Synthetic water soluble di-/tritopic molecular receptors exhibiting Ca^{2+} / Mg^{2+} exchange

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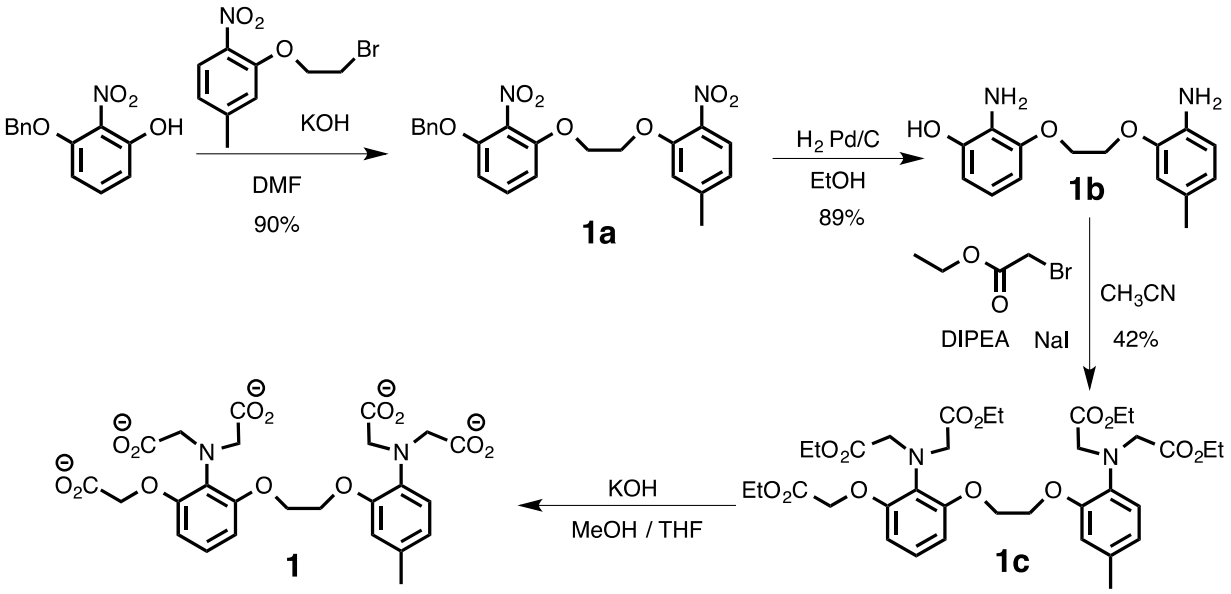
Supporting Information

Contents

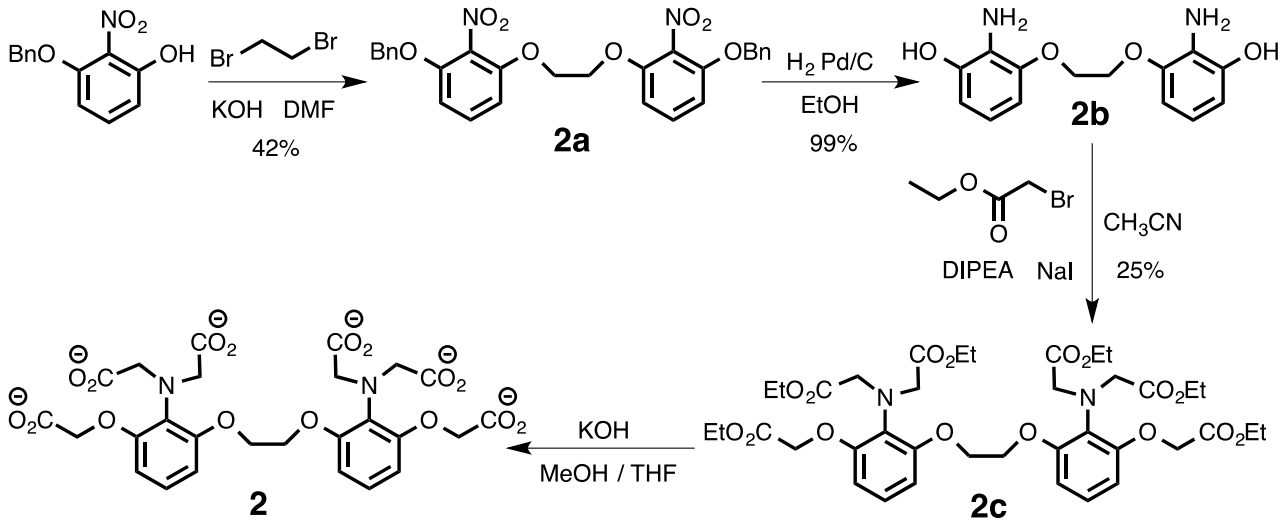
1. Materials and Methods

3-(Benzyloxy)-2-nitrophenol and 1-(2-bromoethoxy)-2-nitrobenzene were synthesized according to literature procedures.[1] All manipulations were performed under a dry nitrogen atmosphere using standard techniques. The reagents and solvents used were commercially available (Sigma-Aldrich, Acros and Alfa Aesar) and were employed without further purification. THF and diethyl ether were distilled over sodium/benzophenone. Acetonitrile and dichloromethane were distilled over calcium hydride immediately before use. The progress of all reactions was monitored by thin layer chromatography on silica gel 40 F_{254}. Column chromatography was performed on silica gel 40 (0.230-0.400 mm or 0.040-0.063 nm, Sigma-Aldrich). ^{1}H and ^{13}C-NMR experiments were performed at 295 K on a Brüker DPX 200 (^{1}H : 200 MHz), AC-250 (^{1}H : 250 MHz, ^{13}C : 62.9 MHz) and a Avance 300 (^{1}H : 300 MHz, ^{13}C : 75 MHz) spectrometer. Chemical shifts are reported in ppm (δ) and are referenced to the NMR solvent residual peaks. Abbreviations used are s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Mass spectra were performed by the CESAMO (Bordeaux, France) on a QStar Elite mass spectrometer (Applied Biosystems). The instrument is equipped with an ESI source and spectra were recorded in the positive mode. The electrospray needle was maintained at 5000 V and operated at room temperature. Samples were introduced by injection through a 20 µL sample loop into a 4500 µL/min flow of methanol from the LC pump. Electronic absorption spectra were measured on a Varian Cary 5000 UV-vis-NIR spectrophotometer.

2. Syntheses of the Compounds



Scheme S1: Synthesis of non-symmetrical receptor **1**.



Scheme S2: Synthesis of symmetrical receptor **2**.

3. Single Crystal X-Ray Crystallographic Information

Crystals of compound **1c** and **2c** were mounted on a short glass fibre attached to a tapered copper pin. A full hemisphere of data were collected on a Brüker Nonius Kappa diffractometer fitted with a CCD-based detector using MoK_{α} radiation (0.71073 Å). The structures were solved by direct methods, completed by subsequent Fourier syntheses and refined with full-matrix least-squares methods against $|F^2|$ data. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were treated as idealized contributions. A summary of crystal data collection, solution and structure refinement parameters are listed in Table S3. Details of the X-ray structure solutions can be found in the CIF format files deposited with the CCDC (numbers are listed in Table S1). This includes any problems with crystal quality, data collection or solution refinement that resulted in high residuals, as well as a description of any restraints necessary to attain the chemically reasonable models shown.

Table S1 A summary of crystal data collection, solution and structure refinement parameters for single-crystal structure determinations

Compounds	**Compound 1c**	**Compound 2c**
CCDC number	CCDC 1413055	CCDC 1413057
Formula	C_{35} H_{48} N_2 O_{13}	C_{38} H_{52} N_2 O_{16}
Formula weight	703.74	792.81
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
T (K)	170(2)	170(2)
a (Å)	12.0268(4)	8.7653(11)
b (Å)	13.3697(6)	15.5191(17)
c (Å)	13.7604(5)	16.6792(18)
α (°)	105.516(3)	67.964(10)
β (°)	103.403(3)	75.967(10)
γ (°)	112.129(4)	74.401(10)
V (Å^3)	1832.71(14)	2000.0(4)
Z	2	2
ρ, g cm^{-3}	1.275	1.316
μ, mm^{-1}	0.096	0.102
Reflections (total)	21318	14206
Reflections (unique)	7478	5734
Parameters/Restraints	537/5	522/38
R_1 [I > 2σ(I)]	0.0424	0.0456
R_1 (all data)	0.0729	0.0882
wR_2 [I > 2σ(I)]	0.1160	0.1089
wR_2 (all data)	0.1364	0.1179
GOF	1.005	0.936

4. Potentiometry study

Carbonate-free 0.1 M KOH and 0.1 M HCl were prepared from Fisher Chemicals concentrates. Potentiometric titrations were performed in 0.1 M aqueous KCl (electrolyte solution) under a nitrogen atmosphere, the temperature was controlled to ± 0.1 °C with a circulating water bath. The p[H] (p[H] = -log[H^+], concentration in molarity) was measured in each titration with a combined pH glass electrode (Metrohm) filled with 3M KCl and the titrant addition was automated by use of a 702 SM titrino (Metrohm). The electrode was calibrated in hydrogen ion concentration by titration of HCl with KOH in 0.1 M electrolyte solution.[2] A plot of meter reading versus pH allows the determination of the electrode standard potential (E°) and the slope factor (f). Continuous potentiometric titrations with KOH 0.1 M were conducted on 5 mL of aqueous solutions containing 0.98 M of **1**, and 0.87 M of **2** in 0.1 M of electrolyte solution, with 2 minutes waiting between 2 points. The titrations of the metal complexes were performed on 5 mL solutions of ligand containing 0.5, 1, 2 and 3 equivalents of metal cation, waiting 2 minutes between 2 points. The exact concentrations of the ligands **1** and **2** were determined from the titrations. Manual titrations were systematically performed on each experiment to check whether thermodynamic equilibrium had been achieved. Experimental data were refined using the computer program Hyperquad 2000.[3] All equilibrium constants are concentration quotients rather than activities and are defined as: $\beta_{mlh} = \frac{[M_m\ L_l H_h]}{[M]^m[L]^l[H]^h}$. The ionic product of water at 25 °C and 0.1 M ionic strength is pK_w = 13.77.[4] Fixed values were used for pK_w, ligand acidity constants and total concentrations of metal, ligand and acid. All values and errors (one standard deviation) reported are at least the average of three independent experiments.

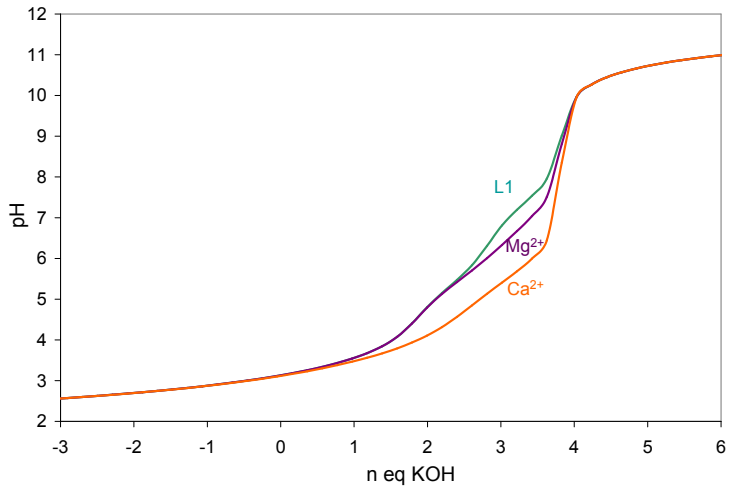


Figure S1: Potentiometric titration curves of solutions containing 0.98 mM of L1 (**1**) with 0 or 1 equivalent of $CaCl_2$ and $MgCl_2$.

5. Complexation of Ca^{2+} and Mg^{2+}: Spectrophotometric and NMR study

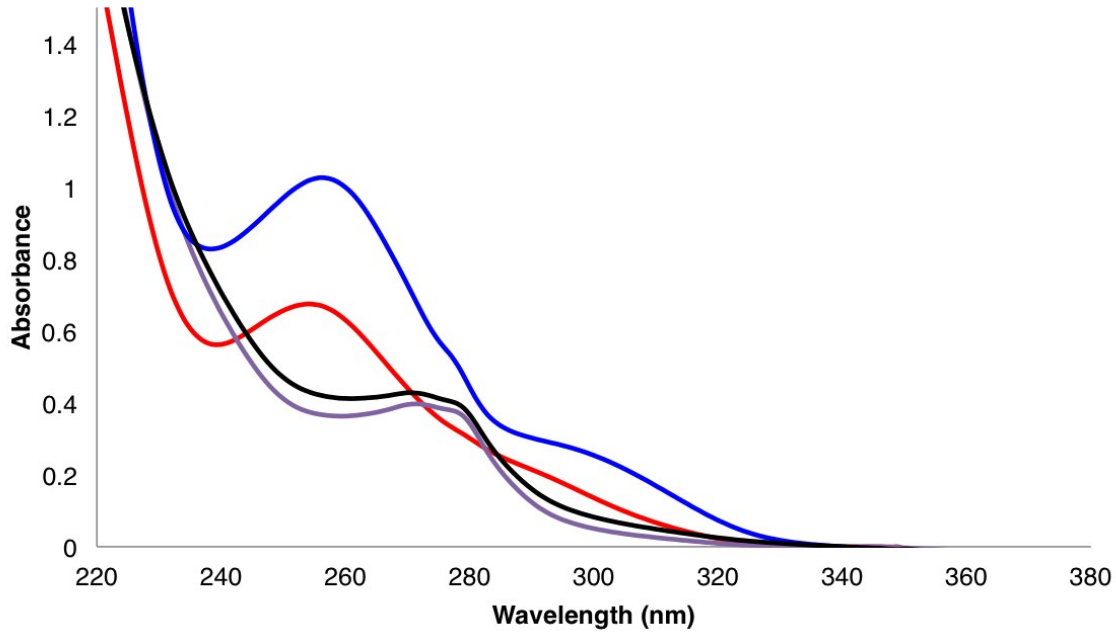


Figure S2: Electronic absorption spectra of non-symmetrical receptor **1** in KCl 0.1 M 298 K at pH 7.2 (concentration =43 μM) in absence of ions (red), with Ca^{2+} ([5 mM], purple), Mg^{2+} ([5 mM], blue), Ca^{2+} and Mg^{2+} (1:1, [5 mM], black).

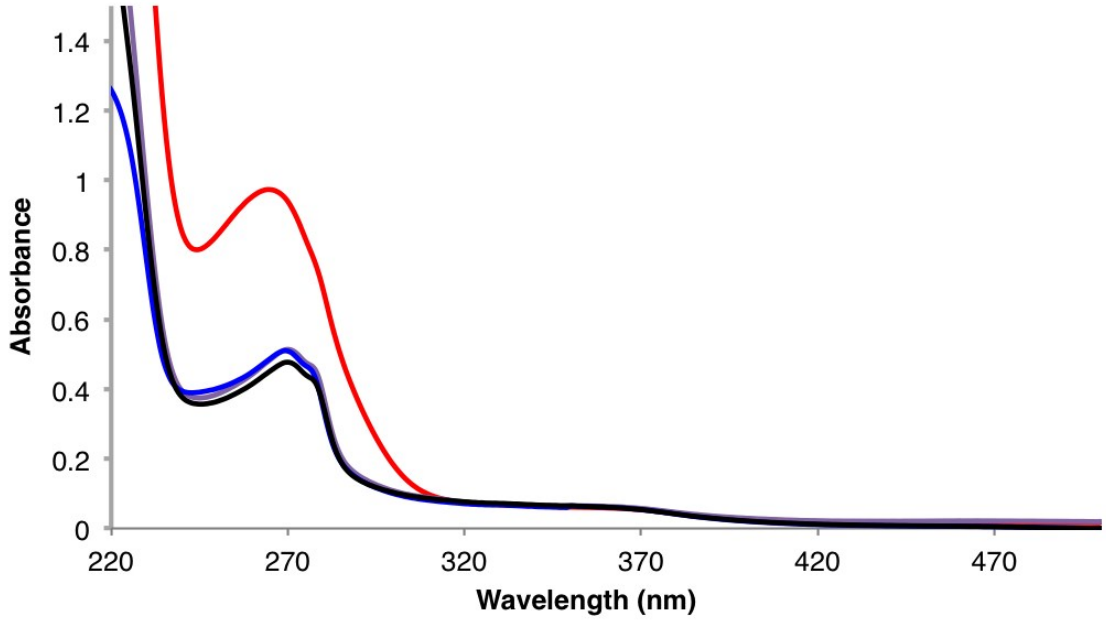


Figure S3: Electronic absorption spectra of symmetrical receptor **2** in KCl 0.1 M 298 K at pH 7.2 (concentration =55 μM) in absence of ions (red), with Ca^{2+} ([5 mM], purple), Mg^{2+} ([5 mM], blue), Ca^{2+} and Mg^{2+} (1:1, [5 mM], black).

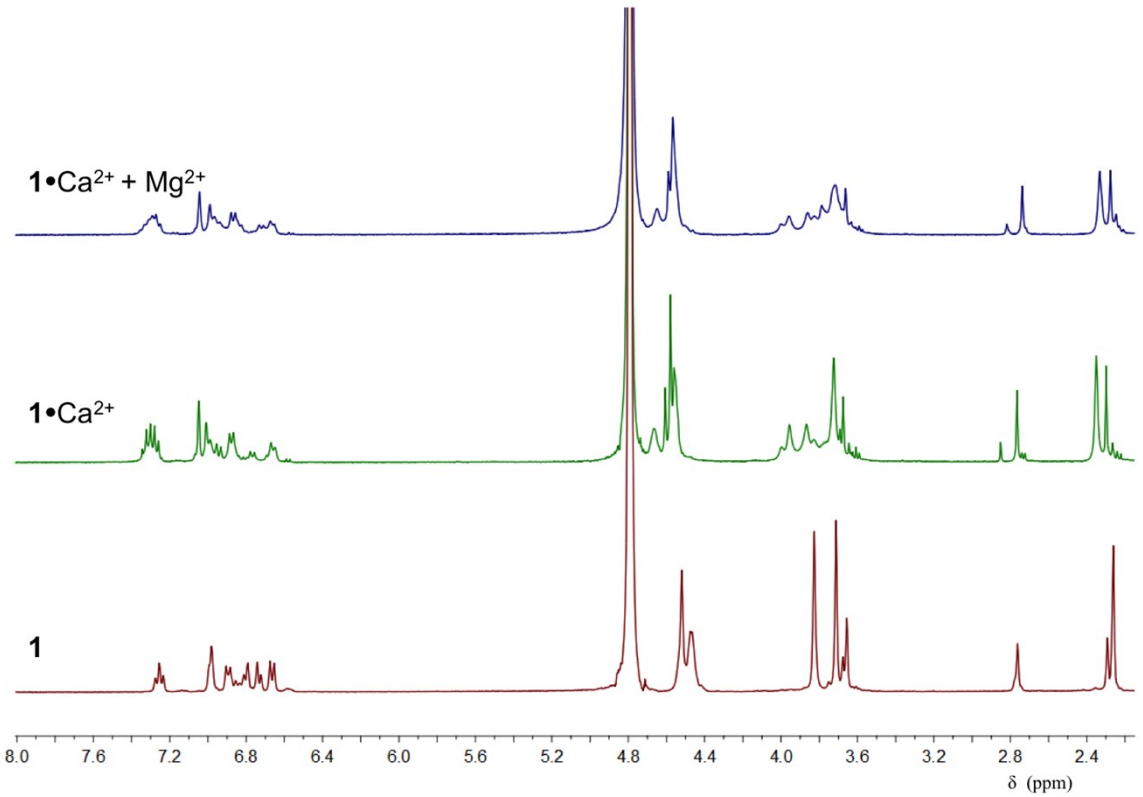


Figure S4: ^{1}H NMR (400 MHz) spectra of non-symmetrical receptor **1** (2mM) in D_2O at 298 K in absence of ions (bottom), with Ca^{2+} (2mM, middle), Ca^{2+} and Mg^{2+} (1:10, top).

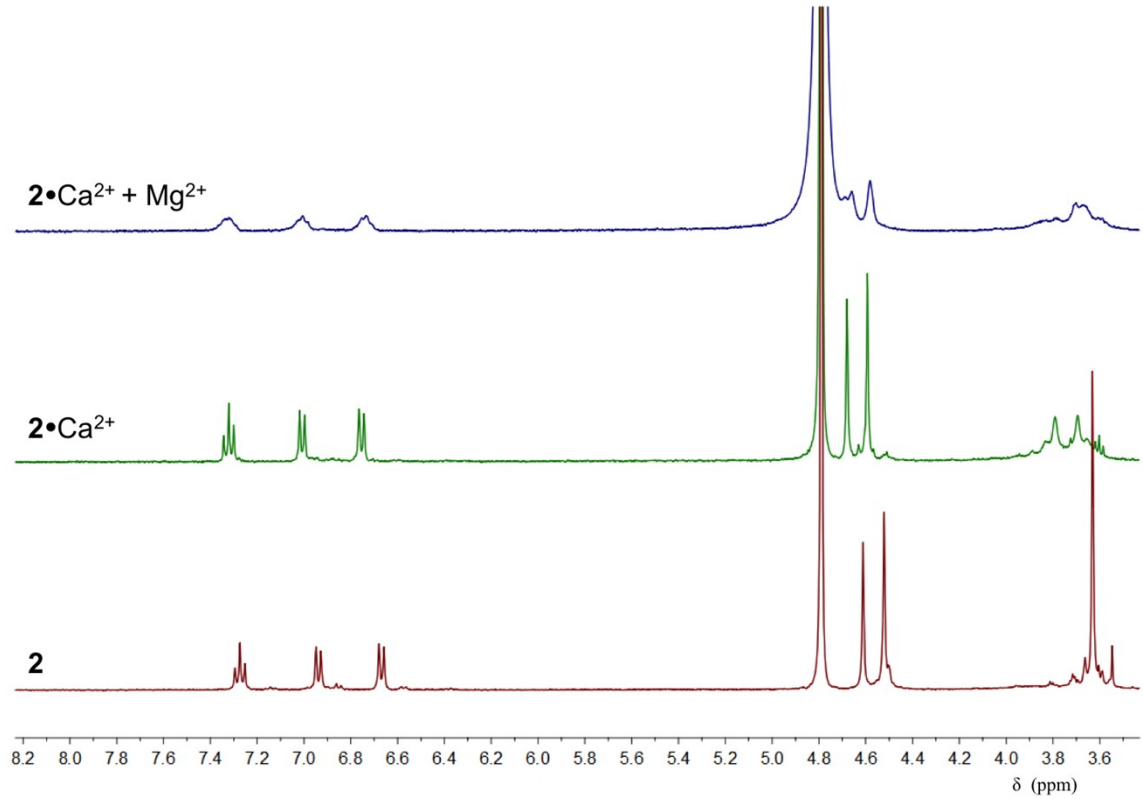


Figure S5: ^{1}H NMR (400 MHz) spectra of symmetrical receptor **2** (2mM) in D_2O at 298 K in absence of ions (bottom), with Ca^{2+} (2mM, middle), Ca^{2+} and Mg^{2+} (1:10, top).

6. Cyclic Voltammetry

The voltammograms were measured on a EGxG Princeton Applied Research Potentiostat/Galvanostat Model 273. CV experiments were performed using a three electrode: silver working electrode, silver wire reference electrode and platinum foil counter electrode. The supporting electrolyte was tetrabutylammonium hexafluorophosphate ($NBu_4^+PF_6^-$). The internal standard used for calibration of voltammograms is either ferrocene or decamethylferrocene. The solution was degassed by nitrogen bubbling for 5 minutes. The scan rate is 200 mV/s.

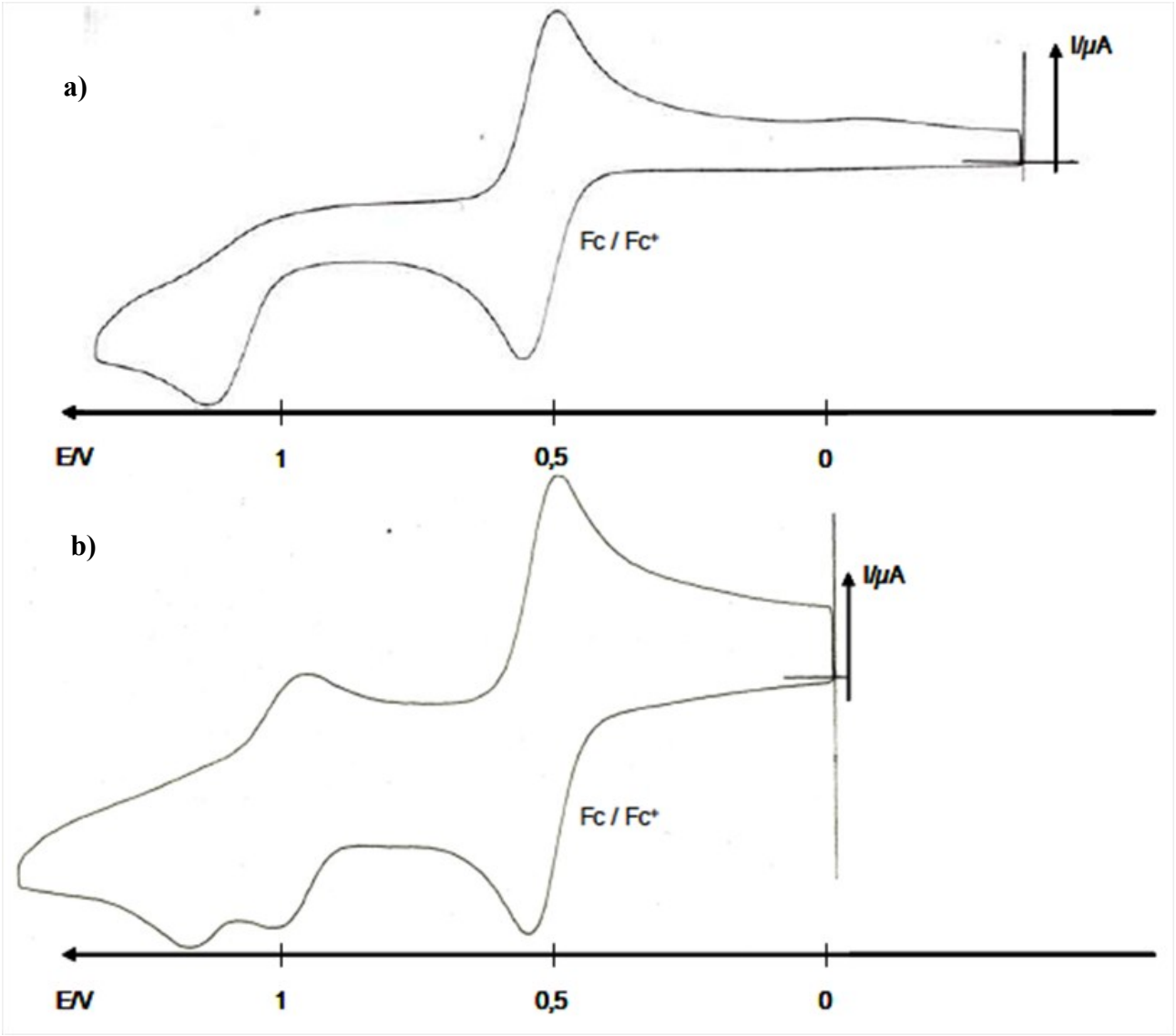


Figure S6: Cyclic voltammetry of symmetrical receptor **2c** (a) non-symmetrical receptor **1c** (b) in acetonitrile. Fc = Ferrocene (Fc/Fc^+ =- 0.022V vs ECS); Fc' = Decamethylferrocene (Fc'/Fc'^+ = +0.41V vs ECS).

7. DFT calculations

Molecular structures were optimized at the density functional theory (DFT) level using the long-range corrected ωB97X-D exchange-correlation functional[5] (which includes 22.20% of HF exchange at short-range and 77.80% at long-range with a range-separation parameter μ = 0.20, as well as empirical dispersion forces), together with the 6-311G(d) basis set. All structures were characterized as real minima of the potential energy surface based on their vibrational frequencies. Solvent effects (water) were included by using the Polarizable Continuum Model in its Integral Equation Formalism (IEF-PCM),[6] and by adding explicit water molecules to complete the coordination of the Ca^{2+} and Mg^{2+} ions. All calculations were performed using the Gaussian 09 package.[7]

Preliminary calculations were first conducted to confirm the preferential coordination of the Ca^{2+} and Mg^{2+} ions in water solution, by varying the number of the surrounding water molecules. The coordination energy of a cation surrounded by *n* explicit water molecules was calculated at the IEFPCM/ωB97X-D/6-311G(d) level, as the Gibb's free energy (ΔG°) of the reaction below, using standard ambient conditions for temperature and pressure, T = 298.15 K and P = 1 atm:

$$M^{2+} + nH_2O \rightarrow \{M^{2+}, (H_2O)_n\}, \text{ with M = Ca or Mg.}$$

These calculations demonstrated that the calcium adopts an octacoordinate environment, whereas the magnesium is hexacoordinated, with respective coordination energies of –57.2 and –202.9 kJ/mol. The complexation energies of the different Ca^{2+} complexes with the asymmetrical BAPTA-APTRA (**1**) and symmetrical APTRA-BAPTA-APTRA (**2**) receptors were then calculated at the same level of approximation, as the Gibb's free energy (ΔG°) of the following reactions:

$$\{Ca^{2+}, (H_2O)_8\} + \mathbf{1} \rightarrow \mathbf{1}\bullet Ca^{2+} + 8H_2O \qquad \text{R1}$$

$$\{Ca^{2+}, (H_2O)_8\} + \mathbf{2} \rightarrow \mathbf{2}\bullet Ca^{2+} + 8H_2O \qquad \text{R2}$$

where Ca^{2+} occupies the BAPTA site and is octacoordinated in both the **1**•Ca^{2+} and **2**•Ca^{2+} chelates, as shown on Figures S5-e and S6-i. In order to address the best complexation site (BAPTA or APTRA) for the calcium cation, the complexation energies of the chelate structures in which Ca^{2+} occupies the peripheral APTRA site in receptors **1** and **2** were also calculated. In this case, 3 water molecules were added to ensure the octacoordination of Ca^{2+}, leading to the following complexation

reactions:

$$\{Ca^{2+}, (H_2O)_8\} + \mathbf{1} \rightarrow \{\mathbf{1}\bullet Ca^{2+}, (H_2O)_3\} + 5H_2O \qquad R3$$

$$\{Ca^{2+}, (H_2O)_8\} + \mathbf{2} \rightarrow \{\mathbf{2}\bullet Ca^{2+}, (H_2O)_3\} + 5H_2O \qquad R4$$

In the $\{\mathbf{1}\bullet Ca^{2+}, (H_2O)_3\}$ and $\{\mathbf{2}\bullet Ca^{2+}, (H_2O)_3\}$ complexes, the coordination of the Ca^{2+} ion implicates three carboxylates, one aniline function, one peripheral ether oxygen and three water molecules (Figures S5-c). The complexation energies calculated for the R1-R4 reactions are gathered in Table S2. The results demonstrate that Ca^{2+} preferentially complexes within the central BAPTA site in both receptors ($\Delta G_{R1} << \Delta G_{R3}$ and $\Delta G_{R2} << \Delta G_{R4}$). It is also found that reactions R3 and R4 are associated to similar complexation energies, which indicates that the presence of a second APTRA group at the other extremity of the molecule in receptor **2** does not impact significantly the cation environment. On the contrary, when Ca^{2+} is complexed within the central BAPTA site, the stabilization energy is markedly larger (by 25 kJ/mol) in the case of receptor **2** than in the case of receptor **1**.

Table S2. Complexation energies (in kJ/mol) calculated for reactions R1-R3 at the IEFPCM/ωB97X-D/6-311G(d) level of approximation.

Reaction	**Complex formed**	**Complexation site**	**Gibbs free energy**
R1	$\mathbf{1}\bullet Ca^{2+}$	BAPTA	–374
R2	$\mathbf{2}\bullet Ca^{2+}$	BAPTA	–399
R3	$\{\mathbf{1}\bullet Ca^{2+}, (H_2O)_3\}$	APTRA	–300
R4	$\{\mathbf{2}\bullet Ca^{2+}, (H_2O)_3\}$	APTRA	–294

Similarly, the complexation energies of the **1**•Mg and **2**•Mg complexes, in which the magnesium occupies the central BAPTA site within a hexacoordinated environment (Figures 5-d and 5-h), were calculated at the IEFPCM/ωB97X-D/6-311G(d) level of approximation as the Gibb's free energies of the following reactions:

$$\{Mg^{2+}, (H_2O)_6\} + \mathbf{1} \rightarrow \mathbf{1}\bullet Mg^{2+} + 6H_2O \qquad R5$$

$$\{Mg^{2+}, (H_2O)_6\} + \mathbf{2} \rightarrow \mathbf{2}\bullet Mg^{2+} + 6H_2O \qquad R6$$

Furthermore, the complexation energy of the $\mathbf{1}\bullet Mg^{2+}$ and $\mathbf{2}\bullet Mg^{2+}$ complexes in which the

magnesium occupies the APTRA site were also determined, by adding one explicit water molecule to ensure the hexacoordination of Mg^{2+}:

$$\{Mg^{2+}, (H_2O)_6\} + \mathbf{1} \rightarrow \{\mathbf{1}\bullet Mg^{2+}, H_2O\} + 5H_2O \qquad R7$$

$$\{Mg^{2+}, (H_2O)_6\} + \mathbf{2} \rightarrow \{\mathbf{2}\bullet Mg^{2+}, H_2O\} + 5H_2O \qquad R8$$

In the {**1**•Mg, H_2O} and {**2**•Mg, H_2O} complexes, the coordination of the Mg^{2+} ion implicates three carboxylates, one aniline function, and one water molecule (Figures S5-b and S6-g). The complexation energies calculated for the R5-R8 reactions are gathered in Table S3. As in the case of Ca^{2+}, the calculations predict that the magnesium ion preferentially complexes within the central BAPTA site rather within the peripheral APTRA sites, independently on the receptor ($\Delta G_{R5} << \Delta G_{R7}$, and $\Delta G_{R6} << \Delta G_{R8}$). Moreover, the energies associated to the complexation of the magnesium by the APTRA sites are very similar in receptor **1** and **2**. Noteworthy, the energies involved in the formation the **1**•Mg and **2**•Mg complexes in which the magnesium occupies the central BAPTA site (reactions R5 and R6), only differ by 3 kJ/mol, which is much smaller than the difference of 25 kJ/mol calculated for **1**•Ca and **2**•Ca. More importantly, the calculations predict that $\Delta G_{R1} < \Delta G_{R5}$, and $\Delta G_{R2} < \Delta G_{R6}$, which indicates that, in presence of the two cations, both receptors **1** and **2** preferentially form complexes with Ca^{2+} rather than with Mg^{2+} in both their BAPTA and APTRA sites.

Table S3. Complexation energies (in kJ/mol) calculated for reactions R4-R7 at the IEFPCM/ωB97X-D/6-311G(d) level of approximation.

Reaction	**Complex formed**	**Complexation site**	**Gibbs free energy**
R5	**1**•Mg^{2+}	BAPTA	–341
R6	**2**•Mg^{2+}	BAPTA	–344
R7	{**1**•Mg^{2+}, H_2O}	APTRA	–279
R8	{**2**•Mg^{2+}, H_2O}	APTRA	–280

Finally, we investigated the possibility for the symmetrical APTRA-BAPTA-APTRA receptor **2** of complexing two Ca^{2+} or Mg^{2+} cations in the peripheral APTRA sites within respectively an octa- or hexacoordination, following the reactions:

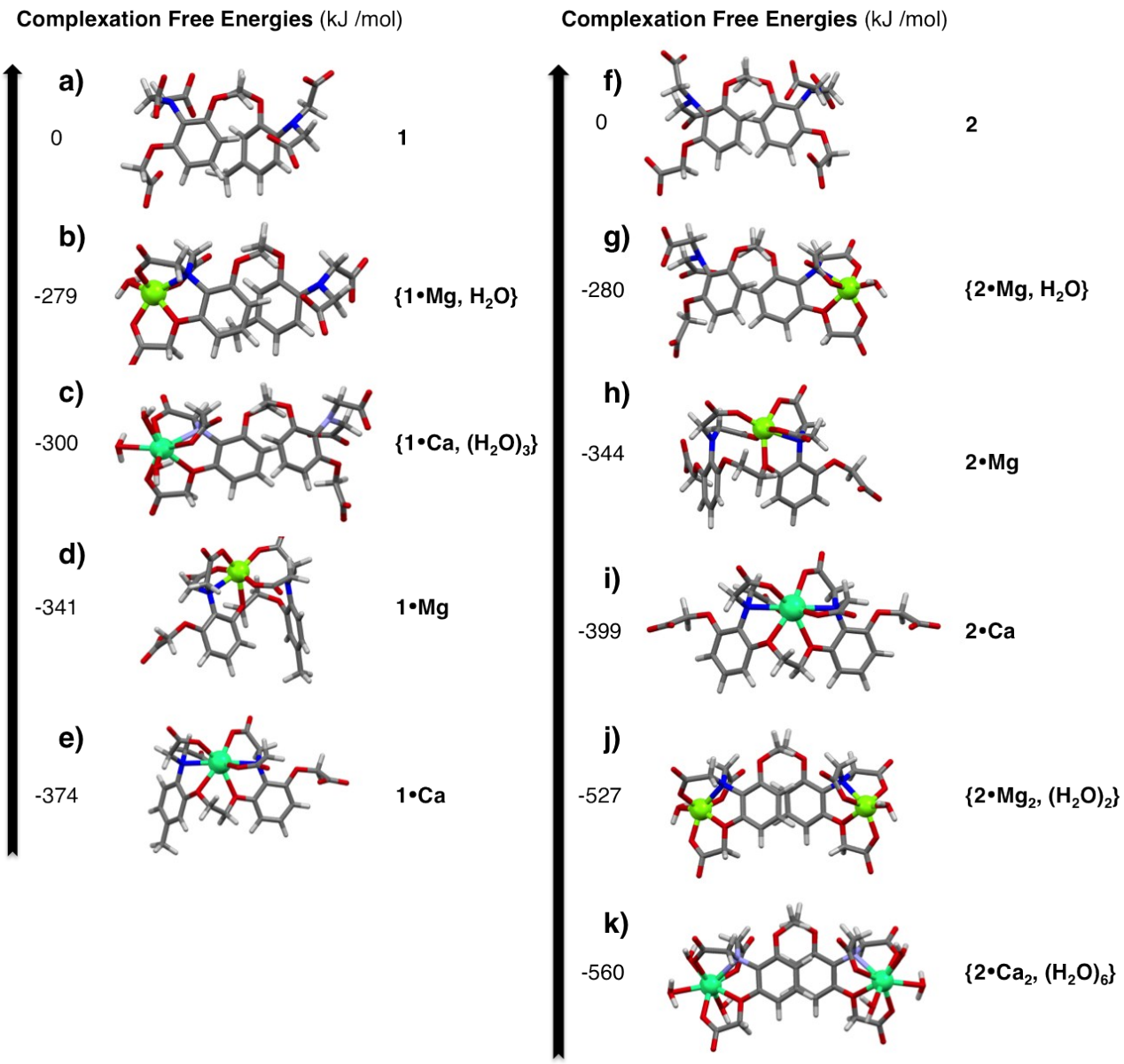
$$2\{Ca^{2+}, (H_2O)_8\} + \mathbf{2} \rightarrow \{\mathbf{2}\bullet\square Ca^{2+}, (H_2O)_6\} + 10H_2O \qquad R9$$

$$2\{Mg^{2+}, (H_2O)_6\} + \mathbf{2} \rightarrow \{\mathbf{2}\bullet\square Mg^{2+}, (H_2O)_2\} + 10H_2O \qquad \text{R10}$$

The final complexes $\{\mathbf{2}\bullet\square Ca^{2+}, (H_2O)_6\}$ and $\{\mathbf{2}\bullet\square Mg^{2+}, (H_2O)_2\}$ have a C_2-symmetry (Figures S5-k and S6-j). The energies calculated for reactions R9 and R10 (Table S4) are larger (by respectively 27 and 32 kJ/mol) than twice those calculated for reactions R4 and R8, involving the complexation of a single cation. As in this case, the formation of $\{\mathbf{2}\bullet\square Ca^{2+}, (H_2O)_6\}$ complexes is favored over $\{\mathbf{2}\bullet\square Mg^{2+}, (H_2O)_2\}$ complexes.

Table S4. Complexation energies (in kJ/Mol) calculated for reactions R8 and R9 at the IEFPCM/ωB97X-D/6-311G(d) level of approximation.

Reaction	**Complex formed**	**Complexation sites**	**Gibbs free energy**
R9	$\{\mathbf{2}\bullet\square Ca^{2+}, (H_2O)_6\}$	APTRA+APTRA	–560
R10	$\{\mathbf{2}\bullet\square Mg^{2+}, (H_2O)_2\}$	APTRA+APTRA	–527



Figures S7: molecular structures optimized at the IEFPCM/ωB97X-D/6-311G(d) level in water.

Molecular structures

Receptor 1

N	2.64513100	-1.97433900	-0.35521300
N	-3.98414500	0.45744900	0.05195700
O	0.00619300	-2.05297900	0.48000300
O	-2.20185700	-0.46201200	-1.86262500
C	-1.23669200	-1.45634300	-1.52899800
C	-1.30536600	-1.88491200	-0.05813200
H	-0.23107600	-1.09812100	-1.75176700
H	-1.44402100	-2.28982500	-2.20094400
H	-1.90097200	-1.17296300	0.51949300
H	-1.77489800	-2.86420300	0.04697600
C	-1.97383500	0.77023800	-1.29025800
C	-0.85341100	1.50132000	-1.64841600
C	-2.89267300	1.25050700	-0.33530500

C	-0.58117800	2.74156600	-1.06825100
H	-0.14303900	1.06225700	-2.34638300
C	-2.61547500	2.49894500	0.22919200
C	-1.47959100	3.22254300	-0.12507000
H	-3.27449100	2.89903800	0.99072300
H	-1.29450000	4.17964200	0.35643100
C	0.72019000	-0.91041600	0.73034100
C	2.06531300	-0.86780400	0.34152200
C	0.12379600	0.15915900	1.40378700
C	2.81622000	0.27616100	0.68945400
C	0.87564600	1.28391500	1.68222400
H	-0.91715900	0.11338700	1.70751200
C	2.21899900	1.35813200	1.33223800
H	0.40632400	2.12899900	2.17588900
H	2.78299100	2.25483600	1.55600400
C	3.59573300	-2.75956100	0.44331600
C	2.99904300	-3.27634200	1.77797500
H	4.51033600	-2.18614400	0.65584600
H	3.87070700	-3.62741700	-0.16377700
C	3.19061900	-1.65024800	-1.68046400
C	2.10016500	-1.22059700	-2.68866900
H	3.64919800	-2.56860900	-2.05707700
H	3.96500100	-0.87509300	-1.62414800
C	-4.92616200	0.09189100	-0.99691100
C	-5.65374900	-1.26979400	-0.83863500
H	-4.40302300	0.04514600	-1.95052200
H	-5.70222300	0.86990800	-1.10521500
C	-4.65576700	0.83120000	1.27730400
C	-3.78139900	0.85323800	2.55658700
H	-5.42684000	0.07334600	1.44373600
H	-5.17560600	1.80057000	1.18910700
O	-5.29125400	-2.05637200	0.06083400
O	-6.55902500	-1.45016400	-1.68588600
O	3.18897500	-2.56287700	2.79007800
O	2.39151500	-4.37147800	1.73243500
O	1.51180900	-2.14027900	-3.30216700
O	1.89535100	0.01271300	-2.80901300
O	-2.88511500	-0.01397000	2.66290500
O	-4.09676600	1.71989000	3.40237800
C	0.67427700	3.49247500	-1.42717900
H	1.56810700	2.94106100	-1.12174200
H	0.75072600	3.65484600	-2.50719600
H	0.70486900	4.47126700	-0.94120700
O	4.13486900	0.23847000	0.37535700
C	4.95548900	1.32019700	0.77475700
C	4.79351700	2.63050200	-0.03805800
H	5.97748800	0.96003500	0.62837300
H	4.82866000	1.52361200	1.84322300
O	5.24992300	3.64159900	0.53816400
O	4.28091800	2.54831100	-1.17079300

Receptor 2

N	3.93394400	-1.33433800	0.24001700
N	-3.43423500	-1.10553700	-0.24002600
O	1.34710500	-1.96742300	1.01540100
O	-1.20190200	-1.93722000	-1.52461100
C	0.02619800	-2.42025700	-0.98661300

C	0.05177900	-2.34630500	0.54376000
H	0.87243600	-1.86732100	-1.39405200
H	0.10693700	-3.44757000	-1.34274500
H	-0.73480300	-1.67486600	0.89851900
H	-0.12648000	-3.32649300	0.98993500
C	-1.39577400	-0.58244600	-1.42801400
C	-0.45813100	0.30398400	-1.95464700
C	-2.57538500	-0.14552900	-0.80662600
C	-0.68964100	1.66406200	-1.86184500
H	0.45955700	-0.07777400	-2.39229200
C	-2.82295200	1.24829300	-0.80972500
C	-1.86581700	2.14218500	-1.29292600
H	-2.04276600	3.20947200	-1.25385100
C	1.68144300	-0.64436800	0.93560900
C	2.98229200	-0.30564500	0.53070700
C	0.75498200	0.34258600	1.28573700
C	3.31205400	1.06639200	0.44905100
C	1.11671100	1.67335700	1.20437900
H	-0.24568700	0.07568400	1.60810400
C	2.38331300	2.05234900	0.77901200
H	0.38966100	2.43859300	1.45877000
H	2.62927500	3.10297900	0.69124300
C	5.07915000	-1.36234100	1.15458600
C	4.69633500	-1.35534400	2.65837900
H	5.77314300	-0.53419300	0.96108000
H	5.61490100	-2.29986400	0.95815700
C	4.36840800	-1.40158800	-1.16015900
C	3.23057500	-1.80644200	-2.12464000
H	5.13763700	-2.17785600	-1.20667700
H	4.81587800	-0.45559800	-1.49223400
C	-4.13503200	-1.96813700	-1.17215600
C	-4.31401200	-3.45809300	-0.77246200
H	-3.60104000	-1.97192800	-2.12357600
H	-5.14277900	-1.57127800	-1.39328600
C	-4.20884900	-0.79533100	0.94680700
C	-3.43894200	-0.23102900	2.15878200
H	-4.62259000	-1.75213200	1.28257400
H	-5.04742500	-0.12237200	0.74308700
O	-3.80742300	-3.87849400	0.28925900
O	-4.97954800	-4.11815400	-1.60598300
O	5.12372300	-0.38980400	3.33489200
O	4.03118600	-2.32859500	3.07579800
O	3.02721800	-3.03329300	-2.26649100
O	2.60516700	-0.87115800	-2.68413600
O	-2.20761900	-0.45156800	2.24590200
O	-4.14871400	0.36378600	3.00172500
O	4.57382500	1.34927100	0.04230700
C	4.94882700	2.70514300	-0.11303900
C	4.30281300	3.45802200	-1.30722900
H	6.02849000	2.67365800	-0.28140200
H	4.78092000	3.26164100	0.81509400
O	4.41828400	4.70087700	-1.23227600
O	3.78782200	2.77943500	-2.21568300
O	-4.03247400	1.64326500	-0.33576400
C	-4.24531900	3.01257300	-0.06230300
C	-5.64398000	3.28112100	0.53960800
H	-4.16367700	3.60811600	-0.98119700
H	-3.48409100	3.38172600	0.63600500

O	-5.80367300	4.47973000	0.86226500
O	-6.45754700	2.34419400	0.62764500
H	0.05483800	2.36442200	-2.22738300

1•Ca^{2+}

Ca	-0.73632600	-1.03424600	-0.46323300
N	1.83024500	-0.72631100	0.14618200
N	-3.31676300	-0.93538000	0.26046300
O	0.22557700	1.37819400	-0.57441300
O	-2.29894600	0.80063200	-1.45953700
C	-1.45181100	1.65924500	-2.21766200
C	-0.44464800	2.37159400	-1.34367100
H	-2.03071000	2.37328000	-2.80764500
H	-0.92799900	0.98542400	-2.89429200
H	0.26330100	2.89411900	-1.99291100
H	-0.91320500	3.09858600	-0.67549000
C	-3.20441400	1.33455100	-0.57957700
C	-3.60506500	2.66131800	-0.58300200
C	-3.73480000	0.42726700	0.35226000
C	-4.52186700	3.13305200	0.36268100
H	-3.20875400	3.35827900	-1.31251100
C	-4.64013300	0.90362400	1.28776300
C	-5.02412200	2.24320900	1.30201500
H	-5.05638800	0.22391300	2.02281200
H	-5.73005100	2.58750700	2.05114900
C	1.45361800	1.69460700	-0.06767800
C	2.29196900	0.62981900	0.28393600
C	1.86150200	3.02014400	0.08475600
C	3.59816800	0.93157200	0.72394200
C	3.13970400	3.28349300	0.55093500
H	1.19763200	3.84013400	-0.15384200
C	4.01597600	2.25699000	0.85969400
H	3.46201500	4.31289300	0.66586500
H	5.02140700	2.48986000	1.18368800
C	1.91387400	-1.48603800	1.40424100
C	1.06297400	-2.76729900	1.44263300
H	1.53357300	-0.84120700	2.20039400
H	2.94129200	-1.75384000	1.65905300
C	2.48483500	-1.39895400	-0.98842800
C	1.85772900	-1.06371000	-2.35792700
H	2.36084200	-2.47710800	-0.85074100
H	3.55581800	-1.18599000	-1.01899300
C	-4.11504000	-1.70040100	-0.69864300
C	-3.33115600	-2.80138900	-1.44015400
H	-4.47613100	-1.01453300	-1.47020900
H	-5.00364900	-2.13890800	-0.22512000
C	-3.15097000	-1.61240600	1.54004500
C	-2.07340700	-0.93885600	2.41869600
H	-2.80632000	-2.63126300	1.32810100
H	-4.08617900	-1.71196700	2.10598300
O	-3.99905900	-3.71676100	-1.93537300
O	-2.07969100	-2.63976500	-1.52699100
O	0.18160300	-2.91844500	0.54522400
O	1.30200100	-3.54438500	2.37543800
O	0.59294100	-0.94906200	-2.39218900
O	2.62356100	-0.99085200	-3.32619300
O	-1.13721500	-0.36074400	1.79056600

O	-2.19438100	-1.04540500	3.64385700
C	-4.92913900	4.58300500	0.34845500
H	-4.06775100	5.23607600	0.51552000
H	-5.36406700	4.86106900	-0.61560800
H	-5.66718200	4.79653600	1.12366000
O	4.38396500	-0.12456900	1.00943200
C	5.76948900	0.08018000	1.24009500
C	6.59121700	0.50653500	-0.00435100
H	6.13545100	-0.89198600	1.57625000
H	5.92976000	0.78623100	2.06081200
O	7.76814700	0.82432500	0.26645400
O	6.02931400	0.46342900	-1.11428800

2•Ca^{2+}

Ca	0.01531700	-0.91177500	0.64675600
N	-2.51031000	-0.66080400	-0.18931900
N	2.67425400	-0.81124300	0.07641700
O	-1.08081900	1.45851000	0.78242600
O	1.42133700	0.90291600	1.66857100
C	0.56067800	1.73761700	2.43525800
C	-0.43071300	2.45972100	1.55371700
H	1.12519700	2.43368800	3.05815900
H	0.02287300	1.04648300	3.08407000
H	-1.14726600	2.98321800	2.19305300
H	0.05168600	3.18386300	0.89079700
C	2.46321400	1.43984400	0.95916000
C	2.86065800	2.76917100	1.06704200
C	3.14649700	0.53709300	0.13518700
C	3.97855900	3.18870900	0.35756400
H	2.33026000	3.47478400	1.69178300
C	4.30470300	0.97727100	-0.52667300
C	4.70696000	2.31287400	-0.42915000
H	5.59924200	2.66152200	-0.93180400
C	-2.27633600	1.75708400	0.20389000
C	-3.02845900	0.67917800	-0.28135900
C	-2.74087400	3.06912800	0.10367800
C	-4.30736600	0.94821900	-0.81236200
C	-3.99200000	3.30158100	-0.44597600
H	-2.14249100	3.90326400	0.44431600
C	-4.78510600	2.25848500	-0.89269800
H	-4.36021000	4.31944500	-0.51836000
H	-5.77179100	2.46519400	-1.28458500
C	-2.43568500	-1.33113400	-1.49672900
C	-1.53559600	-2.57856400	-1.53757500
H	-2.00098100	-0.61832400	-2.20223500
H	-3.41935900	-1.61359900	-1.87676900
C	-3.23021400	-1.43780700	0.83229600
C	-2.74985200	-1.16272100	2.27317800
H	-3.03827000	-2.49815400	0.64245300
H	-4.30952200	-1.27836900	0.77162300
C	3.41801900	-1.72058200	0.94527000
C	2.54632300	-2.77814400	1.65224600
H	3.89021700	-1.13231700	1.73767200
H	4.23133600	-2.22419800	0.40868800
C	2.45967800	-1.35542500	-1.26605900
C	1.48150100	-0.51180200	-2.10626900
H	1.99605700	-2.34222900	-1.13998300

H	3.39137200	-1.49343200	-1.81819600
O	3.14170300	-3.76011700	2.11428500
O	1.30913200	-2.53060900	1.74732200
O	-0.71170000	-2.74550500	-0.58956100
O	-1.67743100	-3.31267800	-2.52386000
O	-1.50149600	-0.99195200	2.43177900
O	-3.60279200	-1.18798500	3.16886600
O	0.53334500	0.03567700	-1.46684400
O	1.67248800	-0.46638600	-3.32766400
O	-5.00615400	-0.12194000	-1.23740500
C	-6.35049100	0.04368100	-1.66084700
C	-7.36932400	0.34849400	-0.53280100
H	-6.61346200	-0.91657900	-2.10895300
H	-6.42033800	0.79865900	-2.44998000
O	-8.50398200	0.64647800	-0.96149200
O	-6.98223600	0.24029900	0.64512700
O	4.96612100	0.04454000	-1.23947700
C	6.24193000	0.36122200	-1.77666100
C	7.37128700	0.54290800	-0.72887600
H	6.18444500	1.23721300	-2.43025900
H	6.49231700	-0.49475700	-2.40648700
O	8.43493200	0.97489400	-1.22132500
O	7.12626000	0.22452500	0.44873300
H	4.29712900	4.22252300	0.43764600

{**1**•Ca^{2+}, $(H_2O)_3$}

N	2.05296800	-0.89759400	0.94002500
N	-5.05124700	-0.16245700	0.33076100
O	-0.57334300	-1.35079500	1.94072400
O	-3.12590900	-2.03588800	-0.37678400
C	-2.08352100	-2.58497900	0.42185500
C	-1.89624000	-1.87381700	1.77200800
H	-1.14161800	-2.60361200	-0.13189800
H	-2.39023800	-3.61941400	0.58364700
H	-2.66018400	-1.10282600	1.89752400
H	-2.00206600	-2.58681800	2.58966900
C	-2.95756800	-0.73303300	-0.79262200
C	-1.84238200	-0.37457700	-1.53514100
C	-3.94128700	0.21277100	-0.44015000
C	-1.61298800	0.94618900	-1.91736800
H	-1.11325700	-1.14062600	-1.78169600
C	-3.70274900	1.53198600	-0.83976100
C	-2.56300000	1.89079500	-1.55010900
H	-4.41150100	2.30270700	-0.56456900
H	-2.41140500	2.93576700	-1.80871000
C	-0.27408700	-0.10356600	1.47673100
C	1.02419200	0.10893400	0.98442400
C	-1.18740400	0.94563400	1.56541000
C	1.37269100	1.41435800	0.59915500
C	-0.81049200	2.20955600	1.15959000
H	-2.18665900	0.79589200	1.96013700
C	0.46454800	2.46168800	0.67137400
H	-1.53109100	3.01797100	1.21748100
H	0.73041700	3.45955800	0.35011100
C	2.65984100	-1.11442100	2.25583500
C	4.09778800	-1.66303800	2.21321800
H	2.04973300	-1.77097800	2.88784500

H	2.71748600	-0.14751000	2.76446600
C	1.68044200	-2.15429600	0.28709900
C	1.38813000	-1.99177200	-1.21242300
H	0.85051200	-2.65751000	0.78218900
H	2.54458100	-2.82350300	0.36055700
C	-5.91907700	-1.20458800	-0.20164600
C	-6.86132200	-0.84506800	-1.38274200
H	-6.54638000	-1.57315500	0.61804900
H	-5.30867300	-2.05272700	-0.51217900
C	-5.75348500	0.89952700	1.02024900
C	-4.90303500	1.66575200	2.06543800
H	-6.57361100	0.42593600	1.57350600
H	-6.21978800	1.61325200	0.33190100
O	-6.79238400	0.29624500	-1.88533100
O	-7.61839400	-1.78381100	-1.72615900
O	4.74089300	-1.48918600	1.12091300
O	4.53460600	-2.18497500	3.23529200
O	0.58567200	-2.77156100	-1.73540600
O	2.05122600	-1.08628900	-1.80644800
O	-4.11606800	0.99127000	2.77100500
O	-5.11733600	2.89547800	2.14510100
C	-0.35221900	1.31948800	-2.65223100
H	0.52941000	1.00406700	-2.08792600
H	-0.29678100	0.83586300	-3.63329400
H	-0.28701300	2.39925300	-2.80790400
O	2.65794500	1.58810600	0.15798600
C	3.15216100	2.91725800	0.03649200
C	4.66574500	2.90430000	-0.20585500
H	2.94547100	3.47666800	0.95231900
H	2.66606600	3.42908900	-0.80042800
O	5.22158400	4.00048900	-0.20267200
O	5.19443100	1.76811900	-0.39973500
O	3.44828900	0.75401400	-2.97373900
H	3.26167600	1.66874800	-3.18665200
H	2.62282200	0.24982200	-3.02151200
Ca	4.02678700	-0.24922600	-0.79086800
O	6.65564300	-0.42935400	-0.46858200
H	6.41436200	-0.86050100	0.36326100
H	6.59022000	0.52459500	-0.31850600
O	4.69800600	-2.59480000	-1.34315100
H	4.08265400	-3.25953500	-1.65577400
H	4.90010100	-2.78258400	-0.41687700

{**2**•Ca^{2+}, $(H_2O)_3$}

N	2.76497300	-0.91238800	0.70791600
N	-4.57884500	-1.40839100	0.39884400
O	0.15300000	-1.56061800	1.51266900
O	-2.40404400	-2.53570100	-0.82531200
C	-1.14600500	-2.73808400	-0.19399700
C	-1.10516700	-2.19173800	1.24046600
H	-0.34597300	-2.28771600	-0.78705200
H	-0.99260400	-3.81850500	-0.20860000
H	-1.94421600	-1.51824600	1.43025600
H	-1.15852800	-2.99989900	1.97023100
C	-2.69476200	-1.21601100	-1.10649800
C	-1.88530000	-0.52488800	-2.00196700
C	-3.79812900	-0.62267000	-0.46029600

C	-2.12571800	0.81526000	-2.25111600
H	-1.05069800	-1.03985500	-2.46712500
C	-3.99923300	0.75392400	-0.72169200
C	-3.17166400	1.45096800	-1.59849700
H	-3.40806400	2.48884700	-1.79987000
C	0.36543000	-0.29200300	1.06477800
C	1.68709600	0.04104300	0.72312700
C	-0.64931100	0.66387900	1.00976800
C	1.97367000	1.37621300	0.40246400
C	-0.33443300	1.95939900	0.64377100
H	-1.66731600	0.41478600	1.28890900
C	0.96935700	2.33556300	0.34558900
H	-1.12489700	2.70050600	0.59311900
H	1.18674900	3.36007200	0.07446900
C	3.18465600	-1.32522000	2.04878500
C	4.63545900	-1.83207200	2.13631100
H	2.51915100	-2.08526700	2.47234700
H	3.12558400	-0.45004000	2.70313300
C	2.50721800	-2.04997200	-0.18285000
C	2.33086400	-1.60376000	-1.64678500
H	1.65349700	-2.64694000	0.14001700
H	3.38624600	-2.70210700	-0.14561700
C	-5.22564700	-2.57276000	-0.18758500
C	-6.50937600	-2.35908200	-1.03553600
H	-5.48215600	-3.26431800	0.62379700
H	-4.51037100	-3.11020600	-0.81042800
C	-5.34124700	-0.81896600	1.48503600
C	-4.57185500	0.06471100	2.48573900
H	-5.72150800	-1.66420000	2.07539700
H	-6.21454600	-0.26980500	1.13125800
O	-6.87838100	-1.19556600	-1.29497500
O	-7.05377200	-3.42998500	-1.39910200
O	5.41991000	-1.49221000	1.18460100
O	4.94350800	-2.48794300	3.12811600
O	1.49050000	-2.17738200	-2.34370700
O	3.11941900	-0.67939100	-2.02446300
O	-3.32019700	-0.00236300	2.51108100
O	-5.29683000	0.75248800	3.23989200
O	3.28623800	1.66923100	0.15279900
C	3.69299700	3.03376900	0.18379000
C	5.22396500	3.12801500	0.20089000
H	3.29596300	3.52092400	1.07786300
H	3.31722800	3.56345000	-0.69723100
O	5.69309300	4.25335500	0.35542500
O	5.85604100	2.04015300	0.03982700
O	5.13699700	0.68734200	-2.97550000
H	5.11724100	1.61083500	-3.23033800
H	4.26766000	0.30125000	-3.16374200
Ca	4.92004800	-0.02331500	-0.62430600
O	7.43435200	-0.09107800	0.04106700
H	7.14140300	-0.63510400	0.78512100
H	7.30803400	0.83485600	0.29144400
O	5.76469400	-2.23335200	-1.39074400
H	5.24031200	-2.85786900	-1.89388300
H	5.83956300	-2.56076700	-0.48460400
O	-5.02199700	1.39176100	-0.09405600
C	-4.76536700	2.67072400	0.47103500
C	-5.21618800	3.89319700	-0.35887700

H	-3.69486200	2.77679700	0.68290400
H	-5.28219700	2.67332800	1.43286700
O	-5.16075700	4.96852400	0.27995200
O	-5.56107100	3.71933700	-1.54483100
H	-1.49805200	1.36748900	-2.94286700

1•Mg^{2+}

N	1.77508900	-1.08827500	0.11070200
N	-3.19350800	-0.41436700	0.52516700
O	-0.39458900	0.39469900	-0.69808400
O	-3.15885900	0.92958100	-2.07813000
C	-2.00582200	0.17125600	-2.46074400
C	-0.68422000	0.76983900	-2.05375700
H	-2.05092900	0.12751300	-3.54962400
H	-2.07859000	-0.84852900	-2.07964600
H	0.10480800	0.38442100	-2.70292500
H	-0.71021000	1.85779800	-2.14000500
C	-3.12359700	1.61496000	-0.88328000
C	-3.06977300	2.99589700	-0.98361300
C	-3.15983900	0.97613400	0.37900600
C	-3.00654700	3.82865300	0.13319000
H	-3.04916400	3.41601600	-1.98528800
C	-3.07999100	1.82362200	1.49334400
C	-2.99833000	3.20736200	1.37357500
H	-3.05856300	1.40084300	2.48900200
H	-2.93326700	3.80475700	2.27876400
C	0.66321100	1.07227400	-0.13481800
C	1.78898700	0.34129300	0.23918700
C	0.58904900	2.45058100	0.03793000
C	2.92163200	1.04809700	0.68628700
C	1.69720100	3.11902800	0.53071700
H	-0.33048500	2.97281800	-0.20217800
C	2.86698800	2.43353700	0.83571000
H	1.65795200	4.19392800	0.67178200
H	3.73316200	2.98352100	1.18008400
C	2.18543100	-1.82029700	1.31707200
C	1.58003300	-3.23340400	1.39970800
H	1.80915400	-1.27367600	2.18362900
H	3.26972600	-1.89488200	1.40958500
C	2.45867300	-1.54605500	-1.11010000
C	1.51057500	-1.82748100	-2.28909200
H	2.96411600	-2.49318300	-0.89467200
H	3.23295900	-0.83775100	-1.41567000
C	-4.05731000	-1.22371300	-0.31548900
C	-3.43888000	-2.58206100	-0.70087500
H	-4.28598000	-0.69644600	-1.23978700
H	-5.01911000	-1.42122900	0.17704600
C	-3.09243800	-0.93999400	1.87305000
C	-1.70708100	-0.77053300	2.52099800
H	-3.26189600	-2.01768800	1.81306900
H	-3.86565000	-0.53703900	2.54052600
O	-4.21013400	-3.42821000	-1.15650200
O	-2.18419300	-2.72748800	-0.54833500
O	0.53570100	-3.45795300	0.70824500
O	2.13793500	-4.03164400	2.15746400
O	0.29400900	-2.06792200	-2.00590900
O	2.00868100	-1.83807100	-3.41852400

O	-0.71397300	-1.02981200	1.77772100
O	-1.65599800	-0.44857500	3.71185300
C	-2.89814900	5.32275400	-0.02176000
H	-1.92490600	5.60824500	-0.43403000
H	-3.66188600	5.71155100	-0.70103500
H	-3.01206100	5.83055500	0.93835000
O	4.01084200	0.30300600	0.96478100
C	5.28758400	0.92390100	0.95652000
C	5.75301500	1.44219000	-0.42912400
H	5.97505300	0.13928600	1.27825700
H	5.34635700	1.72464400	1.69980200
O	6.81647000	2.09416800	-0.37933700
O	5.06664900	1.14364400	-1.42479900
Mg	-0.43536600	-1.82395100	-0.08429400

2•Mg^{2+}

N	-2.32808600	0.63768900	0.76032500
N	2.99704700	0.93438300	0.16310500
O	-0.51297400	0.55859400	-1.28128900
O	1.72542700	1.86715900	-2.00645400
C	0.52984000	2.19818800	-2.68768600
C	-0.55285500	1.13735900	-2.58576900
H	0.71527900	2.41220700	-3.74684600
H	0.19364900	3.11095500	-2.19926300
H	-1.52734800	1.60593100	-2.75428100
H	-0.41281200	0.35244000	-3.32734100
C	2.27677200	0.62711800	-2.13289000
C	2.20786900	-0.11132900	-3.31045800
C	2.94195300	0.14671500	-0.98970200
C	2.73970800	-1.39186000	-3.34266300
H	1.72667900	0.30404200	-4.18821400
C	3.53619100	-1.13228000	-1.07946700
C	3.38481700	-1.91216300	-2.22890600
C	-1.32478100	-0.54201800	-1.12197500
C	-2.29411600	-0.49210600	-0.12283200
C	-1.15961200	-1.66112800	-1.93159700
C	-3.20941100	-1.55984800	-0.02945600
C	-2.03337600	-2.72502400	-1.78078800
H	-0.35267500	-1.69532600	-2.65462500
C	-3.06607700	-2.67695800	-0.85340300
H	-1.92070300	-3.60547700	-2.40428000
H	-3.76544100	-3.50019900	-0.79116000
C	-2.36907800	0.29437900	2.18756100
C	-1.74365300	1.37237100	3.08926000
H	-1.77305100	-0.60895200	2.32981500
H	-3.38147900	0.08653700	2.53755200
C	-3.32152700	1.64591700	0.36765500
C	-2.75642900	2.78699400	-0.50018300
H	-3.71182700	2.12115000	1.27348000
H	-4.17590600	1.19066300	-0.13965500
C	3.45547500	2.29882400	0.07163700
C	2.41883300	3.40888200	0.32750000
H	3.88533500	2.48300900	-0.91333800
H	4.27394000	2.46505900	0.78676000
C	2.89328100	0.36689200	1.49150800
C	1.61391000	-0.44343200	1.75977100
H	2.84963400	1.21133100	2.18809900

H	3.75009600	-0.25095300	1.76431900
O	2.82461400	4.56762600	0.18086500
O	1.25268200	3.08158900	0.70468400
O	-0.94396800	2.19347800	2.54039000
O	-2.04260300	1.33416000	4.28651700
O	-1.51749000	3.03984500	-0.37307400
O	-3.55706600	3.40109100	-1.21145000
O	0.54155000	-0.03046500	1.22117900
O	1.69983800	-1.41444500	2.52065100
O	-4.18422000	-1.42110000	0.88924400
C	-5.20268800	-2.40905800	0.96126900
C	-6.18489700	-2.43985500	-0.23957000
H	-5.76634600	-2.15416400	1.86087300
H	-4.76613900	-3.40011400	1.11948100
O	-6.93785900	-3.43639600	-0.23340900
O	-6.15038300	-1.49097700	-1.04372400
Mg	-0.23671800	1.75436900	0.64427000
H	2.66228200	-1.98635000	-4.24666300
O	4.26393600	-1.52449100	-0.00877100
C	4.58874500	-2.89341600	0.14198200
C	5.31016700	-3.16769700	1.48119600
H	5.25212900	-3.22635600	-0.66602000
H	3.67741300	-3.50142900	0.09524100
O	5.54665800	-4.38292400	1.65843300
O	5.59596700	-2.20784400	2.21930100
H	3.81795400	-2.90293700	-2.27591600

{**1**•Mg^{2+}, H_2O}

N	2.44884200	-1.17445300	0.64474000
N	-4.64736700	-0.27483400	0.29607400
O	-0.19541700	-1.78185400	1.49692500
O	-2.72526300	-1.82631400	-0.98070300
C	-1.65191000	-2.51479000	-0.35258800
C	-1.52073800	-2.20398600	1.14868600
H	-0.71153900	-2.29926000	-0.86626100
H	-1.87596400	-3.57103100	-0.50712000
H	-2.27258800	-1.47085200	1.45114500
H	-1.67511900	-3.10585100	1.74053000
C	-2.60334800	-0.45374400	-1.02580300
C	-1.53167400	0.12432800	-1.69135000
C	-3.58249000	0.33001200	-0.38609200
C	-1.34884200	1.50450300	-1.71496000
H	-0.80141700	-0.52550900	-2.16617600
C	-3.38878700	1.71578400	-0.42369300
C	-2.29523700	2.28702100	-1.06194100
H	-4.09842500	2.36181100	0.07724800
H	-2.18026600	3.36802900	-1.04567200
C	0.13981100	-0.46998500	1.34675200
C	1.44834800	-0.18480700	0.93448600
C	-0.74452300	0.56183700	1.65941100
C	1.83977900	1.15970500	0.85281200
C	-0.32034700	1.87312600	1.56347000
H	-1.75189300	0.35314300	2.00609000
C	0.97148600	2.19479600	1.16217700
H	-1.01593300	2.66858300	1.80692900
H	1.27915900	3.22987700	1.09606600
C	3.05778500	-1.77010400	1.83509500

C	4.55139600	-2.09115200	1.63822000
H	2.52965800	-2.67063400	2.16588000
H	2.99840400	-1.04487800	2.65102600
C	2.08045300	-2.15924900	-0.37291500
C	1.96153000	-1.50399600	-1.75673600
H	1.17894200	-2.71267600	-0.11602600
H	2.89920900	-2.88538700	-0.43875400
C	-5.52145900	-1.15009000	-0.47310300
C	-6.50591700	-0.49494500	-1.47962100
H	-6.11424100	-1.74262400	0.23290200
H	-4.91321300	-1.86689300	-1.02503200
C	-5.33538500	0.53546300	1.27961200
C	-4.44393800	1.02437900	2.44926600
H	-6.10982100	-0.10147800	1.72393200
H	-5.85654000	1.39044500	0.83405500
O	-6.44881500	0.74018400	-1.65770500
O	-7.27705000	-1.31125000	-2.03717600
O	5.13838500	-1.48876600	0.67526100
O	5.07816400	-2.86372200	2.43346800
O	1.11415800	-1.91746400	-2.54662400
O	2.81607400	-0.58107800	-1.98681700
O	-3.60275700	0.21444100	2.90753900
O	-4.67857000	2.17906100	2.86670800
C	-0.12884000	2.10561200	-2.36172100
H	0.72674800	2.06552500	-1.67934900
H	0.15480500	1.56627800	-3.26935000
H	-0.28900100	3.15424900	-2.62489700
O	3.13051400	1.36186000	0.44207200
C	3.63201300	2.68515600	0.29587400
C	5.04190800	2.61042600	-0.30251700
H	3.66471100	3.18597300	1.26601800
H	2.99349500	3.26094100	-0.38050400
O	5.65775600	3.66624300	-0.38883300
O	5.43208500	1.45650300	-0.67393800
Mg	4.26094900	-0.20524400	-0.58857300
O	5.52047200	-0.77381200	-2.25143400
H	6.10072600	-0.02879600	-2.42922900
H	4.91405900	-0.85510300	-2.99314400

{**2**•Mg^{2+}, H_2O}

N	3.22006600	-0.95953600	0.67598600
N	-4.05449200	-1.46861300	0.32251800
O	0.56331500	-1.56272500	1.36145900
O	-1.91127200	-2.36613000	-1.15870700
C	-0.64549600	-2.51432200	-0.53169700
C	-0.68065100	-2.15339700	0.95896600
H	0.10345900	-1.89952400	-1.04137000
H	-0.36674800	-3.55844200	-0.68294000
H	-1.52554900	-1.50134900	1.19361900
H	-0.76696500	-3.04593400	1.57868500
C	-2.31393700	-1.05172600	-1.30595500
C	-1.61673300	-0.24993300	-2.20275800
C	-3.39306500	-0.57830700	-0.53359100
C	-1.93922700	1.08960700	-2.32311700
H	-0.80664000	-0.68816600	-2.77697700
C	-3.68807400	0.80111100	-0.67220900
C	-2.96261200	1.60985400	-1.54314600

C	0.82355200	-0.29324200	0.94614500
C	2.15922300	0.00810300	0.65043500
C	-0.16150700	0.69212600	0.85550800
C	2.49160400	1.32972900	0.32641100
C	0.20263900	1.98043100	0.50593800
H	-1.19365700	0.46598700	1.10032700
C	1.52578900	2.32257700	0.24464500
H	-0.56514900	2.74346600	0.43757000
H	1.78381800	3.34241300	-0.00902800
C	3.63596100	-1.36956700	2.01805700
C	5.15307200	-1.61174500	2.12245800
H	3.09815200	-2.25770900	2.36419400
H	3.39848900	-0.56199600	2.71572300
C	3.01506200	-2.08308600	-0.24399000
C	3.09509600	-1.61505600	-1.70586000
H	2.08397500	-2.61670900	-0.05461400
H	3.83723700	-2.79138000	-0.08854700
C	-4.65423600	-2.64341900	-0.29507700
C	-5.96741300	-2.45667500	-1.10128800
H	-4.85092300	-3.37841600	0.49359900
H	-3.92924700	-3.11466300	-0.95879800
C	-4.79484100	-0.99972500	1.48143000
C	-4.04386900	-0.09726000	2.47919900
H	-5.06587300	-1.90130400	2.04758400
H	-5.73133300	-0.51017900	1.20921600
O	-6.36975300	-1.29899700	-1.33521400
O	-6.49234000	-3.53558000	-1.46852300
O	5.87438600	-1.10884900	1.19460200
O	5.56354700	-2.23141100	3.09973200
O	2.34373500	-2.11301600	-2.53998100
O	4.00014100	-0.73876900	-1.93485600
O	-2.79375400	-0.03630400	2.41318000
O	-4.77616200	0.47192200	3.32020400
O	3.82184400	1.55028100	0.10007800
C	4.28478800	2.84881000	-0.24964600
C	5.79098100	2.76660000	-0.52849700
H	4.09419000	3.55165200	0.56438600
H	3.77699200	3.20185200	-1.15209600
O	6.37346100	3.82776400	-0.71902500
O	6.29093900	1.59554200	-0.55646900
Mg	5.17816000	-0.09861200	-0.38907600
O	6.69908400	-0.87162100	-1.71576400
H	7.29907000	-0.14948000	-1.91977100
H	6.20125400	-1.07123800	-2.51437900
H	-1.39820400	1.72808100	-3.01343700
O	-4.69720200	1.32534900	0.06964800
C	-4.48377700	2.58368700	0.69745300
C	-5.08665500	3.81380000	-0.01479500
H	-3.40962800	2.75296000	0.83609700
H	-4.92204300	2.48808700	1.69300200
O	-5.04666300	4.85368600	0.68117900
O	-5.52441200	3.68059400	-1.17494300
H	-3.26679800	2.64461200	-1.64560400

{**2**•□Ca^{2+}, $(H_2O)_6$}

N	3.69419200	-1.10737500	0.53198300
O	1.31898100	-2.53327500	1.12013500

C	0.15573900	-3.27915100	0.75298100
H	-0.72115800	-2.97839000	1.33198100
H	0.41074100	-4.29595700	1.05146400
C	1.27409900	-1.17494200	1.20018300
C	2.44908600	-0.47681900	0.88473500
C	0.13646000	-0.49870700	1.63758300
C	2.43042700	0.92286400	1.00649800
C	0.14839900	0.87862600	1.72664300
H	-0.74560600	-1.04978100	1.93087000
C	1.28757700	1.60465100	1.40600800
H	-0.74866500	1.39799000	2.04540800
H	1.27237400	2.68403200	1.47091600
C	4.38834200	-1.63452500	1.71039300
C	5.91275000	-1.77416300	1.54183500
H	3.97775000	-2.59907900	2.03242000
H	4.23495200	-0.93102300	2.53416700
C	3.61752400	-2.08846400	-0.55390200
C	3.20557300	-1.45960900	-1.89211900
H	2.96480400	-2.92891500	-0.32062100
H	4.62427800	-2.49573400	-0.69252200
O	6.45156000	-1.06029700	0.62734000
O	6.50028900	-2.52151000	2.31903000
O	2.56312700	-2.15717900	-2.68544900
O	3.59542400	-0.26699100	-2.08325900
O	3.60246800	1.56357500	0.71747400
C	3.74292100	2.92557500	1.10867400
C	5.20422500	3.36901800	0.97327500
H	3.43253400	3.04928600	2.14916000
H	3.11757400	3.56747100	0.48025300
O	5.46360300	4.49702400	1.38628000
O	5.99696600	2.53577500	0.43988200
O	4.58088200	2.11084400	-2.47922500
H	4.20843500	2.98619000	-2.36958000
H	3.87643500	1.50606400	-2.75193000
Ca	5.37018100	0.57721600	-0.73003600
O	7.95037700	0.96158700	-0.38103100
H	7.89060400	0.21247200	0.22765200
H	7.66737000	1.74563300	0.11084500
O	6.57304300	-1.14777800	-2.07608100
H	6.14779800	-1.77717700	-2.66014500
H	6.86353600	-1.61774700	-1.28344700
C	-0.15648800	-3.28008000	-0.75092300
O	-1.31939700	-2.53423700	-1.11922900
H	0.72055900	-2.98036600	-1.33026900
H	-0.41186100	-4.29720200	-1.04802000
C	-1.27410400	-1.17589000	-1.19943100
C	-2.44885600	-0.47732000	-0.88420400
C	-0.13617900	-0.50012100	-1.63677700
N	-3.69414700	-1.10757200	-0.53165400
C	-2.42969400	0.92236000	-1.00595400
C	-0.14754900	0.87722500	-1.72575400
H	0.74564600	-1.05159100	-1.93008500
C	-4.38787500	-1.63537600	-1.71003900
C	-3.61770000	-2.08815600	0.55470700
C	-1.28646600	1.60368800	-1.40517500
O	-3.60157200	1.56348400	-0.71718400
H	0.74981500	1.39622600	-2.04425500
C	-5.91240800	-1.77455900	-1.54217900

H	-3.97735300	-2.60025000	-2.03117900
H	-4.23389300	-0.93250400	-2.53423600
C	-3.20607900	-1.45861200	1.89271800
H	-2.96486800	-2.92866700	0.32188400
H	-4.62446700	-2.49542200	0.69330900
H	-1.27079600	2.68306800	-1.46997600
C	-3.74151600	2.92545800	-1.10862000
Ca	-5.37069800	0.57725100	0.72913000
O	-6.45151800	-1.06028600	-0.62818800
O	-6.49973300	-2.52190100	-2.31954800
O	-2.56324700	-2.15550000	2.68630800
O	-3.59658800	-0.26612300	2.08337800
C	-5.20282700	3.36914400	-0.97420000
H	-3.43051000	3.04900200	-2.14894600
H	-3.11641700	3.56730800	-0.47991200
O	-5.99614800	2.53571500	-0.44197800
O	-4.58416600	2.11095900	2.47974900
O	-6.57464200	-1.14691600	2.07514500
O	-5.46166600	4.49741800	-1.38681500
H	-4.21182900	2.98638500	2.37028500
H	-3.87967900	1.50638500	2.75286800
H	-6.14979100	-1.77630000	2.65951500
H	-6.86481000	-1.61698200	1.28244600
H	-7.66668600	1.74661400	-0.11296700
O	-7.95028900	0.96285300	0.37904500
H	-7.89111500	0.21361500	-0.22951500

{**2**•□Mg^{2+}, $(H_2O)_2$}

N	3.67640500	-1.07970900	0.48383900
O	1.31596200	-2.47531200	1.12257200
O	-1.31868300	-2.48215900	-1.11925000
C	-0.15204000	-3.21697900	-0.75017300
C	0.14954200	-3.21257400	0.75789300
H	0.72271900	-2.89666400	-1.32175500
H	-0.38735100	-4.23535900	-1.05703700
H	-0.72528200	-2.88951600	1.32782400
H	0.38528900	-4.22910500	1.07051900
C	1.27332900	-1.11709500	1.19213900
C	2.44480700	-0.43434800	0.84718400
C	0.15230400	-0.41922900	1.63899100
C	2.44671500	0.96486700	0.93409600
C	0.19105200	0.96041300	1.71285500
H	-0.73875600	-0.94763700	1.95072700
C	1.33015400	1.67184300	1.35575800
H	-0.68741800	1.49733100	2.05303900
H	1.33680400	2.75160200	1.41951200
C	4.38697400	-1.65598500	1.63060100
C	5.91163000	-1.45107500	1.56332600
H	4.16580500	-2.72019300	1.75882300
H	4.04755200	-1.15061200	2.53831900
C	3.59831700	-1.98585200	-0.66497100
C	3.36195400	-1.21440500	-1.96981000
H	2.85421500	-2.77035500	-0.53522900
H	4.57460500	-2.47517400	-0.76180900
O	6.32852800	-0.54064500	0.76980000
O	6.60899000	-2.13941500	2.30277200
O	2.66095000	-1.72537800	-2.84324800

O	3.96073800	-0.08883200	-2.04925300
O	3.62347200	1.56454100	0.58347100
C	3.71319400	2.98502400	0.54410200
C	5.08452300	3.37573000	-0.02048500
H	3.59414500	3.40050700	1.54707400
H	2.93376400	3.39231300	-0.10641600
O	5.35883200	4.56965300	-0.01491100
O	5.80217800	2.42030200	-0.46089800
Mg	5.18829700	0.48674200	-0.51524600
O	6.65781400	0.37625700	-2.09077000
H	7.05581600	1.24801100	-2.16392800
H	6.15005000	0.22304400	-2.89270300
C	-1.27630700	-1.12420100	-1.19444300
C	-2.44715800	-0.43972100	-0.85068600
C	-0.15553900	-0.42844400	-1.64537300
N	-3.67858300	-1.08277100	-0.48239700
C	-2.44852500	0.95919900	-0.94301500
C	-0.19395900	0.95084100	-1.72495800
H	0.73529300	-0.95821500	-1.95564900
C	-4.39318800	-1.66078300	-1.62575600
C	-3.59898000	-1.98632200	0.66846800
C	-1.33239500	1.66403900	-1.36922700
O	-3.62434500	1.56099500	-0.59239200
H	0.68422000	1.48613400	-2.06844800
C	-5.91789400	-1.45825000	-1.55144700
H	-4.17086400	-2.72469200	-1.75458600
H	-4.05871300	-1.15497200	-2.53507700
C	-3.35939400	-1.21202200	1.97100800
H	-2.85593700	-2.77183000	0.53903300
H	-4.57551400	-2.47450800	0.76834700
H	-1.33877100	2.74352300	-1.43744700
C	-3.71164300	2.98173900	-0.55474600
O	-6.33243000	-0.54704800	-0.75732700
O	-6.61781400	-2.14878900	-2.28626900
O	-2.65898400	-1.72258200	2.84516300
O	-3.95481700	-0.08454100	2.04785000
C	-5.07973800	3.37599400	0.01503800
H	-3.59594200	3.39554000	-1.55879200
H	-2.92887400	3.38862800	0.09197300
Mg	-5.18518600	0.48695700	0.51523400
O	-5.35159300	4.57035700	0.00986300
O	-5.79761800	2.42222000	0.45912600
O	-6.65070200	0.41244400	2.10048000
H	-7.00737800	1.30327500	2.16122500
H	-6.14181400	0.25093500	2.90005000

8. Supporting Information References

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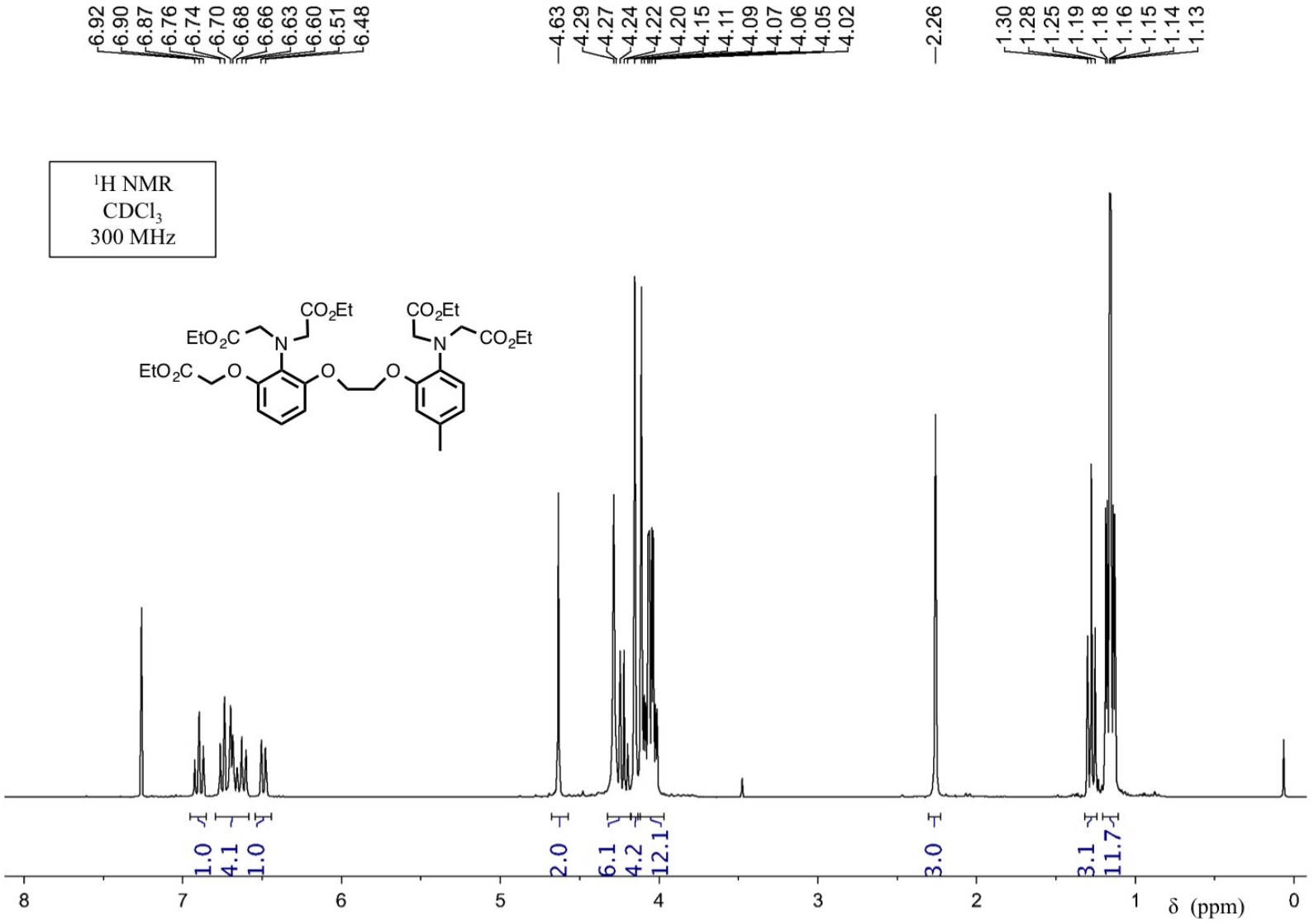

Figure S8: ^{1}H NMR spectrum of **1c** in $CDCl_3$ at 298K on a 300 MHz spectrometer.

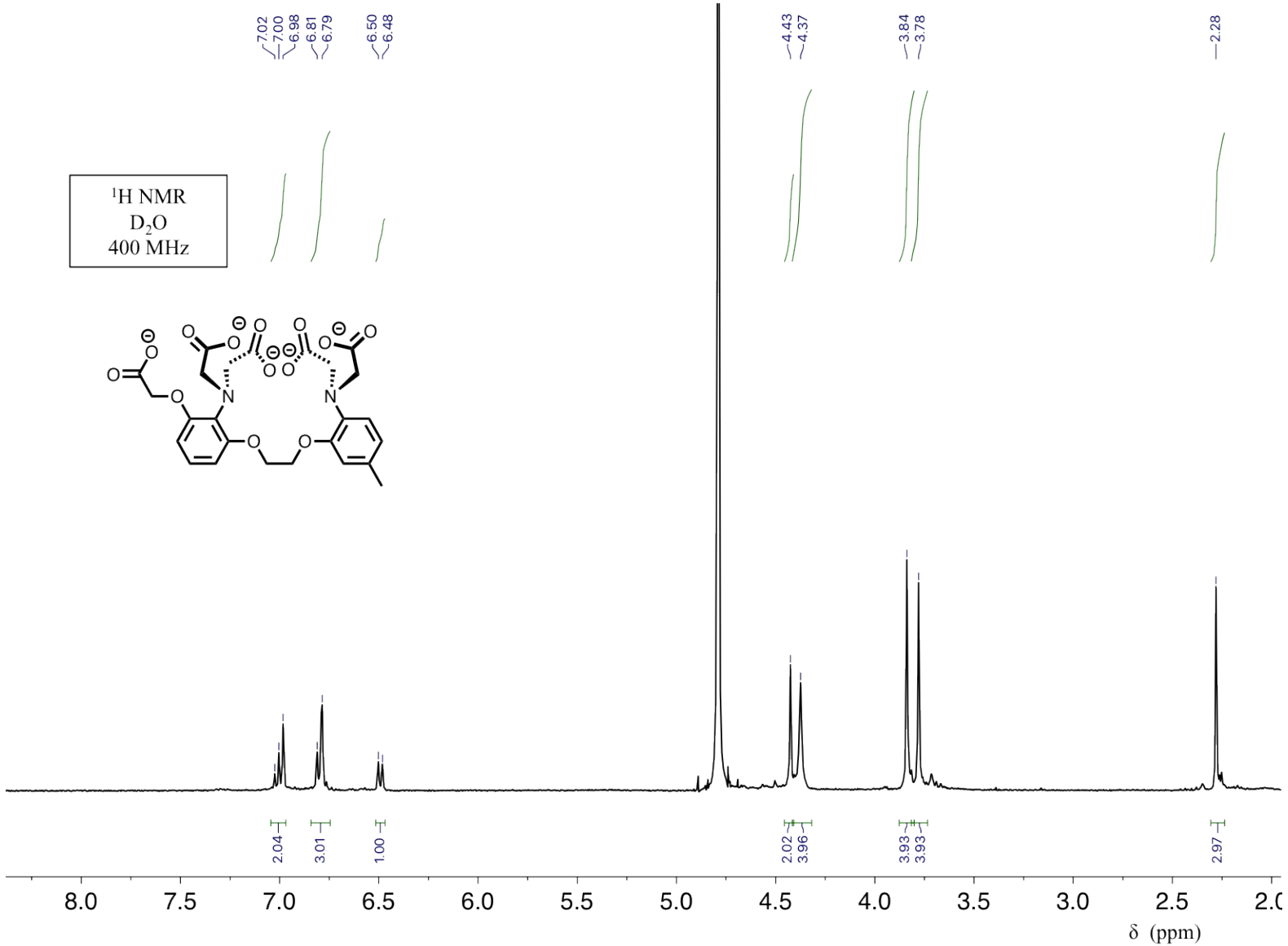

Figure S9: ^{1}H NMR spectrum of **1** in D_2O at 298K on a 400 MHz spectrometer.

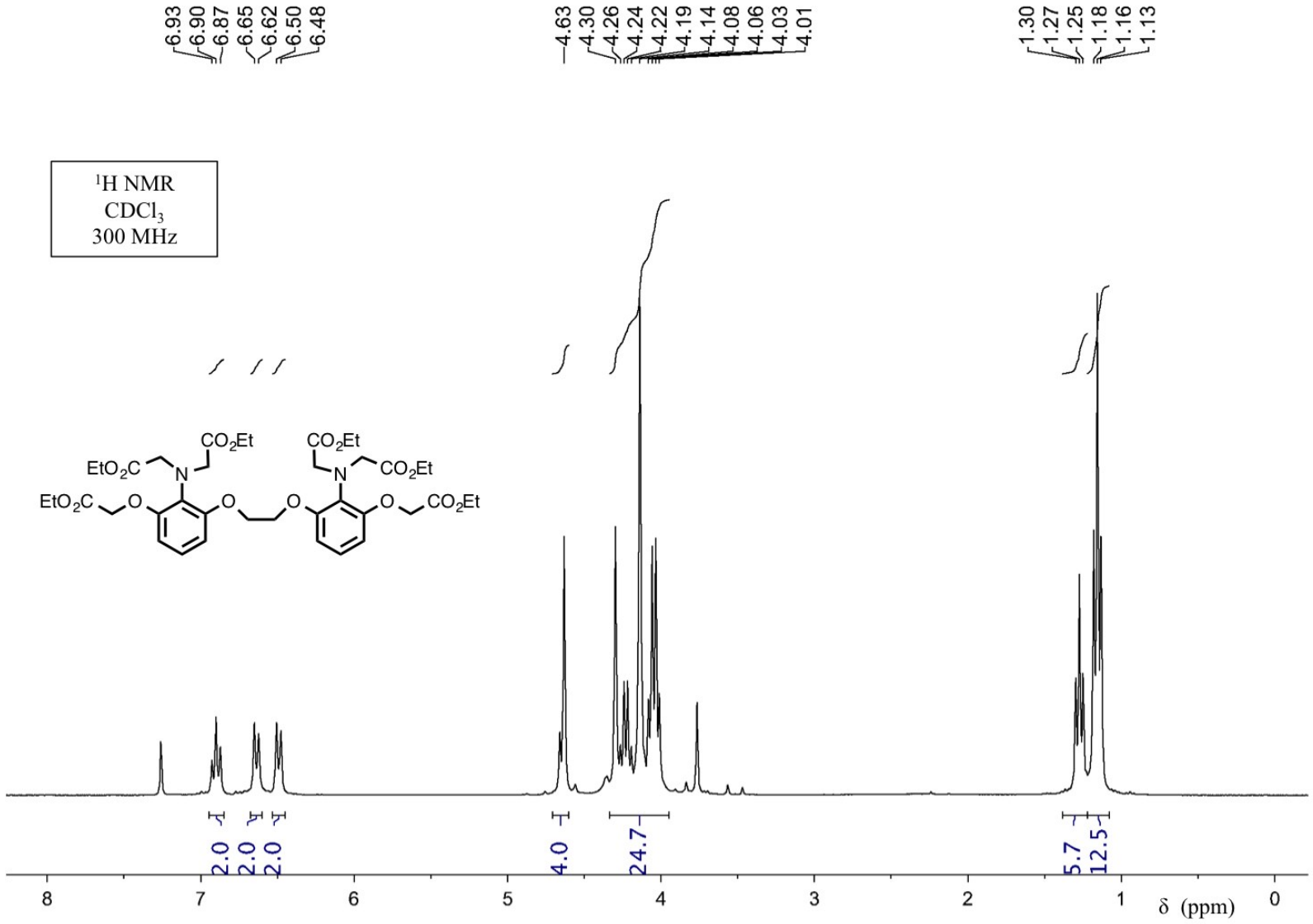

Figure S10: ^{1}H NMR spectrum of **2c** in $CDCl_3$ at 298K on a 300 MHz spectrometer.

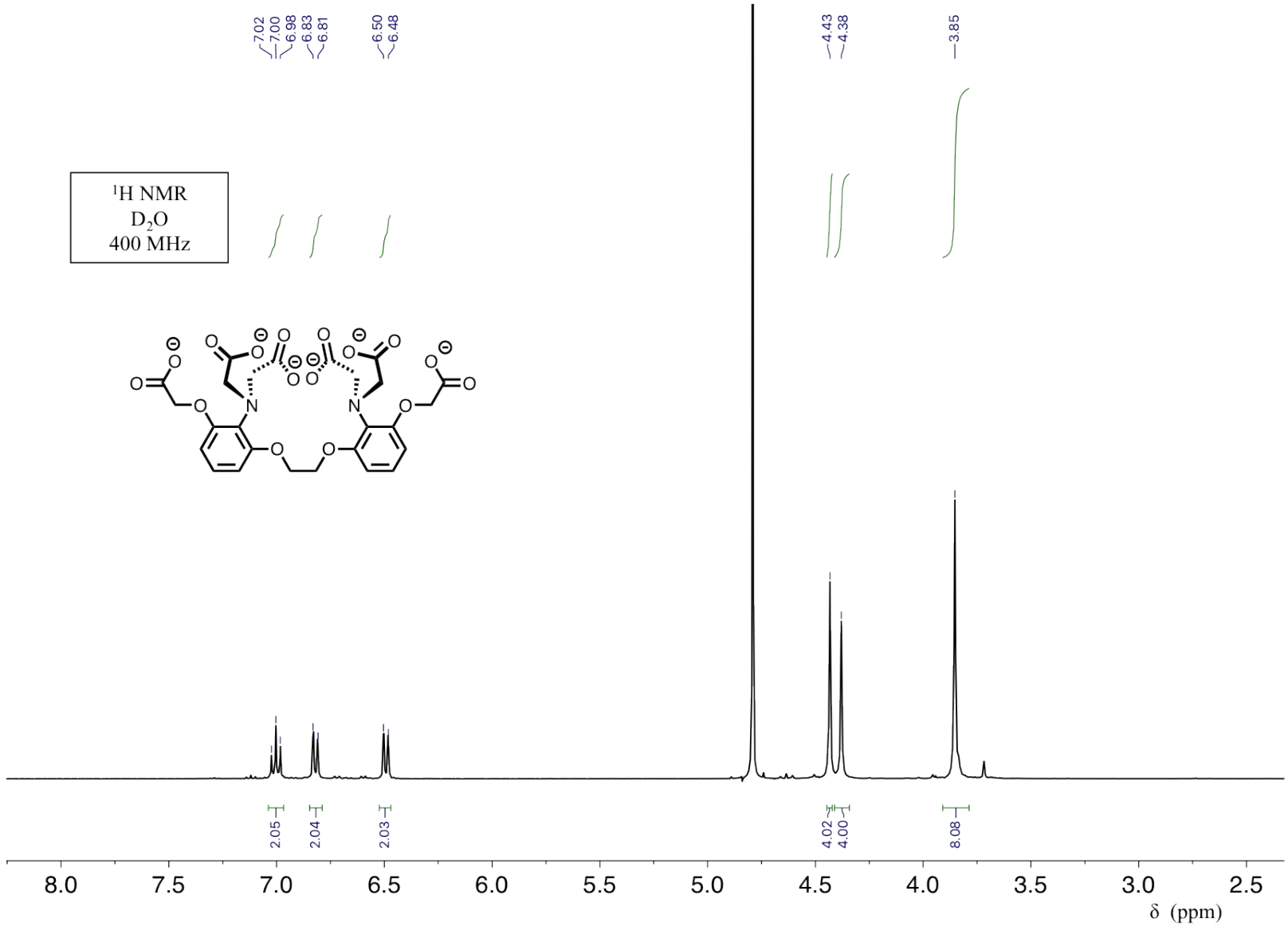

Figure S11: ^{1}H NMR spectrum of **2** in D_2O at 298K on a 400 MHz spectrometer.

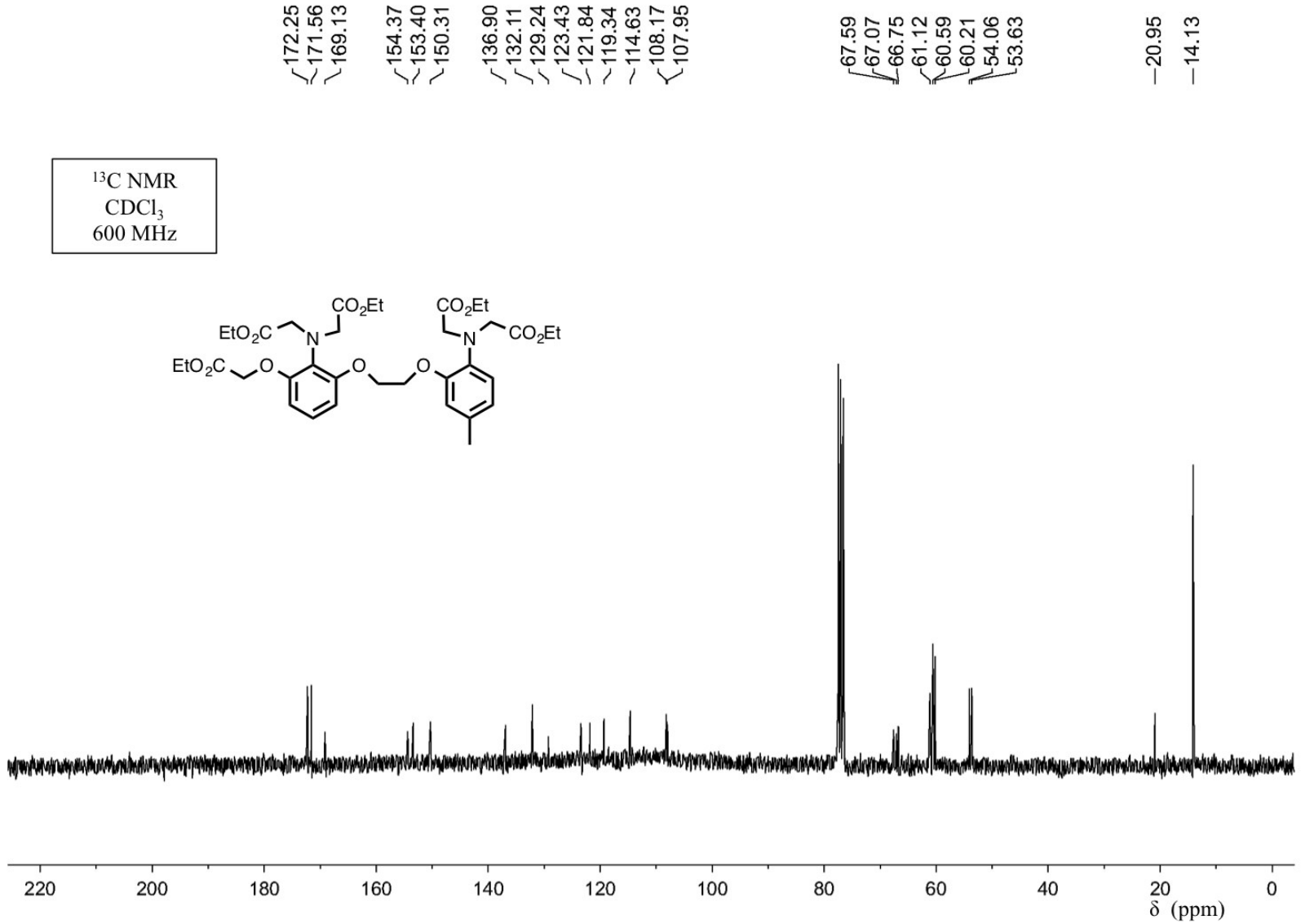

Figure S12: ^{13}C NMR spectrum of **1c** in $CDCl_3$ at 298K on a 300 MHz spectrometer.

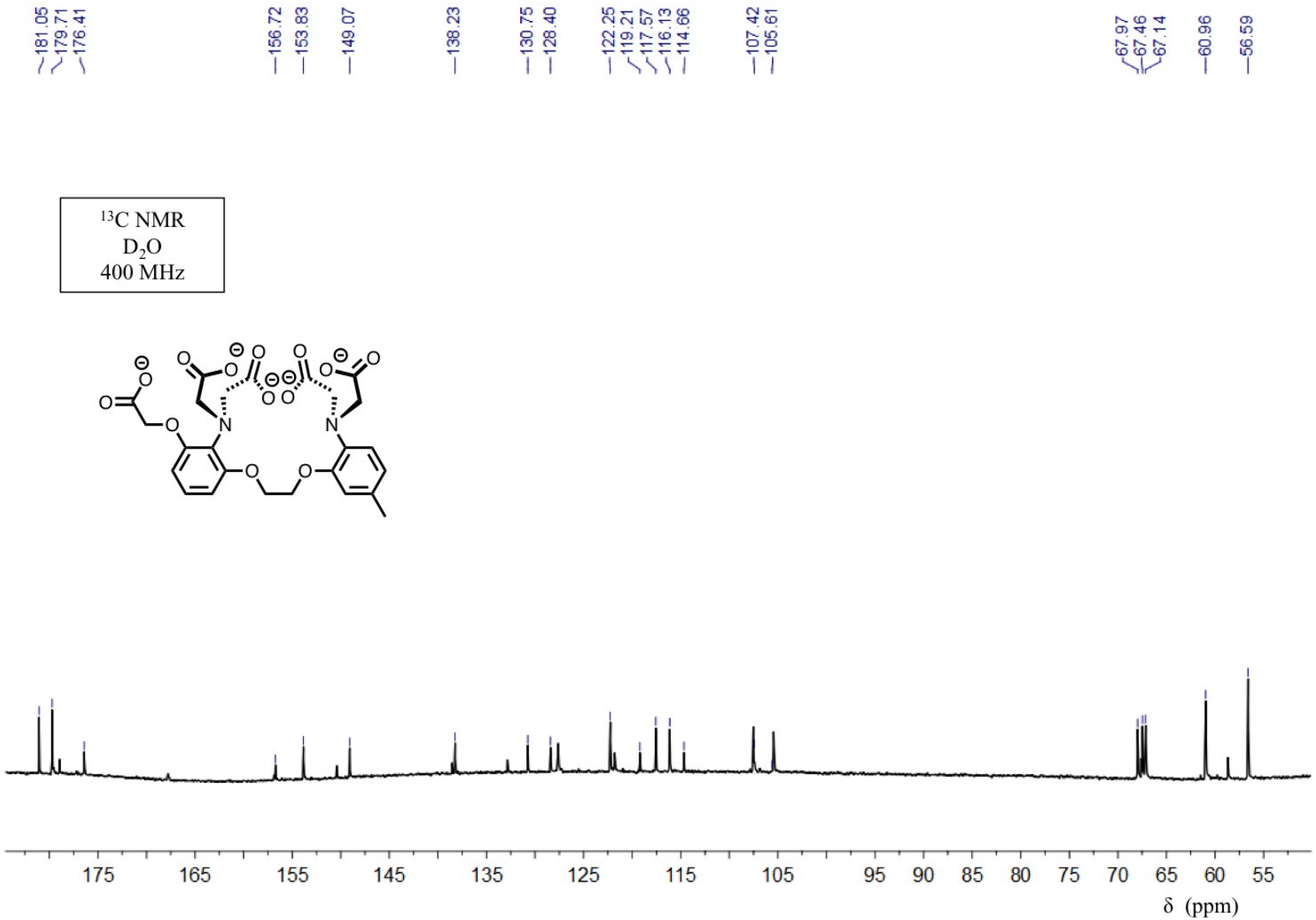

Figure S13: ^{13}C NMR spectrum of **1** in D_2O at 298K on a 400 MHz spectrometer.

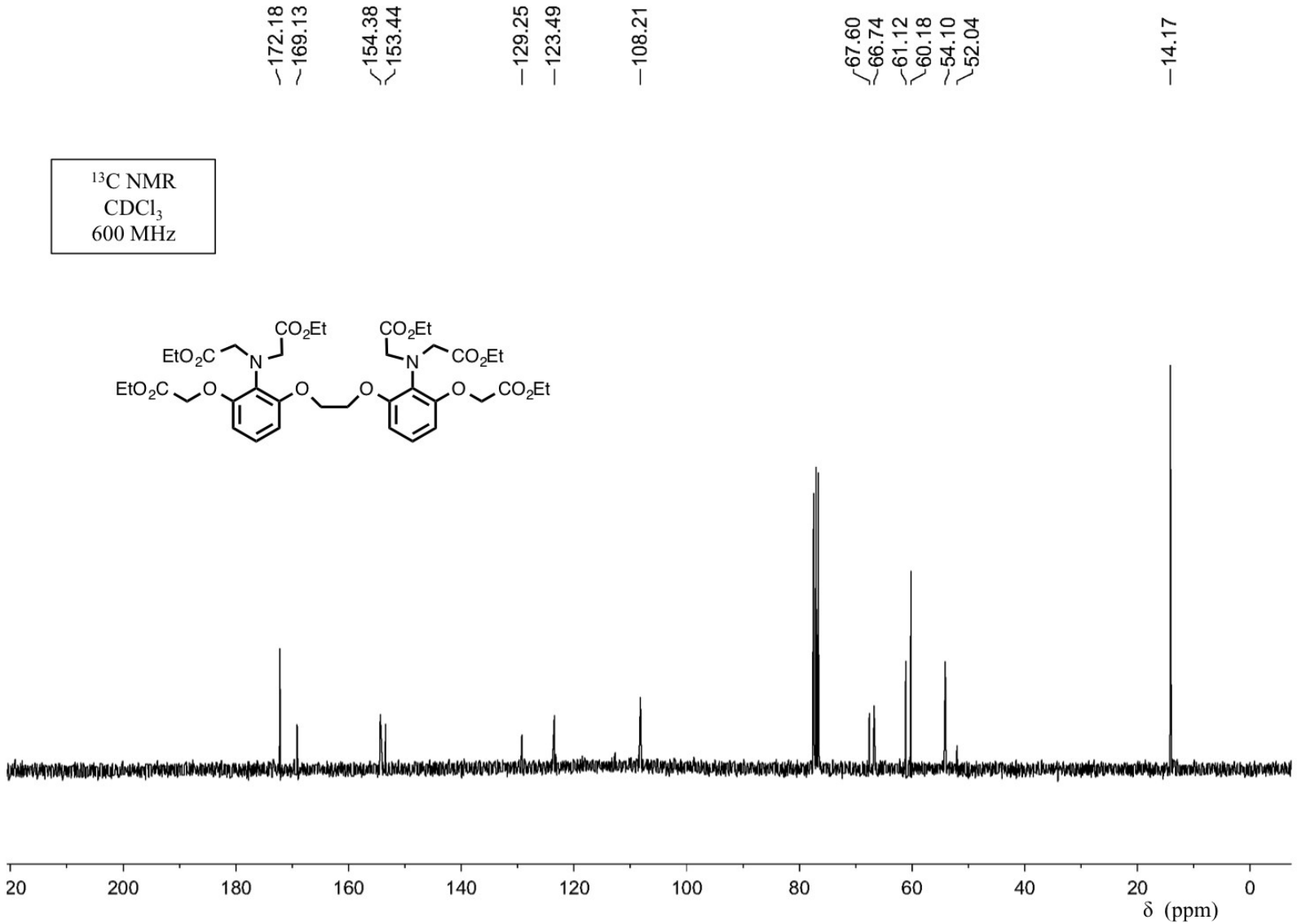

Figure S14: ^{13}C NMR spectrum of **2c** in $CDCl_3$ at 298K on a 300 MHz spectrometer.

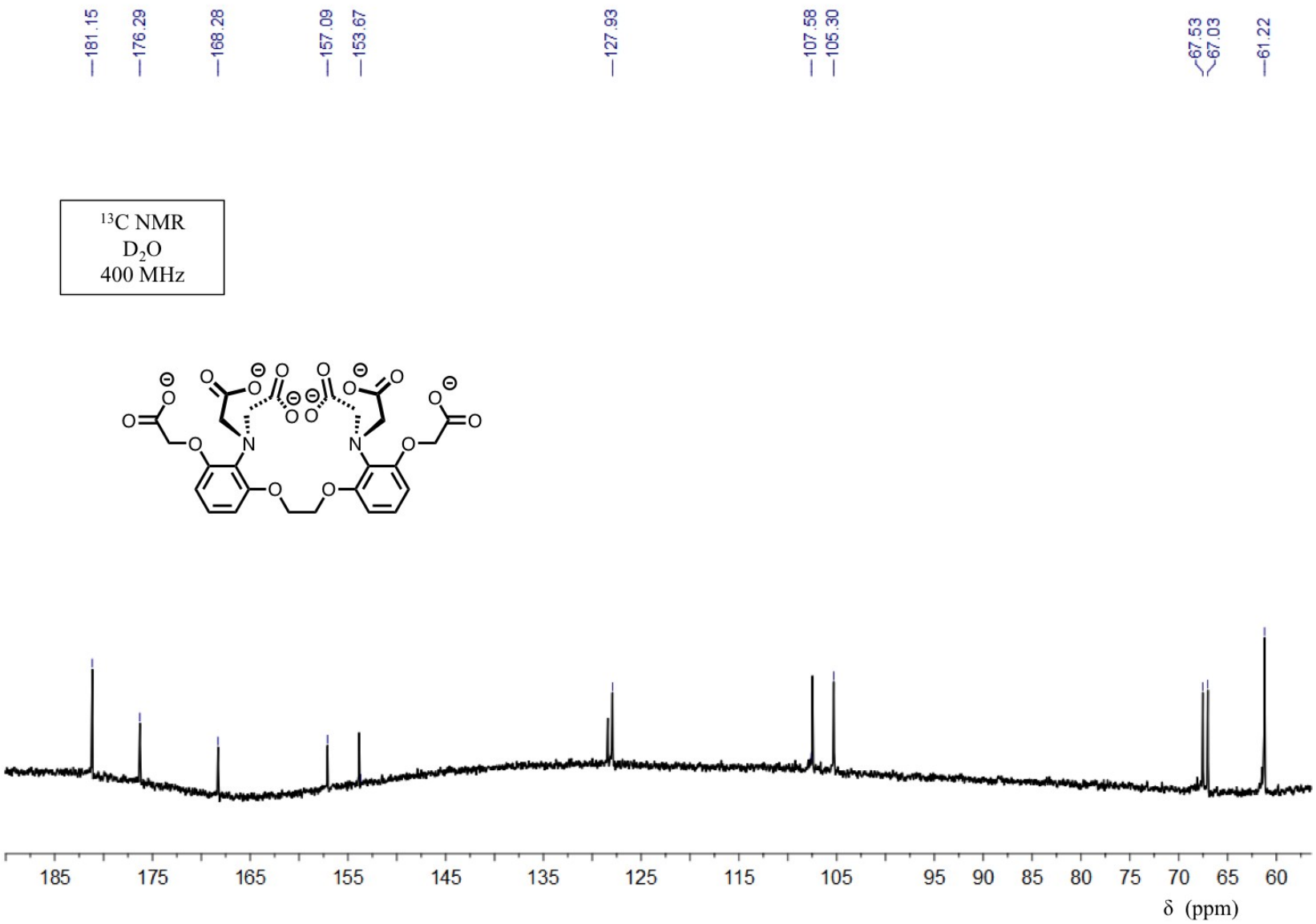

Figure S15: ^{13}C NMR spectrum of **2** in D_2O at 298K on a 400 MHz spectrometer.