Supporting Information

Controlling the reactivity of phthalonitriles for the efficient synthesis of chiral phthalocyanines with self-assembly abilities

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1. General Information

All chemical reagents and solvents were analytical grade and were used without further purification. All reactions were performed in standard glassware, except for the cyclotetramerization reactions that were carried out in high pressure sealed tubes. Analytical TLC was carried out employing aluminum sheets coated with silica gel type 60 F254 (0.2 mm thick, E. Merck). Purification and separation of the synthesized products was performed by column chromatography, using silica gel (230–400 mesh, 0.040-0.063 mm, Merck). Eluents and relative proportions of the solvents are indicated for each particular case. Size exclusion chromatography was performed using Bio-Beads S-X1 (200-400 mesh, Bio-Rad). Anion exchange was performed using of Dowex® resin. Mass Spectrometry (MS) and HighResolution Mass Spectrometry (HRMS) spectra were recorded employing Electrospray Ionization (ESI Positive TOF_MS) mass spectra using an API Q-Star Pulsar i from Sciex, or Matrix Assisted Laser Desorption/Ionization-Time of Flight (MALDI-TOF) using a Bruker Ultraflex III TOF/TOF spectrometer, with a nitrogen laser operating at 337 nm, or with a NdYAG laser operating at 335 nm. The different matrixes employed are indicated for each spectrum. Mass spectrometry data are expressed in m/z units. All MS experiments were carried out at the Servicio Interdepartmental de Investigación (SIdI) of the Universidad Autónoma de Madrid. ^{1}H NMR and ^{13}C NMR were recorded on Bruker XRD-300 (300 MHz) and XRD-500 (500 MHz) instruments. Deuterated solvents employed are indicated in each spectrum.
Compounds **AA-1**,[2] **AA-2**[2] and **2**[3] were prepared following reported procedures.

Spectroscopic and photophysical characterization
UV-vis spectra were recorded on a JASCO-V660 UV-vis spectrophotometer using spectroscopic grade solvents. Absorption coefficients were derived from the slopes of Lambert-Beer plots using solutions from 1.5 µM to 6 µM. Fluorescence spectra were recorded with a JASCO FP-8600 spectrophotometer using spectroscopic grade solvents. UV-Vis and fluorescence measurements were performed using 10 x 10mm quartz cuvettes with a Jasco Peltier ETCS-761 temperature controller incorporated keeping temperature constant at 20ºC. Circular dichroism spectra were recorded on a JASCO J-815 CD-spectrometer including a Jasco Peltier ETCT-762 temperature controller using spectroscopic grade solvents and 10 x 10mm quartz cuvettes. Fluorescence spectra for determining fluorescence quantum yield (Φ_F) were performed using a Fluorolog-3 (FL3-iHR) spectrophotometer (HORIBA JobinYvon). Φ_F was determined by means of Equation 1, comparing the integrated fluorescent intensity of optically matched solutions between sample (S) and reference (R) ZnPc in DMSO (Φ = 0.20).[1] The samples were excited at 630 nm.

$$\Phi F = \frac{Area\ (S)}{Area\ (R)} \times \frac{Abs\ (R)}{Abs\ (S)} \times \frac{n^2(S)}{n^2(R)} \times \Phi R \qquad \text{Eq. 1}$$

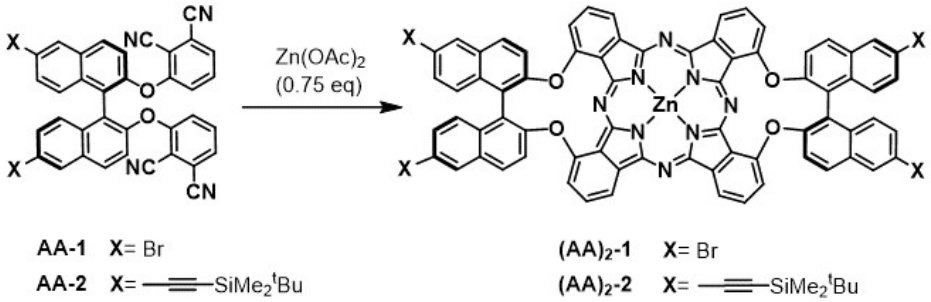
Characterization of nanoaggregates
Samples were imaged using a microscope JEOL JEM 1400 plus from ICTS - Centro Nacional de Microscopía Electrónica, UCM. Samples were prepared over Carbon Film 200 Mesh, CF200-CU grids, with glow-discharge treatment. Solutions were prepared, filtered, sonicated 10 minutes, and left to stand overnight. Dynamic Light Scattering (DLS) measurements were performed in a Malvern Zetasizer Nanoseries Nano- ZS, using quartz cuvettes (1cm). All solutions were prepared using MilliQ water.

Computational method
All the DFT calculations were carried out by employing Gaussian13 software using B3LYP/6-31G(d) level of theory. The counterions of **1** were excluded in the calculations to save

computational cost.

2. Study of the cyclotetramerization reaction conditions

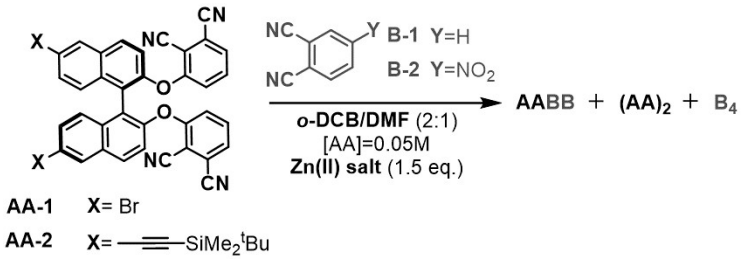
Table S1. Study of the cyclotetramerization reaction conditions of bisphthalonitriles **AA**



Entry	**AA** (eq)	Solvent ([**AA**]=0.05M)	T (ºC)	Time (h)	**(AA)$_2$** (%)[a]
1	**1** (1.0)	o-DCB/DMF (2:1)	150	16	2
2	**2** (1.0)	o-DCB/DMF (2:1)	150	16	7
3	**1** (1.0)	DMAE	120	16	3
4	**1** (1.0)	DMAE/LiOMe (0.5eq)	120	16	4
5[b]	**1** (1.0)	o-DCB/DMF (2:1)	150	2	3
6[b]	**1** (1.0)	DMAE	130	1	3
7[b]	**1** (1.0)	DMAE	130	2	3
8[b]	**1** (1.0)	DBU/1-pentanol (1:1)	150	0.5	4

[a] Isolated yield after purification through flash column chromatography. [b] Reactions performed under MW irradiation.

Table S2 Study of the cross-cyclotetramerization reaction conditions between **AA** and **B** under MW irradiation.



Entry	**AA** (eq)	**B** (eq)	T (ºC)	Time (h)	**(AA)$_2$** (%)	**AABB** (%)
1	**1** (1.0)	**1** (2.0)	150	2	2	15
2	**1** (1.0)	**2** (2.0)	150	2	5	-[a]
3	**2** (1.0)	**2** (2.0)	150	2	3	2

[a] AABB-4 not isolated from the reaction mixture due to solubility issues

3. Experimental procedures and characterization data

3.1 General procedure for the synthesis of AABB and $(AA)_2$ Zn(II)Pcs: Bisphthalonitrile **AA** (1 eq.), phthalonitrile **B** (2 eq.) and anhydrous $Zn(AcO)_2$ (1.5-2 eq.) were placed in a 5 mL high pressure resistant flask equipped with a magnetic stirrer, and then dry *o*-dichlorobenzene/DMF (dried over 4Å molecular sieves) 2:1 were added, for [AA]=0.05 M. The mixture was heated to 150-160°C overnight under argon atmosphere. After cooling, the solvent was removed under vacuum. The mixture of products was then purified as follows.

3.2 Synthesis of $(AA)_2$-1 and AABB-4: Following the general procedure, bisphthalonitrile **AA-1**[2] (60 mg, 0.074 mmol), phthalonitrile **B-2** (29.8 mg, 0.147 mmol) and anhydrous $Zn(AcO)_2$ (23.8 mg, 0.110 mmol). The blue solid containing a mixture of **B_4-2**, **AABB-4** and **$(AA)_2$-1** was purified by flash column chromatography (heptane:THF 1:1). The first eluted product was **$(AA)_2$-1** as a blue solid. The solid was washed with MeOH and isolated in a 14% yield (8.8 mg). **^{1}H-NMR** (500 MHz, Pyridine-d_5): δ 9.62-9.54 (m, 4H, H_{Ar}), 8.26-8.19 (m, 4H, H_{Ar}), 8.15 (s, 4H, H_{Ar}), 8.03-7.97 (m, 8H, H_{Ar}), 7.94-7.86 (m, 4H, H_{Ar}), 7.83-7.80 (d, J = 9.0 Hz, 4H, H_{Ar}), 7.79-7.69 (m, 4H, H_{Ar}) ppm. **^{13}C NMR** (126 MHz, Pyridine-d_5): δ 156.5, 154.3, 153.3, 142.6, 140.0, 134.5, 131.9, 131.6, 131.3, 131.1, 129.4, 128.3, 126.5, 126.3, 121.5, 119.9, 118.5, 115.8 ppm. **HR-MS**: MALDI (ULTRAFLEX III); DCTB + PPGNa 1000 + PPGNa 2000; 1451.8566 (calculated for $C_{72}H_{32}Br_4N_8O_4Zn$); 1451.8524 (experimental). **IR(ATR)** ν^{-1} (cm-1): 1577, 1483, 1330, 1267, 1260, 1198, 1103. **UV-Vis** (THF) log(ε/$M^{-1}cm^{-1}$) (λ): 4.5 (345 nm); 4.2 (613 nm); 5.0 (684 nm). **Fluorescence**: $\lambda_{maximum}$ = 693 nm; $\lambda_{excitation}$ = 674 nm.

3.3 Synthesis of $(AA)_2$-2 and AABB-3: Following the general procedure: Bisphthalonitrile **AA-2**[2] (60 mg, 0.074 mmol), phthalonitrile **B-2** (25.5 mg, 0.147 mmol) and anhydrous $Zn(AcO)_2$ (20.3 mg, 0.110 mmol). The blue solid containing a mixture of **B_4-2**, **AABB-3** and **$(AA)_2$-2** was dissolved in THF (2 mL). The mixture was purified through a silica gel plug in THF, obtaining a mixture of **AABB-3** and **$(AA)_2$-2**. After evaporation of the solvent under reduced pressure, the mixture was dissolved in 4 mL THF, then heptane (10 mL) was added and the precipitate that appears was separated from the solution. The precipitate was submitted to the same procedure two more times, then washed with heptane and MeOH to obtain pure **AABB-3** as a blue solid in a 4% yield (8 mg). **^{1}H NMR** (500 MHz, DMSO-d_6, 353K) δ 9.23-9.02 (m, 1H, H_{Ar}), 9.00-8.84 (m, 1H, H_{Ar}), 8.80-8.68 (m, 1H, H_{Ar}), 8.65-8.42 (m, 3H, H_{Ar}), 8.40-8.20 (m, 3H, H_{Ar}), 8.19 – 7.55 (m, 13H, H_{Ar}), 1.08-0.98 (m, 18H, ^{t}Bu), 0.28-0.17 (m, 12H, Si-CH_3) ppm. **HR-MS**: MALDI (ULTRAFLEX III); DCTB + PPGNa 1000; 1224.2901 (calculated for $C_{68}H_{52}N_{10}O_6Si_2Zn$); 1224.2896 (experimental). UV-vis (THF) log(ε /$M^{-1}cm^{-1}$) (λ): 4.7 (350 nm); 4.5 (639 nm); 4.9 (682 nm). **Fluorescence** (THF): $\lambda_{maximum}$ = 702 nm; $\lambda_{excitation}$ = 650 nm. The supernatant was evaporated under reduced pressure and purified by flash column chromatography (heptane/THF 3:2) obtaining **$(AA)_2$-2** in the first eluting fraction. After washing with MeOH the blue solid was obtained in a 21% yield (13 mg). **^{1}H-NMR** (500 MHz, Pyridine-d_5): δ 9.81-9.40 (m, 4H, H_{Ar}), 8.42-8.18 (m, 4H, H_{Ar}), 8.14 (d, J = 9.4 Hz, 4H, H_{Ar}), 8.09-7.93 (m, 8H, H_{Ar}), 7.91-7.85 (m, 4H, H_{Ar}), 7.83-7.63(m, 4H, H_{Ar}), 1.08 (s, 36H, ^{t}Bu), 0.27 (s, 24H, Si-CH_3) ppm. **^{13}C NMR** (126 MHz, Pyridine-d_5): δ 157.2, 154.3, 153.3, 142.6, 133.7, 131.5, 131.1, 130.7, 130.5, 130.3, 126.6, 126.5, 121.5, 120.0, 119.3, 115.6, 107.7 (C≡), 93.3(≡C-Si), 26.7 (^{t}Bu), 17.4 (C-^{t}Bu), -3.9 (Si-CH_3) ppm. **HR-MS**: MALDI (ULTRAFLEX III); DCTB + PEGNa 1500; 1692.5605 (calculated for $C_{104}H_{92}N_8O_4Si_4Zn$), 1692.5619 (experimental). **IR(ATR)** ν^{-1} (cm^{-1}): 2953, 2147, 1710, 1574, 1470, 1358, 1250, 1219, 1087, 825. UV-Vis (THF) log(ε/$M^{-1}cm^{-1}$) (λ):4.7 (299 nm); 4.7 (349 nm); 4.4 (614 nm); 5.2 (684 nm). **Fluorescence**: $\lambda_{maximum}$ = 683 nm; $\lambda_{excitation}$ = 650 nm.

3.4 Synthesis of 4: $(AA)_2$-2 (17.5 mg, 0.010 mmol) was dissolved in dry THF (0.56 mL), under argon atmosphere. TBAF (purchased from Aldrich, 1 M in THF, 82.5 µL, 0.083 mmol) was added dropwise, and the reaction was stirred for 2h at rt. After that, water (4 mL) was added. The blue precipitate was filtered off, dried and directly added to a Schlenk flask together with $Pd(PPh_3)_4$ (2.4mg, 0.002 mmol) and **2**[3] (37.24 mg, 0.052 mmol). The mixture was dissolved in dry DMF (0.27 mL) and Et_3N (0.11 mL) degassed by three freeze-pump-thaw cycles at room temperature. The reaction mixture was heated at 80 ºC under argon atmosphere, and maintained under continuous stirring 45 min. The disappearance of the product was monitored by TLC in heptane/THF (2:3). After evaporation of the solvent, the product was purified by column chromatography in Bio-Beads using THF as eluent. The product was washed with heptane, obtaining **5** (10.6 mg) as a blue-green solid in a 27% yield over two steps. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 9.6-7.06 (m, 32H, H_{Ar}), 7.00-6.65 (br s, 8H, H_{Ar}), 4.13-3.78 (m, 24H,O-CH_2), 3.41-3.24 (m, 24H, -CH_2-) 2.86-2.70 (br s, 36H, N-CH_3), 2.04-1.69 (m, 24H, N-CH_2), 1.46-1.24 (br s, 108H, CH_3) ppm. **HR-MS**: MALDI (ULTRAFLEX III); DCTB + PMMANa 4300 + NaI; 3785,7904 (calculated for $C_{212}H_{256}N_{20}O_{40}Zn$), 3.808.7796 (experimental for $[M+Na]^+$). **UV-vis** (THF) log(ε /$M^{-1}cm^{-1}$) (λ): 4.6 (350 nm); 4.2 (616 nm); 4.9 (685 nm). **Fluorescence** (THF): $\lambda_{maximum}$ = 691 nm; $\lambda_{excitation}$ = 650 nm.

3.5 Synthesis of 5: 4 (10.5 mg, 0.003 mmol) was dissolved in dry CH_2Cl_2 (3.5 mL). TFA (79 µL, 1.032 mmol) was added dropwise at 0°C, and the reaction was stirred for 5h at rt. After that time a green oily phase appears. The solvent is removed under reduced pressure. The remaining solid is dissolved in water (0.3 mL), turning the product from green to blue, and precipitated by adding acetone (5 mL). After filtration, the product is obtained as a blue solid in a 55 % yield (6 mg). **^{1}H-NMR** (300 MHz, DMSO-d_6): δ 9.53-9.34 (m, 4H, H_{Ar}), 8.93-8.48 (br s, 24H, NH_2); 8.44-8.32 (m, 4H, H_{Ar}); 8.23 (s, 4H, H_{Ar}); 8.14-7.98 (m, 8H, H_{Ar}); 7.86-7.76 (m, 4H, H_{Ar}), 7.72-7.50 (m, 8H, H_{Ar}), 6.92 (s, 8H, H_{Ar}), 4.19-4.04 (m, 16H, O-CH_2), 4.02-3.94 (m, 8H, O-CH_2), 3.15-2.99 (m, 24H, N-CH_2), 2.61 (s, 36H, CH_3), 2.15-1.90 (m, 24H, -CH_2-) ppm. **HR-MS**: MALDI (ULTRAFLEX III); ACC + PPGNa 2000 + PPGNa 2700; 2584,1660 (calculated for C153H161N19O16Zn), 2586.1685 (experimental for [M+H]+).

3.6 Synthesis of 1: 5 (as the trifluoroacetate salt) (6 mg, 0.002 mmol) was dissolved in 0.84 mL of dry DMF (dried over 4Å molecular sieves). Then, an excess of IMe (10.8 µL, 0.174mmol) and PMP (10.1 µL, 0.056mmol) were added and left reacting overnight at rt. Then acetone (5 mL) was added, and the blue solid is separated from the supernatant through centrifugation. The solid is further washed with acetone three more times until the supernatant was colourless. The blue solid was dissolved in 5 mL of MilliQ water and 250mg of Dowex® (1x8 200-400) were added. After stirring for 2h the resin was filtered, and the solvent evaporated under reduced pressure. Yield: 98% (5 mg). **^{1}H-NMR** (300 MHz, DMSO-d_6): δ 9.49-9.31 (m, 4H, H_{Ar}), 8.38-8.29 (m, 4H, H_{Ar}), 8.25-8.17 (m, 4H, H_{Ar}), 8.13-7.95 (m, 8H, H_{Ar}), 7.86-7.75 (m, 4H, H_{Ar}), 7.73-7.62 (m, 4H, H_{Ar}), 7.61-7.50 (m, 4H, H_{Ar}), 6.97 (s, 8H, H_{Ar}), 4.17-4.07 (m, 16H, O-CH_2), 4.02-3.92 (m, 8H, O-CH_2), 3.72-3.43 (m, 24H, N-CH_2), 3.15 (s, 108H, CH_3), 2.26-2.06 (m, 24H, -CH_2-) ppm. **HR-MS**: (ESI Positive ESI+50-3000.m/ Dilution 0.5:0.5:5 H_2O:DMSO: MeOH+0.1% TFA) for $C_{177}H_{221}N_{19}O_{16}Zn$: m/z 1291.8271 $[MTFA_8Cl]^{3+}$ (calculated: 1291.8292); m/z 959.8782 $[MTFA_8]^{4+}$ (calculated: 959.8798); m/z 940.6239 $[MTFA_7Cl]^{4+}$ (calculated: 940.6255); m/z 745.5053 $[MTFA_7]^{5+}$ (calculated: 745.5067); m/z 602.4234 $[MTFA_6]^{6+}$ (calculated: 602.4246); m/z 500.0789 $[MTFA_5]^{7+}$ (calculated: 500.0803); m/z 423.5709 $[MTFA_4]^{8+}$ (calculated: 423.5720). **UV-vis** (DMSO) log(ε /$M^{-1}cm^{-1}$) (λ): 4.0 (323 nm); 4.0 (618 nm); 4.7 (691 nm). **Fluorescence** (THF): $\lambda_{maximum}$ = 697 nm; $\lambda_{excitation}$ = 650 nm.

4. NMR spectra

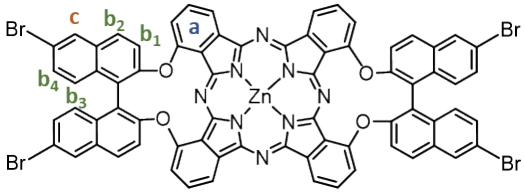


Figure 1 Structure of **$(AA)_2$-1** and H assignation for ^{1}H NMR

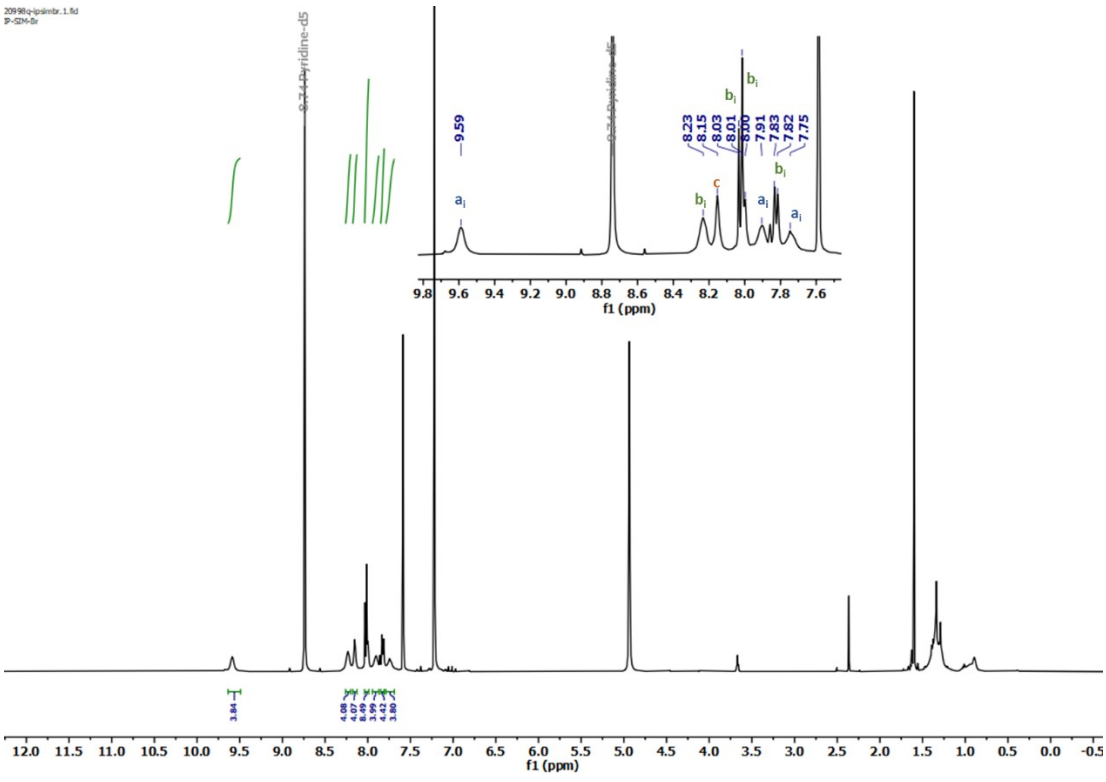


Figure 2 ^{1}H NMR (Pyridine-d_5, 500 MHz) of **$(AA)_2$-1**

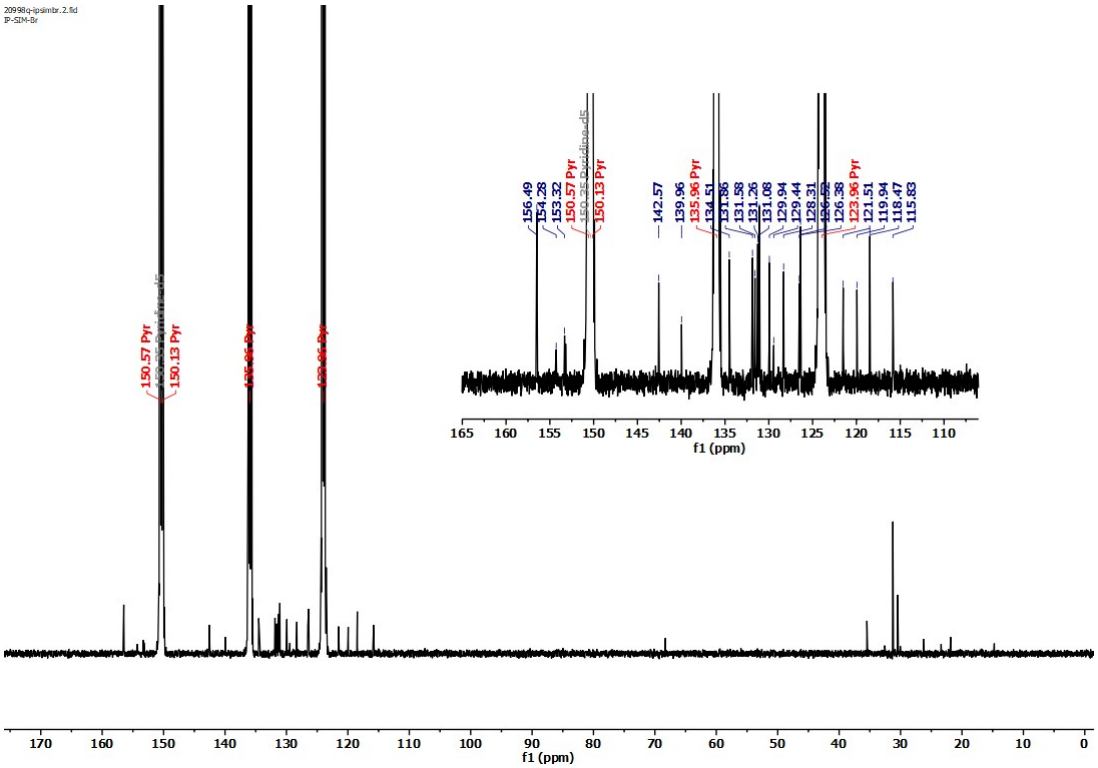


Figure 3 ^{13}C NMR (Pyridine-d_5, 126 MHz) of **$(AA)_2$-1**

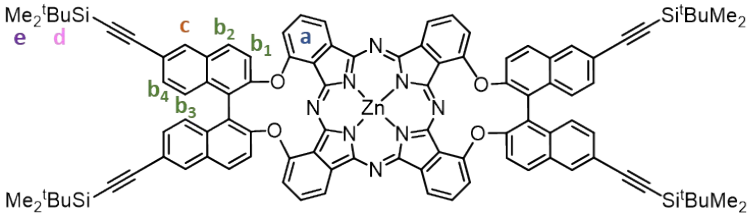


Figure 4 Structure of **$(AA)_2$-2** and H assignation for ^{1}H NMR

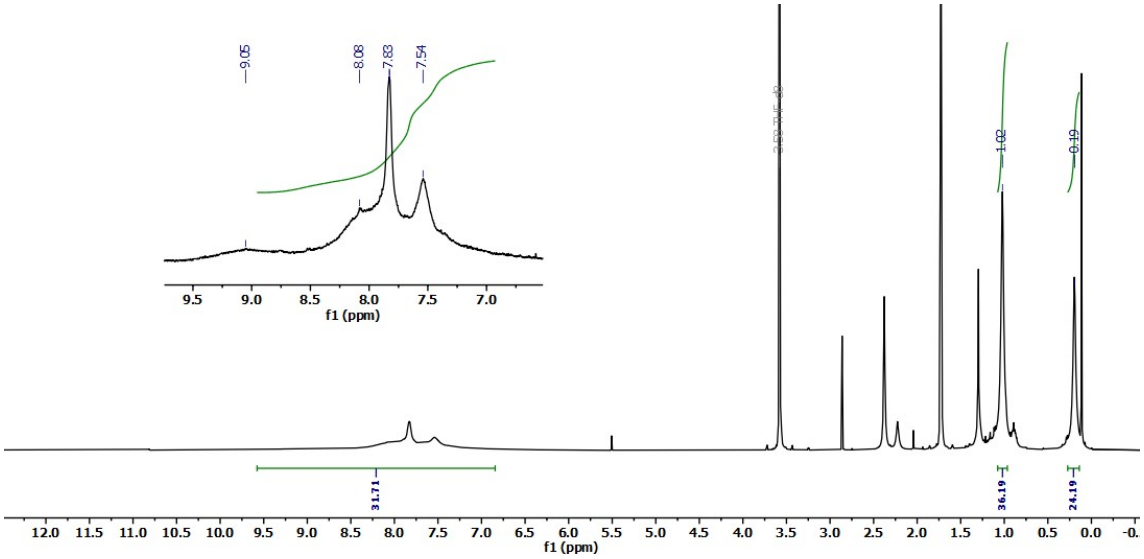


Figure 5 ^{1}H NMR (THF-d_8, 300 MHz) of **$(AA)_2$-2**

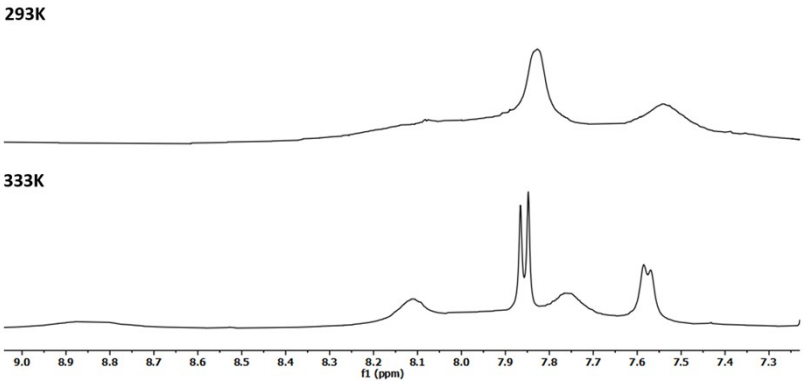


Figure 6 ^{1}H NMR (THF-d_8, 300 MHz) of **$(AA)_2$-2** (disaggregation induced by temperature)

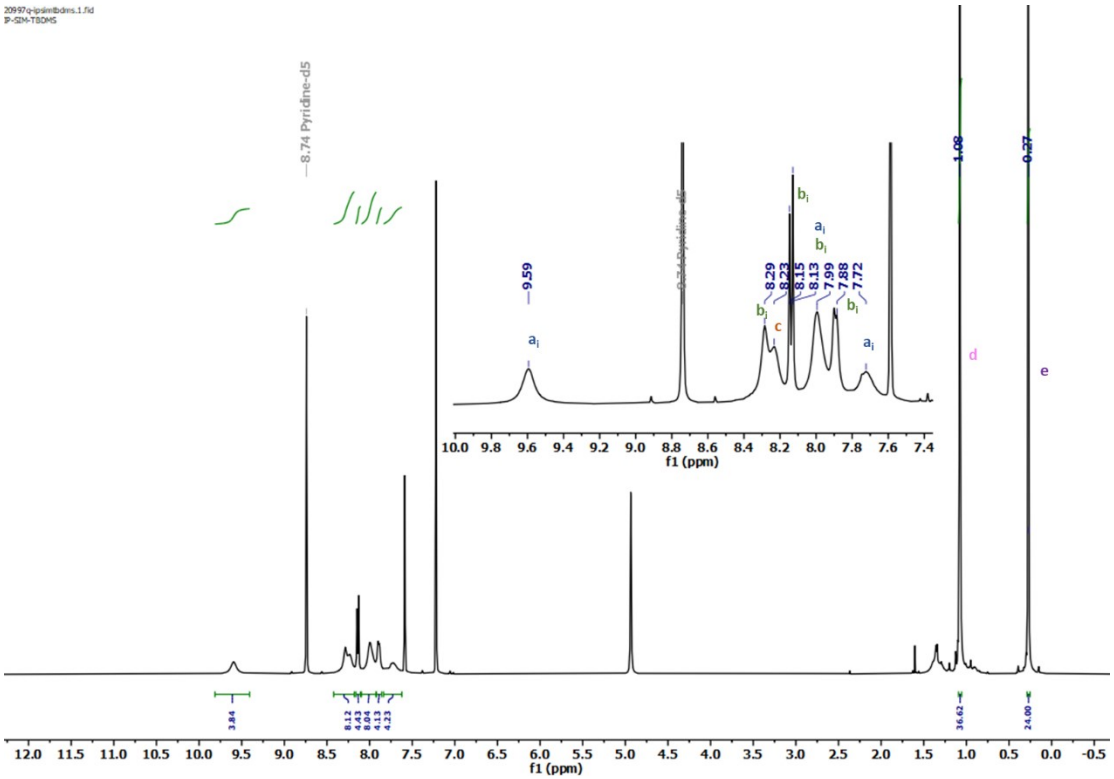


Figure 7 ^{1}H NMR (Pyridine-d_5, 500 MHz) of **$(AA)_2$-2**

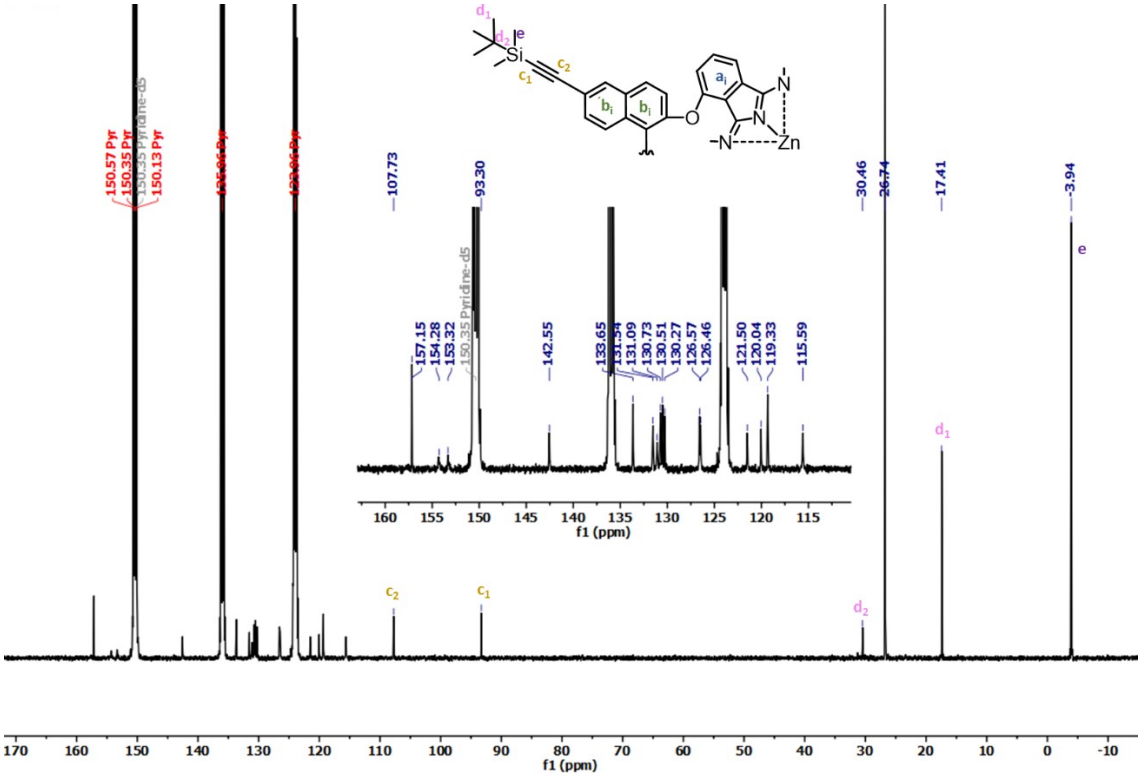


Figure 8 ^{13}C NMR (Pyridine-d_5, 126 MHz) of **$(AA)_2$-2**

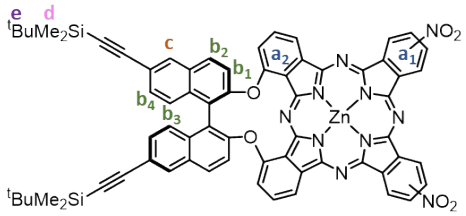


Figure 9 Structure of **AABB-3** and H assignation for ^{1}H NMR.

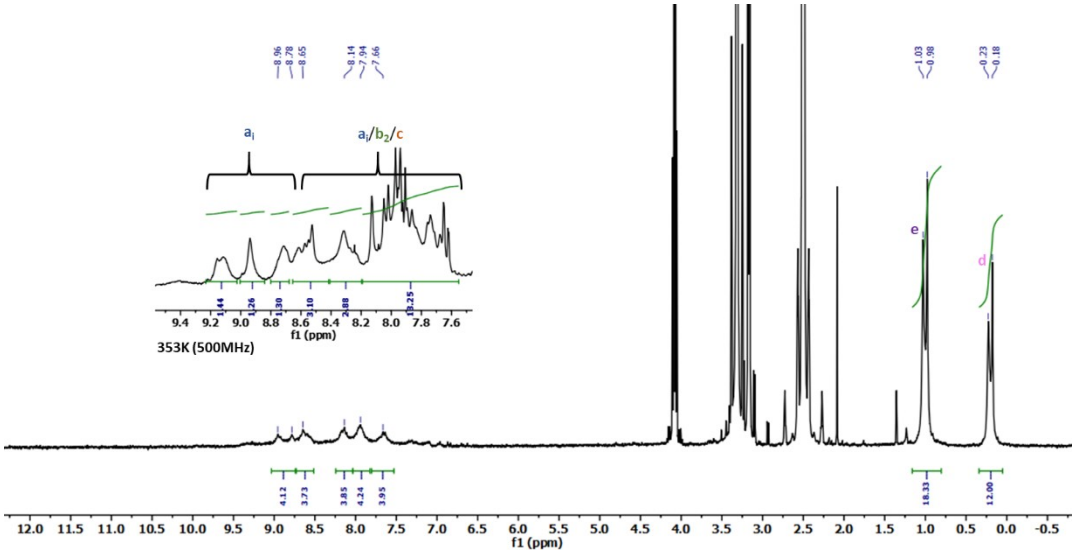


Figure 10 ^{1}H NMR (DMSO-d_6, 300 MHz) of **AABB-3**

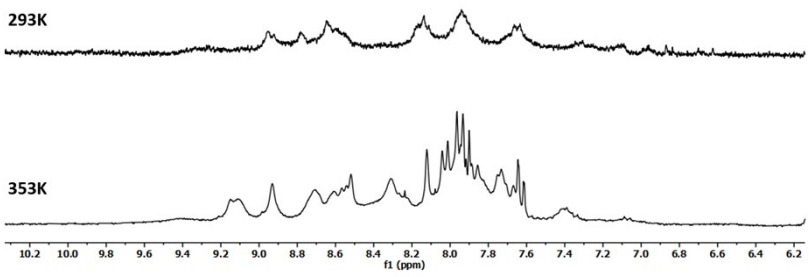


Figure 11 ^{1}H NMR (DMSO-d_6, 500 MHZ) of **AABB-3** (disaggregation induced by temperature).

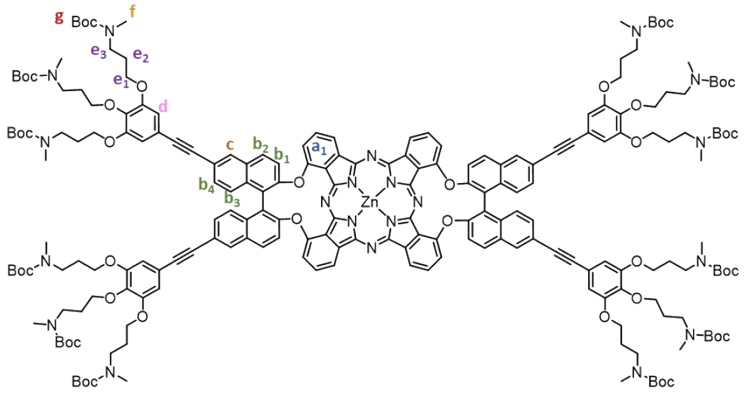


Figure 12 Structure of **4** and H assignation for ^{1}H NMR.

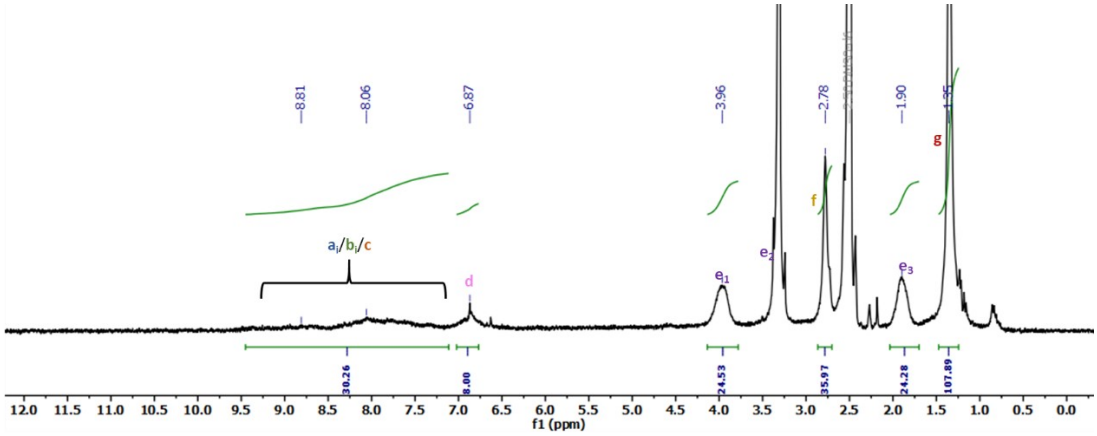


Figure 13 ^{1}H NMR (DMSO-d_6, 300 MHz) of **4**

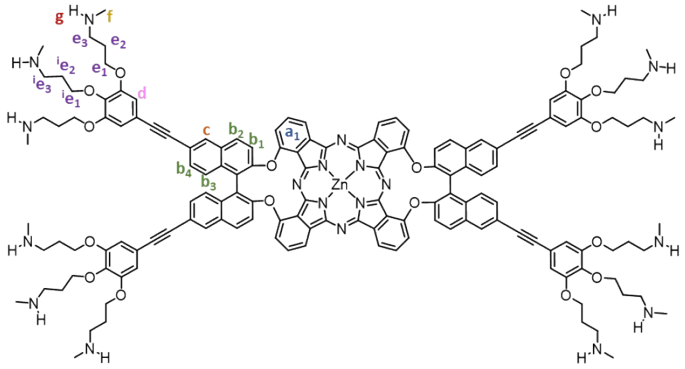


Figure 14 *Structure of* **5** *and H assignation for* ^{1}H *NMR*

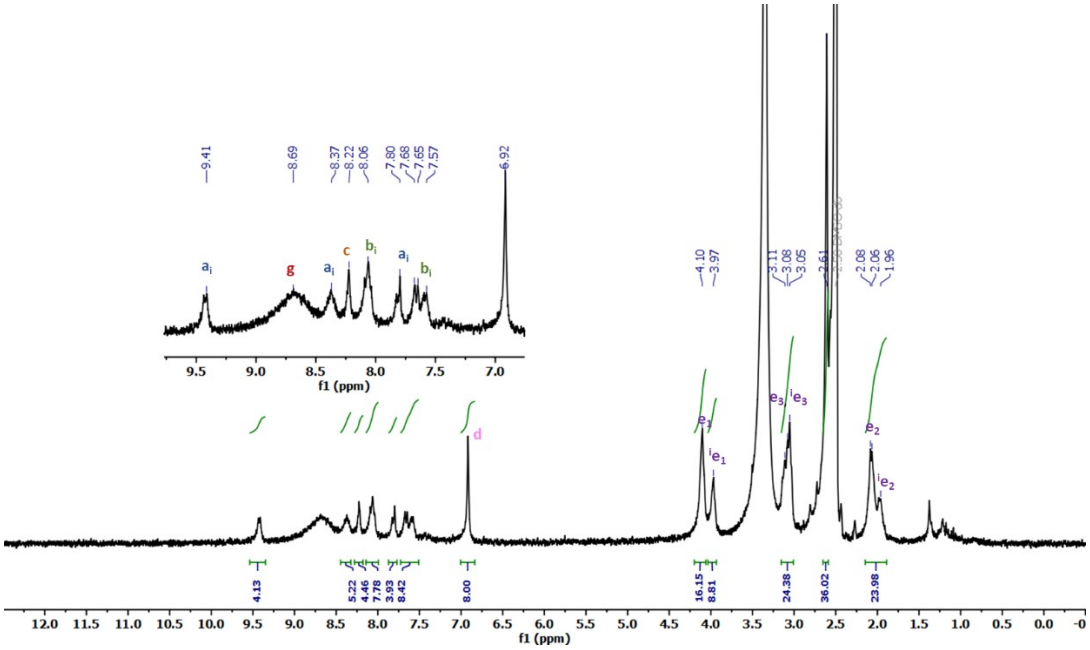


Figure 15 ^{1}H NMR (DMSO-d_6, 300 MHz) of **5**

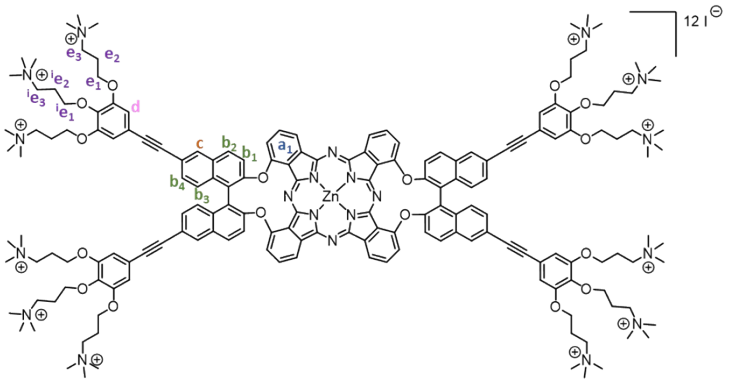


Figure 16 Structure of **1** with I^- as counterion and H assignation for ^{1}H NMR

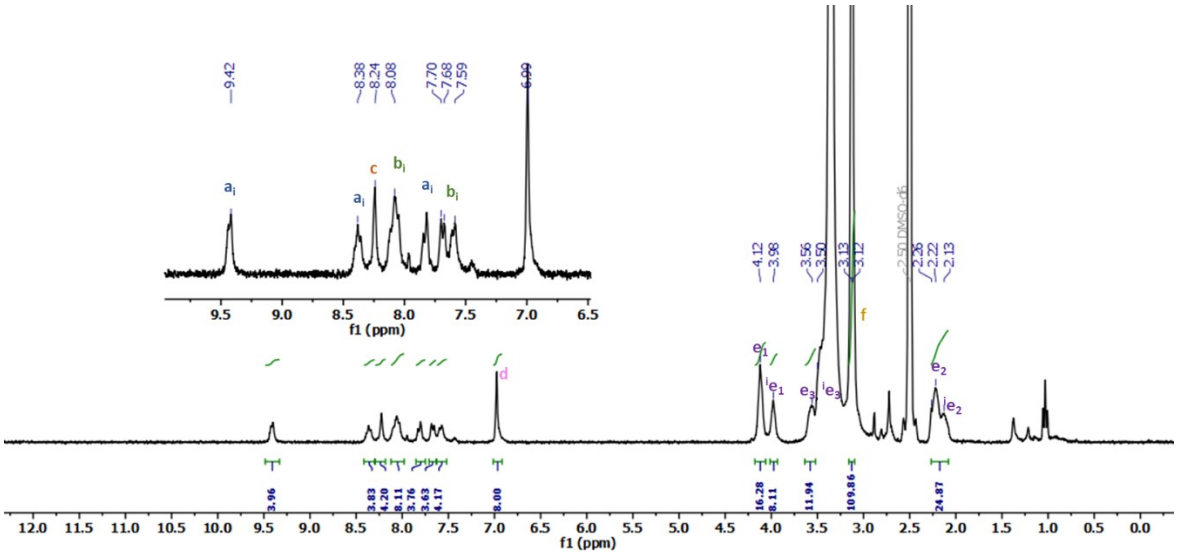


Figure 17 ^{1}H NMR (DMSO-d_6, 300 MHz) of **1**

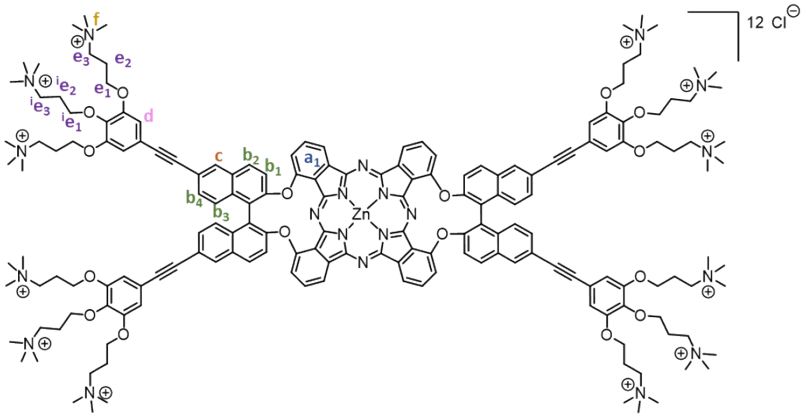


Figure 18 Structure of **1** with Cl^- as counterion and H assignation for ^1H NMR

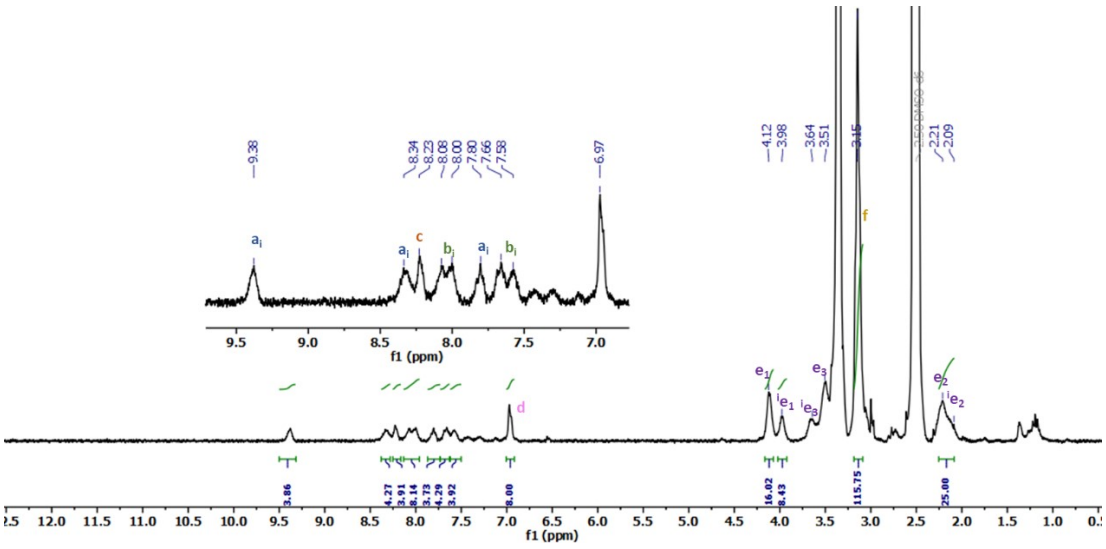


Figure 19 ^1H NMR (DMSO-d_6, 300 MHz) of **1**

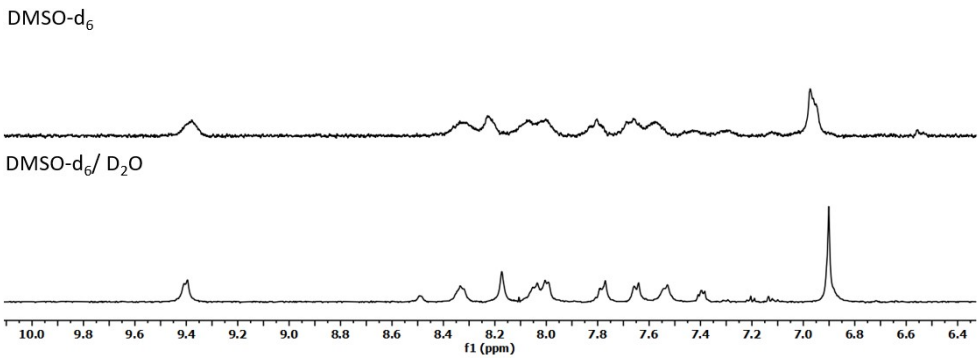


Figure 20 ^1H NMR (DMSO-d_6) of **1** (disaggregation induced by D_2O)

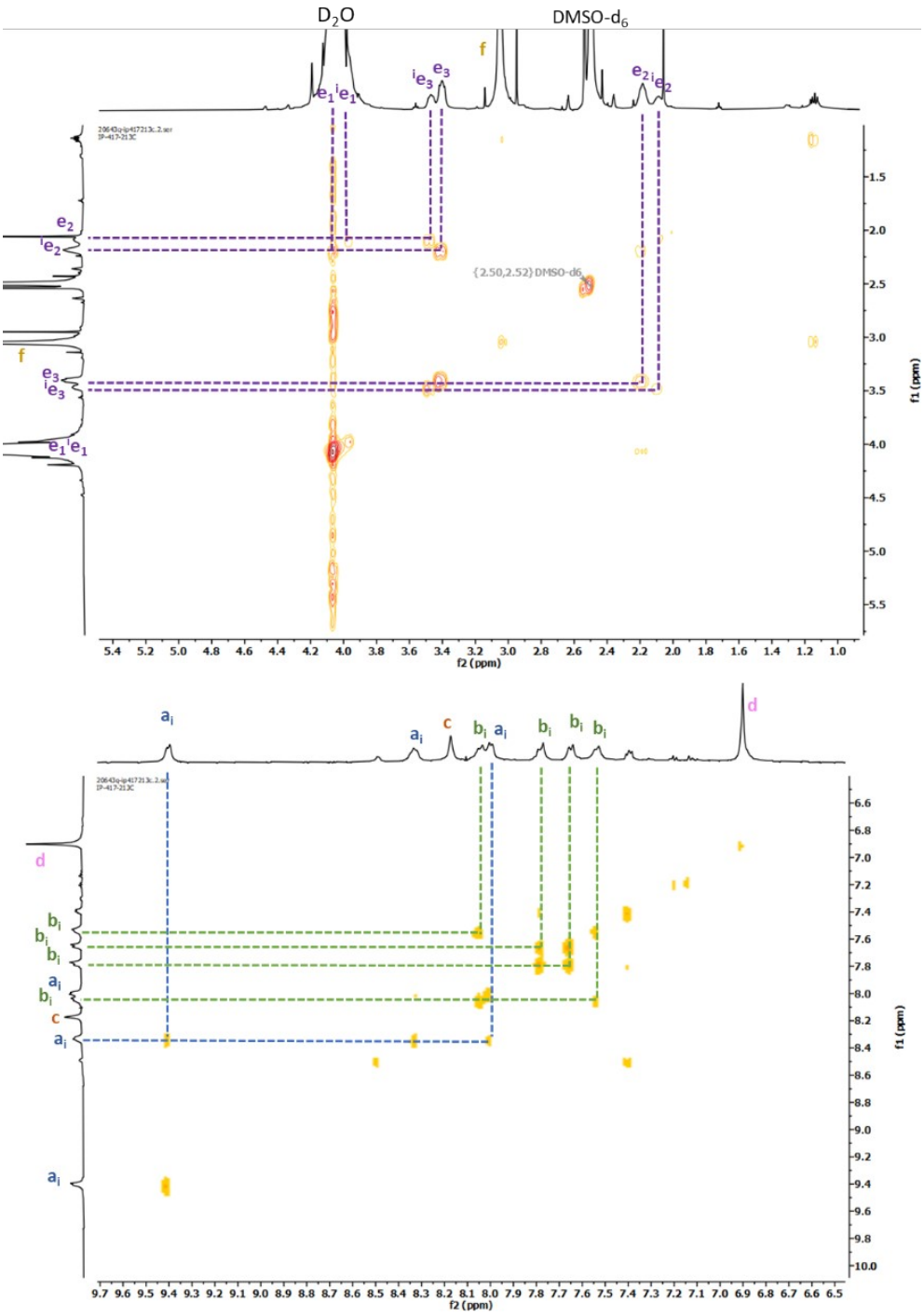


Figure 21 COSY (DMSO-d_6/D_2O, 500 MHz) of **1**

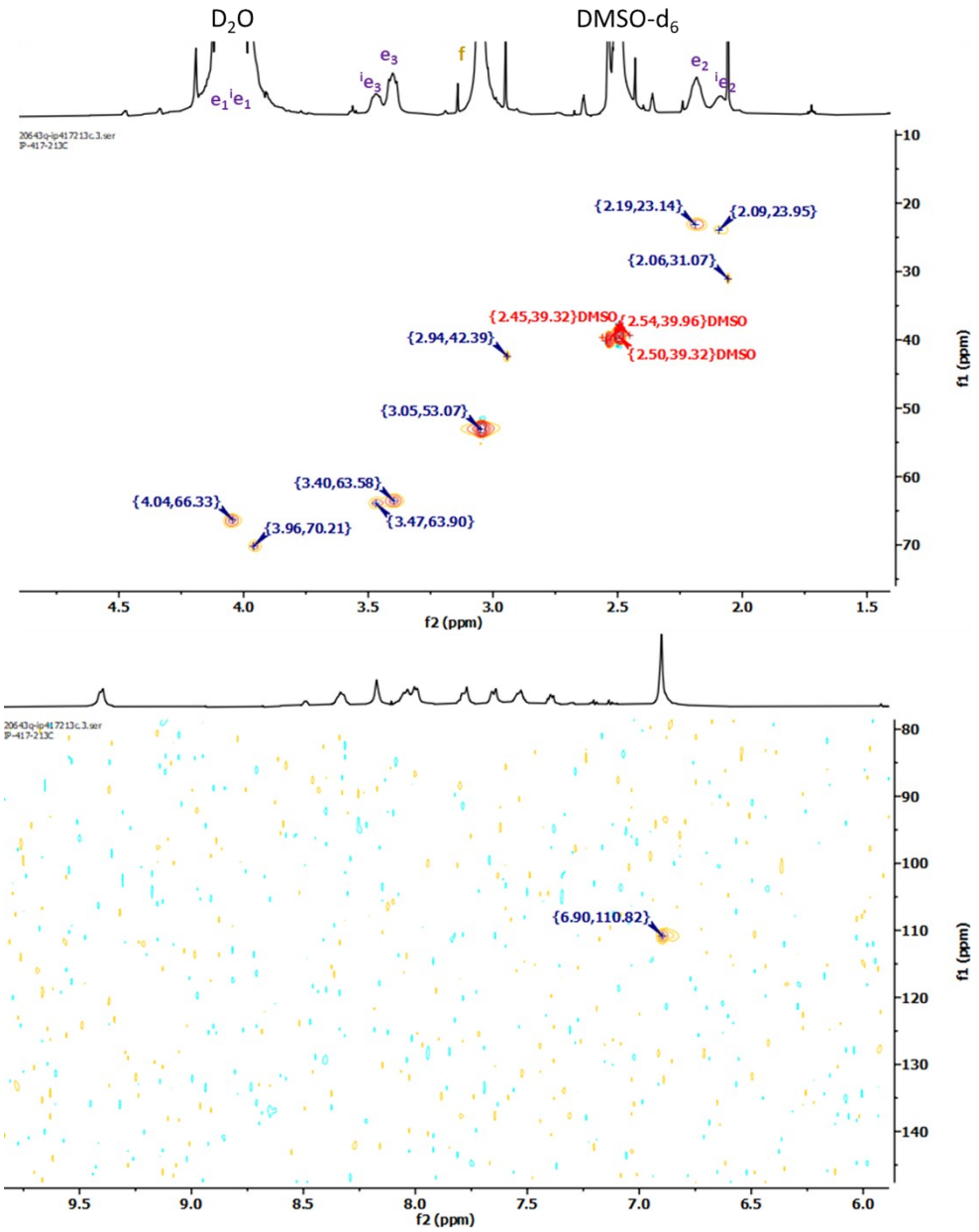


Figure 22 HSQC (DMSO-d_6/D_2O, 126 MHz) of **1**

5. MS and HRMS analysis

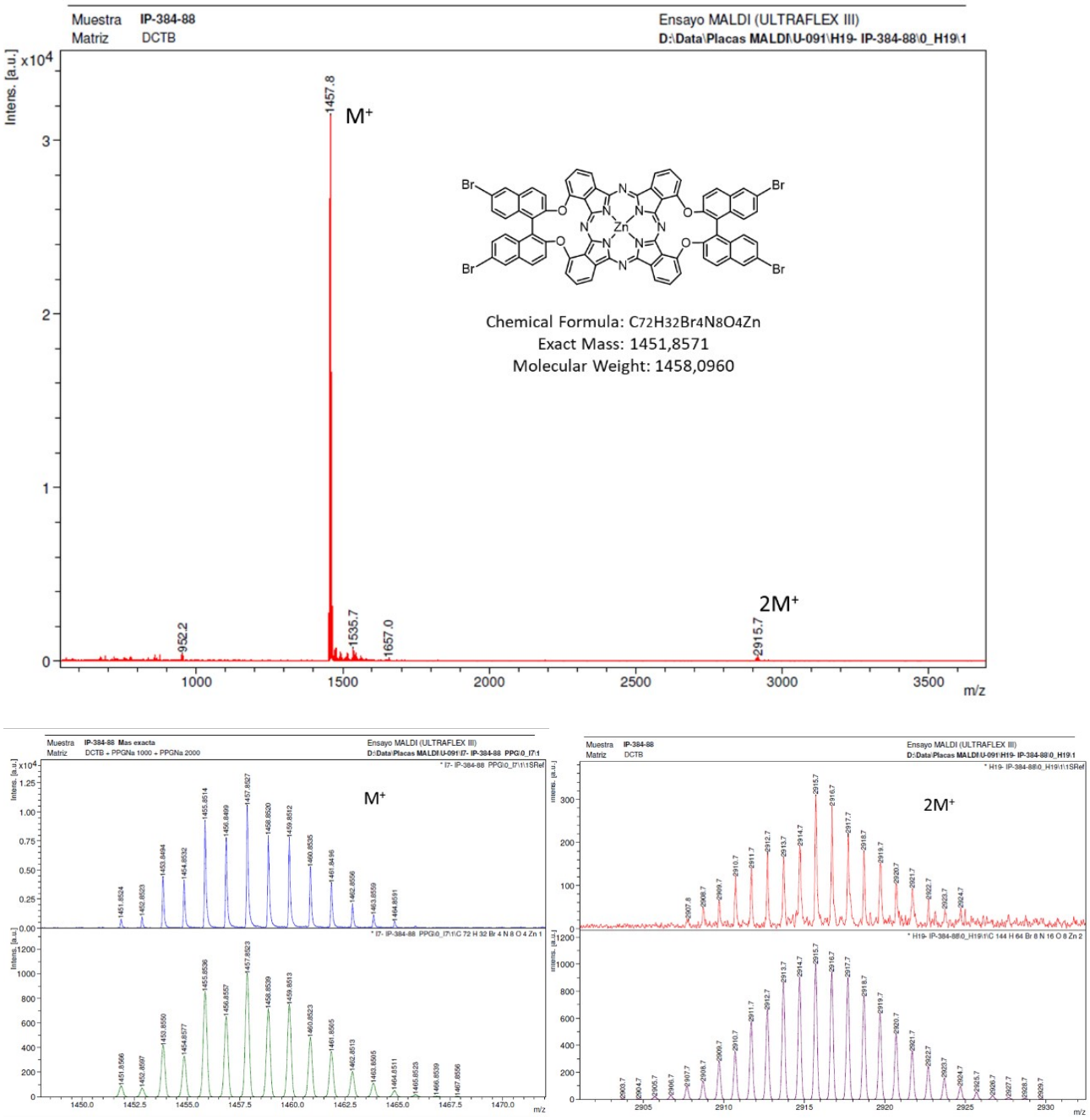


Figure 23 MS and HR-MS spectra of **$(AA)_2$-1**

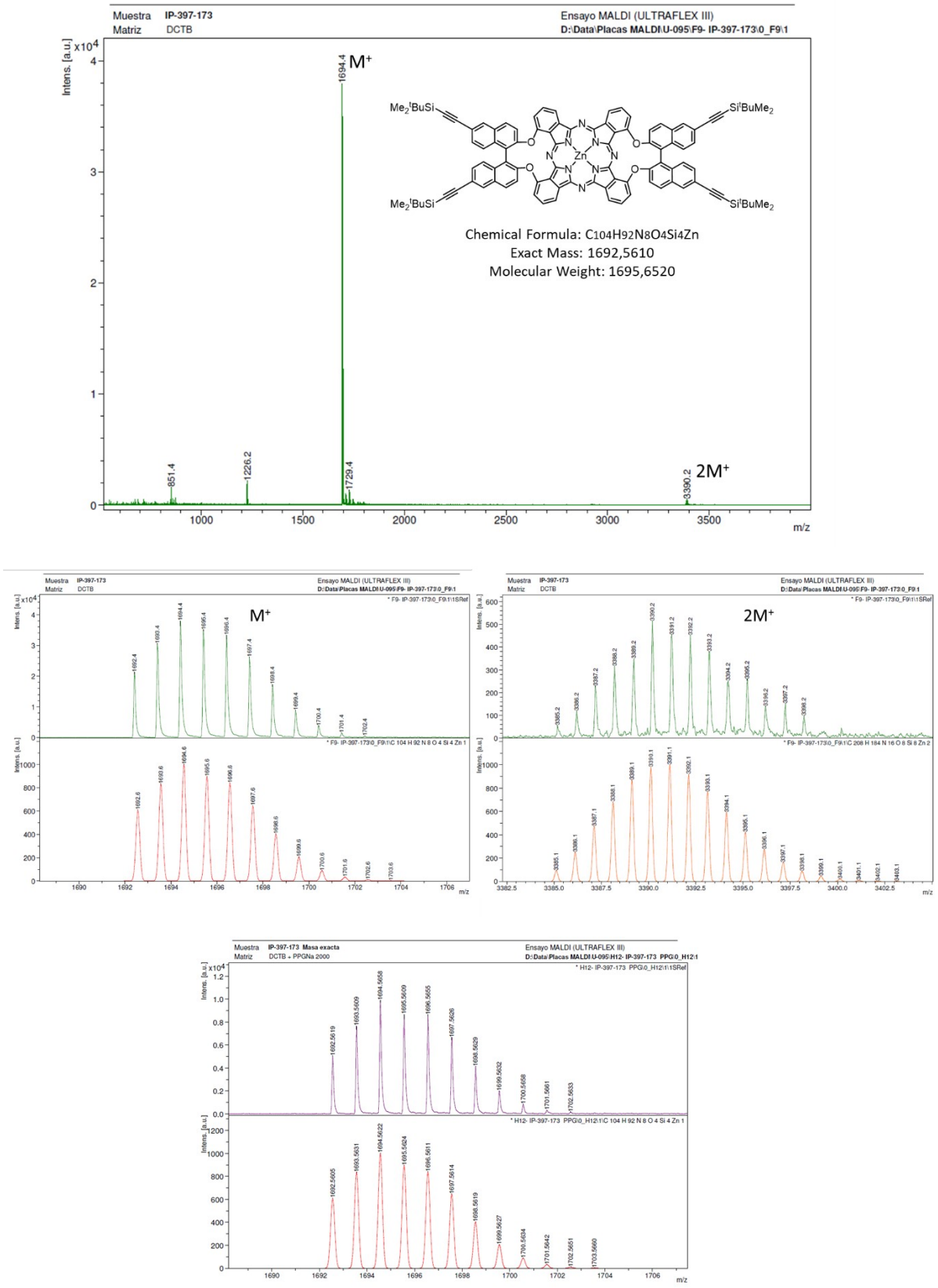


Figure 24 MS and HR-MS spectra of **$(AA)_2$-2**

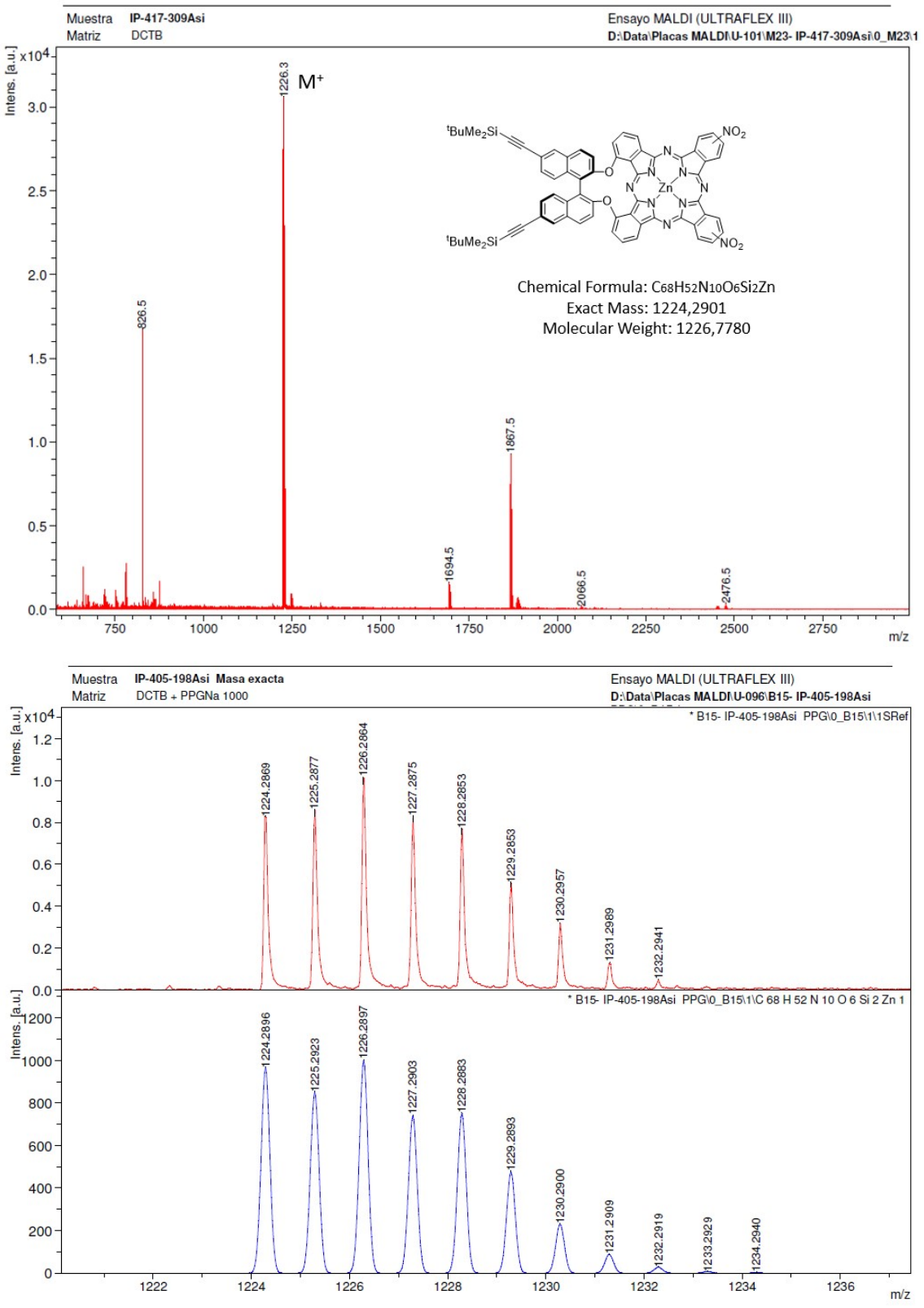


Figure 25 MS and HR-MS spectra of **AABB-3.**

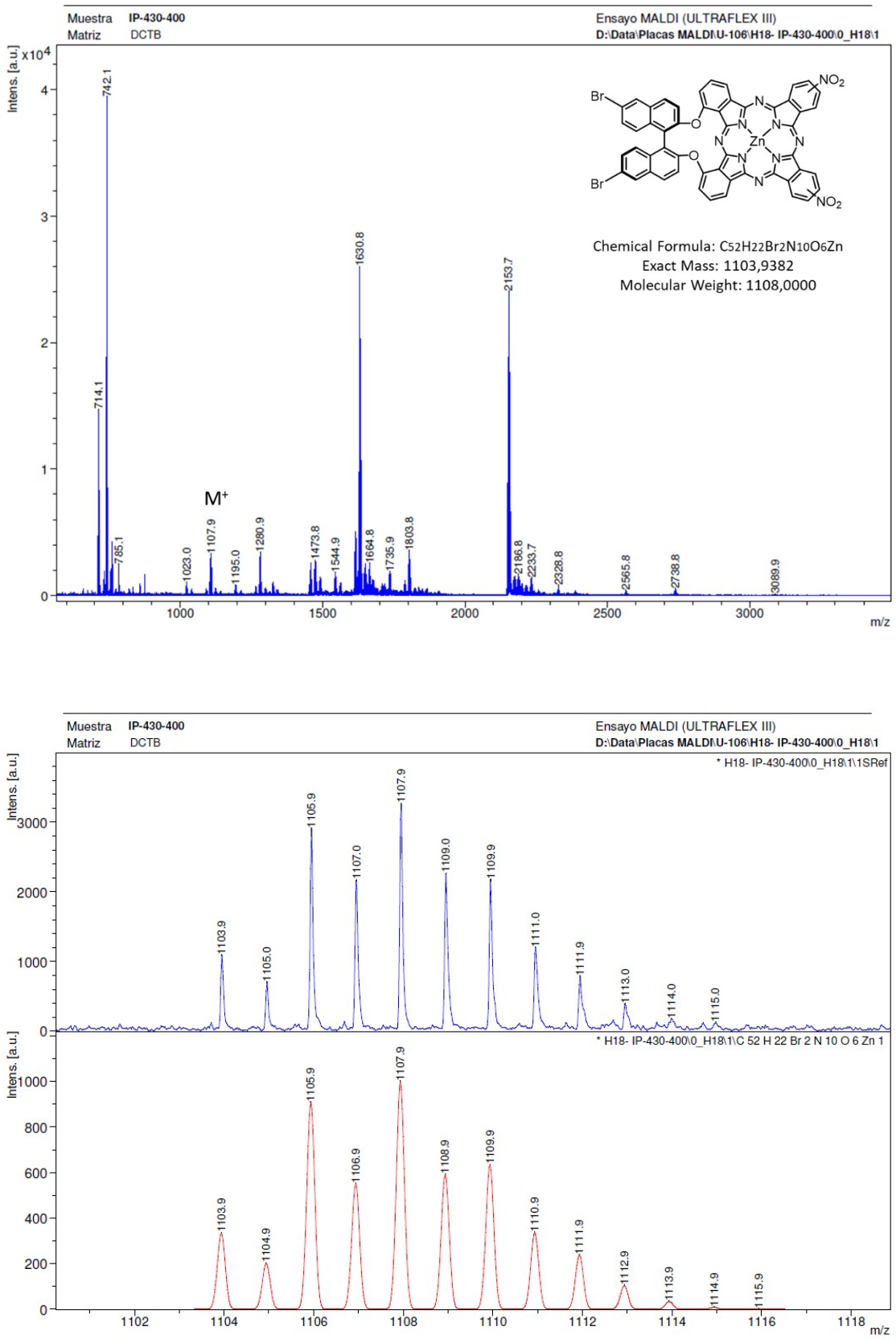


Figure 26 MS spectrum of mixture containing **AABB-4**.

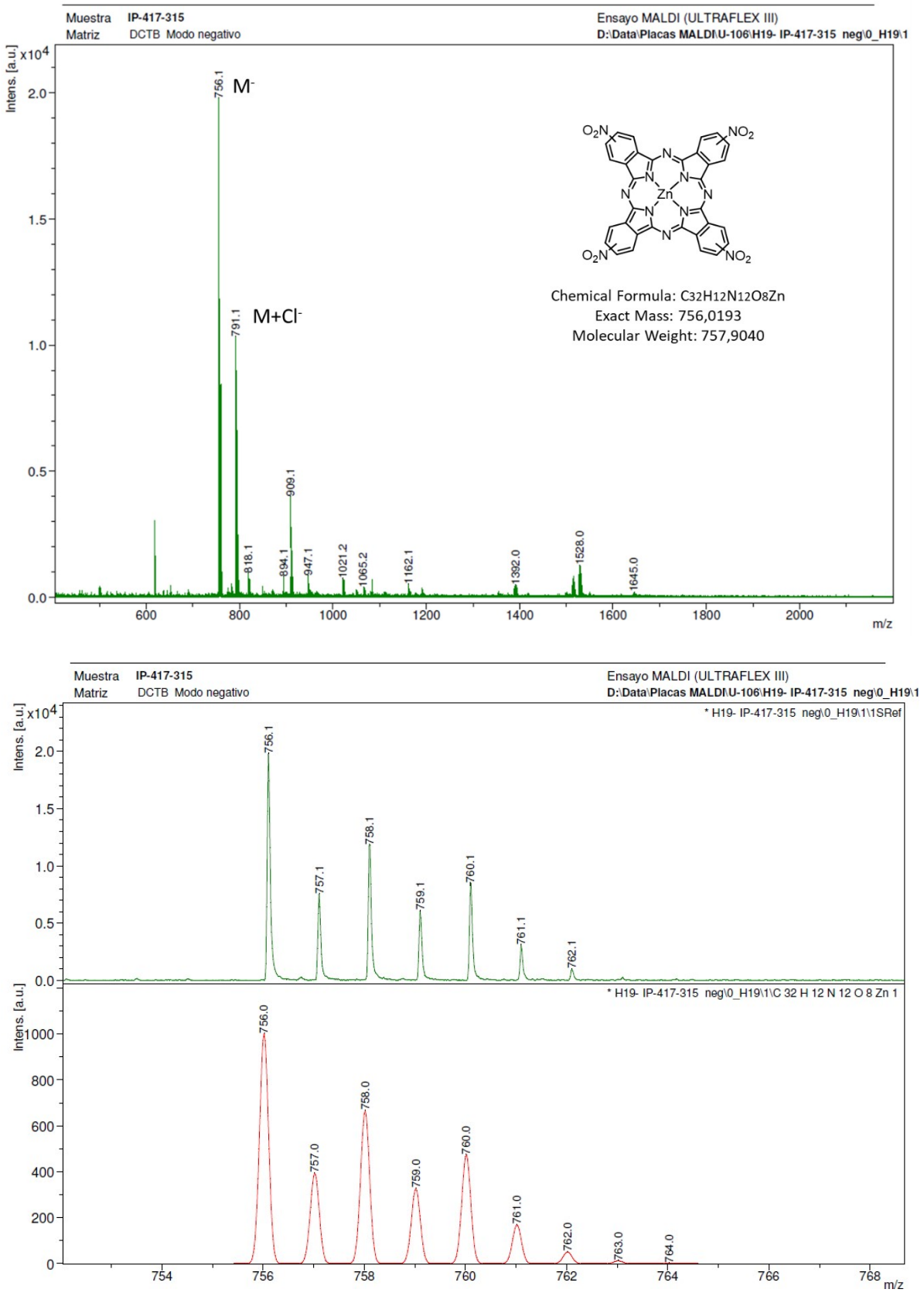


Figure 27 MS spectrum of **B_4**.

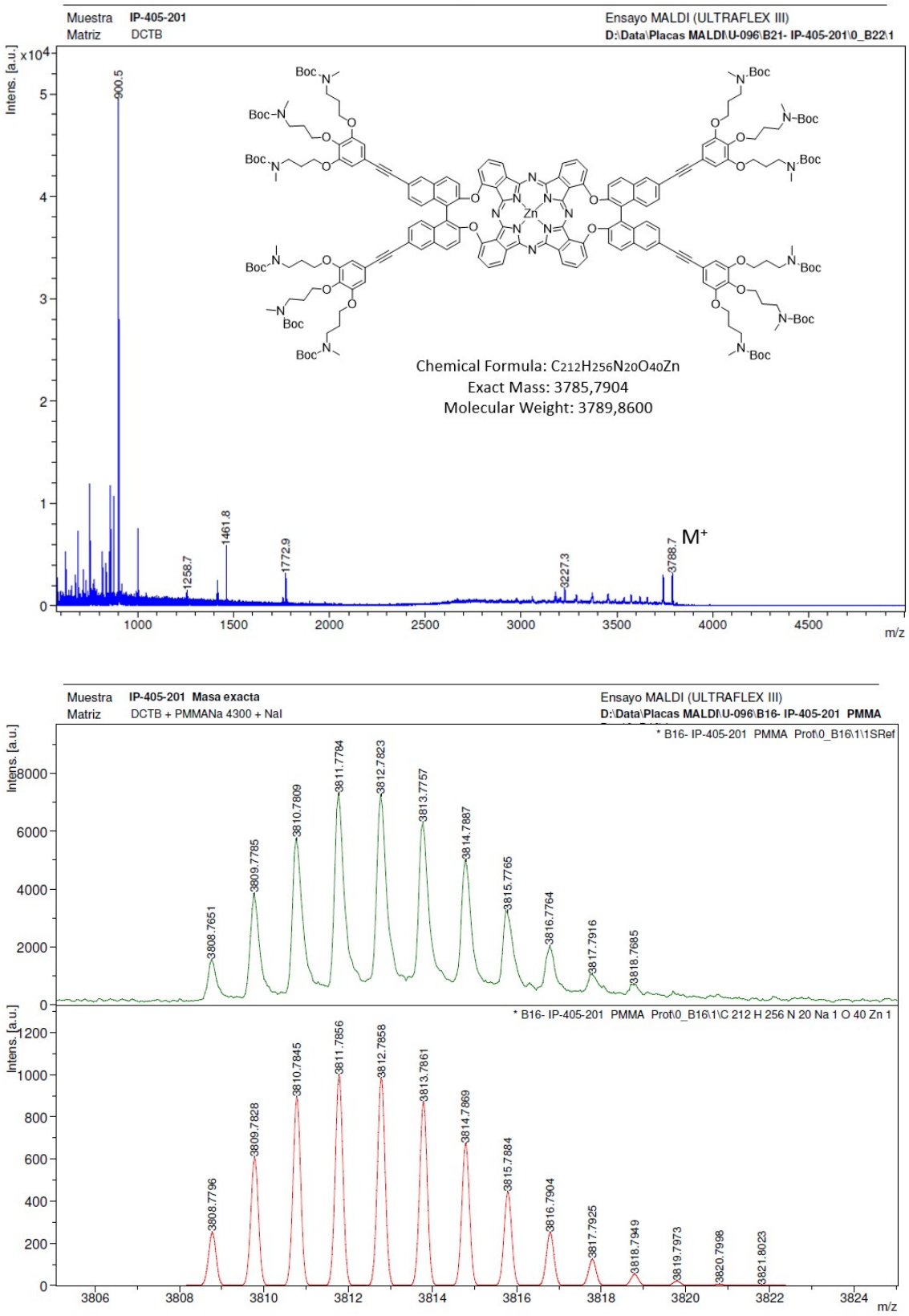


Figure 28 MS and HR-MS spectra of **4.**

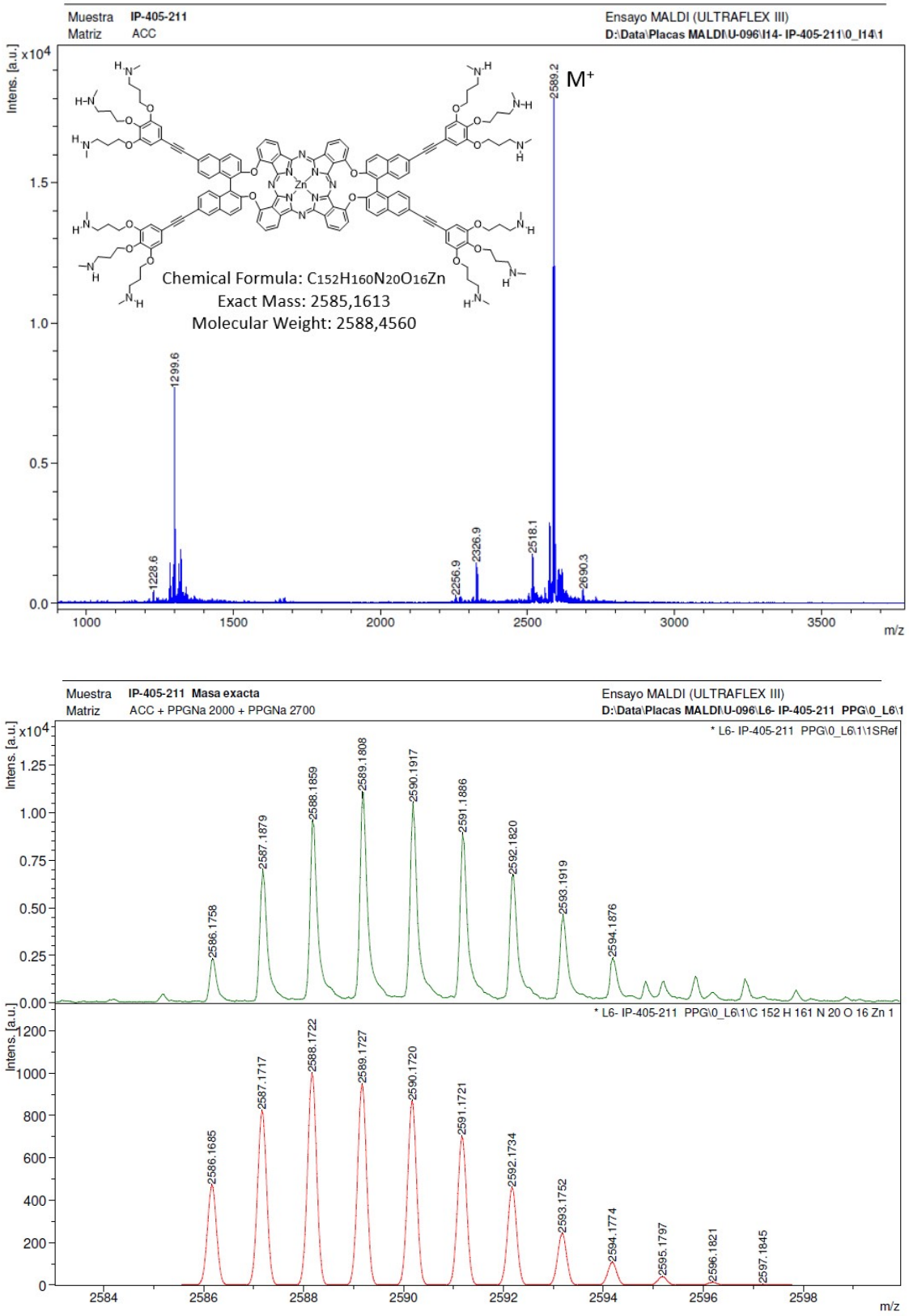


Figure 29 MS and HR-MS spectra of **5.**

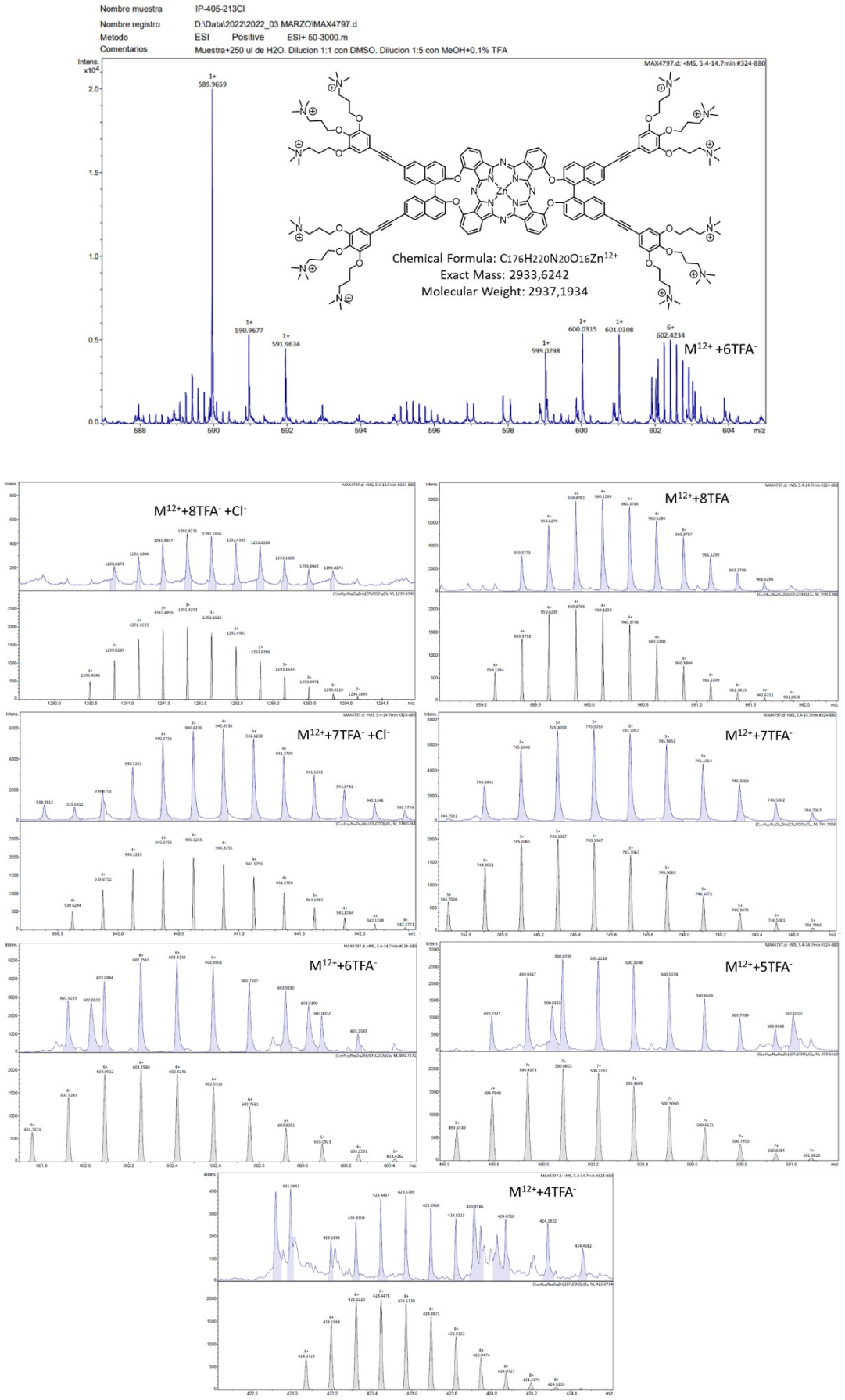


Figure 30 MS and HR-MS spectra of **1**.

6. UV-Vis and fluorescence spectra

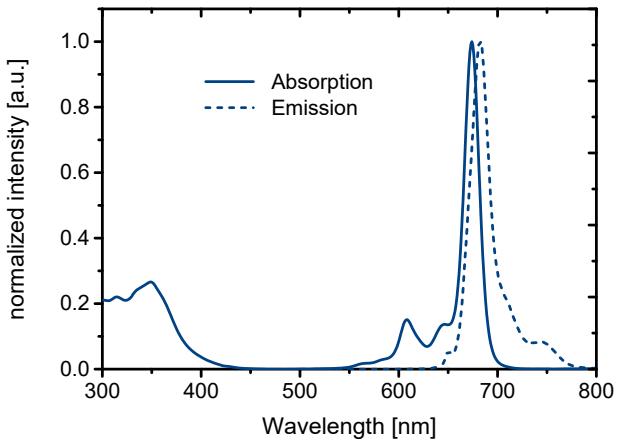


Figure 31 Normalized absorption and emission spectra of **$(AA)_2$-2** from a 5x10^{-6}M solution in THF (λ_{exc} = 650 nm).

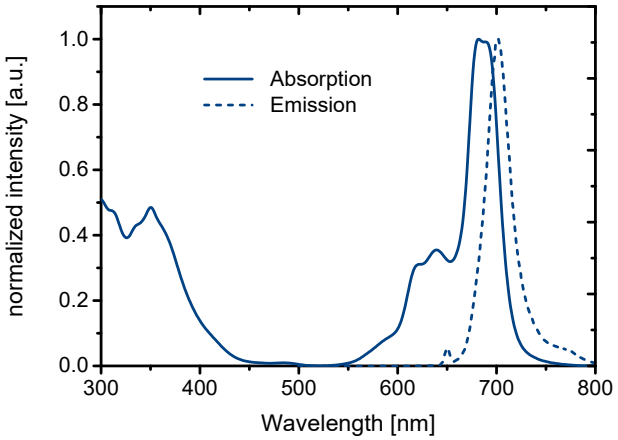


Figure 32 Normalized absorption and emission spectra of **AABB-3** in THF from a 5x10^{-6}M solution in THF (λ_{exc} = 650 nm).

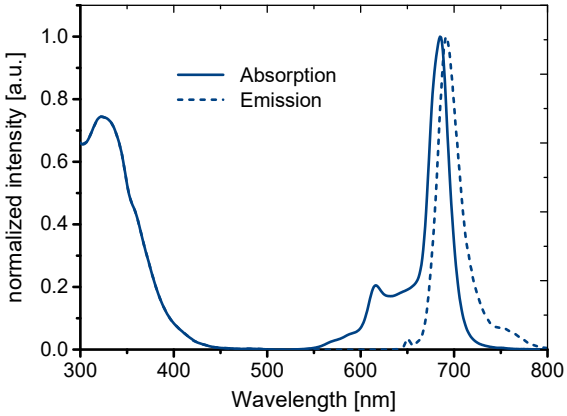


Figure 33 Normalized absorption and emission spectra of **4** in THF from a $2x10^{-6}$M solution in THF (λ_{exc} = 650 nm).

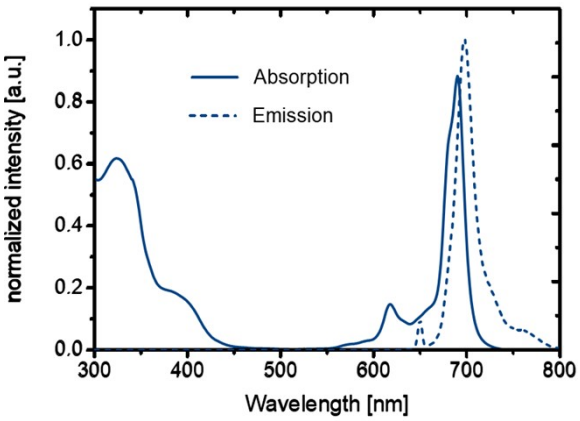


Figure 34 Normalized absorption and emission spectra of **1** in THF from a $5x10^{-6}$M solution in THF (λ_{exc} = 650 nm).

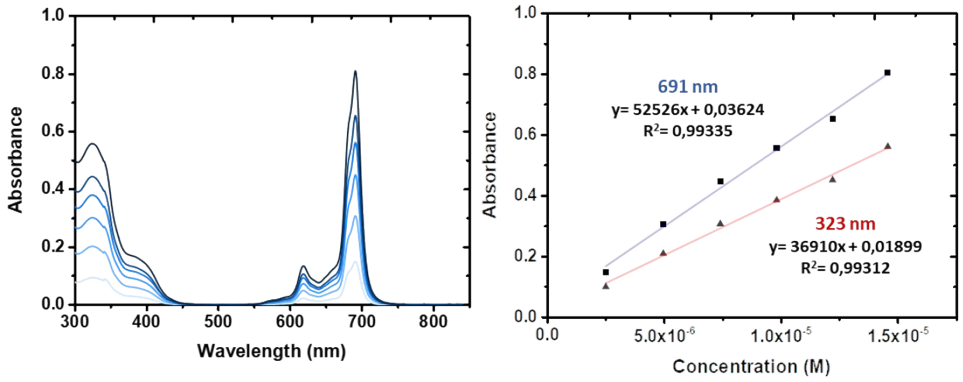


Figure 35 Ground-state absorption experiments. Plotting of absorbance vs concentration and linear regression for **1** in DMSO.

7. DLS analysis of nanoparticles

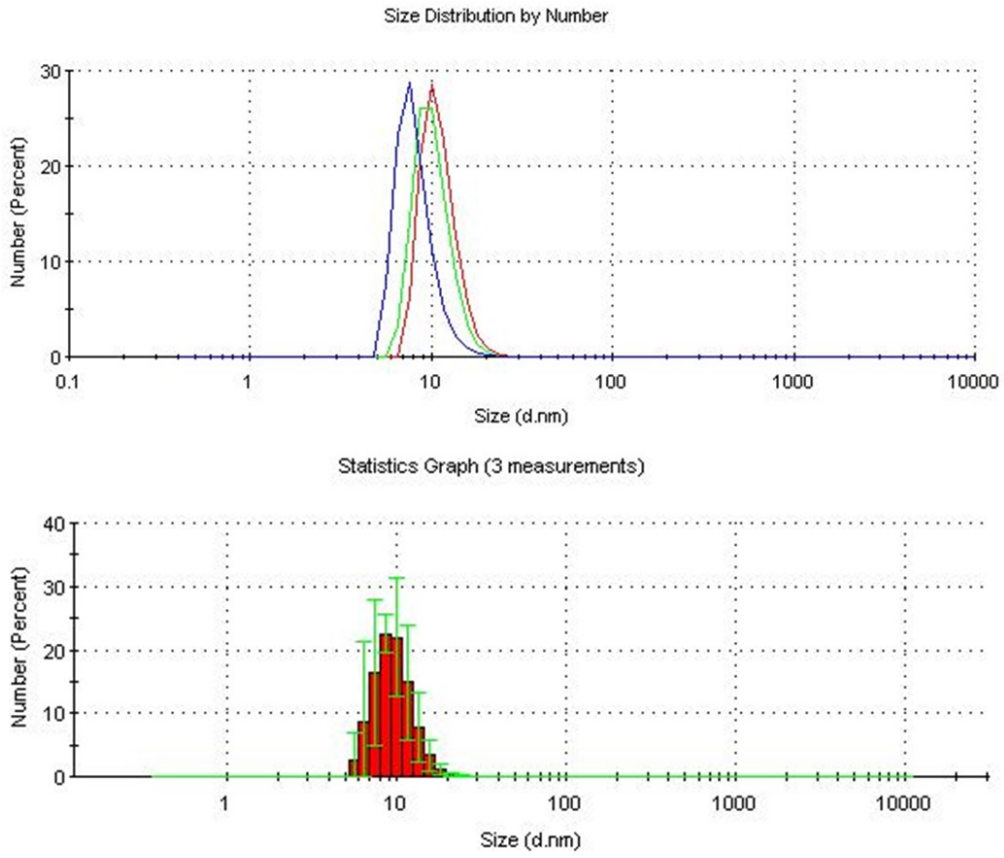


Figure 36. DLS of a freshly prepared $4x10^{-5}$M water solution of **1**, measured after 5 minutes of sonication followed by 10 minutes stabilization at room temperature. Size distribution by number (up) and statistics graph for the three measurements (down).

8. Cartesian coordinates for the optimized structures

General structure AABB

0 1

C	-0.32454361	0.05070994	0.00000000
C	0.67656139	-0.94559306	-0.00851700
C	-0.01505561	-2.23294706	0.01413200
N	0.59950639	-3.40987206	0.01709800
C	-0.01507761	-4.58679506	0.02016100
C	0.67655639	-5.87416006	0.04098600
C	-0.32454861	-6.87048006	0.03207500
C	-1.60495261	-6.16887406	0.00734300
N	-2.78141361	-6.79160606	-0.00155700
C	-3.95611961	-6.17114106	-0.00359200
C	-5.24086961	-6.86686506	-0.01338100
C	-6.23698461	-5.86919606	-0.00736200
C	-5.53955161	-4.58552806	0.00613500
N	-6.16106161	-3.40985406	0.01617700
C	-5.53954661	-2.23419506	0.02667600
C	-6.23696961	-0.95050306	0.03809700
C	-5.24084961	0.04715694	0.04434800
C	-3.95609961	-0.64859206	0.03677500
N	-2.78139161	-0.02812206	0.03470700
C	-1.60492861	-0.65086406	0.02643700
N	-1.37043361	-2.00018706	0.03252700
N	-1.37046761	-4.81953506	0.00242400
N	-4.18654361	-2.00290806	0.02699400
N	-4.18656561	-4.81683106	0.00714000
Zn	-2.77726561	-3.40989906	0.02252900
C	-7.59138061	-0.61655806	0.04218100
C	-7.92578261	0.73678794	0.05291400
C	-6.93133861	1.73282194	0.05911400
C	4.36803739	-1.84493906	3.22299100
C	6.20298439	-4.68547306	1.61933000
C	6.95378139	-5.14394706	2.67772000
C	6.86768139	-4.52388506	3.94783900
C	6.02760739	-3.45008306	4.12832500
C	-5.57730961	1.40085494	0.05481000
C	-0.01447661	1.40965794	-0.03300700
C	1.33203239	1.76466994	-0.08705800
C	2.34050539	0.78724294	-0.10906800
C	2.02488139	-0.57151606	-0.06425700
C	2.02492539	-6.24825106	0.09486000
C	2.34065439	-7.60707706	0.13757300
C	1.33219639	-8.58448706	0.11516900
C	-0.01439561	-8.22944906	0.06285700
C	-5.57733661	-8.22054406	-0.02578800
C	-6.93136461	-8.55248606	-0.03212100
C	-7.92580061	-7.55644406	-0.02615000
C	-7.59139261	-6.20311506	-0.01362400
O	3.01508539	-5.30220006	0.22157500
O	3.01517139	-1.51750606	-0.19059200
C	3.71520939	-4.83736406	-0.87459100
C	3.62250139	-5.45627606	-2.14339900
C	4.36999639	-4.97462506	-3.19120900
C	5.24219039	-3.86995406	-3.02449900
C	5.32446139	-3.24272406	-1.73714000
C	4.53417539	-3.73934206	-0.65475500
C	6.03021939	-3.36952006	-4.09540900
C	6.87021739	-2.29575606	-3.91433900
C	6.95553239	-1.67575306	-2.64414000
C	6.20405139	-2.13425106	-1.58624300
C	4.53372539	-3.08040406	0.68671300
C	5.32332539	-3.57697106	1.76961900
C	5.24026939	-2.94967306	3.05689400
C	3.71460139	-1.98239106	0.90599200
C	3.62119239	-1.36335106	2.17469000
H	-8.35135361	-1.39078706	0.03711400
H	-8.97102961	1.03135394	0.05648200
H	-7.22766461	2.77755394	0.06724100
H	-4.80460161	2.16238494	0.05921500
H	-0.80218961	2.15486694	-0.02628200

H	1.61432339	2.81245894	-0.12316700
H	3.38514239	1.07310694	-0.17475600
H	3.38536339	-7.89298206	0.20193300
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H	-0.80205861	-8.97470806	0.05580200
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H	-7.22769361	-9.59720506	-0.04171200
H	-8.97104661	-7.85099006	-0.03135200
H	-8.35135961	-5.42887806	-0.00881000
H	2.96081639	-6.30345706	-2.28065300
H	4.29825939	-5.44608706	-4.16776900
H	5.95588439	-3.85502106	-5.06530100
H	7.62287939	-0.83002206	-2.50438100
H	6.27851639	-1.65633406	-0.61534300
H	2.95952939	-0.51606606	2.31143000
H	4.29578539	-1.37335506	4.19945400
H	6.27804639	-5.16343806	0.64849900
H	7.62119139	-5.98970506	2.53842200
H	5.95268339	-2.96452606	5.09814400
H	7.46872439	-1.92235806	-4.73994500
H	7.46564839	-4.89726806	4.77384300

General structure $(AA)_2$

0 1

C	0.50709940	-0.04056795	0.00000000
C	1.50682040	-1.03758495	-0.01769000
C	0.81359740	-2.32471795	-0.00700600
N	1.42857940	-3.50137395	-0.01302200
C	0.81358540	-4.67804195	-0.01911800
C	1.50680440	-5.96516495	-0.00705900
C	0.50706840	-6.96217995	-0.02444500
C	-0.77444760	-6.26121795	-0.04574700
N	-1.94929360	-6.88338195	-0.06491400
C	-3.12442660	-6.26074095	-0.06522100
C	-4.40618560	-6.96038595	-0.10701500
C	-5.40528560	-5.96260895	-0.09384800
C	-4.71192060	-4.67731195	-0.04325300
N	-5.32715160	-3.50136395	-0.01280900
C	-4.71192260	-2.32543695	0.01756900
C	-5.40527860	-1.04015595	0.06900200
C	-4.40615860	-0.04239295	0.08233300
C	-3.12441460	-0.74202095	0.03969100
N	-1.94928260	-0.11936695	0.03956200
C	-0.77443860	-0.74154095	0.02004000
N	-0.54115660	-2.09201195	0.01300800
N	-0.54114360	-4.91073695	-0.03972900
N	-3.35727260	-2.09180095	0.00438900
N	-3.35727960	-4.91093495	-0.03035600
Zn	-1.94885360	-3.50133795	-0.01572400
C	-6.75427060	-0.67131395	0.13173500
C	-7.07376860	0.68527405	0.20608600
C	-6.06731560	1.66499905	0.20555200
C	-4.71964160	1.31457505	0.14439700
C	0.81856840	1.31794805	-0.01899700
C	2.16599240	1.67161905	-0.06833700
C	3.17308840	0.69351205	-0.09902600
C	2.85575140	-0.66562495	-0.06799000
C	2.85569540	-6.33714895	0.04439400
C	3.17295140	-7.69626395	0.07685600
C	2.16584740	-8.67437195	0.04651000
C	0.81847440	-8.32068895	-0.00395200
C	-4.71975460	-8.31738195	-0.16802200
C	-6.06747260	-8.66779595	-0.22833200
C	-7.07391260	-7.68805195	-0.22905200
C	-6.75431460	-6.33143395	-0.15569000
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O	3.84375240	-1.61205795	-0.20202000
C	4.54727740	-4.92045095	-0.91428000
C	4.45449840	-5.53029495	-2.18737600
C	5.20396540	-5.04256895	-3.23101800
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C	6.16018740	-3.32272095	-1.76380800
C	5.36811640	-3.82577195	-0.68567800
C	6.86756940	-3.43386095	-4.12238600
C	7.70915040	-2.36281395	-3.93290100
C	7.79450440	-1.75205195	-2.65823300
C	7.04147140	-2.21683095	-1.60418900

C	5.36857640	-3.17699895	0.66074100
C	6.16139840	-3.68002595	1.73832800
C	6.07988240	-3.06217495	3.03025800
C	4.54786840	-2.08233995	0.88989300
C	4.45584940	-1.47256095	2.16307400
C	5.20600640	-1.96029995	3.20621700
C	7.04262140	-4.78587895	1.57810700
C	7.79635640	-5.25065195	2.63165100
C	7.71180540	-4.63992595	3.90639100
C	6.87030140	-3.56891995	4.09645200
O	-7.74069260	-1.62515095	0.23626600
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C	-8.36951760	-1.39739895	-2.11767500
C	-9.13257160	-1.83997195	-3.17266000
C	-10.01208060	-2.93994495	-3.02484400
C	-10.08543660	-3.61055495	-1.75872400
C	-9.27546160	-3.15252995	-0.67341000
C	-10.84161960	-3.39526995	-4.10586200
C	-11.63831260	-4.45956495	-3.86809500
C	-11.75904960	-5.15254595	-2.66707600
C	-10.97244160	-4.71476595	-1.61289600
C	-9.27578260	-3.85018695	0.64860600
C	-10.08621760	-3.39213695	1.73357300
C	-10.01343260	-4.06277295	2.99971200
C	-8.45248660	-4.95013195	0.84264800
C	-8.37047060	-5.60532995	2.09327300
C	-9.13399960	-5.16275295	3.14791600
C	-10.97314260	-2.28791595	1.58736100
C	-11.76022960	-1.85015595	2.64118700
C	-11.64006160	-2.54315595	3.84226100
H	-8.11884660	0.96804205	0.27798500
H	-6.35198660	2.71105805	0.26439900
H	-3.93427660	2.06220505	0.15379900
H	0.03215740	2.06439605	-0.00505100
H	2.44952040	2.71936405	-0.09367100
H	4.21810740	0.97881005	-0.16061300
H	4.21793640	-7.98150995	0.13927000
H	2.44932140	-9.72210295	0.07297600
H	0.03203740	-9.06711595	-0.01763800
H	-3.93443560	-9.06506195	-0.17725600
H	-6.35219360	-9.71388595	-0.28637800
H	-8.11902160	-7.97085895	-0.30032900
H	3.79143940	-6.37524995	-2.33156700
H	5.13235040	-5.50699495	-4.21093200
H	6.79328240	-3.91227595	-5.09577300
H	8.46320040	-0.90851595	-2.51193500
H	7.11610140	-1.74601795	-0.62983700
H	3.79281640	-0.62767095	2.30774700
H	5.13495340	-1.49594595	4.18620600
H	7.11663540	-5.25666495	0.60369500
H	8.46499340	-6.09415695	2.48489900
H	6.79662040	-3.09053895	5.06990000
H	-7.70232660	-0.55173695	-2.23796900
H	-9.06817960	-1.34084095	-4.13549700
H	-10.79972460	-2.87038795	-5.05877200
H	-12.42174460	-6.00534895	-2.54335700
H	-11.02543760	-5.22439195	-0.65484200
H	-7.70326460	-6.45093295	2.21388800
H	-9.07001160	-5.66185495	4.11079500
H	-11.02569960	-1.77827595	0.62928800
H	-12.42286960	-0.99735295	2.51717500
H	8.31216840	-5.01821895	4.72838500
H	8.30896540	-1.98451995	-4.75529500
C	-10.84345860	-3.60744695	4.08035500
H	-10.80199160	-4.13235095	5.03328200

Final Product 1

12 1

C	-2.47036900	-0.03694200	-3.45788500
C	-3.46146700	-0.03138400	-2.44997000
C	-2.75664200	-0.01148400	-1.17477000
N	-3.37125400	-0.00012700	-0.00008200
C	-2.75667100	0.01123200	1.17462000
C	-3.46152900	0.03112600	2.44980300
C	-2.47045500	0.03668000	3.45774400

C	-1.17725700	0.01543400	2.76634500
N	-0.00012800	-0.00013000	3.38842900
C	1.17701600	-0.01568500	2.76637400
C	2.47019700	-0.03693700	3.45780400
C	3.46129600	-0.03135800	2.44988900
C	2.75647000	-0.01145300	1.17468800
N	3.37108100	-0.00007700	0.00000000
C	2.75649800	0.01128200	-1.17470200
C	3.46135500	0.03118700	-2.44988500
C	2.47028100	0.03673300	-3.45782400
C	1.17708400	0.01547200	-2.76642600
N	-0.00004400	-0.00010500	-3.38851000
C	-1.17718800	-0.01568100	-2.76645500
N	-1.40477400	-0.00587900	-1.41398600
N	-1.40480900	0.00563800	1.41387000
N	1.40463700	0.00567600	-1.41395100
N	1.40460200	-0.00586800	1.41390400
Zn	-0.00008600	-0.00010900	-0.00004100
C	4.81839600	0.02628500	-2.79541000
C	5.15906300	0.03149000	-4.14802800
C	4.16328500	0.05214700	-5.14001600
C	2.80797500	0.05156500	-4.81046500
C	-2.80803200	-0.05178500	-4.81053400
C	-4.16333500	-0.05236200	-5.14011500
C	-5.15913600	-0.03168700	-4.14815100
C	-4.81850000	-0.02647300	-2.79552600
C	-4.81857000	0.02621000	2.79532600
C	-5.15923900	0.03141400	4.14794300
C	-4.16346300	0.05208100	5.13993200
C	-2.80815200	0.05151000	4.81038500
C	2.80786100	-0.05178800	4.81045300
C	4.16316400	-0.05235200	5.14003400
C	5.15896500	-0.03165500	4.14807000
C	4.81832900	-0.02643300	2.79544500
O	-5.79135400	-0.11372500	1.81746600
O	-5.79130500	0.11348500	-1.81769000
C	-6.55989700	0.93715800	1.38178800
C	-6.48539000	2.21923100	1.98155800
C	-7.29103500	3.23611400	1.53382400
C	-8.20625900	3.03232700	0.46799300
C	-8.26787600	1.73698300	-0.15059200
C	-7.42866100	0.67813100	0.32105800
C	-9.04095000	4.07907500	0.00644100
C	-9.92417000	3.89565700	-1.05262100
C	-9.97624100	2.60665400	-1.67211900
C	-9.18261200	1.57432000	-1.23361700
C	-7.42867600	-0.67831500	-0.32132500
C	-8.26793700	-1.73713700	0.15030800
C	-8.20634300	-3.03248700	-0.46826500
C	-6.55989200	-0.93737400	-1.38203000
C	-6.48540800	-2.21945300	-1.98179000
C	-7.29109600	-3.23630900	-1.53407000
C	-9.18269800	-1.57443700	1.23330800
C	-9.97636800	-2.60674400	1.67179700
C	-9.92431900	-3.89575300	1.05231100
C	-9.04107500	-4.07920800	-0.00672500
O	5.79118400	-0.11364000	-1.81755300
O	5.79113000	0.11354500	1.81760900
C	6.55971000	0.93725300	-1.38186900
C	6.48518900	2.21932600	-1.98163600
C	7.29081900	3.23621900	-1.53389500
C	8.20603900	3.03244300	-0.46805900
C	8.26767000	1.73709800	0.15052200
C	7.42847300	0.67823600	-0.32113600
C	9.04071300	4.07920100	-0.00649800
C	9.97601100	2.60678600	1.67206400
C	9.18240200	1.57444300	1.23355300
C	7.42851600	-0.67821300	0.32124000
C	8.26780400	-1.73701300	-0.15039400
C	8.20625600	-3.03236100	0.46818800
C	6.55974300	-0.93729400	1.38195000
C	6.48530100	-2.21937300	1.98171600
C	7.29102000	-3.23620500	1.53399900
C	9.18255100	-1.57429100	-1.23340300
C	9.97625100	-2.60657500	-1.67189000
H	6.20780300	0.00477900	-4.42539800

H	4.46317800	0.05700700	-6.18315500
H	2.03882400	0.05628100	-5.57469800
H	-2.03886400	-0.05651000	-5.57474900
H	-4.46320300	-0.05722900	-6.18326200
H	-6.20786900	-0.00496800	-4.42554700
H	-6.20797900	0.00469500	4.42531200
H	-4.46335700	0.05694000	6.18307100
H	-2.03900200	0.05623400	5.57461900
H	2.03869300	-0.05653100	5.57466800
H	4.46303200	-0.05722400	6.18318100
H	6.20769700	-0.00492600	4.42546700
H	-5.78753800	2.38762800	2.79304200
H	-7.22951400	4.21689600	1.99687400
H	-8.97590500	5.04916800	0.49025200
H	-10.65942700	2.45141700	-2.50079100
H	-9.24652300	0.60693700	-1.72015800
H	-5.78753900	-2.38787800	-2.79325400
H	-7.22959100	-4.21709700	-1.99711000
H	-9.24659200	-0.60704800	1.71983800
H	-10.65957100	-2.45148000	2.50045000
H	-8.97604400	-5.04930800	-0.49052400
H	5.78734100	2.38771700	-2.79312400
H	7.22928900	4.21700100	-1.99694500
H	8.97566000	5.04929400	-0.49030800
H	10.65919400	2.45155700	2.50074100
H	9.24632300	0.60705900	1.72008900
H	5.78744200	-2.38781600	2.79318400
H	7.22955100	-4.21699100	1.99704800
H	9.24640900	-0.60690400	-1.71994200
H	10.65944100	-2.45129600	-2.50055200
C	9.04102300	-4.07905500	0.00665400
H	8.97603200	-5.04915300	0.49046500
C	9.92392800	3.89579100	1.05256900
C	9.92425300	-3.89558100	-1.05239000
C	10.74753000	-4.96862200	-1.51582500
C	11.44056000	-5.89114300	-1.91320100
C	12.21888700	-6.99427500	-2.37658200
C	12.53297900	-8.07028000	-1.51793800
C	12.67465700	-7.05712600	-3.71135700
C	13.24480700	-9.17355100	-1.98355600
H	12.19332100	-8.06034300	-0.48834600
C	13.38119800	-8.16525700	-4.17450400
H	12.44024300	-6.25656800	-4.40392300
C	13.67009200	-9.24560700	-3.32194100
C	15.02995900	-7.68595800	-5.82201800
C	15.10459600	-7.55933200	-7.35142100
H	15.14201200	-6.70087400	-5.34895000
H	15.82581300	-8.33985900	-5.43860800
C	16.44443800	-6.95270800	-7.77486600
H	14.96282400	-8.55470900	-7.78332300
H	14.26383600	-6.93725500	-7.67175800
H	16.58356300	-5.96885100	-7.31847800
H	17.27692500	-7.58778200	-7.45972400
C	13.48907200	-11.38295300	-4.28833900
C	14.36599200	-12.54132700	-4.78619800
H	12.82027000	-11.72077100	-3.48615600
H	12.87467800	-10.98388000	-5.10583100
C	13.47699300	-13.66458800	-5.32985200
H	15.03803400	-12.15413900	-5.55801000
H	14.98270400	-12.88728600	-3.95113000
H	12.80369200	-14.03337600	-4.55132500
H	12.86128200	-13.30147700	-6.15720100
C	14.70272900	-10.14667500	-0.37919500
C	14.63003100	-11.20295900	0.73406200
H	15.56852200	-10.31946000	-1.03384700
H	14.79872300	-9.14118100	0.05232700
C	15.88795000	-11.14708800	1.60463900
H	13.72801100	-11.00356100	1.31981500
H	14.51110800	-12.18536200	0.26699100
H	16.78163600	-11.35957100	1.01146400
H	16.00779800	-10.15336000	2.04479500
O	13.74753700	-8.23601200	-5.51182700
O	14.35712400	-10.35396800	-3.79100900
O	13.49019500	-10.24241500	-1.13139100
C	16.57944900	-8.03422700	-10.03813200
H	17.31348700	-8.72530900	-9.62261100

H	15.57597600	-8.44832400	-9.95749500
H	16.81078000	-7.83908900	-11.08552300
C	18.02613000	-6.13360000	-9.47608100
H	18.18886100	-5.96884700	-10.54125900
H	18.08093600	-5.18532000	-8.94124000
H	18.77412600	-6.82650700	-9.09031600
C	15.62386900	-5.77323000	-9.83435400
H	14.63206600	-6.21527400	-9.75876200
H	15.66835200	-4.84181800	-9.26921600
H	15.85991300	-5.58166000	-10.88129900
C	15.00188300	-15.58799200	-4.79669200
H	15.42286700	-16.50700700	-5.20518800
H	15.80699300	-14.92729800	-4.47998100
H	14.34842800	-15.82458300	-3.95646100
C	15.08583300	-14.56631500	-7.03532000
H	15.50403700	-15.48932200	-7.43764900
H	14.49328700	-14.06628900	-7.80203200
H	15.89195400	-13.91963000	-6.69324300
C	13.12651600	-15.87777300	-6.35366800
H	12.48095400	-16.14253200	-5.51613300
H	12.54327600	-15.40146500	-7.14188400
H	13.61509200	-16.77139300	-6.74230500
C	14.82029700	-11.86383600	3.76131400
H	14.86132500	-10.82231600	4.08140100
H	13.86652000	-12.07550500	3.28138200
H	14.95014000	-12.51994900	4.62221900
C	17.26172100	-11.90429700	3.50342800
H	17.31903400	-12.58897200	4.34968000
H	18.08020700	-12.10227600	2.81111100
H	17.30838300	-10.87386600	3.85602200
C	15.88412300	-13.55477200	2.32015600
H	14.91737100	-13.74517100	1.85742900
H	16.69068300	-13.72861300	1.60719600
H	16.01056500	-14.20800900	3.18381700
N	16.64904500	-6.73218200	-9.27830800
N	14.18842000	-14.91006500	-5.87183200
N	15.94487800	-12.12103500	2.78712600
C	10.74711000	4.96889500	1.51603000
C	11.44006900	5.89146000	1.91342500
C	12.21836300	6.99461400	2.37681500
C	12.53249800	8.07059100	1.51815200
C	12.67401200	7.05753400	3.71162600
C	13.24429200	9.17388200	1.98377700
H	12.19288600	8.06060600	0.48854400
C	13.38051700	8.16568700	4.17478100
H	12.43951300	6.25701200	4.40420700
C	13.66950200	9.24598800	3.32218500
O	13.48978700	10.24274000	1.13162900
O	13.74677300	8.23655900	5.51211800
O	14.35660700	10.35429600	3.79123300
C	14.70191100	10.14648500	0.37884000
C	15.02878600	7.68571600	5.82258100
C	13.48867400	11.38346800	4.28836100
C	14.62933700	11.20308800	-0.73411800
H	15.56810700	10.31860700	1.03313800
H	14.79713400	9.14104200	-0.05297200
C	15.10330500	7.55968600	7.35203700
H	15.14016200	6.70035600	5.34992800
H	15.82512000	8.33888900	5.43892100
C	14.36575700	12.54171400	4.78623400
H	12.82003000	11.72134700	3.48607100
H	12.87410700	10.98457900	5.10581400
C	15.88687000	11.14671400	-1.60522300
H	13.72696100	11.00435600	-1.31955000
H	14.51117500	12.18544100	-0.26674700
C	16.44271800	6.95229900	7.77574800
H	14.96223400	8.55534800	7.78351000
H	14.26210400	6.93833700	7.67263000
C	13.47692500	13.66516700	5.32975600
H	15.03766300	12.15443600	5.55811800
H	14.98260300	12.88751500	3.95119900
H	16.78091800	11.35851900	-1.01235100
H	16.00595800	10.15303100	-2.04568700
N	15.94388900	12.12093400	-2.78747900
H	16.58113000	5.96813000	7.31981600
H	17.27565500	7.58663000	7.46029900

N	16.64718800	6.73232400	9.27929000
H	12.80376500	14.03405000	4.55115100
H	12.86107000	13.30221600	6.15706800
N	14.18854600	14.91053200	5.87174300
C	14.81876900	11.86463700	-3.76128300
C	17.26031900	11.90361700	-3.50436400
C	15.88415500	13.55458500	-2.32011500
C	16.57856800	8.03477400	10.03850800
C	18.02383300	6.13281900	9.47731900
C	15.62131200	5.77439000	9.83579800
C	15.00224000	15.58824900	4.79664700
C	15.08578600	14.56665800	7.03532800
C	13.12678800	15.87846800	6.35344000
H	14.85908100	10.82318200	-4.08167400
H	13.86530500	12.07670900	-3.28090500
H	14.94863200	12.52091400	-4.62205900
H	17.31768600	12.58847100	-4.35046800
H	18.07919700	12.10095000	-2.81232600
H	17.30624500	10.87324800	-3.85723500
H	14.91769400	13.74542900	-1.85696400
H	16.69109300	13.72777000	-1.60742400
H	16.01064300	14.20797000	-3.18365700
H	17.31309500	8.72512700	9.62264000
H	15.57539400	8.44956400	9.95771000
H	16.80978900	7.83995600	11.08598200
H	18.18645700	5.96843400	10.54257000
H	18.07793300	5.18425400	8.94291100
H	18.77233500	6.82499800	9.09122500
H	14.62983300	6.21712400	9.76000000
H	15.66510900	4.84267600	9.27110500
H	15.85722000	5.58314500	10.88283400
H	15.42335700	16.50720700	5.20513500
H	15.80725600	14.92738600	4.48004800
H	14.34891100	15.82491900	3.95634100
H	15.50414100	15.48960000	7.43764800
H	14.49307100	14.06679000	7.80201200
H	15.89180700	13.91979300	6.69335500
H	12.48135900	16.14332500	5.51583300
H	12.54337700	15.40230500	7.14161700
H	13.61550400	16.77200600	6.74209100
C	-10.74736800	4.96875600	-1.51606800
C	-11.44033500	5.89132300	-1.91344500
C	-12.21863500	6.99448500	-2.37681300
C	-12.53282100	8.07041000	-1.51810400
C	-12.67420700	7.05748200	-3.71164500
C	-13.24461100	9.17371500	-1.98370200
H	-12.19324900	8.06037700	-0.48848400
C	-13.38071700	8.16564700	-4.17477000
H	-12.43962300	6.25701400	-4.40426100
C	-13.66978000	9.24588600	-3.32212000
O	-13.49017200	10.24252400	-1.13151100
O	-13.74692600	8.23665500	-5.51211400
O	-14.35693600	10.35417300	-3.79111800
C	-14.70227000	10.14614800	-0.37869700
C	-15.02845500	7.68484400	-5.82284200
C	-13.48908200	11.38349200	-4.28806300
C	-14.62977500	11.20275900	0.73425800
H	-15.56849700	10.31818200	-1.03297600
H	-14.79738200	9.14069500	0.05311600
C	-15.10291900	7.55956200	-7.35236000
H	-15.13896300	6.69913800	-5.35070500
H	-15.82535700	8.33711200	-5.43881800
C	-14.36627900	12.54156100	-4.78614800
H	-12.82067300	11.72150700	-3.48563400
H	-12.87426400	10.98470900	-5.10538100
C	-15.88727700	11.14625900	1.60539800
H	-13.72736300	11.00412000	1.31966700
H	-14.51172500	12.18512100	0.26688000
C	-16.44179800	6.95117200	-7.77632300
H	-14.96278600	8.55558400	-7.78330800
H	-14.26116500	6.93915300	-7.67332300
C	-13.47755500	13.66513600	-5.32959200
H	-15.03797600	12.15411600	-5.55813000
H	-14.98333700	12.88729400	-3.95124300
H	-16.78136500	11.35795500	1.01254800
H	-16.00624300	10.15256900	2.04588100

N	-15.94436900	12.12048900	2.78764100
H	-16.57924800	5.96660600	-7.32095900
H	-17.27530100	7.58453800	-7.46043100
N	-16.64618700	6.73189400	-9.27997700
H	-12.80450600	14.03411700	-4.55093700
H	-12.86158600	13.30226600	-6.15685400
N	-14.18930400	14.91040000	-5.87164400
C	-14.81916700	11.86435600	3.76139400
C	-17.26073600	11.90301000	3.50459200
C	-15.88484600	13.55414100	2.32025300
C	-16.57888800	8.03486000	-10.03842500
C	-18.02227500	6.13118500	-9.47824000
C	-15.61944100	5.77527600	-9.83714400
C	-15.00307500	15.58808800	-4.79658600
C	-15.08650400	14.56637100	-7.03521400
C	-13.12764800	15.87842600	-6.35338100
H	-14.85932600	10.82290000	4.08180200
H	-13.86575600	12.07654700	3.28096700
H	-14.94907600	12.52062800	4.62216800
H	-17.31815600	12.58787400	4.35068500
H	-18.07967300	12.10022000	2.81258800
H	-17.30650700	10.87264200	3.85748500
H	-14.91843300	13.74510500	1.85705000
H	-16.69184200	13.72721000	1.60760000
H	-16.01137500	14.20752300	3.18379100
H	-17.31403600	8.72426300	-9.62207800
H	-15.57610300	8.45055900	-9.95747300
H	-16.81001800	7.84044300	-11.08599500
H	-18.18483600	5.96728000	-10.54357500
H	-18.07541300	5.18225000	-8.94439500
H	-18.77140500	6.82241400	-9.09166500
H	-14.62838000	6.21891500	-9.76116100
H	-15.66229700	4.84318300	-9.27300500
H	-15.85525200	5.58443300	-10.88427500
H	-15.42431300	16.50696400	-5.20513400
H	-15.80800600	14.92714700	-4.47993400
H	-14.34976800	15.82489700	-3.95630300
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H	-14.49373700	14.06650800	-7.80186100
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H	-12.48223200	16.14336600	-5.51579000
H	-12.54420200	15.40230100	-7.14155500
H	-13.61645500	16.77190800	-6.74204700
C	-10.74755500	-4.96882400	1.51575800
C	-11.44053000	-5.89137400	1.91316000
C	-12.21883500	-6.99449800	2.37660900
C	-12.53302100	-8.07049900	1.51799600
C	-12.67443300	-7.05736400	3.71143900
C	-13.24482600	-9.17375400	1.98369000
H	-12.19344400	-8.06055900	0.48837600
C	-13.38093200	-8.16549200	4.17466900
H	-12.43987900	-6.25682600	4.40398400
C	-13.66998200	-9.24581200	3.32211700
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O	-14.35710200	-10.35406400	3.79126200
C	-14.70241000	-10.14622500	0.37864000
C	-15.02903500	-7.68532800	5.82256800
C	-13.48917700	-11.38353400	4.28778100
C	-14.62992400	-11.20298000	-0.73417800
H	-15.56872500	-10.31808000	1.03285000
H	-14.79736600	-9.14081500	-0.05330600
C	-15.10349500	-7.55942700	7.35203800
H	-15.14028900	-6.69990800	5.35000700
H	-15.82547200	-8.33835400	5.43887200
C	-14.36632000	-12.54143300	4.78635400
H	-12.82124700	-11.72168200	3.48501100
H	-12.87386100	-10.98484200	5.10476900
C	-15.88735000	-11.14646400	-1.60542800
H	-13.72744200	-11.00450300	-1.31953500
H	-14.51201300	-12.18529800	-0.26667100
C	-16.44279600	-6.95185900	7.77584100
H	-14.96257500	-8.55515200	7.78341300
H	-14.26218300	-6.93824500	7.67266300
C	-13.47751300	-13.66512600	5.32941900
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H	-14.98385300	-12.88710600	3.95177300
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H	-13.61622100	-16.77180100	6.74210200

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