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Supporting Information

# Metal-Backboned Polymers with Well-Defined Lengths

*K. Zeng, Y. Yang, J. Xu, N. Wang, W. Tang, J. Xu, Y. Zhang, Y. Wu, Y. Xu, G. Wang*, P. Chen, B. Wang, X. Sun, G. Jin, H. Peng**

# Contents

SUPPORTING INFORMATION

## 1. General Information

**Materials.** Anhydrous N,N-dimethylformamide (99.8%) was purchased from Sigma-Aldrich. Deuterated chloroform (D, 99.8%) and dimethyl sulfoxide (D, 99.8%) with 0.03% (v/v) tetramethylsilane as internal standard, were purchased from Cambridge Isotope Laboratories. Trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB, 98.0%) and sodium trifluoroacetate (98.0%) were purchased from Tokyo Chemical Industry. All other reagents and solvents including 4-tert-butylcalix[4]arene (98%), 2,6-diaminopyridine (98%), 2,6-dibromopyridine (98%), bis(2,4-dimethoxybenzyl)amine (98%), tris(dibenzylideneacetone) dipalladium ($Pd_2(dba)_3$, 98%), 1,3-bis(diphenylphosphino)propane (DPPP, 98%), potassium tert-butoxide (*t*-BuOK, 98%), 2-chloropyridine (98%), 4-picoline (98%), pyridine (98%), tetrahydrofuran (THF, 99.8%), trifluoroacetic acid (TFA, 99.5%), N,N-Dimethylformamide (DMF, 99.5%) and xylene (99%) were of reagent grade, purchased from Adamas, and used as received.

**Instruments and methods.** $^{1}H$ and $^{13}C$ nuclear magnetic resonance (NMR) spectra were obtained using a Bruker AVANCE III HD spectrometer (400 M). High resolution mass spectrometry (HRMS) measurements were performed using a Bruker McriOTOF11 spectrometer.

Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) was measured using a AB SCIEX 5800 mass spectrometer using trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile as the matrix and sodium trifluoroacetate as the ionization reagent (when necessary).

Fourier transform infrared (FT-IR) spectra were recorded in the region of 400-4000 $cm^{-1}$ on a Thermofisher Nicolet 6700 FT-IR instrument (KBr Discs).

The Raman shifts were recorded by a Renishaw/NT-MDT In Via Qontor/NTEGRA Spectra II with the excitation wavelength of 532 nm.

The Ni K-edge X-ray absorption spectroscopy (XAS) was recorded in a transmission mode at 1W1B beamline in Beijing Synchrotron Radiation Facility. For Ni K-edge data, the absorption edge energy $E_0$ of pure Ni foil was aligned to 8333 eV. $E_0$ of Ni foil was assigned by the first maximum of first-derivative X-ray absorption near-edge structures spectrum. Data reduction and analysis were performed using the Demeter software package[1].

## SUPPORTING INFORMATION

Ultraviolet-visible spectroscopy spectra (UV-Vis) absorption spectra were recorded on a Perkin-Elmer Lambda 750 spectrophotometer and fluorescence spectra were recorded on a PTI QM40 fluorescence spectrophotometer.

The cyclic voltammograms of the nickel-backboned polymers (NBPs) were obtained in dry $CH_2Cl_2$ with a CHI 660D electrochemical workstation using 0.1 M tetrabutyl ammonium perchlorate as the supporting electrolyte, a glassy carbon electrode as the working electrode, a platinum wire as the counter electrode, and a saturated Ag/AgCl electrode as the reference electrode. The scan rate was 100 mV $s^{-1}$.

Crystallographic data was collected using a SMART APEX system ($Ga_{K\alpha}$, $\lambda$ = 1.34138 Å) equipped with CCD detector (Bruker). Indexing was performed using APEX 2 (difference vectors method). Data integration and reduction were performed using SaintPlus 6.01. Absorption correction was performed by the multis-can method implemented in SADABS. The structure was solved and refined using SHELXTL-97.

Cryogenic transmission electron microscope (Cryo-TEM) images were obtained by a JEM-3200FSC from JEOL, Japan. The frozen holey carbon film was transferred to a JEM-3200FSC, and the entire transfer process was carried out in liquid nitrogen. The JEM-3200FSC was equipped with a 300 kV field emission gun and an energy filter. The patterns were collected by a Gatan charge-coupled device (CCD) camera, and the working temperature of the CCD was −5°C. The function of the energy filter was to enhance the contrast of the pattern, and the width of the energy slit was 20 eV. The loss rate of the pattern was 100 $e^{-}$ $nm^{-2}$ $s^{-1}$. A Leica EM GP Grid Plunger (Leica, Germany) was used to prepare the frozen samples for Cryo-TEM characterization. The holey carbon films (Quantifoil, R 2/2) were purchased from Quantifoil, Germany. The holey carbon films were treated by a DII-29020HD plasma cleaning machine from JEOL, Japan. Both the front and the back of the holey carbon films were treated for 10 s.

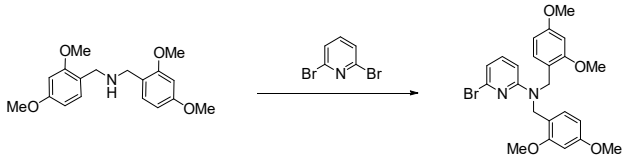
Thermogravimetric Analysis (TGA) was carried out on a Mettler-Toledo TGA 1 and SDT Q600 TG-DTA analyzer under $N_2$ atmosphere from 30 °C to 800 °C along with a ramp rate of 10 °C $min^{-1}$. Before carrying out the TGA, the samples were activated at 100 °C for 30 minutes to eliminate the samples' water.

Theoretical Calculations were employed by density functional theory (DFT) calculations to optimize the ground state geometries of the NBPs using the hybrid B3LYP functional[2] and the 6-31G* basis set[3]. For nickel atoms, the Los Alamos effective core potential basis set (LANL2DZ)[4] was used. All calculations were carried out using

the Gaussian09 program package[5].

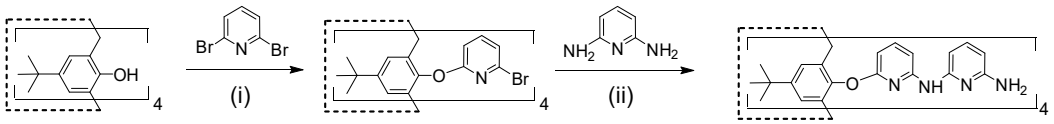
## 2. Synthetic Procedures

### Synthesis of building blocks



**Scheme S1.** Synthetic route to 6-bromo-N,N-bis(2,4-dimethylbenzyl)pyridin-2-amine. Reaction condition: N,N-diisopropylethylamine, xylene, reflux, 24 h.

**6-bromo-N,N-bis(2,4-dimethylbenzyl)pyridin-2-amine**. To a 100 mL flask was added 2,6-dibromopyridine (11.0 g, 0.046 mol), bis(2,4-dimethoxybenzyl)amine (10.0 g, 0.032 mol) and dimethylbenzene (70 mL) under Ar. After the addition of N,N-diisopropylethylamine (16 mL, 0.092 mol), the reaction mixture was degassed with argon for three times. After refluxing at 150 °C for 24 h, the solvent was removed under reduced pressure and purification via column chromatography (silica gel, ethyl acetate : petroleum ether = 1 : 8) afforded 6-bromo-N,N-bis(2,4-dimethoxybenzyl)pyridin-2-amine as white powder (14.3 g, 96% yield). $^1$H NMR (400 MHz, $CDCl_3$, ppm): $\delta$ 7.16 – 7.09 (m, 3H), 6.66 (d, $J$ = 7.5 Hz, 1H), 6.46 (d, $J$ = 2.4 Hz, 2H), 6.42 (dd, $J$ = 8.3, 2.4 Hz, 2H), 6.25 (d, $J$ = 8.4 Hz, 1H), 4.71 (s, 4H), 3.81 (s, 6H), 3.78 (s, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): $\delta$ 159.9, 158.7, 158.4, 139.9, 139.1, 128.8, 118.3, 114.3, 104.4, 103.7, 98.4, 55.4, 55.2, 46.5. HRMS (ESI, m/z): $[M+H]^+$ calcd for $C_{23}H_{25}BrN_2O_4$, 473.1070; Found, 473.1060. FT-IR (KBr, $cm^{-1}$): 3108, 3099, 3074, 3012, 2989,2963, 2940, 2909, 2880, 2831, 1618, 1588, 1539, 1505, 1491, 1464, 1451, 1435, 1423, 1414, 1374, 1363, 1307, 1280, 1254, 1210, 1175, 1166, 1155, 1110, 1081, 1065, 1038, 997, 958, 920, 832, 821, 784, 775, 726, 718, 669, 658, 631, 580, 524, 516, 502, 458.



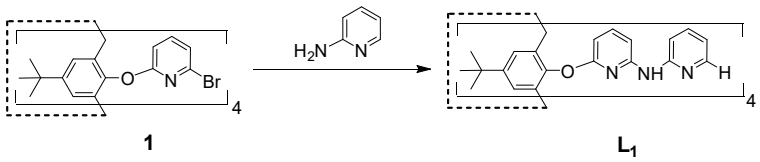
**Scheme S2.** Synthetic route to $\mathbf{P_1}$. (i) NaH, dry DMF, reflux, 12 h; (ii) $Pd_2(dba)_3$, DPPP, *t*-BuOK, xylene, reflux, 12 h.

**1.** It was prepared according to the reported procedure[6]. To a stirred solution of NaH (60%, dispersion in Paraffin Liquid, 3.1 g, 0.078 mol) in dry DMF (150 mL) was added 4-tert-Butylcalix[4]arene (5.0 g, 0.008 mol) in

small portions at 40 °C. Stirring was continued at 50 °C for 30 min and subsequently 2,6-dibromopyridine (29.2 g, 0.123 mol) was added. After refluxing at 150 °C for 12 h, the solvent was removed under reduced pressure and the residue was washed by water and subsequently ethanol. Purification via column chromatography (silica gel, dichloromethane : petroleum ether = 1 : 3) afforded **1** as white powder (3.8 g, 39% yield). Notably, the $^{1}$H NMR spectrum of Compound **1** gives two characteristic signals for the methylene protons at $\delta$ = 3.78 and 3.16 ppm, indicating the desired cone conformation of Compound **1**. In addition, due to the steric hindrance of pyridine structure, this conformation is stable and will not inverse in the subsequent reaction as these signals remained in the spectra of the subsequent products[7]. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm): $\delta$ 7.60 (dd, $J$ = 8.2, 7.5 Hz, 4H), 7.37 (dd, $J$ = 8.2, 0.7 Hz, 4H), 7.08 (dd, $J$ = 7.5, 0.6 Hz, 4H), 7.06 (s, 8H), 3.78 (d, $J$ = 13.0 Hz, 4H), 3.16 (d, $J$ = 13.0 Hz, 4H), 1.18 (s, 36H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): $\delta$ 164.2, 147.2, 145.6, 140.8, 138.5, 133.9, 125.6, 121.1, 110.4, 34.2, 31.4, 31.1. HRMS (ESI, m/z): $[M+H]^+$ calcd for $C_{64}H_{65}Br_4N_4O_4$, 1273.1706; Found, 1273.1714. FT-IR (KBr, $cm^{-1}$): 3077, 3049, 2962, 2933, 2903, 2866, 1577, 1557, 1480, 1429, 1405, 1362, 1301, 1283, 1261, 1236, 1192, 1157, 1137, 1118, 1076, 983, 924, 892, 879, 871, 821, 785, 740, 724, 670, 641, 540, 442.

**$P_1$.** To a 100 mL Schlenk tube was added **1** (1.0 g, 0.079 mmol), 2,6-diaminopyridine (1.72 g, 0.016 mol) and dimethylbenzene (20 mL) under Ar. After the addition of *t*-BuOK (706 mg, 6.290 mmol), $Pd_2(dba)_3$ (72 mg, 0.079 mmol) and DPPP (65 mg, 0.157 mmol), the reaction mixture was degassed with argon for three times. After refluxing at 150 °C for 2 h, the mixture was poured into petroleum ether, and the precipitate was separated by filtration and subsequently washed with distilled water. Then the brown solid was dissolved in THF and the solution was filtered to remove insoluble material. The removal of the solvent under reduced pressure afforded ligand processor **P1** as brown solid (1.02 g, 95% yield). $^{1}$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 8.80 (s, 4H), 7.55 (t, $J$ = 7.9 Hz, 4H), 7.14 (s, 8H), 6.94 (t, $J$ = 8.0 Hz, 4H), 6.78 (d, $J$ = 7.9 Hz, 4H), 6.73 (d, $J$ = 8.0 Hz, 4H), 6.64 (d, $J$ = 8.0 Hz, 4H), 5.87 (d, $J$ = 7.8 Hz, 4H), 5.43 (s, 8H), 3.98 (d, $J$ = 12.5 Hz, 4H), 3.11 (d, $J$ = 12.7 Hz, 4H), 1.18 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.5, 158.4, 153.5, 152.6, 147.3, 146.1, 139.8, 138.6, 134.8, 125.3, 104.3, 101.5, 100.4, 99.6, 34.3, 31.7, 31.5. HRMS (ESI, m/z): $[M+H]^+$ calcd for $C_{84}H_{89}N_{16}O_4$, 1385.7247; Found, 1385.7259. FT-IR (KBr, $cm^{-1}$): 3487, 3197,3122, 3055, 2960, 2925, 2865, 1611, 1574, 1520, 1448, 1436, 1395, 1361, 1317, 1277, 1249, 1215, 1191, 1152, 1120, 1079, 1032, 870, 784, 726.

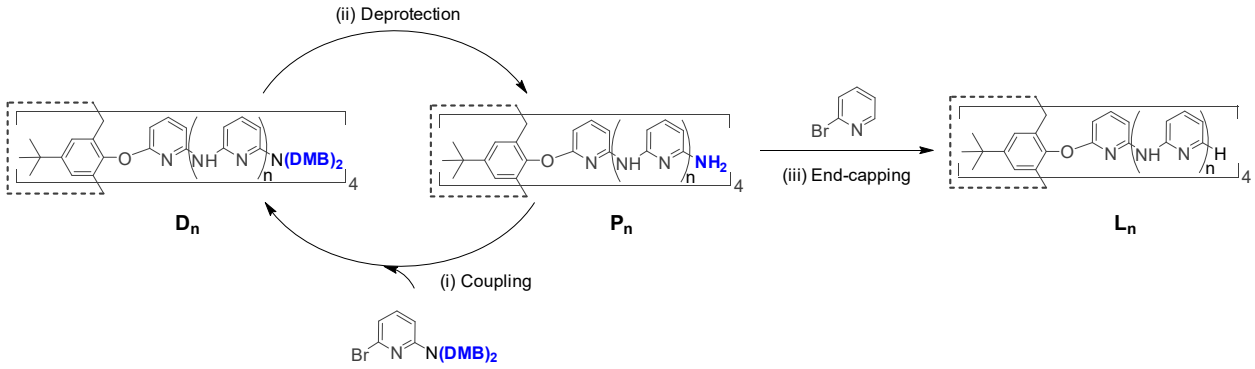
**Synthesis of ligand $L_1$**




**Scheme S3.** Synthetic approach to ligand $\mathbf{L_1}$**.** Reaction conditions: $Pd_2(dba)_3$, DPPP, *t*-BuOK, xylene, reflux, 12 h.

$\mathbf{L_1}$. To a 100 mL Schlenk tube was added Compound **1** (200 mg, 0.157 mmol), 2-aminopyridine (237 mg, 2.500 mmol) and toluene (20 mL) under Ar. After the addition of *t*-BuOK (141 mg, 1.260 mmol), $Pd_2(dba)_3$ (28.8 mg, 0.031 mmol) and DPPP (25.9 mg, 0. 063 mmol), the reaction mixture was degassed with argon for three times, then refluxed at 120 °C for 2 h. Subsequently, the solvent was removed under reduced pressure and the residue was washed by water. Purification via column chromatography (silica gel, dichloromethane : methanol = 10 : 3) afforded $\mathbf{L_1}$ as white powder (191 mg, 92% yield). $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.45 (s, 4H), 8.07 (dd, *J* = 5.1, 1.9 Hz, 4H), 7.64 (t, *J* = 7.9 Hz, 4H), 7.43 (d, *J* = 8.5 Hz, 4H), 7.26 (ddd, *J* = 8.9, 7.2, 2.0 Hz, 4H), 7.19 (s, 8H), 6.86 (d, *J* = 7.9 Hz, 4H), 6.76 – 6.71 (m, 8H), 3.98 (d, *J* = 12.4 Hz, 4H), 3.16 (d, *J* = 12.6 Hz, 4H), 1.19 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.5, 154.2, 153.2, 147.8, 147.3, 146.3, 140.3, 137.4, 134.8, 130.1, 125.4, 116.2, 111.8, 104.4, 102.0, 34.4, 31.7, 31.3. HRMS (ESI, m/z): $[M+Na]^+$ calcd for $C_{84}H_{84}N_{12}NaO_4$, 1347.6631; Found, 1347.6648. FT-IR (KBr, $cm^{-1}$):3266, 3181, 2961, 2929, 2905, 2865, 1597, 1571, 1513 1480, 1459, 1434, 1415, 1362, 1332, 1296, 1281, 1262, 1244, 1215, 1191,1148, 1120, 1102, 1031, 1013, 871, 771, 730, 695.

**Synthesis of ligands $L_n$ (n>1)**




**Scheme S4.** Synthetic approach to ligands via an iterative approach followed by end-capping. Reaction conditions: (i) $Pd_2(dba)_3$, DPPP, *t*-BuOK, Pyridine, 110 °C; (ii) TFA, 0 °C; (iii) $Pd_2(dba)_3$, DPPP, *t*-BuOK, THF, reflux. "DMB" is the abbreviation for 2,6-dimethoxybenzyl group.

**General procedure for $D_n$ (n>1).** To a 100 mL Schlenk tube was added Compound $\mathbf{P_n}$ (0.720 mmol), 6-bromo-N,N-bis(2,4-dimethoxybenzyl)pyridin-2-amine (0.012 mol) and dry 1, 4-dioxane (30 mL) under Ar. After the addition of *t*-BuOK (5.760 mmol), $Pd_2(dba)_3$ (0.290 mmol) and DPPP (0.580 mmol), the reaction mixture was degassed with argon for three times. After refluxing at 110 °C for 2 h, the solvent was removed under reduced pressure and the residue was treated with petroleum ether. Subsequently, the precipitate was separated by filtration and then dissolved in dichloromethane. After filtration to remove insoluble material, the excess solvent was removed under reduced pressure and Compound $\mathbf{D_n}$ was obtained as powder.

**General procedure for $P_n$ (n>1).** To a dichloromethane (30 mL) solution of Compound $\mathbf{D_n}$ (0.680 mmol) was added TFA (0.068 mol) in an ice bath and the mixture was stirred for 1.0 h. After completion, the reaction mixture was concentrated under vacuum. The residue was treated with methanol (30 mL) and filtration. The filtrate was basified with aqueous $NaHCO_3$ solution (20 mL), filtrated, washed with water (100 mL) and then oven-dried to afford Compound $\mathbf{P_n}$ as brown powder.

**General procedure for $L_n$ (n>1).** To a 100 mL Schlenk tube was added Compound $\mathbf{P_{n-1}}$ (0.150 mmol), 2-bromopyridine (1.800 mmol) and THF (10 mL) under Ar. After the addition of *t*-BuOK (1.200 mmol), $Pd_2(dba)_3$ (0.015 mmol) and DPPP (0.030 mmol), the reaction mixture was degassed with argon for three times, then refluxed at 120 °C for 2 h. Subsequently, the solvent was removed under reduced pressure and the residue was treated with petroleum ether. After filtration, the precipitate was washed with water. Then the brown solid was dissolved in THF and the solution was filtered to remove insoluble material. The removal of the solvent under reduced pressure afforded ligands $\mathbf{L_n}$ as brown powder.

**$D_2$**. 2.08 g, 98% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 8.90 (s, 4H), 8.65 (s, 4H), 7.60 (t, $J$ = 7.8 Hz, 4H), 7.28 (t, $J$ = 8.0 Hz, 4H), 7.14 (s, 8H), 6.95 – 6.90 (m, 20H), 6.84 (t, $J$ = 7.9 Hz, 12H), 6.55 (d, $J$ = 2.3 Hz, 8H), 6.43 (dd, $J$ = 8.4, 2.4 Hz, 8H), 5.91 (d, $J$ = 8.2 Hz, 4H), 4.57 (s, 16H), 3.99 (d, $J$ = 12.4 Hz, 4H), 3.76 (s, 24H), 3.71 (s, 24H), 3.13 (d, $J$ = 12.7 Hz, 4H), 1.18 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.5, 159.9, 158.4, 157.5, 153.4, 153.3, 153.0, 152.1, 147.3, 146.2, 140.1, 139.2, 138.4, 134.8, 127.9, 125.4, 118.5, 104.7, 103.9, 103.1, 102.0, 99.5, 98.8, 97.3, 55.7, 55.6, 46.2, 34.3, 31.7, 31.4. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{176}H_{184}N_{24}NaO_{20}$, 2976.4009; Found, 2976.7283. FT-IR (KBr, $cm^{-1}$): 3195, 3124, 3048, 2996, 2954, 2934, 2866, 2834, 1607, 1590, 1569, 1505, 1434, 1362, 1321, 1285, 1244, 1208, 1191, 1155, 1119, 1038, 976, 958, 934, 921, 870, 831, 824, 776, 722, 635, 615, 596, 577, 553, 515, 456, 418.

**$D_3$**. 2.34 g, 98% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 8.98 (s, 4H), 8.77 (s, 4H), 8.74 (s, 4H), 7.63 (t, $J$ = 7.9 Hz, 4H), 7.30 – 7.22 (m, 12H), 7.20 – 7.13 (m, 16H), 7.06 (d, $J$ = 7.6 Hz, 4H), 7.01 (d, $J$ = 7.7 Hz, 4H), 6.94 (d, $J$ = 8.4 Hz, 12H), 6.84 (d, $J$ = 7.6 Hz, 8H), 6.57 (d, $J$ = 2.3 Hz, 8H), 6.44 (dd, $J$ = 8.4, 2.3 Hz, 8H), 5.94 (d, $J$ = 8.2 Hz, 4H), 4.60 (s, 16H), 4.02 (d, $J$ = 9.5 Hz, 4H), 3.78 (s, 24H), 3.72 (s, 24H), 3.17 (d, $J$ = 11.5 Hz, 4H), 1.20 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 159.9, 158.4, 157.4, 153.4, 153.3, 153.1, 153.0, 153.0, 152.1, 147.3, 146.2, 140.1, 139.1, 138.7, 134.8, 130.8, 130.7, 129.2, 129.1, 128.2, 127.8, 125.4, 118.5, 104.8, 104.2, 103.3, 102.0, 99.5, 98.8, 97.2, 55.8, 55.6, 46.5, 34.3, 31.8, 31.5. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{196}H_{200}N_{32}NaO_{20}$, 3344.5508; Found, 3344.9637. FT-IR (KBr, cm$^{-1}$): 3197, 3132, 3055, 3029, 2995, 2954, 2934, 2865, 2834, 1607, 1589, 1575, 1539, 1506, 1430, 1362, 1287, 1246, 1208, 1191, 1155, 1119, 1037, 976, 933, 870, 781, 723, 700, 516, 457, 419.

**$D_4$**. 2.60 g, 98% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.01 (s, 4H), 8.89 (s, 4H), 8.82 (s, 8H), 7.47 (t, $J$ = 7.8 Hz, 8H), 7.37 (d, $J$ = 8.3 Hz, 4H), 7.30 (t, $J$ = 8.0 Hz, 8H), 7.27 – 7.23 (m, 8H), 7.20 – 7.14 (m, 16H), 7.08 (d, $J$ = 7.7 Hz, 8H), 6.95 (d, $J$ = 8.5 Hz, 16H), 6.82 (d, $J$ = 7.6 Hz, 4H), 6.58 (d, $J$ = 2.3 Hz, 8H), 6.45 (dd, $J$ = 8.4, 2.4 Hz, 8H), 5.95 (d, $J$ = 8.3 Hz, 4H), 4.62 (s, 16H), 4.03 (d, $J$ = 8.3 Hz, 4H), 3.78 (s, 24H), 3.72 (s, 24H), 3.18 (d, $J$ = 8.2 Hz, 4H), 1.21 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 162.8, 159.9, 158.4, 157.4, 156.0, 153.4, 153.1, 152.2, 146.3, 140.2, 139.1, 138.6, 134.8, 129.4, 128.7, 127.9, 125.8, 125.5, 118.5, 104.7, 103.5, 103.3, 99.5, 98.8, 97.1, 55.7, 55.6, 46.5, 34.3, 31.8, 31.3. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{216}H_{216}N_{40}NaO_{20}$, 3712.7004; Found, 3712.5855. FT-IR (KBr, cm$^{-1}$): 3195, 3117, 3095, 3053, 3026, 2997, 2955, 2936, 2913, 2867, 2834, 1606, 1590, 1574, 1506, 1427, 1362, 1287, 1247, 1208, 1191, 1155, 1119, 1039, 977, 934, 870, 829, 780, 724, 667, 599, 512, 457, 419.

**$D_5$**. 2.86 g, 98% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.03 (s, 4H), 8.95 (s, 4H), 8.92 (s, 4H), 8.85 (s, 4H), 8.82 (s, 4H), 7.67 (t, $J$ = 7.9 Hz, 4H), 7.49 – 7.45 (m, 8H), 7.39 (d, $J$ = 8.6 Hz, 4H), 7.29 (dd, $J$ = 8.0, 4.4 Hz, 12H), 7.22 – 7.18 (m, 16H), 7.15 (d, $J$ = 7.9 Hz, 8H), 7.06 (dd, $J$ = 10.8, 7.8 Hz, 8H), 6.95 (d, $J$ = 8.3 Hz, 12H), 6.88 (dd, $J$ = 12.8, 8.0 Hz, 8H), 6.82 (d, $J$ = 7.8 Hz, 4H), 6.58 (d, $J$ = 2.2 Hz, 8H), 6.45 (dd, $J$ = 8.4, 2.4 Hz, 8H), 5.96 (d, $J$ = 8.4 Hz, 4H), 4.62 (s, 16H), 4.05 (d, $J$ = 9.2 Hz, 4H), 3.79 (s, 24H), 3.73 (s, 24H), 3.20 (d, $J$ = 9.3 Hz, 4H), 1.22 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 159.9, 158.4, 157.5, 153.4, 153.1, 153.1, 153.1, 152.2, 147.4, 146.3, 140.2, 139.1, 138.7, 134.8, 127.9, 125.5, 118.5, 104.8, 104.3, 103.6, 103.5, 103.3, 102.0, 99.5, 98.8, 97.2, 55.8, 55.6, 46.5, 34.4, 31.8, 31.6. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{236}H_{232}N_{48}NaO_{20}$, 4080.8503; Found, 4081.0104. FT-IR (KBr, cm$^{-1}$): 3197, 3123, 3056, 2996, 2955, 2934, 3908, 2866, 2835, 1606, 1589, 1575, 1540, 1506, 1426, 1363, 1288, 1248, 1207, 1190, 1154, 1122, 1038, 977, 935,

871, 824, 778, 722, 668, 596, 517, 457, 419.

**$P_2$.** 1.16 g, 97% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 8.95 (s, 4H), 8.60 (s, 4H), 7.63 (t, $J$ = 7.9 Hz, 4H), 7.23 (t, $J$ = 7.9 Hz, 4H), 7.17 (s, 8H), 7.09 (d, $J$ = 7.9 Hz, 8H), 6.94 (d, $J$ = 7.9 Hz, 4H), 6.89 (d, $J$ = 8.1 Hz, 4H), 6.85 (t, $J$ = 8.3 Hz, 8H), 5.94 (d, $J$ = 7.8 Hz, 4H), 5.56 (s, 8H), 4.01 (d, $J$ = 12.4 Hz, 4H), 3.16 (d, $J$ = 12.8 Hz, 4H), 1.20 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.5, 158.6, 153.5, 153.4, 153.3, 152.1, 147.3, 146.2, 140.1, 138.9, 138.5, 134.8, 125.4, 104.5, 104.0, 102.8, 101.9, 99.9, 99.5, 34.3, 31.8, 31.4. HRMS (ESI, m/z): $[M+H]^+$ calcd for $C_{104}H_{105}N_{24}O_4$, 1753.8745; Found, 1753.8745. FT-IR (KBr, cm$^{-1}$):3464, 3197, 3112, 3054,2961, 2904, 2866, 1684, 1608, 1575, 1508, 1437, 1361, 1284, 1235, 1208, 1191, 1153, 1082, 1057, 1037, 868, 849, 802, 782, 725, 651, 598.

**$P_3$.** 1.40 g, 97% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.02 (s, 4H), 8.81 (s, 4H), 8.75 (s, 4H), 7.66 (t, $J$ = 7.9 Hz, 4H), 7.43 (t, $J$ = 8.0 Hz, 4H), 7.33 (d, $J$ = 7.9 Hz, 4H), 7.25 (d, $J$ = 7.9 Hz, 4H), 7.23 – 7.20 (m, 8H), 7.17 (d, $J$ = 7.9 Hz, 4H), 7.13 (d, $J$ = 7.9 Hz, 4H), 7.05 (d, $J$ = 7.9 Hz, 4H), 7.00 (d, $J$ = 7.9 Hz, 4H), 6.97 (d, $J$ = 7.8 Hz, 4H), 6.90 (d, $J$ = 7.7 Hz, 4H), 6.86 (d, $J$ = 8.0 Hz, 4H), 5.97 (d, $J$ = 7.8 Hz, 4H), 5.61 (s, 8H), 4.05 (d, $J$ = 12.2 Hz, 4H), 3.20 (d, $J$ = 13.0 Hz, 4H), 1.23 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 158.7, 153.6, 153.4, 153.0, 152.9, 152.2, 147.4, 146.3, 140.1, 138.9, 138.8, 134.8, 125.4, 104.5, 104.3, 103.6, 103.2, 103.0, 102.0, 99.8, 99.7, 34.4, 31.8, 31.4. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{124}H_{120}N_{32}NaO_4$, 2144.0063; Found, 2144.1116. FT-IR (KBr, cm$^{-1}$): 3480, 3196, 3125, 355, 3029, 3002, 2958, 2912, 2865, 2836, 1605, 1575, 1506, 1431, 1361, 1290, 1247, 1207, 1190, 1154, 1119, 1035, 871, 782, 724, 700, 551, 513.

**$P_4$.** 1.64 g, 97% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.02 (s, 4H), 8.92 (s, 4H), 8.84 (s, 4H), 8.76 (s, 4H), 7.65 (t, $J$ = 7.6 Hz, 4H), 7.49 (d, $J$ = 7.9 Hz, 4H), 7.45 (d, $J$ = 4.9 Hz, 4H), 7.43 – 7.38 (m, 8H), 7.26 (t, $J$ = 7.9 Hz, 12H), 7.22 – 7.16 (m, 16H), 7.03 (d, $J$ = 7.9 Hz, 4H), 6.98 (d, $J$ = 8.0 Hz, 8H), 6.88 – 6.84 (m, 4H), 5.97 (d, $J$ = 8.0 Hz, 4H), 5.61 (s, 8H), 4.04 (d, $J$ = 11.1 Hz, 4H), 3.19 (d, $J$ = 11.2 Hz, 4H), 1.22 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 158.7, 153.6, 153.4, 153.2, 153.0, 152.2, 147.3, 146.3, 140.1, 139.1, 138.9, 134.8, 125.4, 104.5, 104.2, 103.8, 103.5, 103.4, 103.3, 103.2, 102.0, 99.6, 34.4, 31.8, 31.3. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{144}H_{136}N_{40}NaO_4$, 2512.1558; Found, 2512.2711. FT-IR (KBr, cm$^{-1}$): 3481, 3196, 3121, 3055, 3030, 2959, 2903, 2865, 1604, 1574, 1515, 1429, 1361, 1289, 1248, 1191, 1154, 1120, 1027, 987, 871, 781, 725, 701, 549, 447.

**$P_5$.** 1.89 g, 97% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.05 (s, 4H), 8.99 (s, 8H), 8.87 (s, 4H), 8.79 (s, 4H), 7.71 – 7.63 (m, 4H), 7.53 – 7.39 (m, 20H), 7.30 – 7.20 (m, 32H), 7.05 – 6.87 (m, 20H), 5.99 (d, $J$ = 8.3 Hz, 4H), 5.63 (s, 8H), 4.06 (d, $J$ = 8.9 Hz, 4H), 3.21 (d, $J$ = 8.7 Hz, 4H), 1.23 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 158.7, 153.6, 153.4, 153.2, 153.1, 152.2, 147.4, 146.3, 140.1, 139.0, 134.8, 125.5, 104.2, 103.7, 103.5, 103.3, 102.1, 99.8, 99.7, 34.4, 31.8, 31.6. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{164}H_{152}N_{48}NaO_4$, 2880.3057; Found, 2880.5253. FT-IR (KBr, cm$^{-1}$): 3481, 3195, 3122, 3054, 2953, 2901, 2864, 1604, 1273, 1507, 1423, 1361, 1290, 1246, 1190, 1151, 1119, 1081, 985, 870, 776, 722, 665, 594, 550, 445.

**$L_2$.** 216 mg, 85% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.24 (s, 4H), 9.07 (s, 4H), 8.16 (ddd, $J$ = 4.9, 2.0, 0.9 Hz, 4H), 8.09 (d, $J$ = 8.5 Hz, 4H), 7.68 – 7.59 (m, 8H), 7.19 (s, 8H), 7.15 (t, $J$ = 8.1 Hz, 4H), 6.96 (d, $J$ = 8.1 Hz, 4H), 6.88 (d, $J$ = 7.9 Hz, 4H), 6.82 (t, $J$ = 6.6 Hz, 12H), 4.02 (d, $J$ = 12.5 Hz, 4H), 3.17 (d, $J$ = 12.7 Hz, 4H), 1.20 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 154.8, 153.3, 153.0, 152.1, 147.9, 147.3, 146.3, 140.2, 138.8, 137.9, 134.8, 125.4, 116.1, 112.2, 104.5, 104.0, 103.2, 102.0, 34.3, 31.7, 31.4. HRMS (ESI, m/z): $[M+H]^+$ calcd for $C_{104}H_{101}N_{20}O_4$, 1693.8309; Found, 1693.8314. FT-IR (KBr, cm$^{-1}$): 3275, 3192, 3108, 3052, 2960, 2866, 1602, 1571, 1511, 1432, 1317, 1299, 1246, 1234, 1190, 1152, 1120, 1057, 870, 779, 727.

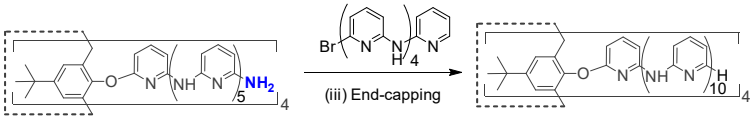
**$L_3$.** 266 mg, 86% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.32 (s, 4H), 9.05 (s, 4H), 8.91 (s, 4H), 8.19 (d, $J$ = 4.6 Hz, 4H), 7.96 (d, $J$ = 8.5 Hz, 4H), 7.64 – 7.56 (m, 8H), 7.50 – 7.41 (m, 12H), 7.22 – 7.14 (m, 12H), 7.01 – 6.94 (m, 12H), 6.83 (t, $J$ = 6.1 Hz, 8H), 4.04 (d, $J$ = 13.1 Hz, 4H), 3.19 (d, $J$ = 12.3 Hz, 4H), 1.22 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 154.9, 153.4, 153.1, 153.0, 152.9, 152.2, 147.9, 147.3, 146.3, 140.2, 139.2, 138.7, 137.7, 134.8, 130.1, 128.9, 128.7, 125.7, 125.4, 125.2, 116.1, 112.4, 104.5, 104.3, 103.6, 103.5, 103.3, 34.4, 31.8, 31.4. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{124}H_{116}N_{28}NaO_4$, 2083.9626; Found, 2084.2292. FT-IR (KBr, cm$^{-1}$): 3266, 3195, 3105, 3054, 3029, 2959, 2928, 2905, 2864, 1601, 1574, 1507, 1480, 1429, 1361, 1306, 1245, 1189, 1152, 1120, 1065, 1052, 1026, 1008, 989, 870, 780, 726, 700.

**$L_4$.** 321 mg, 88%yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.35 (s, 4H), 9.03 (s, 8H), 8.88 (s, 4H), 8.21 (dd, $J$ = 5.3, 2.0 Hz, 4H), 7.96 (d, $J$ = 8.4 Hz, 4H), 7.66 – 7.60 (m, 8H), 7.52 – 7.46 (m, 12H), 7.42 (d, $J$ = 7.9 Hz, 4H), 7.36 (d, $J$ = 8.0 Hz, 4H), 7.22 – 7.16 (m, 12H), 7.11 (d, $J$ = 7.7 Hz, 4H), 7.07 (d, $J$ = 7.9 Hz, 4H), 7.02 (d, $J$ = 7.8 Hz, 4H), 6.98 (d, $J$ = 7.9 Hz, 4H), 6.87 – 6.82 (m, 8H), 4.05 (d, $J$ = 11.7 Hz, 4H), 3.20 (d, $J$ = 11.8 Hz, 4H), 1.22 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 154.9, 153.4, 153.1, 153.0, 152.2, 147.9, 147.4, 146.3, 140.3, 140.1, 139.1, 138.8, 137.8, 134.8, 132.1, 130.8, 130.7, 129.2, 129.1, 128.8, 128.8, 125.5, 116.1, 112.4, 104.6, 104.3, 103.7, 103.5, 101.9, 34.4, 31.8, 31.5. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{144}H_{132}N_{36}NaO_4$,

2452.1123; Found, 2452.3661. FT-IR (KBr, $cm^{-1}$): 3273, 3195, 3107, 3054, 3029, 2959, 2930, 2865, 1601, 1574, 1507, 1480, 1428, 1361, 1305, 1246, 1190, 1152, 1120, 1103, 1072, 1050, 1029, 988, 949, 870, 779, 725, 700, 666, 614, 593, 553, 513, 448, 418.

**$L_5$.** 365 mg, 87% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.37 (s, 8H), 9.08 (d, $J$ = 7.4 Hz, 12H), 8.22 (d, $J$ = 5.0 Hz, 8H), 7.95 (d, $J$ = 8.4 Hz, 8H), 7.65 (t, $J$ = 8.0 Hz, 8H), 7.52 (d, $J$ = 7.7 Hz, 12H), 7.36 – 7.32 (m, 12H), 7.31 – 7.26 (m, 12H), 7.21 (d, $J$ = 8.1 Hz, 8H), 7.11 (d, $J$ = 8.1 Hz, 8H), 6.86 (t, $J$ = 6.0 Hz, 8H), 4.05 (d, $J$ = 12.4 Hz, 4H), 3.20 (d, $J$ = 12.9 Hz, 4H), 1.22 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 154.9, 153.2, 153.1, 152.2, 147.9, 146.4, 139.3, 139.2, 137.9, 134.8, 129.1, 129.0, 125.4, 116.2, 112.4, 107.3, 103.7, 103.5, 91.4, 34.4, 31.8, 31.4. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{164}H_{148}N_{44}NaO_4$, 2820.2620; Found, 2820.6758. FT-IR (KBr, $cm^{-1}$): 3278, 3193, 3104, 3057, 3023, 2954, 2929, 2904, 2866, 1576, 1509, 1423, 1301, 1246, 1190, 1150, 987, 869, 772, 719, 613, 592, 510, 446.

**$L_6$.** 403 mg, 85% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.37 (s, 8H), 9.06 (d, $J$ = 12.9 Hz, 16H), 8.21 (s, 8H), 7.95 (d, $J$ = 8.2 Hz, 8H), 7.64 (s, 12H), 7.51 (s, 16H), 7.36 – 7.30 (m, 16H), 7.23 – 7.18 (m, 16H), 7.12 – 7.08 (m, 8H), 6.85 (s, 12H), 4.04 (d, $J$ = 8.1 Hz, 4H), 3.21 (d, $J$ = 8.1 Hz, 4H), 1.22 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.5, 154.8, 153.1, 152.2, 147.9, 146.3, 142.0, 139.2, 137.9, 134.8, 125.4, 116.2, 112.4, 107.2, 103.7, 34.3, 31.7, 31.5. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{184}H_{164}N_{52}NaO_4$, 3188.4119; Found, 3188.3825. FT-IR (KBr, $cm^{-1}$): 3267, 3195, 3105, 3050, 3025, 2959, 2928, 2903, 2865, 1601, 1574, 1506, 1421, 1302, 1247, 1190, 1151, 1120, 1079, 987, 880, 868, 849, 777, 723, 655, 594, 447.



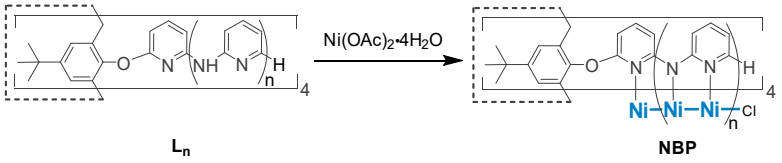

$P_5$ $L_{10}$

**Scheme S5.** Synthetic approach to $L_{10}$ by using a five aminopyridine units-containing end-capping block. Reaction condition: $Pd_2(dba)_3$, DPPP, *t*-BuOK, pyridine, reflux.

**$L_{10}$.** The synthesis procedure was similar to that for **$L_6$** except that five aminopyridine units-containing end-capping block (6-bromo-2-[[6-[[6-[[6-[(pyridin-2-yl)amino]pyridin-2-yl]amino]pyridin-2-yl]amino]py-ridin-2-yl]amino]pyridine[8]) and solvent of pyridine were used instead of 2-bromopyridine and THF. 198 mg, 89% yield. $^1$H NMR (400 MHz, DMSO-$d_6$, ppm): $\delta$ 9.36 (s, 4H), 9.06 (s, 36H), 8.22 (s, 4H), 7.92 (s, 4H), 7.66 (s, 12H), 7.55 – 7.50 (m, 32H), 7.29 (d, $J$ = 7.8 Hz, 48H), 7.21 (d, $J$ = 6.7 Hz, 16H), 7.10 – 7.06 (m, 8H), 6.98 (d, $J$ = 6.0 Hz,

8H), 6.91 – 6.85 (m, 12H), 4.05 (d, *J* = 13.1 Hz, 4H), 3.19 (d, *J* = 13.1 Hz, 4H), 1.22 (s, 36H). $^{13}$C NMR (100 MHz, DMSO-$d_6$, ppm): $\delta$ 163.6, 155.0, 153.1, 152.2, 147.3, 146.3, 139.2, 138.0, 134.8, 129.1, 125.4, 119.1, 116.1, 112.5, 103.7, 34.4, 31.8, 31.4. MS (MALDI, m/z): $[M+Na]^+$ calcd for $C_{264}H_{228}N_{84}NaO_4$, 4644.1260; Found, 4644.5219. FT-IR (KBr, $cm^{-1}$): 3276, 3192, 3122, 3048, 3028, 2954, 2928, 2905, 2863, 1602, 1573, 1509, 1429, 1295, 1247, 1190, 1150, 987, 870, 777, 723, 448.

**Syntheses of Nickel-backboned Polymer (NBP)**




**Scheme S6.** Synthetic approach to **NBP**. Reaction condition: $Ni(OAc)_2{\cdot}4H_2O$, naphthalene, 200 °C.

**General procedure for NBP.** To a 100 mL Schlenk tube was added $\mathbf{L_n}$ (0.015 mmol), nickel(II) acetate tetrahydrate (molar ratio: 1.5 times of quarter-N number in ligands to $\mathbf{L_n}$) and naphthalene (20 g, 0.156 mol). The mixture was degassed with argon for three times and then heated to reflux at 200 °C for 8 h. After cooling to about 80 °C, the dark black solution was treated with petroleum ether and subsequently filtered. After washed with petroleum ether for several times, the precipitate was dissolved with $CH_2Cl_2$. Then the solution was centrifuged and filtered to remove insoluble material. The removal of the solvent under reduced pressure afforded NBP as black powder.

**NBP with 3 nickel atoms.** 22 mg, 95% yield. MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{84}H_{81}ClN_{12}Ni_3O_4$, 1532.4231; Found, 1532.3718. FT-IR (KBr, $cm^{-1}$): 3066, 3026, 2955, 2903, 2866, 1605,1595, 1567, 1556, 1458, 1440, 1423, 1368, 1331, 1266, 1245, 1194, 1157, 1126, 1039, 1007, 909, 899, 870, 845, 811, 765, 743, 732, 699, 658, 643, 482, 433.

**NBP with 5 nickel atoms** 26 mg, 87% yield. MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{104}H_{93}ClN_{20}Ni_5O_4$, 2014.4102; Found, 2014.8466. FT-IR (KBr, $cm^{-1}$): 3064, 3030, 2956, 2906, 2866, 1599, 1550, 1446, 1426, 1554, 1343, 1304, 1277, 1256, 1236, 1195, 1156, 1127, 1010, 991, 772, 729.

**NBP with 7 nickel atoms.** 26 mg, 70% yield. MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{124}H_{105}ClN_{28}Ni_7O_4$, 2496.3970; Found, 2496.0406. FT-IR (KBr, $cm^{-1}$): 3054, 3030, 2955, 2926, 2865, 1683, 1599, 1546, 1418, 1361, 1343, 1326, 1302, 1277, 1256, 1230, 1195, 1155, 1126, 1010, 968, 947, 906, 871, 769, 725, 703.

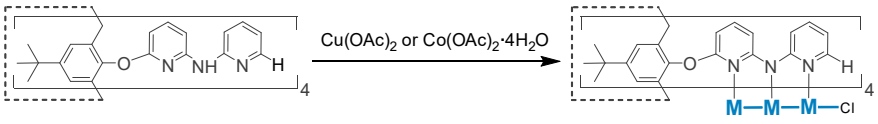
**NBP with 9 nickel atoms.** 25 mg, 55% yield. MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{144}H_{117}ClN_{36}Ni_9O_4$, 2978.3833; Found, 2978.1902. FT-IR (KBr, $cm^{-1}$): 3055, 3029, 2955, 2926, 2857, 1599, 1583, 1558, 1544, 1419, 1361, 1336, 1307, 1279, 1256, 1233, 1194, 1155, 1126,1014, 968, 948, 906, 871, 770, 726, 703, 654, 434, 418.

**NBP with 11 nickel atoms.** 17 mg, 32% yield. MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{164}H_{129}ClN_{44}Ni_{11}O_4$, 3460.3699; Found, 3460.0812. FT-IR (KBr, $cm^{-1}$): 2956, 2923, 2852, 1633, 1600, 1555, 1539, 1417, 1338, 1308, 1259, 1194, 1156, 1125, 1099, 1019, 880, 849, 772, 721, 652, 590, 555, 461, 421.

**NBP with 13 nickel atoms.** 12 mg, 20% yield. MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{184}H_{141}ClN_{52}Ni_{13}O_4$, 3942.3564; Found, 3942.0812. FT-IR (KBr, $cm^{-1}$): 2955, 2925, 2855, 1600, 1553, 1545, 1425, 1353, 1343, 1305, 1277, 1258, 1193, 1155, 1125, 1061, 1011, 845, 774, 723, 704.

**NBP with 21 nickel atoms.** To a 100 mL Schlenk tube was added $\mathbf{L_{10}}$ (20 mg, 0.005 mmol), nickel(II) acetate tetrahydrate (33.8 mg, 0.136 mmol) and dimethyl sulfoxide (20 ml). The mixture was degassed with argon for three times and then heated to reflux at 200 °C for 12 h. After cooling to about 80 °C, the dark black solution was poured into saturated salt water. Subsequently, the precipitate was obtained through filtration and dissolved with $CH_2Cl_2$. The centrifugation and filtration of the solution removed insoluble material, and then the removal of the solvent under reduced pressure afforded product as black solid (2 mg, 8% yield). MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{264}H_{189}ClN_{84}Ni_{21}O_4$, 5870.3324; Found, 5869.7637. FT-IR (KBr, $cm^{-1}$): 2957, 2923, 2853, 1643, 1617, 1558, 1548, 1540, 1522, 1514, 1454, 1426, 1383, 1314, 1262, 1197, 1155, 1098, 1027, 876, 803, 665, 636,598, 560, 509, 501, 465, 424, 405.

**Syntheses of copper- and cobalt-backboned polymer with 3 metal atoms**




$\mathbf{L_1}$ **MBP**

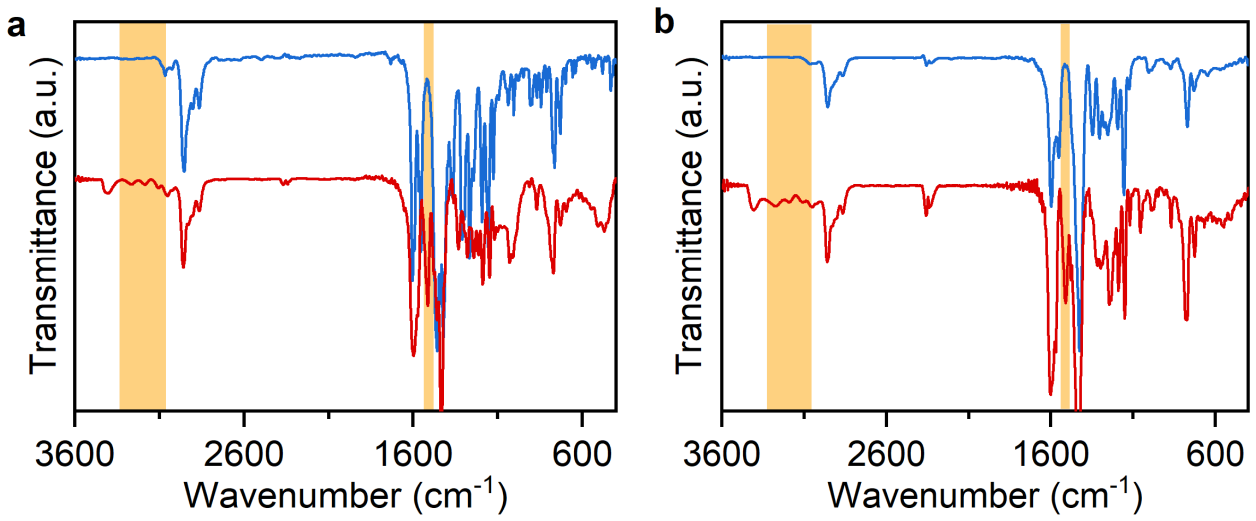
**Scheme S7.** Synthetic approach to copper- and cobalt-backboned polymer with 3 metal atoms. Reaction condition: $Cu(OAc)_2$ or $Co(OAc)_2{\cdot}4H_2O$, naphthalene, 200 °C. M = Cu or Co.

**Copper-backboned polymer with 3 metal atoms.** $\mathbf{L_1}$ (20 mg, 0.015 mmol), anhydrous cupric (II) acetate (12 mg, 0.068 mmol) and naphthalene (20 g, 0.156 mol) were first added to a 100 mL Schlenk tube. The mixture was degassed with argon for three times and then heated to reflux at 200 °C for 8 h. After cooled to about 80

°C, the dark black solution was treated with petroleum ether and subsequently filtered. After washed with petroleum ether for several times, the precipitate was dissolved with $CH_2Cl_2$. The solution was centrifuged and filtered to remove insoluble material. The removal of the solvent under reduced pressure afforded copper-backboned polymer with 3 metal atoms as black powder (22 mg, 94% yield). MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{84}H_{81}ClN_{12}Cu_3O_4$, 1546.4022; Found, 1546.4190. FT-IR (KBr, $cm^{-1}$): 3053, 2957, 2926, 2856, 1596, 1499, 1460, 1435, 1394, 1362, 1299, 1248, 1192, 1158, 1124, 1030, 949, 872, 806, 785, 698, 670, 618, 478.

**Cobalt-backboned polymer with 3 metal atoms.** $\mathbf{L_1}$ (20 mg, 0.015 mmol), cobalt (II) acetate tetrahydrate (17 mg, 0.068 mmol) and naphthalene (20 g, 0.156 mol) were added to a 100 mL Schlenk tube. The mixture was degassed with argon for three times and then heated to reflux at 200 °C for 8 h. After cooled to about 80 °C, the dark black solution was treated with petroleum ether and subsequently filtered. After washed with petroleum ether for several times, the precipitate was dissolved with $CH_2Cl_2$. The solution was centrifuged and filtered to remove insoluble material. The removal of the solvent under reduced pressure afforded cobalt-backboned polymer with 3 metal atoms as black powder (22 mg, 95% yield). MS (MALDI, m/z): $[M+H]^+$ calcd for $C_{84}H_{81}ClN_{12}Co_3O_4$, 1532.4104; Found, 1532.6313. FT-IR (KBr, $cm^{-1}$): 3055, 2957, 2925, 2854, 1604,1570, 1458, 1435, 1384, 1365, 1312, 1296, 1263, 1246, 1193, 1157, 1125, 1035, 950, 909, 890, 872, 810, 773, 732, 698, 673, 657, 617, 504, 482.

## 3. Results and discussion



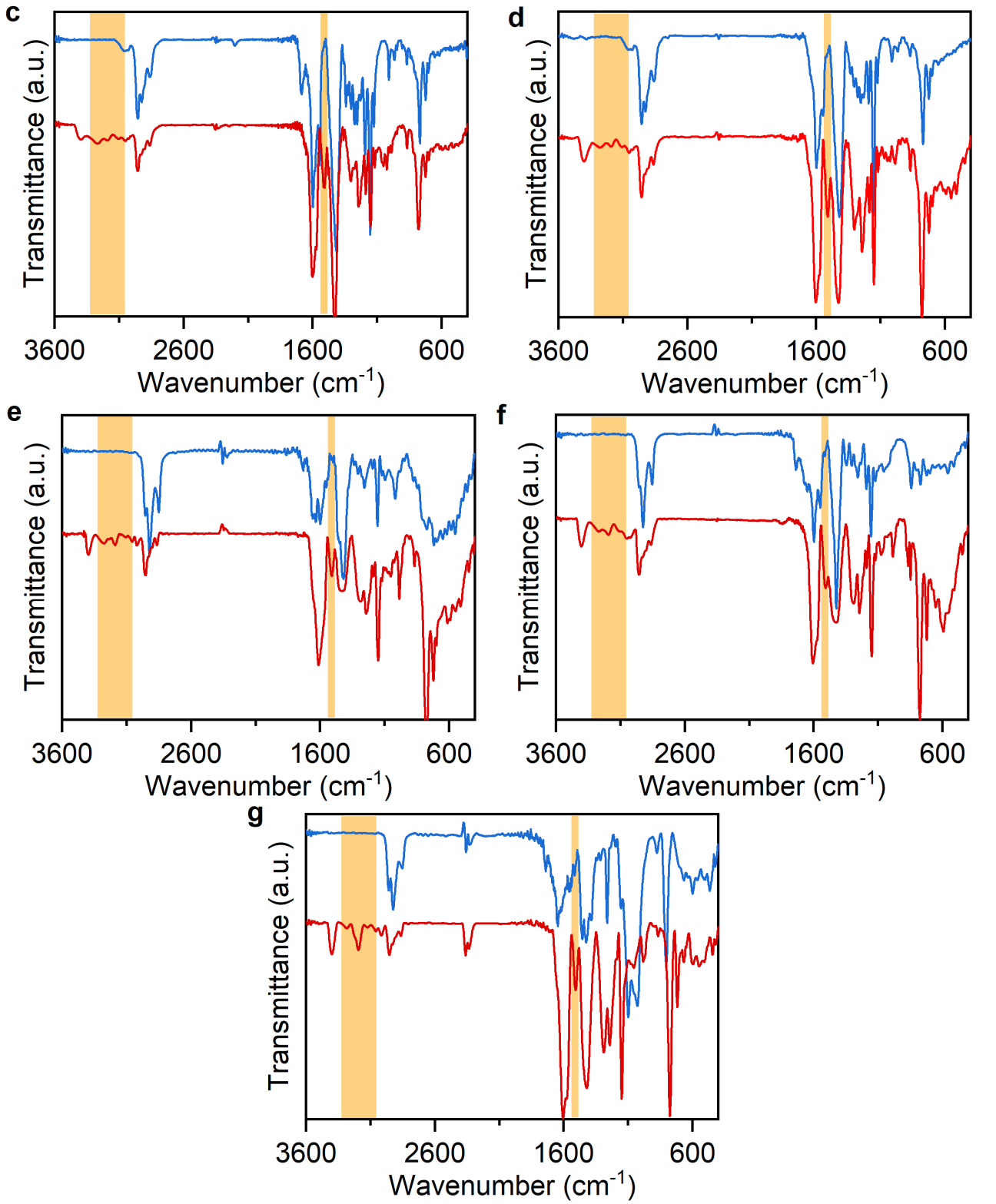



**Figure S1.** FTIR spectra of NBPs with 3–21 nickel atoms (in blue) and corresponding ligands (in red). The stretching vibration peaks of N-H bond at ~3266, 3186 and 3103 $cm^{-1}$ together with the bending vibration peaks of N-H bond at ~1510 $cm^{-1}$ of ligands were found to have disappeared after metalation, well consistent with their structures.

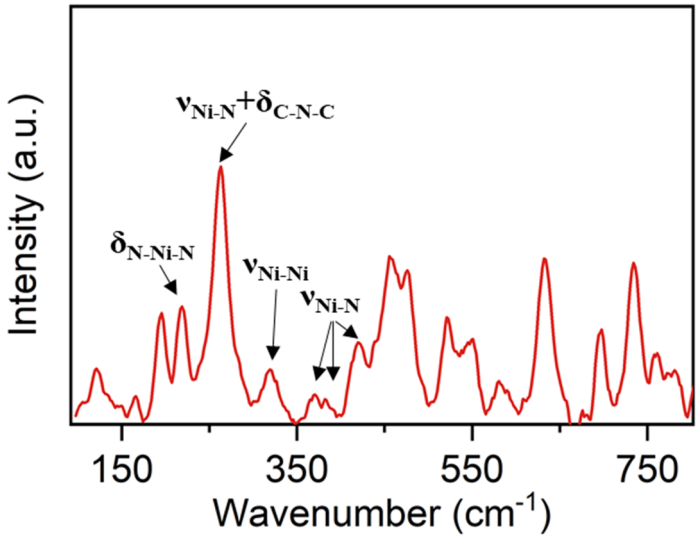



**Figure S2.** The Raman Spectrum of NBP with 3 nickel atoms. The peaks at 319, 420−263 and 219 $cm^{-1}$ could be assigned to the Ni–Ni stretching mode $\nu_{Ni-Ni}$, Ni−N stretching modes $\nu_{Ni-N}$ and N−Ni−N bending $\delta_{N-Ni-N}$, respectively. Excitation wavelength $\lambda_{ex}$ = 532 nm.

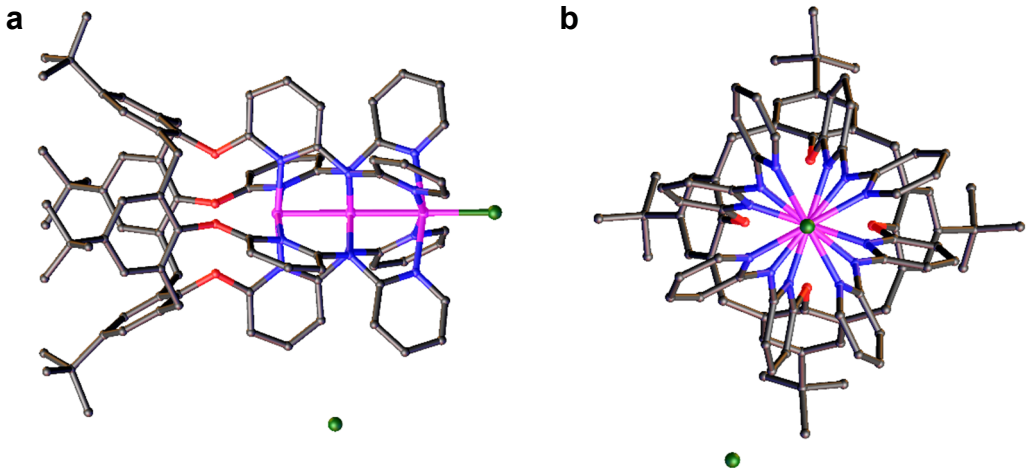



**Figure S3.** Molecular structure of NBP with 3 nickel atoms determined by X-ray crystallographic analysis of a single crystal obtained through slow diffusion of hexane into its dichloromethane solution. (**a**) top view and (**b**) side view. Carbon atoms are colored in gray, oxygen atoms are colored in red, nitrogen atoms are colored in blue, chlorine atoms are colored in green and nickel atoms are colored in pink. Hydrogen atoms and solvent molecules are omitted for clarity. The single-crystal X-ray diffraction data can be obtained free of charge from The Cambridge Crystallographic Data Centre under number CCDC of 2214751 via www.ccdc.cam.ac.uk/data_request/cif.

**Table S1**. Crystal data and structure refinement for NBP with 3 nickel atoms.

| | Data |
|---|---|
| Empirical formula | C84 H80 Cl2 N12 Ni3 O4 |
| Formula weight | 1568.57 |
| Temperature | 173(2) K |
| Wavelength | 1.34138 Å |
| Crystal system | Tetragonal |
| Space group | P4/ncc |
| Unit cell dimensions | a = 15.3620(3) Å α = 90°.<br>b = 15.3620(3) Å β = 90°.<br>c = 42.5288(8) Å γ = 90°. |
| Volume | 10036.4(4) $Å^3$ |
| Z | 4 |
| Density (calculated) | 1.038 $Mg/m^3$ |
| Absorption coefficient | 3.602 $mm^{-1}$ |
| F(000) | 3272 |
| Crystal size | 0.080 × 0.070 × 0.070 $mm^3$ |
| Theta range for data collection | 3.540 to 53.013°. |
| Index ranges | -18<=h<=18, -18<=k<=17, -50<=l<=48 |
| Reflections collected | 100895 |
| Independent reflections | 4443 [R(int) = 0.0420] |
| Completeness to theta = 53.013° | 99.6 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.750 and 0.655 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4443 / 57 / 283 |
| Goodness-of-fit on $F^2$ | 1.034 |
| Final R indices [I>2sigma(I)] | R1 = 0.0662, wR2 = 0.2293 |
| R indices (all data) | R1 = 0.0786, wR2 = 0.2508 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 1.309 and -0.552 e.$Å^{-3}$ |

$R_1 = \Sigma||F_o|-|F_c||$ (based on reflections with $F_o^2 > 2\sigma F^2$). $wR2 = [\Sigma[w(F_o-F_c^2)^2]/\Sigma[w(F_o)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$; $P = [\max(F_o^2, 0) + 2F_c^2]/3$ (also with $F_o^2 > 2\sigma F^2$)

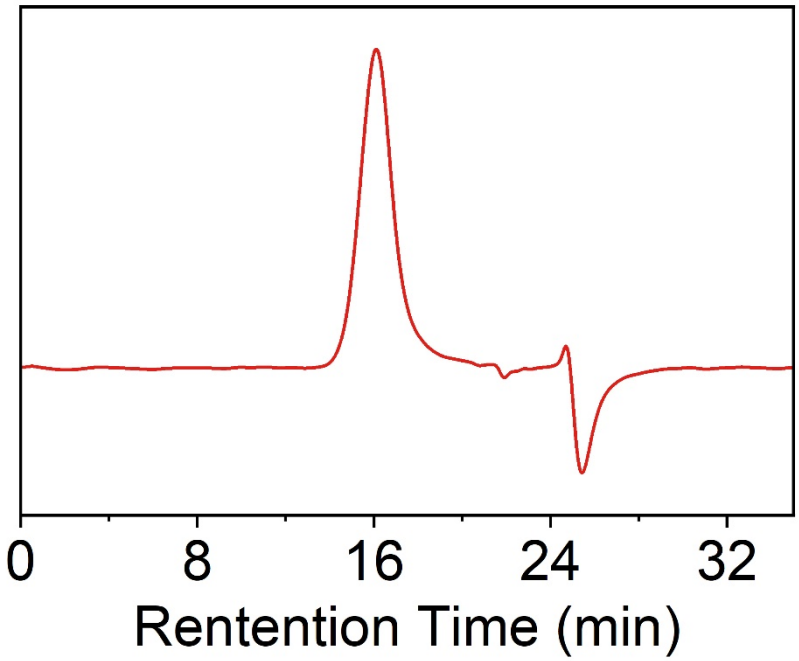



**Figure S4.** Size exclusion chromatography trace of the NBP with 21 nickel atoms. The signal peak at retention time of about 16 min indicates high purity of the isolated product.

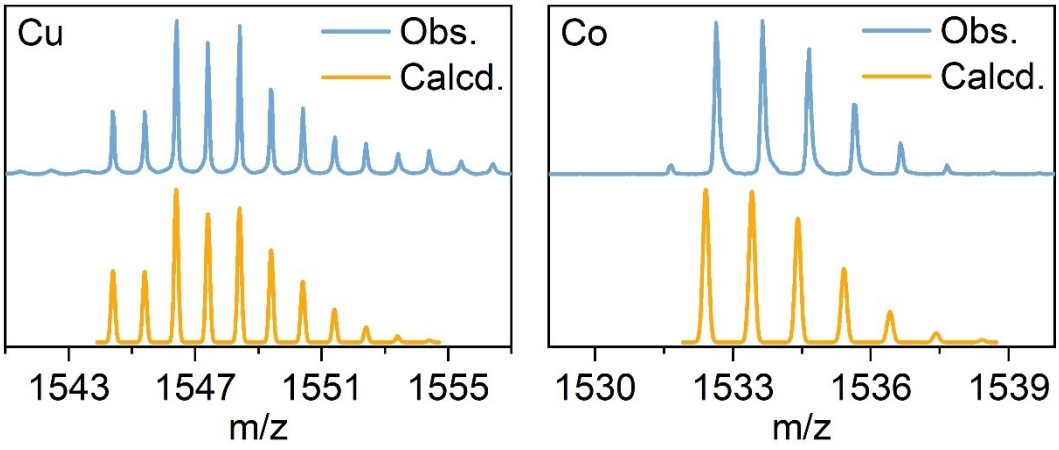



**Figure S5.** Characterization of copper- and cobalt-backboned polymer with 3 metal atoms. Magnified MALDI-TOF MS spectra (top) and simulated isotope patterns (bottom) for copper- and cobalt-backboned polymer with 3 metal atoms. The synthetic procedures are similar to that of NBP with 3 nickel atoms except that $Cu(OAc)_2$ or $Co(OAc)_2{\cdot}4H_2O$ were used instead of $Ni(OAc)_2{\cdot}4H_2O$. These results indicate that the synthesis strategy in this report is extendable to other transition metals such as copper and cobalt to construct other metal-backboned polymers.

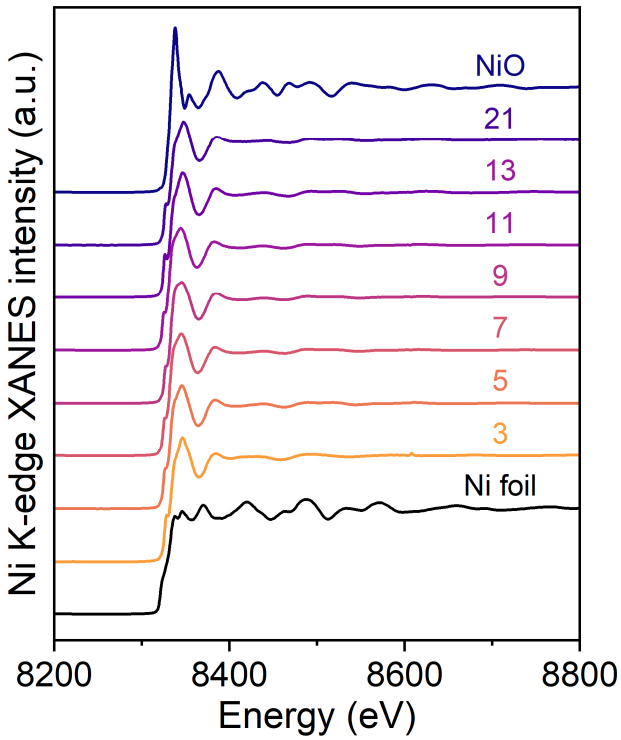



**Figure S6.** The Ni K-edge XANES spectra of NBPs with 3−21 nickel atoms. Ni foil and NiO were adopted as reference samples. The absorption profiles of NBPs are similar with that of the reference NiO rather than Ni foil, implying the +2 oxidation state of Ni atoms after metalation.

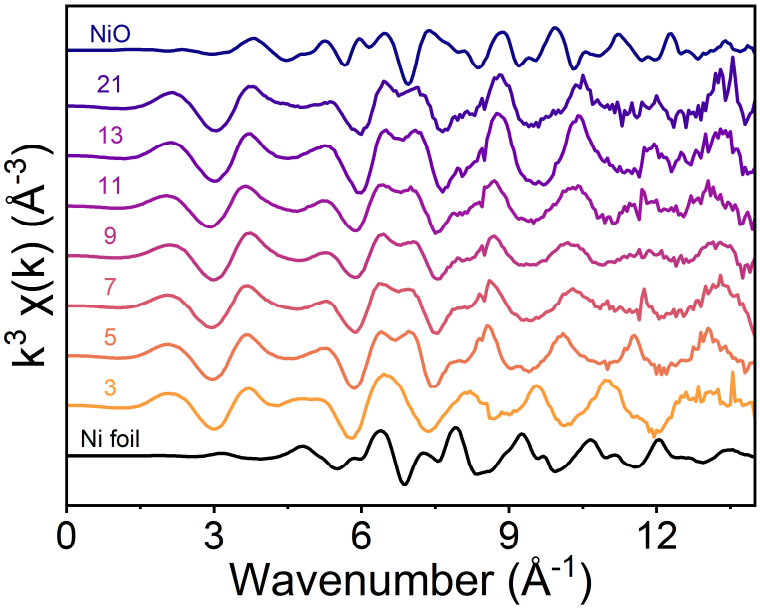



**Figure S7.** The k space EXAFS spectra of NBPs with 3–21 nickel atoms. Ni K-space oscillation, weighted by $k^3$. The absorption profiles of NBPs are similar with that of the reference NiO rather than Ni foil, implying the +2 oxidation state of Ni atoms after metalation.

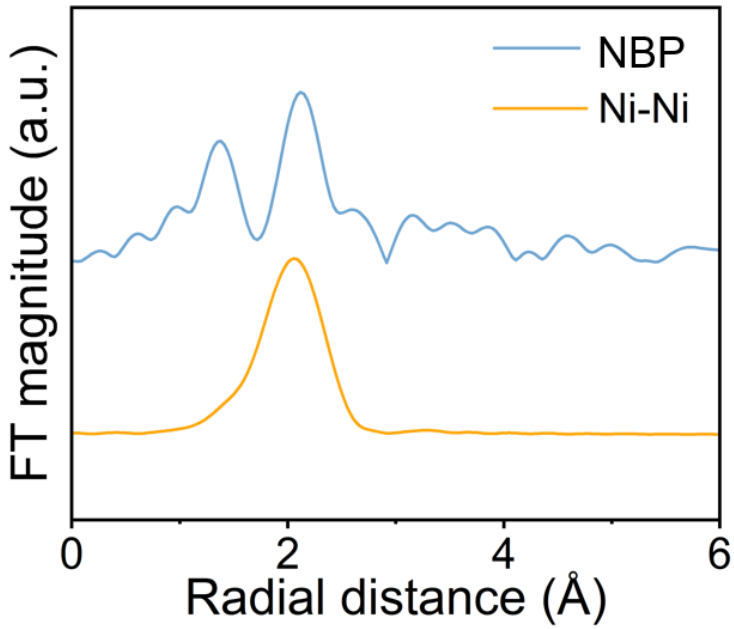
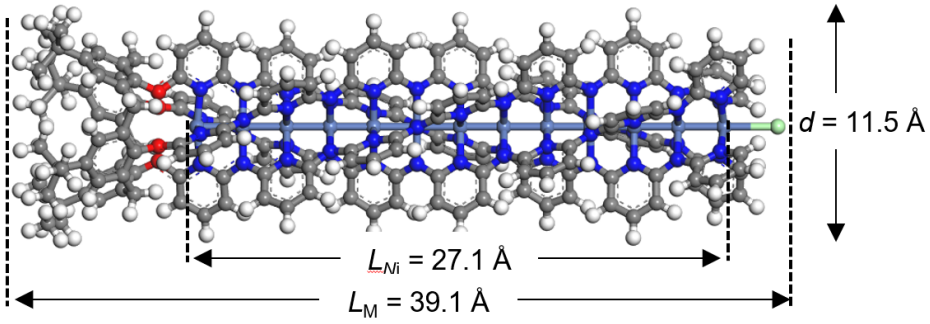



**Figure S8.** The FT-EXAFS spectra of NBP with 3 nickel atoms (top) and the Feff calculation results according to its crystal structure (bottom).

**a**




**b**

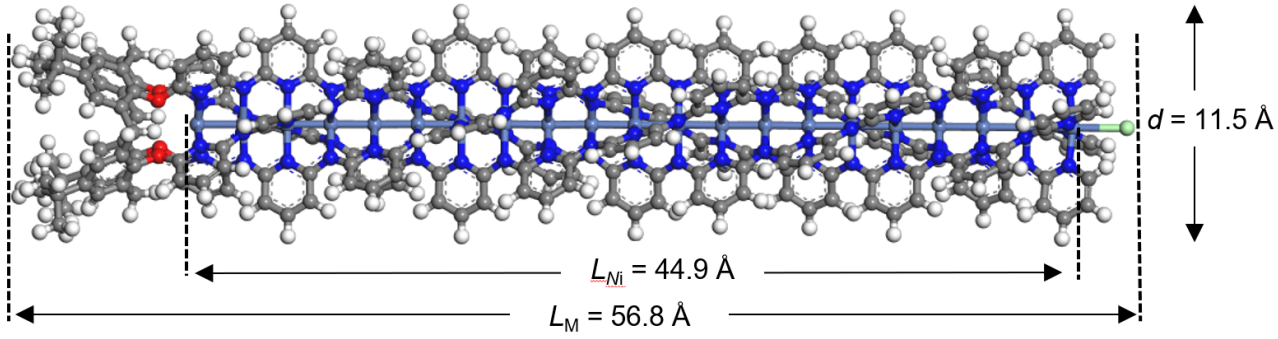



**Figure S9.** Optimized structures for NBPs with 13 and 21 nickel atoms calculated by density functional theory. $L_M$ and $d$ represent the calculated lengths and diameters of NBPs, respectively; $L_{Ni}$ represents the calculated lengths of nickel atom chains. $L_{Ni}$ was used for comparison with the morphologies observed in cryo-TEM because metal atoms have stronger contrast than non-metals.

**Table S2**. The lengths of nickel atom chains ($L_{Ni}$) and molecular lengths ($L_M$) of NBPs with 3–21 nickel atoms calculated by density functional theory (unit: Å).

| n | 3 | 5 | 7 | 9 | 11 | 13 | … | 21 |
|---|---|---|---|---|---|---|---|---|
| $L_M$ | 16.61287 | 21.09916 | 25.57120 | 30.03387 | 34.49952 | 38.96515 | … | 56.80827 |
| $L_{Ni}$ | 4.76846 | 9.25875 | 13.72426 | 18.18085 | 22.64112 | 27.10097 | … | 44.93427 |

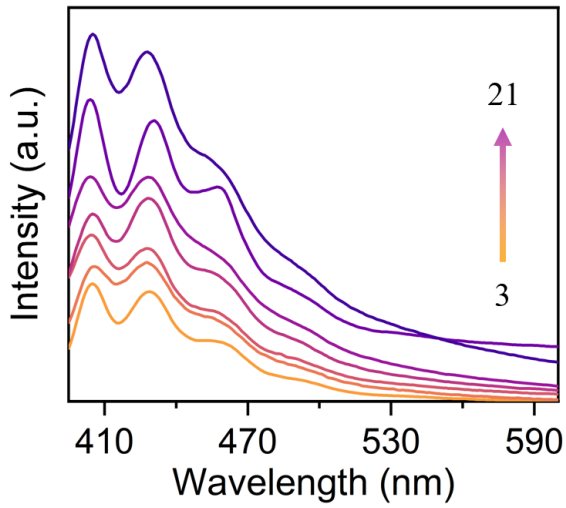



**Figure S10.** The fluorescence emission spectra of NBPs with 3–21 nickel atoms. The spectra show that the NBPs with different nickel atom numbers have almost identical profiles with two main emission peaks at ~405 and ~430 nm and a shoulder peak at ~450 nm. Measured in dichloromethane solution ($10^{-6}$ M) with the excitation wavelength $\lambda_{ex}$ = 380 nm.

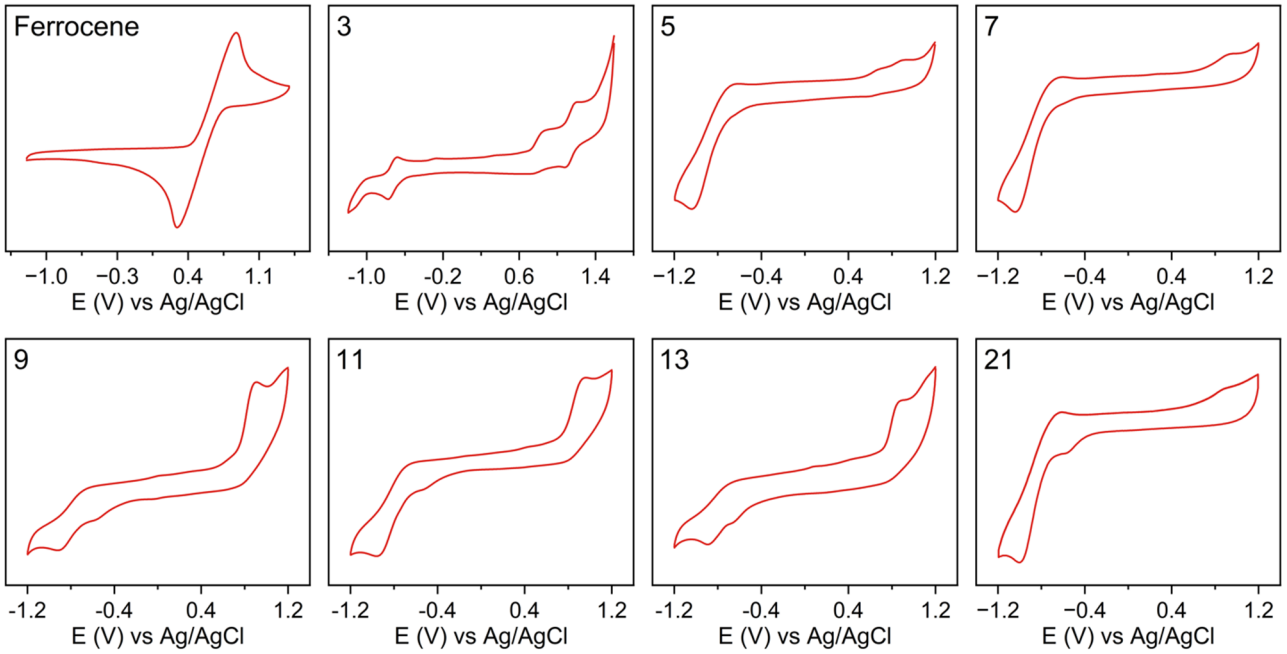



**Figure S11.** Cyclic voltammograms of NBPs with 3–21 nickel atoms. Ferrocene was adopted as the external standard sample.

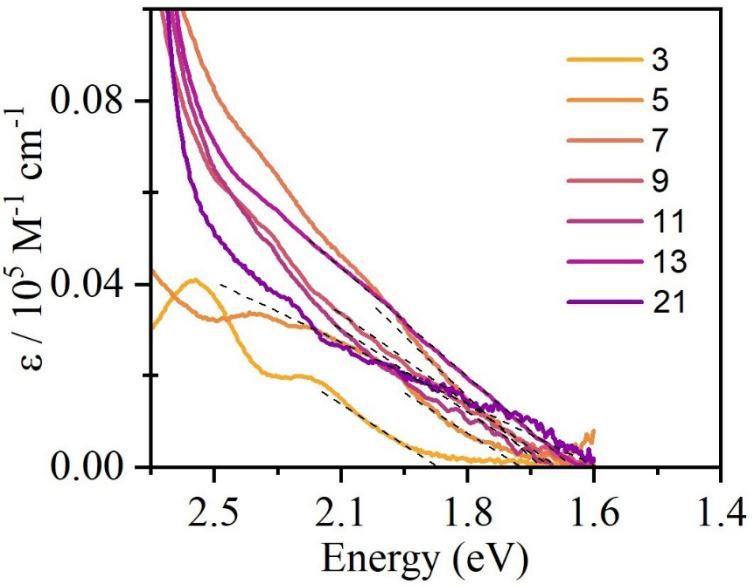



**Figure S12.** Optical bandgaps of NBPs with 3–21 nickel atoms. Tauc plot to determine the optical bandgaps of NBPs with 3–21 nickel atoms, with extrapolation of the linear region (black) estimating of 1.60–1.90 eV that consistent with their cyclic voltammetry results.

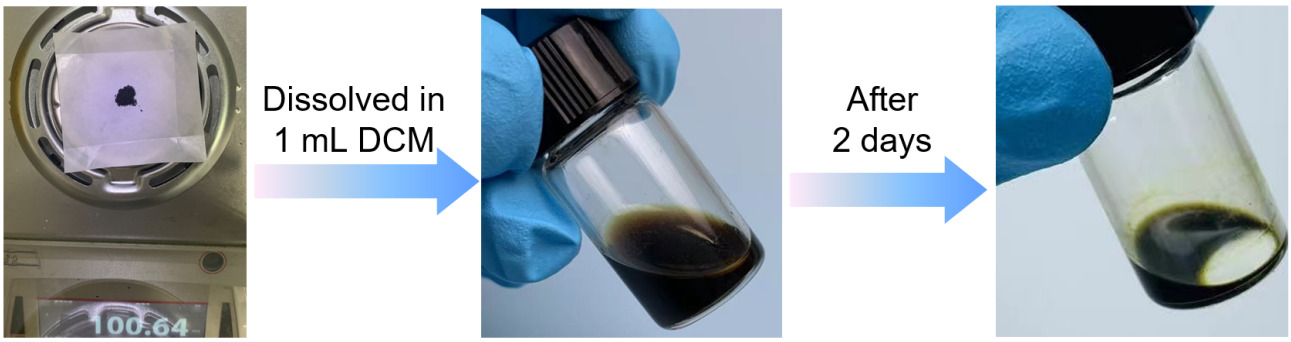



**Figure S13.** The solubility exhibition of NBPs. The photographs show that 100.64 mg of NBP with 21 nickel atoms is well dissolved by 1.0 mL dichloromethane and no precipitation was observed although *ca*. 80% solvent evaporated.

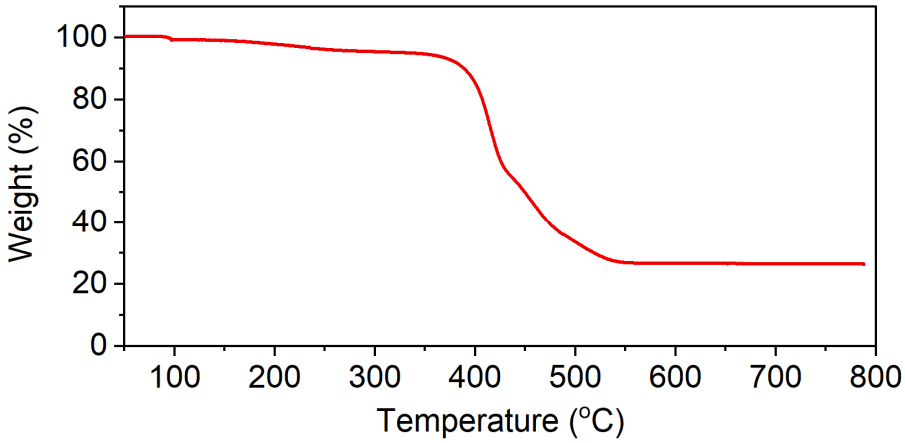



**Figure S14.** TGA of the NBP with 21 nickel atoms (after activation of the sample). The analysis shows that NBP with 21 nickel atoms have excellent thermal stability with decomposition temperature onset above 380 °C. TGA was carried out under $N_2$ atmosphere from 30 °C to 800 °C along with a ramp rate of 10 °C $min^{-1}$. Before carrying out the TGA, the samples were activated at 100 °C for 30 minutes to eliminate the sample's water.

## Characterization Spectra for the Compounds

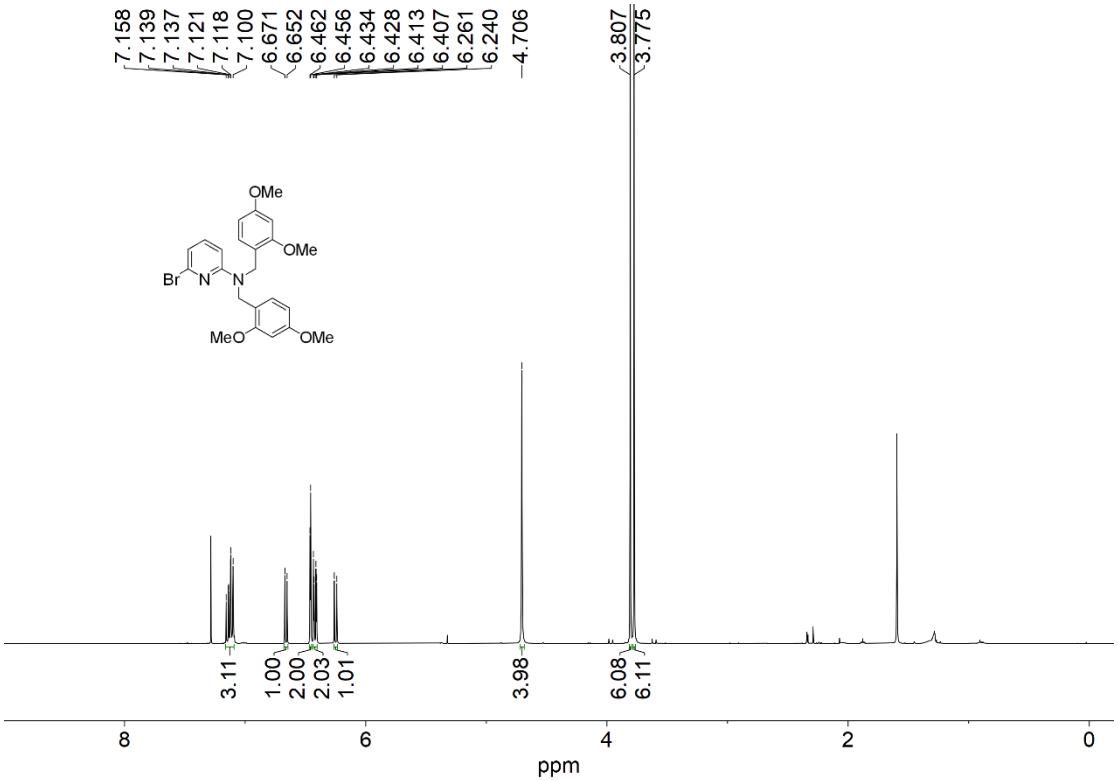



**Figure S15.** $^{1}H$ NMR spectrum of 6-bromo-N,N-bis(2,4-dimethoxybenzyl)pyridin-2-amine in $CDCl_3$.

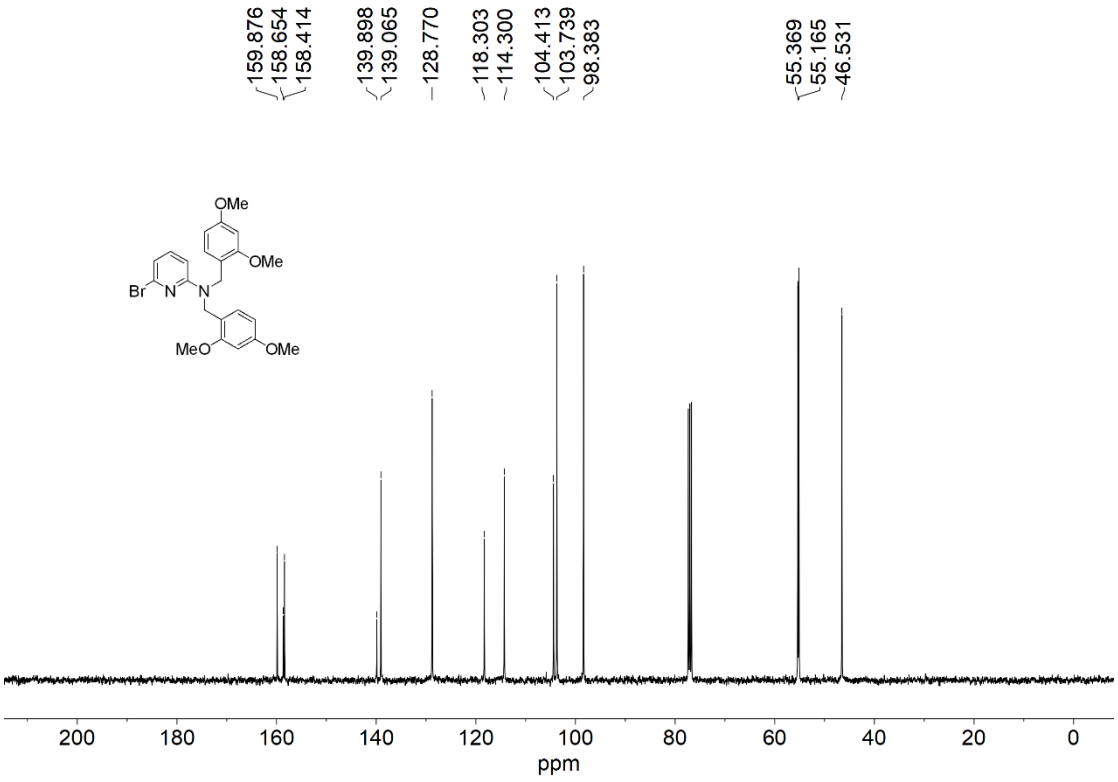



**Figure S16.** $^{13}C$ NMR spectrum of 6-bromo-N,N-bis(2,4-dimethoxybenzyl)pyridin-2-amine in $CDCl_3$.

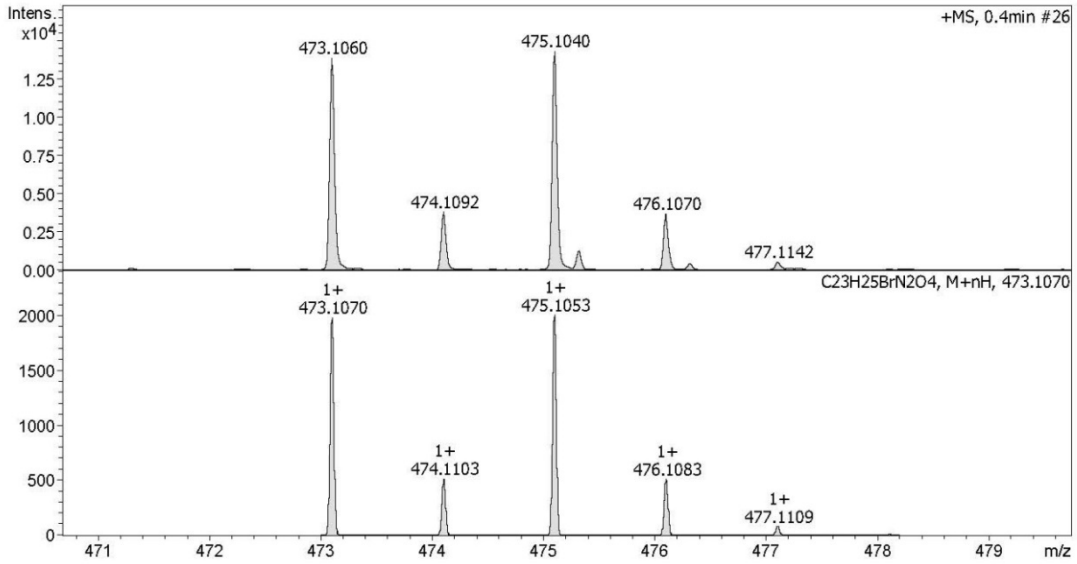



**Figure S17.** HRMS of 6-bromo-N,N-bis(2,4-dimethoxybenzyl)pyridin-2-amine.

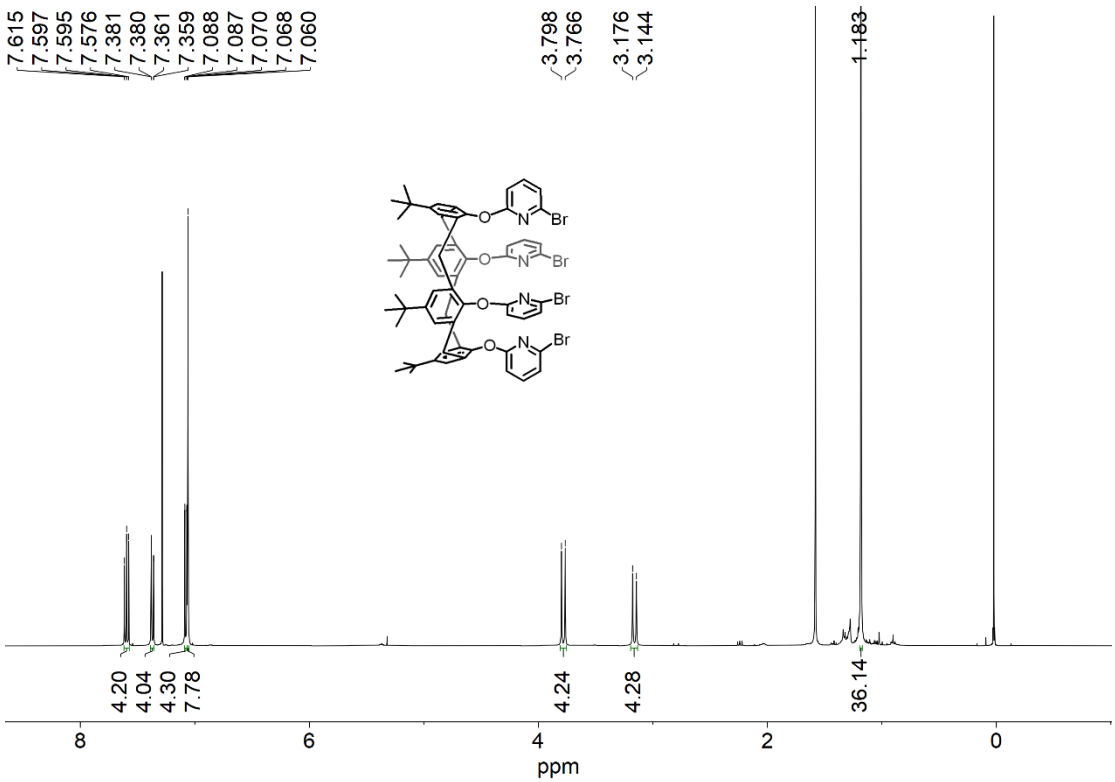



**Figure S18.** $^{1}H$ NMR spectrum of Compound **1** in $CDCl_3$. The two characteristic signals at $\delta$ = 3.78 and 3.16 ppm are attributed to the methylene protons, indicating the cone conformation of the compound.

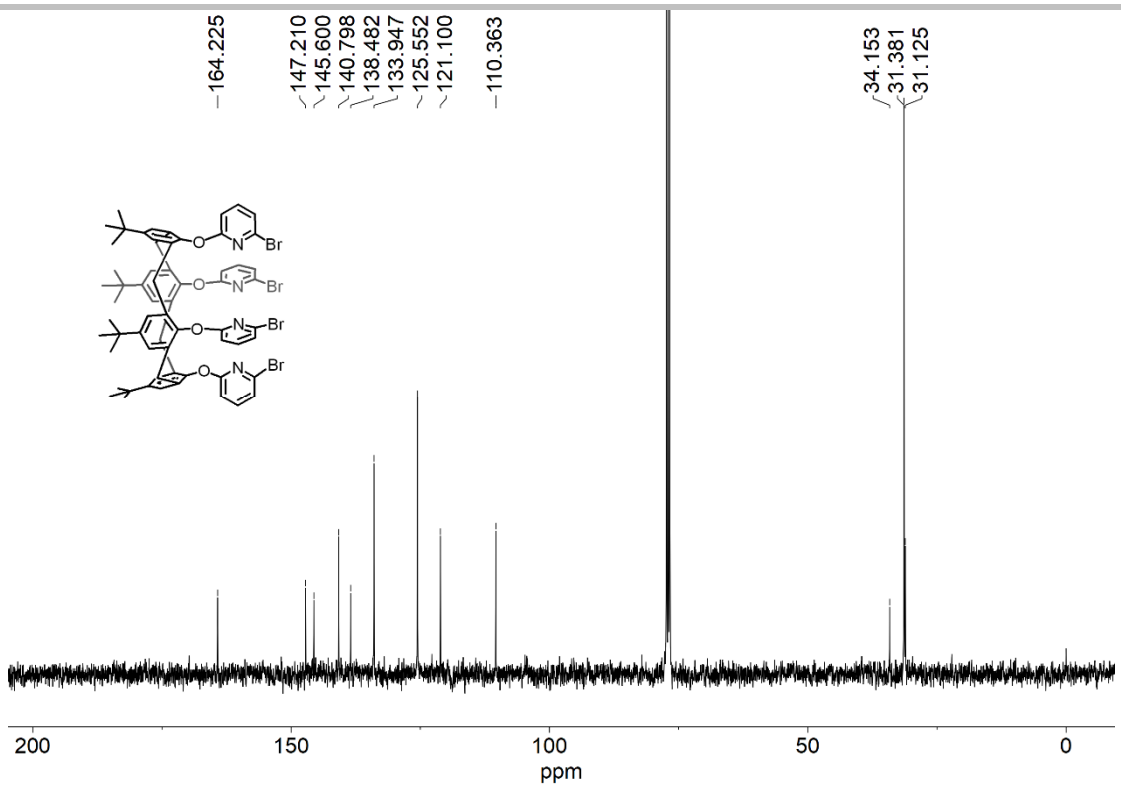



**Figure S19.** $^{13}C$ NMR spectrum of Compound **1** in $CDCl_3$.

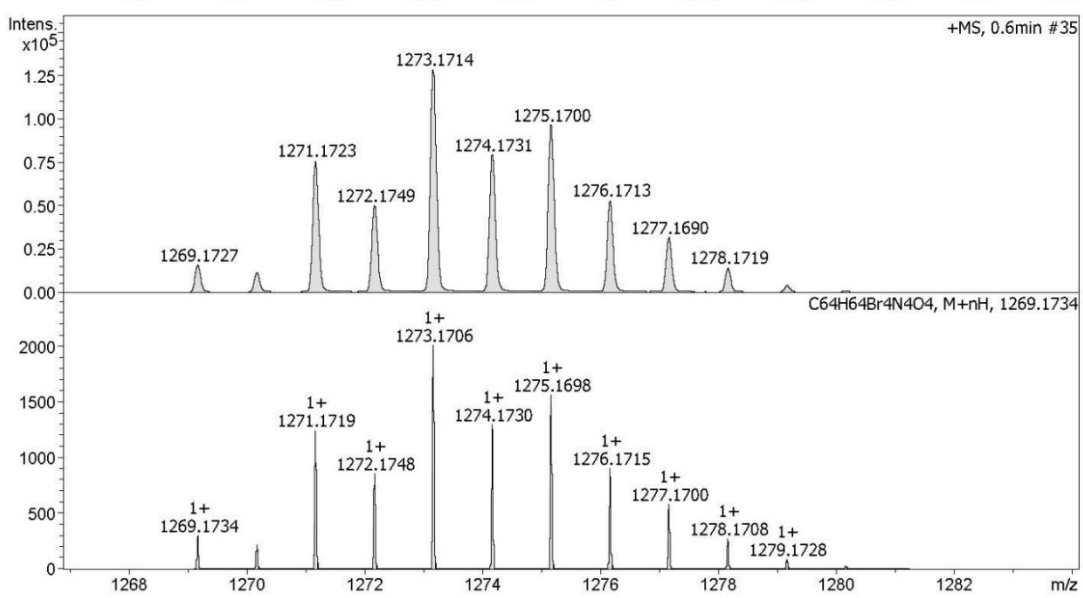



**Figure S20.** HRMS of Compound **1**.

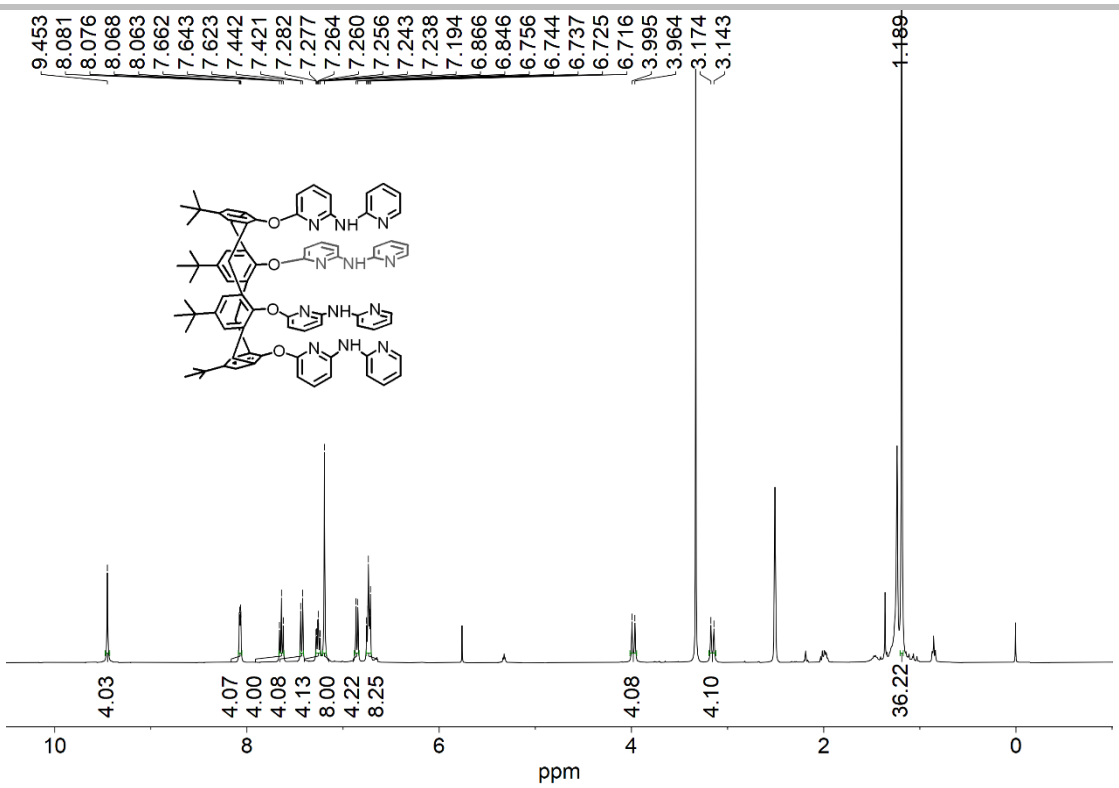



**Figure S21.** $^{1}$H NMR spectrum of $\mathbf{L_1}$ in DMSO-$d_6$.

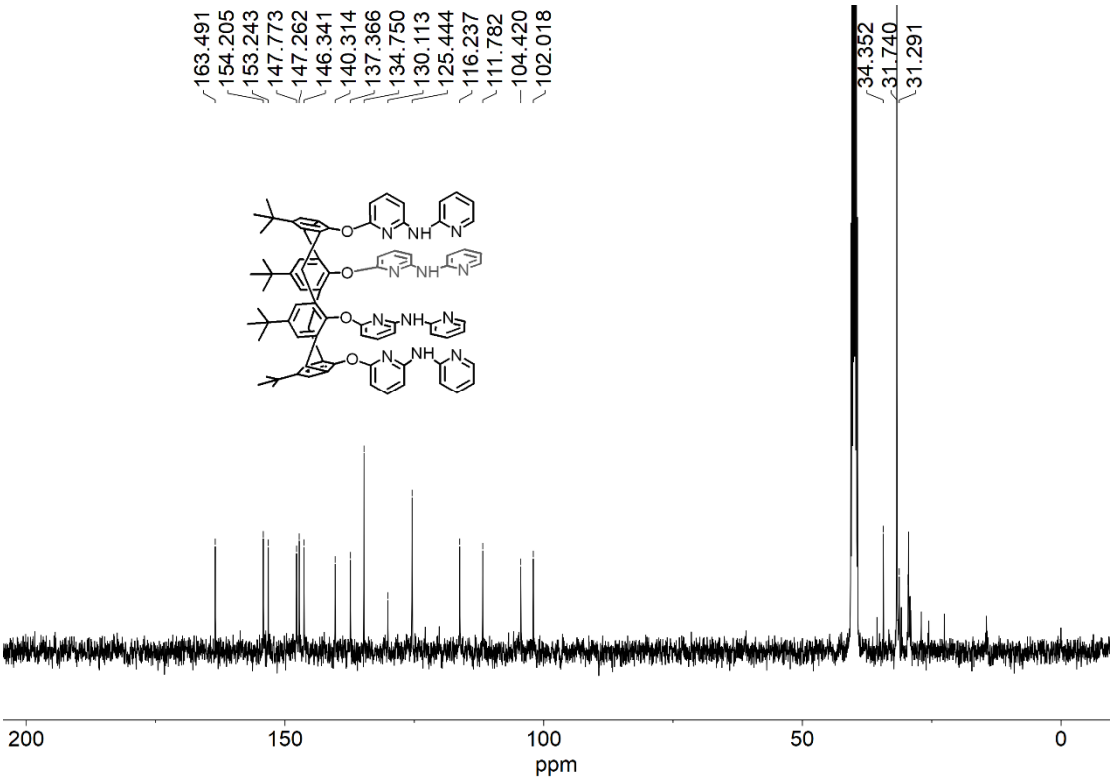



**Figure S22.** $^{13}$C NMR spectrum of $\mathbf{L_1}$ in DMSO-$d_6$.

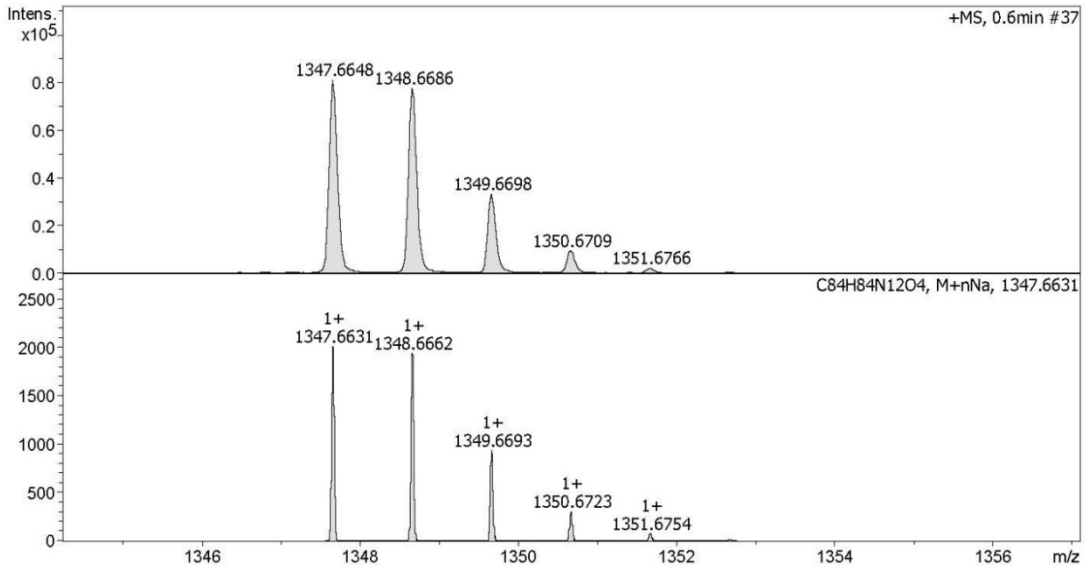



**Figure S23.** HRMS of $\mathbf{L_1}$.

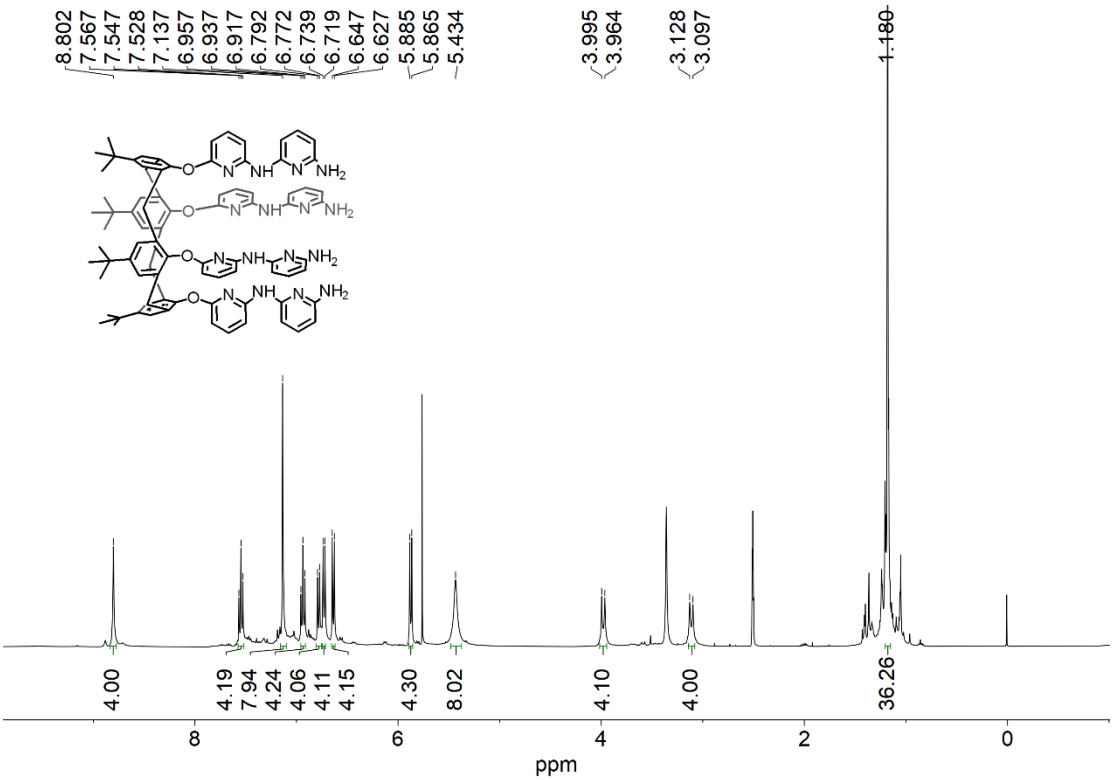



**Figure S24.** $^1$H NMR spectrum of $\mathbf{P_1}$ in DMSO-$d_6$.

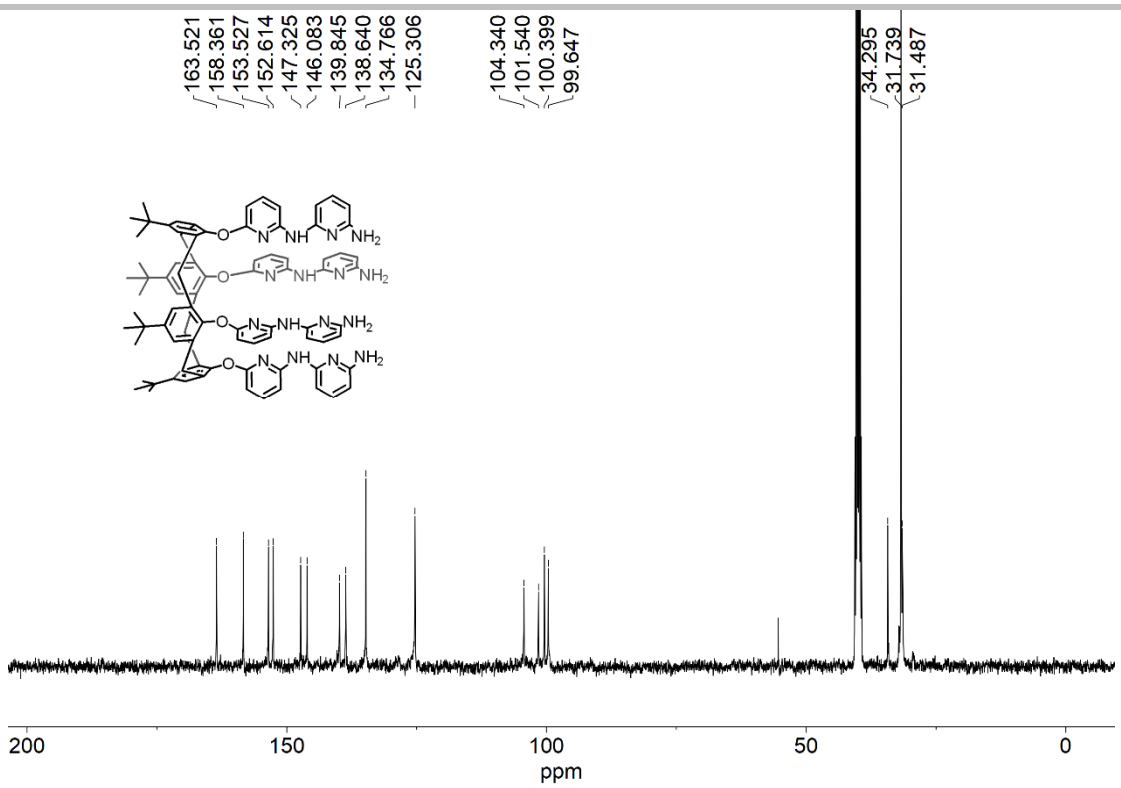



**Figure S25.** $^{13}C$ NMR spectrum of **$P_1$** in DMSO-$d_6$.

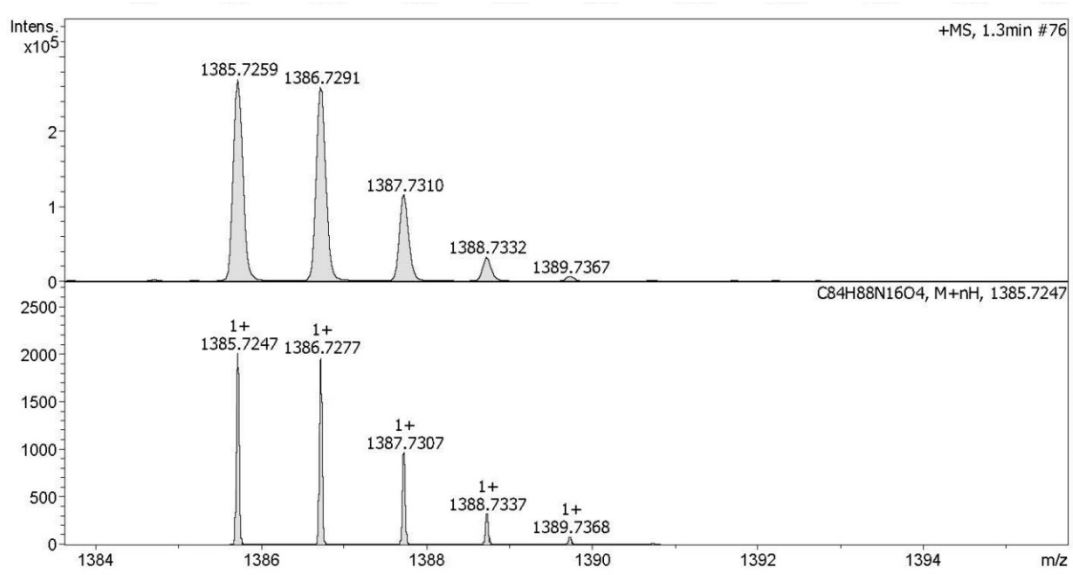



**Figure S26.** HRMS of **$P_1$**.

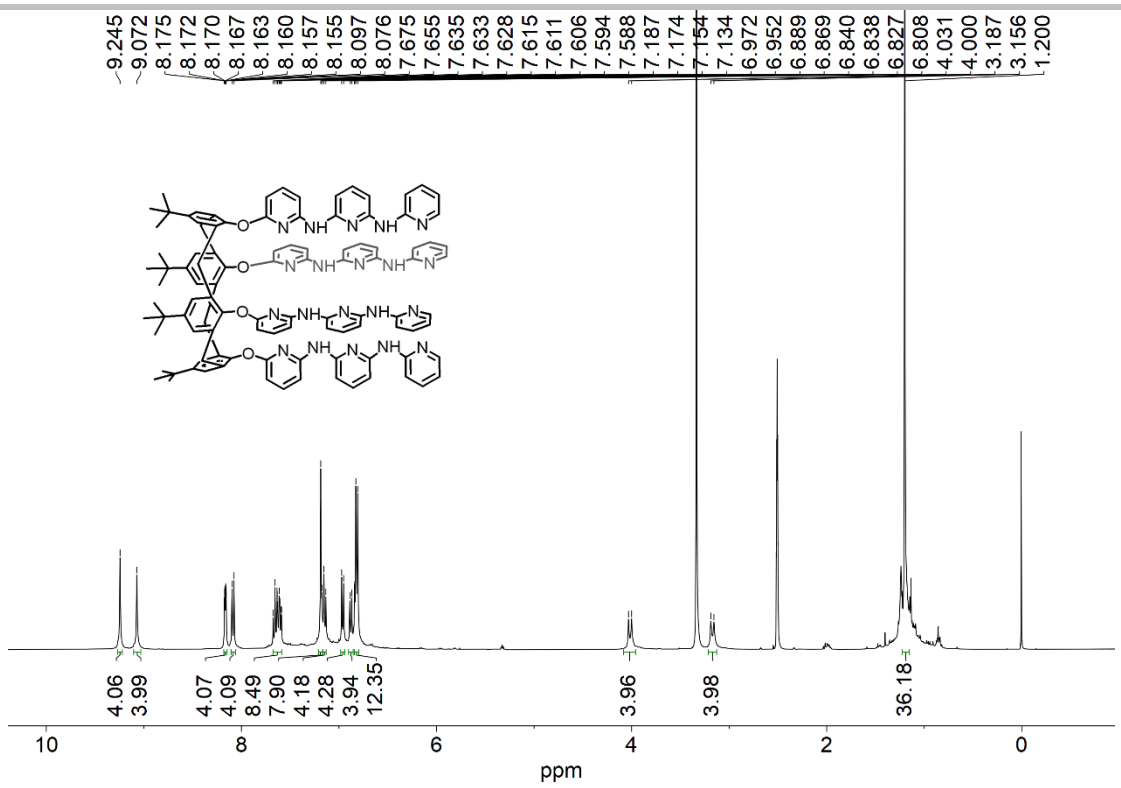



**Figure S27.** $^{1}$H NMR spectrum of **$L_2$** in DMSO-$d_6$.

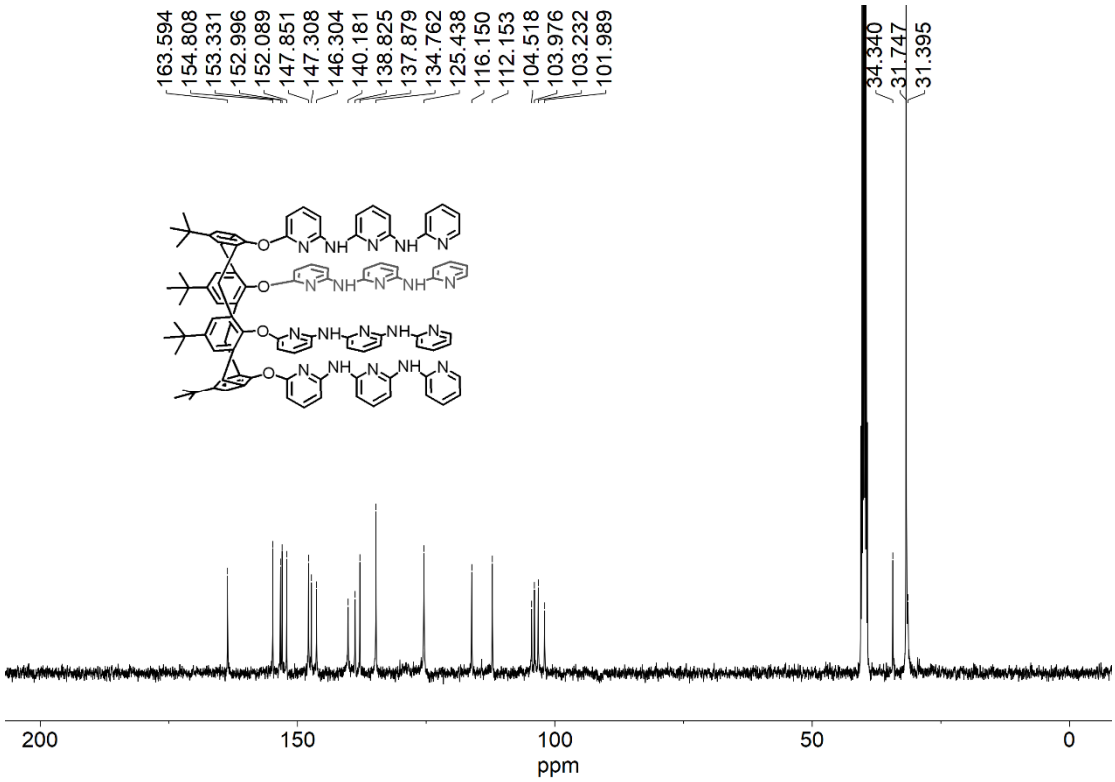



**Figure S28.** $^{13}$C NMR spectrum of **$L_2$** in DMSO-$d_6$.

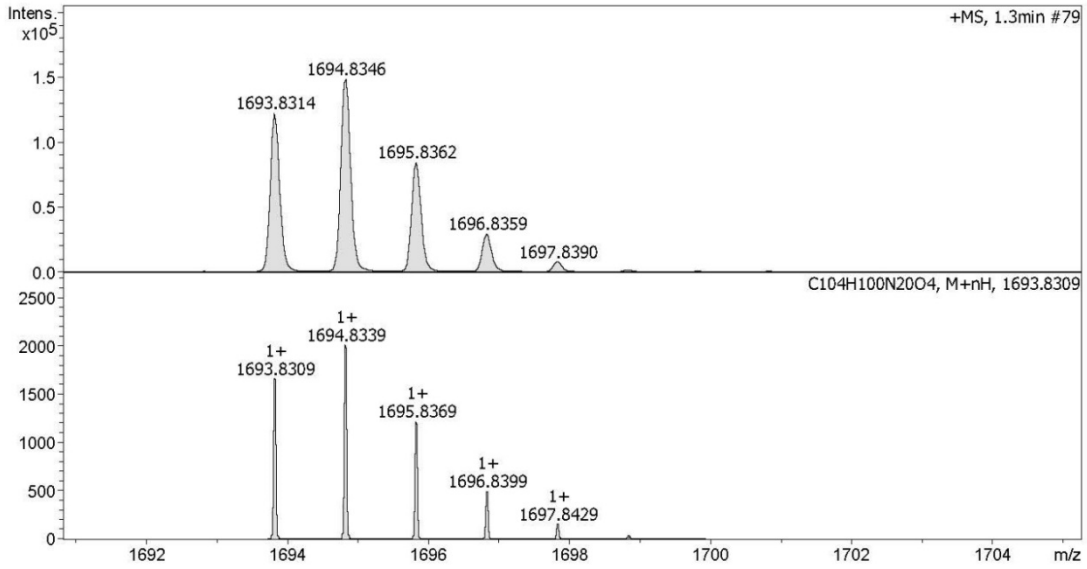



**Figure S29.** HRMS of $\mathbf{L_2}$.

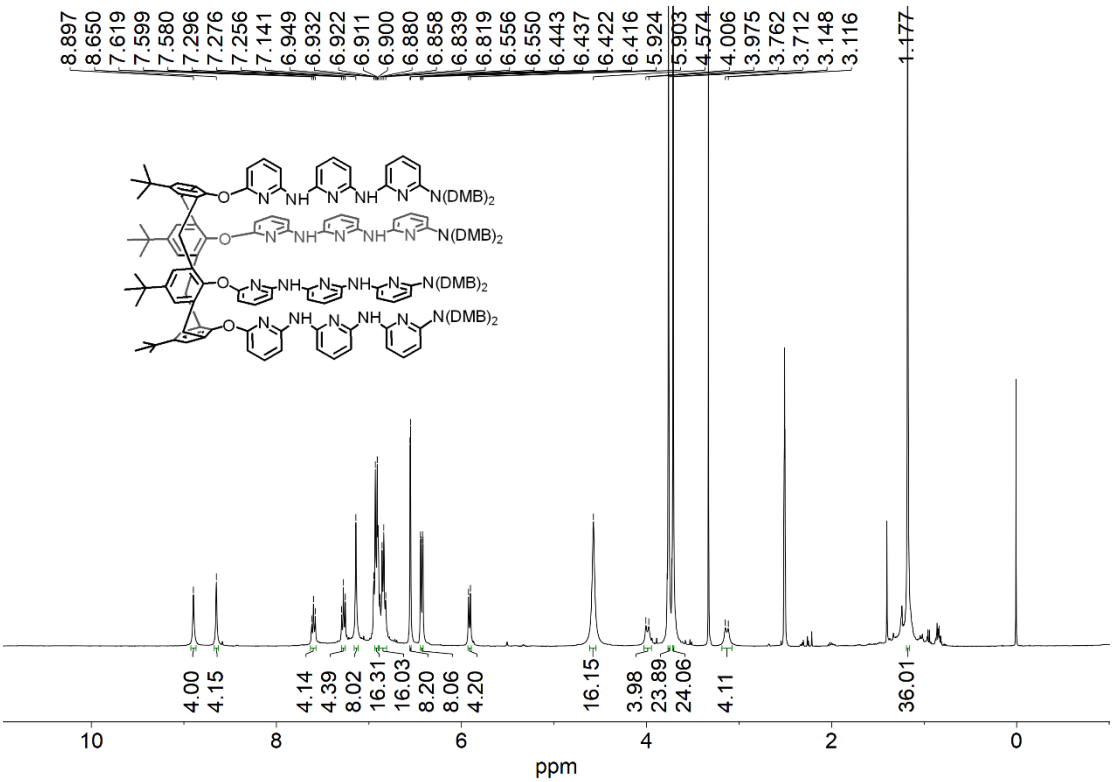



**Figure S30.** $^1$H NMR spectrum of $\mathbf{D_2}$ in DMSO-$d_6$.

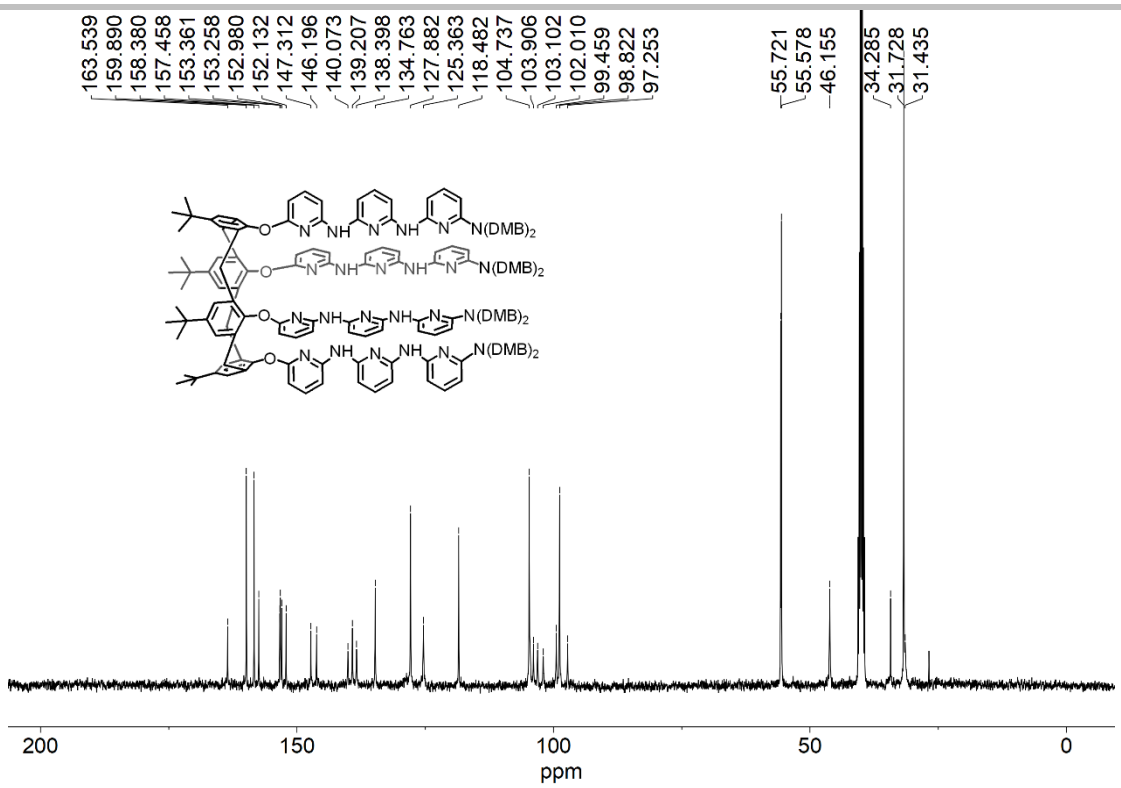



**Figure S31.** $^{13}C$ NMR spectrum of **$D_2$** in DMSO-$d_6$.

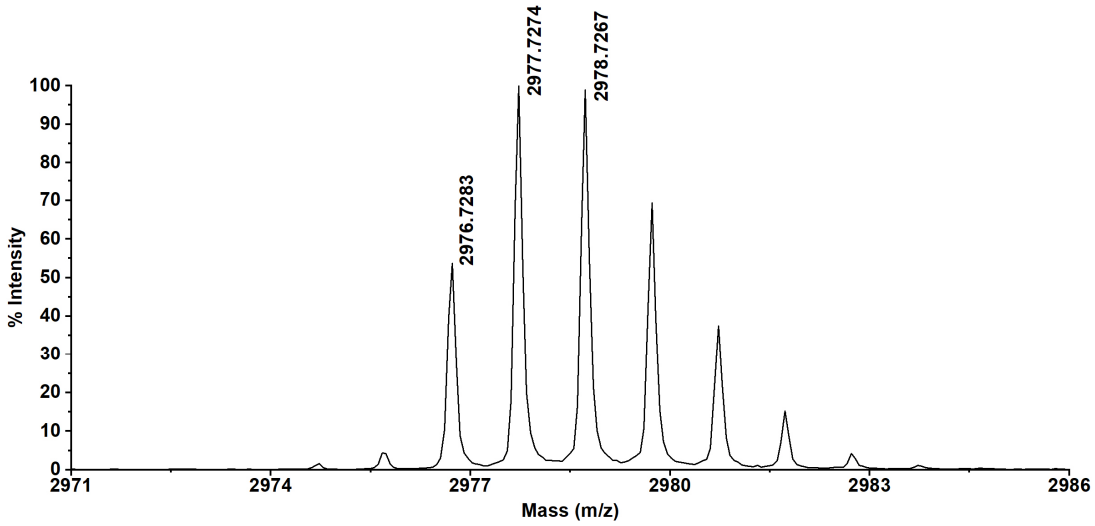



**Figure S32.** MALDI-TOF MS of **$D_2$**.

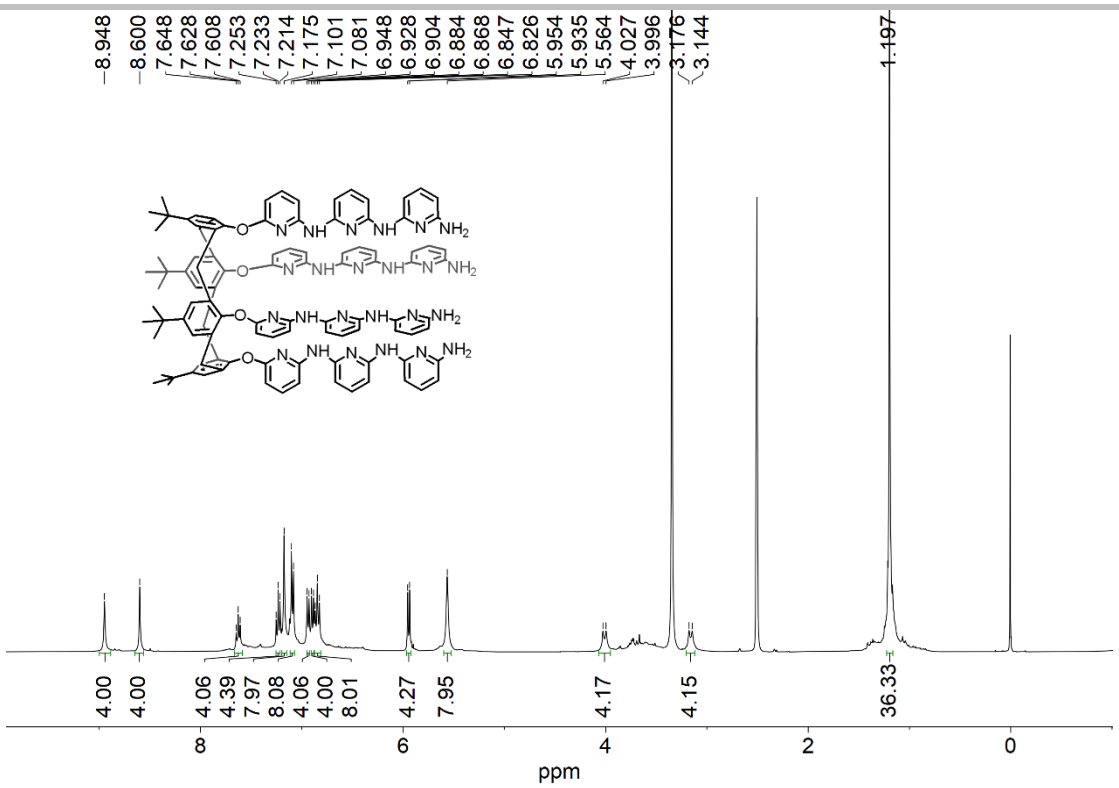



**Figure S33.** $^{1}$H NMR spectrum of **$P_2$** in DMSO-$d_6$.

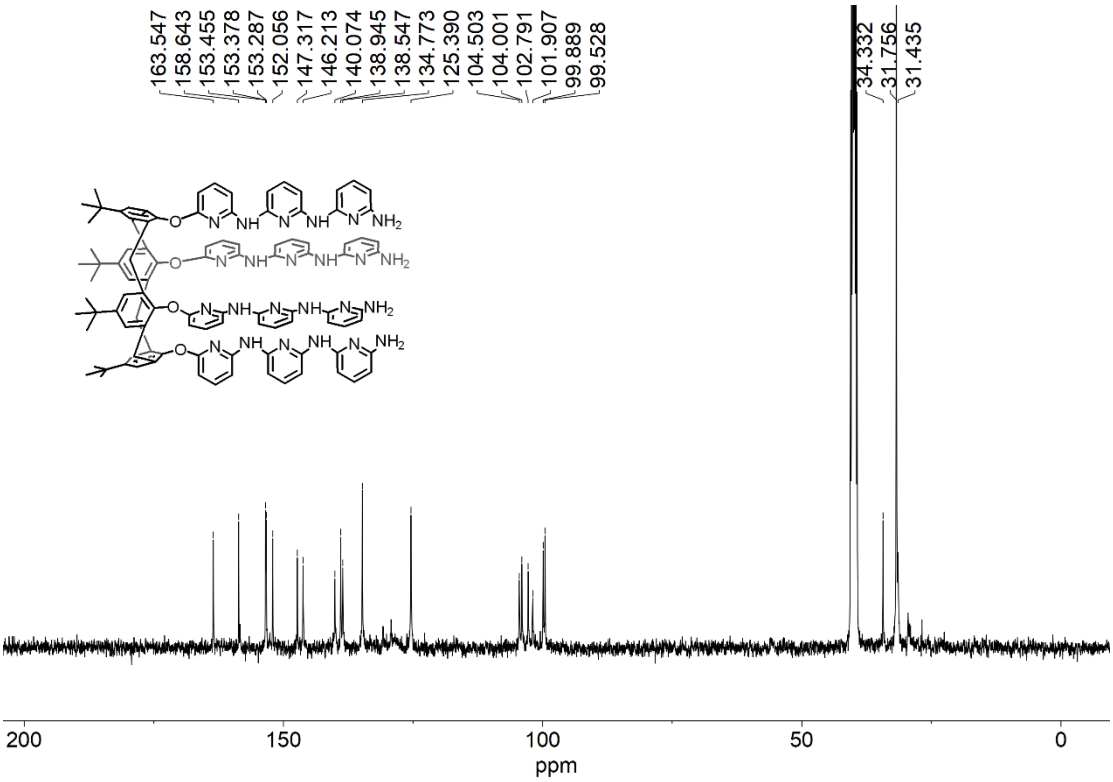



**Figure S34.** $^{13}$C NMR spectrum of **$P_2$** in DMSO-$d_6$.

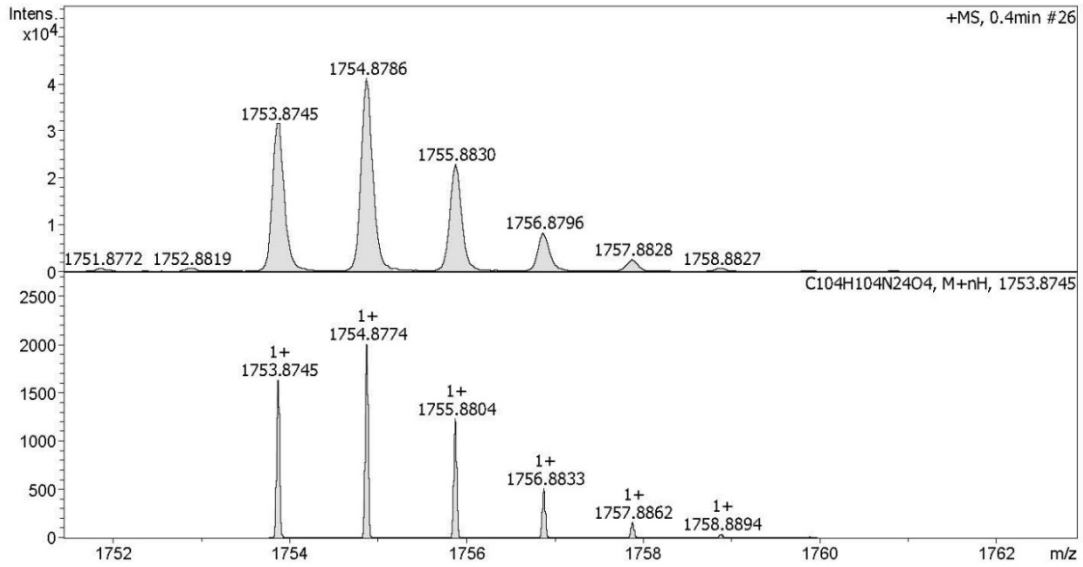



**Figure S35.** HRMS of $\mathbf{P_2}$.

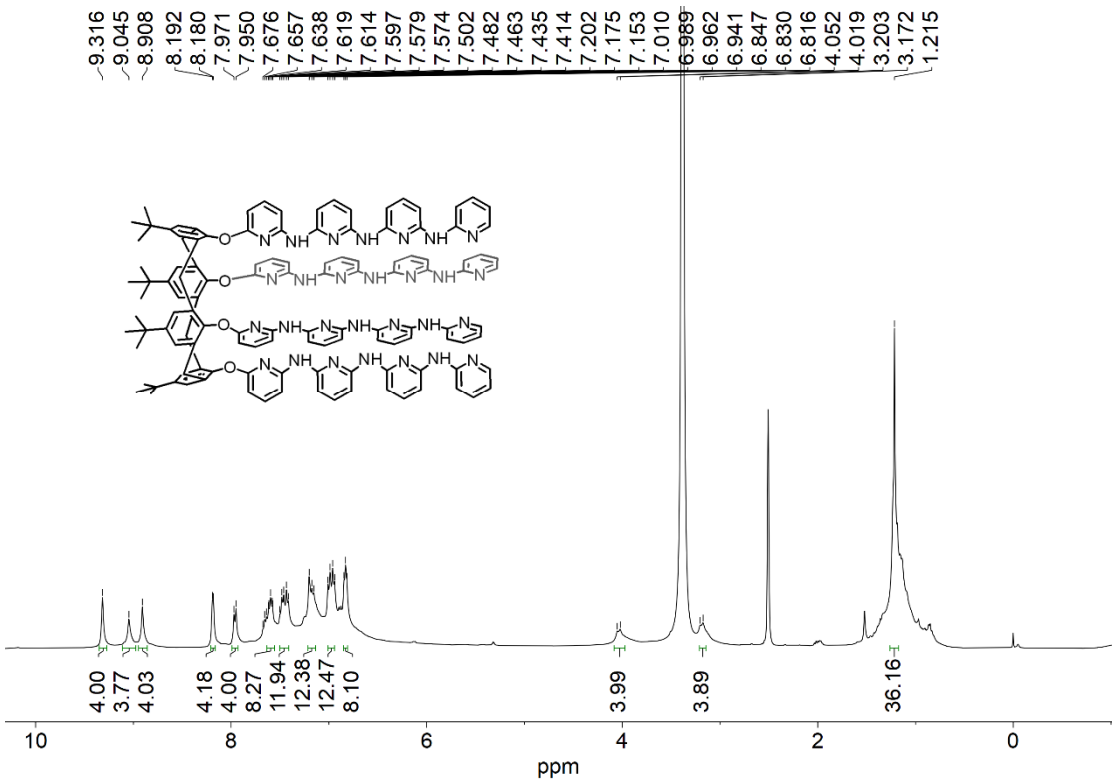



**Figure S36.** $^1$H NMR spectrum of $\mathbf{L_3}$ in DMSO-$d_6$.

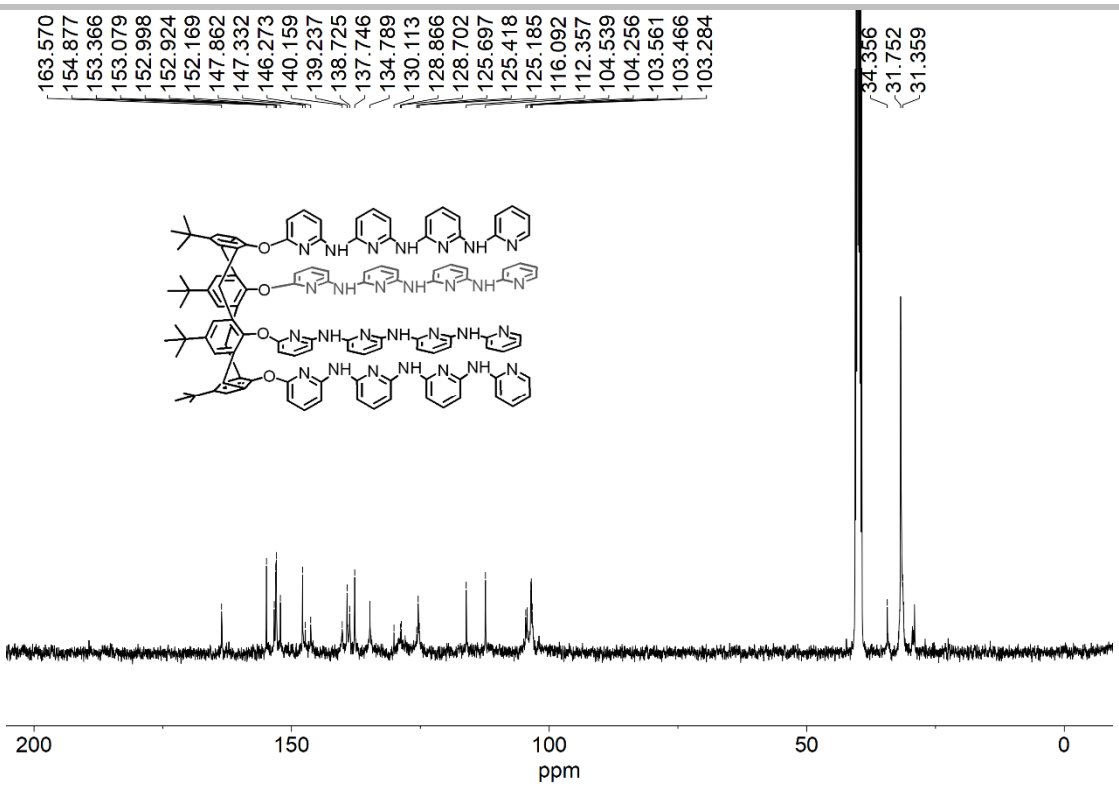



**Figure S37.** $^{13}C$ NMR spectrum of $\mathbf{L_3}$ in DMSO-$d_6$.

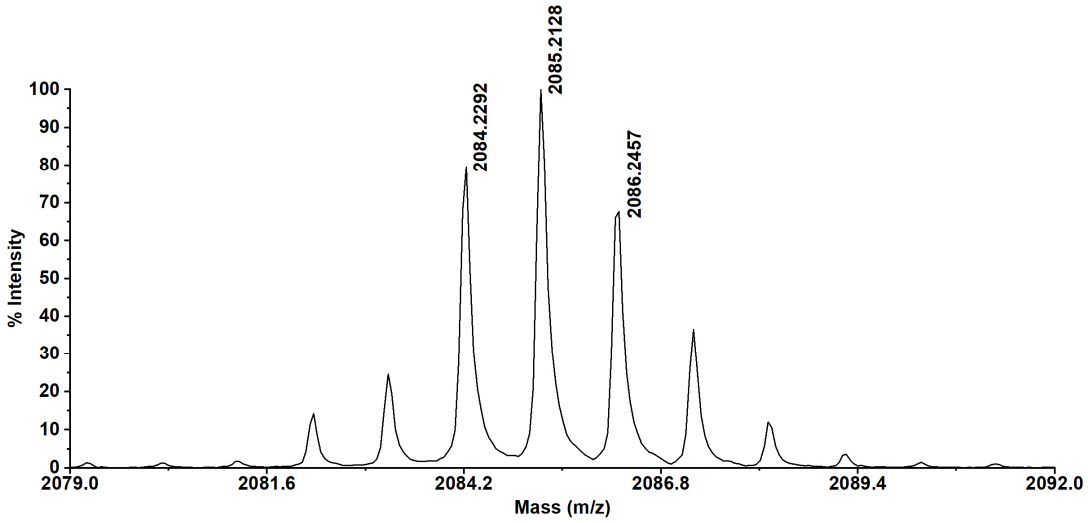



**Figure S38.** MALDI-TOF MS of $\mathbf{L_3}$.

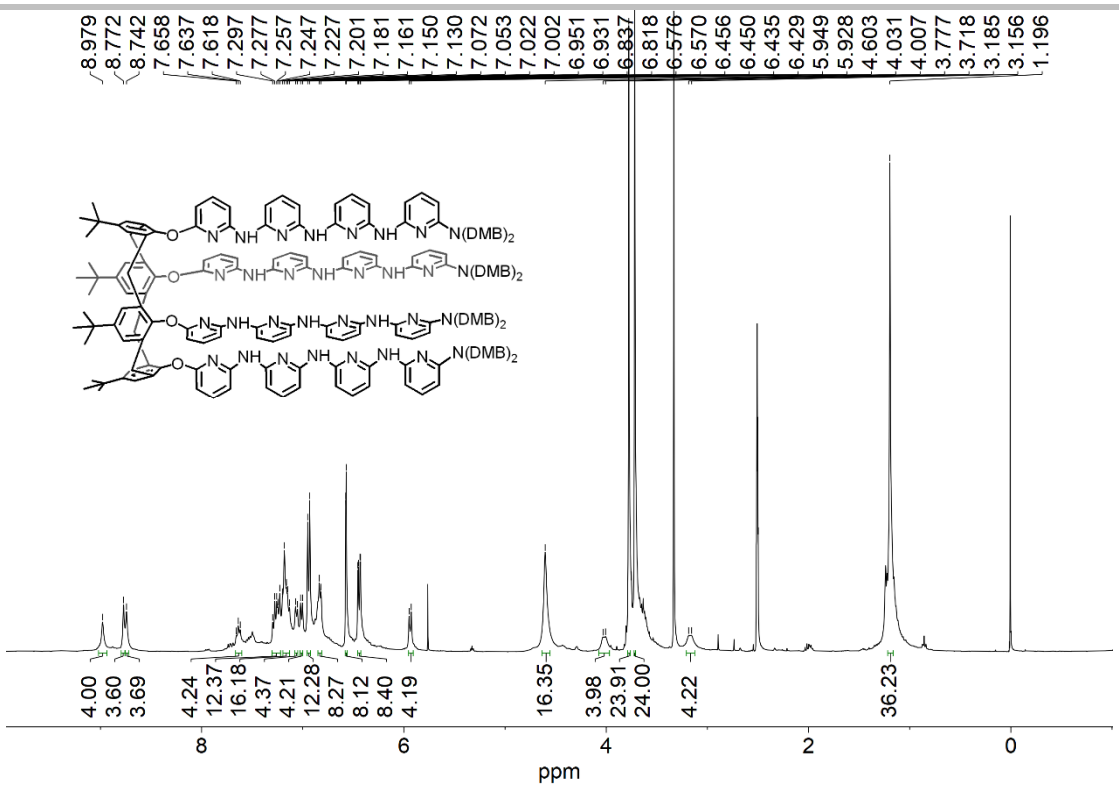



**Figure S39.** $^{1}$H NMR spectrum of **D$_3$** in DMSO-*d*$_6$.

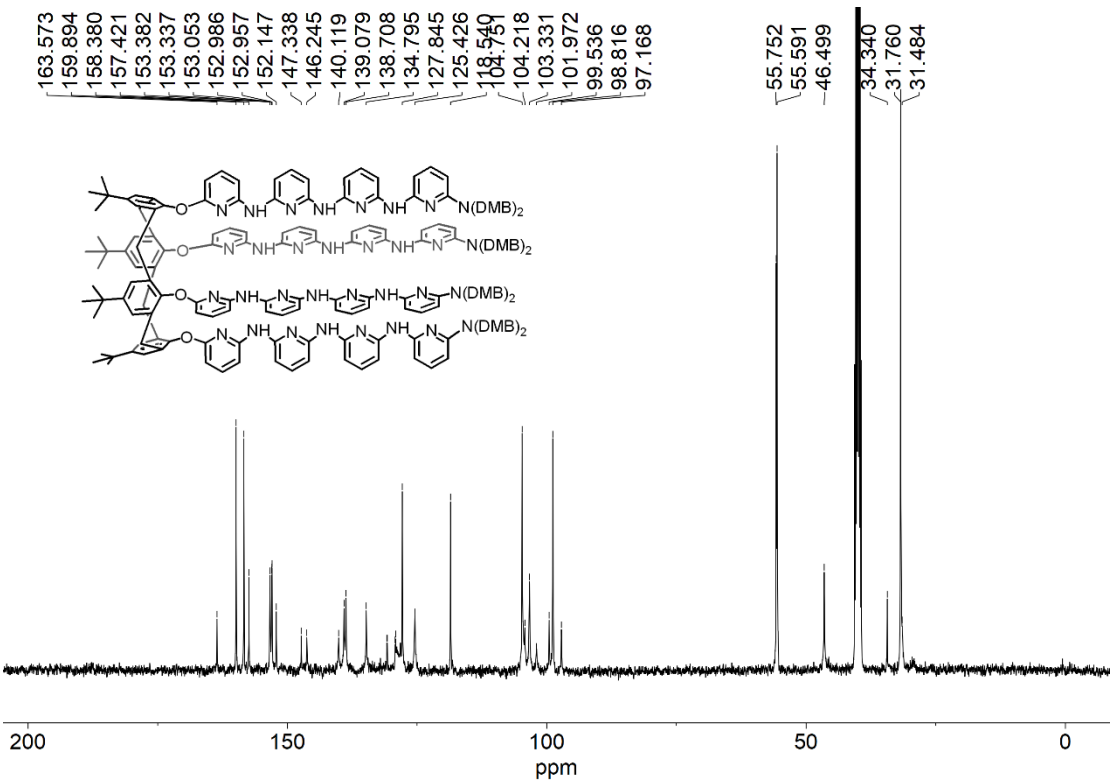



**Figure S40.** $^{13}$C NMR spectrum of **D$_3$** in DMSO-*d*$_6$.

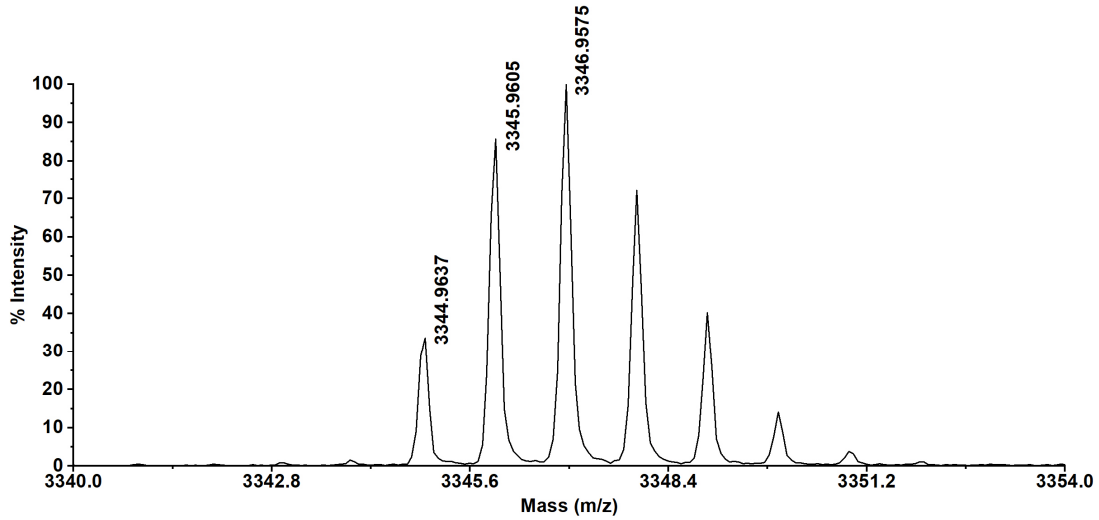



**Figure S41.** MALDI-TOF MS of $\mathbf{D_3}$.

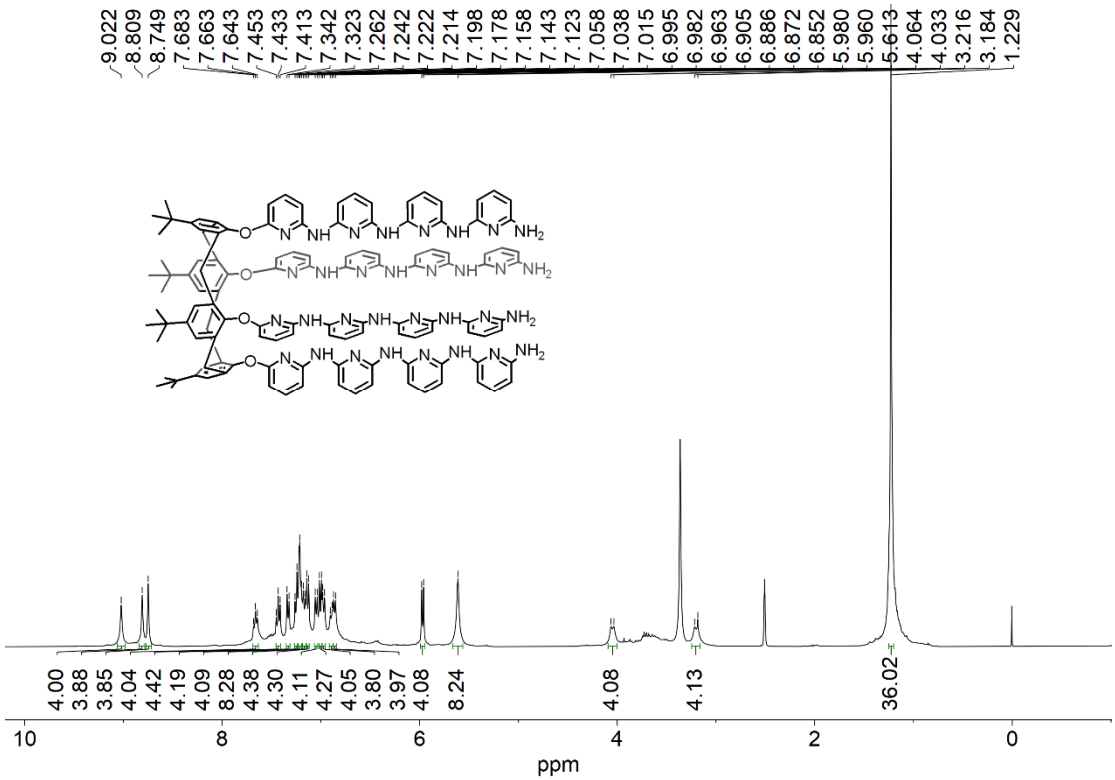



**Figure S42.** $^1$H NMR spectrum of $\mathbf{P_3}$ in DMSO-$d_6$.

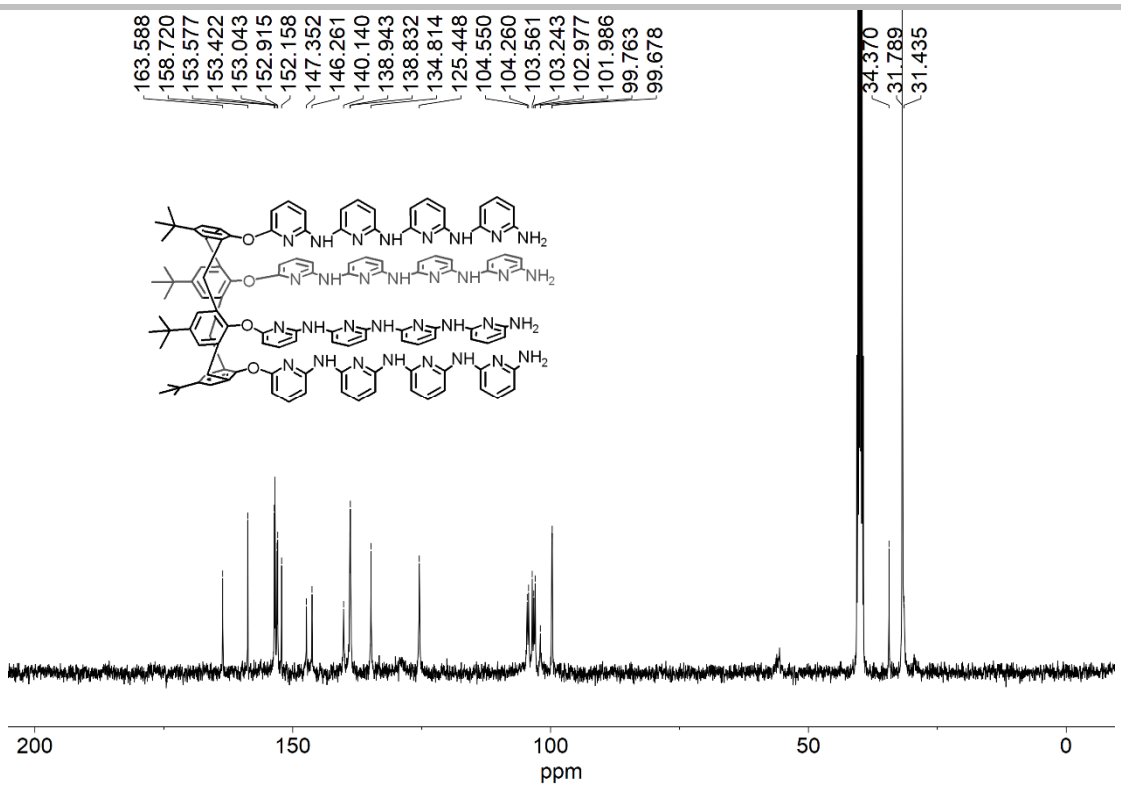



**Figure S43.** $^{13}C$ NMR spectrum of **$P_3$** in DMSO-$d_6$.

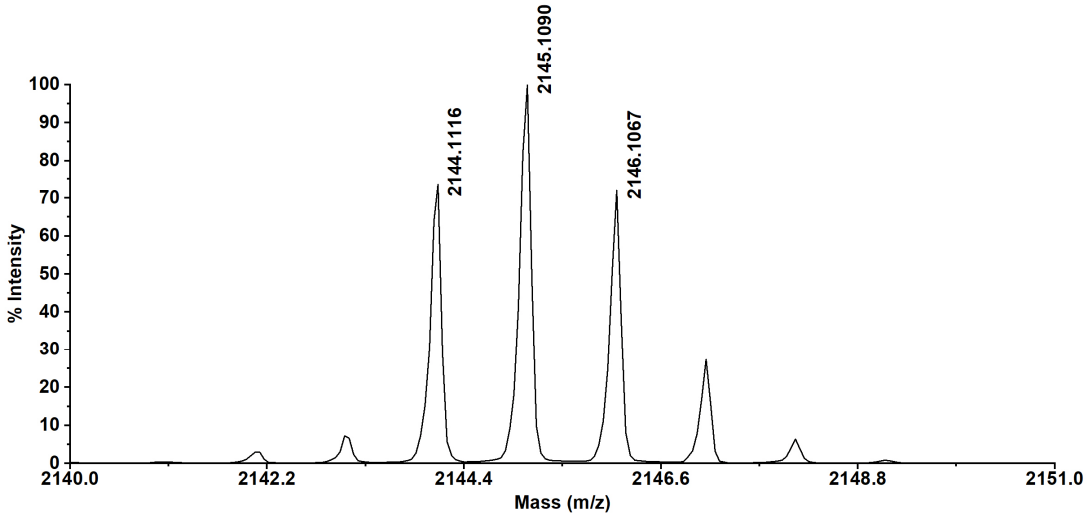



**Figure S44.** MALDI-TOF MS of **$P_3$**.

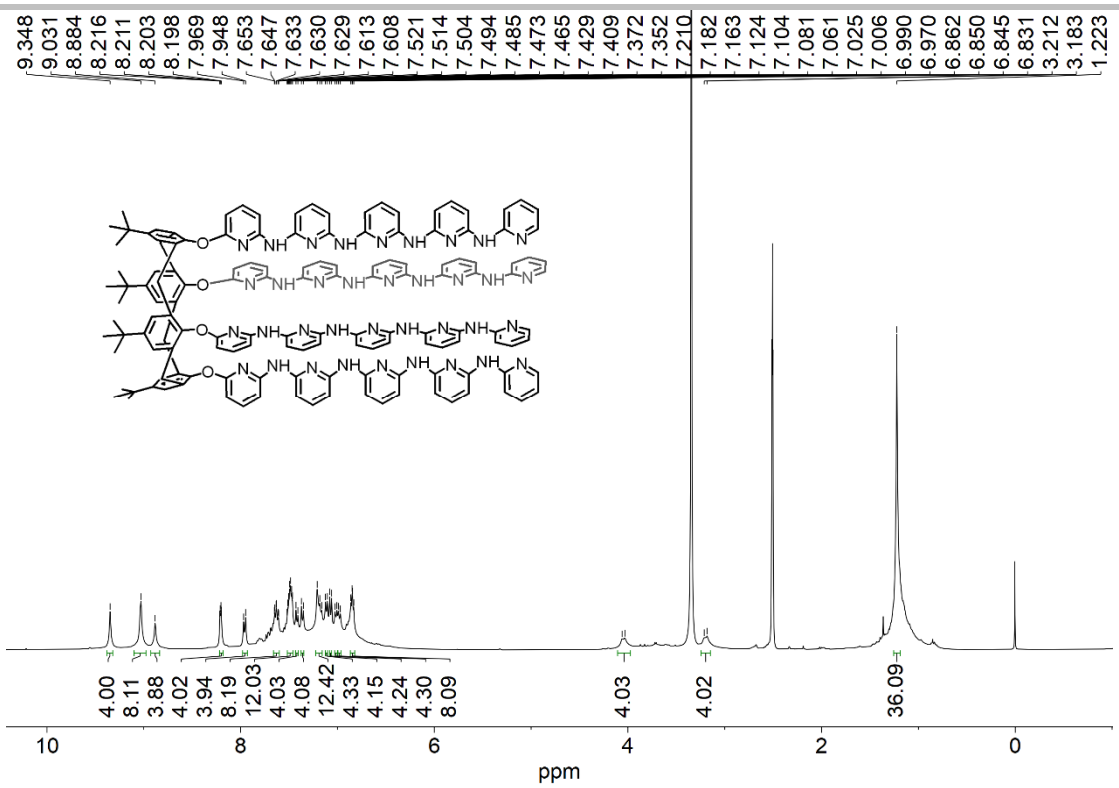



**Figure S45.** $^{1}$H NMR spectrum of **L$_4$** in DMSO-$d_6$.

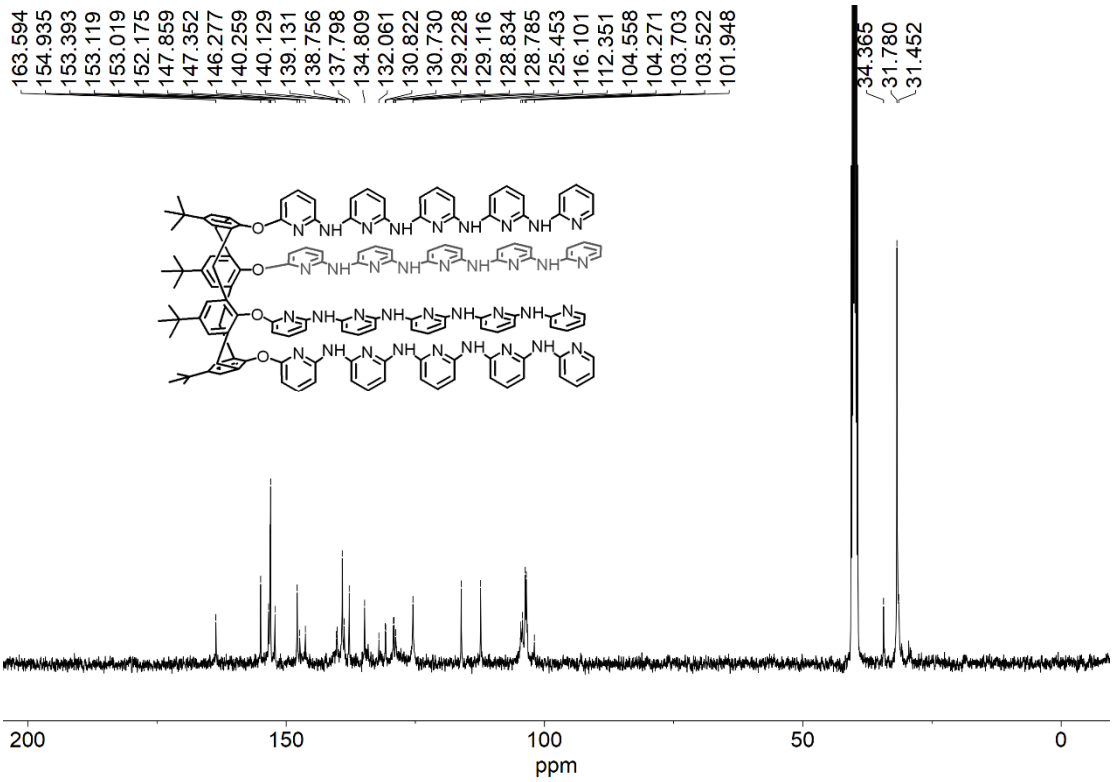



**Figure S46.** $^{13}$C NMR spectrum of **L$_4$** in DMSO-$d_6$.

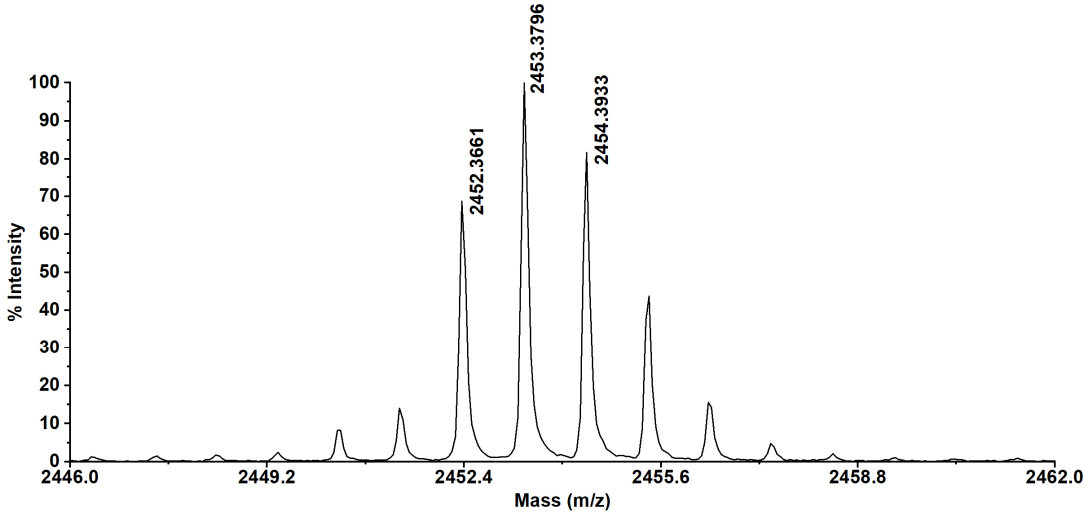



**Figure S47.** MALDI-TOF MS of $\mathbf{L_4}$.

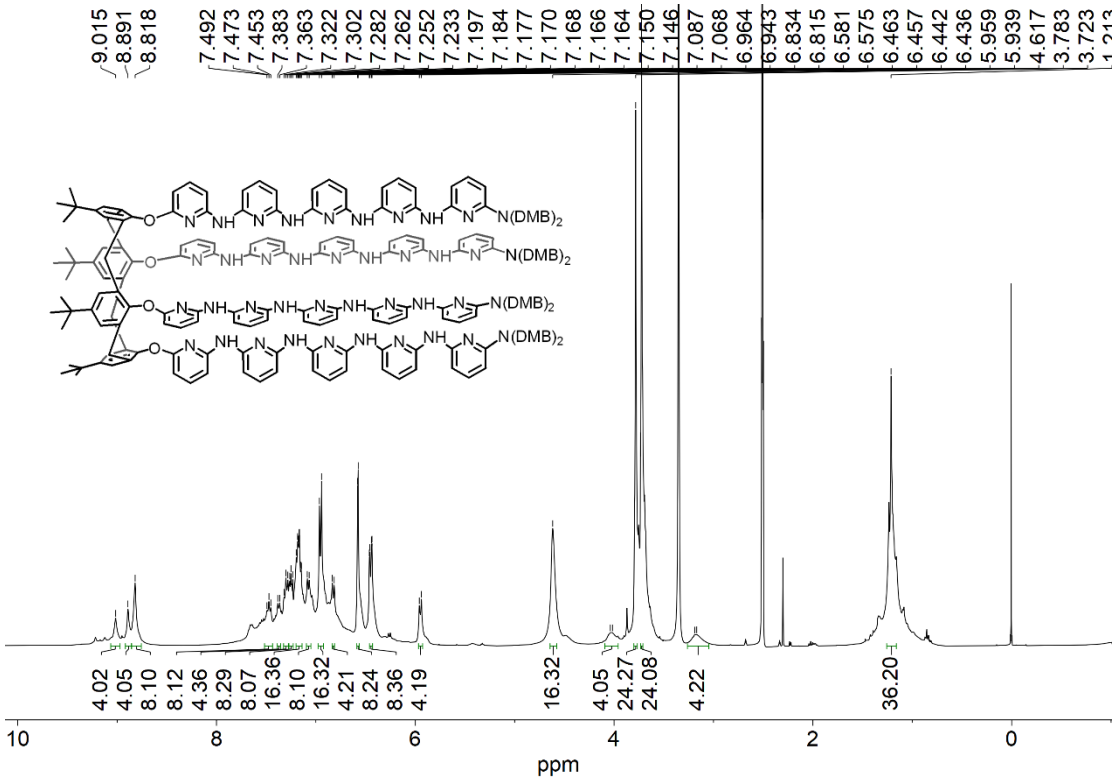



**Figure S48.** $^1$H NMR spectrum of $\mathbf{D_4}$ in DMSO-$d_6$.

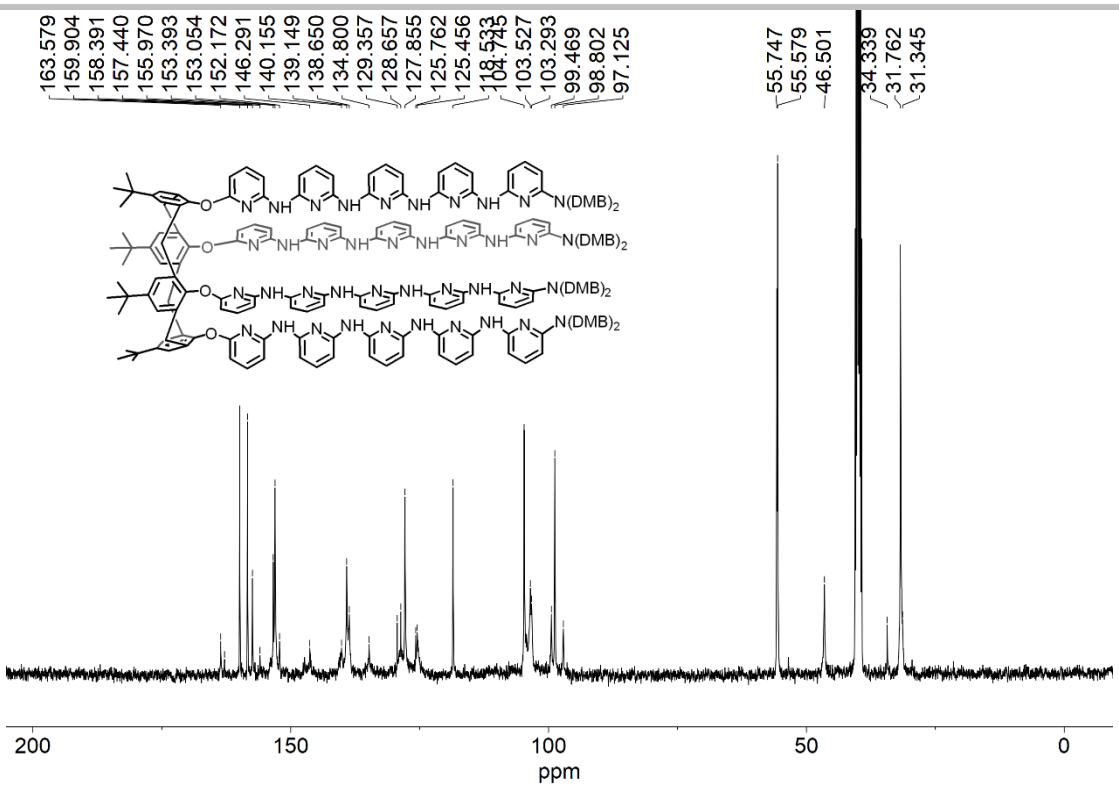



**Figure S49.** $^{13}C$ NMR spectrum of **D₄** in DMSO-$d_6$.

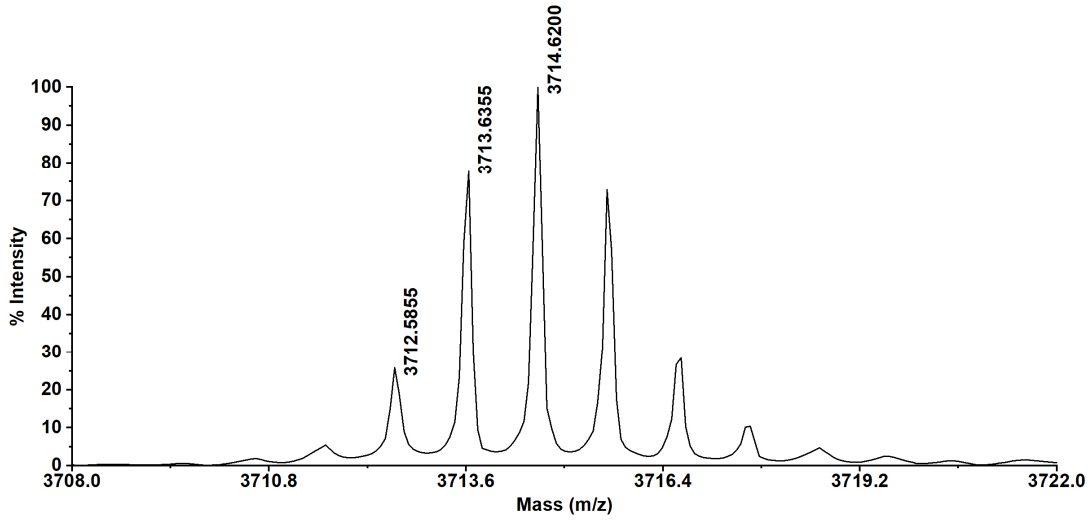



**Figure S50.** MALDI-TOF MS of **D₄**.

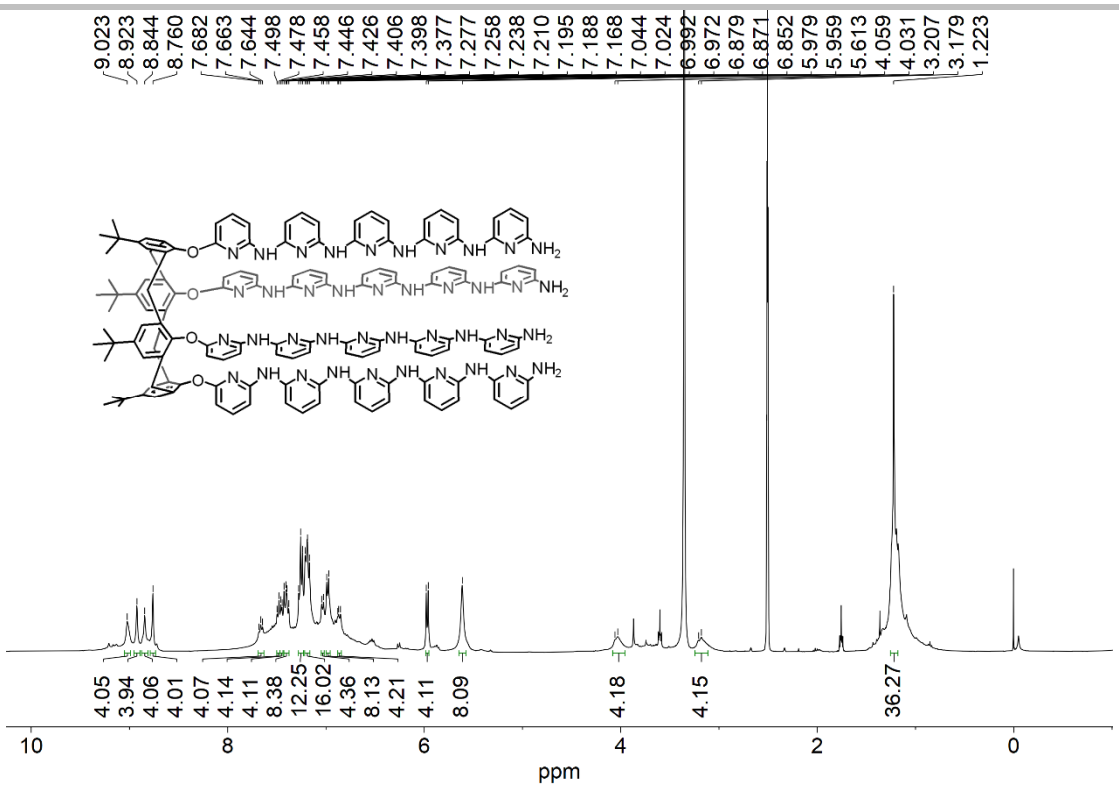



**Figure S51.** $^{1}$H NMR spectrum of **P$_4$** in DMSO-$d_6$.

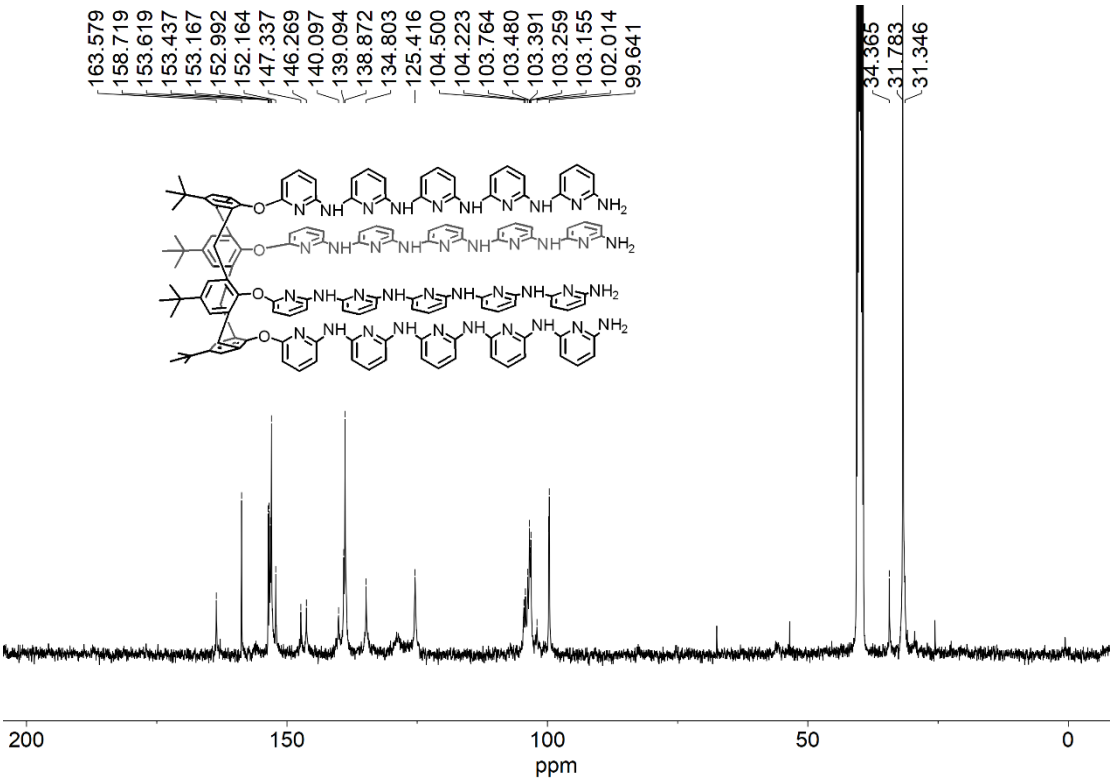



**Figure S52.** $^{13}$C NMR spectrum of **P$_4$** in DMSO-$d_6$.

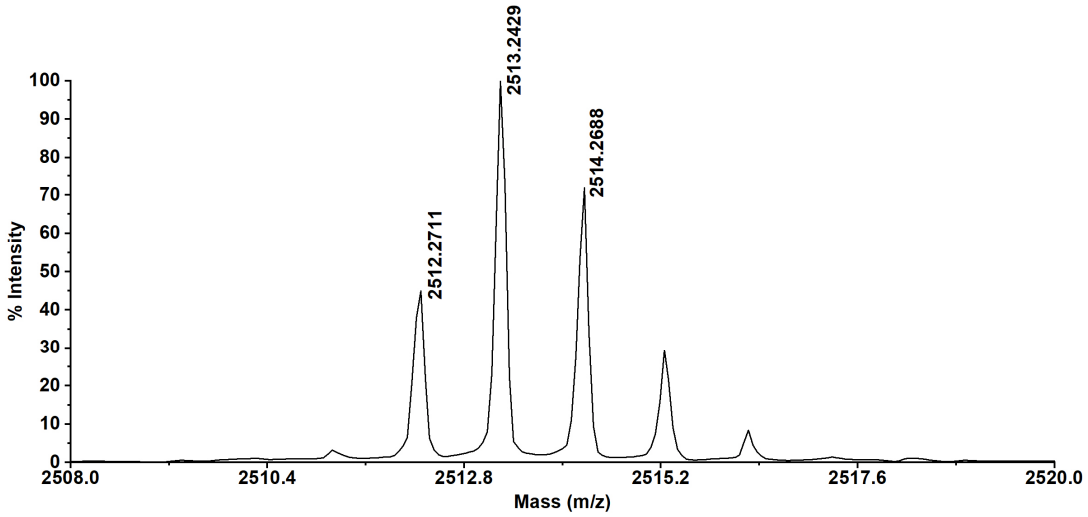



**Figure S53.** MALDI-TOF MS of **$P_4$**.

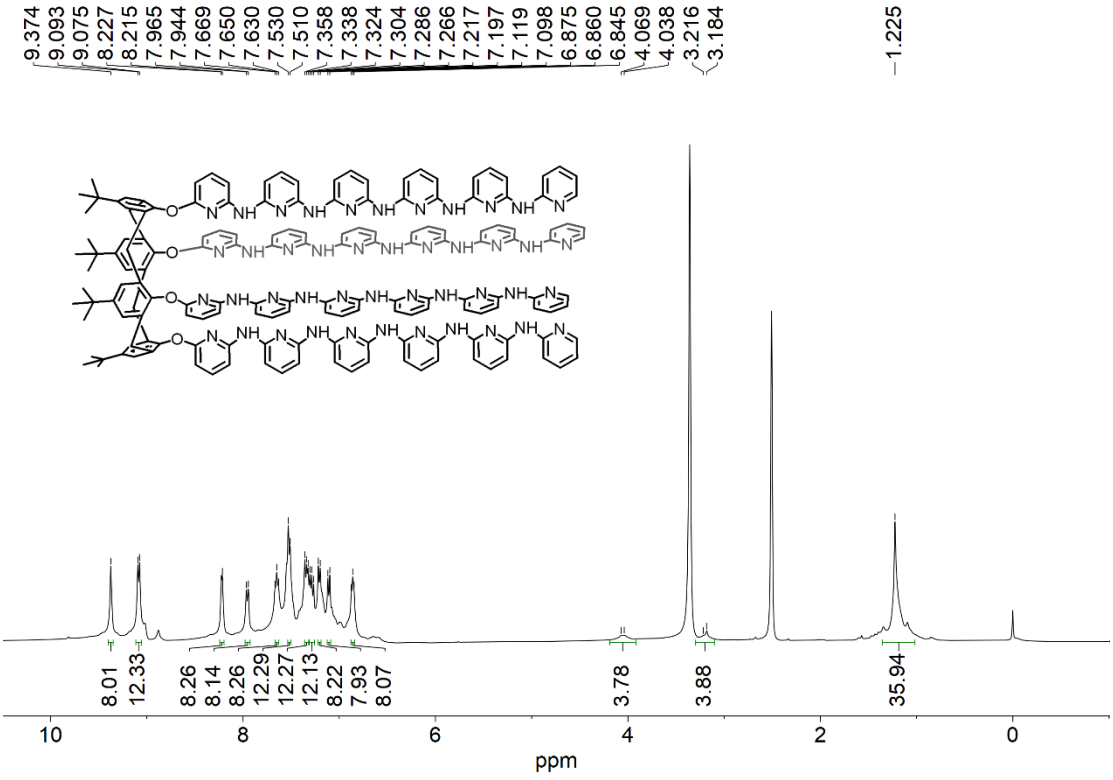



**Figure S54.** $^1$H NMR spectrum of **$L_5$** in DMSO-$d_6$.

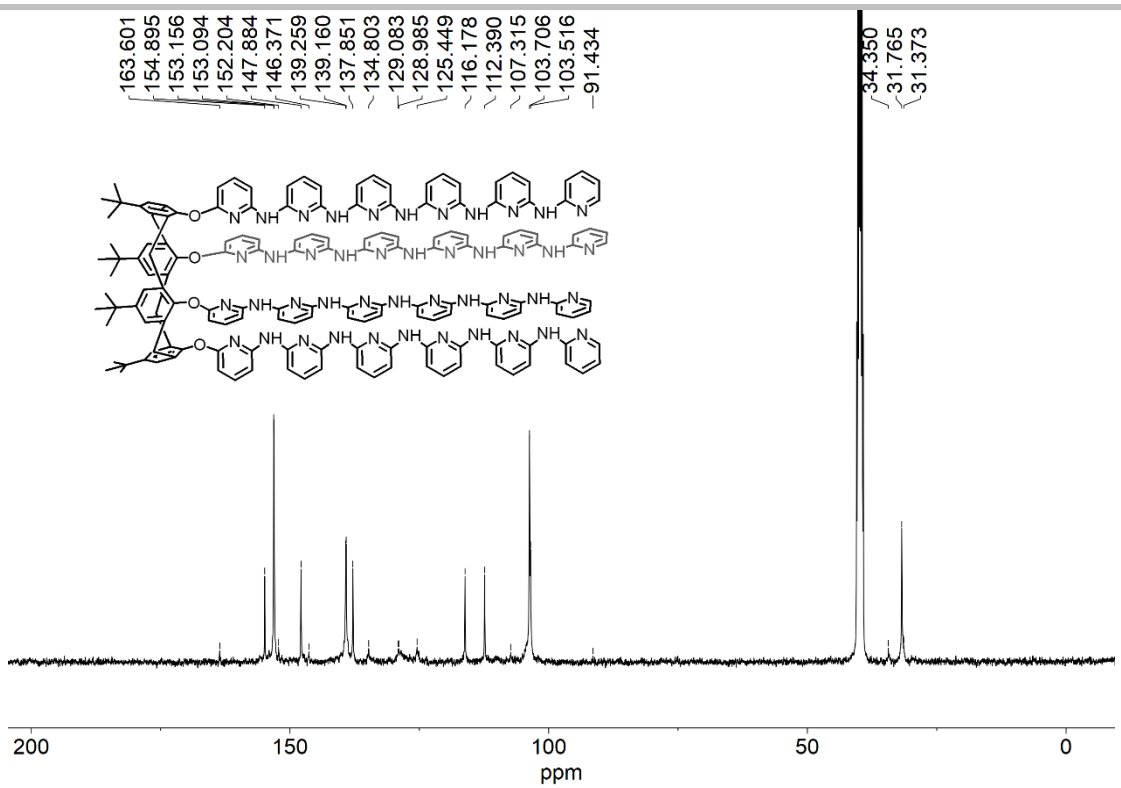



**Figure S55.** $^{13}C$ NMR spectrum of $\mathbf{L_5}$ in DMSO-$d_6$.

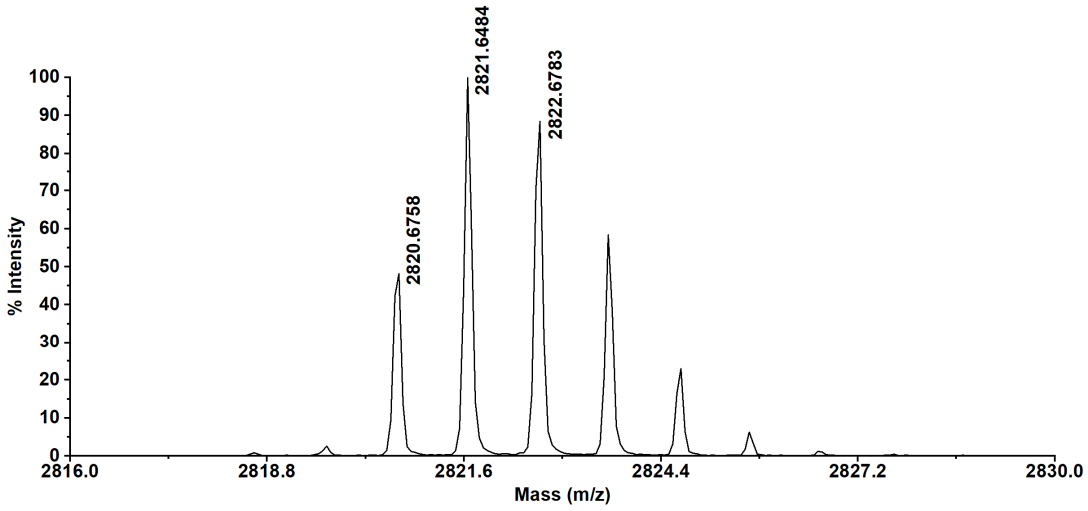



**Figure S56.** MALDI-TOF MS of $\mathbf{L_5}$.

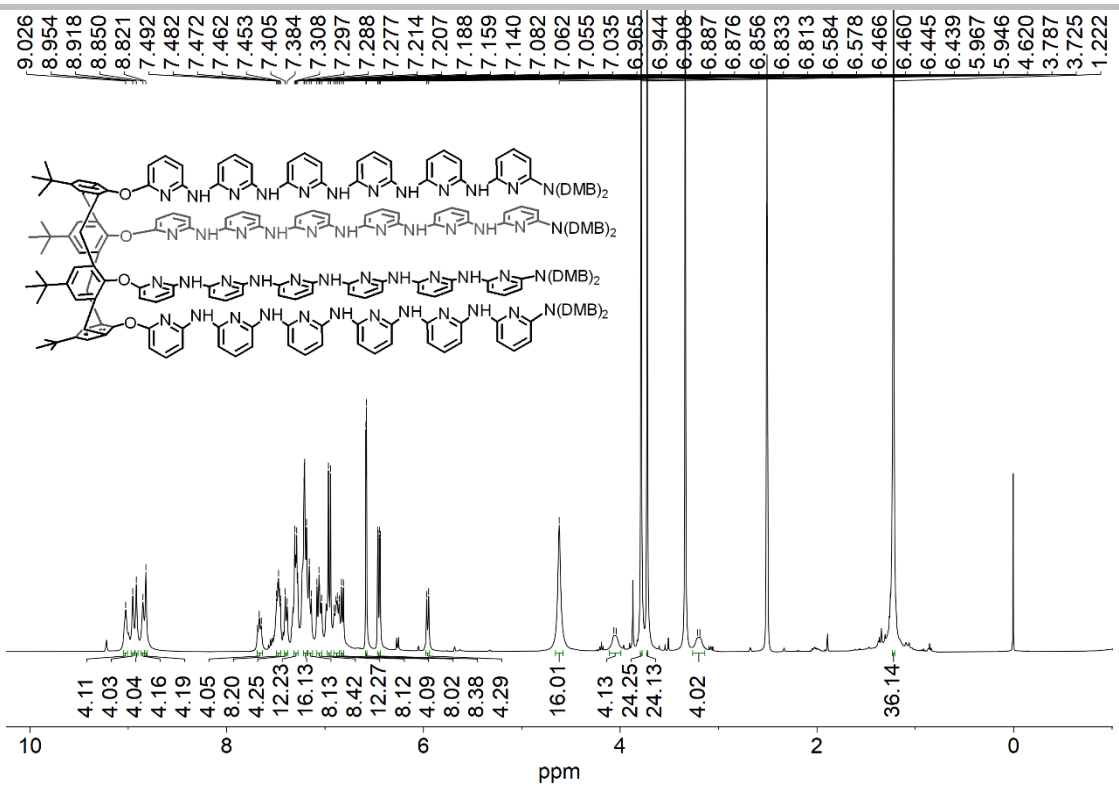



**Figure S57.** [1]H NMR spectrum of **$D_5$** in DMSO-$d_6$.

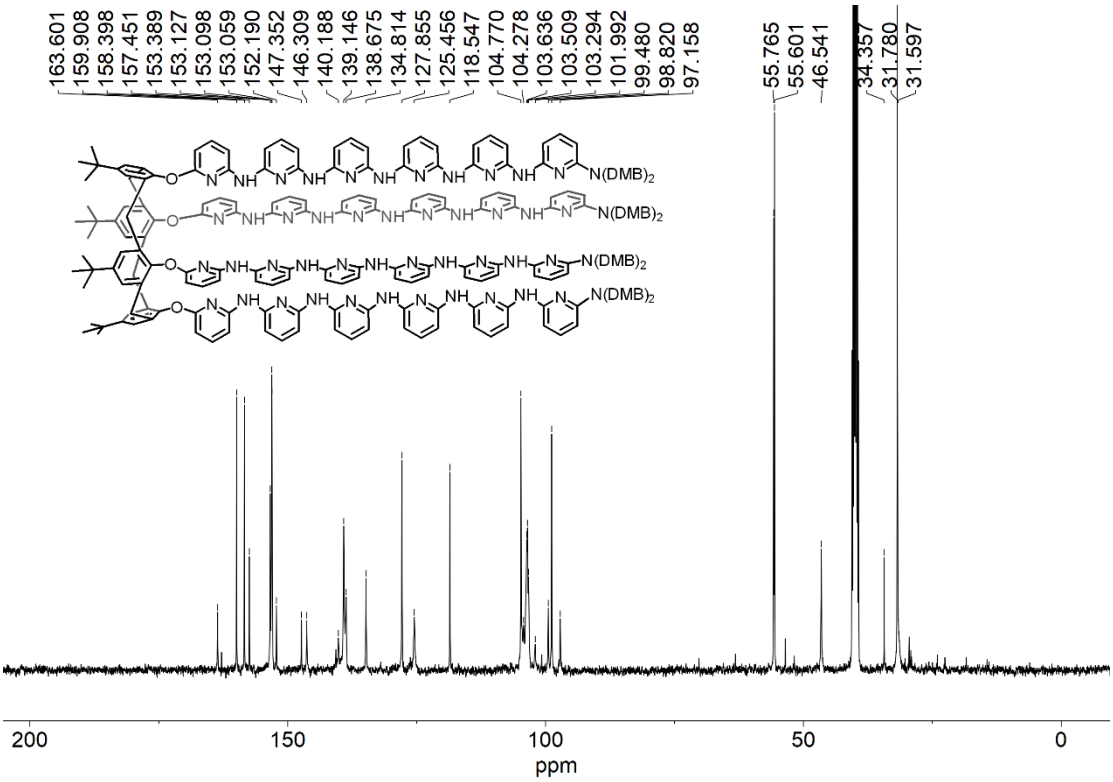



**Figure S58.** [13]C NMR spectrum of Compound **$D_5$** in DMSO-$d_6$.

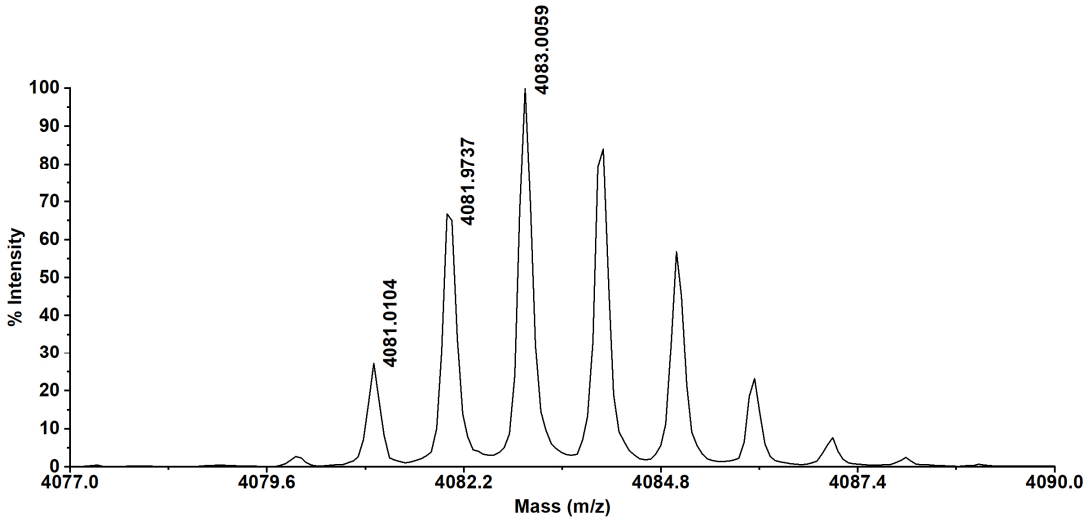



**Figure S59.** MALDI-TOF MS of Compound $\mathbf{D_5}$.

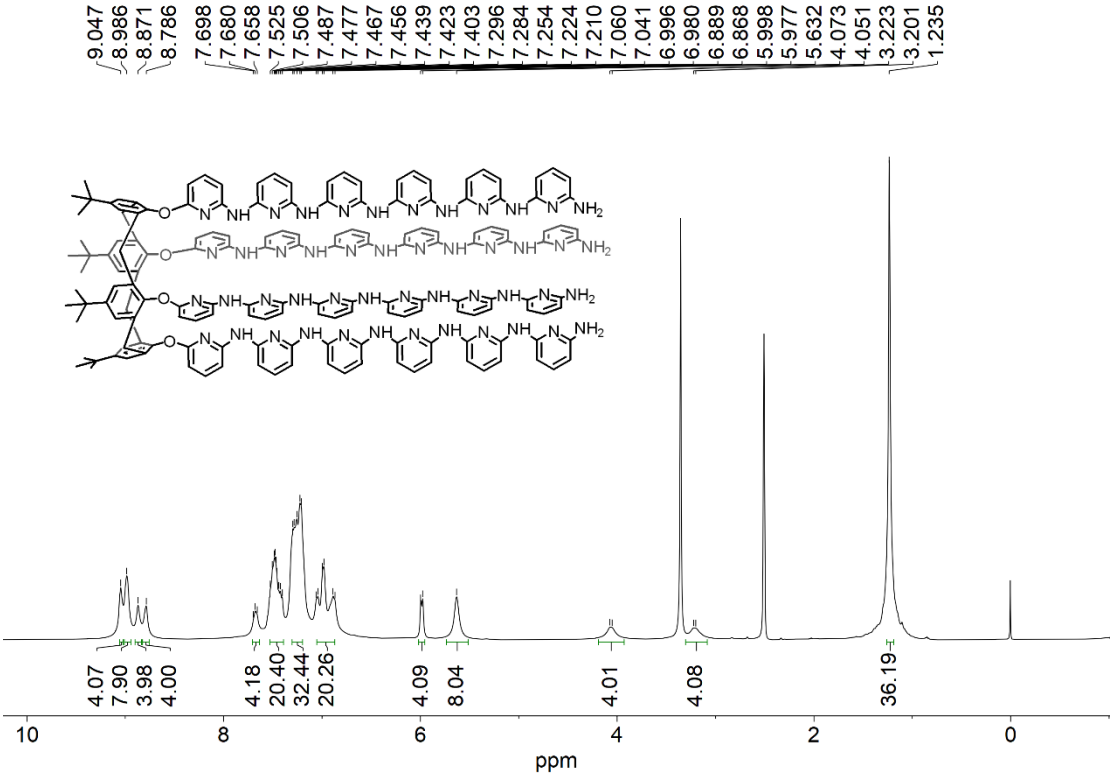



**Figure S60.** $^1$H NMR spectrum of $\mathbf{P_5}$ in DMSO-$d_6$.

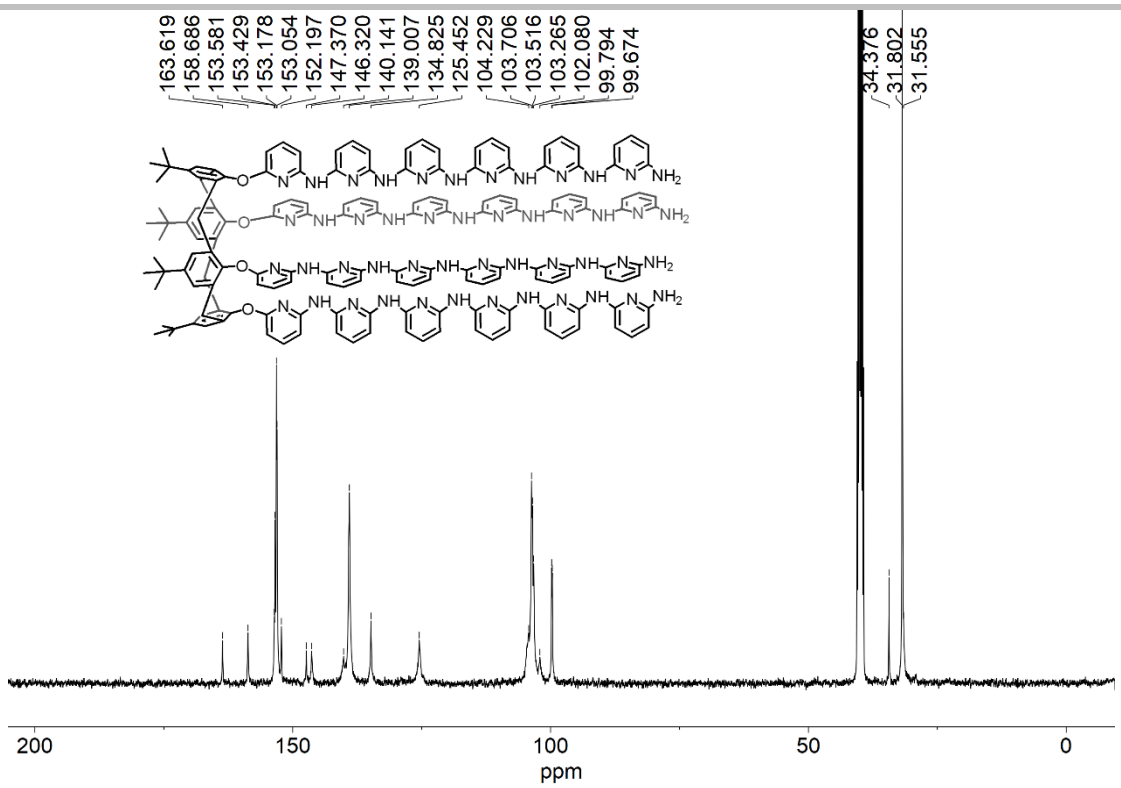



**Figure S61.** $^{13}C$ NMR spectrum of **$P_5$** in DMSO-$d_6$.

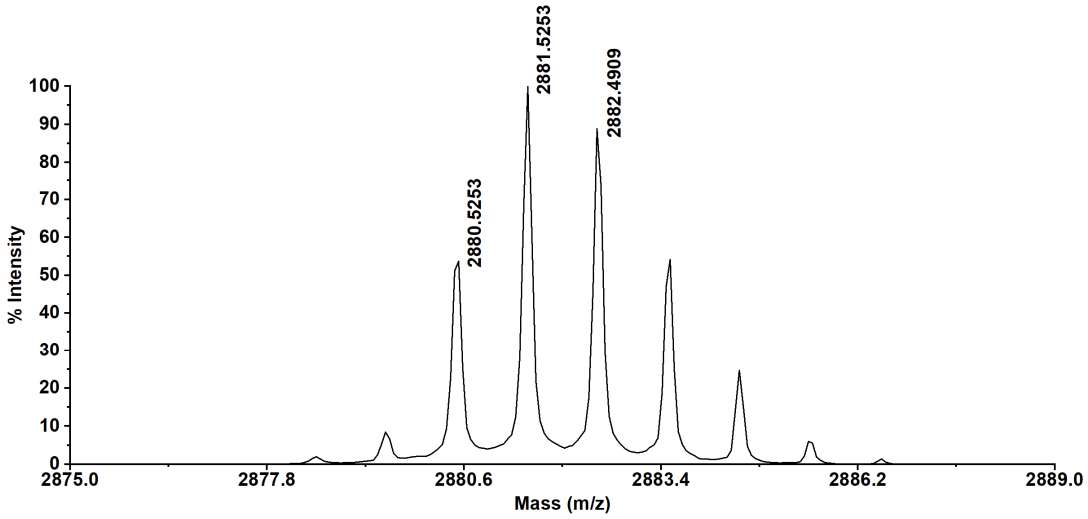



**Figure S62.** MALDI-TOF MS of **$P_5$**.

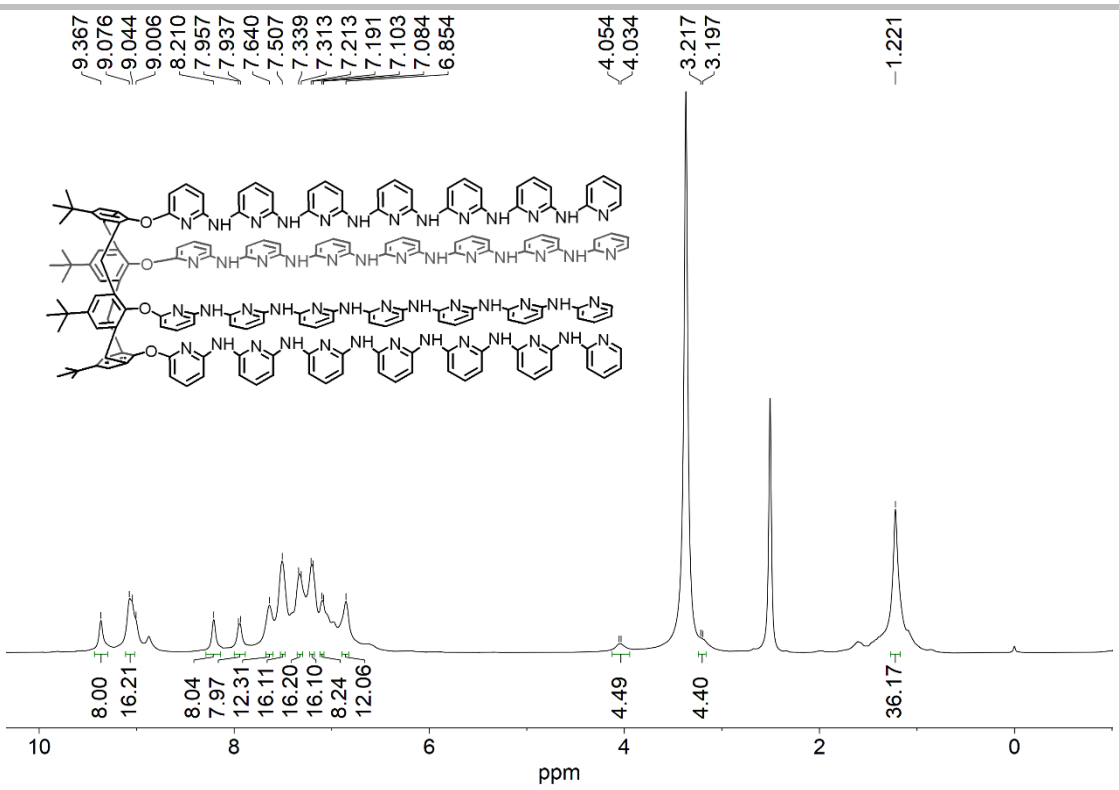



**Figure S63.** $^{1}$H NMR spectrum of **$L_6$** in DMSO-$d_6$.

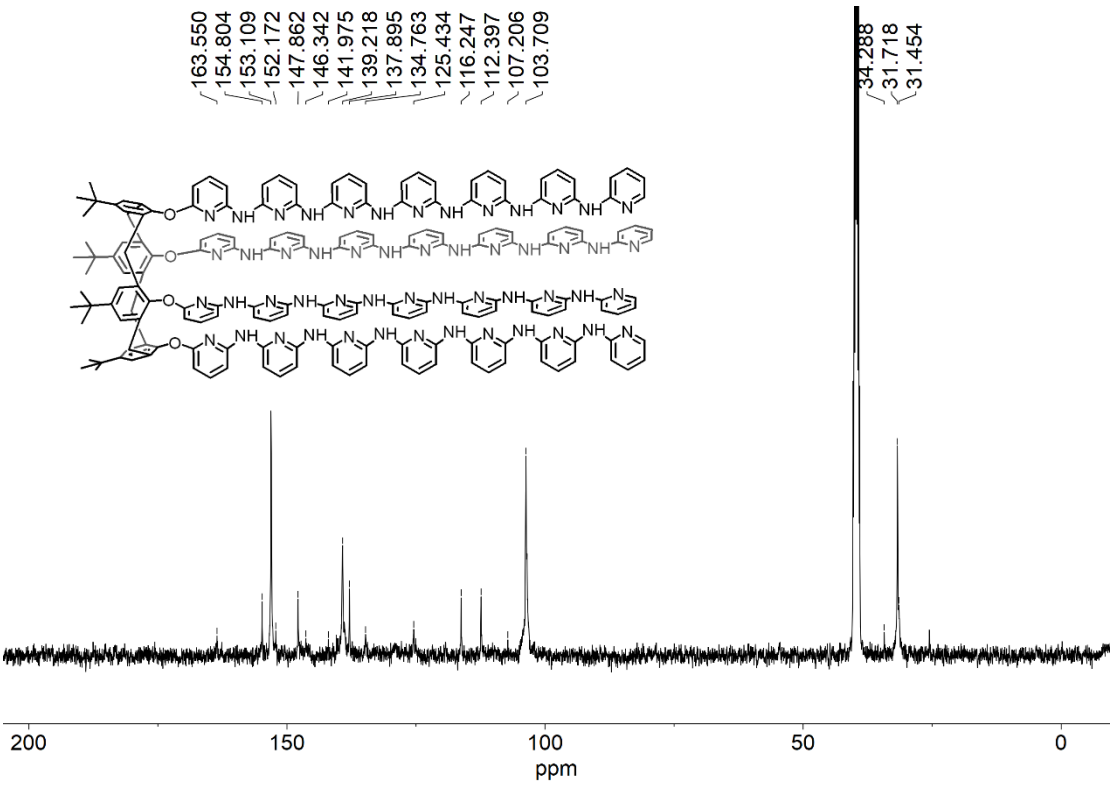



**Figure S64.** $^{13}$C NMR spectrum of **$L_6$** in DMSO-$d_6$.

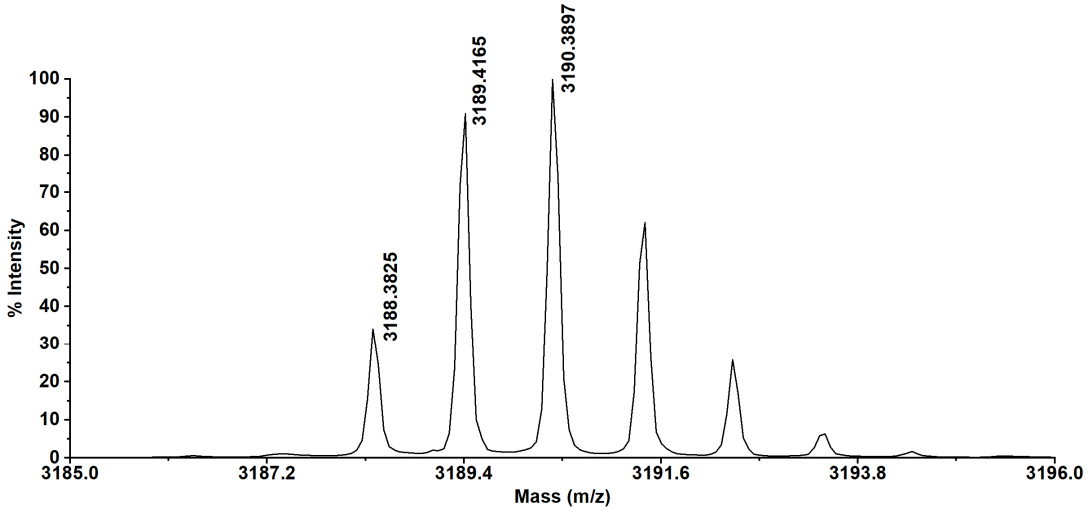



**Figure S65.** MALDI-TOF MS of $\mathbf{L_6}$.

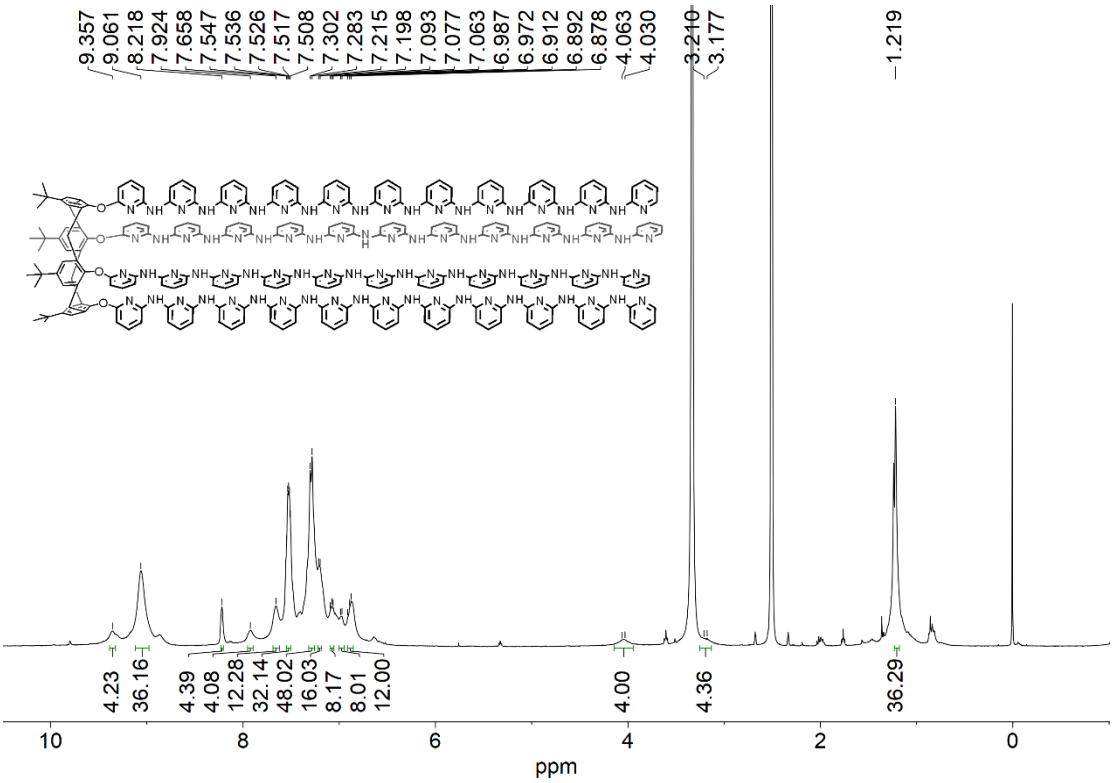



**Figure S66.** $^1$H NMR spectrum of $\mathbf{L_{10}}$ in DMSO-$d_6$.

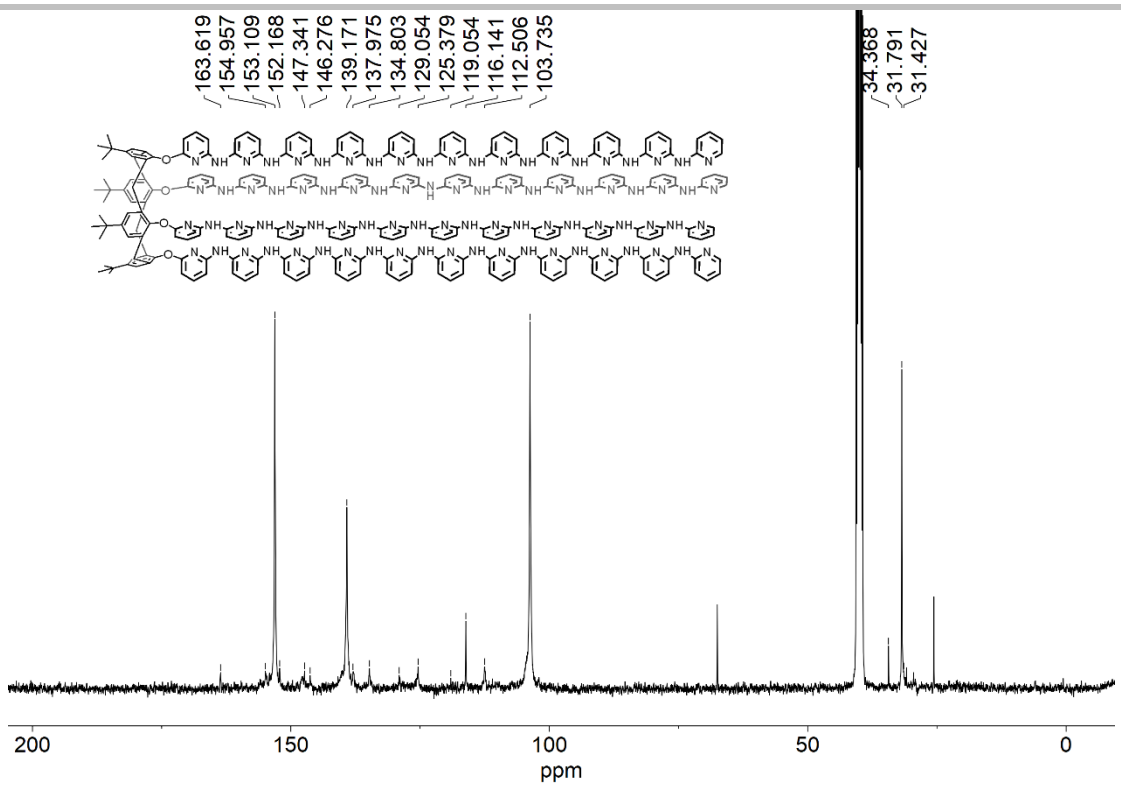



**Figure S67.** $^{13}$C NMR spectrum of $\mathbf{L_{10}}$ in DMSO-$d_6$.

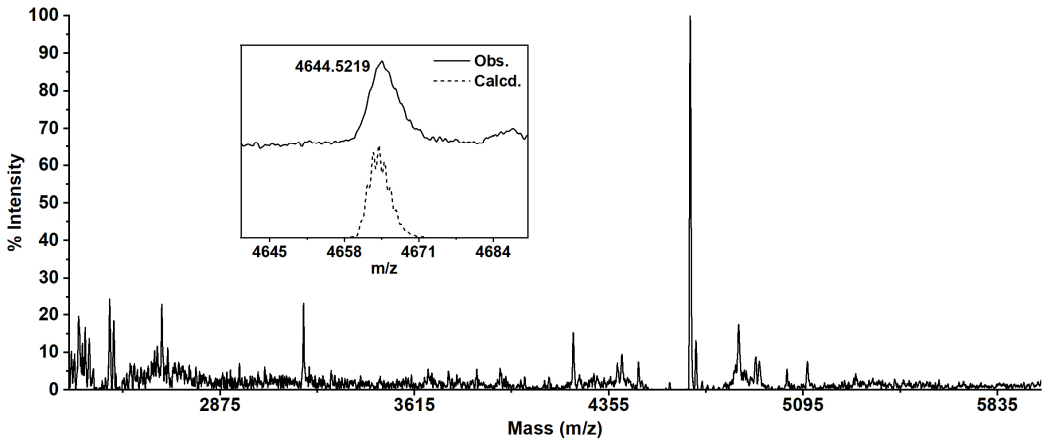



**Figure S68.** MALDI-TOF MS of $\mathbf{L_{10}}$.

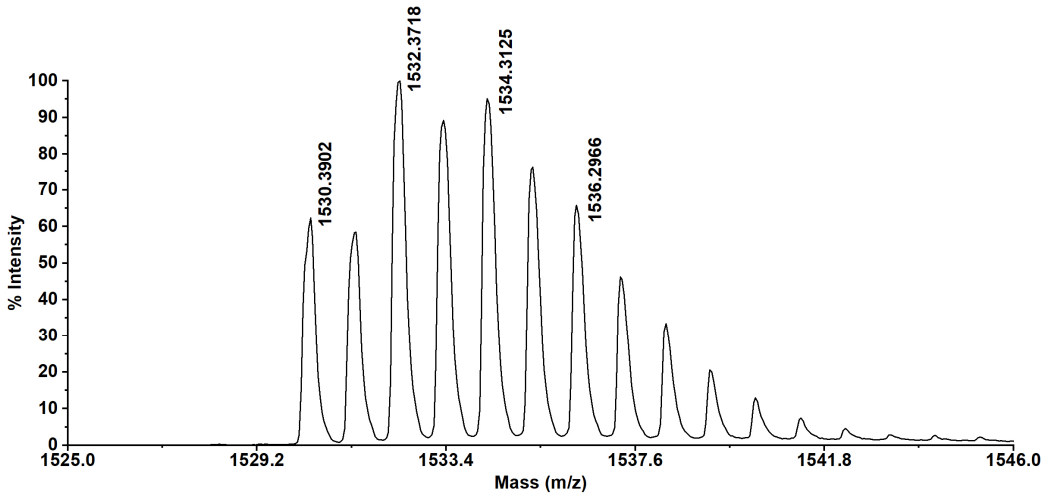



**Figure S69.** MALDI-TOF MS of NBP with 3 nickel atoms.

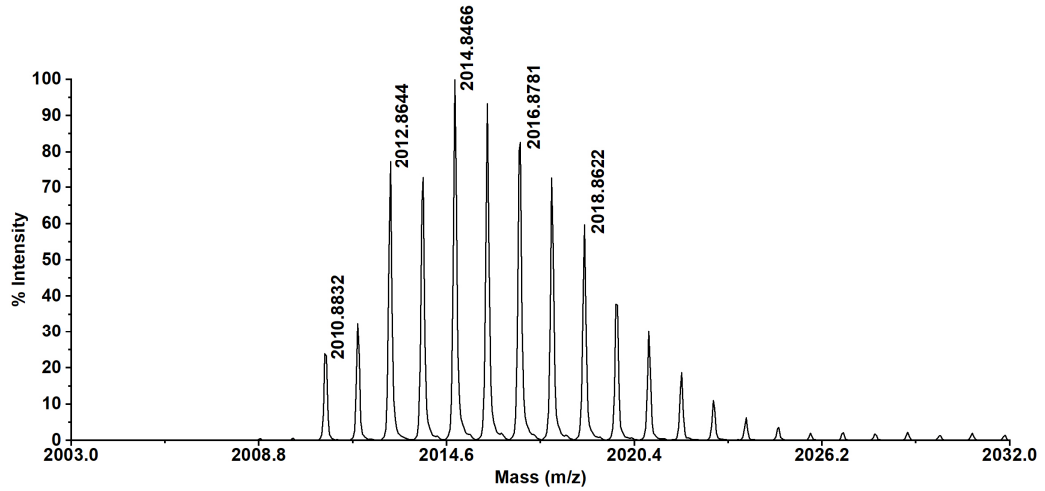



**Figure S70.** MALDI-TOF MS of NBP with 5 nickel atoms.

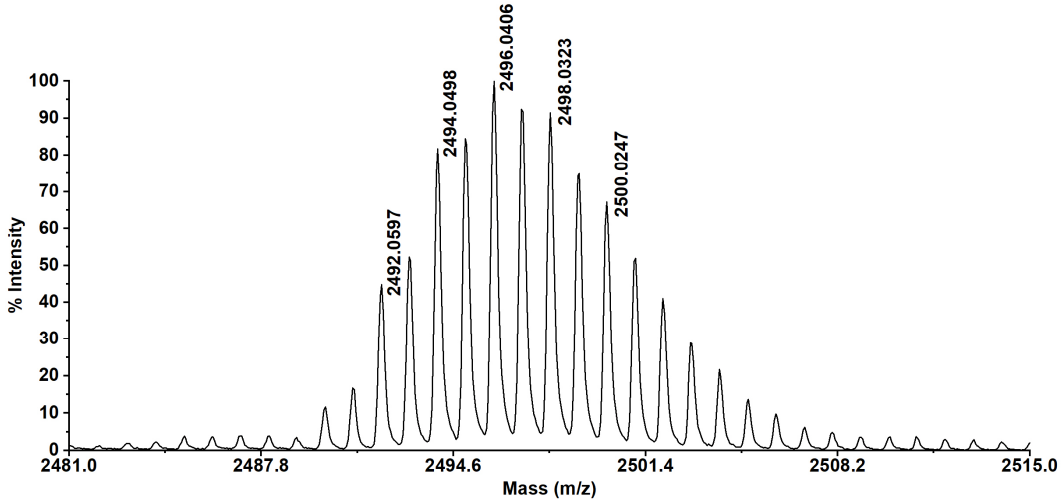



**Figure S71.** MALDI-TOF MS of NBP with 7 nickel atoms.

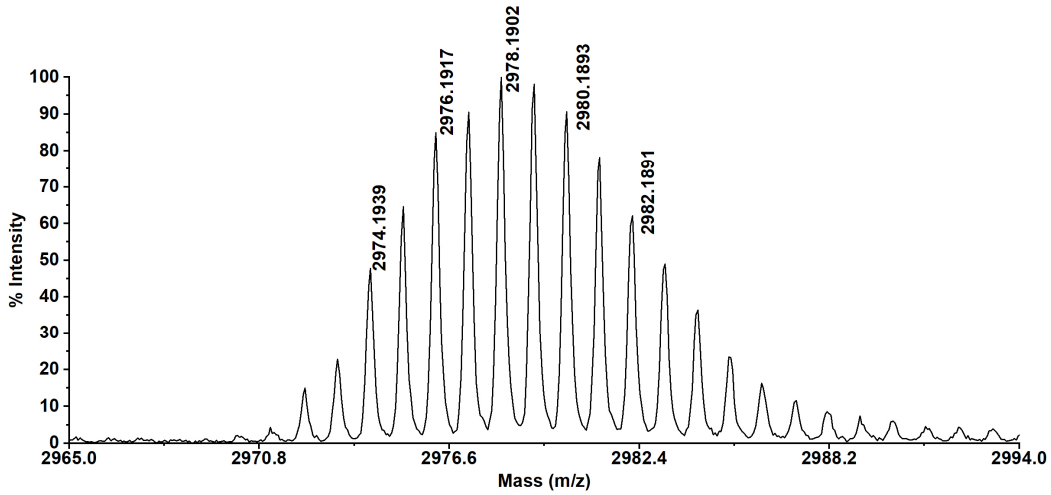



**Figure S72.** MALDI-TOF MS of NBP with 9 nickel atoms.

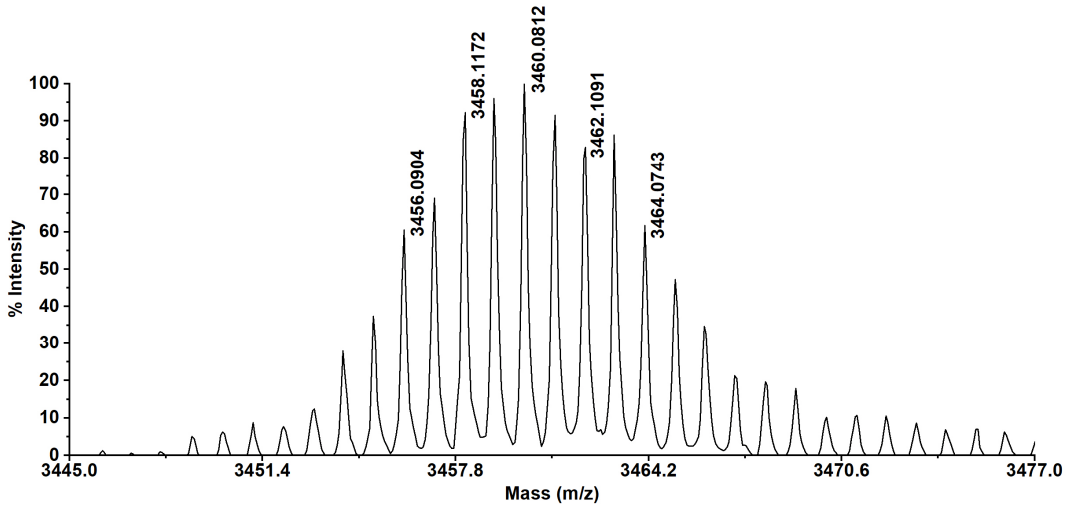



**Figure S73.** MALDI-TOF MS of NBP with 11 nickel atoms.

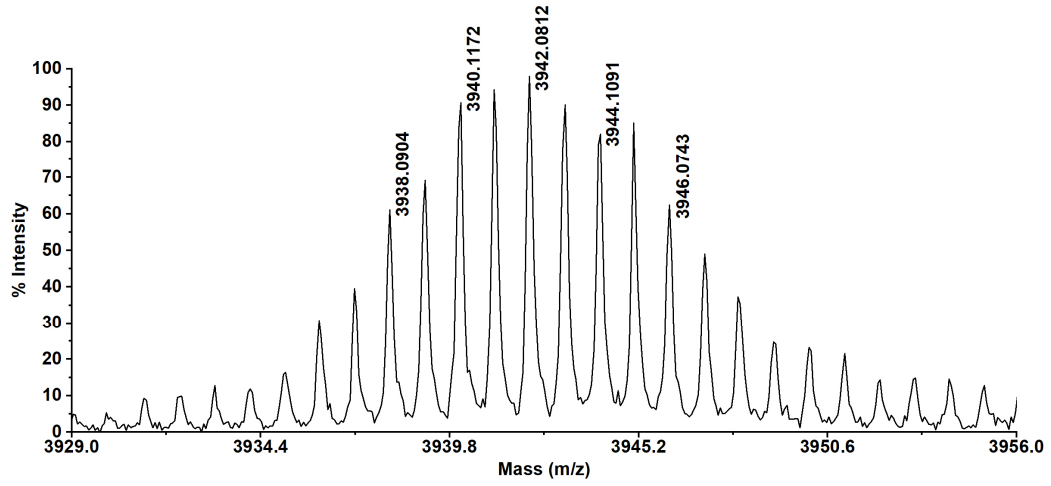



**Figure S74.** MALDI-TOF MS of NBP with 13 nickel atoms.

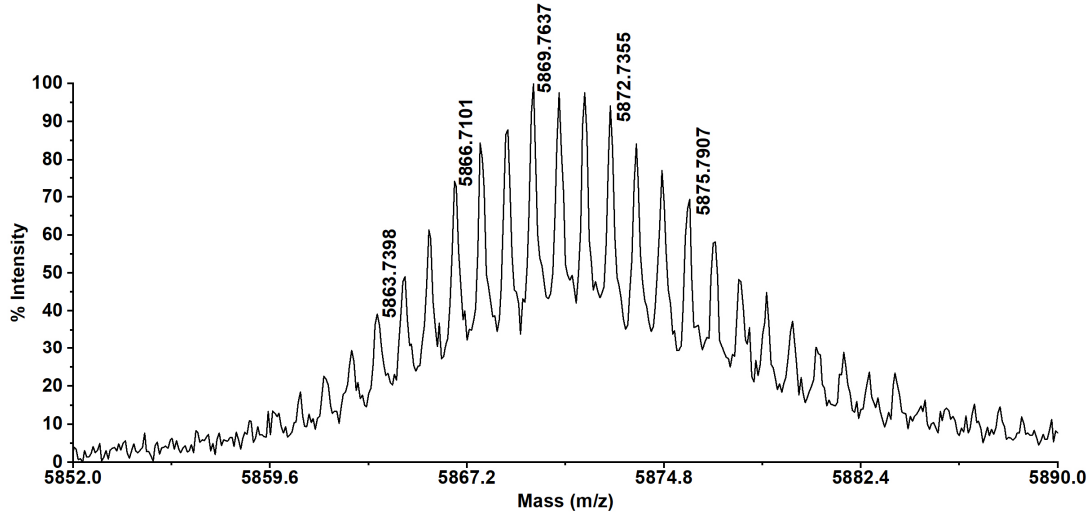



**Figure S75.** MALDI-TOF MS of NBP with 21 nickel atoms.

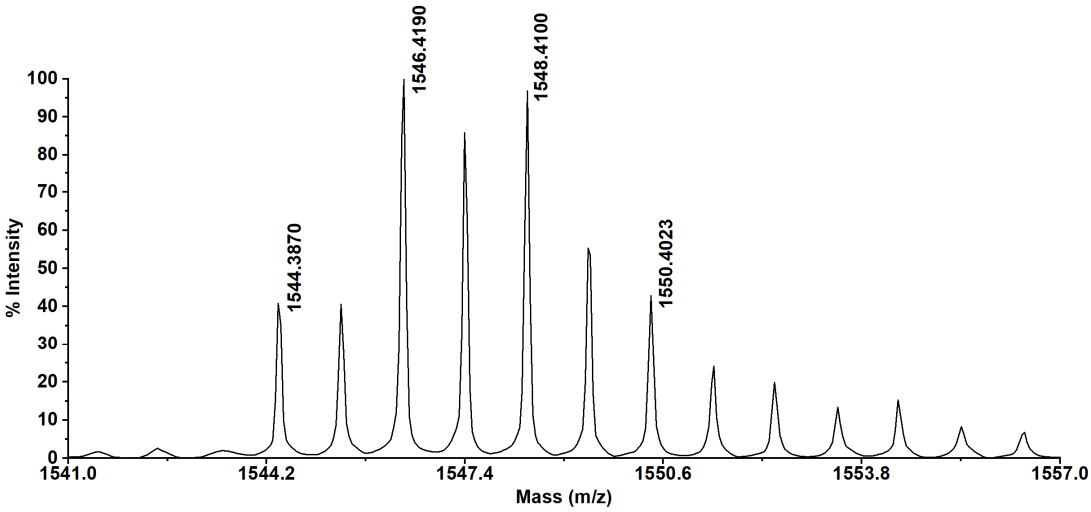



**Figure S76.** MALDI-TOF MS of copper-backboned polymer with 3 metal atoms.

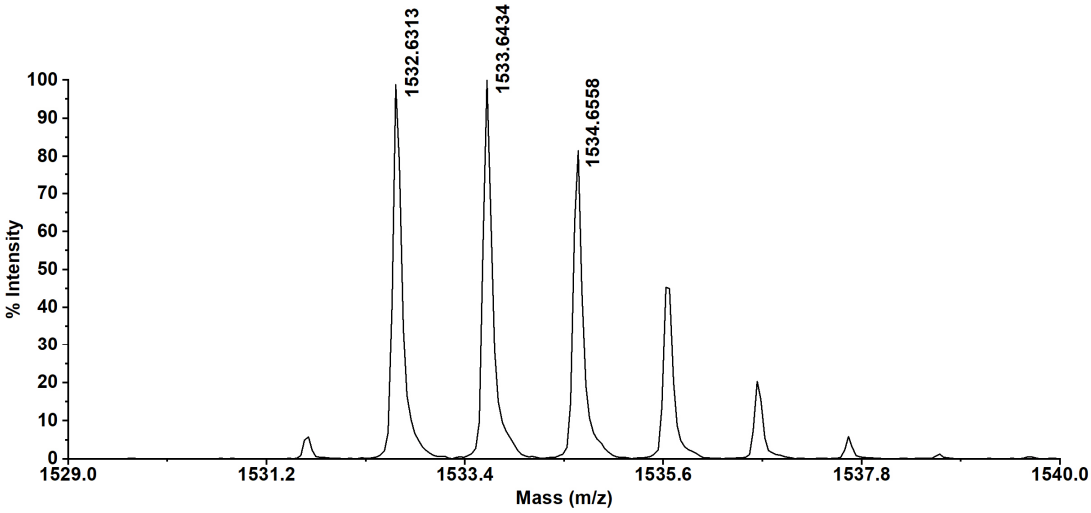



**Figure S77.** MALDI-TOF MS of cobalt-backboned polymer with 3 metal atoms.

SUPPORTING INFORMATION

## Cartesian Coordinates of the Optimized Structures for NBPs

Standard orientation:

| Atomic | X | Y | Z |
|---|---|---|---|
| **NBP with 3 nickel atoms** | | | |
| C | 0.01895631 | -1.41859122 | -3.85467824 |
| C | 0.06675645 | -0.95976425 | -2.54388847 |
| N | -0.98568062 | -0.40417016 | -1.91670909 |
| C | -2.17298812 | -0.23629990 | -2.58612404 |
| C | -2.27934474 | -0.67802438 | -3.92426827 |
| C | -1.19110920 | -1.27009100 | -4.53725283 |
| C | 0.01895373 | 1.41858776 | 3.85467699 |
| C | 0.06675407 | 0.95976272 | 2.54388675 |
| N | -0.98568326 | 0.40416997 | 1.91670622 |
| C | -2.17299029 | 0.23629762 | 2.58612096 |
| C | -2.27934679 | 0.67801918 | 3.92426653 |
| C | -1.19111169 | 1.27008551 | 4.53725170 |
| C | 0.02230307 | -3.85726542 | 1.40864664 |
| C | 0.06909204 | -2.54558010 | 0.95205354 |
| N | -0.98518575 | -1.91688883 | 0.40178941 |
| C | -2.17254838 | -2.58626512 | 0.23457997 |
| C | -2.27813374 | -3.92504296 | 0.67464750 |
| C | -1.18848937 | -4.53919125 | 1.26274523 |
| C | 0.02230281 | 3.85726733 | -1.40864441 |
| C | 0.06909087 | 2.54558083 | -0.95205435 |
| N | -0.98518650 | 1.91688976 | -0.40178991 |
| C | -2.17254904 | 2.58626621 | -0.23457884 |
| C | -2.27813292 | 3.92504565 | -0.67464175 |
| C | -1.18848839 | 4.53919422 | -1.26273916 |
| C | 3.03437130 | -2.49050283 | -2.04306496 |
| C | 2.40642243 | -1.28274818 | -2.36154171 |
| C | 4.28265705 | -2.74963971 | -2.60878489 |
| C | 2.43085304 | -3.45479898 | -1.03930648 |
| C | 3.00444938 | -0.33748757 | -3.19937731 |
| O | 1.17048025 | -1.01613223 | -1.76291558 |
| C | 4.91777736 | -1.84691602 | -3.47065745 |
| C | 3.01353733 | -3.20664282 | 0.34295156 |
| C | 4.25232258 | -0.65122929 | -3.74980434 |
| C | 2.41121748 | 1.03959901 | -3.45006882 |
| C | 6.30068130 | -2.18087649 | -4.04366434 |
| C | 2.40637012 | -2.36463801 | 1.28479830 |
| C | 4.25154890 | -3.75731889 | 0.67375617 |
| C | 3.02085349 | 2.04763484 | -2.49488485 |
| C | 6.84249668 | -1.05931756 | -4.94497956 |
| C | 6.21055363 | -3.47743881 | -4.87681011 |
| C | 7.29085068 | -2.38477997 | -2.87561471 |

| | | | |
|---|---|---|---|
| C | 3.02085257 | -2.04763557 | 2.49488449 |
| O | 1.17369100 | -1.76558632 | 1.00446948 |
| C | 2.40636864 | 2.36463760 | -1.28479986 |
| C | 4.26966504 | 2.61528542 | -2.77222786 |
| C | 4.26966354 | -2.61528637 | 2.77222966 |
| C | 2.41121503 | -1.03959957 | 3.45006726 |
| C | 3.01353434 | 3.20664232 | -0.34295204 |
| O | 1.17368877 | 1.76558597 | -1.00447470 |
| C | 4.90825654 | 3.47760428 | -1.88009496 |
| C | 3.00444672 | 0.33748717 | 3.19937618 |
| C | 4.25154650 | 3.75731826 | -0.67375474 |
| C | 2.43084917 | 3.45479844 | 1.03930569 |
| C | 6.28278749 | 4.09679831 | -2.16160735 |
| C | 2.40641975 | 1.28274771 | 2.36154045 |
| C | 4.25231916 | 0.65122965 | 3.74980435 |
| C | 3.03436772 | 2.49050297 | 2.04306460 |
| C | 6.15298497 | 5.63498976 | -2.18906100 |
| C | 6.86408436 | 3.63159296 | -3.50676047 |
| C | 7.26206656 | 3.68120041 | -1.04152186 |
| O | 1.17047789 | 1.01613084 | 1.76291381 |
| C | 4.91777297 | 1.84691727 | 3.47065871 |
| C | 4.28265270 | 2.74964077 | 2.60878595 |
| C | 6.30067622 | 2.18087857 | 4.04366691 |
| C | 6.84249096 | 1.05932031 | 4.94498330 |
| C | 6.21054749 | 3.47744128 | 4.87681191 |
| C | 7.29084655 | 2.38478165 | 2.87561803 |
| N | -3.20287786 | 0.28734518 | -1.87270238 |
| N | -3.20325293 | -1.87267064 | -0.28718363 |
| N | -3.20325327 | 1.87267006 | 0.28718203 |
| N | -3.20288073 | -0.28734442 | 1.87269876 |
| C | 4.90825668 | -3.47760500 | 1.88009763 |
| C | 6.28278754 | -4.09679834 | 2.16161202 |
| C | 7.26206814 | -3.68119894 | 1.04152841 |
| C | 6.15298608 | -5.63498992 | 2.18906443 |
| C | 6.86408187 | -3.63159350 | 3.50676642 |
| C | -4.17267546 | 1.73851502 | -3.59500373 |
| C | -4.26384014 | 0.96738005 | -2.41664257 |
| N | -5.42858534 | 0.96127506 | -1.70804031 |
| C | -6.45672631 | 2.43110700 | -3.29827644 |
| C | -5.26815789 | 2.46159102 | -4.03438161 |
| C | -4.17268424 | -1.73851216 | 3.59499820 |
| C | -4.26384600 | -0.96737638 | 2.41663750 |
| N | -5.42859312 | -0.96126355 | 1.70803851 |
| C | -6.45674324 | -2.43108162 | 3.29828131 |
| C | -5.26817205 | -2.46157702 | 4.03438135 |
| C | -4.17267124 | -3.59414085 | -1.73971765 |
| C | -4.26405040 | -2.41635598 | -0.96769984 |
| N | -5.42885607 | -1.70787668 | -0.96131580 |

| | | | |
|---|---|---|---|
| C | -6.45674832 | -3.29731202 | -2.43218392 |
| C | -5.26804350 | -4.03317495 | -2.46315520 |
| C | -4.17267428 | 3.59413554 | 1.73972176 |
| C | -4.26405063 | 2.41635199 | 0.96770094 |
| N | -5.42885173 | 1.70786676 | 0.96132123 |
| C | -6.45674493 | 3.29728829 | 2.43220243 |
| C | -5.26804479 | 4.03315928 | 2.46316802 |
| Ni | -0.83647979 | -0.00000045 | -0.00000124 |
| Ni | -3.21659942 | -0.00000154 | -0.00000266 |
| C | -6.48861860 | 1.67788008 | -2.13660728 |
| C | -6.48863141 | -1.67785811 | 2.13660951 |
| C | -6.48881191 | -2.13612575 | -1.67823415 |
| C | -6.48880614 | 2.13610571 | 1.67824682 |
| Ni | -5.60494160 | -0.00000199 | -0.00000853 |
| Cl | -8.34935244 | 0.00000655 | -0.00001254 |
| H | 0.89267782 | -1.86059837 | -4.31167743 |
| H | -3.22970096 | -0.58821193 | -4.43246091 |
| H | -1.28038404 | -1.63683441 | -5.55509770 |
| H | 0.89267511 | 1.86059437 | 4.31167694 |
| H | -3.22970284 | 0.58820499 | 4.43245910 |
| H | -1.28038634 | 1.63682715 | 5.55509723 |
| H | 0.89690132 | -4.31536573 | 1.84769416 |
| H | -3.22879745 | -4.43291420 | 0.58627945 |
| H | -1.27690878 | -5.55763400 | 1.62803266 |
| H | 0.89690079 | 4.31536736 | -1.84769287 |
| H | -3.22879607 | 4.43291767 | -0.58627230 |
| H | -1.27690699 | 5.55763818 | -1.62802351 |
| H | 4.77012301 | -3.68680515 | -2.36149909 |
| H | 1.34556469 | -3.36533041 | -1.03609458 |
| H | 2.67025949 | -4.47878529 | -1.34042663 |
| H | 4.71012018 | 0.07947605 | -4.40459047 |
| H | 2.63932517 | 1.33728340 | -4.47770455 |
| H | 1.32712572 | 1.03209738 | -3.34936234 |
| H | 4.72187961 | -4.41698411 | -0.04794201 |
| H | 6.95588799 | -0.11789153 | -4.39706587 |
| H | 7.82840977 | -1.33907890 | -5.32680868 |
| H | 6.19307813 | -0.88096550 | -5.80788372 |
| H | 7.19310915 | -3.73568032 | -5.28467928 |
| H | 5.51519864 | -3.35611478 | -5.71321682 |
| H | 5.86700139 | -4.32327398 | -4.27440285 |
| H | 8.28966464 | -2.61433324 | -3.26053639 |
| H | 7.35891647 | -1.48230476 | -2.26007298 |
| H | 6.98680305 | -3.20957937 | -2.22546572 |
| H | 4.74121977 | 2.36459584 | -3.71400112 |
| H | 4.74121668 | -2.36459693 | 3.71400376 |
| H | 1.32712336 | -1.03209824 | 3.34935959 |
| H | 2.63932157 | -1.33728367 | 4.47770332 |
| H | 4.72187596 | 4.41698353 | 0.04794419 |

| | | | |
|---|---|---|---|
| H | 2.67025474 | 4.47878505 | 1.34042555 |
| H | 1.34556088 | 3.36532922 | 1.03609366 |
| H | 4.71011686 | -0.07947552 | 4.40459060 |
| H | 7.12812777 | 6.09546822 | -2.37767732 |
| H | 5.46631504 | 5.95430135 | -2.97921003 |
| H | 5.77722504 | 6.02606064 | -1.23910559 |
| H | 7.84496551 | 4.08992194 | -3.66127244 |
| H | 6.22782370 | 3.92361212 | -4.34815724 |
| H | 6.99859116 | 2.54509434 | -3.53558373 |
| H | 8.25540353 | 4.10007742 | -1.23176220 |
| H | 6.93345759 | 4.03861510 | -0.06179160 |
| H | 7.35318733 | 2.59192315 | -0.98649773 |
| H | 4.77011807 | 3.68680675 | 2.36150104 |
| H | 7.82840337 | 1.33908245 | 5.32681376 |
| H | 6.19307126 | 0.88096812 | 5.80788658 |
| H | 6.95588375 | 0.11789416 | 4.39707014 |
| H | 7.19310259 | 3.73568306 | 5.28468193 |
| H | 5.86699583 | 4.32327620 | 4.27440398 |
| H | 5.51519165 | 3.35611761 | 5.71321804 |
| H | 8.28966009 | 2.61433544 | 3.26054042 |
| H | 6.98679913 | 3.20958056 | 2.22546833 |
| H | 7.35891308 | 1.48230611 | 2.26007688 |
| H | 7.35318844 | -2.59192156 | 0.98650543 |
| H | 8.25540501 | -4.10007558 | 1.23176994 |
| H | 6.93346087 | -4.03861288 | 0.06179730 |
| H | 5.77722816 | -6.02606048 | 1.23910813 |
| H | 7.12812894 | -6.09546774 | 2.37768213 |
| H | 5.46631504 | -5.95430251 | 2.97921208 |
| H | 6.22782021 | -3.92361403 | 4.34816197 |
| H | 6.99858746 | -2.54509476 | 3.53559080 |
| H | 7.84496323 | -4.08992160 | 3.66127951 |
| H | -3.22951345 | 1.77876405 | -4.12471599 |
| H | -7.33756258 | 2.97987877 | -3.60849894 |
| H | -5.19182914 | 3.06098434 | -4.93657069 |
| H | -3.22952037 | -1.77876972 | 4.12470669 |
| H | -7.33758380 | -2.97984386 | 3.60850853 |
| H | -5.19184536 | -3.06097038 | 4.93657057 |
| H | -3.22944234 | -4.12368646 | -1.78035344 |
| H | -7.33752273 | -3.60730526 | -2.98118387 |
| H | -5.19151574 | -4.93490700 | -3.06321128 |
| H | -3.22944871 | 4.12368730 | 1.78035374 |
| H | -7.33751765 | 3.60727381 | 2.98120943 |
| H | -5.19151932 | 4.93488976 | 3.06322675 |
| H | -7.37536049 | 1.58691227 | -1.51608110 |
| H | -7.37537341 | -1.58688566 | 1.51608385 |
| H | -7.37559582 | -1.51570443 | -1.58697559 |
| H | -7.37558815 | 1.51568208 | 1.58698854 |

**NBP with 5 nickel atoms**

| | | | |
|---|---|---|---|
| C | 2.28802465 | 3.81875719 | -1.53286505 |
| C | 2.33996009 | 2.52850468 | -1.02221736 |
| N | 1.29226721 | 1.91860787 | -0.43935971 |
| C | 0.10016138 | 2.58873889 | -0.29368679 |
| C | -0.01058153 | 3.90695910 | -0.79427873 |
| C | 1.07297706 | 4.49916701 | -1.41323964 |
| C | 2.30422582 | -3.79963697 | 1.53078740 |
| C | 2.35044327 | -2.50876624 | 1.02108644 |
| N | 1.29926394 | -1.90208649 | 0.44132843 |
| C | 0.10954177 | -2.57661301 | 0.29666573 |
| C | 0.00444674 | -3.89554309 | 0.79662640 |
| C | 1.09129260 | -4.48422564 | 1.41317125 |
| C | 2.29659551 | -1.52939909 | -3.80526443 |
| C | 2.34654270 | -1.01637162 | -2.51583955 |
| N | 1.29732375 | -0.43365962 | -1.90838512 |
| C | 0.10572003 | -0.29094910 | -2.58018353 |
| C | -0.00274999 | -0.79371419 | -3.89768449 |
| C | 1.08231098 | -1.41245730 | -4.48740424 |
| C | 2.29142934 | 1.54536036 | 3.80992784 |
| C | 2.34105169 | 1.03522616 | 2.51946566 |
| N | 1.29353063 | 0.44952564 | 1.91213048 |
| C | 0.10326079 | 0.30131236 | 2.58491416 |
| C | -0.00520071 | 0.80105690 | 3.90369676 |
| C | 1.07843093 | 1.42232802 | 4.49344639 |
| C | 5.29854305 | 1.99054157 | -2.54575911 |
| C | 4.67816049 | 2.34135207 | -1.34797480 |
| C | 6.55212410 | 2.54478178 | -2.83000773 |
| C | 4.69036802 | 0.96016198 | -3.47786850 |
| C | 5.28140133 | 3.20997955 | -0.42805844 |
| O | 3.44693307 | 1.74862934 | -1.05309900 |
| C | 7.18846546 | 3.42828051 | -1.95728441 |
| C | 5.28279394 | -0.41053884 | -3.19419954 |
| C | 6.52261517 | 3.74800242 | -0.76627594 |
| C | 4.69483605 | 3.49207793 | 0.94551439 |
| C | 8.57367904 | 4.02365138 | -2.23724194 |
| C | 4.68587566 | -1.33109171 | -2.32850347 |
| C | 6.52727971 | -0.74197473 | -3.74174921 |
| C | 5.30380318 | 2.55460341 | 1.97091114 |
| C | 8.46802213 | 5.56269960 | -2.29509828 |
| C | 9.16187463 | 3.52426656 | -3.56697363 |
| C | 9.53488448 | 3.61404475 | -1.09861895 |
| C | 5.31231240 | -2.53151213 | -1.98068583 |
| O | 3.45296366 | -1.04485441 | -1.73473703 |
| C | 4.67959011 | 1.35954617 | 2.32460520 |
| C | 6.56289678 | 2.83129506 | 2.51641448 |
| C | 6.55710329 | -2.80949762 | -2.54542994 |
| C | 4.71061664 | -3.46597996 | -0.94826644 |

| | | | |
|---|---|---|---|
| C | 5.28338745 | 0.43649998 | 3.18965271 |
| O | 3.44533402 | 1.06957363 | 1.73614262 |
| C | 7.20116011 | 1.95420572 | 3.39403900 |
| C | 5.29651641 | -3.17822542 | 0.42491436 |
| C | 6.53036830 | 0.76739510 | 3.71862107 |
| C | 4.69210906 | -0.93427282 | 3.47684415 |
| C | 8.59438432 | 2.22303290 | 3.97560385 |
| C | 4.68769299 | -2.31369696 | 1.34521616 |
| C | 6.53787172 | -3.71427981 | 0.76658363 |
| C | 5.30270217 | -1.96465906 | 2.54628386 |
| C | 8.50807969 | 2.26813887 | 5.51620233 |
| C | 9.18336860 | 3.55381723 | 3.48023464 |
| C | 9.54450873 | 1.08330693 | 3.54357465 |
| O | 3.45481096 | -1.72505335 | 1.04922069 |
| C | 7.19561597 | -3.40110233 | 1.96408017 |
| C | 6.55415906 | -2.52044627 | 2.83579528 |
| C | 8.57608923 | -4.00225536 | 2.25543776 |
| C | 8.46495756 | -5.54138910 | 2.30035592 |
| C | 9.15040752 | -3.51519590 | 3.59571419 |
| C | 9.55166427 | -3.58677724 | 1.13205280 |
| N | -0.92124404 | 1.89158742 | 0.26737418 |
| N | -0.91751590 | 0.26946268 | -1.88510535 |
| N | -0.91847798 | -0.26117713 | 1.88953858 |
| N | -0.91499199 | -1.88305443 | -0.26304794 |
| C | 7.19053899 | -1.93192104 | -3.43407943 |
| C | 8.56906366 | -2.28579466 | -4.00578228 |
| C | 9.56439569 | -2.46842142 | -2.83867396 |
| C | 8.46829620 | -3.60043957 | -4.80881747 |
| C | 9.11208165 | -1.18777743 | -4.93492226 |
| C | -1.99810761 | 3.70639912 | 1.52881738 |
| C | -2.02192685 | 2.46927090 | 0.86735138 |
| N | -3.16282642 | 1.72271615 | 0.86998689 |
| C | -4.33634641 | 3.42218751 | 2.08241972 |
| C | -3.17243602 | 4.17488837 | 2.11267795 |
| C | -1.98521455 | -3.70134488 | -1.52520213 |
| C | -2.01340453 | -2.46433312 | -0.86367092 |
| N | -3.15666163 | -1.72137340 | -0.86710429 |
| C | -4.32391371 | -3.42443367 | -2.08057601 |
| C | -3.15762593 | -4.17346963 | -2.10998248 |
| C | -1.99274878 | 1.52825601 | -3.70264010 |
| C | -2.01798202 | 0.86755014 | -2.46512809 |
| N | -3.16026706 | 0.86915901 | -1.72067747 |
| C | -4.33209880 | 2.07945192 | -3.42283292 |
| C | -3.16689576 | 2.11054315 | -4.17351825 |
| C | -1.99072762 | -1.52463690 | 3.70571012 |
| C | -2.01729153 | -0.86319921 | 2.46863513 |
| N | -3.15909883 | -0.86790754 | 1.72346208 |
| C | -4.32826128 | -2.08265101 | 3.42429117 |

| | | | |
|---|---|---|---|
| C | -3.16340558 | -2.11072327 | 4.17559451 |
| Ni | 1.46173420 | 0.00866506 | 0.00154268 |
| Ni | -0.88867768 | 0.00426403 | 0.00223522 |
| C | -4.31367000 | 2.14935122 | 1.47575430 |
| C | -4.30568438 | -2.15157140 | -1.47380790 |
| C | -4.31104083 | 1.47338203 | -2.14969349 |
| C | -4.30826764 | -1.47590287 | 2.15143316 |
| N | -5.39223573 | 1.31612019 | 1.37845487 |
| N | -5.39104678 | 1.37510136 | -1.31842481 |
| N | -5.38800258 | -1.38068802 | 1.31948860 |
| N | -5.38691999 | -1.32171834 | -1.37736549 |
| C | -6.34046717 | 1.68237136 | 3.61656221 |
| C | -6.43787442 | 1.28424432 | 2.26444416 |
| N | -7.60779747 | 0.74090668 | 1.81420536 |
| C | -8.62330920 | 1.01045002 | 3.96977306 |
| C | -7.42909553 | 1.54862026 | 4.45977465 |
| C | -6.33188032 | -1.69056598 | -3.61643089 |
| C | -6.43180163 | -1.29290294 | -2.26436178 |
| N | -7.60379335 | -0.75316526 | -1.81518347 |
| C | -8.61641577 | -1.02555418 | -3.97175557 |
| C | -7.42009751 | -1.56001405 | -4.46067797 |
| C | -6.34100667 | 3.61207697 | -1.68698128 |
| C | -6.43771466 | 2.25994144 | -1.28873585 |
| N | -7.60819065 | 1.80855143 | -0.74754291 |
| C | -8.62545575 | 3.96300982 | -1.01933951 |
| C | -7.43076943 | 4.45416389 | -1.55541148 |
| C | -6.33140967 | -3.62067543 | 1.68672705 |
| C | -6.43191874 | -2.26875373 | 1.28871433 |
| N | -7.60330433 | -1.82082563 | 0.74661791 |
| C | -8.61426656 | -3.97839836 | 1.01724771 |
| C | -7.41851262 | -4.46604101 | 1.55413102 |
| Ni | -3.16575313 | 0.00069527 | 0.00138966 |
| Ni | -5.44034943 | -0.00287480 | 0.00053112 |
| C | -8.66171228 | 0.60800360 | 2.64567553 |
| C | -8.65731699 | -0.62339626 | -2.64764428 |
| C | -8.66322361 | 2.63893949 | -0.61674592 |
| C | -8.65571575 | -2.65437437 | 0.61485384 |
| Ni | -7.79700485 | -0.00641500 | -0.00055867 |
| Cl | -10.53741422 | -0.01057827 | -0.00195374 |
| H | 3.15936774 | 4.26120533 | -1.99391027 |
| H | -0.96205635 | 4.41488061 | -0.72369369 |
| H | 0.97701472 | 5.49970613 | -1.82355302 |
| H | 3.17805492 | -4.23944977 | 1.98962891 |
| H | -0.94527953 | -4.40690066 | 0.72725103 |
| H | 0.99973817 | -5.48540601 | 1.82292876 |
| H | 3.16916723 | -1.98958614 | -4.24614759 |
| H | -0.95367431 | -0.72504929 | -4.40691110 |
| H | 0.98812622 | -1.82468794 | -5.48732423 |

| | | | |
|---|---|---|---|
| H | 3.16293254 | 2.00841722 | 4.25004377 |
| H | -0.95521594 | 0.72818273 | 4.41401961 |
| H | 0.98397447 | 1.83194355 | 5.49441483 |
| H | 7.02974044 | 2.26446351 | -3.76036039 |
| H | 3.60612437 | 0.95491887 | -3.37801250 |
| H | 4.91993635 | 1.23372831 | -4.51191949 |
| H | 6.99018095 | 4.42662843 | -0.06064281 |
| H | 3.61016647 | 3.39659472 | 0.94389476 |
| H | 4.92951664 | 4.52436115 | 1.22133728 |
| H | 6.98370070 | -0.03027157 | -4.41814153 |
| H | 7.79359605 | 5.87702110 | -3.09769514 |
| H | 8.08977841 | 5.97808072 | -1.35656956 |
| H | 9.45187493 | 6.00454593 | -2.48329826 |
| H | 8.53652603 | 3.80673284 | -4.41975574 |
| H | 9.28291716 | 2.43584701 | -3.57267806 |
| H | 10.14984729 | 3.96721205 | -3.72160570 |
| H | 9.19759299 | 3.98968846 | -0.12822127 |
| H | 10.53540975 | 4.01848551 | -1.28275014 |
| H | 9.61236582 | 2.52450451 | -1.02775831 |
| H | 7.04392493 | 3.75899530 | 2.23325234 |
| H | 7.04279127 | -3.74145394 | -2.27580650 |
| H | 3.62543809 | -3.37531286 | -0.94490017 |
| H | 4.94869975 | -4.49846954 | -1.22016791 |
| H | 6.99926496 | 0.05839712 | 4.39274577 |
| H | 3.60788129 | -0.93065982 | 3.37741704 |
| H | 4.92241630 | -1.20554687 | 4.51131031 |
| H | 7.01033895 | -4.38902418 | 0.06033847 |
| H | 7.84137329 | 3.07107308 | 5.84579990 |
| H | 8.13099782 | 1.32790886 | 5.92873616 |
| H | 9.49826065 | 2.44819758 | 5.94712946 |
| H | 8.56320699 | 4.40700004 | 3.77294343 |
| H | 9.29683494 | 3.56505163 | 2.39119439 |
| H | 10.17525145 | 3.70200227 | 3.91662922 |
| H | 9.60977613 | 1.02429188 | 2.45254426 |
| H | 10.55040070 | 1.25728562 | 3.93914374 |
| H | 9.20510651 | 0.11086284 | 3.91205900 |
| H | 7.02595788 | -2.24456934 | 3.77036351 |
| H | 7.78038646 | -5.85983966 | 3.09270367 |
| H | 9.44527323 | -5.98759829 | 2.49649890 |
| H | 8.09641090 | -5.94860412 | 1.35441339 |
| H | 8.51253727 | -3.79840454 | 4.43897315 |
| H | 10.13320821 | -3.96618175 | 3.75979538 |
| H | 9.27998086 | -2.42795227 | 3.60867973 |
| H | 9.22552841 | -3.95444866 | 0.15532100 |
| H | 10.54907543 | -3.99464340 | 1.32538029 |
| H | 9.63217509 | -2.49708392 | 1.06905227 |
| H | 9.26100546 | -3.27871069 | -2.17023913 |
| H | 10.56069029 | -2.70914680 | -3.22343301 |

| | | | |
|---|---|---|---|
| H | 9.63808140 | -1.55373911 | -2.24212204 |
| H | 8.12256083 | -4.43012724 | -4.18555497 |
| H | 9.44756055 | -3.87356629 | -5.21508465 |
| H | 7.76967173 | -3.49426737 | -5.64457597 |
| H | 10.09506501 | -1.48075616 | -5.31451843 |
| H | 8.45957885 | -1.02615798 | -5.79877848 |
| H | 9.23188230 | -0.23458841 | -4.40917866 |
| H | -1.07649509 | 4.26856803 | 1.58988017 |
| H | -5.26093659 | 3.80052734 | 2.49603966 |
| H | -3.17670433 | 5.14623583 | 2.59857283 |
| H | -1.06180562 | -4.26060426 | -1.58571809 |
| H | -5.24699590 | -3.80561747 | -2.49495325 |
| H | -3.15846119 | -5.14478458 | -2.59596174 |
| H | -1.07021039 | 1.58998005 | -4.26322743 |
| H | -5.25646738 | 2.49188476 | -3.80301026 |
| H | -3.16999820 | 2.59588576 | -5.14514665 |
| H | -1.06830962 | -1.58408899 | 4.26672699 |
| H | -5.25161161 | -2.49804921 | 3.80371101 |
| H | -3.16559277 | -2.59665002 | 5.14693280 |
| H | -5.39554283 | 2.05833897 | 3.98589832 |
| H | -9.50043282 | 0.89403633 | 4.59457558 |
| H | -7.34315969 | 1.84648876 | 5.50061234 |
| H | -5.38546570 | -2.06362417 | -3.98489806 |
| H | -9.49329215 | -0.91173816 | -4.59738354 |
| H | -7.33225218 | -1.85748128 | -5.50147130 |
| H | -5.39578212 | 3.98232749 | -2.06129387 |
| H | -9.50344490 | 4.58691602 | -0.90465568 |
| H | -7.34538721 | 5.49503079 | -1.85333782 |
| H | -5.38535569 | -3.98814689 | 2.06167913 |
| H | -9.49028045 | -4.60492923 | 0.90177053 |
| H | -7.33019839 | -5.50670847 | 1.85189882 |
| H | -9.54986708 | 0.18717873 | 2.18346210 |
| H | -9.54719240 | -0.20537196 | -2.18619305 |
| H | -9.55169036 | 2.17585305 | -0.19754067 |
| H | -9.54523296 | -2.19389882 | 0.19499953 |

**NBP with 7 nickel atoms**

| | | | |
|---|---|---|---|
| C | -4.55141086 | -1.49064155 | 3.83248554 |
| C | -4.60342886 | -0.99716411 | 2.53580871 |
| N | -3.55729552 | -0.41905850 | 1.91932381 |
| C | -2.36527814 | -0.26050508 | 2.58769570 |
| C | -2.25444720 | -0.74446482 | 3.91254428 |
| C | -3.33645022 | -1.35910943 | 4.51152383 |
| C | -4.55249816 | 1.47549399 | -3.82572028 |
| C | -4.60400591 | 0.98060961 | -2.52959347 |
| N | -3.55803274 | 0.40059696 | -1.91461049 |
| C | -2.36614901 | 0.24306759 | -2.58345517 |

| | | | |
|---|---|---|---|
| C | -2.25606842 | 0.72784909 | -3.90808800 |
| C | -3.33815762 | 1.34355859 | -4.50580722 |
| C | -4.55019317 | -3.84202506 | -1.47399114 |
| C | -4.60141972 | -2.54458668 | -0.98252029 |
| N | -3.55480514 | -1.92721367 | -0.40643599 |
| C | -2.36260783 | -2.59520872 | -0.24824080 |
| C | -2.25220536 | -3.92069061 | -0.73067965 |
| C | -3.33495448 | -4.52071657 | -1.34299088 |
| C | -4.55734474 | 3.81882005 | 1.48241137 |
| C | -4.60853058 | 2.52250103 | 0.98768193 |
| N | -3.56111080 | 1.90684888 | 0.41090630 |
| C | -2.36936874 | 2.57605776 | 0.25380514 |
| C | -2.25966281 | 3.90063396 | 0.73877981 |
| C | -3.34251775 | 4.49851832 | 1.35281707 |
| C | -7.56399779 | -2.53020566 | 2.01742077 |
| C | -6.94250779 | -1.32275975 | 2.34952463 |
| C | -8.81162735 | -2.80196257 | 2.57799886 |
| C | -6.95819366 | -3.47459535 | 0.99717758 |
| C | -7.54708333 | -0.39012254 | 3.19677227 |
| O | -5.70964138 | -1.04177600 | 1.75435770 |
| C | -9.45633775 | -1.90859446 | 3.44210934 |
| C | -7.54833547 | -3.20101277 | -0.37705792 |
| C | -8.79732919 | -0.71299987 | 3.73688362 |
| C | -6.95511682 | 0.98376365 | 3.46676348 |
| C | -10.84246273 | -2.25452863 | 3.99990594 |
| C | -6.94066260 | -2.35535974 | -1.30913687 |
| C | -8.80199182 | -3.73366130 | -0.69925301 |
| C | -7.56198734 | 2.00543521 | 2.52469116 |
| C | -11.40750110 | -1.13407388 | 4.88809894 |
| C | -10.74759003 | -3.54588367 | 4.84054566 |
| C | -11.81721627 | -2.47578633 | 2.82142412 |
| C | -7.56085268 | -2.01998076 | -2.51635506 |
| O | -5.70704852 | -1.76255857 | -1.02722338 |
| C | -6.94550092 | 2.33764335 | 1.31942833 |
| C | -8.80934829 | 2.57284518 | 2.80951354 |
| C | -8.81223834 | -2.57250151 | -2.78684125 |
| C | -6.94994437 | -1.00264946 | -3.46090590 |
| C | -7.55074613 | 3.19468412 | 0.38982083 |
| O | -5.71525352 | 1.74127185 | 1.02946226 |
| C | -9.44470432 | 3.45022695 | 1.92987559 |
| C | -7.54253288 | 0.37138175 | -3.19250716 |
| C | -8.78680486 | 3.74508736 | 0.72784588 |
| C | -6.96662727 | 3.45744378 | -0.98885696 |
| C | -10.81636297 | 4.07153229 | 2.22067584 |
| C | -6.94347957 | 1.30367544 | -2.34081322 |
| C | -8.79141061 | 0.69217445 | -3.73633972 |
| C | -7.57216426 | 2.50630767 | -2.00386725 |
| C | -10.67796205 | 5.60821816 | 2.27560008 |

| | | | |
|---|---|---|---|
| C | -11.40178535 | 3.58588417 | 3.55681681 |
| C | -11.79721088 | 3.68186036 | 1.09270110 |
| O | -5.70930371 | 1.02649377 | -1.74681207 |
| C | -9.45833698 | 1.88190161 | -3.43643348 |
| C | -8.82247289 | 2.77195486 | -2.56209819 |
| C | -10.84604050 | 2.21988852 | -3.99539564 |
| C | -11.37884653 | 1.12340396 | -4.93219893 |
| C | -10.77404239 | 3.54432273 | -4.78510975 |
| C | -11.83422630 | 2.37220052 | -2.81783836 |
| N | -1.34651394 | 0.29512841 | 1.88315024 |
| N | -1.34359628 | -1.88970573 | 0.30551031 |
| N | -1.34948472 | 1.87279108 | -0.30146712 |
| N | -1.34680091 | -0.31199993 | -1.87936454 |
| C | -9.46134567 | -3.43288008 | -1.89308981 |
| C | -10.85517568 | -3.97424287 | -2.23405922 |
| C | -11.81859996 | -2.78239181 | -2.43280708 |
| C | -10.78070732 | -4.80134960 | -3.53531372 |
| C | -11.42046785 | -4.86868799 | -1.11881208 |
| C | -0.26942670 | 1.57252701 | 3.68498454 |
| C | -0.24490551 | 0.90441279 | 2.45228716 |
| N | 0.89443817 | 0.90450020 | 1.70296124 |
| C | 2.07055721 | 2.11799692 | 3.39949618 |
| C | 0.90793480 | 2.15169552 | 4.15236851 |
| C | -0.26769703 | -1.58660612 | -3.68186726 |
| C | -0.24400728 | -0.91854108 | -2.44916488 |
| N | 0.89580551 | -0.91565312 | -1.70060442 |
| C | 2.07387762 | -2.12597695 | -3.39804625 |
| C | 0.91085181 | -2.16267352 | -4.15013454 |
| C | -0.26304507 | -3.69006475 | 1.58213687 |
| C | -0.24064710 | -2.45766409 | 0.91342916 |
| N | 0.89798381 | -1.70731022 | 0.91135053 |
| C | 2.07762654 | -3.40242856 | 2.12341276 |
| C | 0.91570302 | -4.15624440 | 2.15946586 |
| C | -0.27404527 | 3.67650022 | -1.57751932 |
| C | -0.24813389 | 2.44373458 | -0.90958424 |
| N | 0.89239474 | 1.69623877 | -0.90878605 |
| C | 2.06685564 | 3.39485861 | -2.12098494 |
| C | 0.90306133 | 4.14587577 | -2.15558918 |
| Ni | -3.72745861 | -0.01008704 | 0.00218243 |
| Ni | -1.38139545 | -0.00854908 | 0.00198982 |
| C | 2.04851892 | 1.51336820 | 2.12438043 |
| C | 2.05115221 | -1.52146898 | -2.12286560 |
| C | 2.05342219 | -2.12751294 | 1.51841734 |
| C | 2.04634180 | 2.11964145 | -1.51652527 |
| N | 3.12233543 | 1.41986097 | 1.28420870 |
| N | 3.12626824 | -1.28638939 | 1.42286968 |
| N | 3.12145040 | 1.28123943 | -1.42209733 |
| N | 3.12528974 | -1.42509893 | -1.28346925 |

| | | | |
|---|---|---|---|
| C | 4.17670374 | 3.59353962 | 1.76902646 |
| C | 4.20773446 | 2.26872040 | 1.30168316 |
| N | 5.35717885 | 1.78193005 | 0.74477523 |
| C | 6.51785078 | 3.82655657 | 1.20307491 |
| C | 5.34549075 | 4.34727041 | 1.73037309 |
| C | 4.18508947 | -3.59594132 | -1.76913021 |
| C | 4.21293815 | -2.27103838 | -1.30182476 |
| N | 5.36150435 | -1.78111746 | -0.74589534 |
| C | 6.52736014 | -3.82255702 | -1.20527684 |
| C | 5.35596238 | -4.34647826 | -1.73153008 |
| C | 4.18484247 | -1.76985664 | 3.59482233 |
| C | 4.21312998 | -1.30271796 | 2.26987090 |
| N | 5.36119451 | -0.74486949 | 1.78096163 |
| C | 6.52592840 | -1.20193789 | 3.82355609 |
| C | 5.35494429 | -1.73012649 | 4.34645308 |
| C | 4.17693627 | 1.76800930 | -3.59476975 |
| C | 4.20758667 | 1.30064880 | -2.26994968 |
| N | 5.35754933 | 0.74575155 | -1.78210935 |
| C | 6.51928643 | 1.20619917 | -3.82564927 |
| C | 5.34648254 | 1.73145728 | -4.34742476 |
| Ni | 0.88546229 | -0.00557750 | 0.00119040 |
| Ni | 3.13107242 | -0.00260973 | 0.00037367 |
| C | 6.50199133 | 2.52628952 | 0.65991567 |
| C | 6.50842142 | -2.52234419 | -0.66208180 |
| C | 6.50726321 | -0.65893518 | 2.52325910 |
| C | 6.50319172 | 0.66296143 | -2.52541501 |
| N | 7.58691355 | 1.90798254 | 0.10012076 |
| N | 7.59057254 | -0.09825433 | 1.90295022 |
| N | 7.58853748 | 0.10512397 | -1.90609930 |
| N | 7.59214229 | -1.90106048 | -0.10328389 |
| C | 8.52049297 | 3.83390149 | -1.11059065 |
| C | 8.62533605 | 2.55675198 | -0.51379852 |
| N | 9.79938410 | 1.86595568 | -0.62843567 |
| C | 10.80236517 | 3.66562657 | -1.85534766 |
| C | 9.60383998 | 4.38222529 | -1.77282917 |
| C | 8.53224600 | -3.82443748 | 1.10642552 |
| C | 8.63294864 | -2.54695347 | 0.50963533 |
| N | 9.80516769 | -1.85288066 | 0.62320544 |
| C | 10.81434193 | -3.64984475 | 1.84901452 |
| C | 9.61775634 | -4.36979526 | 1.76757175 |
| C | 8.52658941 | 1.11338347 | 3.82711064 |
| C | 8.62962001 | 0.51665578 | 2.54978392 |
| N | 9.80227891 | 0.63236016 | 1.85681348 |
| C | 10.80742871 | 1.86031591 | 3.65456279 |
| C | 9.61032711 | 1.77666090 | 4.37340421 |
| C | 8.52616564 | -1.10384741 | -3.83114772 |
| C | 8.62870559 | -0.50686254 | -2.55390090 |
| N | 9.80232288 | -0.61930235 | -1.86201215 |

| | | | |
|---|---|---|---|
| C | 10.80931919 | -1.84418359 | -3.66082803 |
| C | 9.61128561 | -1.76397959 | -4.37850698 |
| Ni | 5.37893121 | 0.00044605 | -0.00057952 |
| Ni | 7.64353276 | 0.00353019 | -0.00159538 |
| C | 10.84856541 | 2.40693001 | -1.28101741 |
| C | 10.85646381 | -2.39096455 | 1.27476894 |
| C | 10.85182610 | 1.28600197 | 2.39579312 |
| C | 10.85325900 | -1.26982017 | -2.40206540 |
| Ni | 9.99679505 | 0.00683535 | -0.00269020 |
| Cl | 12.74372366 | 0.01055992 | -0.00388693 |
| H | -5.42191384 | -1.94741164 | 4.28102368 |
| H | -1.30348786 | -0.66502012 | 4.42003860 |
| H | -3.23956658 | -1.75685791 | 5.51706960 |
| H | -5.42288817 | 1.93359841 | -4.27311827 |
| H | -1.30544831 | 0.64860879 | -4.41624267 |
| H | -3.24169130 | 1.74217774 | -5.51104814 |
| H | -5.42125290 | -4.29117738 | -1.92910523 |
| H | -1.30107812 | -4.42795775 | -0.65188744 |
| H | -3.23844243 | -5.52684657 | -1.73935103 |
| H | -5.42813083 | 4.26675732 | 1.93913770 |
| H | -1.30885682 | 4.40862079 | 0.66061503 |
| H | -3.24658800 | 5.50375910 | 1.75156537 |
| H | -9.29257316 | -3.74006332 | 2.32186347 |
| H | -5.87361917 | -3.37926105 | 0.99159222 |
| H | -7.19247102 | -4.50509189 | 1.28002501 |
| H | -9.26186903 | 0.01030368 | 4.39525429 |
| H | -5.87092386 | 0.97680013 | 3.36725179 |
| H | -7.18488150 | 1.26753231 | 4.49804851 |
| H | -9.26977086 | -4.38985938 | 0.02391119 |
| H | -10.77538311 | -0.95033898 | 5.76260789 |
| H | -11.51444365 | -0.19459967 | 4.33553897 |
| H | -12.39898951 | -1.41805068 | 5.25220064 |
| H | -10.06442210 | -3.41172760 | 5.68500421 |
| H | -10.38488512 | -4.38953437 | 4.24625716 |
| H | -11.73198757 | -3.81494035 | 5.23715026 |
| H | -11.88792504 | -1.57696720 | 2.20076353 |
| H | -12.81786002 | -2.71419652 | 3.19622328 |
| H | -11.49686417 | -3.30159977 | 2.17964931 |
| H | -9.28193310 | 2.31016185 | 3.74759484 |
| H | -9.29384371 | -2.31120309 | -3.72313353 |
| H | -5.86589467 | -0.99730774 | -3.36034181 |
| H | -7.17953528 | -1.28799289 | -4.49176258 |
| H | -9.25435032 | 4.41672684 | 0.01540775 |
| H | -5.88174030 | 3.36409559 | -0.98605707 |
| H | -7.20306700 | 4.48554602 | -1.27835581 |
| H | -9.24954528 | -0.02900717 | -4.40136424 |
| H | -9.99161006 | 5.90934980 | 3.07315829 |
| H | -10.29643796 | 6.01301833 | 1.33373295 |

| | | | |
|---|---|---|---|
| H | -11.65091507 | 6.07146881 | 2.46926903 |
| H | -10.76615791 | 3.86188391 | 4.40406382 |
| H | -11.53910955 | 2.49942076 | 3.56735070 |
| H | -12.38162418 | 4.04462781 | 3.71710418 |
| H | -11.89144211 | 2.59423239 | 1.01527229 |
| H | -12.78936563 | 4.09980275 | 1.29139671 |
| H | -11.46759368 | 4.05831168 | 0.12046981 |
| H | -9.31141452 | 3.70380167 | -2.29796248 |
| H | -10.72686592 | 0.97642508 | -5.79914891 |
| H | -12.36640314 | 1.40807563 | -5.30634212 |
| H | -11.48702147 | 0.16515740 | -4.41343733 |
| H | -10.07934135 | 3.45921789 | -5.62655330 |
| H | -11.76080741 | 3.80376507 | -5.18205688 |
| H | -10.43944250 | 4.37420773 | -4.15617993 |
| H | -11.89336705 | 1.44599919 | -2.23759305 |
| H | -12.83615299 | 2.60879825 | -3.19057138 |
| H | -11.53306978 | 3.17329328 | -2.13741158 |
| H | -11.49441233 | -2.13123956 | -3.24983116 |
| H | -12.82431969 | -3.14278429 | -2.67219649 |
| H | -11.87843176 | -2.17535842 | -1.52393580 |
| H | -10.42141698 | -4.20173752 | -4.37657956 |
| H | -11.77142090 | -5.18591086 | -3.79846880 |
| H | -10.10417966 | -5.65352102 | -3.41716574 |
| H | -12.41346933 | -5.22804568 | -1.40358736 |
| H | -10.79017060 | -5.74604142 | -0.94219889 |
| H | -11.52526971 | -4.32161956 | -0.17604337 |
| H | -1.19104951 | 1.63830817 | 4.24649696 |
| H | 2.99521917 | 2.52979451 | 3.77785327 |
| H | 0.91507747 | 2.63743561 | 5.12387900 |
| H | -1.18956802 | -1.65468927 | -4.24271374 |
| H | 2.99935680 | -2.53530927 | -3.77707609 |
| H | 0.91860482 | -2.64830817 | -5.12169152 |
| H | -1.18409086 | -4.25228906 | 1.64979627 |
| H | 3.00333026 | -3.77985770 | 2.53371075 |
| H | 0.92448927 | -5.12755013 | 2.64558693 |
| H | -1.19651014 | 4.23655691 | -1.64395501 |
| H | 2.99127227 | 3.77474819 | -2.53192501 |
| H | 0.90906736 | 5.11746742 | -2.64118107 |
| H | 3.25134926 | 4.01465502 | 2.13538235 |
| H | 7.43946513 | 4.39170029 | 1.21371503 |
| H | 5.33964673 | 5.36067899 | 2.12153053 |
| H | 3.26055773 | -4.01958451 | -2.13464698 |
| H | 7.45050832 | -4.38517292 | -1.21675829 |
| H | 5.35253897 | -5.35989602 | -2.12269182 |
| H | 3.26054949 | -2.13690581 | 4.01765672 |
| H | 7.44856783 | -1.21174604 | 4.38703880 |
| H | 5.35123958 | -2.12114319 | 5.35992581 |
| H | 3.25132078 | 2.13277054 | -4.01669990 |

| | | | |
|---|---|---|---|
| H | 7.44140441 | 1.21850968 | -4.38993441 |
| H | 5.34088776 | 2.12266272 | -5.36081615 |
| H | 7.57271784 | 4.35410222 | -1.07099612 |
| H | 11.67587123 | 4.06167505 | -2.35880523 |
| H | 9.51056392 | 5.35857223 | -2.23943730 |
| H | 7.58589647 | -4.34729334 | 1.06769905 |
| H | 11.68943552 | -4.04348364 | 2.35160545 |
| H | 9.52766179 | -5.34644587 | 2.23416918 |
| H | 7.57982262 | 1.07291642 | 4.34907645 |
| H | 11.68118581 | 2.36463422 | 4.04895992 |
| H | 9.51842797 | 2.24319677 | 5.34991626 |
| H | 7.57879105 | -1.06607181 | -4.35221356 |
| H | 11.68416571 | -2.34592157 | -4.05609970 |
| H | 9.51979467 | -2.23074797 | -5.35494583 |
| H | 11.73940885 | 1.78582487 | -1.29361533 |
| H | 11.74557768 | -1.76737045 | 1.28659709 |
| H | 11.74148344 | 1.29949132 | 1.77300975 |
| H | 11.74356914 | -1.28068476 | -1.78016256 |

**NBP with 9 nickel atoms**

| | | | |
|---|---|---|---|
| C | -6.80905807 | -3.81657783 | -1.48806564 |
| C | -6.85880021 | -2.52132060 | -0.99104154 |
| N | -5.81156886 | -1.90734126 | -0.41283377 |
| C | -4.62009730 | -2.57746928 | -0.25622852 |
| C | -4.51146489 | -3.90148037 | -0.74368954 |
| C | -5.59450278 | -4.49735652 | -1.35919243 |
| C | -6.79801589 | 3.83513180 | 1.49047270 |
| C | -6.85174246 | 2.54041726 | 0.99252712 |
| N | -5.80733856 | 1.92476030 | 0.41083411 |
| C | -4.61457196 | 2.59225837 | 0.25276172 |
| C | -4.50206417 | 3.91573443 | 0.74077784 |
| C | -5.58243405 | 4.51353299 | 1.35910756 |
| C | -6.80057663 | 1.50270505 | -3.82642251 |
| C | -6.85228889 | 1.00513770 | -2.53156417 |
| N | -5.80789303 | 0.42147741 | -1.91787246 |
| C | -4.61642994 | 0.26197821 | -2.58732809 |
| C | -4.50590601 | 0.74929664 | -3.91127928 |
| C | -5.58655570 | 1.36901883 | -4.50722548 |
| C | -6.80205134 | -1.48727664 | 3.82214078 |
| C | -6.85532266 | -0.98696891 | 2.52828300 |
| N | -5.81031566 | -0.40475563 | 1.91408276 |
| C | -4.61749281 | -0.24892153 | 2.58216343 |
| C | -4.50573513 | -0.73900385 | 3.90485846 |
| C | -5.58667678 | -1.35780466 | 4.50117745 |
| C | -9.81236450 | -1.99372421 | -2.52502227 |
| C | -9.19612695 | -2.33054154 | -1.32090262 |
| C | -11.06372132 | -2.55291427 | -2.80828511 |
| C | -9.20248407 | -0.97247296 | -3.46620142 |

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| C | -9.80479642 | -3.18547424 | -0.39135498 |
| O | -7.96433176 | -1.73824214 | -1.03181853 |
| C | -11.70425037 | -3.42513925 | -1.92751090 |
| C | -9.79474612 | 0.40094265 | -3.19363598 |
| C | -11.04596927 | -3.72567543 | -0.72709105 |
| C | -9.21863985 | -3.45794425 | 0.98490384 |
| C | -13.08432257 | -4.03035914 | -2.21244922 |
| C | -9.19095213 | 1.33368670 | -2.33880066 |
| C | -11.04234885 | 0.72503426 | -3.72533247 |
| C | -9.82103089 | -2.51321804 | 2.00766441 |
| C | -12.97158490 | -5.56971030 | -2.24325158 |
| C | -13.65999725 | -3.55637610 | -3.55684571 |
| C | -14.05996105 | -3.60572363 | -1.09258417 |
| C | -9.81694119 | 2.53136974 | -1.99664268 |
| O | -7.95700725 | 1.05155742 | -1.74792160 |
| C | -9.19439776 | -1.30937283 | 2.34378466 |
| C | -11.06598016 | -2.78568685 | 2.57471800 |
| C | -11.07669907 | 2.80097072 | -2.54412677 |
| C | -9.20838736 | 3.47986784 | -0.98105311 |
| C | -9.79237049 | -0.38003871 | 3.19955708 |
| O | -7.96242169 | -1.02922277 | 1.74720004 |
| C | -11.69966706 | -1.89948180 | 3.45452000 |
| C | -9.79441396 | 3.21201189 | 0.39567852 |
| C | -11.03682228 | -0.70630360 | 3.75026250 |
| C | -9.20094289 | 0.99416511 | 3.46834568 |
| C | -13.07832916 | -2.24792211 | 4.02930874 |
| C | -9.18964474 | 2.35399543 | 1.32473172 |
| C | -11.03635666 | 3.75190286 | 0.72819325 |
| C | -9.81035950 | 2.01435303 | 2.52575482 |
| C | -13.62132857 | -1.14150308 | 4.94844742 |
| C | -12.97808383 | -3.55520801 | 4.84430769 |
| C | -14.07367389 | -2.44093193 | 2.86390589 |
| O | -7.95866760 | 1.75954672 | 1.03646251 |
| C | -11.70198893 | 3.44350112 | 1.92228312 |
| C | -11.06477819 | 2.56968788 | 2.80401932 |
| C | -13.08807719 | 4.03986377 | 2.19589869 |
| C | -12.98443994 | 5.57951743 | 2.23873770 |
| C | -13.67622336 | 3.55285553 | 3.53025472 |
| C | -14.04856326 | 3.61800384 | 1.06116470 |
| N | -3.60106842 | -1.87536604 | 0.30095890 |
| N | -3.59925377 | -0.29741793 | -1.88434889 |
| N | -3.59991716 | 0.30988975 | 1.87908114 |
| N | -3.59786206 | 1.88807956 | -0.30613012 |
| C | -11.71426807 | 1.91436522 | -3.41258680 |
| C | -13.10805014 | 2.17573465 | -3.99629353 |
| C | -14.05692575 | 1.03948667 | -3.55258268 |
| C | -13.02242730 | 2.20550172 | -5.53728517 |
| C | -13.69845208 | 3.51077220 | -3.51417920 |

| | | | |
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| C | -2.52066707 | -3.68243502 | 1.56863615 |
| C | -2.49786991 | -2.44691393 | 0.90630793 |
| N | -1.35941687 | -1.69663534 | 0.90810815 |
| C | -0.17957337 | -3.39793716 | 2.11086950 |
| C | -1.34121215 | -4.15190416 | 2.14251587 |
| C | -2.51437115 | 3.69319661 | -1.57384531 |
| C | -2.49360736 | 2.45771956 | -0.91139182 |
| N | -1.35630425 | 1.70572871 | -0.91276154 |
| C | -0.17353890 | 3.40515962 | -2.11528273 |
| C | -1.33403972 | 4.16086241 | -2.14739740 |
| C | -2.51796897 | -1.56595961 | -3.69025875 |
| C | -2.49590618 | -0.90358980 | -2.45477116 |
| N | -1.35814144 | -0.90592743 | -1.70345787 |
| C | -0.17742849 | -2.10946065 | -3.40359644 |
| C | -1.33838801 | -2.14052056 | -4.15862547 |
| C | -2.51695436 | 1.57557064 | 3.68586471 |
| C | -2.49563822 | 0.91390579 | 2.44996990 |
| N | -1.35769357 | 0.91493710 | 1.69892725 |
| C | -0.17562535 | 2.11599595 | 3.39987544 |
| C | -1.33668042 | 2.14824109 | 4.15474083 |
| Ni | -5.97940700 | 0.00897433 | -0.00153475 |
| Ni | -3.63461036 | 0.00632957 | -0.00263693 |
| C | -0.20345242 | -2.11889575 | 1.51386804 |
| C | -0.19950676 | 2.12621688 | -1.51815723 |
| C | -0.20211890 | -1.51235177 | -2.12460711 |
| C | -0.20088733 | 1.51946734 | 2.12064838 |
| N | 0.86759541 | -1.27519926 | 1.42467562 |
| N | 0.86821053 | -1.42364807 | -1.27995067 |
| N | 0.86957053 | 1.42943558 | 1.27626690 |
| N | 0.87026790 | 1.28096616 | -1.42842608 |
| C | 1.92940792 | -1.78150204 | 3.58856246 |
| C | 1.95701963 | -1.29750624 | 2.27043097 |
| N | 3.10400624 | -0.73284031 | 1.78615350 |
| C | 4.27372018 | -1.22748440 | 3.81668249 |
| C | 3.10377276 | -1.76068932 | 4.33449215 |
| C | 1.93393608 | 1.78568225 | -3.59177405 |
| C | 1.96016796 | 1.30172163 | -2.27360039 |
| N | 3.10611716 | 0.73552858 | -1.78865989 |
| C | 4.27763859 | 1.22853896 | -3.81854127 |
| C | 3.10869523 | 1.76328229 | -4.33703535 |
| C | 1.92965311 | -3.58794979 | -1.78529097 |
| C | 1.95732228 | -2.26984206 | -1.30123703 |
| N | 3.10396894 | -1.78603476 | -0.73546172 |
| C | 4.27334701 | -3.81701747 | -1.22903431 |
| C | 3.10370529 | -4.33434434 | -1.76337556 |
| C | 1.93376193 | 3.59217103 | 1.78242003 |
| C | 1.95984732 | 2.27408617 | 1.29820378 |
| N | 3.10610281 | 1.78874963 | 0.73296733 |

| | | | |
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| C | 4.27804196 | 3.81805834 | 1.22733837 |
| C | 3.10884973 | 4.33694399 | 1.76116666 |
| Ni | -1.37011861 | 0.00458554 | -0.00228491 |
| Ni | 0.87123777 | 0.00289474 | -0.00187217 |
| C | 4.25464550 | -0.65713505 | 2.52712320 |
| C | 4.25706823 | 0.65823984 | -2.52898507 |
| C | 4.25424279 | -2.52746769 | -0.65866339 |
| C | 4.25744360 | 2.52858910 | 0.65684974 |
| N | 5.33345679 | -0.07959133 | 1.91335625 |
| N | 5.33274790 | -1.91415695 | -0.08005278 |
| N | 5.33540342 | 1.91379595 | 0.07879553 |
| N | 5.33474475 | 0.07923315 | -1.91460044 |
| C | 6.38390543 | 0.95859359 | 3.88720187 |
| C | 6.41539677 | 0.45793081 | 2.57359473 |
| N | 7.56688366 | 0.57001458 | 1.84422706 |
| C | 8.72593217 | 1.53972015 | 3.70225687 |
| C | 7.55143655 | 1.47496337 | 4.43836821 |
| C | 6.38502951 | -0.96027919 | -3.88784361 |
| C | 6.41636347 | -0.45972860 | -2.57418885 |
| N | 7.56723874 | -0.57341504 | -1.84410006 |
| C | 8.72615406 | -1.54457840 | -3.70144815 |
| C | 7.55221301 | -1.47819201 | -4.43829943 |
| C | 6.38147344 | -3.88844789 | 0.95904041 |
| C | 6.41392391 | -2.57482039 | 0.45849127 |
| N | 7.56556892 | -1.84587519 | 0.57175782 |
| C | 8.72299132 | -3.70437232 | 1.54250357 |
| C | 7.54829747 | -4.44005973 | 1.47653464 |
| C | 6.38747357 | 3.88667219 | -0.95958491 |
| C | 6.41781119 | 2.57298240 | -0.45906438 |
| N | 7.56851728 | 1.84245671 | -0.57164161 |
| C | 8.72909173 | 3.69938960 | -1.54161927 |
| C | 7.55537125 | 4.43669444 | -1.47634399 |
| Ni | 3.10856938 | 0.00136280 | -0.00124758 |
| Ni | 5.34394884 | -0.00019053 | -0.00062966 |
| C | 8.71066927 | 1.11494226 | 2.35938675 |
| C | 8.71061323 | -1.11985759 | -2.35856448 |
| C | 8.70863199 | -2.36147364 | 1.11778574 |
| C | 8.71262421 | 2.35650196 | -1.11694741 |
| N | 9.79744006 | 1.14207113 | 1.52631839 |
| N | 9.79568240 | -1.52880056 | 1.14603645 |
| N | 9.79854398 | 1.52233495 | -1.14452773 |
| N | 9.79682198 | -1.14850319 | -1.52480975 |
| C | 10.73239328 | 3.30878703 | 2.21751640 |
| C | 10.83516432 | 2.02902061 | 1.62488833 |
| N | 12.00860296 | 1.67131332 | 1.02069751 |
| C | 13.01326512 | 3.76900024 | 1.60380774 |
| C | 11.81573669 | 4.16806834 | 2.20729718 |
| C | 10.72923743 | -3.31647063 | -2.21550632 |

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| C | 10.83338570 | -2.03687632 | -1.62274567 |
| N | 12.00692430 | -1.68081657 | -1.01777400 |
| C | 13.00907536 | -3.77985428 | -1.60034166 |
| C | 11.81139040 | -4.17724222 | -2.20462896 |
| C | 10.72818272 | -2.22040820 | 3.31367663 |
| C | 10.83247112 | -1.62777659 | 2.03403448 |
| N | 12.00649419 | -1.02400163 | 1.67753993 |
| C | 13.00880072 | -1.60752218 | 3.77623982 |
| C | 11.81065035 | -2.21059741 | 4.17406538 |
| C | 10.73344068 | 2.21274009 | -3.31151811 |
| C | 10.83605408 | 1.61990618 | -2.03183353 |
| N | 12.00900275 | 1.01448981 | -1.67458475 |
| C | 13.01352548 | 1.59674287 | -3.77257606 |
| C | 11.81647410 | 2.20148678 | -4.17117711 |
| Ni | 7.58763349 | -0.00171975 | 0.00006959 |
| Ni | 9.85010738 | -0.00326344 | 0.00077625 |
| C | 13.05783682 | 2.51861717 | 1.01169140 |
| C | 13.05498530 | -2.52956381 | -1.00813225 |
| C | 13.05486433 | -1.01539228 | 2.52591723 |
| C | 13.05793038 | 1.00448253 | -2.52225525 |
| Ni | 12.20143721 | -0.00489401 | 0.00154175 |
| Cl | 14.95446344 | -0.00681597 | 0.00244388 |
| H | -7.68024184 | -4.26255810 | -1.94603569 |
| H | -3.56087275 | -4.41001972 | -0.66665428 |
| H | -5.49897253 | -5.50183956 | -1.75996873 |
| H | -7.66717915 | 4.28244399 | 1.95099346 |
| H | -3.55052764 | 4.42224958 | 0.66213146 |
| H | -5.48382949 | 5.51751718 | 1.76038701 |
| H | -7.67004644 | 1.96451874 | -4.27189098 |
| H | -3.55547559 | 0.66922910 | -4.41964227 |
| H | -5.48924736 | 1.76973253 | -5.51156219 |
| H | -7.67174627 | -1.94749388 | 4.26869789 |
| H | -3.55432247 | -0.66167039 | 4.41182068 |
| H | -5.48866691 | -1.76093038 | 5.50448026 |
| H | -11.53610636 | -2.28651755 | -3.74532472 |
| H | -8.11836726 | -0.96699794 | -3.36635541 |
| H | -9.43236004 | -1.25473157 | -4.49787336 |
| H | -11.51787954 | -4.39325631 | -0.01365583 |
| H | -8.13363445 | -3.36601406 | 0.98047882 |
| H | -9.45568284 | -4.48778886 | 1.26772865 |
| H | -11.51086762 | 0.00848864 | -4.39174225 |
| H | -12.28718033 | -5.89457650 | -3.03314870 |
| H | -12.60154104 | -5.96752284 | -1.29390367 |
| H | -13.95153020 | -6.01902433 | -2.43440209 |
| H | -13.02238316 | -3.84689636 | -4.39780642 |
| H | -13.79024317 | -2.46939376 | -3.57987900 |
| H | -14.64259224 | -4.00965865 | -3.71605121 |
| H | -13.73302879 | -3.96415539 | -0.11270203 |

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| H | -15.05713065 | -4.01625418 | -1.28175182 |
| H | -14.14136910 | -2.51558045 | -1.03939070 |
| H | -11.55153617 | -3.72029587 | 2.31406510 |
| H | -11.55873599 | 3.73084136 | -2.26987173 |
| H | -8.12375291 | 3.38473867 | -0.97864639 |
| H | -9.44366517 | 4.50913447 | -1.26763176 |
| H | -11.49359591 | 0.01224306 | 4.41916612 |
| H | -8.11683926 | 0.98871139 | 3.36769432 |
| H | -9.43014586 | 1.27842928 | 4.49964204 |
| H | -11.50472911 | 4.42251001 | 0.01541975 |
| H | -12.96855663 | -0.97187728 | 5.81056654 |
| H | -13.74114473 | -0.19317748 | 4.41401096 |
| H | -14.60427817 | -1.43103541 | 5.33089700 |
| H | -12.27942275 | -3.44153836 | 5.67906097 |
| H | -12.63232349 | -4.39053221 | 4.22864799 |
| H | -13.95745810 | -3.82452387 | 5.25298724 |
| H | -13.76993969 | -3.25685533 | 2.20254106 |
| H | -15.07005347 | -2.67843442 | 3.25059670 |
| H | -14.14730028 | -1.53150118 | 2.25937390 |
| H | -11.54229371 | 2.29796740 | 3.73698697 |
| H | -12.31075285 | 5.90240779 | 3.03856292 |
| H | -13.96892098 | 6.02217891 | 2.42198210 |
| H | -12.60591072 | 5.98594250 | 1.29641650 |
| H | -13.05152570 | 3.84448346 | 4.38042640 |
| H | -14.66491003 | 3.99594935 | 3.68013490 |
| H | -13.79559209 | 2.46436983 | 3.54661345 |
| H | -13.71139142 | 3.98450818 | 0.08725296 |
| H | -15.04974095 | 4.02289193 | 1.24101914 |
| H | -14.12446887 | 2.52771917 | 1.00089862 |
| H | -14.12164169 | 0.99137322 | -2.46098894 |
| H | -15.06321201 | 1.20832964 | -3.94951500 |
| H | -13.71648538 | 0.06376323 | -3.91127249 |
| H | -12.64398090 | 1.26171188 | -5.94031292 |
| H | -12.35680138 | 3.00595090 | -5.87504446 |
| H | -14.01298186 | 2.37984733 | -5.96983408 |
| H | -13.81126457 | 3.53286691 | -2.42525415 |
| H | -13.07932131 | 4.36163190 | -3.81570475 |
| H | -14.69074742 | 3.65340035 | -3.95159711 |
| H | -3.44172851 | -4.24490841 | 1.63399607 |
| H | 0.74622051 | -3.77792872 | 2.51840866 |
| H | -1.33190289 | -5.12638077 | 2.62229175 |
| H | -3.43458606 | 4.25704298 | -1.63942058 |
| H | 0.75295287 | 3.78375015 | -2.52253738 |
| H | -1.32310885 | 5.13527924 | -2.62725890 |
| H | -3.43857841 | -1.63082756 | -4.25354062 |
| H | 0.74848323 | -2.51752796 | -3.78273339 |
| H | -1.32843772 | -2.62034934 | -5.13306898 |
| H | -3.43756952 | 1.64126734 | 4.24905535 |

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| H | 0.75077817 | 2.52261706 | 3.77936891 |
| H | -1.32623071 | 2.62753682 | 5.12944156 |
| H | 1.00513044 | -2.15076976 | 4.00931365 |
| H | 5.19722394 | -1.25128383 | 4.37708763 |
| H | 3.10387748 | -2.17080676 | 5.34047484 |
| H | 1.01038582 | 2.15615456 | -4.01306275 |
| H | 5.20149187 | 1.25109893 | -4.37842077 |
| H | 3.10991744 | 2.17336170 | -5.34303262 |
| H | 1.00556239 | -4.00833906 | -2.15543668 |
| H | 5.19664891 | -4.37779171 | -1.25196582 |
| H | 3.10380288 | -5.34031487 | -2.17352250 |
| H | 1.01006688 | 4.01376467 | 2.15219009 |
| H | 5.20210662 | 4.37755327 | 1.25078928 |
| H | 3.11013881 | 5.34286757 | 2.17142672 |
| H | 5.45773316 | 0.95173288 | 4.44378460 |
| H | 9.64719425 | 1.89584317 | 4.14197211 |
| H | 7.54378893 | 1.83274137 | 5.46410652 |
| H | 5.45922253 | -0.95214044 | -4.44501554 |
| H | 9.64721442 | -1.90191796 | -4.14059925 |
| H | 7.54473214 | -1.83589771 | -5.46406408 |
| H | 5.45511321 | -4.44470497 | 0.95123042 |
| H | 9.64374248 | -4.14443725 | 1.89951580 |
| H | 7.53992943 | -5.46581772 | 1.83424006 |
| H | 5.46187218 | 4.44419957 | -0.95231601 |
| H | 9.65066698 | 4.13819881 | -1.89804965 |
| H | 7.54863588 | 5.46247486 | -1.83401941 |
| H | 9.78535847 | 3.61382112 | 2.64234116 |
| H | 13.88687522 | 4.40902989 | 1.58029735 |
| H | 11.72340791 | 5.15440105 | 2.65274006 |
| H | 9.78205973 | -3.62017663 | -2.64096367 |
| H | 13.88178850 | -4.42108671 | -1.57629878 |
| H | 11.71799411 | -5.16342334 | -2.65018496 |
| H | 9.78068572 | -2.64490650 | 3.61772871 |
| H | 13.88176310 | -1.58433844 | 4.41716455 |
| H | 11.71715531 | -2.65603592 | 5.16029026 |
| H | 9.78673332 | 2.63855716 | -3.61618568 |
| H | 13.88688855 | 1.57239491 | -4.41291144 |
| H | 11.72425697 | 2.64710655 | -5.15744033 |
| H | 13.94770943 | 2.12785197 | 0.52692233 |
| H | 13.94508339 | -2.14004779 | -0.52277038 |
| H | 13.94531242 | -0.53093630 | 2.13607452 |
| H | 13.94744818 | 0.51878273 | -2.13183695 |

**NBP with 11 nickel atoms**

| | | | |
|---|---|---|---|
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| H | 0.87049230 | -2.23165404 | 5.31912413 |
| H | 3.21999580 | -4.46043556 | 0.89804509 |
| H | 7.41357085 | -4.17433342 | 1.82065057 |
| H | 5.31675860 | -5.49933666 | 1.73320885 |
| H | 3.21494983 | 4.45778994 | -0.89555770 |
| H | 7.40832691 | 4.17589610 | -1.82033137 |
| H | 5.31022633 | 5.49878144 | -1.73182157 |
| H | 3.21673537 | -0.89832077 | -4.45778008 |
| H | 7.41076436 | -1.81983943 | -4.17490400 |
| H | 5.31289111 | -1.73302839 | -5.49826592 |
| H | 3.21817487 | 0.89558780 | 4.46035328 |
| H | 7.41112753 | 1.82130935 | 4.17527662 |
| H | 5.31404672 | 1.73234490 | 5.49975143 |
| H | 7.67613246 | -2.82670603 | 3.55870417 |
| H | 11.86435596 | -1.98746162 | 4.09706621 |
| H | 9.76124957 | -3.05051981 | 4.88856338 |
| H | 7.67121730 | 2.82845569 | -3.55853917 |
| H | 11.85999570 | 1.99349598 | -4.09924278 |
| H | 9.75534994 | 3.05435722 | -4.88959225 |
| H | 7.67470585 | -3.55777915 | -2.82736120 |
| H | 11.86373328 | -4.09512854 | -1.99149021 |
| H | 9.75994669 | -4.88717427 | -3.05279294 |
| H | 7.67263296 | 3.55954512 | 2.82767194 |
| H | 11.86061923 | 4.10123160 | 1.98938560 |
| H | 9.75663462 | 4.89107773 | 3.05193154 |
| H | 12.00076955 | 0.25992889 | 4.47118118 |
| H | 16.09780094 | 1.59963147 | 4.40728644 |
| H | 13.93618258 | 1.23776077 | 5.66572888 |
| H | 11.99847726 | -0.25378984 | -4.47335822 |

| | | | |
|---|---|---|---|
| H | 16.09692611 | -1.58925774 | -4.41178206 |
| H | 13.93420499 | -1.22967887 | -5.66898506 |
| H | 12.00200026 | -4.46912800 | 0.25580728 |
| H | 16.10008910 | -4.40428739 | 1.59222561 |
| H | 13.93845725 | -5.66321608 | 1.23213504 |
| H | 11.99725020 | 4.47539166 | -0.25799482 |
| H | 16.09464636 | 4.41474972 | -1.59673060 |
| H | 13.93192937 | 5.67146246 | -1.23541489 |
| H | 16.15939342 | 0.96241257 | 1.97680191 |
| H | 16.15926382 | -0.95188615 | -1.98135508 |
| H | 16.16063307 | -1.97380641 | 0.95488381 |
| H | 16.15804275 | 1.98433444 | -0.95942414 |

**NBP with 13 nickel atoms**

| | | | |
|---|---|---|---|
| C | 11.29599139 | 3.85170275 | -1.41905649 |
| C | 11.34696137 | 2.54827933 | -0.94435820 |
| N | 10.30020734 | 1.92292248 | -0.37759292 |
| C | 9.10764026 | 2.58879189 | -0.21020265 |
| C | 8.99778227 | 3.92105641 | -0.67505817 |
| C | 10.08024894 | 4.52865041 | -1.27950866 |
| C | 11.29599372 | -3.85169924 | 1.41905876 |
| C | 11.34696280 | -2.54827584 | 0.94436019 |
| N | 10.30020835 | -1.92291989 | 0.37759515 |
| C | 9.10764127 | -2.58878934 | 0.21020599 |
| C | 8.99778402 | -3.92105384 | 0.67506175 |
| C | 10.08025132 | -4.52864720 | 1.27951182 |
| C | 11.29239611 | -1.42865394 | -3.84928947 |
| C | 11.34446286 | -0.95191624 | -2.54673703 |
| N | 10.29963662 | -0.37987668 | -1.92284878 |
| C | 9.10709161 | -0.21173654 | -2.58869173 |
| C | 8.99640747 | -0.67794253 | -3.92038966 |
| C | 10.07739366 | -1.28627450 | -4.52689474 |
| C | 11.29239198 | 1.42866181 | 3.84929332 |
| C | 11.34446001 | 0.95192231 | 2.54674150 |
| N | 10.29963477 | 0.37988106 | 1.92285343 |
| C | 9.10708965 | 0.21174034 | 2.58869576 |
| C | 8.99640424 | 0.67794712 | 3.92039329 |
| C | 10.07738938 | 1.28628129 | 4.52689816 |
| N | 8.08924944 | 1.87654218 | 0.33420911 |
| N | 8.08949382 | 0.33437388 | -1.87655525 |
| N | 8.08949276 | -0.33437137 | 1.87655890 |
| N | 8.08924997 | -1.87653993 | -0.33420537 |
| C | 7.00739768 | 3.66129669 | 1.63188956 |
| C | 6.98519594 | 2.43724449 | 0.94906564 |
| N | 5.84739363 | 1.68631867 | 0.93762146 |
| C | 4.66593628 | 3.36713957 | 2.16748678 |
| C | 5.82693151 | 4.12092262 | 2.21225186 |
| C | 7.00739985 | -3.66129521 | -1.63188608 |

| | | | |
|---|---|---|---|
| C | 6.98519721 | -2.43724288 | -0.94906226 |
| N | 5.84739447 | -1.68631775 | -0.93761858 |
| C | 4.66593858 | -3.36713932 | -2.16748446 |
| C | 5.82693431 | -4.12092177 | -2.21224897 |
| C | 7.00739942 | 1.63132887 | -3.66160977 |
| C | 6.98531696 | 0.94897865 | -2.43731031 |
| N | 5.84752650 | 0.93763326 | -1.68633165 |
| C | 4.66597191 | 2.16708588 | -3.36737592 |
| C | 5.82688631 | 2.21156603 | -4.12130558 |
| C | 7.00739926 | -1.63132793 | 3.66161266 |
| C | 6.98531648 | -0.94897735 | 2.43731338 |
| N | 5.84752613 | -0.93763258 | 1.68633449 |
| C | 4.66597241 | -2.16708728 | 3.36737786 |
| C | 5.82688668 | -2.21156651 | 4.12130785 |
| Ni | 10.46956380 | 0.00000164 | 0.00000204 |
| Ni | 8.12468701 | 0.00000128 | 0.00000194 |
| C | 4.69058437 | 2.09742827 | 1.55011299 |
| C | 4.69058575 | -2.09742817 | -1.55011054 |
| C | 4.69067206 | 1.55000272 | -2.09751622 |
| C | 4.69067212 | -1.55000328 | 2.09751855 |
| N | 3.62112593 | 1.25412304 | 1.44798965 |
| N | 3.62121617 | 1.44798110 | -1.25417246 |
| N | 3.62121623 | -1.44798174 | 1.25417483 |
| N | 3.62112674 | -1.25412361 | -1.44798738 |
| C | 2.55463932 | 1.73092936 | 3.61656289 |
| C | 2.52967722 | 1.26378431 | 2.29274682 |
| N | 1.38464553 | 0.70378237 | 1.79912470 |
| C | 0.20953740 | 1.17434074 | 3.83209916 |
| C | 1.37755858 | 1.70209202 | 4.35866425 |
| C | 2.55464127 | -1.73092979 | -3.61656111 |
| C | 2.52967851 | -1.26378478 | -2.29274499 |
| N | 1.38464657 | -0.70378277 | -1.79912344 |
| C | 0.20953939 | -1.17434160 | -3.83209849 |
| C | 1.37756100 | -1.70209243 | -4.35866314 |
| C | 2.55461628 | 3.61643202 | -1.73126595 |
| C | 2.52971740 | 2.29268211 | -1.26392991 |
| N | 1.38470486 | 1.79910394 | -0.70382791 |
| C | 0.20953891 | 3.83200481 | -1.17456365 |
| C | 1.37752344 | 4.35851721 | -1.70245152 |
| C | 2.55461716 | -3.61643307 | 1.73126679 |
| C | 2.52971763 | -2.29268294 | 1.26393139 |
| N | 1.38470506 | -1.79910470 | 0.70382929 |
| C | 0.20954018 | -3.83200685 | 1.17456407 |
| C | 1.37752482 | -4.35851895 | 1.70245192 |
| Ni | 5.86007986 | 0.00000058 | 0.00000151 |
| Ni | 3.61938186 | -0.00000067 | 0.00000120 |
| C | 0.23170794 | 0.61652726 | 2.53655679 |
| C | 0.23170917 | -0.61652868 | -2.53655590 |

| | | | |
|---|---|---|---|
| C | 0.23174733 | 2.53652016 | -0.61661978 |
| C | 0.23174809 | -2.53652198 | 0.61662073 |
| N | -0.84280504 | 0.04088812 | 1.91459863 |
| N | -0.84275516 | 1.91459440 | -0.04090779 |
| N | -0.84275481 | -1.91459713 | 0.04090864 |
| N | -0.84280459 | -0.04089101 | -1.91459771 |
| C | -1.90247855 | -1.00125604 | 3.88005598 |
| C | -1.92926618 | -0.50154950 | 2.56698658 |
| N | -3.07696084 | -0.61386194 | 1.83134040 |
| C | -4.24813090 | -1.56554253 | 3.69032908 |
| C | -3.07711766 | -1.50309696 | 4.43017618 |
| C | -1.90247744 | 1.00125383 | -3.88005495 |
| C | -1.92926526 | 0.50154761 | -2.56698543 |
| N | -3.07695979 | 0.61386111 | -1.83133914 |
| C | -4.24812969 | 1.56554088 | -3.69032833 |
| C | -3.07711633 | 1.50309504 | -4.43017528 |
| C | -1.90247419 | 3.88010013 | 1.00109722 |
| C | -1.92923636 | 2.56699642 | 0.50147957 |
| N | -3.07692653 | 1.83134139 | 0.61384074 |
| C | -4.24811662 | 3.69035968 | 1.56543665 |
| C | -3.07711717 | 4.43022506 | 1.50292521 |
| C | -1.90247469 | -3.88010241 | -1.00109531 |
| C | -1.92923657 | -2.56699847 | -0.50147823 |
| N | -3.07692637 | -1.83134259 | -0.61383959 |
| C | -4.24811666 | -3.69036147 | -1.56543533 |
| C | -3.07711758 | -4.43022731 | -1.50292341 |
| Ni | 1.38388852 | 0.00000041 | 0.00000061 |
| Ni | -0.84706786 | -0.00000235 | 0.00000028 |
| C | -4.22764655 | -1.15651028 | 2.34141621 |
| C | -4.22764556 | 1.15650883 | -2.34141542 |
| C | -4.22762036 | 2.34142847 | 1.15646755 |
| C | -4.22762007 | -2.34143017 | -1.15646658 |
| N | -5.30548331 | -1.19535070 | 1.49631874 |
| N | -5.30545532 | 1.49632280 | 1.19534247 |
| N | -5.30545527 | -1.49632488 | -1.19534214 |
| N | -5.30548273 | 1.19534846 | -1.49631832 |
| C | -6.36041165 | -3.26145512 | 2.32715137 |
| C | -6.38858944 | -2.03208666 | 1.64511322 |
| N | -7.53798624 | -1.64656974 | 1.01039907 |
| C | -8.70501342 | -3.57560437 | 1.81686359 |
| C | -7.53217995 | -4.00305111 | 2.42215479 |
| C | -6.36040895 | 3.26145470 | -2.32714921 |
| C | -6.38858796 | 2.03208573 | -1.64511199 |
| N | -7.53798518 | 1.64656967 | -1.01039811 |
| C | -8.70501078 | 3.57560531 | -1.81686226 |
| C | -7.53217667 | 4.00305157 | -2.42215264 |
| C | -6.36040705 | 2.32722148 | 3.26140792 |
| C | -6.38857182 | 1.64514022 | 2.03206298 |

| | | | |
|---|---|---|---|
| N | -7.53796703 | 1.01040698 | 1.64656231 |
| C | -8.70500416 | 1.81691337 | 3.57557280 |
| C | -7.53217741 | 2.42223271 | 4.00299981 |
| C | -6.36040811 | -2.32722409 | -3.26140659 |
| C | -6.38857214 | -1.64514192 | -2.03206214 |
| N | -7.53796666 | -1.01040727 | -1.64656155 |
| C | -8.70500464 | -1.81691381 | -3.57557178 |
| C | -7.53217852 | -2.42223455 | -4.00299849 |
| Ni | -3.07907891 | 0.00000046 | 0.00000089 |
| Ni | -5.30949675 | -0.00000183 | -0.00000014 |
| C | -8.68634225 | -2.39220510 | 1.05249491 |
| C | -8.68634077 | 2.39220569 | -1.05249410 |
| C | -8.68632706 | 1.05251514 | 2.39219306 |
| C | -8.68632680 | -1.05251514 | -2.39219232 |
| N | -9.76808358 | -1.87673274 | 0.38584782 |
| N | -9.76806792 | 0.38585308 | 1.87673208 |
| N | -9.76806733 | -0.38585224 | -1.87673184 |
| N | -9.76808257 | 1.87673350 | -0.38584769 |
| C | -10.81654225 | -3.99099956 | -0.32730248 |
| C | -10.84692830 | -2.61312497 | -0.04255836 |
| N | -11.99886869 | -1.91146109 | -0.27286862 |
| C | -13.15767738 | -3.89997677 | -0.93464942 |
| C | -11.98256760 | -4.61656748 | -0.75157046 |
| C | -10.81654146 | 3.99100040 | 0.32730233 |
| C | -10.84692734 | 2.61312592 | 0.04255792 |
| N | -11.99886784 | 1.91146207 | 0.27286765 |
| C | -13.15767685 | 3.89997748 | 0.93464847 |
| C | -11.98256707 | 4.61656817 | 0.75157006 |
| C | -10.81654040 | -0.32725686 | 3.99100583 |
| C | -10.84691845 | -0.04253765 | 2.61312574 |
| N | -11.99885768 | -0.27286085 | 1.91146120 |
| C | -13.15767400 | -0.93461276 | 3.89998187 |
| C | -11.98256786 | -0.75151770 | 4.61657481 |
| C | -10.81653807 | 0.32725890 | -3.99100582 |
| C | -10.84691729 | 0.04253917 | -2.61312592 |
| N | -11.99885684 | 0.27286245 | -1.91146200 |
| C | -13.15767124 | 0.93461664 | -3.89998298 |
| C | -11.98256485 | 0.75152111 | -4.61657525 |
| Ni | -7.54231941 | 0.00000035 | 0.00000061 |
| Ni | -9.77657624 | 0.00000023 | -0.00000002 |
| C | -13.14159415 | -2.50738103 | -0.72916773 |
| C | -13.14159362 | 2.50738170 | 0.72916642 |
| C | -13.14158579 | -0.72915170 | 2.50738334 |
| C | -13.14158441 | 0.72915418 | -2.50738456 |
| N | -14.22961237 | -1.68856960 | -0.88841125 |
| N | -14.22960263 | -0.88840661 | 1.68857042 |
| N | -14.22960168 | 0.88840827 | -1.68857230 |
| N | -14.22961168 | 1.68857022 | 0.88840902 |

| | | | |
|---|---|---|---|
| C | -15.16361704 | -2.71532289 | -2.91832864 |
| C | -15.26555134 | -1.92555105 | -1.74903698 |
| N | -16.43900893 | -1.27036362 | -1.49388729 |
| C | -17.44227481 | -2.17589124 | -3.47443579 |
| C | -16.24551051 | -2.83842251 | -3.77006187 |
| C | -15.16361603 | 2.71532162 | 2.91832742 |
| C | -15.26555060 | 1.92555110 | 1.74903502 |
| N | -16.43900845 | 1.27036481 | 1.49388424 |
| C | -17.44227602 | 2.17589551 | 3.47443058 |
| C | -16.24551045 | 2.83842314 | 3.77005924 |
| C | -15.16361222 | -2.91830958 | 2.71534579 |
| C | -15.26554362 | -1.74902757 | 1.92555929 |
| N | -16.43900036 | -1.49388431 | 1.27036625 |
| C | -17.44226846 | -3.47442266 | 2.17591464 |
| C | -16.24550617 | -3.77004112 | 2.83845285 |
| C | -15.16361286 | 2.91831108 | -2.71534733 |
| C | -15.26554330 | 1.74902830 | -1.92556189 |
| N | -16.43900046 | 1.49388312 | -1.27037084 |
| C | -17.44227100 | 3.47442028 | -2.17591846 |
| C | -16.24550818 | 3.77004091 | -2.83845474 |
| Ni | -12.01967340 | 0.00000077 | -0.00000031 |
| Ni | -14.28199959 | 0.00000020 | -0.00000090 |
| Ni | -16.63141010 | -0.00000047 | -0.00000156 |
| C | -17.48685063 | 1.39312790 | 2.33386788 |
| C | -17.48684127 | -2.33386888 | 1.39313400 |
| C | -17.48684291 | 2.33386574 | -1.39313878 |
| C | -17.48684963 | -1.39312337 | -2.33387339 |
| C | 14.29866238 | 2.05339179 | -2.48927309 |
| C | 13.68396263 | 2.36703039 | -1.27815482 |
| C | 15.54728235 | 2.62200856 | -2.76578692 |
| C | 13.68834580 | 1.04781491 | -3.44664764 |
| C | 14.29185208 | 3.20739021 | -0.33506208 |
| O | 12.45401373 | 1.76750352 | -0.99747405 |
| C | 16.18593991 | 3.48224165 | -1.87177583 |
| C | 14.28245791 | -0.32957294 | -3.20057958 |
| C | 15.52965090 | 3.75913637 | -0.66458189 |
| C | 13.70830160 | 3.45112196 | 1.04747216 |
| C | 17.56073203 | 4.10168457 | -2.15170358 |
| C | 13.68388304 | -1.27600086 | -2.36415962 |
| C | 15.53002175 | -0.64198759 | -3.75223748 |
| C | 14.31226096 | 2.48464438 | 2.04888599 |
| C | 17.43252540 | 5.64005478 | -2.17341568 |
| C | 18.14119476 | 3.64138294 | -3.49889608 |
| C | 18.54056943 | 3.68124100 | -1.03399246 |
| C | 14.31226223 | -2.48464003 | -2.04888478 |
| O | 12.45065557 | -1.00918431 | -1.76500233 |
| C | 13.68388145 | 1.27600577 | 2.36416262 |
| C | 15.56035985 | 2.74284643 | 2.61563158 |

| | | | |
|---|---|---|---|
| C | 15.56036022 | -2.74284233 | -2.61563259 |
| C | 13.70830361 | -3.45111903 | -1.04747158 |
| C | 14.28245897 | 0.32957632 | 3.20057894 |
| O | 12.45065303 | 1.00919002 | 1.76500678 |
| C | 16.19529338 | 1.83836939 | 3.47569478 |
| C | 14.29185335 | -3.20738817 | 0.33506342 |
| C | 15.53002545 | 0.64198926 | 3.75223224 |
| C | 13.68834628 | -1.04781107 | 3.44664785 |
| C | 17.57837147 | 2.17113914 | 4.04911681 |
| C | 13.68396384 | -2.36702705 | 1.27815531 |
| C | 15.52965048 | -3.75913699 | 0.66458578 |
| C | 14.29866249 | -2.05338878 | 2.48927412 |
| C | 18.11998438 | 1.04833156 | 4.94900391 |
| C | 17.48924363 | 3.46653902 | 4.88409197 |
| C | 18.56890280 | 2.37612557 | 2.88164432 |
| O | 12.45401531 | -1.76749989 | 0.99747387 |
| C | 16.18593790 | -3.48224309 | 1.87178104 |
| C | 15.54728065 | -2.62200805 | 2.76579025 |
| C | 17.56072611 | -4.10169190 | 2.15171535 |
| C | 17.43251350 | -5.64006177 | 2.17342067 |
| C | 18.14118026 | -3.64139745 | 3.49891396 |
| C | 18.54057404 | -3.68124764 | 1.03401379 |
| C | 16.19529354 | -1.83836443 | -3.47569519 |
| C | 17.57835829 | -2.17114415 | -4.04914418 |
| C | 18.56893524 | -2.37608573 | -2.88170178 |
| C | 17.48920584 | -3.46657219 | -4.88407210 |
| C | 18.11993385 | -1.04836281 | -4.94908637 |
| Cl | -19.39558752 | -0.00000160 | -0.00000003 |
| H | 12.16681960 | 4.30677402 | -1.86863649 |
| H | 8.04639005 | 4.42677988 | -0.58980404 |
| H | 9.98369241 | 5.53966779 | -1.66326673 |
| H | 12.16682230 | -4.30677038 | 1.86863806 |
| H | 8.04639201 | -4.42677785 | 0.58980836 |
| H | 9.98369542 | -5.53966467 | 1.66326987 |
| H | 12.16230075 | -1.88116769 | -4.30329815 |
| H | 8.04532985 | -0.59105696 | -4.42642685 |
| H | 9.97992779 | -1.67126009 | -5.53735778 |
| H | 12.16229561 | 1.88117724 | 4.30330209 |
| H | 8.04532662 | 0.59106039 | 4.42643030 |
| H | 9.97992255 | 1.67126774 | 5.53736079 |
| H | 7.92819805 | 4.22295137 | 1.70727840 |
| H | 3.73957116 | 3.74002965 | 2.58019199 |
| H | 5.81661371 | 5.08765116 | 2.70748044 |
| H | 7.92820054 | -4.22294944 | -1.70727445 |
| H | 3.73957385 | -3.74002991 | -2.58019009 |
| H | 5.81661731 | -5.08765028 | -2.70747762 |
| H | 7.92817641 | 1.70649093 | -4.22335283 |
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| H | 1.37422009 | 2.10189401 | 5.36882382 |
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| H | -3.07734737 | -1.85172786 | 5.45919232 |
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| H | -0.97794271 | 4.43926240 | 0.99935185 |
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| H | -0.97794329 | -4.43926480 | -0.99934951 |
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| H | 16.79386186 | 3.34412114 | 5.72034949 |

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| C | 19.00717560 | 1.30051564 | 4.53736078 |
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| N | 14.78737329 | 1.68808603 | 0.93821789 |
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| C | 15.94141293 | -2.43084233 | -0.94863359 |
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| C | 15.92830933 | -0.94542890 | 2.43914020 |
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| Ni | 17.07133473 | 0.00878351 | 0.00547356 |
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| C | 9.18653604 | -0.62729698 | -2.55018862 |
| C | 9.17371900 | 2.52231780 | -0.62688155 |
| C | 9.18423946 | -2.55188978 | 0.59961675 |
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| N | 8.10880524 | -0.05729006 | -1.92956379 |
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| C | 4.72262369 | 1.13717563 | -2.35849977 |
| C | 4.71352608 | 2.31552249 | 1.14093128 |
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| N | 3.64415042 | 1.17132191 | -1.51478870 |
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| C | 2.55663566 | -2.06274542 | 1.62060101 |
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| N | 1.41359645 | 1.62621743 | -1.02270666 |
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| N | 1.40837271 | 0.98078113 | 1.62977664 |
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| C | 0.26027721 | -2.42145422 | 1.02155106 |
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| C | -1.89615534 | 2.58610138 | 0.03315992 |
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| C | -1.87399877 | -0.35213152 | 3.97304551 |
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| N | -3.04994282 | -0.31810293 | 1.89014923 |
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| C | -1.87478399 | 0.29071675 | -4.01607040 |
| C | -1.89933994 | 0.02603402 | -2.63499467 |

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| C | -3.04748981 | 0.69503895 | -4.64267923 |
| Ni | 1.40965088 | -0.01535008 | -0.01461355 |
| Ni | -0.81919765 | -0.03873253 | -0.02880498 |
| C | -4.19963640 | -2.53038782 | -0.76419315 |
| C | -4.19528872 | 2.47807151 | 0.72262931 |
| C | -4.19933396 | -0.77005429 | 2.48320539 |
| C | -4.19545827 | 0.71690043 | -2.52479712 |
| N | -5.27859316 | -1.70486210 | -0.94856851 |
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| C | 22.62631596 | 2.39051707 | -1.26074116 |
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| O | 21.39743489 | 1.78790405 | -0.98291035 |
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| H | -27.19818191 | 3.16696945 | -3.46700144 |
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| H | -27.25344532 | 1.52691268 | 1.65763170 |
| H | -27.26659114 | -1.57767473 | 1.51170993 |
| H | -27.26049438 | 1.67278225 | -1.44673025 |
| H | -27.27365984 | -1.43148277 | -1.59278083 |
| C | -6.34409908 | -2.87581436 | -2.83445621 |
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| C | -6.33636663 | -2.84386781 | 2.83025729 |
| H | -5.41143222 | -3.12523800 | 3.31264146 |

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## Author Contributions

H. P. figured out the conception of metal-backboned polymer and directed all aspects of the project. H. P., G. W. and K. Z. designed the experiments. K. Z. and Y. Y. performed the experiments on the syntheses, characterizations, theoretical calculations and property studies and contributed equally to this work. Y. X. carried out Cryo-TEM measurements. W. T. provided guidance on the theoretical calculations. J. X., N. W., J. X., Y. Z., Y. W. and all other authors discussed the data and wrote the paper.