Supporting Information

Synthesis and properties of helically-folded poly(arylenediethynylene)s

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1. Experimental Section

General

Unless otherwise noted, all materials including dry solvents were obtained from commercial suppliers and used as received. All reactions were performed with dry solvents under an atmosphere of argon or nitrogen in glassware dried with a heat-gun by standard vacuum-line techniques. All work-up and purification procedures were carried out with reagent-grade solvents in air. (*S*)-2,5,8,11-tetraoxa-13-tetradecanamine (**S5**)[S1] was prepared according to previous reports.

Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F254 precoated plates (0.25 mm). The developed chromatogram was analyzed by UV lamp (254 nm). LCMS analysis was conducted on Agilent Technologies 1200 series. Flash column chromatography was performed with KANTO Silica Gel 60N (spherical, neutral, 40-100 μm). Preparative recycling size-exclusion chromatography (SEC) was performed with LC-9210II NEXT instrument (Japan Analytical Industry Ltd.) equipped with an in-line JAIGEL-3H and 5H columns using $CHCl_3$ as an eluent at the flow rate of 3.5 mL/min, UV and RI detectors. Molecular weight and its distribution of synthesized polymers were measured by SEC on a Shimadzu Prominence 2000 instrument equipped with two in-line linear polystyrene gel columns (TOSOH TSKgel Multipore H_{XL}-M SEC columns 7.8 mm × 300 mm) at 40 °C, and tetrahydrofuran (THF) containing 0.1wt% tetra-*n*-butylammonium bromide (TBAB) was used as the eluent at the flow rate of 1.0 mL/min. The molecular weight calibration curve was obtained with standard polystyrenes (TOSOH TSKgel polystyrene standard). The absorption, fluorescence and CD spectra were obtained in a 1 cm quartz cell at 25 °C using a JASCO V570 spectrophotometer, JASCO FP-6600, and JASCO J720WN spectropolarimeter. High-resolution mass spectra (HRMS) were obtained from a Thermo Fisher Scientific Exactive (ESI). Nuclear magnetic resonance (NMR) spectra were recorded on JEOL JNM-ECA-600 (^{1}H 600 MHz, ^{13}C 150 MHz) and a JEOL JMN-ECA-600II with Ultra COOL™ probe (^{1}H NMR: 600 MHz, ^{13}C NMR: 150 MHz). Chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to Me_4Si (δ 0.00 ppm) or residual peak of $C_2D_2Cl_4$ (δ 5.98 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm) or $C_2D_2Cl_4$ (δ 73.79 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, dt = doublet of triplets, t = triplet, td = triplet of doublets, q = quintet, m = multiplet, brs = broad signal), coupling constant (Hz), and integration.

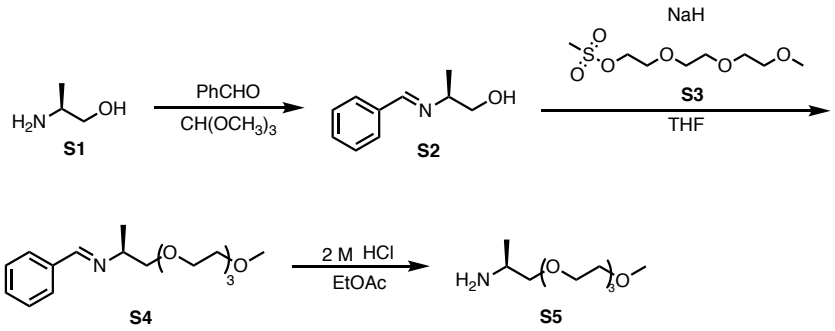
1-1. Measurement of UV-Vis Absorption, Fluorescence, and CD Spectra

Measurements of UV-Vis absorption, fluorescence, and CD spectra were performed with degassed sample solution in spectroscopic-grade solvents using 1 cm quartz cell. Unless otherwise stated, all experiments were carried out at 25 °C. Solutions of poly-ArDEs in solvent, which were filtered

through a 0.45 μm membrane filter, were used for measurements. Each spectrum was recorded on the corresponding device with a resoluteion of 0.5 nm or 1 nm.

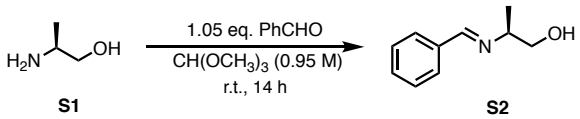
1-2. Synthesis and Characterization of Compounds

1-2-1. Synthesis of chiral amine side chain



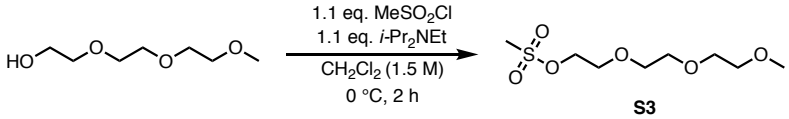
Scheme S1. Synthesis of chiral amine side chain **S5**.

Synthesis of (*S*)-2-(benzylideneamino)-1-propanol (S2)



To a 200-mL round-bottomed flask containing a magnetic stirring bar were added (*S*)-2-amino-1-propanol (**S1**; 5.00 g, 66.8 mmol) and benzaldehyde (7.42 g, 69.6 mmol) in trimethyl orthoformate (70 mL). The mixture was stirred at room temperature for 14 h. The reaction mixture was extracted with saturated NaCl aqueous solution and CH_2Cl_2, and the organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The purification by three-time-repeated recrystallizations from toluene afforded **S2** as a white crystal (9.56 g, 96%). ^{1}H NMR spectrum of **S2** was identical to that reported in the literature.[S1]

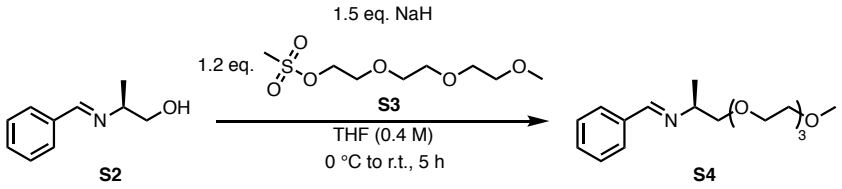
Synthesis of 2-{2-(2-methoxyethoxy)ethoxy}ethyl methanesulfonate (S3)



To a 300-mL round-bottomed flask containing a magnetic stirring bar were added *N,N*-diisopropylethylamine (7.2 mL, 42 mmol) and triethylene glycol monomethyl ether (6.0 mL, 38 mmol) in CH_2Cl_2 (75 mL). Then, a solution of $MeSO_2Cl$ (4.88 g, 42.6 mmol) in CH_2Cl_2 (25 mL) was added at 0 °C. After stirring the reaction mixture at 0 °C for 2 h, saturated NaCl aqueous solution was added to the mixture. The mixture was extracted with CH_2Cl_2, and the organic layer was dried over

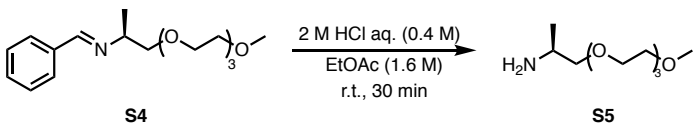
Na_2SO_4, filtered and concentrated under reduced pressure. The residue was extracted with hexane and H_2O, and CH_2Cl_2 and saturated NaCl aqueous solution were added to the water layer. The organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure, and directly used for the next step without further purification. ^{1}H NMR spectrum of **S3** was identical to that reported in the literature.[S1]

Synthesis of (*S*)-1-phenyl-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)-methanimine (S4)



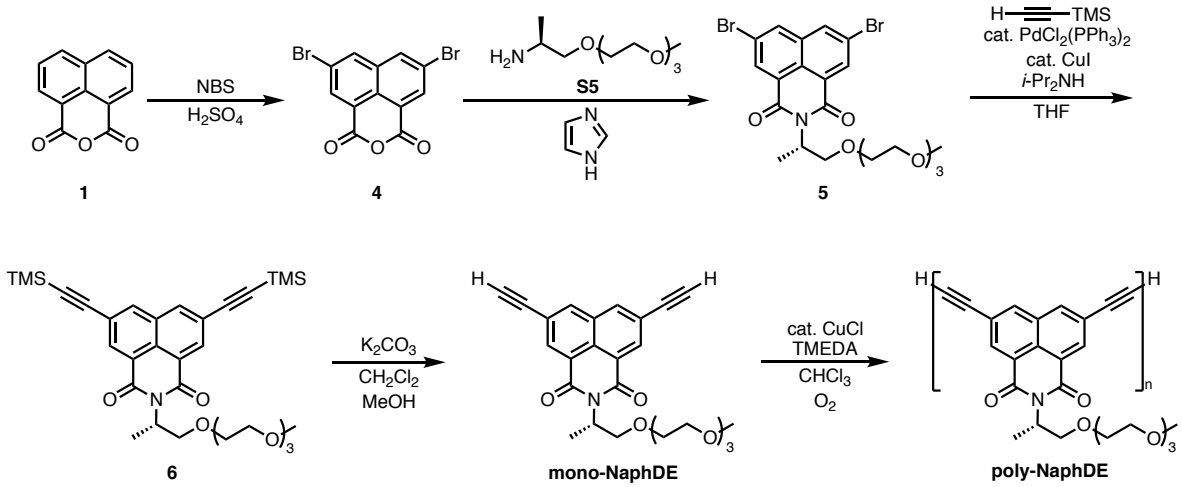
To a 200-mL round-bottomed flask containing a magnetic stirring bar were added sodium hydride (60% oil dispersion, 1.1 g, 27 mmol) and **S2** (3.00 g, 18 mmol) in dry THF (45 mL) at 0 °C under N_2. After stirring the mixture for 1 h, **S3** (5.3 g, 22 mmol) was added. The mixture was stirred at room temperature for 5 h, and poured into a mixture of ice water, NaCl, and diethyl ether. The organic layer was then separated, and the aqueous phase was extracted with EtOAc. The combined organic layers were washed with saturated NH_4Cl aqueous solution and brine, and then dried over Na_2SO_4. After filtration, the solvents were removed under reduced pressure, and directly used for the next step without further purification.

Synthesis of (*S*)-2,5,8,11-tetraoxa-13-tetradecanamine (S5)



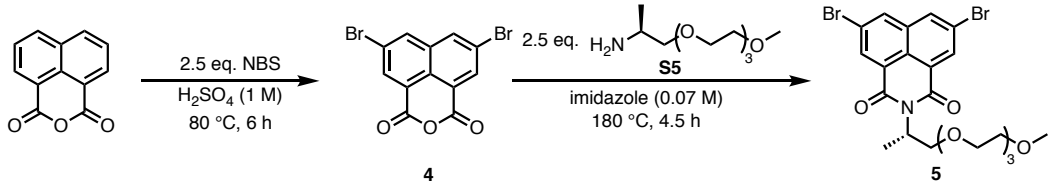
To a 300-mL round-bottomed flask containing a magnetic stirring bar were added the material obtained above **S4** and 2M HCl aqueous solution (70 mL) in EtOAc (40 mL). The mixture was stirred at room temperature for 30 min, and the mixture was extracted with H_2O. Then, the volatiles of water layer were removed under reduced pressure. Once again, the residue was extracted with H_2O and EtOAc, and the volatiles of water layer were removed under reduced pressure. The crude product was rinsed with $CHCl_3$ and filtered. The solvent was concentrated under reduced pressure to yield **S5**, which was directly used for the next step without further purification. ^{1}H NMR spectrum of **S5** was identical to that reported in the literature.[S1]

1-2-2. Synthesis of poly-NaphDE



Scheme S2. Synthesis of **poly-NaphDE**.

Synthesis of (*S*)-2,7-dibromo-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)naphtaleneimide (5)



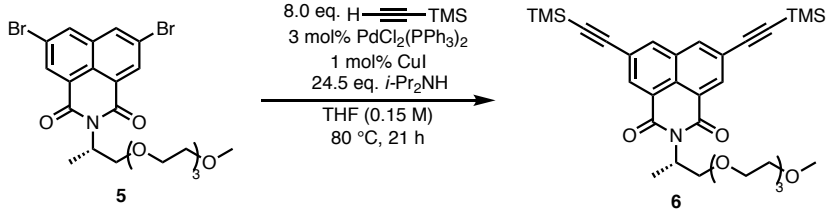
To a 200-mL two-necked round-bottomed flask containing a magnetic stirring bar were added sulfuric acid (50.5 mL), 1,8-naphthalenedicarboxylic anhydride (**1**; 10.0 g, 50.5 mmol) and *N*-bromosuccinimide (22.5 g, 126.2 mmol) under N_2. The reaction mixture was stirred at 80 °C for 6 h. After cooling down to room temperature, the reaction mixture was poured into ice water (100 mL). The precipitate was collected by filtration, washed with water and acetonitrile and dried under vacuum. The collected solid (**4**; 25.2 g, quant.) was used to the subsequent reaction without further purification.

To a 200-mL round-bottomed flask containing a magnetic stirring bar were added compound **4** (4.50 g, 13.4 mmol), **S5** (7.11 g, 33.4 mmol) and imidazole (13.7 g, 0.20 mol) under N_2. After stirring at 180 °C for 4.5 h, the reaction mixture was diluted with ethanol before complete cooling. The reaction mixture was treated with 2 M HCl aqueous solution and chloroform, and the organic layer was separated. The aqueous layer was extracted with chloroform. Then, the combined organic layers were dried over Na_2SO_4, filtered and concentrated in *vacuo*. The purification with flash column chromatography on silica gel (eluent: chloroform/methanol = 10:1) afforded imide **5** as a brown oil (2.02 g, 2 steps overall 27%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 1.52 (d, J = 6.6 Hz, 3H), 3.35 (s, 3H), 3.48–3.60 (m, 11H), 3.63–3.68 (m, 1H), 3.79 (dd, J = 10.5, 5.7 Hz, 1H), 4.20 (dd, J = 10.2, 8.4 Hz, 1H), 5.42–5.51 (m, 1H), 8.25 (d, J = 1.8 Hz, 2H), 8.61 (d, J = 1.8 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ15.0, 48.8, 59.0, 70.3, 70.51 (2C), 70.49 (2C), 71.8, 71.9, 122.3, 124.7, 125.2, 133.8, 134.0, 134.1, 162.9. HRMS (ESI) *m/z* calcd for

$C_{22}H_{25}Br_2NNaO_6^+$ $[M+Na]^+$: 581.9920, found 581.9926.

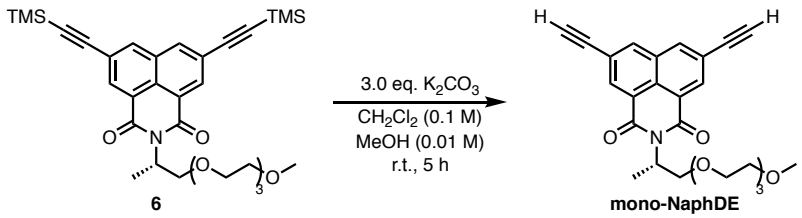
Synthesis of (*S*)-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)-3,5-bis{(trimethylsilyl)ethynyl}naphthalimide (6)



To a 100-mL two-necked round-bottomed flask containing a magnetic stirring bar were added **5** (2.00 g, 3.58 mmol), bis(triphenylphosphine)palladium dichloride (75.6 mg, 0.11 mmol), copper(I) iodide (6.4 mg, 0.03 mmol) and diisopropylamine (12.3 mL, 87.6 mmol) in THF (24 mL) under N_2. Then, trimethylsilylacetylene (4.00 mL, 28.9 mmol) was added to the mixture. The reaction mixture was stirred at 80 °C for 21 h. After cooling down to room temperature, Et_2O and activated carbon were added to the reaction mixture. After stirring at room temperature for 1 h, the mixture was filtered and the solvents were removed by evaporation. H_2O was added to the residue, and the organic layer was extracted with $CHCl_3$, dried over Na_2SO_4, filtered and concentrated in *vacuo*. The purification by flash column chromatography on silica gel (eluent: chloroform/methanol = 10:1) afforded **6** as a brown oil (1.76 g, 83%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 0.30 (s, 18H), 1.52 (d, J = 7.2 Hz, 3H), 3.35 (s, 3H), 3.45–3.59 (m, 11H), 3.63–3.68 (m, 1H), 3.81 (dd, J = 10.5, 5.7 Hz, 1H), 4.19 (dd, J = 9.9, 8.7 Hz, 1H), 5.44–5.51 (m, 1H), 8.17 (s, 2H), 8.54 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ –0.2, 15.1, 48.5, 59.0, 70.3, 70.43, 70.45, 70.48, 70.51, 71.9, 72.0, 97.8, 103.0, 123.0, 123.2, 126.6, 131.1, 134.4, 135.8, 163.6. HRMS (ESI) *m/z* calcd for $C_{32}H_{43}NNaO_6Si_2^+$ $[M+Na]^+$: 616.2521, found 616.2501.

Synthesis of (*S*)-3,5-diethynyl-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)naphtalimide (mono-NaphDE)



To a 15-mL Schlenk tube containing a magnetic stirring bar were added **6** (0.20 g, 0.34 mmol) and potassium carbonate (0.14 g, 1.0 mmol) in 3.7 mL of a CH_2Cl_2/MeOH mixture (10:1). After stirring the mixture at room temperature for 5.5 h, the reaction mixture was diluted with CH_2Cl_2 and filtered through a Celite® pad. The filtrate was concentrated by evaporation and crude product was purified by flash column chromatography on silica gel (eluent: chloroform/methanol = 10:1) and PTLC (eluent: chloroform/methanol = 95:5) to afford **mono-NaphDE** as a yellow solid (0.14 g, 92%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 1.53 (d, J = 6.6 Hz, 3H), 3.29 (s, 2H), 3.35 (s, 3H), 3.45–3.51 (m, 4H), 3.52–3.60 (m, 7H), 3.64–3.69 (m, 1H), 3.81 (dd, J = 10.2, 6.0 Hz, 1H), 4.20 (dd, J = 10.2, 8.4 Hz, 1H), 5.45–5.53 (m, 1H), 8.25 (d, J = 1.8 Hz, 2H), 8.58 (d, J = 1.2 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 15.1, 48.6, 59.0, 70.3, 70.45 (2C), 70.49, 70.51, 71.87, 71.94, 80.1, 81.8, 122.1, 123.4, 127.0, 131.0 134.4, 136.3, 163.5. HRMS (ESI) *m/z* calcd for $C_{26}H_{27}NNaO_6^+$ $[M+Na]^+$: 472.1731 found 472.1733.

Synthesis of poly-(*S*)-3,5-diethynyl-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)naphtalimide (poly-NaphDE)

To a 30-mL round-bottomed flask containing a magnetic stirring bar were added **mono-NaphDE** (117.0 mg, 0.26 mmol), copper(I) chloride (7.7 mg, 0.08 mmol) and tetramethylethylenediamine (0.12 mL, 0.78 mmol) in $CHCl_3$ (2.6 mL) under O_2. After stirring at room temperature for 24 h, the reaction mixture was quenched with saturated NH_4Cl aqueous solution. The mixture was extracted with $CHCl_3$, and the organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The purification by gel permeation chromatography (SEC) afforded **poly-NaphDE** as a brown solid (101.9 mg, 87% by weight).

^{1}H NMR (600 MHz, $C_2D_2Cl_4$, 140 °C) δ 1.45 (br s, 3H), 3.39 (br s, 3H), 3.50–3.73 (m, 11H), 3.88–3.95 (m, 1H), 4.18–4.24 (m, 1H), 5.45–5.53 (m, 1H), 8.38 (s, 2H), 8.70 (s, 2H). ^{13}C NMR (150 MHz, $C_2D_2Cl_4$, 140 °C) δ 15.0, 49.3, 58.4, 70.2, 70.37, 70.39, 70.44 (2C), 71.9, 72.1, 76.4, 81.3, 121.7, 124.0, 127.4, 131.1, 134.2, 136.4, 162.8

The average molecular number (M_n) and the average molecular weight (M_w) and polydispersity index (PDI = M_w/M_n) were estimated by SEC (see Figure S1 for details).

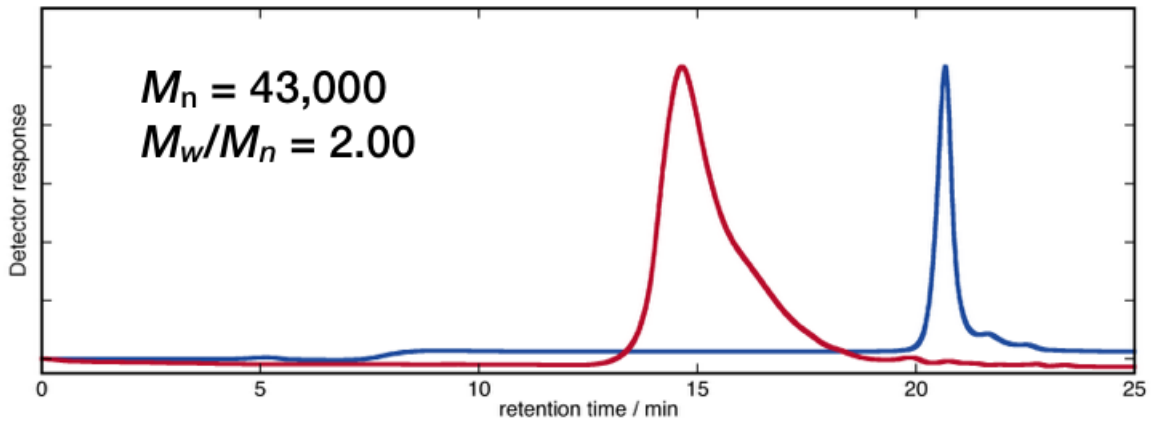
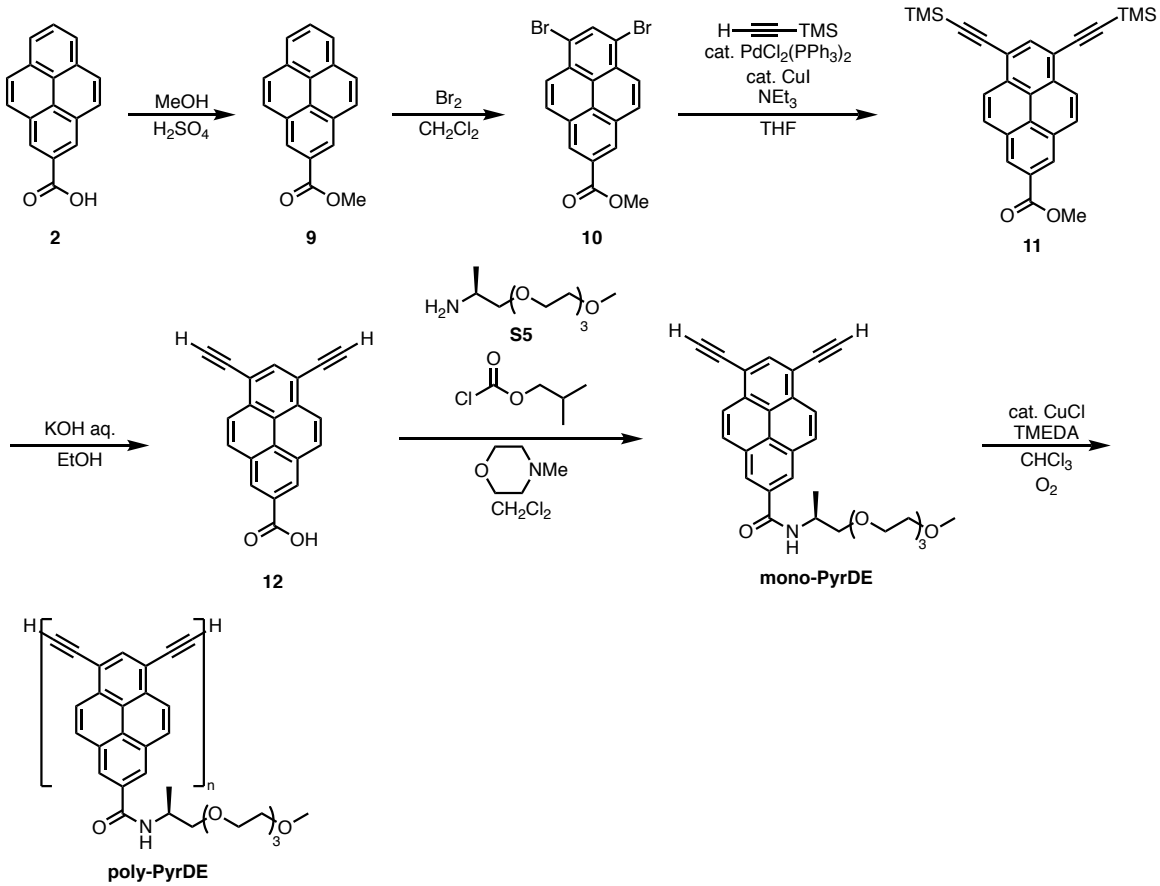


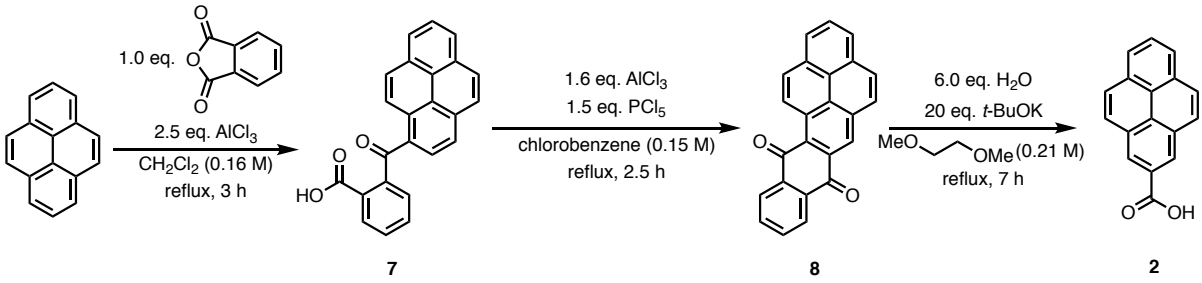
Figure S1. SEC chart of **mono-NaphDE** (blue line) and **poly-NaphDE** (red line) for the analysis of M_n and M_w/M_n. M_n and M_w/M_n were determined by SEC analysis equipped with a polystyrene column eluted with THF containing TBAB (0.1 wt%) and polystyrenes standards (see General section for details) at the 1.0 mL/min of flow rate.

1-2-3. Synthesis of poly-PyrDE



Scheme S3. Synthesis of **poly-PyrDE**.

Synthesis of pyrene-2-carboxylic acid (2)



Pyrene-2-carboxylic acid (**2**) was synthesized by the reported procedure.[S2]

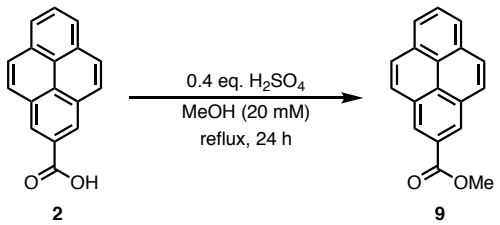
To a 1-L three-necked round-bottomed flask containing a magnetic stirring bar were added pyrene (9.4 g, 46 mmol) and phthalic anhydride (6.9 g, 46 mmol) in dehydrated CH_2Cl_2 (280 mL). Then $AlCl_3$ (15.5 g, 116 mmol) was added portionwise to the solution under N_2 atmosphere. The mixture was heated under reflux for 3 h. The solvent was then evaporated and the residue was cooled to 0 °C and suspended in H_2O (300 mL). The pH of the solution was adjusted to 0–1 by adding conc. HCl aqueous solution, and the resulting solid was collected by filtration, washed with ice water. Then, remaining water in the solid was azeotropically removed by adding toluene and evaporation. The

solid was suspended in AcOH and heated at 130 °C for 5 min, after which the insoluble material was removed by hot filtration and washing with hot AcOH. The filtrate was poured into 1 L ice water and the resulting solid was isolated by filtration, washed with ice water. Then, remaining water in the solid was azeotropically removed by adding toluene and evaporation to afford 1-(*o*-carboxy-benzoyl)pyrene (**7**) (17.6 g, quant.) as a bright yellow powder. This compound was used directly in the next step without further purification.

To a 1-L three-necked round-bottomed flask containing a magnetic stirring bar was added a solution of **7** (16.0 g, 45.7 mmol) in chlorobenzene (300 mL) under N_2 atmosphere. Then PCl_5 (14.5 g, 69.6 mmol) and $AlCl_3$ (9.70 g, 72.8 mmol) were added portionwise to the solution. The resulting dark green mixture was heated under reflux for 2.5 h. The solvent was removed by evaporation, and the residue was cooled to 0 °C and suspended in H_2O. The dark red precipitate was collected by filtration, washed with H_2O. Then, remaining water in the solid was azeotropically removed by adding toluene and dried in *vacuo* to give **8** (18.4 g, quant.). This material was used directly in the next step without further purification.

To a 300-mL three-necked round-bottomed flask containing a magnetic stirring bar was added crude **8** (5.0 g, 15 mmol) in 1,2-dimethoxyethane (70 mL). H_2O (1.7 mL, 90 mmol) was added, and then potassium *tert*-butoxide (33.8 g, 300 mmol) was added portionwise with vigorous stirring. The mixture was vigorously stirred under reflux for 7 h, and then the solvent was evaporated. The residue was cooled to 0 °C, suspended in H_2O, and acidified to pH 1–2 with conc. HCl aqueous solution. The resulting solid was removed by filtration, suspended in H_2O, stirred overnight, collected by filtration, washed with H_2O and dried in *vacuo*. The purification with flash column chromatography on silica gel (eluent: CH_2Cl_2/methanol/aq. NH_3 = 90:9:1) afforded pyrene-2-carboxylic acid (**2**; 1.96 g, 7.95 mmol, overall 53% yield from pyrene) as a light grey solid along with pyrene, starting material **8**. ^{1}H-NMR spectrum of **2** was identical to that reported in the literature.[S2]

Synthesis of pyrene-2-carboxylic acid methyl ester (9)

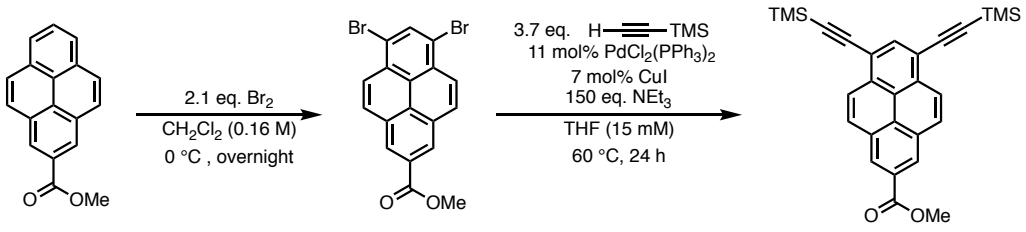


2 **9**

To a 1-L round-bottomed flask containing a magnetic stirring bar was added pyrene-2-carboxylic acid (**2**; 1.87 g, 7.59 mmol) in methanol (375 mL) containing conc. H_2SO_4 (3.8 mL, 3.0 mmol), and the resulting mixture was heated at reflux for 24 h. The solution was cooled to room temperature, and the solvent was removed to afford a residue that was redissolved in CH_2Cl_2. The mixture was washed

with H_2O, Na_2CO_3 solution and H_2O again. Then the organic layer was separated, dried over Na_2SO_4, filtered and evaporated. The purification with flash column chromatography on silica gel (eluent: hexane/CH_2Cl_2 = 5:1) afforded **9** as white solid (1.37 g, 72 %). ^{1}H-NMR spectrum of **9** was identical to that reported in the literature. [S3]

Synthesis of 6,8-bis{(trimethylsilyl)ethynyl}pyrene-2-carboxylic acid methyl ester (11)



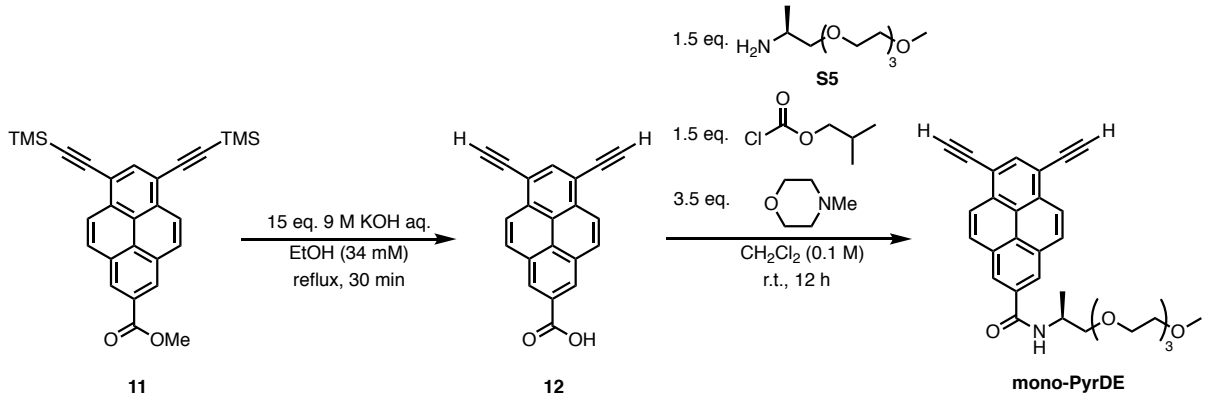
9 **10** **11**

To a 200-mL two-necked round-bottomed flask containing a magnetic stirring bar was added a solution of pyrene-2-carboxylic acid methyl ester (**9**; 1.00 g, 3.84 mmol) in dehydrated CH_2Cl_2 (24 mL) under N_2. A solution of Br_2 (0.42 mL, 8.07 mmol) in dehydrated CH_2Cl_2 (24 mL) was added dropwise over 1 h at 0 °C. The mixture was stirred overnight at room temperature and the solvent was evaporated. The product was difficult to isolate because of the low solubility, so it was used for the next step without purification.

To a 1-L round-bottomed flask containing a magnetic stirring bar were added compound **10**, copper(I) iodide (53.8 mg, 0.28 mmol) and dichlorobis(triphenylphosphine)palladium(II) (297 mg, 0.42 mmol) under N_2. The solid was dissolved in THF (255 mL) containing Et_3N (80 mL, 0.58 mol), and the solution was thoroughly purged with N_2 for 1 h. Then trimethylsilylacetylene (1.93 mL, 14.0 mmol) was added dropwise to the stirred solution. After stirring the mixture for 20 min, the temperature of the reaction mixture was raised to 60 °C and maintained for 24 h. After cooling to room temperature, the solvent was removed and the residue was extracted with CH_2Cl_2 and H_2O, and the organic layer was dried over Na_2SO_4, filtered and concentrated in *vacuo*. The purification with flash column chromatography on silica gel (eluent: hexane/CH_2Cl_2 = 1:1) afforded **11** as a yellow solid (1.16 g, 2 steps overall 67 %).

^{1}H NMR (600 MHz, $CDCl_3$) δ 0.39 (s, 18H), 4.07 (s, 3H), 8.11 (d, J = 9.0 Hz, 2H), 8.28 (s, 1H), 8.46 (d, J = 9.0 Hz, 2H), 8.75 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 0.1, 52.5, 101.1, 102.7, 118.0, 123.7, 125.9, 126.1, 126.7, 127.7, 129.2, 130.8, 132.5, 134.7, 167.2. HRMS (ESI) *m/z* calcd for $C_{28}H_{29}O_2Si_2^+$ $[M+H]^+$: 453.1701, found 453.1711.

Synthesis of *N*-((*S*)-1-methyl-3,6,9,12-tetraoxatridecyl)-pyrene-2-carboxamide (mono-PyrDE)

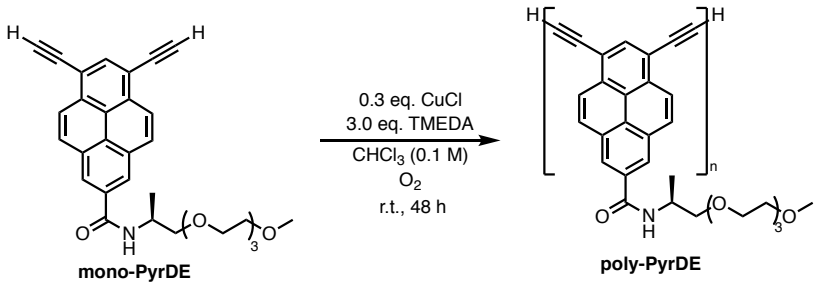


To a 100-mL round-bottomed flask containing a magnetic stirring bar were added **11** (0.50 g, 1.10 mmol) and 9.0 M aq. potassium hydroxide (1.84 mL, 16.6 mmol) in ethanol (32 mL). The mixture was stirred under reflux for 30 min and the solvent was evaporated. H_2O and 2.0 M HCl aqueous solution was added to the residue, and the resulting solid was collected by filtration, washed with ice water and dried in *vacuo*. The crude product **12** was used directly in the next step without further purification.

To a 50-mL two-necked round-bottomed flask containing a magnetic stirring bar were added *i*-BuOCOCl (0.22 mL, 1.7 mmol), crude **5** and *N*-methylmorpholine (0.24 mL, 2.2 mmol) in CH_2Cl_2 (11 mL). After stirring the mixture at room temperature for 20 min, chiral amine **S5** (0.36 g, 1.66 mmol) and *N*-methylmorpholine (0.18 mL, 1.6 mmol) were added. After stirring at room temperature for 12 h, the reaction mixture was added to saturated $NaHCO_3$ aqueous solution. The mixture was extracted with CH_2Cl_2, and the organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The purification with flash column chromatography (eluent: $CHCl_3$/MeOH = 10:0 to 10:1) and PTLC ($CHCl_3$/methanol = 95:5) afforded **mono-PyrDE** as a yellow solid (0.17 g, 2 steps overall 32%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 1.42 (d, J = 6.6 Hz, 3H), 3.26 (s, 3H), 3.43 (t, J = 4.2 Hz, 2H), 3.49–3.56 (m, 2H), 3.58–3.61 (m, 2H), 3.63 (s, 2H), 3.65–3.76 (m, 8H), 4.53–4.55 (m, 1H), 7.15 (d, J = 7.8 Hz, 1H), 8.22 (d, J = 9.6 Hz, 2H), 8.34 (s, 1H), 8.56 (d, J = 9.0 Hz, 2H), 8.66 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 17.8, 46.0, 58.9, 70.46, 70.55, 70.58, 70.61, 70.8, 71.8, 74.1, 81.5, 83.3, 116.9, 123.9, 124.7, 125.0, 125.9, 129.6, 130.9, 132.9, 133.0, 134.8, 167.0. HRMS (ESI) *m/z* calcd for $C_{31}H_{31}NNaO_5^+$ $[M+Na]^+$: 520.2094 found 520.2081.

Synthesis of poly-*N*-((*S*)-1-methyl-3,6,9,12-tetraoxatridecyl)-pyrene-2-carboxamide (poly-PyrDE)



To a 20-mL Schlenk tube containing a magnetic stirring bar were added **mono-PyrDE** (100 mg, 0.20 mmol), copper(I) chloride (6.0 mg, 0.06 mmol) and tetramethylethylenediamine (0.09 mL, 0.6 mmol) in $CHCl_3$ (2.0 mL) under O_2. After stirring at room temperature for 48 h, the reaction mixture was quenched with saturated NH_4Cl aqueous solution. The mixture was extracted with $CHCl_3$, and the organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The purification by SEC (eluent: $CHCl_3$) afforded **poly-PyrDE** as a brown solid (18.6 mg, 19% by weight).

^{1}H NMR (600 MHz, $C_2D_2Cl_4$, 140 °C) δ 1.42 (br s, 3H), 3.20–4.16 (m, 17 H), 4.20–4.78 (br s, 1H) 6.10–8.60 (brs, 8H) ^{13}C NMR spectrum (150 MHz, $C_2D_2Cl_4$, 140 °C) was not obtained with a good S/N ratio due to low solubility of the compound.

The M_n, the M_w and PDI were estimated by SEC (see Figure S2 for details).

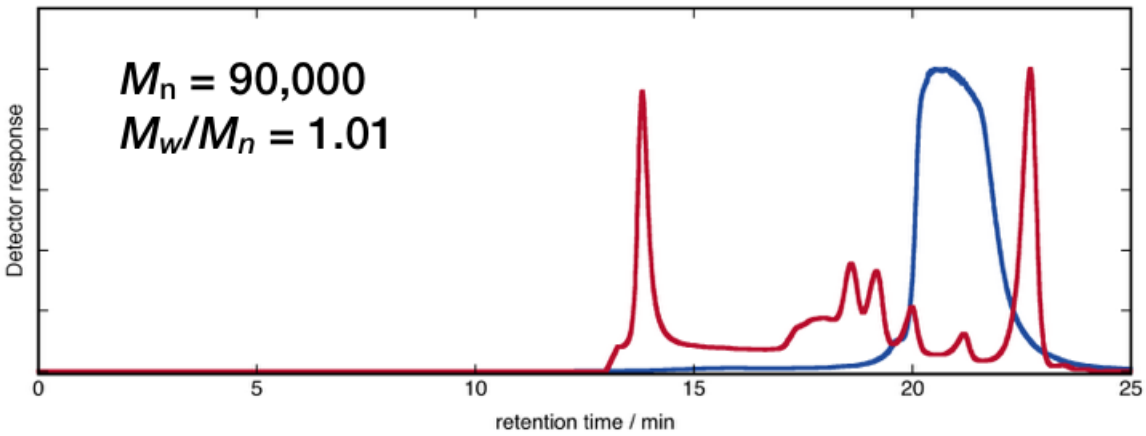
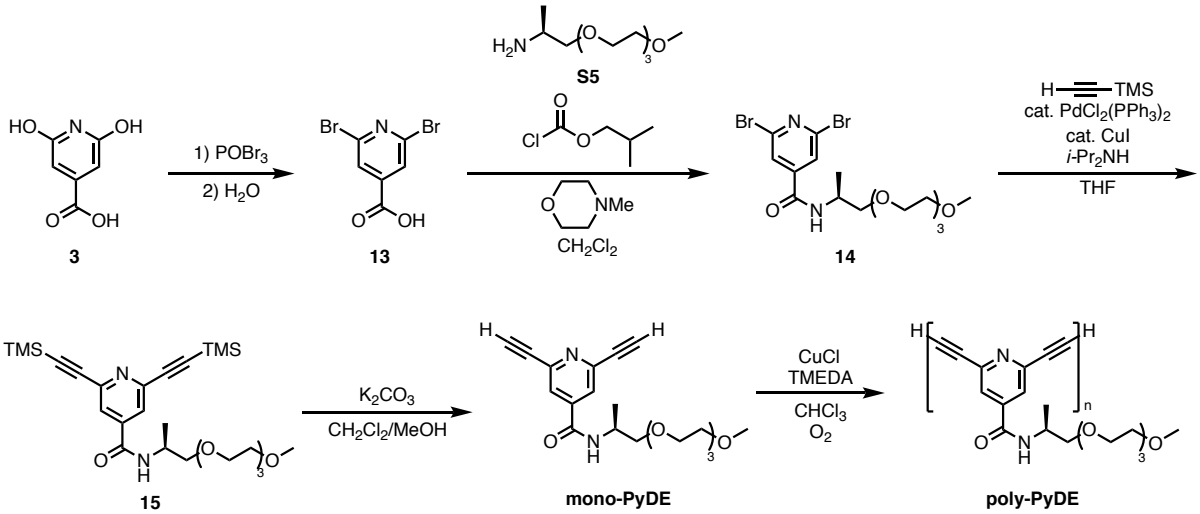


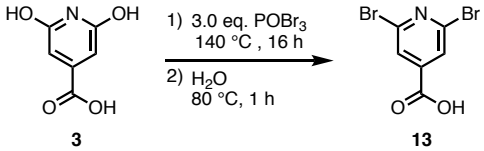
Figure S2. SEC chart of **mono-PyrDE** (blue line) and **poly-PyrDE** (red line) for the analysis of M_n and M_w/M_n. M_n and M_w/M_n were determined by SEC analysis equipped with a polystyrene column eluted with THF containing TBAB (0.1 wt%) and polystyrenes standards (see General section for details) at the 1.0 mL/min of flow rate.

1-2-4. Synthesis of poly-PyDE



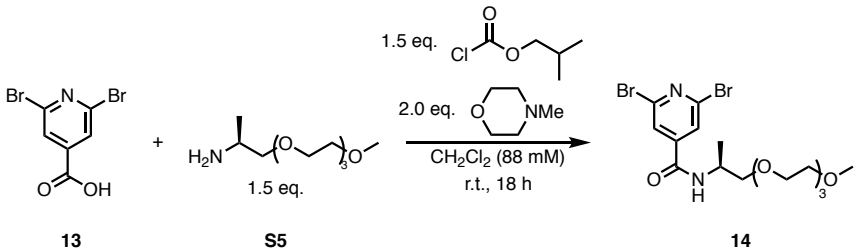
Scheme S4. Synthesis of **poly-PyDE**.

Synthesis of 2,6-dibromocitrazinic acid (13)



To a 30-mL Schlenk tube containing a magnetic stirring bar were added citrazinic acid (**3**; 2.01 g, 13.0 mmol) and $POBr_3$ (11.3 g, 39.3 mmol) under N_2. After stirring at 140 °C for 16 h, the reaction mixture was cooled to room temperature and quenched with deionized water. The solution was stirred at 80 °C for 1 h, then cooled to room temperature again. The resulting precipitate was filtered, washed with water. After drying, the obtained crude product **13** was used without further purification (3.02 g, 83%). ^{1}H-NMR spectrum of **13** was identical to that reported in the literature. [S4]

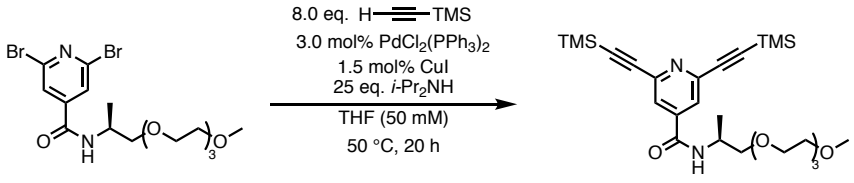
Synthesis of *N*-((*S*)-1-methyl-3,6,9,12-tetraoxatridecyl)-2,6-dibromoisonicotinamide (14)



To a 300-mL round-bottom flask containing a magnetic stirring bar were added *i*-BuOCOCl (0.70 mL, 5.3 mmol), 2,6-dibromocitrazinic acid **13** (1.0 g, 3.5 mmol) and *N*-methylmorpholine (0.80 mL, 7.1 mmol) in CH_2Cl_2 (40 mL). After stirring the mixture at room temperature for 20 min, chiral amine **S5** (1.2 g, 5.3 mmol) and *N*-methylmorpholine (0.60 mL, 5.3 mmol) was added. After stirring at room temperature for 18 h, saturated $NaHCO_3$ aqueous solution was added to the reaction mixture.

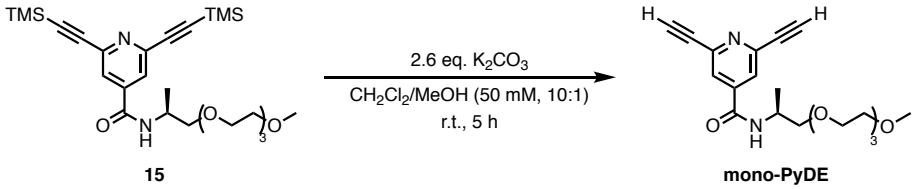
The mixture was extracted with CH_2Cl_2, and the organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The purification with flash column chromatography (eluent: $CHCl_3$/MeOH = 10:0 to 10:1) afforded **14** as a yellow oil (1.10 g, 64%). ^{1}H-NMR spectrum of **14** was identical to that reported in the literature. [S4]

Synthesis of *N*-((*S*)-1-methyl-3,6,9,12-tetraoxatridecyl)-2,6-bis(trimethylsilylethynyl) isonicotinamide (15)



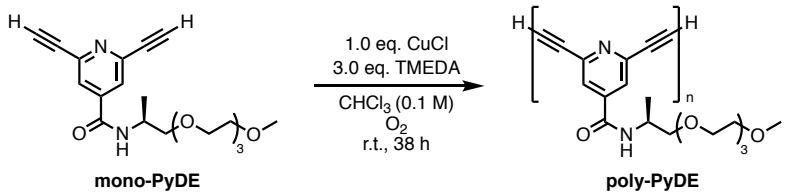
To a 200-mL round-bottomed flask containing a magnetic stirring bar were added **14** (1.0 g, 2.1 mmol), *N,N*-diisopropylethylamine (7.1 mL, 51 mmol) and trimethylsilylacetylene (2.3 mL, 17 mmol) in THF (40 mL) under N_2. The mixture was degassed five times by freeze-pump-thaw method. Then, bis(triphenylphosphine)palladium dichloride (44 mg, 0.062 mmol), copper(I) iodide (6.5 mg, 0.034 mmol) were added. The reaction mixture was stirred at 50 °C for 20 h. After cooled down to room temperature, Et_2O was added to the reaction mixture. After the filtration, the solvent was removed by evaporation. The purification with flash column chromatography (eluent: $CHCl_3$/MeOH = 10:0 to 10:1) afford **15** as a brown oil (0.96 g, 90%). ^{1}H-NMR spectrum of **15** was identical to that reported in the literature.[S4]

Synthesis of *N*-((*S*)-1-methyl-3,6,9,12-tetraoxatridecyl)-2,6-diethynylisonicotinamide (mono-PyDE)



To a 20-mL Schlenk tube containing a magnetic stirring bar were added **15** (0.20 g, 0.38 mmol) and potassium carbonate (0.14 g, 0.99 mmol) in 7.6 mL of a CH_2Cl_2-MeOH mixture (10:1). After stirring at room temperature for 5 h, the reaction mixture was diluted with CH_2Cl_2 and filtered through a Celite® pad. The solvent was removed under reduced pressure. The purification with flash column chromatography (eluent: $CHCl_3$/MeOH = 10:1) afforded **mono-PyDE** as a brown oil (0.12 g, 82%). ^{1}H-NMR spectrum was identical to that reported in the literature.[S4]

Synthesis of poly-*N*-((*S*)-1-methyl-3,6,9,12-tetraoxatridecyl)-2,6-diethynylisonicotinamide (poly-PyDE)



mono-PyDE **poly-PyDE**

To a 20-mL Schlenk tube containing a magnetic stirring bar were added **mono-PyDE** (100 mg, 0.27 mmol), copper(I) chloride (27.0 mg, 0.27 mmol) and tetramethylethylenediamine (0.12 mL, 0.80 mmol) in $CHCl_3$ (3.0 mL) under O_2. After stirring at room temperature for 38 h, the reaction mixture was quenched with saturated NH_4Cl aqueous solution. The mixture was extracted with $CHCl_3$, and the organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The purification by SEC (eluent: $CHCl_3$) afforded **poly-PyDE** as a yellow solid (34.2 mg, 34% by weight).

^{1}H NMR (600 Hz, $C_2D_2Cl_4$) δ 1.29 (d, J = 6.6 Hz, 2H), 3.26 (s, 3H), 3.45–3.70 (m, 14H), 4.32 (br s, 1H), 7.68 (d, J = 7.8 Hz, 1H), 8.02 (s, 2H). ^{13}C NMR (150 Hz, $C_2D_2Cl_4$) δ 17.1, 46.4, 58.6, 70.0, 70.19, 70.22, 70.4, 71.6, 76.9, 77.1, 77.3, 80.5, 120.2, 126.5, 142.5, 143.1, 162.8. In ^{13}C NMR spectra in d_2-1,1,2,2-tetrachloroethane at 25 °C, there are some unidentified extra peaks around an acetylene region (77 ppm) and an aromatic region (120 ppm) probably due to the existence of various conformers. We were not able to obtain the ^{13}C NMR spectrum at higher temperature because of the decomposition of poly-PyDE.

The average molecular number (M_n) and the average molecular weight (M_w) and polymer dispersion index (PDI = M_w/M_n) were estimated by SEC (see Figure S3 for details).

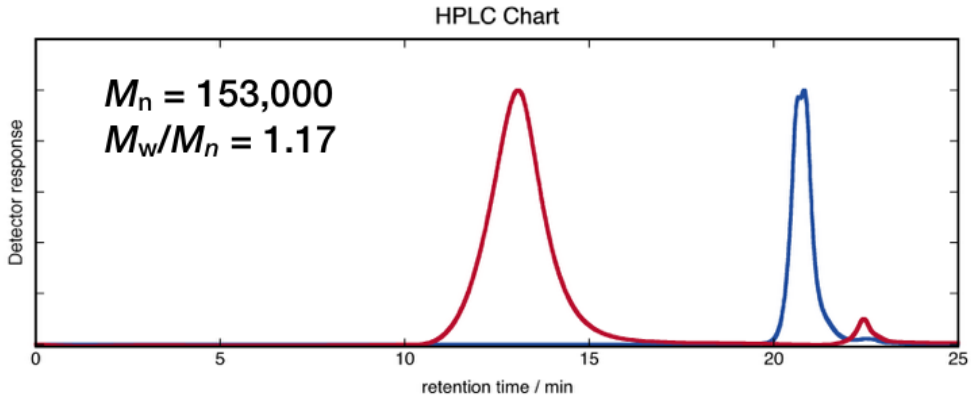


Figure S3. SEC chart of **mono-PyDE** (blue line) and **poly-PyDE** (red line) for the analysis of M_n and M_w/M_n. M_n and M_w/M_n were determined by SEC analysis equipped with a polystyrene column eluted with THF containing TBAB (0.1 wt%) and polystyrenes standards (see General section for details) at the 1.0 mL/min of flow rate.

2. Spectroscopic Data

UV-Vis absorption and fluorescence spectra of **mono-PyrDE** and **poly-PyrDE** in various solvents were measured to discuss the changes in properties due to polymerization and the formation of the helical structure of **poly-PyrDE**. No significant solvent-dependent change of spectrum was observed in mono-PyrDE, whereas the marked changes of spectra were confirmed in **poly-PyrDE** depending on the polarity of the solvents.

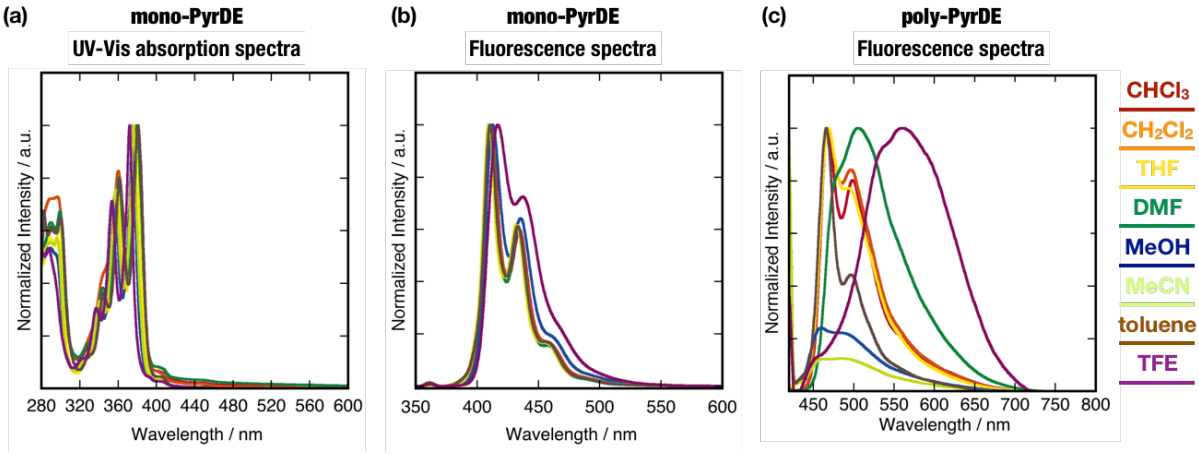


Figure S4. Spectroscopic analysis of **mono-PyrDE** and **poly-PyrDE** (M_n = 5.6 × 10^4, PDI = 1.03) in various solvents. (a) UV-Vis absorption spectra of **mono-PyrDE**, (b) fluorescence spectra of **mono-PyrDE** (excitation laser: 360 nm), and (c) fluorescence spectra of **poly-PyrDE** (excitation laser: 410 nm). The color of each line indicates; red = $CHCl_3$, orange = CH_2Cl_2, yellow = tetrahydrofurane (THF), green = *N,N*-dimethylformamide (DMF), blue = methanol (MeOH), light green = acetonitrile, brown = toluene, and purple = 2,2,2-trifluoroethanol (TFE)

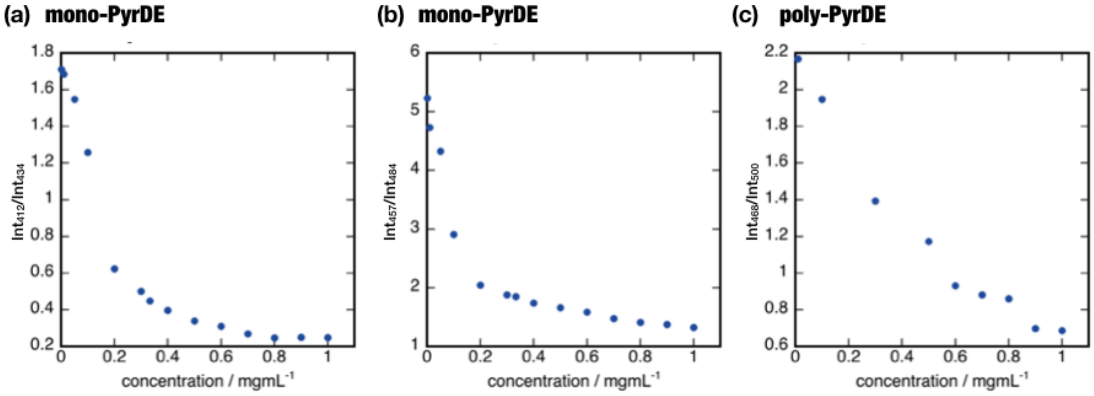


Figure S5. Changes of the fluorescence intensity ratios at (a) 412 nm/434 nm (Int_{412}/Int_{434}) and (b) 457 nm/484 nm (Int_{457}/Int_{484}) in **mono-PyrDE**, and (c) 457 nm/484 nm (Int_{457}/Int_{484}) in **poly-PyrDE** at each concentrations in $CHCl_3$.

3. Computational Study

Molecular modeling and calculations of helical structures of poly-ArDEs[S5]

The MM calculations were conducted using the COMPUSS II force field as contained in the MS Modeling software (version 4.4, Accelrys, Inc., San Diego, CA) operated using a PC running under Windows® 7. The polymer models (40 repeating monomer units) of **poly-ArDEs** were constructed using the Polymer Builder module in the MS Modeling software so as to maintain the intramolecular hydrogen bonding networks between the amide residues (NH and CO) of the neighboring pendants (*n* and *n* + 6) and to satisfy the helical parameters (~4.0 Å for the π–π stacking and ~6 monomer units per turn). The triethylene glycol side groups were replaced with the terminal methyl groups for clarity. The geometrical parameters for the **poly-ArDEs** backbone were fixed during the following force field optimization. The dielectric constant was set to 1.0. The geometry optimizations were carried out without any cutoff by the smart minimizer in three steps. First, the starting conformations were subject to the steepest decent optimization in order to eliminate the worse steric conflicts. Second, subsequent optimization until the convergence using a conjugate gradient algorithm was performed. The fully-optimized **poly-ArDEs** models were obtained by the further energy minimization using the Newton method with the 0.1 kcal/mol/Å convergence criterion.

Cartesian coordinates of optimized helical **poly-NaphDE** are shown as follows;

C	-9.828000	0.337000	-1.109000	C	-10.671000	-0.558000	-8.838000	H	-20.564000	-1.204000	-18.095000
C	-8.656000	0.054000	-1.036000	N	-11.995000	-2.629000	-8.869000	C	-13.246000	2.184000	-17.555000
C	-7.242000	-0.069000	-0.732000	O	-14.257000	-2.537000	-8.571000	H	-22.688000	-1.058000	-19.079000
C	-6.618000	-1.303000	-0.495000	C	-9.365000	1.497000	-8.929000	H	-21.725000	0.309000	-19.699000
C	-6.487000	1.086000	-0.630000	H	-10.478000	3.342000	-8.795000	H	-23.001000	0.596000	-18.500000
C	-5.249000	-1.402000	-0.250000	C	-9.452000	0.100000	-8.937000	O	-20.851000	-1.354000	-15.462000
H	-7.240000	-2.208000	-0.543000	C	-10.720000	-2.061000	-8.935000	H	-22.414000	-1.933000	-16.722000
C	-5.106000	1.028000	-0.345000	C	-12.097000	-4.021000	-9.403000	H	-22.606000	-0.335000	-15.966000
H	-6.960000	2.072000	-0.759000	C	-8.062000	2.125000	-8.966000	C	-21.405000	-1.814000	-14.246000
C	-4.463000	-0.247000	-0.218000	H	-8.507000	-0.464000	-9.013000	H	-20.572000	-1.955000	-13.538000
C	-4.598000	-2.752000	-0.048000	O	-9.693000	-2.720000	-9.025000	H	-21.935000	-2.773000	-14.383000
C	-4.349000	2.197000	-0.129000	C	-13.069000	-4.182000	-10.593000	H	-22.104000	-1.082000	-13.805000
C	-3.078000	-0.302000	-0.016000	C	-12.407000	-5.076000	-8.262000	C	-20.181000	18.473000	-18.147000
N	-3.204000	-2.748000	-0.092000	H	-11.112000	-4.303000	-9.807000	C	-20.893000	17.541000	-17.870000
O	-5.259000	-3.778000	-0.006000	C	-6.932000	2.468000	-8.730000	C	-21.726000	16.380000	-17.633000
C	-3.000000	2.111000	0.158000	H	-12.812000	-5.127000	-11.097000	C	-23.107000	16.490000	-17.406000
H	-4.844000	3.177000	-0.155000	H	-12.987000	-3.371000	-11.332000	C	-21.156000	15.118000	-17.642000
C	-2.364000	0.867000	0.186000	H	-14.124000	-4.248000	-10.285000	C	-23.924000	15.372000	-17.257000
C	-2.367000	-1.620000	0.017000	O	-11.383000	-5.056000	-7.275000	H	-23.526000	17.510000	-17.370000
C	-2.434000	-4.009000	-0.290000	H	-12.468000	-6.063000	-8.756000	C	-21.945000	13.968000	-17.417000
C	-2.277000	3.311000	0.498000	H	-13.396000	-4.885000	-7.808000	H	-20.073000	15.000000	-17.789000
H	-1.288000	0.831000	0.408000	C	-11.627000	-5.995000	-6.248000	C	-23.369000	14.095000	-17.301000
O	-1.163000	-1.763000	0.119000	H	-10.812000	-5.883000	-5.516000	C	-25.413000	15.525000	-17.028000
C	-3.140000	-5.193000	-0.991000	H	-11.626000	-7.033000	-6.629000	C	-21.361000	12.695000	-17.267000
C	-1.680000	-4.580000	1.014000	H	-12.586000	-5.810000	-5.733000	C	-24.162000	12.949000	-17.184000
H	-1.613000	-3.758000	-0.991000	C	-21.267000	12.459000	-7.818000	N	-26.195000	14.352000	-17.110000
C	-1.740000	4.308000	0.910000	C	-21.553000	11.289000	-7.810000	O	-25.888000	16.630000	-16.826000
H	-2.366000	-5.934000	-1.257000	C	-21.661000	9.857000	-7.986000	C	-22.151000	11.581000	-17.033000
H	-3.653000	-4.901000	-1.919000	C	-22.875000	9.151000	-7.998000	H	-20.272000	12.580000	-17.363000
H	-3.863000	-5.709000	-0.339000	C	-20.486000	9.145000	-8.159000	C	-23.546000	11.719000	-17.012000
O	-0.692000	-5.448000	0.488000	C	-22.932000	7.775000	-8.187000	C	-25.672000	13.047000	-17.221000
H	-2.384000	-5.116000	1.675000	H	-23.807000	9.713000	-7.854000	C	-27.699000	14.400000	-17.098000
H	-1.221000	-3.771000	1.608000	C	-20.497000	7.743000	-8.322000	C	-21.544000	10.272000	-16.889000

H	-1.293000	5.187000	1.305000	H	-19.516000	9.665000	-8.137000	H	-24.150000	10.816000	-16.839000
C	0.218000	-5.935000	1.451000	C	-21.751000	7.048000	-8.345000	O	-26.401000	12.067000	-17.265000
H	0.928000	-6.578000	0.909000	C	-24.263000	7.066000	-8.287000	C	-28.411000	15.775000	-17.185000
H	-0.275000	-6.539000	2.233000	C	-19.302000	7.002000	-8.446000	C	-28.442000	13.618000	-15.844000
H	0.784000	-5.117000	1.930000	C	-21.765000	5.663000	-8.529000	H	-28.026000	13.840000	-17.994000
C	-18.876000	6.263000	-0.504000	N	-24.210000	5.694000	-8.568000	C	-21.085000	9.154000	-16.869000
C	-18.203000	5.263000	-0.440000	O	-25.325000	7.668000	-8.266000	H	-29.490000	15.578000	-17.302000
C	-17.536000	3.978000	-0.403000	C	-19.335000	5.625000	-8.583000	H	-28.097000	16.378000	-18.051000
C	-18.285000	2.828000	-0.138000	H	-18.332000	7.518000	-8.443000	H	-28.282000	16.363000	-16.260000
C	-16.168000	3.857000	-0.603000	C	-20.569000	4.973000	-8.649000	O	-29.762000	13.306000	-16.285000
C	-17.721000	1.565000	-0.137000	C	-23.063000	4.904000	-8.600000	H	-28.457000	14.301000	-14.974000
H	-19.360000	2.948000	0.062000	C	-25.421000	5.075000	-9.175000	H	-27.928000	12.695000	-15.522000
C	-15.552000	2.582000	-0.625000	C	-18.117000	4.852000	-8.621000	C	-30.652000	12.959000	-15.243000
H	-15.553000	4.758000	-0.746000	H	-20.560000	3.878000	-8.778000	H	-30.405000	11.986000	-14.784000
C	-16.359000	1.416000	-0.401000	O	-23.085000	3.684000	-8.706000	H	-31.652000	12.892000	-15.696000
C	-18.595000	0.370000	0.127000	C	-26.144000	5.896000	-10.266000	H	-30.688000	13.727000	-14.453000
C	-14.167000	2.417000	-0.860000	C	-26.427000	4.446000	-8.111000	C	-10.908000	23.369000	-19.386000
C	-15.768000	0.152000	-0.440000	H	-25.068000	4.202000	-9.750000	C	-12.096000	23.406000	-19.188000
N	-17.948000	-0.865000	0.119000	C	-17.197000	4.084000	-8.496000	C	-13.516000	23.526000	-18.970000
O	-19.800000	0.461000	0.279000	H	-26.819000	5.198000	-10.790000	C	-14.081000	24.760000	-18.617000
C	-13.594000	1.150000	-0.906000	H	-25.438000	6.293000	-11.012000	C	-14.329000	22.417000	-19.123000
H	-13.536000	3.308000	-0.987000	H	-26.758000	6.728000	-9.892000	C	-15.453000	24.925000	-18.474000
C	-14.412000	0.035000	-0.698000	O	-26.221000	3.042000	-8.177000	H	-13.392000	25.609000	-18.486000
C	-16.588000	-1.081000	-0.178000	H	-27.471000	4.708000	-8.359000	C	-15.716000	22.526000	-18.907000
C	-18.652000	-2.070000	0.655000	H	-26.245000	4.847000	-7.095000	H	-13.890000	21.446000	-19.404000
C	-12.164000	0.944000	-1.100000	C	-26.948000	2.313000	-7.209000	C	-16.287000	23.816000	-18.628000
H	-13.942000	-0.958000	-0.734000	H	-26.670000	1.257000	-7.344000	C	-16.035000	26.294000	-18.167000
O	-16.127000	-2.207000	-0.205000	H	-28.041000	2.402000	-7.340000	C	-16.549000	21.388000	-18.928000
C	-20.188000	-2.186000	0.468000	H	-26.692000	2.619000	-6.179000	C	-17.669000	23.928000	-18.490000
C	-18.255000	-2.343000	2.228000	C	-15.912000	21.655000	-8.306000	N	-17.442000	26.372000	-18.117000
H	-18.274000	-2.933000	0.082000	C	-17.000000	21.161000	-8.149000	O	-15.301000	27.255000	-17.998000
C	-10.995000	0.645000	-1.128000	C	-18.257000	20.444000	-8.120000	C	-17.913000	21.516000	-18.730000
H	-20.481000	-3.224000	0.697000	C	-19.483000	21.093000	-8.323000	H	-16.114000	20.393000	-19.103000
H	-20.489000	-1.972000	-0.570000	C	-18.246000	19.067000	-7.977000	C	-18.458000	22.791000	-18.545000
H	-20.759000	-1.532000	1.144000	C	-20.680000	20.404000	-8.418000	C	-18.309000	25.269000	-18.250000
O	-18.581000	-3.653000	2.681000	H	-19.480000	22.183000	-8.449000	C	-18.182000	27.683000	-18.114000
H	-18.837000	-1.652000	2.856000	C	-19.443000	18.327000	-8.066000	C	-18.750000	20.343000	-18.661000
H	-17.187000	-2.123000	2.410000	H	-17.294000	18.536000	-7.837000	H	-19.549000	22.858000	-18.407000
C	-17.555000	-4.580000	2.361000	C	-20.675000	19.016000	-8.331000	O	-19.520000	25.386000	-18.142000
H	-17.933000	-5.580000	2.608000	C	-21.963000	21.146000	-8.699000	C	-17.371000	28.991000	-18.280000
H	-16.634000	-4.394000	2.943000	C	-19.452000	16.920000	-7.962000	C	-19.217000	27.967000	-16.845000
H	-17.291000	-4.570000	1.289000	C	-21.840000	18.284000	-8.551000	H	-18.858000	27.659000	-18.989000
C	-19.494000	16.630000	-0.546000	N	-23.072000	20.354000	-9.017000	C	-19.466000	19.404000	-18.420000
C	-20.044000	15.579000	-0.350000	O	-22.000000	22.362000	-8.790000	H	-18.096000	29.822000	-18.327000
C	-20.775000	14.347000	-0.217000	C	-20.638000	16.224000	-8.110000	H	-16.774000	29.018000	-19.205000
C	-22.157000	14.373000	-0.003000	H	-18.527000	16.374000	-7.727000	H	-16.706000	29.169000	-17.420000
C	-20.126000	13.127000	-0.319000	C	-21.817000	16.909000	-8.409000	O	-20.202000	28.875000	-17.335000
C	-22.915000	13.216000	0.043000	C	-23.120000	18.965000	-8.955000	H	-18.634000	28.410000	-16.017000
H	-22.646000	15.356000	0.078000	C	-24.210000	21.007000	-9.740000	H	-19.706000	27.056000	-16.455000
C	-20.861000	11.924000	-0.260000	C	-20.688000	14.795000	-7.954000	C	-21.030000	29.463000	-16.354000
H	-19.036000	13.066000	-0.454000	H	-22.743000	16.320000	-8.512000	H	-21.608000	30.243000	-16.874000
C	-22.287000	11.977000	-0.106000	O	-24.138000	18.320000	-9.159000	H	-20.452000	29.946000	-15.547000
C	-24.413000	13.315000	0.170000	C	-23.828000	21.977000	-10.878000	H	-21.736000	28.738000	-15.912000
C	-20.222000	10.674000	-0.406000	C	-25.333000	21.660000	-8.806000	C	-1.655000	18.523000	-20.824000
C	-23.021000	10.791000	-0.158000	H	-24.751000	20.208000	-10.277000	C	-2.280000	19.528000	-20.596000
N	-25.104000	12.111000	0.076000	C	-20.963000	13.624000	-7.871000	C	-2.973000	20.770000	-20.345000
O	-25.008000	14.379000	0.209000	H	-24.748000	22.160000	-11.457000	C	-2.264000	21.938000	-20.027000
C	-20.959000	9.504000	-0.449000	H	-23.087000	21.543000	-11.566000	C	-4.355000	20.826000	-20.441000
H	-19.126000	10.646000	-0.494000	H	-23.459000	22.954000	-10.535000	C	-2.889000	23.166000	-19.864000
C	-22.358000	9.582000	-0.335000	O	-26.268000	20.648000	-8.469000	H	-1.172000	21.854000	-19.937000
C	-24.527000	10.840000	-0.037000	H	-25.829000	22.460000	-9.387000	C	-5.035000	22.039000	-20.207000
C	-26.580000	12.203000	-0.208000	H	-24.886000	22.142000	-7.918000	H	-4.929000	19.920000	-20.696000
C	-20.246000	8.249000	-0.577000	C	-27.386000	21.120000	-7.746000	C	-4.277000	23.237000	-19.976000
H	-22.936000	8.649000	-0.381000	H	-27.990000	20.237000	-7.482000	C	-2.069000	24.410000	-19.568000
O	-25.232000	9.846000	-0.064000	H	-28.019000	21.787000	-8.354000	C	-6.445000	22.092000	-20.157000
C	-26.962000	13.079000	-1.430000	H	-27.101000	21.643000	-6.814000	C	-4.949000	24.449000	-19.833000
C	-27.505000	12.568000	1.067000	C	-5.478000	22.274000	-9.736000	N	-2.780000	25.631000	-19.559000
H	-26.930000	11.199000	-0.499000	C	-6.460000	22.961000	-9.591000	O	-0.869000	24.325000	-19.365000
C	-19.564000	7.253000	-0.555000	C	-7.729000	23.664000	-9.468000	C	-7.097000	23.294000	-19.927000

H	-28.028000	12.903000	-1.655000	C	-7.863000	25.052000	-9.642000	H	-7.020000	21.163000	-20.290000
H	-26.384000	12.801000	-2.325000	C	-8.872000	22.929000	-9.199000	C	-6.335000	24.463000	-19.816000
H	-26.838000	14.161000	-1.268000	C	-9.092000	25.695000	-9.609000	C	-4.182000	25.736000	-19.659000
O	-28.837000	12.261000	0.686000	H	-6.960000	25.637000	-9.861000	C	-2.098000	26.969000	-19.646000
H	-27.408000	13.634000	1.343000	C	-10.139000	23.543000	-9.139000	C	-8.532000	23.326000	-19.783000
H	-27.200000	11.968000	1.944000	H	-8.818000	21.840000	-9.076000	H	-6.880000	25.408000	-19.671000
C	-29.773000	12.453000	1.726000	C	-10.251000	24.947000	-9.407000	O	-4.764000	26.808000	-19.568000
H	-30.758000	12.195000	1.311000	C	-9.184000	27.177000	-9.880000	C	-0.572000	26.992000	-19.887000
H	-29.802000	13.499000	2.077000	C	-11.310000	22.791000	-8.905000	C	-2.377000	28.055000	-18.413000
H	-29.576000	11.795000	2.591000	C	-11.519000	25.518000	-9.539000	H	-2.527000	27.474000	-20.530000
C	-11.177000	23.101000	-1.492000	N	-10.476000	27.660000	-10.122000	C	-9.721000	23.346000	-19.588000
C	-12.343000	22.826000	-1.346000	O	-8.200000	27.889000	-10.015000	H	-0.281000	28.048000	-20.019000
C	-13.766000	22.688000	-1.165000	C	-12.552000	23.392000	-8.985000	H	-0.267000	26.452000	-20.797000
C	-14.525000	23.835000	-0.924000	H	-11.252000	21.721000	-8.653000	H	-0.017000	26.593000	-19.024000
C	-14.385000	21.451000	-1.203000	C	-12.648000	24.744000	-9.326000	O	-2.167000	29.358000	-18.964000
C	-15.896000	23.784000	-0.771000	C	-11.668000	26.956000	-9.955000	H	-1.663000	27.844000	-17.595000
H	-14.003000	24.800000	-0.858000	C	-10.589000	28.902000	-10.954000	H	-3.394000	27.989000	-17.985000
C	-15.778000	21.358000	-1.034000	C	-13.751000	22.638000	-8.713000	C	-2.044000	30.398000	-18.015000
H	-13.794000	20.537000	-1.346000	H	-13.658000	25.175000	-9.417000	H	-3.000000	30.613000	-17.504000
C	-16.552000	22.554000	-0.855000	O	-12.764000	27.468000	-10.123000	H	-1.735000	31.291000	-18.580000
C	-16.660000	25.055000	-0.549000	C	-9.595000	29.037000	-12.127000	H	-1.268000	30.194000	-17.255000
C	-16.423000	20.109000	-1.048000	C	-10.672000	30.256000	-10.129000	C	-1.144000	8.113000	-21.787000
C	-17.944000	22.466000	-0.787000	H	-11.564000	28.857000	-11.471000	C	-0.576000	9.163000	-21.620000
N	-18.032000	24.891000	-0.393000	C	-14.826000	22.138000	-8.499000	C	0.159000	10.400000	-21.442000
O	-16.141000	26.161000	-0.582000	H	-9.979000	29.844000	-12.772000	C	1.518000	10.386000	-21.094000
C	-17.799000	20.043000	-0.956000	H	-9.559000	28.123000	-12.740000	C	-0.460000	11.625000	-21.643000
H	-15.822000	19.193000	-1.141000	H	-8.571000	29.312000	-11.839000	C	2.272000	11.548000	-21.002000
C	-18.551000	21.221000	-0.852000	O	-12.024000	30.444000	-9.748000	H	1.981000	9.401000	-20.929000
C	-18.762000	23.719000	-0.616000	H	-10.345000	31.075000	-10.795000	C	0.259000	12.830000	-21.489000
C	-18.795000	26.077000	0.084000	H	-9.979000	30.246000	-9.269000	H	-1.524000	11.664000	-21.926000
C	-18.429000	18.754000	-0.920000	C	-12.259000	31.687000	-9.119000	C	1.667000	12.786000	-21.225000
H	-19.644000	21.128000	-0.793000	H	-13.311000	31.686000	-8.794000	C	3.740000	11.483000	-20.669000
O	-19.980000	23.736000	-0.639000	H	-12.124000	32.529000	-9.816000	C	-0.394000	14.079000	-21.526000
C	-19.008000	27.097000	-1.038000	H	-11.610000	31.851000	-8.237000	C	2.388000	13.981000	-21.140000
C	-18.219000	26.726000	1.420000	C	0.530000	13.717000	-11.002000	N	4.458000	12.689000	-20.789000
H	-19.794000	25.731000	0.401000	C	0.646000	14.911000	-10.872000	O	4.285000	10.438000	-20.354000
C	-18.958000	17.688000	-0.745000	C	0.577000	16.357000	-10.788000	C	0.315000	15.255000	-21.349000
H	-19.589000	27.949000	-0.653000	C	1.679000	17.207000	-10.994000	H	-1.483000	14.094000	-21.662000
H	-19.575000	26.659000	-1.876000	C	-0.660000	16.937000	-10.560000	C	1.708000	15.188000	-21.203000
H	-18.059000	27.494000	-1.423000	C	1.559000	18.591000	-11.024000	C	3.887000	13.966000	-20.927000
O	-18.217000	25.747000	2.449000	H	2.654000	16.745000	-11.198000	C	5.958000	12.611000	-20.759000
H	-18.901000	27.558000	1.676000	C	-0.818000	18.336000	-10.544000	C	-0.398000	16.511000	-21.253000
H	-17.217000	27.163000	1.271000	H	-1.557000	16.319000	-10.421000	H	2.262000	16.132000	-21.097000
C	-17.735000	26.273000	3.668000	C	0.305000	19.176000	-10.837000	O	4.543000	14.995000	-20.835000
H	-17.848000	25.485000	4.428000	C	2.756000	19.463000	-11.332000	C	6.600000	11.452000	-21.547000
H	-18.310000	27.156000	3.997000	C	-2.080000	18.917000	-10.306000	C	6.593000	12.620000	-19.271000
H	-16.669000	26.547000	3.600000	C	0.102000	20.552000	-10.987000	H	6.327000	13.510000	-21.277000
C	-1.556000	19.505000	-2.780000	N	2.454000	20.803000	-11.651000	C	-1.025000	17.520000	-21.048000
C	-2.297000	20.443000	-2.603000	O	3.890000	19.025000	-11.438000	H	7.678000	11.672000	-21.633000
C	-3.102000	21.634000	-2.395000	C	-2.241000	20.290000	-10.367000	H	6.193000	11.369000	-22.568000
C	-2.482000	22.885000	-2.277000	H	-2.937000	18.273000	-10.056000	H	6.505000	10.472000	-21.056000
C	-4.479000	21.555000	-2.278000	C	-1.149000	21.089000	-10.726000	O	6.527000	13.851000	-18.553000
C	-3.198000	24.058000	-2.107000	C	1.223000	21.442000	-11.462000	H	7.639000	12.273000	-19.356000
H	-1.385000	22.921000	-2.332000	C	3.403000	21.565000	-12.531000	H	6.079000	11.867000	-18.657000
C	-5.247000	22.725000	-2.095000	C	-3.519000	20.909000	-10.084000	C	7.527000	14.766000	-18.965000
H	-4.968000	20.570000	-2.311000	H	-1.323000	22.175000	-10.793000	H	7.351000	15.701000	-18.416000
C	-4.594000	24.005000	-2.055000	O	1.060000	22.637000	-11.657000	H	7.477000	14.988000	-20.044000
C	-2.459000	25.373000	-2.015000	C	4.036000	20.748000	-13.679000	H	8.544000	14.407000	-18.726000
C	-6.648000	22.656000	-1.970000	C	4.508000	22.445000	-11.790000	C	-9.749000	1.909000	-22.216000
C	-5.373000	25.162000	-1.974000	H	2.805000	22.322000	-13.069000	C	-8.569000	2.153000	-22.160000
N	-3.279000	26.513000	-1.963000	C	-4.504000	21.581000	-9.900000	C	-7.123000	2.241000	-22.070000
O	-1.245000	25.446000	-2.071000	H	4.507000	21.470000	-14.366000	C	-6.382000	1.091000	-21.767000
C	-7.411000	23.808000	-1.879000	H	3.274000	20.197000	-14.254000	C	-6.447000	3.436000	-22.280000
H	-7.116000	21.661000	-1.973000	H	4.815000	20.041000	-13.359000	C	-4.998000	1.084000	-21.730000
C	-6.758000	25.053000	-1.898000	O	3.915000	23.658000	-11.356000	H	-6.945000	0.165000	-21.584000
C	-4.701000	26.516000	-1.960000	H	5.298000	22.664000	-12.533000	C	-5.039000	3.486000	-22.172000
C	-2.681000	27.896000	-1.904000	H	4.986000	21.886000	-10.967000	H	-7.002000	4.355000	-22.524000
C	-8.848000	23.667000	-1.761000	C	4.857000	24.537000	-10.777000	C	-4.305000	2.269000	-21.962000
H	-7.363000	25.966000	-1.834000	H	4.301000	25.427000	-10.446000	C	-4.252000	-0.200000	-21.445000

O	-5.306000	27.571000	-1.930000	H	5.612000	24.863000	-11.508000	C	-4.336000	4.708000	-22.221000
C	-1.185000	28.114000	-2.246000	H	5.377000	24.091000	-9.908000	C	-2.912000	2.300000	-21.952000
C	-2.946000	28.721000	-0.514000	C	-3.863000	4.075000	-11.803000	N	-2.850000	-0.150000	-21.604000
H	-3.208000	28.484000	-2.681000	C	-2.800000	4.634000	-11.687000	O	-4.850000	-1.213000	-21.128000
C	-10.015000	23.393000	-1.631000	C	-1.595000	5.448000	-11.638000	C	-2.954000	4.732000	-22.126000
H	-1.022000	29.202000	-2.337000	C	-0.312000	4.929000	-11.885000	H	-4.888000	5.652000	-22.327000
H	-0.895000	27.668000	-3.207000	C	-1.718000	6.812000	-11.414000	C	-2.260000	3.519000	-22.037000
H	-0.510000	27.742000	-1.458000	C	0.812000	5.742000	-12.000000	C	-2.114000	1.025000	-21.814000
O	-2.560000	30.065000	-0.764000	H	-0.231000	3.843000	-12.035000	C	-2.043000	-1.413000	-21.738000
H	-2.344000	28.280000	0.299000	C	-0.602000	7.672000	-11.506000	C	-2.266000	5.999000	-22.088000
H	-4.004000	28.675000	-0.201000	H	-2.707000	7.248000	-11.216000	H	-1.162000	3.557000	-21.993000
C	-2.781000	30.909000	0.346000	C	0.673000	7.127000	-11.870000	O	-0.891000	1.040000	-21.849000
H	-2.465000	31.915000	0.038000	C	2.161000	5.154000	-12.360000	C	-2.807000	-2.680000	-22.180000
H	-2.188000	30.605000	1.226000	C	-0.726000	9.066000	-11.323000	C	-1.082000	-1.868000	-20.484000
H	-3.847000	30.953000	0.633000	C	1.728000	8.002000	-12.150000	H	-1.354000	-1.232000	-22.580000
C	0.039000	9.183000	-4.035000	N	3.146000	6.087000	-12.735000	C	-1.705000	7.057000	-21.947000
C	0.434000	10.321000	-3.932000	O	2.350000	3.950000	-12.465000	H	-2.052000	-3.438000	-22.449000
C	1.063000	11.616000	-3.755000	C	0.353000	9.910000	-11.539000	H	-3.431000	-2.505000	-23.071000
C	2.458000	11.702000	-3.633000	H	-1.684000	9.498000	-10.999000	H	-3.439000	-3.109000	-21.388000
C	0.300000	12.764000	-3.641000	C	1.559000	9.368000	-11.987000	O	0.183000	-1.226000	-20.303000
C	3.115000	12.916000	-3.483000	C	3.052000	7.480000	-12.638000	H	-0.913000	-2.952000	-20.623000
H	3.020000	10.754000	-3.670000	C	4.316000	5.589000	-13.520000	H	-1.621000	-1.760000	-19.530000
C	0.924000	14.019000	-3.474000	C	0.278000	11.339000	-11.312000	C	1.099000	-1.478000	-21.356000
H	-0.799000	12.701000	-3.646000	H	2.382000	10.077000	-12.183000	H	2.086000	-1.148000	-21.001000
C	2.357000	14.095000	-3.449000	O	3.981000	8.234000	-12.887000	H	0.851000	-0.896000	-22.261000
C	4.631000	12.966000	-3.399000	C	3.990000	4.605000	-14.665000	H	1.166000	-2.548000	-21.631000
C	0.156000	15.196000	-3.334000	C	5.549000	5.072000	-12.640000	C	-19.347000	5.714000	-22.502000
C	2.955000	15.354000	-3.390000	H	4.741000	6.458000	-14.053000	C	-18.656000	4.724000	-22.493000
N	5.183000	14.252000	-3.383000	C	0.394000	12.528000	-11.150000	C	-17.866000	3.516000	-22.349000
O	5.336000	11.976000	-3.466000	H	4.894000	4.549000	-15.293000	C	-18.464000	2.302000	-21.985000
C	0.759000	16.443000	-3.266000	H	3.160000	4.957000	-15.299000	C	-16.493000	3.551000	-22.535000
H	-0.939000	15.092000	-3.299000	H	3.760000	3.582000	-14.336000	C	-17.734000	1.128000	-21.859000
C	2.163000	16.495000	-3.318000	O	6.422000	6.176000	-12.447000	H	-19.551000	2.299000	-21.820000
C	4.459000	15.468000	-3.382000	H	6.066000	4.266000	-13.190000	C	-15.710000	2.388000	-22.363000
C	6.679000	14.446000	-3.353000	H	5.210000	4.638000	-11.683000	H	-16.003000	4.499000	-22.807000
C	-0.064000	17.634000	-3.115000	C	7.634000	5.831000	-11.807000	C	-16.357000	1.142000	-22.078000
H	2.647000	17.480000	-3.278000	H	8.178000	6.772000	-11.632000	C	-18.429000	-0.155000	-21.482000
O	5.055000	16.531000	-3.346000	H	8.265000	5.191000	-12.445000	C	-14.302000	2.430000	-22.427000
C	7.629000	13.338000	-3.873000	H	7.478000	5.322000	-10.838000	C	-15.591000	-0.021000	-21.985000
C	7.277000	14.946000	-1.925000	C	-14.324000	2.194000	-12.073000	N	-17.651000	-1.320000	-21.532000
H	6.887000	15.285000	-4.045000	C	-13.247000	1.654000	-12.050000	O	-19.610000	-0.181000	-21.179000
C	-0.807000	18.572000	-2.952000	C	-11.896000	1.143000	-12.105000	C	-13.545000	1.280000	-22.289000
H	8.638000	13.784000	-3.941000	C	-11.603000	-0.221000	-12.233000	H	-13.809000	3.399000	-22.585000
H	7.361000	12.976000	-4.876000	C	-10.849000	2.049000	-12.085000	C	-14.208000	0.058000	-22.098000
H	7.694000	12.478000	-3.189000	C	-10.307000	-0.684000	-12.406000	C	-16.263000	-1.352000	-21.725000
O	8.621000	15.330000	-2.168000	H	-12.446000	-0.925000	-12.233000	C	-18.311000	-2.661000	-21.360000
H	7.224000	14.126000	-1.187000	C	-9.510000	1.621000	-12.195000	C	-12.105000	1.397000	-22.305000
H	6.693000	15.793000	-1.523000	H	-11.060000	3.120000	-11.964000	H	-13.591000	-0.851000	-22.008000
C	9.242000	15.887000	-1.029000	C	-9.247000	0.226000	-12.407000	O	-15.612000	-2.385000	-21.633000
H	10.271000	16.134000	-1.325000	C	-10.054000	-2.147000	-12.694000	C	-19.706000	-2.816000	-21.999000
H	9.276000	15.177000	-0.185000	C	-8.427000	2.527000	-12.112000	C	-18.444000	-3.164000	-19.826000
H	8.743000	16.814000	-0.695000	C	-7.936000	-0.187000	-12.636000	H	-17.689000	-3.393000	-21.899000
C	-7.708000	2.088000	-4.434000	N	-8.739000	-2.472000	-13.073000	C	-10.925000	1.645000	-22.266000
C	-6.549000	2.404000	-4.320000	O	-10.963000	-2.957000	-12.803000	H	-19.938000	-3.893000	-22.034000
C	-5.120000	2.609000	-4.237000	C	-7.122000	2.070000	-12.221000	H	-19.740000	-2.432000	-23.032000
C	-4.268000	1.508000	-4.091000	H	-8.610000	3.600000	-11.948000	H	-20.507000	-2.326000	-21.424000
C	-4.584000	3.882000	-4.270000	C	-6.897000	0.724000	-12.521000	O	-17.268000	-3.408000	-19.052000
C	-2.888000	1.646000	-4.058000	C	-7.639000	-1.614000	-13.015000	H	-19.080000	-4.067000	-19.849000
H	-4.742000	0.514000	-4.023000	C	-8.505000	-3.703000	-13.903000	H	-19.016000	-2.407000	-19.272000
C	-3.188000	4.070000	-4.209000	C	-5.981000	2.950000	-12.067000	C	-16.585000	-4.613000	-19.348000
H	-5.257000	4.749000	-4.310000	H	-5.848000	0.410000	-12.652000	H	-15.873000	-4.771000	-18.525000
C	-2.326000	2.923000	-4.149000	O	-6.491000	-1.968000	-13.255000	H	-16.015000	-4.543000	-20.288000
C	-2.012000	0.416000	-3.961000	C	-9.560000	-3.998000	-14.993000	H	-17.258000	-5.485000	-19.402000
C	-2.631000	5.365000	-4.214000	C	-8.154000	-5.032000	-13.095000	C	-20.735000	15.984000	-21.523000
C	-0.944000	3.114000	-4.190000	H	-7.592000	-3.518000	-14.495000	C	-21.199000	14.900000	-21.288000
N	-0.639000	0.649000	-4.031000	C	-4.929000	3.524000	-11.933000	C	-21.842000	13.618000	-21.327000
O	-2.493000	-0.706000	-3.914000	H	-9.120000	-4.751000	-15.667000	C	-23.239000	13.536000	-21.339000
C	-1.257000	5.544000	-4.223000	H	-9.799000	-3.111000	-15.602000	C	-21.075000	12.476000	-21.463000
H	-3.311000	6.228000	-4.240000	H	-10.500000	-4.416000	-14.603000	C	-23.895000	12.329000	-21.527000

C	-0.431000	4.406000	-4.234000	O	-6.758000	-5.034000	-12.845000	H	-23.803000	14.474000	-21.226000
C	-0.027000	1.914000	-4.167000	H	-8.423000	-5.896000	-13.730000	C	-21.703000	11.236000	-21.687000
C	0.344000	-0.481000	-3.936000	H	-8.752000	-5.118000	-12.173000	H	-19.976000	12.537000	-21.460000
C	-0.715000	6.892000	-4.192000	C	-6.315000	-6.237000	-12.251000	C	-23.136000	11.173000	-21.743000
H	0.656000	4.568000	-4.261000	H	-5.243000	-6.112000	-12.040000	C	-25.407000	12.278000	-21.541000
O	1.186000	2.000000	-4.245000	H	-6.428000	-7.096000	-12.933000	C	-20.939000	10.074000	-21.916000
C	-0.117000	-1.938000	-4.185000	H	-6.842000	-6.462000	-11.305000	C	-23.735000	9.951000	-22.036000
C	1.211000	-0.497000	-2.560000	C	-21.348000	10.061000	-13.103000	N	-25.966000	11.027000	-21.880000
H	1.091000	-0.307000	-4.734000	C	-21.188000	8.902000	-12.814000	O	-26.108000	13.238000	-21.285000
C	-0.336000	8.038000	-4.122000	C	-20.953000	7.499000	-12.593000	C	-21.549000	8.867000	-22.215000
H	0.792000	-2.560000	-4.252000	C	-22.005000	6.581000	-12.668000	H	-19.846000	10.157000	-21.848000
H	-0.669000	-2.064000	-5.126000	C	-19.660000	7.052000	-12.378000	C	-22.950000	8.826000	-22.262000
H	-0.730000	-2.330000	-3.358000	C	-21.773000	5.215000	-12.641000	C	-25.238000	9.839000	-22.074000
O	2.291000	-1.389000	-2.782000	H	-23.016000	6.991000	-12.815000	C	-27.452000	10.824000	-21.888000
H	0.577000	-0.837000	-1.722000	C	-19.382000	5.670000	-12.337000	C	-20.737000	7.686000	-22.432000
H	1.587000	0.511000	-2.301000	H	-18.836000	7.773000	-12.283000	H	-23.433000	7.860000	-22.476000
C	3.131000	-1.499000	-1.652000	C	-20.460000	4.748000	-12.550000	O	-25.770000	8.742000	-22.135000
H	3.938000	-2.193000	-1.927000	C	-22.915000	4.241000	-12.797000	C	-28.346000	12.003000	-22.325000
H	2.598000	-1.909000	-0.776000	C	-18.063000	5.179000	-12.205000	C	-28.039000	10.172000	-20.507000
H	3.581000	-0.530000	-1.375000	C	-20.164000	3.400000	-12.744000	H	-27.651000	10.049000	-22.650000
C	-17.692000	4.763000	-4.730000	N	-22.539000	2.944000	-13.164000	C	-20.042000	6.701000	-22.483000
C	-16.921000	3.846000	-4.600000	O	-24.085000	4.582000	-12.705000	H	-29.363000	11.607000	-22.484000
C	-15.993000	2.750000	-4.505000	C	-17.805000	3.821000	-12.320000	H	-28.007000	12.453000	-23.272000
C	-16.448000	1.439000	-4.319000	H	-17.230000	5.873000	-12.020000	H	-28.421000	12.801000	-21.571000
C	-14.636000	2.998000	-4.591000	C	-18.861000	2.954000	-12.611000	O	-29.260000	9.521000	-20.829000
C	-15.573000	0.360000	-4.293000	C	-21.244000	2.428000	-13.133000	H	-28.193000	10.959000	-19.745000
H	-17.536000	1.292000	-4.223000	C	-23.571000	2.082000	-13.800000	H	-27.323000	9.443000	-20.085000
C	-13.720000	1.929000	-4.546000	C	-16.466000	3.293000	-12.184000	C	-29.885000	8.948000	-19.698000
H	-14.268000	4.032000	-4.677000	H	-18.630000	1.884000	-12.722000	H	-30.778000	8.413000	-20.060000
C	-14.204000	0.582000	-4.456000	O	-20.968000	1.263000	-13.379000	H	-30.213000	9.714000	-18.973000
C	-16.109000	-1.041000	-4.106000	C	-24.456000	2.738000	-14.886000	H	-29.229000	8.226000	-19.179000
C	-12.335000	2.173000	-4.582000	C	-24.448000	1.274000	-12.752000	C	-13.214000	23.081000	-22.619000
C	-13.293000	-0.474000	-4.517000	H	-23.033000	1.296000	-14.358000	C	-14.409000	22.975000	-22.502000
N	-15.183000	-2.077000	-4.254000	C	-15.393000	2.748000	-12.118000	C	-15.830000	22.728000	-22.463000
O	-17.296000	-1.231000	-3.897000	H	-24.983000	1.916000	-15.401000	C	-16.775000	23.766000	-22.425000
C	-11.434000	1.123000	-4.617000	H	-23.876000	3.291000	-15.642000	C	-16.264000	21.416000	-22.496000
H	-11.997000	3.218000	-4.594000	H	-25.215000	3.422000	-14.479000	C	-18.143000	23.508000	-22.471000
C	-11.934000	-0.192000	-4.614000	O	-23.829000	0.008000	-12.588000	H	-16.393000	24.797000	-22.378000
C	-13.793000	-1.902000	-4.446000	H	-25.473000	1.161000	-13.152000	C	-17.638000	21.118000	-22.467000
C	-15.619000	-3.514000	-4.137000	H	-24.540000	1.820000	-11.794000	H	-15.546000	20.582000	-22.505000
C	-10.016000	1.420000	-4.636000	C	-24.457000	-0.773000	-11.589000	C	-18.594000	22.185000	-22.513000
H	-11.204000	-1.011000	-4.662000	H	-23.995000	-1.772000	-11.629000	C	-19.154000	24.630000	-22.495000
O	-13.048000	-2.865000	-4.497000	H	-25.544000	-0.886000	-11.749000	C	-18.084000	19.787000	-22.348000
C	-17.116000	-3.881000	-4.283000	H	-24.304000	-0.351000	-10.581000	C	-19.957000	21.876000	-22.561000
C	-15.102000	-4.304000	-2.803000	C	-18.503000	20.198000	-14.596000	N	-20.489000	24.265000	-22.720000
H	-15.137000	-4.040000	-4.985000	C	-19.328000	19.328000	-14.453000	O	-18.861000	25.804000	-22.383000
C	-8.860000	1.752000	-4.545000	C	-20.394000	18.360000	-14.249000	C	-19.437000	19.509000	-22.316000
H	-17.180000	-4.979000	-4.377000	C	-21.668000	18.784000	-13.840000	H	-17.342000	18.977000	-22.284000
H	-17.578000	-3.449000	-5.183000	C	-20.162000	17.001000	-14.409000	C	-20.359000	20.552000	-22.460000
H	-17.714000	-3.583000	-3.406000	C	-22.718000	17.895000	-13.650000	C	-20.988000	22.968000	-22.688000
O	-15.346000	-5.690000	-3.020000	H	-21.814000	19.865000	-13.695000	C	-21.488000	25.359000	-22.983000
H	-15.668000	-3.933000	-1.935000	C	-21.190000	16.064000	-14.162000	C	-19.882000	18.156000	-22.106000
H	-14.031000	-4.139000	-2.595000	H	-19.147000	16.656000	-14.673000	H	-21.429000	20.287000	-22.453000
C	-15.412000	-6.435000	-1.820000	C	-22.511000	16.532000	-13.853000	O	-22.186000	22.735000	-22.710000
H	-14.472000	-6.384000	-1.243000	C	-24.080000	18.400000	-13.234000	C	-21.130000	26.293000	-24.161000
H	-15.600000	-7.480000	-2.107000	C	-20.929000	14.677000	-14.118000	C	-21.900000	26.208000	-21.683000
H	-16.243000	-6.101000	-1.173000	C	-23.549000	15.614000	-13.685000	H	-22.417000	24.871000	-23.318000
C	-20.928000	14.753000	-3.948000	N	-25.133000	17.469000	-13.263000	C	-20.298000	17.067000	-21.811000
C	-21.242000	13.590000	-3.917000	O	-24.275000	19.586000	-13.029000	H	-22.008000	26.922000	-24.386000
C	-21.595000	12.194000	-4.007000	C	-21.949000	13.782000	-13.840000	H	-20.893000	25.721000	-25.073000
C	-22.931000	11.778000	-3.949000	H	-19.896000	14.330000	-14.258000	H	-20.288000	26.969000	-23.949000
C	-20.605000	11.249000	-4.215000	C	-23.254000	14.258000	-13.667000	O	-22.484000	25.450000	-20.623000
C	-23.298000	10.451000	-4.106000	C	-24.971000	16.087000	-13.463000	H	-22.589000	27.004000	-22.017000
H	-23.700000	12.554000	-3.826000	C	-26.535000	17.948000	-12.976000	H	-21.022000	26.707000	-21.251000
C	-20.933000	9.887000	-4.363000	C	-21.672000	12.378000	-13.678000	C	-23.870000	25.226000	-20.807000
H	-19.553000	11.551000	-4.306000	H	-24.034000	13.506000	-13.459000	H	-24.189000	24.567000	-19.988000
C	-22.310000	9.485000	-4.306000	O	-25.893000	15.277000	-13.406000	H	-24.097000	24.730000	-21.768000
C	-24.762000	10.077000	-4.136000	C	-26.959000	19.338000	-13.498000	H	-24.444000	26.167000	-20.748000
C	-19.936000	8.918000	-4.604000	C	-26.931000	17.918000	-11.401000	C	-3.155000	20.449000	-24.096000

C	-22.634000	8.142000	-4.496000	H	-27.205000	17.252000	-13.508000	C	-3.831000	21.432000	-23.933000
N	-25.038000	8.707000	-4.285000	C	-21.505000	11.218000	-13.400000	C	-4.810000	22.487000	-23.799000
O	-25.631000	10.936000	-4.173000	H	-28.060000	19.383000	-13.433000	C	-4.502000	23.855000	-23.904000
C	-20.280000	7.589000	-4.774000	H	-26.679000	19.507000	-14.548000	C	-6.128000	22.115000	-23.599000
H	-18.883000	9.222000	-4.659000	H	-26.563000	20.167000	-12.889000	C	-5.484000	24.837000	-23.844000
C	-21.627000	7.215000	-4.717000	O	-27.201000	16.641000	-10.832000	H	-3.461000	24.156000	-24.074000
C	-24.067000	7.690000	-4.440000	H	-27.788000	18.598000	-11.251000	C	-7.143000	23.083000	-23.491000
C	-26.437000	8.166000	-4.247000	H	-26.110000	18.364000	-10.822000	H	-6.418000	21.061000	-23.504000
C	-19.263000	6.579000	-4.926000	C	-28.534000	16.226000	-11.086000	C	-6.818000	24.468000	-23.669000
H	-21.859000	6.147000	-4.849000	H	-28.626000	15.186000	-10.740000	C	-5.135000	26.298000	-23.993000
O	-24.365000	6.506000	-4.502000	H	-28.790000	16.250000	-12.160000	C	-8.476000	22.710000	-23.228000
C	-27.552000	9.031000	-4.864000	H	-29.266000	16.847000	-10.539000	C	-7.847000	25.413000	-23.672000
C	-26.905000	7.618000	-2.794000	C	-8.489000	23.271000	-15.633000	N	-6.215000	27.172000	-24.146000
H	-26.449000	7.273000	-4.895000	C	-9.660000	23.500000	-15.454000	O	-3.993000	26.720000	-24.028000
C	-18.470000	5.675000	-4.848000	C	-11.033000	23.923000	-15.240000	C	-9.464000	23.674000	-23.168000
H	-28.454000	8.400000	-4.932000	C	-11.315000	25.260000	-14.927000	H	-8.733000	21.647000	-23.116000
H	-27.303000	9.373000	-5.879000	C	-12.085000	23.020000	-15.326000	C	-9.146000	25.011000	-23.418000
H	-27.814000	9.905000	-4.251000	C	-12.609000	25.724000	-14.742000	C	-7.558000	26.861000	-23.935000
O	-28.008000	6.752000	-3.015000	H	-10.455000	25.945000	-14.854000	C	-5.991000	28.621000	-24.442000
H	-27.181000	8.469000	-2.144000	C	-13.412000	23.440000	-15.088000	C	-10.835000	23.315000	-22.920000
H	-26.079000	7.070000	-2.301000	H	-11.888000	21.959000	-15.554000	H	-9.964000	25.748000	-23.397000
C	-28.598000	6.273000	-1.826000	C	-13.676000	24.827000	-14.834000	O	-8.418000	27.727000	-23.899000
H	-27.898000	5.652000	-1.240000	C	-12.857000	27.192000	-14.463000	C	-4.843000	29.020000	-25.398000
H	-29.453000	5.650000	-2.131000	C	-14.479000	22.516000	-15.069000	C	-5.983000	29.536000	-23.114000
H	-28.979000	7.090000	-1.185000	C	-14.998000	25.241000	-14.668000	H	-6.880000	28.966000	-25.002000
C	-13.984000	22.680000	-4.690000	N	-14.206000	27.573000	-14.344000	C	-12.022000	23.184000	-22.760000
C	-15.116000	22.311000	-4.498000	O	-11.953000	28.008000	-14.429000	H	-5.003000	30.077000	-25.667000
C	-16.508000	21.917000	-4.429000	C	-15.788000	22.930000	-14.868000	H	-4.854000	28.436000	-26.332000
C	-17.513000	22.874000	-4.632000	H	-14.258000	21.448000	-15.204000	H	-3.844000	28.947000	-24.946000
C	-16.852000	20.589000	-4.238000	C	-16.022000	24.302000	-14.688000	O	-6.440000	30.824000	-23.491000
C	-18.854000	22.533000	-4.662000	C	-15.312000	26.704000	-14.448000	H	-4.971000	29.561000	-22.671000
H	-17.206000	23.918000	-4.794000	C	-14.568000	29.017000	-14.100000	H	-6.661000	29.117000	-22.350000
C	-18.203000	20.194000	-4.279000	C	-16.856000	21.948000	-14.826000	C	-6.243000	31.777000	-22.466000
H	-16.070000	19.833000	-4.082000	H	-17.060000	24.628000	-14.534000	H	-6.637000	32.733000	-22.840000
C	-19.209000	21.188000	-4.525000	O	-16.466000	27.102000	-14.351000	H	-5.174000	31.917000	-22.230000
C	-19.911000	23.594000	-4.911000	C	-13.533000	30.143000	-14.389000	H	-6.777000	31.511000	-21.537000
C	-18.579000	18.840000	-4.136000	C	-15.227000	29.314000	-12.630000	C	-0.587000	10.323000	-25.212000
C	-20.525000	20.774000	-4.694000	H	-15.377000	29.232000	-14.819000	C	-0.026000	11.383000	-25.098000
N	-21.224000	23.126000	-5.015000	C	-17.684000	21.075000	-14.721000	C	0.418000	12.751000	-24.984000
O	-19.619000	24.764000	-5.111000	H	-14.075000	31.102000	-14.322000	C	1.764000	13.145000	-25.034000
C	-19.906000	18.458000	-4.250000	H	-13.118000	30.076000	-15.406000	C	-0.558000	13.722000	-24.851000
H	-17.811000	18.080000	-3.930000	H	-12.714000	30.173000	-13.652000	C	2.136000	14.487000	-25.019000
C	-20.855000	19.435000	-4.566000	O	-16.655000	29.405000	-12.633000	H	2.527000	12.358000	-25.117000
C	-21.597000	21.773000	-5.019000	H	-14.779000	30.231000	-12.210000	C	-0.217000	15.089000	-24.793000
C	-22.415000	24.020000	-5.092000	H	-14.973000	28.513000	-11.918000	H	-1.621000	13.451000	-24.783000
C	-20.289000	17.074000	-4.087000	C	-17.120000	30.659000	-13.105000	C	1.154000	15.476000	-24.935000
H	-21.898000	19.114000	-4.698000	H	-18.217000	30.605000	-13.114000	C	3.586000	14.898000	-25.118000
O	-22.746000	21.413000	-5.227000	H	-16.779000	30.888000	-14.132000	C	-1.201000	16.085000	-24.613000
C	-22.230000	25.517000	-5.418000	H	-16.816000	31.491000	-12.445000	C	1.475000	16.836000	-24.988000
C	-23.462000	23.901000	-3.851000	C	-0.867000	16.339000	-17.125000	N	3.820000	16.264000	-25.334000
H	-23.005000	23.647000	-5.953000	C	-1.191000	17.481000	-16.897000	O	4.507000	14.103000	-25.045000
C	-20.610000	15.914000	-4.007000	C	-1.489000	18.877000	-16.606000	C	-0.848000	17.424000	-24.629000
H	-23.239000	25.946000	-5.526000	C	-0.464000	19.799000	-16.318000	H	-2.251000	15.781000	-24.494000
H	-21.687000	25.682000	-6.361000	C	-2.805000	19.307000	-16.587000	C	0.481000	17.785000	-24.847000
H	-21.716000	26.064000	-4.613000	C	-0.723000	21.150000	-16.095000	C	2.886000	17.291000	-25.195000
O	-24.739000	23.900000	-4.473000	H	0.565000	19.399000	-16.303000	C	5.167000	16.685000	-25.826000
H	-23.346000	24.756000	-3.158000	C	-3.111000	20.652000	-16.307000	C	-1.822000	18.472000	-24.446000
H	-23.328000	22.984000	-3.248000	H	-3.621000	18.587000	-16.768000	H	0.729000	18.858000	-24.876000
C	-25.826000	23.942000	-3.572000	C	-2.047000	21.598000	-16.124000	O	3.217000	18.466000	-25.200000
H	-26.734000	24.039000	-4.187000	C	0.403000	22.149000	-15.842000	C	5.724000	15.841000	-26.996000
H	-25.782000	24.815000	-2.895000	C	-4.449000	21.083000	-16.208000	C	6.285000	16.963000	-24.693000
H	-25.903000	23.019000	-2.969000	C	-2.366000	22.947000	-15.967000	H	5.034000	17.670000	-26.305000
C	-3.763000	20.857000	-5.953000	N	0.035000	23.496000	-15.766000	C	-2.497000	19.455000	-24.270000
C	-4.633000	21.664000	-5.737000	O	1.569000	21.789000	-15.800000	H	6.611000	16.364000	-27.386000
C	-5.657000	22.681000	-5.631000	C	-4.751000	22.422000	-16.028000	H	4.997000	15.756000	-27.818000
C	-5.346000	24.028000	-5.883000	H	-5.255000	20.341000	-16.292000	H	6.042000	14.829000	-26.708000
C	-6.957000	22.318000	-5.326000	C	-3.696000	23.339000	-15.919000	O	6.556000	18.358000	-24.726000
C	-6.316000	25.020000	-5.863000	C	-1.276000	23.980000	-15.838000	H	7.202000	16.389000	-24.914000
H	-4.300000	24.278000	-6.122000	C	1.068000	24.575000	-15.590000	H	5.956000	16.636000	-23.688000

C	-7.977000	23.287000	-5.335000	C	-6.139000	22.827000	-15.946000	C	7.555000	18.751000	-23.808000
H	-7.229000	21.270000	-5.124000	H	-3.951000	24.398000	-15.759000	H	7.717000	19.829000	-23.960000
C	-7.647000	24.648000	-5.650000	O	-1.518000	25.177000	-15.758000	H	8.513000	18.233000	-23.982000
C	-5.946000	26.471000	-6.145000	C	2.551000	24.287000	-15.943000	H	7.246000	18.580000	-22.761000
C	-9.324000	22.912000	-5.140000	C	1.020000	25.327000	-14.124000	C	-7.854000	2.485000	-25.653000
C	-8.686000	25.554000	-5.834000	H	0.786000	25.359000	-16.316000	C	-6.684000	2.761000	-25.559000
N	-7.026000	27.358000	-6.260000	C	-7.315000	23.055000	-15.800000	C	-5.303000	3.184000	-25.577000
O	-4.793000	26.811000	-6.354000	H	3.086000	25.251000	-15.911000	C	-4.237000	2.275000	-25.680000
C	-10.348000	23.830000	-5.306000	H	2.669000	23.877000	-16.957000	C	-5.030000	4.539000	-25.508000
H	-9.550000	21.869000	-4.873000	H	3.037000	23.617000	-15.216000	C	-2.914000	2.703000	-25.746000
C	-10.006000	25.142000	-5.672000	O	0.494000	26.659000	-14.171000	H	-4.469000	1.201000	-25.732000
C	-8.376000	26.976000	-6.237000	H	2.022000	25.315000	-13.662000	C	-3.703000	5.011000	-25.556000
C	-6.881000	28.837000	-6.444000	H	0.367000	24.782000	-13.421000	H	-5.849000	5.264000	-25.397000
C	-11.728000	23.422000	-5.112000	C	1.412000	27.598000	-14.702000	C	-2.635000	4.069000	-25.727000
H	-10.826000	25.859000	-5.823000	H	0.918000	28.578000	-14.642000	C	-1.772000	1.712000	-25.841000
O	-9.287000	27.754000	-6.480000	H	1.661000	27.404000	-15.762000	C	-3.400000	6.386000	-25.434000
C	-5.505000	29.439000	-6.800000	H	2.351000	27.639000	-14.122000	C	-1.329000	4.539000	-25.861000
C	-7.510000	29.782000	-5.266000	C	-2.622000	6.146000	-16.198000	N	-0.511000	2.248000	-26.119000
H	-7.507000	29.091000	-7.323000	C	-1.822000	7.031000	-16.352000	O	-1.941000	0.516000	-25.684000
C	-12.857000	23.052000	-4.902000	C	-0.837000	8.036000	-16.665000	C	-2.088000	6.819000	-25.544000
H	-5.669000	30.518000	-6.971000	C	0.530000	7.751000	-16.560000	H	-4.221000	7.106000	-25.301000
H	-5.069000	29.014000	-7.717000	C	-1.227000	9.304000	-17.069000	C	-1.074000	5.893000	-25.783000
H	-4.776000	29.337000	-5.981000	C	1.508000	8.703000	-16.799000	C	-0.183000	3.599000	-26.070000
O	-8.094000	30.881000	-5.957000	H	0.822000	6.737000	-16.260000	C	0.658000	1.382000	-26.469000
H	-6.708000	30.108000	-4.577000	C	-0.262000	10.309000	-17.298000	C	-1.712000	8.205000	-25.443000
H	-8.276000	29.277000	-4.650000	H	-2.290000	9.581000	-17.152000	H	-0.046000	6.273000	-25.891000
C	-8.370000	32.006000	-5.146000	C	1.129000	10.005000	-17.121000	O	0.976000	3.989000	-26.120000
H	-8.753000	32.786000	-5.819000	C	2.971000	8.330000	-16.678000	C	0.395000	0.157000	-27.374000
H	-7.465000	32.401000	-4.649000	C	-0.659000	11.644000	-17.512000	C	1.597000	1.003000	-25.206000
H	-9.133000	31.796000	-4.376000	C	2.062000	11.040000	-17.113000	H	1.321000	1.995000	-27.105000
C	0.295000	11.297000	-7.597000	N	3.883000	9.374000	-16.770000	C	-1.165000	9.272000	-25.329000
C	0.545000	12.467000	-7.442000	O	3.319000	7.162000	-16.602000	H	1.375000	-0.220000	-27.714000
C	0.806000	13.878000	-7.271000	C	0.270000	12.669000	-17.462000	H	-0.184000	0.422000	-28.273000
C	2.105000	14.399000	-7.348000	H	-1.734000	11.865000	-17.605000	H	-0.114000	-0.672000	-26.866000
C	-0.247000	14.736000	-6.998000	C	1.624000	12.353000	-17.248000	O	2.904000	0.771000	-25.715000
C	2.364000	15.760000	-7.243000	C	3.521000	10.727000	-16.854000	H	1.191000	0.123000	-24.675000
H	2.923000	13.682000	-7.527000	C	5.375000	9.113000	-16.769000	H	1.627000	1.836000	-24.480000
C	-0.021000	16.119000	-6.837000	C	-0.176000	14.051000	-17.490000	C	3.760000	0.175000	-24.761000
H	-1.274000	14.354000	-6.904000	H	2.338000	13.185000	-17.152000	H	3.903000	0.811000	-23.870000
C	1.302000	16.640000	-7.032000	O	4.351000	11.603000	-16.686000	H	4.731000	0.027000	-25.257000
C	3.777000	16.289000	-7.418000	C	5.884000	7.671000	-17.042000	H	3.391000	-0.812000	-24.432000
C	-1.086000	17.004000	-6.569000	C	6.218000	9.668000	-15.450000	C	-18.239000	4.176000	-25.866000
C	1.486000	18.022000	-7.072000	H	5.780000	9.711000	-17.608000	C	-17.412000	3.298000	-25.806000
N	3.900000	17.681000	-7.520000	C	-0.527000	15.197000	-17.329000	C	-16.336000	2.333000	-25.754000
O	4.723000	15.528000	-7.543000	H	6.971000	7.734000	-17.215000	C	-16.556000	0.948000	-25.701000
C	-0.889000	18.374000	-6.624000	H	5.438000	7.212000	-17.936000	C	-15.034000	2.800000	-25.775000
H	-2.090000	16.603000	-6.366000	H	5.724000	7.005000	-16.178000	C	-15.508000	0.034000	-25.723000
C	0.396000	18.865000	-6.892000	O	7.610000	9.564000	-15.754000	H	-17.594000	0.590000	-25.663000
C	2.853000	18.598000	-7.357000	H	5.981000	9.049000	-14.568000	C	-13.945000	1.903000	-25.787000
C	5.149000	18.341000	-8.015000	H	5.952000	10.709000	-15.207000	H	-14.827000	3.879000	-25.782000
C	-1.999000	19.277000	-6.416000	C	8.444000	10.401000	-14.978000	C	-14.195000	0.492000	-25.816000
H	0.521000	19.956000	-6.956000	H	8.339000	11.464000	-15.263000	C	-15.780000	-1.449000	-25.649000
O	3.025000	19.801000	-7.478000	H	9.477000	10.086000	-15.186000	C	-12.613000	2.367000	-25.775000
C	6.221000	17.492000	-8.733000	H	8.254000	10.293000	-13.897000	C	-13.120000	-0.394000	-25.922000
C	5.913000	19.300000	-6.950000	C	-12.104000	1.911000	-17.296000	N	-14.693000	-2.290000	-25.925000
H	4.825000	19.049000	-8.803000	C	-10.963000	1.644000	-17.024000	O	-16.886000	-1.881000	-25.371000
C	-2.886000	20.062000	-6.186000	C	-9.560000	1.403000	-16.801000	C	-11.560000	1.471000	-25.863000
H	6.944000	18.189000	-9.190000	C	-9.001000	0.127000	-16.944000	H	-12.437000	3.453000	-25.753000
H	5.807000	16.865000	-9.536000	C	-8.736000	2.469000	-16.478000	C	-11.829000	0.101000	-25.964000
H	6.778000	16.841000	-8.043000	C	-7.629000	-0.078000	-16.855000	C	-13.349000	-1.881000	-25.960000
O	6.546000	20.278000	-7.761000	H	-9.697000	-0.700000	-17.172000	C	-14.878000	-3.772000	-26.030000
H	6.645000	18.718000	-6.357000	C	-7.337000	2.300000	-16.384000	C	-10.193000	1.933000	-25.857000
H	5.225000	19.783000	-6.231000	H	-9.156000	3.472000	-16.307000	H	-10.978000	-0.592000	-26.060000
C	7.376000	21.162000	-7.035000	C	-6.777000	1.007000	-16.646000	O	-12.433000	-2.687000	-25.928000
H	7.861000	21.816000	-7.775000	C	-7.042000	-1.450000	-17.065000	C	-16.227000	-4.302000	-26.562000
H	8.171000	20.636000	-6.474000	C	-6.471000	3.394000	-16.160000	C	-14.481000	-4.569000	-24.673000
H	6.802000	21.793000	-6.333000	C	-5.391000	0.871000	-16.772000	H	-14.140000	-4.117000	-26.777000
C	-5.800000	2.783000	-8.462000	N	-5.690000	-1.480000	-17.398000	C	-9.024000	2.216000	-25.759000
C	-4.667000	3.107000	-8.210000	O	-7.739000	-2.451000	-17.092000	H	-16.099000	-5.373000	-26.788000

C	-3.327000	3.646000	-8.118000	C	-5.096000	3.221000	-16.217000	H	-16.540000	-3.797000	-27.489000
C	-2.193000	2.824000	-8.015000	H	-6.903000	4.391000	-15.979000	H	-17.044000	-4.222000	-25.828000
C	-3.146000	5.019000	-8.180000	C	-4.575000	1.963000	-16.532000	O	-14.064000	-5.872000	-25.052000
C	-0.898000	3.331000	-8.014000	C	-4.790000	-0.433000	-17.229000	H	-15.343000	-4.592000	-23.980000
H	-2.369000	1.740000	-7.941000	C	-5.210000	-2.632000	-18.226000	H	-13.658000	-4.060000	-24.142000
C	-1.855000	5.582000	-8.100000	C	-4.200000	4.335000	-16.050000	C	-13.840000	-6.698000	-23.928000
H	-4.016000	5.685000	-8.269000	H	-3.477000	1.877000	-16.601000	H	-13.492000	-7.671000	-24.309000
C	-0.712000	4.713000	-8.055000	O	-3.592000	-0.577000	-17.419000	H	-14.763000	-6.861000	-23.343000
C	0.304000	2.392000	-8.002000	C	-6.194000	-3.191000	-19.281000	H	-13.070000	-6.283000	-23.254000
C	-1.668000	6.982000	-8.053000	C	-4.542000	-3.830000	-17.414000	H	-22.242000	14.984000	-24.865000
C	0.564000	5.273000	-8.038000	H	-4.373000	-2.246000	-18.836000	C	-22.415000	13.938000	-24.911000
N	1.566000	3.000000	-8.055000	C	-3.415000	5.246000	-16.095000	C	-22.595000	12.752000	-25.012000
O	0.147000	1.183000	-8.049000	H	-5.600000	-3.801000	-19.982000	C	-22.803000	11.344000	-25.249000
C	-0.393000	7.519000	-7.978000	H	-6.679000	-2.398000	-19.870000	C	-24.094000	10.812000	-25.285000
H	-2.543000	7.649000	-8.074000	H	-6.978000	-3.839000	-18.863000	C	-21.710000	10.521000	-25.460000
C	0.707000	6.651000	-7.983000	O	-3.176000	-3.501000	-17.238000	C	-24.315000	9.470000	-25.528000
C	1.786000	4.390000	-8.043000	H	-4.635000	-4.749000	-18.021000	H	-24.934000	11.498000	-25.106000
C	2.847000	2.205000	-8.174000	H	-5.073000	-4.018000	-16.463000	C	-21.889000	9.137000	-25.669000
C	-0.193000	8.953000	-7.890000	C	-2.432000	-4.488000	-16.553000	H	-20.699000	10.950000	-25.435000
H	1.713000	7.089000	-7.932000	H	-1.413000	-4.087000	-16.440000	C	-23.225000	8.612000	-25.701000
O	2.917000	4.842000	-8.003000	H	-2.367000	-5.430000	-17.129000	C	-25.721000	8.947000	-25.586000
C	2.776000	0.688000	-8.467000	H	-2.836000	-4.700000	-15.544000	C	-20.789000	8.255000	-25.777000
C	3.961000	2.348000	-6.947000	C	-20.635000	8.034000	-16.878000	C	-23.405000	7.237000	-25.839000
H	3.374000	2.620000	-9.057000	C	-20.185000	6.913000	-16.911000	N	-25.840000	7.575000	-25.825000
C	0.046000	10.127000	-7.749000	C	-19.632000	5.579000	-17.024000	O	-26.718000	9.632000	-25.448000
H	3.808000	0.346000	-8.657000	C	-20.442000	4.440000	-16.901000	C	-20.990000	6.883000	-25.882000
H	2.186000	0.442000	-9.361000	C	-18.282000	5.403000	-17.284000	H	-19.779000	8.688000	-25.750000
H	2.389000	0.112000	-7.614000	C	-19.942000	3.153000	-17.064000	C	-22.304000	6.403000	-25.919000
O	5.222000	1.973000	-7.497000	H	-21.512000	4.594000	-16.695000	C	-24.790000	6.658000	-25.864000
H	3.669000	1.672000	-6.124000	C	-17.734000	4.110000	-17.433000	C	-27.226000	7.002000	-25.926000
H	4.023000	3.366000	-6.525000	H	-17.611000	6.271000	-17.357000	C	-19.889000	5.938000	-25.944000
C	6.273000	1.899000	-6.556000	C	-18.587000	2.962000	-17.328000	H	-22.446000	5.314000	-25.992000
H	7.161000	1.562000	-7.112000	C	-20.869000	1.962000	-16.997000	O	-25.003000	5.456000	-25.888000
H	6.073000	1.163000	-5.755000	C	-16.351000	3.922000	-17.634000	C	-28.102000	7.597000	-27.046000
H	6.499000	2.882000	-6.106000	C	-18.044000	1.678000	-17.444000	C	-27.978000	6.936000	-24.513000
C	-16.292000	3.302000	-8.357000	N	-20.305000	0.736000	-17.306000	H	-27.122000	5.951000	-26.241000
C	-15.377000	2.528000	-8.241000	O	-22.069000	2.106000	-16.822000	C	-19.058000	5.062000	-25.915000
C	-14.180000	1.722000	-8.315000	C	-15.824000	2.643000	-17.694000	H	-28.982000	6.945000	-27.189000
C	-14.217000	0.320000	-8.275000	H	-15.694000	4.803000	-17.681000	H	-27.559000	7.630000	-28.004000
C	-12.959000	2.354000	-8.484000	C	-16.674000	1.534000	-17.607000	H	-28.472000	8.609000	-26.828000
C	-13.077000	-0.452000	-8.453000	C	-18.943000	0.466000	-17.363000	O	-27.312000	6.191000	-23.488000
H	-15.197000	-0.162000	-8.141000	C	-21.195000	-0.407000	-17.675000	H	-28.992000	6.539000	-24.696000
C	-11.773000	1.608000	-8.632000	C	-14.403000	2.445000	-17.762000	H	-28.103000	7.947000	-24.099000
H	-12.903000	3.450000	-8.533000	H	-16.202000	0.538000	-17.648000	C	-27.452000	4.785000	-23.588000
C	-11.841000	0.175000	-8.634000	O	-18.514000	-0.678000	-17.366000	H	-27.056000	4.367000	-22.652000
C	-13.181000	-1.958000	-8.551000	C	-22.208000	-0.105000	-18.799000	H	-26.864000	4.365000	-24.421000
C	-10.526000	2.245000	-8.806000	C	-21.867000	-1.029000	-16.403000	H	-28.504000	4.469000	-23.694000

Table S1. Cartesian coordinates of optimized helical **poly-NaphDE**

Cartesian coordinates of optimized helical **poly-PyrDE** are shown as follows;

C	-1.989000	9.314000	2.749000	C	-2.818000	23.203000	-3.460000	C	14.899000	27.119000	-8.959000
C	-1.382000	8.272000	2.638000	H	-0.683000	23.049000	-3.578000	H	12.941000	28.095000	-8.708000
C	-0.798000	6.959000	2.361000	C	-4.157000	18.318000	-4.008000	H	16.640000	25.837000	-9.288000
C	0.500000	6.655000	2.730000	C	-1.801000	15.694000	-4.674000	C	15.730000	28.235000	-8.424000
C	-1.571000	5.981000	1.662000	C	-5.302000	20.444000	-3.919000	O	16.799000	28.134000	-7.848000
C	1.046000	5.403000	2.497000	C	-4.057000	22.506000	-3.525000	N	15.177000	29.469000	-8.677000
H	1.111000	7.412000	3.238000	H	-2.817000	24.291000	-3.282000	H	14.320000	29.570000	-9.190000
C	-1.020000	4.702000	1.407000	C	-5.325000	19.025000	-4.030000	C	15.936000	30.651000	-8.274000
C	-2.905000	6.252000	1.248000	H	-4.196000	17.216000	-4.088000	H	16.213000	30.585000	-7.210000
C	0.297000	4.405000	1.810000	C	-6.506000	21.176000	-3.802000	H	16.855000	30.774000	-8.870000
C	2.381000	5.106000	2.975000	C	-5.284000	23.177000	-3.320000	H	15.314000	31.549000	-8.411000
C	-1.785000	3.717000	0.812000	H	-6.288000	18.502000	-4.079000	C	12.313000	11.719000	-14.501000
C	-3.689000	5.256000	0.739000	C	-6.498000	22.525000	-3.471000	C	13.177000	12.536000	-14.310000
H	-3.349000	7.253000	1.387000	H	-7.428000	20.574000	-3.874000	C	14.126000	13.510000	-13.831000
C	0.838000	3.114000	1.545000	H	-5.248000	24.252000	-3.071000	C	13.630000	14.770000	-13.557000

C	3.466000	4.806000	3.407000	C	-7.756000	23.300000	-3.242000	C	15.491000	13.187000	-13.588000
C	-1.235000	2.440000	0.530000	O	-7.895000	24.300000	-2.560000	C	14.431000	15.756000	-13.023000
C	-3.151000	3.955000	0.538000	N	-8.819000	22.771000	-3.925000	H	12.569000	14.988000	-13.747000
H	-4.739000	5.468000	0.491000	H	-8.720000	21.943000	-4.477000	C	16.300000	14.170000	-12.978000
C	0.100000	2.148000	0.921000	C	-10.124000	23.401000	-3.761000	C	16.038000	11.903000	-13.892000
H	1.869000	2.884000	1.855000	H	-10.440000	23.387000	-2.705000	C	15.771000	15.445000	-12.654000
H	4.420000	4.566000	3.809000	H	-10.105000	24.446000	-4.111000	C	13.905000	17.085000	-12.788000
C	-2.048000	1.445000	-0.061000	H	-10.872000	22.852000	-4.354000	C	17.614000	13.874000	-12.685000
C	-3.949000	2.894000	0.056000	C	9.995000	20.664000	-3.953000	C	17.311000	11.574000	-13.509000
H	0.524000	1.143000	0.745000	C	9.162000	21.520000	-3.812000	H	15.407000	11.159000	-14.402000
C	-3.405000	1.661000	-0.262000	C	8.045000	22.363000	-3.502000	C	16.580000	16.393000	-11.964000
H	-1.569000	0.474000	-0.271000	C	6.799000	21.785000	-3.639000	C	13.619000	18.242000	-12.600000
H	-5.015000	3.111000	-0.100000	C	8.208000	23.691000	-3.027000	C	18.455000	14.882000	-12.163000
C	-4.301000	0.608000	-0.820000	C	5.661000	22.475000	-3.301000	C	18.132000	12.575000	-12.918000
O	-5.507000	0.510000	-0.709000	H	6.697000	20.753000	-4.004000	H	17.724000	10.567000	-13.709000
N	-3.605000	-0.273000	-1.623000	C	7.037000	24.409000	-2.690000	C	17.901000	16.129000	-11.761000
H	-2.646000	-0.059000	-1.852000	C	9.495000	24.304000	-2.901000	H	16.171000	17.367000	-11.633000
C	-4.359000	-1.228000	-2.428000	C	5.760000	23.808000	-2.802000	C	19.835000	14.627000	-12.018000
H	-4.704000	-2.071000	-1.807000	C	4.356000	21.876000	-3.436000	C	19.497000	12.334000	-12.656000
H	-5.234000	-0.755000	-2.902000	C	7.142000	25.716000	-2.270000	H	18.543000	16.891000	-11.299000
H	-3.709000	-1.622000	-3.226000	C	9.595000	25.585000	-2.441000	C	20.344000	13.360000	-12.264000
C	-2.373000	17.068000	3.366000	H	10.412000	23.753000	-3.179000	H	20.437000	15.469000	-11.645000
C	-3.185000	16.186000	3.228000	C	4.595000	24.558000	-2.462000	H	19.904000	11.323000	-12.837000
C	-4.016000	15.020000	2.990000	C	3.203000	21.542000	-3.563000	C	21.786000	13.046000	-12.106000
C	-3.373000	13.802000	3.062000	C	5.978000	26.499000	-2.072000	O	22.275000	11.953000	-11.880000
C	-5.409000	15.084000	2.715000	C	8.418000	26.292000	-2.070000	N	22.573000	14.153000	-12.271000
C	-4.029000	12.608000	2.843000	H	10.577000	26.081000	-2.359000	H	22.162000	15.062000	-12.368000
H	-2.299000	13.789000	3.302000	C	4.698000	25.885000	-2.158000	C	24.017000	14.000000	-12.111000
C	-6.100000	13.876000	2.458000	H	3.590000	24.103000	-2.522000	H	24.268000	13.584000	-11.123000
C	-6.117000	16.319000	2.735000	C	6.110000	27.867000	-1.737000	H	24.431000	13.338000	-12.889000
C	-5.421000	12.630000	2.512000	C	8.488000	27.609000	-1.581000	H	24.501000	14.984000	-12.205000
C	-3.270000	11.364000	2.887000	H	3.798000	26.478000	-1.947000	C	4.832000	9.665000	-16.201000
C	-7.454000	13.914000	2.192000	C	7.360000	28.397000	-1.467000	C	5.964000	9.261000	-16.111000
C	-7.469000	16.349000	2.533000	H	5.175000	28.442000	-1.632000	C	7.303000	8.746000	-15.965000
H	-5.583000	17.260000	2.953000	H	9.477000	28.048000	-1.388000	C	8.292000	9.574000	-15.474000
C	-6.140000	11.434000	2.225000	C	7.559000	29.816000	-1.081000	C	7.619000	7.422000	-16.371000
C	-2.624000	10.341000	2.831000	O	8.156000	30.233000	-0.104000	C	9.595000	9.142000	-15.328000
C	-8.158000	12.724000	1.889000	N	7.093000	30.633000	-2.080000	H	8.026000	10.609000	-15.211000
C	-8.168000	15.132000	2.306000	H	6.696000	30.237000	-2.925000	C	8.955000	6.976000	-16.252000
H	-8.021000	17.302000	2.585000	C	7.322000	32.074000	-1.976000	C	6.632000	6.564000	-16.932000
C	-7.466000	11.479000	1.895000	H	7.001000	32.443000	-0.989000	C	9.949000	7.813000	-15.696000
H	-5.627000	10.455000	2.246000	H	8.383000	32.337000	-2.123000	C	10.570000	10.095000	-14.857000
C	-9.563000	12.774000	1.719000	H	6.723000	32.588000	-2.746000	C	9.292000	5.717000	-16.699000
C	-9.579000	15.111000	2.240000	C	13.143000	13.454000	-5.335000	C	6.969000	5.324000	-17.380000
H	-8.021000	10.547000	1.703000	C	13.504000	14.589000	-5.140000	H	5.575000	6.871000	-16.984000
C	-10.271000	13.948000	1.956000	C	13.774000	15.953000	-4.743000	C	11.279000	7.328000	-15.557000
H	-10.060000	11.813000	1.502000	C	12.671000	16.775000	-4.642000	C	11.440000	10.906000	-14.667000
H	-10.120000	16.058000	2.391000	C	15.088000	16.461000	-4.509000	C	10.632000	5.273000	-16.641000
C	-11.761000	14.015000	1.909000	C	12.805000	18.078000	-4.231000	C	8.294000	4.851000	-17.200000
O	-12.505000	14.782000	2.490000	H	11.666000	16.402000	-4.876000	H	6.214000	4.662000	-17.826000
N	-12.267000	13.115000	1.003000	C	15.218000	17.800000	-4.070000	C	11.622000	6.096000	-16.038000
H	-11.668000	12.532000	0.444000	C	16.261000	15.687000	-4.750000	H	12.050000	7.960000	-15.094000
C	-13.691000	13.173000	0.688000	C	14.069000	18.579000	-3.817000	C	10.946000	3.978000	-17.105000
H	-14.294000	12.714000	1.487000	C	11.656000	18.934000	-4.145000	C	8.625000	3.515000	-17.503000
H	-14.025000	14.212000	0.543000	C	16.466000	18.332000	-3.831000	H	12.648000	5.717000	-15.930000
H	-13.873000	12.627000	-0.252000	C	17.503000	16.248000	-4.629000	C	9.941000	3.094000	-17.474000
C	4.925000	20.403000	3.825000	H	16.170000	14.625000	-5.026000	H	12.005000	3.681000	-17.065000
C	3.750000	20.686000	3.795000	C	14.190000	19.824000	-3.127000	H	7.790000	2.861000	-17.814000
C	2.325000	20.955000	3.875000	C	10.816000	19.791000	-4.060000	C	10.244000	1.697000	-17.864000
C	1.480000	19.886000	3.641000	C	16.591000	19.617000	-3.246000	O	9.651000	0.689000	-17.515000
C	1.790000	22.222000	4.246000	C	17.623000	17.551000	-4.065000	N	11.256000	1.688000	-18.787000
C	0.115000	19.980000	3.818000	H	18.407000	15.655000	-4.858000	H	11.630000	2.572000	-19.101000
H	1.909000	18.921000	3.334000	C	15.425000	20.343000	-2.865000	C	11.522000	0.447000	-19.509000
C	0.387000	22.360000	4.354000	H	13.288000	20.392000	-2.826000	H	11.759000	-0.362000	-18.800000
C	2.622000	23.347000	4.497000	C	17.878000	20.114000	-2.938000	H	10.664000	0.134000	-20.127000
C	-0.453000	21.230000	4.208000	C	18.868000	18.043000	-3.615000	H	12.390000	0.598000	-20.170000
C	-0.734000	18.819000	3.638000	H	15.517000	21.304000	-2.331000	C	-1.125000	14.789000	-16.623000
C	-0.165000	23.598000	4.619000	C	19.001000	19.311000	-3.078000	C	-1.049000	13.594000	-16.756000
C	2.078000	24.570000	4.771000	H	17.903000	21.122000	-2.489000	C	-0.687000	12.198000	-16.744000

H	3.719000	23.253000	4.432000	H	19.743000	17.384000	-3.711000	C	0.658000	11.930000	-16.615000
C	-1.851000	21.372000	4.428000	C	20.359000	19.759000	-2.662000	C	-1.637000	11.140000	-16.825000
C	-1.547000	17.937000	3.500000	O	21.278000	19.063000	-2.259000	C	1.130000	10.639000	-16.555000
C	-1.568000	23.754000	4.695000	N	20.507000	21.110000	-2.814000	H	1.379000	12.755000	-16.530000
C	0.668000	24.722000	4.836000	H	19.753000	21.699000	-3.113000	C	-1.155000	9.808000	-16.838000
H	2.729000	25.441000	4.926000	C	21.751000	21.714000	-2.345000	C	-3.039000	11.391000	-16.894000
C	-2.401000	22.604000	4.638000	H	21.901000	21.542000	-1.266000	C	0.225000	9.541000	-16.661000
H	-2.521000	20.500000	4.354000	H	22.614000	21.304000	-2.894000	C	2.541000	10.390000	-16.386000
C	-2.118000	25.045000	4.877000	H	21.715000	22.800000	-2.520000	C	-2.038000	8.763000	-17.014000
C	0.078000	25.978000	5.102000	C	8.421000	7.365000	-7.841000	C	-3.918000	10.355000	-17.029000
H	-3.492000	22.711000	4.750000	C	9.545000	7.612000	-7.489000	H	-3.421000	12.424000	-16.833000
C	-1.297000	26.143000	5.106000	C	10.851000	8.084000	-7.094000	C	0.681000	8.189000	-16.624000
H	-3.218000	25.107000	4.898000	C	10.998000	9.352000	-6.562000	C	3.692000	10.046000	-16.290000
H	0.742000	26.841000	5.270000	C	11.999000	7.299000	-7.422000	C	-1.566000	7.428000	-17.092000
C	-1.840000	27.505000	5.366000	C	12.252000	9.844000	-6.260000	C	-3.428000	9.021000	-17.082000
O	-1.309000	28.424000	5.961000	H	10.108000	9.966000	-6.376000	H	-5.003000	10.537000	-17.113000
N	-3.060000	27.691000	4.759000	C	13.272000	7.754000	-7.026000	C	-0.182000	7.161000	-16.880000
H	-3.527000	26.954000	4.263000	C	11.906000	6.067000	-8.131000	H	1.749000	7.953000	-16.462000
C	-3.706000	28.992000	4.909000	C	13.410000	9.026000	-6.429000	C	-2.495000	6.376000	-17.296000
H	-3.836000	29.246000	5.973000	C	12.435000	11.182000	-5.742000	C	-4.319000	7.939000	-17.221000
H	-3.117000	29.787000	4.424000	C	14.371000	6.926000	-7.179000	H	0.179000	6.122000	-16.857000
H	-4.700000	28.961000	4.437000	C	12.981000	5.232000	-8.246000	C	-3.858000	6.642000	-17.348000
C	11.635000	15.624000	3.566000	H	10.933000	5.710000	-8.492000	H	-2.083000	5.352000	-17.319000
C	11.020000	16.650000	3.726000	C	14.701000	9.447000	-5.991000	H	-5.398000	8.157000	-17.291000
C	10.519000	17.990000	3.958000	C	12.774000	12.320000	-5.522000	C	-4.879000	5.580000	-17.550000
C	9.177000	18.298000	3.799000	C	15.641000	7.349000	-6.735000	O	-5.978000	5.505000	-17.029000
C	11.448000	19.011000	4.309000	C	14.215000	5.601000	-7.651000	N	-4.480000	4.713000	-18.548000
C	8.698000	19.577000	4.042000	H	12.844000	4.235000	-8.692000	H	-3.815000	5.127000	-19.192000
H	8.486000	17.500000	3.501000	C	15.788000	8.644000	-6.182000	C	-5.561000	3.890000	-19.113000
C	10.977000	20.320000	4.548000	H	14.849000	10.434000	-5.519000	H	-6.002000	3.270000	-18.317000
C	12.841000	18.741000	4.419000	C	16.700000	6.418000	-6.667000	H	-6.363000	4.492000	-19.570000
C	9.593000	20.592000	4.504000	C	15.255000	4.662000	-7.422000	H	-5.154000	3.219000	-19.883000
C	7.271000	19.836000	3.943000	H	16.772000	8.946000	-5.795000	C	1.548000	22.260000	-15.645000
C	11.871000	21.325000	4.866000	C	16.484000	5.073000	-6.933000	C	0.507000	21.665000	-15.795000
C	13.724000	19.734000	4.725000	H	17.665000	6.798000	-6.297000	C	-0.682000	20.835000	-15.851000
H	13.237000	17.727000	4.251000	H	15.079000	3.602000	-7.664000	C	-0.461000	19.483000	-16.057000
C	9.133000	21.858000	4.966000	C	17.583000	4.095000	-6.699000	C	-2.017000	21.314000	-15.653000
C	6.097000	20.116000	3.877000	O	17.529000	2.993000	-6.178000	C	-1.490000	18.569000	-16.052000
C	11.414000	22.627000	5.170000	N	18.766000	4.625000	-7.193000	H	0.553000	19.086000	-16.221000
C	13.257000	21.057000	4.926000	H	18.590000	5.217000	-8.004000	C	-3.083000	20.383000	-15.689000
H	14.797000	19.517000	4.807000	C	19.880000	3.671000	-7.288000	C	-2.312000	22.680000	-15.379000
C	10.014000	22.853000	5.294000	H	19.687000	2.856000	-8.007000	C	-2.828000	19.002000	-15.853000
H	8.053000	22.063000	5.015000	H	20.792000	4.203000	-7.599000	C	-1.226000	17.169000	-16.272000
C	12.359000	23.667000	5.358000	H	20.060000	3.231000	-6.295000	C	-4.386000	20.818000	-15.564000
C	14.162000	22.110000	5.173000	C	0.932000	9.802000	-9.280000	C	-3.590000	23.086000	-15.095000
H	9.630000	23.834000	5.622000	C	1.746000	8.907000	-9.293000	H	-1.484000	23.404000	-15.324000
C	13.726000	23.409000	5.361000	C	2.599000	7.734000	-9.275000	C	-3.911000	18.077000	-15.897000
H	11.937000	24.665000	5.545000	C	3.943000	7.852000	-8.969000	C	-1.167000	15.981000	-16.457000
H	15.232000	21.852000	5.181000	C	2.049000	6.455000	-9.559000	C	-5.455000	19.918000	-15.791000
C	14.770000	24.456000	5.555000	C	4.778000	6.752000	-8.909000	C	-4.665000	22.158000	-15.203000
O	15.972000	24.294000	5.683000	H	4.374000	8.846000	-8.776000	H	-3.804000	24.138000	-14.846000
N	14.263000	25.735000	5.507000	C	2.910000	5.337000	-9.601000	C	-5.194000	18.533000	-15.957000
H	13.284000	25.935000	5.364000	C	0.667000	6.299000	-9.864000	H	-3.733000	16.993000	-16.004000
C	15.190000	26.837000	5.761000	C	4.274000	5.459000	-9.237000	C	-6.783000	20.388000	-15.764000
H	15.547000	26.829000	6.803000	C	6.153000	6.965000	-8.535000	C	-6.017000	22.555000	-15.062000
H	16.062000	26.779000	5.091000	C	2.420000	4.126000	-10.046000	H	-6.026000	17.831000	-16.089000
H	14.678000	27.793000	5.572000	C	0.185000	5.100000	-10.292000	C	-7.052000	21.695000	-15.404000
C	10.855000	8.347000	1.281000	H	-0.018000	7.160000	-9.795000	H	-7.578000	19.644000	-15.918000
C	11.605000	9.183000	1.721000	C	5.111000	4.306000	-9.273000	H	-6.240000	23.589000	-14.750000
C	12.658000	10.100000	2.089000	C	7.290000	7.155000	-8.192000	C	-8.447000	22.201000	-15.357000
C	12.349000	11.360000	2.547000	C	3.296000	3.033000	-10.222000	O	-8.873000	23.043000	-14.588000
C	14.017000	9.733000	1.865000	C	1.049000	3.977000	-10.366000	N	-9.242000	21.657000	-16.341000
C	13.345000	12.277000	2.824000	H	-0.858000	4.999000	-10.615000	H	-8.915000	20.862000	-16.868000
H	11.292000	11.639000	2.675000	C	4.644000	3.131000	-9.794000	C	-10.644000	22.069000	-16.389000
C	15.049000	10.629000	2.231000	H	6.158000	4.342000	-8.930000	H	-11.224000	21.660000	-15.547000
C	14.352000	8.491000	1.252000	C	2.799000	1.830000	-10.763000	H	-10.717000	23.168000	-16.363000
C	14.726000	11.926000	2.696000	C	0.569000	2.722000	-10.804000	H	-11.097000	21.725000	-17.331000
C	12.891000	13.592000	3.223000	H	5.291000	2.242000	-9.868000	C	9.294000	24.445000	-15.399000
C	16.371000	10.260000	2.069000	C	1.446000	1.674000	-11.013000	C	8.228000	24.987000	-15.253000

C	15.657000	8.107000	1.138000	H	3.508000	0.997000	-10.893000	C	6.861000	25.300000	-14.920000
H	13.562000	7.806000	0.897000	H	-0.508000	2.630000	-11.028000	C	5.907000	24.347000	-15.235000
C	15.783000	12.830000	3.010000	C	0.913000	0.367000	-11.461000	C	6.493000	26.509000	-14.256000
C	12.276000	14.614000	3.407000	O	-0.078000	-0.191000	-11.029000	C	4.576000	24.502000	-14.906000
C	17.414000	11.181000	2.333000	N	1.708000	-0.176000	-12.438000	H	6.214000	23.436000	-15.769000
C	16.694000	8.978000	1.562000	H	2.360000	0.452000	-12.895000	C	5.123000	26.708000	-13.964000
H	15.912000	7.140000	0.683000	C	1.261000	-1.386000	-13.130000	C	7.446000	27.508000	-13.885000
C	17.093000	12.466000	2.854000	H	0.520000	-1.177000	-13.919000	C	4.174000	25.688000	-14.226000
H	15.552000	13.847000	3.369000	H	2.132000	-1.880000	-13.592000	C	3.583000	23.498000	-15.246000
C	18.752000	10.809000	2.047000	H	0.818000	-2.086000	-12.404000	C	4.707000	27.908000	-13.425000
C	18.047000	8.617000	1.380000	C	-1.636000	17.263000	-8.789000	C	7.037000	28.668000	-13.282000
H	17.908000	13.170000	3.112000	C	-2.123000	16.171000	-8.948000	H	8.519000	27.344000	-14.089000
C	19.062000	9.533000	1.591000	C	-2.555000	14.800000	-9.036000	C	2.823000	25.879000	-13.829000
H	19.542000	11.554000	2.239000	C	-1.561000	13.846000	-9.146000	C	2.581000	22.858000	-15.462000
H	18.254000	7.614000	0.974000	C	-3.924000	14.424000	-8.957000	C	3.331000	28.154000	-13.203000
C	20.462000	9.104000	1.316000	C	-1.849000	12.500000	-9.208000	C	5.652000	28.895000	-13.061000
O	20.948000	8.000000	1.452000	H	-0.509000	14.160000	-9.189000	H	7.735000	29.468000	-12.984000
N	21.203000	10.136000	0.778000	C	-4.237000	13.050000	-9.053000	C	2.411000	27.080000	-13.340000
H	20.699000	10.930000	0.396000	C	-4.966000	15.381000	-8.781000	H	2.062000	25.088000	-13.966000
C	22.558000	9.859000	0.295000	C	-3.210000	12.089000	-9.191000	C	2.904000	29.438000	-12.786000
H	23.109000	9.279000	1.052000	C	-0.767000	11.524000	-9.255000	C	5.193000	30.117000	-12.521000
H	22.571000	9.302000	-0.657000	C	-5.552000	12.637000	-9.002000	H	1.357000	27.213000	-13.067000
H	23.087000	10.814000	0.143000	C	-6.269000	14.967000	-8.707000	C	3.838000	30.396000	-12.426000
C	3.530000	6.590000	-0.922000	H	-4.724000	16.458000	-8.717000	H	1.818000	29.586000	-12.670000
C	4.698000	6.290000	-0.845000	C	-3.543000	10.718000	-9.291000	H	5.928000	30.881000	-12.227000
C	6.023000	5.710000	-0.846000	C	0.092000	10.672000	-9.268000	C	3.437000	31.722000	-11.888000
C	7.089000	6.420000	-0.332000	C	-5.875000	11.266000	-9.155000	O	3.995000	32.334000	-10.995000
C	6.234000	4.438000	-1.455000	C	-6.582000	13.583000	-8.792000	N	2.348000	32.240000	-12.561000
C	8.362000	5.885000	-0.305000	H	-7.091000	15.691000	-8.600000	H	2.143000	31.851000	-13.472000
H	6.918000	7.425000	0.079000	C	-4.836000	10.300000	-9.227000	C	2.117000	33.678000	-12.360000
C	7.526000	3.863000	-1.397000	H	-2.741000	9.983000	-9.433000	H	2.065000	33.899000	-11.283000
C	5.185000	3.738000	-2.124000	C	-7.230000	10.878000	-9.229000	H	2.907000	34.305000	-12.806000
C	8.599000	4.567000	-0.798000	C	-7.917000	13.129000	-8.728000	H	1.155000	33.960000	-12.811000
C	9.387000	6.691000	0.322000	H	-5.043000	9.221000	-9.265000	C	14.395000	18.462000	-16.682000
C	7.726000	2.586000	-1.881000	C	-8.233000	11.808000	-9.001000	C	14.448000	19.621000	-16.356000
C	5.404000	2.494000	-2.642000	H	-7.420000	9.802000	-9.396000	C	14.298000	20.963000	-15.843000
H	4.165000	4.158000	-2.212000	H	-8.720000	13.855000	-8.523000	C	13.031000	21.501000	-15.947000
C	9.860000	3.920000	-0.642000	C	-9.664000	11.425000	-9.046000	C	15.360000	21.692000	-15.230000
C	10.127000	7.509000	0.811000	O	-10.549000	11.799000	-8.292000	C	12.728000	22.737000	-15.429000
C	8.981000	1.957000	-1.726000	N	-9.924000	10.699000	-10.196000	H	12.222000	20.931000	-16.428000
C	6.668000	1.866000	-2.484000	H	-9.259000	10.712000	-10.977000	C	15.068000	22.984000	-14.730000
H	4.588000	1.952000	-3.140000	C	-11.327000	10.413000	-10.498000	C	16.693000	21.188000	-15.140000
C	10.033000	2.632000	-1.054000	H	-11.763000	9.791000	-9.699000	C	13.737000	23.466000	-14.728000
H	10.710000	4.457000	-0.190000	H	-11.930000	11.329000	-10.606000	C	11.395000	23.277000	-15.550000
C	9.173000	0.652000	-2.224000	H	-11.374000	9.852000	-11.445000	C	16.082000	23.769000	-14.219000
C	6.881000	0.525000	-2.891000	C	4.230000	22.667000	-7.748000	C	17.707000	21.996000	-14.705000
H	10.981000	2.101000	-0.890000	C	3.033000	22.541000	-7.814000	H	16.938000	20.162000	-15.459000
C	8.131000	-0.065000	-2.791000	C	1.602000	22.345000	-7.773000	C	13.432000	24.676000	-14.040000
H	10.174000	0.215000	-2.088000	C	1.139000	21.092000	-8.128000	C	10.342000	23.859000	-15.500000
H	6.019000	-0.010000	-3.319000	C	0.708000	23.371000	-7.343000	C	15.786000	25.033000	-13.655000
C	8.329000	-1.461000	-3.276000	C	-0.198000	20.769000	-8.070000	C	17.416000	23.297000	-14.211000
O	7.475000	-2.309000	-3.453000	H	1.849000	20.317000	-8.454000	H	18.750000	21.637000	-14.702000
N	9.658000	-1.729000	-3.551000	C	-0.666000	23.047000	-7.267000	C	14.436000	25.468000	-13.563000
H	10.376000	-1.029000	-3.409000	C	1.144000	24.684000	-6.974000	H	12.387000	25.017000	-13.951000
C	10.032000	-3.109000	-3.849000	C	-1.121000	21.741000	-7.580000	C	16.833000	25.823000	-13.130000
H	9.935000	-3.760000	-2.964000	C	-0.647000	19.429000	-8.394000	C	18.430000	24.112000	-13.656000
H	9.401000	-3.514000	-4.657000	C	-1.574000	24.012000	-6.884000	H	14.221000	26.443000	-13.103000
H	11.080000	-3.134000	-4.187000	C	0.249000	25.613000	-6.514000	C	18.141000	25.364000	-13.136000
C	-2.197000	11.947000	-1.052000	H	2.210000	24.968000	-7.032000	H	16.545000	26.774000	-12.654000
C	-2.022000	10.762000	-1.208000	C	-2.497000	21.419000	-7.420000	H	19.463000	23.722000	-13.638000
C	-1.773000	9.341000	-1.419000	C	-1.135000	18.345000	-8.604000	C	19.253000	26.172000	-12.565000
C	-0.518000	8.822000	-1.168000	C	-2.958000	23.724000	-6.906000	O	20.273000	25.746000	-12.055000
C	-2.794000	8.459000	-1.898000	C	-1.137000	25.302000	-6.492000	N	19.035000	27.526000	-12.680000
C	-0.197000	7.502000	-1.405000	H	0.577000	26.623000	-6.216000	H	18.259000	27.868000	-13.220000
H	0.262000	9.494000	-0.781000	C	-3.405000	22.398000	-7.150000	C	20.155000	28.417000	-12.364000
C	-2.477000	7.102000	-2.167000	H	-2.852000	20.392000	-7.608000	H	20.602000	28.128000	-11.399000
C	-4.130000	8.909000	-2.102000	C	-3.886000	24.753000	-6.650000	H	20.943000	28.396000	-13.135000
C	-1.173000	6.609000	-1.937000	C	-2.100000	26.286000	-6.170000	H	19.791000	29.451000	-12.270000
C	1.182000	7.111000	-1.153000	H	-4.480000	22.169000	-7.107000	C	11.136000	11.628000	-19.381000

C	-3.447000	6.249000	-2.656000	C	-3.458000	26.017000	-6.277000	C	12.203000	12.106000	-19.078000
C	-5.096000	8.060000	-2.554000	H	-4.947000	24.466000	-6.714000	C	13.383000	12.729000	-18.526000
H	-4.406000	9.944000	-1.863000	H	-1.745000	27.303000	-5.904000	C	13.291000	14.058000	-18.158000
C	-0.869000	5.252000	-2.252000	C	-4.420000	27.110000	-5.984000	C	14.603000	12.014000	-18.354000
C	2.355000	6.853000	-1.025000	O	-4.226000	28.084000	-5.276000	C	14.361000	14.722000	-17.593000
C	-3.146000	4.902000	-2.967000	N	-5.584000	26.968000	-6.694000	H	12.355000	14.608000	-18.325000
C	-4.771000	6.709000	-2.827000	H	-5.777000	26.149000	-7.244000	C	15.686000	12.675000	-17.726000
H	-6.130000	8.395000	-2.725000	C	-6.614000	27.990000	-6.528000	C	14.753000	10.669000	-18.809000
C	-1.825000	4.413000	-2.759000	H	-6.829000	28.163000	-5.461000	C	15.555000	14.011000	-17.283000
H	0.154000	4.874000	-2.090000	H	-6.305000	28.946000	-6.984000	C	14.257000	16.127000	-17.265000
C	-4.178000	4.048000	-3.434000	H	-7.543000	27.657000	-7.015000	C	16.887000	12.021000	-17.560000
C	-5.771000	5.815000	-3.256000	C	11.760000	20.148000	-8.040000	C	15.937000	10.012000	-18.634000
H	-1.594000	3.358000	-2.985000	C	11.141000	21.171000	-7.864000	H	13.907000	10.153000	-19.298000
C	-5.488000	4.498000	-3.559000	C	10.314000	22.315000	-7.519000	C	16.618000	14.627000	-16.557000
H	-3.877000	3.007000	-3.633000	C	8.953000	22.183000	-7.737000	C	14.318000	17.297000	-16.982000
H	-6.792000	6.209000	-3.363000	C	10.843000	23.518000	-6.968000	C	18.003000	12.704000	-17.008000
C	-6.639000	3.643000	-3.980000	C	8.040000	23.135000	-7.334000	C	17.017000	10.674000	-17.982000
O	-7.825000	3.918000	-3.909000	H	8.547000	21.278000	-8.209000	H	16.075000	8.982000	-19.007000
N	-6.227000	2.429000	-4.467000	C	9.923000	24.503000	-6.542000	C	17.833000	14.010000	-16.456000
H	-5.249000	2.223000	-4.628000	C	12.246000	23.772000	-6.869000	H	16.480000	15.639000	-16.133000
C	-7.213000	1.391000	-4.751000	C	8.524000	24.268000	-6.615000	C	19.265000	12.062000	-17.009000
H	-8.169000	1.838000	-5.062000	C	6.620000	22.917000	-7.538000	C	18.263000	10.036000	-17.826000
H	-6.851000	0.760000	-5.579000	C	10.396000	25.698000	-6.039000	H	18.672000	14.529000	-15.963000
H	-7.396000	0.754000	-3.870000	C	12.715000	24.966000	-6.393000	C	19.378000	10.742000	-17.414000
C	-0.179000	19.437000	-0.117000	H	12.963000	23.015000	-7.229000	H	20.121000	12.618000	-16.604000
C	-1.255000	18.918000	-0.284000	C	7.631000	25.171000	-5.974000	H	18.364000	8.984000	-18.134000
C	-2.386000	18.040000	-0.484000	C	5.427000	22.789000	-7.655000	C	20.682000	10.031000	-17.433000
C	-2.045000	16.705000	-0.539000	C	9.482000	26.681000	-5.603000	O	20.909000	8.923000	-16.982000
C	-3.745000	18.464000	-0.610000	C	11.788000	25.949000	-5.944000	N	21.612000	10.748000	-18.151000
C	-2.982000	15.713000	-0.713000	H	13.803000	25.166000	-6.346000	H	21.246000	11.516000	-18.701000
H	-0.991000	16.409000	-0.421000	C	8.098000	26.372000	-5.527000	C	22.796000	10.014000	-18.612000
C	-4.729000	17.448000	-0.715000	H	6.546000	24.970000	-5.900000	H	23.256000	9.485000	-17.762000
C	-4.149000	19.839000	-0.587000	C	9.959000	27.943000	-5.189000	H	22.562000	9.277000	-19.400000
C	-4.359000	16.080000	-0.813000	C	12.222000	27.192000	-5.423000	H	23.538000	10.724000	-19.007000
C	-2.588000	14.317000	-0.777000	H	7.393000	27.106000	-5.125000	C	3.211000	11.032000	-20.558000
C	-6.065000	17.791000	-0.692000	C	11.317000	28.190000	-5.086000	C	4.194000	10.330000	-20.595000
C	-5.474000	20.168000	-0.506000	H	9.182000	28.670000	-4.903000	C	5.457000	9.621000	-20.490000
H	-3.411000	20.659000	-0.569000	H	13.309000	27.362000	-5.342000	C	6.593000	10.380000	-20.268000
C	-5.372000	15.087000	-0.955000	C	11.820000	29.498000	-4.583000	C	5.550000	8.196000	-20.589000
C	-2.380000	13.133000	-0.906000	O	12.841000	29.689000	-3.948000	C	7.836000	9.798000	-20.134000
C	-7.065000	16.797000	-0.811000	N	10.995000	30.544000	-4.930000	H	6.516000	11.475000	-20.188000
C	-6.455000	19.140000	-0.525000	H	10.141000	30.394000	-5.439000	C	6.824000	7.595000	-20.451000
H	-5.807000	21.218000	-0.429000	C	11.387000	31.893000	-4.531000	C	4.406000	7.365000	-20.795000
C	-6.689000	15.431000	-0.912000	H	11.650000	31.919000	-3.461000	C	7.969000	8.385000	-20.197000
H	-5.112000	14.021000	-1.091000	H	12.250000	32.254000	-5.115000	C	9.004000	10.618000	-19.888000
C	-8.431000	17.167000	-0.800000	H	10.544000	32.582000	-4.695000	C	6.952000	6.224000	-20.529000
C	-7.827000	19.448000	-0.418000	C	13.070000	12.457000	-9.985000	C	4.524000	6.000000	-20.809000
H	-7.473000	14.663000	-0.954000	C	13.663000	13.482000	-9.765000	H	3.414000	7.827000	-20.918000
C	-8.807000	18.483000	-0.576000	C	14.263000	14.698000	-9.291000	C	9.231000	7.759000	-19.992000
H	-9.146000	16.335000	-0.909000	C	13.417000	15.768000	-9.068000	C	10.064000	11.142000	-19.646000
H	-8.116000	20.500000	-0.277000	C	15.651000	14.786000	-9.019000	C	8.227000	5.617000	-20.421000
C	-10.231000	18.916000	-0.495000	C	13.885000	16.960000	-8.552000	C	5.806000	5.406000	-20.660000
O	-10.682000	19.891000	0.080000	H	12.349000	15.654000	-9.298000	H	3.654000	5.334000	-20.949000
N	-11.047000	18.100000	-1.245000	C	16.143000	15.990000	-8.475000	C	9.361000	6.407000	-20.109000
H	-10.693000	17.270000	-1.694000	C	16.535000	13.696000	-9.274000	H	10.129000	8.356000	-19.761000
C	-12.486000	18.337000	-1.177000	C	15.262000	17.060000	-8.176000	C	8.354000	4.218000	-20.552000
H	-12.736000	19.336000	-1.570000	C	13.004000	18.097000	-8.342000	C	5.969000	4.004000	-20.685000
H	-13.009000	17.586000	-1.788000	C	17.492000	16.109000	-8.226000	H	10.327000	5.914000	-19.938000
H	-12.856000	18.260000	-0.141000	C	17.864000	13.795000	-8.982000	C	7.228000	3.427000	-20.691000
C	7.883000	20.738000	0.455000	H	16.142000	12.764000	-9.711000	H	9.366000	3.797000	-20.436000
C	6.811000	21.298000	0.506000	C	15.778000	18.218000	-7.522000	H	5.076000	3.370000	-20.791000
C	5.456000	21.842000	0.558000	C	12.374000	19.118000	-8.194000	C	7.320000	1.954000	-20.842000
C	4.397000	20.959000	0.387000	C	18.016000	17.332000	-7.749000	O	6.533000	1.136000	-20.398000
C	5.188000	23.236000	0.744000	C	18.359000	15.007000	-8.430000	N	8.320000	1.588000	-21.726000
C	3.082000	21.387000	0.407000	H	18.554000	12.960000	-9.193000	H	8.691000	2.275000	-22.366000
H	4.580000	19.885000	0.253000	C	17.127000	18.376000	-7.376000	C	8.346000	0.175000	-22.115000
C	3.846000	23.673000	0.839000	H	15.104000	19.033000	-7.198000	H	8.452000	-0.454000	-21.216000
C	6.228000	24.202000	0.849000	C	19.411000	17.459000	-7.561000	H	7.438000	-0.132000	-22.660000
C	2.788000	22.752000	0.682000	C	19.726000	15.146000	-8.122000	H	9.216000	-0.008000	-22.762000

C	1.974000	20.472000	0.223000	H	17.539000	19.292000	-6.932000	C	-1.039000	17.625000	-20.186000
C	3.562000	24.991000	1.146000	C	20.243000	16.364000	-7.722000	C	-1.398000	16.480000	-20.295000
C	5.952000	25.515000	1.111000	H	19.781000	18.433000	-7.198000	C	-1.424000	15.038000	-20.317000
H	7.276000	23.879000	0.761000	H	20.378000	14.271000	-8.270000	C	-0.184000	14.429000	-20.366000
C	1.447000	23.188000	0.879000	C	21.704000	16.465000	-7.488000	C	-2.627000	14.269000	-20.318000
C	0.907000	19.935000	0.051000	O	22.372000	15.806000	-6.711000	C	-0.068000	13.059000	-20.394000
C	2.223000	25.413000	1.340000	N	22.247000	17.354000	-8.376000	H	0.727000	15.044000	-20.381000
C	4.610000	25.918000	1.347000	H	21.649000	17.815000	-9.050000	C	-2.517000	12.860000	-20.323000
H	6.767000	26.249000	1.217000	C	23.700000	17.495000	-8.483000	C	-3.921000	14.871000	-20.318000
C	1.166000	24.472000	1.226000	H	24.167000	17.360000	-7.495000	C	-1.240000	12.248000	-20.319000
H	0.603000	22.489000	0.766000	H	24.143000	16.768000	-9.185000	C	1.238000	12.424000	-20.442000
C	1.955000	26.746000	1.724000	H	23.940000	18.510000	-8.838000	C	-3.658000	12.082000	-20.338000
C	4.301000	27.209000	1.838000	C	6.341000	8.656000	-11.948000	C	-5.051000	14.101000	-20.282000
H	0.124000	24.765000	1.426000	C	7.535000	8.549000	-11.785000	H	-4.003000	15.969000	-20.320000
C	2.990000	27.621000	2.016000	C	8.969000	8.377000	-11.580000	C	-1.146000	10.829000	-20.247000
H	0.892000	27.001000	1.864000	C	9.719000	9.422000	-11.079000	C	2.233000	11.740000	-20.502000
H	5.129000	27.906000	2.029000	C	9.638000	7.187000	-12.008000	C	-3.557000	10.672000	-20.388000
C	2.732000	28.998000	2.525000	C	11.088000	9.314000	-10.928000	C	-4.941000	12.682000	-20.290000
O	3.452000	29.679000	3.231000	H	9.215000	10.364000	-10.830000	H	-6.055000	14.562000	-20.263000
N	1.539000	29.483000	2.042000	C	11.038000	7.060000	-11.830000	C	-2.275000	10.062000	-20.297000
H	0.909000	28.874000	1.548000	C	8.940000	6.146000	-12.675000	H	-0.163000	10.325000	-20.209000
C	1.032000	30.722000	2.629000	C	11.773000	8.110000	-11.249000	C	-4.734000	9.889000	-20.479000
H	1.781000	31.524000	2.522000	C	11.833000	10.435000	-10.415000	C	-6.090000	11.855000	-20.288000
H	0.121000	31.032000	2.093000	C	11.702000	5.929000	-12.264000	H	-2.189000	8.970000	-20.281000
H	0.783000	30.605000	3.698000	C	9.590000	5.025000	-13.094000	C	-5.987000	10.475000	-20.411000
C	12.979000	14.619000	-0.915000	H	7.860000	6.236000	-12.856000	H	-4.597000	8.799000	-20.510000
C	12.973000	15.803000	-0.658000	C	13.172000	7.949000	-11.026000	H	-7.082000	12.340000	-20.233000
C	12.861000	17.213000	-0.267000	C	12.457000	11.440000	-10.187000	C	-7.242000	9.664000	-20.431000
C	11.597000	17.774000	-0.121000	C	13.104000	5.800000	-12.105000	O	-8.307000	9.978000	-19.923000
C	14.001000	18.029000	-0.017000	C	10.980000	4.873000	-12.857000	N	-7.119000	8.490000	-21.142000
C	11.384000	19.084000	0.280000	H	9.017000	4.227000	-13.584000	H	-6.274000	8.334000	-21.667000
H	10.711000	17.154000	-0.314000	C	13.827000	6.826000	-11.445000	C	-8.349000	7.772000	-21.485000
C	13.810000	19.360000	0.433000	H	13.756000	8.751000	-10.550000	H	-8.934000	7.577000	-20.573000
C	15.322000	17.530000	-0.188000	C	13.756000	4.628000	-12.556000	H	-8.981000	8.332000	-22.195000
C	12.508000	19.890000	0.610000	C	11.654000	3.682000	-13.196000	H	-8.094000	6.804000	-21.941000
C	10.021000	19.611000	0.354000	H	14.907000	6.714000	-11.251000	C	3.892000	24.133000	-19.203000
C	14.907000	20.154000	0.697000	C	13.028000	3.565000	-13.073000	C	2.759000	23.732000	-19.347000
C	16.403000	18.287000	0.152000	H	14.847000	4.586000	-12.412000	C	1.400000	23.203000	-19.360000
H	15.489000	16.510000	-0.566000	H	11.039000	2.852000	-13.578000	C	1.211000	21.858000	-19.641000
C	12.345000	21.216000	1.100000	C	13.646000	2.264000	-13.457000	C	0.264000	24.040000	-19.109000
C	8.948000	20.167000	0.405000	O	13.057000	1.199000	-13.576000	C	-0.048000	21.291000	-19.629000
C	14.735000	21.509000	1.070000	N	15.020000	2.347000	-13.586000	H	2.067000	21.208000	-19.871000
C	16.215000	19.621000	0.601000	H	15.549000	3.186000	-13.385000	C	-1.026000	23.457000	-19.074000
H	17.422000	17.884000	0.051000	C	15.740000	1.074000	-13.598000	C	0.379000	25.450000	-18.927000
C	13.428000	22.018000	1.304000	H	15.550000	0.488000	-12.684000	C	-1.181000	22.069000	-19.271000
H	11.340000	21.633000	1.276000	H	15.445000	0.471000	-14.469000	C	-0.249000	19.885000	-19.897000
C	15.872000	22.321000	1.273000	H	16.821000	1.269000	-13.668000	C	-2.147000	24.239000	-18.869000
C	17.320000	20.441000	0.912000	C	-0.828000	11.959000	-12.898000	C	-0.731000	26.223000	-18.736000
H	13.295000	23.051000	1.663000	C	-0.413000	10.830000	-12.864000	H	1.371000	25.930000	-18.933000
C	17.148000	21.775000	1.239000	C	0.364000	9.613000	-12.922000	C	-2.466000	21.472000	-19.121000
H	15.676000	23.370000	1.548000	C	1.696000	9.697000	-12.566000	C	-0.633000	18.752000	-20.053000
H	18.328000	20.003000	0.815000	C	-0.171000	8.366000	-13.355000	C	-3.439000	23.661000	-18.864000
C	18.357000	22.577000	1.571000	C	2.550000	8.615000	-12.639000	C	-2.019000	25.631000	-18.671000
O	19.369000	22.189000	2.126000	H	2.091000	10.658000	-12.203000	H	-0.630000	27.313000	-18.614000
N	18.248000	23.867000	1.099000	C	0.682000	7.231000	-13.381000	C	-3.570000	22.249000	-18.924000
H	17.352000	24.210000	0.804000	C	-1.545000	8.217000	-13.690000	H	-2.604000	20.383000	-19.242000
C	19.232000	24.819000	1.613000	C	2.048000	7.354000	-13.054000	C	-4.580000	24.493000	-18.792000
H	20.247000	24.488000	1.345000	C	3.952000	8.772000	-12.304000	C	-3.179000	26.409000	-18.450000
H	19.059000	25.804000	1.153000	C	0.167000	5.975000	-13.637000	H	-4.564000	21.783000	-18.877000
H	19.171000	24.928000	2.708000	C	-2.063000	6.966000	-13.872000	C	-4.448000	25.854000	-18.569000
C	10.032000	7.668000	-3.413000	H	-2.241000	9.074000	-13.709000	H	-5.554000	23.987000	-18.814000
C	11.107000	8.058000	-3.046000	C	2.881000	6.206000	-13.049000	H	-3.031000	27.483000	-18.225000
C	12.299000	8.770000	-2.659000	C	5.147000	8.736000	-12.118000	C	-5.633000	26.745000	-18.413000
C	12.160000	10.076000	-2.225000	C	0.990000	4.820000	-13.587000	O	-5.645000	27.820000	-17.840000
C	13.592000	8.176000	-2.684000	C	-1.225000	5.826000	-13.799000	N	-6.782000	26.242000	-18.976000
C	13.228000	10.855000	-1.816000	H	-3.138000	6.813000	-14.046000	H	-6.754000	25.401000	-19.525000
H	11.142000	10.496000	-2.201000	C	2.370000	4.962000	-13.264000	C	-7.972000	27.090000	-18.975000
C	14.701000	8.944000	-2.258000	H	3.954000	6.306000	-12.815000	H	-8.215000	27.403000	-17.947000
C	13.781000	6.817000	-3.060000	C	0.399000	3.539000	-13.723000	H	-7.836000	27.990000	-19.597000

C	14.533000	10.279000	-1.810000	C	-1.780000	4.533000	-13.816000	H	-8.827000	26.522000	-19.371000
C	13.009000	12.250000	-1.422000	H	3.026000	4.089000	-13.134000	C	11.826000	24.461000	-19.194000
C	15.958000	8.374000	-2.257000	C	-0.980000	3.408000	-13.783000	C	10.966000	25.254000	-18.899000
C	14.999000	6.214000	-2.926000	H	1.084000	2.673000	-13.651000	C	9.733000	25.919000	-18.534000
H	12.924000	6.215000	-3.392000	H	-2.876000	4.445000	-13.874000	C	8.572000	25.226000	-18.823000
C	15.668000	11.014000	-1.365000	C	-1.659000	2.089000	-13.798000	C	9.675000	27.203000	-17.905000
C	12.982000	13.433000	-1.165000	O	-2.676000	1.787000	-13.187000	C	7.330000	25.744000	-18.521000
C	17.093000	9.151000	-1.932000	N	-1.052000	1.248000	-14.707000	H	8.643000	24.244000	-19.315000
C	16.124000	6.999000	-2.552000	H	-0.354000	1.590000	-15.352000	C	8.404000	27.764000	-17.635000
H	15.129000	5.148000	-3.171000	C	-1.819000	0.056000	-15.081000	C	10.845000	27.934000	-17.540000
C	16.918000	10.475000	-1.440000	H	-2.077000	-0.525000	-14.181000	C	7.225000	27.037000	-17.927000
H	15.562000	12.044000	-0.985000	H	-2.750000	0.307000	-15.614000	C	6.120000	25.001000	-18.835000
C	18.382000	8.584000	-2.053000	H	-1.205000	-0.579000	-15.736000	C	8.311000	29.042000	-17.119000
C	17.424000	6.452000	-2.557000	C	-0.769000	19.968000	-12.342000	C	10.747000	29.149000	-16.919000
H	17.793000	11.053000	-1.106000	C	-1.544000	19.063000	-12.516000	H	11.838000	27.500000	-17.737000
C	18.546000	7.240000	-2.365000	C	-2.349000	17.872000	-12.593000	C	5.954000	27.642000	-17.707000
H	19.218000	9.260000	-1.817000	C	-1.677000	16.686000	-12.830000	C	5.015000	24.547000	-19.031000
H	17.541000	5.379000	-2.766000	C	-3.757000	17.900000	-12.374000	C	7.052000	29.681000	-17.017000
C	19.884000	6.592000	-2.504000	C	-2.339000	15.479000	-12.822000	C	9.471000	29.730000	-16.691000
O	20.151000	5.405000	-2.488000	H	-0.588000	16.676000	-12.995000	H	11.643000	29.714000	-16.614000
N	20.880000	7.519000	-2.698000	C	-4.448000	16.670000	-12.412000	C	5.874000	28.954000	-17.339000
H	20.693000	8.505000	-2.639000	C	-4.476000	19.109000	-12.116000	H	5.022000	27.099000	-17.945000
C	22.258000	7.039000	-2.623000	C	-3.738000	15.454000	-12.551000	C	6.978000	30.997000	-16.502000
H	22.434000	6.261000	-3.383000	C	-1.623000	14.231000	-12.947000	C	9.338000	31.004000	-16.087000
H	22.946000	7.874000	-2.822000	C	-5.817000	16.645000	-12.259000	H	4.889000	29.425000	-17.242000
H	22.490000	6.623000	-1.629000	C	-5.836000	19.077000	-11.959000	C	8.104000	31.634000	-16.010000
C	2.092000	8.010000	-5.359000	H	-3.932000	20.072000	-12.068000	H	5.971000	31.428000	-16.424000
C	3.177000	7.485000	-5.327000	C	-4.432000	14.222000	-12.395000	H	10.245000	31.525000	-15.729000
C	4.353000	6.647000	-5.259000	C	-1.212000	13.099000	-12.934000	C	8.031000	32.967000	-15.341000
C	5.548000	7.146000	-4.782000	C	-6.513000	15.414000	-12.292000	O	8.812000	33.372000	-14.498000
C	4.264000	5.287000	-5.681000	C	-6.535000	17.843000	-12.032000	N	6.964000	33.744000	-15.791000
C	6.672000	6.352000	-4.706000	H	-6.412000	20.006000	-11.798000	H	6.731000	33.504000	-16.750000
H	5.622000	8.197000	-4.463000	C	-5.789000	14.196000	-12.299000	C	7.117000	35.179000	-15.499000
C	5.434000	4.486000	-5.664000	H	-3.891000	13.264000	-12.427000	H	7.198000	35.330000	-14.412000
C	3.033000	4.712000	-6.122000	C	-7.922000	15.407000	-12.269000	H	8.008000	35.623000	-15.976000
C	6.642000	5.002000	-5.149000	C	-7.941000	17.781000	-11.908000	H	6.232000	35.725000	-15.857000
C	7.876000	6.952000	-4.194000	H	-6.321000	13.234000	-12.229000	C	15.088000	17.414000	-21.201000
C	5.399000	3.186000	-6.124000	C	-8.620000	16.583000	-12.070000	C	15.494000	18.493000	-20.837000
C	3.008000	3.421000	-6.554000	H	-8.418000	14.429000	-12.342000	C	15.695000	19.819000	-20.277000
H	2.071000	5.257000	-6.089000	H	-8.502000	18.709000	-11.713000	C	14.604000	20.675000	-20.278000
C	7.806000	4.184000	-5.125000	C	-10.099000	16.583000	-12.006000	C	16.935000	20.230000	-19.689000
C	8.950000	7.315000	-3.796000	O	-10.797000	17.272000	-11.288000	C	14.668000	21.927000	-19.702000
C	6.569000	2.391000	-6.150000	N	-10.647000	15.765000	-12.966000	H	13.654000	20.363000	-20.736000
C	4.170000	2.611000	-6.508000	H	-10.058000	15.518000	-13.745000	C	16.997000	21.499000	-19.064000
H	2.074000	2.972000	-6.906000	C	-12.078000	15.966000	-13.231000	C	18.100000	19.404000	-19.688000
C	7.793000	2.930000	-5.672000	H	-12.658000	15.772000	-12.315000	C	15.849000	22.325000	-19.014000
H	8.744000	4.593000	-4.721000	H	-12.310000	16.984000	-13.581000	C	13.510000	22.804000	-19.690000
C	6.475000	1.031000	-6.527000	H	-12.408000	15.254000	-14.002000	C	18.167000	21.922000	-18.465000
C	4.106000	1.227000	-6.792000	C	6.642000	23.318000	-11.642000	C	19.258000	19.816000	-19.082000
H	8.715000	2.328000	-5.678000	C	5.435000	23.416000	-11.623000	H	18.072000	18.417000	-20.177000
C	5.248000	0.445000	-6.809000	C	4.011000	23.627000	-11.401000	C	15.879000	23.531000	-18.256000
H	7.417000	0.462000	-6.484000	C	3.106000	22.644000	-11.770000	C	12.660000	23.632000	-19.467000
H	3.111000	0.810000	-7.012000	C	3.544000	24.823000	-10.779000	C	18.225000	23.186000	-17.832000
C	5.110000	-1.011000	-7.104000	C	1.749000	22.765000	-11.531000	C	19.314000	21.091000	-18.454000
O	4.117000	-1.699000	-6.925000	H	3.469000	21.732000	-12.267000	H	20.164000	19.186000	-19.078000
N	6.287000	-1.532000	-7.593000	C	2.156000	24.991000	-10.591000	C	17.048000	23.970000	-17.705000
H	7.136000	-0.981000	-7.541000	C	4.430000	25.871000	-10.399000	H	14.970000	24.144000	-18.142000
C	6.402000	-2.991000	-7.600000	C	1.261000	23.924000	-10.847000	C	19.449000	23.640000	-17.293000
H	6.459000	-3.412000	-6.582000	C	0.824000	21.721000	-11.904000	C	20.505000	21.562000	-17.847000
H	5.535000	-3.433000	-8.115000	C	1.664000	26.230000	-10.225000	H	17.080000	24.932000	-17.175000
H	7.309000	-3.281000	-8.151000	C	3.942000	27.076000	-9.980000	C	20.578000	22.842000	-17.311000
C	-1.952000	14.526000	-4.941000	H	5.519000	25.715000	-10.473000	H	19.435000	24.623000	-16.803000
C	-2.120000	13.355000	-5.190000	C	-0.112000	24.083000	-10.504000	H	21.392000	20.902000	-17.850000
C	-2.341000	11.933000	-5.343000	C	0.026000	20.849000	-12.138000	C	21.865000	23.314000	-16.723000
C	-1.248000	11.096000	-5.310000	C	0.272000	26.458000	-10.225000	O	22.728000	22.607000	-16.233000
C	-3.647000	11.392000	-5.491000	C	2.541000	27.297000	-9.916000	N	22.033000	24.683000	-16.788000
C	-1.359000	9.729000	-5.444000	H	4.640000	27.892000	-9.746000	H	21.421000	25.210000	-17.391000
H	-0.247000	11.537000	-5.192000	C	-0.609000	25.344000	-10.294000	C	23.369000	25.207000	-16.488000
C	-3.787000	9.998000	-5.669000	H	-0.826000	23.241000	-10.551000	H	23.706000	24.830000	-15.510000

C	-4.795000	12.233000	-5.510000	C	-0.212000	27.779000	-10.096000	H	24.117000	24.927000	-17.250000
C	-2.649000	9.146000	-5.643000	C	2.004000	28.581000	-9.648000	H	23.327000	26.305000	-16.432000
C	-0.107000	9.001000	-5.413000	H	-1.686000	25.514000	-10.172000	H	8.984000	11.468000	-24.389000
C	-5.039000	9.486000	-5.948000	C	0.646000	28.818000	-9.778000	C	9.938000	11.648000	-23.957000
C	-6.031000	11.722000	-5.770000	H	-1.299000	27.928000	-10.167000	C	11.015000	11.889000	-23.472000
H	-4.671000	13.315000	-5.357000	H	2.717000	29.394000	-9.423000	C	12.349000	12.203000	-22.997000
C	-2.823000	7.754000	-5.879000	C	0.110000	30.184000	-9.514000	C	12.635000	13.501000	-22.601000
C	0.991000	8.503000	-5.387000	O	0.195000	30.801000	-8.470000	C	13.362000	11.197000	-22.985000
C	-5.183000	8.126000	-6.289000	N	-0.424000	30.739000	-10.653000	C	13.917000	13.882000	-22.248000
C	-6.177000	10.329000	-5.991000	H	-0.209000	30.325000	-11.556000	H	11.834000	14.252000	-22.604000
H	-6.914000	12.370000	-5.864000	C	-0.755000	32.161000	-10.586000	C	14.683000	11.589000	-22.672000
C	-4.056000	7.266000	-6.212000	H	-1.639000	32.317000	-9.947000	C	13.097000	9.832000	-23.323000
H	-1.967000	7.059000	-5.844000	H	0.078000	32.760000	-10.186000	C	14.971000	12.930000	-22.330000
C	-6.443000	7.651000	-6.719000	H	-0.989000	32.524000	-11.598000	C	14.233000	15.256000	-21.879000
C	-7.437000	9.801000	-6.354000	C	13.352000	19.401000	-12.398000	C	15.709000	10.668000	-22.739000
H	-4.199000	6.194000	-6.415000	C	13.067000	20.551000	-12.166000	C	14.120000	8.930000	-23.405000
C	-7.556000	8.479000	-6.747000	C	12.547000	21.827000	-11.734000	H	12.069000	9.471000	-23.506000
H	-6.504000	6.585000	-6.991000	C	11.184000	21.994000	-11.892000	C	16.322000	13.325000	-22.121000
H	-8.286000	10.515000	-6.377000	C	13.346000	22.831000	-11.119000	C	14.652000	16.340000	-21.545000
C	-8.892000	7.956000	-7.161000	C	10.507000	23.097000	-11.422000	C	17.044000	11.059000	-22.476000
O	-9.955000	8.181000	-6.616000	H	10.585000	21.212000	-12.378000	C	15.436000	9.317000	-23.045000
N	-8.795000	7.134000	-8.256000	C	12.672000	23.970000	-10.615000	H	13.931000	7.886000	-23.704000
H	-7.917000	7.136000	-8.770000	C	14.770000	22.720000	-10.996000	C	17.336000	12.417000	-22.189000
C	-10.023000	6.693000	-8.922000	C	11.257000	24.082000	-10.704000	H	16.568000	14.375000	-21.905000
H	-10.783000	6.435000	-8.167000	C	9.056000	23.169000	-11.567000	C	18.063000	10.082000	-22.439000
H	-10.444000	7.458000	-9.598000	C	13.403000	24.975000	-10.015000	C	16.472000	8.363000	-22.928000
H	-9.810000	5.785000	-9.508000	C	15.486000	23.714000	-10.387000	H	18.369000	12.730000	-21.991000
C	2.043000	21.234000	-3.687000	H	15.310000	21.848000	-11.409000	C	17.770000	8.746000	-22.633000
C	0.885000	20.913000	-3.803000	C	10.602000	25.169000	-10.062000	H	19.063000	10.436000	-22.156000
C	-0.446000	20.350000	-3.895000	C	7.849000	23.238000	-11.620000	H	16.225000	7.305000	-23.101000
C	-0.490000	18.989000	-4.110000	C	12.747000	26.127000	-9.521000	C	18.807000	7.689000	-22.499000
C	-1.651000	21.104000	-3.791000	C	14.811000	24.868000	-9.899000	O	18.623000	6.540000	-22.127000
C	-1.678000	18.299000	-4.180000	H	16.586000	23.655000	-10.302000	N	20.057000	8.112000	-22.876000
H	0.455000	18.435000	-4.208000	C	11.324000	26.176000	-9.494000	H	20.194000	8.994000	-23.339000
C	-2.882000	20.412000	-3.870000	H	9.504000	25.243000	-10.098000	C	21.121000	7.108000	-22.908000
C	-1.646000	22.516000	-3.610000	C	13.516000	27.215000	-9.049000	H	21.198000	6.606000	-21.930000
C	-2.908000	19.002000	-4.009000	C	15.538000	25.947000	-9.346000	H	20.946000	6.346000	-23.685000
C	-1.678000	16.867000	-4.410000	H	10.812000	27.046000	-9.062000	H	22.081000	7.602000	-23.115000
C	-4.066000	21.117000	-3.794000								

Table S2. Cartesian coordinates of optimized helical **poly-PyrDE**

Cartesian coordinates of optimized helical **poly-PyDE** are shown as follows;

C	1.858000	4.057000	1.844000	H	0.441000	17.339000	-3.175000	O	14.877000	21.785000	-11.980000
C	2.504000	3.090000	1.573000	C	-0.965000	14.306000	-3.568000	N	13.943000	22.696000	-10.144000
C	3.200000	2.051000	1.226000	C	0.218000	12.266000	-3.739000	H	13.325000	22.552000	-9.409000
N	4.523000	2.018000	1.517000	C	-0.965000	14.306000	-3.568000	C	14.677000	23.931000	-10.145000
C	2.621000	0.982000	0.514000	C	0.218000	12.266000	-3.739000	H	15.367000	24.015000	-10.991000
C	5.335000	0.997000	1.150000	C	-2.065000	16.512000	-3.540000	H	13.978000	24.768000	-10.188000
C	3.421000	-0.109000	0.088000	H	-1.868000	13.837000	-3.698000	H	15.256000	24.007000	-9.222000
H	1.619000	1.001000	0.295000	C	0.204000	11.093000	-3.962000	C	13.072000	8.792000	-14.694000
C	4.799000	-0.090000	0.428000	O	-1.991000	17.622000	-4.118000	C	13.859000	9.652000	-14.435000
C	6.597000	1.066000	1.458000	N	-3.255000	16.109000	-3.029000	C	14.732000	10.584000	-14.203000
C	2.853000	-1.160000	-0.672000	H	-3.256000	15.273000	-2.535000	N	14.336000	11.731000	-13.598000
H	5.418000	-0.853000	0.135000	C	-4.507000	16.808000	-3.117000	C	16.073000	10.443000	-14.611000
C	7.757000	1.134000	1.732000	H	-4.429000	17.757000	-3.656000	C	15.179000	12.767000	-13.356000
O	1.808000	-0.948000	-1.334000	H	-5.236000	16.180000	-3.634000	C	16.995000	11.493000	-14.385000
N	3.408000	-2.399000	-0.702000	H	-4.877000	17.015000	-2.111000	H	16.379000	9.584000	-15.082000
H	8.653000	1.188000	1.943000	C	11.378000	16.626000	-3.904000	C	16.535000	12.663000	-13.732000
H	4.201000	-2.526000	-0.159000	C	10.434000	17.306000	-3.637000	C	14.697000	13.851000	-12.829000
C	2.938000	-3.536000	-1.444000	C	9.415000	18.070000	-3.382000	C	18.325000	11.381000	-14.844000
H	2.047000	-3.315000	-2.040000	N	8.185000	17.513000	-3.262000	H	17.177000	13.444000	-13.556000
H	3.724000	-3.878000	-2.120000	C	9.555000	19.467000	-3.273000	C	14.252000	14.869000	-12.392000
H	2.695000	-4.346000	-0.753000	C	7.063000	18.241000	-3.037000	O	18.539000	10.815000	-15.942000
C	1.163000	11.481000	3.388000	C	8.416000	20.277000	-3.042000	N	19.371000	11.870000	-14.134000

C	0.538000	10.493000	3.145000	H	10.481000	19.900000	-3.372000	H	19.164000	12.251000	-13.266000
C	-0.150000	9.440000	2.825000	C	7.157000	19.642000	-2.906000	C	20.755000	11.851000	-14.521000
N	0.483000	8.245000	2.733000	C	5.919000	17.628000	-2.999000	H	20.918000	11.382000	-15.496000
C	-1.523000	9.523000	2.517000	C	8.537000	21.682000	-2.996000	H	21.132000	12.874000	-14.565000
C	-0.144000	7.107000	2.350000	H	6.312000	20.198000	-2.741000	H	21.330000	11.300000	-13.774000
C	-2.231000	8.367000	2.099000	C	4.857000	17.082000	-3.008000	C	6.014000	6.173000	-15.886000
H	-2.005000	10.426000	2.583000	O	9.366000	22.242000	-3.752000	C	7.170000	5.885000	-15.965000
C	-1.517000	7.142000	2.031000	N	7.784000	22.441000	-2.162000	C	8.422000	5.571000	-16.100000
C	0.558000	6.021000	2.231000	H	7.199000	21.966000	-1.549000	N	9.370000	6.418000	-15.631000
C	-3.596000	8.454000	1.737000	C	7.785000	23.875000	-2.071000	C	8.814000	4.394000	-16.768000
H	-1.986000	6.284000	1.724000	H	8.486000	24.346000	-2.767000	C	10.700000	6.188000	-15.769000
C	1.208000	5.034000	2.064000	H	6.783000	24.251000	-2.286000	C	10.190000	4.106000	-16.945000
O	-4.059000	9.553000	1.344000	H	8.057000	24.173000	-1.056000	H	8.104000	3.752000	-17.137000
N	-4.423000	7.379000	1.803000	C	14.729000	10.268000	-6.516000	C	11.140000	5.015000	-16.418000
H	-4.024000	6.553000	2.117000	C	14.935000	11.387000	-6.153000	C	11.531000	7.088000	-15.341000
C	-5.820000	7.344000	1.472000	C	15.175000	12.613000	-5.799000	C	10.589000	2.964000	-17.672000
H	-6.207000	8.319000	1.159000	N	14.166000	13.368000	-5.300000	H	12.144000	4.839000	-16.531000
H	-5.985000	6.634000	0.660000	C	16.451000	13.187000	-5.967000	C	12.298000	7.935000	-14.996000
H	-6.391000	7.016000	2.343000	C	14.321000	14.668000	-4.946000	O	9.910000	2.614000	-18.667000
C	7.600000	15.596000	3.741000	C	16.669000	14.542000	-5.616000	N	11.686000	2.243000	-17.333000
C	6.410000	15.657000	3.823000	H	17.219000	12.628000	-6.355000	H	12.154000	2.518000	-16.528000
C	5.116000	15.754000	3.859000	C	15.585000	15.280000	-5.082000	C	12.210000	1.098000	-18.026000
N	4.369000	14.624000	3.829000	C	13.284000	15.333000	-4.536000	H	11.619000	0.825000	-18.906000
C	4.475000	17.009000	3.872000	C	17.926000	15.144000	-5.841000	H	13.231000	1.308000	-18.351000
C	3.014000	14.637000	3.808000	H	15.707000	16.264000	-4.821000	H	12.230000	0.244000	-17.347000
C	3.059000	17.087000	3.839000	C	12.329000	15.968000	-4.203000	C	0.258000	11.108000	-14.947000
H	5.037000	17.867000	3.893000	O	18.585000	14.807000	-6.854000	C	0.524000	9.982000	-15.243000
C	2.330000	15.871000	3.818000	N	18.438000	16.073000	-4.997000	C	0.794000	8.765000	-15.608000
C	2.377000	13.509000	3.719000	H	17.927000	16.261000	-4.193000	N	2.070000	8.315000	-15.525000
C	2.410000	18.344000	3.799000	C	19.675000	16.787000	-5.155000	C	-0.204000	7.920000	-16.133000
H	1.306000	15.879000	3.784000	H	20.216000	16.506000	-6.064000	C	2.443000	7.073000	-15.922000
C	1.776000	12.487000	3.580000	H	19.471000	17.859000	-5.195000	C	0.130000	6.615000	-16.569000
O	3.023000	19.339000	3.342000	H	20.320000	16.587000	-4.297000	H	-1.172000	8.255000	-16.210000
N	1.136000	18.504000	4.241000	C	10.214000	4.506000	-8.691000	C	1.475000	6.188000	-16.442000
H	0.703000	17.711000	4.591000	C	11.354000	4.846000	-8.587000	C	3.698000	6.750000	-15.859000
C	0.375000	19.723000	4.256000	C	12.597000	5.215000	-8.519000	C	-0.851000	5.786000	-17.154000
H	0.941000	20.581000	3.881000	N	12.902000	6.402000	-7.940000	H	1.752000	5.250000	-16.749000
H	-0.516000	19.604000	3.636000	C	13.628000	4.432000	-9.076000	C	4.856000	6.460000	-15.851000
H	0.062000	19.942000	5.278000	C	14.167000	6.885000	-7.865000	O	-1.723000	6.308000	-17.889000
C	14.170000	12.162000	1.891000	C	14.969000	4.889000	-9.029000	N	-0.873000	4.446000	-16.948000
C	13.692000	13.201000	2.234000	H	13.407000	3.537000	-9.527000	H	-0.206000	4.091000	-16.338000
C	13.179000	14.350000	2.551000	C	15.232000	6.129000	-8.398000	C	-1.800000	3.505000	-17.511000
N	11.868000	14.416000	2.887000	C	14.357000	8.060000	-7.347000	H	-2.553000	3.978000	-18.149000
C	13.942000	15.534000	2.497000	C	16.000000	4.143000	-9.640000	H	-1.255000	2.773000	-18.110000
C	11.240000	15.581000	3.177000	H	16.190000	6.492000	-8.350000	H	-2.315000	2.980000	-16.704000
C	13.336000	16.786000	2.777000	C	14.538000	9.158000	-6.913000	C	2.024000	18.408000	-13.521000
H	14.934000	15.489000	2.240000	O	15.747000	3.511000	-10.694000	C	1.117000	17.646000	-13.674000
C	11.963000	16.791000	3.134000	N	17.254000	4.092000	-9.124000	C	0.116000	16.845000	-13.882000
C	9.967000	15.559000	3.432000	H	17.386000	4.532000	-8.269000	N	0.347000	15.517000	-14.029000
C	14.083000	17.983000	2.673000	C	18.392000	3.426000	-9.695000	C	-1.199000	17.337000	-14.006000
H	11.482000	17.673000	3.335000	H	18.162000	2.924000	-10.640000	C	-0.637000	14.621000	-14.292000
C	8.786000	15.564000	3.612000	H	19.183000	4.156000	-9.878000	C	-2.265000	16.447000	-14.286000
O	15.086000	18.018000	1.920000	H	18.763000	2.678000	-8.991000	H	-1.383000	18.341000	-13.904000
N	13.742000	19.101000	3.366000	C	2.682000	5.789000	-8.729000	C	-1.970000	15.067000	-14.414000
H	12.963000	19.027000	3.939000	C	3.520000	4.968000	-8.952000	C	-0.315000	13.377000	-14.475000
C	14.421000	20.366000	3.348000	C	4.418000	4.075000	-9.239000	C	-3.574000	16.941000	-14.474000
H	15.310000	20.363000	2.710000	N	5.719000	4.332000	-8.959000	H	-2.717000	14.396000	-14.620000
H	13.741000	21.139000	2.984000	C	4.072000	2.866000	-9.876000	C	-0.023000	12.239000	-14.690000
H	14.733000	20.625000	4.362000	C	6.723000	3.473000	-9.263000	O	-3.728000	18.046000	-15.048000
C	13.663000	5.051000	-0.796000	C	5.081000	1.932000	-10.218000	N	-4.665000	16.252000	-14.056000
C	14.438000	5.926000	-0.546000	H	3.091000	2.667000	-10.102000	H	-4.497000	15.425000	-13.577000
C	15.283000	6.887000	-0.331000	C	6.423000	2.244000	-9.887000	C	-6.039000	16.637000	-14.221000
N	14.852000	8.013000	0.288000	C	7.947000	3.829000	-9.014000	H	-6.153000	17.601000	-14.726000
C	16.618000	6.809000	-0.775000	C	4.753000	0.746000	-10.910000	H	-6.559000	15.878000	-14.808000
C	15.650000	9.088000	0.503000	H	7.179000	1.593000	-10.124000	H	-6.514000	16.704000	-13.240000
C	17.498000	7.907000	-0.589000	C	9.078000	4.166000	-8.832000	C	9.392000	20.378000	-13.824000
H	16.949000	5.960000	-1.246000	O	3.829000	0.776000	-11.758000	C	8.292000	20.799000	-13.625000
C	16.993000	9.055000	0.074000	N	5.406000	-0.420000	-10.683000	C	7.100000	21.283000	-13.451000
C	15.132000	10.146000	1.049000	H	6.063000	-0.415000	-9.968000	N	6.040000	20.439000	-13.419000

C	18.825000	7.855000	-1.080000	C	5.201000	-1.667000	-11.368000	C	6.883000	22.671000	-13.344000
H	17.589000	9.876000	0.221000	H	4.423000	-1.607000	-12.136000	C	4.759000	20.865000	-13.287000
C	14.652000	11.143000	1.497000	H	6.133000	-1.973000	-11.847000	C	5.565000	23.174000	-13.211000
O	19.097000	7.085000	-2.033000	H	4.912000	-2.433000	-10.646000	H	7.678000	23.319000	-13.375000
N	19.815000	8.618000	-0.549000	C	0.233000	12.887000	-7.257000	C	4.495000	22.246000	-13.169000
H	19.561000	9.194000	0.188000	C	-0.125000	11.780000	-7.531000	C	3.804000	19.987000	-13.325000
C	21.193000	8.648000	-0.955000	C	-0.531000	10.593000	-7.868000	C	5.334000	24.566000	-13.166000
H	21.412000	7.945000	-1.765000	N	0.368000	9.580000	-7.932000	H	3.528000	22.575000	-13.077000
H	21.451000	9.653000	-1.294000	C	-1.876000	10.346000	-8.210000	C	2.919000	19.189000	-13.404000
H	21.828000	8.393000	-0.104000	C	0.037000	8.320000	-8.310000	O	6.052000	25.322000	-13.863000
C	6.646000	2.264000	-2.072000	C	-2.277000	9.049000	-8.615000	N	4.358000	25.104000	-12.395000
C	7.812000	2.016000	-2.130000	H	-2.562000	11.109000	-8.179000	H	3.857000	24.487000	-11.837000
C	9.075000	1.743000	-2.257000	C	-1.301000	8.023000	-8.644000	C	4.010000	26.494000	-12.295000
N	9.993000	2.609000	-1.763000	C	0.975000	7.427000	-8.406000	H	4.643000	27.137000	-12.914000
C	9.507000	0.594000	-2.950000	C	-3.606000	8.806000	-9.023000	H	2.972000	26.631000	-12.606000
C	11.329000	2.427000	-1.907000	H	-1.557000	7.074000	-8.935000	H	4.106000	26.816000	-11.256000
C	10.891000	0.356000	-3.143000	C	1.833000	6.608000	-8.546000	C	14.301000	15.042000	-16.192000
H	8.815000	-0.063000	-3.327000	O	-4.212000	9.696000	-9.666000	C	14.222000	16.173000	-15.817000
C	11.806000	1.292000	-2.596000	N	-4.241000	7.641000	-8.745000	C	14.148000	17.417000	-15.451000
C	12.139000	3.336000	-1.456000	H	-3.759000	7.008000	-8.188000	N	12.959000	17.912000	-15.026000
C	11.329000	-0.766000	-3.887000	C	-5.564000	7.264000	-9.160000	C	15.265000	18.274000	-15.527000
H	12.816000	1.165000	-2.719000	H	-6.058000	8.035000	-9.759000	C	12.782000	19.207000	-14.666000
C	12.896000	4.188000	-1.099000	H	-5.510000	6.350000	-9.754000	C	15.138000	19.639000	-15.167000
O	10.559000	-1.281000	-4.734000	H	-6.177000	7.070000	-8.278000	H	16.168000	17.912000	-15.854000
N	12.565000	-1.301000	-3.710000	C	5.531000	18.337000	-6.476000	C	13.874000	20.098000	-14.719000
H	13.123000	-0.874000	-3.042000	C	4.355000	18.128000	-6.465000	C	11.593000	19.601000	-14.327000
C	13.121000	-2.434000	-4.396000	C	3.071000	17.929000	-6.490000	C	16.236000	20.518000	-15.295000
H	12.417000	-2.892000	-5.099000	N	2.596000	16.663000	-6.590000	H	13.744000	21.081000	-14.456000
H	14.008000	-2.125000	-4.951000	C	2.163000	19.007000	-6.461000	C	10.493000	19.980000	-14.057000
H	13.412000	-3.192000	-3.666000	C	1.273000	16.372000	-6.661000	O	17.035000	20.356000	-16.248000
C	0.682000	6.944000	-1.227000	C	0.770000	18.762000	-6.535000	N	16.447000	21.534000	-14.423000
C	0.987000	5.827000	-1.516000	H	2.512000	19.970000	-6.400000	H	15.832000	21.596000	-13.675000
C	1.310000	4.623000	-1.875000	C	0.328000	17.419000	-6.617000	C	17.503000	22.507000	-14.474000
N	2.606000	4.237000	-1.785000	C	0.915000	15.134000	-6.821000	H	18.187000	22.348000	-15.313000
C	0.355000	3.729000	-2.400000	C	-0.142000	19.839000	-6.574000	H	17.072000	23.505000	-14.565000
C	3.042000	3.018000	-2.184000	H	-0.673000	17.206000	-6.674000	H	18.080000	22.460000	-13.547000
C	0.757000	2.443000	-2.839000	C	0.579000	14.004000	-7.018000	C	11.408000	8.399000	-18.685000
H	-0.628000	4.014000	-2.475000	O	0.179000	20.880000	-7.194000	C	12.422000	9.004000	-18.502000
C	2.123000	2.090000	-2.717000	N	-1.352000	19.780000	-5.964000	C	13.533000	9.662000	-18.349000
C	4.310000	2.752000	-2.100000	H	-1.530000	18.984000	-5.438000	N	13.510000	10.877000	-17.747000
C	-0.181000	1.560000	-3.416000	C	-2.376000	20.787000	-5.988000	C	14.756000	9.156000	-18.835000
H	2.451000	1.171000	-3.034000	H	-2.097000	21.665000	-6.579000	C	14.618000	11.643000	-17.583000
C	5.478000	2.509000	-2.064000	H	-3.289000	20.365000	-6.411000	C	15.945000	9.915000	-18.694000
O	-1.115000	2.036000	-4.106000	H	-2.584000	21.114000	-4.967000	H	14.784000	8.242000	-19.300000
N	-0.097000	0.217000	-3.241000	C	12.795000	16.428000	-7.900000	C	15.865000	11.170000	-18.042000
H	0.611000	-0.100000	-2.656000	C	12.077000	17.327000	-7.578000	C	14.494000	12.821000	-17.049000
C	-0.965000	-0.778000	-3.805000	C	11.314000	18.331000	-7.266000	C	17.162000	9.443000	-19.232000
H	-1.779000	-0.348000	-4.397000	N	9.995000	18.117000	-7.037000	H	16.705000	11.747000	-17.927000
H	-0.385000	-1.441000	-4.450000	C	11.822000	19.644000	-7.207000	C	14.391000	13.924000	-16.601000
H	-1.406000	-1.372000	-3.001000	C	9.124000	19.115000	-6.742000	O	17.142000	8.804000	-20.311000
C	2.265000	14.270000	0.213000	C	10.958000	20.726000	-6.908000	N	18.352000	9.667000	-18.620000
C	1.372000	13.493000	0.059000	H	12.816000	19.819000	-7.393000	H	18.323000	10.126000	-17.765000
C	0.389000	12.671000	-0.150000	C	9.593000	20.443000	-6.655000	C	19.649000	9.267000	-19.091000
N	0.654000	11.352000	-0.307000	C	7.866000	18.823000	-6.601000	H	19.609000	8.718000	-20.036000
C	-0.939000	13.129000	-0.265000	C	11.447000	22.050000	-6.913000	H	20.272000	10.153000	-19.234000
C	-0.306000	10.432000	-0.575000	H	8.939000	21.203000	-6.437000	H	20.122000	8.627000	-18.342000
C	-1.981000	12.213000	-0.550000	C	6.701000	18.570000	-6.519000	C	3.809000	7.944000	-19.284000
H	-1.149000	14.128000	-0.155000	O	12.319000	22.369000	-7.756000	C	4.826000	7.336000	-19.439000
C	-1.650000	10.843000	-0.692000	N	11.004000	22.985000	-6.037000	C	5.921000	6.663000	-19.645000
C	0.049000	9.198000	-0.761000	H	10.383000	22.679000	-5.357000	N	7.114000	7.206000	-19.294000
C	-3.305000	12.669000	-0.728000	C	11.390000	24.368000	-5.988000	C	5.897000	5.391000	-20.253000
H	-2.379000	10.153000	-0.904000	H	12.112000	24.636000	-6.765000	C	8.301000	6.582000	-19.495000
C	0.370000	8.068000	-0.975000	H	10.505000	24.995000	-6.112000	C	7.106000	4.687000	-20.487000
O	-3.490000	13.782000	-1.276000	H	11.837000	24.585000	-5.016000	H	5.000000	4.976000	-20.530000
N	-4.372000	11.936000	-0.325000	C	14.189000	9.431000	-10.639000	C	8.320000	5.301000	-20.088000
H	-4.178000	11.109000	0.146000	C	14.703000	10.461000	-10.320000	C	9.394000	7.207000	-19.168000
C	-5.758000	12.275000	-0.490000	C	15.277000	11.587000	-10.017000	C	7.084000	3.426000	-21.129000
H	-5.904000	13.248000	-0.968000	N	14.542000	12.574000	-9.448000	H	9.216000	4.829000	-20.248000
H	-6.246000	11.514000	-1.104000	C	16.637000	11.817000	-10.308000	C	10.400000	7.798000	-18.906000

H	-6.244000	12.298000	0.487000	C	15.054000	13.790000	-9.133000	O	6.169000	3.173000	-21.948000
C	9.600000	16.406000	-0.028000	C	17.224000	13.070000	-10.002000	N	8.018000	2.472000	-20.882000
C	8.488000	16.797000	0.163000	H	17.199000	11.082000	-10.752000	H	8.672000	2.667000	-20.191000
C	7.284000	17.251000	0.331000	C	16.415000	14.058000	-9.389000	C	8.117000	1.182000	-21.509000
N	6.244000	16.382000	0.345000	C	14.257000	14.696000	-8.652000	H	7.326000	1.003000	-22.245000
C	7.033000	18.633000	0.449000	C	18.567000	13.330000	-10.348000	H	9.081000	1.099000	-22.014000
C	4.953000	16.777000	0.468000	H	16.808000	14.976000	-9.156000	H	8.056000	0.405000	-20.744000
C	5.702000	19.102000	0.573000	C	13.523000	15.551000	-8.256000	C	-0.178000	14.326000	-17.961000
H	7.813000	19.300000	0.431000	O	19.018000	12.861000	-11.420000	C	-0.277000	13.168000	-18.240000
C	4.654000	18.149000	0.596000	N	19.381000	14.073000	-9.558000	C	-0.410000	11.916000	-18.572000
C	4.018000	15.878000	0.419000	H	19.012000	14.358000	-8.706000	N	0.688000	11.124000	-18.635000
C	5.437000	20.487000	0.629000	C	20.740000	14.447000	-9.835000	C	-1.671000	11.372000	-18.892000
H	3.679000	18.455000	0.680000	H	21.100000	14.065000	-10.795000	C	0.641000	9.817000	-18.996000
C	3.147000	15.065000	0.333000	H	20.820000	15.536000	-9.848000	C	-1.787000	10.010000	-19.272000
O	6.152000	21.266000	-0.046000	H	21.390000	14.060000	-9.047000	H	-2.507000	11.966000	-18.855000
N	4.435000	20.992000	1.390000	C	8.180000	5.042000	-12.371000	C	-0.603000	9.230000	-19.312000
H	3.948000	20.358000	1.943000	C	9.374000	5.078000	-12.362000	C	1.757000	9.151000	-19.066000
C	4.045000	22.371000	1.494000	C	10.673000	5.115000	-12.399000	C	-3.047000	9.472000	-19.626000
H	4.677000	23.037000	0.898000	N	11.320000	6.175000	-11.854000	H	-0.642000	8.244000	-19.591000
H	3.013000	22.482000	1.155000	C	11.419000	4.102000	-13.035000	C	2.785000	8.547000	-19.160000
H	4.106000	22.687000	2.537000	C	12.669000	6.313000	-11.882000	O	-3.919000	10.229000	-20.117000
C	14.728000	11.241000	-2.339000	C	12.831000	4.196000	-13.096000	N	-3.353000	8.161000	-19.443000
C	14.600000	12.367000	-1.962000	H	10.939000	3.304000	-13.465000	H	-2.688000	7.612000	-18.998000
C	14.475000	13.607000	-1.598000	C	13.457000	5.313000	-12.491000	C	-4.579000	7.506000	-19.806000
N	13.263000	14.057000	-1.190000	C	13.197000	7.394000	-11.394000	H	-5.307000	8.182000	-20.264000
C	15.560000	14.503000	-1.664000	C	13.582000	3.222000	-13.789000	H	-4.364000	6.703000	-20.514000
C	13.034000	15.346000	-0.838000	H	14.478000	5.412000	-12.519000	H	-5.032000	7.068000	-18.914000
C	15.376000	15.864000	-1.314000	C	13.688000	8.407000	-10.995000	C	3.771000	20.781000	-16.851000
H	16.479000	14.174000	-1.979000	O	13.116000	2.742000	-14.849000	C	2.669000	20.319000	-16.895000
C	14.092000	16.278000	-0.882000	N	14.792000	2.799000	-13.347000	C	1.459000	19.845000	-16.964000
C	11.828000	15.697000	-0.513000	H	15.083000	3.148000	-12.490000	N	1.275000	18.514000	-17.152000
C	16.441000	16.782000	-1.440000	C	15.667000	1.865000	-14.000000	C	0.333000	20.689000	-16.873000
H	13.923000	17.256000	-0.625000	H	15.268000	1.502000	-14.953000	C	0.049000	17.942000	-17.260000
C	10.714000	16.041000	-0.253000	H	16.629000	2.343000	-14.191000	C	-0.976000	20.151000	-16.972000
O	17.253000	16.635000	-2.385000	H	15.829000	1.005000	-13.347000	H	0.463000	21.698000	-16.739000
N	16.607000	17.810000	-0.571000	C	1.262000	8.263000	-11.879000	C	-1.104000	18.751000	-17.162000
H	15.991000	17.851000	0.179000	C	1.844000	7.256000	-12.151000	C	-0.024000	16.662000	-17.479000
C	17.624000	18.824000	-0.625000	C	2.453000	6.160000	-12.493000	C	-2.106000	21.001000	-16.914000
H	18.324000	18.681000	-1.454000	N	3.792000	6.056000	-12.307000	H	-2.031000	18.324000	-17.249000
H	17.154000	19.803000	-0.737000	C	1.754000	5.095000	-13.096000	C	-0.095000	15.491000	-17.707000
H	18.192000	18.815000	0.307000	C	4.507000	4.961000	-12.670000	O	-1.996000	22.191000	-17.296000
C	12.077000	4.537000	-4.846000	C	2.450000	3.928000	-13.496000	N	-3.309000	20.577000	-16.447000
C	13.075000	5.163000	-4.655000	H	0.743000	5.169000	-13.256000	H	-3.350000	19.674000	-16.091000
C	14.167000	5.847000	-4.495000	C	3.845000	3.863000	-13.259000	C	-4.526000	21.340000	-16.388000
N	14.103000	7.062000	-3.899000	C	5.797000	4.978000	-12.513000	H	-4.410000	22.361000	-16.765000
C	15.406000	5.373000	-4.973000	C	1.767000	2.885000	-14.156000	H	-5.293000	20.840000	-16.982000
C	15.185000	7.862000	-3.734000	H	4.379000	3.033000	-13.540000	H	-4.868000	21.394000	-15.352000
C	16.569000	6.170000	-4.832000	C	6.987000	5.007000	-12.420000	C	11.366000	20.543000	-17.814000
H	15.463000	4.458000	-5.434000	O	0.871000	3.177000	-14.983000	C	10.450000	21.252000	-17.519000
C	16.448000	7.426000	-4.188000	N	2.056000	1.581000	-13.924000	C	9.466000	22.052000	-17.222000
C	15.018000	9.034000	-3.201000	H	2.715000	1.400000	-13.234000	N	8.207000	21.556000	-17.132000
C	17.802000	5.732000	-5.361000	C	1.464000	0.442000	-14.571000	C	9.679000	23.430000	-17.017000
H	17.269000	8.030000	-4.073000	H	0.721000	0.720000	-15.325000	C	7.124000	22.325000	-16.853000
C	14.869000	10.130000	-2.752000	H	2.246000	-0.143000	-15.059000	C	8.589000	24.286000	-16.714000
O	17.804000	5.083000	-6.435000	H	0.976000	-0.185000	-13.822000	H	10.627000	23.816000	-17.091000
N	18.979000	5.996000	-4.741000	C	0.870000	15.743000	-10.344000	C	7.297000	23.708000	-16.627000
H	18.927000	6.448000	-3.883000	C	0.219000	14.769000	-10.574000	C	5.949000	21.765000	-16.827000
C	20.292000	5.641000	-5.203000	C	-0.509000	13.733000	-10.864000	C	8.797000	25.676000	-16.538000
H	20.275000	5.070000	-6.136000	N	0.080000	12.516000	-10.976000	H	6.481000	24.293000	-16.422000
H	20.876000	6.548000	-5.366000	C	-1.891000	13.857000	-11.110000	C	4.864000	21.264000	-16.828000
H	20.791000	5.036000	-4.443000	C	-0.601000	11.393000	-11.313000	O	9.748000	26.233000	-17.137000
C	4.508000	3.759000	-5.492000	C	-2.652000	12.717000	-11.467000	N	8.005000	26.431000	-15.734000
C	5.548000	3.193000	-5.645000	H	-2.344000	14.775000	-11.042000	H	7.320000	25.964000	-15.227000
C	6.670000	2.578000	-5.855000	C	-1.990000	11.467000	-11.550000	C	8.097000	27.849000	-15.522000
N	7.828000	3.173000	-5.478000	C	0.060000	10.284000	-11.460000	H	8.912000	28.314000	-16.086000
C	6.713000	1.329000	-6.507000	C	-4.023000	12.846000	-11.774000	H	7.159000	28.321000	-15.824000
C	9.047000	2.622000	-5.697000	H	-2.511000	10.622000	-11.809000	H	8.259000	28.046000	-14.461000
C	7.961000	0.709000	-6.764000	C	0.666000	9.272000	-11.647000	C	14.419000	14.058000	-20.461000
H	5.843000	0.874000	-6.805000	O	-4.411000	13.864000	-12.394000	C	14.683000	15.163000	-20.091000

C	9.139000	1.368000	-6.335000	N	-4.928000	11.900000	-11.423000	C	14.986000	16.372000	-19.720000
C	10.105000	3.290000	-5.351000	H	-4.594000	11.156000	-10.897000	N	14.008000	17.186000	-19.250000
C	8.020000	-0.511000	-7.469000	C	-6.334000	11.904000	-11.720000	C	16.304000	16.862000	-19.822000
H	10.059000	0.949000	-6.509000	H	-6.646000	12.781000	-12.295000	C	14.232000	18.468000	-18.868000
C	11.087000	3.912000	-5.078000	H	-6.585000	11.010000	-12.294000	C	16.603000	18.191000	-19.429000
O	7.209000	-0.711000	-8.404000	H	-6.899000	11.887000	-10.786000	H	17.047000	16.255000	-20.185000
N	8.933000	-1.466000	-7.162000	C	7.433000	19.632000	-10.060000	C	15.540000	18.994000	-18.940000
H	9.500000	-1.293000	-6.392000	C	6.247000	19.735000	-9.959000	C	13.221000	19.185000	-18.470000
C	9.121000	-2.721000	-7.836000	C	4.958000	19.879000	-9.889000	C	17.919000	18.693000	-19.556000
H	8.422000	-2.868000	-8.665000	N	4.165000	18.780000	-9.924000	H	15.714000	19.964000	-18.658000
H	10.138000	-2.770000	-8.232000	C	4.367000	21.156000	-9.827000	C	12.291000	19.856000	-18.130000
H	8.984000	-3.538000	-7.125000	C	2.811000	18.844000	-9.897000	O	18.657000	18.260000	-20.474000
C	0.178000	9.928000	-4.222000	C	2.956000	21.283000	-9.797000	N	18.418000	19.626000	-18.705000
C	0.140000	8.771000	-4.516000	H	4.958000	21.996000	-9.816000	H	17.848000	19.887000	-17.964000
C	0.085000	7.524000	-4.872000	C	2.175000	20.101000	-9.817000	C	19.716000	20.239000	-18.764000
N	1.224000	6.790000	-4.876000	C	2.134000	17.740000	-10.003000	H	20.326000	19.870000	-19.595000
C	-1.122000	6.933000	-5.297000	C	2.357000	22.560000	-9.795000	H	19.601000	21.319000	-18.876000
C	1.265000	5.493000	-5.272000	H	1.151000	20.157000	-9.800000	H	20.251000	20.041000	-17.833000
C	-1.135000	5.582000	-5.725000	C	1.507000	16.735000	-10.153000	H	8.492000	8.549000	-22.355000
H	-1.988000	7.484000	-5.309000	O	2.879000	23.476000	-10.475000	C	9.398000	8.719000	-22.351000
C	0.080000	4.855000	-5.692000	N	1.233000	22.823000	-9.085000	C	10.572000	8.941000	-22.342000
C	2.410000	4.883000	-5.301000	H	0.896000	22.101000	-8.530000	C	11.850000	9.184000	-22.332000
C	-2.324000	4.998000	-6.212000	C	0.512000	24.065000	-9.044000	N	12.284000	10.359000	-21.816000
H	0.106000	3.877000	-5.997000	H	0.958000	24.837000	-9.678000	C	12.789000	8.267000	-22.846000
C	3.462000	4.323000	-5.376000	H	-0.515000	23.899000	-9.377000	C	13.592000	10.708000	-21.764000
O	-3.115000	5.708000	-6.878000	H	0.489000	24.434000	-8.017000	C	14.174000	8.570000	-22.809000
N	-2.628000	3.696000	-5.984000	C	13.813000	15.906000	-11.996000	H	12.467000	7.378000	-23.246000
H	-2.018000	3.199000	-5.414000	C	13.384000	16.962000	-11.639000	C	14.568000	9.813000	-22.252000
C	-3.777000	2.986000	-6.475000	C	12.934000	18.130000	-11.293000	C	13.896000	11.876000	-21.280000
H	-4.441000	3.615000	-7.076000	N	11.628000	18.264000	-10.953000	C	15.119000	7.661000	-23.340000
H	-3.447000	2.148000	-7.091000	C	13.765000	19.268000	-11.311000	H	15.559000	10.075000	-22.218000
H	-4.348000	2.595000	-5.631000	C	11.070000	19.455000	-10.620000	C	14.160000	12.962000	-20.859000
C	3.787000	16.555000	-3.051000	C	13.234000	20.537000	-10.973000	O	14.788000	6.924000	-24.299000
C	2.708000	16.048000	-3.125000	H	14.751000	19.181000	-11.581000	N	16.373000	7.550000	-22.832000
C	1.527000	15.521000	-3.240000	C	11.868000	20.618000	-10.607000	H	16.573000	8.082000	-22.045000
N	1.415000	14.178000	-3.381000	C	9.796000	19.497000	-10.373000	C	17.424000	6.698000	-23.315000
C	0.366000	16.320000	-3.269000	C	14.044000	21.690000	-11.047000	H	17.124000	6.095000	-24.178000
C	0.225000	13.550000	-3.549000	H	11.451000	21.522000	-10.360000	H	18.280000	7.310000	-23.606000
C	-0.904000	15.716000	-3.445000	C	8.616000	19.554000	-10.196000	H	17.736000	6.022000	-22.516000

Table S3. Cartesian coordinates of optimized helical **poly-PyDE**

4. References

[S1] K. Maeda, L. Hong, T. Nishihara, Y. Nakanishi, Y. Miyauchi, R. Kitaura, N. Ousaka, E. Yashima, H. Ito, K. Itami, *J. Am. Chem. Soc.* 2016, **138**, 11001–11008.

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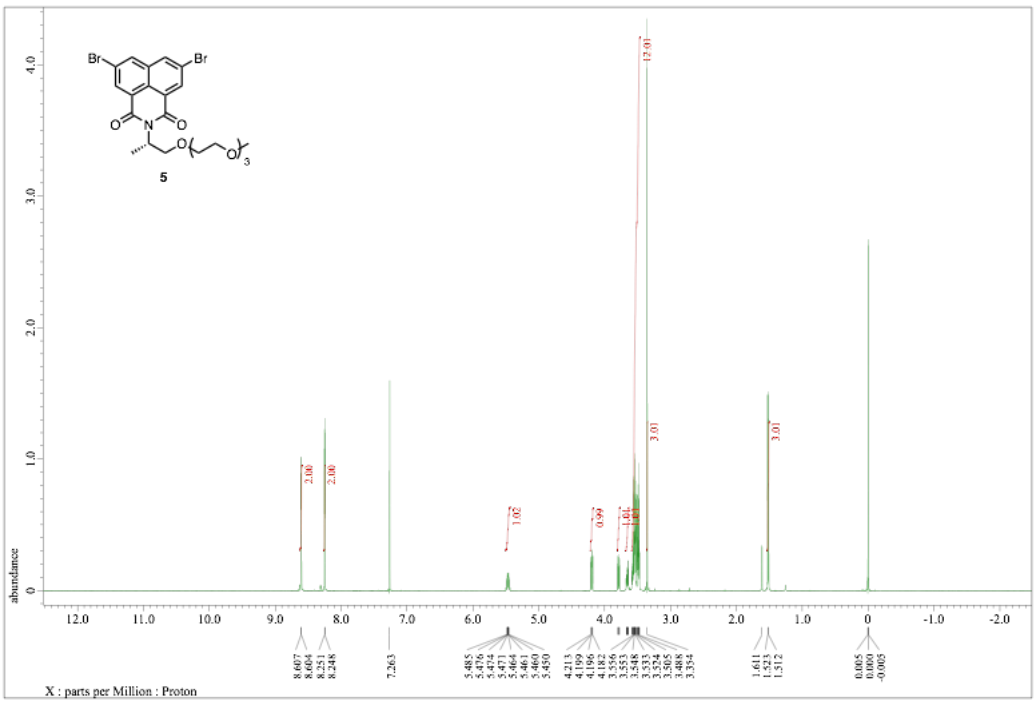
[S3] A. C. Benniston, A. Harriman, S. L. Howell, C. A. Sams, Y. –G. Zhi, *Chem. –Eur. J.* 2007, **13**, 4665–4674.

[S4] H. Makida, H. Abe, M. Inouye, *Org. Biomol. Chem.*, 2015, **13**, 1700–1707.

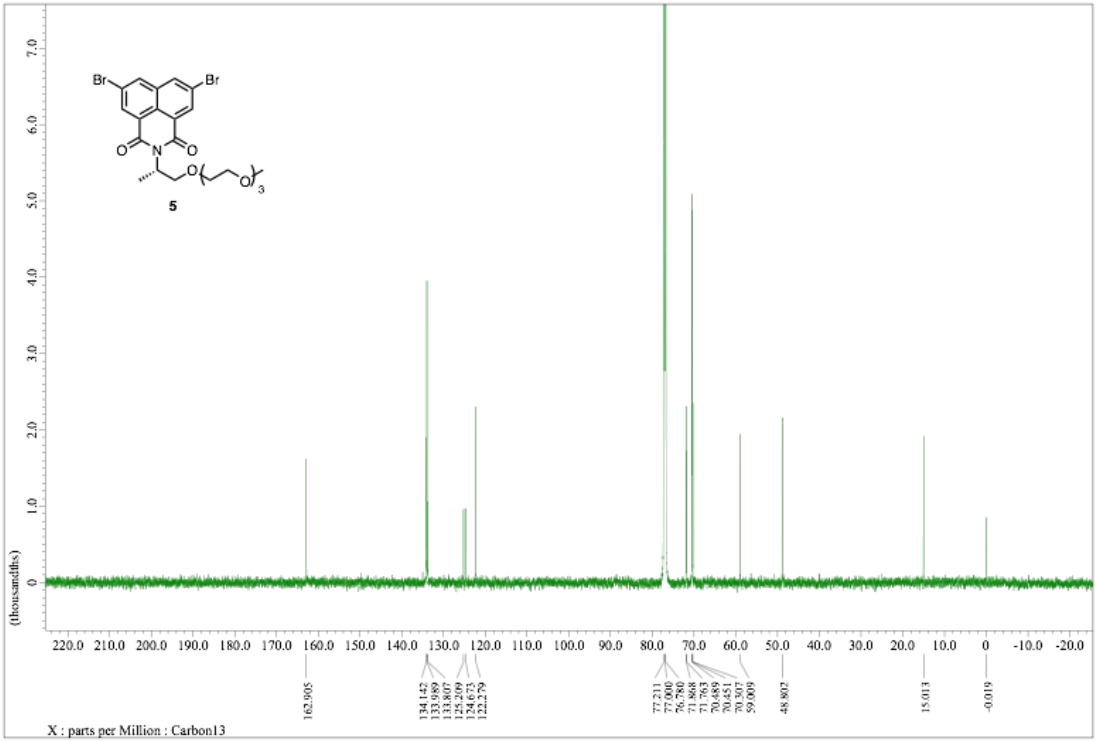
[S5] M. Banno, T. Yamaguchi, K. Nagai, C. Kaiser, S. Hecht, E. Yashima, *J. Am. Chem. Soc*. 2012, **134**, 8718–8728.

5. ^{1}H NMR, ^{13}C NMR Spectra of Products

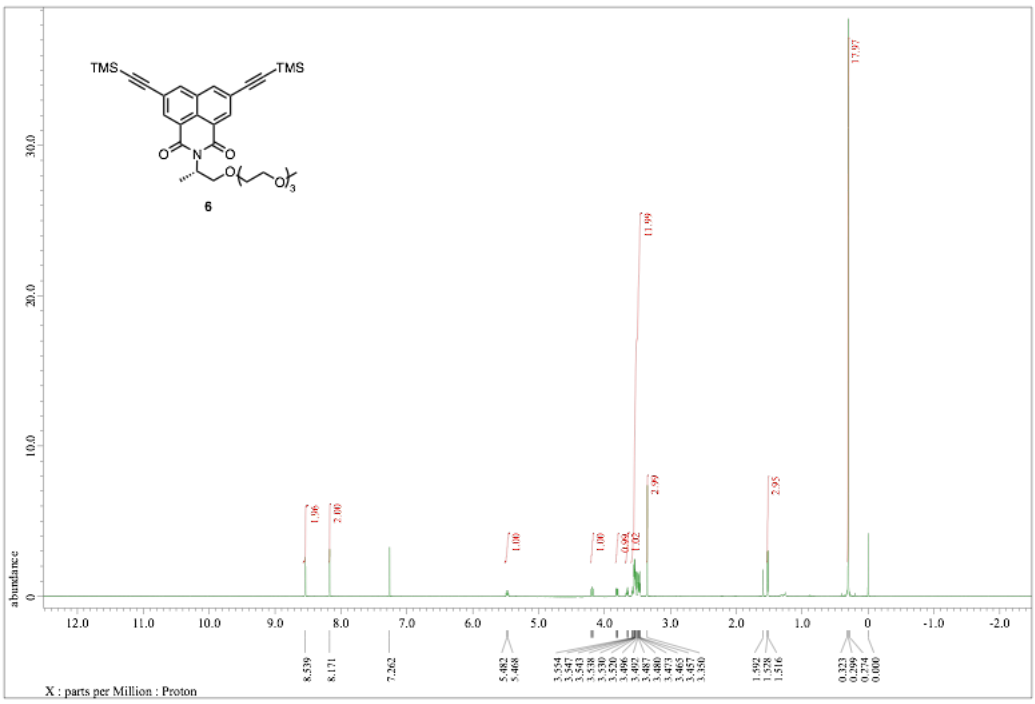
^{1}H NMR spectrum of **5** (600 MHz, $CDCl_3$, 25 °C)



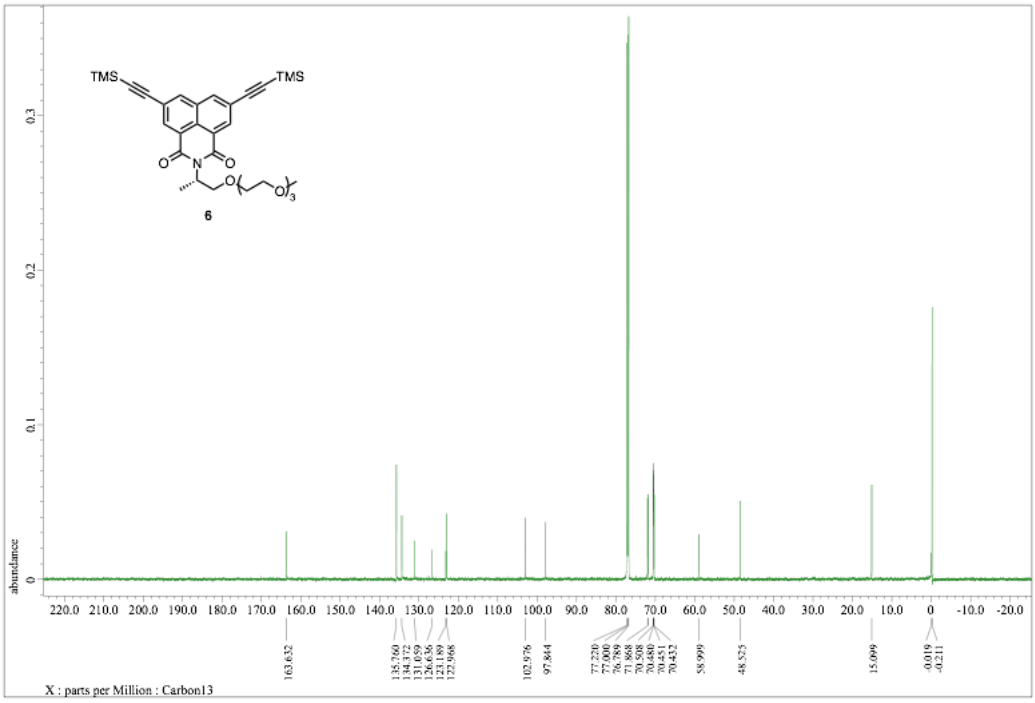
^{13}C NMR spectrum of **5** (150 MHz, $CDCl_3$, 25 °C)



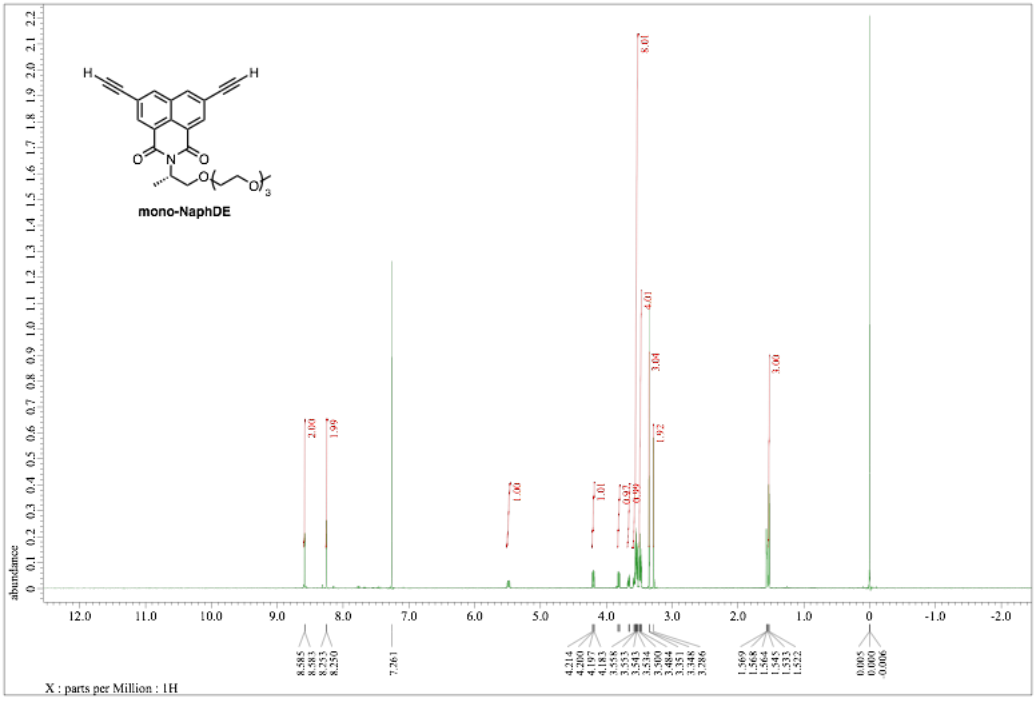
^{1}H NMR spectrum of **6** (600 MHz, $CDCl_3$, 25 °C)



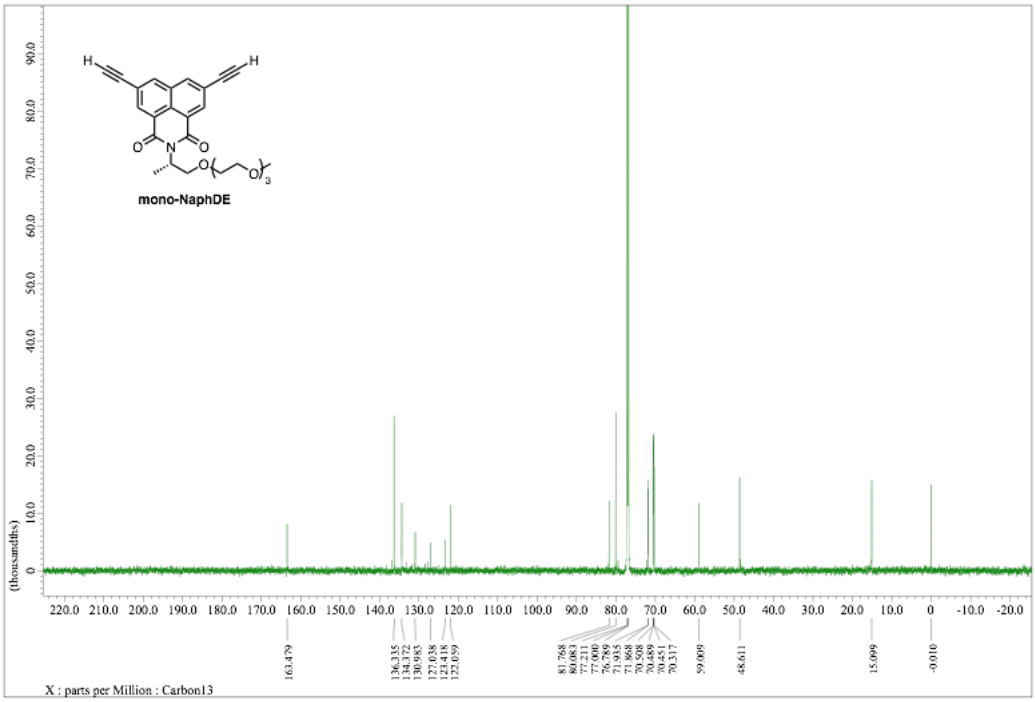
^{13}C NMR spectrum of **6** (150 MHz, $CDCl_3$, 25 °C)



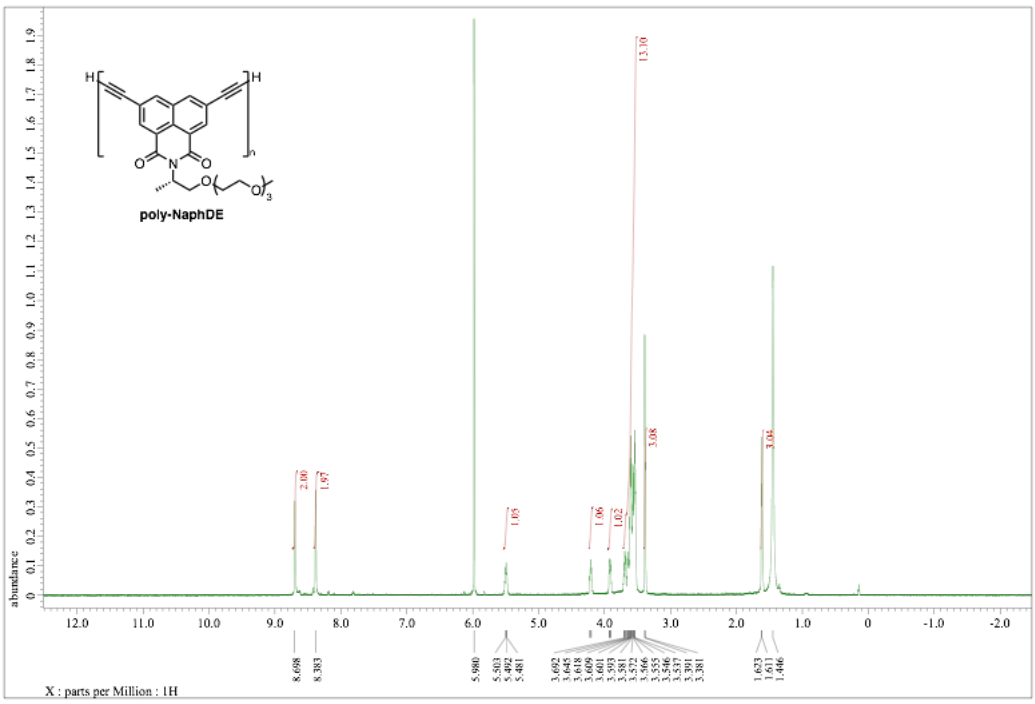
^{1}H NMR spectrum of **mono-NaphDE** (600 MHz, $CDCl_3$, 25 °C)



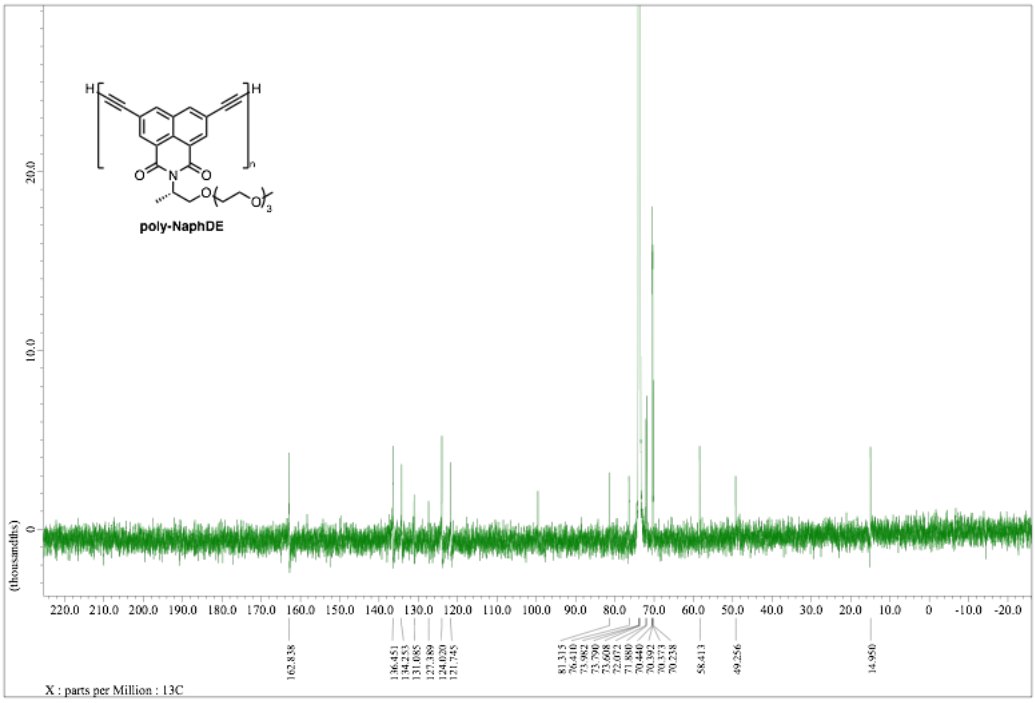
^{13}C NMR spectrum of **mono-NaphDE** (150 MHz, $CDCl_3$, 25 °C)



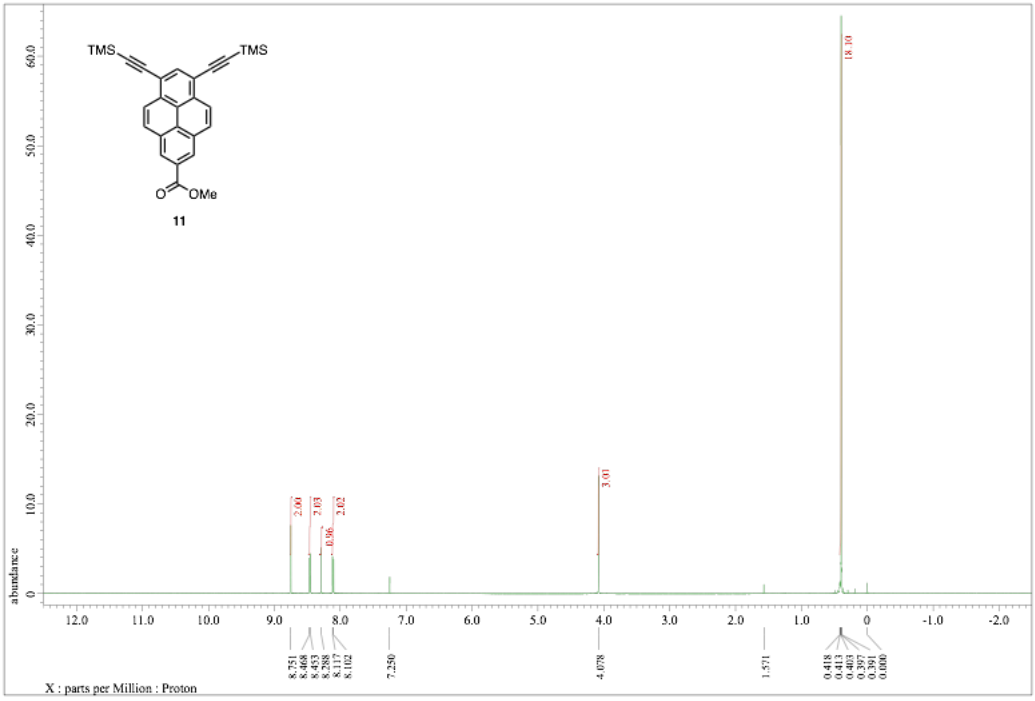
^{1}H NMR spectrum of **poly-NaphDE** (600 MHz, $C_2D_2Cl_4$, 140 °C)



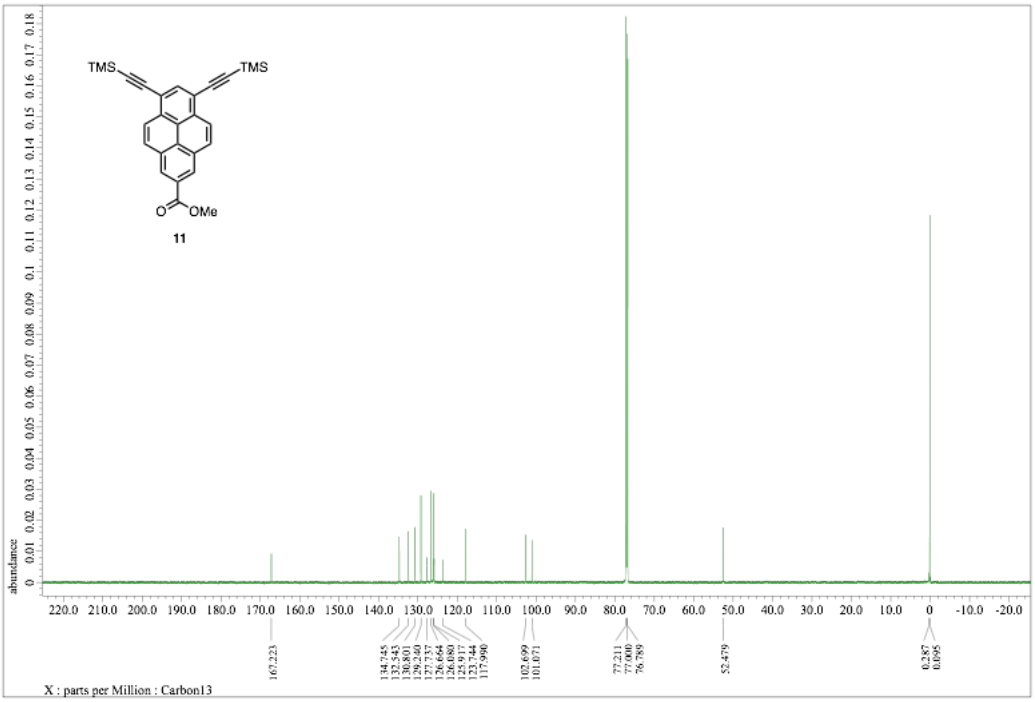
^{13}C NMR spectrum of **poly-NaphDE** (150 MHz, $C_2D_2Cl_4$, 140 °C)



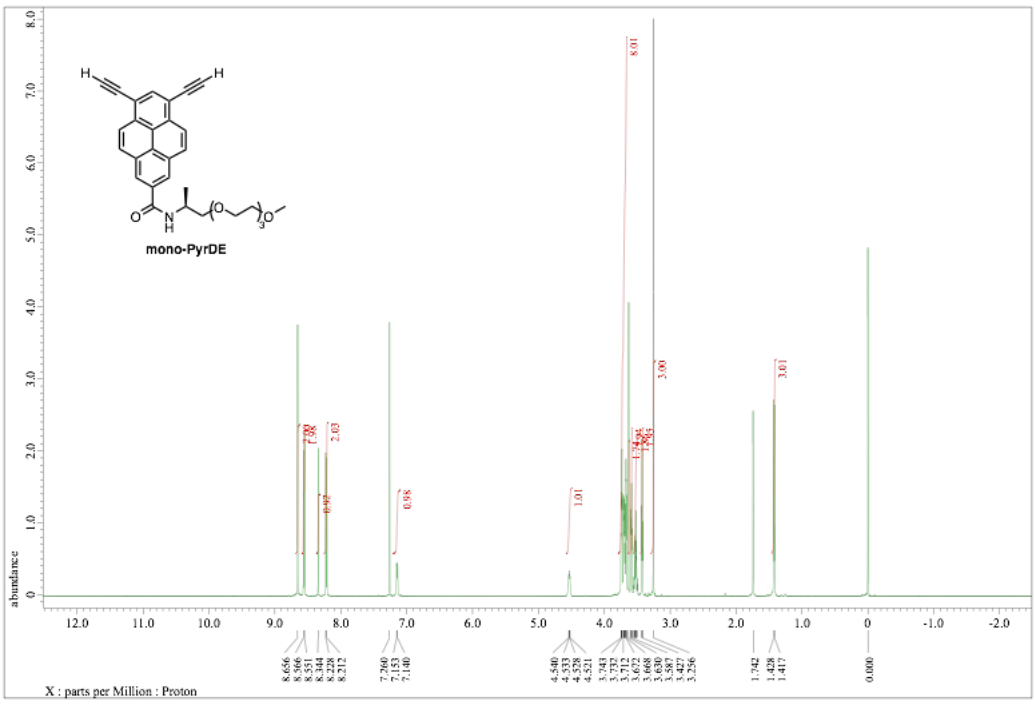
^{1}H NMR spectrum of **11** (600 MHz, $CDCl_3$, 25 °C)



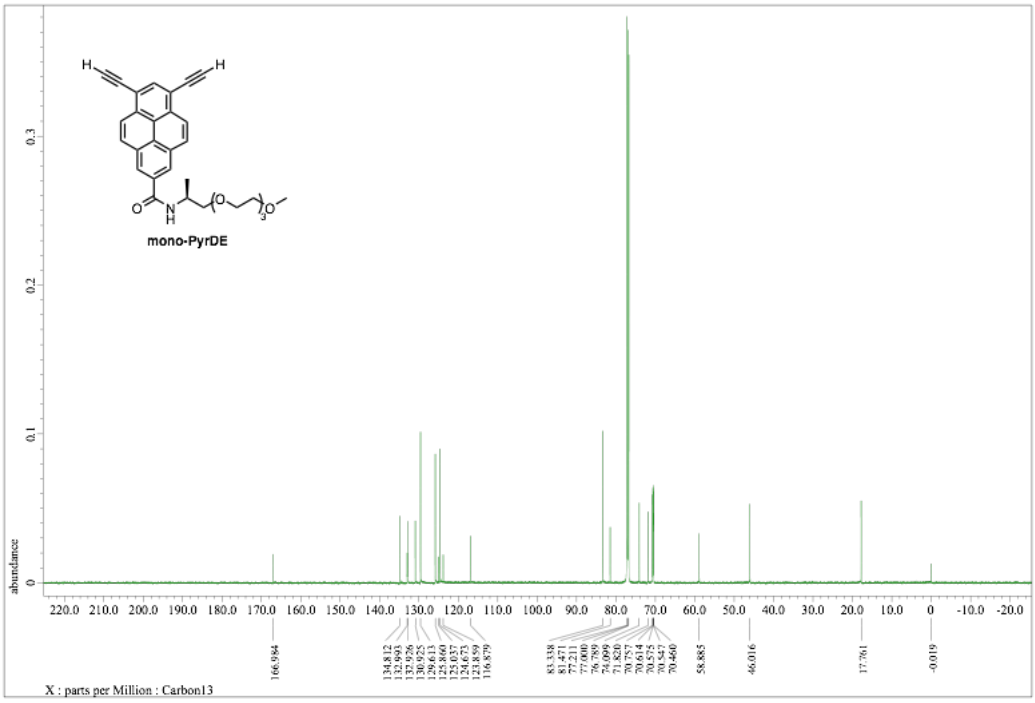
^{13}C NMR spectrum of **11** (150 MHz, $CDCl_3$, 25 °C)



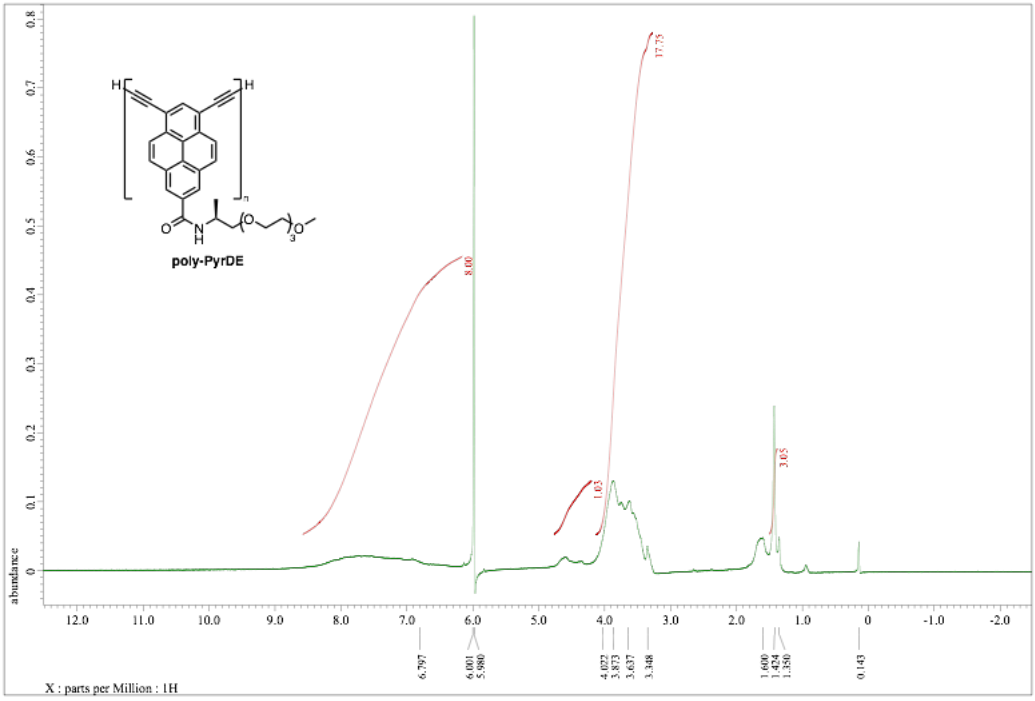
^{1}H NMR spectrum of **mono-PyrDE** (600 MHz, $CDCl_3$, 25 °C)



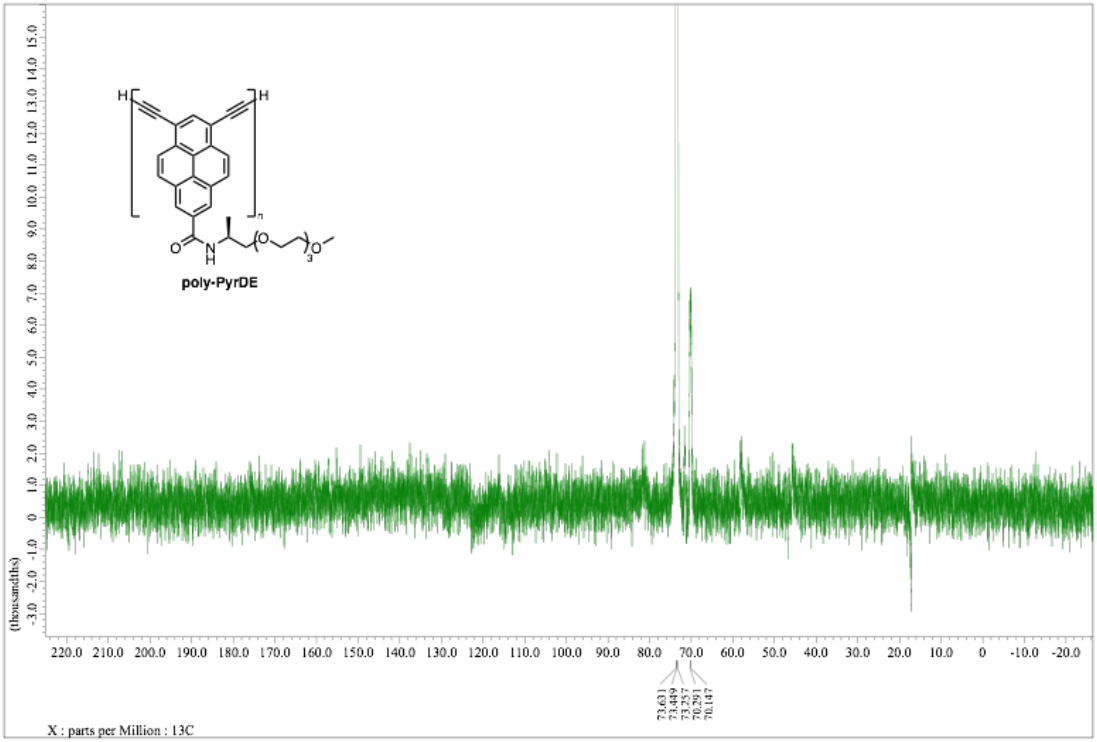
^{13}C NMR spectrum of **mono-PyrDE** (150 MHz, $CDCl_3$, 25 °C)



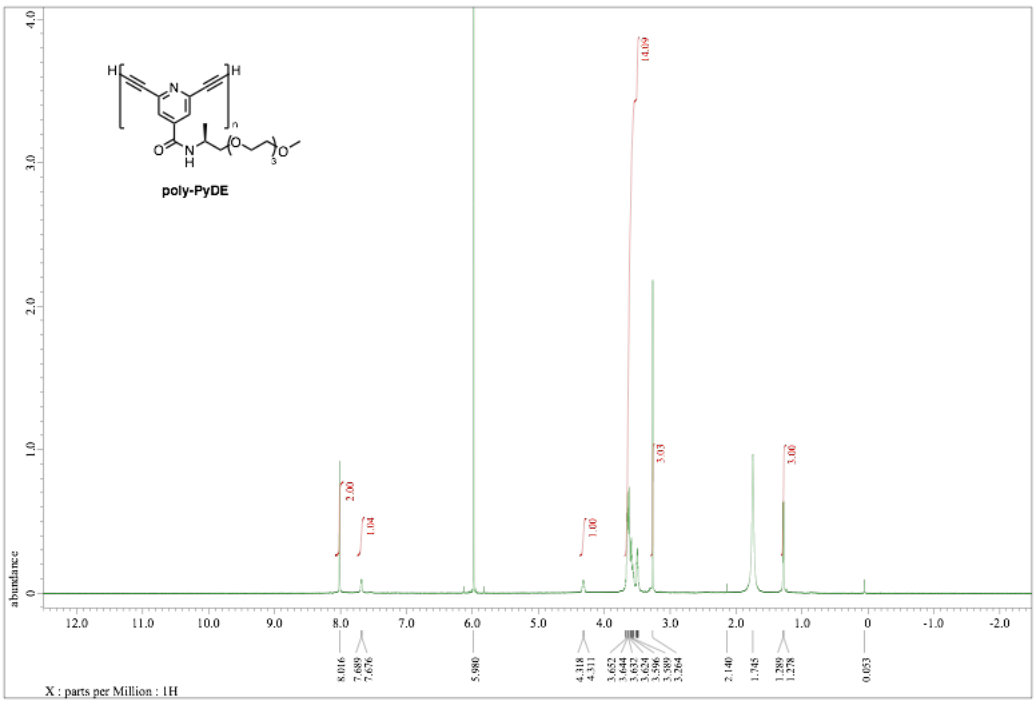
^{1}H NMR spectrum of **poly-PyrDE** (600 MHz, $C_2D_2Cl_4$, 140 °C)



^{13}C NMR spectrum of **poly-PyrDE** (150 MHz, $C_2D_2Cl_4$, 140 °C)



^{1}H NMR spectrum of **poly-PyDE** (600 MHz, $C_2D_2Cl_4$, 25 °C)



^{13}C NMR spectrum of **poly-PyDE** (150 MHz, $C_2D_2Cl_4$, 25 °C)