Supplementary Information

Cyclic arylopeptoid oligomers: Synthesis and structure of peptide-mimetic aromatic macrocycles

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Abbreviation: DIC = *N*,*N*'-diisopropylcarbodiimide, NMP = *N*-Methyl-2-pyrrolidone, DMF = *N*,*N*-dimethylformamide, DMSO = dimethylsulfoxide, DMAP = *N*,*N*-Dimethylpyridin-4-amine, DIEA = *N*,*N*-diisopropylethylamine, DVB = divinylbenzene.

1. General experimental

Unless stated otherwise, all commercial reagents were used as received. All water used in the experiments refers to ultra-pure water obtained from a Millipore system having a specific resistance of 18 MΩ•cm. Thin layer chromatography (TLC) was performed on silica gel $60F_{254}$ (Merck). Column chromatography was performed on silica gel PSQ-100B (Fuji Silysia Chemical, 100 μm). Analytical size exclusion chromatography (SEC) was conducted with a Shimadzu Prominence instrument LC-20AT and SPD-20A equipped with a Tosoh TSKgel $G2500H_{xL}$ (5 μm, 300 mm × 7.8 mm I. D.). ^{1}H and ^{13}C NMR spectra were obtained on a JEOL JNM ECS-400 spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C) or a JEOL JNM ECA-600 spectrometer (600 MHz for ^{1}H, 150 MHz for ^{13}C) with tetramethylsilane (TMS) or residual non-deuterated solvents as the internal references. Multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = double doublet, br = broad. MALDI-TOF mass spectra were recorded using a Shimadzu AXIMA-CFR plus mass spectrometer (CHCA as matrix). Electron-splay ionization (ESI) TOF mass spectrometry was performed on a Waters Xevo G1 QTof or a JEOL JMS-T100LP AccuTOF LC-plus mass spectrometer.

2. Synthesis

2.1 Solid-phase synthesis of linear arylopeptoid oligomers

Syntheses of arylopeptoid oligomers were carried out on the solid phase by using a multiple reaction device (HiPep Laboratories, PetiSyzer) according to the method reported previously[s1]. All reactions were carried out in cartridges with polypropylene frits (HiPep Laboratories, LibraTube). The solid phase synthesis was performed on 2-chlorotrityl chloride resin (Watanabe, 100–200 mesh, 1% DVB, 1.6 mmol/g). Each obtained arylopeptoid after cleavage from the resin was purified by silica gel column chromatography and size exclusion column chromatography (Biobeads SX-1, chloroform) and analyzed by ^{1}H and ^{13}C NMR and MALDI-TOF-MS.

Coupling of 4-chloromethyl benzoic acid on trityl resin: Typically, 100 mg of 2-chlorotrityl chloride resin (0.16 mmol) were washed twice with CH_2Cl_2 (2.0 mL), followed by swelling in CH_2Cl_2 (2.0 mL) overnight. The first monomer was introduced upon the addition of 4-chloromethyl benzoic acid (31 mg, 0.18 mmol, 1.1 equiv) and *N*,*N*-diisopropylethylamine (DIEA) (126 μL, 0.72 mmol) in CH_2Cl_2 (1.3 mL) for 1 h at room temperature (rt), followed by extensive washes with CH_2Cl_2 and DMF.

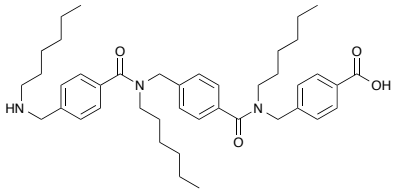
General procedure for nucleophilic displacement: Amine (3 mmol, 20 equiv) was added in dry DMSO (1.3 mL) to the resin in the synthesis cartridge and the mixture was agitated at 50 °C for 2 h,

followed by extensive washes with DMSO and CH_2Cl_2. The reaction was monitored by a chloranil test (positive).

General procedure for acylation: To a solution of 4-(chloromethyl)benzoyl chloride (71 mg, 0.38 mmol, 2 equiv) in CH_2Cl_2 (0.8 mL) was added DIEA (132 μL, 0.76 mmol) at rt. The mixture was added to the resin in the synthesis cartridge and the mixture was agitated at rt for 1 h, followed by extensive washes with DMSO and CH_2Cl_2. The reaction was monitored by a chloranil test (negative).

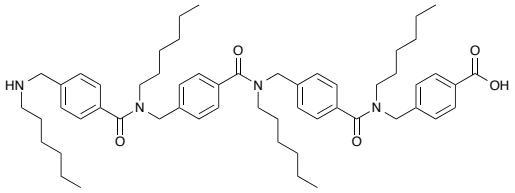
General procedure for cleavage from trityl resin: The cleavage from the resin was carried out in HFIP/CH_2Cl_2 (1:4 (*v*/*v*), 1.0 mL). The resin was drained and washed with CH_2Cl_2 (3 × 3.0 mL). The collected solvents were evaporated under reduced procedure to yield crude arylopeptoid.

L[3]pAP(Hex$_3$): The titled linear arylopeptoid was synthesized according to the method described above. Purification by column chromatography (SiO_2, chloroform-methanol = 60:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, chloroform) gave **L[3]pAP(Hex$_3$)** as a white powder.



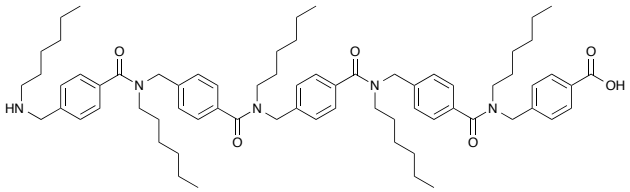
Isolated yield: 65 mg (63%, 0.16 mmol scale); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 0.73–0.92 (m, 9H), 0.99–1.56 (m, 20H), 1.58–1.82 (br, 4H), 2.66–3.12 (br, 4H), 3.44–3.83 (br, 4H), 4.10 (br, 1H), 2.98–4.28–4.50 (m, 2H), 4.56–4.89 (br, 2H), 6.83–7.56 (m, 10H), 7.70–8.12 (br, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 14.0, 22.4, 26.1, 26.5, 31.3, 127.2, 127.7, 128.1, 130.1, 178.6; HRMS (ESI, positive): Calcd. for $[M(C_{42}H_{60}N_3O_4) + H]^+$: m/z = 670.4584; Found: 670.4575.

L[4]pAP(Hex$_4$): The titled linear arylopeptoid was synthesized according to the method described above. Purification by column chromatography (SiO_2, chloroform-methanol = 60:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, chloroform) gave **L[4]pAP(Hex$_4$)** as a white powder.



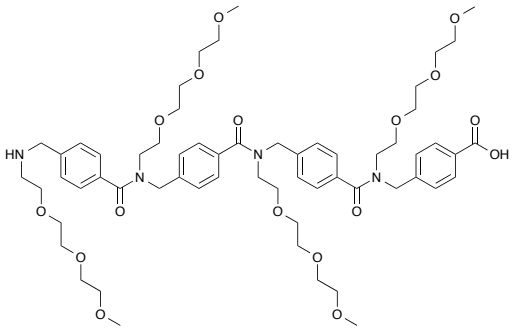
Isolated yield: 110 mg (76%, 0.16 mmol scale); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 0.69–0.92 (m, 12H), 0.99–1.37 (m, 24H), 1.46 (br, 2H), 1.64 (br, 2H), 1.80 (br, 3H), 2.82 (br, 2H), 2.98–3.28 (m, 3H), 3.45 (br, 3H), 4.06–4.25 (br, 2H), 4.49 (br, 3H), 4.78 (br, 3H), 6.98–7.73 (m, 14H), 8.02 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 13.9, 14.0, 22.3, 22.6, 26.0, 26.3, 26.7, 27.2, 28.1, 29.7, 31.1, 31.6, 127.0, 130.1, 137.0, 171.8; HRMS (ESI, positive): Calcd. for $[M(C_{56}H_{78}N_4O_5) + Na]^+$: m/z = 909.5870; Found: 909.5852.

L[5]pAP(Hex$_5$): The titled linear arylopeptoid was synthesized according to the method described above. Purification by column chromatography (SiO_2, chloroform-methanol = 60:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, chloroform) gave **L[5]pAP(Hex$_5$)** as a white powder.



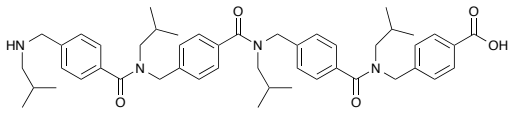
Isolated yield: 86 mg (48%, 0.16 mmol scale); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 0.68–0.96 (m, 15H), 0.98–1.82 (m, 20H), 2.59–3.57 (m, 10H), 3.88–4.87 (m, 10H), 7.04–7.70 (m, 18H), 8.06 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 13.9, 14.1, 22.4, 22.7, 26.2, 26.5, 26.7, 27.0, 28.2, 29.8, 31.3, 31.6, 127.1, 127.7, 130.1, 135.7, 137.0, 171.7; HRMS (ESI, positive): Calcd. for $[M(C_{70}H_{97}N_5O_6) + K]^+$: m/z = 1142.7076; Found: 1142.7093.

L[4]pAP(mTEG$_4$): The titled linear arylopeptoid was synthesized according to the method described above. Purification by column chromatography (SiO_2, chloroform-methanol = 60:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, chloroform) gave **L[4]pAP(mTEG$_4$)** as a white powder.



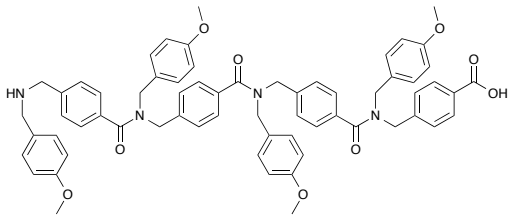
Isolated yield: 67 mg (37%, 0.16 mmol scale); ^{1}H NMR (400 MHz, $CDCl_3$, rt): δ (ppm) = 3.36 (s, 12H), 3.40–3.92 (m, 40H), 4.27–4.42 (m, 3H), 4.55–4.92 (m, 8H), 7.26 (s, 13H), 7.84–8.12 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, rt): δ (ppm) = 59.1, 66.0, 69.4, 70.5, 70.6, 70.7, 72.0, 127.5, 127.8, 128.0, 130.5, 166.4; HRMS (ESI, positive): Calcd. for [M ($C_{64}H_{62}N_4O_9$) + Na]$^+$: m/z = 1157.5861; Found: 1157.5886.

L[4]pAP(iBt$_4$): The titled linear arylopeptoid was synthesized according to the method described above. Purification by column chromatography (SiO_2, chloroform-methanol = 60:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, chloroform) gave **L[4]pAP(iBt$_4$)** as a white powder.



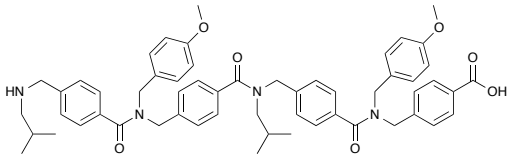
Isolated yield: 92 mg (74%, 0.16 mmol scale); ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 0.58–1.05 (m, 24H), 2.04–2.19 (m, 3H), 2.56–2.69 (m, 2H), 2.80–2.89 (m, 1H), 3.24–3.47 (m, 4H), 3.95–4.11 (m, 3H), 4.39–4.60 (m, 5H), 4.66–4.81 (m, 3H), 6.93–7.24 (m, 5H), 7.27–7.57 (m, 8H), 7.83–8.10 (m, 3H); 13C NMR (100 MHz, $CDCl_3$): δ (ppm) = 19.8, 20.2, 20.6, 26.7, 51.5, 52.7, 126.2, 126.9, 127.2, 127.4, 127.9, 130.3, 135.9, 172.4; HRMS (ESI, positive): Calcd. for [M($C_{48}H_{62}N_4O_5$) + Na]$^+$: m/z = 775.4799; Found: 775.4798.

L[4]pAP(mBzl$_4$): The titled linear arylopeptoid was synthesized according to the method described above. Purification by column chromatography (SiO_2, chloroform-methanol = 60:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, chloroform) gave **L[4]pAP(mBzl$_4$)** as a white powder.



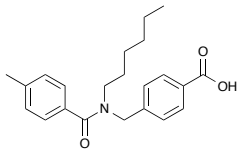
Isolated yield: 120 mg (72%, 0.16 mmol scale); ^{1}H NMR (400 MHz, $CDCl_3$, rt): δ (ppm) = 3.81 (m, 16H), 4.15–4.79 (m, 12H), 7.26 (m, 30H), 7.85–8.16 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 46.6, 126.4, 114.2, 55.3, 51.2, 127.1, 127.7, 128.0, 128.3, 129.8, 130.2, 131.1, 159.1, 171.6, 171.8; HRMS (ESI, positive): Calcd. for $[M(C_{64}H_{62}N_4O_9) + H]^+$: m/z = 1031.4595; Found: 1031.4601.

L[4]pAP(iBt-mBzl-iBt-mBzl): The titled compound was synthesized from the corresponding linear compound and purification by column chromatography (SiO_2, chloroform-methanol = 60:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, chloroform) gave **L[4]pAP(iBt-mBzl-iBt-mBzl)** as a white powder.



Isolated yield: 110 mg (75%, 0.16 mmol scale); ^{1}H NMR (400 MHz, $CDCl_3$, rt): δ (ppm) = 0.79–1.08 (m, 12H), 2.59–2.74 (br, 2H), 2.90–3.44 (br, 4H), 3.82 (s, 6H), 4.05 (s, 2H), 4.13–4.23 (m, 1H), 4.26–4.35 (br, 1H), 4.36–4.83 (br, 8H), 7.26 (br, 21H), 7.81–8.17 (br, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 20.1, 20.5, 26.4, 46.2, 51.2, 55.3, 114.1, 114.3, 127.2, 128.3, 129.7, 129.8, 129.9, 130.0, 159.2, 171.5, 171.8; HRMS (ESI, positive): Calcd. for $[M(C_{56}H_{62}N_4O_7) + Na]^+$: m/z = 925.4516; Found: 925.4492.

L[2]pAP(Hex) (Dimer model compound for NMR analysis): The titled linear arylopeptoid dimer was synthesized according to the general method described above except for acylation at the final step using *p*-toluoyl chloride instead of 4-(chloromethyl)benzoyl chloride. After cleavage from resin according to the general method, purification by column chromatography (SiO_2, *n*-hexane-ethyl acetate = 1:1 (*v*/*v*)) gave **L[2]pAP(Hex)** as yellow amorphous solid.



Isolated yield: 57 mg (92%, 0.16 mmol scale); ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 0.77–0.91 (m, 4H), 1.02–1.35 (m, 9H), 2.31–2.43 (m, 2H), 3.14–3.48 (m, 2H), 4.59–4.87 (m, 2H), 7.15 (d, J = 7.6 Hz, 1H), 7.24 (d, J = 7.6 Hz, 1H), 7.30 (d, J = 5.5 Hz, 2H), 7.35 (d, J = 7.9 Hz, 1H), 7.45 (d, J = 7.9 Hz, 1H), 8.10 (d, J = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 13.9, 21.3, 22.4, 26.1, 28.1, 29.6, 31.5, 47.5, 48.7, 126.6, 127.7, 129.0, 130.5, 133.2, 139.6, 171.1, 172.54; HRMS (ESI, positive): Calcd. for $[M(C_{22}H_{27}NO_3) + Na]^+$: m/z = 376.1889; Found: 376.1900.

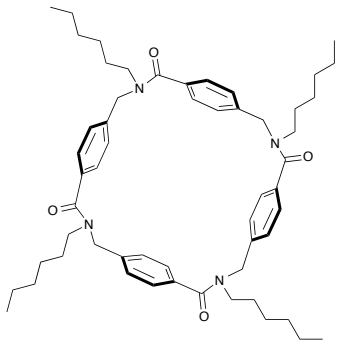
2.2. General procedure for macrocyclization (Synthesis of C[n]pAP(R_n))

Method A (High dilution without slow addition): Macrocyclization reactions were conducted in dry DMF according to the slightly modified method reported previously[s2,3]. The reaction vessel containing PyBOP, DIEA and linear arylopeptoid was flushed with Ar and sealed from air. The reaction proceeded at room temperature. After the almost complete consumption of starting material (linear arylopeptoid), the resulting mixture was evaporated under reduced pressure. Purification by column chromatography (SiO_2, $CHCl_3$–MeOH) and size exclusion column chromatography (Biobeads SX-1, $CHCl_3$) gave the desired products (cyclic arylopeptoid).

Method B (High dilution with slow addition via syringe pump): PyBOP, DIEA of DMF was charged to a 50-mL round bottom flask with a magnetic stirrer under Ar. A solution of linear arylopeptoid in DMF was added to this reaction solution by dropwise addition via syringe pump (YMC YSP-101) at rt. The reaction proceeded at room temperature. After the almost complete consumption of starting material (linear arylopeptoid), the resulting mixture was evaporated under reduced pressure. Purification by column chromatography (SiO_2, $CHCl_3$–MeOH) and size exclusion column chromatography (Biobeads SX-1, $CHCl_3$) gave the desired product (cyclic arylopeptoid).

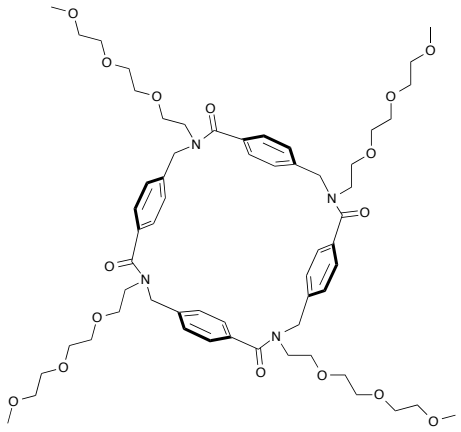
C[4]pAP(Hex$_4$): The titled compound was synthesized according to the **method A** and **method B**. **Method B**: PyBOP (37 mg, 0.72 mmol), DIEA (25 μL, 0.14 mmol) and 11 mL of DMF was charged to a 50 mL round bottom flask with a magnetic stirrer under Ar. A solution of **L[4]pAP(Hex$_4$)** (21 mg, 24 μmol) and 1.2 mL of DMF was added to this reaction solution by dropwise addition via syringe pump at rt (50 μL/h). After stirring for 10 h, PyBOP (37 mg, 0.72 mmol) was added to reaction solution. After another 12 h, the resulting mixture was evaporated under reduced pressure. Purification by

column chromatography (SiO_2, $CHCl_3$–MeOH = 15:1 (*v*/*v*)) and size exclusion column chromatography (Biobeads SX-1, $CHCl_3$) gave **C[4]pAP(Hex$_4$)** as a white powder.



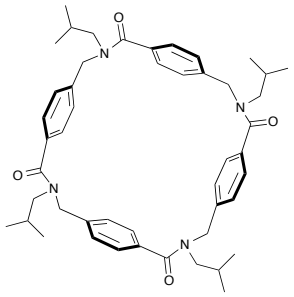
Isolated yield: 19 mg (92%); ^{1}H NMR (600 MHz, $CDCl_3$, –20 °C): δ (ppm) = 0.86 (s, 12H), 1.27 (s, 24H), 1.56–1.64 (br, 8H), 3.36 (br, 8H), 4.37 (s, 8H), 7.06 (d, J = 7.6 Hz, 8H), 7.38 (d, J = 7.6 Hz, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 14.0, 22.5, 26.6, 27.1, 31.5, 45.0, 52.0, 126.7, 127.0, 136.0, 138.2, 171.1; HRMS (ESI, positive): Calcd. for [M($C_{56}H_{76}N_4O_4$) + H]$^+$: m/z = 891.5764; Found: 891.5790. Structure was confirmed by single crystal X-ray diffraction (**Fig. S32**).

C[4]pAP(mTEG$_4$): The titled compound was synthesized from **L[4]pAP(mTEG$_4$)** (49 mg, 43 μmol) according to the **method B**.



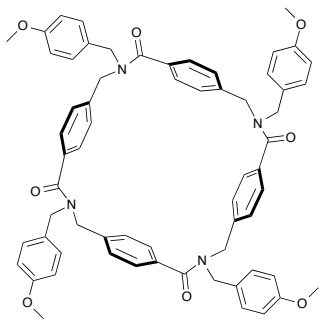
Isolated yield: 35 mg (72%); ^{1}H NMR (600 MHz, $CDCl_3$, –20 °C): δ (ppm) = 3.37 (s, 12H), 3.57 (s, 8H), 3.66 (s, 32H), 3.77 (s, 8H), 4.55 (s., 8H), 7.08 (d, J = 8.3 Hz, 8H), 7.40 (d, J = 8.3 Hz, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 44.6, 53.3, 59.0, 69.5, 70.3, 70.5, 70.6, 71.9, 126.9, 127.1, 135.8, 138.5, 171.6; HRMS (ESI, positive): Calcd. for [M ($C_{60}H_{84}N_4O_{16}$) + H]$^+$: m/z = 1117.5961; Found: 1117.5944.

C[4]pAP(iBt$_4$): The titled compound was synthesized from **L[4]pAP(iBt$_4$)** (23 mg, 30 μmol) according to the **method B**.



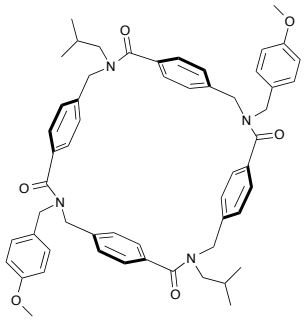
Isolated yield: 18 mg (80%); ^{1}H NMR (600 MHz, $CDCl_3$, –20 °C): δ (ppm) = 0.94 (d, J = 6.2 Hz, 24H), 2.07 (s, 4H), 3.11–3.33 (br, 8H), 4.40 (s., 8H), 7.05 (d, J = 8.3 Hz, 8H), 7.40 (d, J = 8.3 Hz, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 20.0, 26.4, 51.4, 52.7, 126.8, 127.1, 136.2, 138.1, 171.7; HRMS (ESI, positive): Calcd. for $[M(C_{48}H_{60}N_4O_4) + Na]^+$: m/z = 779.4512; Found: 779.4504.

C[4]pAP(mBzl$_4$): The titled compound was synthesized from **L[4]pAP(iBt-mBzl-iBt-mBzl)** (27 mg, 26 μmol) according to the **method B**.



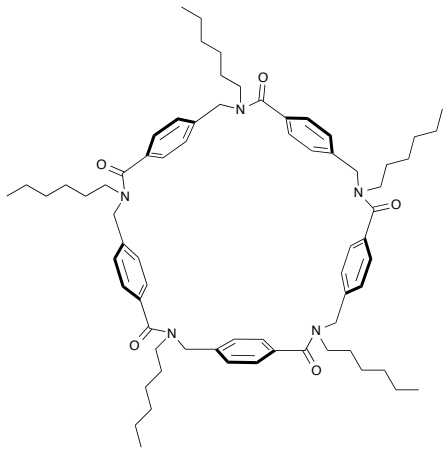
Isolated yield: 22 mg (85%); ^{1}H NMR (600 MHz, $CDCl_3$, –20 °C): δ (ppm) = 3.82 (s, 12H), 4.13–4.78 (m, 16H), 6.88 (d, J = 7.6 Hz, 8H), 7.06 (d, J = 6.9 Hz, 8H), 7.18 (d, J = 7.6 Hz, 8H), 7.46 (d, J = 7.6 Hz, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 46.4, 50.7, 55.4, 114.3, 127.2, 127.3, 128.7, 130.1, 136.0, 137.9, 159.3, 171.6; HRMS (ESI, positive): Calcd. for $[M(C_{64}H_{60}N_4O_8) + Na]^+$: m/z = 1035.4309; Found: 1035.4324.

C[4]pAP(iBt-mBzl-iBt-mBzl): The titled compound was synthesized from **L[4]pAP(iBt-mBzl-iBt-mBzl)** (23 mg, 26 μmol) according to the **method B**.



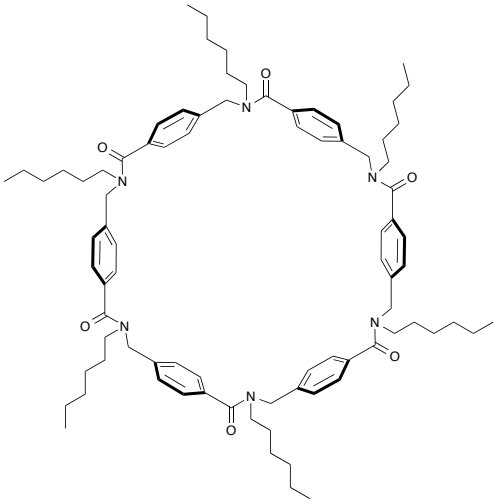
Isolated yield: 17 mg (76%); ^{1}H NMR (600 MHz, $CDCl_3$, –20 °C): δ (ppm) = 0.96 (d, J = 6.9 Hz, 12H), 2.05–2.14 (br, 2H), 3.11–3.40 (br, 4H), 3.81 (s, 8H), 4.19 (br, 4H), 4.40 (br, 8H), 6.87 (d, J = 8.3 Hz, 4H), 7.06 (d, J = 4.8 Hz, 8H), 7.16 (d, J = 8.3 Hz, 4H), 7.43 (d, J = 7.6 Hz, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 20.1, 26.5, 46.2, 50.5, 51.6, 52.5, 55.3, 114.1, 126.9, 127.1, 127.3, 128.5, 129.9, 135.7, 136.4, 137.5, 138.3, 159.2, 171.4, 171.8; HRMS (ESI, positive): Calcd. for $[M(C_{56}H_{60}N_4O_6) + Na]^+$: m/z = 907.4411; Found: 907.4385. Structure was confirmed by single crystal X-ray diffraction (**Fig. S34**).

C[5]pAP(Hex$_5$): The titled compound was synthesized from **L[5]pAP(Hex$_5$)** (59 mg, 53 μmol) according to the **method A**.



Isolated yield: 36 mg (62%); ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) = 0.73–0.96 (br, 15H), 1.01–1.41 (br, 30H), 1.44–1.99 (br, 10H (overlapped with water)), 3.06–3.67 (m, 10H), 4.27–4.90 (m, 10H), 7.03–7.61 (m, 20H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 14.1, 22.6, 22.7, 26.2, 26.4, 26.7, 27.0, 31.3, 31.6, 46.5, 46.5, 52.2. 127.4, 135.4, 139.3, 171.8; HRMS (ESI, positive): Calcd. for $[M(C_{70}H_{95}N_5O_5) + Na]^+$: m/z = 1108.7231; Found: 1108.7240.

C[6]pAP(Hex$_6$): The titled compound was obtained from **L[3]pAP(Hex$_3$)** (34 mg, 31 μmol) according to the **method A.**



Isolated yield: 27 mg (81%); ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) = 0.73–0.95 (br, 18H), 1.00–1.39 (br, 36H (overlapped with water)), 1.41–1.76 (br, 12H), 3.02–3.56 (m, 12H), 4.41–4.89 (m, 12H), 7.04–7.55 (m, 24H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 14.0, 22.5, 22.7, 26.2, 26.7, 28.2, 29.8, 31.3, 31.7, 127.1, 127.8, 135.7, 139.2, 172.0; HRMS (ESI, positive): Calcd. for $[M(C_{84}H_{114}N_6O_6) + Na]^+$: m/z = 1325.8734; Found: 1325.8698.

3. Characterization of compounds

3.1. Size exclusion chromatography of macrocyclic oligomers (cyclo[n]-*p*-arylopeptoids)

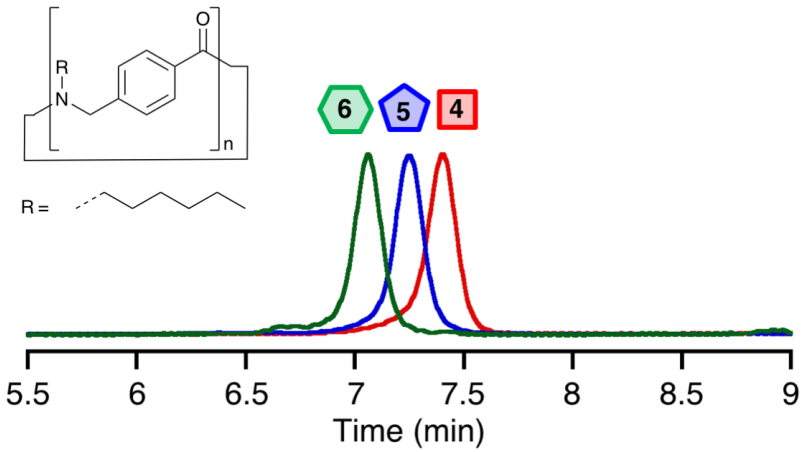


Fig. S1 SEC charts of macrocyclic oligomers (**C[4]pAP(Hex$_4$)**, **C[5]pAP(Hex$_5$)**, and **C[6]pAP(Hex$_6$)**). *Conditions* Column: Tosoh TSKgel G2500H$_{XL}$ (5 μm, 300 mm × 7.8 mm I. D.), Eluent: THF, Flow rate: 1.0 mL/min, detection wavelength: 254 nm.

3.2. ^{1}H and ^{13}C NMR spectra of compounds

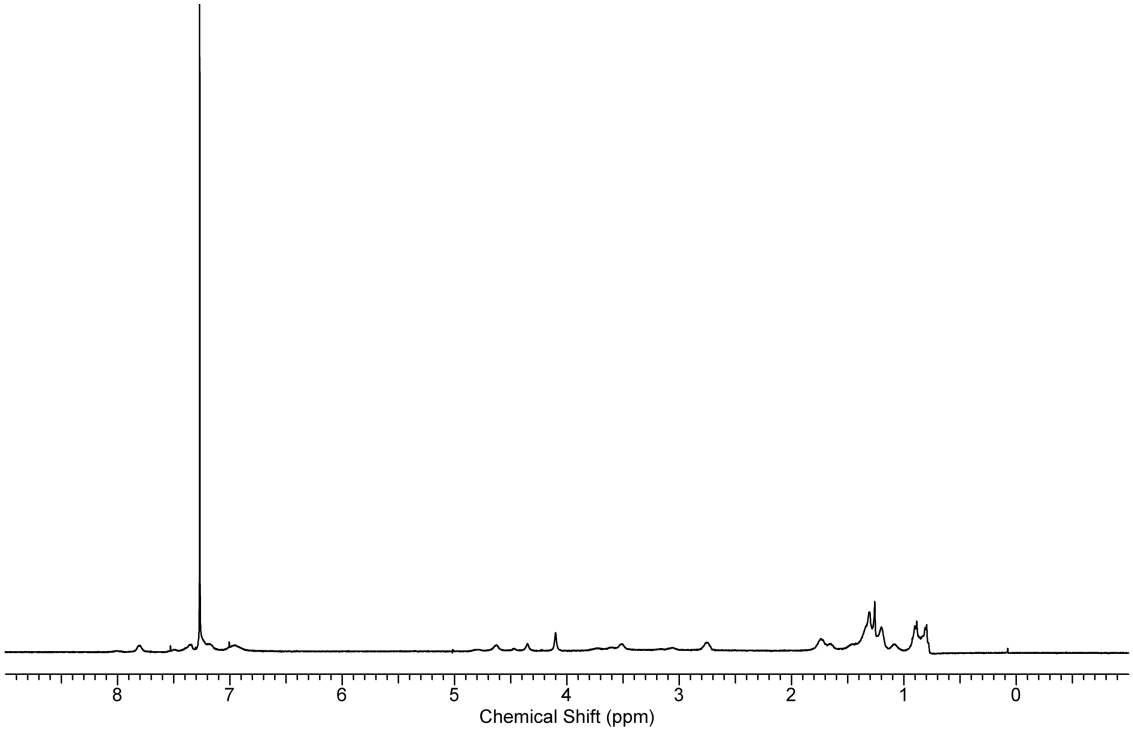


Fig. S2 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L[3]pAP(Hex$_3$)**.

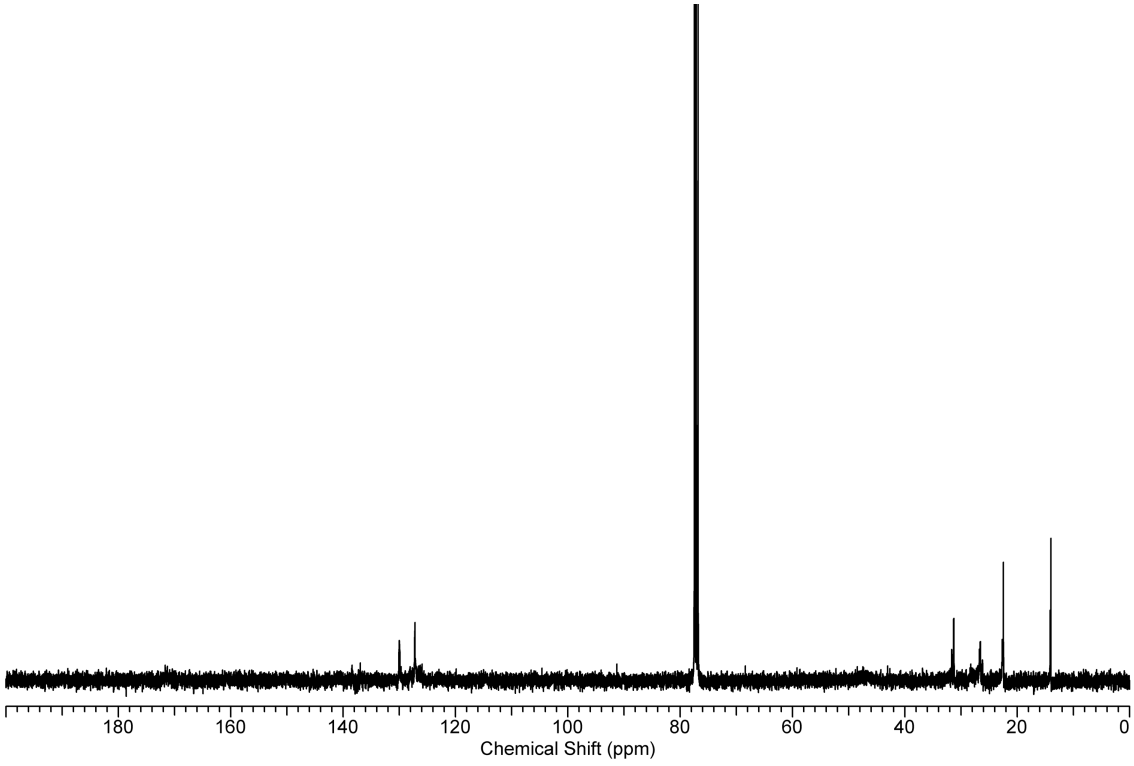


Fig. S3 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[3]pAP(Hex$_3$)**.

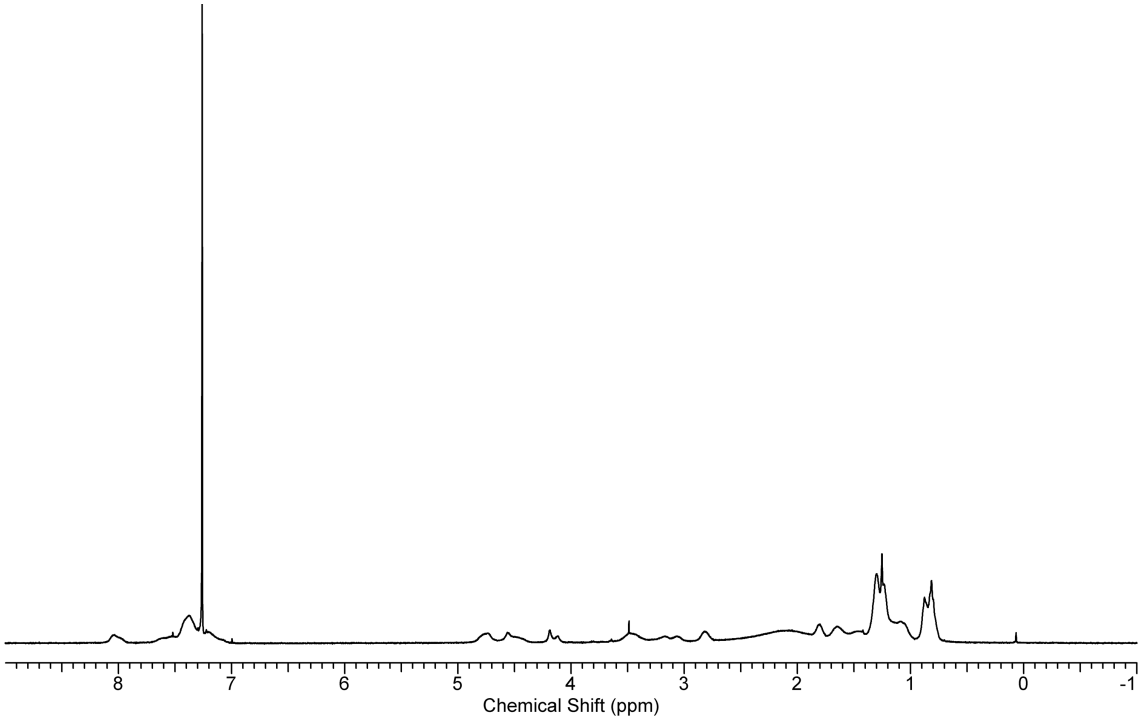


Fig. S4 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L[4]pAP(Hex$_4$)**.

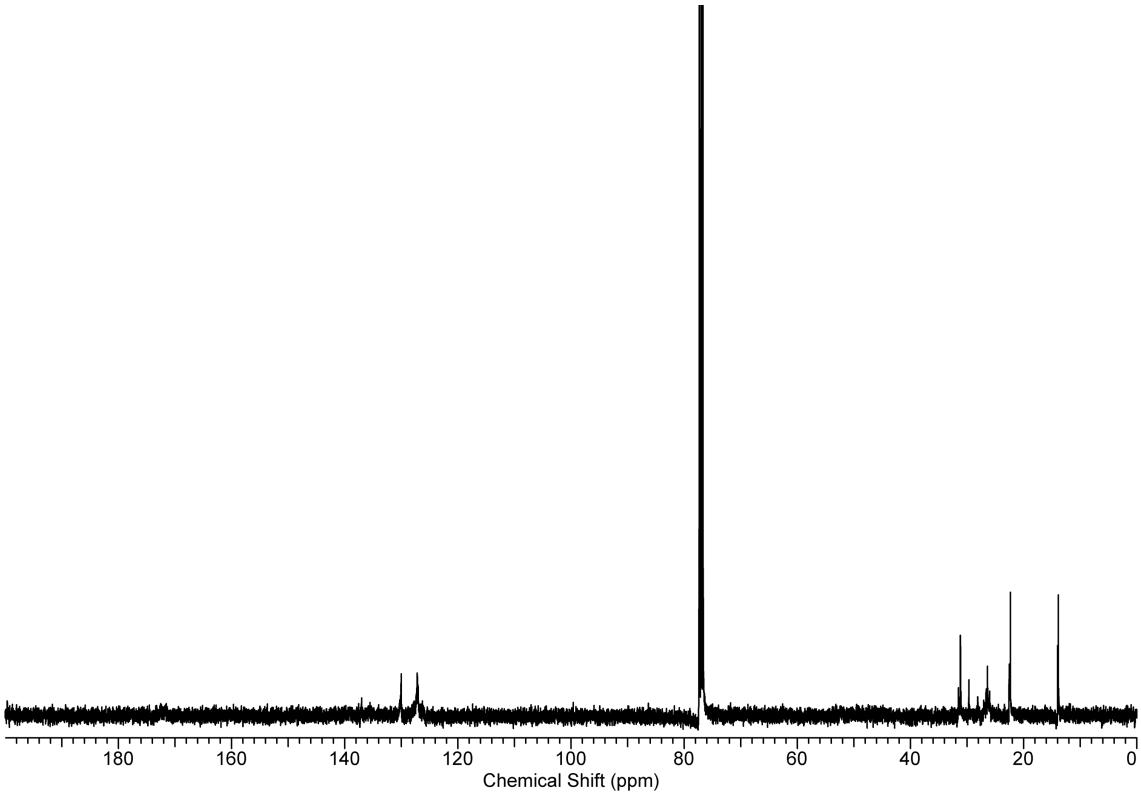


Fig. S5 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[4]pAP(Hex$_4$)**.

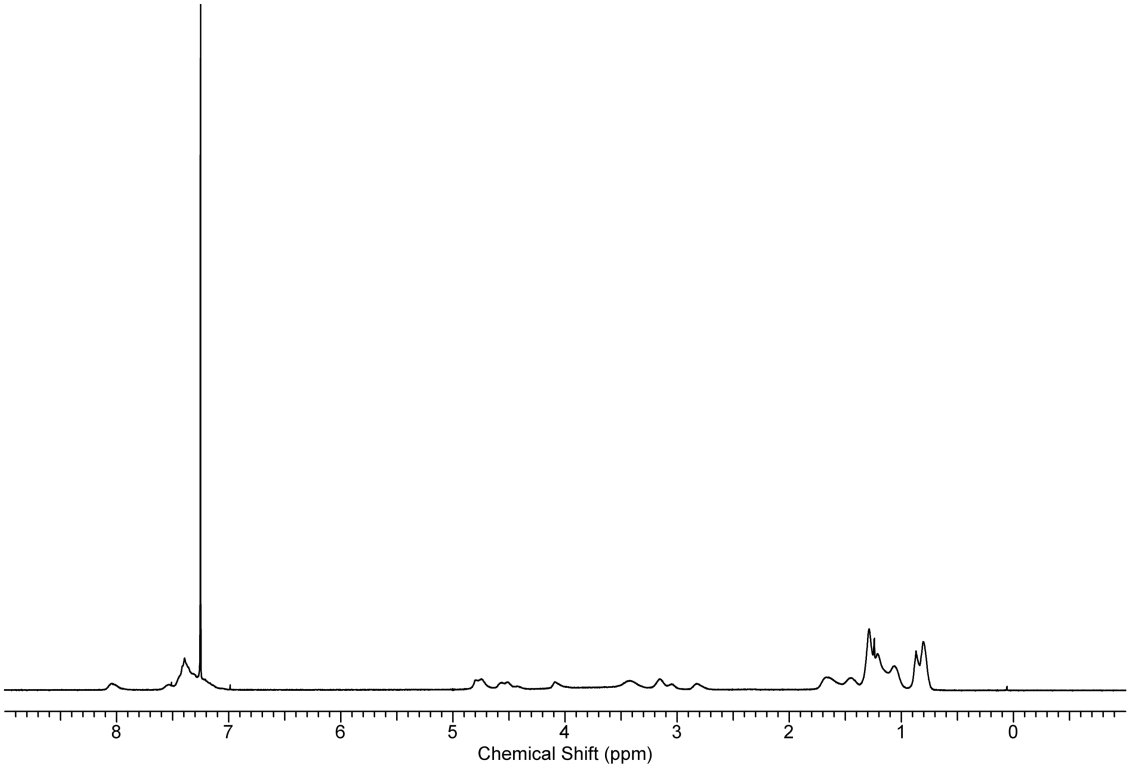


Fig. S6 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L[5]pAP(Hex$_5$)**.

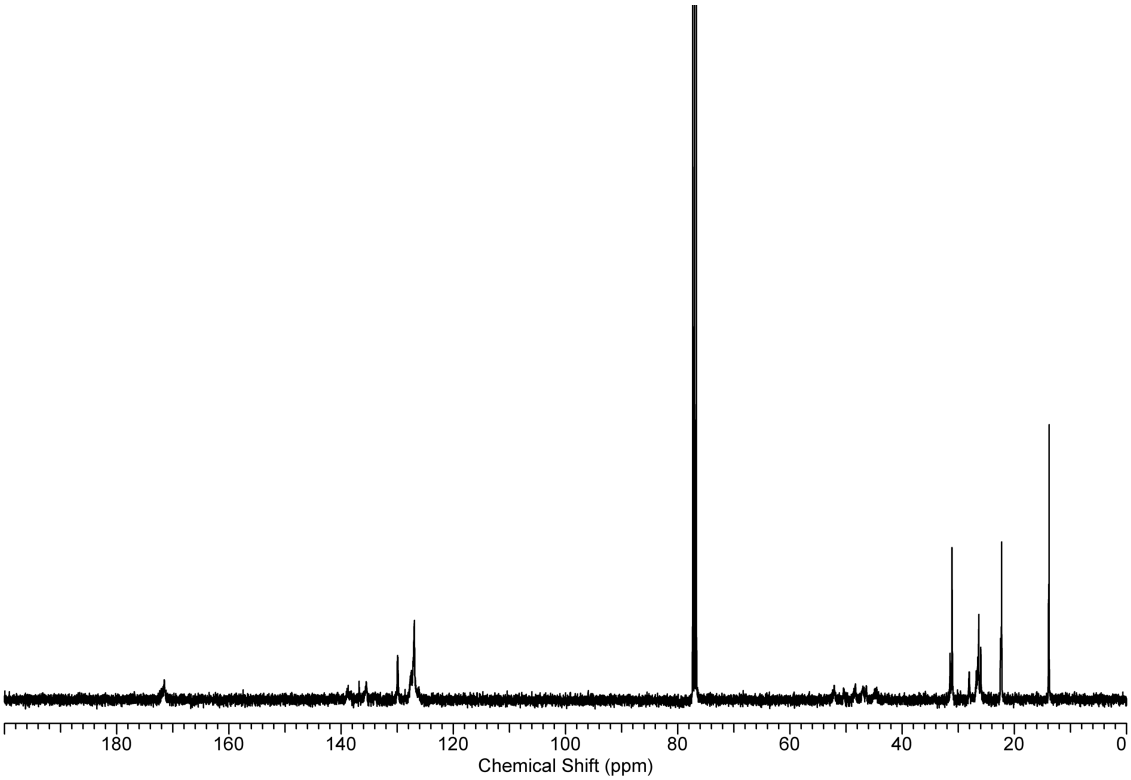


Fig. S7 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[5]pAP(Hex$_5$)**.

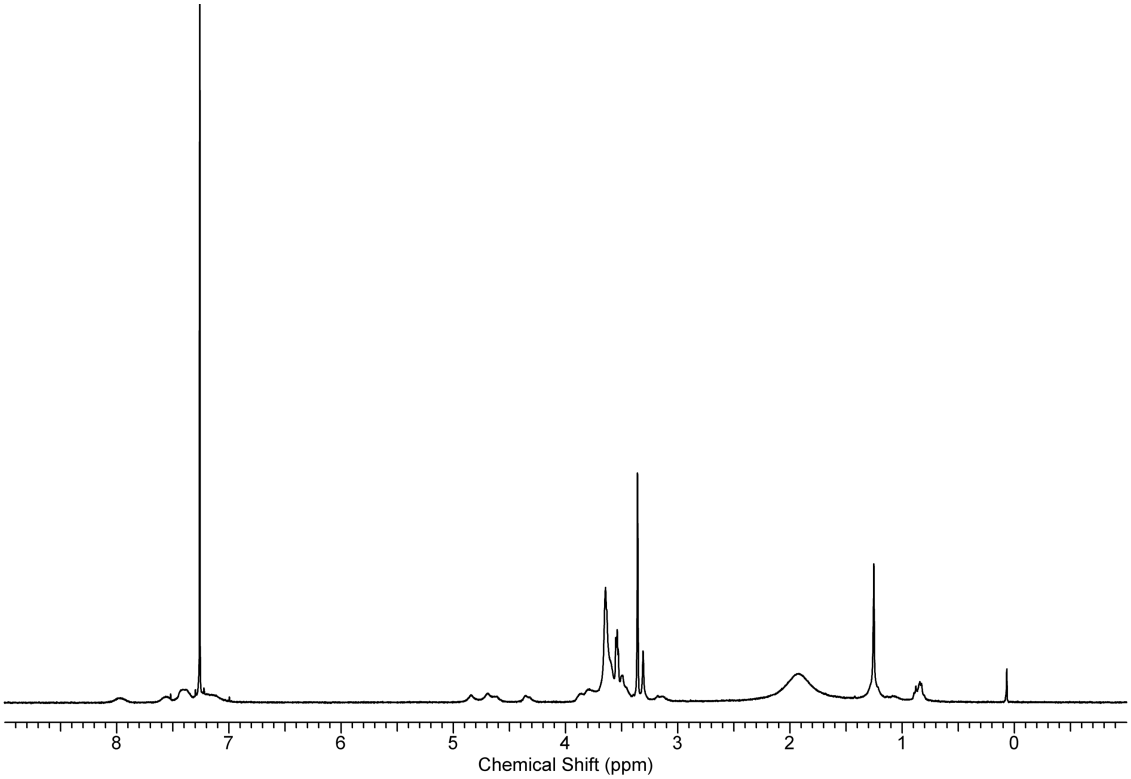


Fig. S8 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L[4]pAP(mTEG$_4$)**.

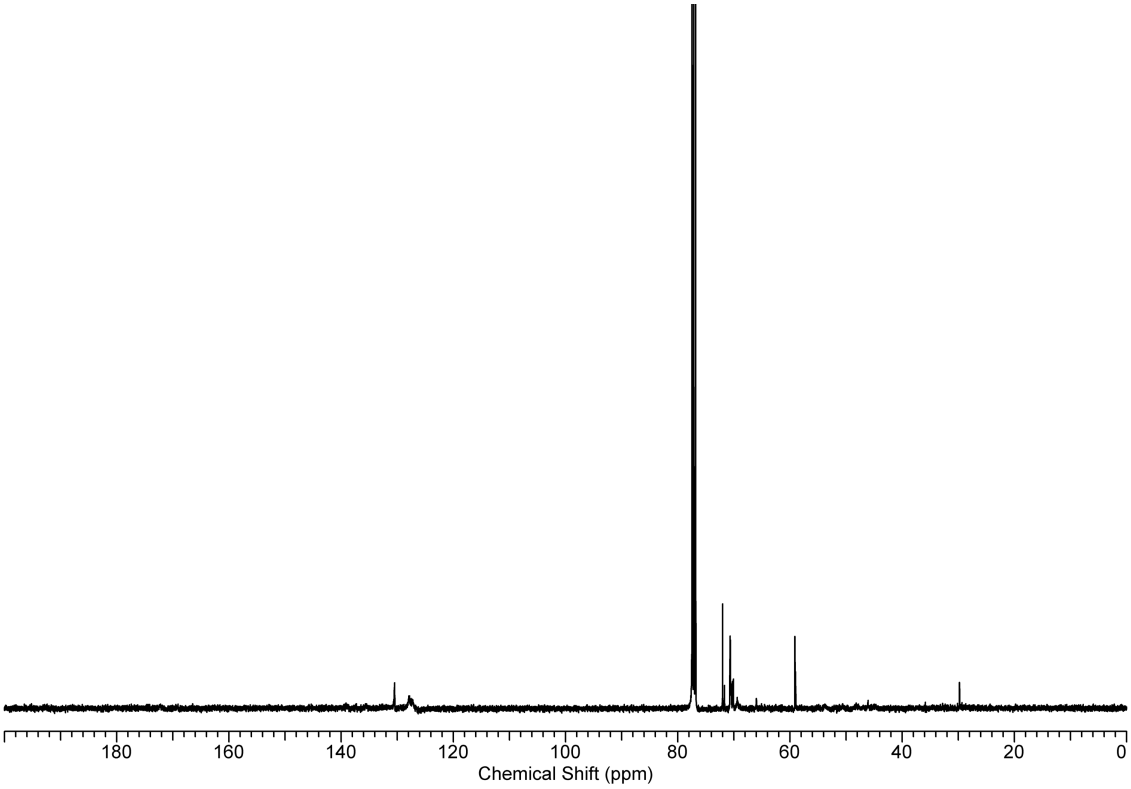


Fig. S9 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[4]pAP(mTEG$_4$)**.

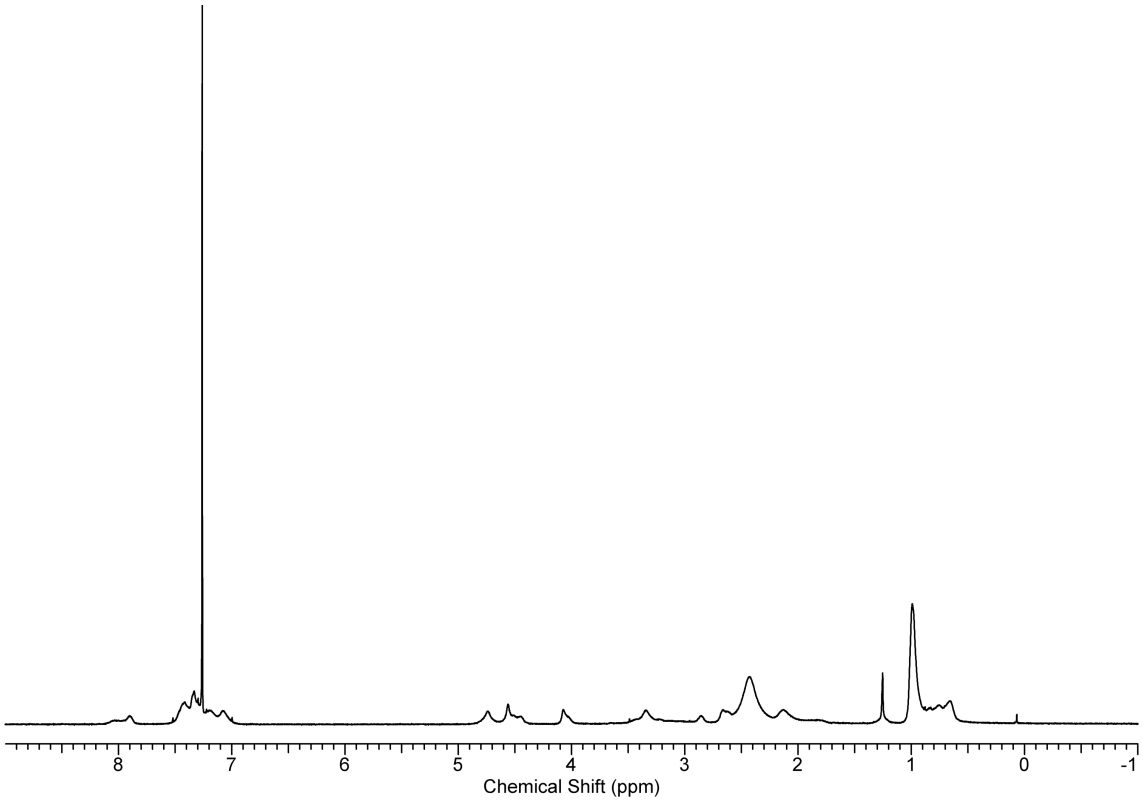


Fig. S10 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L[4]pAP(iBt$_4$)**.

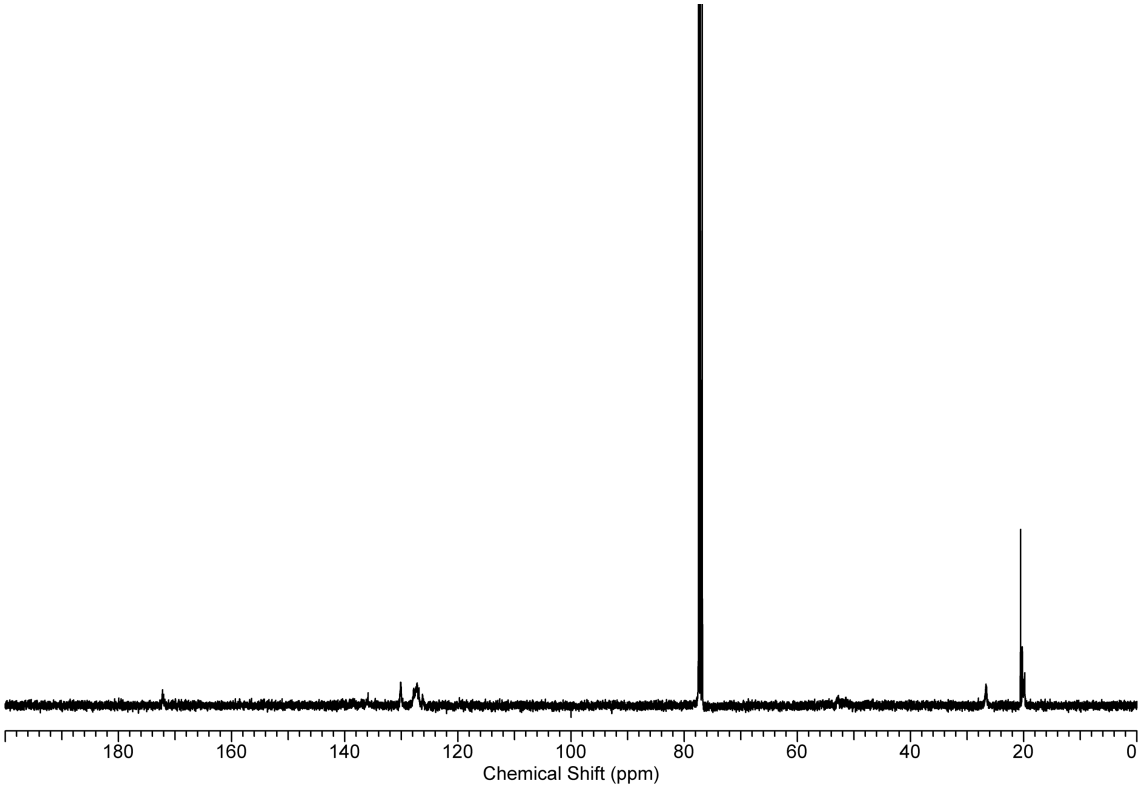


Fig. S11 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[4]pAP(iBt$_4$)**.

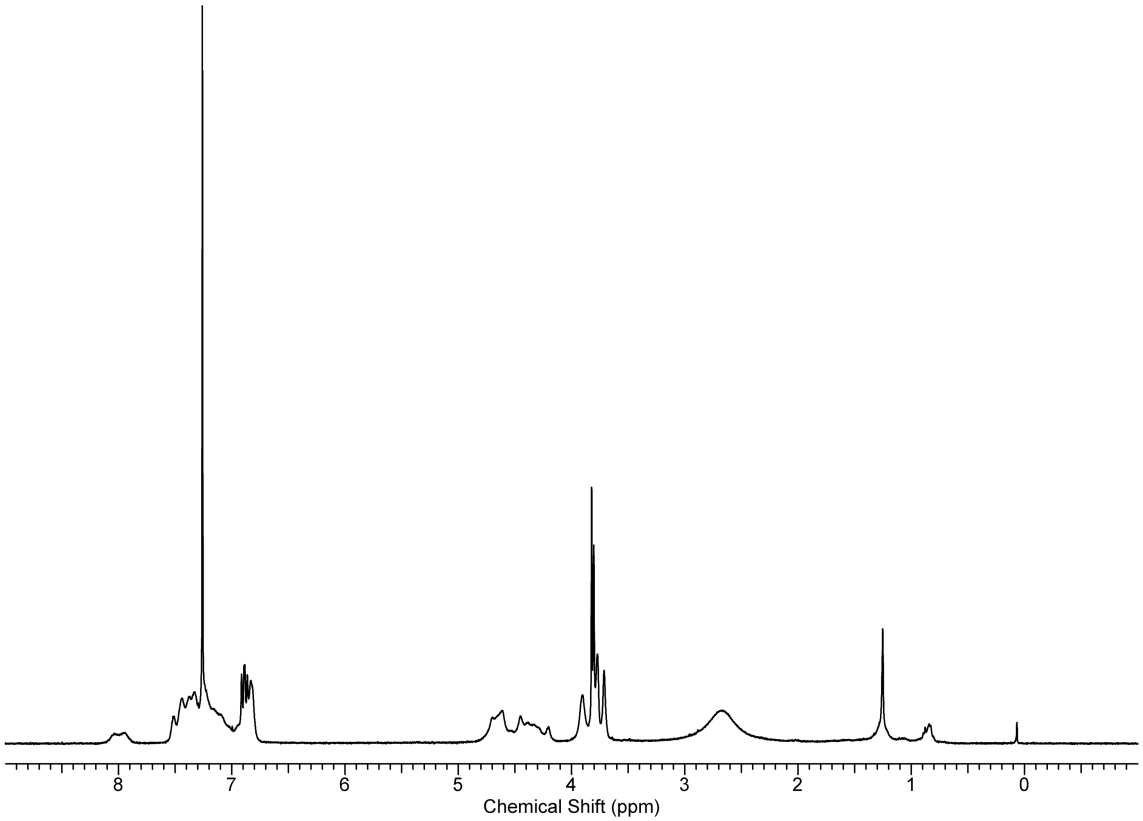


Fig. S12 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L[4]pAP(mBzl$_4$)**.

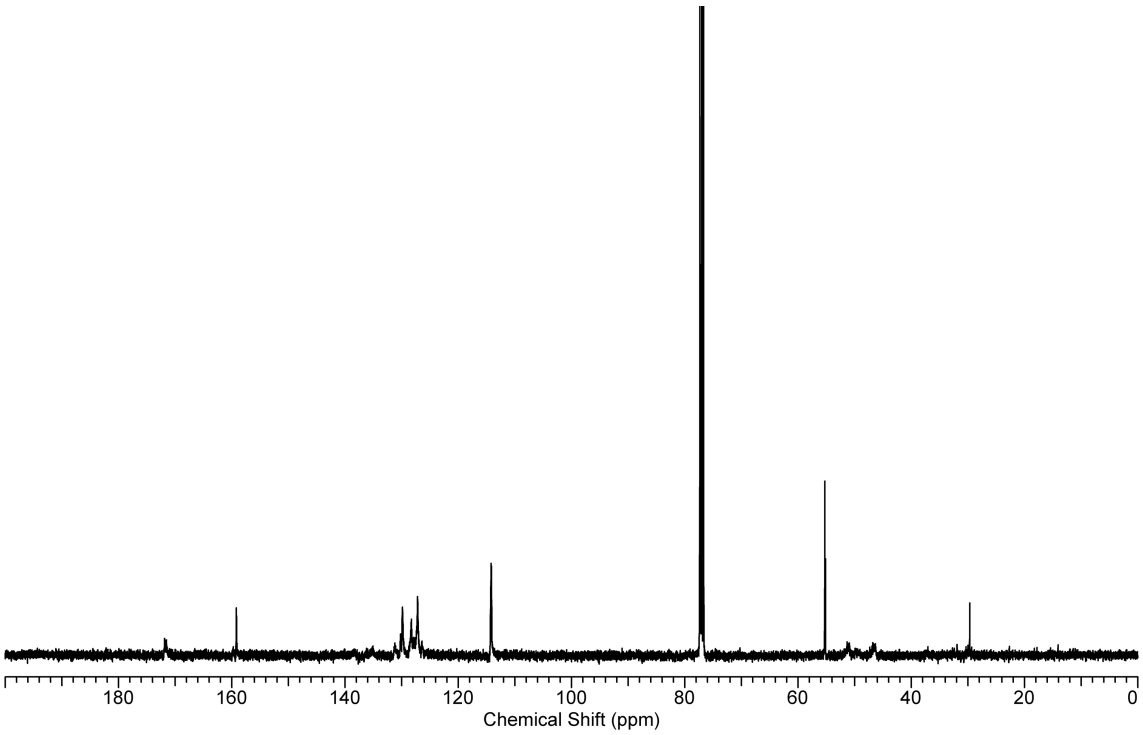


Fig. S13 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[4]pAP(mBzl$_4$)**.

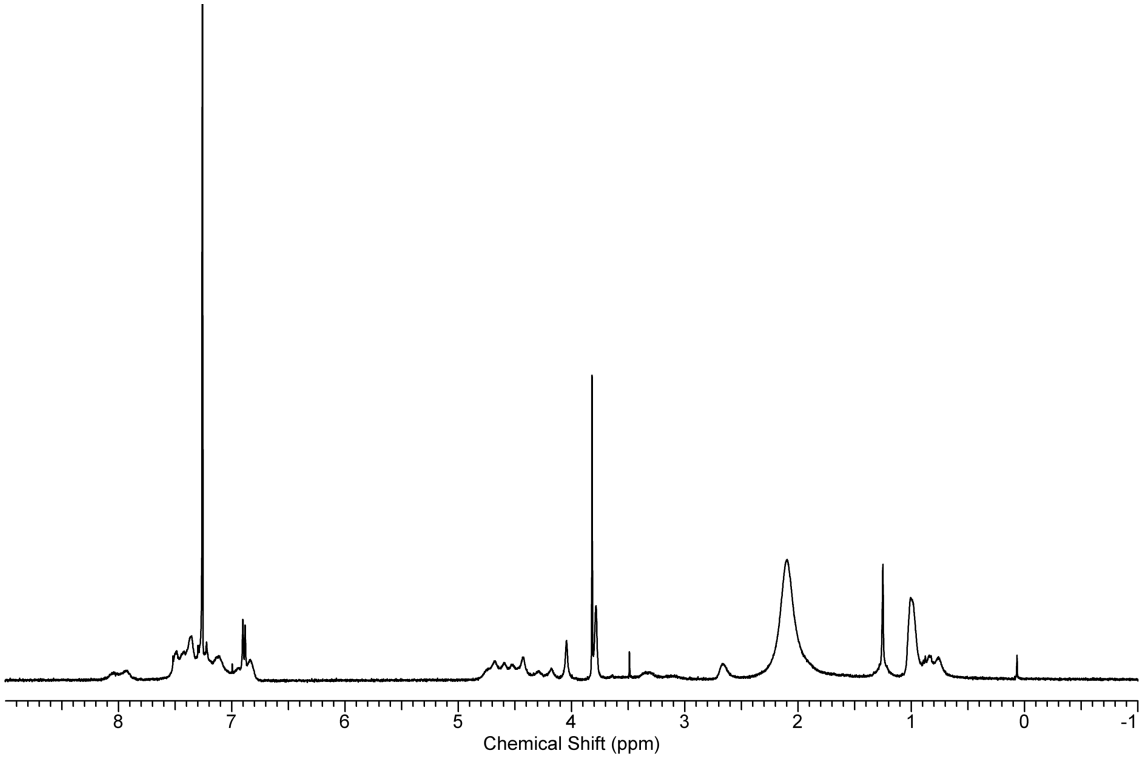


Fig. S14 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L[4]pAP(iBt-mBzl-iBt-mBzl)**.

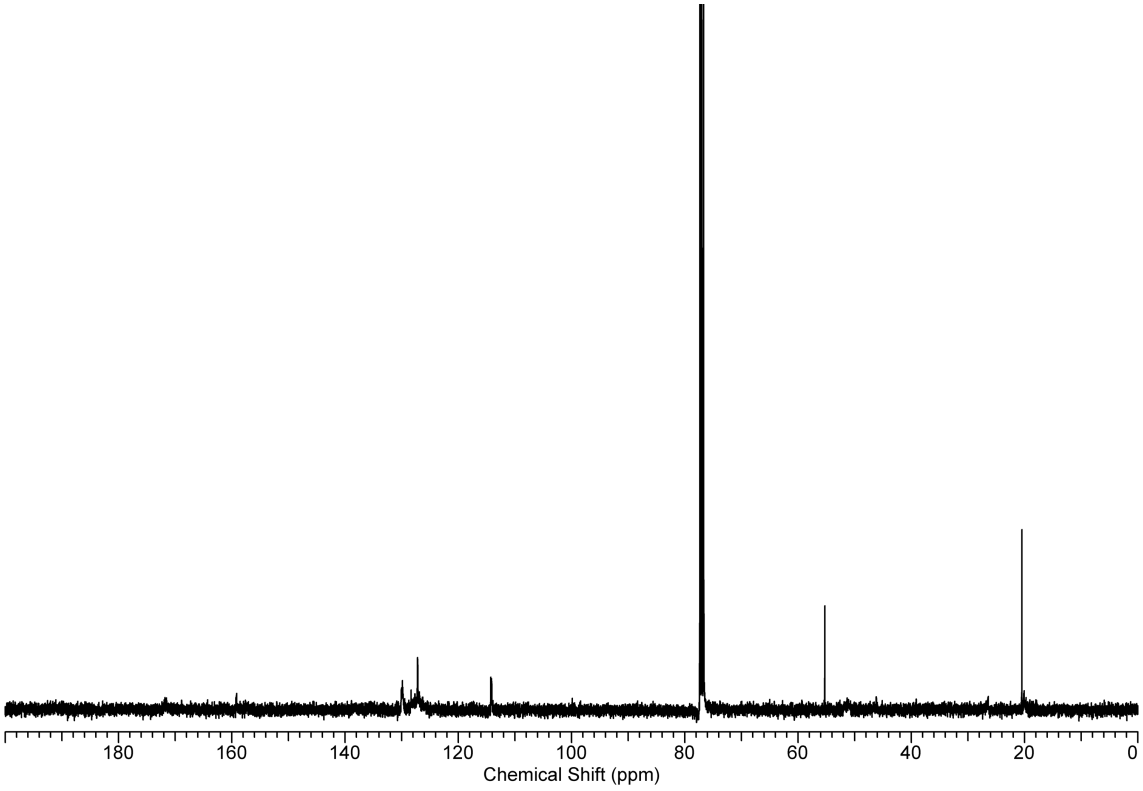


Fig. S15 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[4]pAP(iBt-mBzl-iBt-mBzl)**.

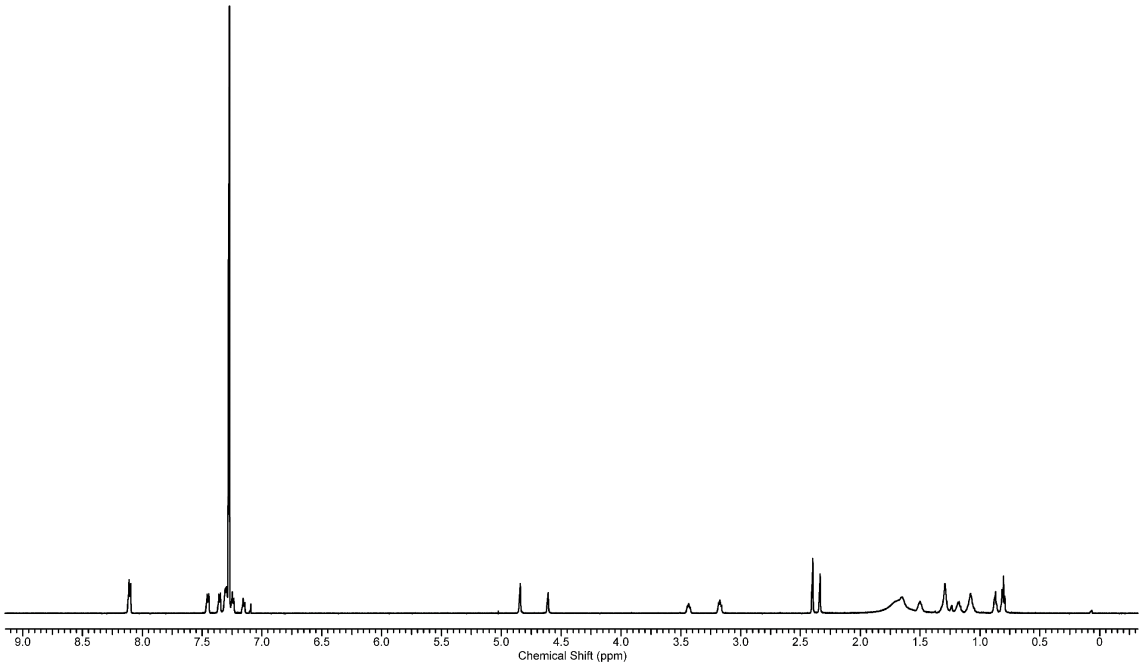


Fig. S16 ^{1}H NMR spectrum (600 MHz, $CDCl_3$, –20 °C) of **L[2]pAP(Hex)**.

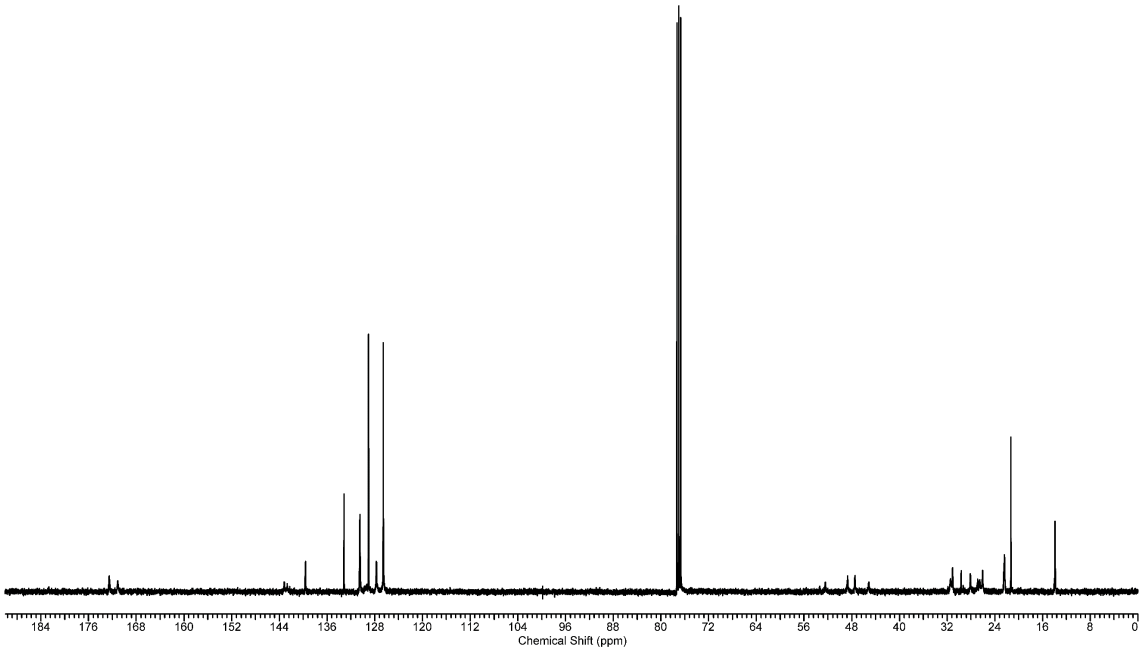


Fig. S17 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **L[2]pAP(Hex)**.

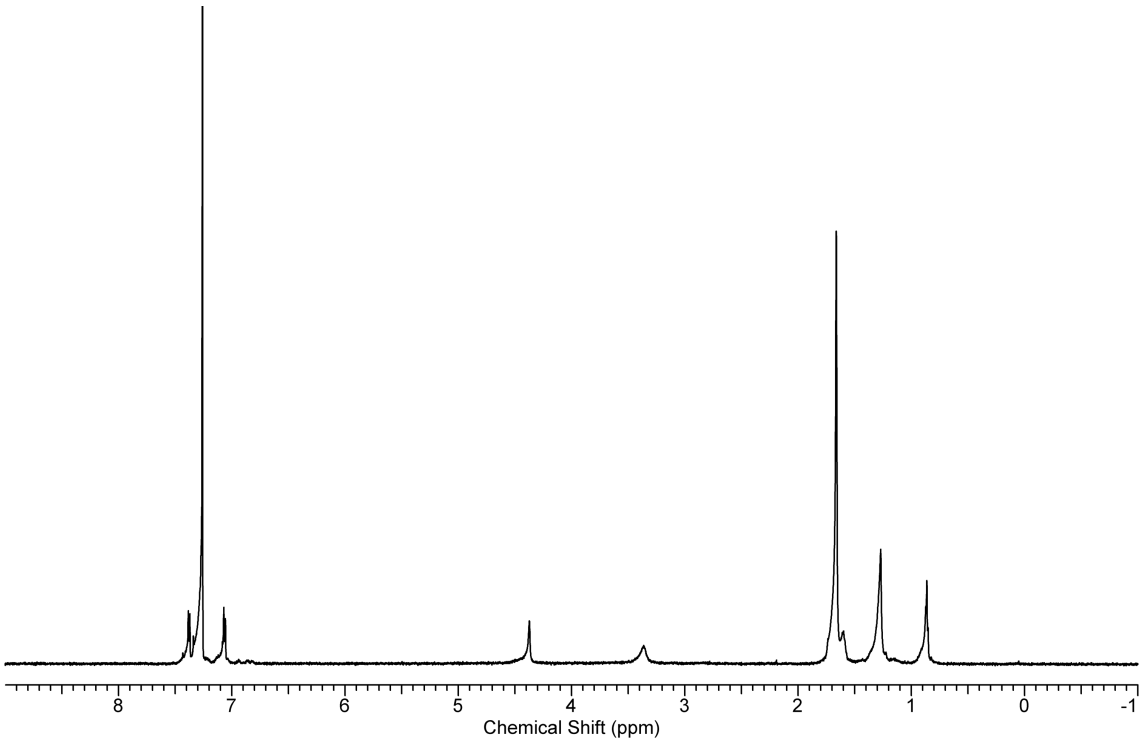


Fig. S18 ^{1}H NMR spectrum (600 MHz, $CDCl_3$, –20 °C) of **C[4]pAP(Hex$_4$)**.

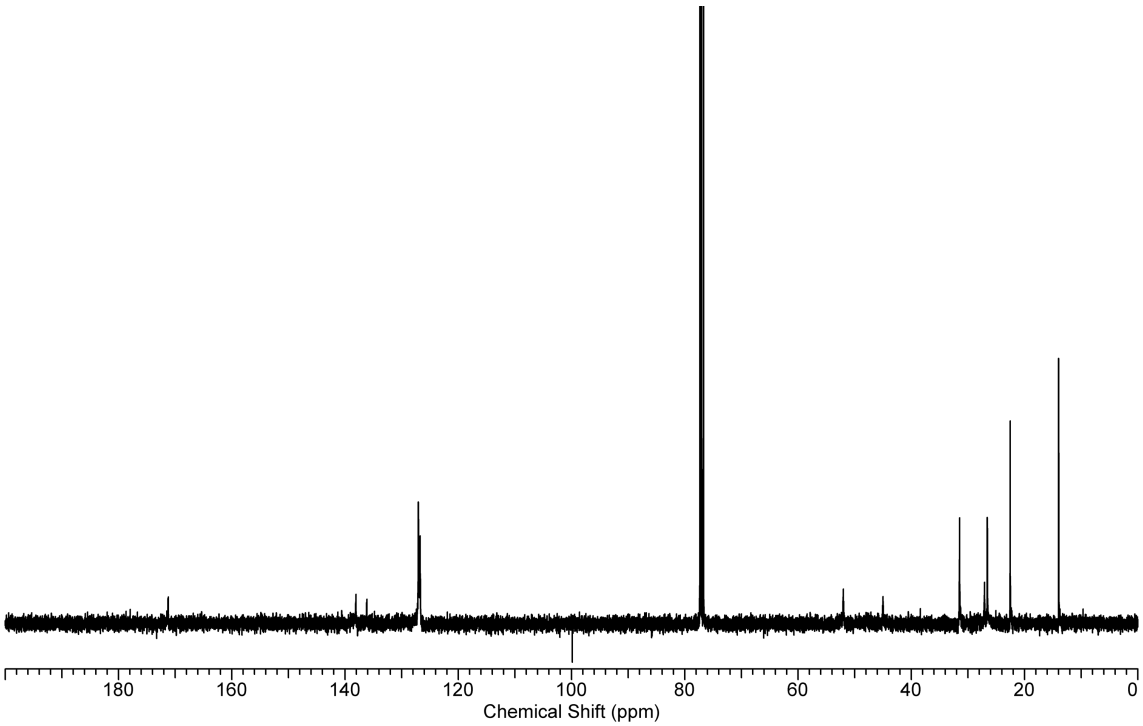


Fig. S19 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **C[4]pAP(Hex$_4$)**.

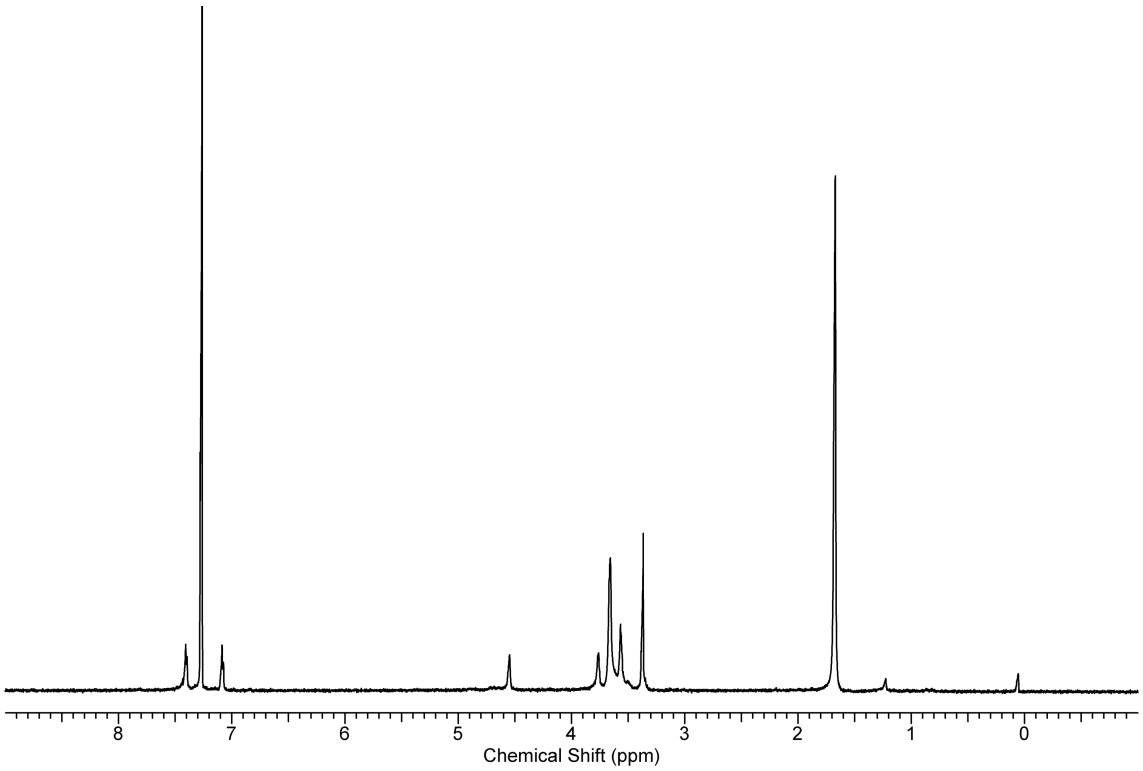


Fig. S20 ^{1}H NMR spectrum (600 MHz, $CDCl_3$, –20 °C) of **C[4]pAP(mTEG$_4$)**.

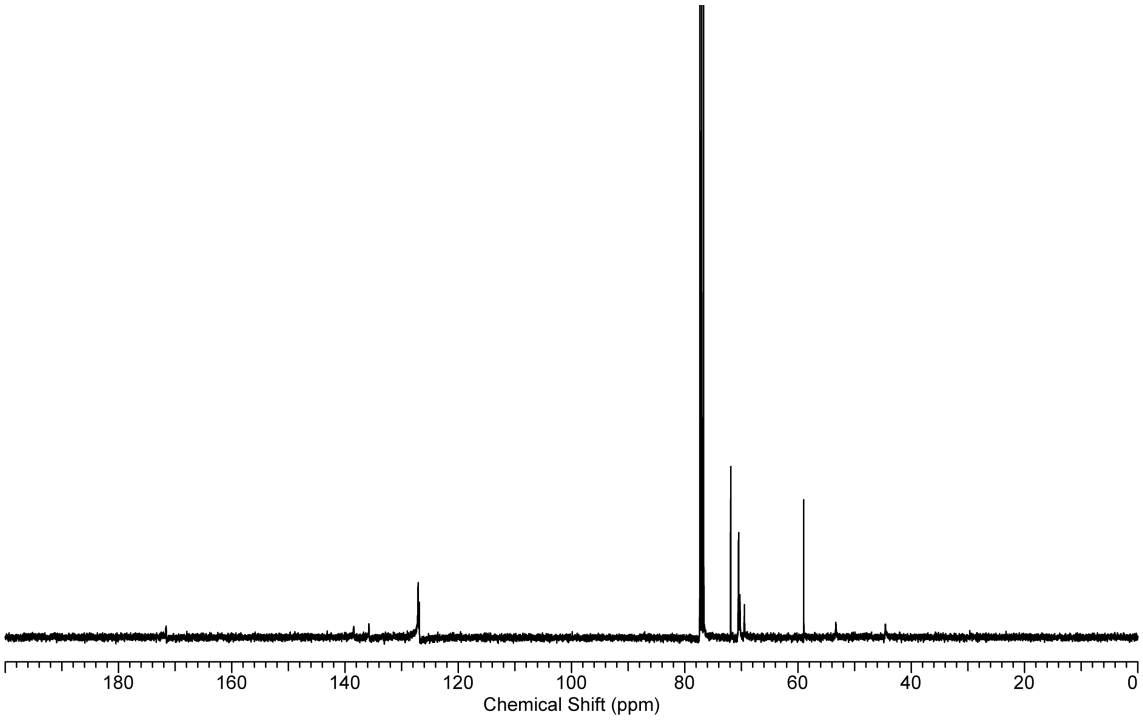


Fig. S21 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **C[4]pAP(mTEG$_4$)**.

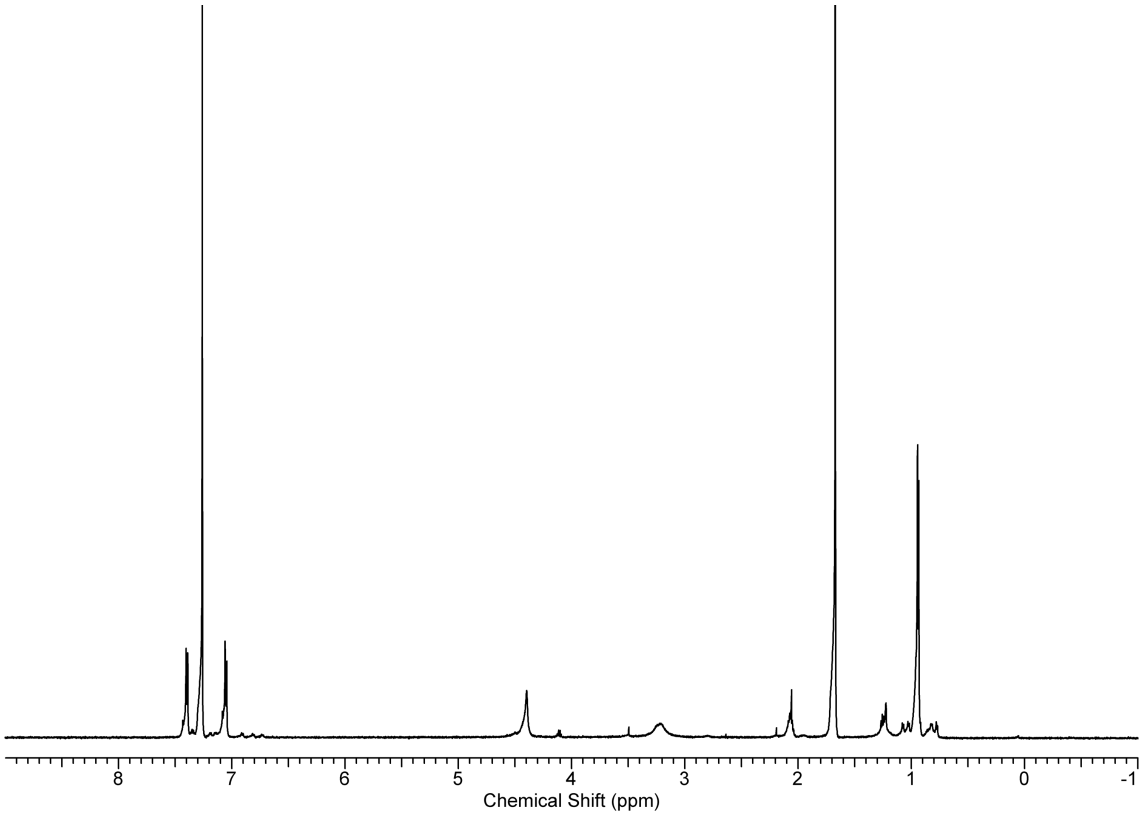


Fig. S22 ^{1}H NMR spectrum (600 MHz, $CDCl_3$, –20 ºC) of **C[4]pAP(iBt$_4$)**.

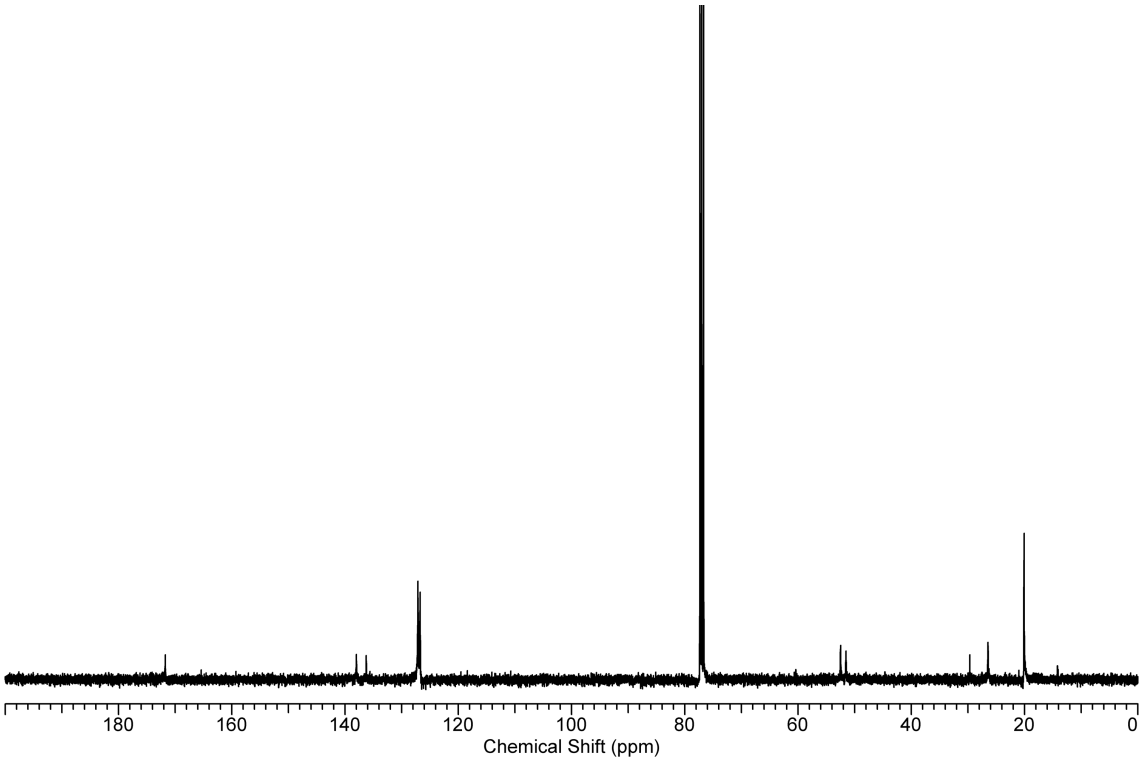


Fig. S23 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **C[4]pAP(iBt$_4$)**.

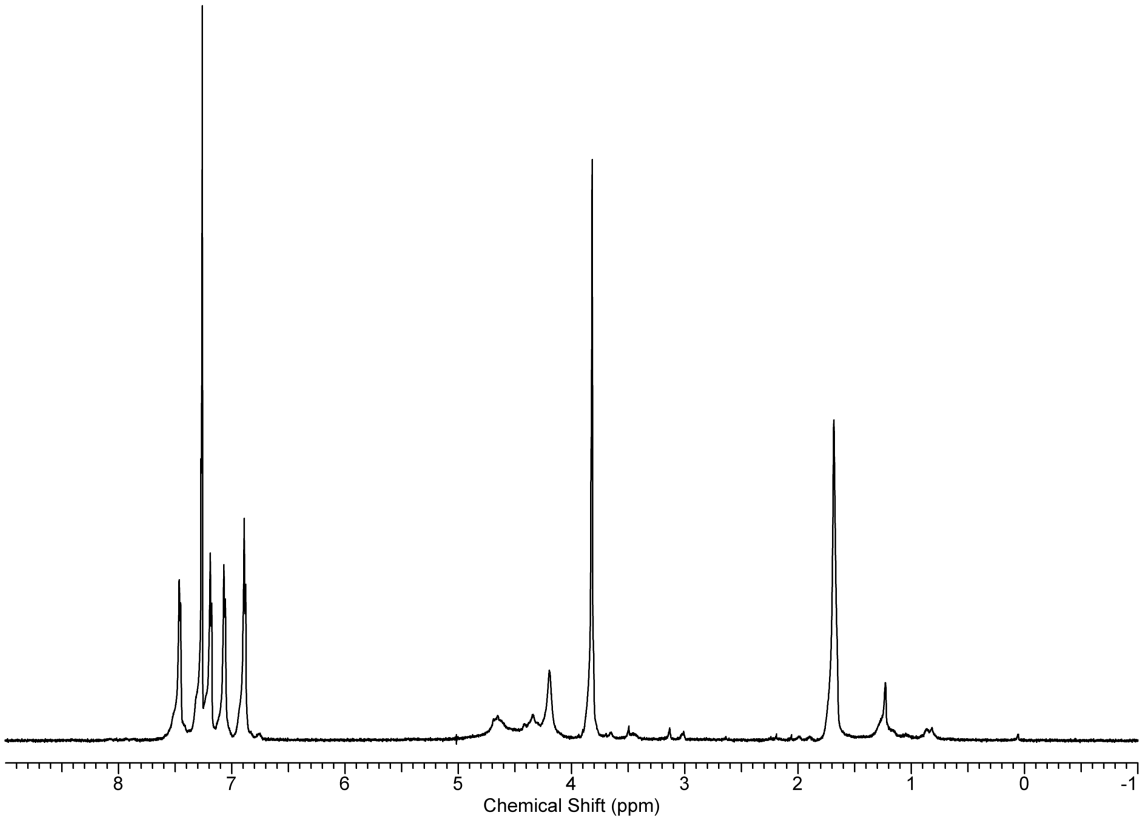


Fig. S24 ^{1}H NMR spectrum (600 MHz, $CDCl_3$, –20 °C) of **C[4]pAP(mBzl$_4$)**.

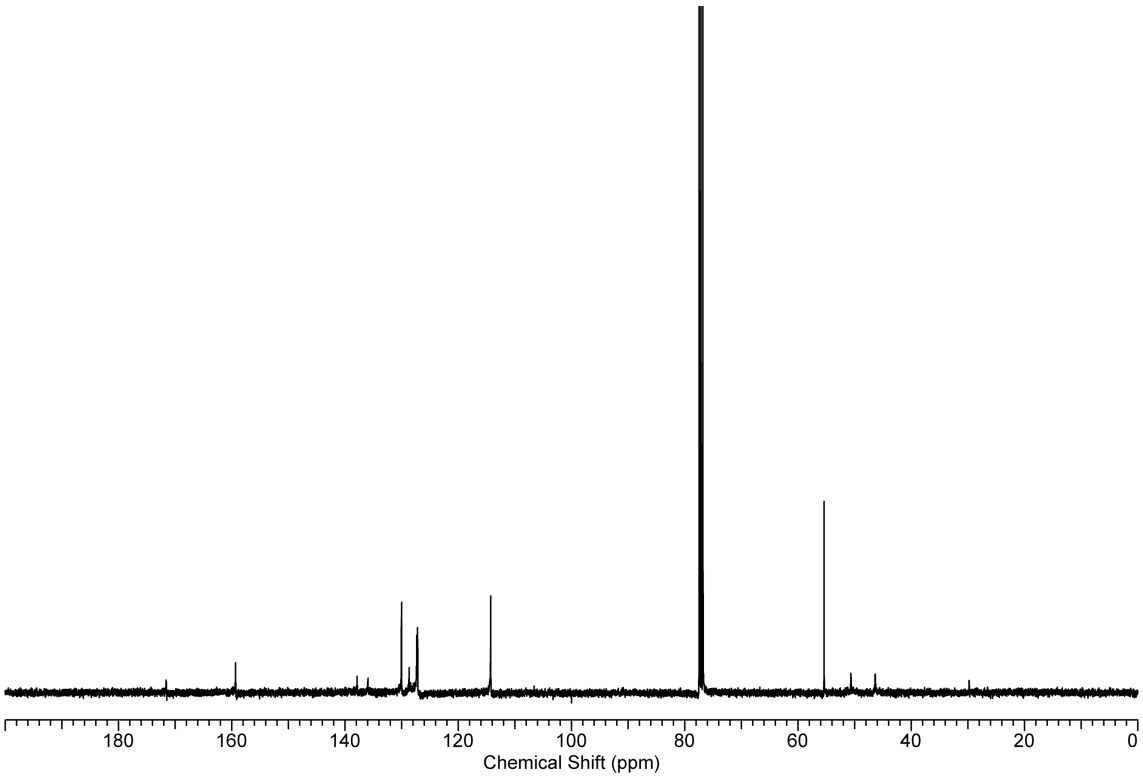


Fig. S25 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **C[4]pAP(mBzl$_4$)**.

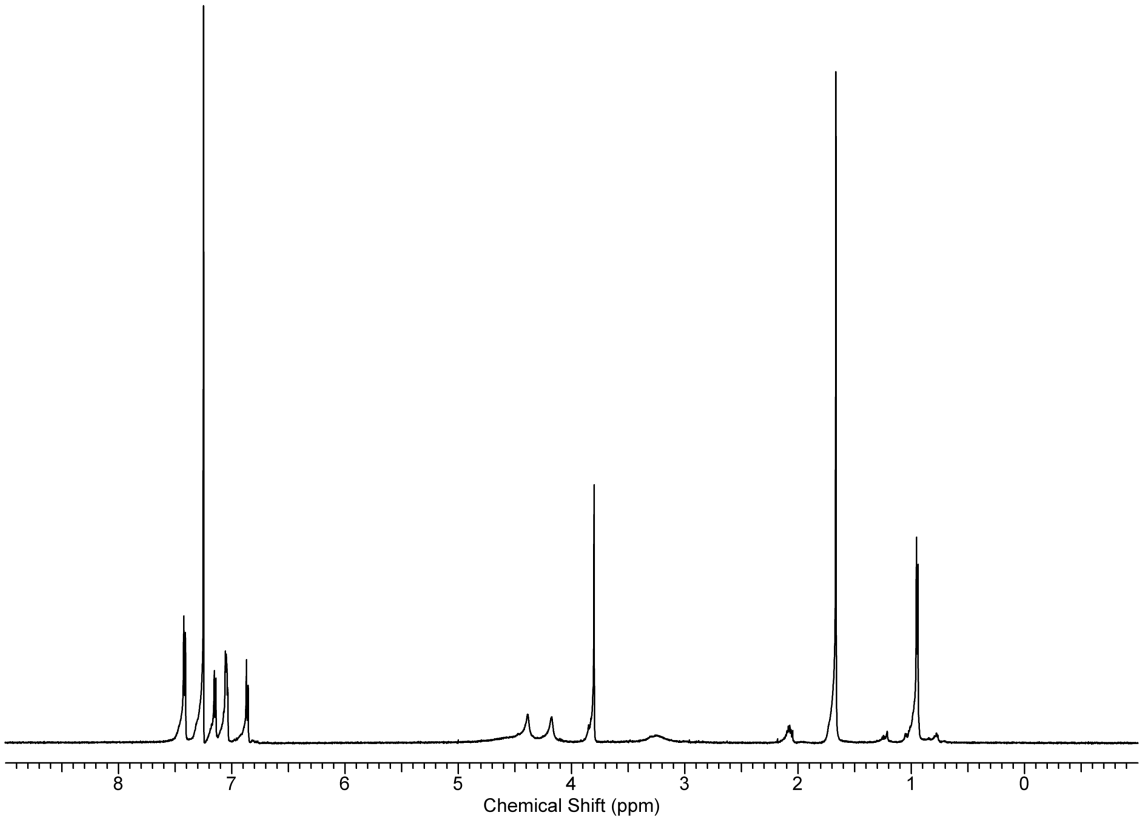


Fig. S26 ^{1}H NMR spectrum (600 MHz, $CDCl_3$, –20 °C) of **C[4]pAP(iBt-mBzl-iBt-mBzl)**.

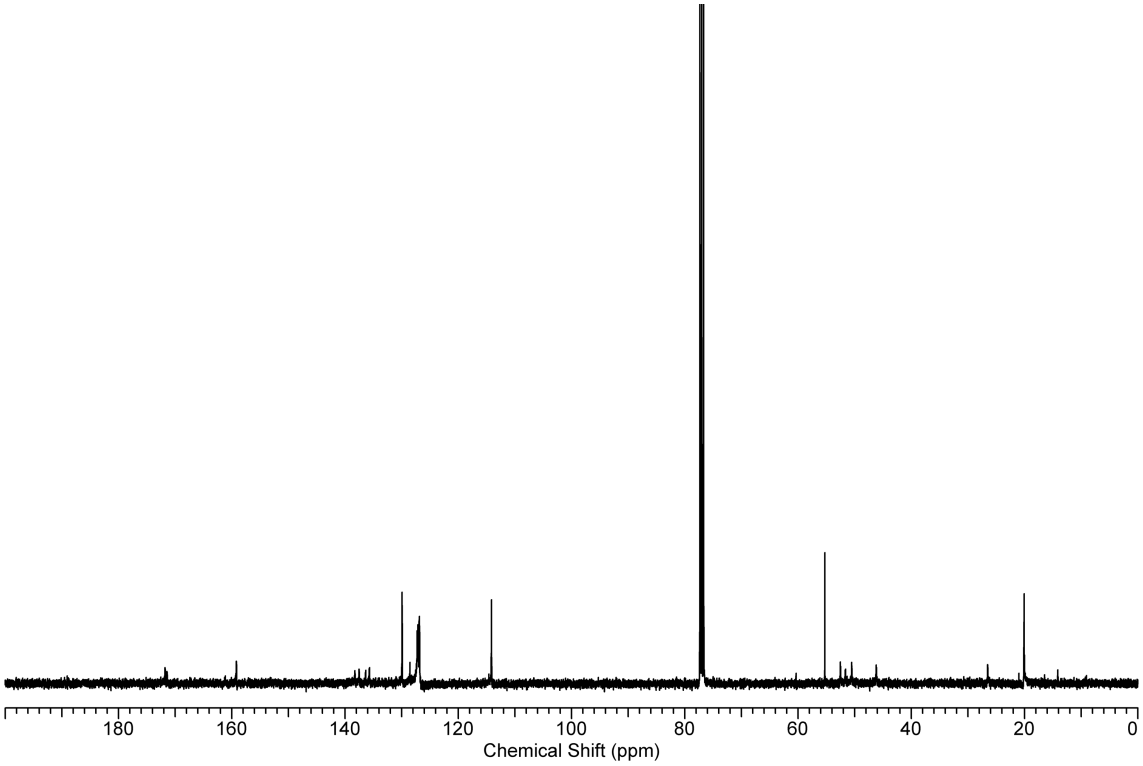


Fig. S27 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **C[4]pAP(iBt-mBzl-iBt-mBzl)**.

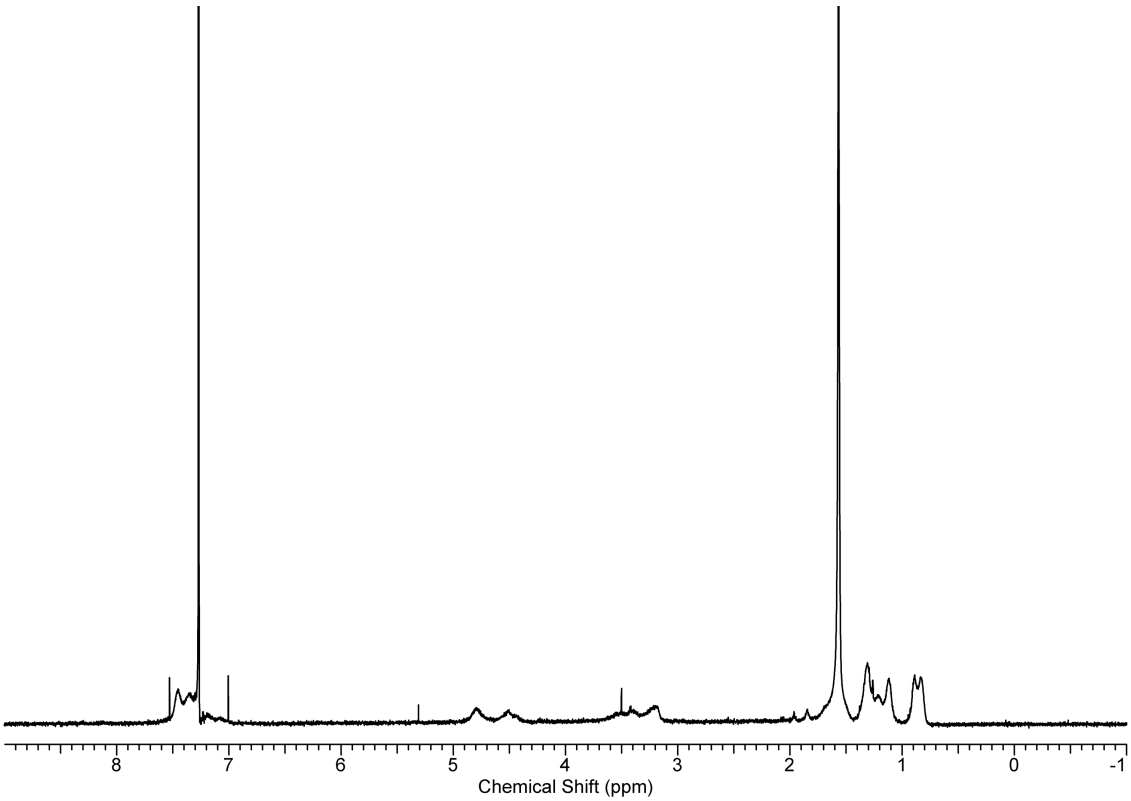


Fig. S28 ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **C[5]pAP(Hex$_5$)**.

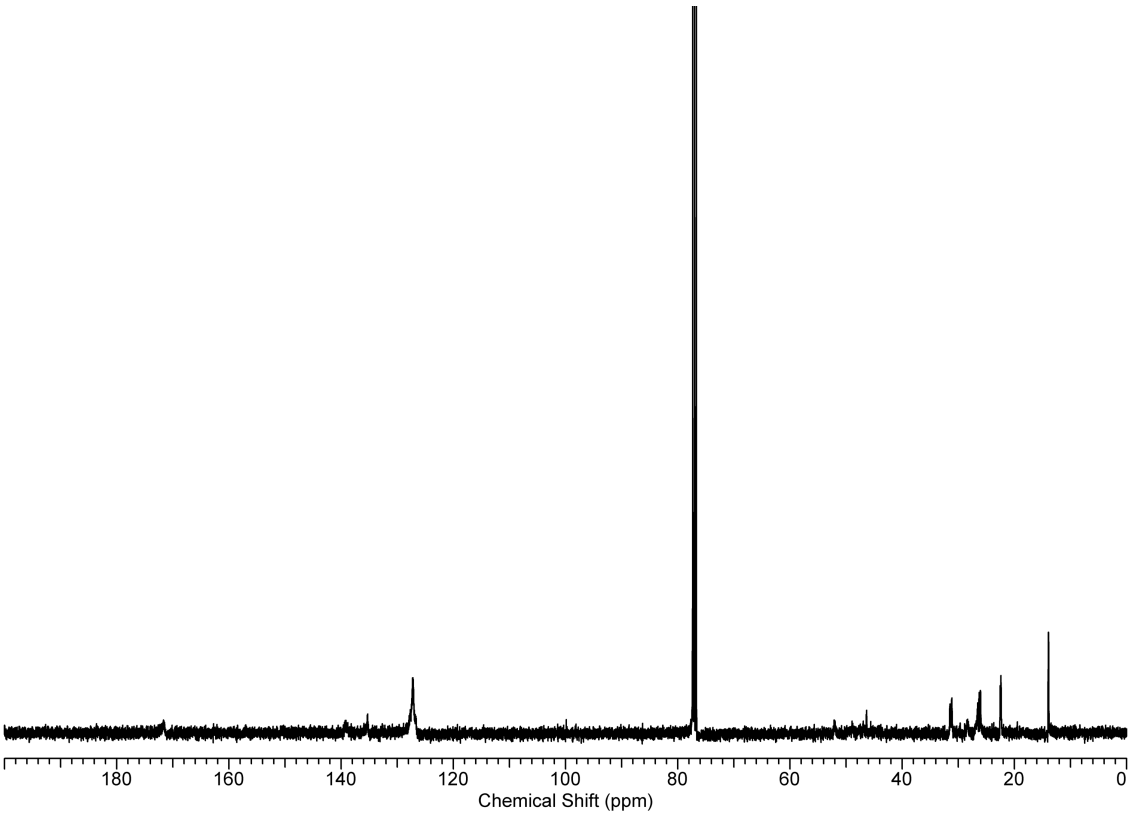


Fig. S29 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **C[5]pAP(Hex$_5$)**.

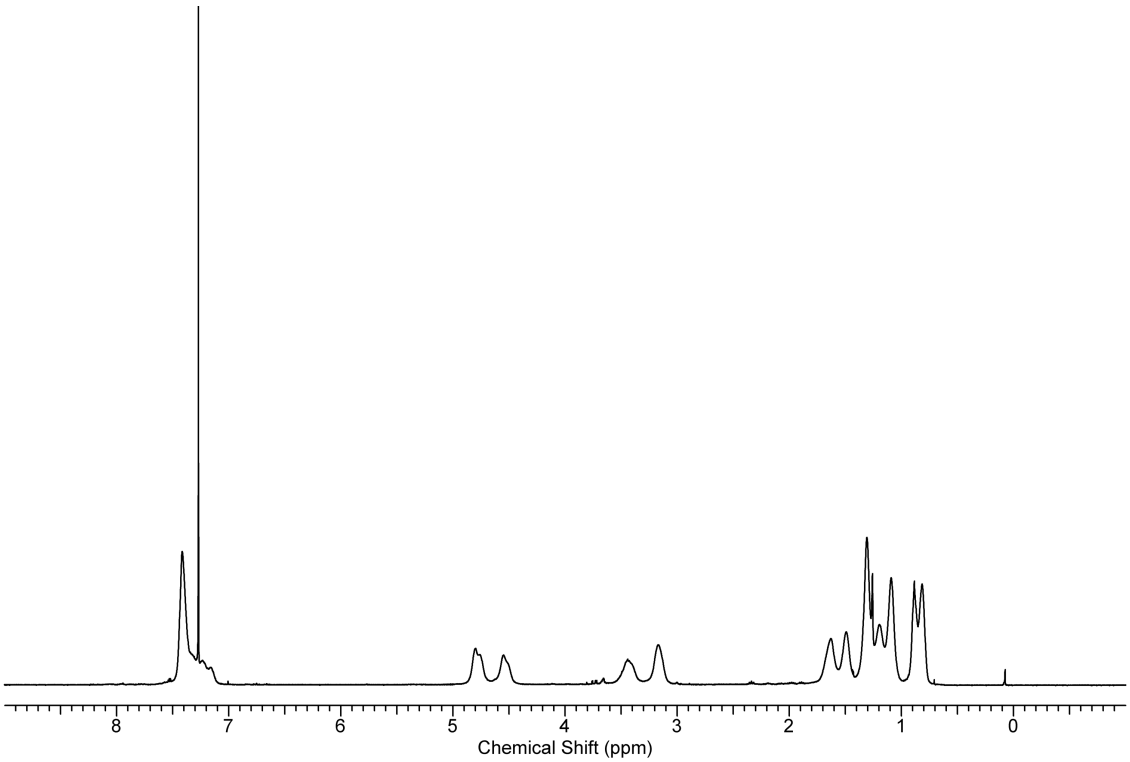


Fig. S30 ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **C[6]pAP(Hex$_6$)**.

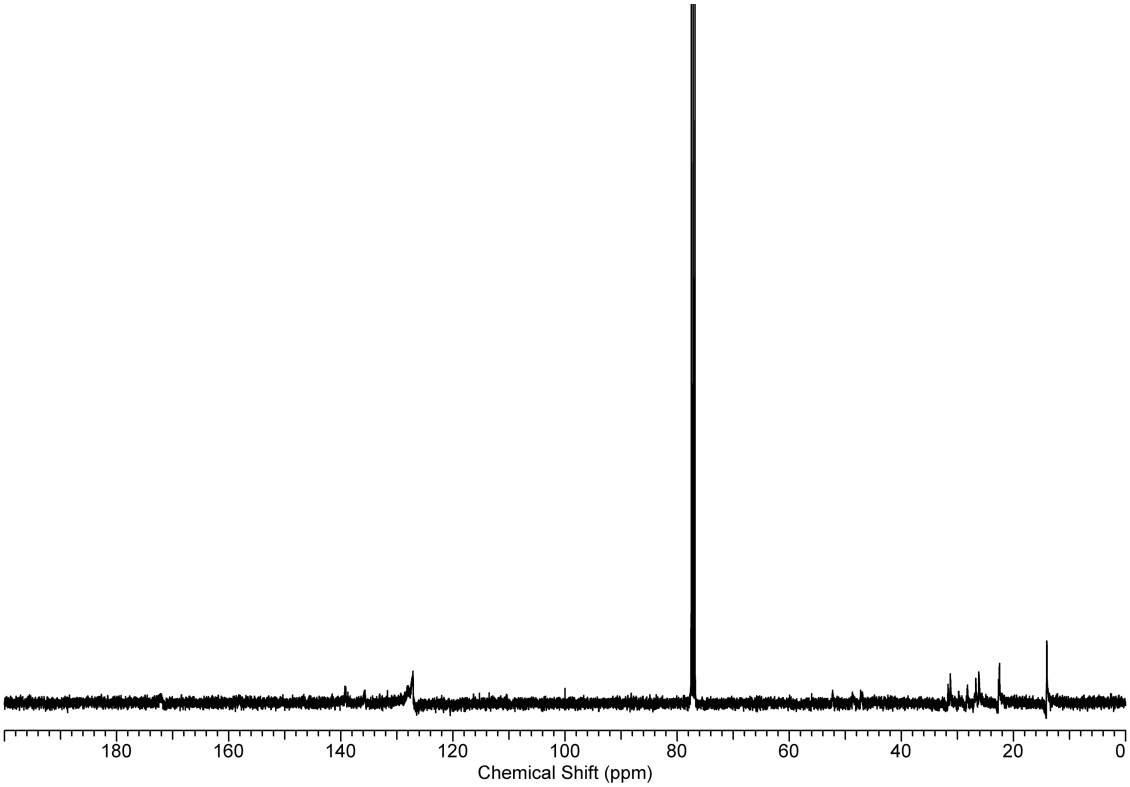


Fig. S31 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **C[6]pAP(Hex$_6$)**.

4. X-ray crystallographic structures

4.1 X-ray Crystallographic Structure Determination for C[4]pAP(Hex$_4$)•isopropanol. X-ray diffraction data for **C[4]pAP(Hex$_4$)**•2(isopropanol) was collected using a Rigaku Saturn 724 CCD diffractometer with Mo-Kα radiation (λ = 0.71075 Å) at 93 K. A Single crystals (size: 0.23 × 0.23 × 0.07 mm^3) of **C[4]pAP(Hex$_4$)**•2(isopropanol) ($C_{62}H_{92}N_4O_6$, Mw = 989.39) suitable for X-ray analysis were grown by the recrystallization of a solution of **C[4]pAP(Hex$_4$)** in isopropanol at ambient temperature. The unit cell was monoclinic with the space group $P2_1/c$. Lattice constants with Z = 2, Density = 1.124 g cm^{-3}, μ = 0.71 cm^{-1}, $F(000)$ = 1080, θ_{max} = 27.485° were a = 19.493(5), b = 17.572(5), c = 8.547(2) Å, α = 90°, β = 93.428(4)°, γ = 90°, and V = 2922.4(13) Å^3. A total of 39194 reflections were collected, of which 6691 were independent (Rint = 0.0491). The structure was refined to final R_1 = 0.0491 for 5617 data [I > 2sigma(I)] with 332 parameters and wR_2 = 0.1136 for all data, GOF = 1.095, and residual electron density max./min. = 0.258 and –0.210 e.Å^{-3}. The ORTEP diagram is shown in **Fig. S32**, and the crystal data and structure refinement are listed in **Table S1**. Data collection, cell refinement, and data reduction were conducted using the CrystalClear-SM Expert 2.0 software[S4]. The structure was solved by direct methods using the program SHELXS-97[S5] and refined by full-matrix least-squares methods on $F2$ using SHELXL2014[S6]. All materials for publication were prepared by Yadokari-XG 2009 software[S7]. All non-hydrogen atoms were refined anisotropically. The H1S attached to O1S of isopropanol was located by differential Fourier analysis and refined with U_{iso}(H) = 1.5U_{eq}(O). The positions of other H atoms were calculated geometrically and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). Tables of positional and thermal parameters, bond lengths and angles, torsion angles and Fig.s may be found from the Cambridge Crystallographic Centre by referencing CCDC number 1847583.

Table S1 Crystal data and structure refinement parameters for **C[4]pAP(Hex$_4$)**•2(isopropanol)

Empirical formula	C_{56} H_{76} N_4 O_4, 2(C_3 H_8 O)	
Formula weight	989.39	
Temperature	93 K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 19.493(5) Å	α = 90°
	b = 17.572(5) Å	β = 93.428(4)°
	c = 8.547(2) Å	γ = 90°
Volume	2922.4(13) Å^3	
Z	2	
Density (calculated)	1.124 g cm^{-3}	
Absorption coefficient	0.071 mm^{-1}	
F(000)	1080	
Crystal size	0.23 × 0.23 × 0.07 mm^3	
Theta range for data collection	2.093 to 27.485°	
Index ranges	$-25 \le h \le 25$, $-22 \le k \le 22$, $-11 \le l \le 11$	
Reflections collected	39194	
Independent reflections	6691	
Completeness to theta = 27.485°	99.8	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmissions	1.000 and 0.898	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	6691/0/332	
Goodness-of-fit on F^2	1.095	
Final R indices [I > 2sigma(I)]	R_1 = 0.0491, wR_2 = 0.1065	
R indices (all data)	R_1 = 0.0628, wR_2 = 0.1136	
Largest diff. peak and hole	0.258 and –0.210 e.Å^{-3}	

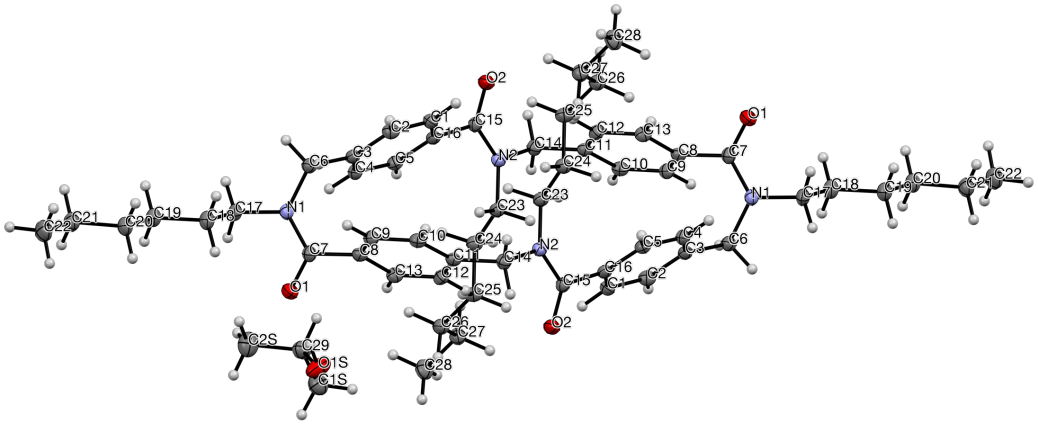


Fig. S32 ORTEP diagram of **C[4]pAP(Hex$_4$)**•2(isopropanol) with thermal ellipsoids at 50% probability.

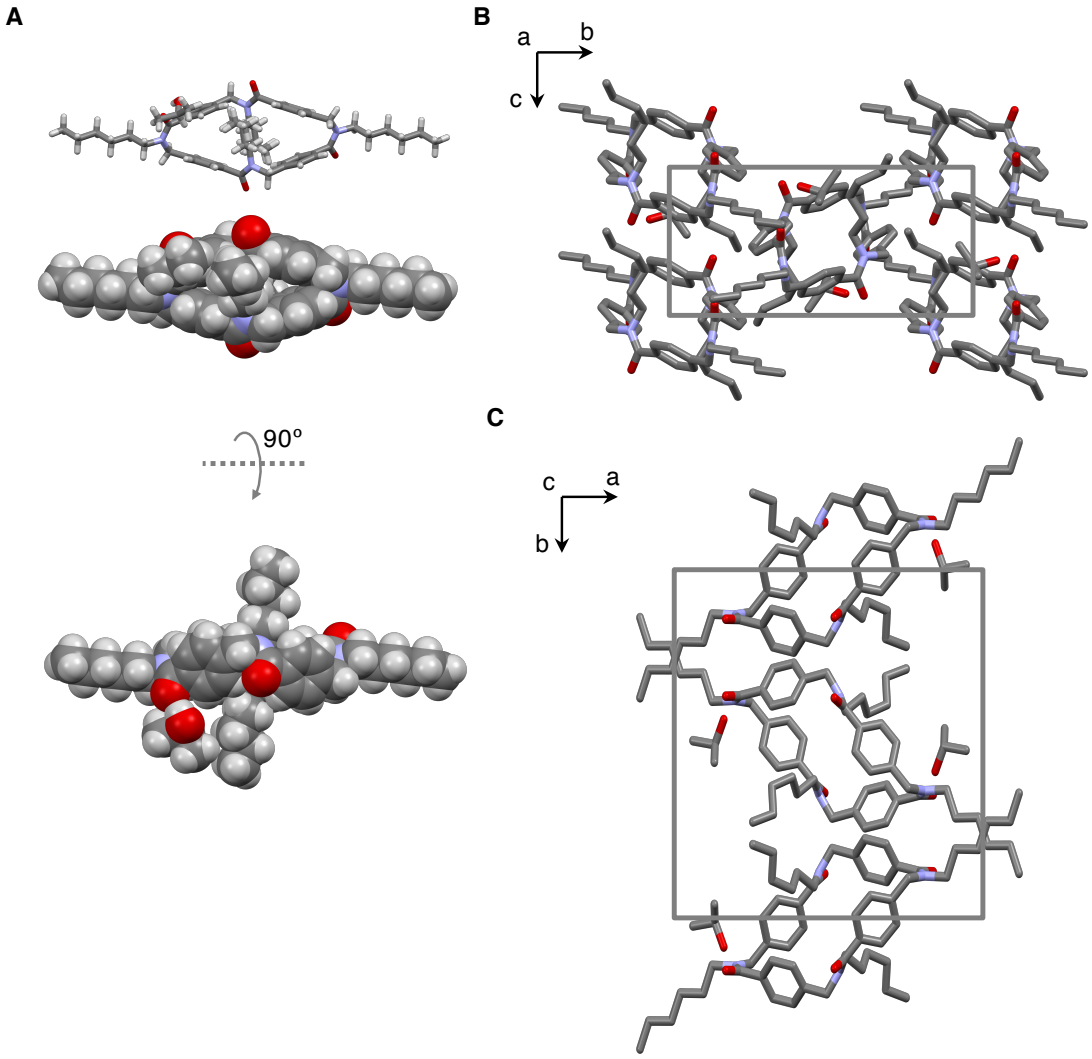


Fig. S33 Crystal structure of **C[4]pAP(Hex$_4$)**•2(isopropanol)**.** (**A**) **C[4]pAP(Hex$_4$)**•2(isopropanol) as viewed along the cavity axis (top, middle) and perpendicular to the cavity axis (bottom). Isopropanol forms hydrogen-bond with the one carbonyl group of **C[4]pAP(Hex$_4$)**. (**B**) Packing structure along the *a* axis. (**C**) Packing structure along the *c* axis. Hydrogen atoms are omitted for clarity in (**B**) and (**C**).

4.2 X-ray Crystallographic Structure Determination for C[4]pAP(iBt-mBzl-iBt-mBzl)•3(chloroform). X-ray diffraction data for **C[4]pAP(iBt-mBzl-iBt-mBzl)•**3(chloroform) was collected using a Rigaku Saturn 724 CCD diffractometer with Mo-Kα radiation (λ = 0.71075 Å) at 93 K. Single crystals (size: 0.20 × 0.20 × 0.08 mm^3) of **C[4]pAP(iBt-mBzl-iBt-mBzl)•**3(chloroform) ($C_{59}H_{63}Cl_9N_4O_6$, Mw = 1243.18) suitable for X-ray analysis were grown by the recrystallization of a solution of **C[4]pAP(iBt-mBzl-iBt-mBzl)** in chloroform at ambient temperature. The unit cell was monoclinic with the space group *C*2/*c*. Lattice constants with Z = 4, Density = 1.407 g cm^{-3}, μ = 4.83 cm^{-1}, *F*(000) = 2584, θ_{max} = 24.998° were *a* = 40.5482(9), *b* = 5.74900(10), *c* = 26.1364(7) Å, α = 90°, β = 105.526(2)°, γ = 90°, and *V* = 5870.4(2) $Å^3$. A total of 31702 reflections were collected, of which 5145 were independent (*R*int = 0.0444?). The structure was refined to final R_1 = 0.0865 for 4417 data [*I* > 2sigma(*I*)] with 363 parameters and wR_2 = 0.2767 for all data, GOF = 1.130, and residual electron density max./min. = 1.091 and –1.735 e.$Å^{-3}$. The ORTEP diagram is shown in **Fig. S34**, and the crystal data and structure refinement are listed in **Table S2**. Data collection, cell refinement, and data reduction were conducted using the CrysAlisPro software.[S8] The structure was solved by direct methods using the program SHELXT[S9] and refined by full-matrix least-squares methods on *F*2 using SHELXL2014[S6]. All materials for publication were prepared by Yadokari-XG 2009 software[S7]. All non-hydrogen atoms were refined anisotropically. The H30 attached to C30 of disordered chloroform was located by differential Fourier analysis and refined with U_{iso}(H) values of 1.2U_{eq}(C). The positions of other H atoms were calculated geometrically and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). Tables of positional and thermal parameters, bond lengths and angles, torsion angles and Fig.s may be found from the Cambridge Crystallographic Centre by referencing CCDC number 1847584.

Table S2 Crystal data and structure refinement parameters for **C[4]pAP(iBt-mBzl-iBt-mBzl)•**3(chloroform)

Empirical formula	$C_{56}\ H_{60}\ N_4\ O_6$, 3(C H Cl_3)	
Formula weight	1243.18	
Temperature	93 K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	*a* = 40.5482(9) Å	α = 90°
	b = 5.74900(10) Å	β = 105.526(2)°
	c = 26.1364(7) Å	γ = 90°
Volume	5870.4(2) Å^3	
Z	4	
Density (calculated)	1.407 g cm^{-3}	
Absorption coefficient	0.483 mm^{-1}	
F(000)	2584	
Crystal size	0.20 × 0.20 × 0.08 mm^3	
Theta range for data collection	1.673 to 24.998°	
Index ranges	–48 ≤ h ≤ 48, –6 ≤ k ≤ 6, –31 ≤ l ≤ 31	
Reflections collected	31702	
Independent reflections	5145	
Completeness to theta = 24.998°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmissions	1.000 and 0.9449	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	5145/3/363	
Goodness-of-fit on F^2	1.130	
Final R indices [$I > 2\text{sigma}(I)$]	R_1 = 0.0865, wR_2 = 0.2679	
R indices (all data)	R_1 = 0.0964, wR_2 = 0.2767	
Largest diff. peak and hole	1.091 and –1.735 e.Å^{-3}	

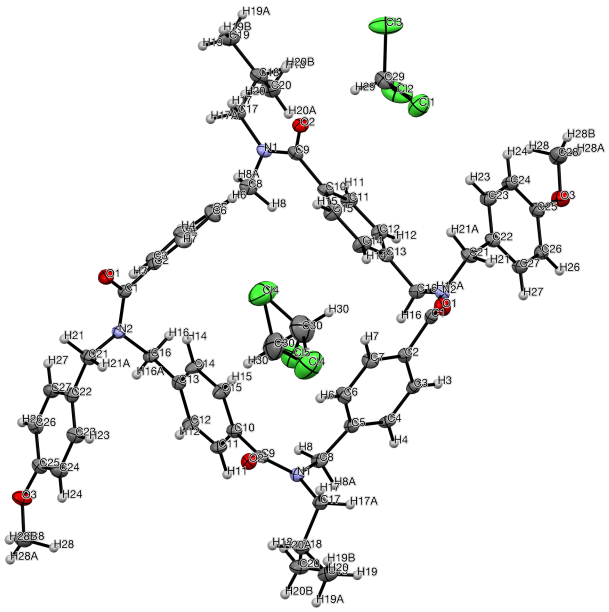


Fig. S34 ORTEP diagram of **C[4]pAP(iBt-mBzl-iBt-mBzl)•**3(chloroform) with thermal ellipsoids at 50% probability.

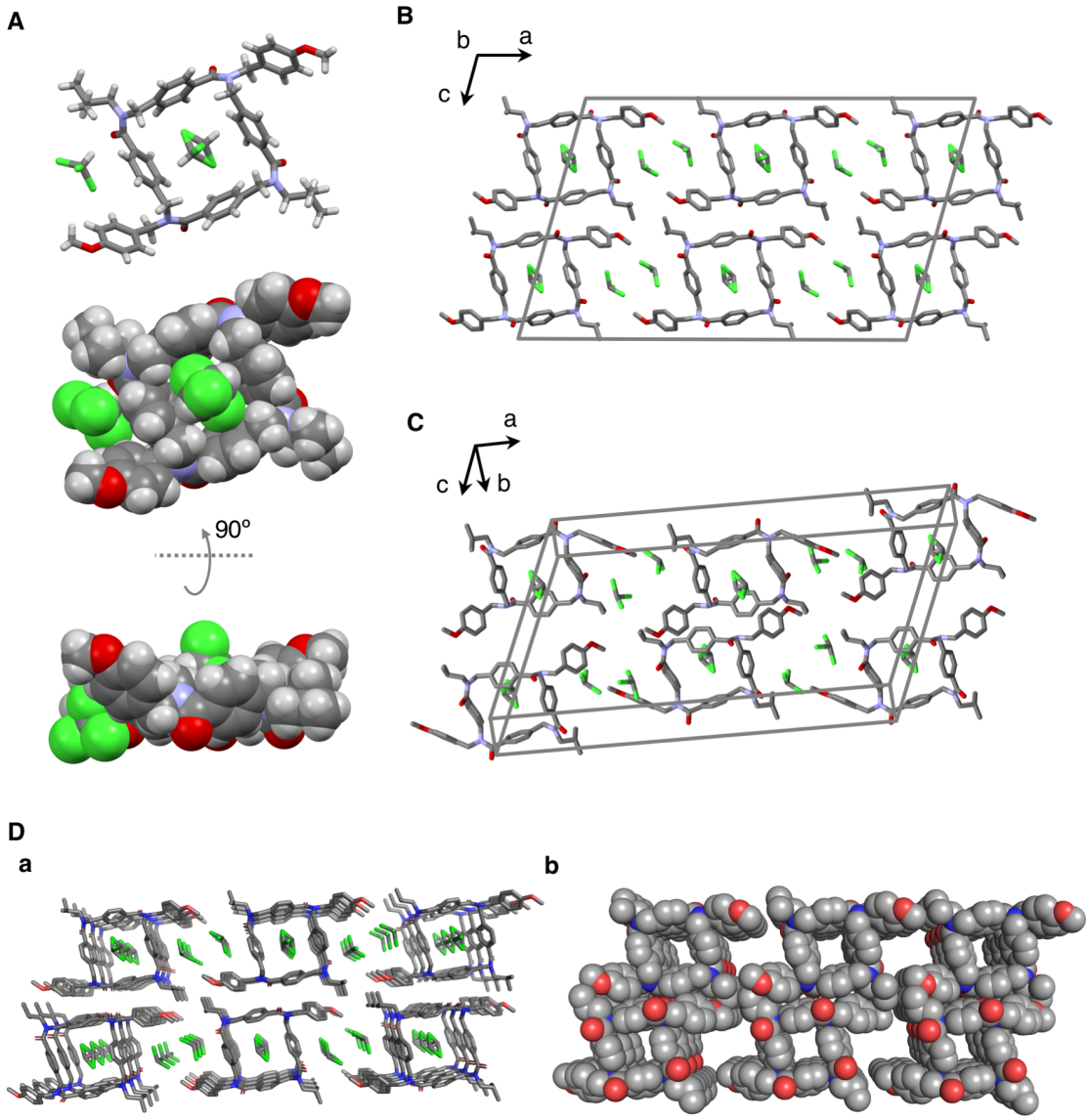


Fig. S35 Crystal structure of **C[4]pAP(iBt-mBzl-iBt-mBzl)**•3(chloroform)**.** Chloroform molecule in the cavity is disordered. (**A**) **C[4]pAP(iBt-mBzl-iBt-mBzl)**•3(chloroform) as viewed along the cavity axis (top, middle) and perpendicular to the cavity axis (bottom). (**B**, **C**) Packing structure along (**B**) *b* axis and (**C**) slightly tilted *b* axis. (**D**) Perspective views (**a**: stick model, **b**: CPK model (Chloroform molecules omitted for clarity)) of one-dimensional channel. Hydrogen atoms are omitted for clarity (**B**, **C**, **D**).

5. Characterization of model dimer compound

5.1 Variable temperature ^{1}H NMR spectra of L[2]pAP(Hex) in $CDCl_2CDCl_2$

Variable temperature (VT) ^{1}H NMR spectra were measured to evaluate the exchange rate of the equilibrium between the two conformations (*cis* and *trans*) of **L[2]pAP(Hex)** in tetrachloroethene-d_2 ($CDCl_2CDCl_2$). As shown in **Fig. S36A**, the resonances separate into two sets of distinct signals at 273K, since the exchange rates of two conformation is slower than that of the ^{1}H NMR timescale. As the temperature was raised two sets of signals coalescence into one set of signals indicating the rapid conversion between the two conformations.

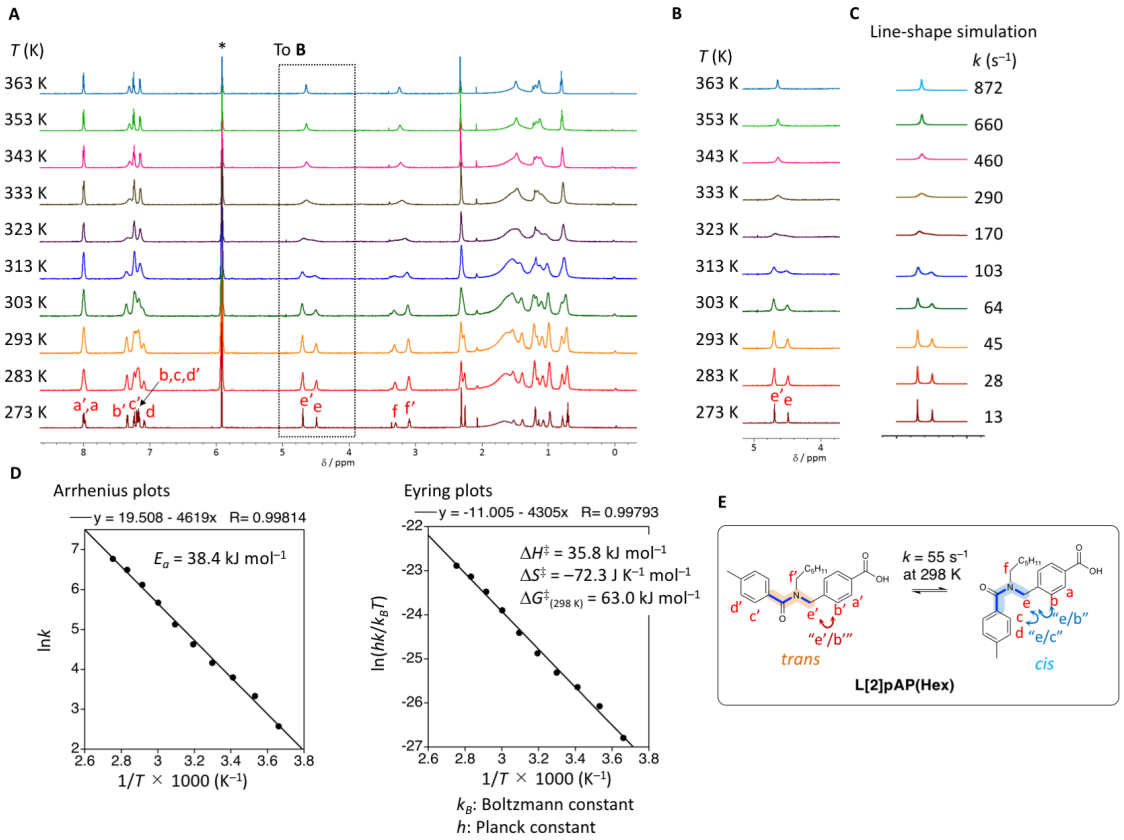


Fig. S36 (**A**) VT ^{1}H NMR spectra (400 MHz, $CDCl_2CDCl_2$) of **L[2]pAP(Hex)** (4.0 mM). Asterisk denotes a peak of solvent. (**B**) Part of VT ^{1}H NMR spectra marked with a broken line frame in panel (**A**) and (**C**) the corresponding line-shape simulation. The coalescence temperature for *cis*-e and *trans*-e' protons was observed at ca. 333 K. Values of temperature and exchange rate constant are given for every trace. (**D**) Arrhenius plots and (**E**) Eyring plots based on line-shape analysis (**C**). (**E**) Chemical structure of **L[2]pAP(Hex)** and equilibrium between the two possible conformations (*cis* and *trans*). Exchange rate constant (k) at room temperature (298 K) evaluated on the basis of Eyring plots analysis is shown. The assignments of the signals are also shown.

We carried out NOESY measurements of **L[2]pAP(Hex)** to assign signals for the two conformations as shown in **Fig. S37**. Due to the significant overlaps of the signals, it was difficult to assign them unambiguously. We thus assigned the signal based on the comparisons of chemical shifts reported previously for the similar compounds[S10] and the absence of the correlation (e'/c') under the experimental conditions we conducted.

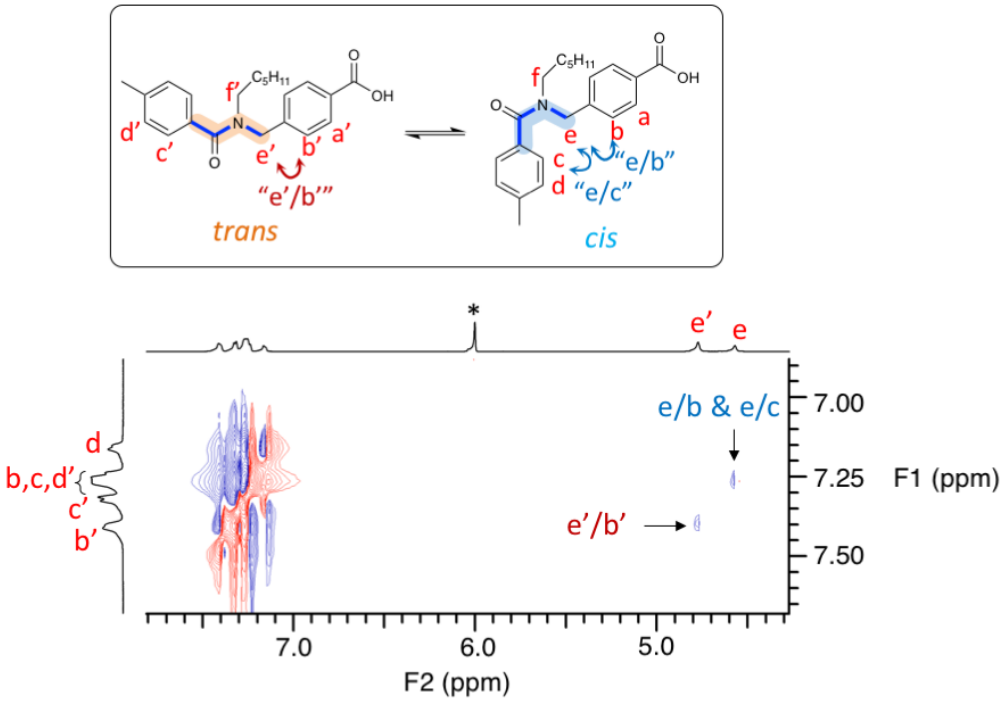


Fig. S37 Part of NOESY spectrum (600 MHz, $CDCl_2CDCl_2$, –30 ºC, mixing time = 1.2 s) of **L[2]pAP(Hex)** (20 mM). The arrows shown with chemical structures of **L[2]pAP(Hex)** indicate possible assignments of the observed NOE correlations (e/b, e/c, and e'/b'). Asterisk denotes a peak of solvent.

5.2 ^{1}H NMR spectra of L[2]pAP(Hex) in various solvent systems

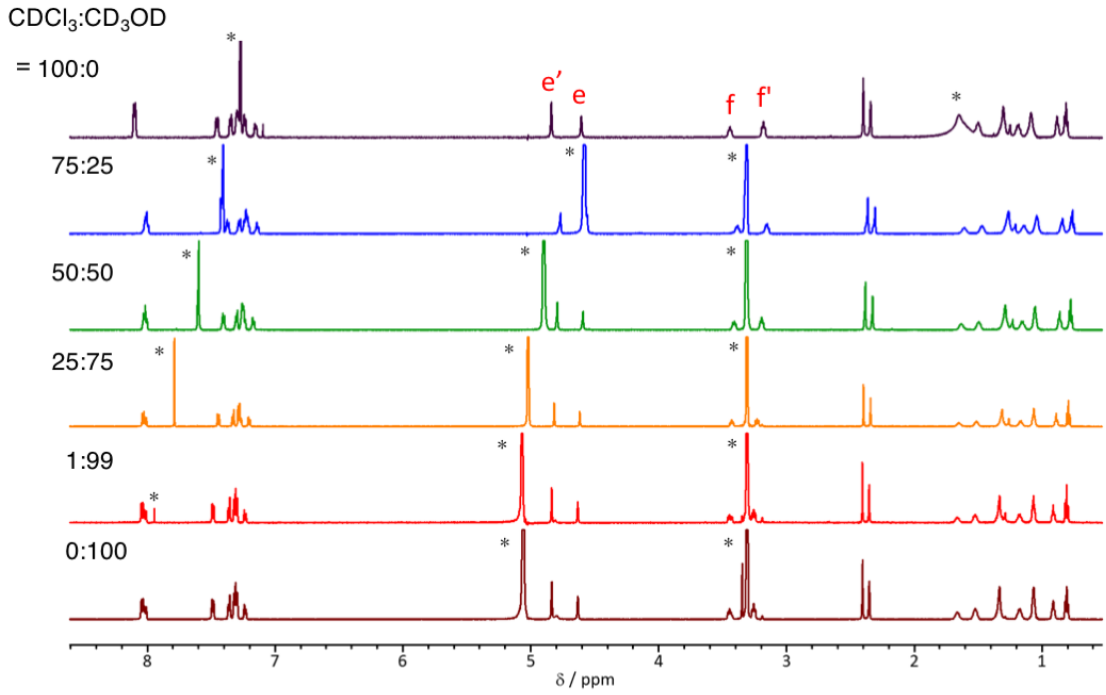


Fig. S38 ^{1}H NMR spectrum (600 MHz, 0 °C) of **L[2]pAP(Hex)** (4.0 mM) in CD_3OD-$CDCl_3$ systems at different ratios. Asterisks denote peaks of solvent.

6. Theoretical analysis

Computational methods

The Gaussian 16 program[S11] was used in all DFT calculations. The structures were optimized at B3LYP/6-31G(d,p) level followed by frequency calculation at the same level under gas phase. The effect of solvents was investigated at the same level by means of the default solvent option (SCRF calculations) implemented in the Gaussian 16 program, which is based on the inclusion of the polarizable continuum model using the integral equation formalism variant (IEFPCM). The structures were confirmed to have zero imaginary frequencies. The energies shown in the main text are calculated using Gibbs free energies of the results containing zero-point, thermal, and entropy effects at 298.15 K at 1 atm (**Table S3**).

Table S3 Uncorrected and thermal-corrected (298.15 K, 1 atm) energies of stationary points (Hartree).

Conformation	E	G
cccc (gas phase)	-1913.51276030	-1912.930769
cccc (scrf = chloroform)	-1913.53339803	-1912.952373
cccc (scrf = methanol)	-1913.54231415	-1912.961316
cccc (scrf = water)	-1913.54338275	-1912.962440
ctct (gas phase)	-1913.51242522	-1912.928732
ctct (scrf = chloroform)	-1913.53254193	-1912.949466
ctct (scrf = methanol)	-1913.54144801	-1912.958653
ctct (scrf = water)	-1913.54252717	-1912.959901
tttt (gas phase)	-1913.50151987	-1912.917558

Cartesian coordinates of each conformation

·*cccc conformation* (gas phase)

O	20.93314300	1.09596900	1.11620500
C	20.79669600	2.16330400	1.70869200
C	19.41089000	2.66849100	2.01868500
C	18.97005100	3.95929700	1.69863600
H	19.64890200	4.66194600	1.22390800
C	17.65427400	4.33916300	1.95967400
H	17.32550700	5.34210400	1.69757700
C	16.75505200	3.45133700	2.56160900
C	17.18798100	2.15017700	2.84388100
H	16.49889000	1.43387300	3.28031600
C	18.49353400	1.75913900	2.55940900
H	18.81641500	0.74173500	2.75420900
C	15.36899500	3.94089600	2.96396000
H	15.43242800	4.35306500	3.97232100
H	15.07278000	4.76697800	2.30538800
N	14.31669600	2.92978700	2.93680200
C	13.93798100	2.16585600	4.02514500
O	13.34446600	1.09897900	3.88958300

C	14.24845800	2.67190100	5.41052900
C	13.92964600	3.96338200	5.85028600
H	13.45558600	4.66591500	5.17084800
C	14.19105500	4.34410200	7.16574300
H	13.92992000	5.34756900	7.49367100
C	14.79214600	3.45645500	8.06570500
C	15.07317000	2.15466100	7.63386900
H	15.50892200	1.43852000	8.32356000
C	14.78831700	1.76280100	6.32864400
H	14.98214500	0.74494200	6.00661400
C	15.19497900	3.94679200	9.45134700
H	16.20373700	4.35793300	9.38755900
H	14.53720700	4.77375800	9.74687300
N	15.16685400	2.93659600	10.50449800
C	13.93765600	2.44249300	1.61162200
C	13.84121000	2.45089100	10.88395100
H	13.93776700	1.82859600	11.77145900
H	13.38261000	1.85360000	10.08701900
O	16.11786200	1.10566100	11.47821800
C	16.25446000	2.17192000	10.88383000
C	17.64033500	2.67636300	10.57294100
C	18.08133800	3.96769100	10.89064800
H	17.40257500	4.67129000	11.36409200
C	19.39716700	4.34691100	10.62893400
H	19.72606100	5.35028500	10.88920900
C	20.29628100	3.45787600	10.02862400
C	19.86318800	2.15625800	9.74871900
H	20.55219200	1.43906900	9.31360200
C	18.55758000	1.76590900	10.03388600
H	18.23456800	0.74819400	9.84093400
C	21.68240200	3.94652500	9.62539000
H	21.61902300	4.35688300	8.61628700
H	21.97872800	4.77375400	10.28247100
N	22.73456600	2.93532800	9.65437200
C	23.11320000	2.16939800	8.56740700
O	23.70660300	1.10270500	8.70488900
C	22.80277100	2.67296900	7.18111000
C	23.12171000	3.96361900	6.73901000
H	23.59583500	4.66733900	7.41717400
C	22.86034800	4.34197700	5.42286300
H	23.12158300	5.34482200	5.09311800
C	22.25917800	3.45275700	4.52450600
C	21.97802700	2.15177700	4.95870400
H	21.54221200	1.43442200	4.27031500
C	22.26283400	1.76225800	6.26464000
H	22.06891100	0.74500200	6.58851100
C	21.85640500	3.94062100	3.13797400
H	20.84769900	4.35200600	3.20101200
H	22.51428200	4.76696400	2.84094300
N	21.88440500	2.92850600	2.08666600
C	23.11355500	2.45038900	10.98043000
C	23.20999000	2.44196000	1.70808500
H	13.19296000	3.30747500	11.09434700
H	13.72649900	3.29827700	0.96256200
H	13.05069600	1.81951000	1.70878100
H	23.11333600	1.81798000	0.82177200
H	23.66856700	1.84615600	2.50614000
H	23.32487500	3.30731800	11.62792400
H	24.00040300	1.82707600	10.88438500
H	22.31600600	1.85434400	11.43957600
H	23.85831000	3.29808200	1.49602400
H	14.73511000	1.84547100	1.15358100

• *cccc conformation* (scrf = chloroform)

O	20.94156600	1.17144100	1.01894700
C	20.79459600	2.20621100	1.67413400
C	19.40271400	2.68830200	1.99256700
C	18.94726400	3.97594000	1.67809100
H	19.61790900	4.69073600	1.21026200
C	17.62726100	4.33951900	1.94177700
H	17.28740500	5.33960700	1.68473300
C	16.73913100	3.43874200	2.54223000
C	17.18833100	2.14287900	2.82322000
H	16.51119600	1.41784900	3.26361600
C	18.49825900	1.76705000	2.53549200
H	18.83113400	0.75412600	2.73759500
C	15.34828900	3.91280700	2.94457200
H	15.40625500	4.33131100	3.95019700
H	15.03773600	4.72951300	2.28288100
N	14.31161000	2.88319400	2.92278100
C	13.91338100	2.15016100	4.01587000

O	13.28265600	1.09700900	3.89526800
C	14.24592400	2.65885100	5.39503500
C	13.90207200	3.94202400	5.84089800
H	13.40048600	4.63424700	5.17096300
C	14.17951600	4.32958800	7.15159500
H	13.89959200	5.32582700	7.48443300
C	14.82156200	3.45767100	8.03888200
C	15.13343100	2.16522900	7.59921300
H	15.60824500	1.46218000	8.27637600
C	14.83389600	1.76525900	6.29952700
H	15.06159500	0.75529200	5.97437700
C	15.23413900	3.95485400	9.41835200
H	16.25145700	4.34285300	9.35419600
H	14.59410300	4.79656200	9.70689200
N	15.18107900	2.95001300	10.47853100
C	13.92164700	2.39761600	1.59920000
C	13.84452300	2.49098900	10.85591600
H	13.90973500	1.94953000	11.79759000
H	13.41480600	1.82569000	10.09822100
O	16.10924100	1.18154500	11.57560500
C	16.25649900	2.21504000	10.91847400
C	17.64850000	2.69629200	10.59930000
C	18.10409000	3.98448900	10.91127800
H	17.43350600	4.70028300	11.37766800
C	19.42413800	4.34740300	10.64691400
H	19.76409500	5.34796100	10.90198800
C	20.31217800	3.44535700	10.04823100
C	19.86285700	2.14898100	9.76981500
H	20.53992000	1.42300400	9.33086900
C	18.55287600	1.77386500	10.05824700
H	18.21988600	0.76058300	9.85812700
C	21.70302400	3.91854800	9.64488100
H	21.64496900	4.33519200	8.63848800
H	22.01371500	4.73645800	10.30501600
N	22.73963100	2.88890300	9.66843600
C	23.13757100	2.15373100	8.57668000
O	23.76794600	1.10059500	8.69926700
C	22.80521700	2.65996500	7.19657600
C	23.14902900	3.94236400	6.74844700
H	23.65050300	4.63582700	7.41718200
C	22.87173200	4.32754500	5.43701900
H	23.15163000	5.32320100	5.10241900
C	22.22988100	3.45397900	4.55120800
C	21.91808700	2.16229700	4.99315000
H	21.44346400	1.45797300	4.31718000
C	22.21747200	1.76469700	6.29359800
H	21.98985700	0.75529000	6.62053200
C	21.81745100	3.94867900	3.17080000
H	20.80024700	4.33710500	3.23422700
H	22.45772800	4.78966200	2.88068100
N	21.87020700	2.94183900	2.11250700
C	23.12964400	2.40555600	10.99282100
C	23.20663300	2.48187300	1.73580400
H	13.18925100	3.35899800	10.96990900
H	13.76098000	3.25433200	0.93888000
H	13.00232600	1.82263600	1.69082100
H	23.14115100	1.93844100	0.79528400
H	23.63643200	1.81812000	2.49480600
H	23.28924000	3.26337600	11.65195400
H	24.04958400	1.83137700	10.90232600
H	22.35826600	1.76413900	11.43442300
H	23.86198200	3.34956100	1.61983900
H	14.69356200	1.75636900	1.15829300

• *cccc conformation* (scrf = methanol)

O	20.94093300	1.19490800	0.99042300
C	20.79144900	2.21864200	1.66655100
C	19.39776800	2.69395900	1.98634200
C	18.94006200	3.98250100	1.67769400
H	19.61009200	4.70266800	1.21755600
C	17.61866600	4.34161700	1.94065300
H	17.27774800	5.34260700	1.68959400
C	16.73129500	3.43541200	2.53458500
C	17.18315900	2.13936900	2.81072800
H	16.50808900	1.41082300	3.24842500
C	18.49480300	1.76780000	2.52387300
H	18.82923900	0.75536600	2.72649600
C	15.33933300	3.90591200	2.93621500
H	15.39581600	4.32641400	3.94085200
H	15.02493500	4.71986400	2.27398900
N	14.30686300	2.87082300	2.91553700

C	13.90303300	2.14701000	4.00882200
O	13.26004900	1.09814200	3.89176800
C	14.24250400	2.65424200	5.38662600
C	13.89306200	3.93501700	5.83554000
H	13.38536900	4.62597900	5.16908600
C	14.17629400	4.32329900	7.14492700
H	13.89338000	5.31781200	7.47958500
C	14.82954200	3.45465700	8.02742400
C	15.14833700	2.16487100	7.58435200
H	15.63485400	1.46506300	8.25657600
C	14.84365400	1.76381900	6.28599500
H	15.08160100	0.75685200	5.95848800
C	15.24743200	3.95371200	9.40423500
H	16.26712500	4.33431100	9.33804100
H	14.61390500	4.79978600	9.69208700
N	15.18797300	2.94976200	10.46631400
C	13.90992500	2.38932400	1.59218800
C	13.84826900	2.50119700	10.84619900
H	13.90320200	1.99131300	11.80605600
H	13.42658100	1.81150900	10.10605600
O	16.11001200	1.20515900	11.60423200
C	16.25969200	2.22752400	10.92608000
C	17.65345600	2.70203400	10.60546200
C	18.11131500	3.99110400	10.91166400
H	17.44136500	4.71222700	11.37041900
C	19.43275200	4.34956400	10.64801600
H	19.77378900	5.35099300	10.89715400
C	20.32000800	3.44212700	10.05579300
C	19.86799900	2.14560800	9.78214100
H	20.54298100	1.41614900	9.34582900
C	18.55631200	1.77473900	10.06971200
H	18.22175200	0.76196100	9.86901800
C	21.71199000	3.91172600	9.65318500
H	21.65545700	4.33035000	8.64776700
H	22.02652600	4.72688800	10.31385700
N	22.74435400	2.87657100	9.67570100
C	23.14803800	2.15069100	8.58373300
O	23.79083100	1.10192300	8.70273200
C	22.80868000	2.65545000	7.20499600
C	23.15813800	3.93541700	6.75378800
H	23.66578300	4.62759300	7.41901700
C	22.87500800	4.32132300	5.44367700
H	23.15793700	5.31523300	5.10724600
C	22.22185800	3.45106900	4.56269300
C	21.90306700	2.16207700	5.00807000
H	21.41665000	1.46102900	4.33706700
C	22.20764200	1.76338700	6.30718200
H	21.96970400	0.75700500	6.63648500
C	21.80407900	3.94763100	3.18494500
H	20.78447400	4.32859400	3.25042700
H	22.43779400	4.79302200	2.89550400
N	21.86330500	2.94167600	2.12475300
C	23.14130200	2.39740200	10.99989300
C	23.20291500	2.49221200	1.74559500
H	13.19177900	3.37151500	10.92590900
H	13.77682600	3.24684500	0.92762500
H	12.97364500	1.84155900	1.67986800
H	23.14777800	1.98029800	0.78683200
H	23.62467700	1.80406800	2.48713000
H	23.27394600	3.25607700	11.66305000
H	24.07783000	1.84989100	10.91326500
H	22.38553900	1.73309500	11.43456700
H	23.85945700	3.36231100	1.66392400
H	14.66591700	1.72462400	1.15851700

·*cccc conformation* (scrf = water)

O	20.94013000	1.19582000	0.98847400
C	20.79109000	2.21881900	1.66634300
C	19.39750600	2.69402900	1.98656700
C	18.93993100	3.98275900	1.67838500
H	19.61004100	4.70322200	1.21886700
C	17.61853300	4.34186700	1.94138300
H	17.27782100	5.34303900	1.69091300
C	16.73101200	3.43545500	2.53482300
C	17.18279200	2.13929300	2.81063400
H	16.50777300	1.41067700	3.24829300
C	18.49447000	1.76772100	2.52381500
H	18.82880100	0.75528900	2.72671000
C	15.33910500	3.90602000	2.93640900
H	15.39545400	4.32615400	3.94117600
H	15.02476400	4.72017700	2.27453800

N	14.30663900	2.87076500	2.91511100
C	13.90141000	2.14783700	4.00799900
O	13.25666900	1.09973600	3.89070500
C	14.24125100	2.65430000	5.38595700
C	13.89171500	3.93488000	5.83543500
H	13.38405100	4.62619800	5.16935200
C	14.17532000	4.32273500	7.14487500
H	13.89255000	5.31714400	7.47986500
C	14.82905200	3.45387700	8.02683500
C	15.14800700	2.16431200	7.58318000
H	15.63522300	1.46443800	8.25483100
C	14.84299100	1.76364800	6.28474700
H	15.08167400	0.75698500	5.95678100
C	15.24751600	3.95276000	9.40349000
H	16.26719200	4.33324700	9.33693900
H	14.61427500	4.79878900	9.69180900
N	15.18826200	2.94839700	10.46536000
C	13.90919500	2.39027400	1.59150500
C	13.84855900	2.50045200	10.84612100
H	13.90304200	1.99357600	11.80761300
H	13.42742500	1.80842000	10.10784900
O	16.11083700	1.20608000	11.60618200
C	16.26005800	2.22770400	10.92628200
C	17.65372000	2.70211000	10.60521800
C	18.11144900	3.99136700	10.91095400
H	17.44141800	4.71278500	11.36909100
C	19.43288800	4.34981800	10.64726900
H	19.77372000	5.35142800	10.89582100
C	20.32029500	3.44217400	10.05554100
C	19.86836800	2.14553800	9.78221600
H	20.54330000	1.41601000	9.34594300
C	18.55664600	1.77466600	10.06975000
H	18.22219200	0.76189000	9.86878500
C	21.71222600	3.91183400	9.65298800
H	21.65583700	4.33009600	8.64744400
H	22.02670500	4.72719200	10.31331300
N	22.74458000	2.87650700	9.67612800
C	23.14968200	2.15153000	8.58455100
O	23.79426100	1.10354400	8.70376900
C	22.80993300	2.65552000	7.20566700
C	23.15948000	3.93529100	6.75389300
H	23.66710000	4.62782400	7.41874800
C	22.87597000	4.32077000	5.44373100
H	23.15875400	5.31457500	5.10696700
C	22.22233200	3.45030100	4.56328800
C	21.90338200	2.16153200	5.00925100
H	21.41626000	1.46041900	4.33882300
C	22.20829800	1.76322900	6.30843600
H	21.96962600	0.75715200	6.63819700
C	21.80397600	3.94668600	3.18569500
H	20.78438200	4.32752200	3.25153200
H	22.43739300	4.79204100	2.89579000
N	21.86301300	2.94031800	2.12571500
C	23.14203200	2.39837100	11.00058500
C	23.20262700	2.49147200	1.74569900
H	13.19180300	3.37075300	10.92297300
H	13.78151700	3.24797700	0.92622500
H	12.96985700	1.84751400	1.67786100
H	23.14796800	1.98262000	0.78526200
H	23.62380200	1.80093000	2.48534100
H	23.26950400	3.25725200	11.66438100
H	24.08148400	1.85564600	10.91523800
H	22.38893500	1.73007200	11.43377500
H	23.85945100	3.36155600	1.66695900
H	14.66240100	1.72137300	1.15943600

• *ctct conformation* (gas phase)

C	7.70063200	8.77863000	7.36778000
H	8.64734000	8.73314500	7.89528800
C	6.78675900	7.73514700	7.45605500
H	7.03721400	6.85157200	8.03818300
C	5.54715000	7.80670700	6.80738100
C	5.24449200	8.95423300	6.06807800
H	4.28662100	9.03470800	5.56322200
C	6.16943000	9.99304200	5.95659300
H	5.90947800	10.87776900	5.38362100
C	4.56405700	6.65719700	6.97504400
H	5.12817000	5.73910200	7.15748900
H	3.97763300	6.82757700	7.88482400
N	3.58984600	6.47153400	5.89646400
C	3.91906600	6.22547100	4.57680100

O	3.09742700	6.35454700	3.67178500
C	5.32598400	5.80267800	4.24510000
C	6.01030800	4.77366600	4.89947000
H	5.53462800	4.22665900	5.70755700
C	7.30324700	4.42391400	4.50370700
H	7.82452900	3.62516700	5.02596300
C	7.93419500	5.08489700	3.44592500
C	7.22419100	6.08091900	2.75670300
H	7.68991000	6.56697800	1.90537600
C	5.93636000	6.42668000	3.14645900
H	5.37943700	7.18164700	2.60169300
C	9.35592400	4.74035600	3.03816200
H	9.74838800	3.95051500	3.68950600
H	9.37733500	4.38268200	2.00711400
N	10.27697300	5.88385300	3.10579100
C	10.54433400	6.55734500	1.93628000
O	9.97117000	6.27385900	0.88193400
C	11.56787500	7.66071300	1.93807400
C	2.20497500	6.83317500	6.19492800
H	1.59644800	6.61118500	5.32070800
H	2.10907500	7.90124500	6.42868600
C	10.59223400	6.36084500	4.44816700
H	9.67075300	6.43912800	5.03618900
H	11.05414400	7.34500200	4.40934600
C	11.28134400	8.79338500	1.16402800
H	10.33463500	8.83888000	0.63652300
C	12.19522300	9.83686500	1.07575900
H	11.94477000	10.72044600	0.49363900
C	13.43483400	9.76529200	1.72442700
C	13.73748800	8.61775800	2.46372000
H	14.69536000	8.53727400	2.96857200
C	12.81254400	7.57895400	2.57520000
H	13.07249300	6.69422100	3.14816400
C	14.41793500	10.91479400	1.55676700
H	13.85383200	11.83289200	1.37431000
H	15.00436800	10.74440300	0.64699400
N	15.39213800	11.10045600	2.63535600
C	15.06290800	11.34652600	3.95501500
O	15.88454200	11.21746300	4.86003700
C	13.65598700	11.76931800	4.28670400
C	12.97166900	12.79833000	3.63232700
H	13.44735500	13.34533500	2.82424200
C	11.67872700	13.14808500	4.02808000
H	11.15745000	13.94683100	3.50581900
C	11.04777100	12.48710400	5.08585900
C	11.75776800	11.49108200	5.77508700
H	11.29204300	11.00502500	6.62641200
C	13.04560300	11.14531800	5.38534200
H	13.60252000	10.39035200	5.93011300
C	9.62604100	12.83164900	5.49361300
H	9.23357800	13.62148400	4.84226100
H	9.60462700	13.18933000	6.52465800
N	8.70499400	11.68814900	5.42599300
C	8.43763500	11.01466600	6.59550900
O	9.01080100	11.29816100	7.64985200
C	7.41409800	9.91129500	6.59372400
C	16.77701300	10.73882500	2.33690000
H	17.38552800	10.96079800	3.21113300
H	16.87291700	9.67076100	2.10311900
C	8.38973300	11.21114700	4.08362000
H	9.31121300	11.13286300	3.49559700
H	7.92782600	10.22698800	4.12244900
H	17.13776900	11.31513000	1.47818100
H	7.70982300	11.90022800	3.56641300
H	11.27214000	5.67175800	4.96537100
H	1.84422900	6.25689000	7.05366400

·*ctct conformation* (scrf = chloroform)

C	7.70602600	8.75606300	7.32317200
H	8.66747100	8.68401200	7.82034700
C	6.78789000	7.71514100	7.41071900
H	7.04806100	6.81655200	7.96413600
C	5.53215800	7.81045000	6.79668100
C	5.21873900	8.97659800	6.09043200
H	4.24838800	9.07685900	5.61391200
C	6.14720600	10.01207500	5.97775900
H	5.88016900	10.90929000	5.42809800
C	4.54290500	6.66785100	6.96871500
H	5.09639600	5.74471400	7.15415900
H	3.95475400	6.84637900	7.87482900
N	3.56895900	6.48838700	5.88548300

C	3.89646600	6.19676900	4.58374500
O	3.06873600	6.26233300	3.67033800
C	5.31403700	5.80082300	4.26174900
C	5.99031400	4.75457100	4.89781000
H	5.50715300	4.18923700	5.68861100
C	7.28833600	4.41496400	4.50866600
H	7.80283800	3.60312800	5.01635900
C	7.93282100	5.10493200	3.47747300
C	7.23438900	6.12492000	2.81237100
H	7.71165400	6.64239300	1.98643700
C	5.94065300	6.46050900	3.19345700
H	5.39983400	7.23956100	2.66625400
C	9.35500700	4.75976900	3.07066100
H	9.75193700	3.98120800	3.73132200
H	9.37376700	4.38457400	2.04591400
N	10.27052500	5.90805600	3.11986000
C	10.55485200	6.55805800	1.94799200
O	9.99738400	6.25642100	0.88509500
C	11.57581500	7.66340000	1.94775600
C	2.17779700	6.81979200	6.19569400
H	1.56899800	6.61124300	5.31890000
H	2.07297200	7.87879300	6.45905500
C	10.61477200	6.38072500	4.45851400
H	9.70414500	6.45532500	5.06242400
H	11.07430900	7.36532300	4.41377900
C	11.27596100	8.81589600	1.20859400
H	10.31452500	8.88792500	0.71140000
C	12.19408600	9.85682800	1.12104200
H	11.93391500	10.75540100	0.56760000
C	13.44980700	9.76154800	1.73510700
C	13.76322900	8.59541900	2.44138400
H	14.73357200	8.49518100	2.91792500
C	12.83477300	7.55993300	2.55406200
H	13.10181100	6.66273300	3.10374800
C	14.43904100	10.90416500	1.56307600
H	13.88553100	11.82729600	1.37766100
H	15.02717700	10.72566600	0.65694600
N	15.41300300	11.08362600	2.64629300
C	15.08551200	11.37524000	3.94803500
O	15.91325100	11.30967000	4.86143300
C	13.66794400	11.77118500	4.27004800
C	12.99166300	12.81744400	3.63400300
H	13.47481900	13.38278600	2.84320600
C	11.69364300	13.15704600	4.02316000
H	11.17913800	13.96888800	3.51548000
C	11.04916500	12.46706700	5.05435000
C	11.74760300	11.44707100	5.71943700
H	11.27034300	10.92959000	6.54536800
C	13.04133500	11.11148700	5.33833800
H	13.58215800	10.33242900	5.86552800
C	9.62698200	12.81222400	5.46117700
H	9.23005000	13.59079900	4.80053300
H	9.60822900	13.18740100	6.48593100
N	8.71146100	11.66394100	5.41196200
C	8.42714600	11.01391200	6.58381800
O	8.98462900	11.31552100	7.64671500
C	7.40617400	9.90857900	6.58404200
C	16.80415800	10.75220600	2.33606700
H	17.41297000	10.96075900	3.21285000
H	16.90897100	9.69320100	2.07271600
C	8.36720000	11.19130100	4.07330200
H	9.27782100	11.11669900	3.46938300
H	7.90764900	10.20670800	4.11802200
H	17.15401900	11.35627000	1.49265700
H	7.67818700	11.88341300	3.57493800
H	11.30379000	5.68863100	4.95689500
H	1.82792800	6.21571600	7.03909200

• *ctct conformation* (scrf = methanol)

C	7.70123200	8.73830700	7.30667300
H	8.67029100	8.65297100	7.78697800
C	6.77893200	7.70059100	7.39738500
H	7.04285400	6.79532900	7.93765100
C	5.51523300	7.80855200	6.80170100
C	5.19800300	8.98336800	6.11088200
H	4.22153500	9.09386400	5.64947900
C	6.13010700	10.01497800	5.99398900
H	5.86107000	10.91755400	5.45427800
C	4.52150700	6.67029900	6.97386900
H	5.06827900	5.74436400	7.16413500
H	3.92871700	6.85456000	7.87534000

N	3.55243100	6.49328600	5.88398200
C	3.88710300	6.19636800	4.58913800
O	3.06242500	6.24333800	3.66870100
C	5.31025500	5.81461100	4.27448500
C	5.98211800	4.75911600	4.90026000
H	5.49472000	4.18404200	5.68124800
C	7.28311100	4.42550400	4.51540600
H	7.79407500	3.60703800	5.01546500
C	7.93533100	5.13136400	3.49962900
C	7.24350300	6.16493000	2.84860600
H	7.72728100	6.70105500	2.03855100
C	5.94623200	6.49437800	3.22436300
H	5.41355500	7.28664900	2.70839200
C	9.35771900	4.78444400	3.09406000
H	9.75616600	4.01284200	3.76121300
H	9.37511900	4.39776800	2.07351700
N	10.27165700	5.93388000	3.13045900
C	10.56290800	6.56905700	1.95529600
O	10.01042200	6.25709300	0.89044900
C	11.58533000	7.67278200	1.94917100
C	2.15605600	6.80465800	6.19377500
H	1.54936000	6.58731000	5.31775700
H	2.03773100	7.86170300	6.45752700
C	10.63250900	6.40753800	4.46527200
H	9.72903400	6.47838600	5.07965600
H	11.08763500	7.39377400	4.41472800
C	11.28074100	8.83369600	1.22513400
H	10.31168000	8.91903400	0.74483200
C	12.20304200	9.87141200	1.13442200
H	11.93912000	10.77667500	0.59415800
C	13.46674200	9.76344800	1.73010200
C	13.78397300	8.58863000	2.42091800
H	14.76044200	8.47813200	2.88231800
C	12.85186700	7.55702200	2.53781200
H	13.12090500	6.65444500	3.07752100
C	14.46047200	10.90169600	1.55792900
H	13.91370500	11.82763300	1.36765400
H	15.05326500	10.71742600	0.65646200
N	15.42954600	11.07871300	2.64781800
C	15.09487200	11.37563400	3.94266000
O	15.91954800	11.32866900	4.86310000
C	13.67171800	11.75738700	4.25731100
C	12.99985300	12.81287900	3.63153300
H	13.48725000	13.38795100	2.85054200
C	11.69886000	13.14649100	4.01638800
H	11.18789500	13.96495600	3.51632700
C	11.04664300	12.44063500	5.03216800
C	11.73847200	11.40707000	5.68319300
H	11.25469600	10.87094800	6.49325000
C	13.03574300	11.07762400	5.30743600
H	13.56842200	10.28535500	5.82340900
C	9.62425600	12.78755500	5.43773900
H	9.22580700	13.55915600	4.77058500
H	9.60685700	13.17423200	6.45828100
N	8.71031700	11.63811900	5.40134200
C	8.41906600	11.00294500	6.57650600
O	8.97154900	11.31491300	7.64135300
C	7.39664400	9.89922100	6.58263300
C	16.82592300	10.76734800	2.33802500
H	17.43261500	10.98468200	3.21405000
H	16.94424900	9.71030800	2.07425500
C	8.34946500	11.16445800	4.06653000
H	9.25293900	11.09361100	3.45214500
H	7.89434000	10.17822200	4.11707600
H	17.16605800	11.37658700	1.49478900
H	7.65268300	11.85509300	3.57810600
H	11.32928900	5.71690100	4.95369600
H	1.81592500	6.19543400	7.03702400

ctct conformation (scrf = water)

C	7.70016800	8.73444700	7.30445500
H	8.67025500	8.64703600	7.78235300
C	6.77685200	7.69758900	7.39592000
H	7.04093000	6.79141700	7.93453500
C	5.51207300	7.80770500	6.80289300
C	5.19473300	8.98373900	6.11408100
H	4.21742300	9.09594400	5.65489500
C	6.12776400	10.01438300	5.99628700
H	5.85878300	10.91773600	5.45785800
C	4.51727900	6.67048700	6.97525500
H	5.06275500	5.74408600	7.16692500

H	3.92356600	6.85627300	7.87574600
N	3.54922500	6.49354100	5.88418300
C	3.88533300	6.19709300	4.59005900
O	3.06130900	6.24226300	3.66857000
C	5.30929900	5.81753500	4.27646300
C	5.98092800	4.76125400	4.90120500
H	5.49315900	4.18500200	5.68106700
C	7.28240400	4.42871000	4.51702400
H	7.79313500	3.60966600	5.01630400
C	7.93542800	5.13653800	3.50309300
C	7.24412000	6.17142800	2.85357500
H	7.72858300	6.70989100	2.04548800
C	5.94624800	6.49972600	3.22847000
H	5.41432200	7.29331800	2.71371600
C	9.35795900	4.78965000	3.09788400
H	9.75669400	4.01919500	3.76609800
H	9.37535500	4.40125600	2.07798100
N	10.27153900	5.93933800	3.13241700
C	10.56359400	6.57238800	1.95668800
O	10.01152300	6.25907800	0.89174300
C	11.58661500	7.67551600	1.94948700
C	2.15190100	6.80132300	6.19356000
H	1.54563100	6.58085000	5.31803100
H	2.03057400	7.85837100	6.45576800
C	10.63449400	6.41348800	4.46659400
H	9.73194800	6.48413600	5.08229600
H	11.08914800	7.39987700	4.41501500
C	11.28180800	8.83755900	1.22734900
H	10.31171900	8.92497400	0.74945400
C	12.20512400	9.87441700	1.13588600
H	11.94104700	10.78059100	0.59727500
C	13.46990500	9.76429700	1.72891100
C	13.78724400	8.58826000	2.41771800
H	14.76455500	8.47605200	2.87690200
C	12.85421200	7.55761600	2.53550900
H	13.12319400	6.65426100	3.07393400
C	14.46470000	10.90151400	1.55655100
H	13.91922600	11.82791700	1.36488200
H	15.05841300	10.71572800	0.65605900
N	15.43275300	11.07845800	2.64762400
C	15.09664400	11.37490800	3.94174700
O	15.92066400	11.32973300	4.86323900
C	13.67267600	11.75446500	4.25533800
C	13.00104600	12.81074100	3.63058800
H	13.48881600	13.38698900	2.85072300
C	11.69956900	13.14328500	4.01476500
H	11.18883800	13.96232500	3.51548000
C	11.04654500	12.43546200	5.02870000
C	11.73785300	11.40057800	5.67822500
H	11.25339000	10.86211900	6.48631500
C	13.03572600	11.07228000	5.30333400
H	13.56765300	10.27869100	5.81809400
C	9.62401300	12.78235100	5.43390500
H	9.22527800	13.55280200	4.76568700
H	9.60661500	13.17075100	6.45380600
N	8.71043400	11.63266300	5.39937700
C	8.41837900	10.99961700	6.57510900
O	8.97044900	11.31293200	7.64005300
C	7.39536000	9.89648800	6.58231300
C	16.83007700	10.77067100	2.33825000
H	17.43634600	10.99114400	3.21377900
H	16.95140100	9.71362200	2.07604300
C	8.34747900	11.15850600	4.06520300
H	9.25002400	11.08785600	3.44950100
H	7.89282400	10.17211800	4.11678700
H	17.16814200	11.37967400	1.49408000
H	7.64979700	11.84886600	3.57780400
H	11.33217500	5.72312600	4.95399000
H	1.81383800	6.19231800	7.03772900

· *tttt conformation* (gas phase)

C	7.98006300	10.14936100	8.01999700
H	9.05775500	10.08937900	7.90884100
C	7.24057200	8.97292100	8.11226500
H	7.74899500	8.01456100	8.08690900
C	5.84494200	9.00821400	8.18095700
C	5.20769900	10.25545000	8.17230900
H	4.12222200	10.30252800	8.20309900
C	5.94236900	11.43324300	8.07757000
H	5.44223000	12.39392100	8.01592800
C	5.02552200	7.73163000	8.27750700

H	4.92480400	7.44499700	9.33106100
H	4.01681500	7.91965000	7.88906400
N	5.63861000	6.58953600	7.58993200
C	5.72881300	6.71054500	6.20610600
O	5.19067800	7.64652800	5.62458800
C	6.61222600	5.75754300	5.44889600
C	7.73220600	5.12888000	6.01351600
H	7.94418200	5.24068200	7.07183800
C	8.60745800	4.39631800	5.21454500
H	9.47443200	3.92312000	5.66934400
C	8.39978300	4.28652900	3.83321200
C	7.27339600	4.90516300	3.27365200
H	7.11935600	4.85041100	2.20124900
C	6.39440300	5.63293500	4.07012100
H	5.54849500	6.15142600	3.63216500
C	9.42441300	3.60209600	2.94564700
H	9.80744000	2.69679900	3.42592400
H	8.97358100	3.32481500	1.99074100
N	10.57460500	4.48358300	2.67869100
C	10.40358700	5.44762400	1.70608700
O	9.44113800	5.40690500	0.93968100
C	11.36111300	6.60539800	1.64289800
C	5.49634300	5.29641100	8.25667700
H	5.79125900	4.49161500	7.58571800
H	4.45222200	5.12164000	8.55108200
C	11.81639100	4.20370700	3.38394300
H	11.75901500	4.45651700	4.45116000
H	12.63569600	4.76766800	2.94121700
C	11.61635300	7.19038000	0.39534600
H	11.19332000	6.73146700	-0.49193400
C	12.35508600	8.36579600	0.30296900
H	12.52392900	8.81694600	-0.67136100
C	12.84351800	9.00114500	1.45159000
C	12.58930500	8.41621100	2.69545000
H	12.93399200	8.91108500	3.59765700
C	11.85252800	7.23844400	2.79244200
H	11.62055100	6.83880200	3.77421200
C	13.64205100	10.28883400	1.33250800
H	13.37834000	10.79227900	0.39397700
H	14.71114700	10.04914000	1.28870600
N	13.46347200	11.19531700	2.47262600
C	12.18080300	11.71652500	2.61878300
O	11.32880400	11.52987200	1.75680300
C	11.81308500	12.39125700	3.91164100
C	10.69219400	13.23250600	3.90383400
H	10.20198600	13.43049400	2.95689800
C	10.18840400	13.75793900	5.08984200
H	9.29510900	14.37330600	5.07743900
C	10.78828000	13.45145200	6.31909400
C	11.92005700	12.62540800	6.32467100
H	12.40204600	12.37648800	7.26707500
C	12.42297000	12.09301200	5.13938600
H	13.26909700	11.41469900	5.17709700
C	10.16118100	13.91983700	7.62042700
H	9.52169300	14.78658400	7.44272100
H	10.93385600	14.19903700	8.34293900
N	9.34360000	12.85752800	8.23217900
C	8.07631600	12.67589000	7.71693400
O	7.57259100	13.51438800	6.96953500
C	7.34152500	11.39660900	8.00809100
C	14.65798500	11.92489400	2.89469200
H	15.37804700	11.25538100	3.37931200
H	15.15344500	12.39445800	2.03358900
C	9.90126800	12.15384600	9.37732800
H	10.28852000	12.87998800	10.10258300
H	10.72434100	11.48278600	9.09735900
H	6.11788000	5.24710400	9.15828900
H	12.05439800	3.13607600	3.30147100
H	14.39026000	12.71427500	3.59473200
H	9.12950500	11.56392100	9.86895900

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