

Electronic Supporting Information

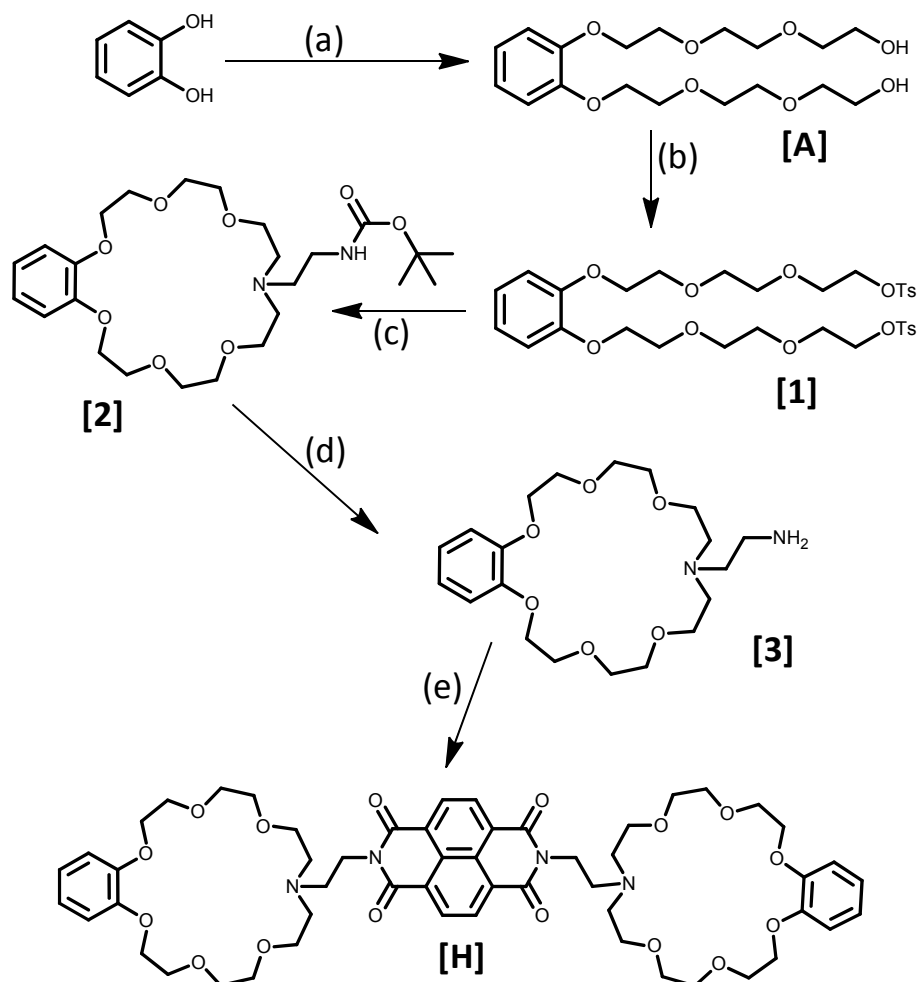
Studies on [3]pseudorotaxane Formation from a Bis-azacrown Derivative as Host and Imidazolium Ion-derivatives as Guest

Amal Kumar Mandal, Moorthy Suresh, Amitava Das.*

*Central Salt & Marine Chemicals Research Institute (CSIR),
Bhavnagar: 364002, Gujarat, India,
E-Mail: amitava@csmcri.org*

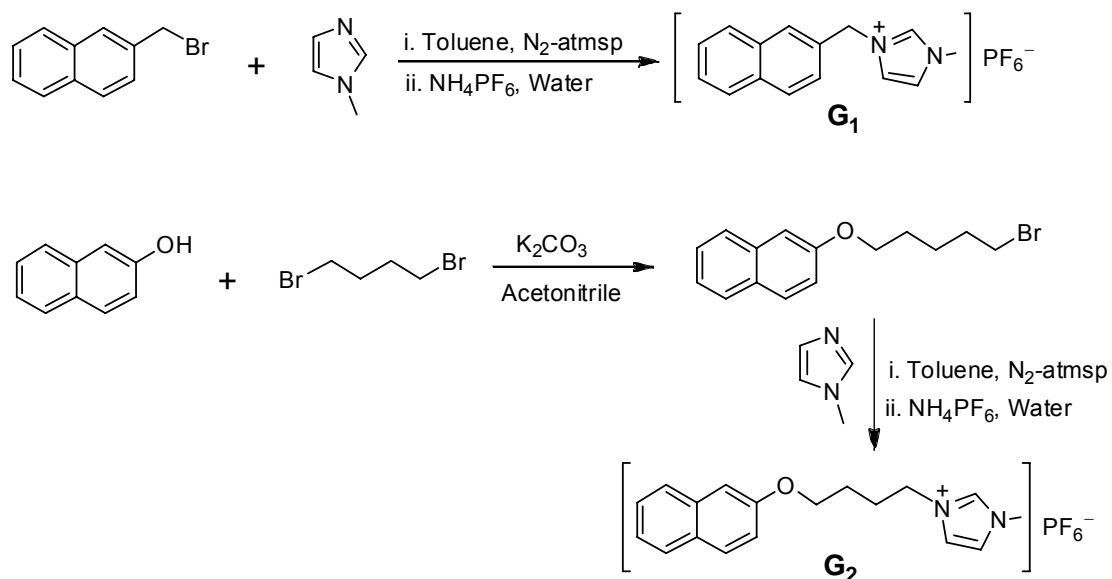
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1. Synthetic route for H:



Reagents and conditions: (a) $\text{Cl}(\text{CH}_2\text{O})_3\text{H}$, K_2CO_3 , KI , DMF , 90°C (b) TsCl , NaOH , $\text{THF}/\text{H}_2\text{O}$, 0°C - RT . (c) K_2CO_3 , KI , $\text{H}_2\text{N}(\text{CH}_2)_2\text{NHBoc}$, MeCN , 81°C . (d) HCl , Et_2O , DCM , RT . (e) 1,4,5,8-Naphthalene dianhydride, MeCN , 81°C .

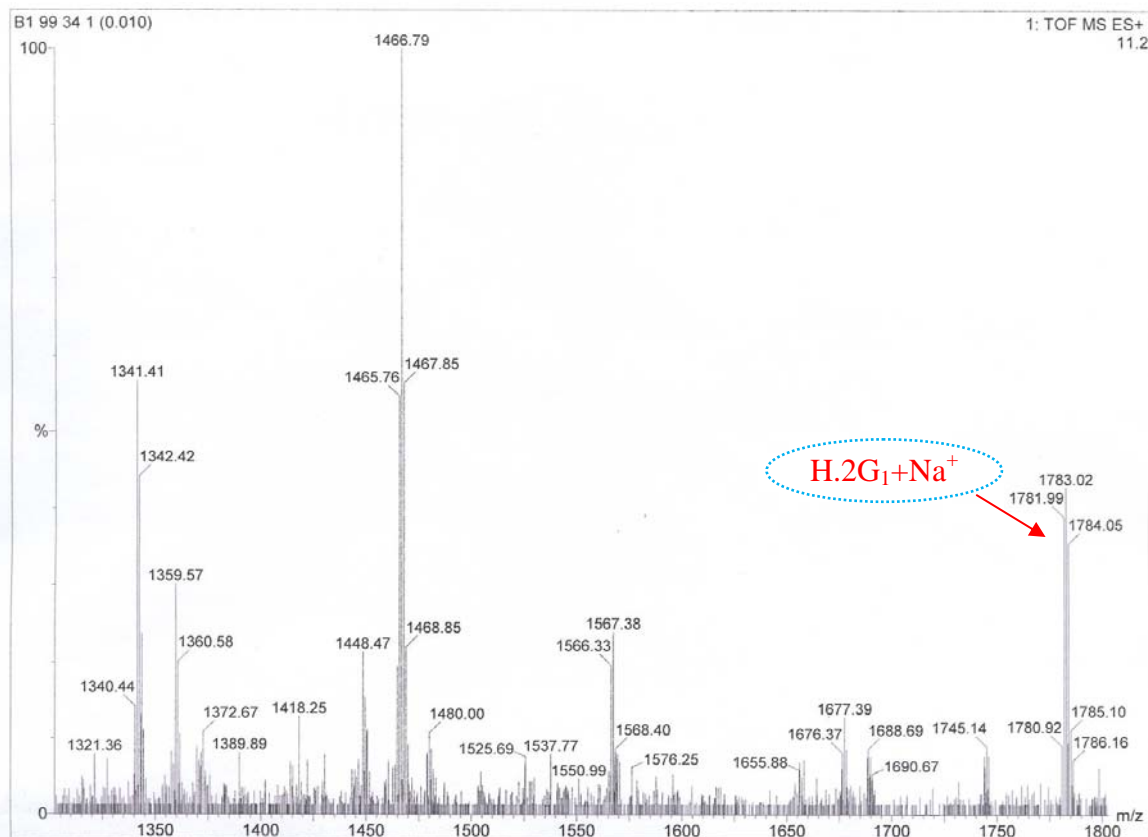
2. Synthetic route for G1 & G2:



3. Synthesis of I:

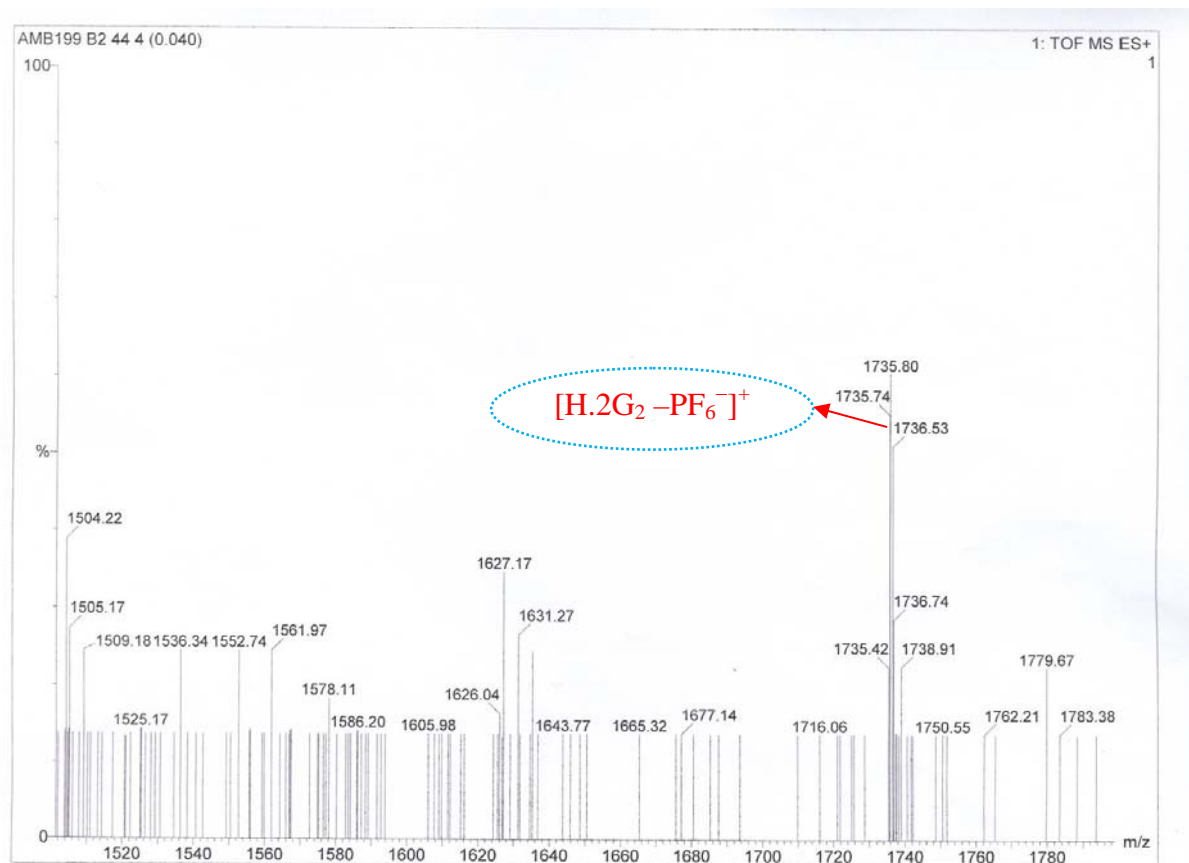
2- Naphthol (2gm, 13.87mM) was dissolved in 40 ml of freshly dried acetonitrile in two neck round bottom flask in N₂-atmosphere. To this solution K₂CO₃ powder (3.25g, 23.57 mM) was added and the reaction mixture was stirred for 30 mint. After 30 mint. The colourless solution turned to light green solution. Then dibromobutane (14.97gm, 69.36mM) was added and the reaction mixture was refluxed for 24hr. After one day, the solvent was removed under reduced pressure and extracted three times with CHCl₃ and water. Organic layers were combined and dried over anhydrous sodium sulphate. Solvent was removed under reduced pressure to give crude product which was purified on Silica-gel column, using methanol:chloroform (1:99 v/v) as an eluent to yield **I** (2.3 gm, 60%), as a white solid. ¹H-NMR (200MHz, CDCl₃, δ ppm) 7.79 - 7.72 (3H, m), 7.46 - 7.34 (2H, m), 7.17 (1H, s), 7.13 (1H, s), 4.11 (2H, t, *J* = 5.8), 3.52 (2H, t, *J* = 6.4), 2.04 - 2.01 (4H, m). (ESI – MS) calcd for C₁₄H₁₅BrO : 279.17, found : 279.43.

4. Mass spectrum for H.2G₁.



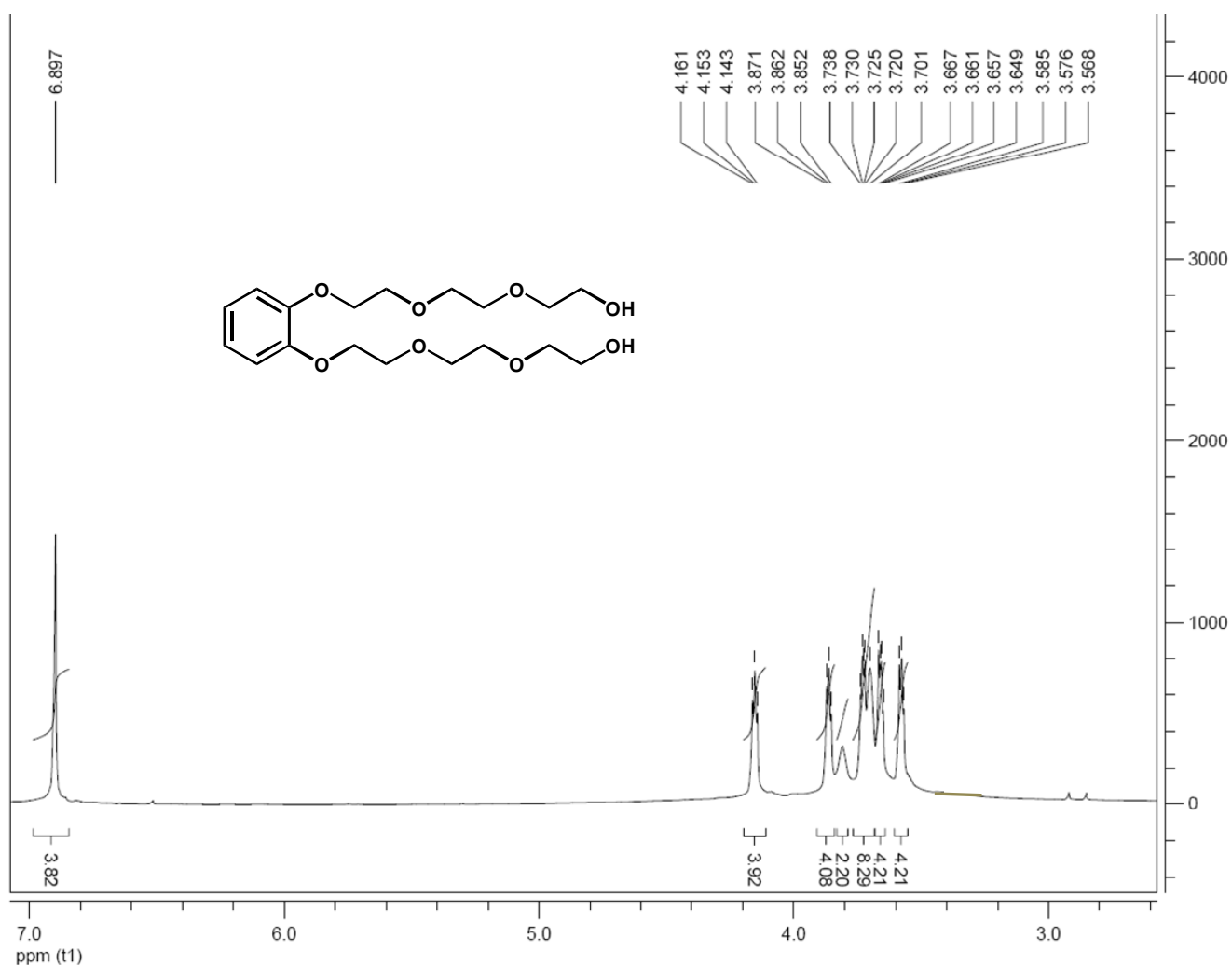
ESI Figure 1: ESI-mass spectrum for **H.2G₁** using Micromass Q-ToF microTM, equipped with ESI source and Q-ToF analyzer.

5. Mass spectrum For H.2G₂:



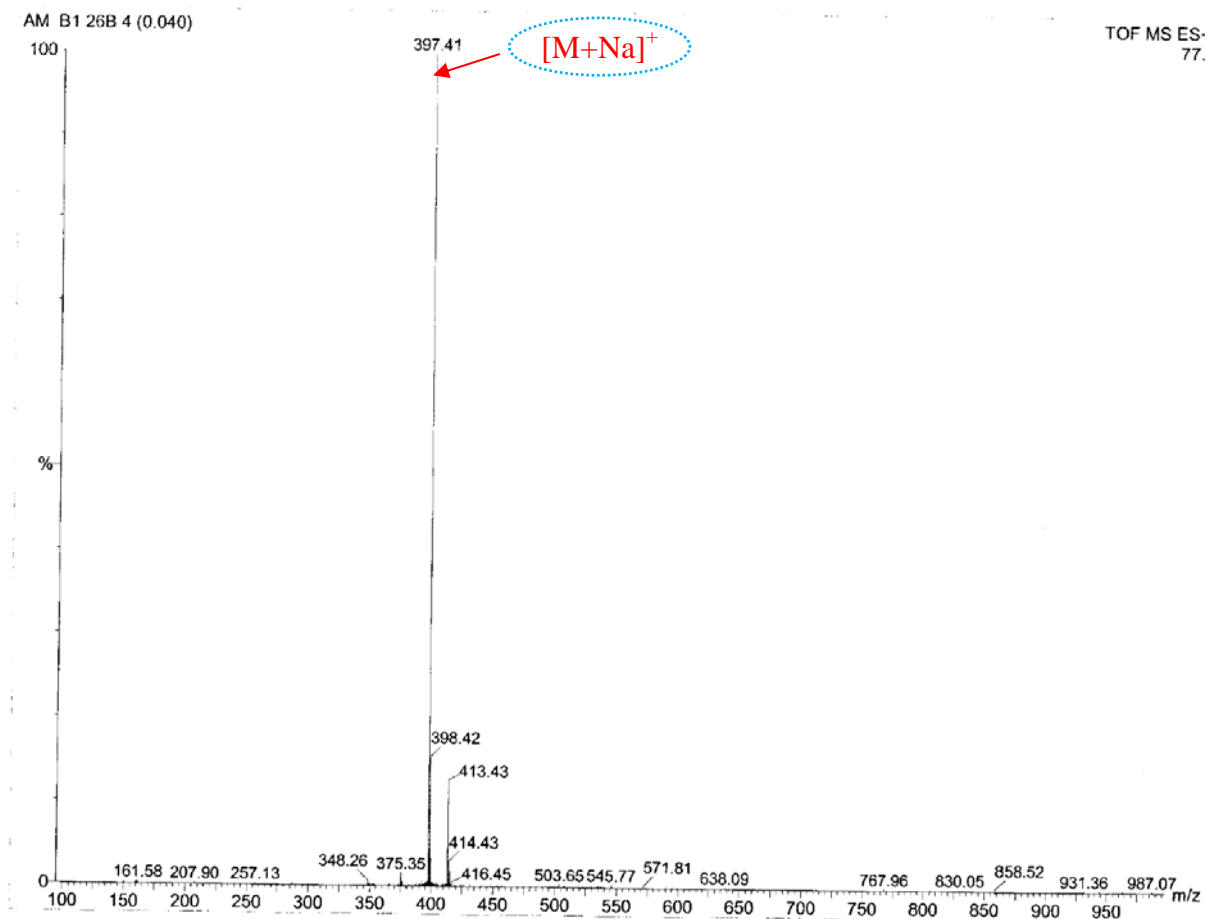
ESI Figure 2: ESI-mass spectrum for **H.2G₂** using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

6. ^1H - NMR spectrum of A:



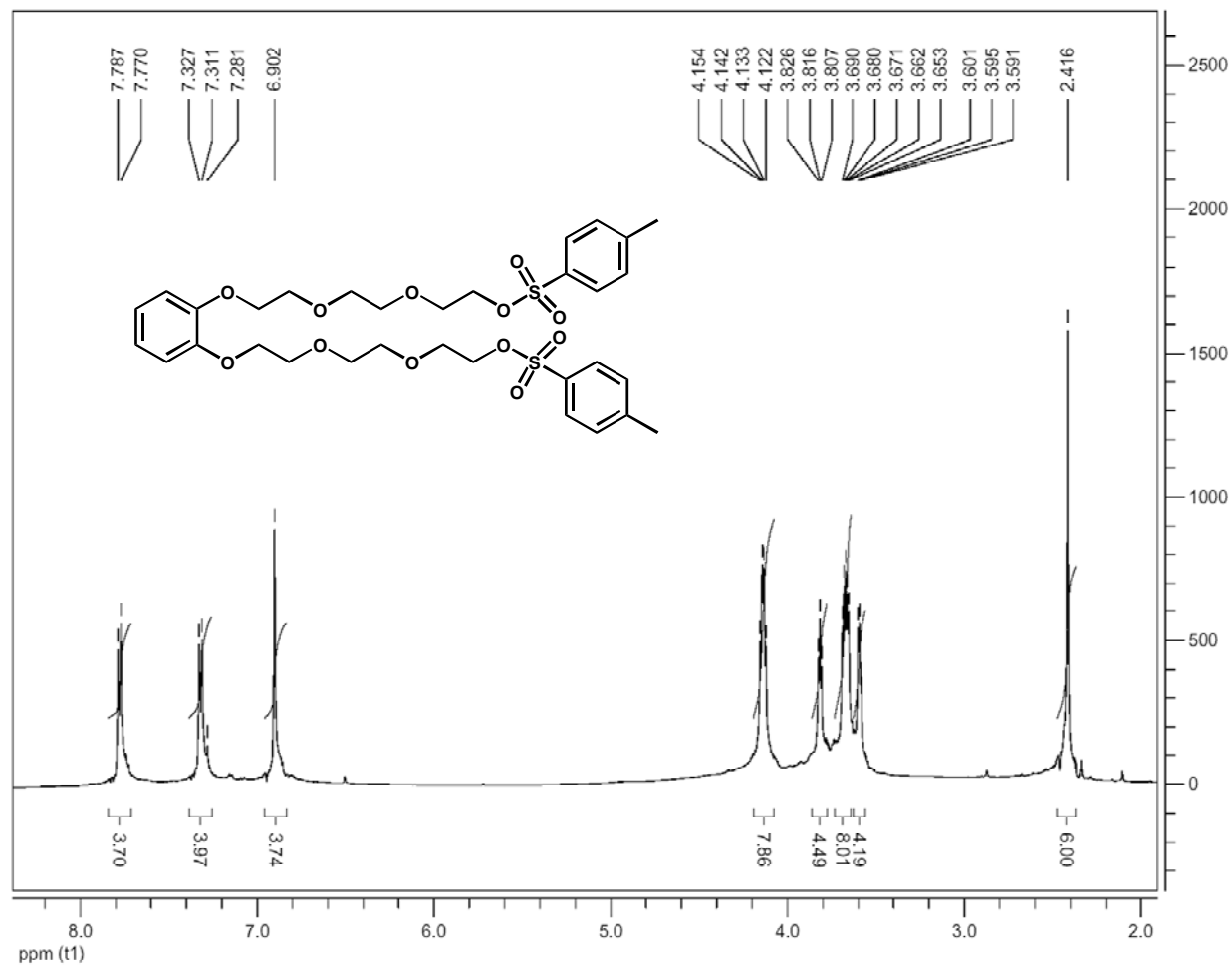
ESI Figure 3: ^1H NMR spectrum of compound **A** in CDCl_3

7. Mass spectrum of A:



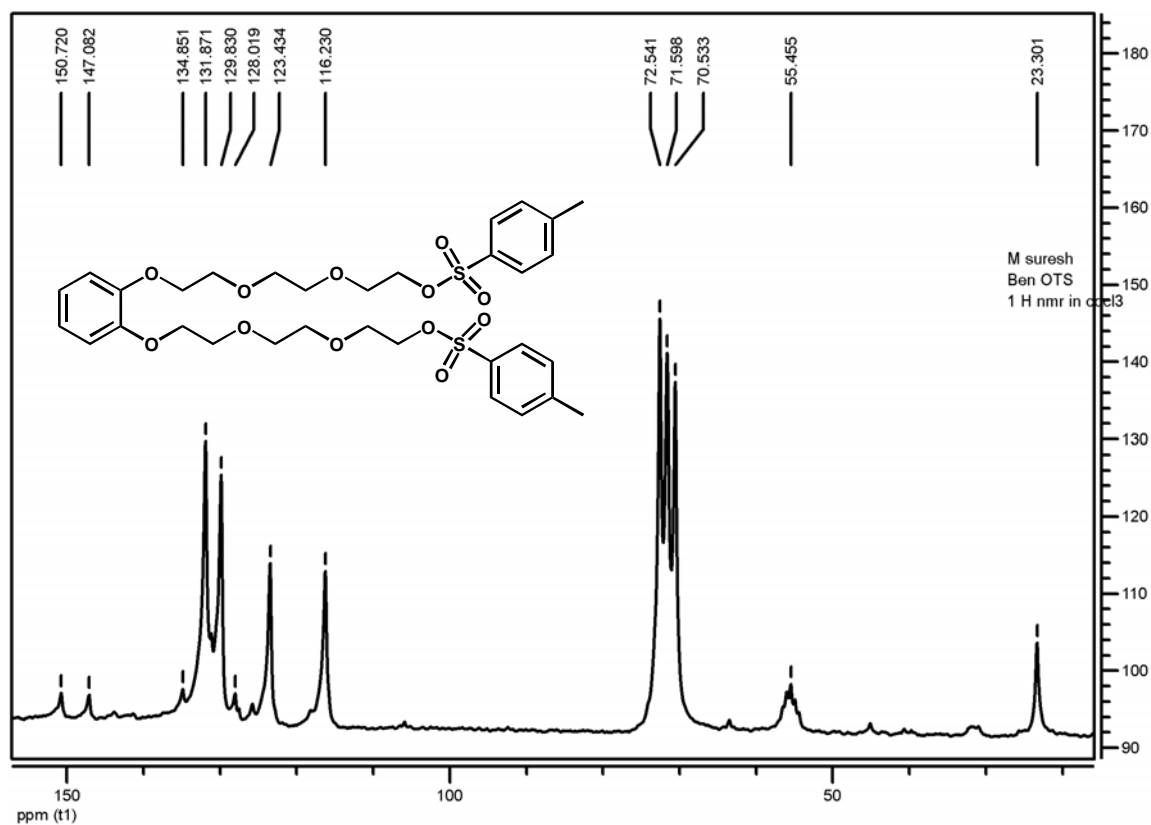
ESI Figure 4: ESI-mass spectrum of compound **A** using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

8. ¹H-NMR spectrum of 1:



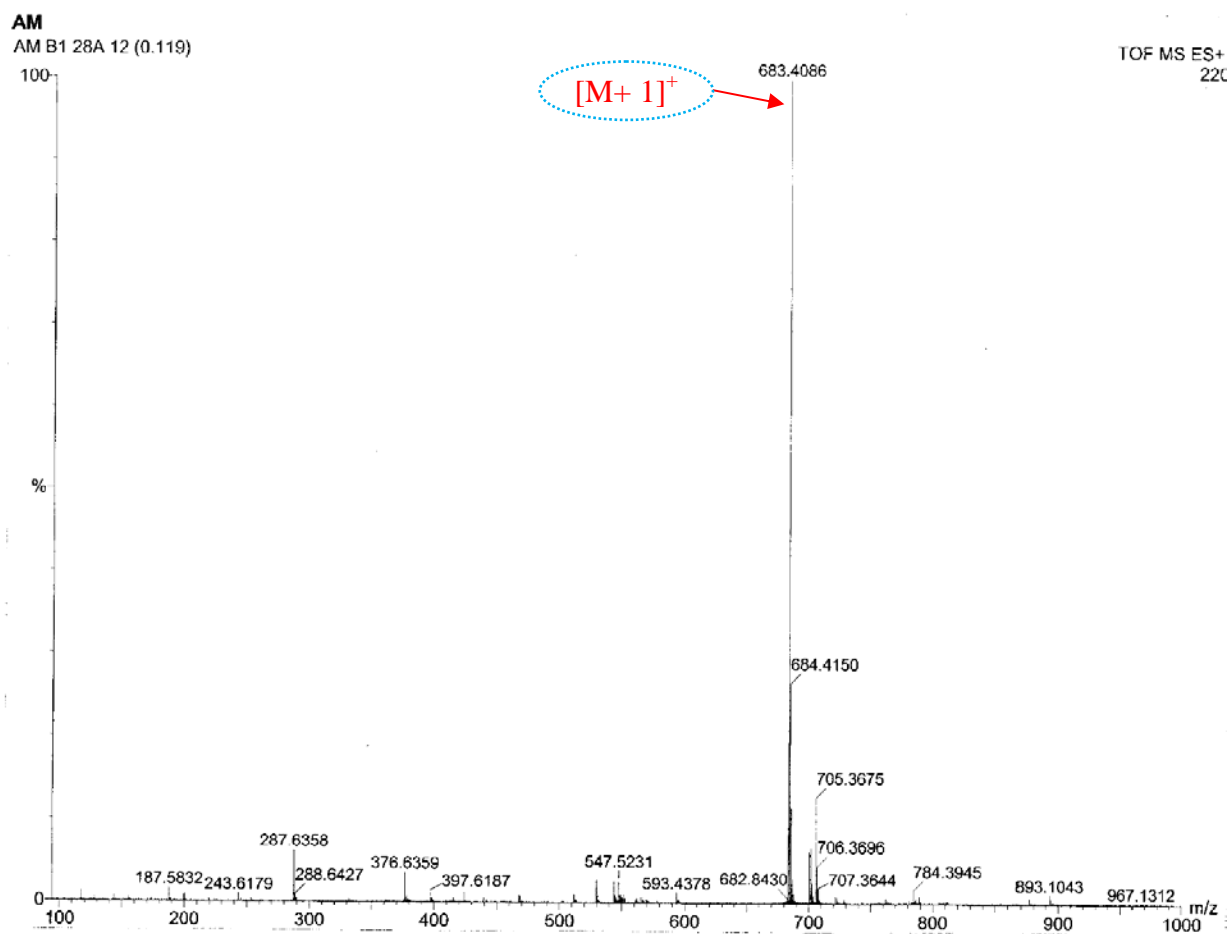
ESI Figure 5: ¹H NMR spectrum of compound 1 in CDCl₃.

9. ^{13}C -NMR spectrum of **1**:



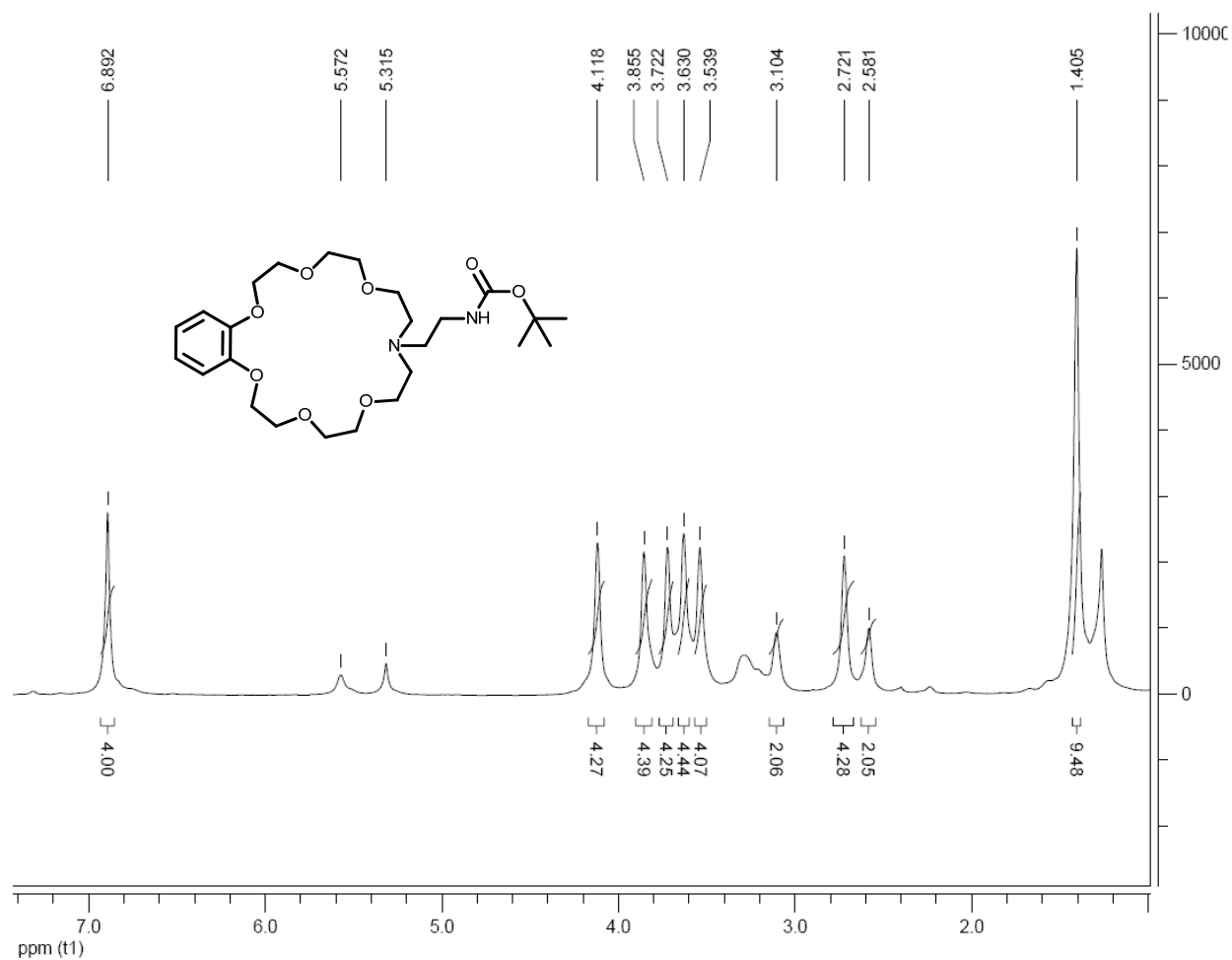
ESI Figure 6: ^{13}C -NMR spectrum of compound **1** in CDCl_3 .

10. Mass spectrum of 1:

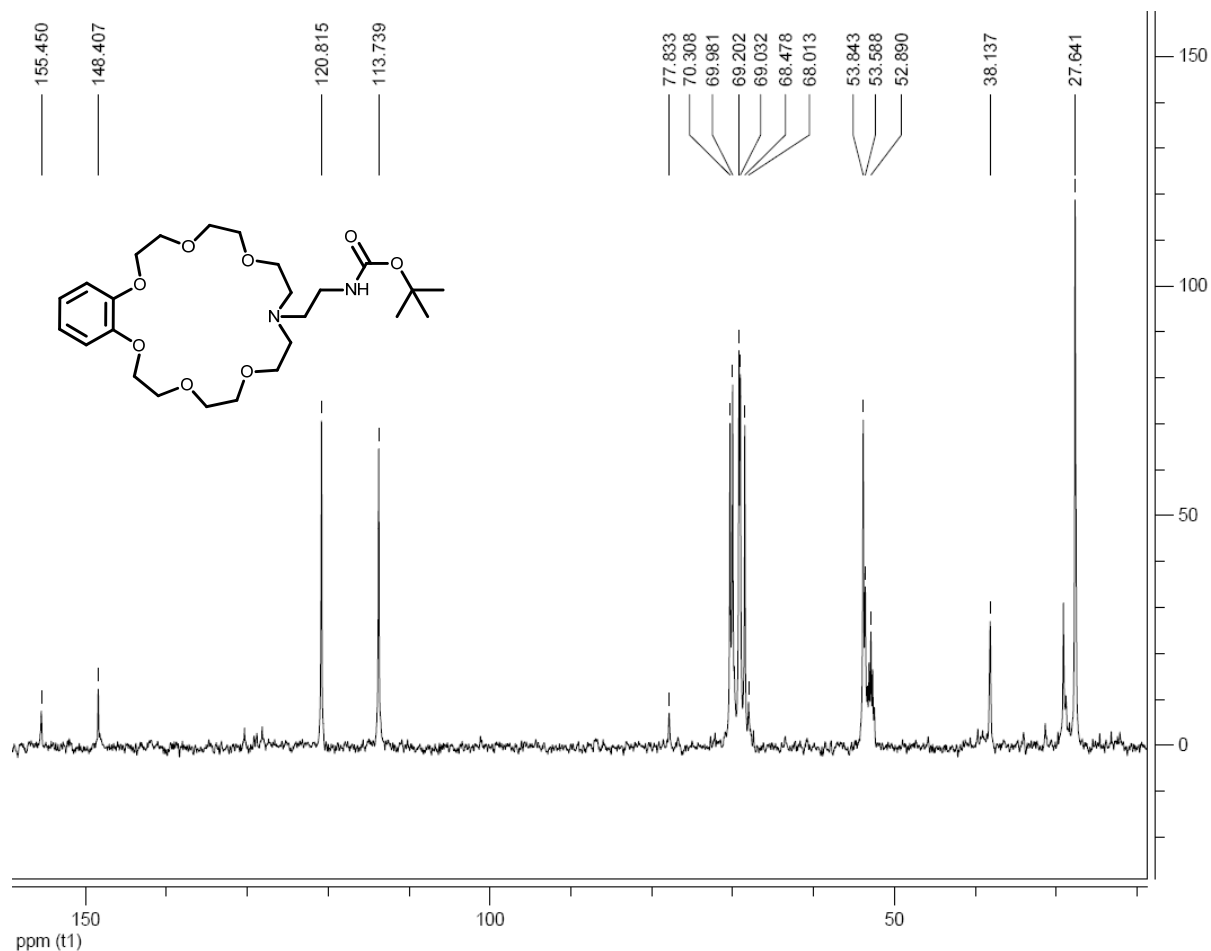


ESI Figure 7: ESI-mass spectrum of compound **1** using Micromass Q-ToF microTM, equipped with ESI source and Q-ToF analyzer.

11. ¹H-NMR spectrum of 2:

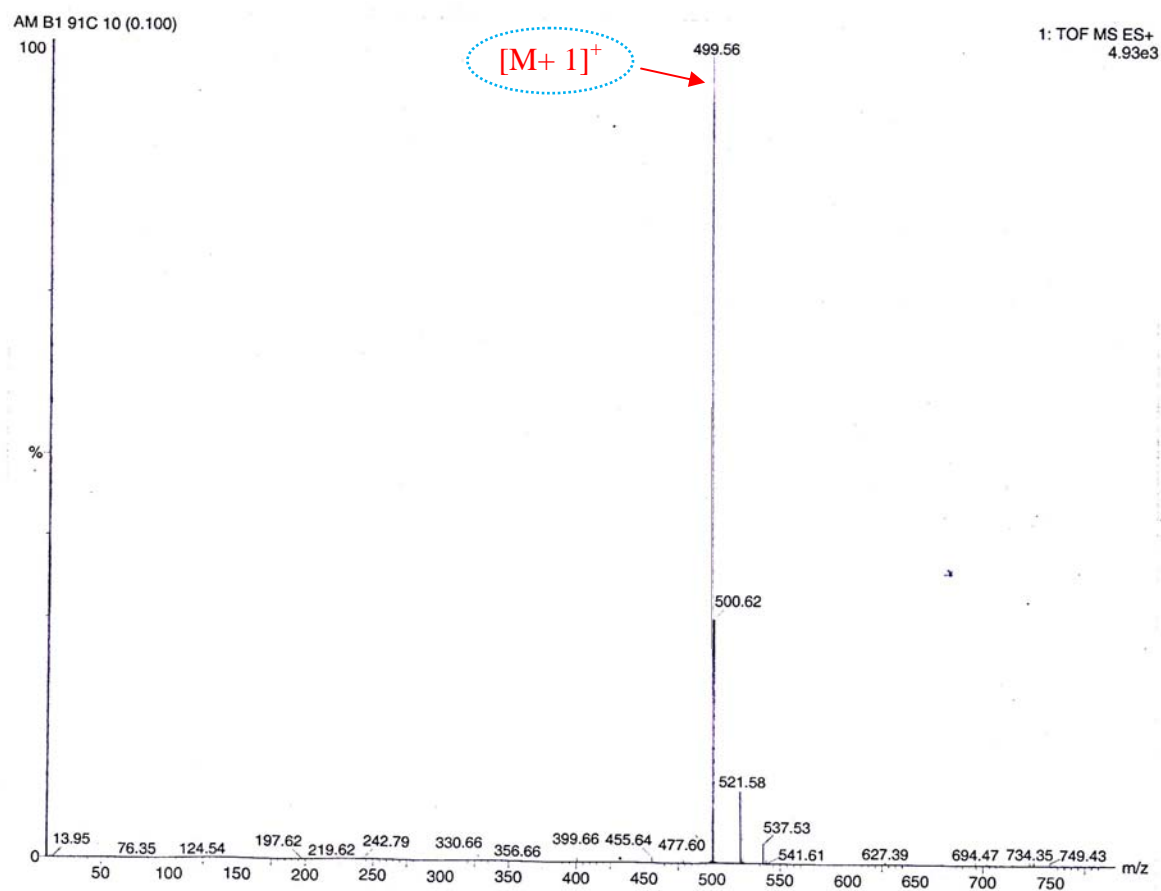


12. ¹³C-NMR spectrum of 2:



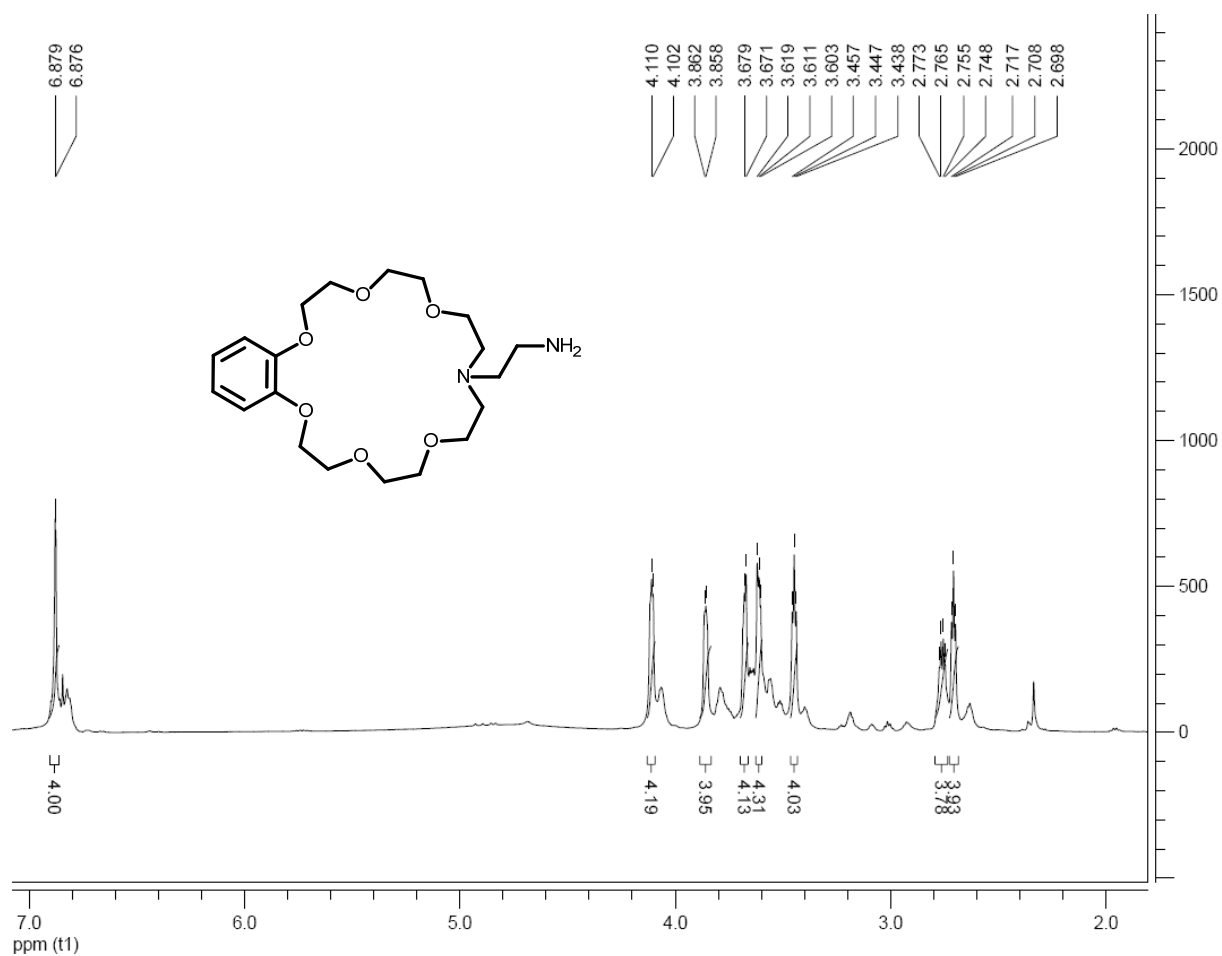
ESI Figure 9: ¹³C-NMR spectrum of compound 2 in CD₂Cl₂.

13. Mass spectrum of 2:



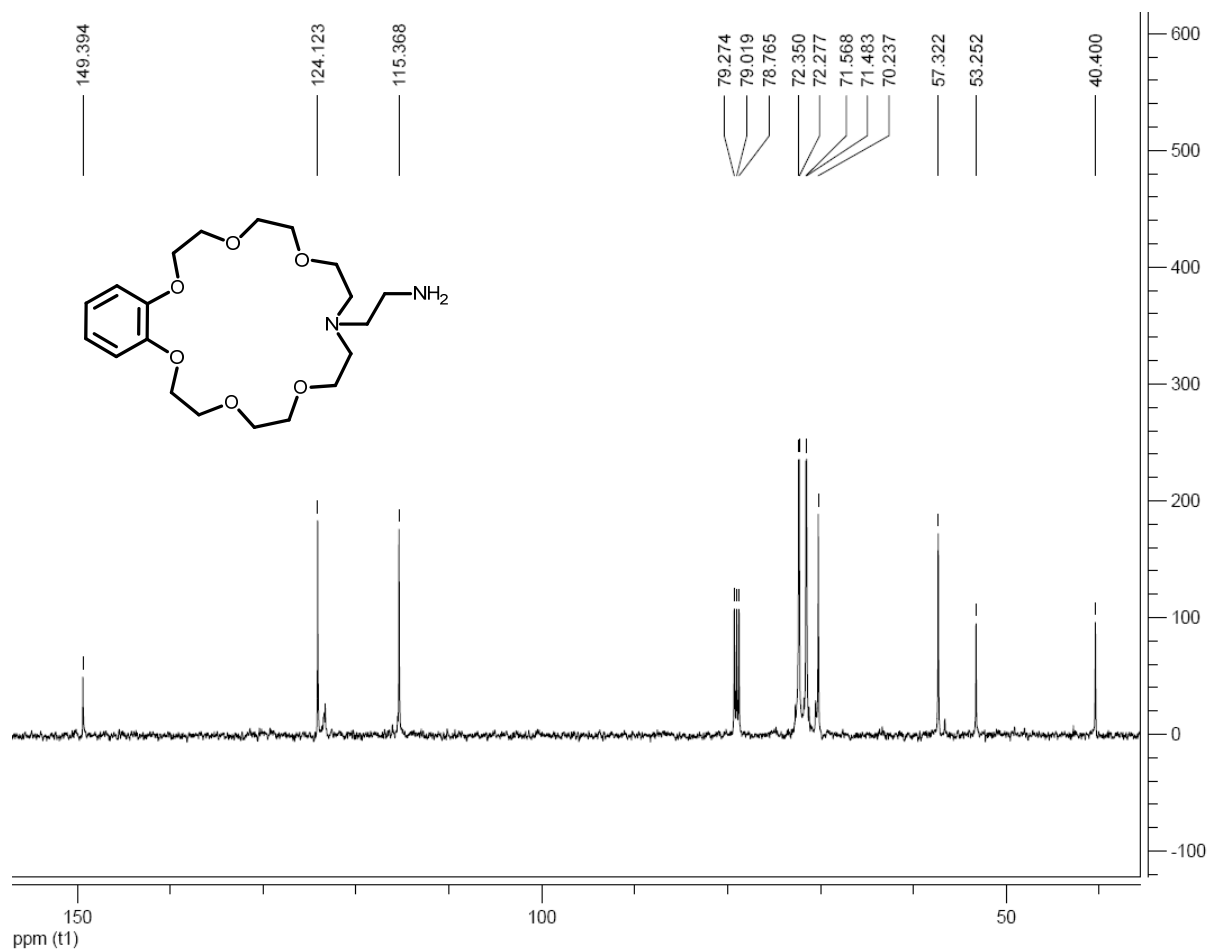
ESI Figure 10: ESI-mass spectrum of compound **2** using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

14. ¹H- NMR spectrum of 3:



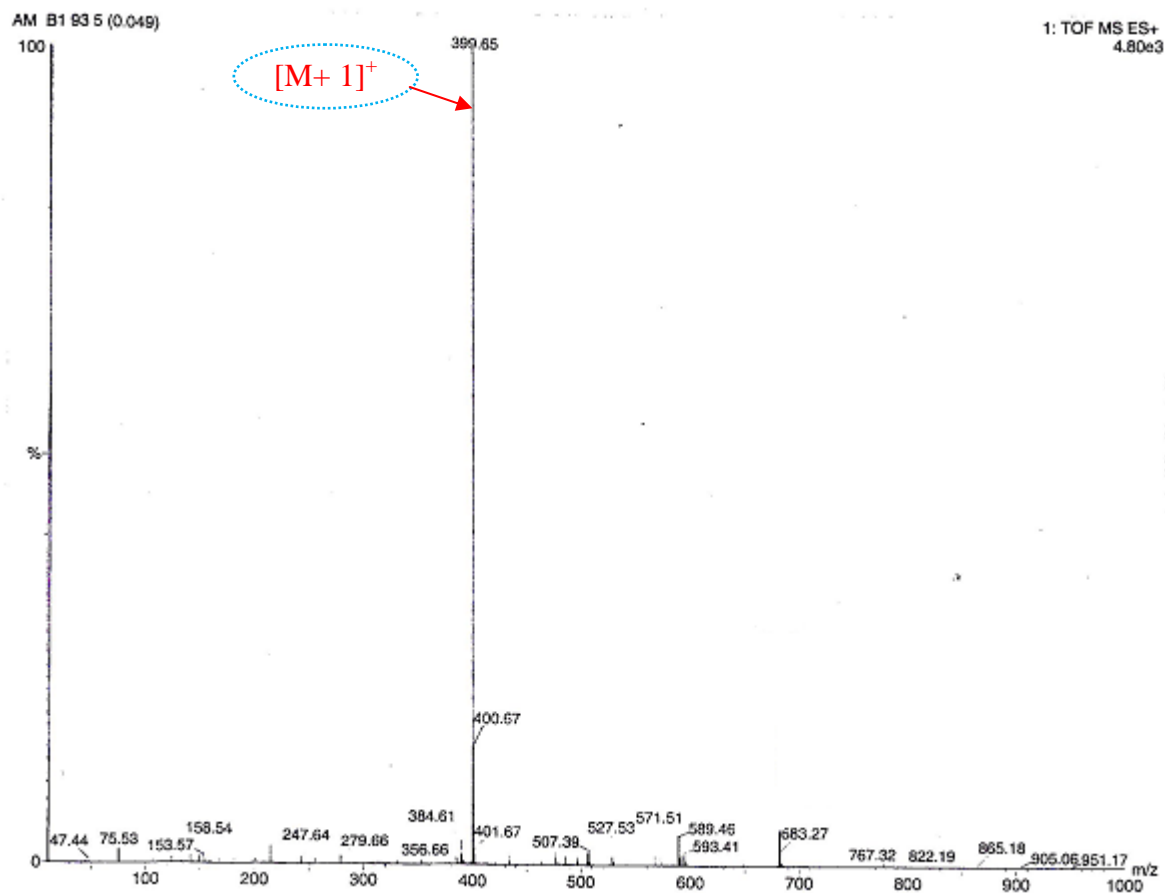
ESI Figure 11: ¹H NMR spectrum of compound **3** in CDCl₃.

15. ^{13}C - NMR spectrum of **3:**



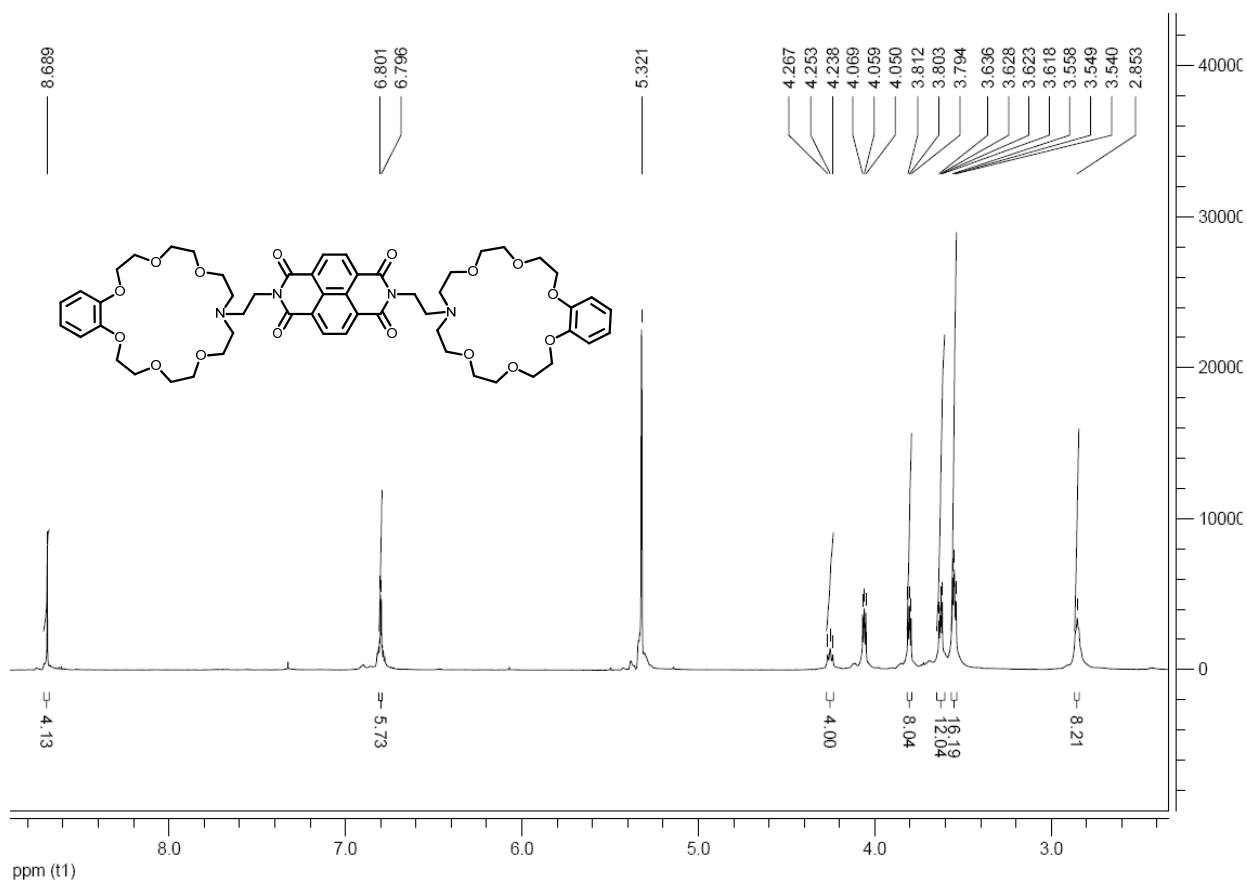
ESI Figure 12: ^{13}C -NMR spectrum of compound **3** in CDCl_3 .

16. Mass spectrum of 3:



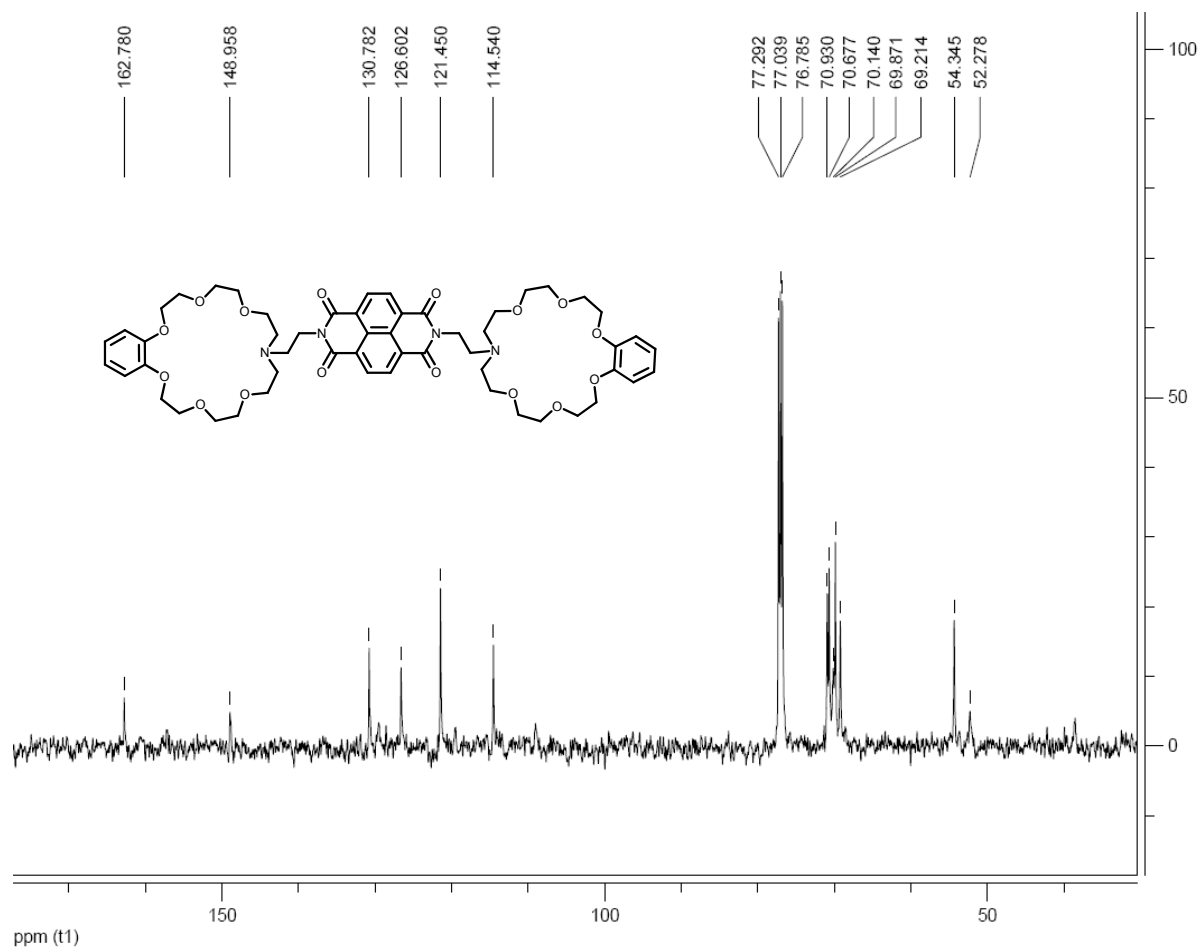
ESI Figure 13: ESI-mass spectrum of compound **3** using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

17. ¹H- NMR spectrum of H:



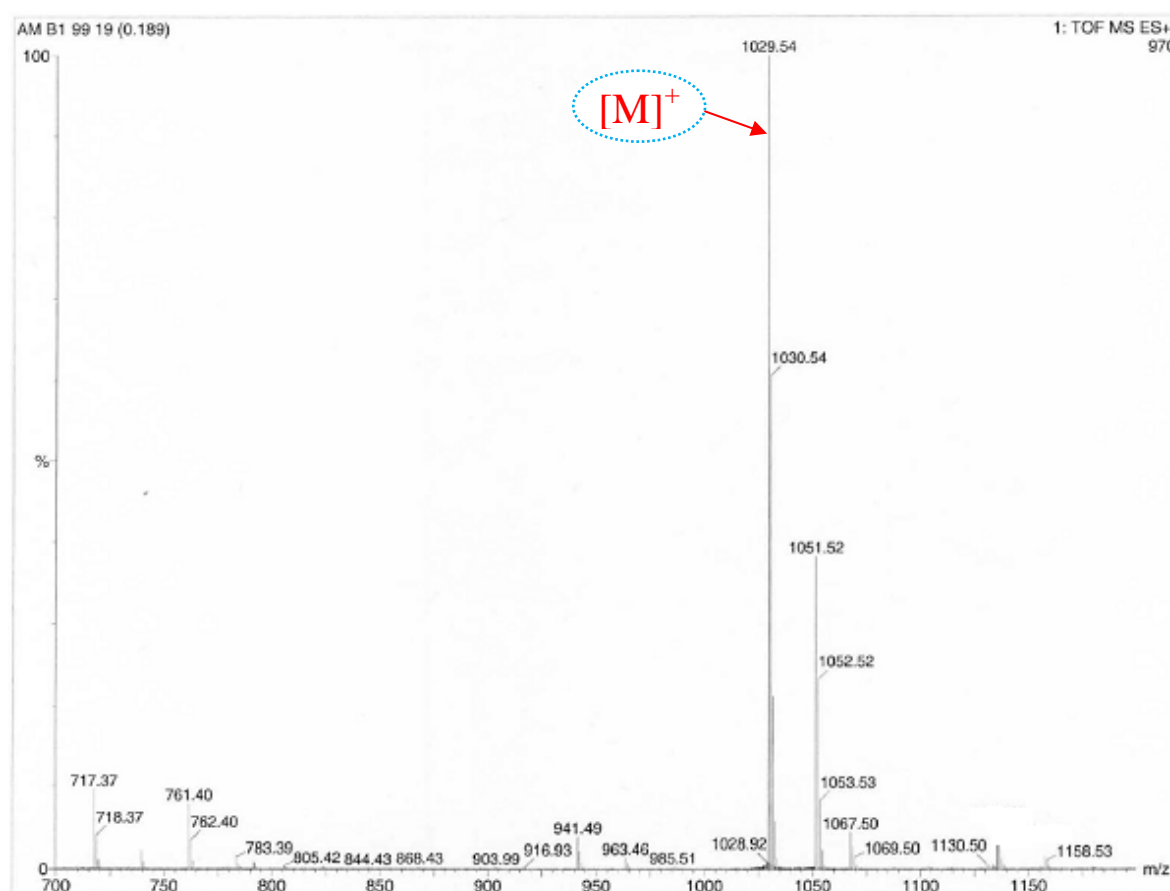
ESI Figure 14: ¹H NMR spectrum of compound **H** in CDCl₃.

18. ^{13}C -NMR spectrum of H:



ESI Figure 15: ^{13}C -NMR spectrum of compound H in CDCl_3 .

19. Mass spectrum of H:



ESI Figure 16: ESI-mass spectrum of compound **H** using Micromass Q-Tof micro™, equipped with ESI source and Q-Tof analyzer.

20. HRMS spectrum of H.

Elemental Composition Report

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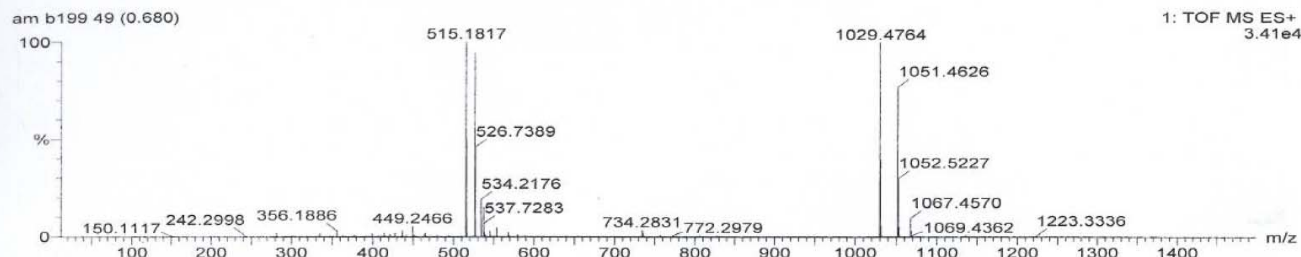
Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

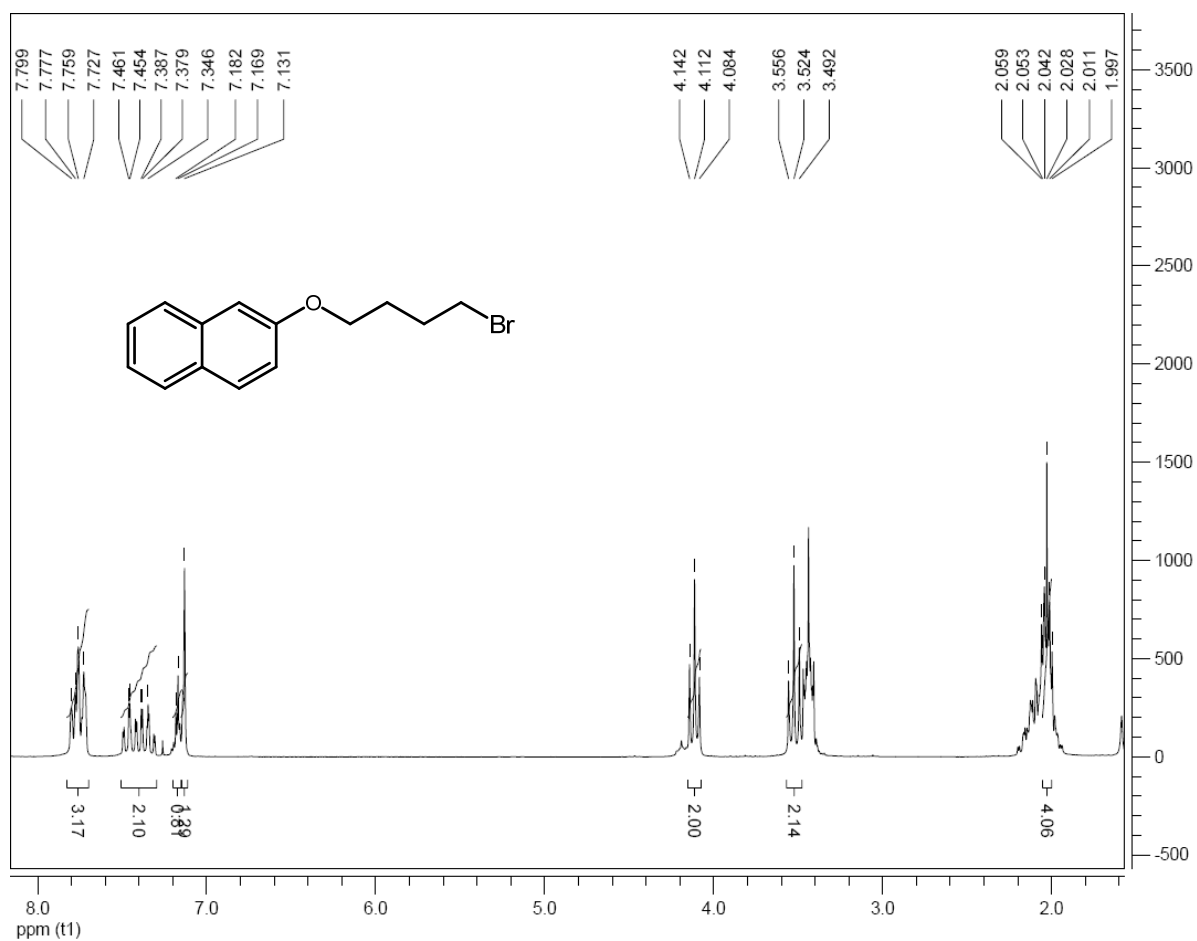
3224 formula(e) evaluated with 50 results within limits (up to 50 closest results for each mass)



| Minimum: | | | | | -1.5 | | | | |
|-----------|------------|------|------|------|-------|---------|-----|-----|--------|
| Maximum: | | 10.0 | 10.0 | | 50.0 | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula | | | |
| 1029.4764 | 1029.4765 | -0.1 | -0.1 | 27.5 | 24 | C62 | H70 | O12 | Na |
| | 1029.4762 | 0.2 | 0.2 | 31.5 | 23 | C60 | H65 | N6 | O10 |
| | 1029.4760 | 0.4 | 0.4 | 45.5 | 48 | C75 | H62 | N2 | O Na |
| | 1029.4770 | -0.6 | -0.6 | 15.0 | 1 | C48 | H72 | N5 | O18 Na |
| | 1029.4770 | -0.6 | -0.6 | 49.0 | 49 | C75 | H59 | N5 | |
| | 1029.4757 | 0.7 | 0.7 | 44.0 | 47 | C74 | H63 | N | O4 |
| | 1029.4776 | -1.2 | -1.1 | 31.0 | 25 | C62 | H67 | N3 | O11 |
| | 1029.4752 | 1.2 | 1.2 | 28.0 | 22 | C60 | H68 | N3 | O11 Na |
| | 1029.4778 | -1.4 | -1.4 | 32.5 | 26 | C63 | H66 | N4 | O8 Na |
| | 1029.4749 | 1.5 | 1.5 | 26.5 | 21 | C59 | H69 | N2 | O14 |
| | 1029.4746 | 1.8 | 1.7 | 46.0 | 46 | C73 | H60 | N5 | Na |
| | 1029.4783 | -1.9 | -1.9 | 14.5 | 2 | C50 | H74 | N2 | O19 Na |
| | 1029.4784 | -2.0 | -1.9 | 48.5 | 50 | C77 | H61 | N2 | O |
| | 1029.4744 | 2.0 | 2.0 | 44.5 | 45 | C72 | H61 | N4 | O3 |
| | 1029.4789 | -2.5 | -2.4 | 30.5 | 27 | C64 | H69 | O12 | |
| | 1029.4738 | 2.6 | 2.5 | 28.5 | 20 | C58 | H66 | N6 | O10 Na |
| | 1029.4792 | -2.8 | -2.7 | 32.0 | 28 | C65 | H68 | N | O9 Na |
| | 1029.4735 | 2.9 | 2.8 | 27.0 | 19 | C57 | H67 | N5 | O13 |
| | 1029.4794 | -3.0 | -2.9 | 18.0 | 3 | C50 | H71 | N5 | O18 |
| | 1029.4733 | 3.1 | 3.0 | 41.0 | 44 | C72 | H64 | N | O4 Na |
| | 1029.4797 | -3.3 | -3.2 | 19.5 | 5 | C51 | H70 | N6 | O15 Na |
| | 1029.4730 | 3.4 | 3.3 | 39.5 | 42 | C71 | H65 | O7 | |
| | 1029.4802 | -3.8 | -3.7 | 35.5 | 29 | C65 | H65 | N4 | O8 |
| | 1029.4725 | 3.9 | 3.8 | 23.5 | 18 | C57 | H70 | N2 | O14 Na |
| | 1029.4805 | -4.1 | -4.0 | 37.0 | 31 | C66 | H64 | N5 | O5 Na |
| | 1029.4722 | 4.2 | 4.1 | 22.0 | 16 | C56 | H71 | N | O17 |
| | 1029.4808 | -4.4 | -4.2 | 17.5 | 6 | C52 | H73 | N2 | O19 |
| | 1029.4720 | 4.4 | 4.3 | 41.5 | 41 | C70 | H62 | N4 | O3 Na |
| | 1029.4810 | -4.6 | -4.5 | 19.0 | 9 | C53 | H72 | N3 | O16 Na |
| | 1029.4717 | 4.7 | 4.6 | 40.0 | 38 | C69 | H63 | N3 | O6 |
| | 1029.4816 | -5.2 | -5.0 | 35.0 | 32 | C67 | H67 | N | O9 |
| | 1029.4711 | 5.3 | 5.1 | 24.0 | 15 | C55 | H68 | N5 | O13 Na |
| | 1029.4819 | -5.5 | -5.3 | 36.5 | 34 | C68 | H66 | N2 | O6 Na |
| | 1029.4709 | 5.5 | 5.4 | 22.5 | 13 | C54 | H69 | N4 | O16 |
| | 1029.4821 | -5.7 | -5.5 | 22.5 | 11 | C53 | H69 | N6 | O15 |
| | 1029.4706 | 5.8 | 5.6 | 36.5 | 36 | C69 | H66 | O7 | Na |
| | 1029.4824 | -6.0 | -5.8 | 18.5 | 12 | C55 | H74 | O17 | Na |
| | 1029.4703 | 6.1 | 5.9 | 40.5 | 35 | C67 | H61 | N6 | O5 |
| | 1029.4829 | -6.5 | -6.3 | 40.0 | 37 | C68 | H63 | N5 | O5 |
| | 1029.4698 | 6.6 | 6.4 | 19.0 | 10 | C54 | H72 | N | O17 Na |
| | 1029.4832 | -6.8 | -6.6 | 41.5 | 39 | C69 | H62 | N6 | O2 Na |
| | 1029.4695 | 6.9 | 6.7 | 17.5 | 8 | C53 | H73 | O20 | |
| | 1029.4834 | -7.0 | -6.8 | 22.0 | 14 | C55 | H71 | N3 | O16 |

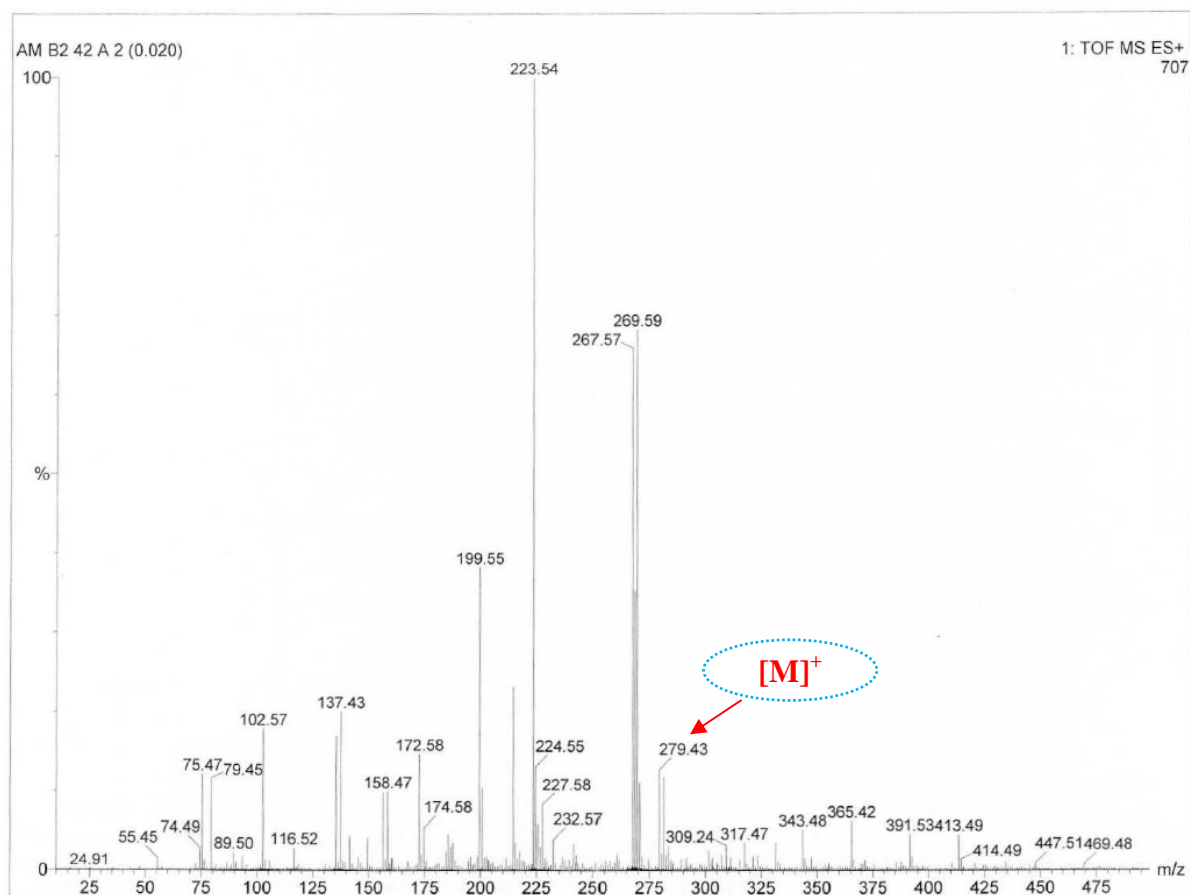
ESI Figure 17: HRMS spectrum of compound H using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

21. ¹H- NMR spectrum of I:



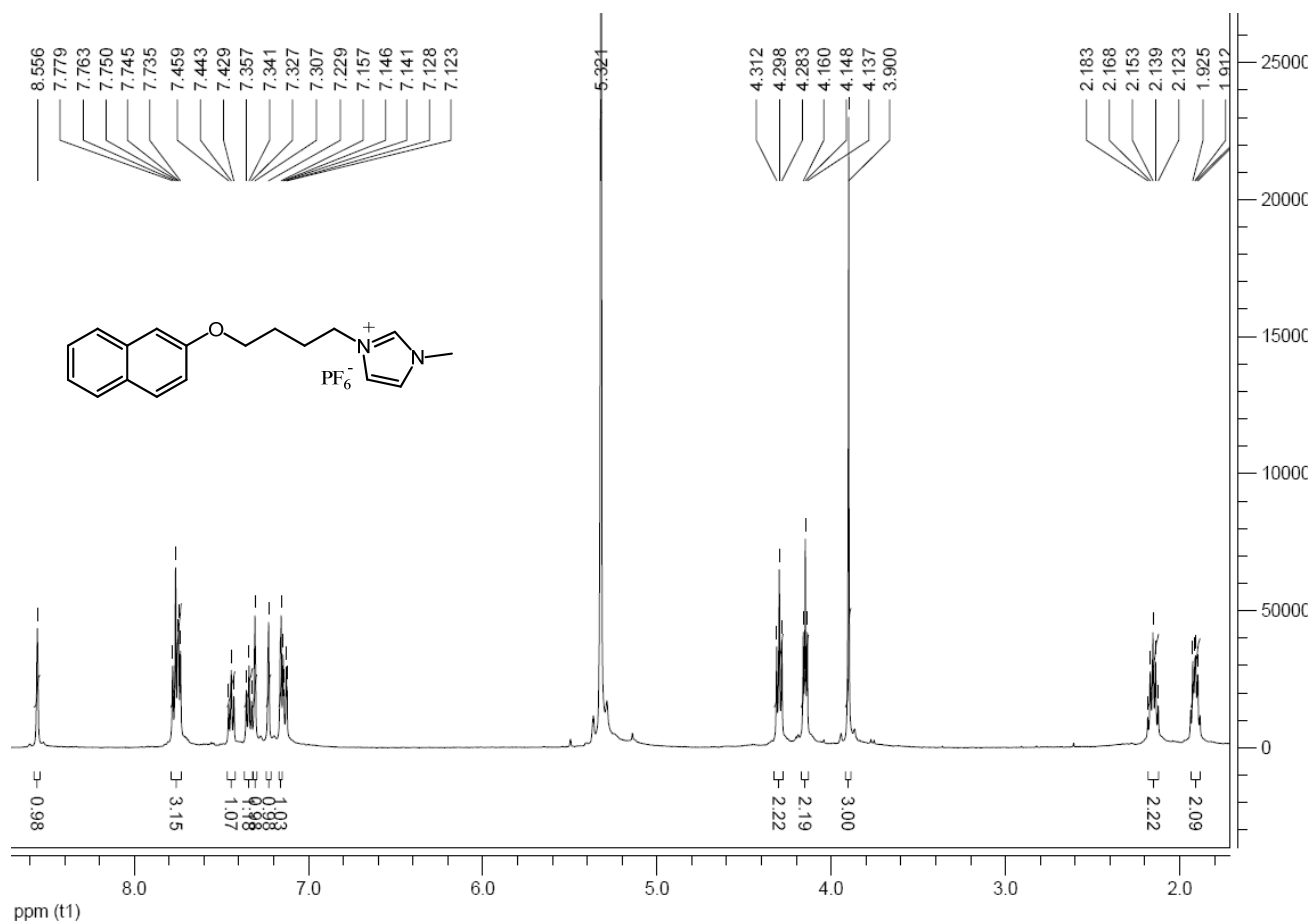
ESI Figure 18: ¹H-NMR spectrum of compound I in CDCl₃.

22. Mass spectrum of I:



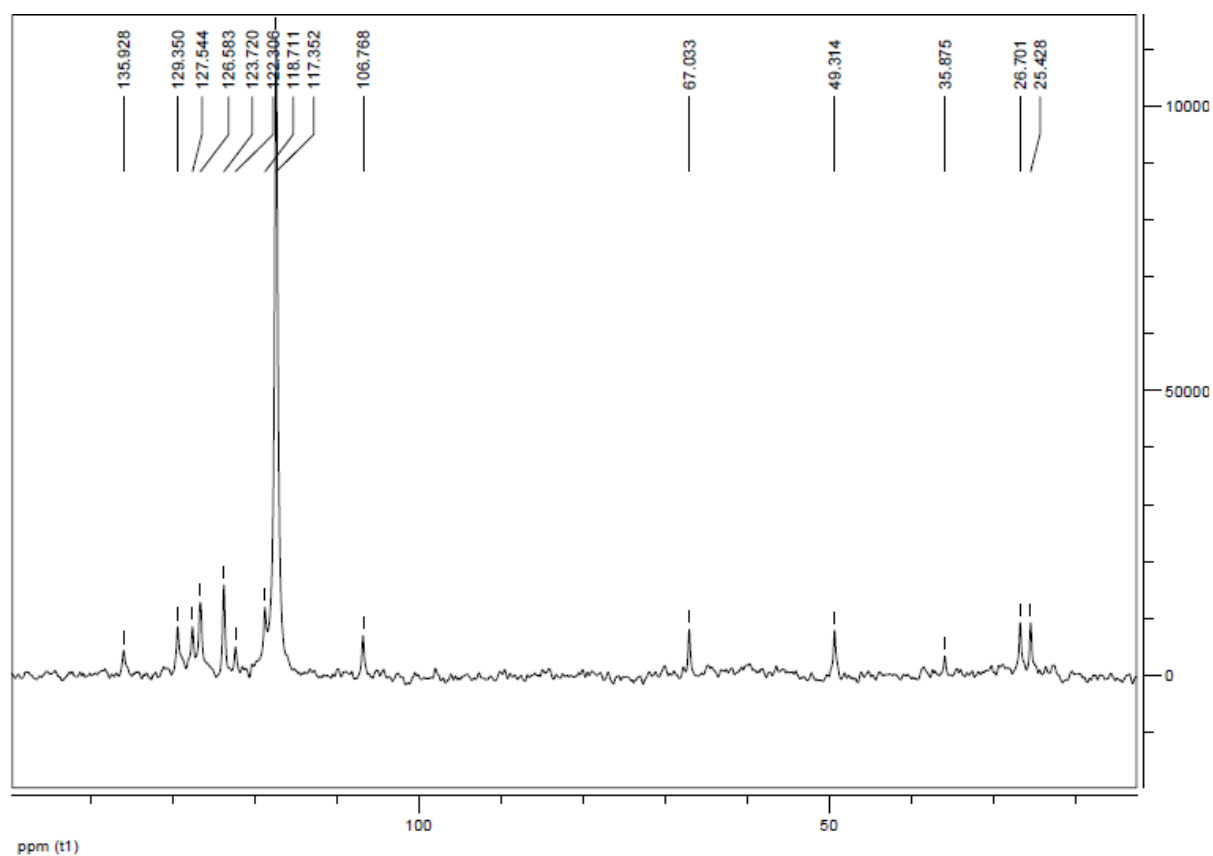
ESI Figure 19: ESI-mass spectrum of compound **I** using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

23. ^1H -NMR spectrum of **G₂**:



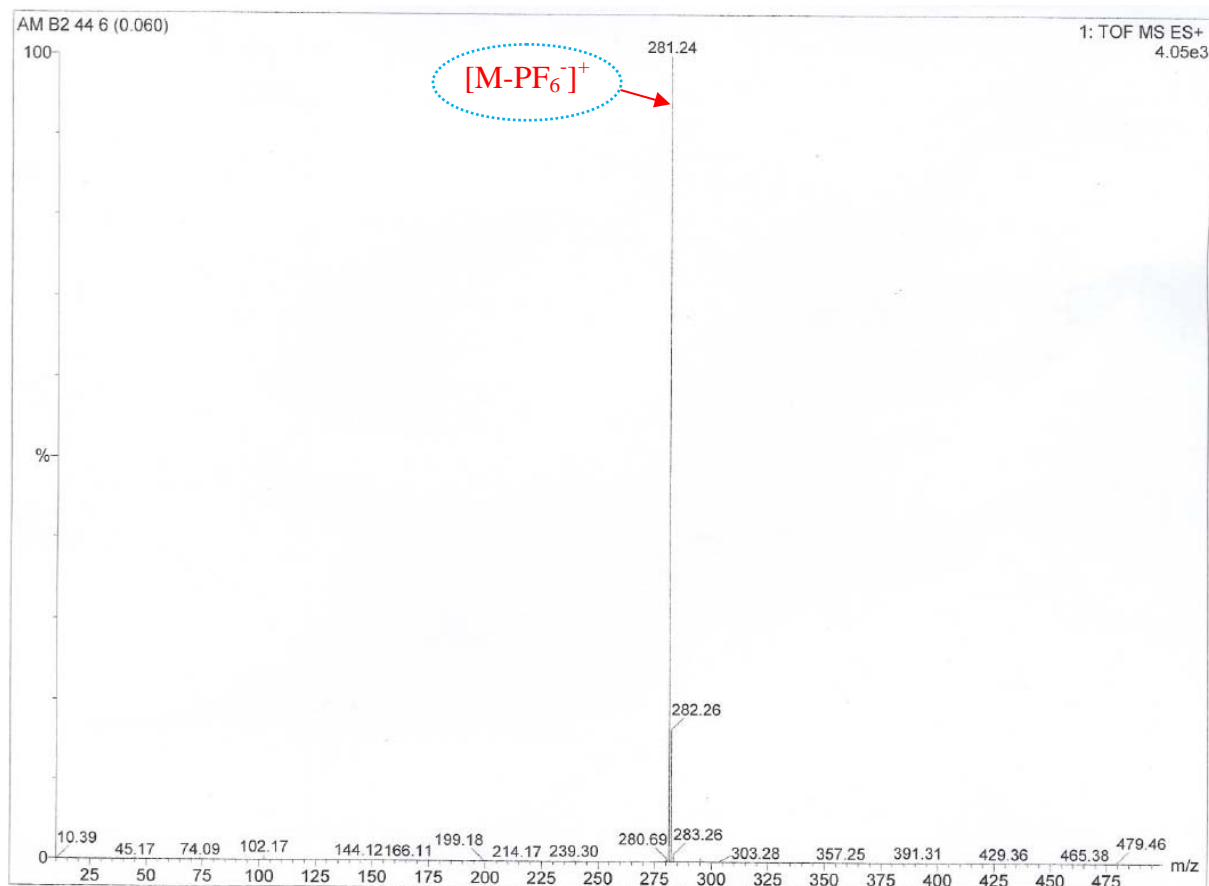
ESI Figure 20: ^1H -NMR spectrum of compound **G₂** in CD_2Cl_2 .

24. ^{13}C - NMR spectrum of G_2 :



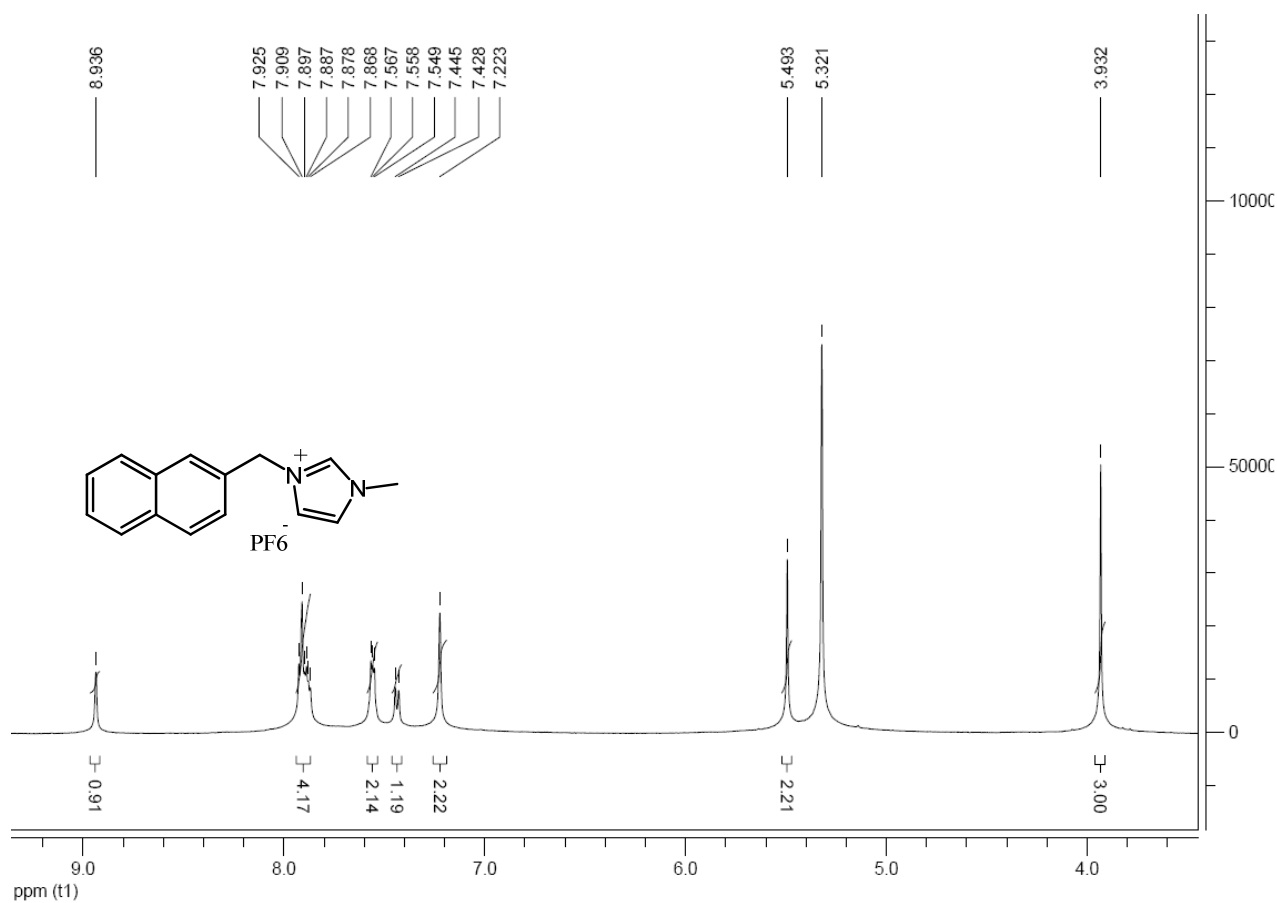
ESI Figure 21: ^{13}C -NMR spectrum of compound G_2 in CD_3CN .

25. Mass spectrum of G₂:



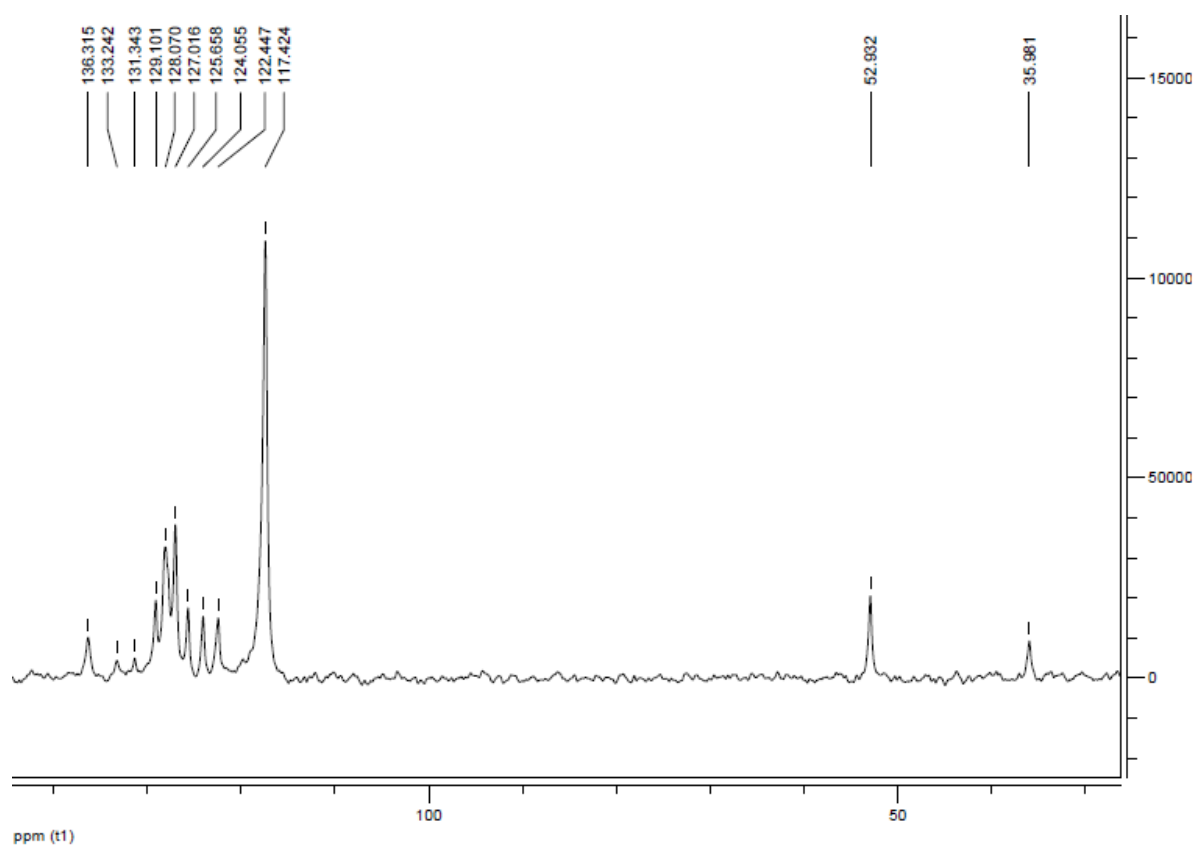
ESI Figure 22: ESI-mass spectrum of compound **G₂** using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

26. ^1H - NMR spectrum of **G₁**:



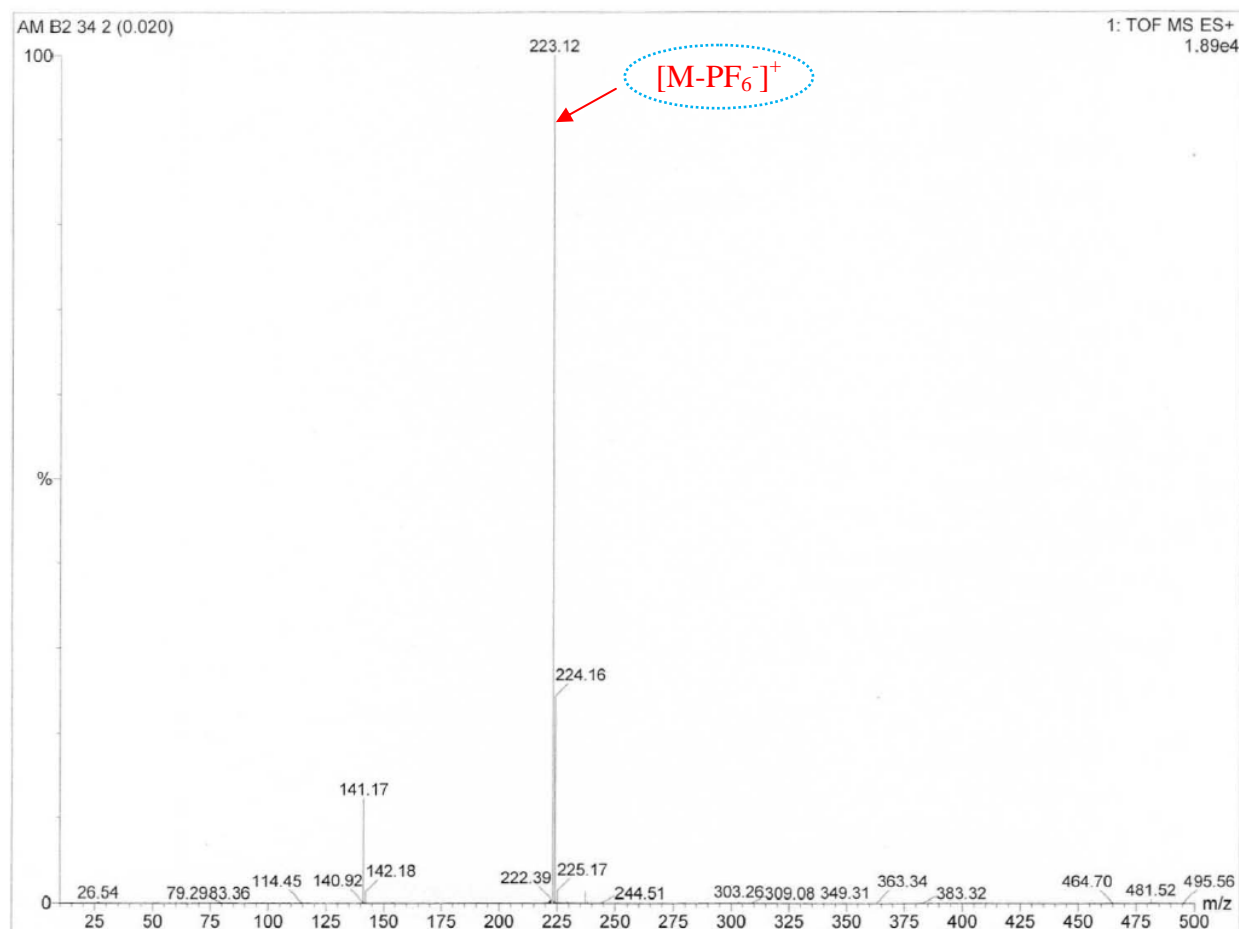
ESI Figure 23: ^1H -NMR spectrum of compound **G₁** in CD_2Cl_2 .

27. ^{13}C - NMR spectrum of G_1 :



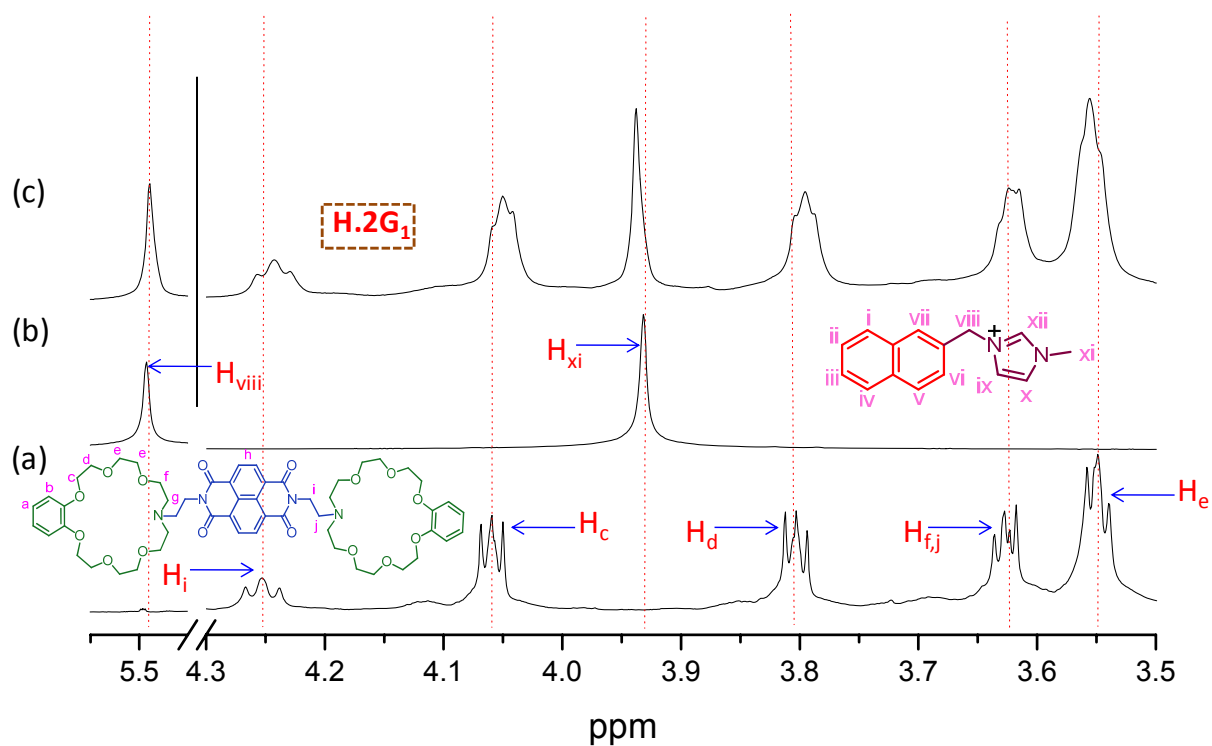
ESI Figure 24: ^{13}C -NMR spectrum of compound G_1 in CD_3CN .

28. Mass spectrum of G₁:



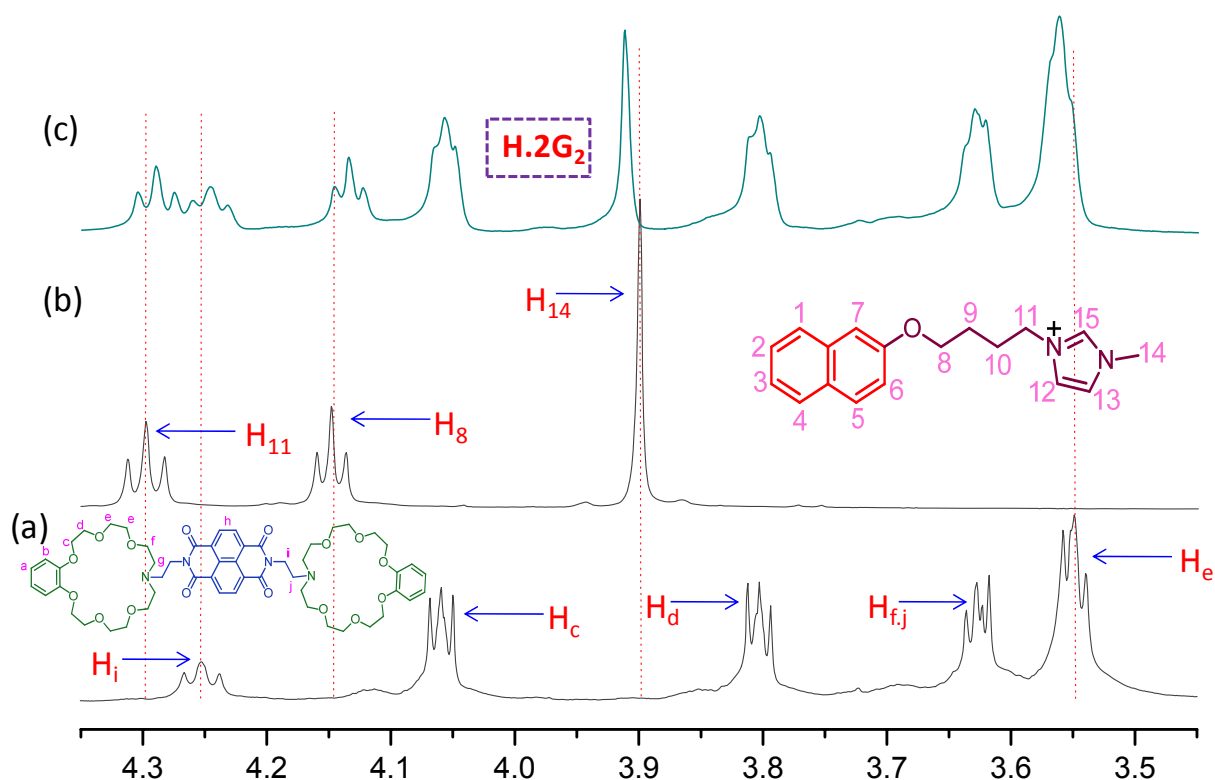
ESI Figure 25: ESI-mass spectrum of compound **G₁** using Micromass Q-Tof microTM, equipped with ESI source and Q-Tof analyzer.

29. ^1H -NMR spectrum of H, G_1 and $\text{H} \cdot 2\text{G}_1$.



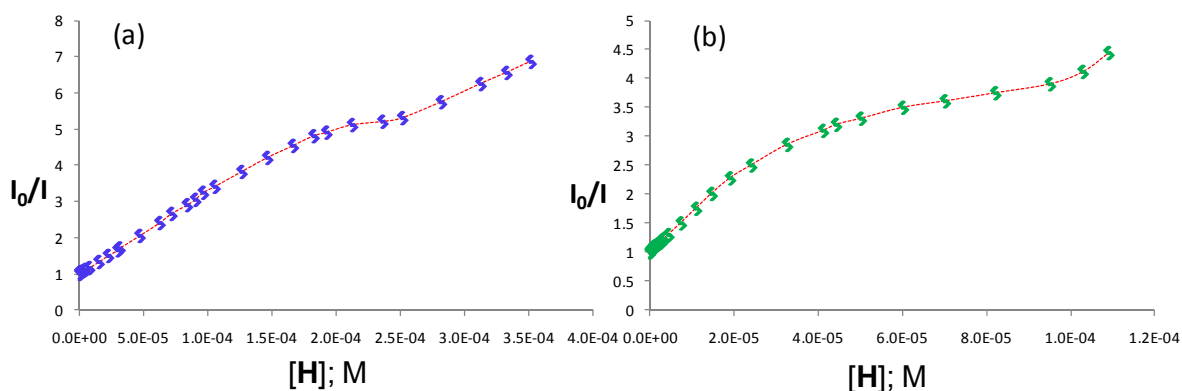
ESI Figure 26: ^1H -NMR spectra recorded in CD_2Cl_2 at 25°C of (a) 5.43mM **H**; (b) in presence of 10.89 mM **G**₁ and (c) in presence of 10.89mM of **G**₁.

30. ^1H -NMR spectrum of H , G_2 and $\text{H} \cdot 2\text{G}_2$.



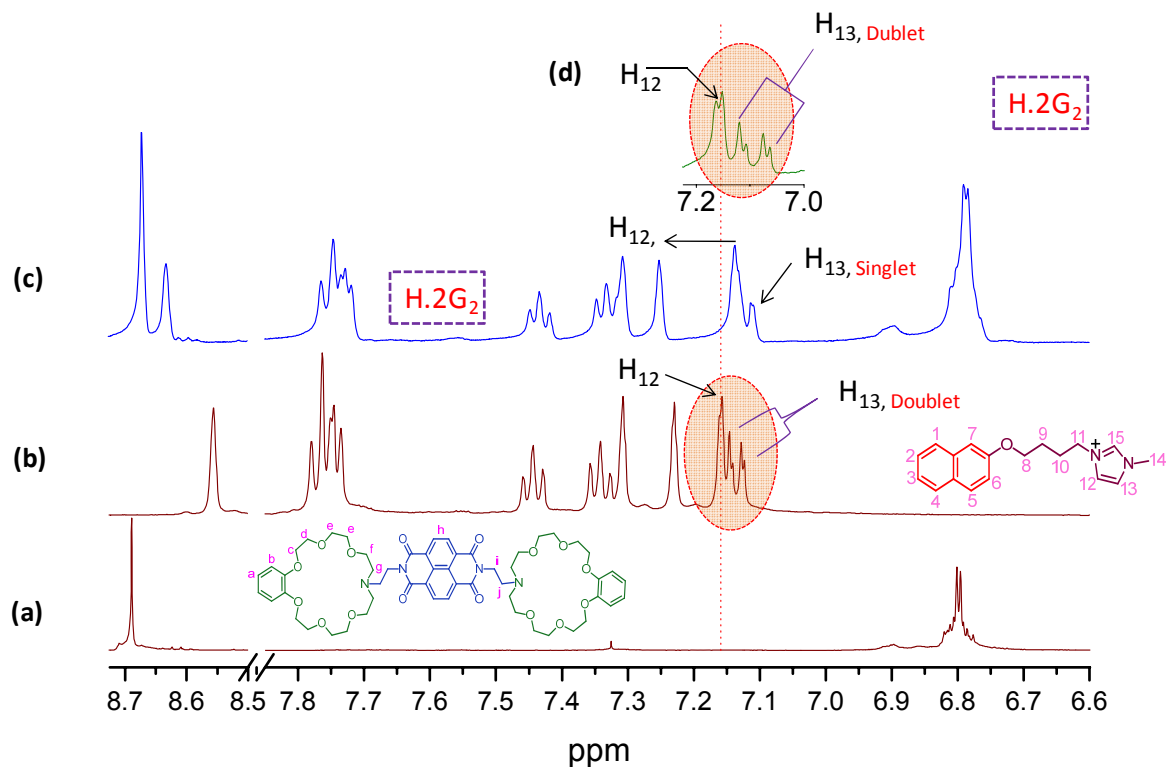
ESI Figure 27: ^1H -NMR spectra recorded in CD_2Cl_2 at 25°C of (a) 4.68mM H ; (b)) in presence of 9.38mM G_2 and (c)) in presence of 9.38mM G_2 and 4.68mM H .

31. Stern-Volmer plot of H.2G₁ & H.2G₂:



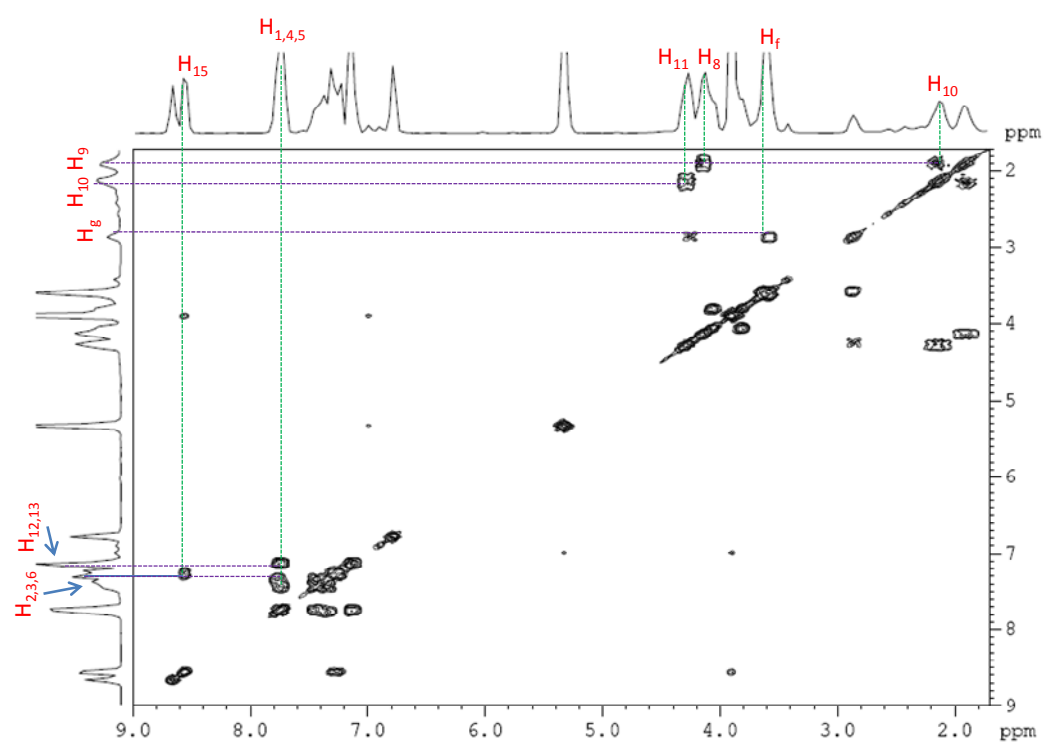
ESI Figure 28: Stern-Volmer Plots for emission quenching for (a) H.2G₁ system and (b) H.2G₂ system upon addition of H.

32. ^1H -NMR spectrum of H.2G_2 in the presence of methanol.



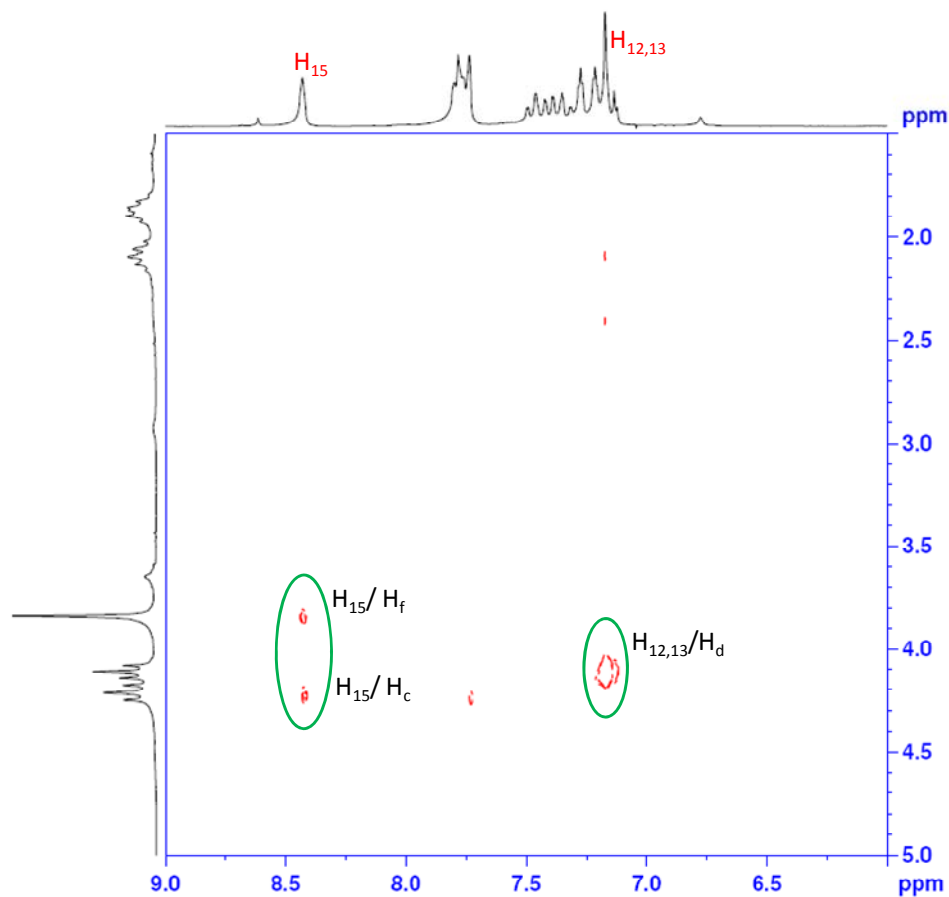
ESI Figure 29: ^1H -NMR spectra recorded in CD_2Cl_2 at 25°C of (a) 4.68mM H ; (b) 9.38mM G_2 and (c) in presence of 9.38mM G_2 and 4.68mM H ; (d) Partial spectra of H.2G_2 in the presence of CH_3OD . The doublet for H_{13} of G_2 , which disappeared due to the formation of the threaded complex H.2G_2 , reappeared on addition of polar solvent like CH_3OD —supporting the de-threading phenomena in polar solvent.

33. 2D-COSY spectrum of H.2G₂



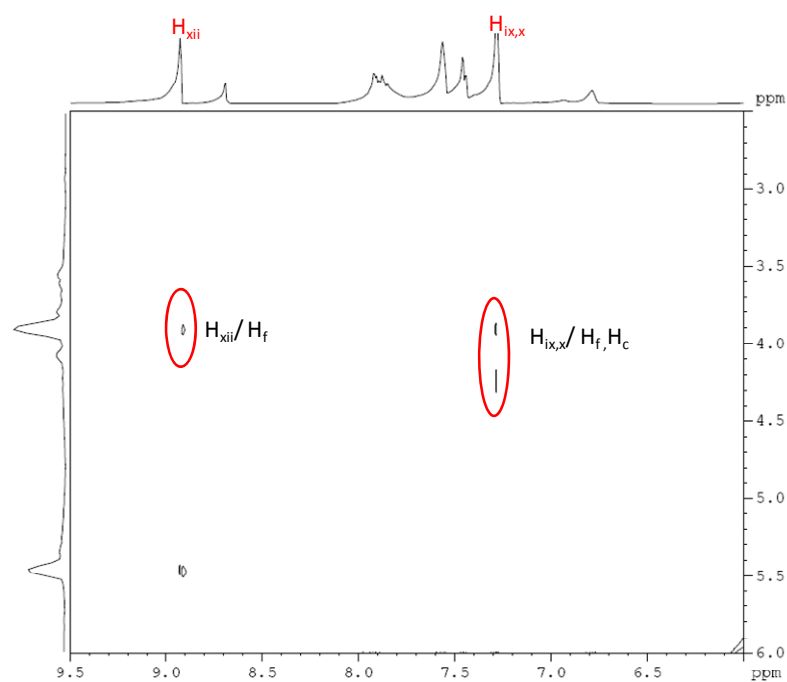
ESI Figure 30: 2D-COSY spectra OF **H.2G₂** recorded in CD₂Cl₂ at 25°C.

34. 2D-NOSEY spectrum of H.2G₂



ESI Figure 31: 2D-NOSEY spectra OF **H.2G₂** recorded in CD₂Cl₂ at 25°C.

35. 2D-NOSEY spectrum of H.2G₁



ESI Figure 31: 2D-NOSEY spectra OF **H.2G₁** recorded in CD₂Cl₂ at 25°C.