Supporting Information

Naphthalene Diimides as Red Fluorescent pH Sensors for Functional Cells Imaging.

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Supplemental Experimental Procedures

Materials and General Procedures.

Reagents, solvents and chemicals were purchased from Alfa Aesar, or Sigma-Aldrich and were used as supplied without further purification. For cell cultures experiments naphthalene diimide derivatives and Bafilomycin A1 (Sigma Aldrich Co., St. Louis, MO) were dissolved in DMSO at appropriate concentrations and stored as stock solutions at -20°C. TLC analysis was carried out on silica gel (Merck 60F-254) with visualization at 254 and 366 nm. HPLC analysis and purifications were performed using two different HPLC: Waters system combining a Delta 600 PUMP, a 2489 UV/VIS detector and Fraction Collector III (for preparative and analytical) and an Agilent system SERIES 1260 (for analytical). The analytical column was XSelect CSH Phenyl-Hexyl (150 x 4.6 mm) (Waters). The preparative column was XSelect CSH Prep Phenyl-Hexyl 5µm (150 x 30 mm) (Waters). Flows were 1 ml/min for analytical and 27 ml/min for preparative. For the analytical analysis was used the following method: (Aqueous solvent: 0.1% trifluoroacetic acid in water; Organic solvent: Acetonitrile; Gradient: 95% aqueous, gradually to 40% aqueous over 8 minutes and at the end an isocratic flow over 4 minutes). Preparative HPLC were performed using an upgrade of the analytical method. ^{1}H-, ^{13}C-NMR spectra have been recorded on a Bruker ADVANCE 300 MHz spectrometer. The potentiometric titrations have been made with a Radiometer TitraLab 90 titration system. UV/Vis spectra have been recorded on a Varian Cary 100 SCAN spectrophotometer with quartz cuvettes of the appropriate path length (0.1-1 cm) at 25.0 ± 0.1 °C. Emission spectra have been recorded on a Perkin Elmer LS 50B instrument.

Synthesis of intermediates and final ligands:

The NDI intermediate **6** has been synthesized according to the published procedure.[S1] The following nucleophilic aromatic substitution (S_NAr) was performed according to an efficient protocol described below, in order to synthesized the ligands **7** in good yield.

Nucleophilic aromatic substitution reaction.

N,N'-Bis-(hydroxyethyl)-2-bromo-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide (7): The NDI **6** (0.02 mmol) was dissolved into 10 ml of acetonitrile in a round bottom flask together with the ethanolamine 0.054 mmol. The mixture was stirred at 70°C for 4h, under argon. The resulting red solution was concentrated under vacuum and a red solid was obtained. The

crude product was purified by column chromatography ($CHCl_3$:CH_3OH 9:1). Red solid. Yield 53%. M.P. dec. >200°C. ^{1}H-NMR (300 MHz, DMSO-d_6): δ (ppm) =10.13 (s, 1NH); 8.40 (s, 1H); 8.08 (s, 1H); 5.13 (bs, 1H); 4.85 (bs, 2H); 4.11 (m, 4H); 3.75 (m, 2H); 3.65 (m, 6H). ^{13}C-NMR (75 MHz, DMSO-d_6): δ (ppm) =164.9; 161.3; 161.1; 160.7; 151.3; 136.2; 127.8; 126.9; 122.8; 122.6; 120.8; 120.4; 118.2; 98.5; 59.5; 57.6; 57.5; 44.8; 42.6; 41.8. Anal. Calcd. for $C_{20}H_{18}BrN_3O_7$: C, 48.80; H, 3.69; N, 8.54. Found: C, 40.77; H, 3.72; N, 8.63.

Absorption and fluorescence spectra. UV-visible absorption spectra were recorded on a standard commercial spectrophotometer. Fluorescence spectra were measured using 1 nm steps. Slits were kept narrow to 2 nm in emission. Right angle detection was used. All the measurements were carried out at 295 K in quartz cuvettes with path length of 1 cm. All fluorescence spectra have been obtained for air-equilibrated solutions absorbing 0.07 at the excitation wavelength (540 nm) to avoid inner filter effects and re-absorption of emission. The compound **8** dissolved in air-equilibrated water with known fluorescence quantum yield (Φ_F) of 0.29 was used as standard for the determination of the fluorescence quantum yield of the NDI samples. Using the same solvents for all compounds and iso-absorbing solutions at the excitation wavelength no corrections had to be made for absorbance neither solvent refraction index and we calculated the fluorescence quantum yields, Φ_F, using the formula below, with A being the integrated area of the corrected fluorescence spectra:

$$\Phi_F = \Phi_F^{ref} \times A/A^{ref}$$

Potentiometric titrations.

All measurements were performed at 25.0 ± 0.1 °C in aqueous solution (0.1 M $NaNO_3$). Titrations were performed under nitrogen atmosphere, in the presence of a SCE reference electrode. In a typical experiment, 10 mL of a 5.0×10^{-4} M solution of **1**·3HCl or **2**·4HCl was treated with an excess of 1.0 M HNO_3 standard solution. Titrations were run by addition of 10 μL portions of standard 0.1 M NaOH, collecting 80-100 points for each titration. Prior to each potentiometric titration, the standard electrochemical potential (E°) of the glass electrode was determined in 0.1 M $NaNO_3$, by a titration experiment according to the Gran method. [S2] Titration data (emf *vs.* mL of NaOH) were processed with the Hyperquad® package to determine the equilibrium constants.[S3]

Spectrophotometric and spectrofluorimetric titrations.

Spectrofluorimetric studies were performed with on a commercial spectrophotometer. All titrations were performed at 25.0 ± 0.1 °C. Protonation constants of ligand L were determined in a water mixture, made 0.1 M in $NaNO_3$. In a typical experiment, 15 mL of a 5×10^{-4} M ligand solution were treated with an excess of a 1.0 M HNO_3 standard solution. Titrations were run by addition of 10 μL aliquots of carbonate-free standard 0.1 M NaOH. For the spectrofluorimetric titrations, samples were excited at a wavelength corresponding to an isosbestic point in the UV-vis spectra. Titration data were processed with non-linear least-squares procedure (Hyperquad® package),[S3] in order to determine the equilibrium constants.

Cell cultures and imaging studies

Human prostate normal (PNT-1A, #95012614-1V) and cancer cells (PC-3, CRL-1435™) were purchased from Sigma-Aldrich and the American Type Culture Collection (Rockville, MD), respectively. The cell lines were routinely tested for the absence of *Mycoplasma* and authenticated by the AmpFISTR Identifiler PCR amplification kit (PN4322288; Applied Biosystems, Carlsbad, CA, USA). Cells were cultured in Roswell Park Memorial Institute 1640 medium (Lonza Milano S.r.l., Treviglio, Italy) supplemented with 10% fetal bovine serum and maintained in a logarithmic growth phase at 37°C, 5% CO_2 in humidified atmosphere.

NDI cellular uptake was assessed on PC-3 cells seeded on glass cover slips in 6-well plates (1×10^5cell/well), incubated at 37°C for 24 h, subsequently exposed to 60 μmol L^{-1} of the compound and incubated for 90 min at 37 °C or 4 °C. At the end of treatments, cells were washed in cold PBS and fixed in 4% formaldehyde/PBS for 15 min. The intracellular distribution of NDI was monitored by fluorescence microscopy (Nikon Eclipse E600 microscope, Nikon Instruments S.p.A., Firenze, Italy) using a tetramethylrhodamine isothiocyanate filter. Nuclei were counterstained by Fluoroshield mounting medium containing 0.0002% 4’6’-diamidino-2-phenylindole (DAPI) (ab104139, Abcam, Cambridge, UK), according to the manufacturer’s instruction.

To assess the possible localization of NDI within lysosomes, fixed cells were permeabilized in a 1:1 methanol/acetone solution for 15 min at room temperature, probed with a mouse monoclonal primary antibody (ab25631, Abcam) raised against LAMP2A, a lysosome specific marker, and subsequently with a rabbit anti-mouse AlexaFluor® 488 secondary antibody (Life Technologies, Monza, Italy). The NDI/lysosomes co-localization was verified by fluorescence microscopy (Nikon) using tetramethylrhodamine isothiocyanate and fluorescein isothiocyanate filters.

The capability of NDI derivative to act as a pH sensor and hence to detect any change in the intracellular pH was investigated by fluorescence microscopy (according to the procedure described above) in PC-3 and PTNA-1 cells grown on glass cover slips, exposed to NDI (see above) and subsequently treated for 3 h with 50 nM Bafilomycin A1 (the optimization of such experimental conditions was carried out by preliminary experiments, data not shown).

All images were acquired at the indicated magnifications using ACT-1 software (Nikon) and processed by Adobe Photoshop Image Reader 7.0.

Absorption spectra

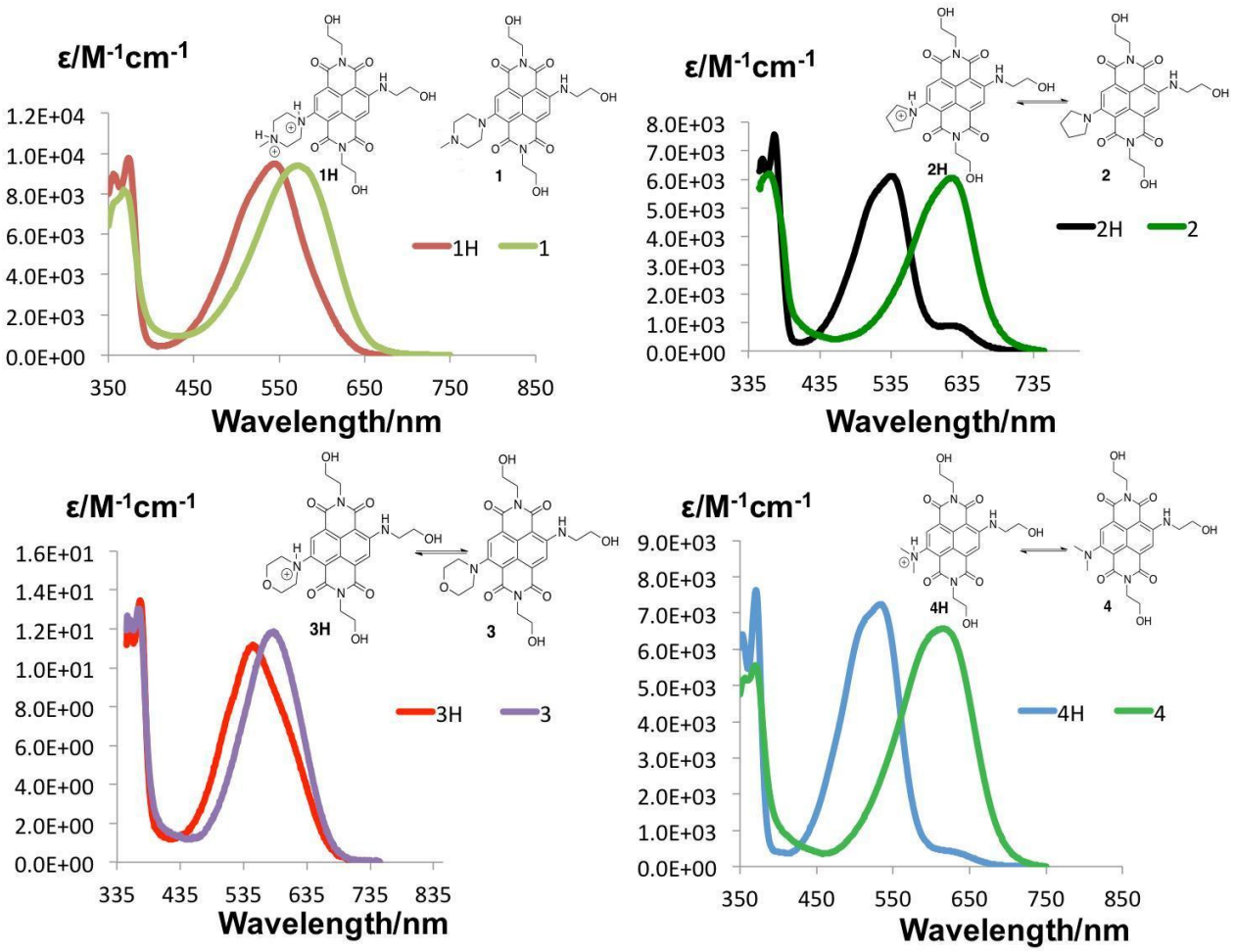


Figure 1S: Absorption spectra of the NDI sensors **1H**, **1; 2H, 2; 3H, 3;** and **4H, 4** measured in pure water.

Titration

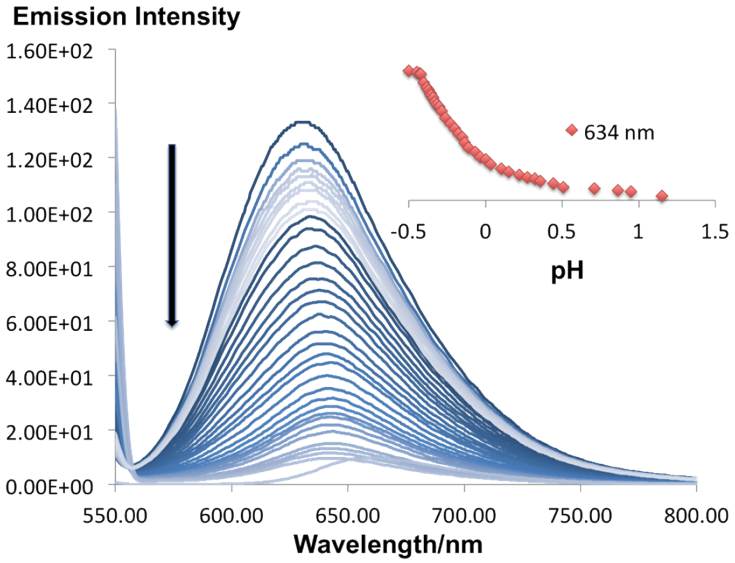


Figure 2S. Fluorimetric titration of NDI **1** in water.

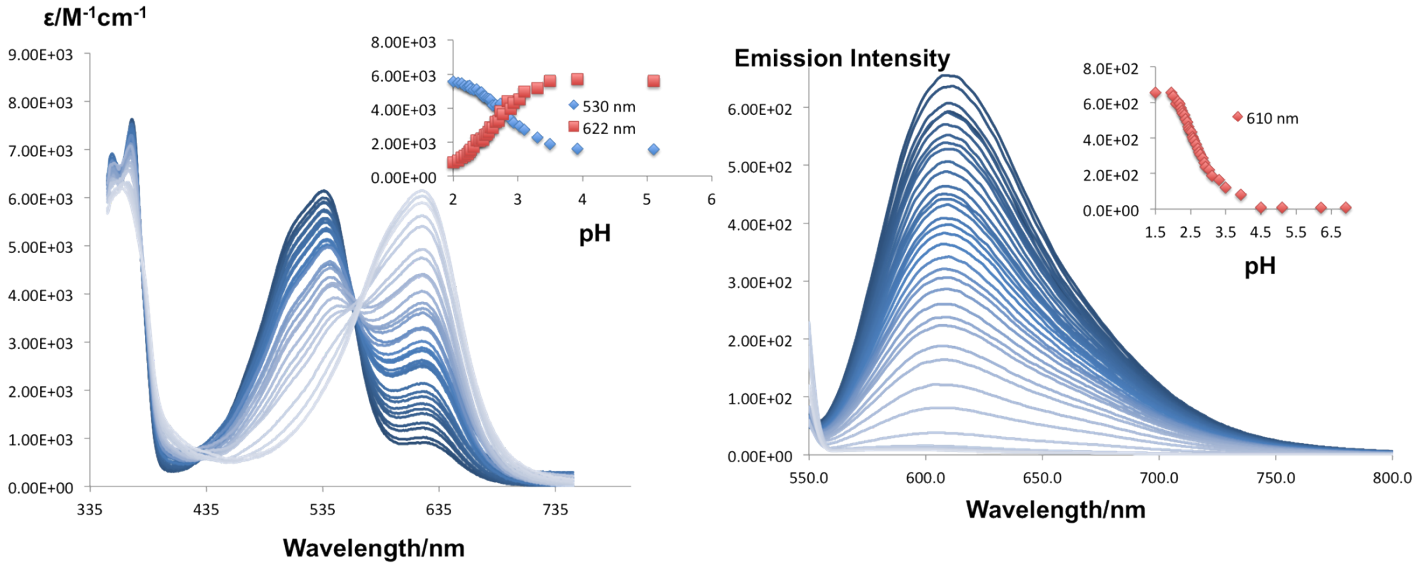


Figure 3S. (a) Spectrophotometric titration of NDI **2** in water. (b) Fluorimetric titration of NDI **2** in water.

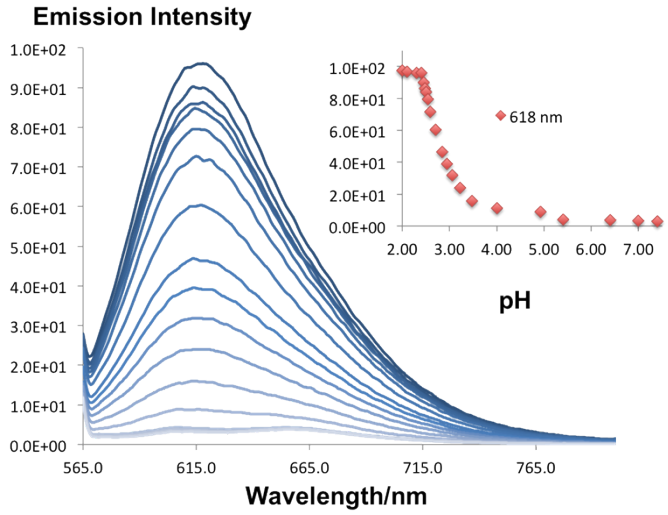


Figure 4S. Fluorimetric titration of NDI **3** in water.

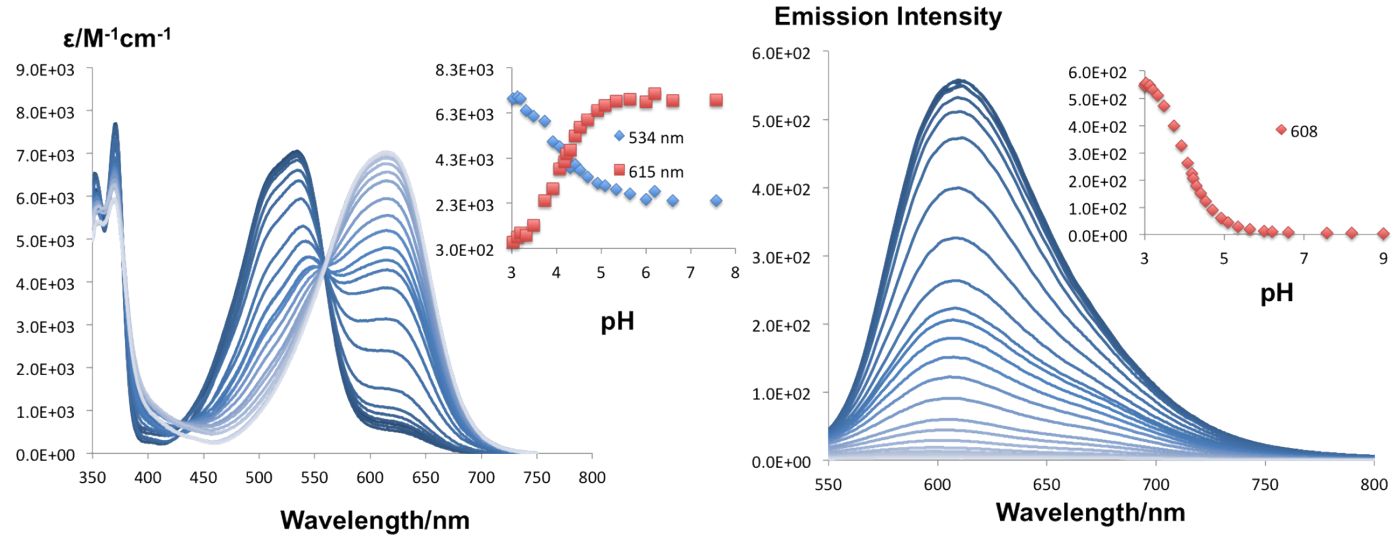


Figure 5S. (a) Spectrophotometric titration of NDI **2** in water. (b) Fluorimetric titration of NDI **4** in water.

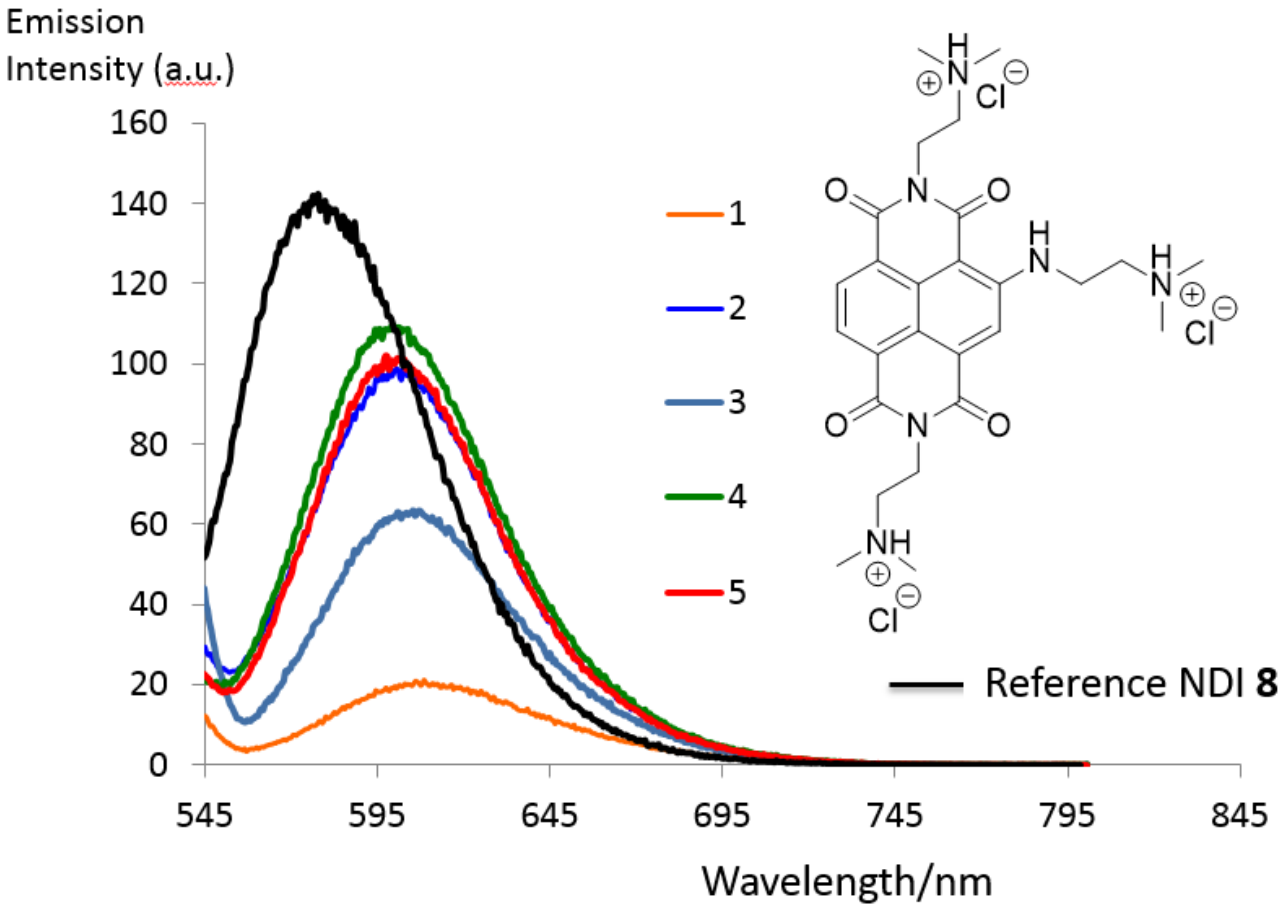


Figure 6S: Fluorescence spectra of NDI **1-5** in aqueous phosphate buffer of pH 2.0. All samples were excited at 540 nm where their absorbance was 0.07. The NDI **8** (structure shown in figure) dissolved in aqueous buffer of pH 2.0 with known fluorescence quantum yield (Φ_F) of 0.29 was used as standard for the determination of the fluorescence quantum yields of the new NDIs.

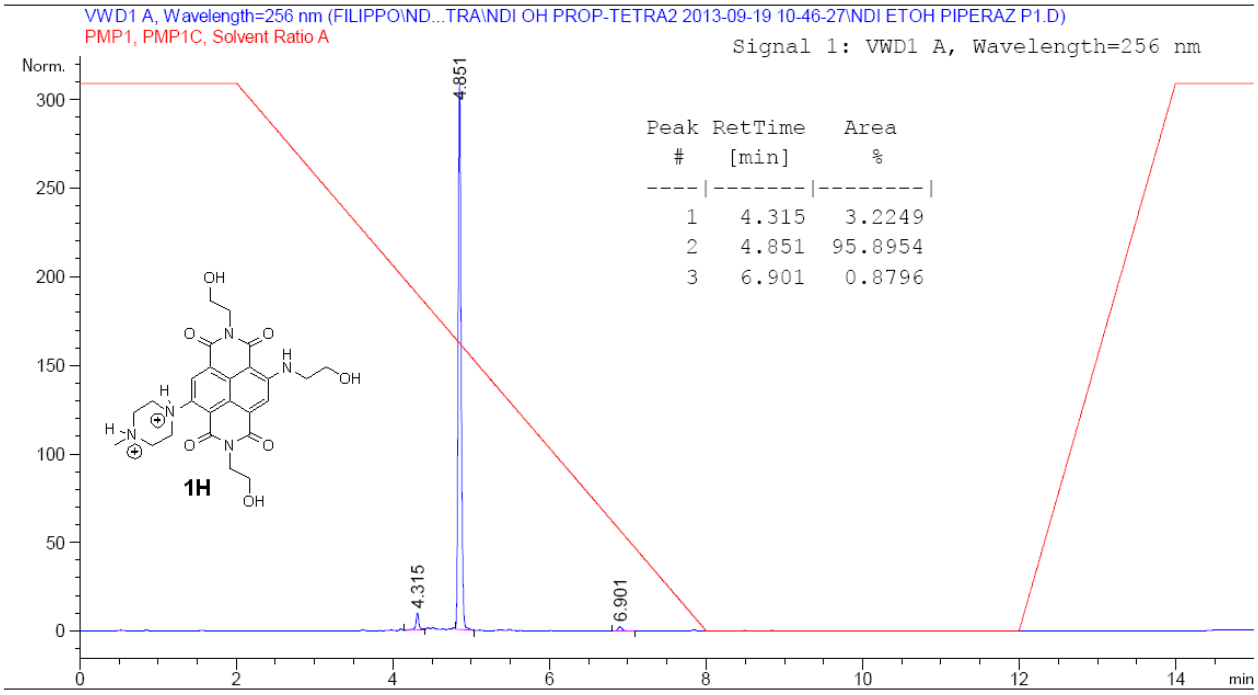
Table 1S. Maximum absorbance wavelength (λ_{max}/nm) for the NDIs **1H-4H** and their conjugate bases **1-4**

λ_{max}/nm							
1H	**1**	**2H**	**2**	**3H**	**3**	**4H**	**4**
546	571	536	622	556	584	533	615

HPLC PURITY DATA:

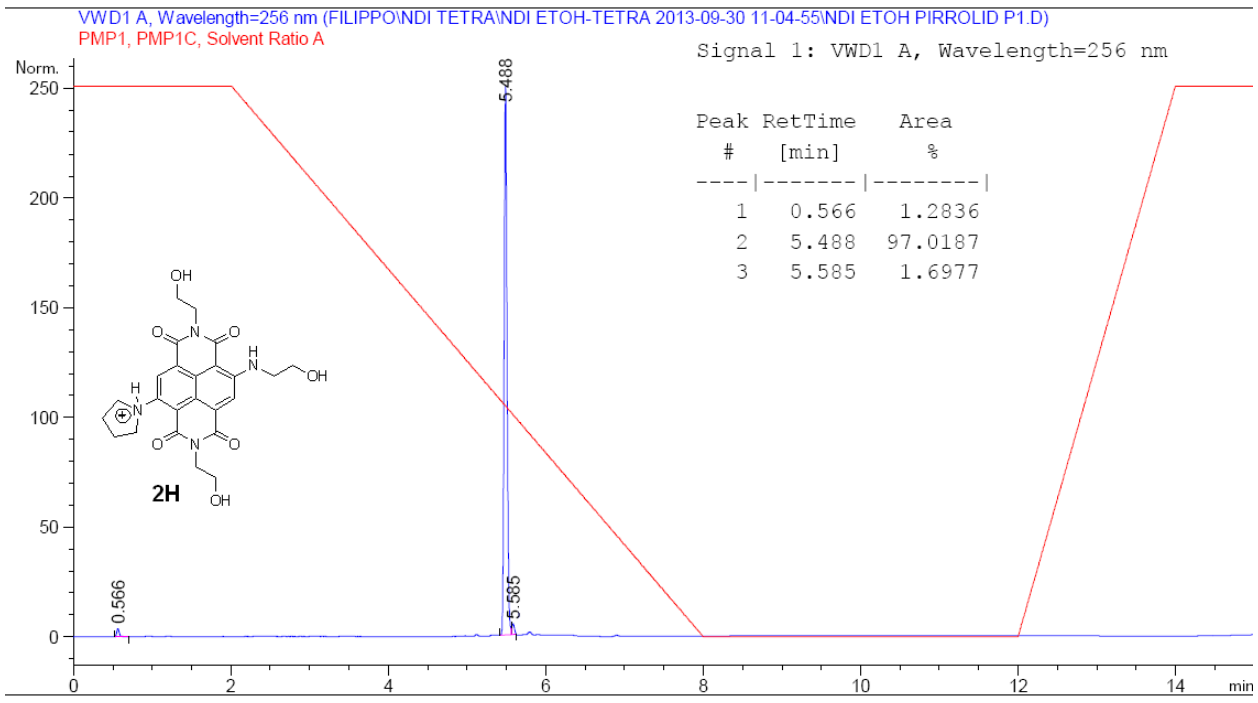
N,N'-Bis-(hydroxyethyl)-2-(N'-methyl-N-piperazinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (1·1HCl)

Analytical Method



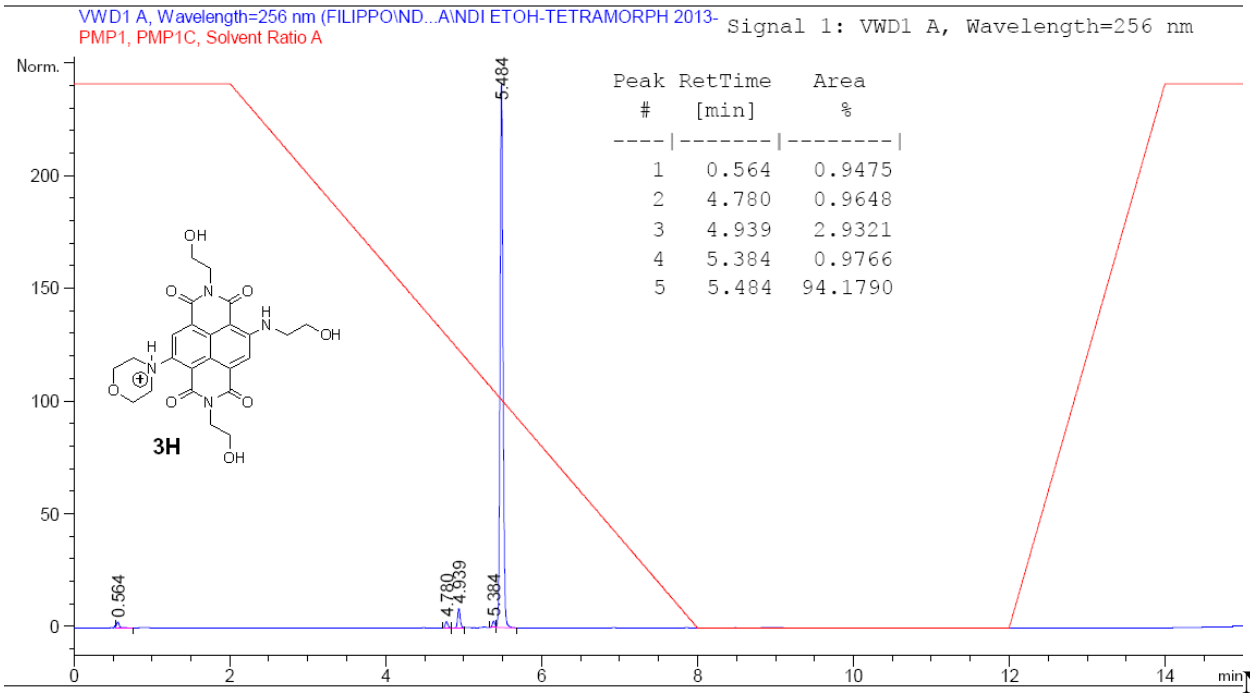
N,N'-Bis-(hydroxyethyl)-2-(N-pirrodinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (2·1HCl)

Analytical Method



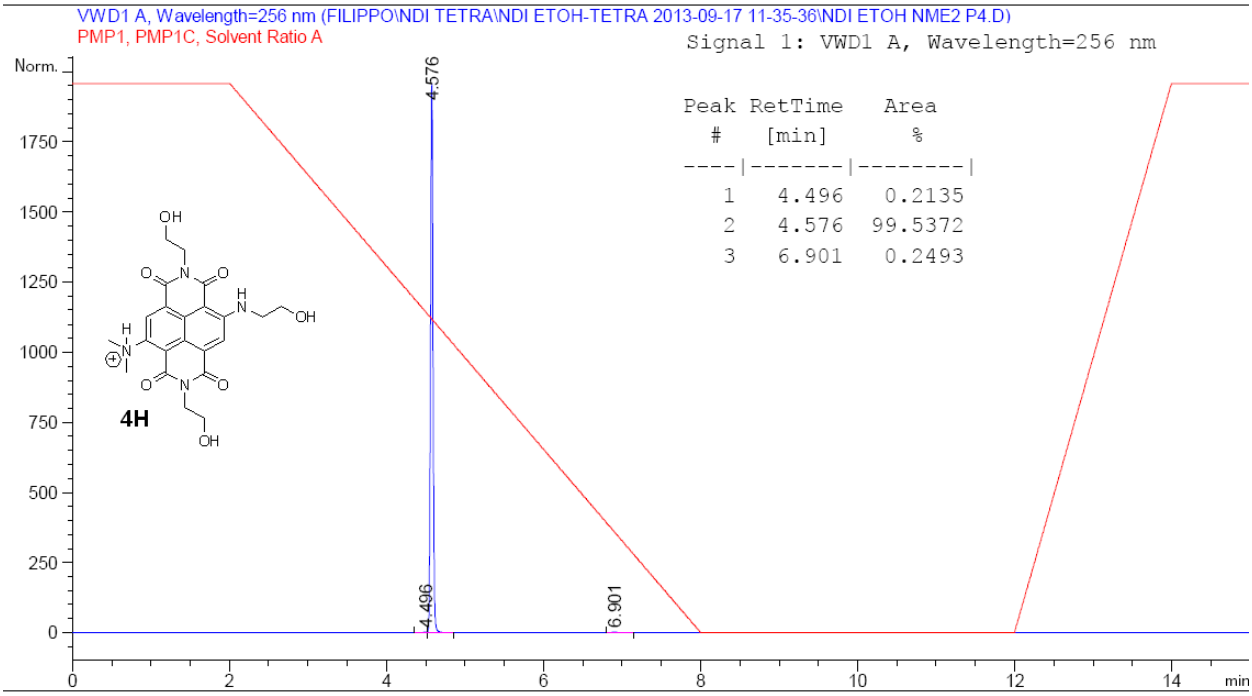
N,N'-Bis-(hydroxyethyl)-2-(N-morpholinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (3·1HCl)

Analytical Method



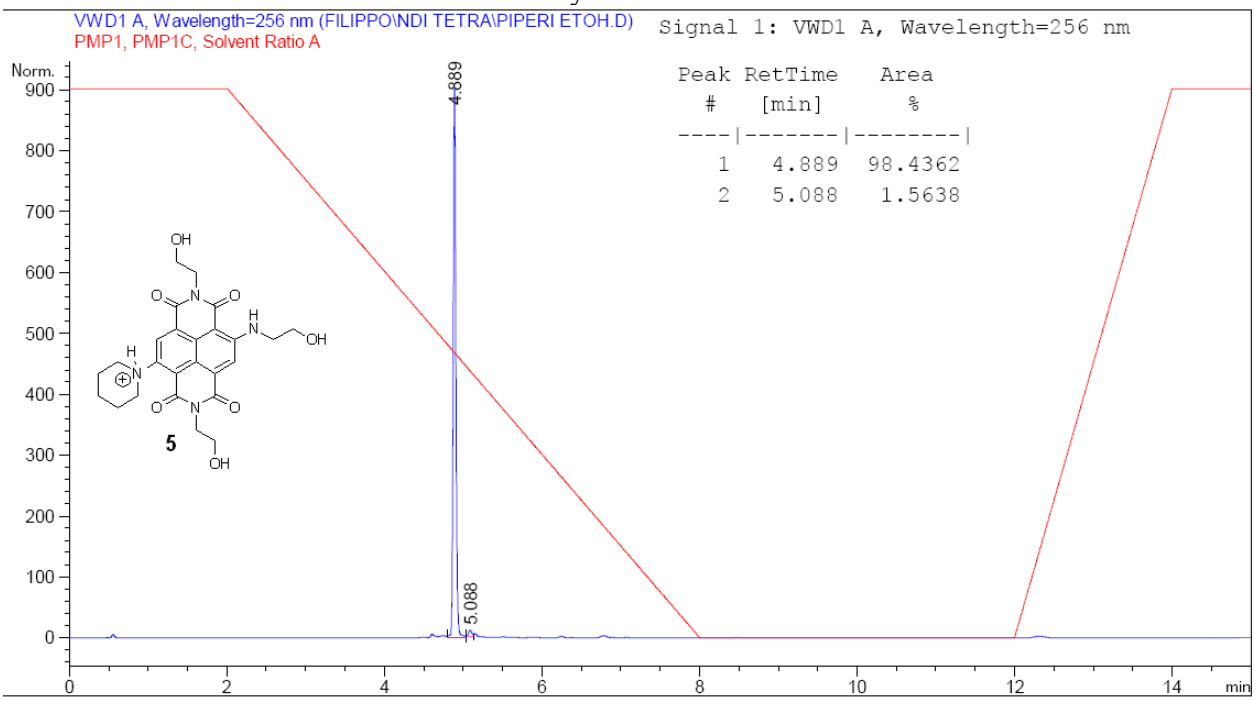
N,N'-Bis-(hydroxyethyl)-2-(N-dimethylamino)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (4·1HCl)

Analytical Method



N,N'-Bis-(hydroxyethyl)-2-(N-piperidinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (5·1HCl)

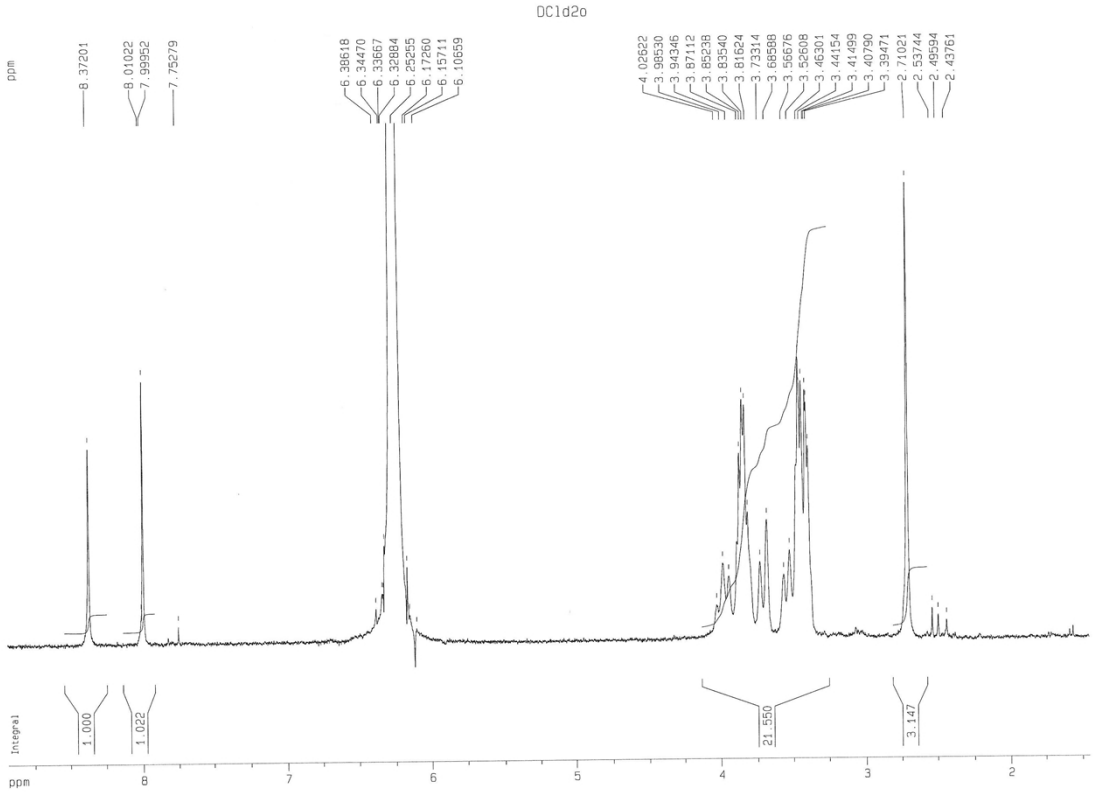
Analytical Method



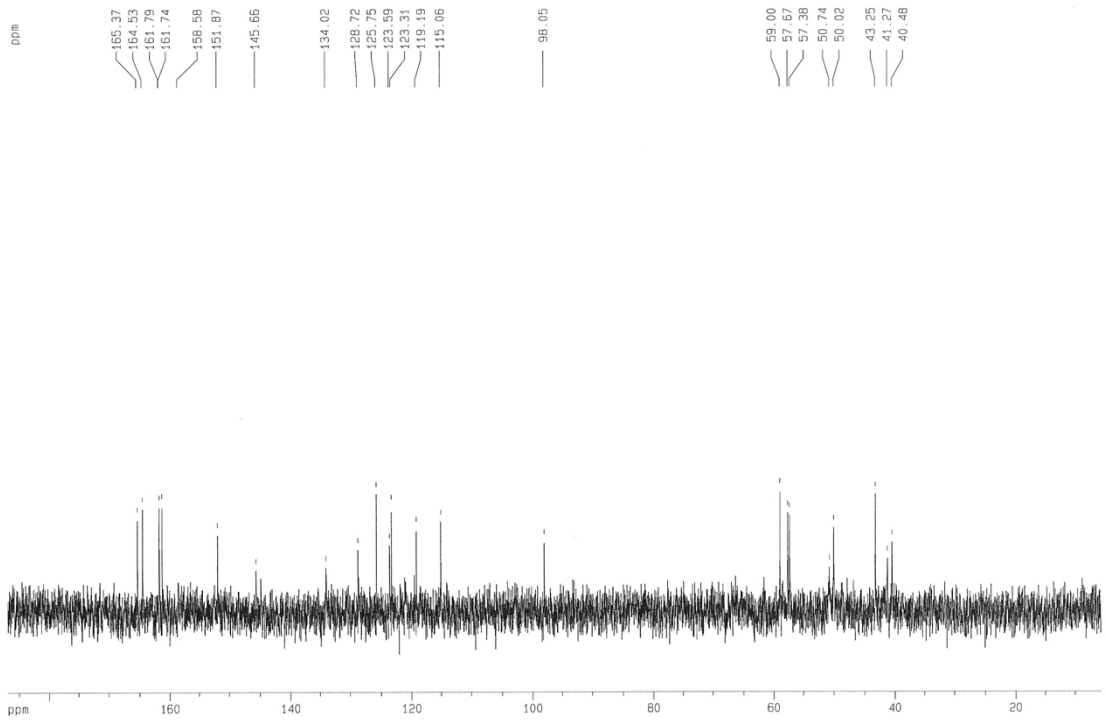
NMR Spectra:

N,N'-Bis-(hydroxyethyl)-2-(N'-methyl-N-piperazinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (1·2HCl)

(D_2O-DCl) ^1H NMR 300MHz

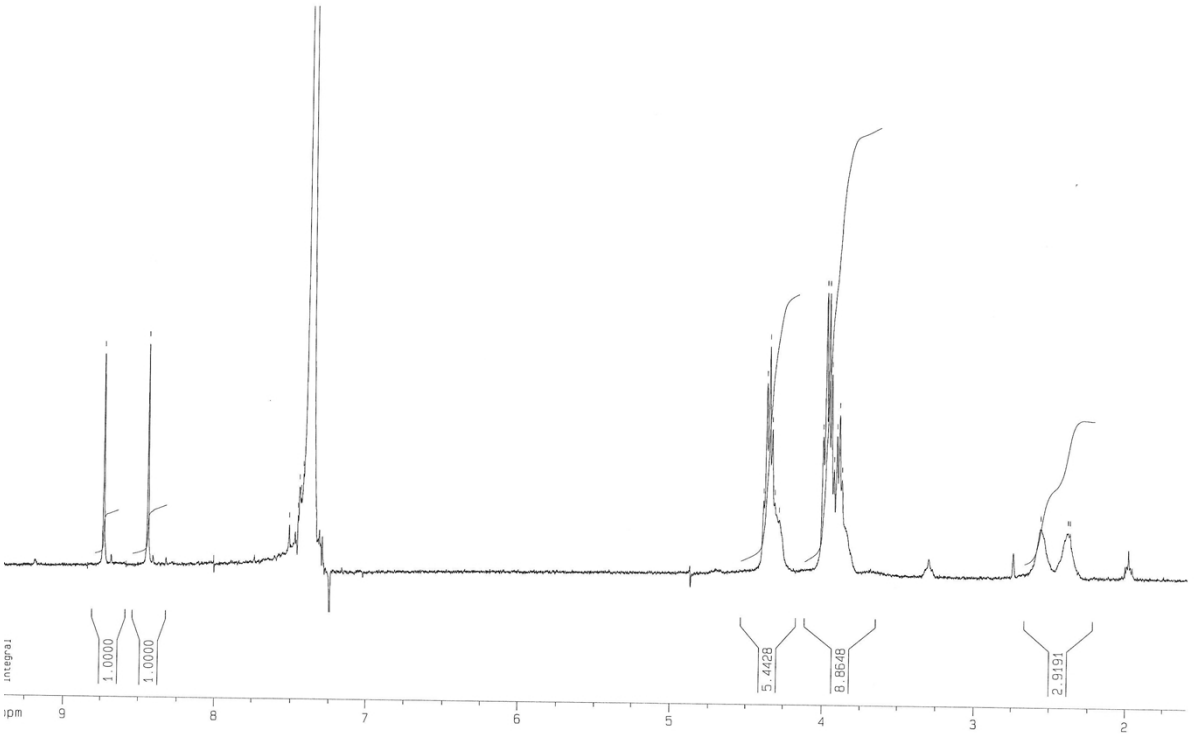


(D_2O-DCl) ^{13}C NMR 75MHz

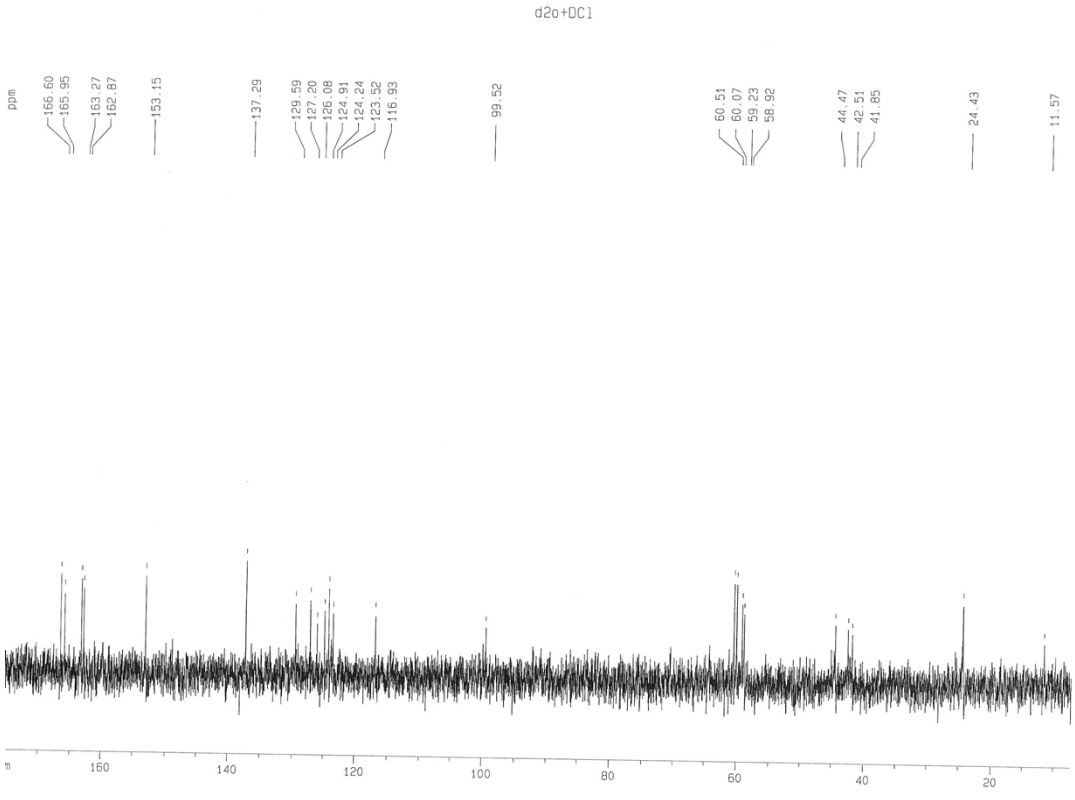


N,N'-Bis-(hydroxyethyl)-2-(N-pirrodinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (2·1HCl)

(D_2O-DCl) ^1H NMR 300MHz

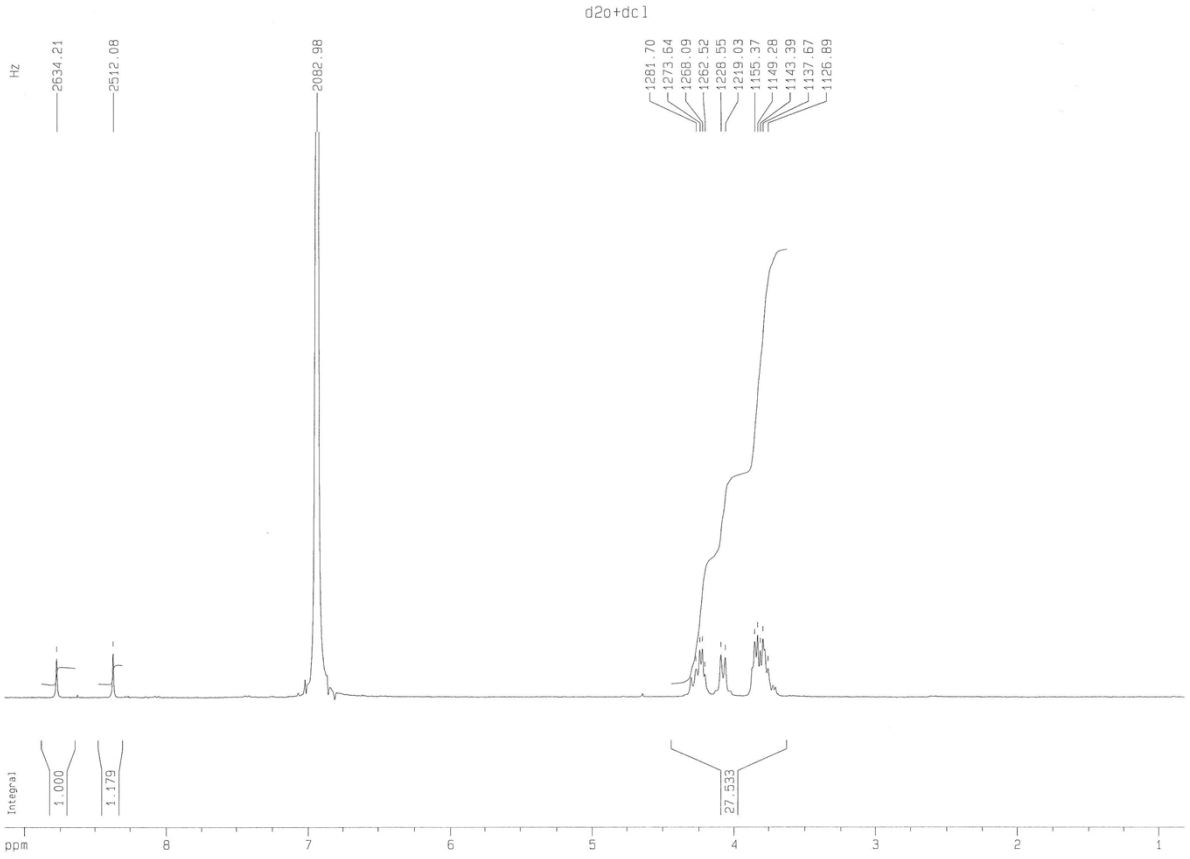


(D_2O-DCl) ^{13}C NMR 75MHz

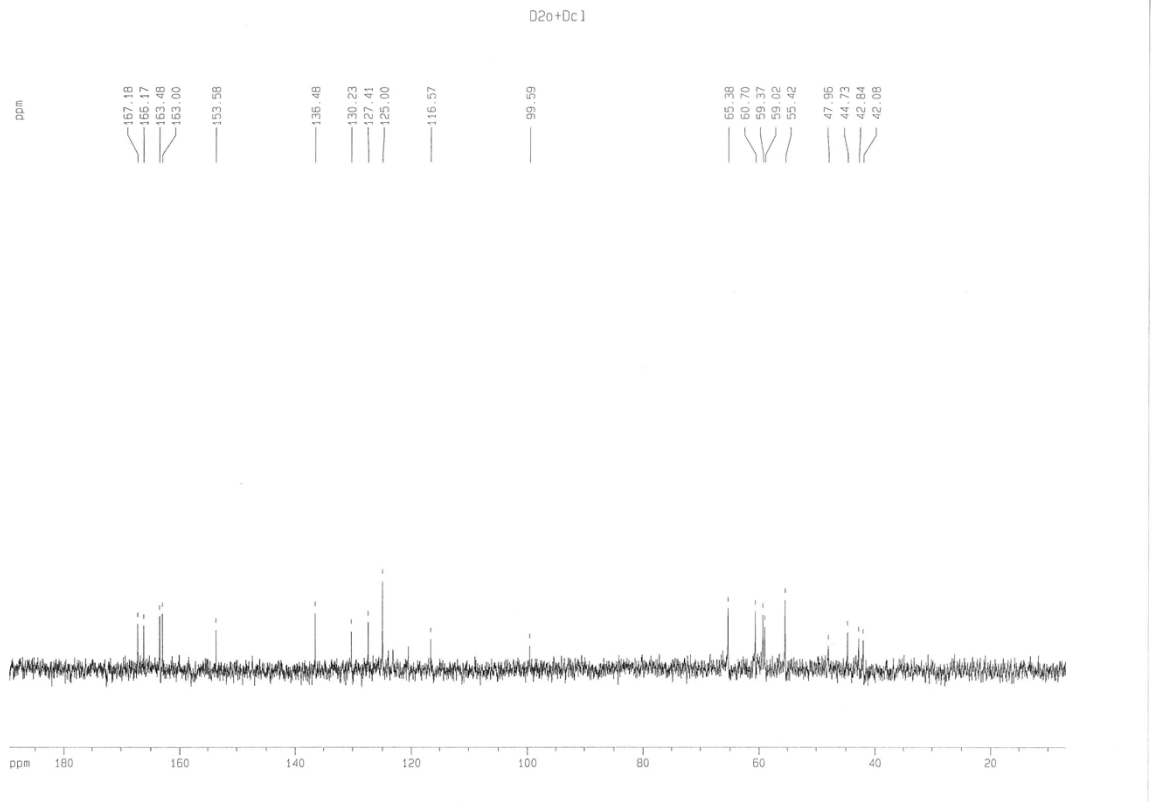


N,N'-Bis-(hydroxyethyl)-2-(N-morpholinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (3·1HCl)

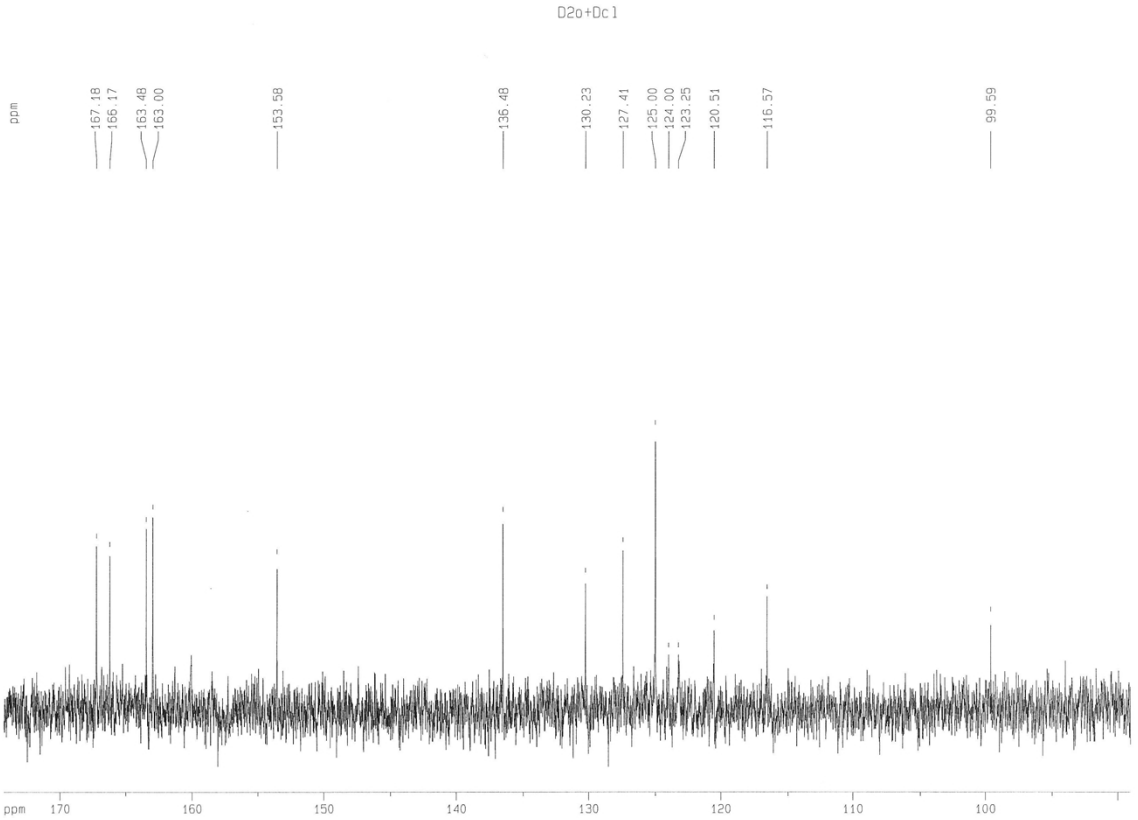
(D_2O-DCl) ^1H NMR 300MHz



(D_2O-DCl) ^{13}C NMR 75MHz

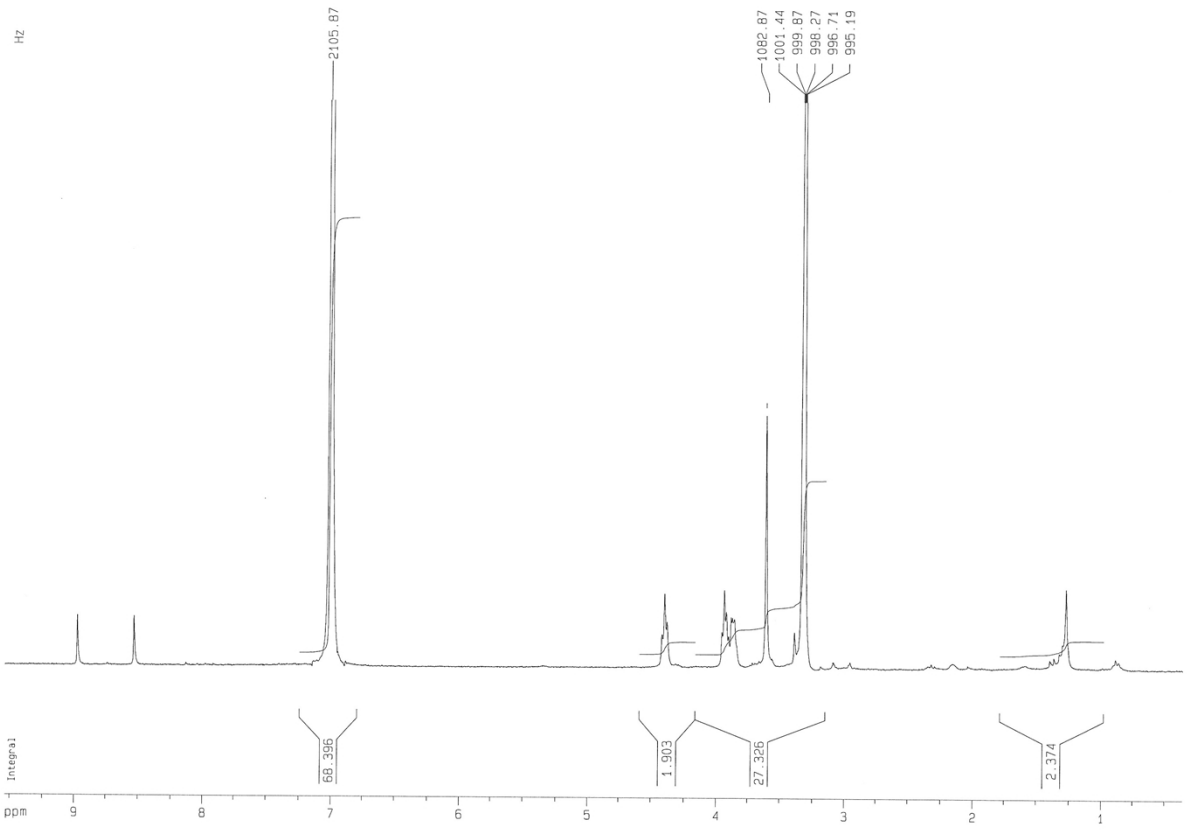


(D_2O-DCl) ^{13}C NMR 75MHz- Enlarged

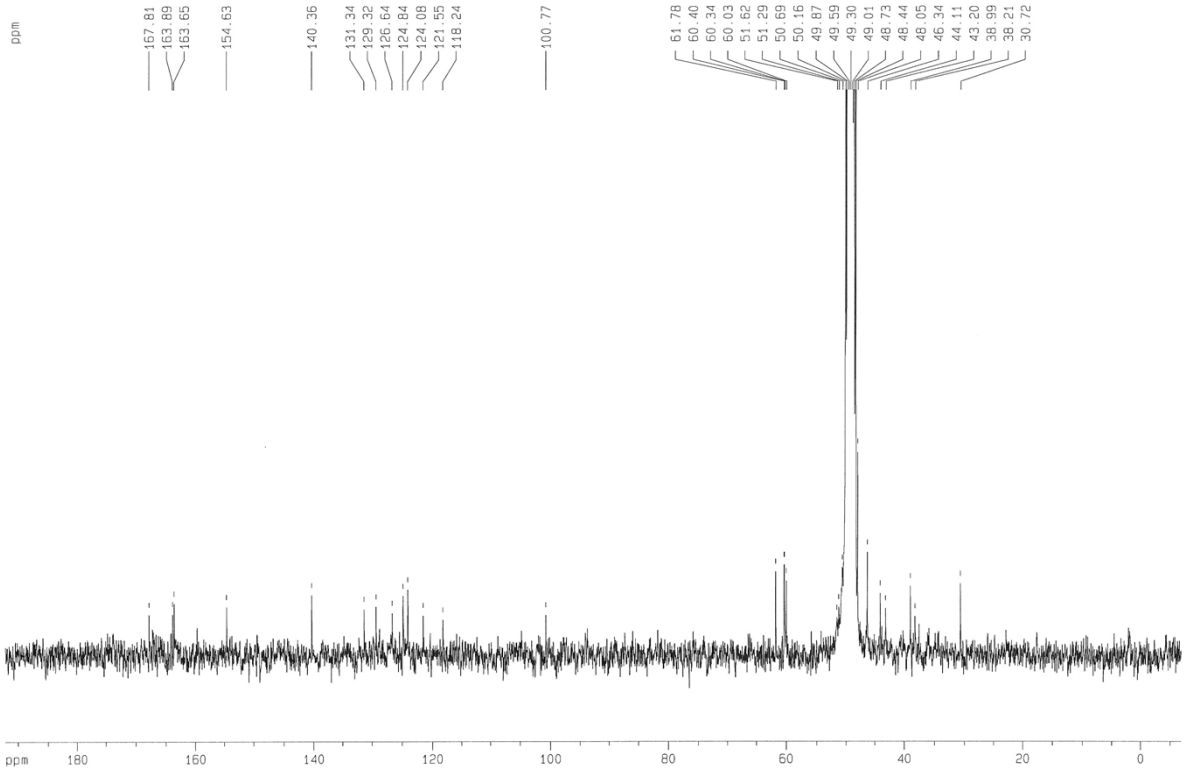


N,N'-Bis-(hydroxyethyl)-2-(N-dimethylamino)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (4·1HCl)

(CD_3OD-DCl) ^{1}H NMR 300MHz

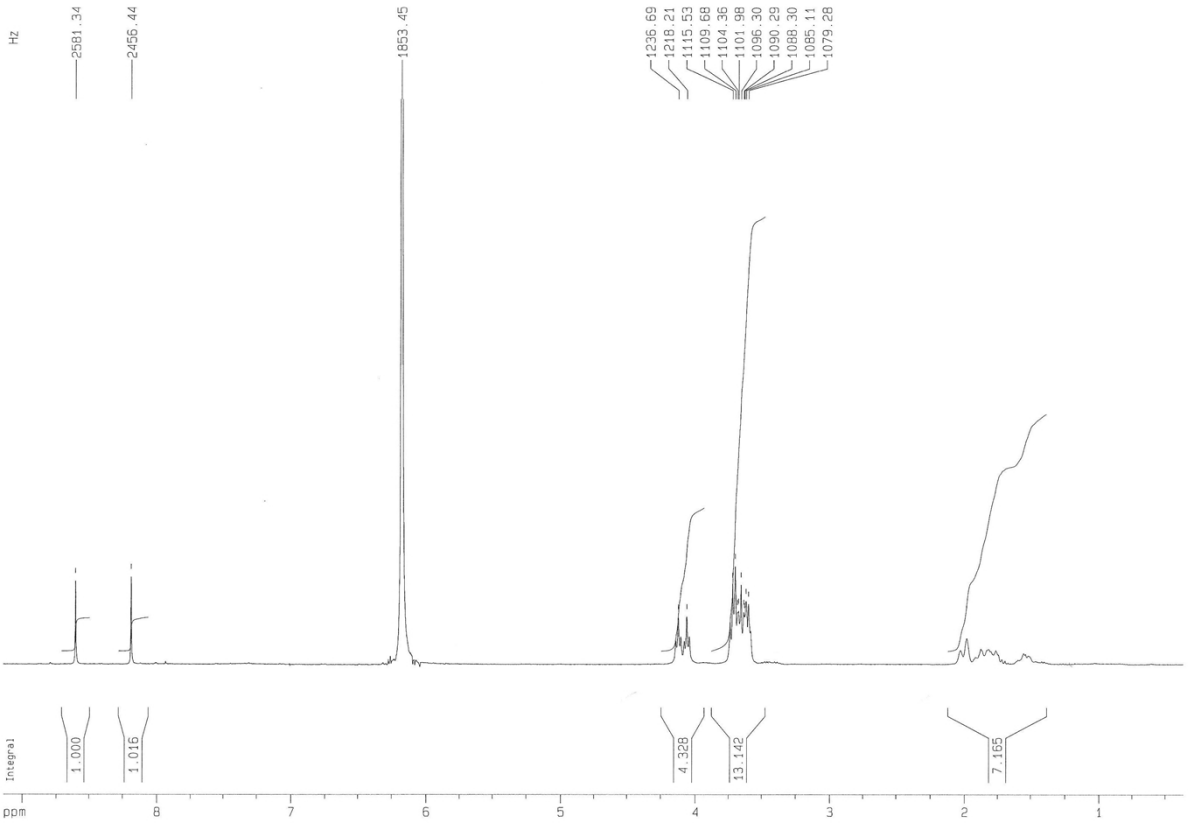


(CD_3OD-DCl) ^{13}C NMR 75MHz

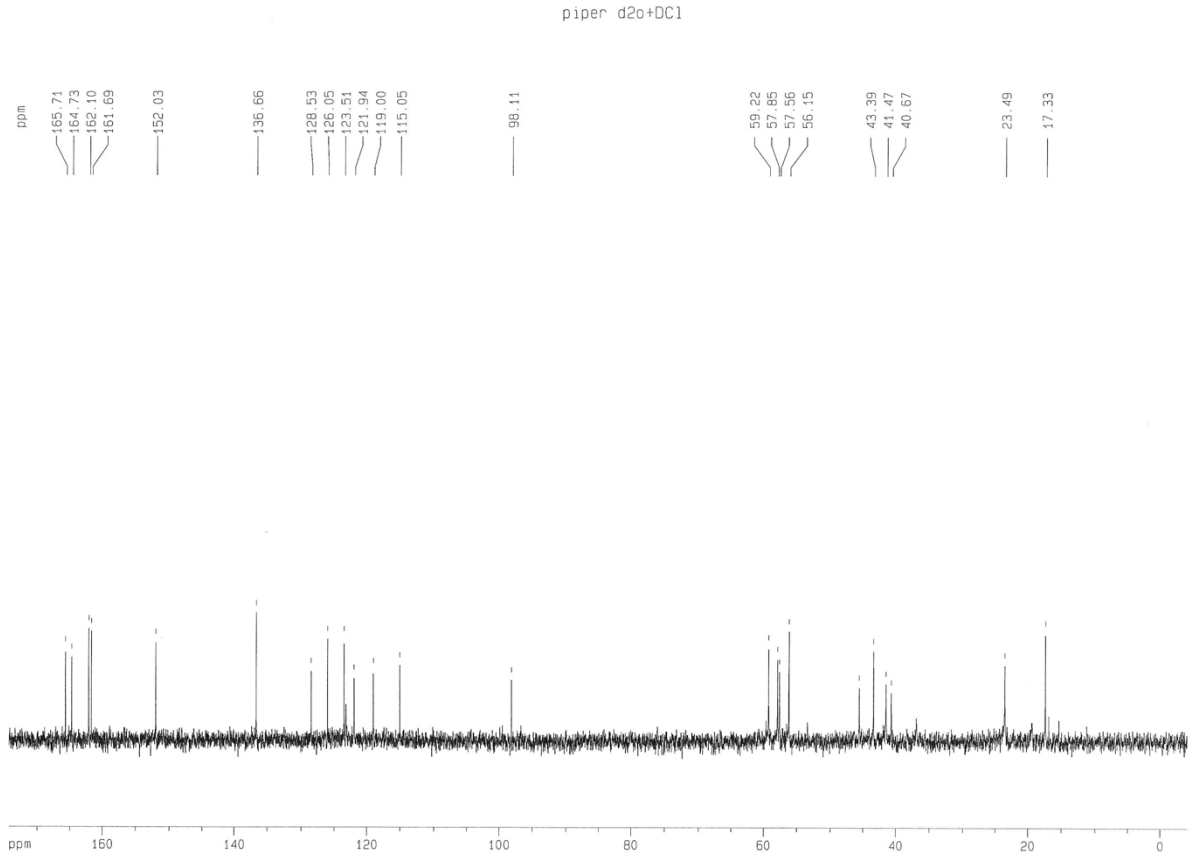


N,N'-Bis-(hydroxyethyl)-2-(N-piperidinyl)-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide hydrochloride (5·1HCl)

(D_2O-DCl) ^{1}H NMR 300MHz

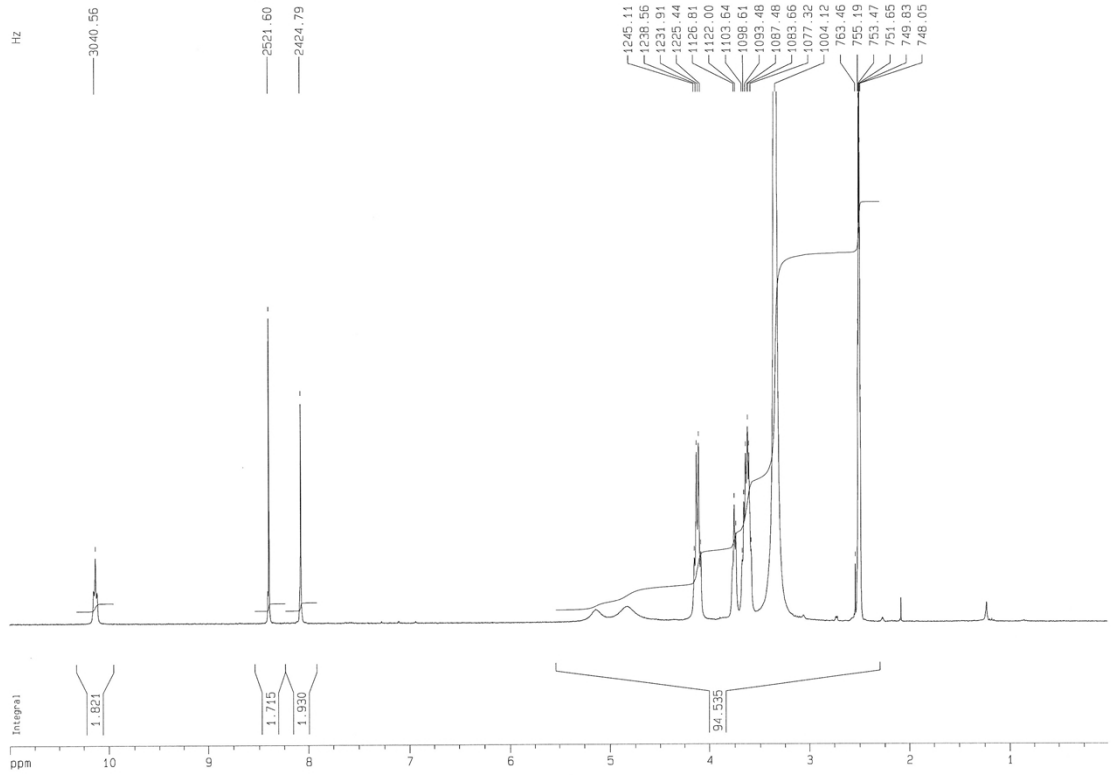


(D_2O-DCl) ^{13}C NMR 75MHz

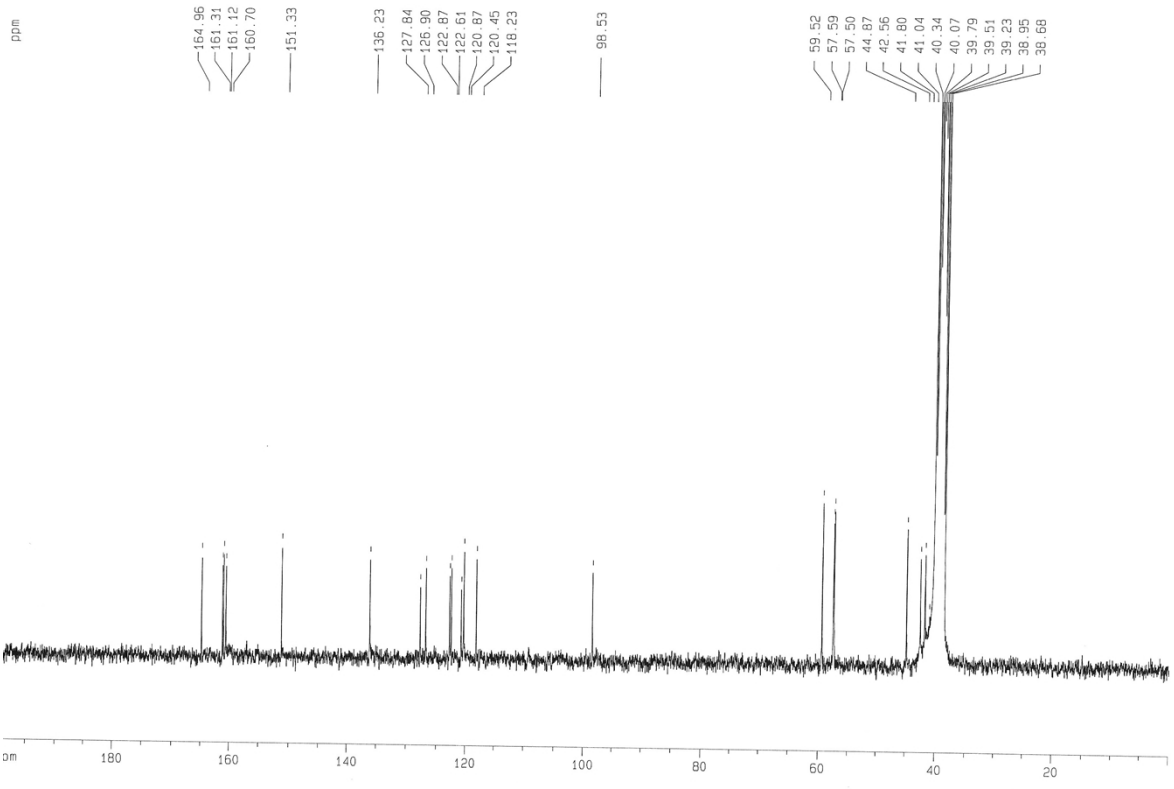


N,N'-Bis-(hydroxyethyl)-2-bromo-6-(hydroxyethylamino)-1,4,5,8-tetracarboxylic acid bisimide (7)

(DMSO) ^{1}H NMR 300MHz



(DMSO) ^{13}C NMR 75MHz



Gas Phase DFT Optimization

DFT calculations were run with Gaussian 09 (Revision A.02),[S4] with 6-31+G(d,p) as the basis set.
The excited states were investigated at a TD-B3LYP level of theory.

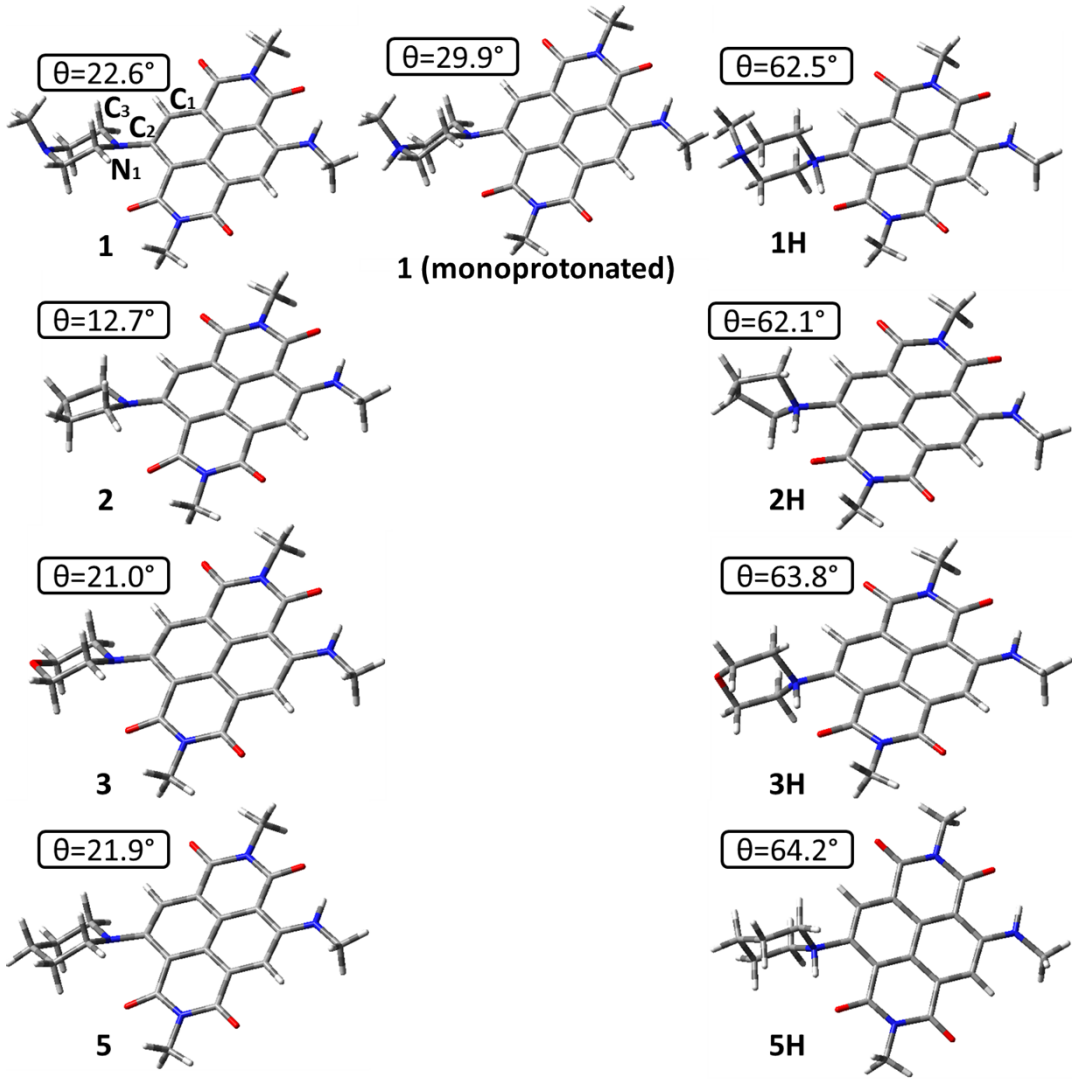


Figure 7S. Optimized geometry of compounds **1**, **2**, **3** and **5** and their protonated species in gas phase at B3LYP/6-31+G(d,p) level of theory. In the picture the dihedral angle $\theta=C_1C_2N_1C_3$ is reported.

1. **1**

Electronic Energy= -1427.009436 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	-1.360761	-2.988497	-0.136330
2	6	0	-0.678854	-1.671545	-0.114169
3	6	0	-1.422708	-0.468478	-0.016497
4	6	0	-2.840644	-0.500096	0.060121
5	6	0	-3.527327	-1.790675	0.051368
6	6	0	0.699514	-1.648502	-0.155790
7	6	0	-0.694957	0.753371	-0.012989
8	6	0	0.729148	0.781459	-0.076116
9	6	0	1.387824	2.095681	-0.258163
10	6	0	-0.794829	3.280357	-0.029505
11	6	0	-1.459808	1.954271	0.033828

12	6	0	-2.833718	1.935437	0.112658
13	6	0	-3.574627	0.717099	0.139630
14	1	0	-3.343164	2.890373	0.146623
15	1	0	1.202919	-2.606052	-0.184621
16	8	0	-1.419200	4.334323	0.050734
17	8	0	2.588789	2.245090	-0.466859
18	8	0	-4.761162	-1.909565	0.123992
19	8	0	-0.749146	-4.048797	-0.226566
20	7	0	-2.756498	-2.957433	-0.046181
21	7	0	0.584660	3.256183	-0.213910
22	6	0	-3.491679	-4.230021	-0.056579
23	6	0	1.291269	4.534492	-0.379262
24	1	0	1.793283	4.556036	-1.348578
25	1	0	2.047962	4.643837	0.400474
26	1	0	-2.761712	-5.031826	-0.134529
27	1	0	-4.179877	-4.252481	-0.904091
28	1	0	0.554157	5.330448	-0.309613
29	1	0	-4.074187	-4.327307	0.861841
30	6	0	1.454879	-0.445238	-0.099423
31	7	0	-4.926055	0.740567	0.228029
32	1	0	-5.368863	-0.175201	0.225132
33	6	0	-5.732781	1.944349	0.300952
34	1	0	-6.779957	1.645970	0.371248
35	1	0	-5.489581	2.547509	1.184399
36	1	0	-5.615532	2.572759	-0.590857
37	6	0	3.607909	0.082678	1.018858
38	6	0	3.499953	-1.732820	-0.602335
39	6	0	5.031834	0.412455	0.550920
40	1	0	3.636552	-0.628365	1.863163
41	1	0	3.112226	0.987543	1.359860
42	6	0	4.932495	-1.371170	-1.045085
43	1	0	3.523519	-2.541669	0.148660
44	1	0	2.945920	-2.098663	-1.470814
45	1	0	5.611223	0.817876	1.387677
46	1	0	4.963095	1.184240	-0.222453
47	1	0	5.440046	-2.274854	-1.400590
48	1	0	4.860598	-0.671084	-1.886813
49	7	0	2.841026	-0.531284	-0.079532
50	7	0	5.743750	-0.743022	-0.004455
51	6	0	6.267429	-1.669218	0.995221
52	1	0	6.852250	-2.446595	0.492357
53	1	0	6.941709	-1.126095	1.665624
54	1	0	5.507633	-2.172227	1.619950

2. **1** (monoprotonated)

Electronic Energy= -1427.3963299 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	1.410284	-2.991139	0.037499
2	6	0	0.723271	-1.674440	0.033937
3	6	0	1.456838	-0.466176	-0.006177
4	6	0	2.874488	-0.488851	-0.038233
5	6	0	3.568824	-1.777807	-0.045236
6	6	0	-0.660117	-1.656870	0.053210
7	6	0	0.722715	0.755645	-0.005141
8	6	0	-0.696724	0.773053	0.018019
9	6	0	-1.387667	2.091371	0.079265
10	6	0	0.794968	3.282750	0.066578
11	6	0	1.477589	1.965262	0.001154
12	6	0	2.849479	1.954942	-0.026549
13	6	0	3.603136	0.735197	-0.060055

14	1	0	3.358429	2.911040	-0.014794
15	1	0	-1.160439	-2.618674	0.058935
16	8	0	1.403755	4.341589	0.067662
17	8	0	-2.614617	2.215648	0.086377
18	8	0	4.801934	-1.881249	-0.081794
19	8	0	0.785993	-4.046912	0.077920
20	7	0	2.802379	-2.953201	-0.008263
21	7	0	-0.606384	3.246336	0.139045
22	6	0	3.547011	-4.223785	-0.012944
23	6	0	-1.330268	4.525951	0.226712
24	1	0	-1.984296	4.516515	1.099923
25	1	0	-1.941557	4.670480	-0.666721
26	1	0	2.821568	-5.032655	0.015756
27	1	0	4.205574	-4.266828	0.856442
28	1	0	-0.591130	5.318421	0.308870
29	1	0	4.158848	-4.286878	-0.914548
30	6	0	-1.398029	-0.457864	0.038745
31	7	0	4.948206	0.772449	-0.100730
32	1	0	5.398066	-0.141766	-0.111529
33	6	0	5.759470	1.980913	-0.118403
34	1	0	6.806890	1.681220	-0.161688
35	1	0	5.544239	2.601007	-0.995826
36	1	0	5.612409	2.582543	0.785769
37	6	0	-3.568561	-0.135701	-1.105398
38	6	0	-3.443260	-1.646391	0.763856
39	6	0	-4.939049	0.374309	-0.684771
40	1	0	-3.649156	-0.970403	-1.824607
41	1	0	-3.069321	0.687638	-1.612329
42	6	0	-4.818638	-1.205432	1.265356
43	1	0	-3.531296	-2.554079	0.140220
44	1	0	-2.857488	-1.921295	1.644579
45	1	0	-5.572609	0.630783	-1.536818
46	1	0	-4.804611	1.241134	-0.035638
47	1	0	-5.365452	-2.023429	1.740509
48	1	0	-4.707936	-0.377267	1.968440
49	7	0	-2.815807	-0.529402	0.079663
50	7	0	-5.688987	-0.681666	0.127512
51	6	0	-6.281160	-1.775897	-0.718451
52	1	0	-6.852456	-2.445872	-0.074679
53	1	0	-6.936016	-1.322698	-1.463607
54	1	0	-5.484642	-2.327643	-1.213343
55	1	0	-6.477587	-0.199737	0.566936

3. **1H**

Electronic Energy= -1427.6720232 Hartree/ Molecule

Standard Orientation Coordinates:

1	6	0	-1.083731	-2.999590	-0.000074
2	6	0	-0.543500	-1.608802	-0.000092
3	6	0	-1.412451	-0.490694	-0.000026
4	6	0	-2.811947	-0.667887	0.000019
5	6	0	-3.359754	-2.033025	-0.000041
6	6	0	0.837813	-1.446924	-0.000141
7	6	0	-0.824259	0.808127	-0.000017
8	6	0	0.579087	0.962576	-0.000084
9	6	0	1.107924	2.318053	-0.000179
10	6	0	-1.132708	3.304447	0.000018
11	6	0	-1.690730	1.936173	0.000033
12	6	0	-3.056359	1.776368	0.000094
13	6	0	-3.674973	0.473353	0.000108
14	1	0	-3.675704	2.665975	0.000126
15	1	0	1.433190	-2.354827	-0.000160
16	8	0	-1.782723	4.321559	0.000149

17	8	0	2.397346	2.519531	-0.000328
18	8	0	-4.571351	-2.257903	0.000021
19	8	0	-0.328483	-3.963497	-0.000072
20	7	0	-2.467263	-3.116919	-0.000121
21	7	0	0.322204	3.395405	-0.000145
22	6	0	-3.068753	-4.467155	-0.000154
23	6	0	0.931962	4.747650	-0.000271
24	1	0	1.546641	4.869353	-0.893341
25	1	0	1.547777	4.869004	0.892053
26	1	0	-2.258819	-5.191580	-0.000331
27	1	0	-3.692431	-4.586870	-0.887258
28	1	0	0.118011	5.467793	0.000361
29	1	0	-3.692182	-4.587042	0.887103
30	6	0	1.416021	-0.176129	-0.000130
31	7	0	-5.007921	0.365863	0.000207
32	1	0	-5.354082	-0.595082	0.000158
33	6	0	-5.963382	1.471810	0.000273
34	1	0	-6.965826	1.045019	0.000653
35	1	0	-5.855429	2.094527	0.894276
36	1	0	-5.855948	2.094197	-0.894028
37	6	0	3.512573	-0.567136	1.220033
38	6	0	3.512752	-0.567633	-1.219940
39	6	0	5.005437	-0.251953	1.244962
40	1	0	3.333360	-1.647284	1.295320
41	1	0	3.060827	-0.105985	2.102468
42	6	0	5.005571	-0.252316	-1.244764
43	1	0	3.333624	-1.647831	-1.294817
44	1	0	3.061100	-0.106944	-2.102667
45	1	0	5.485441	-0.704641	2.115083
46	1	0	5.179148	0.827211	1.270062
47	1	0	5.485794	-0.705102	-2.114712
48	1	0	5.179138	0.826873	-1.270065
49	7	0	2.873275	-0.003696	-0.000131
50	7	0	5.713172	-0.769757	0.000201
51	6	0	5.939419	-2.264666	0.000415
52	1	0	6.507556	-2.527465	-0.892664
53	1	0	6.507409	-2.527239	0.893649
54	1	0	4.983954	-2.784981	0.000393
55	1	0	6.646613	-0.345633	0.000169
56	1	0	2.832178	1.576861	-0.000324

4. **2**

Electronic Energy= -1332.3540797 Hartree/ Molecule

Standard Orientation Coordinates:

1	6	0	-1.343158	-2.895912	-0.169359
2	6	0	-0.473393	-1.695570	-0.110071
3	6	0	-1.033577	-0.396825	-0.011672
4	6	0	-2.441077	-0.218426	0.050552
5	6	0	-3.310908	-1.392819	0.019281
6	6	0	0.892682	-1.879578	-0.115368
7	6	0	-0.132980	0.702728	-0.002898
8	6	0	1.280427	0.520502	-0.053845
9	6	0	2.114382	1.715546	-0.300755
10	6	0	0.144107	3.215525	-0.016511
11	6	0	-0.711457	2.003737	0.041458
12	6	0	-2.073704	2.188480	0.116332
13	6	0	-2.987048	1.093616	0.133025
14	1	0	-2.436034	3.208244	0.153478
15	1	0	1.243989	-2.901658	-0.153899
16	8	0	-0.313074	4.351016	0.079382
17	8	0	3.307521	1.677686	-0.594550
18	8	0	-4.549332	-1.329323	0.082666

19	8	0	-0.894686	-4.033696	-0.273086
20	7	0	-2.719962	-2.659233	-0.094828
21	7	0	1.501255	2.985095	-0.224042
22	6	0	-3.635291	-3.808259	-0.137315
23	6	0	2.384597	4.141980	-0.427621
24	1	0	2.824780	4.101223	-1.426212
25	1	0	3.194450	4.122603	0.304377
26	1	0	-3.031411	-4.707513	-0.229687
27	1	0	-4.312064	-3.710276	-0.988629
28	1	0	1.783968	5.040385	-0.309198
29	1	0	-4.233551	-3.838116	0.775688
30	6	0	1.820079	-0.801368	-0.022260
31	7	0	-4.321279	1.316577	0.213724
32	1	0	-4.895145	0.477045	0.201284
33	6	0	-4.940530	2.626483	0.285855
34	1	0	-6.020960	2.487101	0.347946
35	1	0	-4.616637	3.184279	1.173257
36	1	0	-4.724667	3.233625	-0.602440
37	6	0	4.083408	-0.493104	1.044857
38	6	0	3.659863	-2.460856	-0.193001
39	6	0	5.458035	-0.948058	0.547808
40	1	0	3.868070	-0.898866	2.048860
41	1	0	3.988346	0.587744	1.068065
42	6	0	5.199152	-2.337702	-0.091112
43	1	0	3.323204	-2.798426	-1.177223
44	1	0	3.287206	-3.178697	0.555534
45	1	0	5.816381	-0.239981	-0.204631
46	1	0	6.193071	-0.984584	1.356876
47	1	0	5.665670	-2.411070	-1.077079
48	1	0	5.603811	-3.149299	0.520472
49	7	0	3.161761	-1.103859	0.074229

5. **2H**

Electronic Energy= -1332.7496196 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	-1.093269	-2.941215	0.002683
2	6	0	-0.333771	-1.662567	0.000105
3	6	0	-1.007249	-0.416095	0.001274
4	6	0	-2.420103	-0.360177	0.005491
5	6	0	-3.184271	-1.611983	0.008958
6	6	0	1.052337	-1.722694	-0.005182
7	6	0	-0.218124	0.770874	-0.003471
8	6	0	1.189906	0.707779	-0.008698
9	6	0	1.970607	1.971547	-0.016054
10	6	0	-0.115094	3.294995	-0.009122
11	6	0	-0.891011	2.025928	-0.003852
12	6	0	-2.260162	2.090628	0.000501
13	6	0	-3.079341	0.906336	0.005106
14	1	0	-2.722080	3.070629	0.000105
15	1	0	1.510923	-2.706839	-0.009010
16	8	0	-0.640078	4.391688	-0.007677
17	8	0	3.217014	1.963856	-0.021895
18	8	0	-4.420053	-1.642225	0.012889
19	8	0	-0.521004	-4.024332	0.000559
20	7	0	-2.481695	-2.826315	0.007593
21	7	0	1.298796	3.168672	-0.016423
22	6	0	-3.294186	-4.056995	0.010515
23	6	0	2.114864	4.399952	-0.023747
24	1	0	2.751315	4.410412	-0.909954
25	1	0	2.745491	4.425730	0.866501
26	1	0	-2.612905	-4.903767	0.010428

27	1	0	-3.931797	-4.076112	-0.874919
28	1	0	1.433324	5.246178	-0.032627
29	1	0	-3.928860	-4.073674	0.898064
30	6	0	1.811189	-0.550431	-0.009286
31	7	0	-4.416538	1.015852	0.008742
32	1	0	-4.913491	0.124585	0.011619
33	6	0	-5.170267	2.263824	0.007797
34	1	0	-6.231058	2.013407	0.011595
35	1	0	-4.956667	2.865206	0.898045
36	1	0	-4.961954	2.860666	-0.886762
37	6	0	3.911118	-1.269674	1.221013
38	6	0	3.916012	-1.324911	-1.231283
39	6	0	5.331907	-1.565334	0.754418
40	1	0	3.354782	-2.179729	1.456672
41	1	0	3.824198	-0.566187	2.051078
42	6	0	5.130614	-2.097663	-0.678879
43	1	0	4.180613	-0.534415	-1.936201
44	1	0	3.166627	-1.967965	-1.691626
45	1	0	5.930659	-0.647815	0.755554
46	1	0	5.828038	-2.287226	1.406841
47	1	0	6.013989	-1.953689	-1.304196
48	1	0	4.912469	-3.169295	-0.657397
49	7	0	3.281357	-0.636980	-0.011497
50	1	0	3.575689	0.376651	-0.023450

6. **3**

Electronic Energy= -1407.5660531 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	-1.394010	-2.936986	-0.096264
2	6	0	-0.594253	-1.687924	-0.070008
3	6	0	-1.225915	-0.420819	-0.005434
4	6	0	-2.641989	-0.321348	0.040890
5	6	0	-3.444309	-1.543573	0.033551
6	6	0	0.781359	-1.792393	-0.074349
7	6	0	-0.389221	0.729177	-0.003248
8	6	0	1.031817	0.625414	-0.032484
9	6	0	1.814001	1.870792	-0.218452
10	6	0	-0.254605	3.254084	-0.061590
11	6	0	-1.040628	1.996146	0.008840
12	6	0	-2.411273	2.104385	0.060133
13	6	0	-3.261877	0.959118	0.089955
14	1	0	-2.831453	3.102338	0.069405
15	1	0	1.193871	-2.792893	-0.078354
16	8	0	-0.779890	4.362129	-0.011683
17	8	0	3.028763	1.904040	-0.395532
18	8	0	-4.684858	-1.547013	0.083304
19	8	0	-0.879901	-4.049147	-0.164517
20	7	0	-2.782465	-2.777192	-0.036772
21	7	0	1.120575	3.099889	-0.216908
22	6	0	-3.630978	-3.977306	-0.050828
23	6	0	1.944911	4.304859	-0.389304
24	1	0	2.486514	4.247569	-1.335321
25	1	0	2.675110	4.375249	0.419875
26	1	0	-2.976107	-4.843204	-0.107293
27	1	0	-4.301842	-3.945477	-0.911805
28	1	0	1.279601	5.164443	-0.376378
29	1	0	-4.237287	-4.011328	0.856623
30	6	0	1.640923	-0.662470	-0.014599
31	7	0	-4.606193	1.108469	0.152035
32	1	0	-5.131456	0.237245	0.154024

33	6	0	-5.299588	2.382568	0.194508
34	1	0	-6.370881	2.182936	0.248380
35	1	0	-5.017411	2.973179	1.074820
36	1	0	-5.108646	2.984660	-0.702656
37	6	0	3.797393	-0.315005	1.161161
38	6	0	3.573182	-2.148832	-0.406418
39	6	0	5.259034	-0.175714	0.752121
40	1	0	3.724661	-1.000526	2.023101
41	1	0	3.404451	0.655059	1.453323
42	6	0	5.048504	-1.952763	-0.765969
43	1	0	3.491784	-2.927891	0.370896
44	1	0	3.035725	-2.488507	-1.296028
45	1	0	5.865598	0.141716	1.604502
46	1	0	5.343832	0.565877	-0.053598
47	1	0	5.501868	-2.914636	-1.021230
48	1	0	5.128827	-1.277190	-1.632035
49	7	0	3.014660	-0.871783	0.045971
50	8	0	5.791179	-1.431606	0.327954

7. **3H**

Electronic Energy= -1407.9561551 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	-1.203482	-2.964651	-0.000383
2	6	0	-0.492995	-1.657768	-0.000085
3	6	0	-1.213103	-0.438148	-0.000005
4	6	0	-2.627016	-0.435824	0.000072
5	6	0	-3.343268	-1.716035	0.000086
6	6	0	0.895147	-1.666578	-0.000010
7	6	0	-0.469478	0.778473	-0.000006
8	6	0	0.939565	0.769058	0.000089
9	6	0	1.671119	2.061591	0.000103
10	6	0	-0.462952	3.304721	-0.000515
11	6	0	-1.189842	2.007175	-0.000162
12	6	0	-2.560331	2.019473	-0.000156
13	6	0	-3.334042	0.804553	0.000218
14	1	0	-3.059607	2.981042	-0.000528
15	1	0	1.388159	-2.633430	-0.000060
16	8	0	-1.028250	4.380865	-0.000842
17	8	0	2.917816	2.099970	0.000094
18	8	0	-4.576960	-1.792392	0.000192
19	8	0	-0.590268	-4.024703	-0.000596
20	7	0	-2.595369	-2.902482	-0.000206
21	7	0	0.955549	3.231884	0.000006
22	6	0	-3.360441	-4.163434	-0.000350
23	6	0	1.724332	4.493548	0.000000
24	1	0	2.356061	4.536174	-0.888700
25	1	0	2.357015	4.535519	0.888036
26	1	0	-2.647426	-4.983660	-0.000845
27	1	0	-3.995607	-4.205210	-0.886712
28	1	0	1.011077	5.313262	0.000626
29	1	0	-3.995022	-4.205779	0.886406
30	6	0	1.607123	-0.466135	0.000092
31	7	0	-4.674129	0.863242	0.000638
32	1	0	-5.136777	-0.046494	0.000289
33	6	0	-5.475594	2.081351	0.000653
34	1	0	-6.525851	1.789967	0.003449
35	1	0	-5.285967	2.689048	0.891932
36	1	0	-5.289909	2.686586	-0.893169
37	6	0	3.680097	-1.117212	1.249554
38	6	0	3.680235	-1.116691	-1.249340

39	6	0	5.204282	-1.047933	1.171997
40	1	0	3.338083	-2.152852	1.298339
41	1	0	3.290736	-0.563936	2.107493
42	6	0	5.204449	-1.047584	-1.171566
43	1	0	3.338134	-2.152270	-1.298778
44	1	0	3.291173	-0.562994	-2.107156
45	1	0	5.633014	-1.576545	2.026091
46	1	0	5.546289	-0.001372	1.204649
47	1	0	5.633225	-1.576020	-2.025744
48	1	0	5.546504	-0.001033	-1.203888
49	7	0	3.085131	-0.492232	0.000155
50	8	0	5.681216	-1.689002	0.000160
51	1	0	3.337158	0.537500	0.000336

8. **4**

Electronic Energy= -1254.9278033 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	1.942551	-2.508320	-0.141455
2	6	0	0.706134	-1.690822	-0.082103
3	6	0	0.776055	-0.275043	-0.002347
4	6	0	2.030560	0.388585	0.035460
5	6	0	3.257528	-0.404952	-0.002344
6	6	0	-0.507219	-2.344157	-0.060025
7	6	0	-0.451110	0.439331	0.016483
8	6	0	-1.709154	-0.229674	-0.016371
9	6	0	-2.911725	0.583876	-0.288910
10	6	0	-1.605844	2.686217	0.009778
11	6	0	-0.371926	1.859883	0.049557
12	6	0	0.838946	2.514189	0.100162
13	6	0	2.079148	1.810412	0.102221
14	1	0	0.820282	3.596414	0.131680
15	1	0	-0.479961	-3.426154	-0.066110
16	8	0	-1.582140	3.909906	0.107166
17	8	0	-3.996781	0.119779	-0.630890
18	8	0	4.395284	0.090396	0.038296
19	8	0	1.922816	-3.732943	-0.223304
20	7	0	3.148298	-1.800341	-0.095049
21	7	0	-2.795800	1.988064	-0.184203
22	6	0	4.408950	-2.554329	-0.141985
23	6	0	-4.031983	2.755991	-0.388404
24	1	0	-4.804413	2.395005	0.292841
25	1	0	-4.389631	2.624252	-1.412402
26	1	0	4.159174	-3.609197	-0.223721
27	1	0	4.987144	-2.365114	0.764906
28	1	0	-3.806834	3.802116	-0.196049
29	1	0	5.000858	-2.230926	-1.000625
30	6	0	-1.748932	-1.652444	0.042679
31	7	0	-2.899700	-2.386751	0.220021
32	7	0	3.251173	2.489291	0.156934
33	1	0	4.083532	1.905442	0.139055
34	6	0	3.370832	3.933886	0.211598
35	1	0	4.432144	4.184446	0.250695
36	1	0	2.938261	4.416833	-0.673848
37	1	0	2.888212	4.351914	1.103815
38	6	0	-2.948206	-3.796021	-0.149037
39	1	0	-2.392663	-3.974859	-1.071572
40	1	0	-2.556709	-4.457988	0.639125
41	1	0	-3.991727	-4.066488	-0.332560
42	6	0	-3.963509	-1.965135	1.125241
43	1	0	-3.645998	-1.099901	1.708850

44	1	0	-4.877150	-1.697354	0.587198
45	1	0	-4.172322	-2.786222	1.823468

9. **4** at the first excited state S_1

Electronic Energy= -1254.9013123 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	1.938807	-2.542315	-0.000707
2	6	0	0.721689	-1.720753	-0.003204
3	6	0	0.786096	-0.286569	-0.001132
4	6	0	2.062084	0.367150	0.001137
5	6	0	3.271351	-0.424209	0.001520
6	6	0	-0.512140	-2.356899	-0.006503
7	6	0	-0.407863	0.455003	-0.001349
8	6	0	-1.665454	-0.189614	-0.002781
9	6	0	-2.911166	0.574366	-0.006178
10	6	0	-1.593768	2.685126	-0.004273
11	6	0	-0.358285	1.892054	-0.001404
12	6	0	0.873071	2.531691	-0.001914
13	6	0	2.100508	1.798215	0.001515
14	1	0	0.872453	3.614702	-0.004478
15	1	0	-0.535420	-3.442113	-0.006481
16	8	0	-1.605603	3.914722	-0.007218
17	8	0	-4.032035	0.020957	-0.015605
18	8	0	4.431018	0.070629	0.003173
19	8	0	1.920165	-3.779365	-0.001446
20	7	0	3.155795	-1.836014	0.000028
21	7	0	-2.825642	1.967356	0.002613
22	6	0	4.407273	-2.603875	0.000456
23	6	0	-4.090193	2.714816	0.004716
24	1	0	-4.730985	2.356283	0.813433
25	1	0	-4.621723	2.567757	-0.941203
26	1	0	4.146805	-3.659617	-0.008471
27	1	0	4.993811	-2.360647	0.890053
28	1	0	-3.849444	3.766703	0.136978
29	1	0	5.001826	-2.346687	-0.879609
30	6	0	-1.686867	-1.603685	-0.003957
31	7	0	-2.964902	-2.280285	0.005129
32	7	0	3.292234	2.430381	0.004482
33	1	0	4.092495	1.787586	0.002688
34	6	0	3.468473	3.868334	0.001702
35	1	0	4.538395	4.082475	0.009263
36	1	0	3.028461	4.334021	-0.889951
37	1	0	3.015225	4.338298	0.884302
38	6	0	-3.542822	-2.747209	-1.234386
39	1	0	-3.270749	-2.066670	-2.038957
40	1	0	-3.149262	-3.747911	-1.461803
41	1	0	-4.629081	-2.800037	-1.146040
42	6	0	-3.549359	-2.703670	1.257373
43	1	0	-3.174360	-2.078538	2.064134
44	1	0	-4.636206	-2.628710	1.202234
45	1	0	-3.271602	-3.750255	1.453116

10. **4H**

Electronic Energy= -1255.3186694 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	1.875013	-2.544192	-0.000365
2	6	0	0.664996	-1.679111	-0.000068
3	6	0	0.779875	-0.267567	-0.000135

4	6	0	2.050903	0.352167	-0.000108
5	6	0	3.254390	-0.486604	-0.000356
6	6	0	-0.580327	-2.292484	0.000311
7	6	0	-0.420195	0.502637	-0.000068
8	6	0	-1.684938	-0.119499	-0.000106
9	6	0	-2.913279	0.720139	-0.000570
10	6	0	-1.530404	2.765228	0.000657
11	6	0	-0.307422	1.922084	0.000251
12	6	0	0.919425	2.532609	0.000623
13	6	0	2.145677	1.776912	0.000263
14	1	0	0.948802	3.615747	0.001165
15	1	0	-0.602382	-3.377768	0.000511
16	8	0	-1.508532	3.980940	0.003209
17	8	0	-4.044422	0.194375	0.000367
18	8	0	4.397647	-0.016681	-0.000090
19	8	0	1.785732	-3.765706	-0.000070
20	7	0	3.099864	-1.880717	-0.000998
21	7	0	-2.774691	2.086018	-0.002520
22	6	0	4.338792	-2.680999	-0.001561
23	6	0	-3.979080	2.942895	-0.003842
24	1	0	-4.855504	2.302304	-0.033322
25	1	0	-3.949622	3.598341	-0.875218
26	1	0	4.055617	-3.730253	-0.007940
27	1	0	4.925706	-2.446598	0.888100
28	1	0	-3.982811	3.558735	0.896911
29	1	0	4.930811	-2.436635	-0.885025
30	6	0	-1.743585	-1.522317	0.000389
31	7	0	-3.064364	-2.194791	0.001016
32	7	0	3.325936	2.413922	0.000350
33	1	0	4.138682	1.796540	0.000330
34	6	0	3.516363	3.859568	0.000855
35	1	0	4.588604	4.055155	0.000826
36	1	0	3.083049	4.324201	-0.891396
37	1	0	3.083201	4.323587	0.893503
38	6	0	-3.317885	-2.994730	-1.247717
39	1	0	-3.178134	-2.344612	-2.111325
40	1	0	-2.623595	-3.833970	-1.293991
41	1	0	-4.345318	-3.360161	-1.216988
42	6	0	-3.316560	-2.994704	1.250041
43	1	0	-3.175637	-2.344664	2.113514
44	1	0	-4.344074	-3.360006	1.220535
45	1	0	-2.622352	-3.834063	1.295373
46	1	0	-3.736197	-1.372526	0.001209

11. **4H** at the first excited state S_1

Electronic Energy= -1255.3124245 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	1.862447	-2.537878	-0.000185
2	6	0	0.663101	-1.687662	-0.000056
3	6	0	0.761705	-0.282112	-0.000149
4	6	0	2.046273	0.347272	-0.000108
5	6	0	3.268296	-0.499675	-0.000274
6	6	0	-0.601955	-2.301768	0.000268
7	6	0	-0.413505	0.513060	-0.000199
8	6	0	-1.701363	-0.108440	-0.000220
9	6	0	-2.900958	0.703578	-0.000430
10	6	0	-1.532193	2.760429	0.000327
11	6	0	-0.302843	1.931400	0.000049
12	6	0	0.926149	2.563829	0.000420
13	6	0	2.118595	1.784242	0.000209

14	1	0	0.955589	3.644911	0.000837
15	1	0	-0.637821	-3.385896	0.000501
16	8	0	-1.494803	3.985618	0.002305
17	8	0	-4.057119	0.178852	0.000473
18	8	0	4.409632	-0.014497	-0.000021
19	8	0	1.803870	-3.759244	-0.000135
20	7	0	3.110172	-1.870418	-0.000643
21	7	0	-2.759000	2.081334	-0.001784
22	6	0	4.344217	-2.678849	-0.000985
23	6	0	-3.964786	2.931804	-0.002695
24	1	0	-4.837824	2.286224	-0.027138
25	1	0	-3.940808	3.586297	-0.875474
26	1	0	4.052924	-3.725666	-0.003231
27	1	0	4.933982	-2.444643	0.887182
28	1	0	-3.968333	3.552837	0.894939
29	1	0	4.935634	-2.441070	-0.887061
30	6	0	-1.746534	-1.525425	0.000276
31	7	0	-3.083248	-2.160598	0.000696
32	7	0	3.339394	2.362258	0.000314
33	1	0	4.121379	1.684725	0.000185
34	6	0	3.593136	3.786561	0.000594
35	1	0	4.670259	3.947535	0.000464
36	1	0	3.154249	4.259853	-0.886921
37	1	0	3.154536	4.259454	0.888469
38	6	0	-3.360861	-2.947997	-1.246075
39	1	0	-3.198878	-2.302352	-2.109347
40	1	0	-2.699138	-3.813749	-1.296096
41	1	0	-4.401683	-3.274619	-1.219090
42	6	0	-3.360049	-2.947989	1.247644
43	1	0	-3.197538	-2.302327	2.110803
44	1	0	-4.400877	-3.274645	1.221321
45	1	0	-2.698261	-3.813716	1.297236
46	1	0	-3.734491	-1.283303	0.000905

12. **5**

Electronic Energy= -1371.676097 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	-1.401359	-2.938343	-0.092507
2	6	0	-0.600579	-1.690132	-0.071098
3	6	0	-1.231509	-0.422398	-0.007797
4	6	0	-2.647500	-0.321473	0.040420
5	6	0	-3.450850	-1.542782	0.035027
6	6	0	0.774798	-1.795836	-0.076527
7	6	0	-0.393497	0.726560	-0.007433
8	6	0	1.027511	0.621216	-0.038645
9	6	0	1.809739	1.865355	-0.228621
10	6	0	-0.257318	3.251499	-0.063934
11	6	0	-1.044045	1.994016	0.006017
12	6	0	-2.414785	2.103631	0.059267
13	6	0	-3.266152	0.959553	0.089900
14	1	0	-2.833708	3.102089	0.069741
15	1	0	1.185348	-2.796924	-0.076552
16	8	0	-0.782285	4.360096	-0.011326
17	8	0	3.022727	1.898452	-0.413420
18	8	0	-4.691609	-1.545652	0.085581
19	8	0	-0.889397	-4.051953	-0.156319
20	7	0	-2.790019	-2.777002	-0.033953
21	7	0	1.116658	3.096266	-0.221861
22	6	0	-3.639542	-3.976183	-0.045742
23	6	0	1.941988	4.300140	-0.394485

24	1	0	2.474255	4.248280	-1.346230
25	1	0	2.680589	4.362825	0.407633
26	1	0	-2.985589	-4.842581	-0.105332
27	1	0	-4.313737	-3.942889	-0.904053
28	1	0	1.278960	5.161266	-0.369406
29	1	0	-4.242630	-4.010826	0.863922
30	6	0	1.638041	-0.667038	-0.019043
31	7	0	-4.610824	1.109914	0.153576
32	1	0	-5.136790	0.239237	0.156001
33	6	0	-5.302415	2.384631	0.197420
34	1	0	-6.373994	2.186507	0.252256
35	1	0	-5.018607	2.974693	1.077683
36	1	0	-5.111594	2.987260	-0.699503
37	6	0	3.772227	-0.309733	1.176501
38	6	0	3.563950	-2.153044	-0.417649
39	6	0	5.239368	-0.087269	0.807537
40	1	0	3.706497	-1.019050	2.022903
41	1	0	3.314359	0.623755	1.492105
42	6	0	5.030484	-1.980159	-0.836416
43	1	0	3.496807	-2.926491	0.369786
44	1	0	2.980753	-2.498944	-1.274162
45	6	0	5.875737	-1.386640	0.297716
46	1	0	5.774354	0.284904	1.689810
47	1	0	5.285628	0.689505	0.037304
48	1	0	5.422356	-2.956729	-1.145656
49	1	0	5.069487	-1.319019	-1.711050
50	1	0	6.901144	-1.206146	-0.045134
51	1	0	5.941009	-2.112279	1.121886
52	7	0	3.010451	-0.876238	0.048020

13. **5H**

Electronic Energy= -1372.0745984 Hartree/ Molecule
Standard Orientation Coordinates:

1	6	0	-1.208275	-2.966428	-0.000069
2	6	0	-0.498288	-1.659735	-0.000047
3	6	0	-1.218234	-0.440251	0.000027
4	6	0	-2.632563	-0.438083	0.000083
5	6	0	-3.348457	-1.718023	0.000079
6	6	0	0.889540	-1.667592	-0.000087
7	6	0	-0.474282	0.775923	0.000014
8	6	0	0.935497	0.766784	0.000015
9	6	0	1.666299	2.060638	-0.000063
10	6	0	-0.469806	3.302515	-0.000253
11	6	0	-1.195513	2.004173	-0.000037
12	6	0	-2.566062	2.016451	-0.000019
13	6	0	-3.339624	0.801952	0.000170
14	1	0	-3.064933	2.978196	-0.000237
15	1	0	1.382822	-2.633978	-0.000113
16	8	0	-1.037462	4.377967	-0.000536
17	8	0	2.911236	2.103166	-0.000189
18	8	0	-4.582287	-1.795450	0.000178
19	8	0	-0.595573	-4.027185	-0.000266
20	7	0	-2.600201	-2.904527	-0.000077
21	7	0	0.947148	3.230960	0.000021
22	6	0	-3.365134	-4.165258	-0.000171
23	6	0	1.714698	4.492949	-0.000060
24	1	0	2.347052	4.535791	-0.888325
25	1	0	2.347213	4.535764	0.888091
26	1	0	-2.652072	-4.985450	-0.000347
27	1	0	-4.000233	-4.207351	-0.886596

28	1	0	1.000883	5.312189	0.000014
29	1	0	-4.000068	-4.207590	0.886362
30	6	0	1.603662	-0.468010	-0.000068
31	7	0	-4.680153	0.860488	0.000289
32	1	0	-5.142856	-0.049044	0.000007
33	6	0	-5.480915	2.078766	0.000293
34	1	0	-6.531385	1.788000	0.001920
35	1	0	-5.291883	2.686124	0.891998
36	1	0	-5.294159	2.684685	-0.892893
37	6	0	3.662641	-1.123962	1.260418
38	6	0	3.662704	-1.124665	-1.260150
39	6	0	5.184943	-0.996453	1.262024
40	1	0	3.344963	-2.169966	1.277557
41	1	0	3.201558	-0.605831	2.104172
42	6	0	5.185024	-0.997111	-1.261764
43	1	0	3.345103	-2.170697	-1.276724
44	1	0	3.201667	-0.607042	-2.104241
45	6	0	5.806581	-1.611620	0.000306
46	1	0	5.559490	-1.489472	2.165019
47	1	0	5.462549	0.062377	1.344844
48	1	0	5.559618	-1.490581	-2.164489
49	1	0	5.462584	0.061690	-1.345097
50	1	0	6.888705	-1.452477	0.000308
51	1	0	5.647093	-2.698084	0.000586
52	7	0	3.080264	-0.501679	-0.000075
53	1	0	3.342956	0.520300	-0.000269

Supplementary References

S1 F. Doria, M. Nadai, M. Folini, M. Scalabrin, L. Germani, G. Sattin, M. Mella, M. Palumbo, N. Zaffaroni, D. Fabris, M. Freccero and S.N. Richter. *Chem. Eur. J.* **2013**, 19, 78.

S2 F. J. C. Rossotti, and H. Rossotti, *J. Chem. Educ.* **1965**, 42, 375-378.

S3 P. Gans, A. Sabatini and A. Vacca, *Talanta* **1996**, 43, 1739.

S4 M. J. Frisch, Gaussian, Inc., Wallingford CT, 2009.