

Electronic Supplementary Information (ESI)

Encapsulation and removal of aniline by di-cyclohexanocucurbit[6]uril

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Table of Contents

Figure S1: ¹H NMR of the guest 1⁺ binding with the Cy6Q[6].....	2
Figure S2: ¹H NMR of the guests 2⁺ binding with Cy6Q[6].....	3
Figure S3: ¹H NMR of the guest 3²⁺ binding with Cy6Q[6].....	4
Figure S4: The chemical shifts and splitting of the Cy2Q[6] protons.....	5
Figure S5-S7: ORTEP diagram of the compounds 1-3.....	6-8
Figure S8-S10: ¹H NMR of the compounds 1-3	9-11

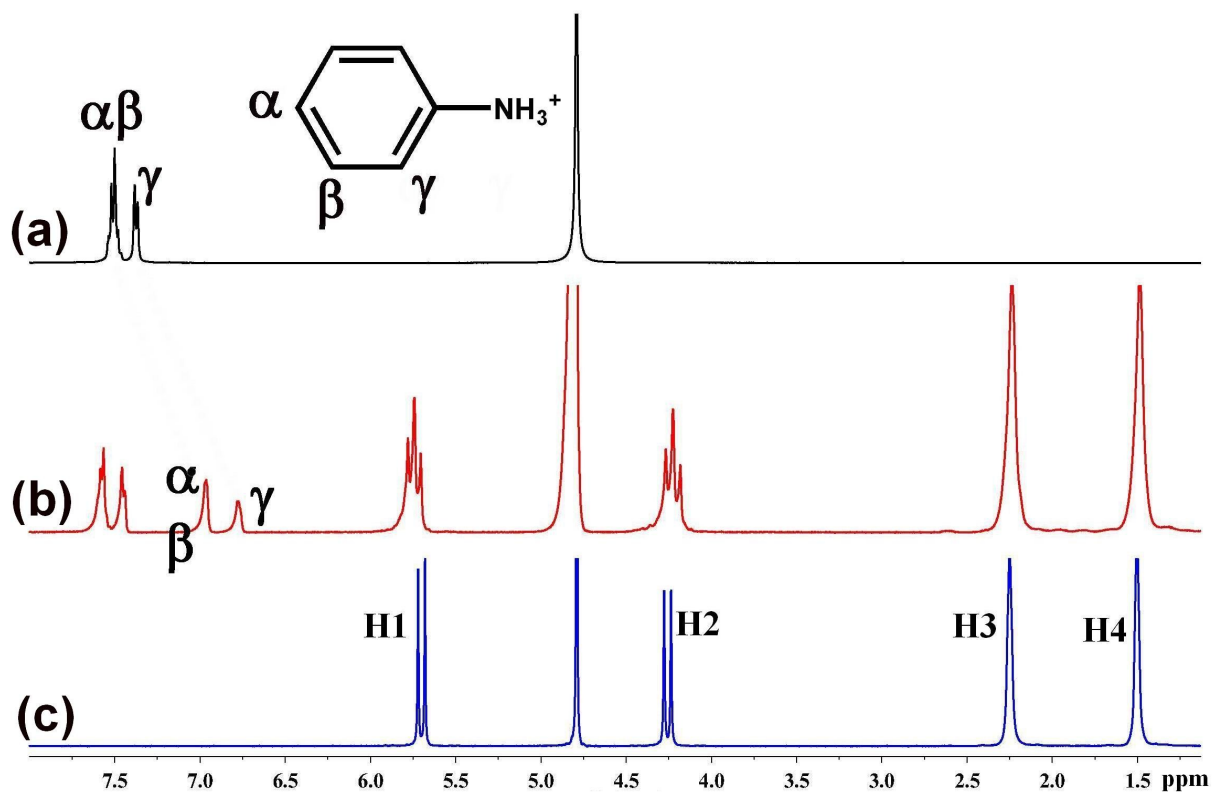


Figure S1. ^1H NMR spectra (400 MHz) of guest 1^+ (2.0 mM) in absence (a) and presence of 0.37 (b) equiv of Cy6Q[6] in D_2O at $20\text{ }^\circ\text{C}$. (c) shows the ^1H NMR spectrum (400 MHz) of Cy6Q[6] (2.0 mM) in 0.50 ml D_2O at $20\text{ }^\circ\text{C}$.

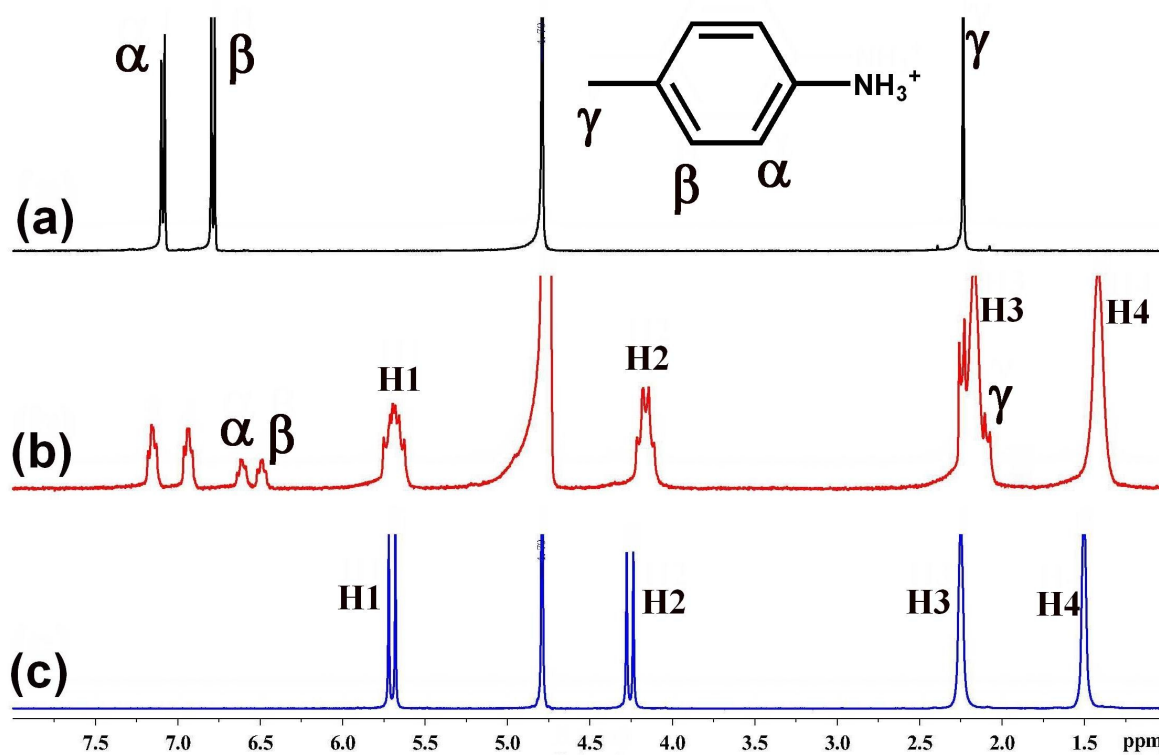


Figure S2. ^1H NMR spectra (400 MHz) of guest 2^+ (2.0 mM) in absence (a) and presence of 0.32 (b) equiv of Cy6Q[6] in D_2O at 20 $^\circ\text{C}$. (c) shows the ^1H NMR spectrum (400 MHz) of Cy6Q[6] (2.0 mM) in 0.50 ml D_2O at 20 $^\circ\text{C}$.

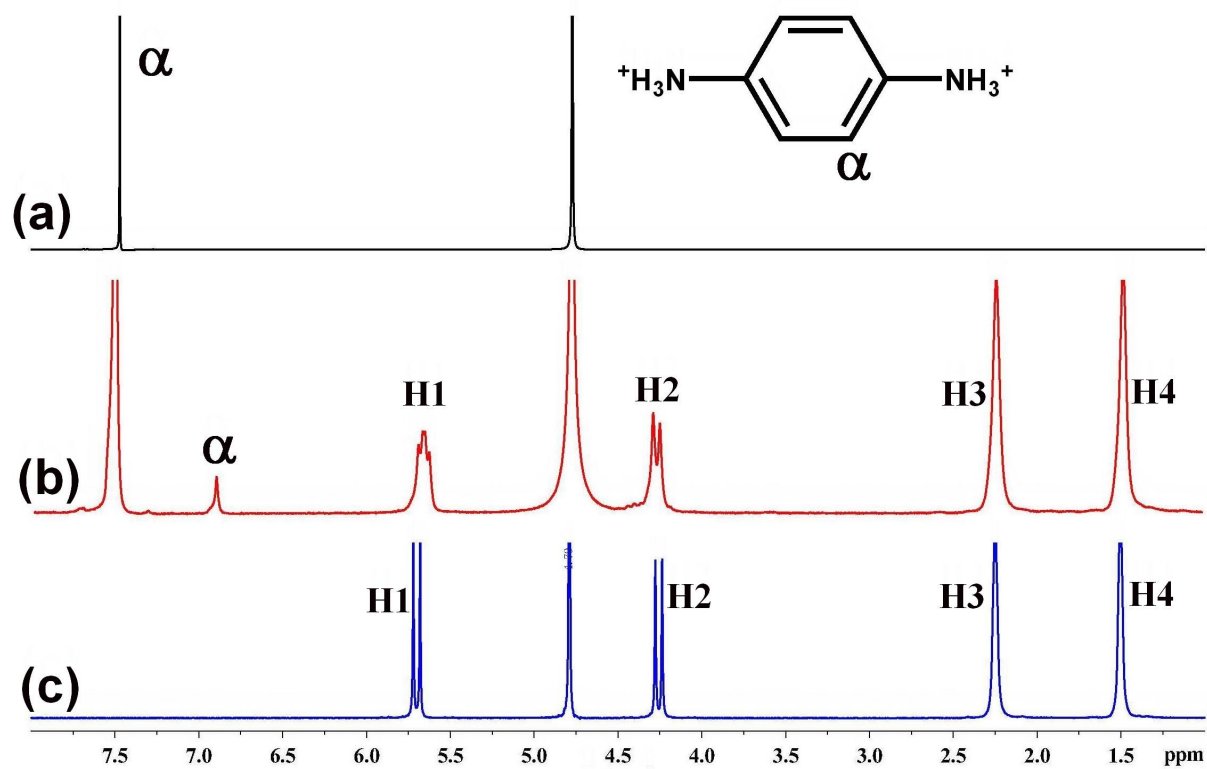


Figure S3. ^1H NMR spectra (400 MHz) of guest 3^{2+} (2.0 mM) in absence (a) and presence of 0.12 (b) equiv of Cy6Q[6] in D_2O at 20°C . (c) shows the ^1H NMR spectrum (400 MHz) of Cy6Q[6] (2.0 mM) in 0.50 ml D_2O at 20°C .

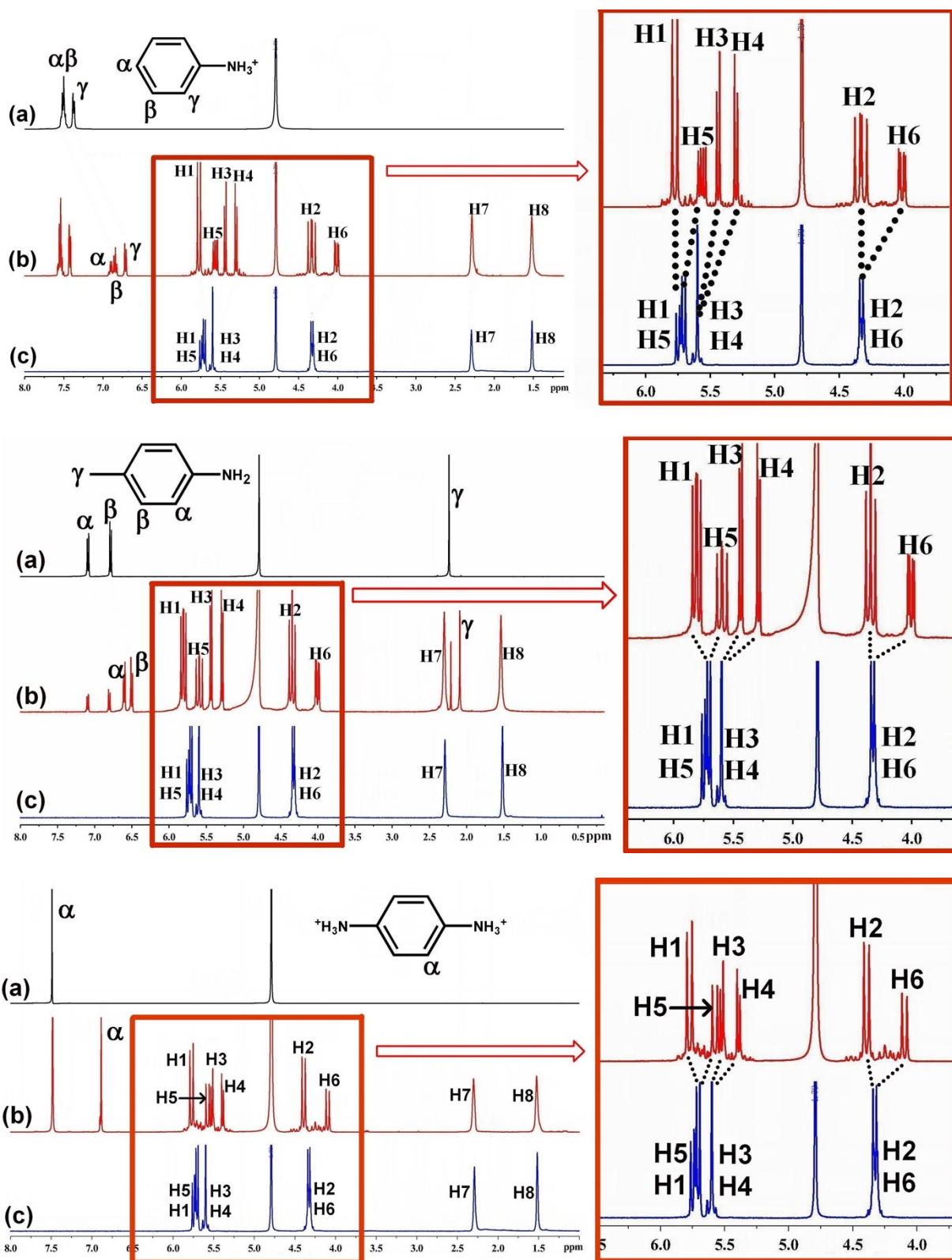


Figure S4. The chemical shifts and splitting of the Cy2Q[6] protons.

1

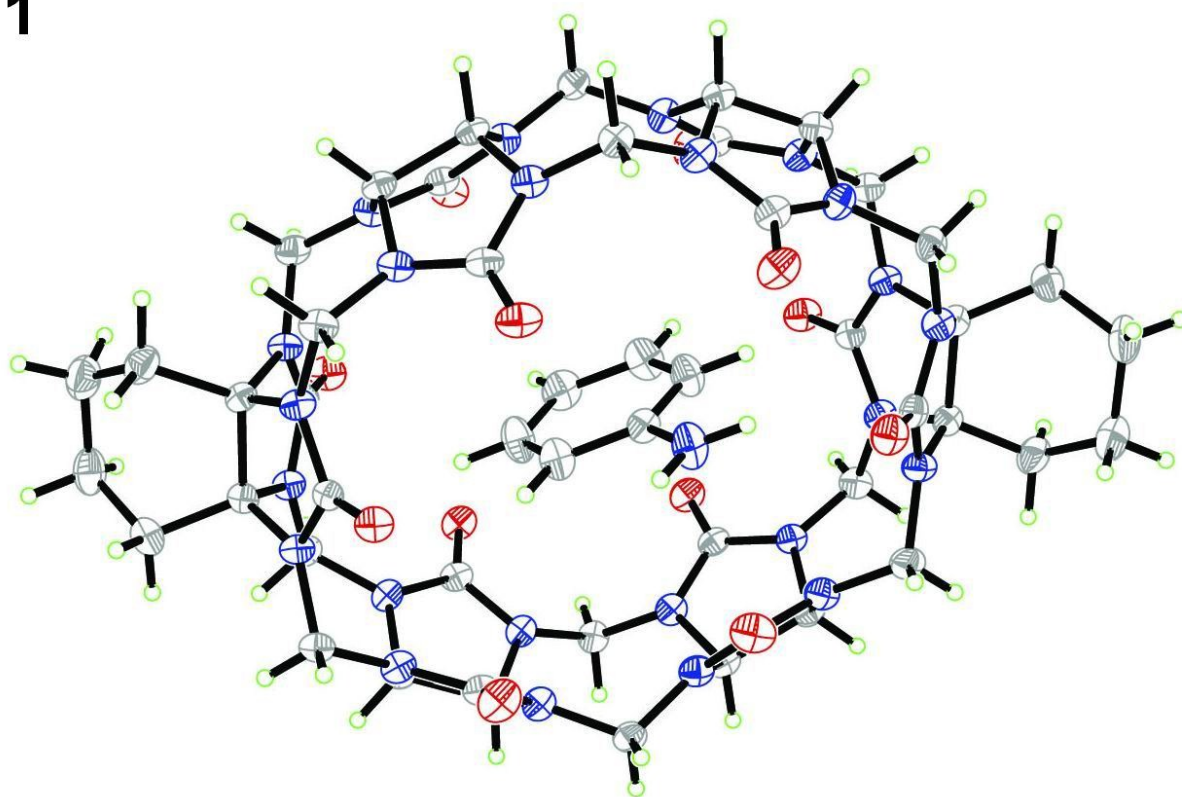


Figure S5. ORTEP diagram of the compound **1**; displacement ellipsoids are drawn at the 30% probability level. Solvate water molecules are omitted for clarity.

2

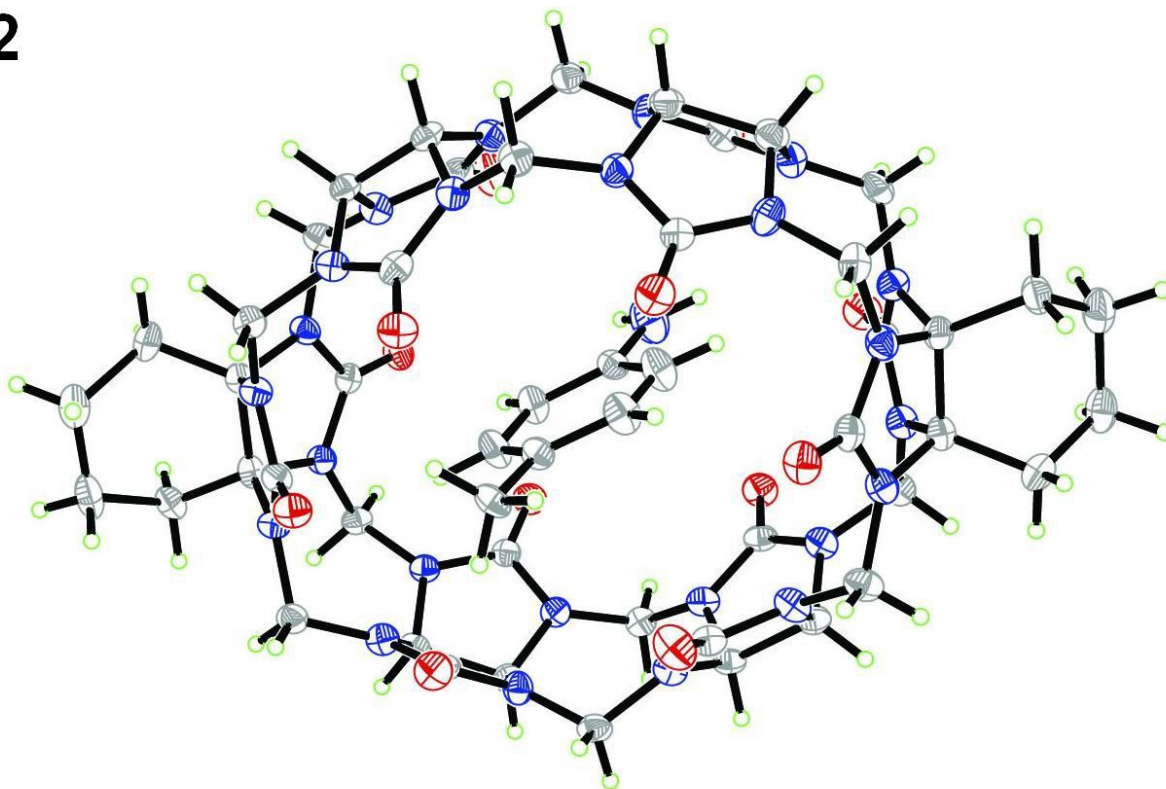


Figure S6. ORTEP diagram of the compound **2**; displacement ellipsoids are drawn at the 30% probability level. Solvate water molecules are omitted for clarity.

3

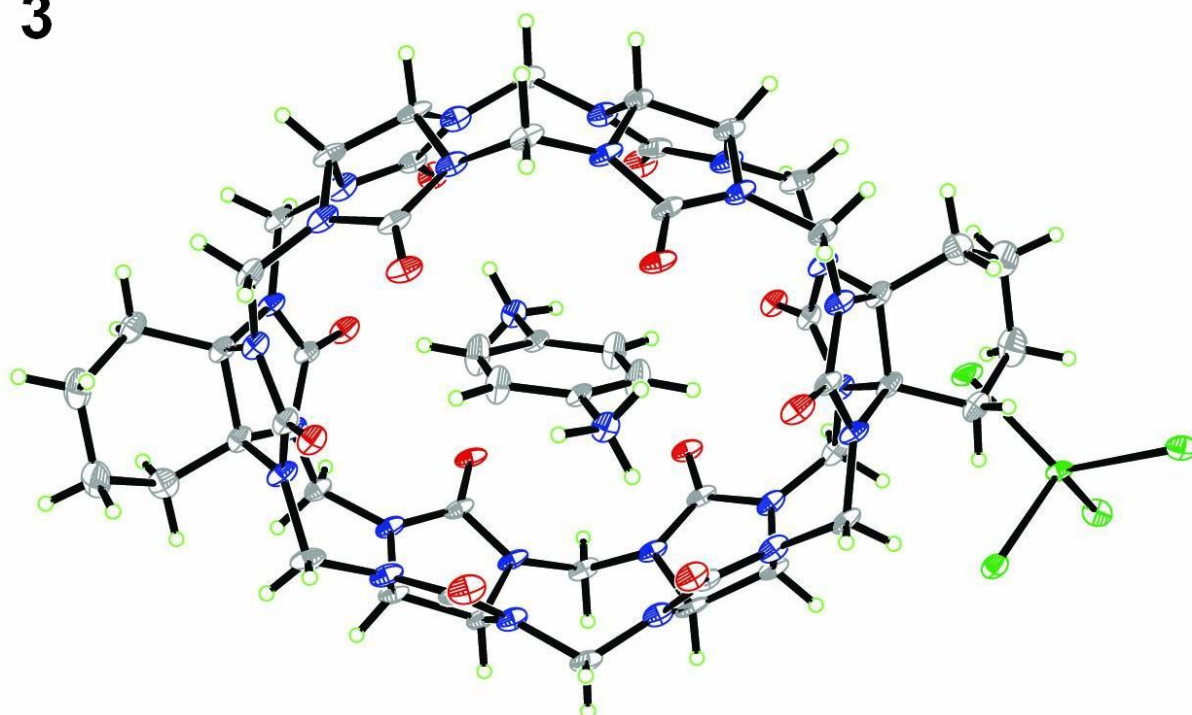


Figure S7. ORTEP diagram of the compound **3**; displacement ellipsoids are drawn at the 30% probability level. Solvate water molecules are omitted for clarity.

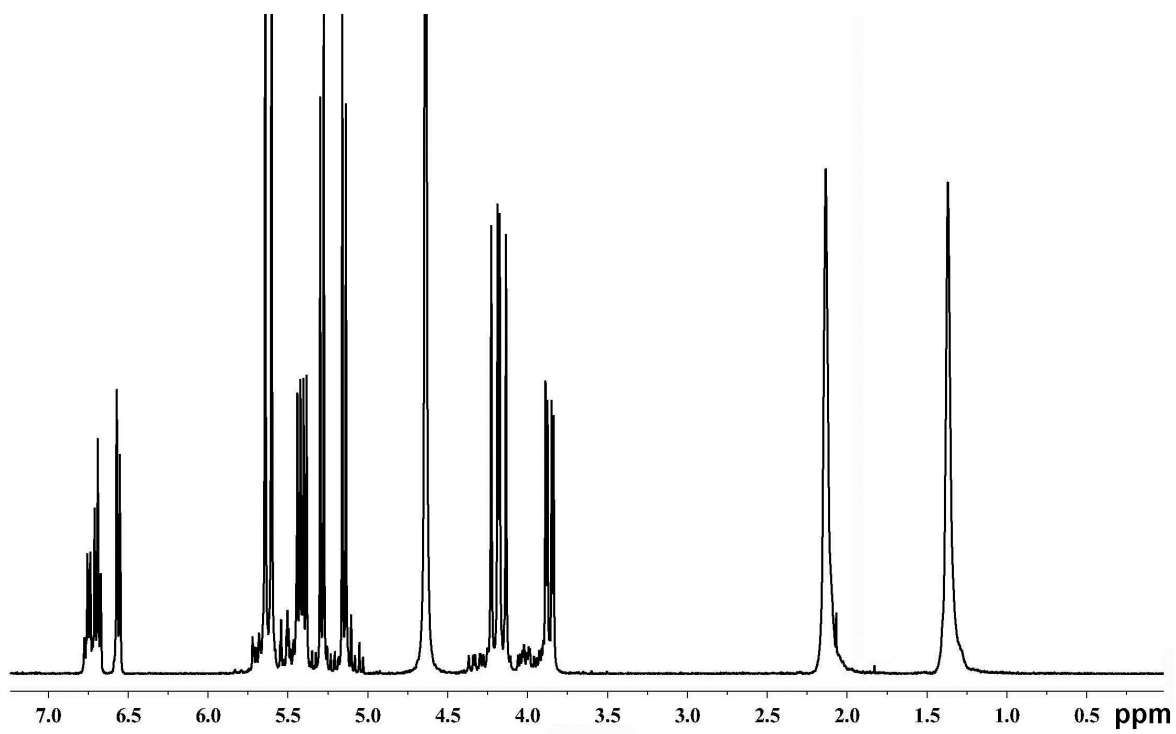


Figure S8. ¹H NMR spectrum of the compound **1** (2.0 mM) in D₂O at 20 °C.

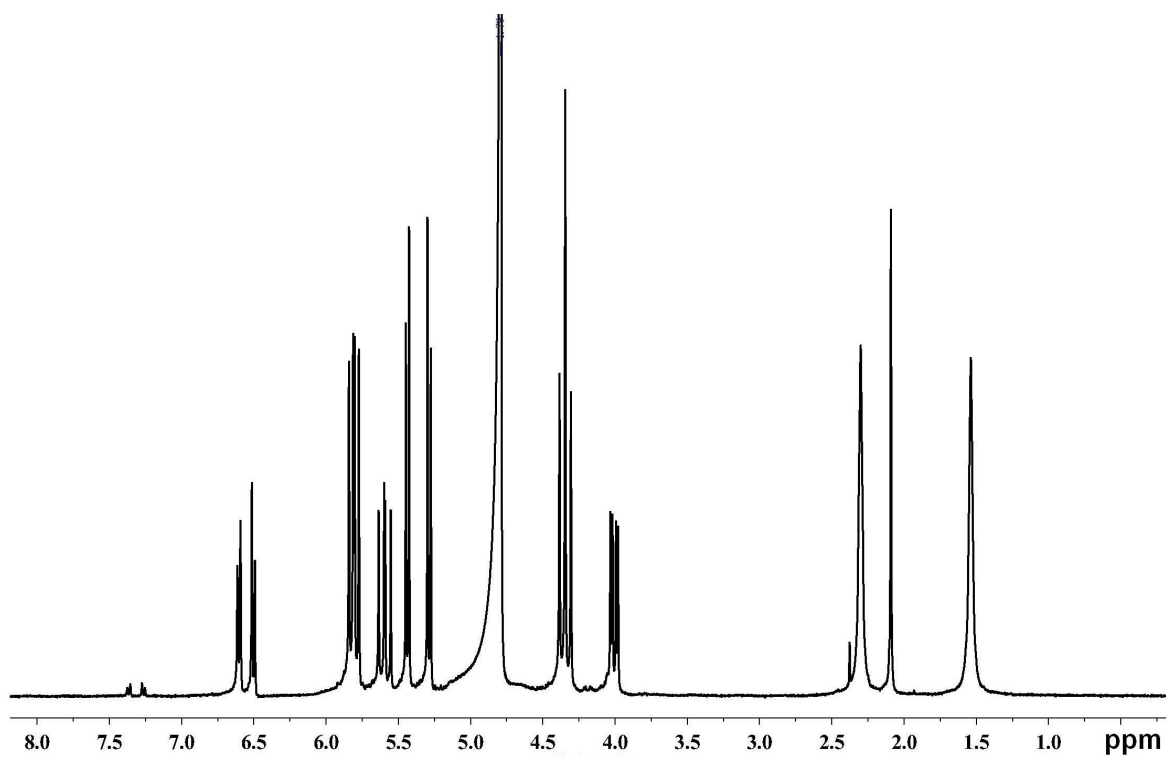


Figure S9. ¹H NMR spectrum of the compound **2** (2.0 mM) in D₂O at 20 °C.

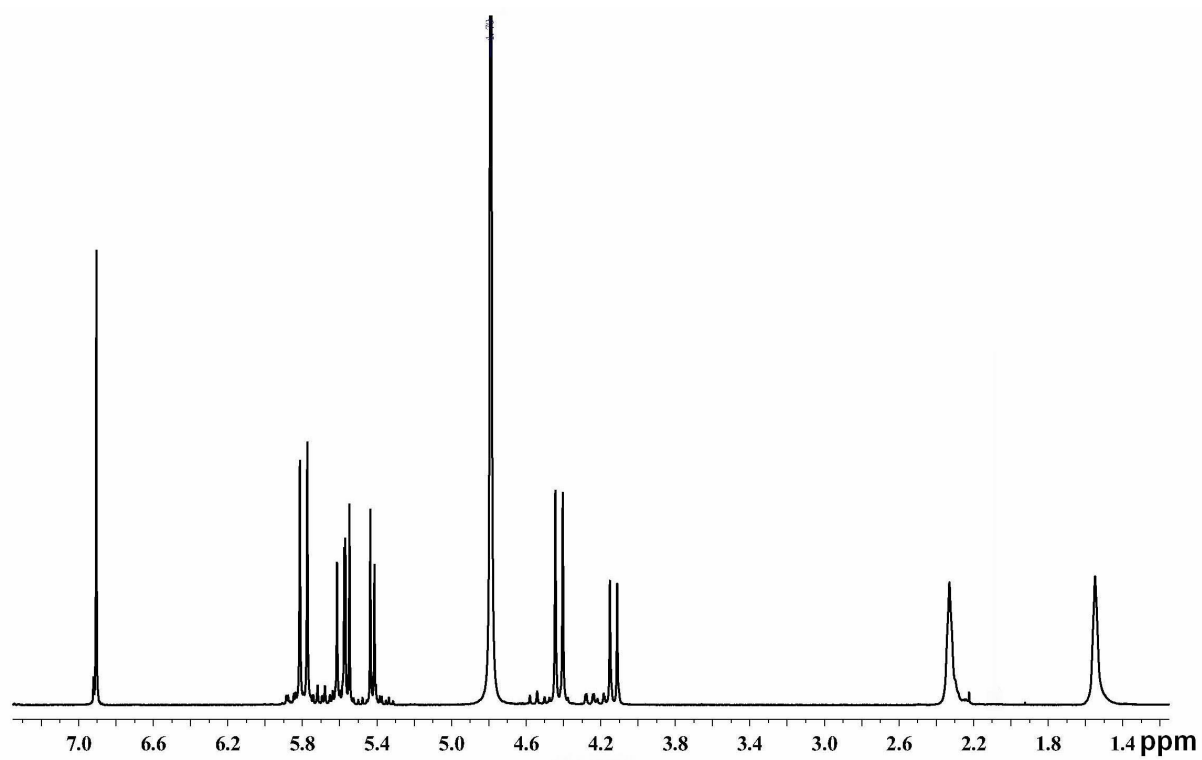


Figure S10. ^1H NMR spectrum of the compound **3** (2.0 mM) in D_2O at $20\text{ }^\circ\text{C}$.