

Supplementary Materials: Stabilization of Supramolecular Networks of Polyiodides with Protonated Small Tetraazacyclophanes

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Table S1 - Hydrogen bonds found in the [(H₂L1)₂I₂(I₅)(I₃)₃] crystal structure

D-H	D(D-H)	D(H..A)	<DHA	D(D...A)	A
N2-H2A	0.910	3.048	128.54	3.684	I9
N2-H2B	0.910	3.043	134.84	3.741	I7
N2-H2B	0.910	2.909	133.38	3.595	I8
N3-H3A	0.912	3.122	128.94	3.763	I9 [-x+1, -y+2, -z+1]
N3-H3A	0.912	3.066	139.07	3.802	I15 [x-1, y, z]
N4-H4B	0.910	2.791	154.35	3.632	I8 [-x+1, -y+2, -z+1]
N4-H4B	0.910	3.284	111.20	3.712	I15
N6-H6A	0.910	3.067	120.70	3.618	I5
N6-H6A	0.910	2.948	126.57	3.566	I11 [x-1, y-1, z]
N7-H7A	0.912	3.086	128.07	3.718	I10 [-x-1, -y, -z]
N7-H7A	0.912	3.203	137.27	3.922	I12 [x-1, y, z]
N8-H8A	0.910	2.796	143.60	3.569	I11 [-x, -y+1, -z]
N8-H8B	0.910	3.091	124.24	3.681	I10
C8-H8D	0.990	3.323	135.48	4.088	I16 [-x, -y+2, -z+1]
C10-H10A	0.990	3.092	155.23	4.013	I16 [x+1, y+1, z]
C19-H19B	0.990	3.288	125.07	3.941	I13 [-x, -y+1, -z]
C21-H21B	0.990	3.028	162.40	3.982	I13 [x-1, y, z]

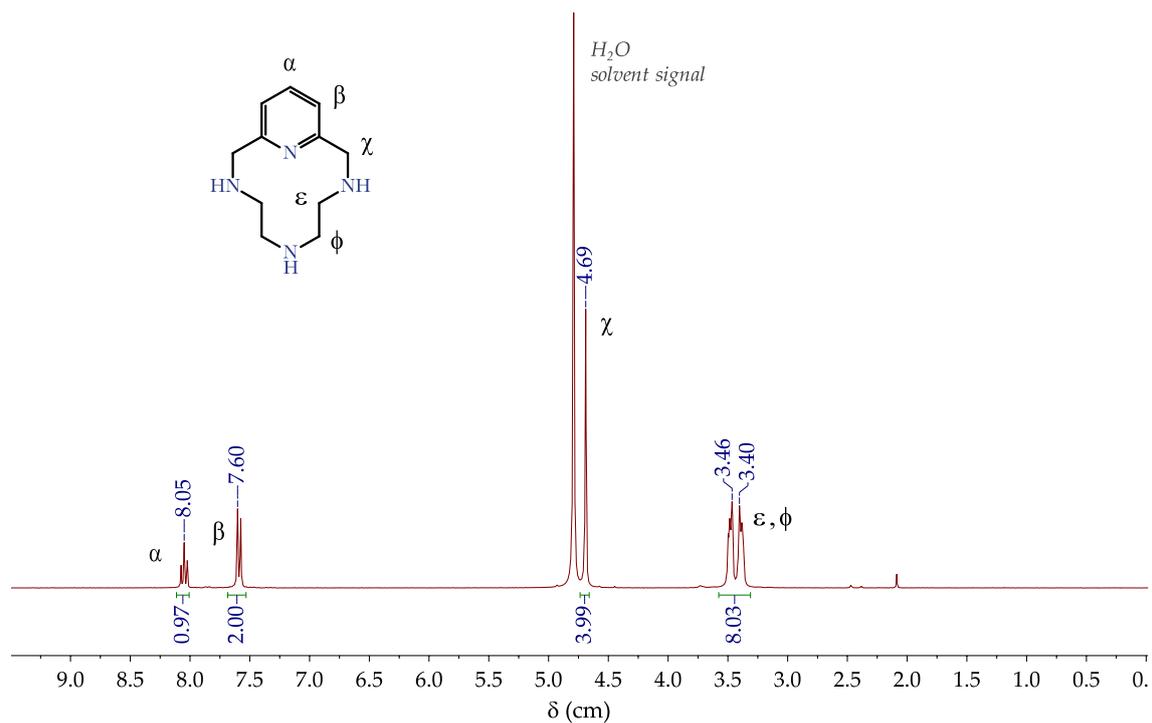


Figure S1. $^1\text{H-NMR}$ spectrum of L1 in D_2O at 298 K.

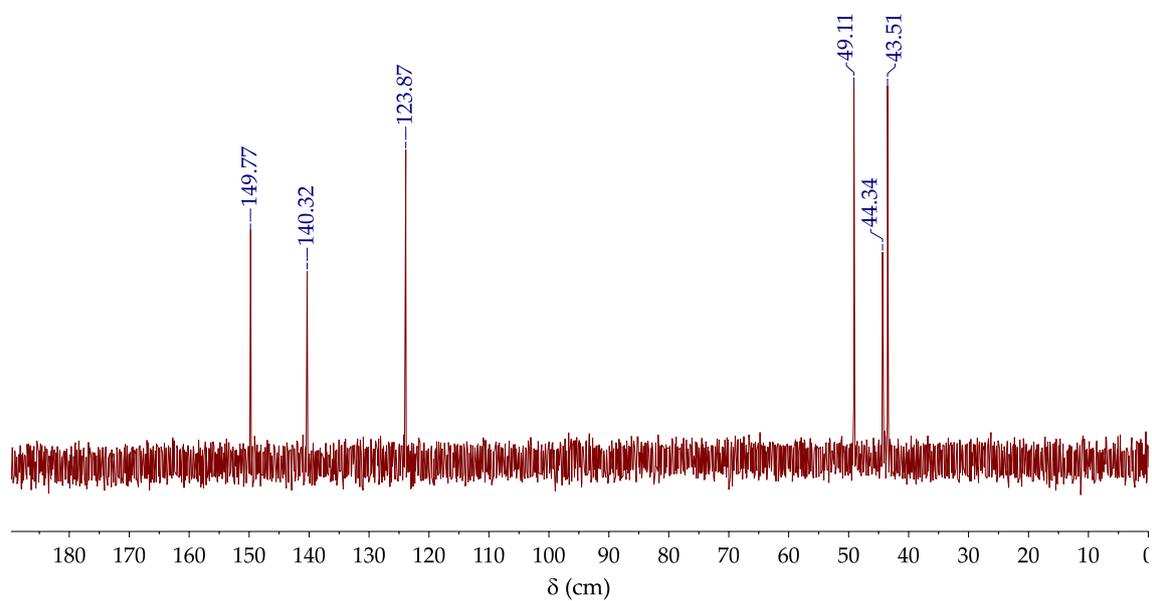


Figure S2. $^{13}\text{C-NMR}$ spectrum of L1 in D_2O at 298 K.

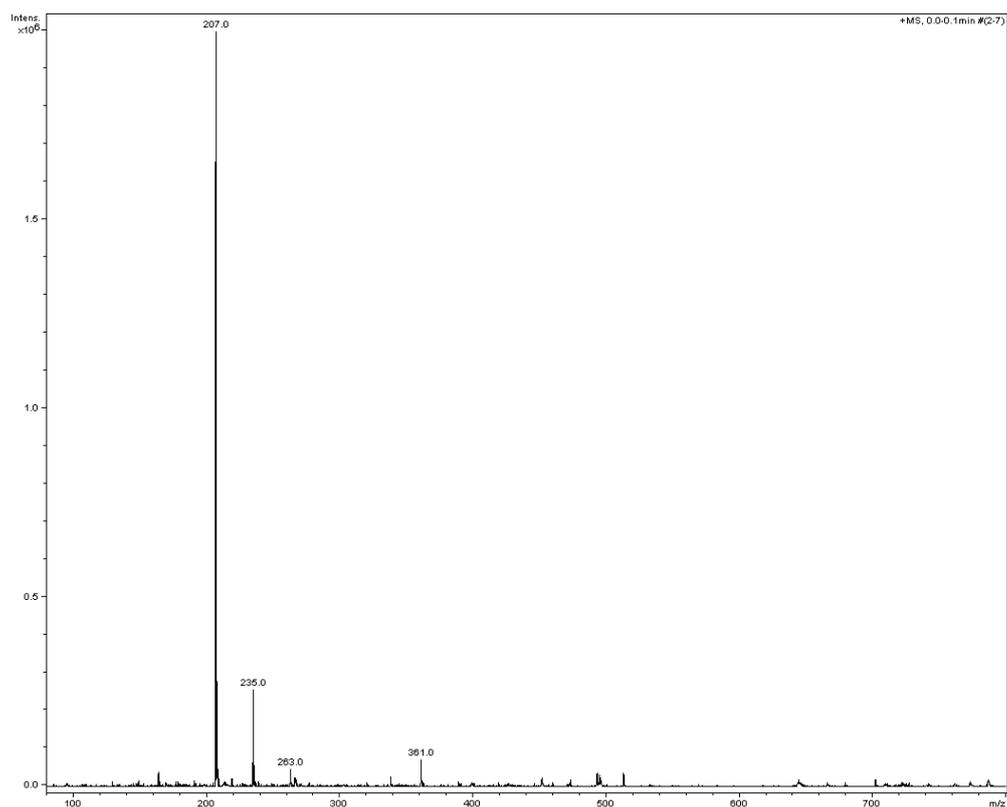


Figure S3. LC-MS (ESI/APCI-TOF) of L1 in H₂O.

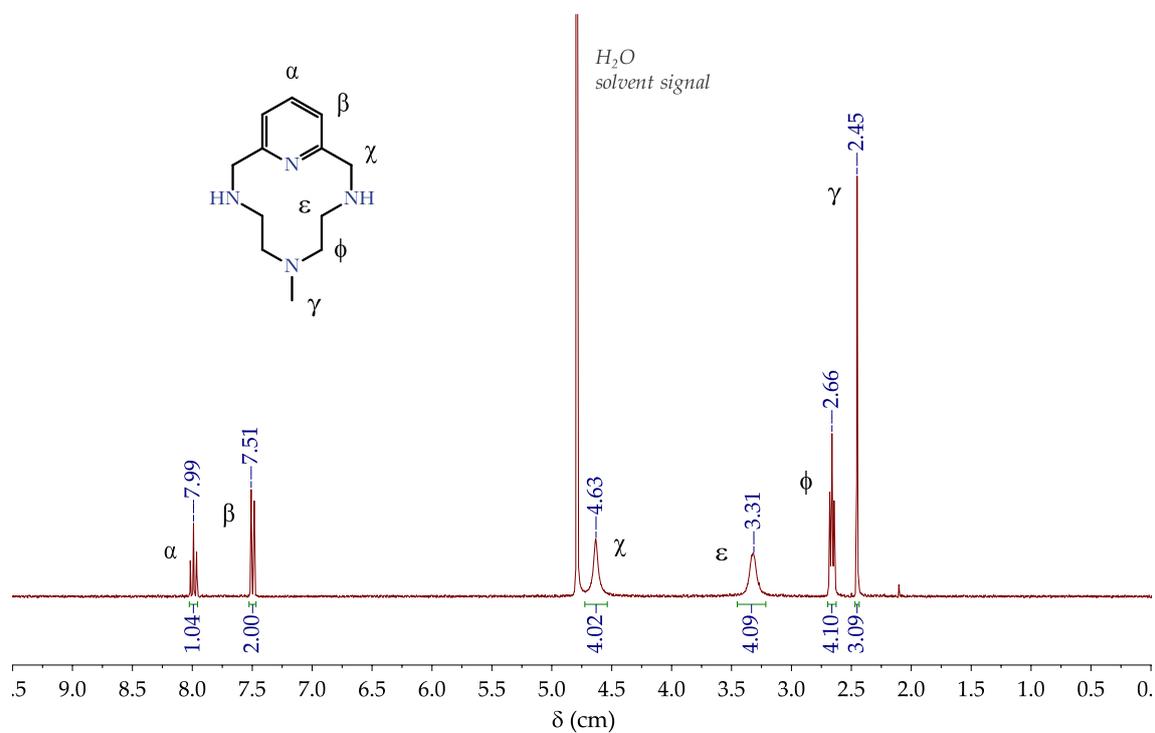


Figure S4. ¹H-NMR spectrum of L1-Me in D₂O at 298 K.

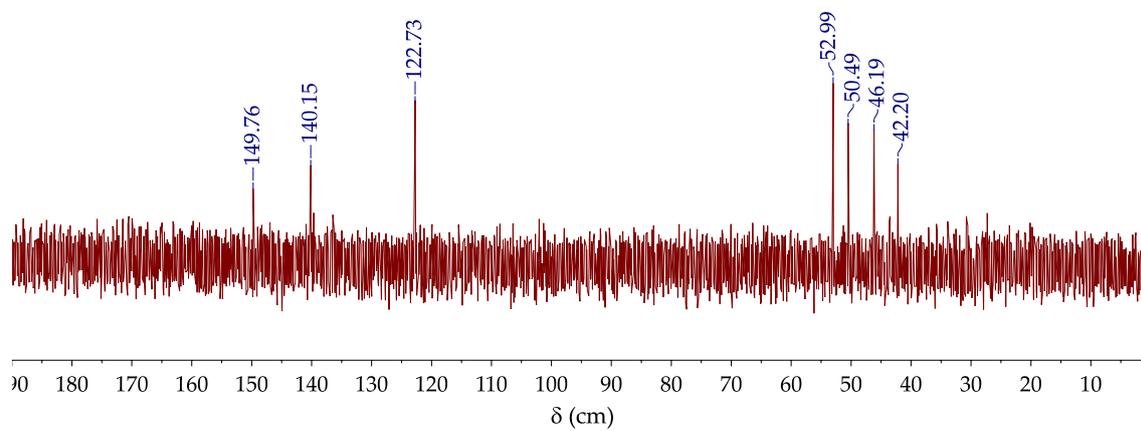


Figure S5. ^{13}C -NMR spectrum of L1-Me in D_2O at 298 K.

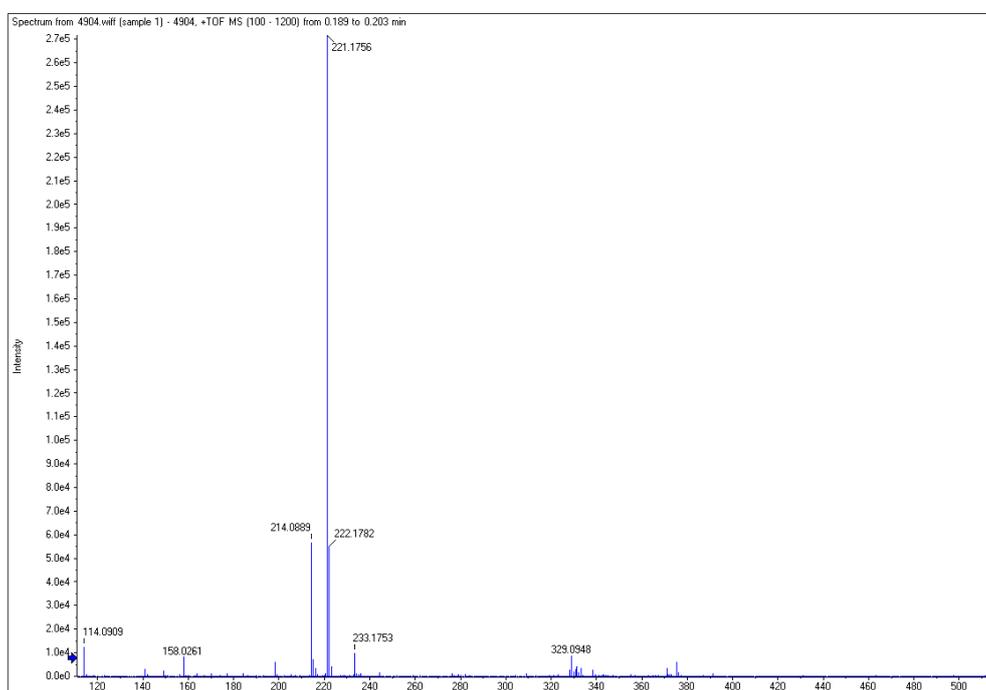


Figure S6. LC-MS (ESI/APCI-TOF) of L1-Me in D_2O .

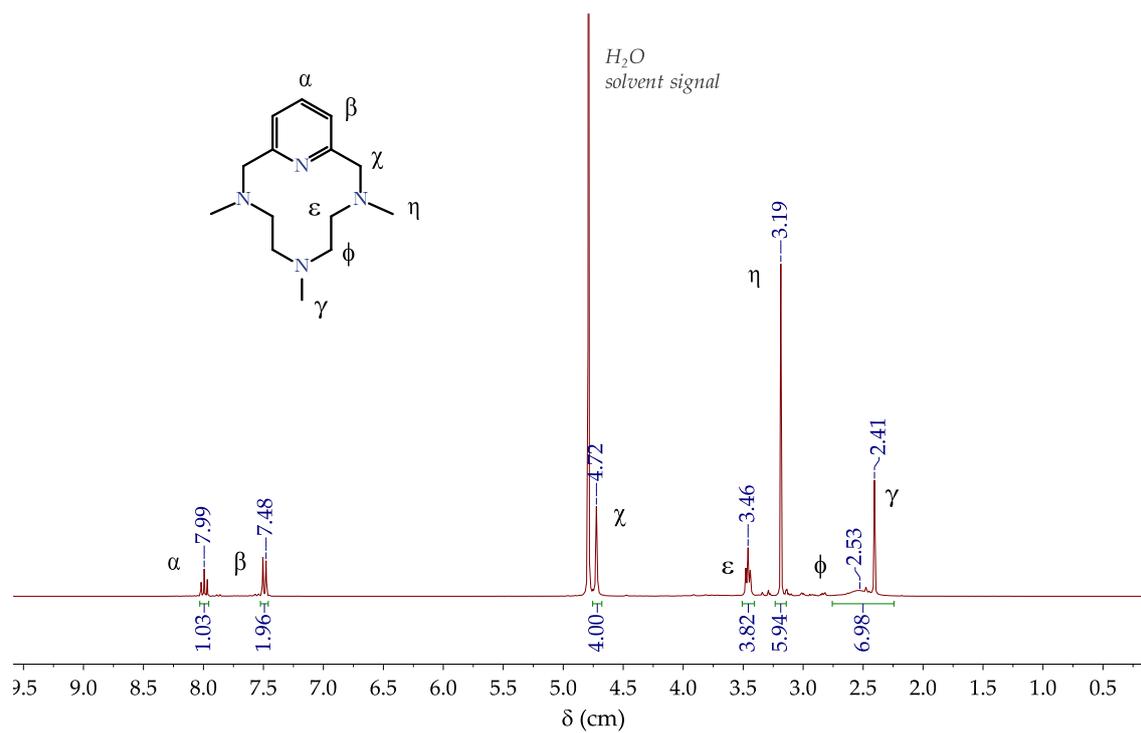


Figure S7. ¹H-NMR spectrum of L1-Me₃ in D₂O at 298 K.

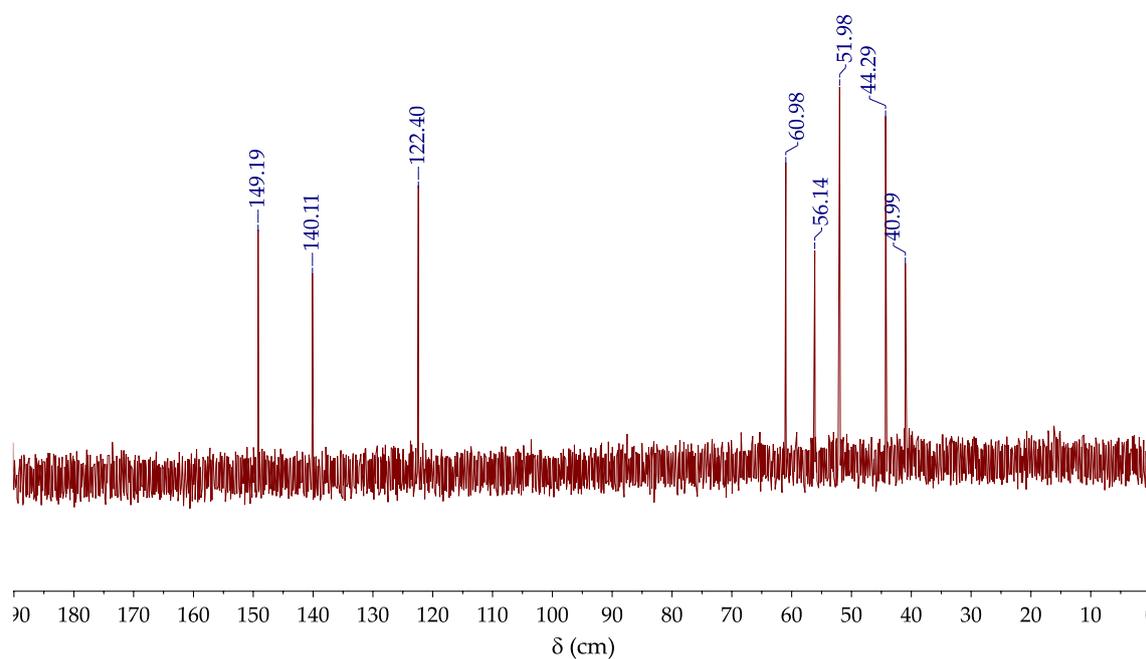


Figure S8. ¹³C-NMR spectrum of L1-Me₃ in D₂O at 298 K.

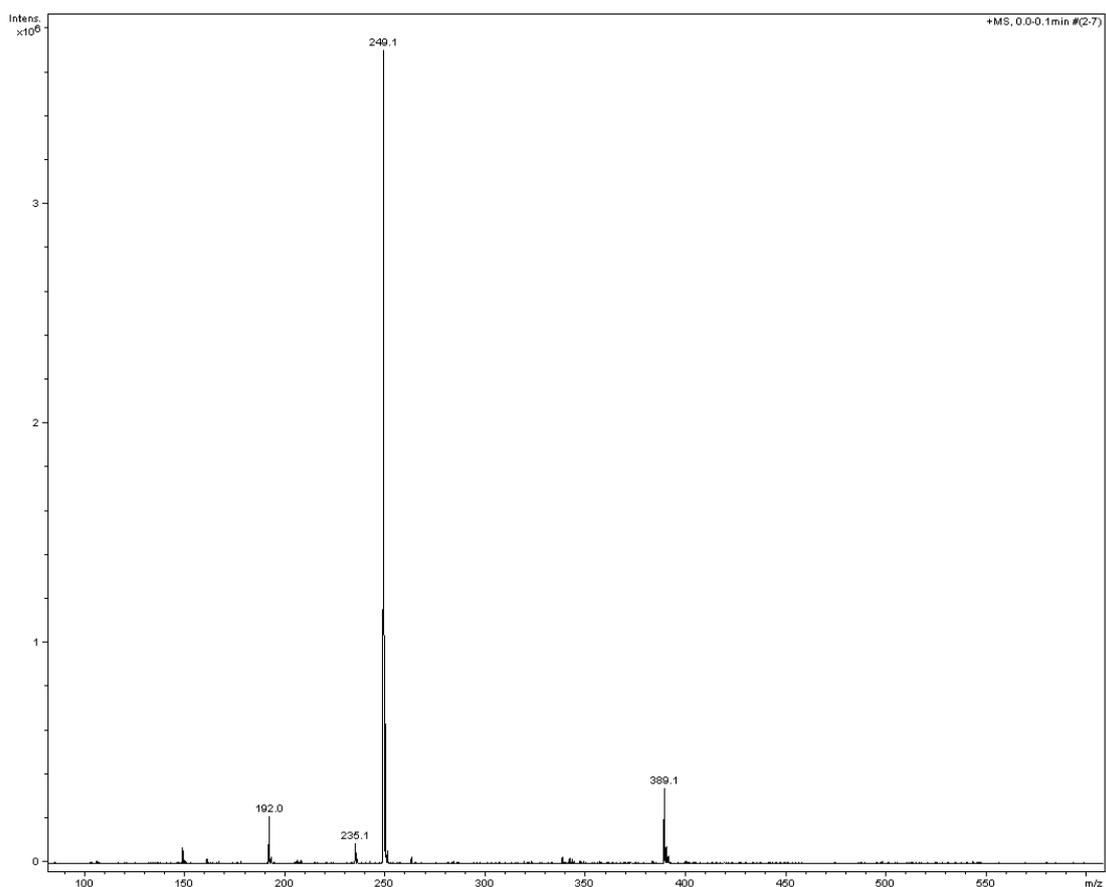


Figure S9. LC-MS (ESI/APCI-TOF) of L1-Me₃ in D₂O.

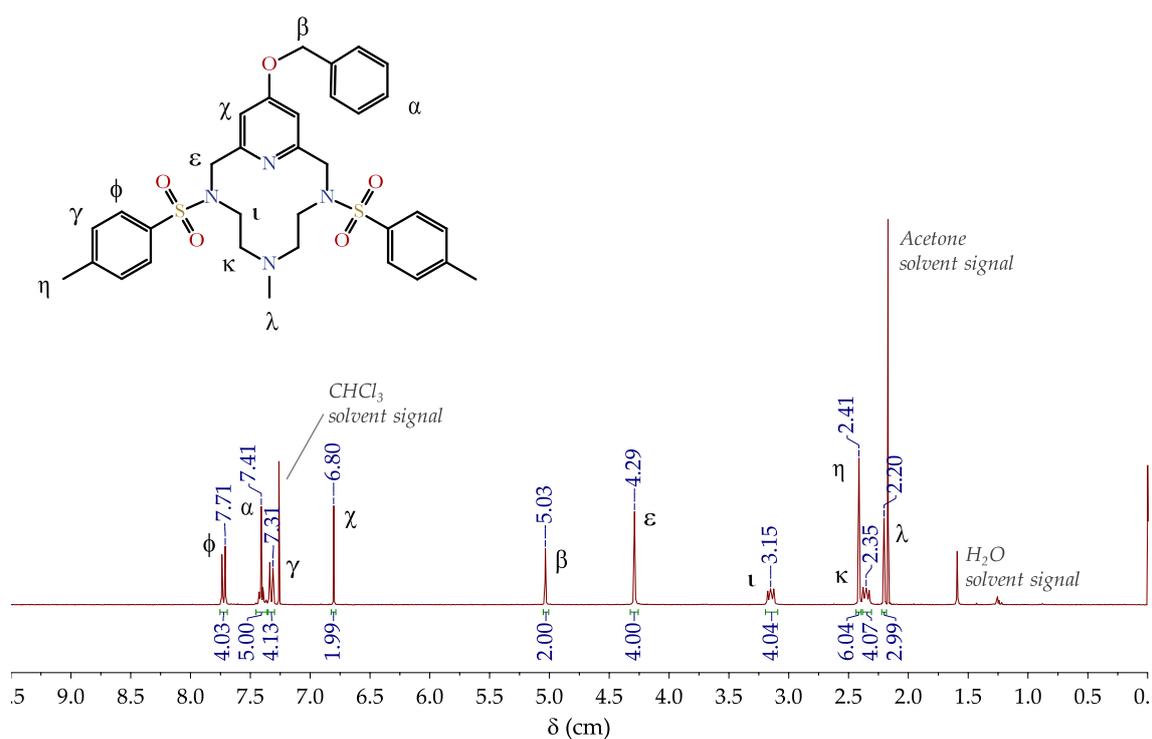


Figure S10. ¹H-NMR spectrum of **3** in CDCl₃ at 298 K.

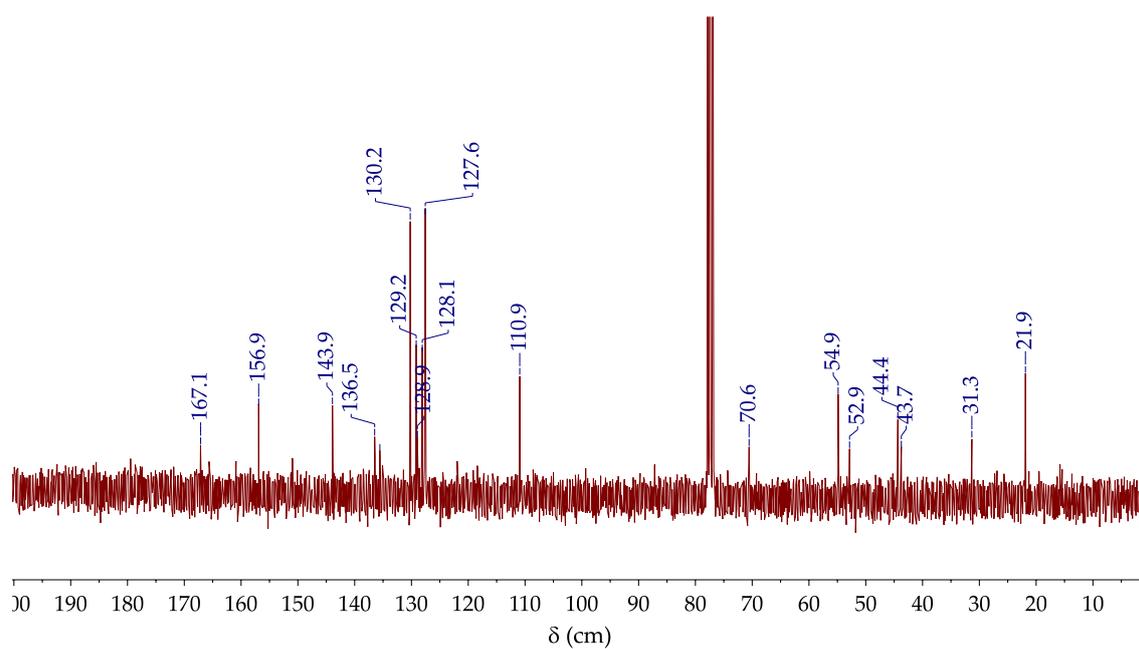


Figure S11. ^{13}C -NMR spectrum of **3** in CDCl_3 at 298 K.

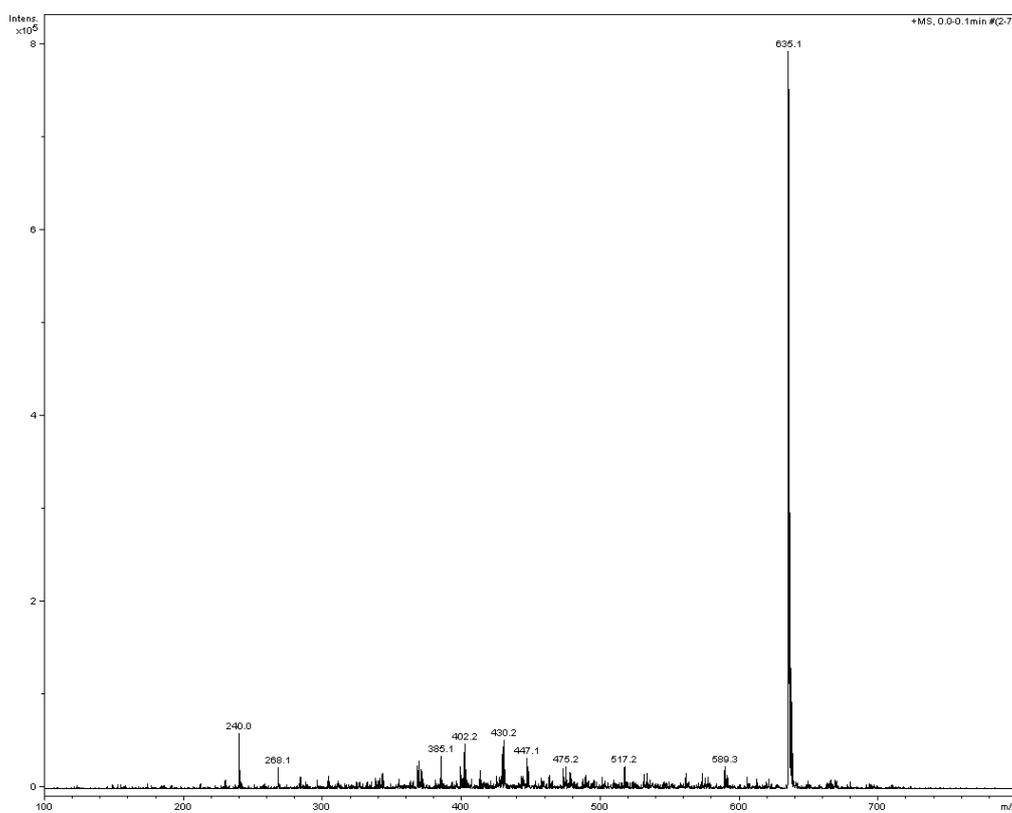


Figure S12. LC-MS (ESI/APCI-TOF) of **3** in CHCl_3 .

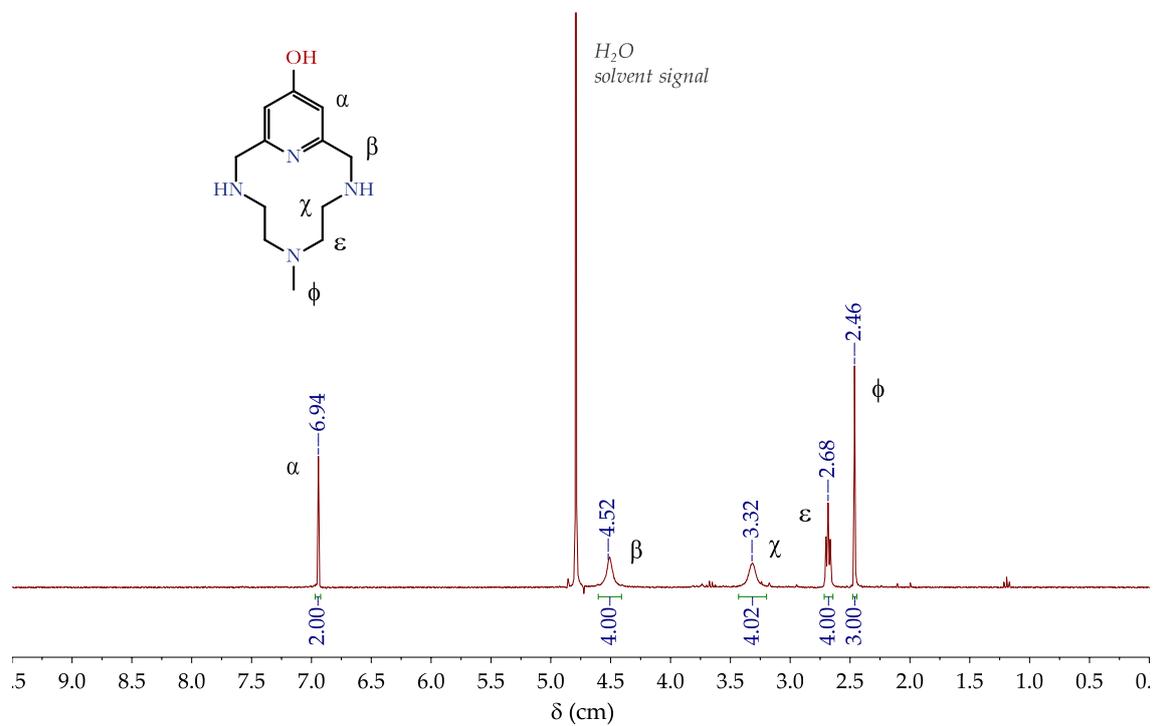


Figure S13. $^1\text{H-NMR}$ spectrum of **4** in D_2O at 298 K.

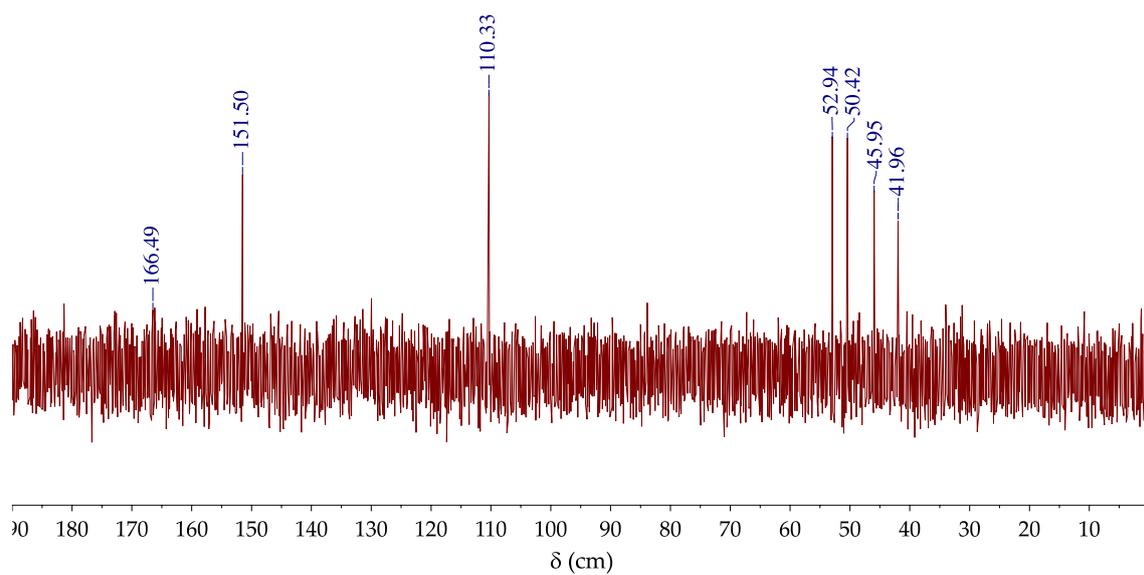


Figure S14. $^{13}\text{C-NMR}$ spectrum of **4** in D_2O at 298 K.

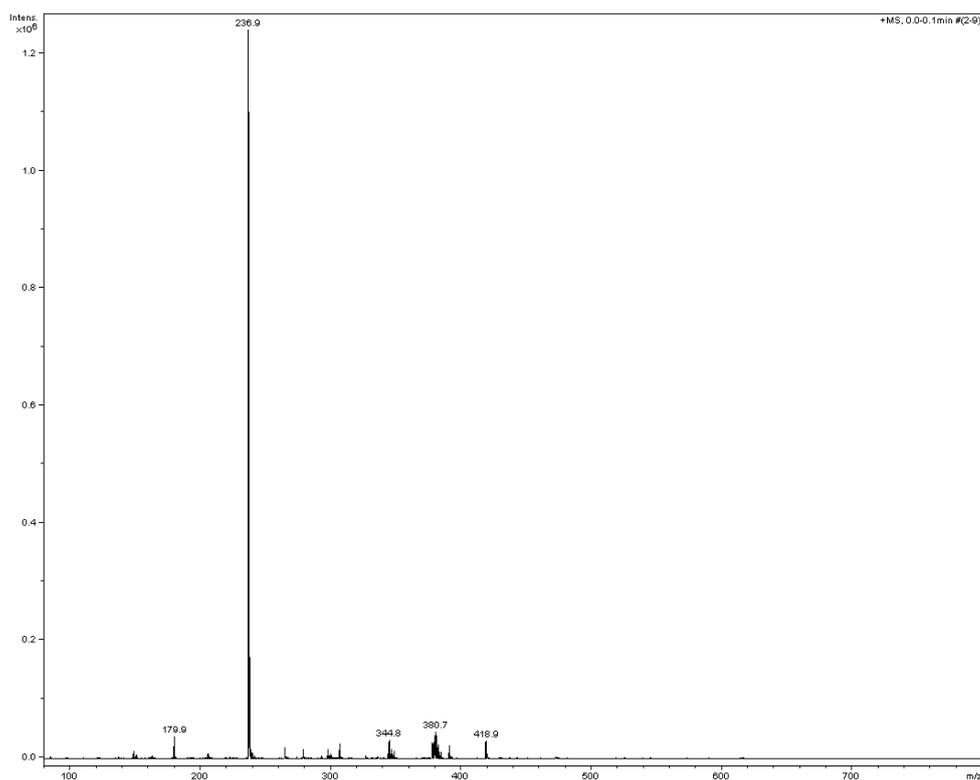


Figure S15. LC-MS (ESI/APCI-TOF) of 4 in CHCl₃.

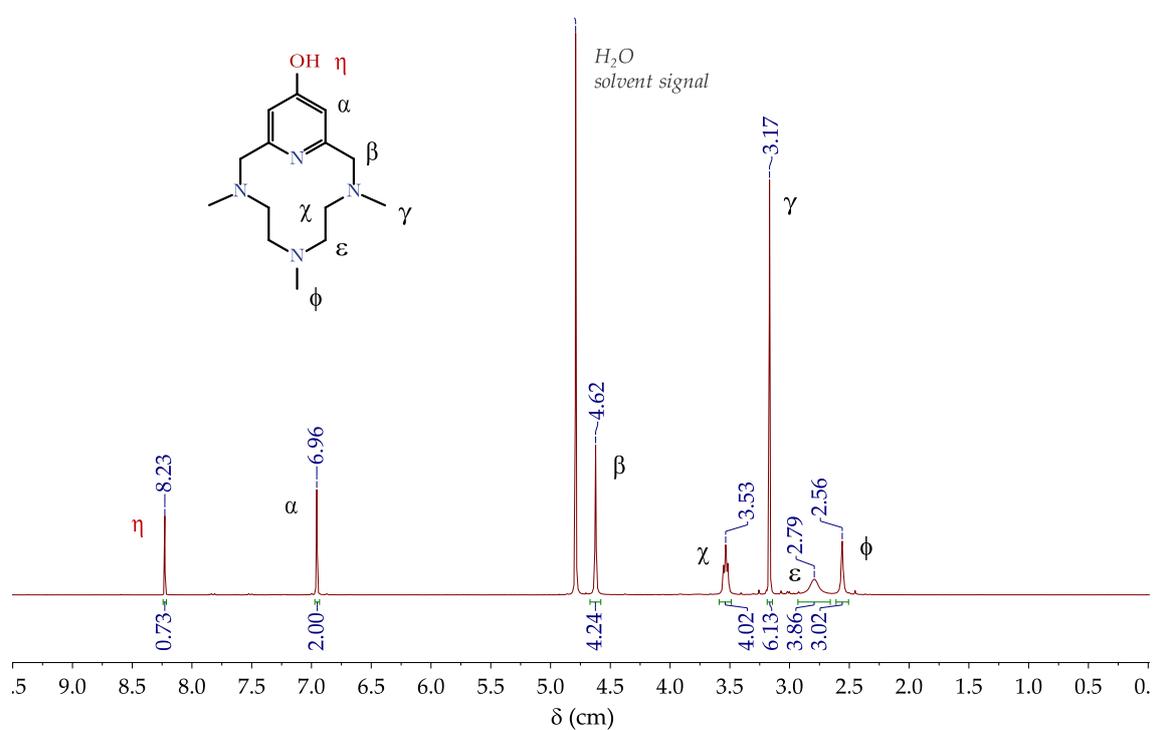


Figure S16. ¹H-NMR spectrum of L2 in D₂O at 298 K.

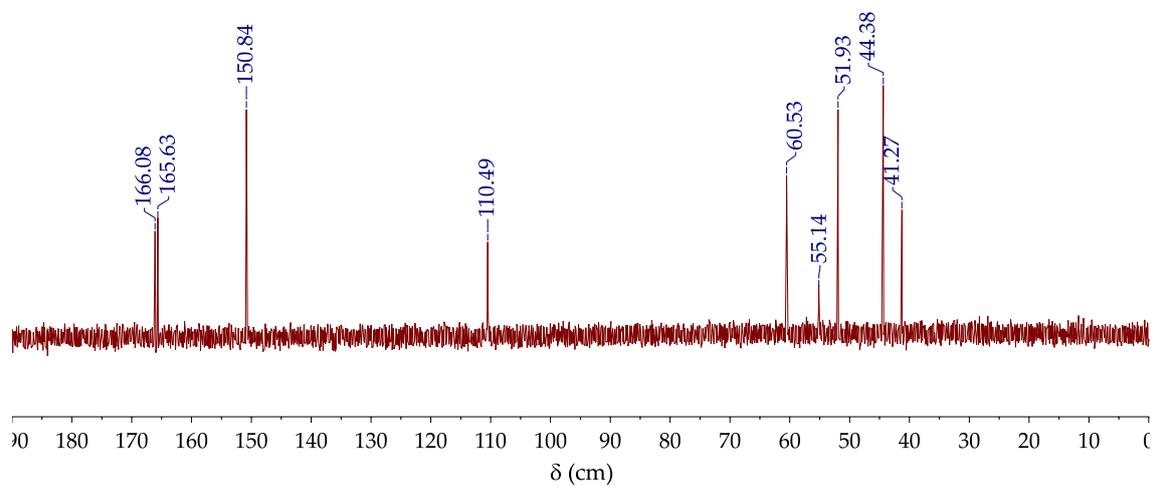


Figure S17. ^{13}C -NMR spectrum of L2 in D_2O at 298 K.

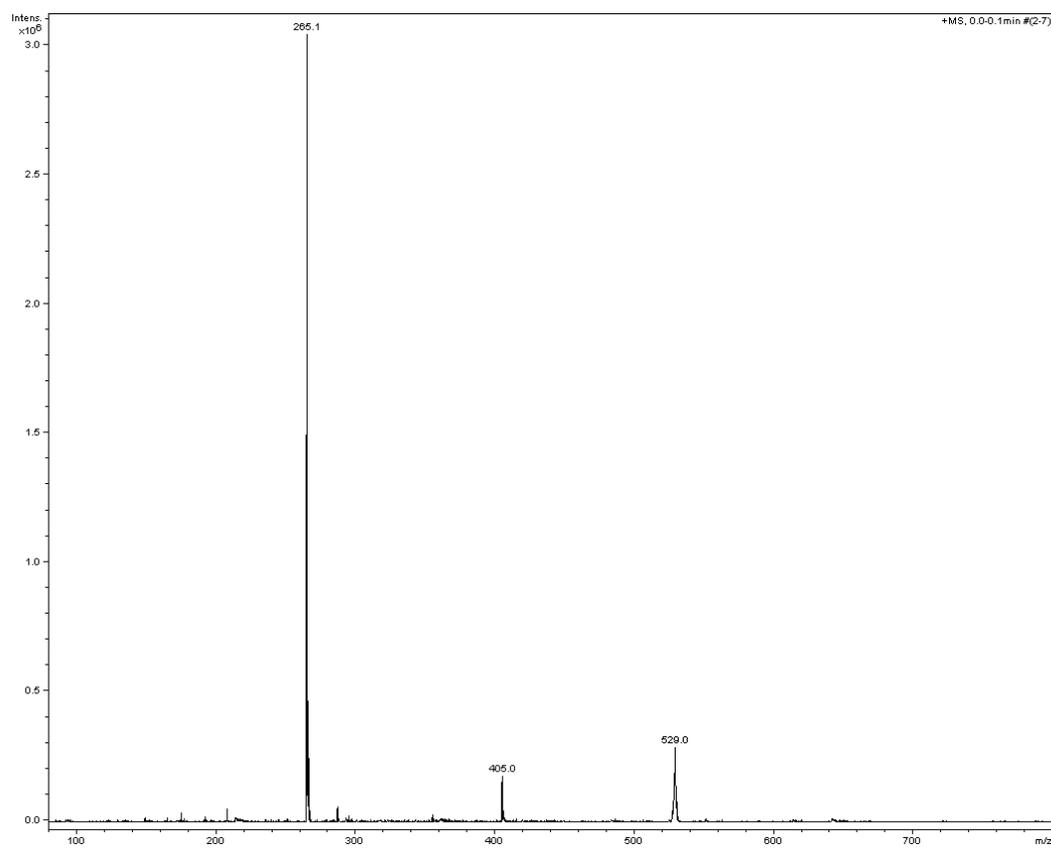


Figure S18. LC-MS (ESI/APCI-TOF) of L2 in CHCl_3 .