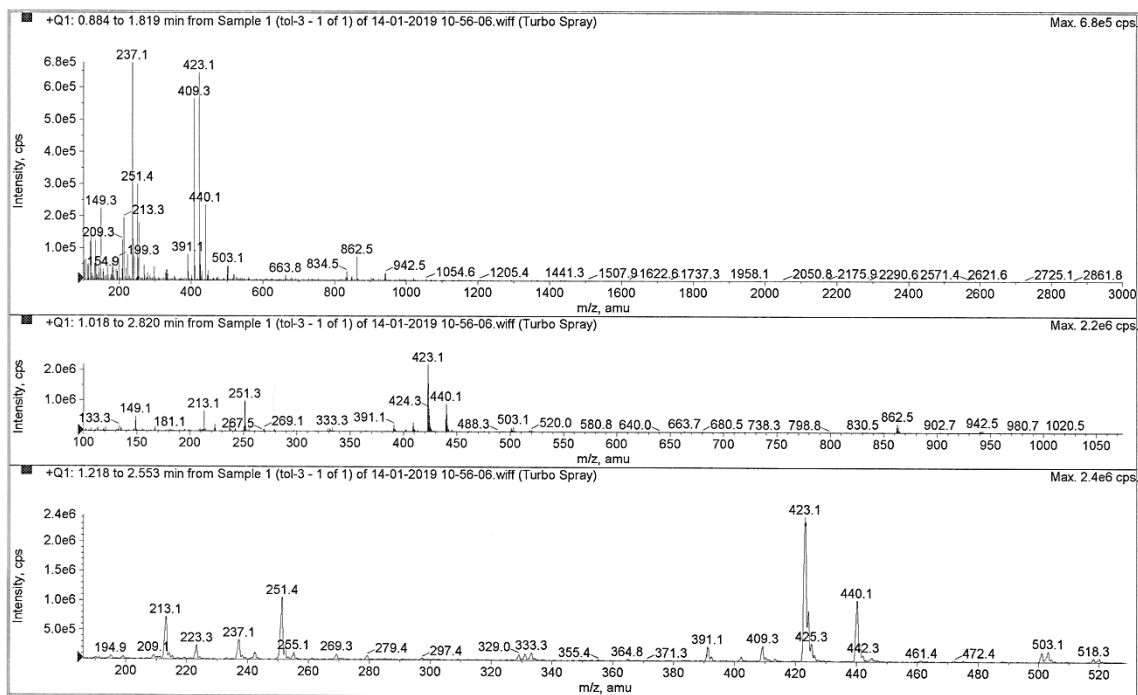
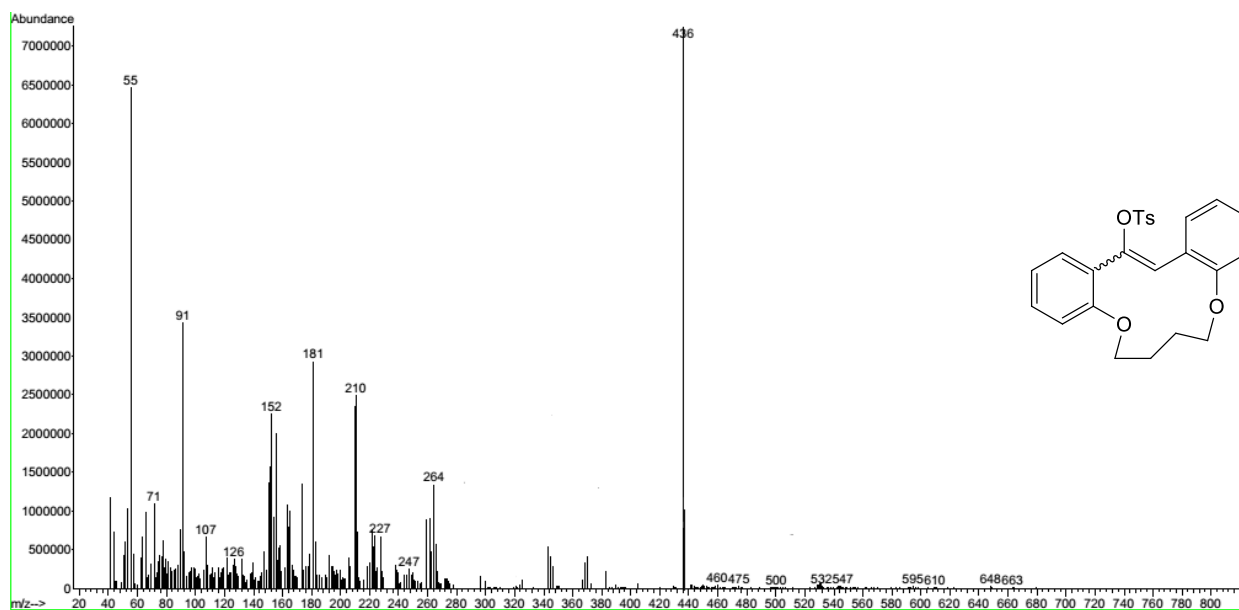


Fig S10. Mass spectrum and LC-Mass spectrum of **5b**



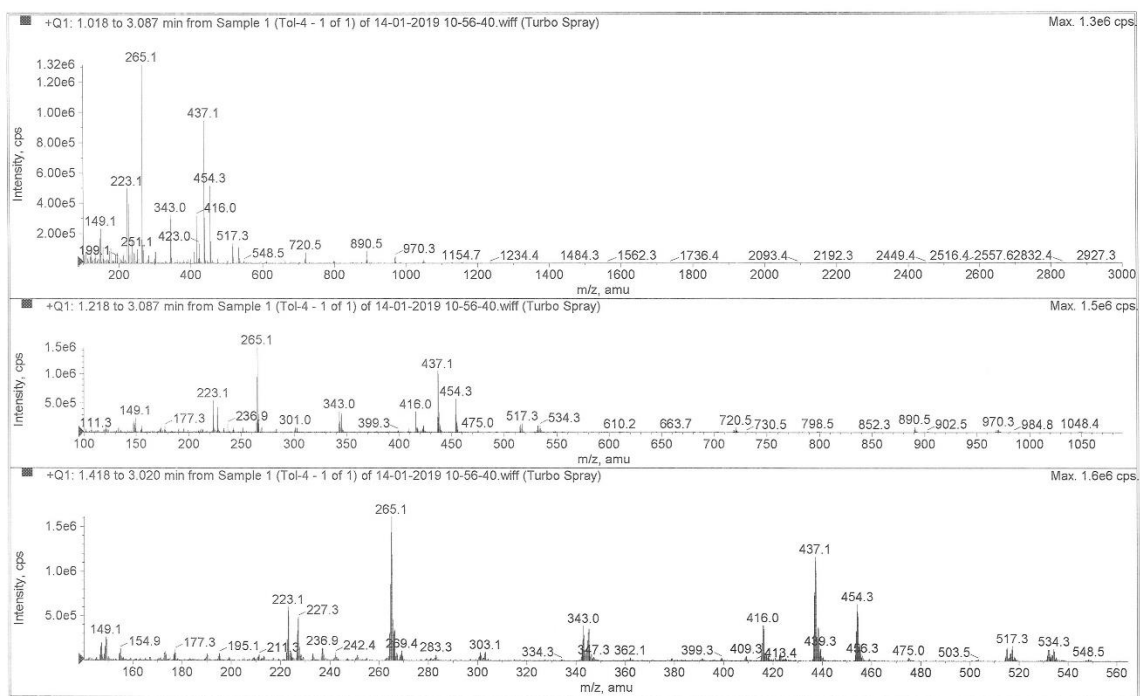


Fig S11. Mass spectrum and LC-Mass spectrum of **5c**

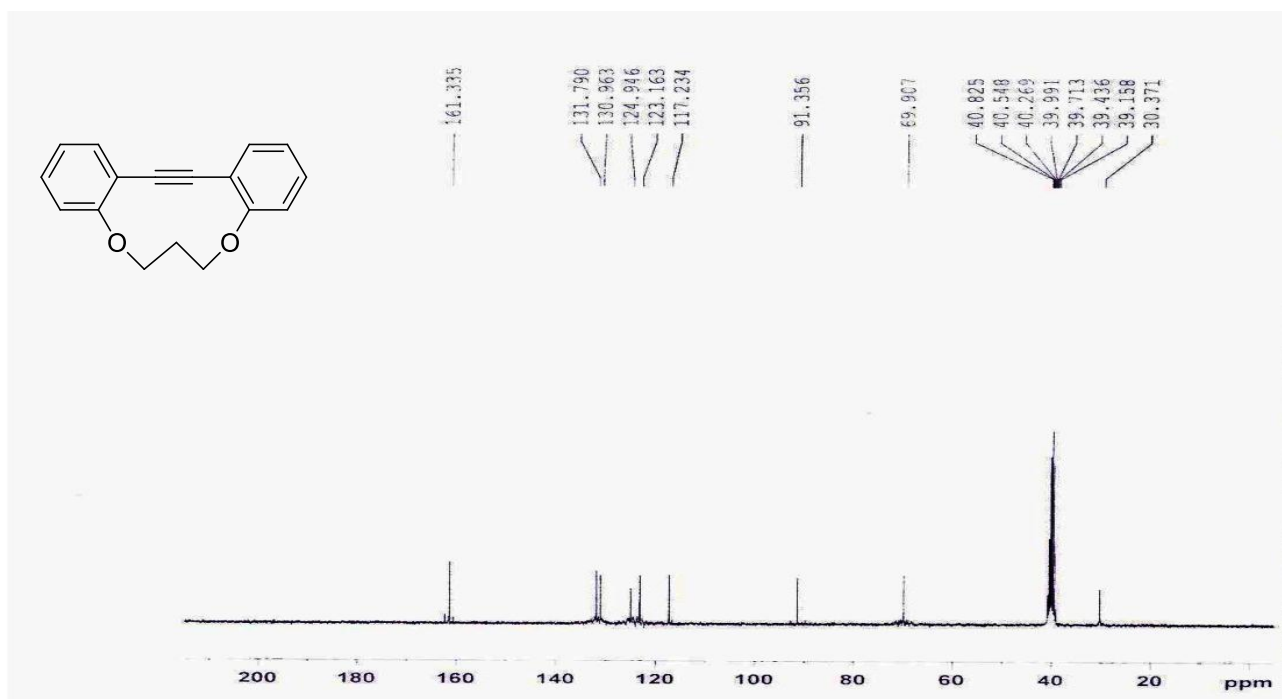


Fig S12. ^{13}C NMR spectrum of **1b**

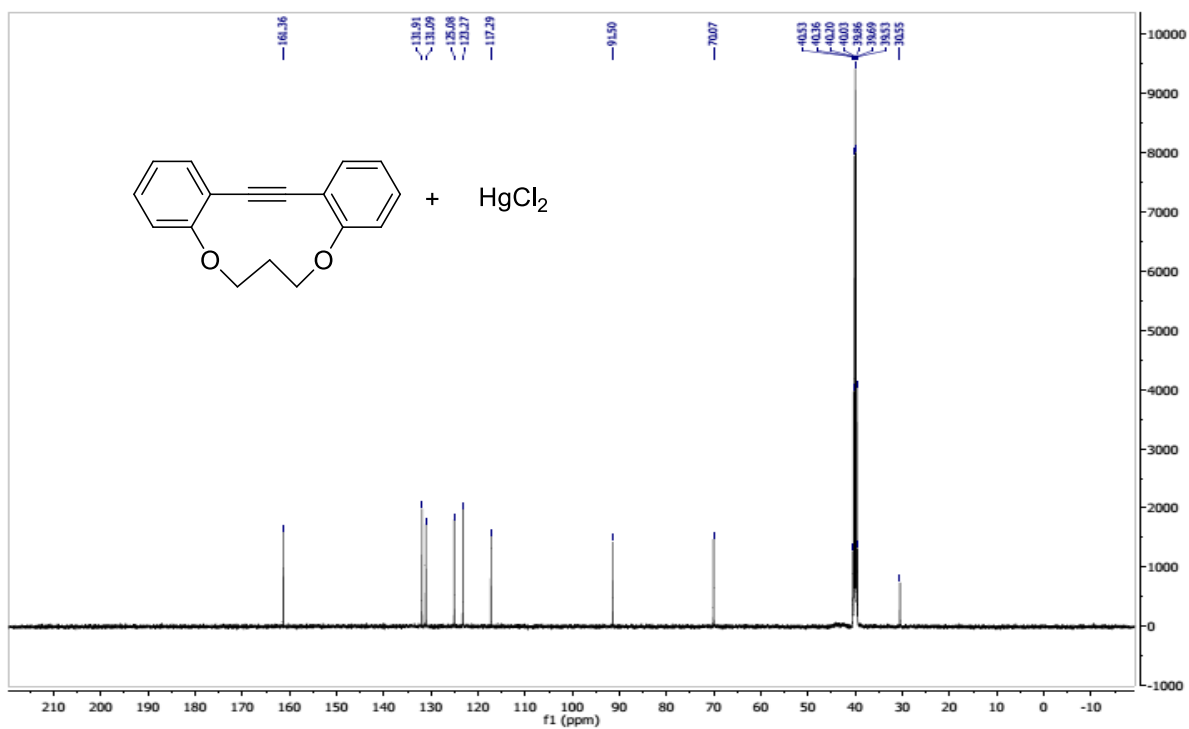


Fig S13. ^{13}C NMR spectrum of **1b**@ HgCl_2

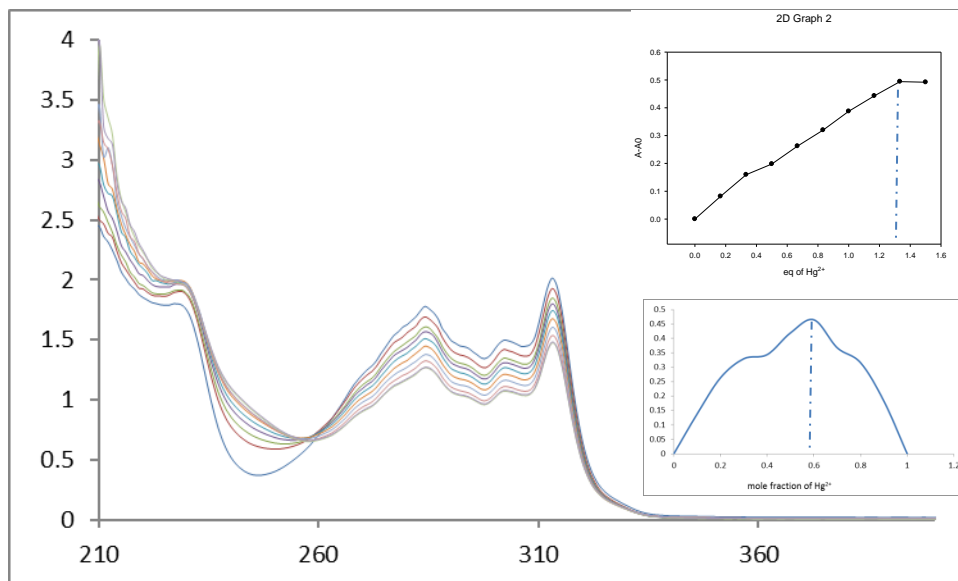


Fig S14. UV-vis spectrum of **1a** upon addition of HgCl_2 in CH_3CN . Above inset: the changes in absorbance intensity of the solution. Below inset: Job Plot.

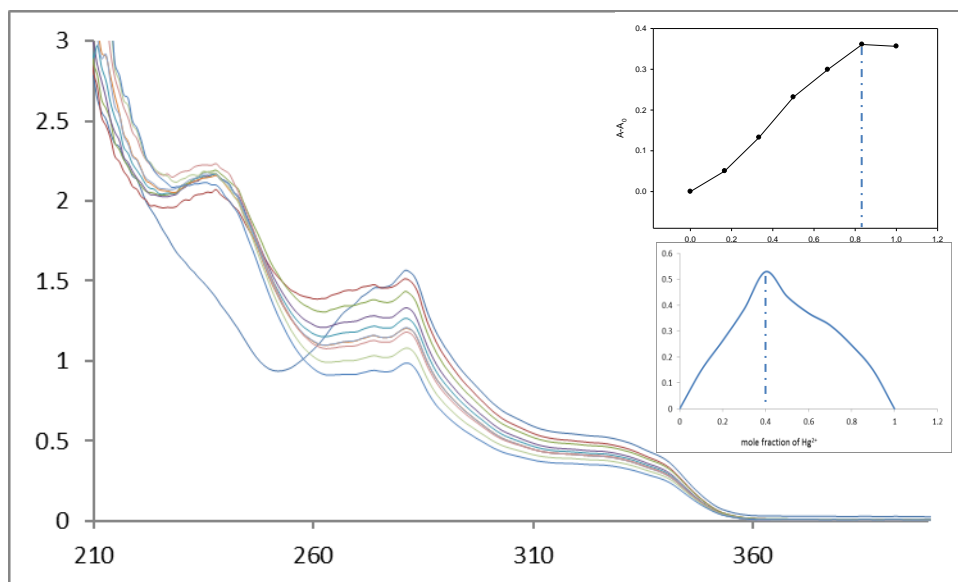
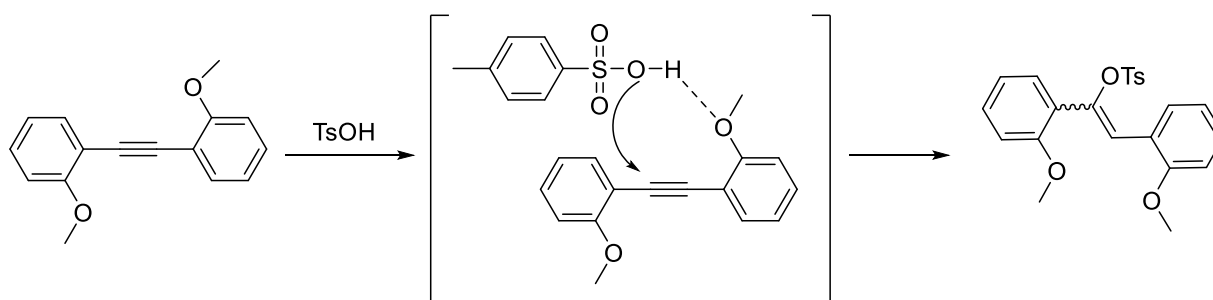
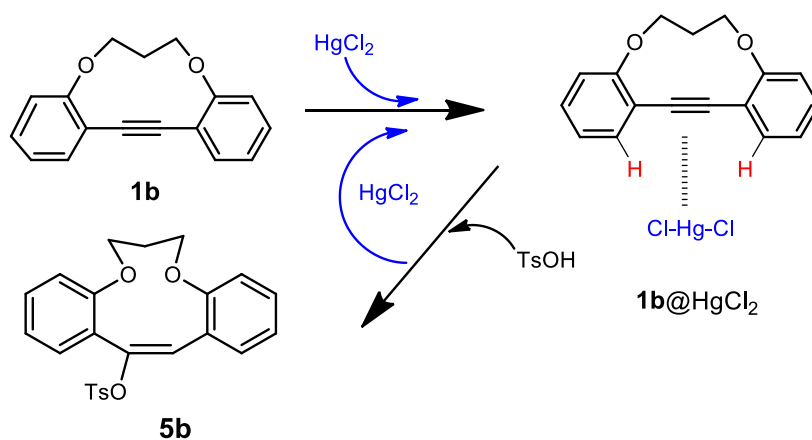


Fig S15. UV-vis spectrum of **1c** upon addition of HgCl_2 in CH_3CN . Above inset: the changes in absorbance intensity of the solution. Below inset: Job Plot.



Scheme S1. Plausible mechanism of hydration of alkyne.



Scheme S2. Proposed mechanism for HgCl_2 -catalyzed synthesis of **5**.

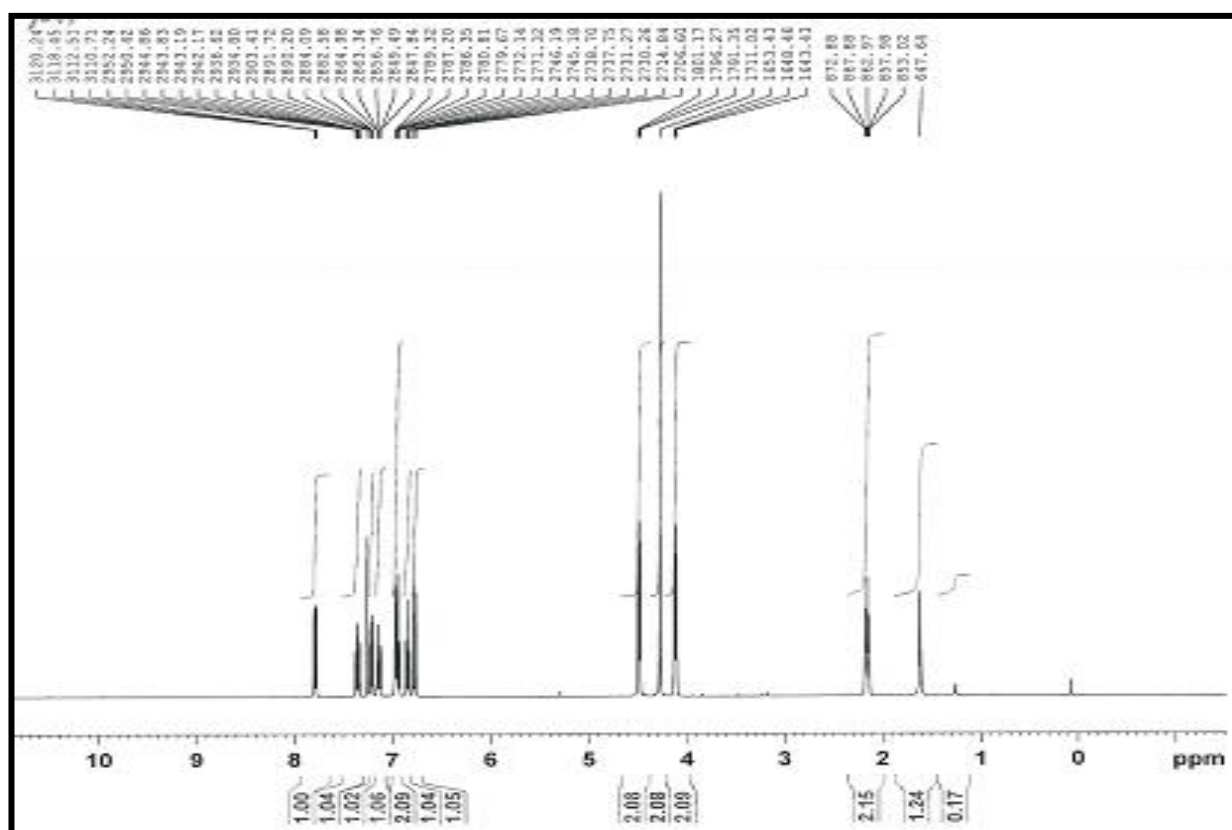


Fig S16. $^1\text{H-NMR}$ spectrum of **4b**

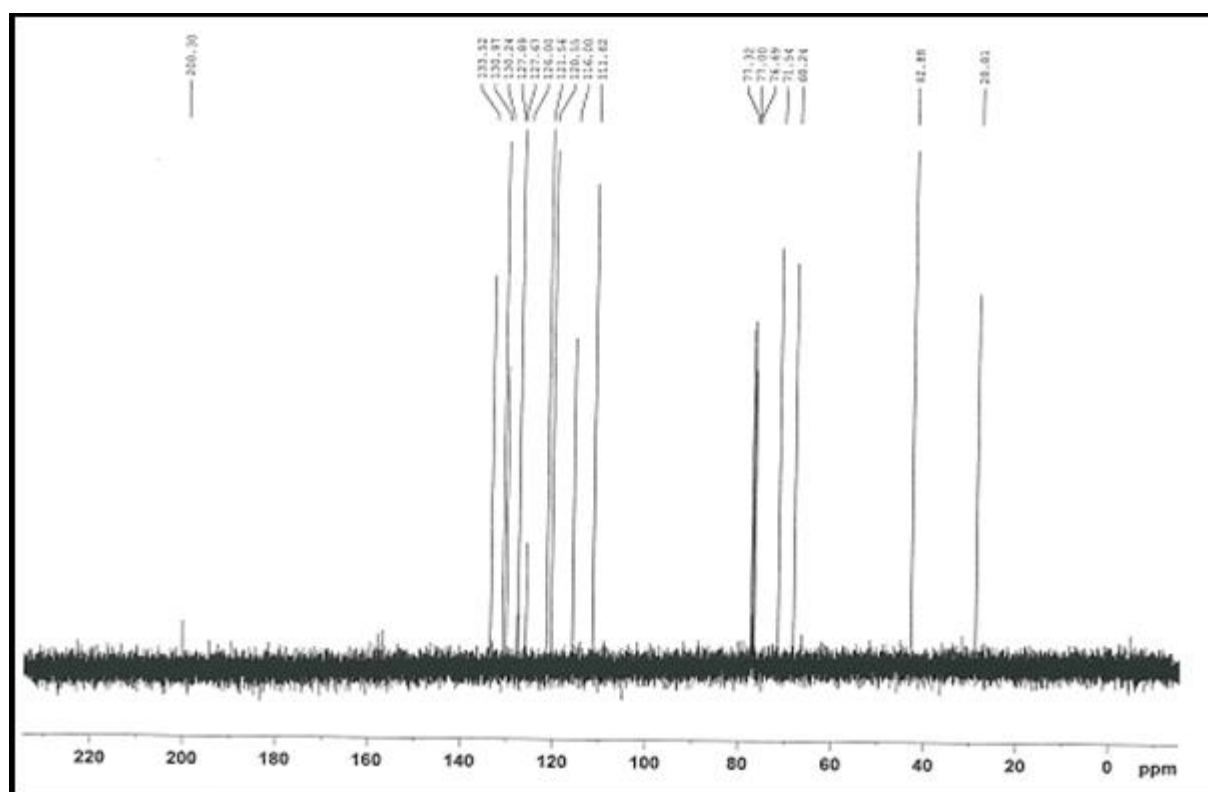


Fig S17. ^{13}C -NMR spectrum of **4b**

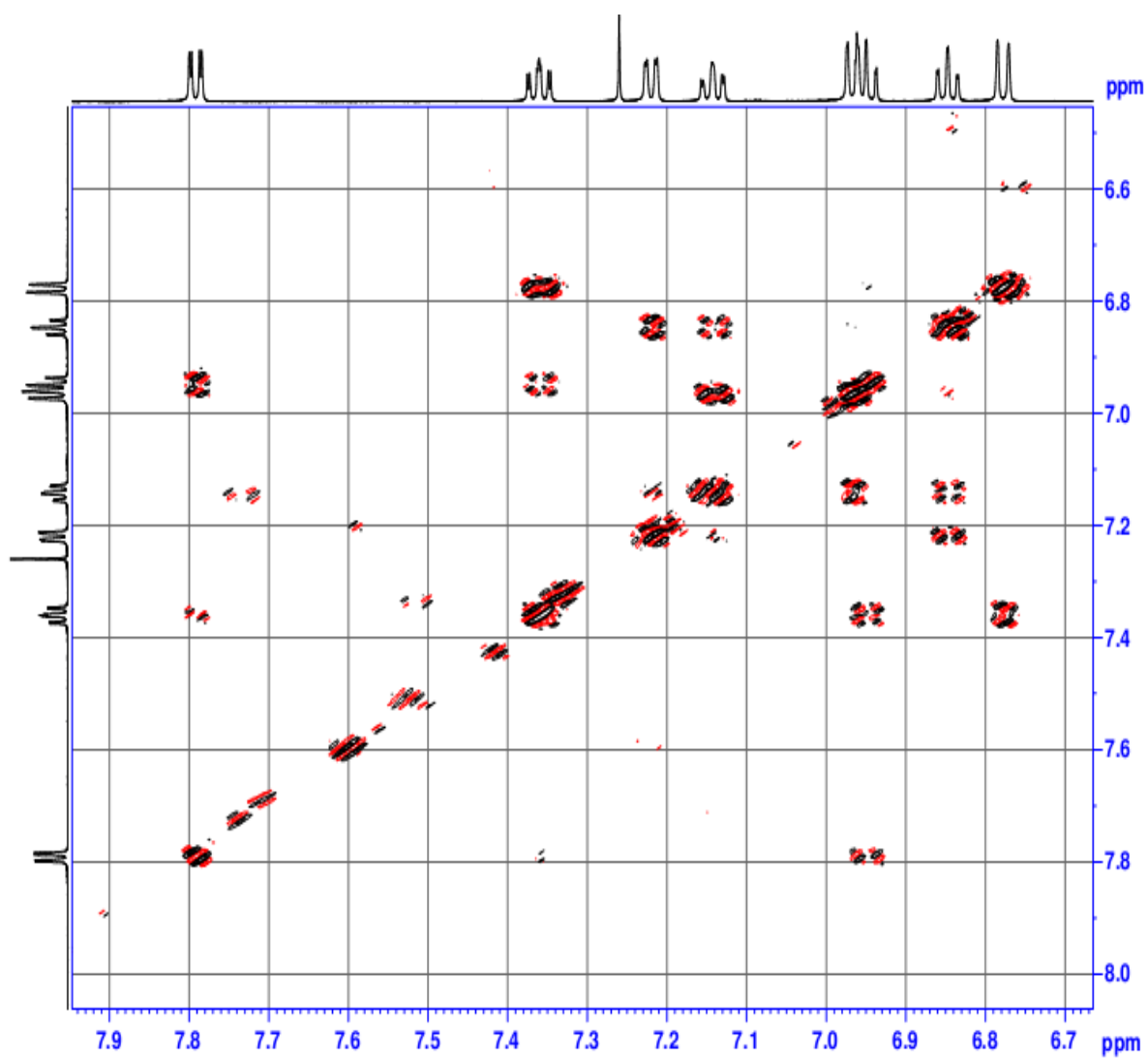


Fig S18. HH-COSY spectrum of **4b**

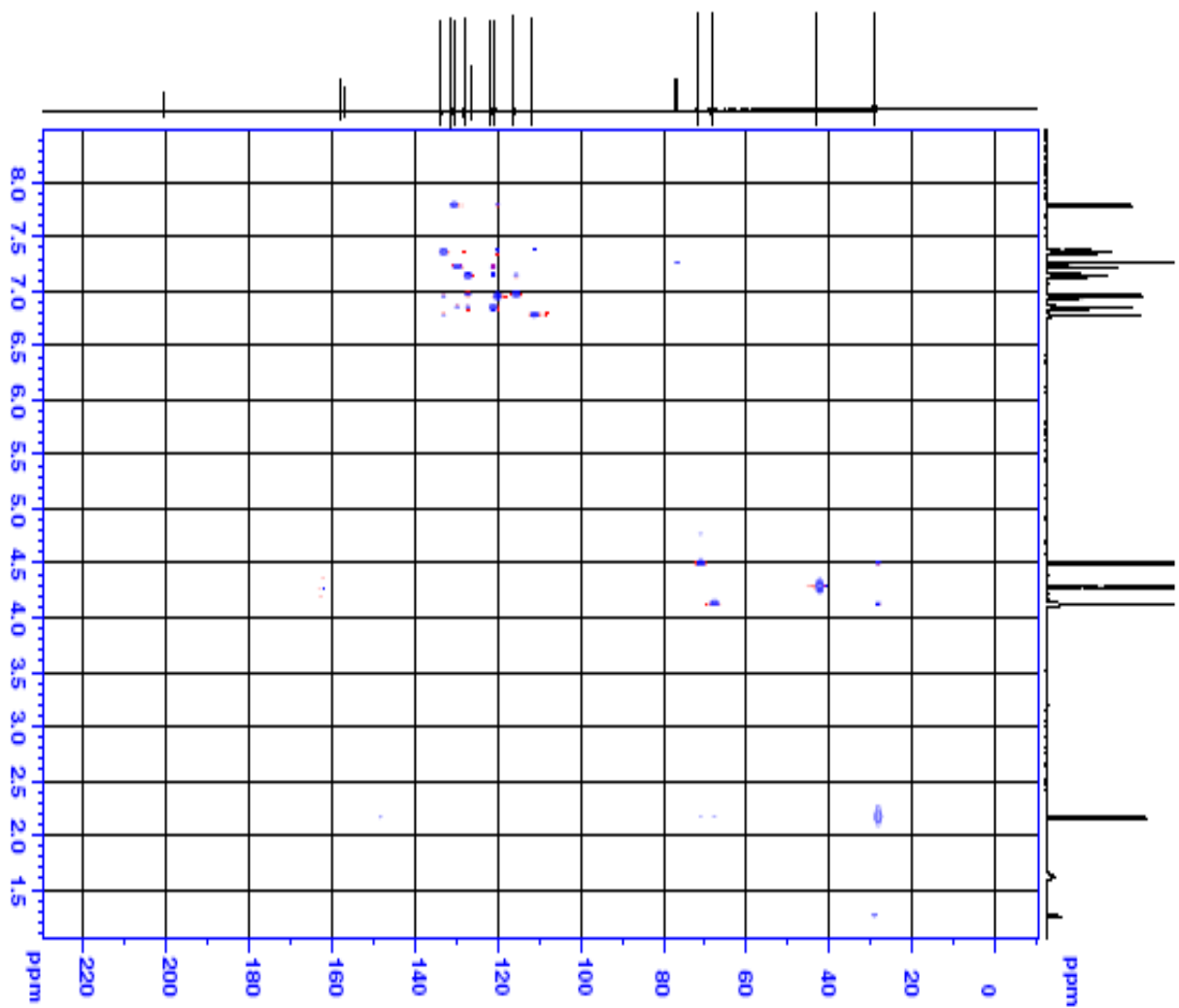


Fig S19. HSQC spectrum of **4b**

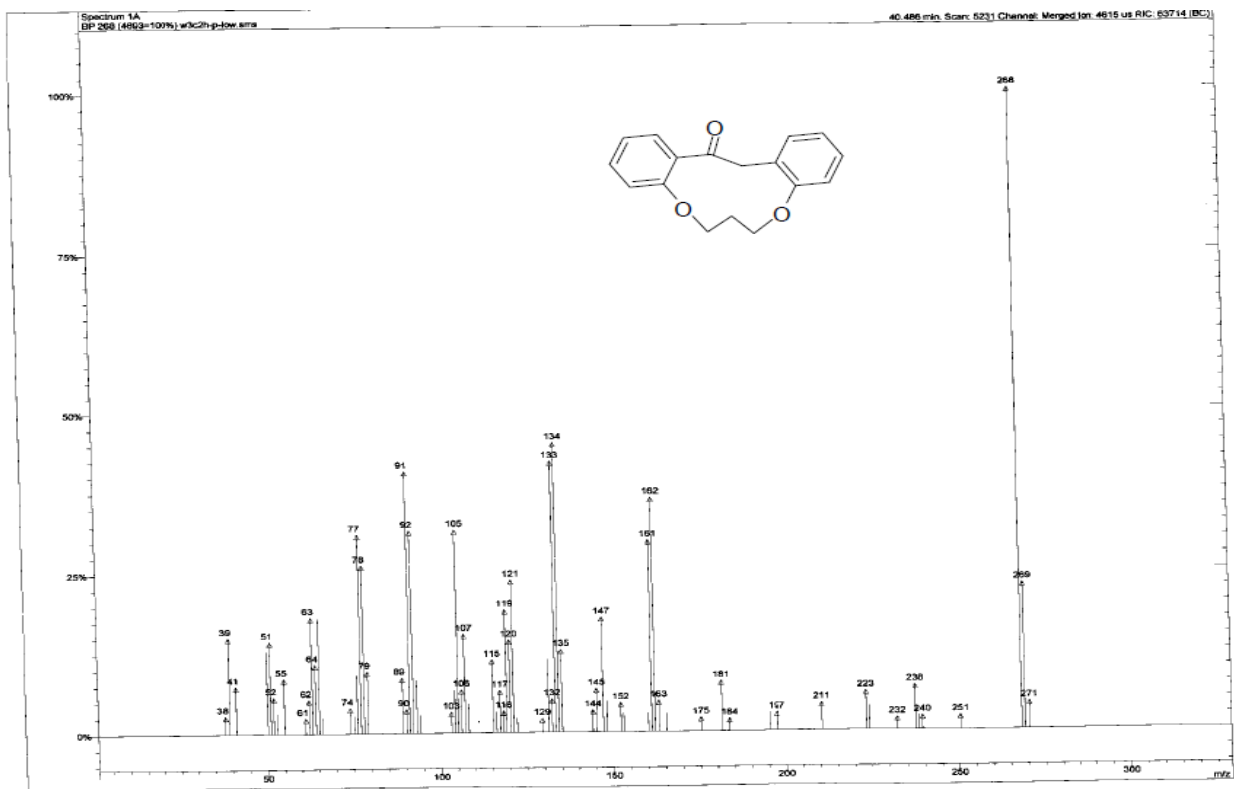


Fig S20. Mass spectrum of 4b

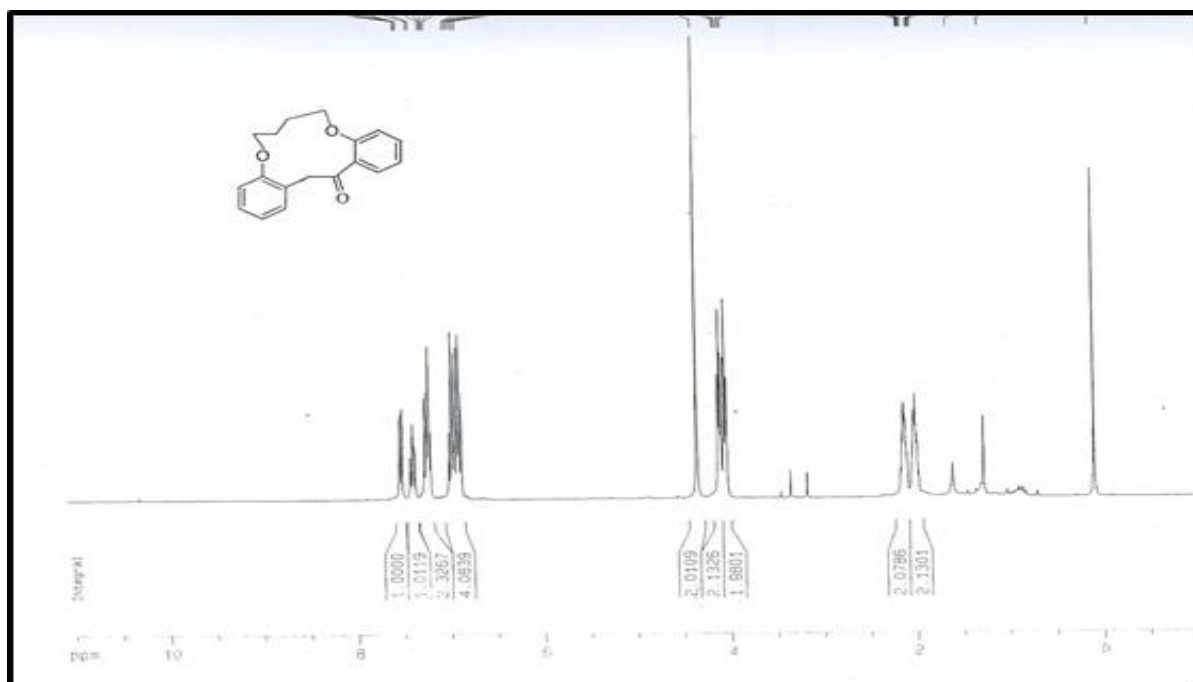


Fig S21. ¹H NMR spectrum of 4c

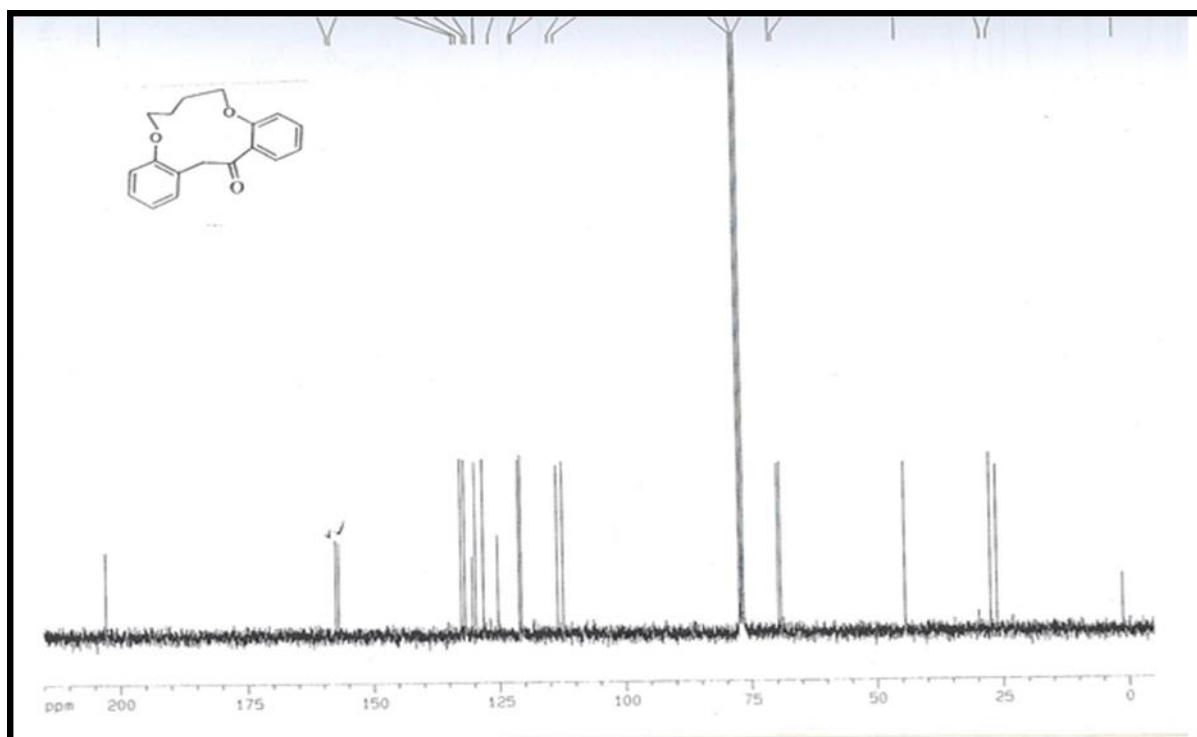


Fig S22. ^{13}C NMR spectrum of **4c**

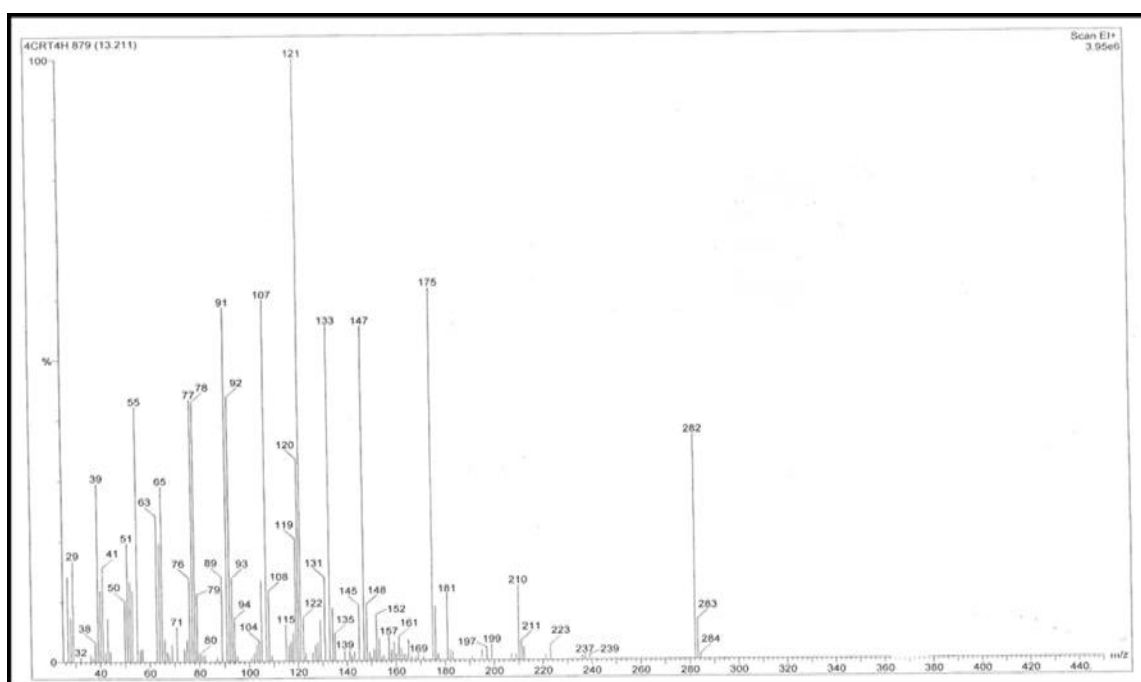


Fig S23. Mass spectrum of **4c**

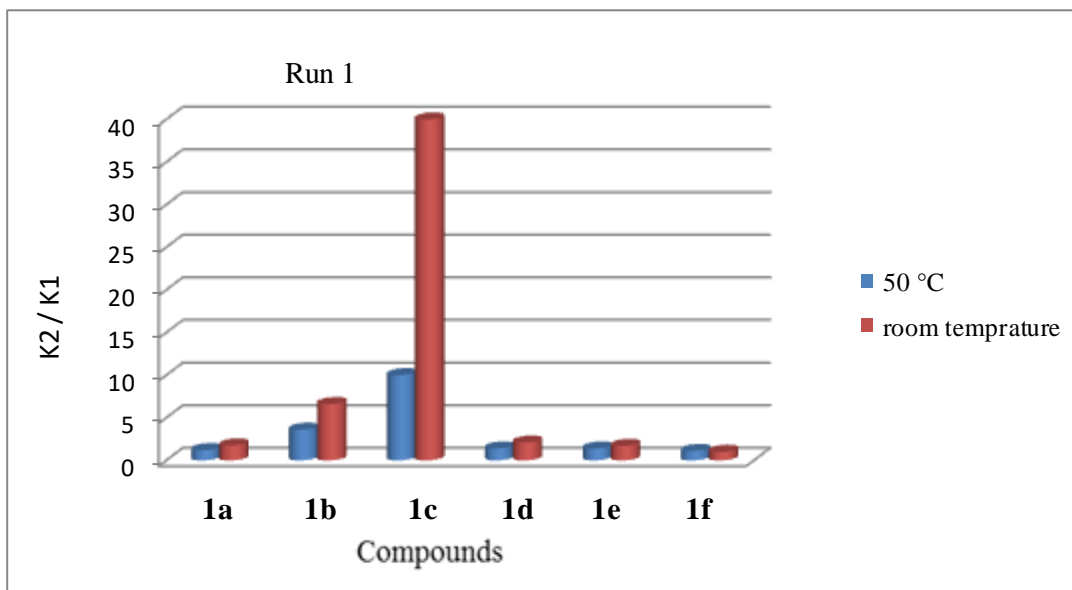


Fig S24. The reaction rate (K_2 / K_1) of **1** at 50 °C (blue) and room temperature (red) conditions (The first run).

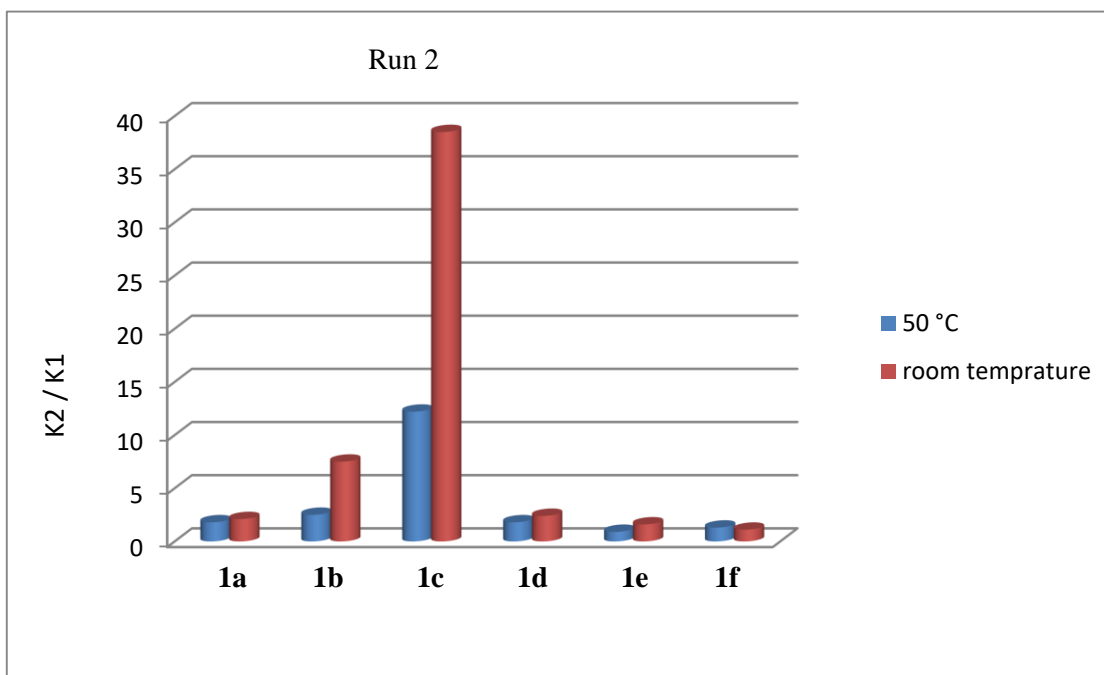


Fig S25. The reaction rate (K_2 / K_1) of **1** at 50 °C (blue) and room temperature (red) conditions (The second run).

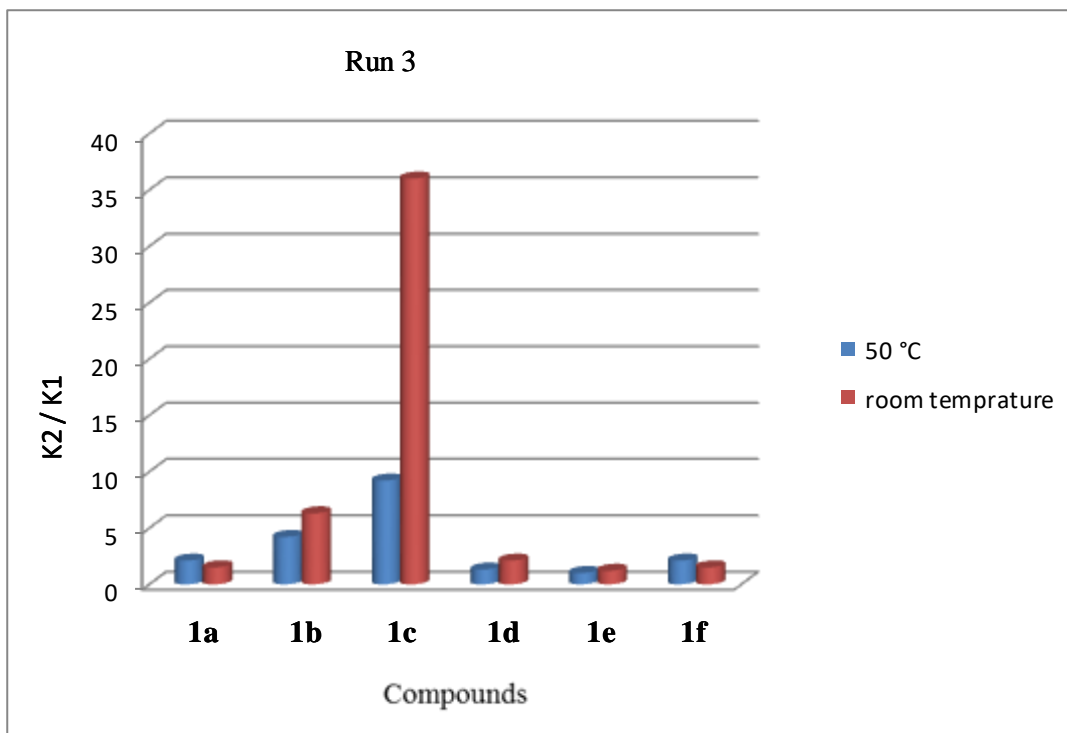


Fig S26. The reaction rate (K_2 / K_1) of **1** at 50 °C (blue) and room temperature (red) conditions (The third run).

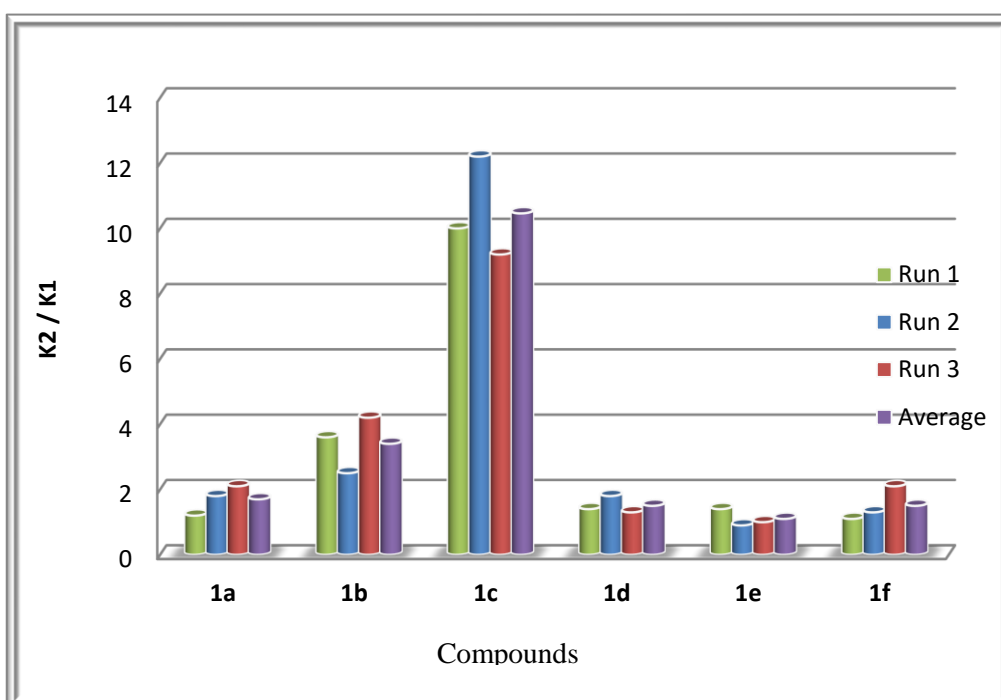


Fig S27. The comparison of three runs and their average reaction rate (K_2 / K_1) of **1** at 50 °C.

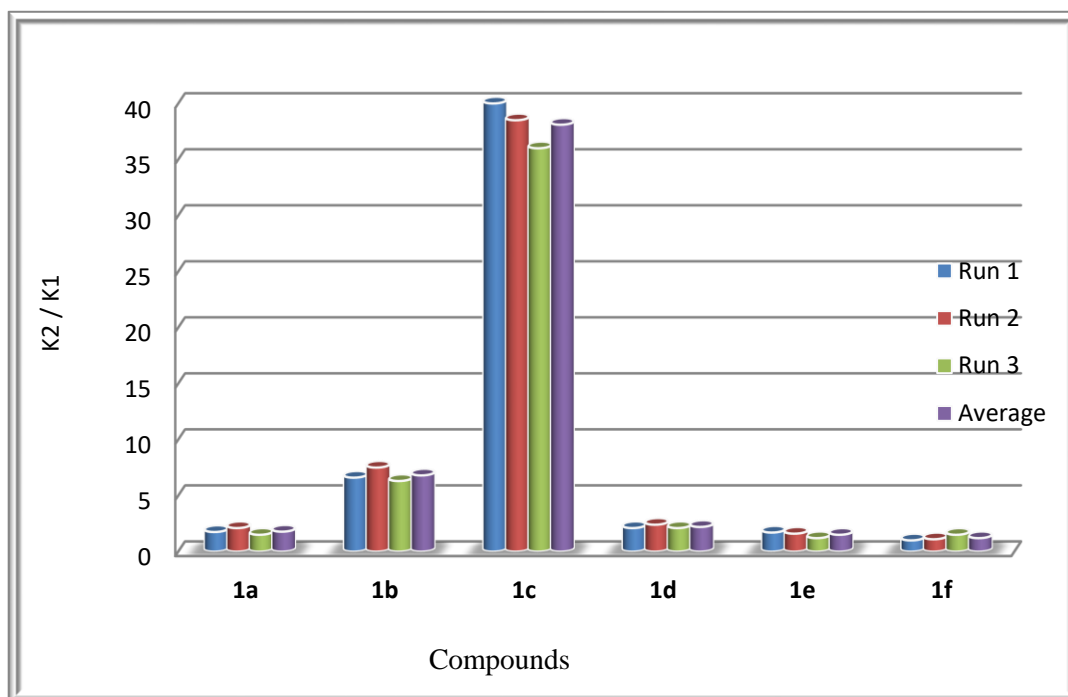


Fig S28. The comparison of three runs and their average reaction rate (K_2 / K_1) of **1** at room temperature.