

# *Catechol-based macrocyclic aromatic ether-sulfones: Synthesis, characterization and ring-opening polymerization*

Article

Supplemental Material

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## Supplementary Material

### Catechol-based macrocyclic aromatic ether-sulfones: Synthesis, characterization and ring-opening polymerization

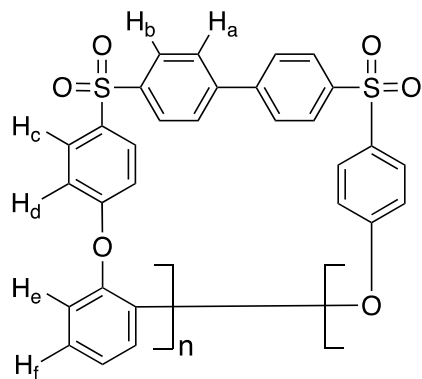
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Via Torino 155, 30172 Venice, Italy*

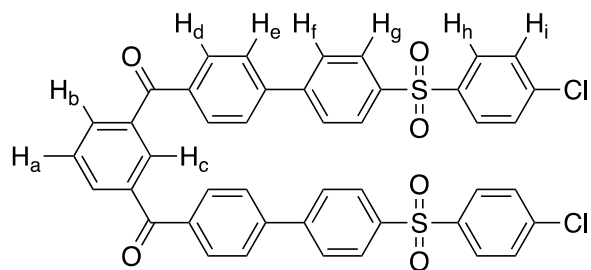
<sup>b</sup>*Department of Chemistry, University of Reading, Whiteknights, Reading, RG6 6AD, UK  
Email: [fabio.arico@unive.it](mailto:fabio.arico@unive.it); [h.m.colquhoun@rdg.ac.uk](mailto:h.m.colquhoun@rdg.ac.uk)*

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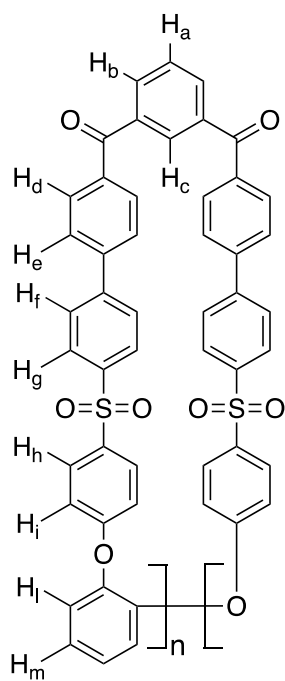
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**2** ( $n = 2$ ), **3** ( $n = 3$ ), **4** ( $n = 4$ ), **5** ( $n = 5$ )

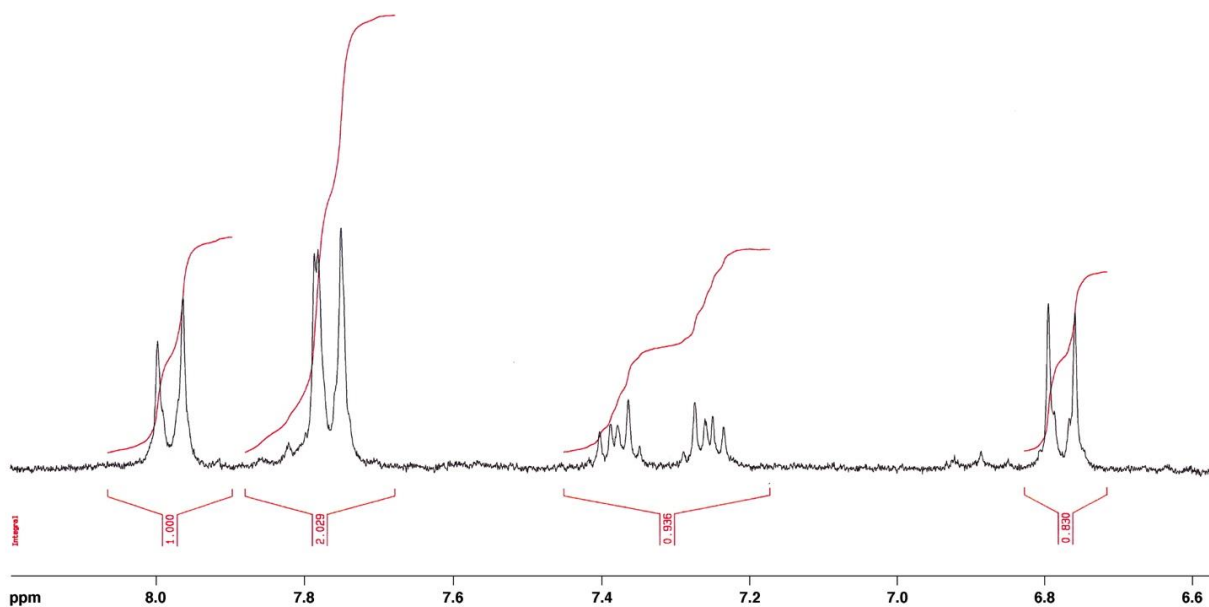


**7**

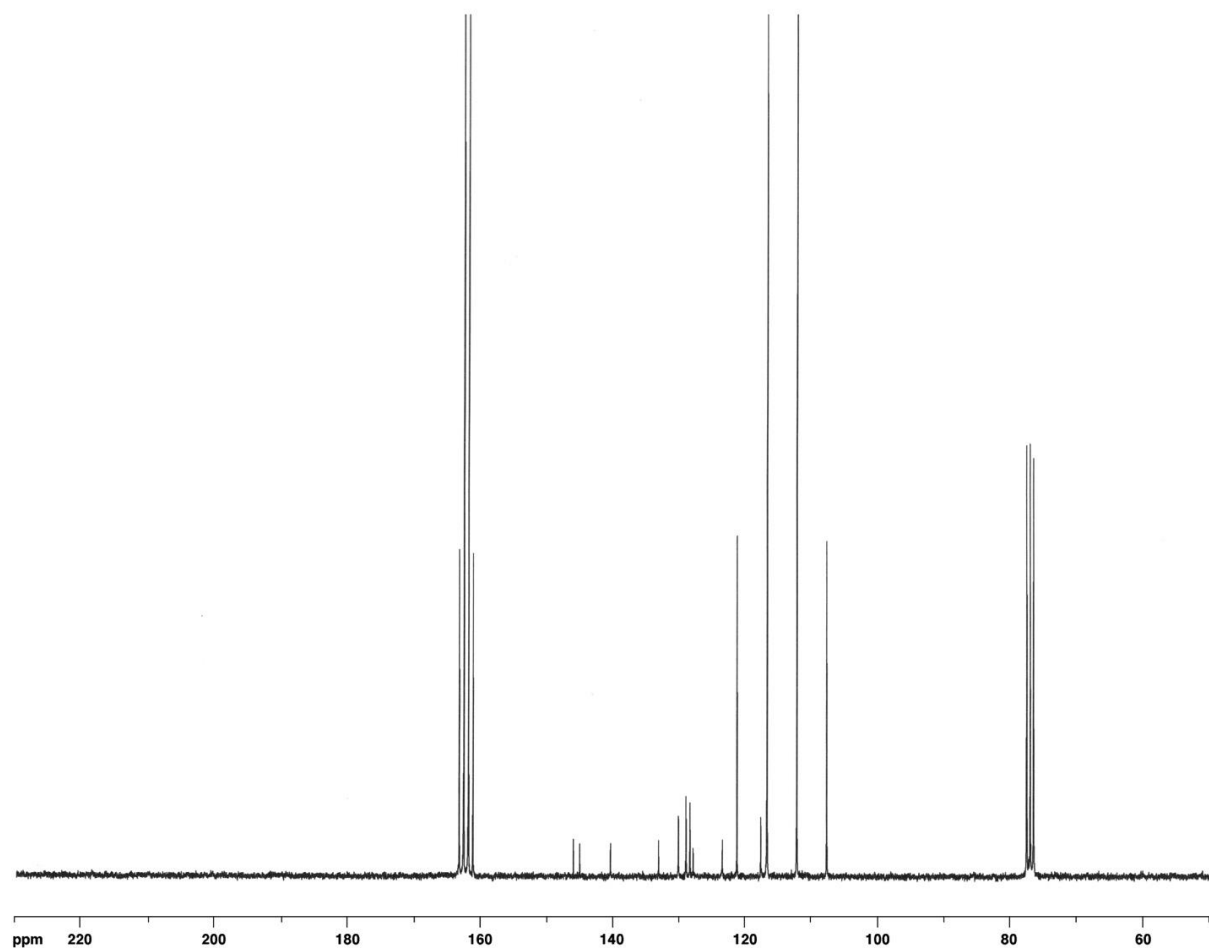


**8** ( $n = 1$ ), **9** ( $n = 2$ )

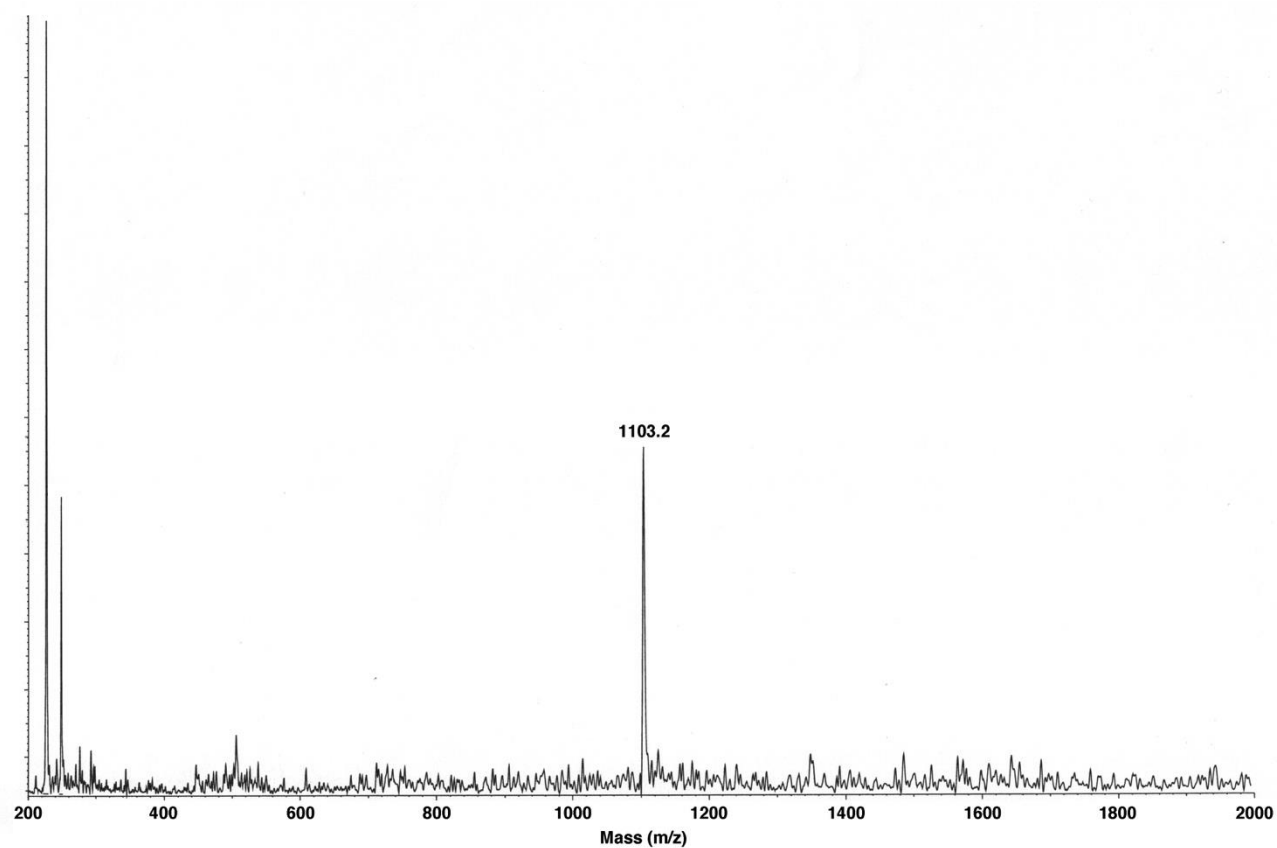
**Chart S1:** Labelled structures for  $^1\text{H}$  NMR assignments (refer to Experimental Section).



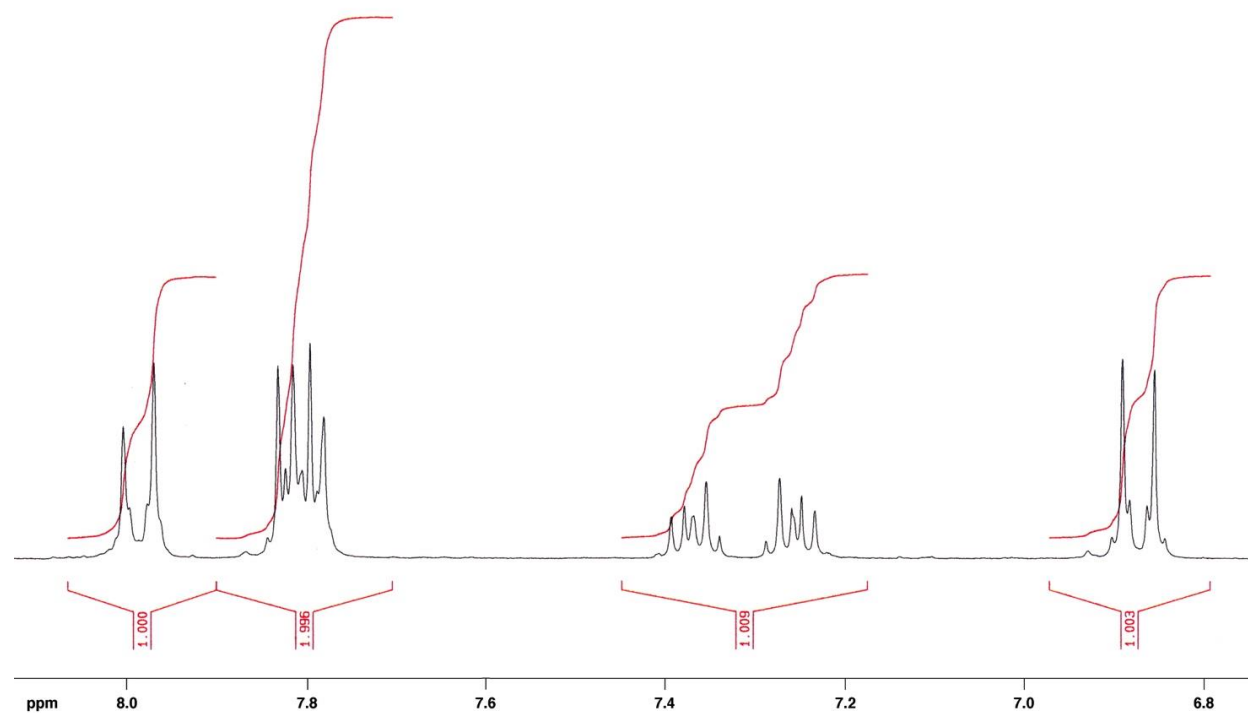
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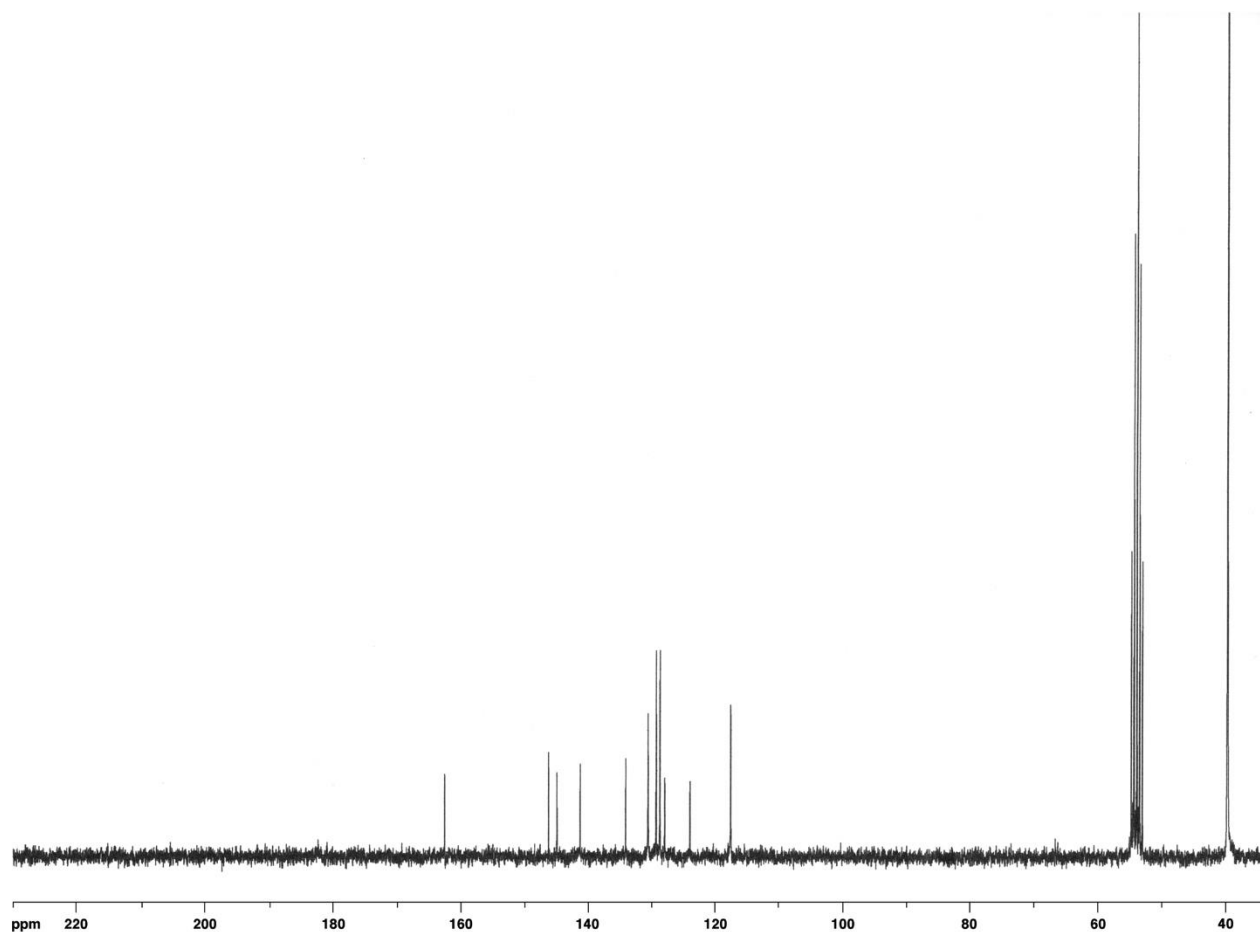
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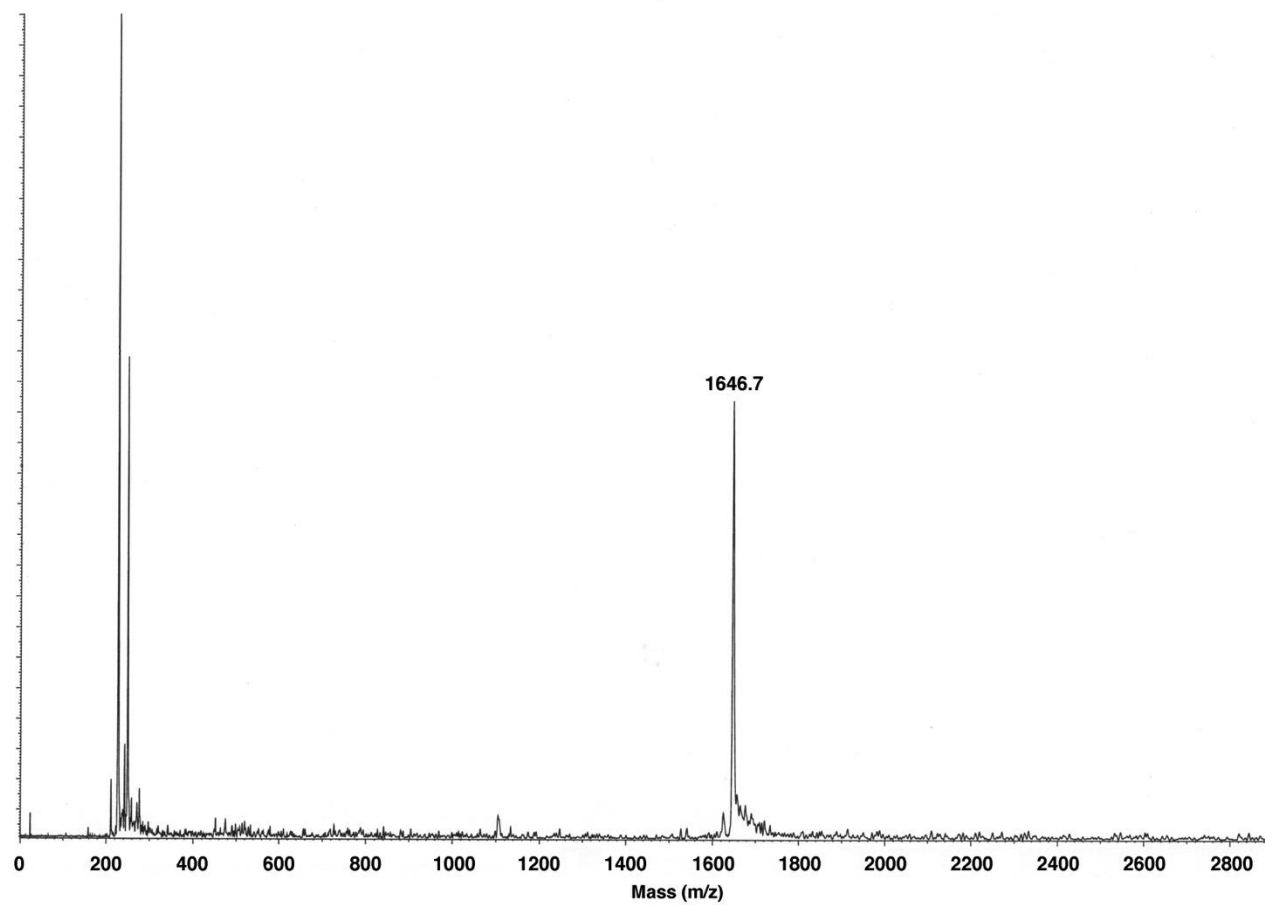
**Figure S3:** MALDI-TOF mass spectrum of macrocycle **2**. (Calc.  $m/z$  for  $[\text{C}_{60}\text{H}_{40}\text{S}_4\text{O}_{12}\text{Na}]^+ = 1104.2$ ).



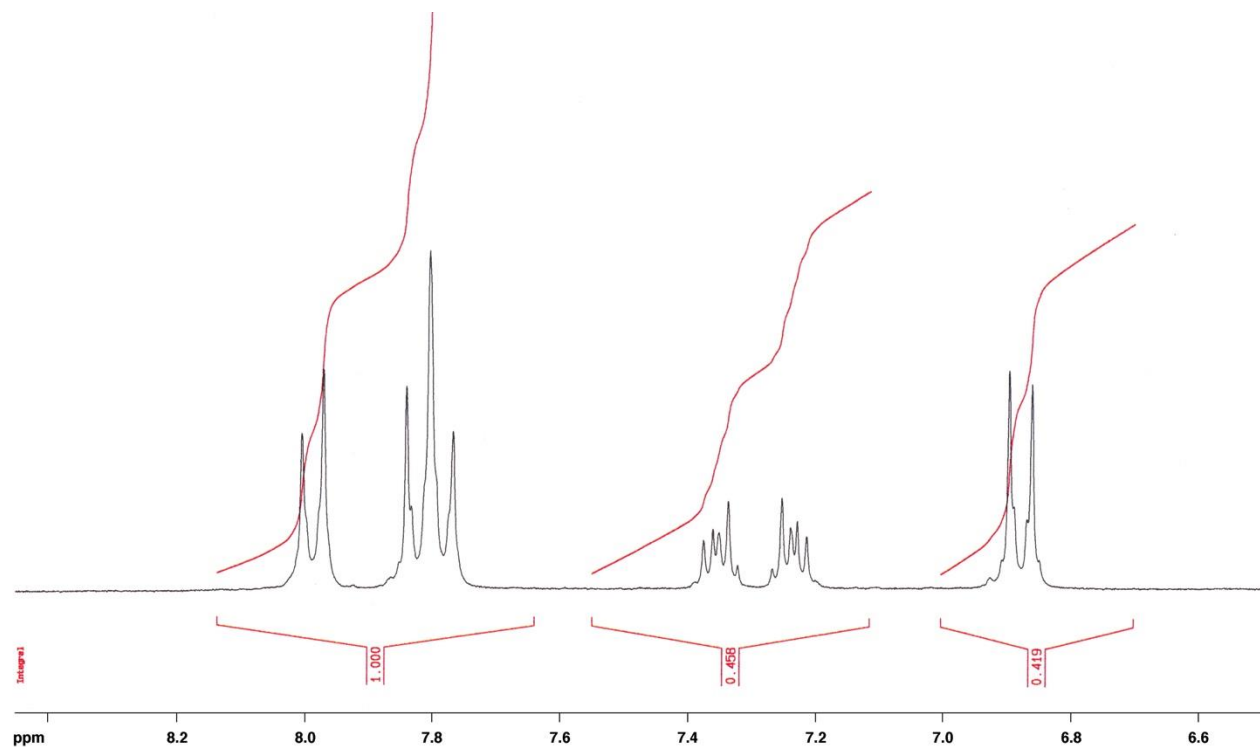
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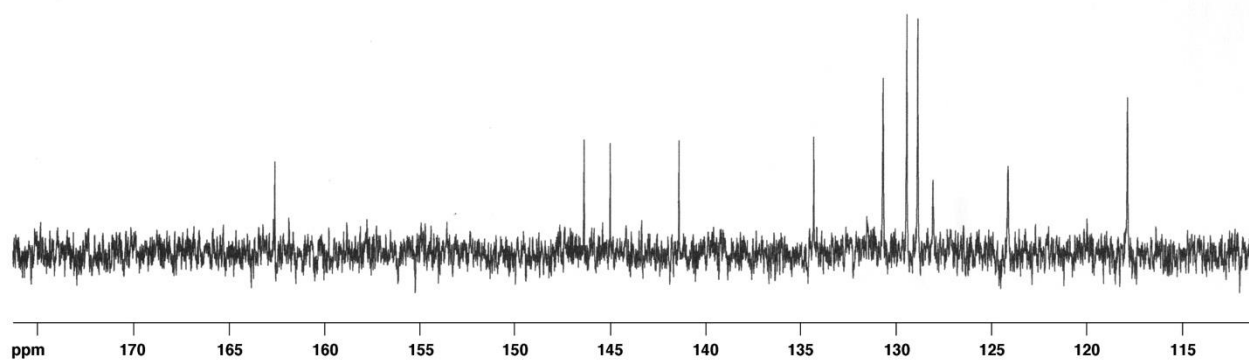
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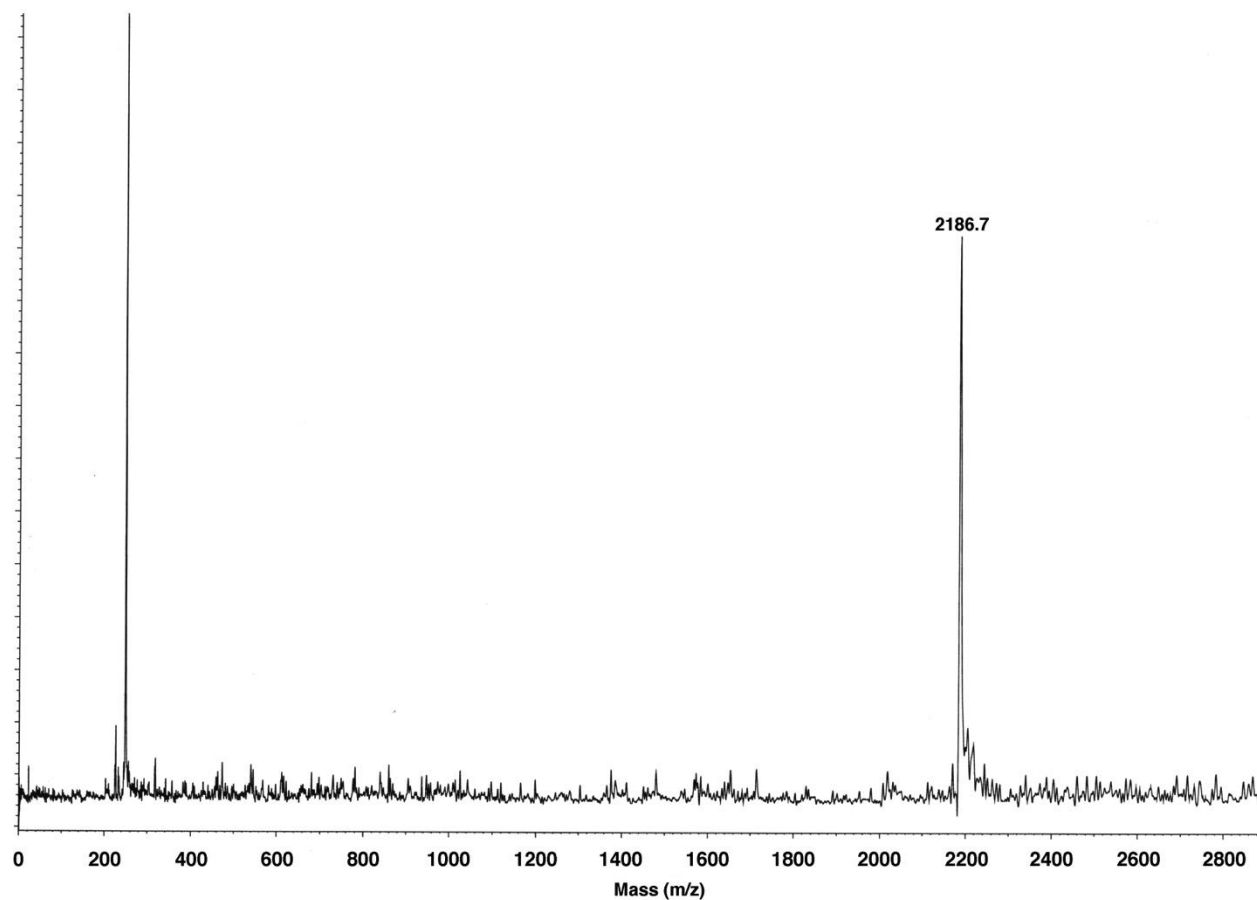
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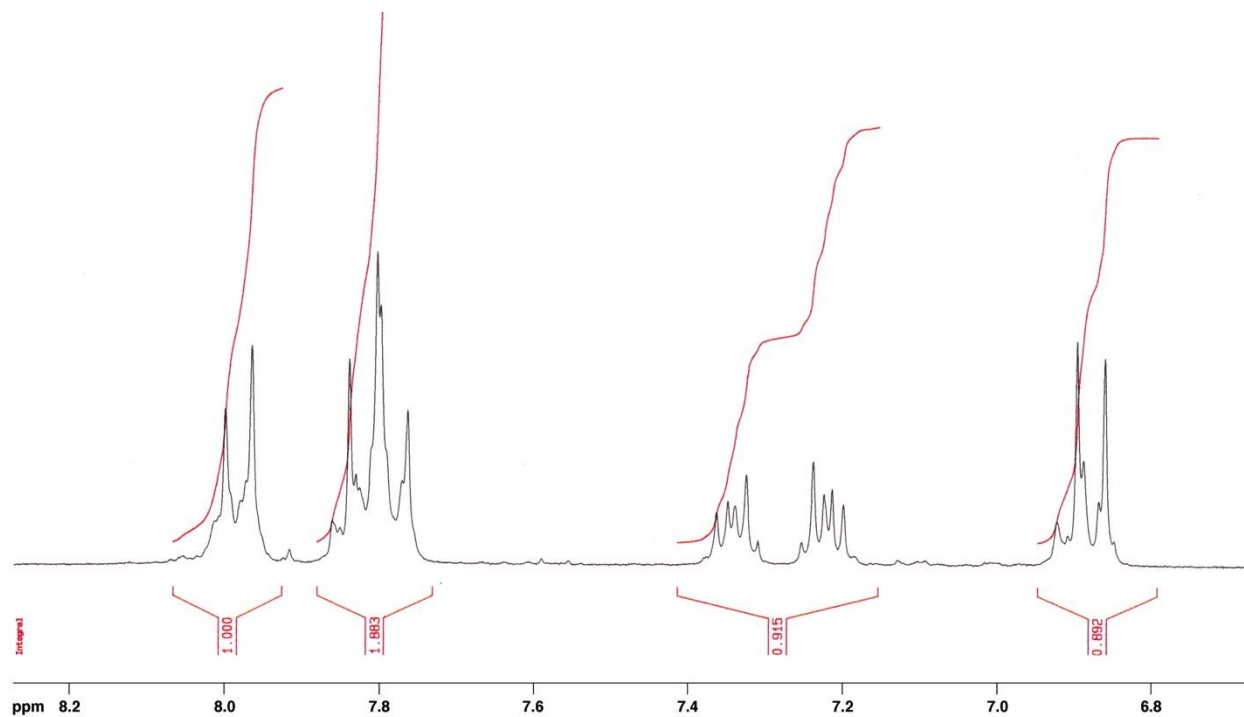
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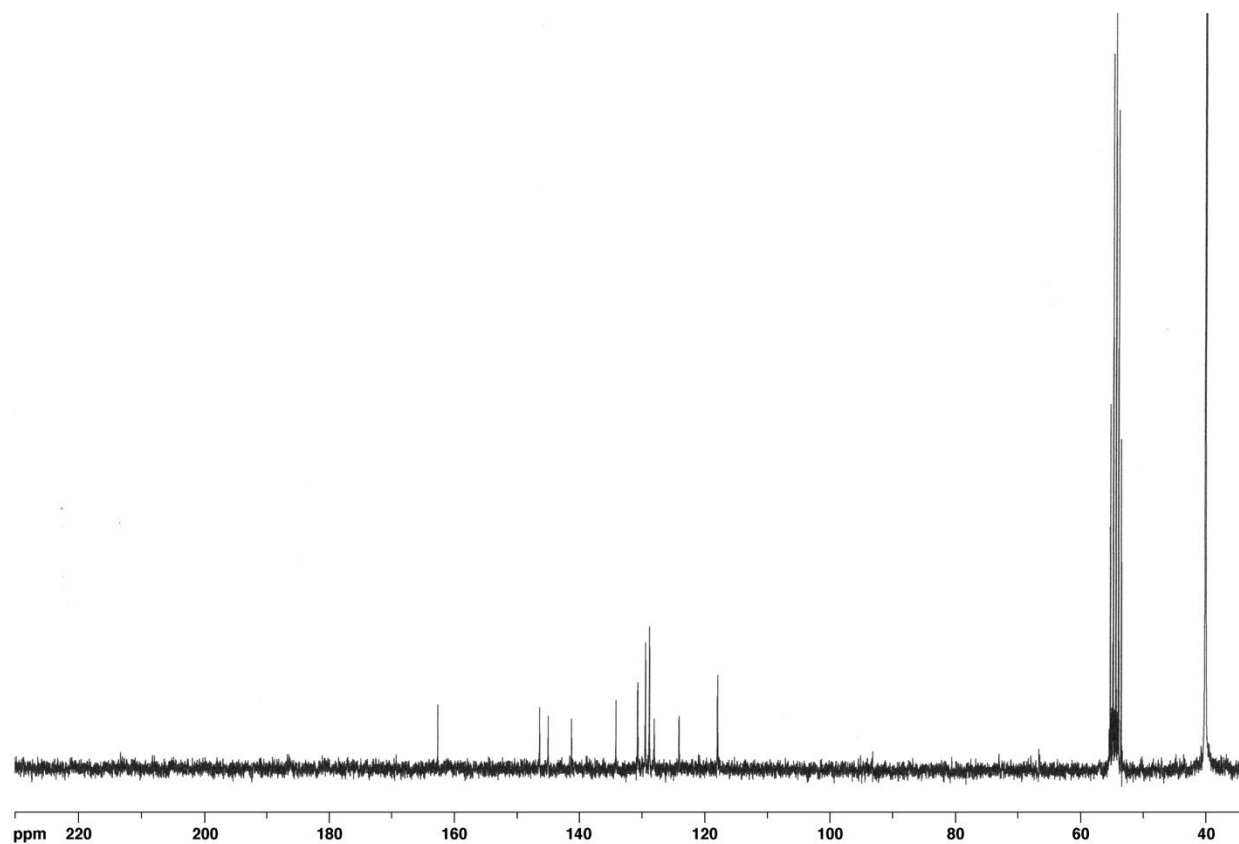
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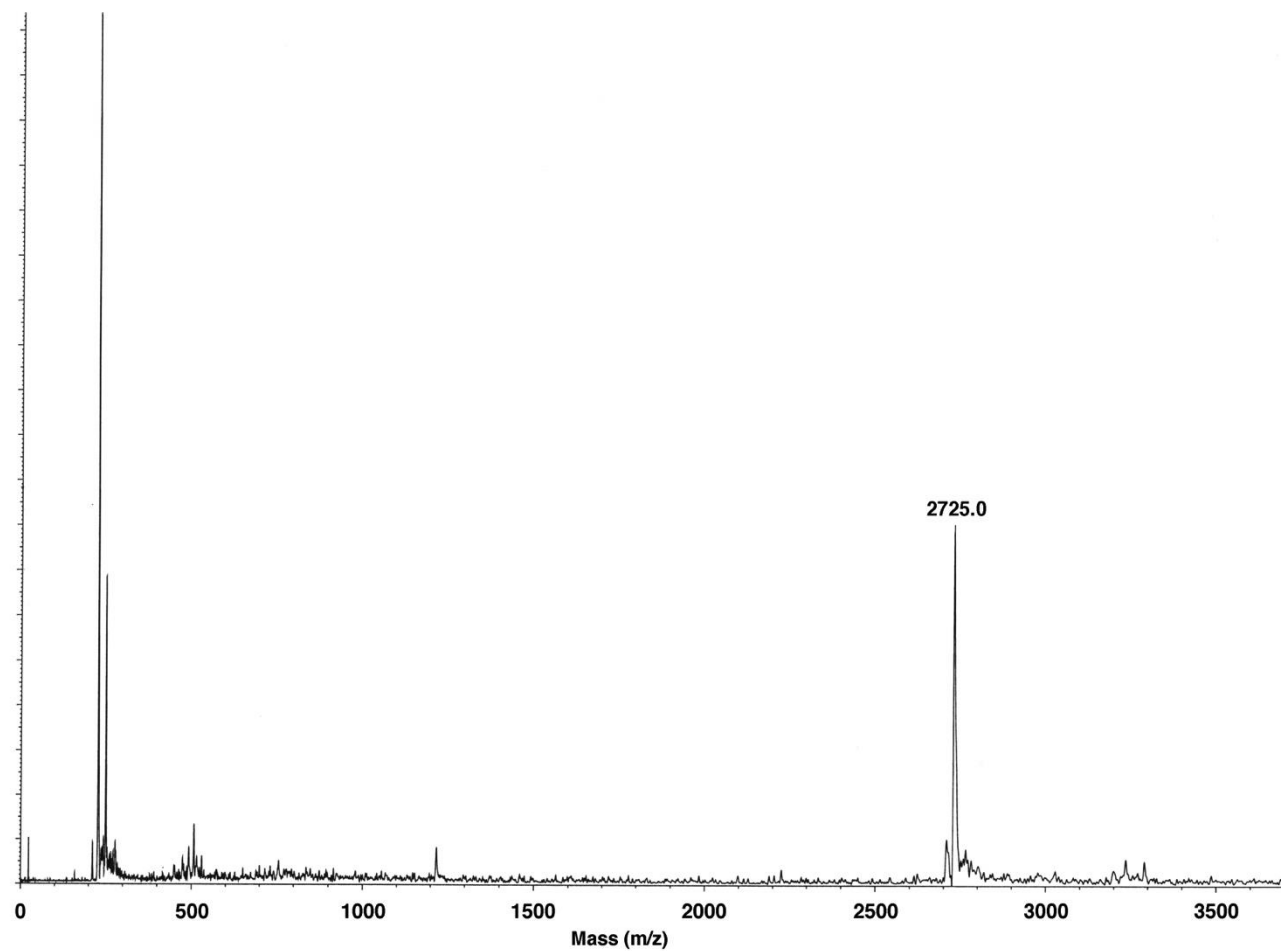
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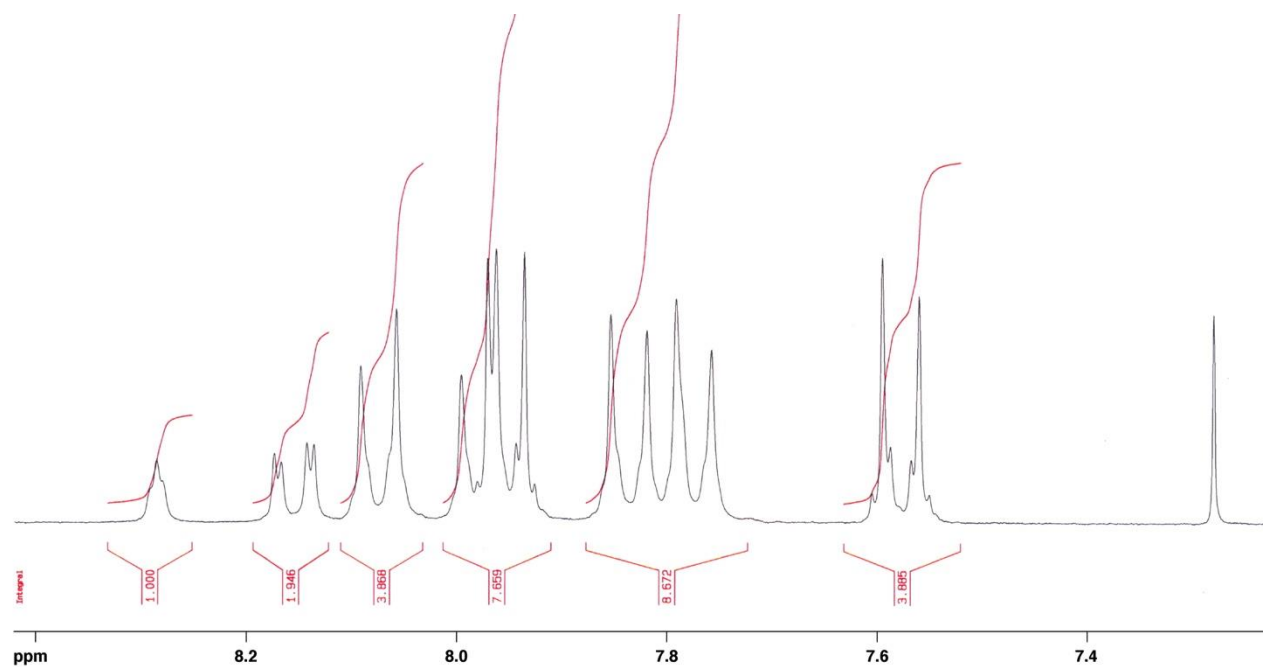
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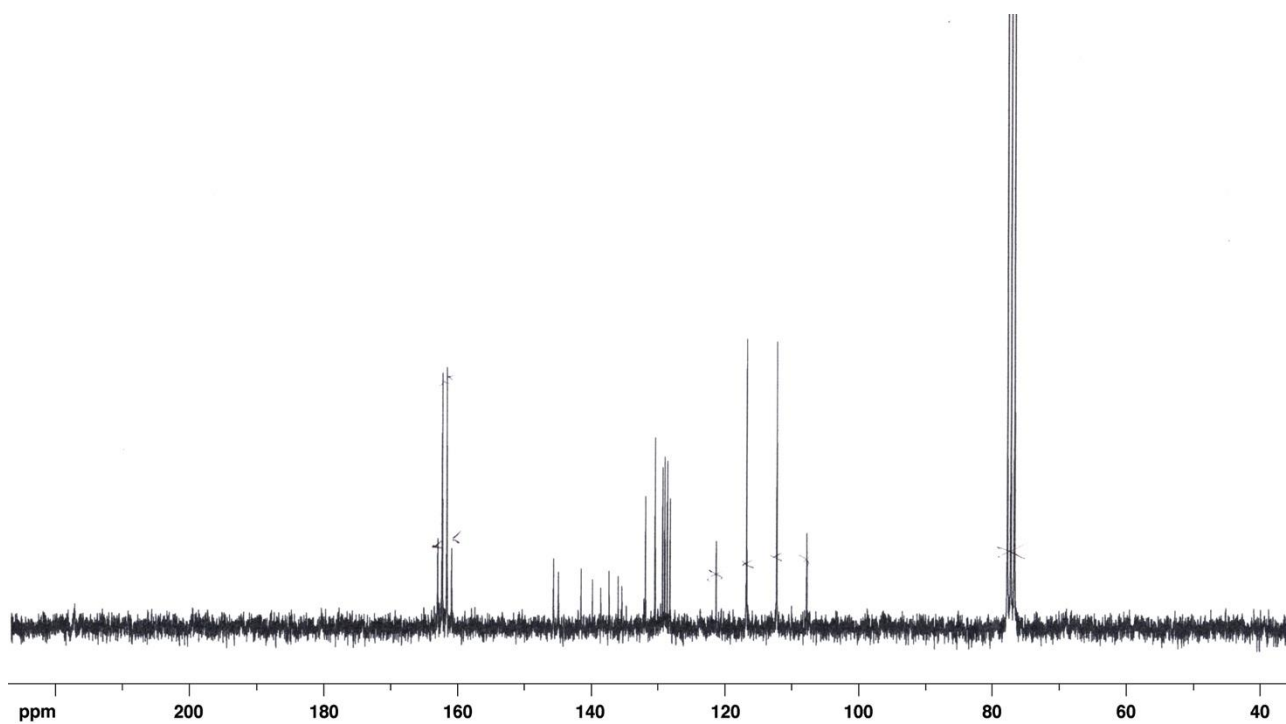
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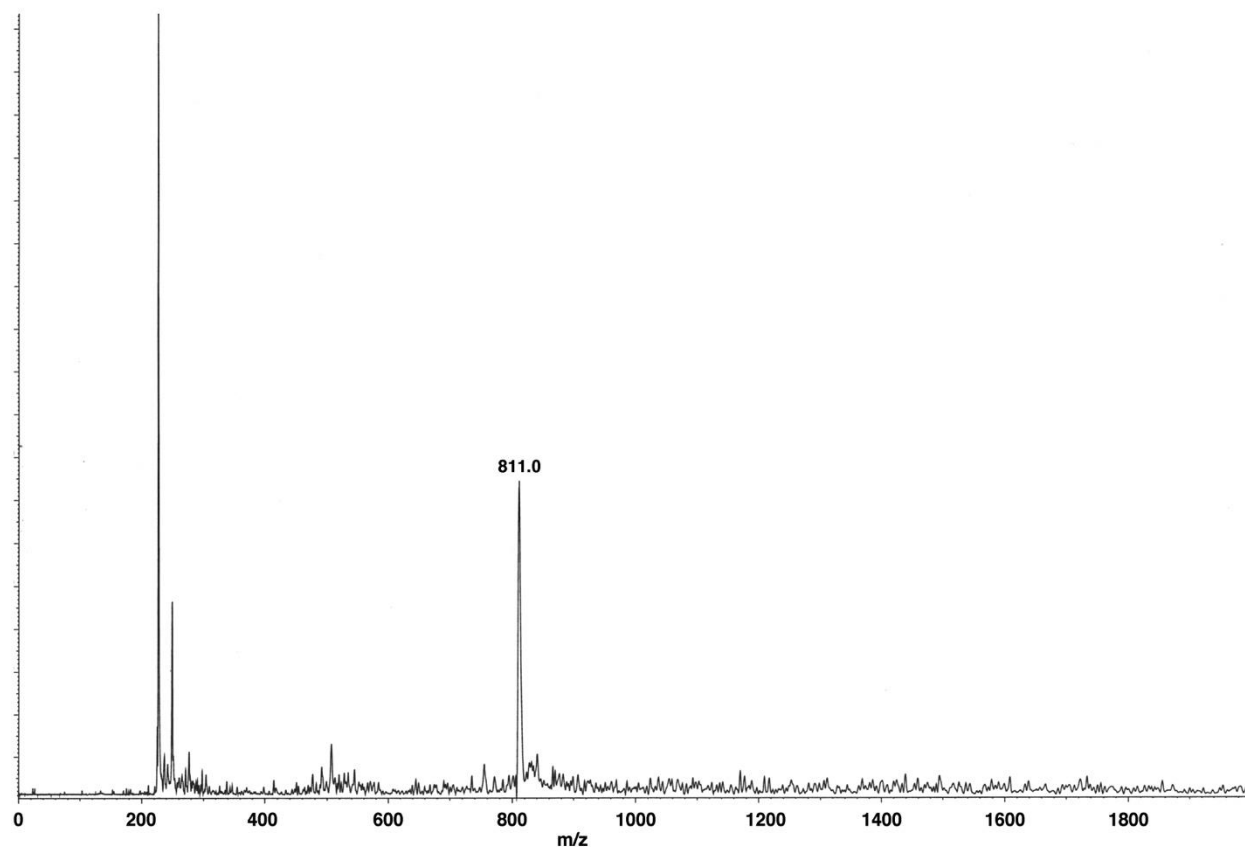
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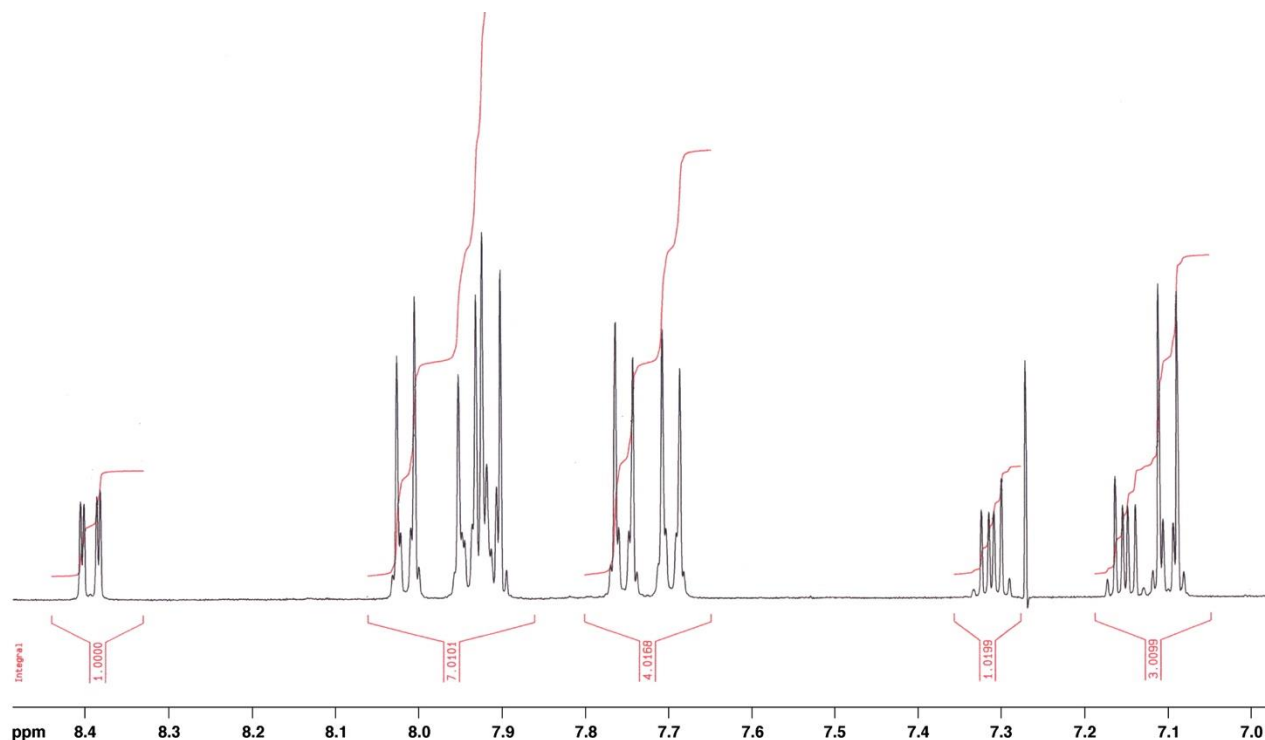
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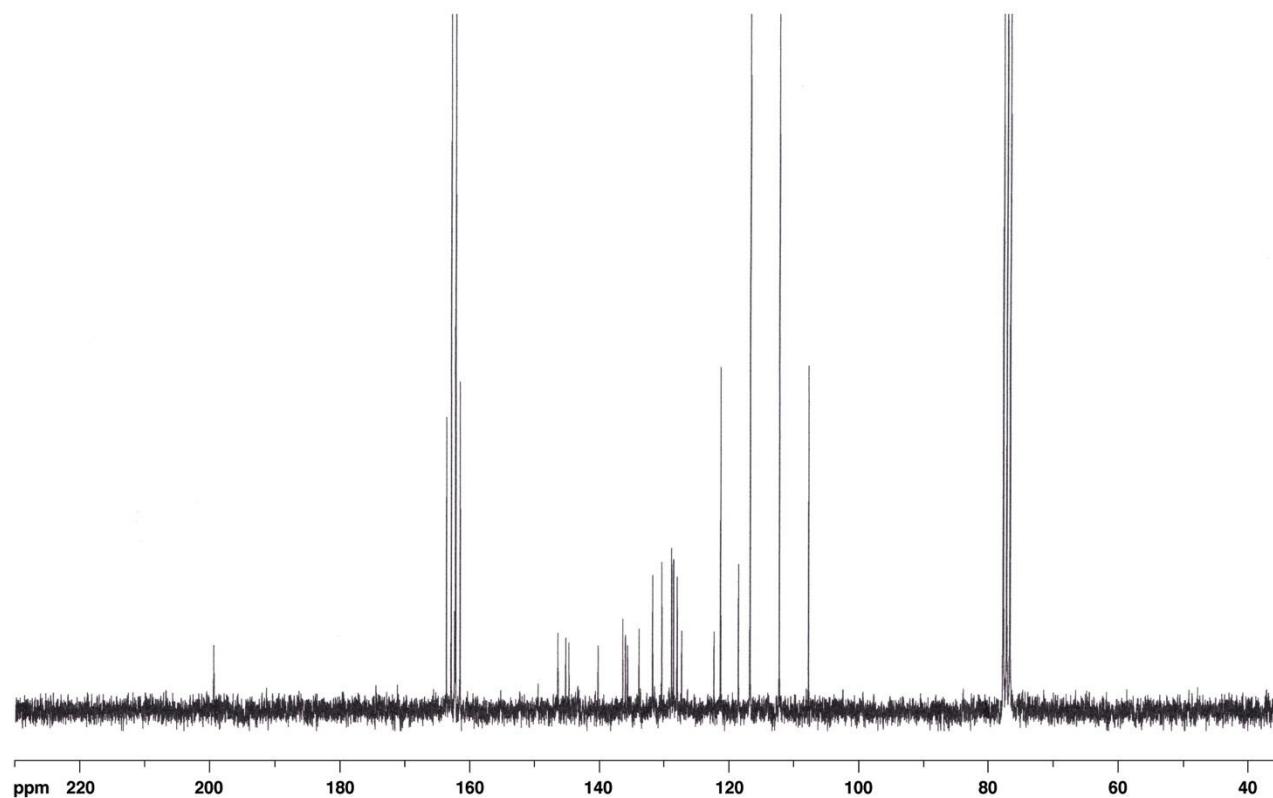
**Figure S14:** <sup>13</sup>C NMR spectrum of linear oligomer **7** (62.5 MHz, CDCl<sub>3</sub>/CF<sub>3</sub>COOH 5/1 v/v). *Note:* the strong quartet resonances centred at 114 and 162 ppm are due to trifluoroacetic acid co-solvent.



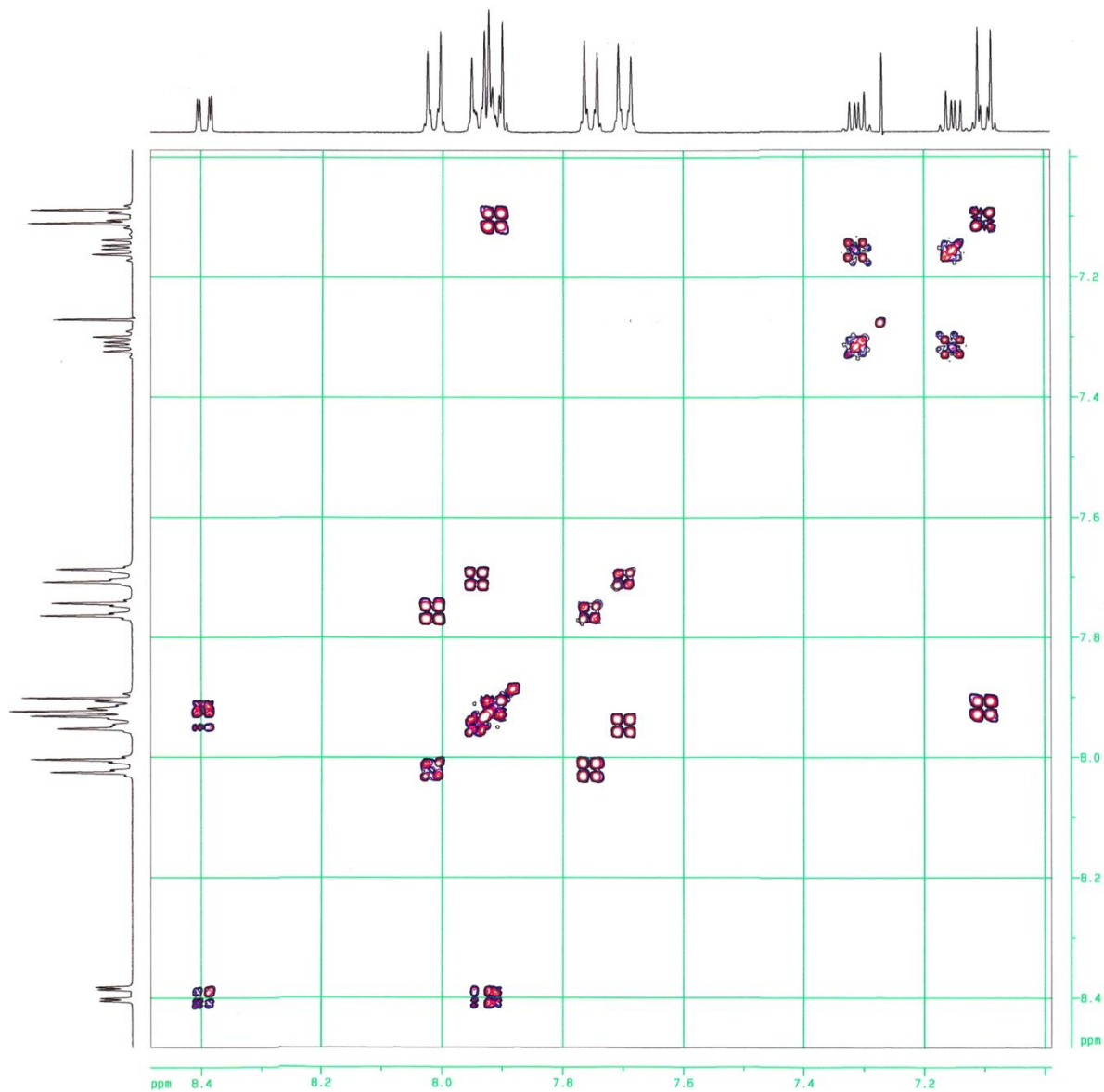
**Figure S15:** MALDI-TOF mass spectrum of linear oligomer **7**. (Calc.  $m/z$  for  $[C_{44}H_{28}S_2O_6Cl_2Na]^+ = 810.7$ ).



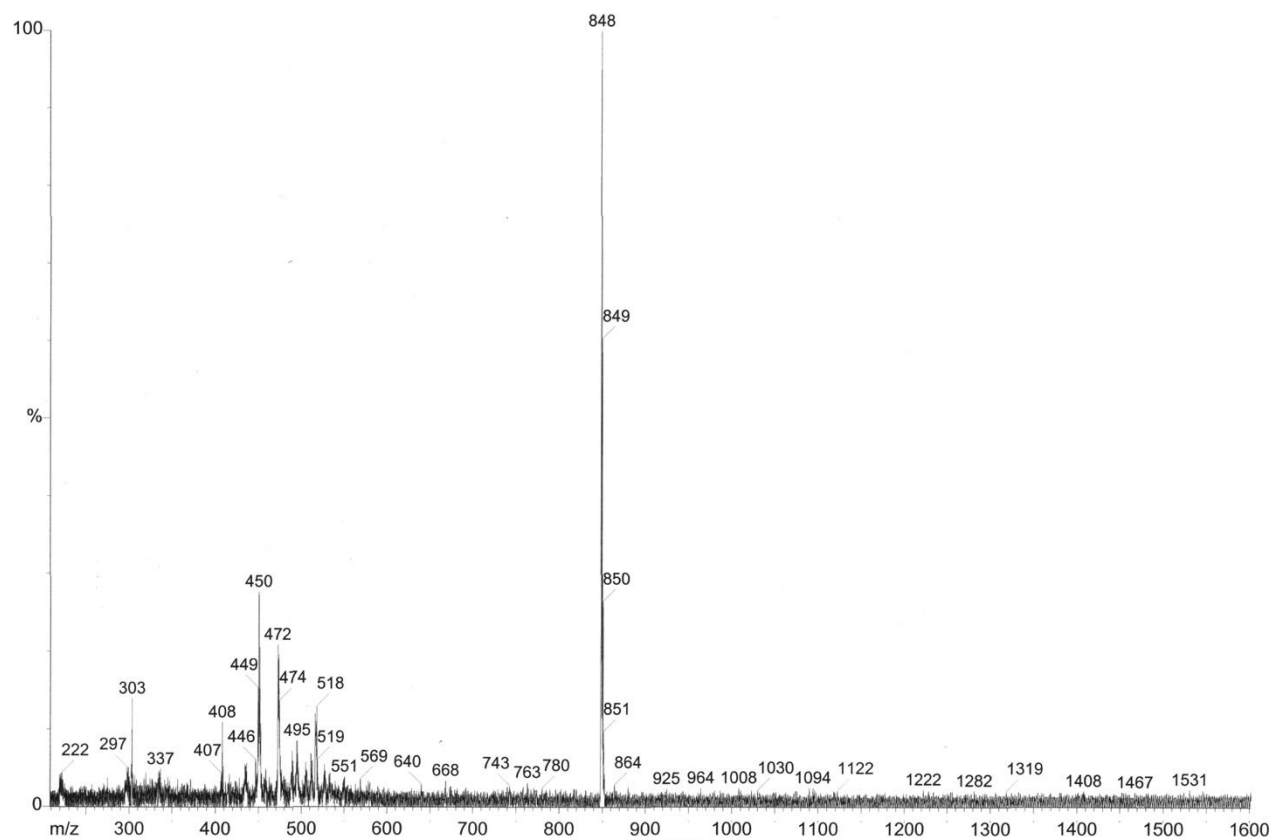
**Figure S16:**  $^1\text{H}$  NMR spectrum of macrocycle **8** (400 MHz,  $\text{CDCl}_3/\text{CF}_3\text{COOH}$  5/1 v/v).



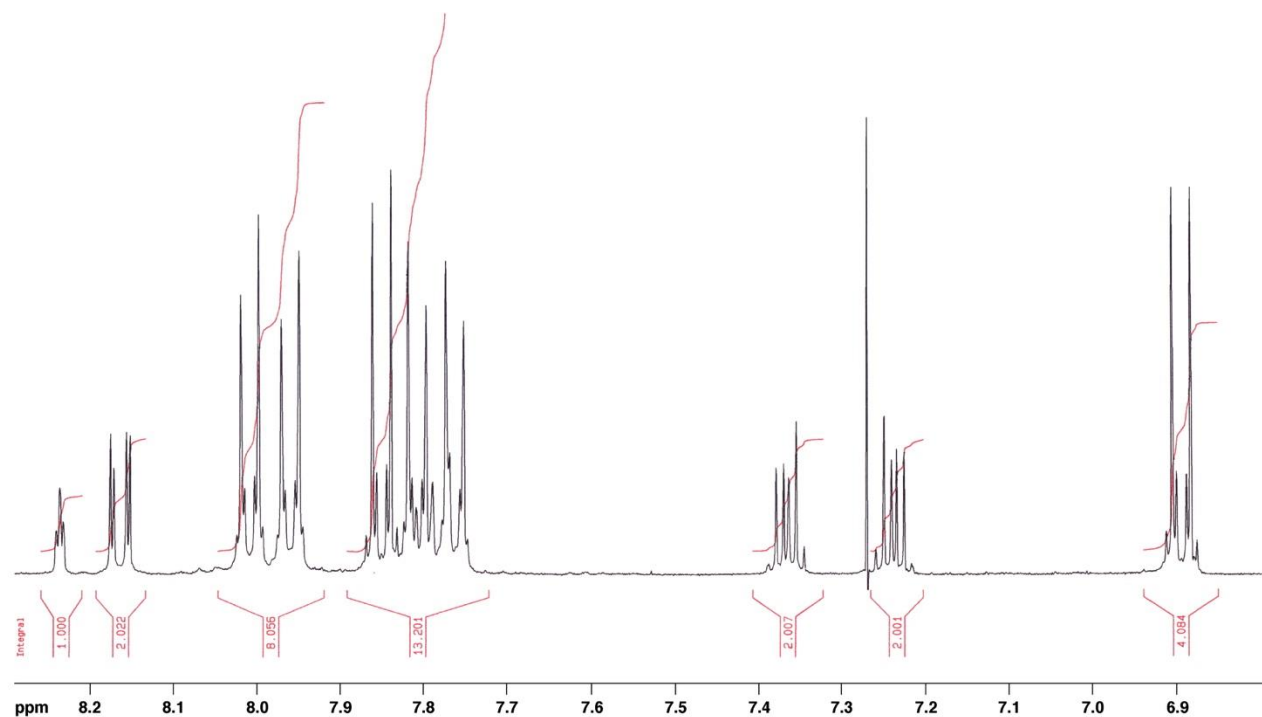
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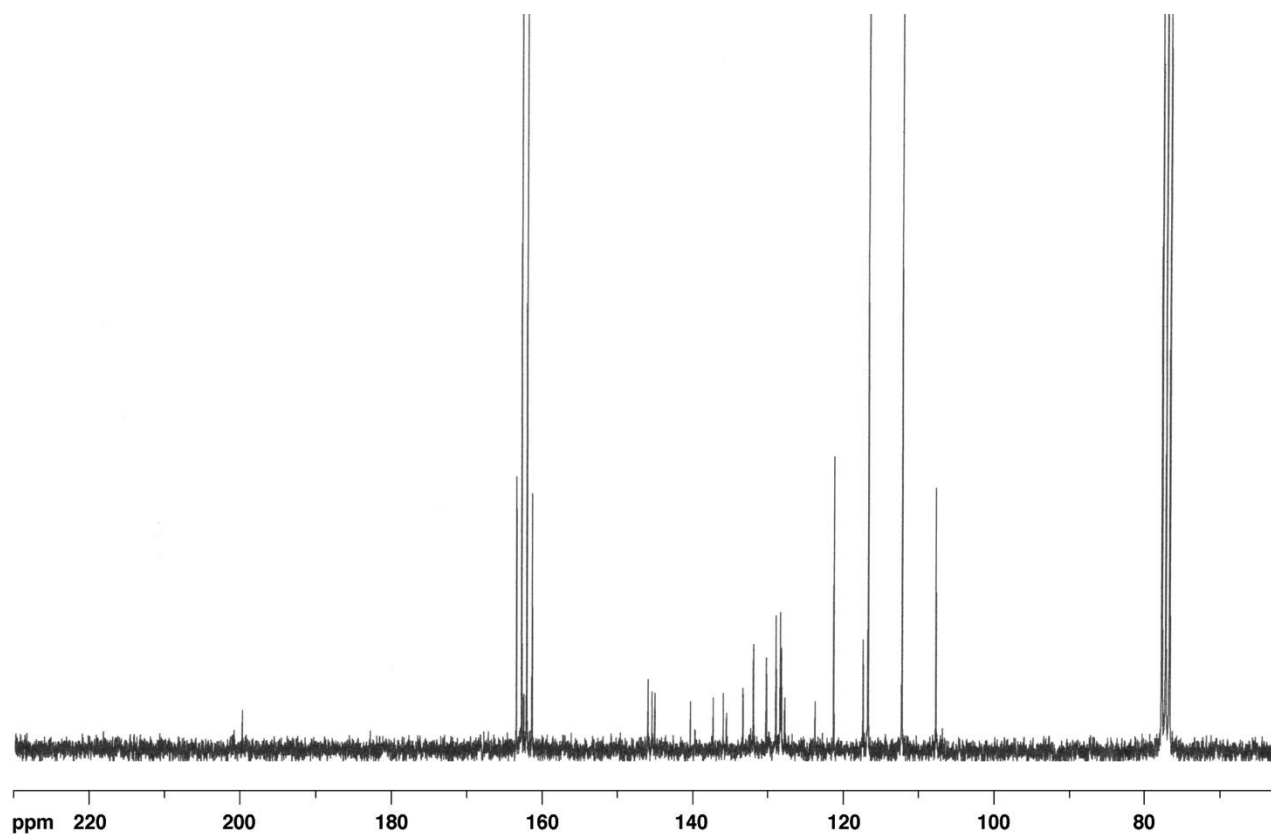
**Figure S18:**  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of macrocycle **8** (400 MHz,  $\text{CDCl}_3/\text{CF}_3\text{COOH}$  5/1 v/v).



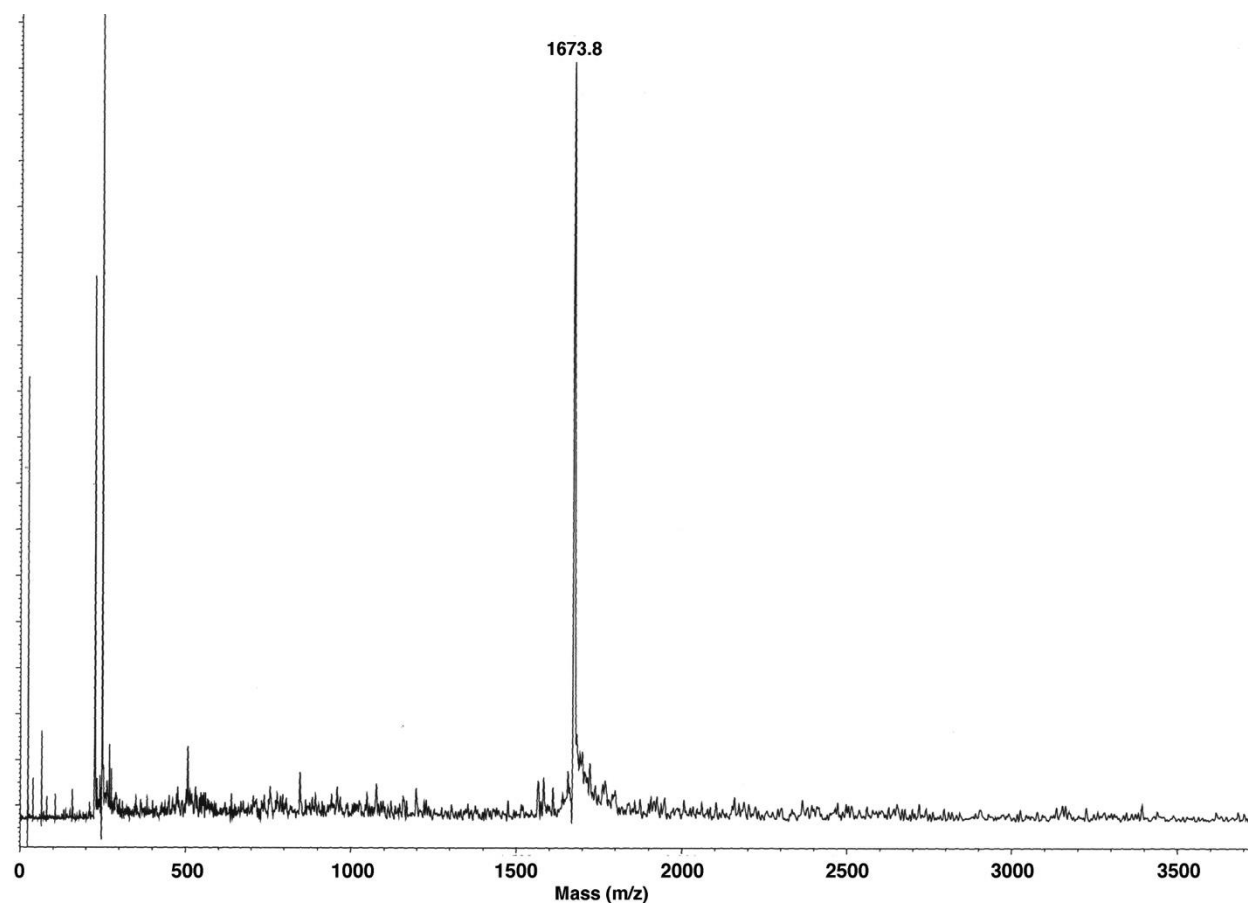
**Figure S19:** MALDI-TOF mass spectrum of macrocycle **8** (Calc.  $m/z$  for  $[C_{50}H_{32}S_2O_8Na]^+ = 847.9$ ).



**Figure S20:** <sup>1</sup>H NMR spectrum of macrocycle **9** (400 MHz, CDCl<sub>3</sub>/CF<sub>3</sub>COOH 5/1 v/v).



**Figure S21:** <sup>13</sup>C NMR spectrum of macrocycle **9** (100 MHz, CDCl<sub>3</sub>/CF<sub>3</sub>COOH 5/1 v/v). *Note:* the strong quartet resonances centred at 114 and 162 ppm are due to trifluoroacetic acid co-solvent.



**Figure S19:** MALDI-TOF mass spectrum of macrocycle **9** (Calc.  $m/z$  for  $[\text{C}_{100}\text{H}_{64}\text{S}_4\text{O}_{16}\text{Na}]^+ = 1672.8$ ).

### Computational modelling of macrocycles **8** and **9**

Models of macrocycles **8** and **9** were constructed on a SGI-O2 workstation using the *Cerius2* suite of programs, v. 3.5, Accelrys, San Diego. Models were minimised initially using the Dreiding-II force field (molecular mechanics with charge-equilibration),<sup>S1</sup> and the resulting models were then re-minimised with a modified version of this force field in which aromatic ether, ketone, and sulfone linkages were constrained to experimentally-established bond lengths and bond angles.

Atomic coordinates of the final models for **8** and **9** are available from the authors as electronic data files in pdb format. Email: [fabio.arico@unive.it](mailto:fabio.arico@unive.it); or [h.m.colquhoun@rdg.ac.uk](mailto:h.m.colquhoun@rdg.ac.uk)

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S1. Mayo, S. L.; Olafson, B. D.; Goddard III, W. A. *J. Phys. Chem.* **1990**, *94*, 8897-8909.