Chemistry–A European Journal

Supporting Information

Manifold-Fused Porphyrin-Nanographene Conjugates

Christoph Oleszak, Christian L. Ritterhoff, Max M. Martin, Bernd Meyer,* and Norbert Jux*

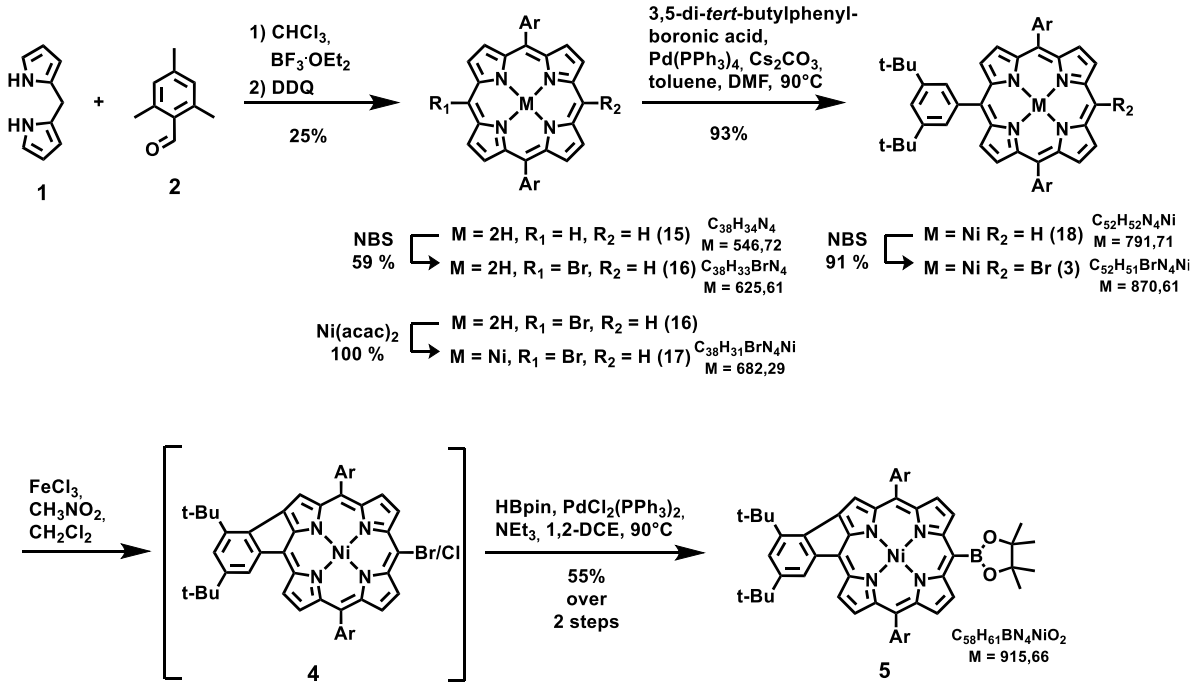
Table of Content

1 General Information

All chemicals were purchased from Sigma-Aldrich and used without any further purification. Solvents were distilled prior to usage. Dichloromethane was neutralized with K_2CO_3 before distillation. Thin layer chromatography (TLC) was performed on Merck silica gel 60 F524, detected by UV-light (254 nm, 366 nm). Column chromatography and flash column chromatography were performed on Macherey-Nagel silica gel 60 M (deactivated, 230−400 mesh, 0.04−0.063 mm). NMR spectroscopy was performed on Bruker Avance Neo Cryo-Probe DCH (^{1}H: 600 MHz, ^{13}C: 150 MHz), Bruker Avance Neo 500 (^{1}H: 500 MHz, ^{13}C: 126 MHz) and Bruker Avance 400 (^{1}H: 400 MHz, ^{13}C{^{1}H}: 101 MHz). Deuterated solvents were purchased from Sigma-Aldrich and used as received. Chemical shifts are referenced to residual protic impurities in the solvents (^{1}H: $CHCl_3$: 7.24 ppm) and (^{1}H: CH_2Cl_2: 5.32 ppm) or the deuterated solvent itself (^{13}C{^{1}H}: $CDCl_3$: 77.0 ppm) and (^{13}C{^{1}H}: CD_2Cl_2: 53.8 ppm). The resonance multiplicities are indicated as “s” (singlet), “d” (doublet), “t” (triplet), “q” (quartet) and “m” (multiplet). Signals referred to as “bs” (broad singlet) are not clearly resolved or significantly broadened. IR spectra were recorded on a Bruker FT-IR Tensor 27 spectrometer with a Pike MIRacle ATR unit. LDI/MALDI-ToF mass spectrometry was performed on a Bruker Ultraflex Extreme machine. In case of MALDI, the following matrix were used: 2,5-dihydroxybenzoic acid (DHB) or trans-2-[3-(4-*tert*-butylphenyl)-2-methyl-2propenyl-idene]malononitrile (DCTB). High resolution mass spectrometry was performed on a ESI/APPI-ToF mass spectrometer Bruker maXis 4G UHR MS/MS spectrometer, a Bruker micrOTOF II focus TOF MSspectrometer, or on a MALDI-ToF Bruker Ultraflex Extreme spectrometer. Microwave reactions were carried out in a monomode microwave reactor Biotage Initiator+ with an external IR surface temperature sensor. The microwave assisted reactions were carried out exclusively in the fixed hold time mode using an external IR temperature sensor. UV/vis spectroscopy was carried out on a Varian Cary 5000 UV−vis−NIR spectrometer.

2 Synthetic Procedures

2.1 Synthesis of Phenyl-Fused Porphyrin-Precursor



Scheme S1. Synthesis of phenyl-fused porphyrin building block **5**. Ar = mesityl.

5,15-Dimesitylporphyrin 15

Adapting a procedure from Chen *et al.*[1], Ethanol (4.5 mL) stabilized $CHCl_3$ (600 mL) was degassed for 15 min (bubbling N_2 through the solution). Dipyrromethane **1** (890 mg, 6.00 mmol, 1 equiv) and mesitaldehyde **2** (885 µL, 6.00 mmol, 1 equiv) were added to the solution, and the reaction was degassed for another 10 min. $BF_3{\cdot}OEt_2$ (500 µL) was added, and the solution was stirred for 3 h at rt under the exclusion of light. DDQ (2.04 g, 9.00 mmol, 3 equiv) was added, and the mixture was stirred for a further 30 min. The acid was quenched via the addition of NEt_3 (8 mL), and the solvent was removed under reduced pressure. The crude was purified by filtration through silica (SiO_2, hexanes/CH_2Cl_2, 1:1, Ø 13 x 8 cm). The product **15** was obtained as a purple crystalline solid in 25% yield (407 mg, 744 µmol).

^{1}H NMR (400 MHz, CD_2Cl_2, rt): δ [ppm]: 10.25 (s, 2H), 9.37 (d, *J* = 4.6 Hz, 4H), 8.86 (d, *J* = 4.6 Hz, 4H), 7.35 (s, 4H), 2.66 (s, 6H), 1.84 (s, 12H), -3.13 (s, 2H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 139.34, 138.00, 137.47, 131.85, 129.92, 127.80, 117.31, 104.45, 21.36, 21.19.

HRMS (MALDI, DCTB) for $C_{38}H_{34}N_4$ (M^+), calcd.: 546.2778, found: 546.2793.

Nickel-5,15-Dimesityl-10-Bromoporphyrin 17

Adapting a procedure from Mishra *et al*.[2], 5,15-Dimesitylporphyrin **15** (410 mg, 750 µmol, 1 equiv) was dissolved in $CHCl_3$ (200 mL) and pyridine (320 µL). The mixture was cooled to 0 °C, and NBS (133 mg, 750 µmol, 1 equiv) was added. After stirring for 25 min, the reaction was quenched with acetone (10 mL). The solution was washed with H_2O (100 mL) and subsequently dried over Na_2SO_4. The crude was separated by column chromatography (SiO_2, hexanes/CH_2Cl_2, 3:1, Ø 10 x 30 cm, 2nd band). The product was obtained as a purple crystalline solid in 59% yield (278 mg, 444 µmol). 5,15-Dimesityl-10-Bromoporphyrin **16** (226 mg, 361 µmol, 1 equiv) and $Ni(acac)_2$ (464 mg, 1.81 mmol, 5 equiv) were dissolved in toluene (40 mL). The mixture was heated to reflux for 6 h (heat-on temperature: 140 °C). The solvent was removed under reduced pressure, and the crude was purified by silica plug filtration (SiO_2, CH_2Cl_2, Ø 3.5 cm x 12 cm). After removal of the solvent, the residue was dissolved in CH_2Cl_2 (10 mL), and the product precipitated with MeOH (50 mL). The precipitate was filtered off and dried *in vacuo*. The product **17** was obtained as a red-brown solid in 100% yield (246 mg, 361 µmol).

^{1}H NMR (400 MHz, CD_2Cl_2, rt): δ [ppm]: 9.80 (s, 1H), 9.55 (d, *J* = 4.9 Hz, 2H), 9.10 (d, *J* = 4.8 Hz, 2H), 8.67 (dd, *J* = 4.9, 1.4 Hz, 4H), 7.26 (s, 4H), 2.59 (s, 6H), 1.78 (s, 12H).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2, rt): δ [ppm]: 143.45, 143.26, 142.85, 142.19, 138.86, 138.08, 136.72, 133.30, 132.94, 131.99, 131.85, 127.79, 117.69, 104.86, 21.12, 21.00.

UV/Vis (CH_2Cl_2): λ [nm] (ε [$M^{-1}cm^{-1}$]): 409 (150000), 523 (12000).

HRMS (MALDI, DCTB) for $C_{38}H_{31}N_4NiBr$ (M^+), calcd.: 680.1080, found:680.1041.

TLC: R_f [%]: 0.60 (hexanes/CH_2Cl_2 4:1).

Nickel-5,15-Dimesityl-10-(3,5-di-*tert*-butylphenyl)-Porphyrin 18

Nickel-5,15-Dimesityl-10-Bromoporphyrin **17** (260 mg, 382 µmol, 1 equiv), 3,5-di-*tert*-butylphenyl boronic acid (179 mg, 764 µmol, 2 equiv), Cs_2CO_3 (375 mg, 1.15 mmol, 3 equiv) and $Pd(PPh_3)_4$ (88 mg, 76 µmol, 0.2 equiv) were dissolved in toluene (20 mL) and DMF (10 mL) and were degassed. The reaction mixture was heated to 90 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure, and the crude was subjected to silica plug filtration (hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm). The product **18** was obtained in 93% yield (242 mg, 355 µmol).

^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.78 (s, 1H), 9.09 (d, *J* = 4.7 Hz, 2H), 8.77 (d, *J* = 4.9, 2H), 8.71 (d, *J* = 4.7 Hz, 2H), 8.62 (d, *J* = 4.9, 2H), 7.91 (d, *J* = 1.8, 1H), 7.72 (m, 1H), 7.20 (s, 4H), 2.57 (s, 6H), 1.80 (s, 12H), 1.46 (s, 18H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 148.80, 142.87, 142.81, 142.67, 142.49, 140.23, 139.08, 137.66, 137.42, 132.75, 132.34, 131.40, 130.79, 129.00, 127.74, 121.00, 120.42, 116.92, 104.10, 35.03, 31.70, 21.43, 21.40.

UV/Vis (CH_2Cl_2): *λ* [nm] (ε [$M^{-1}cm^{-1}$]): 408 (225000), 521 (16000).

HRMS (MALDI, DCTB) for $C_{52}H_{52}N_4Ni$ (M^+), calcd.: 790.3540, found: 790.3911.

TLC: R_f [%]: 0.70 (hexanes/CH_2Cl_2 3:1).

Nickel-5,15-Dimesityl-10-(3,5-di-*tert*-butylphenyl)-20-Bromoporphyrin 3

To a solution of $CHCl_3$ (25 mL), pyridine (600 µL) and Nickel-5,15-Dimesityl-10-(3,5-di-*tert*-butylphenyl)-porphyrin **18** (300 mg, 380 µmol, 1 equiv) NBS (68 mg, 380 µmol, 1 equiv) in $CHCl_3$ (7.5 mL) was added slowly at rt. The mixture was stirred for 15 min at rt before the reaction was quenched with acetone (8 mL). The solvents were removed under reduced pressure and the crude was purified by silica plug filtration (hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm). The product **3** was obtained as a dark-orange solid in 91% yield (301 mg, 346 µmol).

^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.47 (d, *J* = 4.9 Hz, 2H), 8.70 (d, *J* = 4.9 Hz, 2H), 8.63 (d, *J* = 4.9 Hz, 2H), 8.53 (d, *J* = 4.9 Hz, 2H), 7.86 (d, *J* = 1.8 Hz, 2H), 7.70 (t, *J* = 1.9 Hz, 1H), 7.20 (s, 4H), 2.56 (s, 6H), 1.80 (s, 12H), 1.45 (s, 18H).

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 148.95, 143.42, 142.88, 142.67, 142.36, 139.68, 138.95, 137.80, 136.91, 133.34, 133.20, 132.17, 131.42, 128.80, 127.77, 121.13, 120.61, 117.81, 101.68, 35.00, 31.65, 21.38, 21.34.

UV/Vis (CH_2Cl_2): λ [nm] (ε [$M^{-1}cm^{-1}$]): 417 (180000), 531 (13000).

HRMS (MALDI, DCTB) for $C_{52}H_{51}BrN_4Ni$ (M^+), calcd.: 868.2645, found: 868.2879.

TLC: R_f [%]: 0.80 (hexanes/CH_2Cl_2 3:1).

Fused Nickel-5,15-Dimesityl-10-(3,5-di-*tert*-butylphenyl)-20-Boronic-Ester-Porphyrin 5

A 20 mL vial was filled with a solution of Nickel-5,15-Dimesityl-10-(3,5-di-*tert*-butylphenyl)-20-bromoporphyrin **3** (100 mg, 115 µmol, 1 equiv) in CH_2Cl_2 (20 mL) and cooled with an ice bath. The solution was degassed (bubbling N_2 through the solution for 15 min). The N_2 flow through the solution was increased, and a solution of dry $FeCl_3$ (149 mg, 920 µmol, 8 equiv) in CH_3NO_2 (0.5 mL) was added. The N_2 bubbling through the solution was stopped 15 min after $FeCl_3$ was added, and the solution was stirred under slow warming to rt for 24 h. MeOH (10 mL) was added to quench the reaction. After adding NEt_3 (1 mL), the solvent was removed, and the crude was purified by filtration through silica (SiO_2, hexanes/ CH_2Cl_2 - 1:1, Ø 3 x 12 cm). The obtained dark-green solid was used in the next step without further purification. The porphyrin mixture **4** from the previous step, $PdCl_2(PPh_3)_2$ (4.2 mg, 5.9 µmol, 0.05 equiv.) and NEt_3 (0.4 mL) were dissolved in dry 1,2 dichloroethane (10 mL) in a 20 mL microwave vial. The vial was sealed, and the reaction mixture was degassed before pinacolborane (142 µL, 983 µmol, 8.33 equiv) was added via a syringe. The reaction mixture was stirred for 18 h at 90 °C under the exclusion of light. The solvent was removed under reduced pressure, and the crude product was subjected to column chromatography (SiO_2, hexanes/CH_2Cl_2 - 4:1 → 2:1, Ø 7 x 25 cm, 3rd band). **5** was obtained in 55% yield across the two reaction steps (58 mg, 63 µmol).

^1H NMR (400 MHz, CD_2Cl_2, rt): δ [ppm]: 9.27 (d, *J* = 4.9 Hz, 1H), 9.21 (d, *J* = 4.9 Hz, 1H), 9.12 (d, *J* = 5.0 Hz, 1H), 8.45 (d, *J* = 4.9 Hz, 1H), 8.26 (d, *J* = 4.9 Hz, 2H), 7.97

(d, *J* = 1.7 Hz, 1H), 7.68 (s, 1H), 7.22 (d, *J* = 4.4 Hz, 4H), 7.04 (d, *J* = 1.6 Hz, 1H), 2.57 (s, 6H), 1.92 (s, 6H), 1.82 (s, 6H), 1.68 (s, 12H), 1.56 (s, 9H), 1.47 (s, 9H).

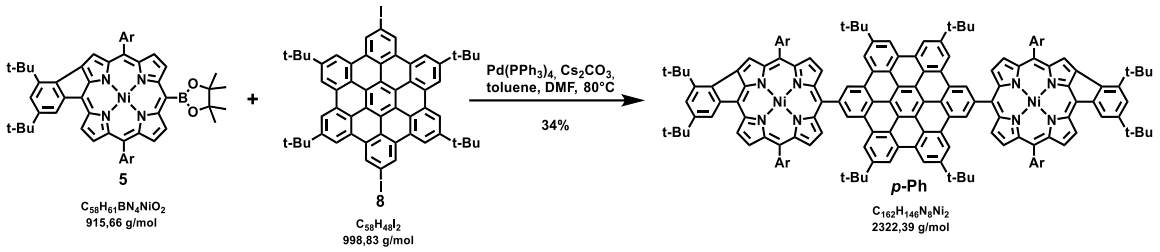
$^{13}C\{^{1}H\}$ NMR (151 MHz, CD_2Cl_2, rt): δ [ppm]: 153.88, 153.02, 150.91, 148.84, 147.77, 147.65, 147.17, 146.54, 145.26, 144.71, 144.17, 140.40, 139.16, 138.94, 138.27, 138.18, 137.42, 135.91, 134.52, 133.74, 133.46, 132.32, 131.38, 130.59, 128.12, 127.39, 126.27, 123.45, 121.50, 121.15, 117.85, 113.96, 85.51, 35.51, 35.32, 31.17, 29.01, 25.30, 21.53, 21.49, 21.46, 21.33.

UV/Vis (CH_2Cl_2): *λ* [nm] (ε [$M^{-1}cm^{-1}$]): 377 (39000),437 (93000), 572 (9000), 620 (6000)

HRMS (MALDI, DCTB) for $C_{58}H_{61}BN_4NiO_2$ (M^+), calcd.: 914.4236, found: 914.4227.

TLC: R_f [%] = 0.40 (hexanes/CH_2Cl_2 2:1).

2.2 Synthesis of Phenyl-Fused Porphyrin-HBC Conjugates



Scheme S2. Synthesis of *para*-Phenyl-Fused porphyrin ***p*-Ph**. Ar = mesityl.

Iodinated HBCs **6-9** were synthesized following the procedures given in [3].

para-Phenyl-Fused-Porphyrin *p*-Ph

Fused nickel-5,15-dimesityl-10-(3,5-di-*tert*-butylphenyl)-20-boronic ester-porphyrin **5** (15 mg, 17 µmol, 2.1 equiv), *para*-I-HBC **8** (8 mg, 8 µmol, 1 equiv), Cs_2CO_3 (9.8 mg, 24 µmol, 3 equiv) and $Pd(PPh_3)_4$ (1.8 mg, 1.6 µmol, 0.2 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure, and the crude was subjected to silica plug filtration (SiO_2, hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm) to remove the inorganics. The crude was further purified by size exclusion chromatography (Biobeads SX1, toluene, Ø 3 x 30 cm) followed by filtration through silica (SiO_2, hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm) to obtain ***p*-Ph** as a dark-green crystalline solid in 34% yield (6.4 mg, 2.8 µmol).

^{1}H NMR (601 MHz, CD_2Cl_2, rt): δ [ppm]: 9.93 (s, 4H), 9.42 (d, *J* = 1.6 Hz, 4H), 9.35 (d, *J* = 1.6 Hz, 4H), 9.18 (d, *J* = 5.0 Hz, 2H), 8.58 (d, *J* = 4.8 Hz, 2H), 8.54 (d, *J* = 4.8 Hz, 2H) 8.52 (d, *J* = 4.8 Hz, 2H), 8.24 (d, *J* = 4.9 Hz, 2H), 8.20 (d, *J* = 4.8 Hz, 2H), 8.03 (d, *J* = 1.6 Hz, 2H), 7.77 (s, 2H), 7.22 (d, *J* = 8.3 Hz, 8H), 7.08 (d, *J* = 1.7 Hz, 2H), 2.53 (d, J = 3.3 Hz, 12H), 2.00 (s, 12H), 1.91 (s, 12H), 1.65 (s, 36H), 1.61 (s, 18H), 1.51 (s,18H).

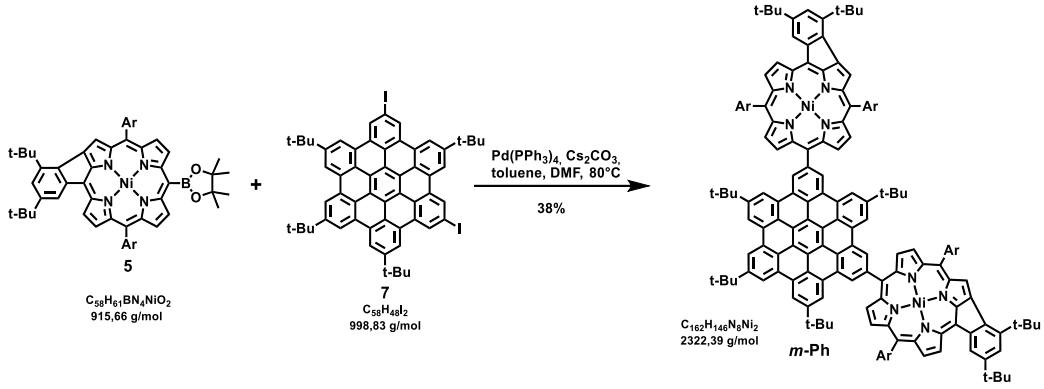
^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2, rt): δ [ppm]: 154.89, 153.24, 150.99, 150.27, 148.76, 147.99, 146.68, 146.06, 145.01, 144.66, 144.51, 141.31, 139.85, 139.13, 138.90, 138.36, 138.26, 135.82, 134.08, 133.85, 133.43, 131.78, 130.95, 130.88, 130.21, 130.02, 128.19, 128.17, 127.40, 126.94, 126.72, 124.57, 123.36, 122.84, 122.26,

121.56, 121.35, 121.04, 120.28, 120.06, 118.45, 113.20, 54.19, 54.01, 53.90, 31.96, 31.21, 29.02, 21.53, 21.48, 21.45, 21.39, 14.25, 1.13.

UV/Vis (CH_2Cl_2): λ [nm] (ε [$M^{-1}cm^{-1}$]): 360 (120000), 453 (180000), 475 (180000), 572 (20000).

HRMS (MALDI, DCTB) for $C_{182}H_{148}N_8Ni_2$ (M^+), calcd.: 2319.0372, found: 2319.0335.

TLC: R_f [%]: 0.40 (hexanes/CH_2Cl_2 4:1).



Scheme S3. Synthesis of *meta*-Phenyl-Fused porphyrin ***m*-Ph**. Ar = mesityl.

meta-Phenyl-Fused-Porphyrin *m*-Ph

Fused nickel-5,15-dimesityl-10-(3,5-di-*tert*-butylphenyl)-20-boronic ester-porphyrin **5** (15 mg, 17 µmol, 2.1 equiv), *meta*-I-HBC **7** (8 mg, 8 µmol, 1 equiv), Cs_2CO_3 (9.8 mg, 24 µmol, 3 equiv) and $Pd(PPh_3)_4$ (1.8 mg, 1.6 µmol, 0.2 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure, and the crude was subjected to silica plug filtration (SiO_2, hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm) to remove the inorganics. The crude was further purified by size exclusion chromatography (Biobeads SX1, toluene, Ø 3 x 30 cm) followed by filtration through silica (SiO_2, hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm) to obtain ***m*-Ph** as a dark-green crystalline solid in 38% yield (7.1 mg, 3.1 µmol).

^{1}H NMR (601 MHz, CD_2Cl_2, rt): δ [ppm]: δ 9.94 - 9.89 (m, 4H), 9.44 (m, 2H), 9.36 - 9.31 (m, 4H), 9.16 (d, *J* = 5.1 Hz, 2H), 8.57 (d, *J* = 4.9 Hz, 2H), 8.52 (d, *J* = 4.9 Hz, 2H), 8.51 (d, *J* = 4.9 Hz, 2H), 8.23 (d, *J* = 5.0 Hz, 2H), 8.19 (d, *J* = 4.9 Hz, 2H), 8.02

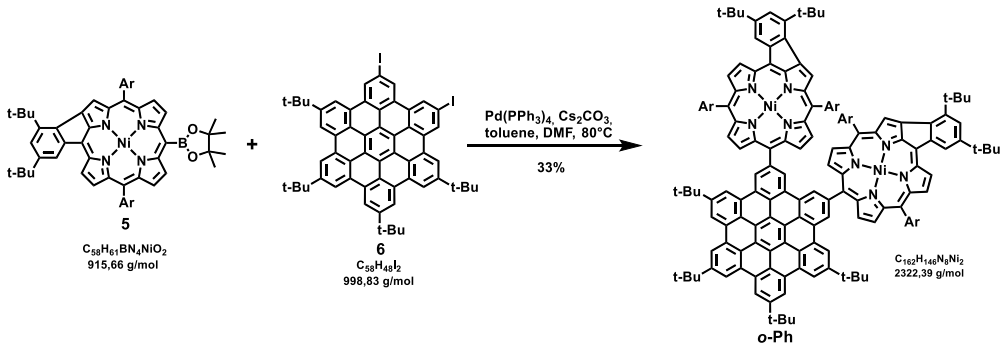
(d, *J* = 1.6 Hz, 2H), 7.75 (s, 2H), 7.20 (m, 8H), 7.07 (d, *J* = 1.6 Hz, 2H), 2.52 (m, 12H), 1.99 (m, 12H), 1.91 (m, 12H), 1.86 (s, 9H), 1.67 (s, 18H), 1.59 (s, 18H), 1.50 (s, 18H), 1.44 (s, 9H).

$^{13}C\{^1H\}$ NMR (151 MHz, CD_2Cl_2, rt): δ [ppm]: 154.85, 153.21, 150.96, 150.41, 150.33, 150.09, 148.72, 147.96, 146.65, 146.02, 144.98, 144.63, 144.49, 141.28, 139.75, 139.11, 138.87, 138.33, 138.23, 137.33, 135.79, 134.05, 133.82, 133.41, 131.75, 130.97, 130.92, 130.90, 130.69, 130.61, 130.18, 129.95, 129.90, 128.16, 127.37, 126.96, 126.91, 126.69, 125.76, 124.87, 124.49, 124.23, 123.33, 122.81, 122.23, 121.82, 121.76, 121.33, 121.06, 121.01, 120.54, 120.22, 120.06, 119.76, 118.42, 113.17, 32.07, 31.97, 31.84, 31.20, 29.01.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 360 (130000), 452 (190000), 475 (180000), 572 (20000)

HRMS (MALDI, DCTB) for $C_{182}H_{148}N_8Ni_2$ (M^+), calcd.: 2319.0372, found: 2319.0430.

TLC: R_f [%]: 0.40 (hexanes/CH_2Cl_2 4:1).



Scheme S4. Synthesis of *ortho*-Phenyl-Fused porphyrin ***o*-Ph**. Ar = mesityl.

ortho-Phenyl-Fused-Porphyrin *o*-Ph

Fused nickel-5,15-dimesityl-10-(3,5-di-*tert*-butylphenyl)-20-boronic ester-porphyrin **5** (19 mg, 21 µmol, 2.1 equiv), *ortho*-I-HBC **6** (10 mg, 10 µmol, 1 equiv), Cs_2CO_3 (9.8 mg, 24 µmol, 3 equiv) and $Pd(PPh_3)_4$ (1.8 mg, 1.6 µmol, 0.2 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure and the crude was subjected to silica plug filtration (SiO_2, hexanes/CH_2Cl_2 -

1:1, Ø 3 x 12 cm) to remove the inorganics. The crude was further purified by size exclusion chromatography (Biobeads SX1, toluene, Ø 3 x 30 cm) followed by filtration through silica (SiO_2, hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm) to obtain ***o*-Ph** as a dark-green crystalline solid in 33% yield (6.8 mg, 2.9 µmol).

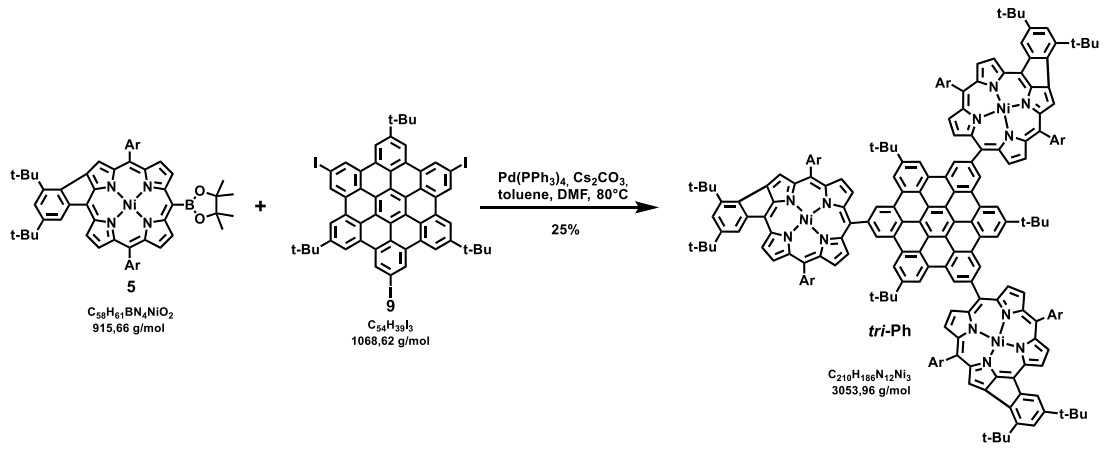
^{1}H NMR (601 MHz, CD_2Cl_2, rt): δ [ppm]: 9.91 (d, *J* = 1.4 Hz, 2H), 9.81 (d, *J* = 1.5 Hz, 2H), 9.47 - 9.42 (m, 6H), 9.33 (d, *J* = 1.7 Hz, 2H), 9.05 (d, *J* = 5.0 Hz, 2H), 8.49 (d, *J* = 4.9 Hz, 2H), 8.43 (d, *J* = 4.9 Hz, 2H), 8.40 (d, *J* = 4.9 Hz, 2H), 8.09 (d, *J* = 4.9 Hz, 2H), 8.06 (d, *J* = 4.9 Hz, 2H), 7.92 (d, *J* = 1.7 Hz, 2H), 7.63 (s, 2H), 7.17 - 7.13 (m, 4H), 7.08 (d, *J* = 6.2 Hz, 4H), 7.00 (d, *J* = 1.7 Hz, 2H), 2.49 (m, 12H), 1.92 (s, 6H), 1.88 (s, 18H), 1.82 (s, 6H), 1.72 (s, 6H), 1.66 (s, 18H), 1.62 (s, 6H), 1.52 (s, 18H), 1.44 (s, 18H).

^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2, rt): δ [ppm]: 154.74, 153.08, 150.87, 150.26, 150.18, 148.54, 147.82, 146.51, 145.86, 144.82, 144.47, 144.26, 144.25, 141.14, 139.80, 139.08, 138.98, 138.85, 138.75, 138.19, 138.09, 137.26, 135.72, 133.87, 133.57, 133.32, 131.50, 131.00, 130.93, 130.86, 130.61, 130.10, 129.99, 129.65, 128.04, 127.50, 127.39, 127.19, 126.53, 125.99, 124.56, 124.18, 123.22, 122.53, 122.07, 121.60, 121.54, 121.24, 120.90, 120.23, 120.10, 119.78, 119.72, 118.26, 113.00, 35.47, 35.30, 32.09, 31.95, 31.14, 30.05, 28.94, 21.44.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 367 (140000), 448 (160000), 472 (140000), 572 (16000).

HRMS (MALDI, DCTB) for $C_{182}H_{148}N_8Ni_2$ (M^+), calcd.: 2319.0372, found: 2319.0420.

TLC: R_f [%]: 0.40 (hexanes/CH_2Cl_2 4:1).



Scheme S5. Synthesis of *tri*-Phenyl-Fused porphyrin ***tri*-Ph**. Ar = mesityl.

tri-Phenyl-Fused-Porphyrin *tri*-Ph

Fused nickel-5,15-dimesityl-10-(3,5-di-*tert*-butylphenyl)-20-boronic-ester porphyrin **5** (18.9 mg, 20.6 µmol, 3.15 equiv), *tri*-I-HBC **9** (7.0 mg, 6.6 µmol, 1 equiv), Cs_2CO_3 (9.6 mg, 29.5 µmol, 4.5 equiv) and $Pd(PPh_3)_4$ (2.3 mg, 2.0 µmol, 0.3 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure, and the crude was subjected to silica plug filtration (SiO_2, hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm) to remove the inorganics. The crude was further purified by size exclusion chromatography (Biobeads SX1, toluene, Ø 3 x 30 cm) followed by filtration through silica (SiO_2, hexanes/CH_2Cl_2 - 1:1, Ø 3 x 12 cm) to obtain ***tri*-Ph** as a dark-green crystalline solid in 25% yield (4.9 mg, 1.6 µmol).

^{1}H NMR (601 MHz, CD_2Cl_2, rt): δ [ppm]: 9.96 (s, 6H), 9.38 (s, 6H), 9.17 (d, *J* = 5.1 Hz, 3H), 8.60 (d, *J* = 5.0 Hz, 3H), 8.54 - 8.52 (m, 6H), 8.25 (d, *J* = 5.0 Hz, 3H), 8.21 (d, *J* = 4.9 Hz, 3H), 8.02 (d, *J* = 1.7 Hz, 3H), 7.76 (s, 3H), 7.25 - 7.18 (m, 12H), 7.07 (d, *J* = 1.6 Hz, 3H), 2.53 (m, 18H), 1.99 (s, 18H), 1.90 (s, 18H), 1.59 (s, 27H), 1.47 - 1.50 (m, 54H).

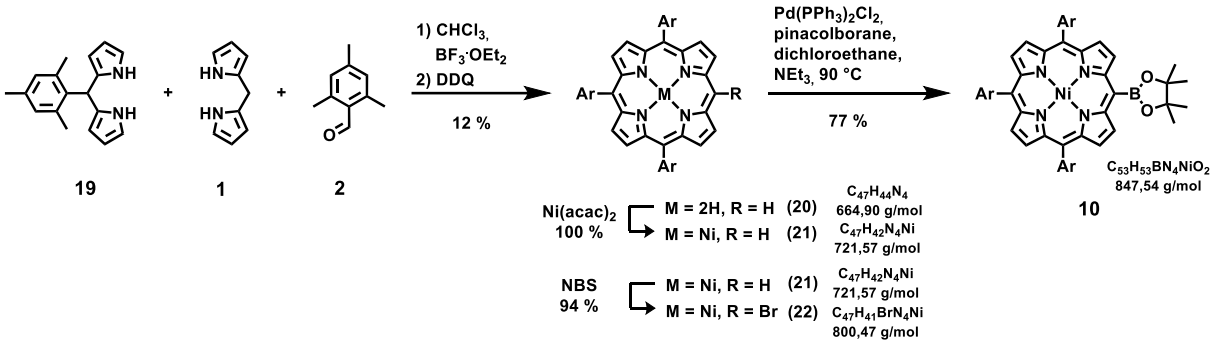
^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2, rt): δ [ppm]: 154.87, 153.22, 150.96, 150.65, 148.74, 147.97, 146.66, 146.04, 144.99, 144.65, 144.49, 144.48, 141.29, 139.91, 139.11, 138.88, 138.34, 138.24, 137.34, 135.80, 134.06, 133.83, 133.41, 131.75, 130.95, 130.76, 130.21, 130.00, 128.17, 127.38, 127.03, 126.70, 125.82, 124.87, 123.34, 122.75, 122.32, 122.25, 121.34, 121.02, 120.65, 118.44, 113.20, 31.86, 31.20, 29.01, 21.52, 21.38.

UV/Vis (CH_2Cl_2): *λ* [nm] (ε [$M^{-1}cm^{-1}$]): 360 (152000), 454 (319000), 475 (317000), 572 (33000).

HRMS (MALDI, DCTB) for $C_{182}H_{148}N_8Ni_2$ (M^+), calcd.: 3049.2978, found: 3049.2933.

TLC: R_f [%]: 0.30 (hexanes/CH_2Cl_2 3:1).

2.3 Synthesis of Trimesityl-Porphyrin Precursor



Scheme S6. Synthesis of Trimesityl-Porphyrin **10**. Ar = mesityl.

Nickel-5,10,15-Trimesitylporphyrin 21

Ethanol (2 mL) stabilized $CHCl_3$ (775 mL) was degassed for 20 min (bubbling N_2 through the solution). Dipyrromethane **1** (284 mg, 1.94 mmol, 1 equiv), mesitaldehyde **2** (572 µL, 3.88 mmol, 2 equiv) and mesityl-dipyrromethane **19*** (513 mg, 1.94 mmol, 1 equiv) were added to the solution and the reaction was stirred for 5 min at rt. $BF_3{\cdot}OEt_2$ (316 µL, 2.57 mmol, 0.66 equiv) was added, and the solution was stirred for 1 h at rt under the exclusion of light. DDQ (1.32 g, 5.81 mmol, 1.5 equiv) was added, and the mixture was stirred for a further 45 min. The acid was quenched via the addition of NEt_3 (3.6 mL), and the solvent was removed. The crude was purified by column chromatography (SiO_2, hexanes/CH_2Cl_2, 3:1, Ø 8 x 40 cm). The first isolated fraction contained both A_4-porphyrin and the target A_3B porphyrin, which were subsequently separated by a second column (SiO_2, hexanes/toluene, 3:1, Ø 8 x 40 cm, 2nd band). The product **20** was obtained as a purple solid. Free-base porphyrin **20** (125 mg, 188 µmol, 1 equiv) and $Ni(acac)_2$ (241 mg, 940 µmol, 5 equiv.) were dissolved in toluene (30 mL) and heated to reflux (heat-on temperature: 140 °C) for 5 h. The solvent was removed under reduced pressure, the product was poured over a plug (SiO_2, CH_2Cl_2, Ø 3 x 6 cm), and afterwards recryst. from CH_2Cl_2/MeOH yielding 12% of nickel-porphyrin **21** (136 mg, 188 µmol).

^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.79 (s, 1H), 9.07 (d, *J* = 4.8 Hz, 2H), 8.69 (d, *J* = 4.7 Hz, 2H), 8.57 (s, 4H), 7.22 (m, 6H), 2.56 (m, 9H), 1.79 (s, 18H).

^{13}C NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 142.93, 142.74, 142.59, 142.37, 139.11, 139.08, 137.88, 137.63, 137.59, 137.52, 137.44, 132.17, 131.24, 131.21, 131.15, 129.04, 128.23, 127.72, 127.69, 125.30, 117.32, 116.81, 104.26, 21.48, 21.39.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 407 (250000), 521 (18000), 553 (5000).

HRMS (MALDI, CH_2Cl_2) for $C_{47}H_{42}N_4Ni$ (M^+) calcd.: 720.2757, found: 720.2775.

TLC: R_f [%]: 0.74 (hexanes/CH_2Cl_2 - 2:1).

*Synthesized adapting a procedure from the literature [4].

Nickel-(5-Bromo)-10,15,20-Trimesitylporphyrin 22

To a solution of $CHCl_3$ (11 mL), pyridine (250 µL) and porphyrin **21** (130 mg, 180 µmol, 1 equiv) NBS (32 mg, 180 µmol, 1 equiv) in $CHCl_3$ (3 mL) was added slowly at rt. The mixture was stirred for 15 min at rt before the reaction was quenched with acetone (3 mL). The solvents were removed under reduced pressure, and the crude was purified by silica plug filtration (hexanes/CH_2Cl_2 - 2:1, Ø 3 x 12 cm). The product **22** was obtained as a dark-orange solid in 94% yield (135 mg, 169 µmol).

^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.46 (d, *J* = 5.0 Hz, 2H), 8.60 (d, *J* = 5.0 Hz, 2H), 8.48 (s, 4H), 7.19 - 7.17 (m, 6H), 2.55 (m, 9H), 1.79 (m, 18H).

^{13}C NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 143.04, 143.00, 142.76, 142.43, 139.00, 138.95, 137.80, 137.75, 136.94, 133.20, 132.03, 131.84, 131.80, 127.77, 117.71, 117.54, 101.91, 21.46, 21.37.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 415 (225000), 530 (17000).

HRMS (MALDI, CH_2Cl_2) for $C_{47}H_{41}BrN_4Ni$ (M^+) calcd.: 798.1863, found: 798.1853.

TLC: R_f [%]: 0.77 (hexanes/CH_2Cl_2 - 2:1).

Boronic-Ester-Porphyrin 10

Bromo-porphyrin **22** (135 mg, 169 µmol, 1 equiv), $PdCl_2(PPh_3)_2$ (6.0 mg, 8.5 µmol, 0.05 equiv.) and NEt_3 (0.5 mL) were dissolved in dry 1,2 dichloroethane (22 mL) in a 20 mL microwave vial. The vial was sealed, and the reaction mixture was degassed before pinacolborane (205 µL, 180 mg, 1.41 mmol, 8.33 equiv) was added via syringe. The reaction mixture was stirred for 2.5 h at 90 °C under exclusion of light. The solvent was removed under reduced pressure, and the crude product was subjected to column chromatography (SiO_2, hexanes/CH_2Cl_2 - 3:1, Ø 5 x 25 cm). The 3rd isolated band contained the pure product **10** in 77% (110 mg, 130 µmol).

^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.66 (d, *J* = 4.9 Hz, 2H), 8.65 (d, *J* = 4.8 Hz, 2H), 8.51 (d, *J* = 4.8 Hz, 2H), 8.48 (d, *J* = 4.8 Hz, 2H), 7.19 - 7.16 (m, 6H), 2.56 - 2.54 (m, 9H), 1.79 (m, 18H), 1.70 (s, 12H).

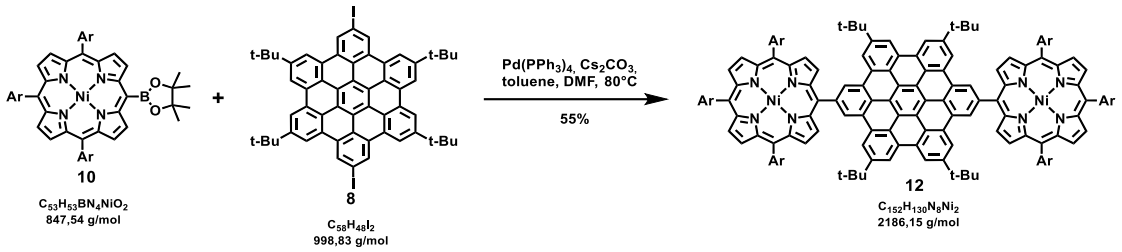
^{13}C NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 146.87, 142.79, 141.92, 141.71, 139.12, 139.03, 137.59, 137.54, 137.43, 137.29, 133.73, 131.84, 131.54, 130.84, 127.68, 118.19, 116.89, 25.21, 21.47, 21.42.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 412 (240000), 528 (16000), 561 (7000).

HRMS (MALDI, CH_2Cl_2) for $C_{53}H_{53}BN_4NiO_2$ (M^+) calcd.: 846.3615, found: 846.3601.

TLC: R_f [%]: 0.23 (hexanes/CH_2Cl_2 - 2:1).

2.4 Synthesis of Trimesityl-Porphyrin-HBC Conjugates



Scheme S7. Synthesis of *para*-bis-porphyrin-HBC **12**. Ar = mesityl.

para-Bis-Porphyrin-HBC 12

para-I-HBC **8** (21 mg, 21 µmol, 1 equiv), boronic-ester-porphyrin **10** (37 mg, 44 µmol, 2.1 equiv), Cs_2CO_3 (21 mg, 63 µmol, 3 equiv) and $Pd(PPh_3)_4$ (4.9 mg, 4.2 µmol, 0.2 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure, and the crude was subjected to silica plug filtration (cyclohexane/CH_2Cl_2 - 1:1, Ø 3 x 12 cm). Further purification was achieved by size exclusion chromatography (Biobeads SX1, toluene, Ø 3 x 30 cm, 1st band) followed by silica plug filtration (cyclohexane/CH_2Cl_2 - 2:1, Ø 3 x 10 cm). The pure product **12** was obtained in 55% yield (25 mg, 12 µmol).

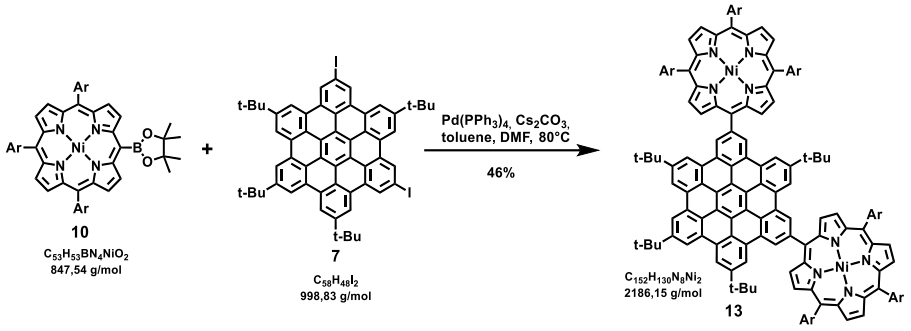
^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.96 (s, 4H), 9.36 (d, *J* = 2.0 Hz, 4H), 9.30 (d, *J* = 1.7 Hz, 4H), 8.95 (d, *J* = 4.8 Hz, 4H), 8.67 (d, *J* = 4.9 Hz, 4H), 8.62 (s, 8H), 7.24 - 7.19 (m, 12H), 2.62 (s, 6H), 2.57 (s, 12H), 1.94 - 1.93 (m, 36H), 1.68 (s, 36H).

^{13}C NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 149.12, 143.14, 142.45, 142.33, 139.67, 138.76, 138.73, 137.41, 137.17, 137.14, 132.76, 131.34, 131.15, 130.53, 130.28, 129.33, 127.77, 126.65, 125.28, 124.36, 123.15, 121.19, 121.00, 119.65, 119.35, 118.51, 117.24, 116.93, 35.39, 31.71, 31.23, 21.45, 21.40.

UV/Vis (CH_2Cl_2): λ [nm] (ε [$M^{-1}cm^{-1}$]): 357 (105000), 427 (393000), 528 (42800).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{130}N_8Ni_2$ (M^+) calcd.: 2182.9120, found: 2182.9134.

TLC: R_f [%]: 0.80 (hexanes/CH_2Cl_2 - 2:1).



Scheme S8. Synthesis of *meta*-bis-porphyrin-HBC **13**. Ar = mesityl.

meta-Bis-Porphyrin-HBC 13

meta-I-HBC **7** (20 mg, 20 µmol, 1 equiv), boronic-ester-porphyrin **10** (36 mg, 42 µmol, 2.1 equiv), Cs_2CO_3 (20 mg, 60 µmol, 3 equiv) and $Pd(PPh_3)_4$ (4.6 mg, 4.0 µmol, 0.2 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure, and the crude was subjected to silica plug filtration (cyclohexane/CH_2Cl_2 - 1:1, Ø 3 x 12 cm). Further purification was achieved by size exclusion chromatography (Biobeads SX1, toluene, Ø 3 x 30 cm, 1st band) followed by silica plug filtration (cyclohexane/CH_2Cl_2 - 2:1, Ø 3 x 10 cm). The pure product **13** was obtained in 46% yield (20 mg, 9.3 µmol).

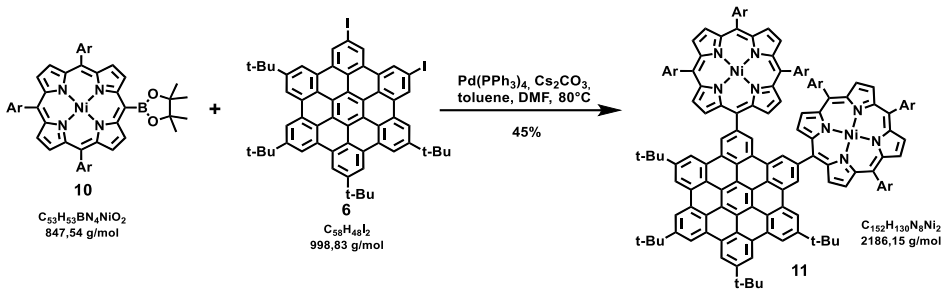
^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.99 (m, 4H), 9.40 (m, 4H), 9.35 - 9.27 (m, 4H), 8.96 (d, *J* = 5.0 Hz, 4H), 8.67 (d, *J* = 4.9 Hz, 4H), 8.60 (s, 8H), 7.21 (m, 12H), 2.56 (m, 18H), 1.88 (m, 36H).

^{13}C NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 149.70, 143.17, 142.71, 142.61, 139.67, 139.11, 139.08, 137.70, 137.28, 132.91, 131.66, 131.44, 130.69, 130.49, 130.42, 129.47, 127.80, 125.51, 124.45, 121.57, 120.86, 118.53, 117.43, 117.08, 32.08, 31.96, 31.82, 21.60, 21.49, 21.41.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 419 (410000), 529 (50000).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{130}N_8Ni_2$ (M^+) calcd.: 2182.9120, found: 2182.9111.

TLC: R_f [%]: 0.50 (hexanes/CH_2Cl_2 - 3:1).



Scheme S9. Synthesis of *ortho*-bis-porphyrin-HBC **13**. Ar = mesityl.

ortho-Bis-Porphyrin-HBC 11

ortho-I-HBC **6** (21 mg, 21 µmol, 1 equiv), boronic-ester-porphyrin **10** (37 mg, 44 µmol, 2.1 equiv), Cs_2CO_3 (21 mg, 63 µmol, 3 equiv) and $Pd(PPh_3)_4$ (4.9 mg, 4.2 µmol, 0.2 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure and the crude was subjected to silica plug filtration (cyclohexane/CH_2Cl_2 - 1:1, Ø 3 x 12 cm). Further purification was achieved by size exclusion chromatography (Biobeads SX1, toluene, Ø 3 x 30 cm, 1st band) followed by silica plug filtration (SiO_2, cyclohexane/CH_2Cl_2 - 3:1, Ø 3 x 12 cm). The pure product **11** was obtained in 45% yield (21 mg, 9.5 µmol).

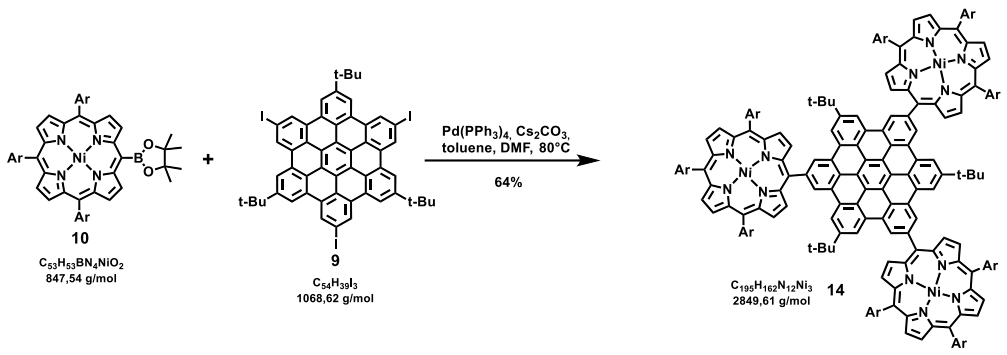
^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 9.91 (s, 4H), 9.41 - 9.33 (m, 6H), 9.25 (d, *J* = 1.7 Hz, 2H), 8.84 (d, *J* = 4.8 Hz, 4H), 8.48 (d, *J* = 5.0 Hz, 4H), 8.45 (s, 8H), 7.14 - 7.10 (m, 8H), 7.04 (s, 4H), 2.53 - 2.50 (m, 18H), 1.89 (s, 18H), 1.84 (s, 12H), 1.78 (s, 6H), 1.71 (s, 6H), 1.64 (s, 18H), 1.58 (s, 12H).

^{13}C NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 142.95, 142.25, 142.13, 142.11, 138.72, 137.32, 137.25, 137.14, 137.09, 132.56, 131.13, 131.04, 130.66, 130.58, 129.31, 127.64, 127.62, 127.22, 127.19, 125.65, 125.12, 124.74, 124.37, 123.97, 123.84, 121.19, 121.01, 119.40, 119.04, 118.28, 117.02, 116.69, 35.43, 31.90, 31.73, 27.05, 21.34, 21.19.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 358 (90000), 417 (365000), 528 (35000).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{130}N_8Ni_2$ (M^+) calcd.: 2182.9120, found: 2182.9085.

TLC: R_f [%]: 0.80 (hexanes/CH_2Cl_2 - 2:1).



Scheme S10. Synthesis of Tris-porphyrin-HBC **13**. Ar = mesityl.

Tris-Porphyrin-HBC 14

Tris-I-HBC **9** (20 mg, 19 µmol, 1 equiv), boronic-ester-porphyrin **10** (50 mg, 59 µmol, 3.15 equiv), Cs_2CO_3 (27 mg, 84 µmol, 4.5 equiv) and $Pd(PPh_3)_4$ (6.5 mg, 5.6 µmol, 0.3 equiv) were dissolved in toluene (2 mL) and DMF (1 mL) and were degassed. The reaction mixture was heated to 80 °C for 18 h. After cooling to rt, the solvent was removed under reduced pressure, and the crude was subjected to silica plug filtration (cyclohexane/CH_2Cl_2 - 1:1, Ø 3 x 12 cm). Further purification was achieved by size exclusion chromatography (bio-beads SX1, toluene, Ø 3 x 30 cm, 1st band) followed by silica plug filtration (cyclohexane/CH_2Cl_2 - 2:1, Ø 3 x 10 cm). The pure product **14** was obtained in 64% yield (34 mg, 12 µmol).

^{1}H NMR (400 MHz, $CDCl_3$, rt): δ [ppm]: 10.02 (s, 6H), 9.33 (s, 6H), 8.98 (d, *J* = 4.9 Hz, 6H), 8.67 (d, *J* = 5.0 Hz, 6H), 8.59 (s, 12H), 7.24 - 7.14 (m, 18H), 2.55 (m, 27H), 1.87 (m, 54H),

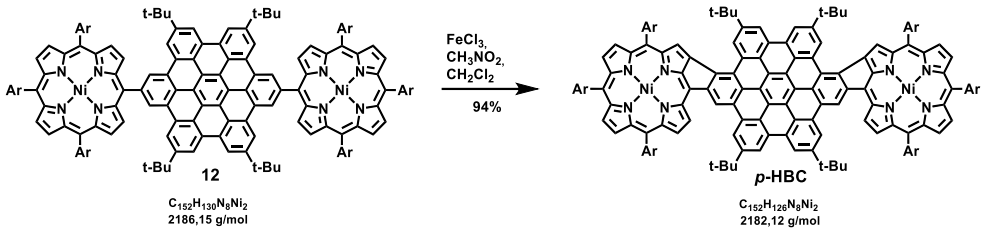
^{13}C NMR (101 MHz, $CDCl_3$, rt): δ [ppm]: 143.16, 142.62, 139.08, 137.70, 131.67, 131.47, 130.57, 127.79, 117.43, 31.83, 21.58, 21.48, 21.40.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 418 (610000), 528 (72000).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{130}N_8Ni_2$ (M^+) calcd.: 2845.1100, found: 2845.1126.

TLC: R_f [%]: 0.25 (hexanes/CH_2Cl_2 - 3:1).

2.5 Synthesis of HBC-Fused Porphyrin Conjugates



Scheme S11. Synthesis of fused *para*-bis-porphyrin-HBC ***p*-HBC**. Ar = mesityl.

Fused *para*-Bis-Porphyrin-HBC *p*-HBC

A 20 mL vial was filled with a solution of *para*-bis-porphyrin-HBC **12** (20 mg, 9.2 µmol, 1 equiv) in CH_2Cl_2 (10 mL) and cooled with an ice bath. The solution was degassed (bubbling N_2 through the solution for 15 min). The N_2 flow through the solution was increased and a solution of dry $FeCl_3$ (89 mg, 549 µmol, 60 equiv) in CH_3NO_2 (0.5 mL) was added. The N_2 bubbling through the solution was stopped 15 min after $FeCl_3$ was added and the solution was stirred under slow warming to rt for 24 h. MeOH (10 mL) was added to quench the reaction. After adding NEt_3 (1 mL) the solvent was removed and the crude was purified by a silica plug (hexanes/ CH_2Cl_2 - 1:1, Ø 3 x 8 cm). The product ***p*-HBC** was obtained as a purple-black solid in 94% yield (19 mg, 8.55 µmol).

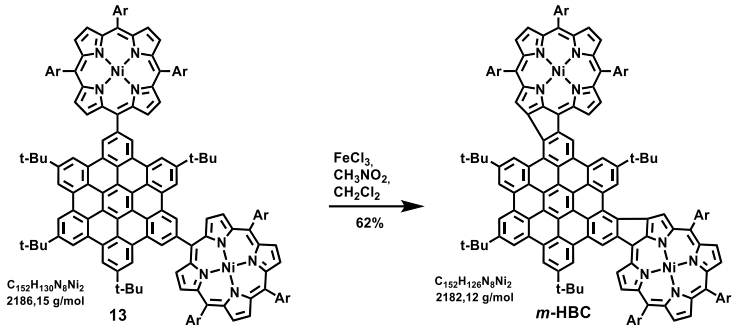
^{1}H NMR (500 MHz, CD_2Cl_2, rt): δ [ppm]: 9.86 (m, 4H), 9.61 (d, *J* = 5.0 Hz, 2H), 9.44 (s, 2H), 9.38 (s, 2H), 9.27 (s, 2H), 8.66 (d, *J* = 4.8 Hz, 2H), 8.48 (s, 2H), 8.25 - 8.15 (m, 6H), 8.13 (d, *J* = 4.8 Hz, 2H), 7.27 (s, 4H), 7.24 (s, 4H), 7.20 (s, 4H), 2.63 - 2.43 (m, 18H), 2.07 - 1.79 (m, 54H), 1.61 (s, 18H).

^{13}C NMR (126 MHz, CD_2Cl_2, rt): δ [ppm]: 156.15, 150.15, 149.87, 149.55, 148.67, 146.61, 146.24, 145.33, 144.72, 144.39, 144.28, 141.72, 139.23, 138.99, 138.79, 138.42, 138.34, 138.26, 137.45, 137.12, 135.98, 134.46, 133.66, 132.26, 131.65, 131.33, 131.11, 131.09, 130.79, 130.67, 130.62, 130.30, 130.16, 128.69, 128.37, 128.20, 128.16, 126.99, 124.91, 124.19, 124.04, 123.07, 122.67, 121.79, 121.60, 121.49, 121.43, 120.97, 119.83, 119.58, 119.33, 118.74, 112.47, 32.39, 32.15, 21.64, 21.50, 21.44, 21.43, 21.29.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 381 (100000), 441 (110000), 523 (145000), 544 (160000), 596 (50000), 641 (30000), 700 (10000).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{126}N_8Ni_2$ (M^+) calcd.: 2178.8807, found: 2178.8811.

TLC: R_f [%]: 0.68 (hexanes/CH_2Cl_2 - 2:1).



Scheme S12. Synthesis of fused *meta*-bis-porphyrin-HBC ***m*-HBC**. Ar = mesityl.

Fused *meta*-Bis-Porphyrin-HBC *m*-HBC

A 20 mL vial was filled with a solution of *meta*-bis-porphyrin-HBC **13** (12 mg, 5.5 µmol, 1 equiv) in CH_2Cl_2 (8 mL) and cooled with an ice bath. The solution was degassed (bubbling N_2 through the solution for 15 min). The N_2 flow through the solution was increased and a solution of dry $FeCl_3$ (53 mg, 329 µmol, 60 equiv) in CH_3NO_2 (0.3 mL) was added. The N_2 bubbling through the solution was stopped 15 min after $FeCl_3$ was added and the solution was stirred under slow warming to rt for 72 h. MeOH (10 mL) was added to quench the reaction. After adding NEt_3 (1 mL) the solvent was removed and the crude was purified by a silica plug (hexanes/ CH_2Cl_2 - 1:1, Ø 3 x 8 cm). Further purification was achieved by column chromatography (SiO_2, hexanes/CH_2Cl_2 - 4:1, Ø 7 x 40 cm) The product ***m*-HBC** was obtained as a purple-black solid in 62% yield (7.4 mg, 3.41 µmol).

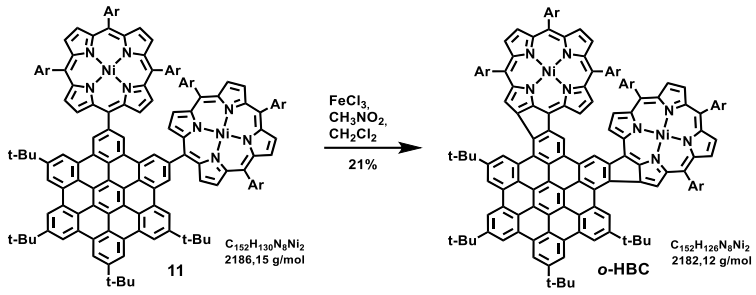
^{1}H NMR (600 MHz, CD_2Cl_2, rt): δ [ppm]: 9.89 - 9.78 (m, 5H), 9.62 - 9.60 (m, 2H), 9.43 (s, 1H), 9.39 - 9.34 (m, 3H), 9.29 (s, 1H), 9.25 (s, 1H), 8.68 (d, *J* = 4.7 Hz, 1H), 8.66 (d, *J* = 4.8 Hz, 1H), 8.49 - 8.46 (m, 2H), 8.21 - 8.16 (m, 5H), 8.13 - 8.12 (m, 2H), 7.31 (s, 2H), 7.27 (s, 2H), 7.24 - 7.23 (m, 4H), 7.20 (m, 4H), 2.67 - 2.49 (m, 18H), 2.01 - 1.85 (m, 45H), 1.65 (s, 9H), 1.59 (s, 9H), 1.55 (s, 9H).

^{13}C NMR (151 MHz, CD_2Cl_2, rt): δ [ppm]: 156.14, 156.10, 150.18, 150.07, 149.84, 149.76, 149.53, 149.48, 148.70, 148.63, 146.61, 146.57, 146.23, 146.21, 145.31, 144.71, 144.69, 144.36, 144.25, 141.73, 141.69, 139.23, 139.20, 138.97, 138.76, 138.43, 138.39, 138.34, 138.31, 138.23, 137.44, 137.42, 137.09, 135.93, 134.42, 133.71, 133.63, 132.25, 132.23, 131.63, 131.45, 131.30, 131.06, 130.97, 130.89, 130.77, 130.74, 130.63, 130.60, 130.53, 130.28, 130.17, 128.68, 128.66, 128.32, 128.20, 128.18, 128.13, 128.07, 127.02, 126.97, 125.09, 125.06, 124.10, 124.07, 124.00, 123.98, 123.31, 123.12, 122.67, 122.66, 121.89, 121.72, 121.52, 121.49, 121.46, 121.42, 121.36, 121.33, 121.21, 119.84, 119.78, 119.50, 119.46, 119.31, 119.21, 118.71, 118.70, 112.42, 54.16, 32.44, 32.35, 32.29, 32.13, 32.07, 30.05, 30.01, 23.06, 21.62, 21.52, 21.50, 21.49, 21.47, 21.44, 21.44, 21.42, 21.29.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 392 (55000), 448 (70000), 506 (80000), 594 (27000), 639 (17000), 693 (5000).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{126}N_8Ni_2$ (M^+) calcd.: 2178.8807, found:2178.8815.

TLC: R_f [%]: 0.30 (hexanes/CH_2Cl_2 - 4:1).



Scheme S13. Synthesis of fused *ortho*-bis-porphyrin-HBC ***o*-HBC**. Ar = mesityl.

Fused *ortho*-Bis-Porphyrin-HBC *o*-HBC

A 20 mL vial was filled with a solution of *ortho*-bis-porphyrin-HBC **11** (20 mg, 9.2 µmol, 1 equiv) in CH_2Cl_2 (10 mL) and cooled with an ice bath. The solution was degassed (bubbling N_2 through the solution for 15 min). The N_2 flow through the solution was increased, and a solution of dry $FeCl_3$ (89 mg, 549 µmol, 60 equiv) in CH_3NO_2 (0.3 mL) was added. The N_2 bubbling through the solution was stopped 15 min after $FeCl_3$ was

added and the solution was stirred under slow warming to rt for 148 h. MeOH (10 mL) was added to quench the reaction. After adding NEt_3 (1 mL), the solvent was removed, and the crude was purified by a silica plug (hexanes/ CH_2Cl_2 - 1:1, Ø 3 x 8 cm). Further purification was achieved by column chromatography (SiO_2, hexanes/CH_2Cl_2 - 3:1, Ø 7 x 40 cm). The product ***o*-HBC** was obtained as a purple-black solid in 21% yield (4.2 mg, 1.9 µmol).

^{1}H NMR (601 MHz, CD_2Cl_2/CS_2, rt): δ [ppm]: 9.81 (s, 2H), 9.76 (s, 2H), 9.74 (d, *J* = 4.8 Hz, 2H), 9.25 (s, 2H), 9.21 (s, 2H), 9.18 (s, 2H), 8.81 (d, *J* = 4.7 Hz, 2H), 8.39 (s, 2H), 8.19 (s, 4H), 8.17 (d, *J* = 4.6 Hz, 2H), 8.12 (d, *J* = 4.6 Hz, 2H), 7.31 (s, 4H), 7.22 (s, 4H), 7.18 (s, 4H), 2.73 (s, 6H), 2.64 (s, 6H), 2.60 (s, 6H), 2.06 (s, 12H), 2.03 (s, 12H), 1.96 (s, 12H), 1.92 (s, 18H), 1.63 (s, 18H).

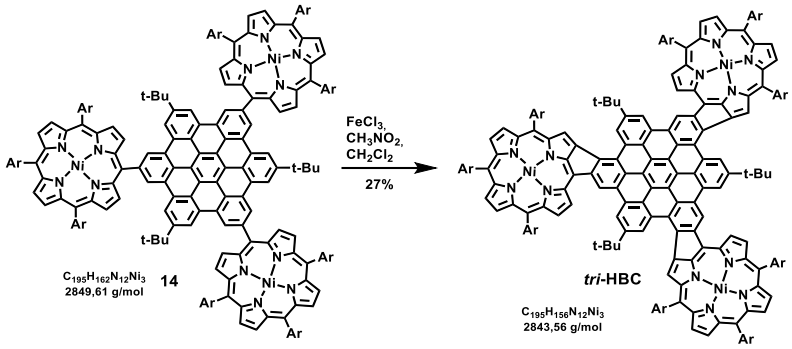
^{13}C NMR (151 MHz, CD_2Cl_2/CS_2, rt): δ [ppm]: 156.60, 149.92, 149.31, 148.82, 148.68, 146.55, 146.05, 145.12, 144.65, 144.17, 144.09, 142.06, 139.22, 138.91, 138.79, 138.08, 138.02, 137.74, 137.28, 136.18, 134.49, 133.80, 132.18, 131.68, 131.38, 131.24, 131.21, 131.09, 130.98, 130.70, 130.68, 130.35, 128.86, 128.79, 128.68, 128.53, 127.21, 125.42, 124.30, 123.62, 123.24, 122.38, 122.01, 121.68, 121.59, 121.36, 121.35, 119.61, 119.55, 119.44, 118.78, 113.19, 32.66, 32.49, 30.64, 22.24, 22.15, 22.14, 22.12, 21.86.

UV/Vis (CH_2Cl_2): *λ* [nm] (*ε* [$M^{-1}cm^{-1}$]): 387 (49000), 452 (61000), 484 (72000), 561 (43000), 707 (4000).

MS (MALDI, DCTB): m/z (rel. Int.) = 2182 (M^+, 100 %).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{126}N_8Ni_2$ (M^+) calcd.: 2178.8807, found: 2178.8821.

TLC: R_f [%]: 0.30 (hexanes/CH_2Cl_2 - 4:1).



Scheme S13. Synthesis of fused tris-porphyrin-HBC ***tri*-HBC**. Ar = mesityl.

Fused Tris-Porphyrin-HBC *tri*-HBC

A 20 mL vial was filled with a solution of tris-porphyrin-HBC **14** (20 mg, 7.0 µmol, 1 equiv) in CH_2Cl_2 (10 mL) and cooled with an ice bath. The solution was degassed (bubbling N_2 through the solution for 15 min). The N_2 flow through the solution was increased, and a solution of dry $FeCl_3$ (68 mg, 421 µmol, 60 equiv) in CH_3NO_2 (0.2 mL) was added. The N_2 bubbling through the solution was stopped 15 min after $FeCl_3$ was added and the solution was stirred under slow warming to rt for 72 h. MeOH (10 mL) was added to quench the reaction. After adding NEt_3 (1 mL) the solvent was removed and the crude was purified by a silica plug (hexanes/ CH_2Cl_2 - 1:1, Ø 3 x 8 cm). Further purification was achieved by column chromatography (SiO_2, hexanes/CH_2Cl_2 - 3:1, Ø 7 x 40 cm). The product ***tri*-HBC** was obtained as a purple-black solid in 27% yield (4.6 mg, 1.6 µmol).

^{1}H NMR (601 MHz, CD_2Cl_2, rt): δ [ppm]: 9.88 (s, 3H), 9.81 (s, 3H), 9.63 - 9.62 (m, 3H), 9.38 (s, 3H), 8.69 - 8.69 (m, 3H), 8.51 (s, 3H), 8.22 - 8.20 (m, 6H), 8.19 (d, *J* = 4.6 Hz, 3H), 8.13 (d, *J* = 4.6 Hz, 3H), 7.30 (m, 6H), 7.25 (s, 6H), 7.21 (m, 6H), 2.63 - 2.55 (m, 18H), 2.55 (s, 9H), 2.00 (s, 18H), 1.95 (s, 18H), 1.90 (s, 18H), 1.64 (s, 27H).

^{13}C NMR (151 MHz, CD_2Cl_2, rt): δ [ppm]: 156.09, 149.91, 149.75, 148.60, 146.59, 146.25, 145.33, 144.73, 144.39, 144.28, 141.74, 139.23, 138.97, 138.78, 138.44, 138.35, 138.24, 137.44, 137.09, 135.93, 134.44, 133.71, 132.27, 131.57, 131.32, 131.08, 130.83, 130.81, 130.34, 130.31, 128.70, 128.20, 128.14, 127.02, 125.07, 124.05, 123.38, 122.71, 121.92, 121.74, 121.51, 121.47, 121.45, 119.32, 112.36, 32.45, 23.06, 21.64, 21.52, 21.51, 21.45, 21.30.

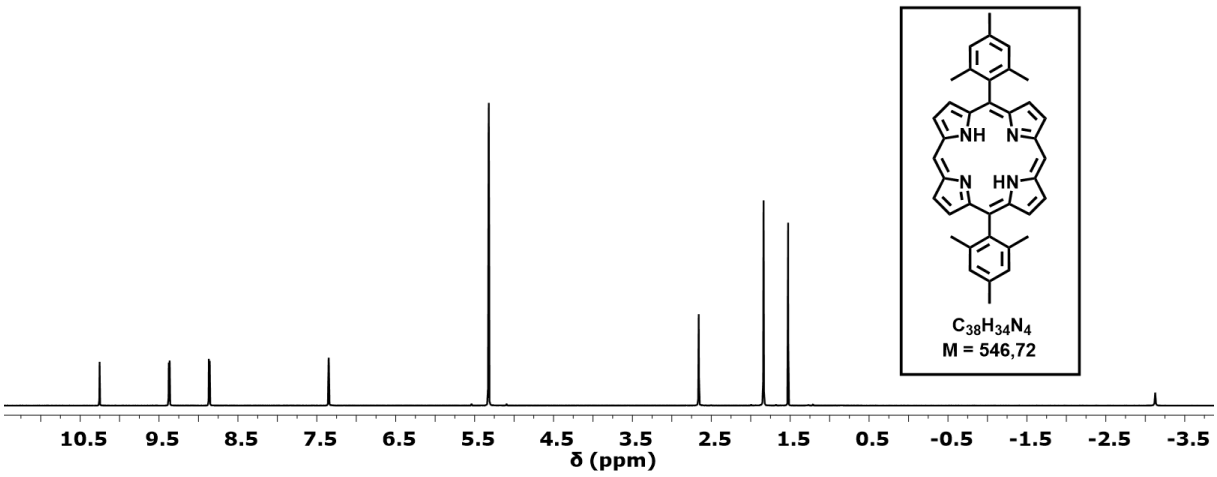
UV/Vis (CH_2Cl_2): λ [nm] (ε [$M^{-1}cm^{-1}$]): 400 (63000), 458 (74000), 519 (87000), 554 (76000), 643 (24000).

HRMS (MALDI, CH_2Cl_2) for $C_{152}H_{126}N_8Ni_2$ (M^+) calcd.: 2839.0631, found: 2839.0737.

TLC: R_f [%]: 0.30 (hexanes/CH_2Cl_2 - 2:1).

3 Spectral Appendix

^{1}H NMR (400 MHz, CD_2Cl_2, rt)



^{13}C NMR (101 MHz, CD_2Cl_2, rt)

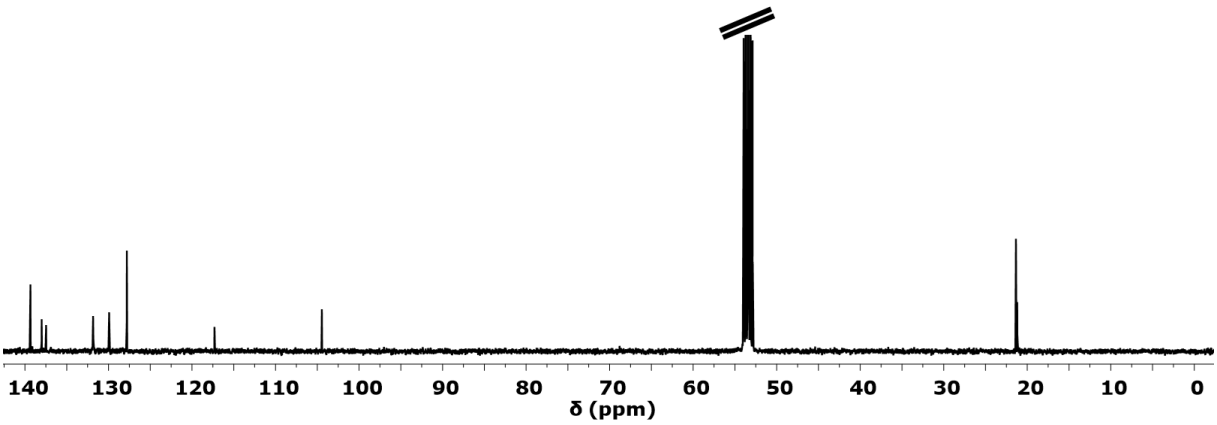
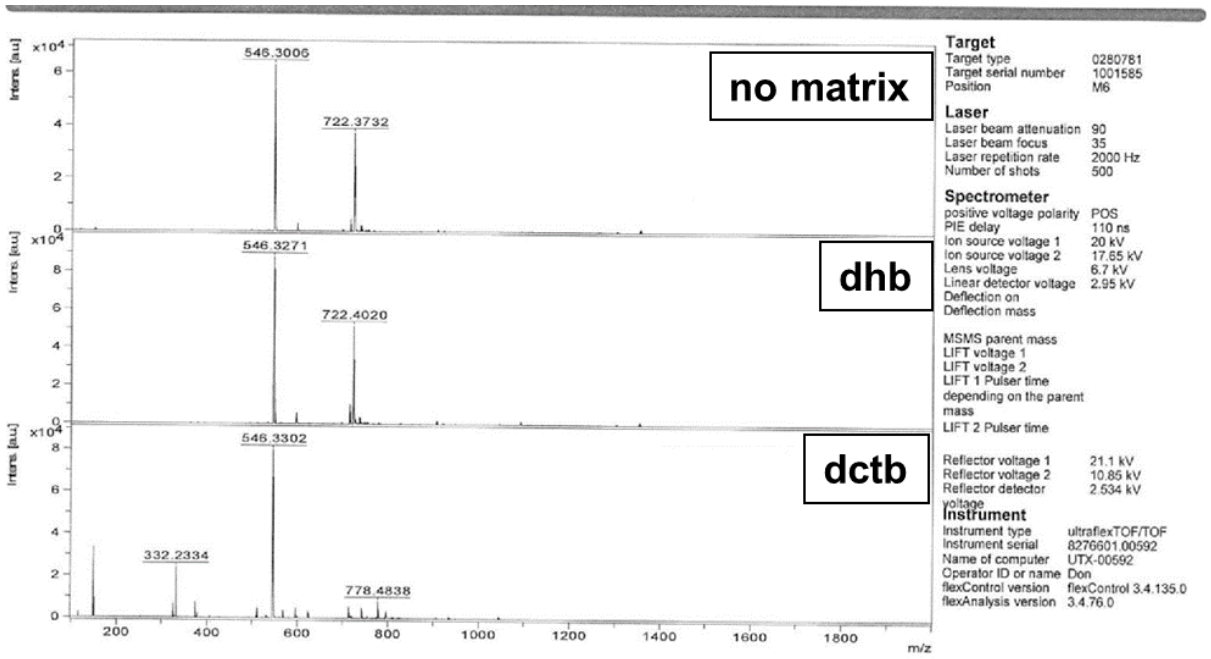
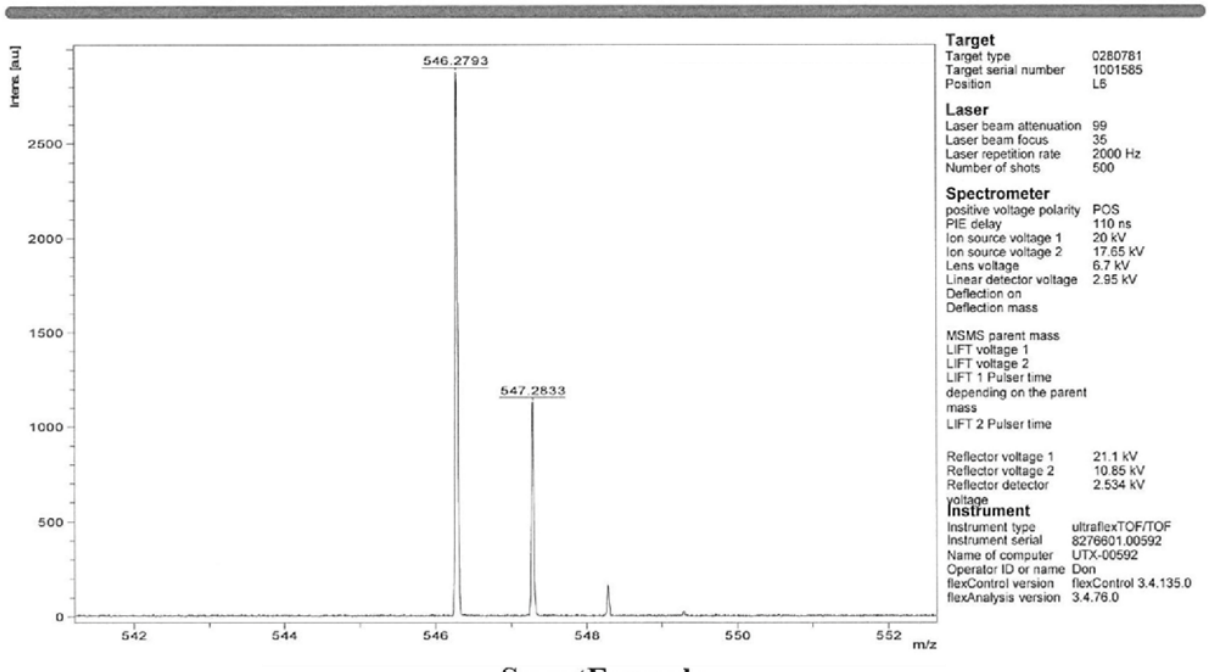


Figure S1. ^{1}H and ^{13}C NMR of **15**.

MS (MALDI)



HRMS (MALDI)

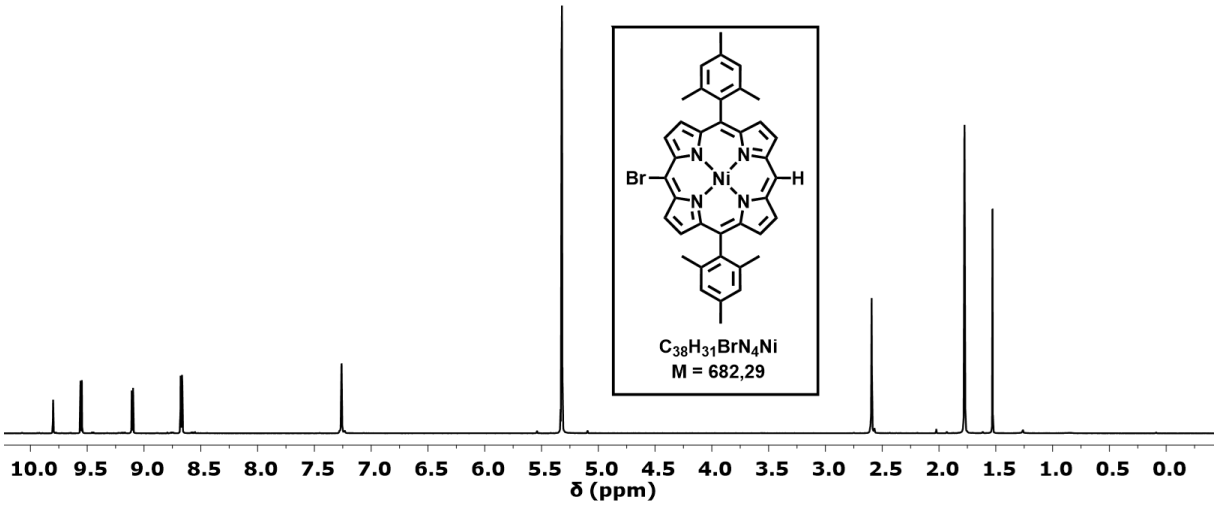


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 38 H 34 N 4	546.2778	2.8010	48.8215	24.00	ok	odd

Figure S2. MS/HRMS (MALDI) of **15**.

^{1}H NMR (400 MHz, CD_2Cl_2, rt)



^{13}C NMR (101 MHz, CD_2Cl_2, rt)

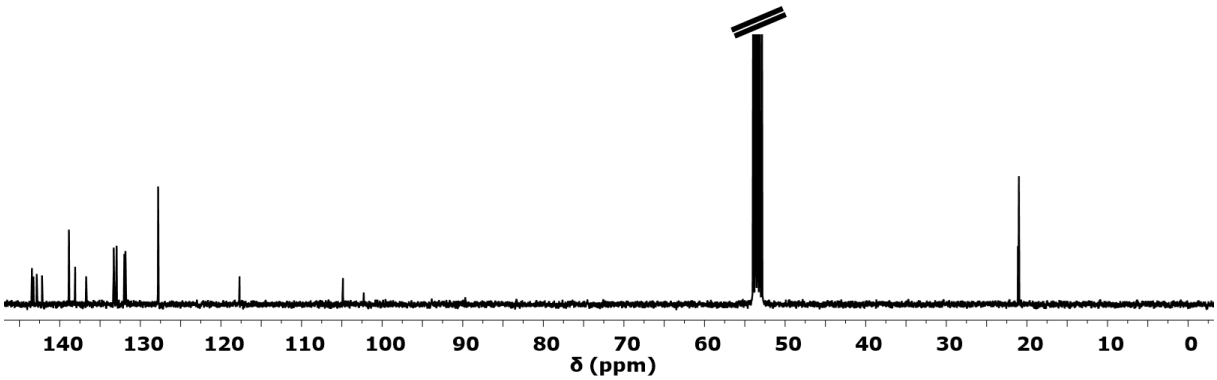
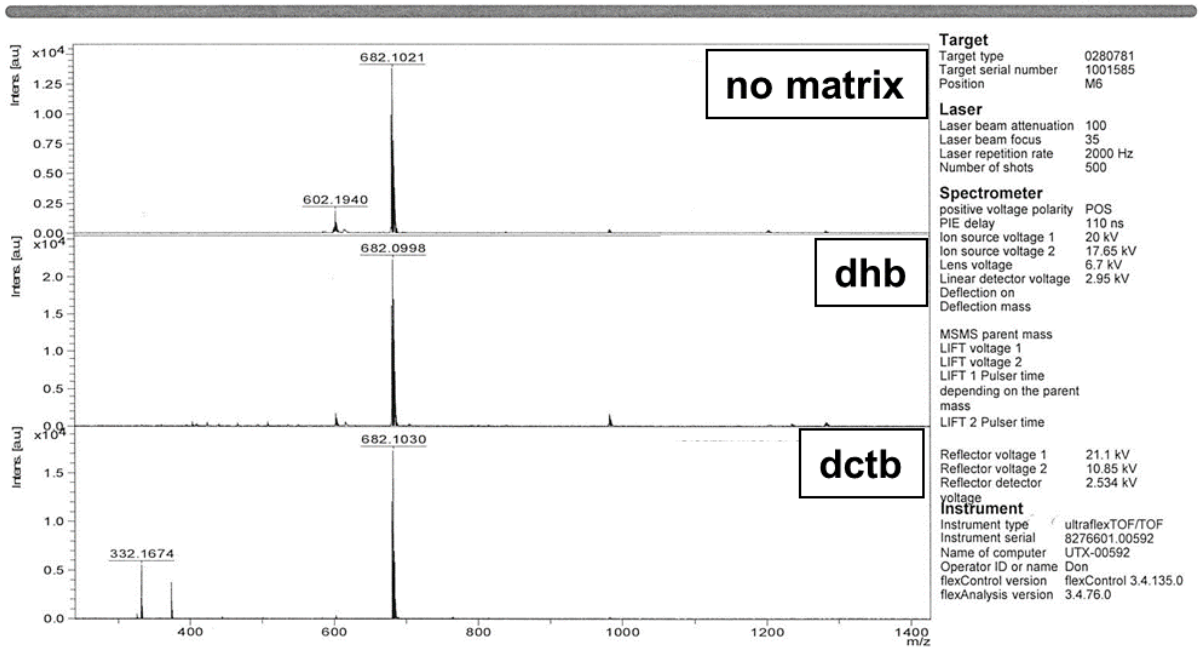
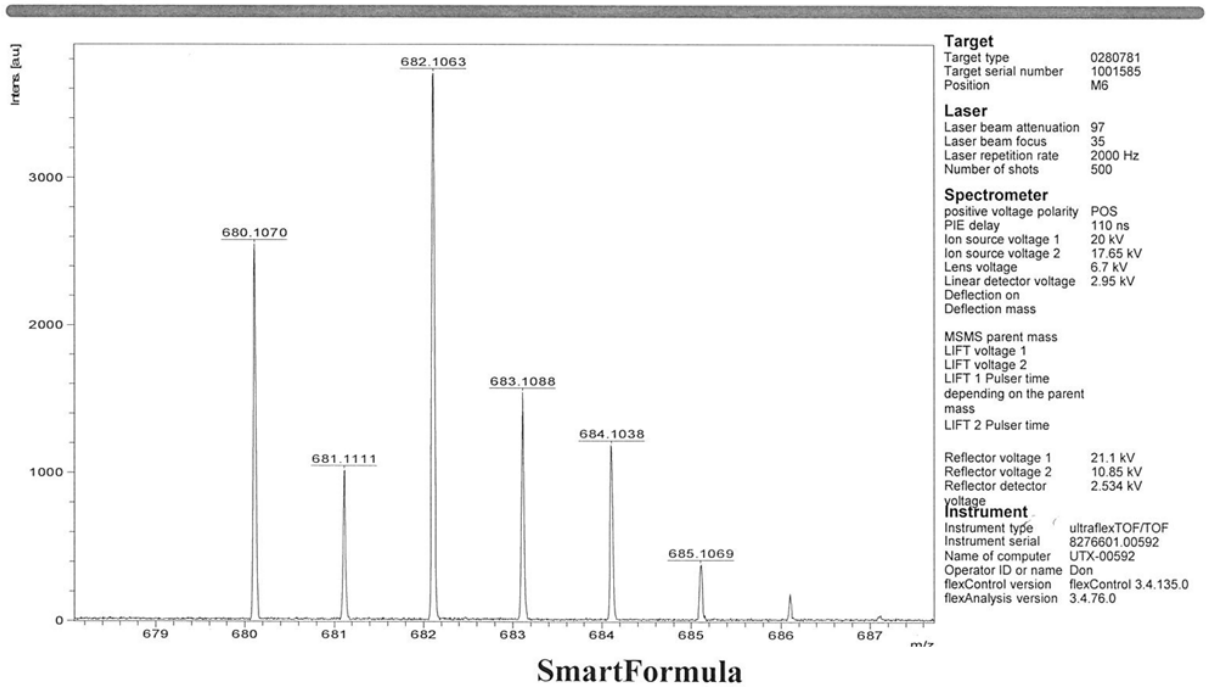


Figure S3. ^{1}H and ^{13}C NMR of **17**.

MS (MALDI)



HRMS (MALDI)

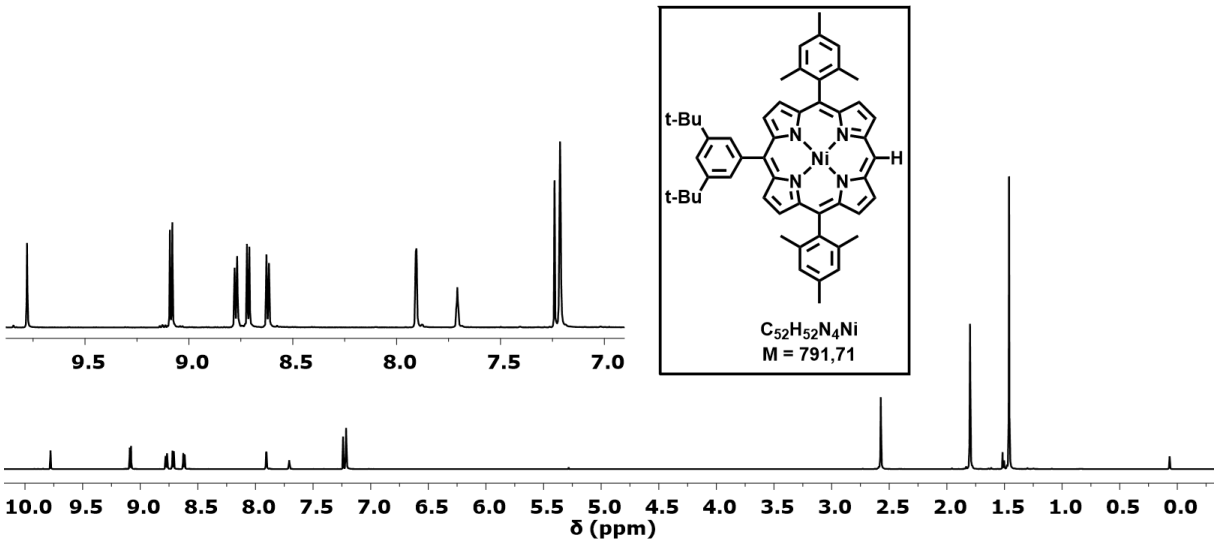


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 38 H 31 Br N 4 Ni	680.1080	1.4813	36.9206	25.00	ok	odd

Figure S4. MS/HRMS (MALDI) of **17**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

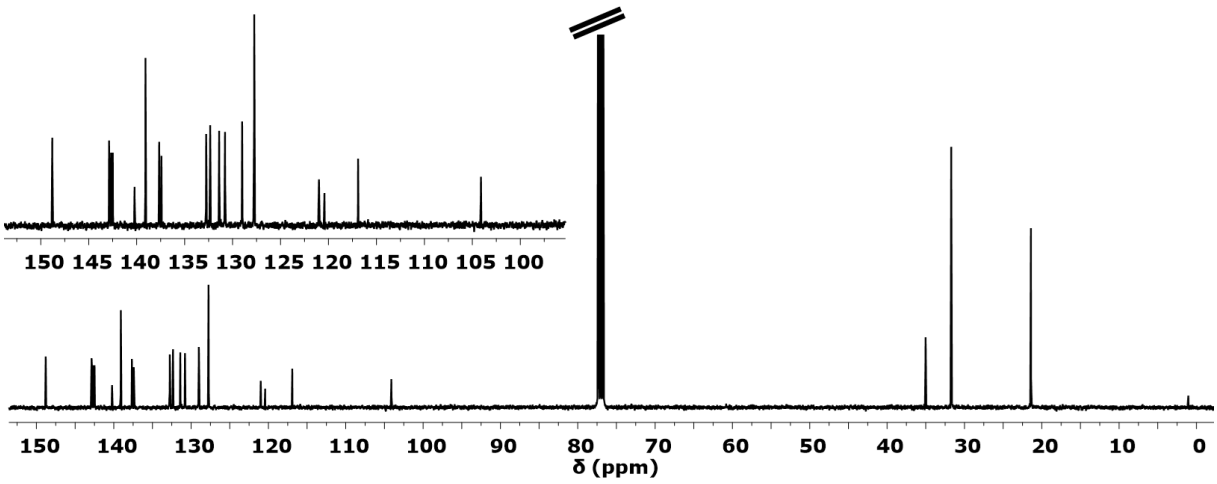
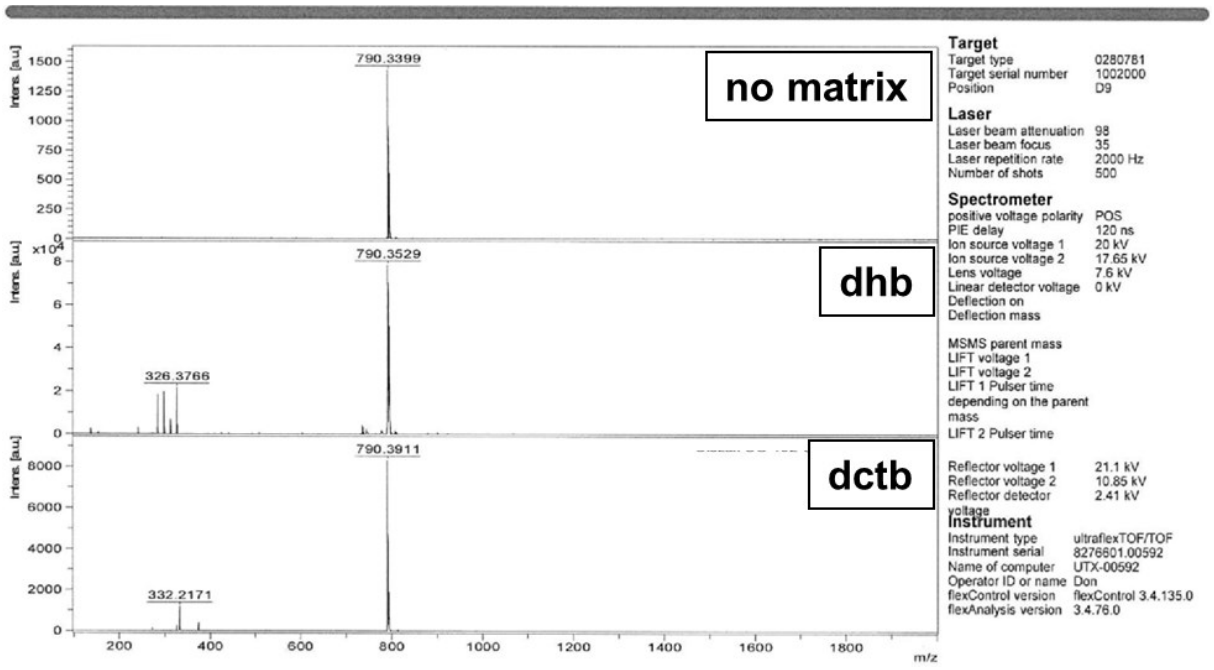
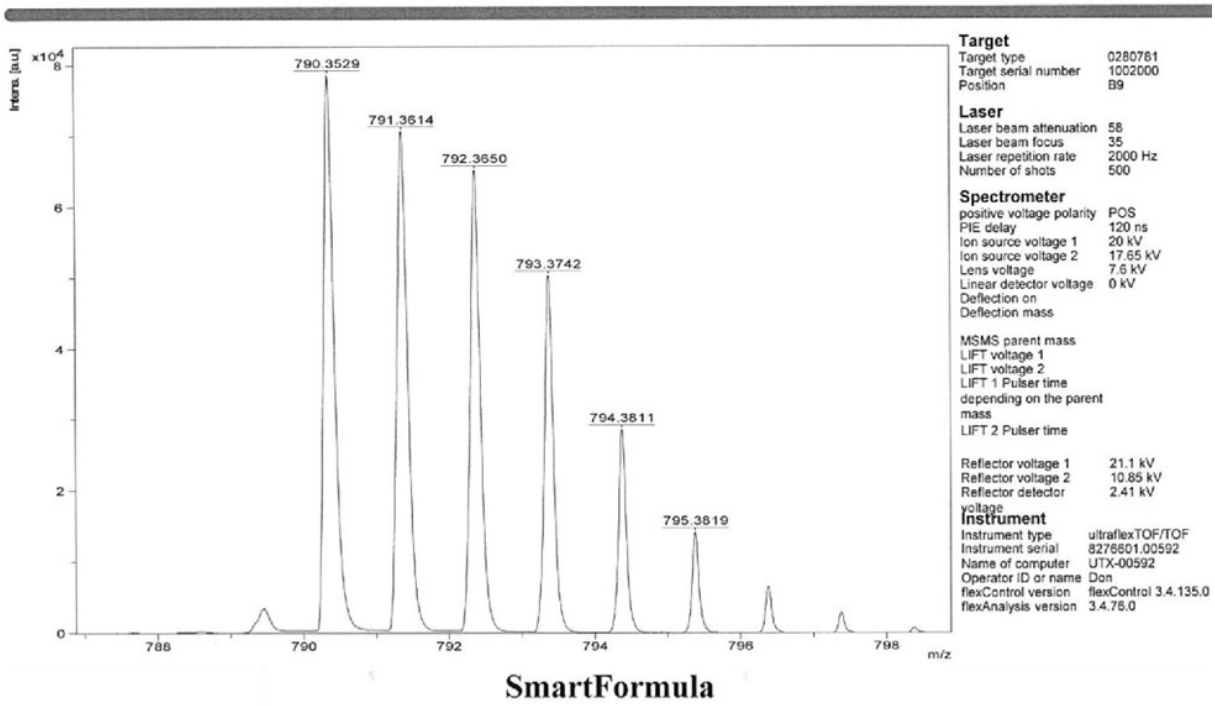


Figure S5. ^{1}H and ^{13}C NMR of **18**.

MS (MALDI)



HRMS (MALDI)

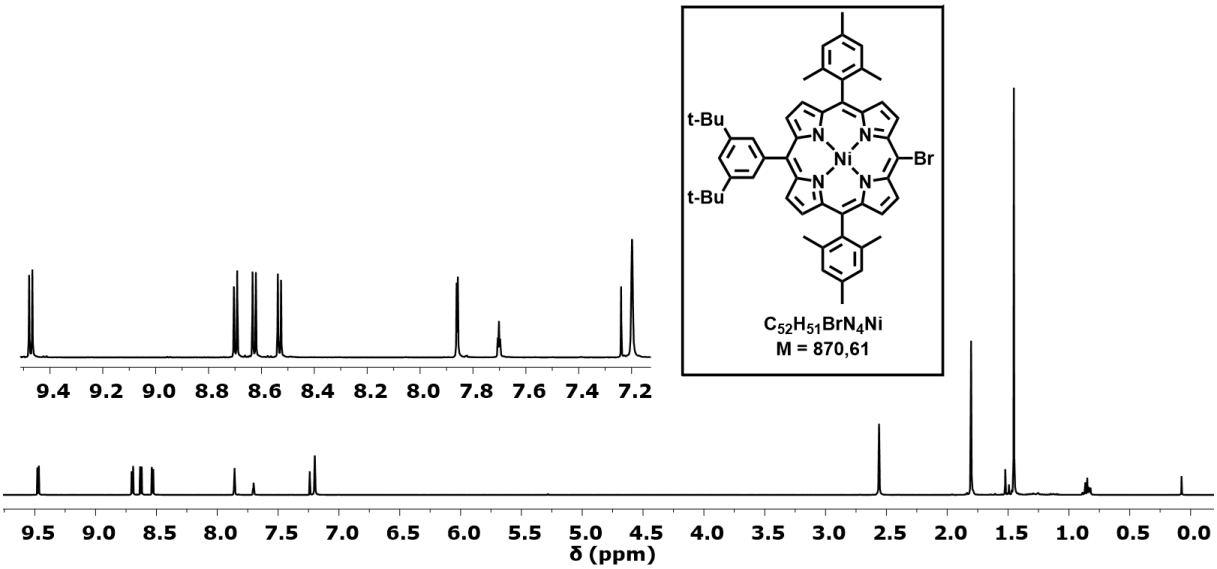


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 52 H 52 N 4 Ni	790.3540	1.3846	219.2905	29.00	ok	odd

Figure S6. MS/HRMS (MALDI) of **18**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

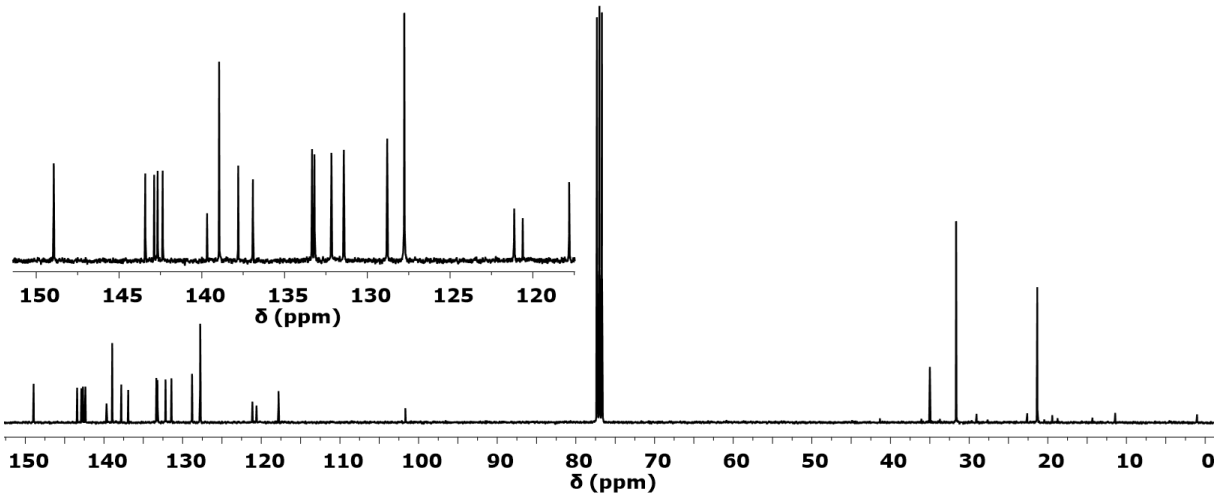
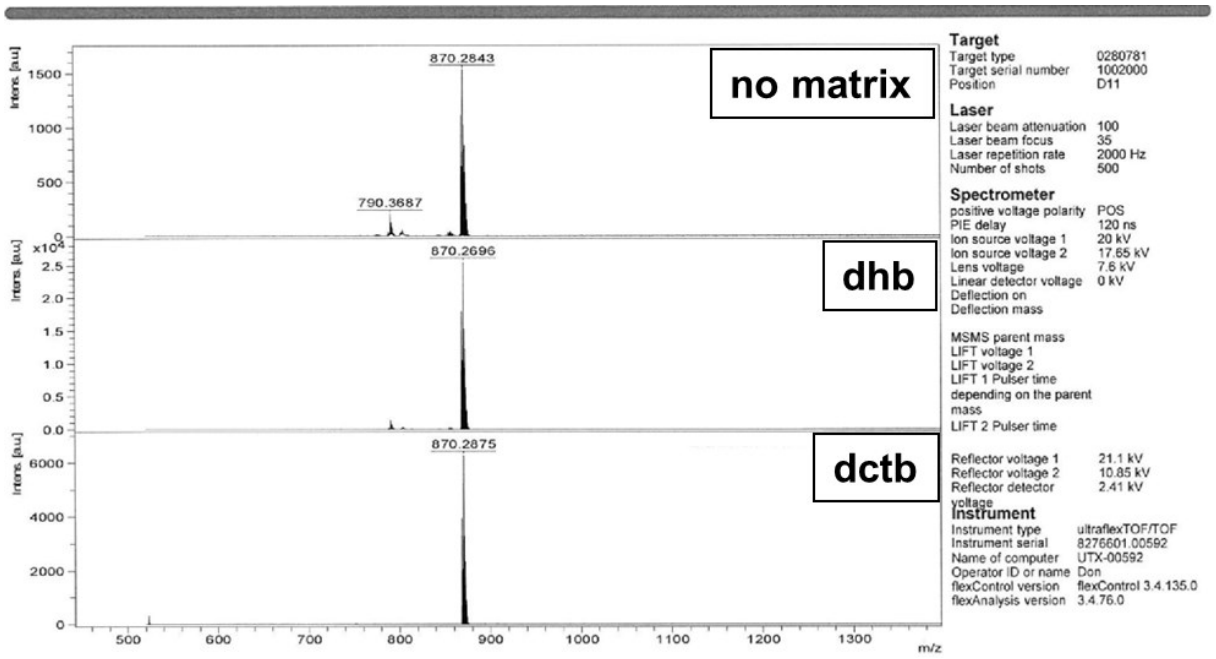
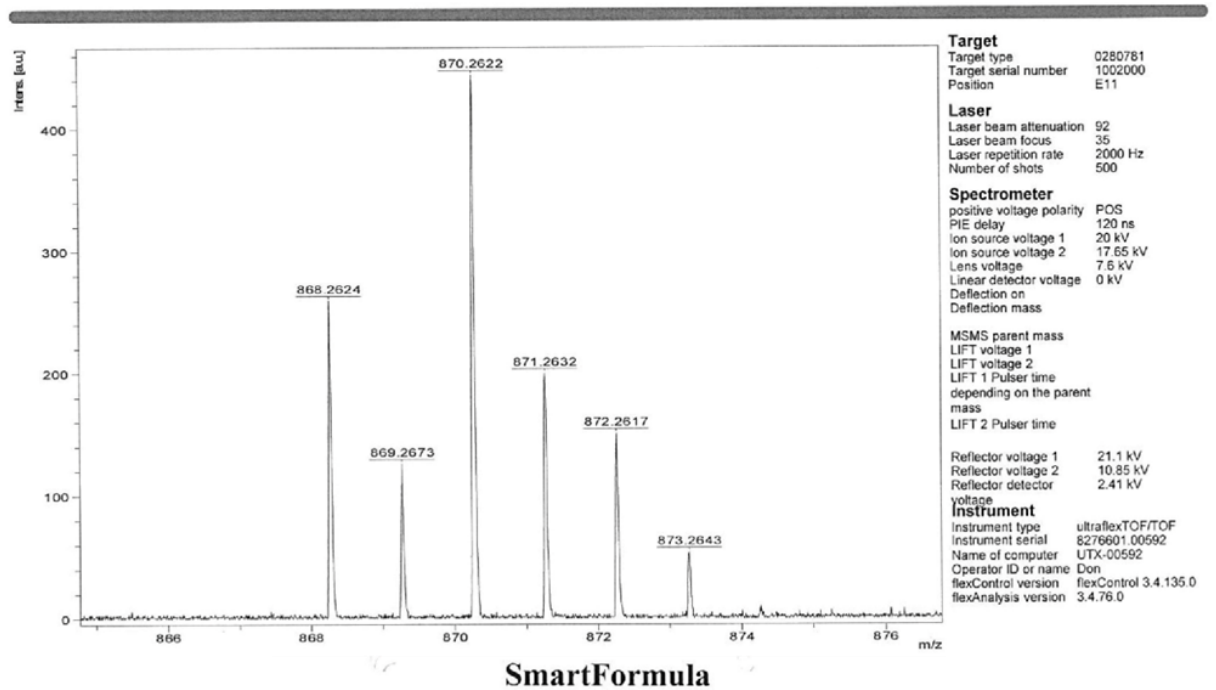


Figure S7. ^{1}H and ^{13}C NMR of **3**.

MS (MALDI)



HRMS (MALDI)

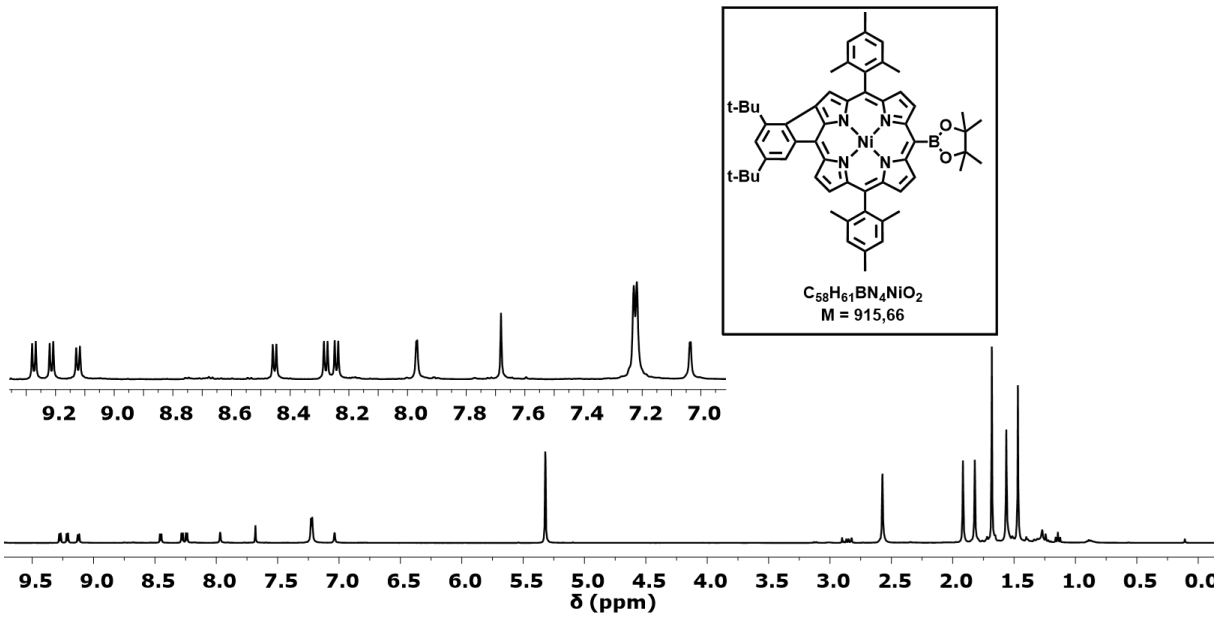


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 52 H 51 Br N 4 Ni	868.2645	2.4787	72.7265	29.00	ok	odd

Figure S8. MS/HRMS (MALDI) of **3**.

^{1}H NMR (400 MHz, CD_2Cl_2, rt)



^{13}C NMR (101 MHz, CD_2Cl_2, rt)

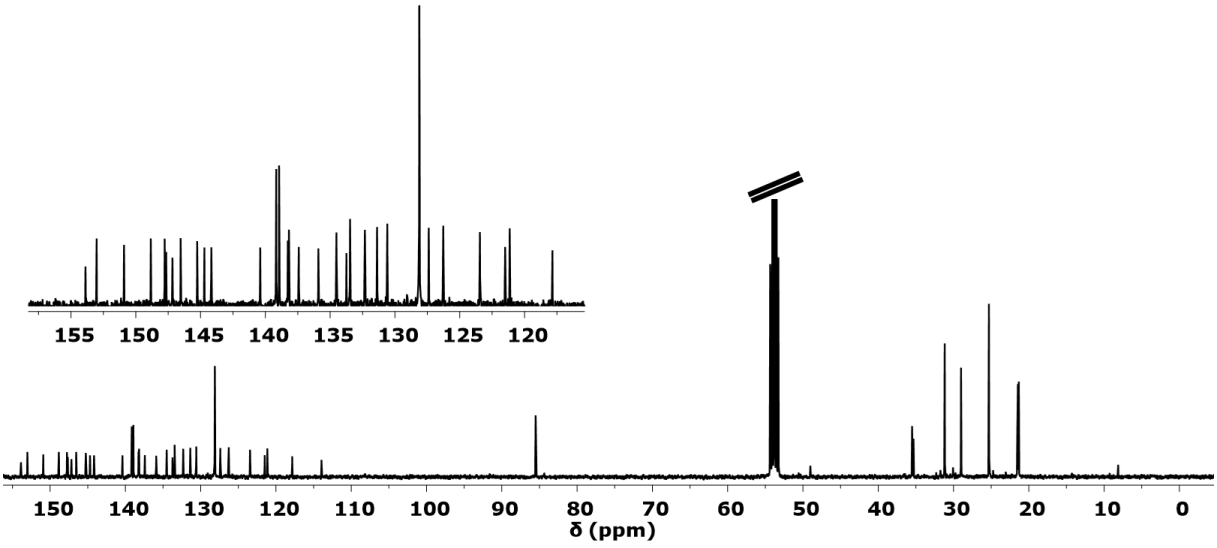
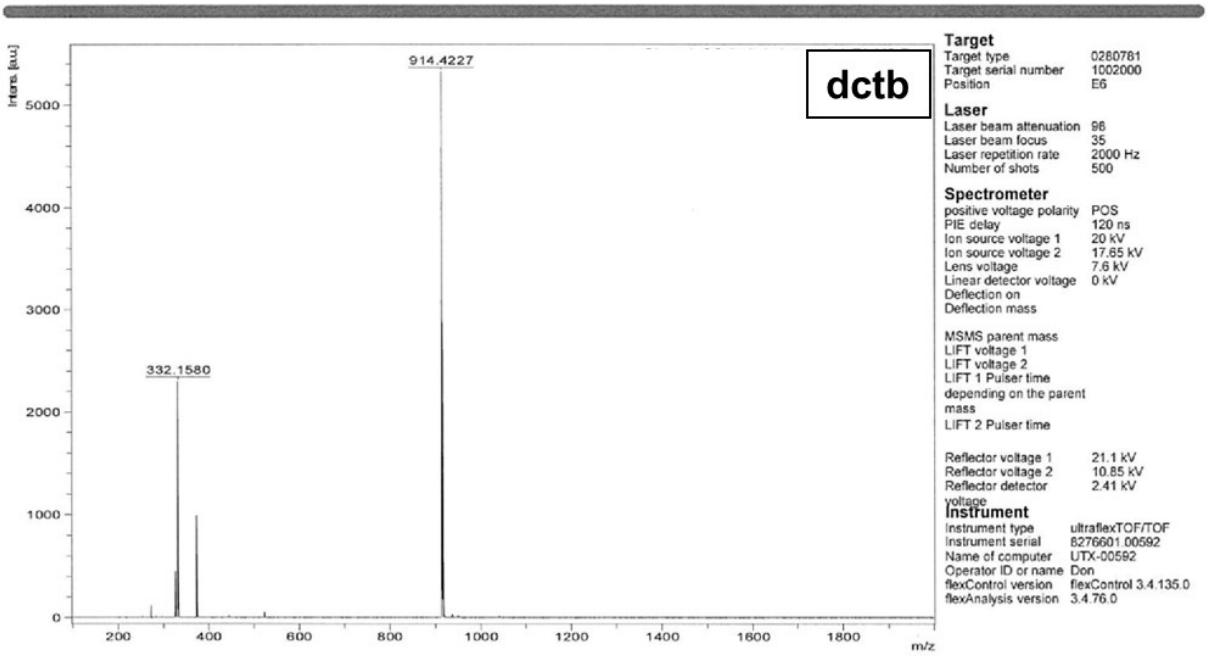
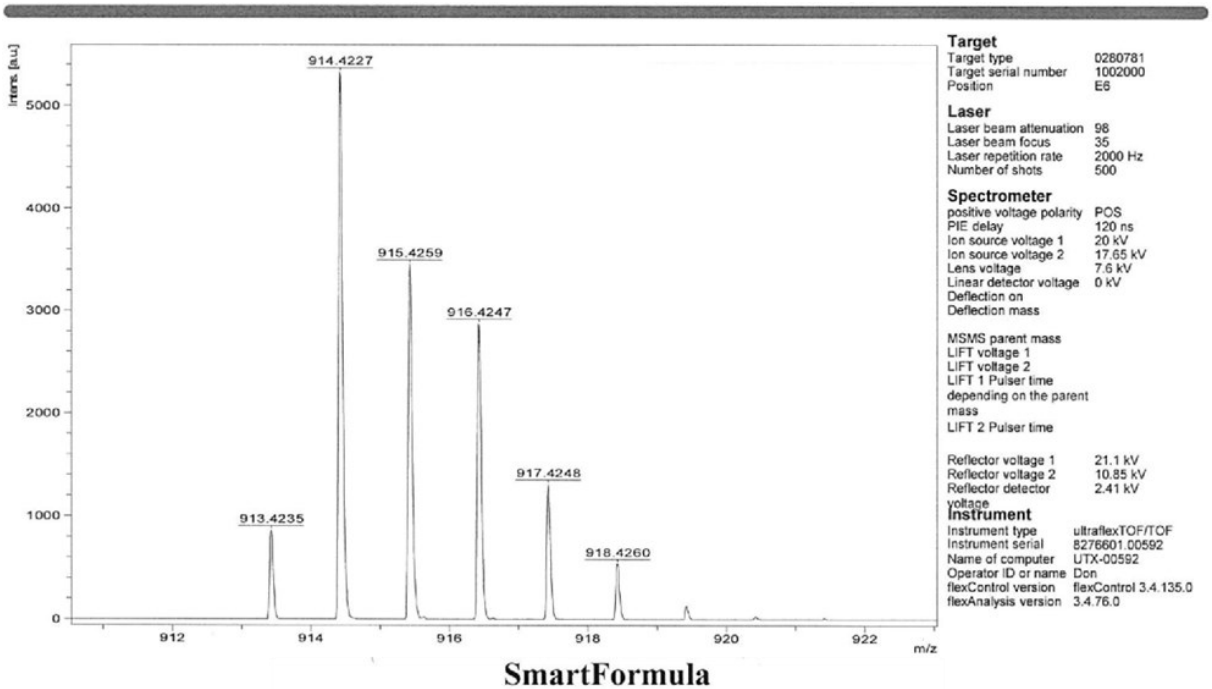


Figure S9. ^{1}H and ^{13}C NMR of **5**.

MS (MALDI)



HRMS (MALDI)

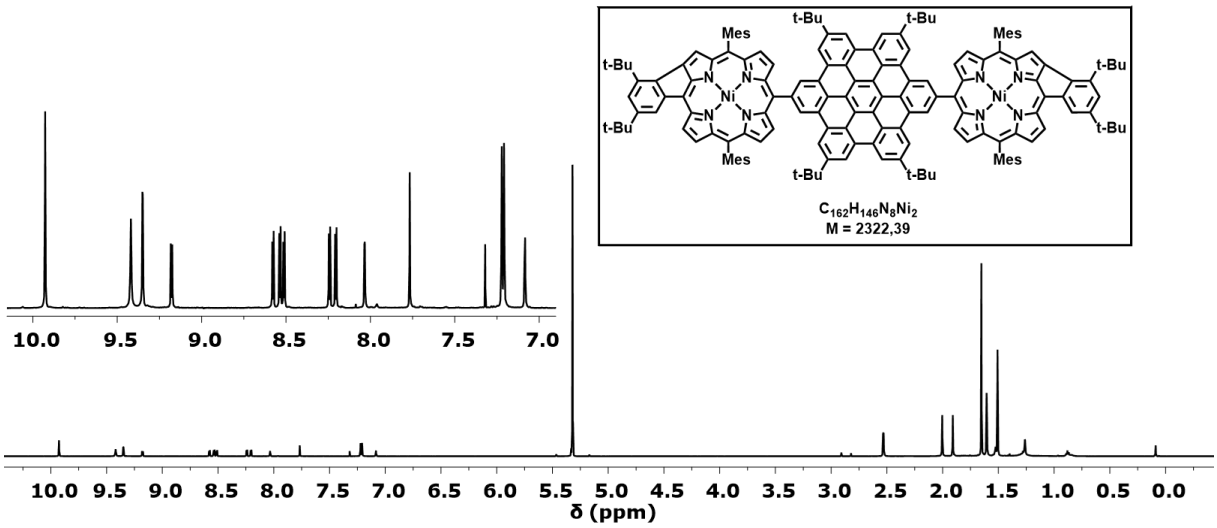


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 58 H 61 B N 4 Ni O 2	914.4236	0.9784	40.2851	31.00	ok	odd

Figure S10. MS/HRMS (MALDI) of **5**.

^{1}H NMR (601 MHz, CD_2Cl_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2, rt)

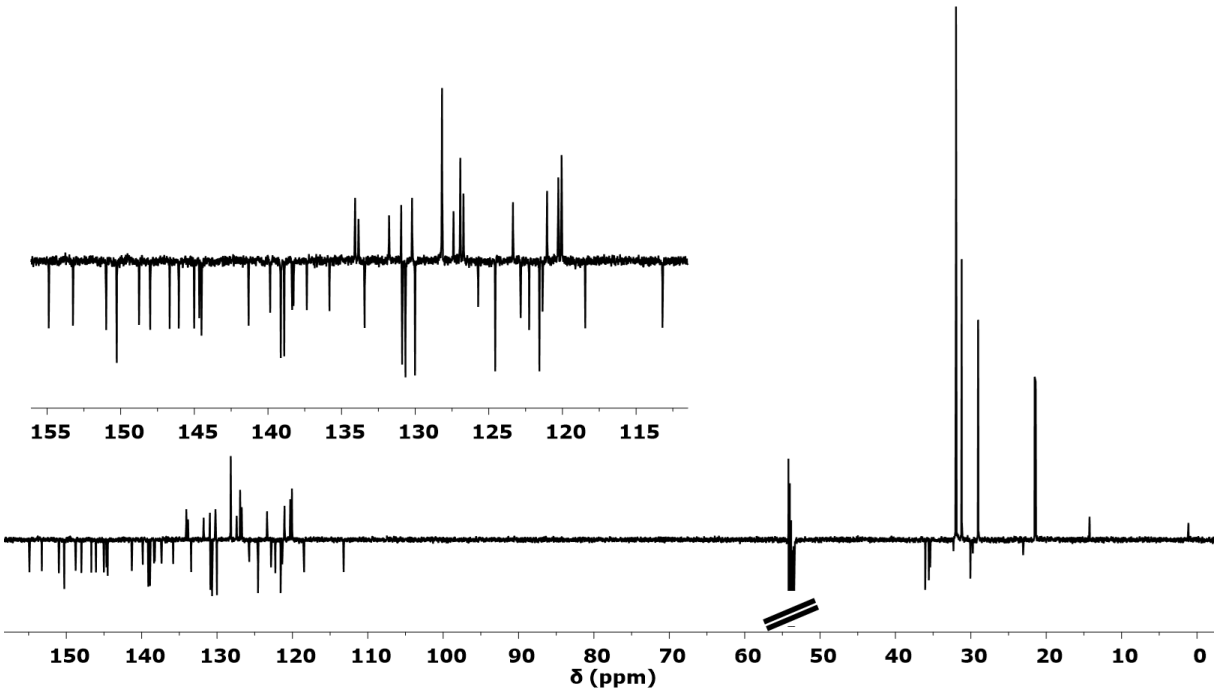


Figure S11. ^{1}H and ^{13}C NMR (DEPTQ135) of ***p*-Ph**.

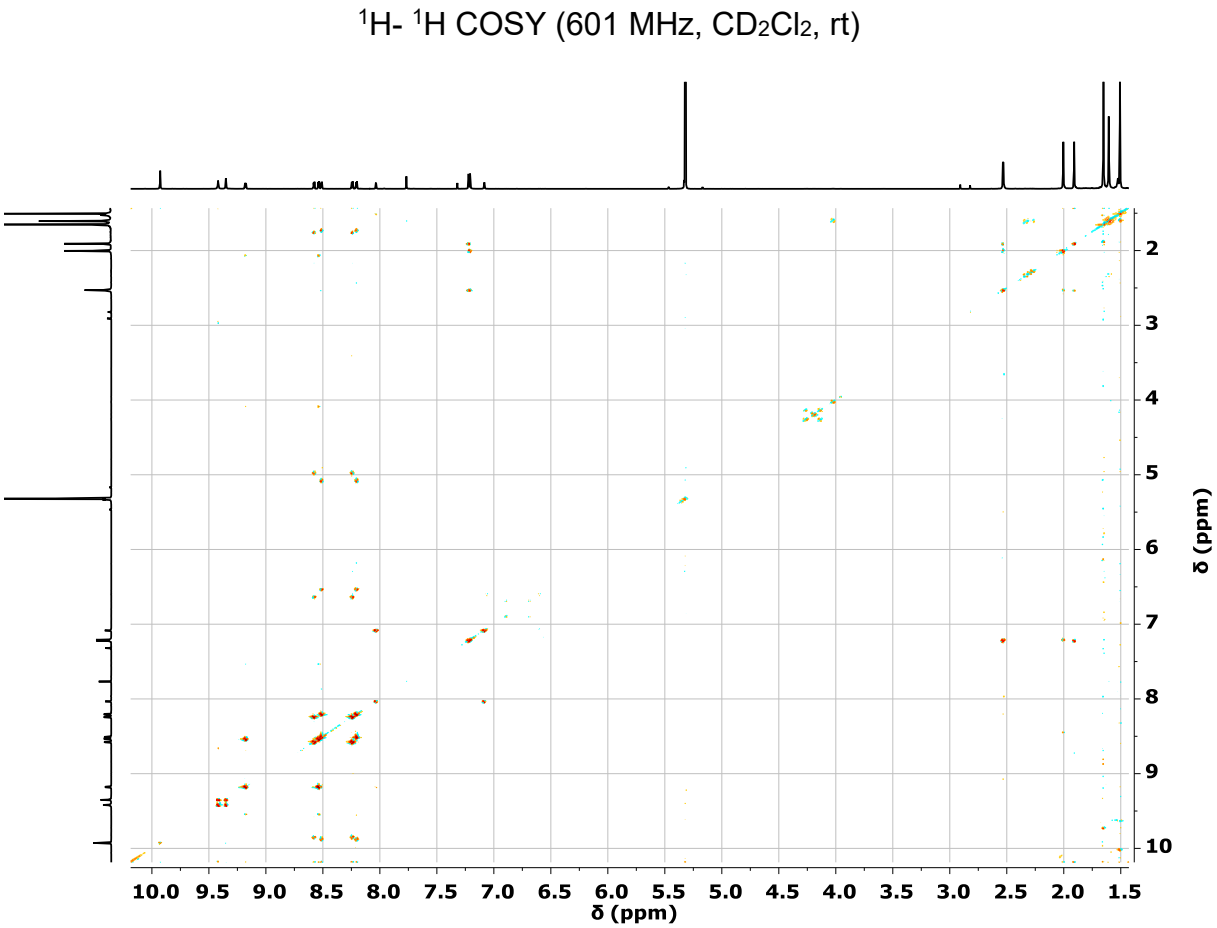


Figure S12. ^{1}H- ^{1}H COSY of ***p*-Ph**.

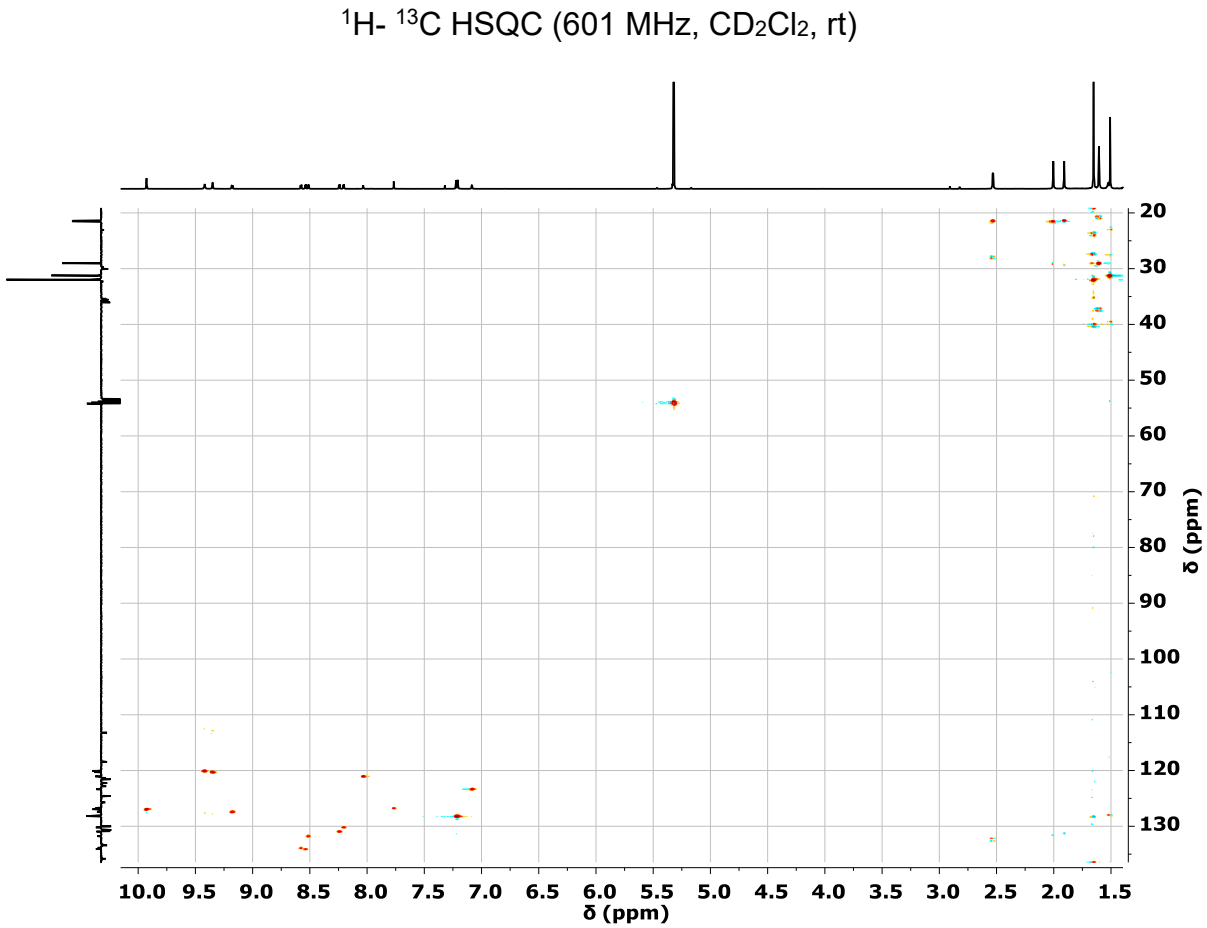


Figure S13. ^{1}H- ^{13}C HSQC of ***p*-Ph**.

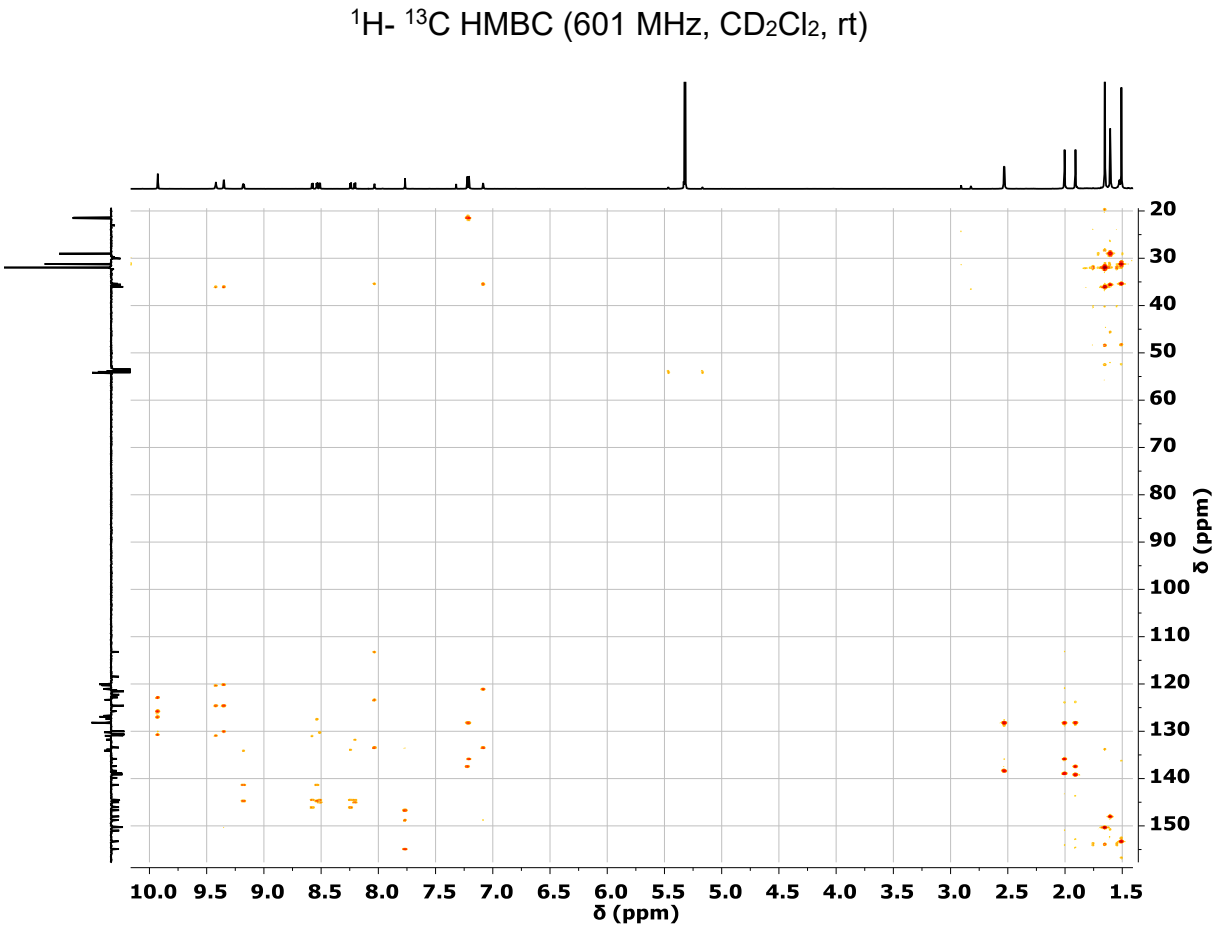


Figure S14. ^{1}H- ^{13}C HMBC of ***p*-Ph**.

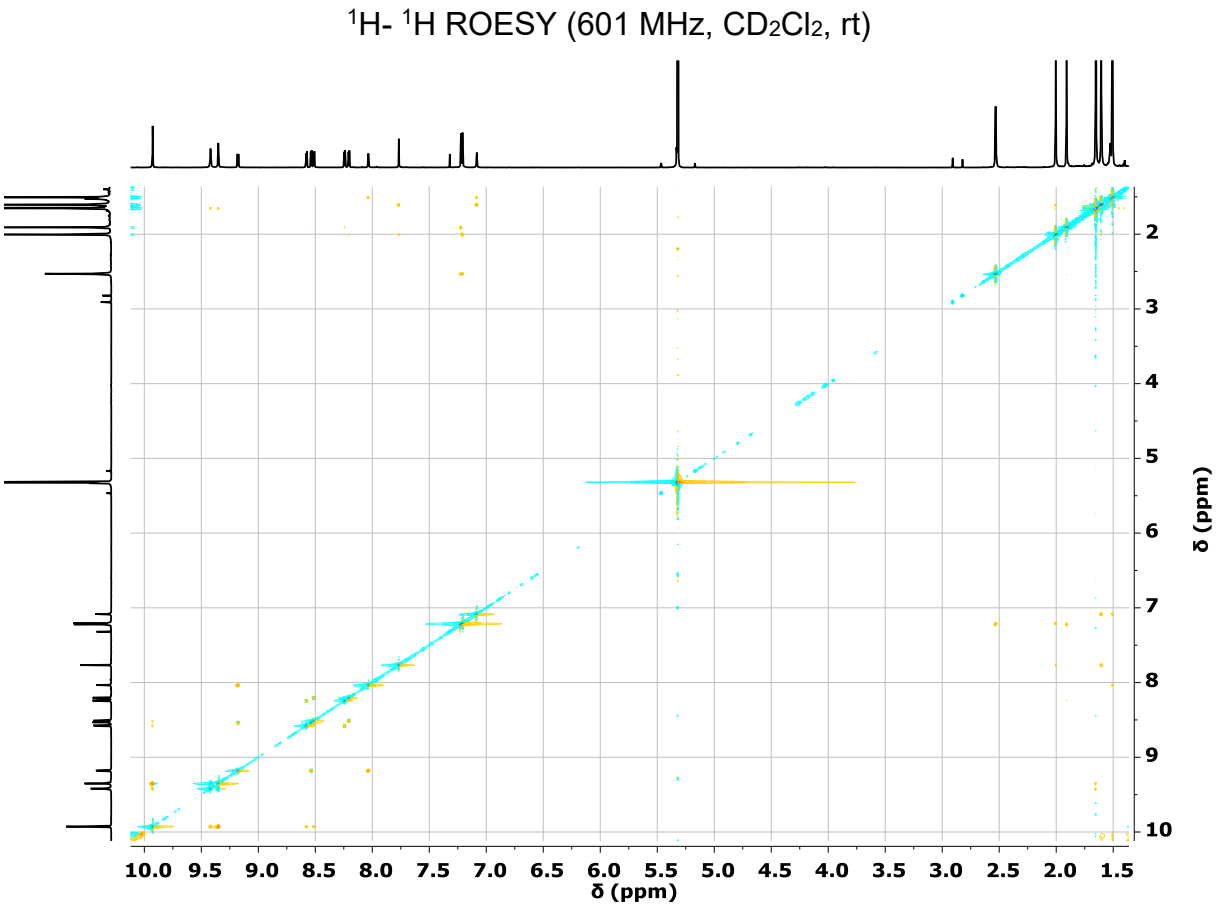
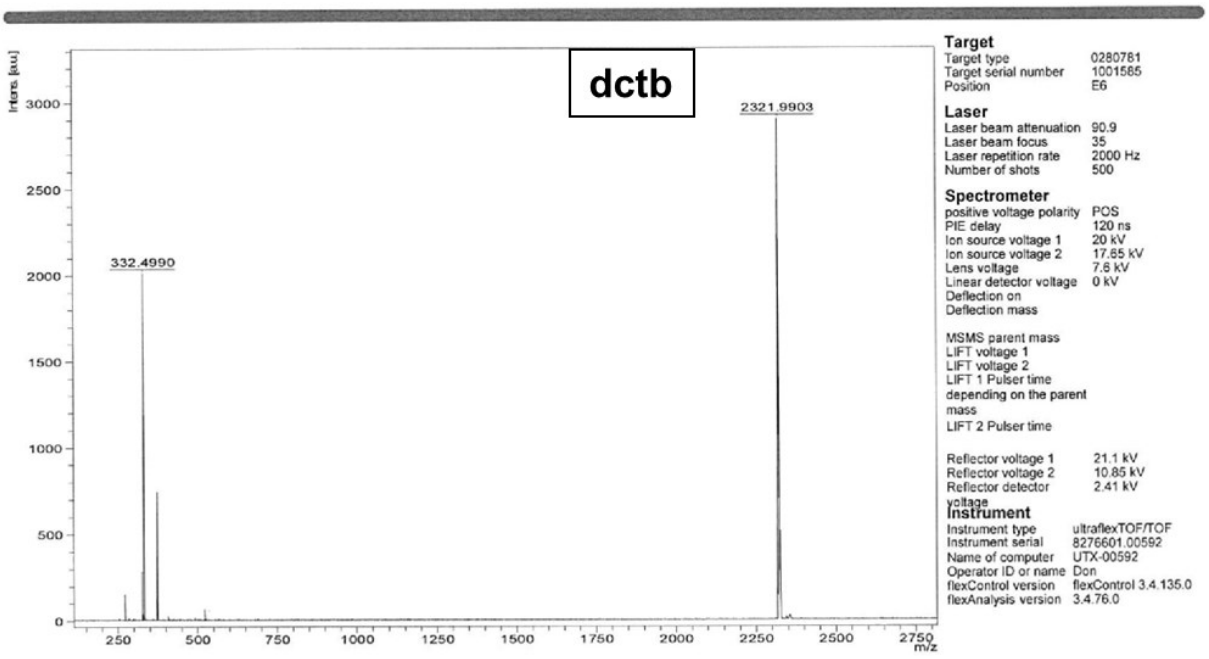
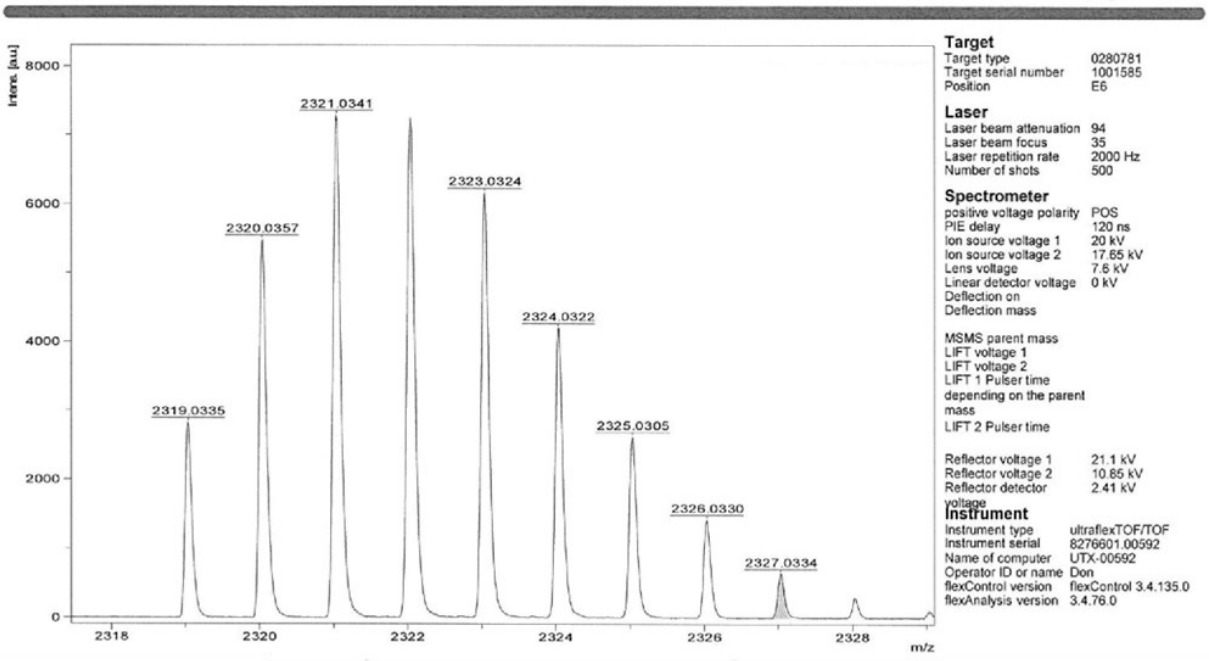


Figure S15. ^{1}H- ^{1}H ROESY of ***p*-Ph**.

MS (MALDI)



HRMS (MALDI)

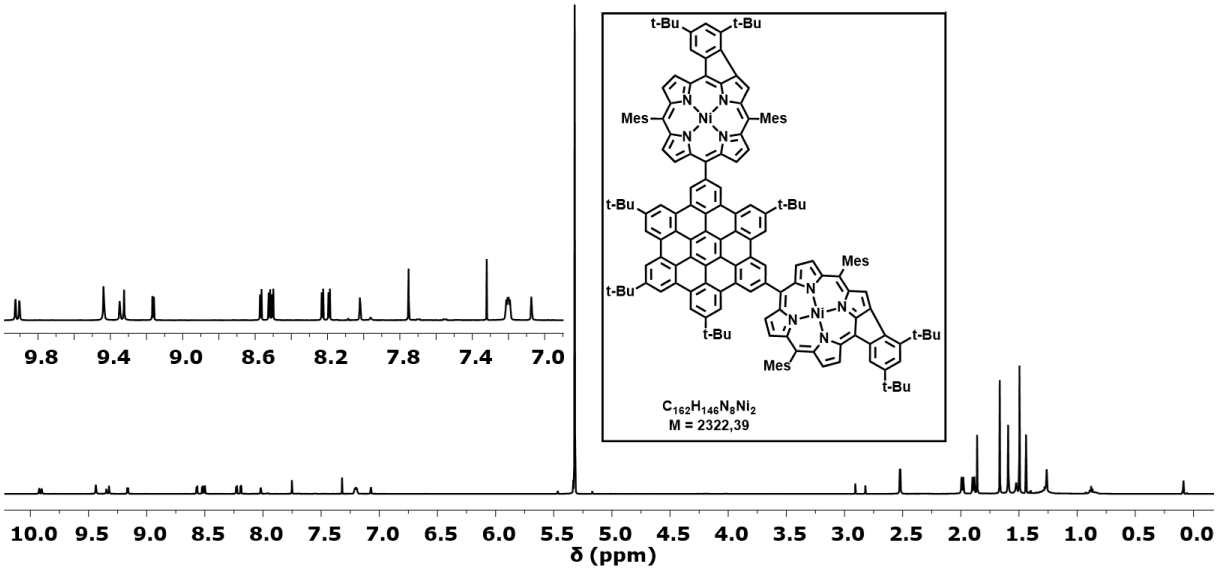


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 162 H 146 N 8 Ni 2	2,319.0372	1.5870	25.5332	94.00	ok	odd

Figure S16. MS/HRMS (MALDI) of ***p*-Ph**.

^{1}H NMR (601 MHz, CD_2Cl_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2, rt)

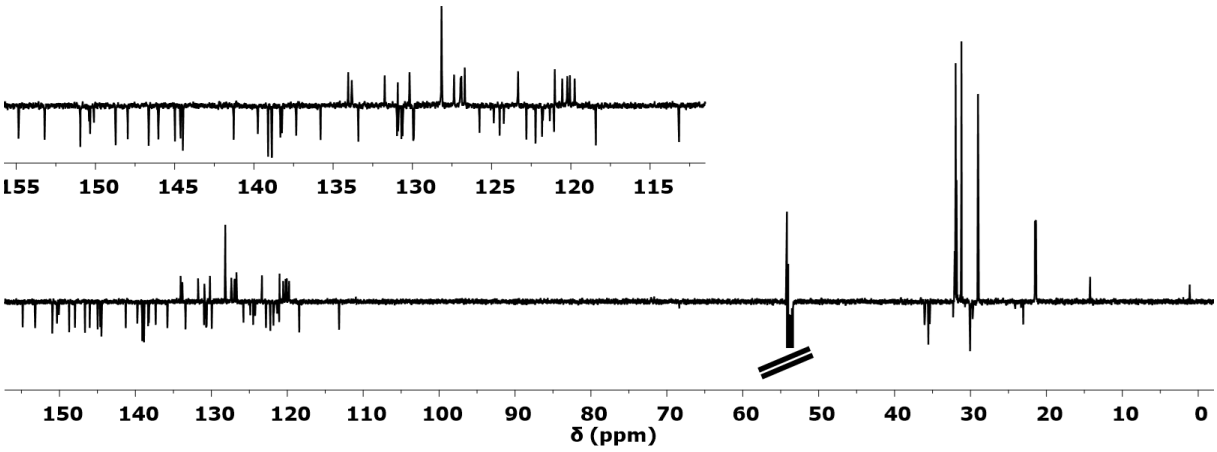


Figure S17. ^{1}H and ^{13}C NMR (DEPTQ135) of ***m*-Ph**.

^{1}H- ^{1}H COSY (601 MHz, CD_2Cl_2, rt)

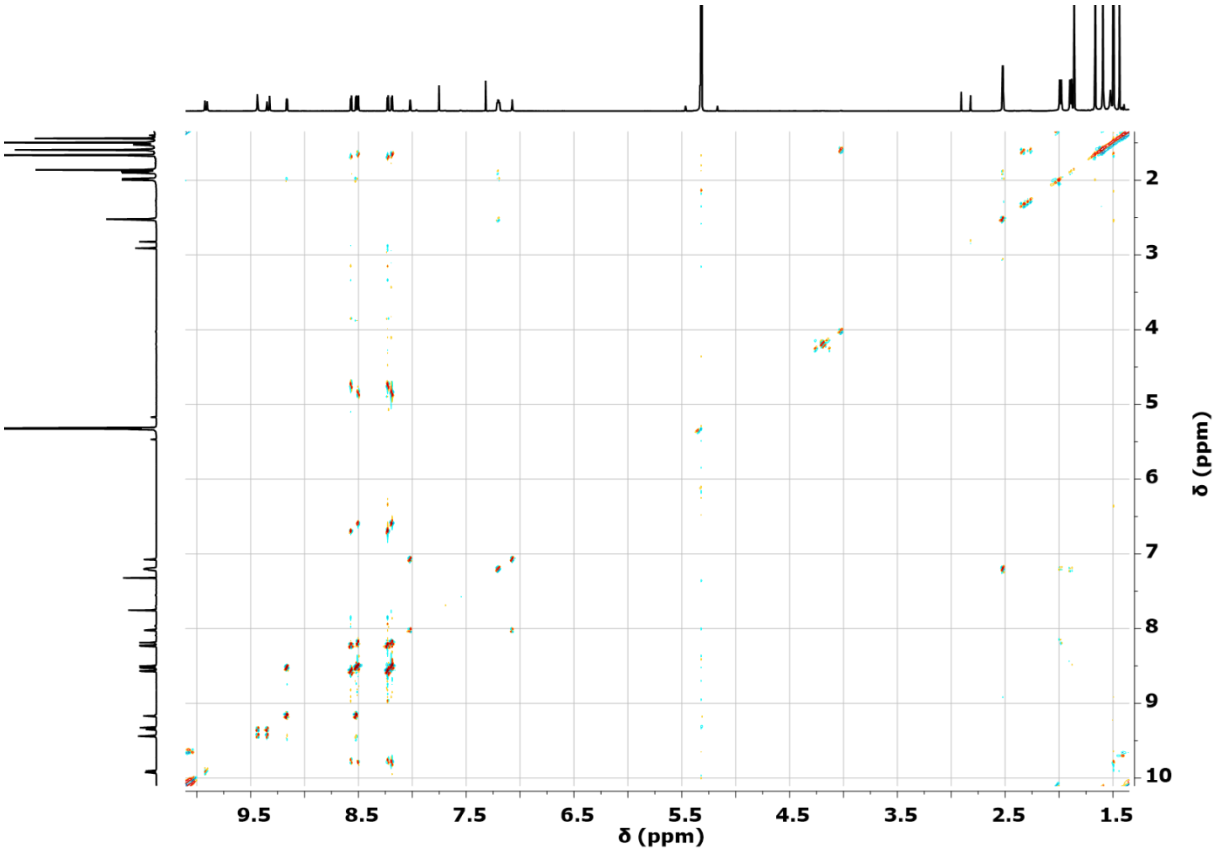


Figure S18. ^{1}H- ^{1}H COSY of ***m*-Ph**.

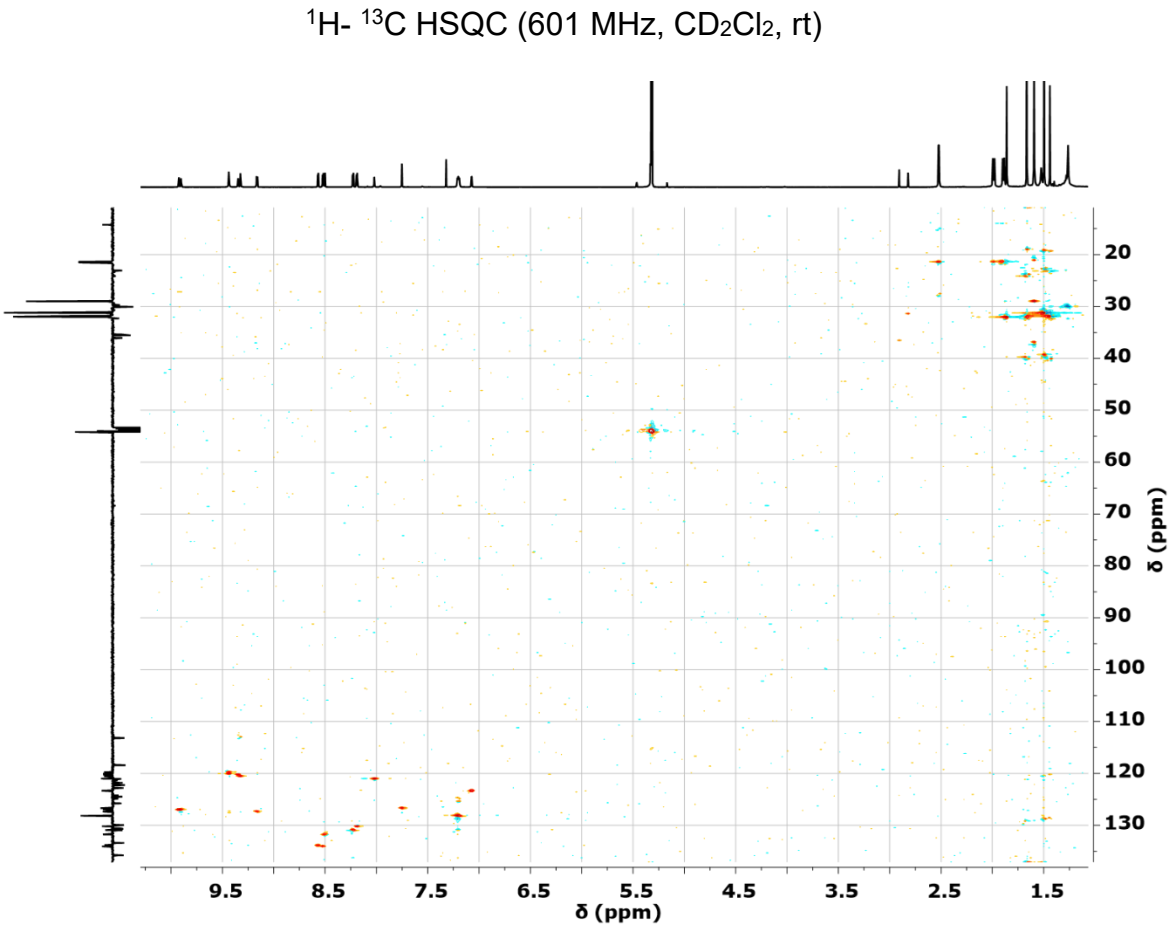


Figure S19. ^{1}H- ^{13}C HSQC of ***m*-Ph**.

^{1}H- ^{13}C HMBC (601 MHz, CD_2Cl_2, rt)

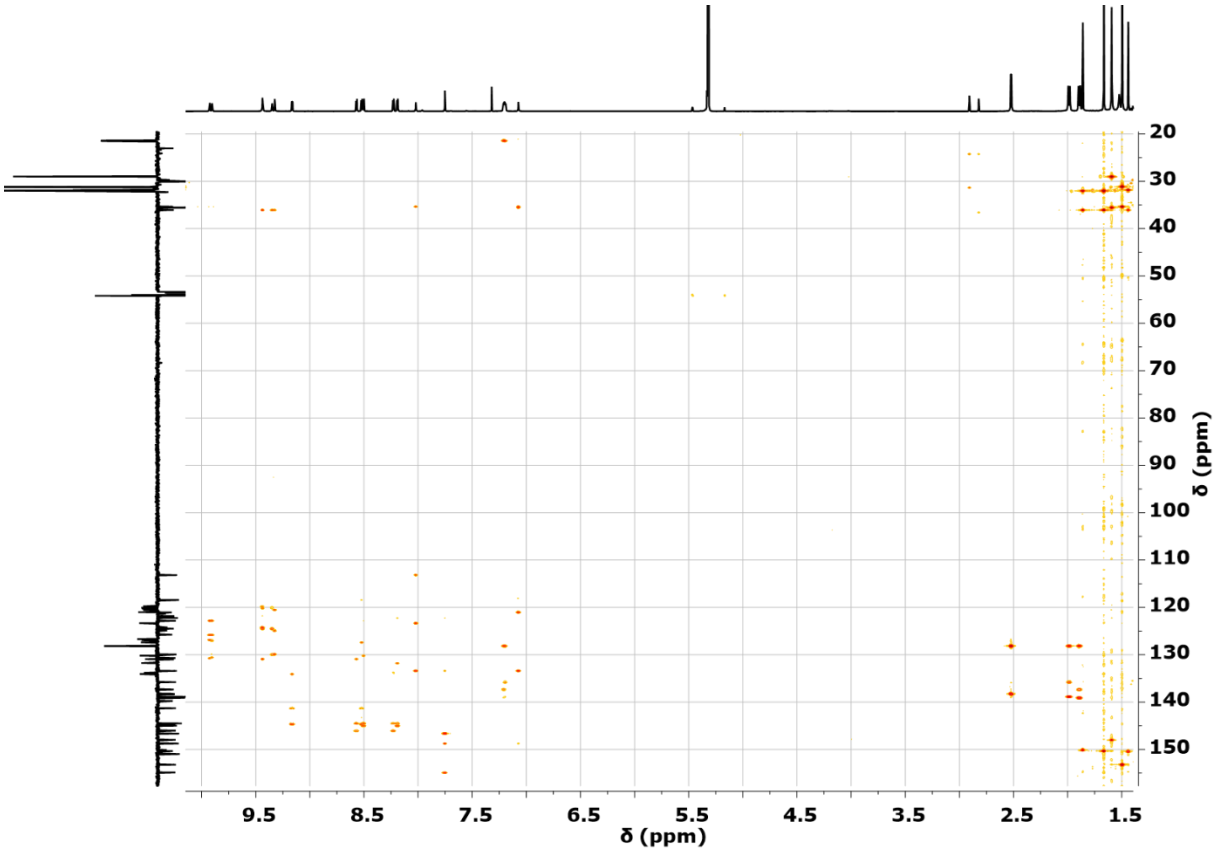


Figure S20. ^{1}H- ^{13}C HMBC of ***m*-Ph**.

^{1}H- ^{1}H ROESY (601 MHz, CD_2Cl_2, rt)

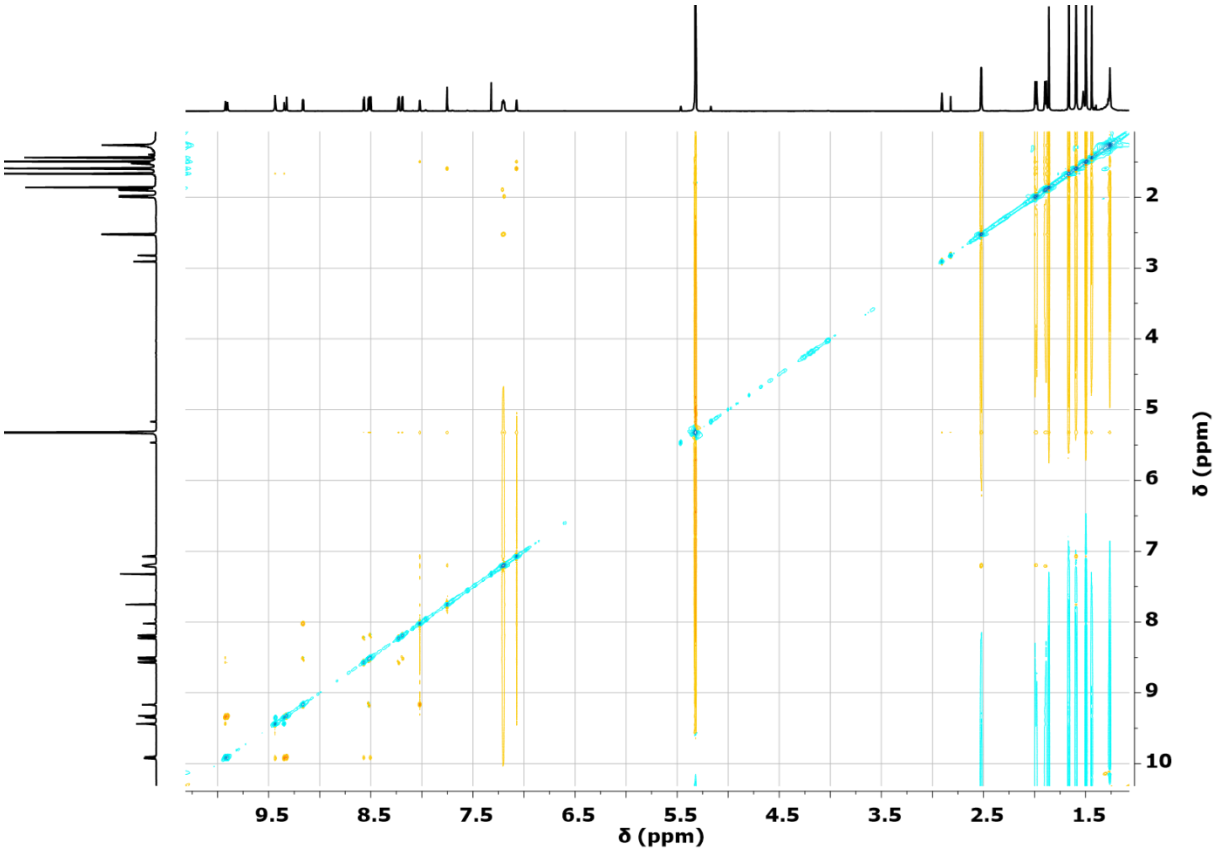
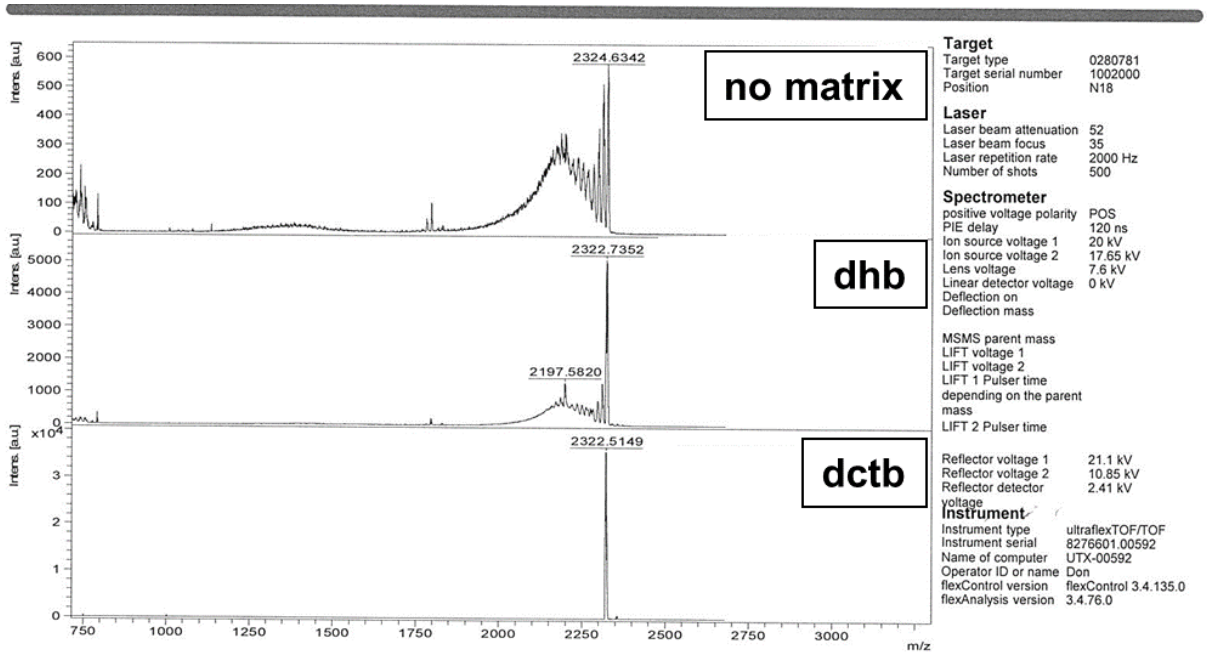
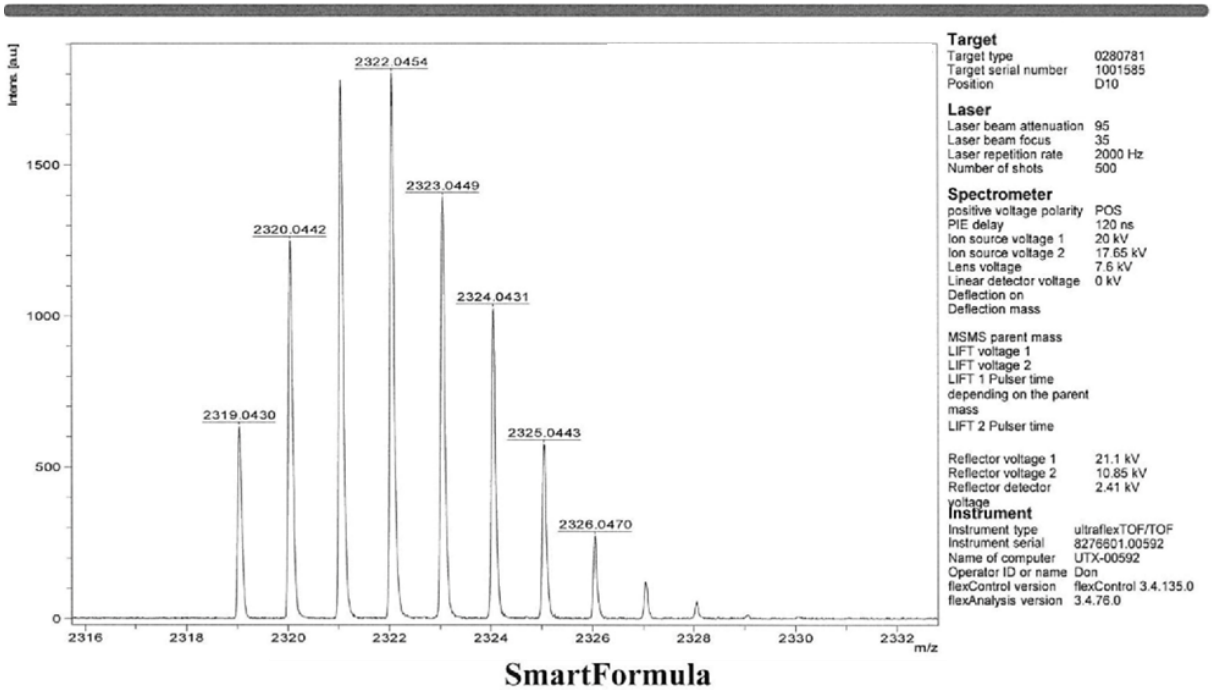


Figure S21. ^{1}H- ^{1}H ROESY of ***m*-Ph**.

MS (MALDI)



HRMS (MALDI)

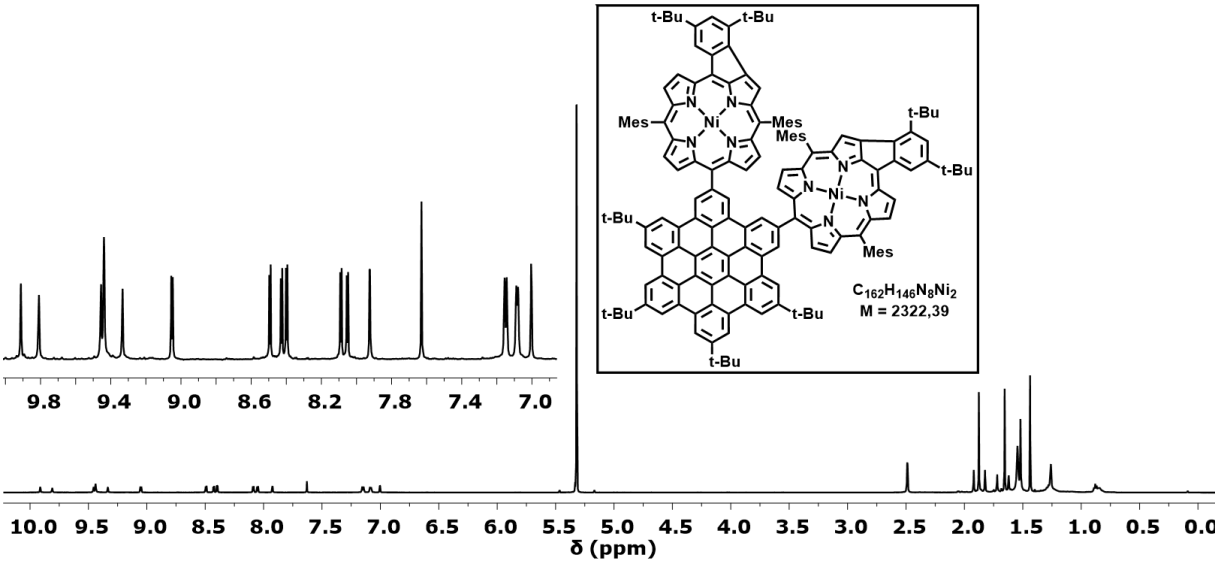


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 162 H 146 N 8 Ni 2	2,319.0372	2.5074	55.7052	94.00	ok	odd

Figure S22. MS/HRMS (MALDI) of ***m*-Ph**.

^{1}H NMR (601 MHz, CD_2Cl_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2, rt)

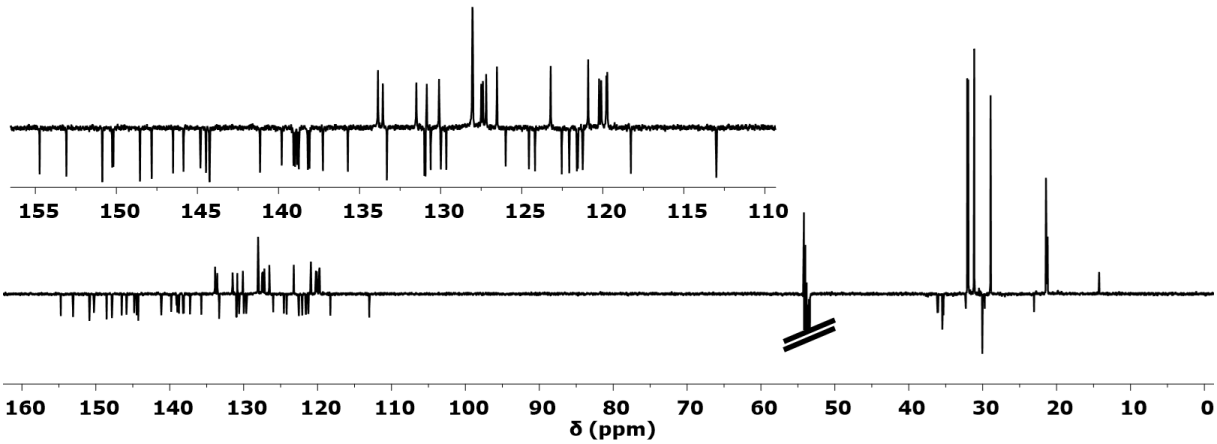


Figure S23. ^{1}H and ^{13}C NMR (DEPTQ135) of ***o*-Ph**.

^{1}H- ^{1}H COSY (601 MHz, CD_2Cl_2, rt)

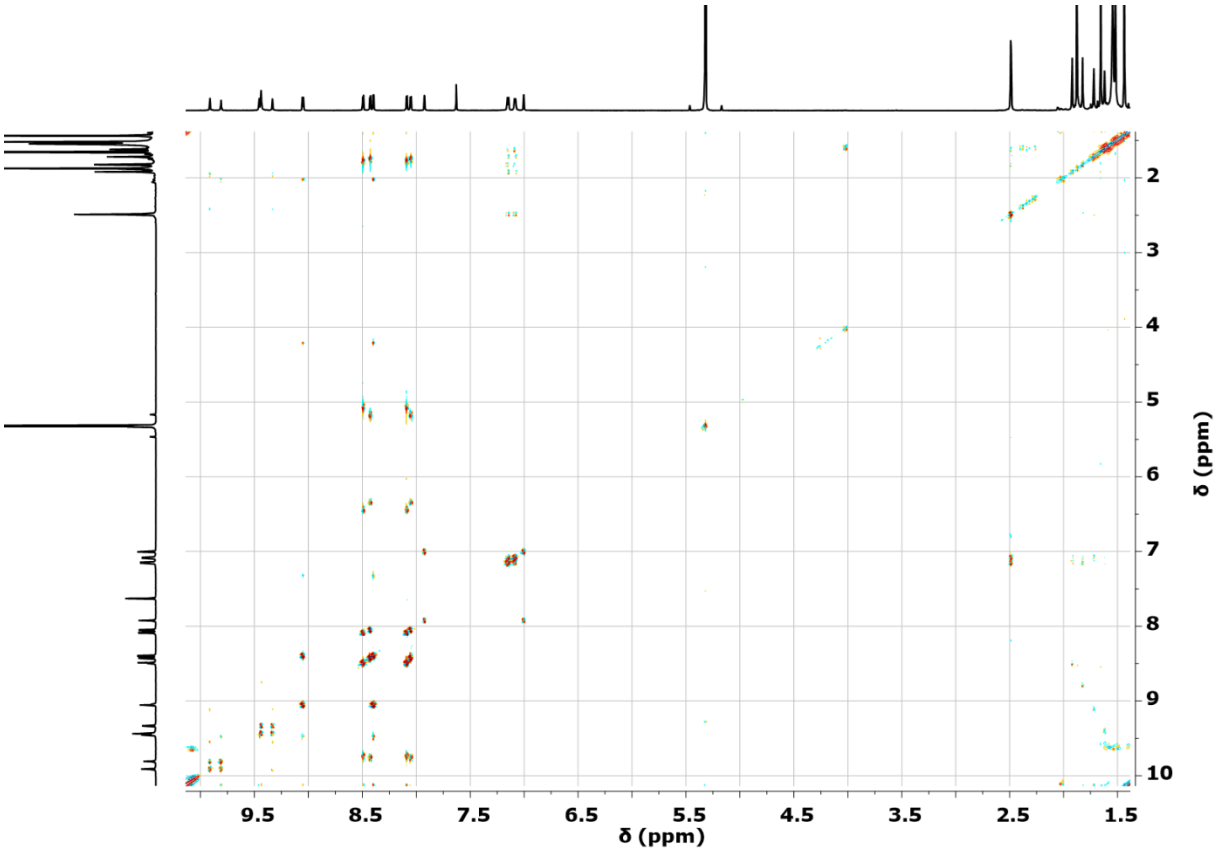


Figure S24. ^{1}H- ^{1}H COSY of ***o*-Ph**.

^{1}H- ^{13}C HSQC (601 MHz, CD_2Cl_2, rt)

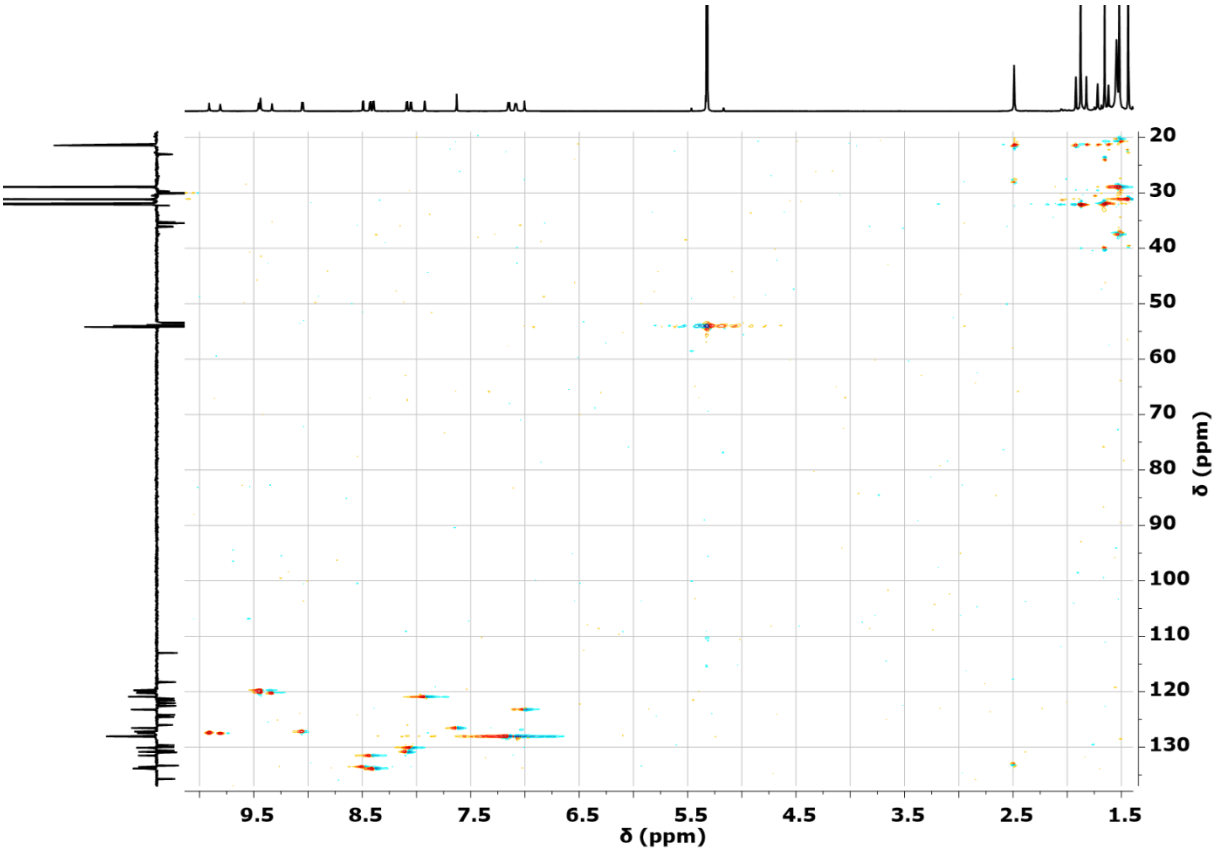


Figure S25. ^{1}H- ^{13}C HSQC of ***o*-Ph**.

^{1}H- ^{13}C HMBC (601 MHz, CD_2Cl_2, rt)

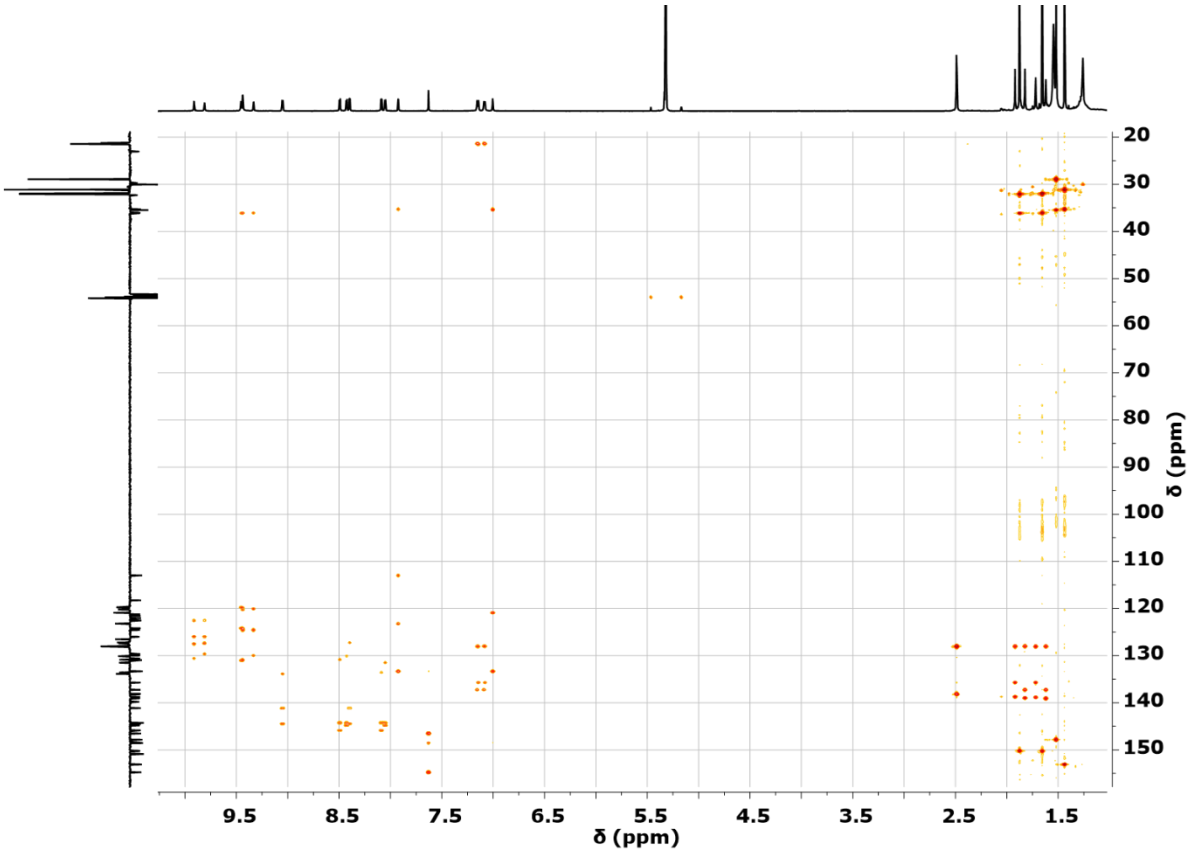


Figure S26. ^{1}H- ^{13}C HMBC of ***o*-Ph**.

^{1}H- ^{1}H ROESY (601 MHz, CD_2Cl_2, rt)

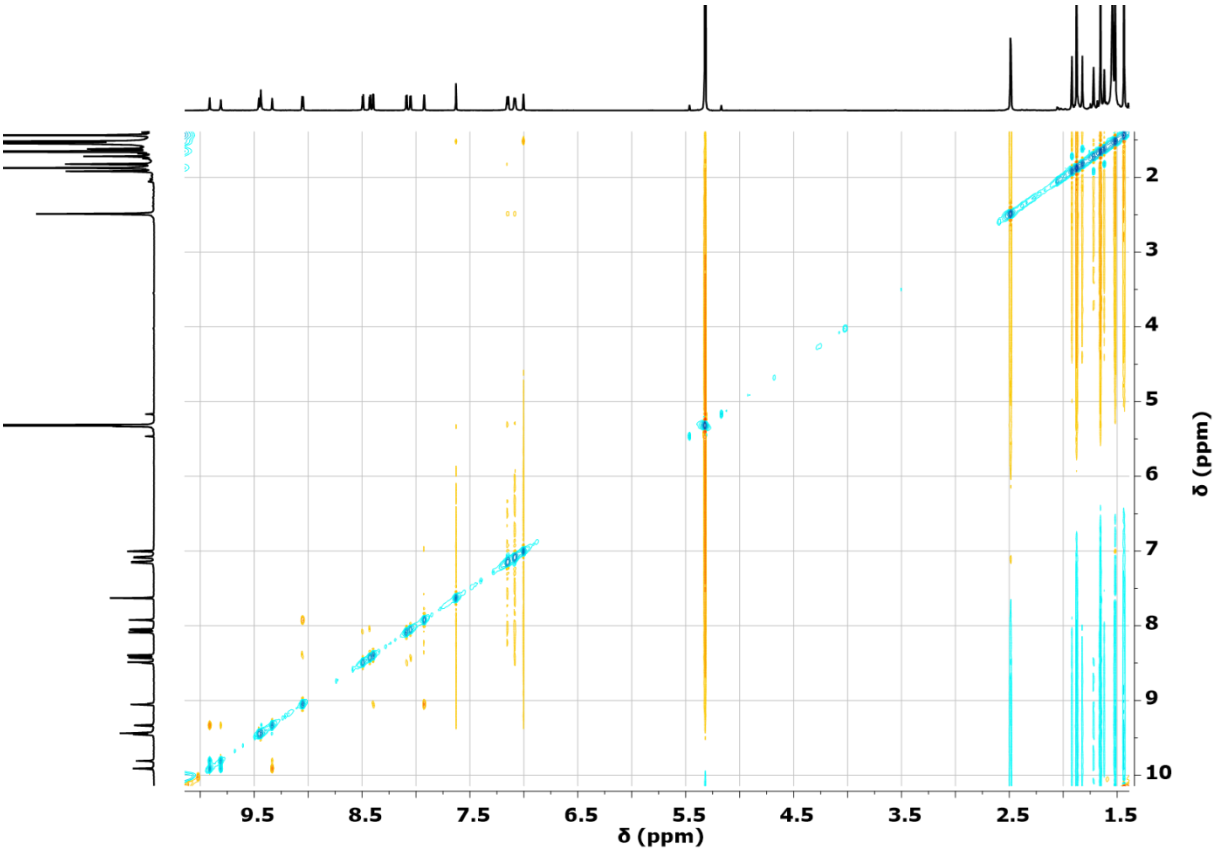
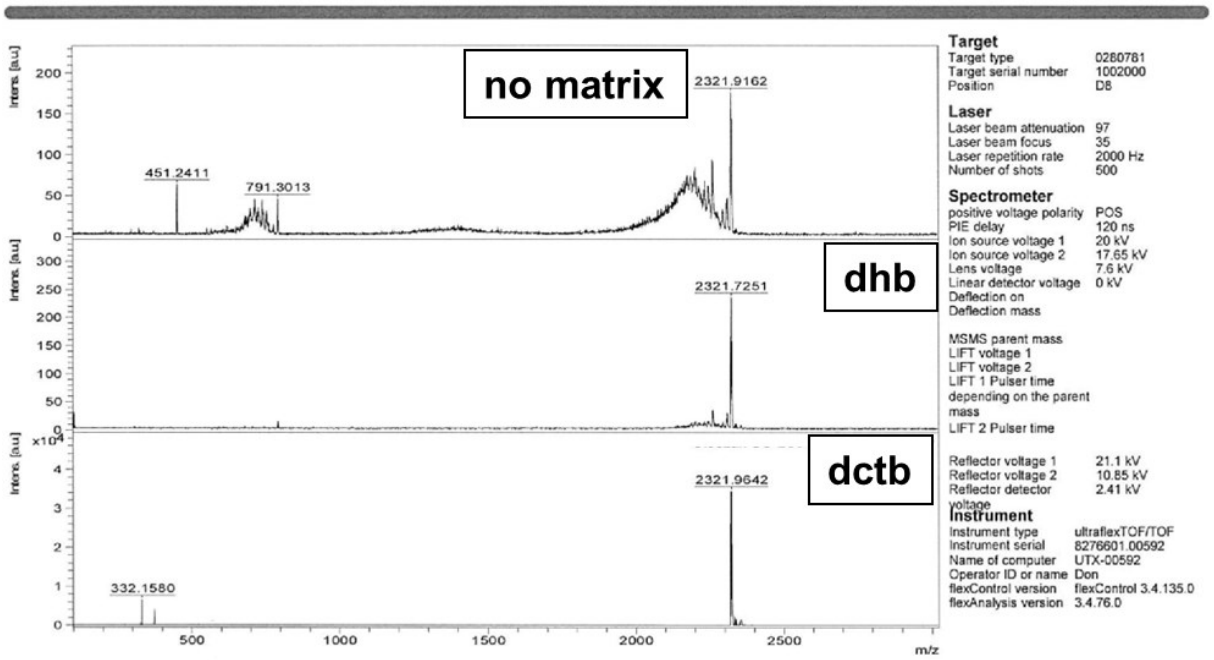
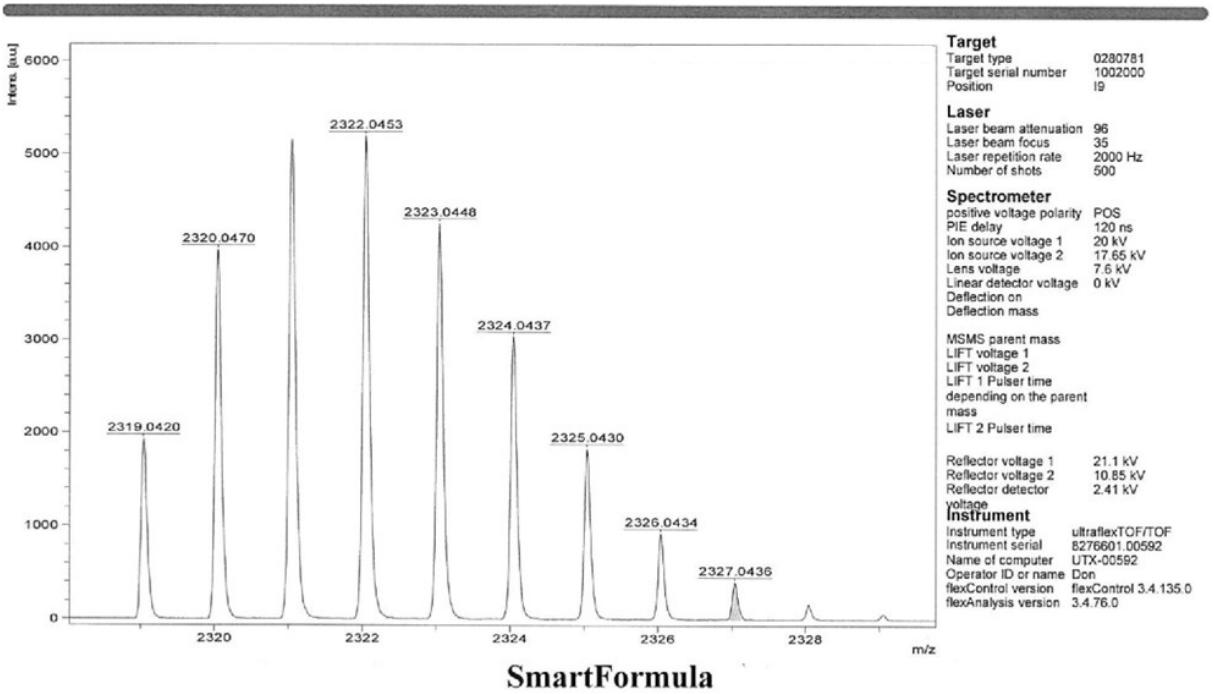


Figure S27. ^{1}H- ^{1}H ROESY of ***o*-Ph**.

MS (MALDI)



HRMS (MALDI)

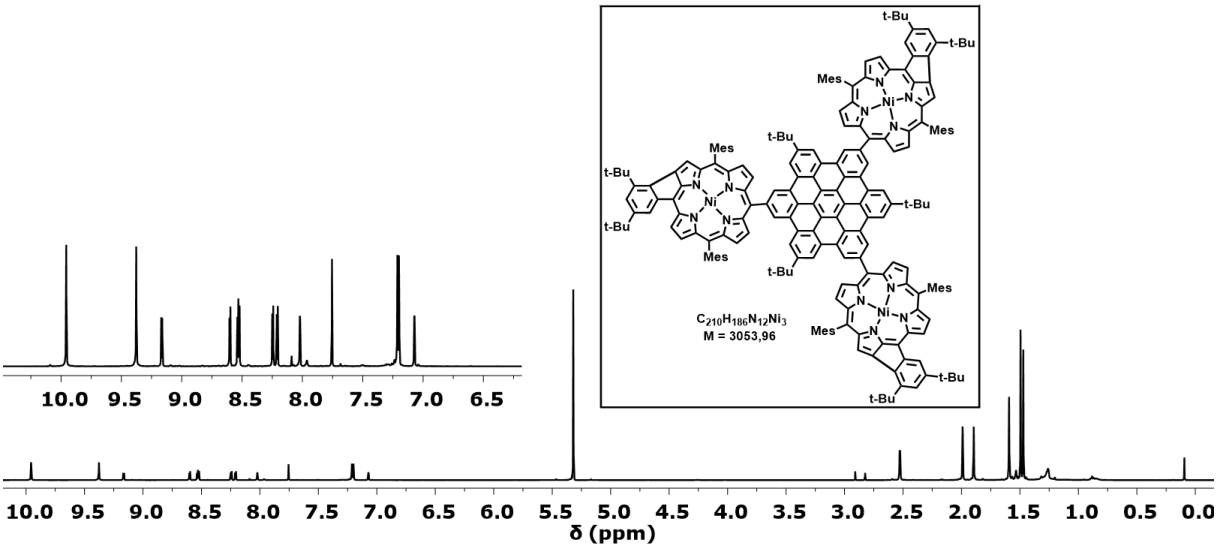


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 162 H 146 N 8 Ni 2	2,319.0372	2.0654	43.6349	94.00	ok	odd

Figure S28. MS/HRMS (MALDI) of ***o*-Ph**.

^{1}H NMR (601 MHz, CD_2Cl_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2, rt)

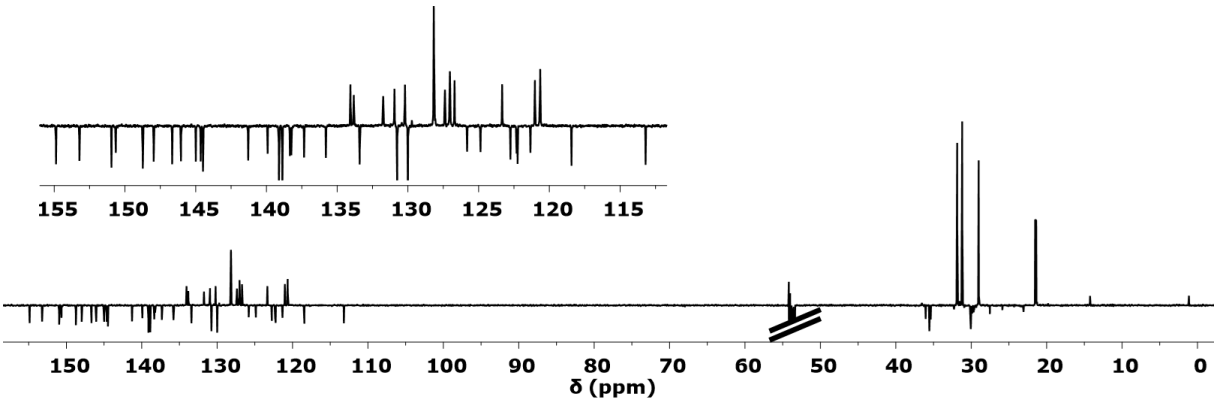


Figure S29. ^{1}H and ^{13}C NMR (DEPTQ135) of ***tri*-Ph**.

^{1}H- ^{1}H COSY (601 MHz, CD_2Cl_2, rt)

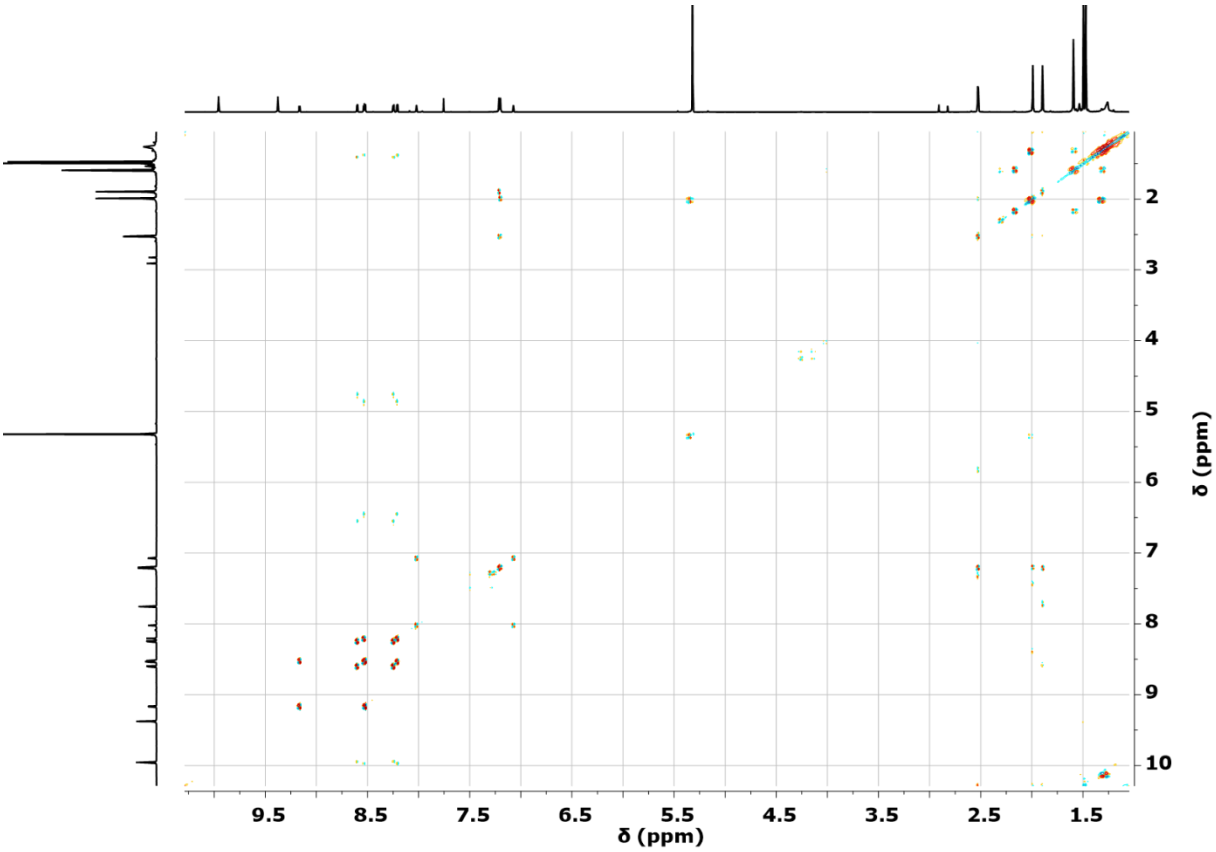


Figure S30. ^{1}H- ^{1}H COSY of ***tri*-Ph**.

^{1}H- ^{13}C HSQC (601 MHz, CD_2Cl_2, rt)

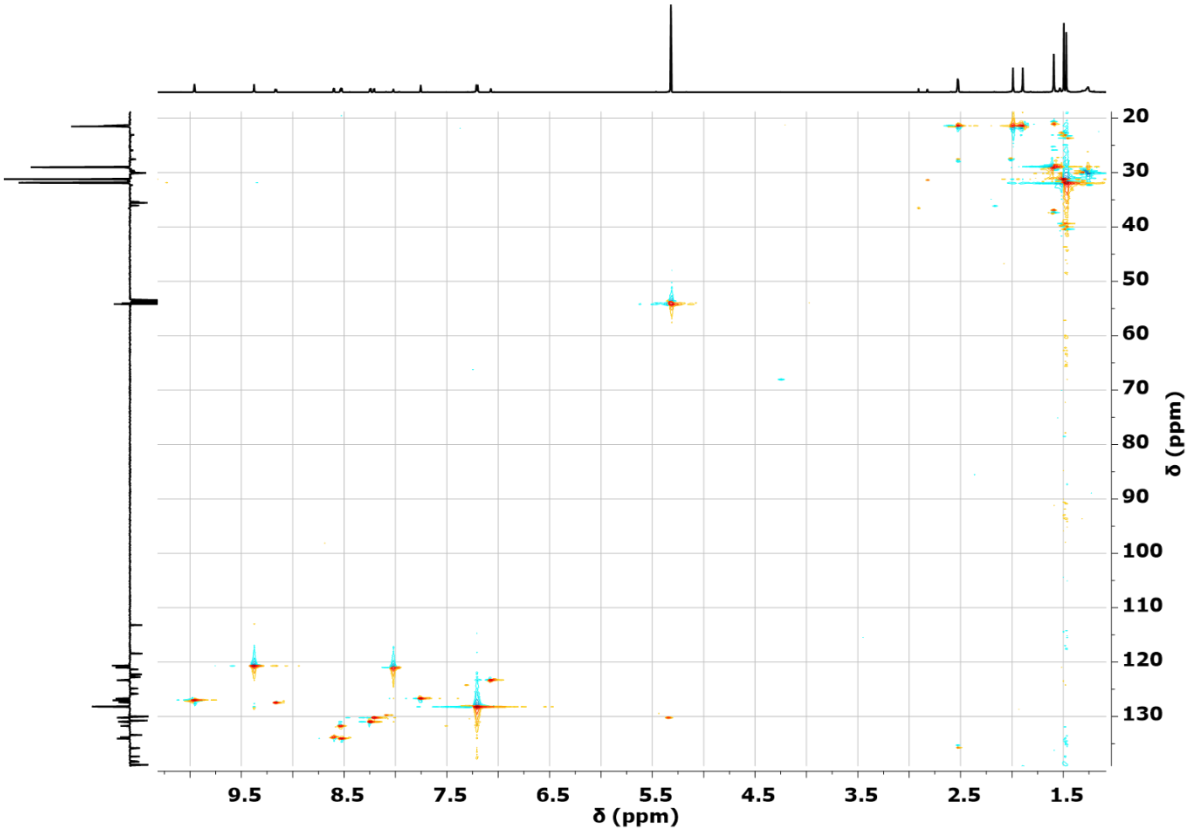


Figure S31. ^{1}H- ^{13}C HSQC of ***tri*-Ph**.

^{1}H- ^{13}C HMBC (601 MHz, CD_2Cl_2, rt)

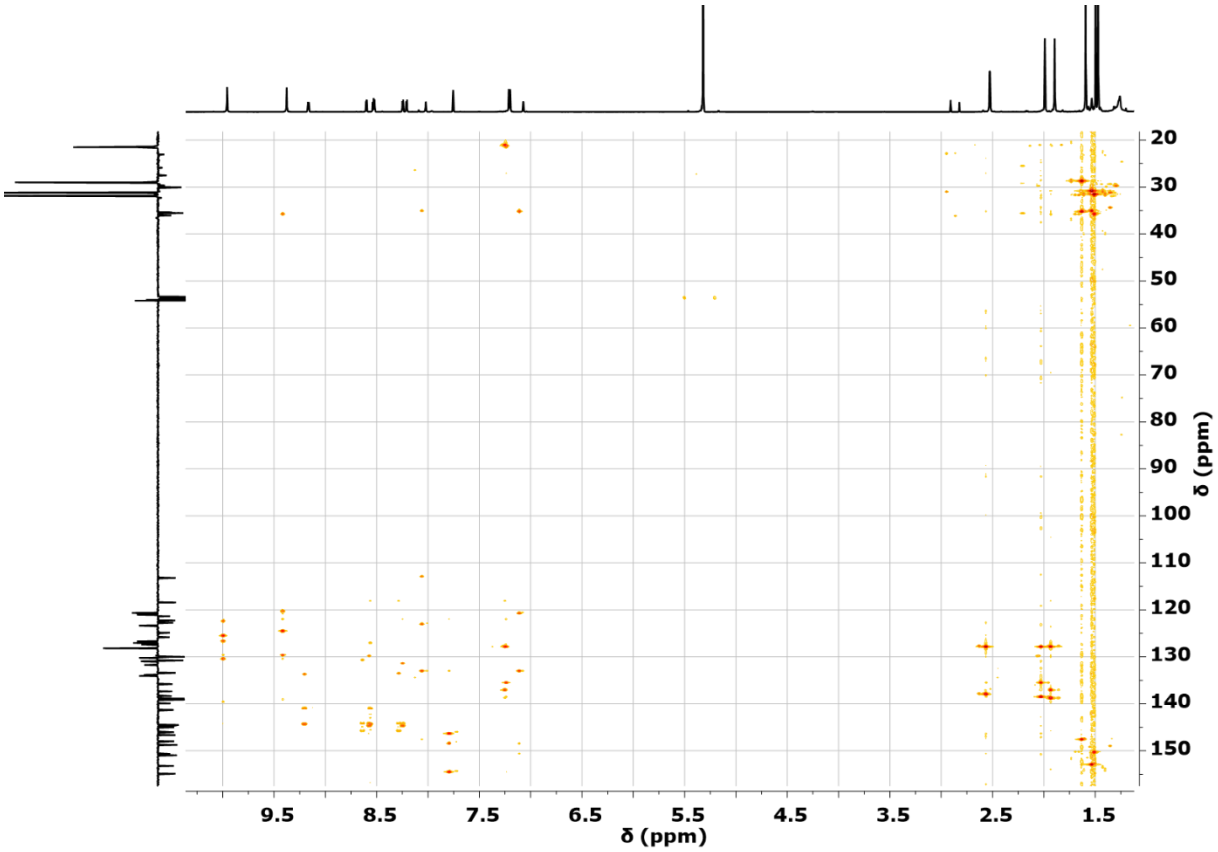


Figure S32. ^{1}H- ^{13}C HMBC of ***tri*-Ph**.

^{1}H- ^{1}H ROESY (601 MHz, CD_2Cl_2, rt)

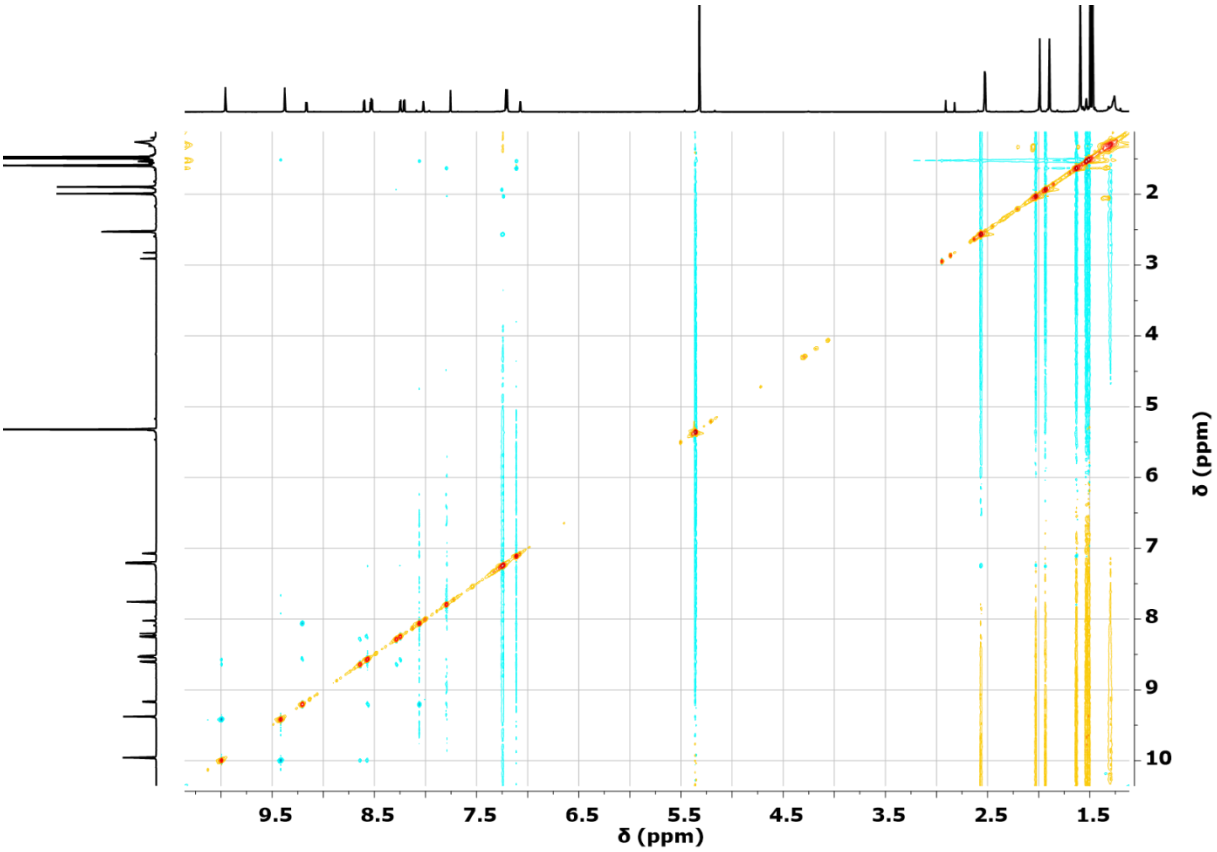
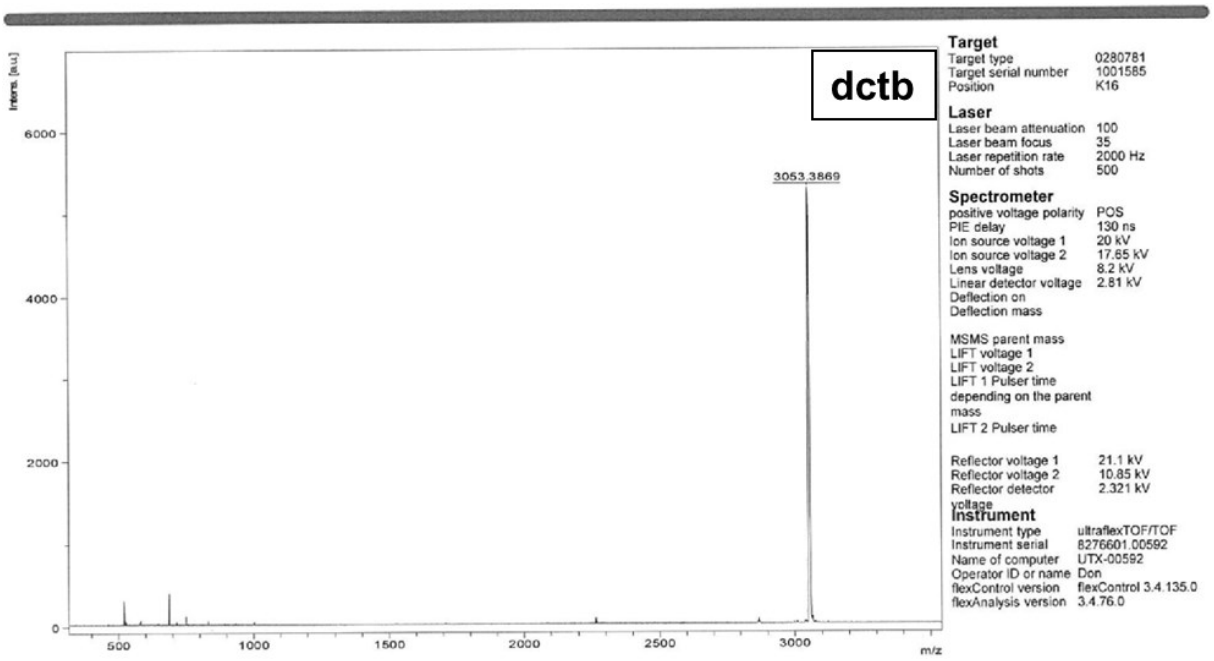
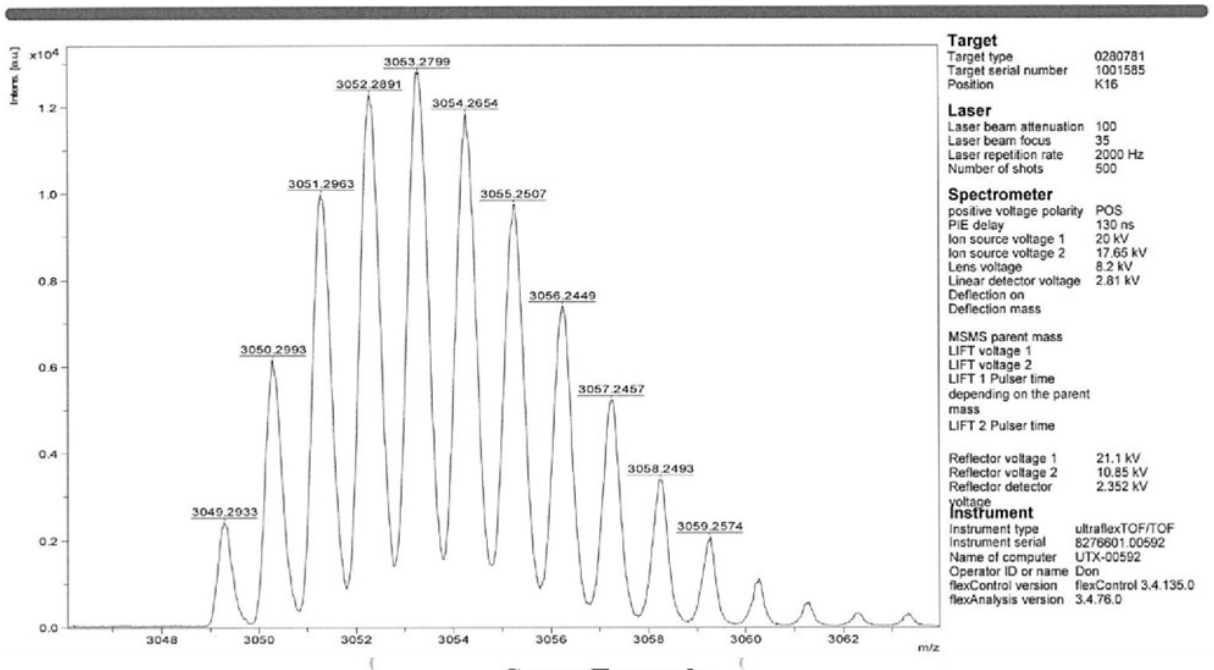


Figure S33. ^{1}H- ^{1}H ROESY of ***tri*-Ph**.

MS (MALDI)



HRMS (MALDI)

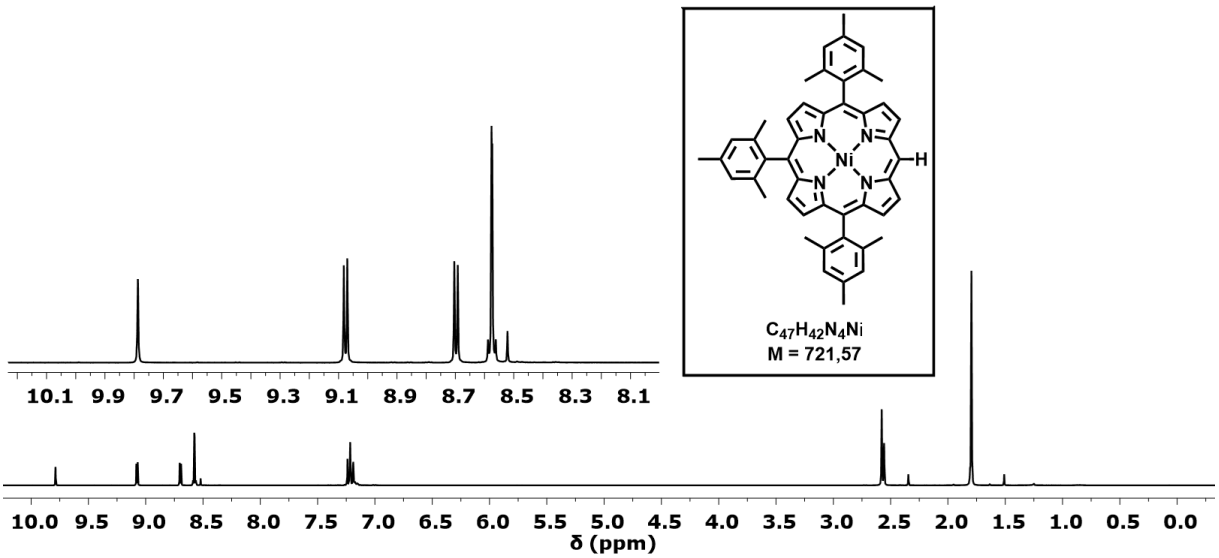


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 210 H 186 N 12 Ni 3	3,049.2978	1.4948	34.4860	124.00	ok	odd

Figure S34. MS/HRMS (MALDI) of ***tri*-Ph**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

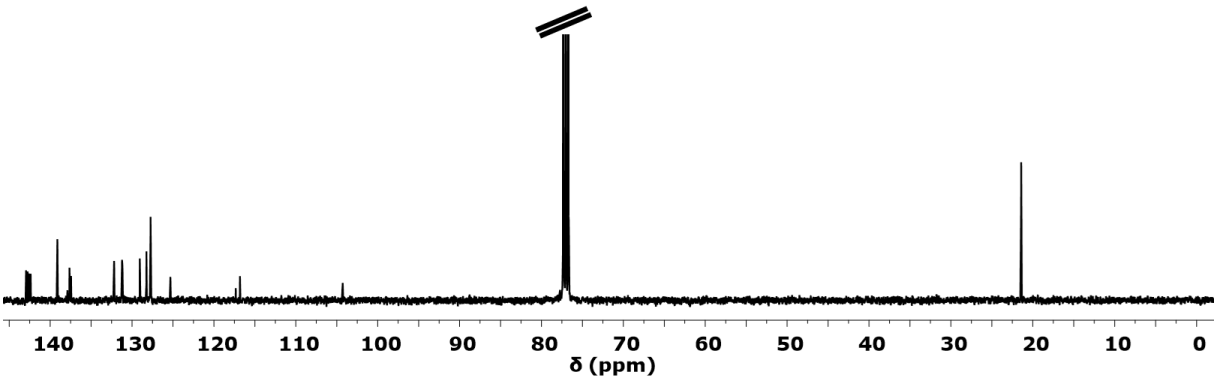
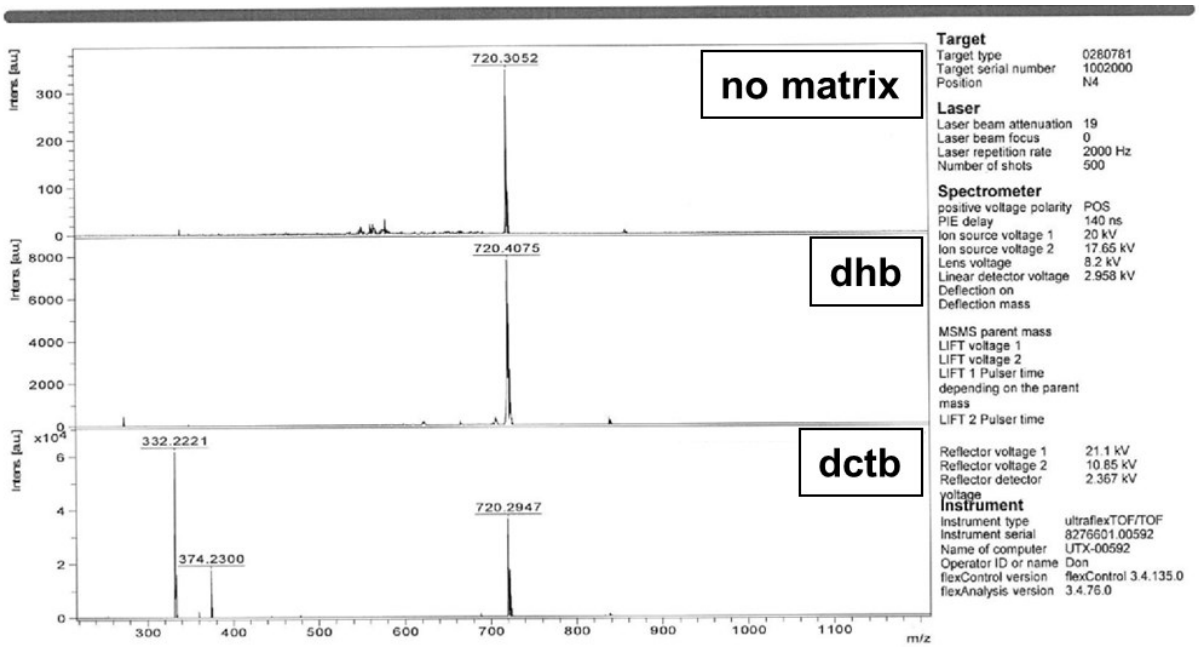
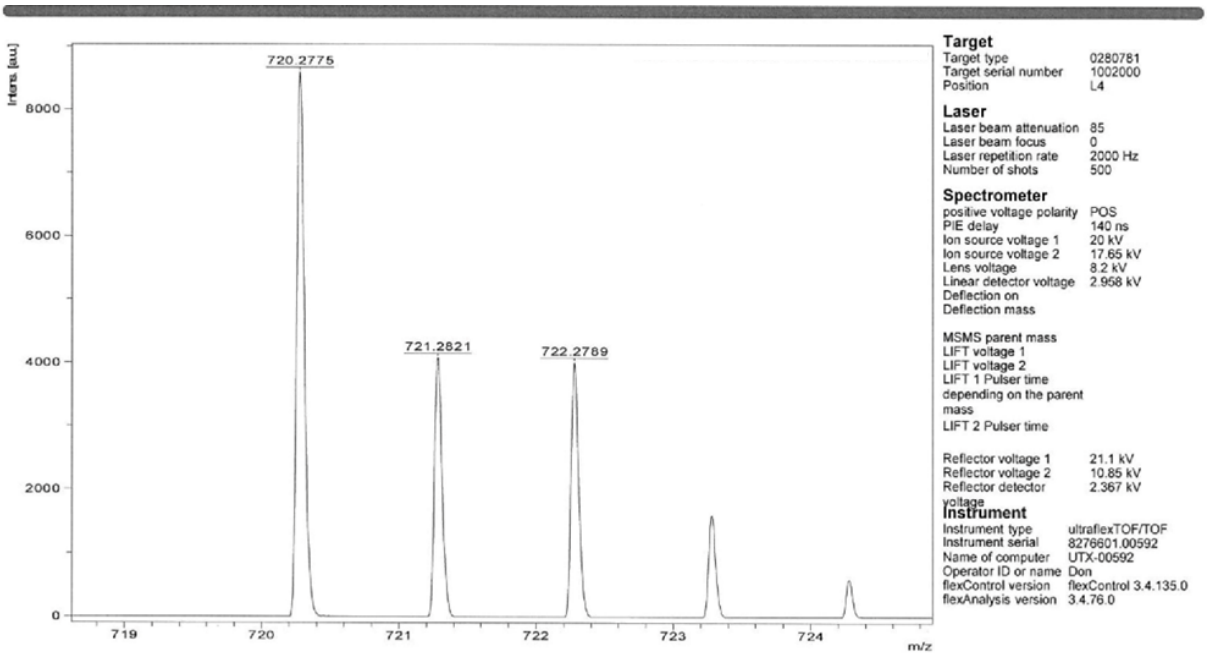


Figure S35. ^{1}H and ^{13}C NMR of **21**.

MS (MALDI)



HRMS (MALDI)

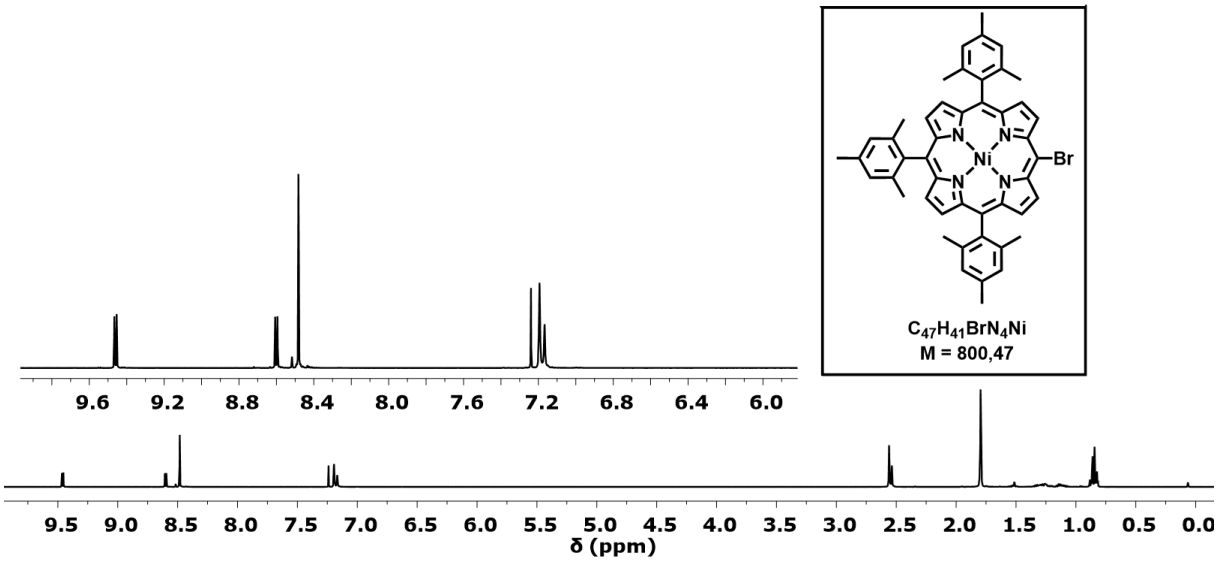


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 47 H 42 N 4 Ni	720.2757	2.3975	100.6242	29.00	ok	odd

Figure S36. MS/HRMS (MALDI) of **21**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

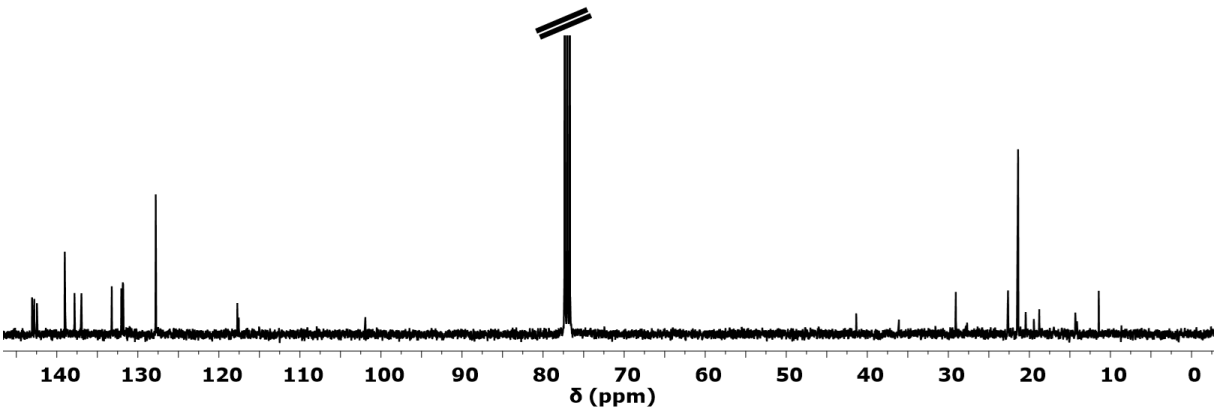
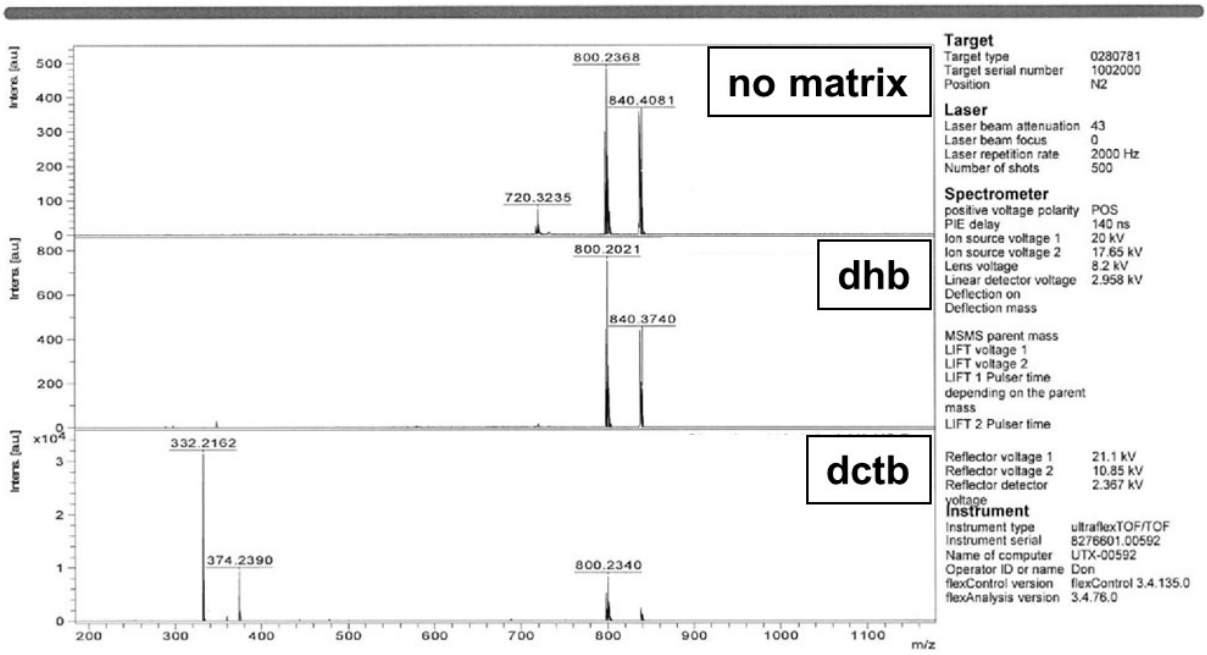
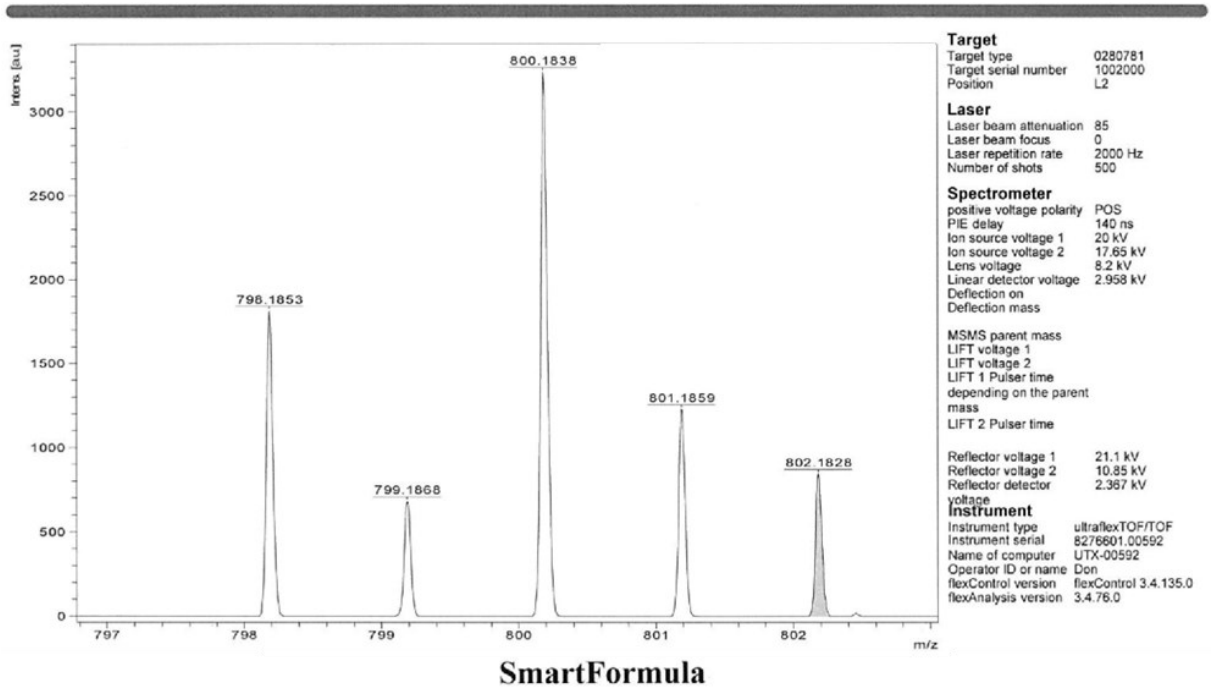


Figure S37. ^{1}H and ^{13}C NMR of **22**.

MS (MALDI)



HRMS (MALDI)

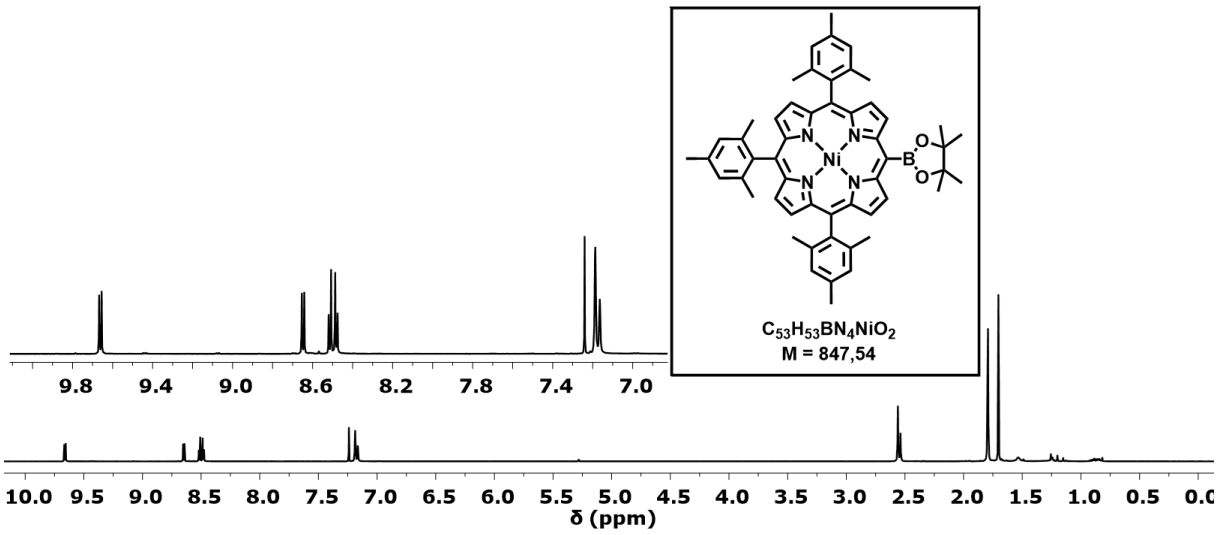


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 47 H 41 Br N 4 Ni	798.1863	1.1747	247.2498	29.00	ok	odd

Figure S38. MS/HRMS (MALDI) of **22**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

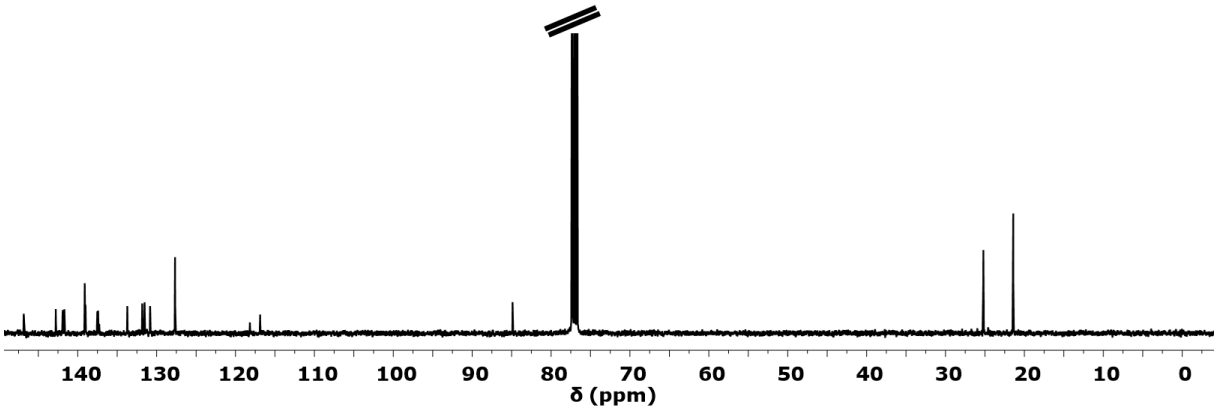
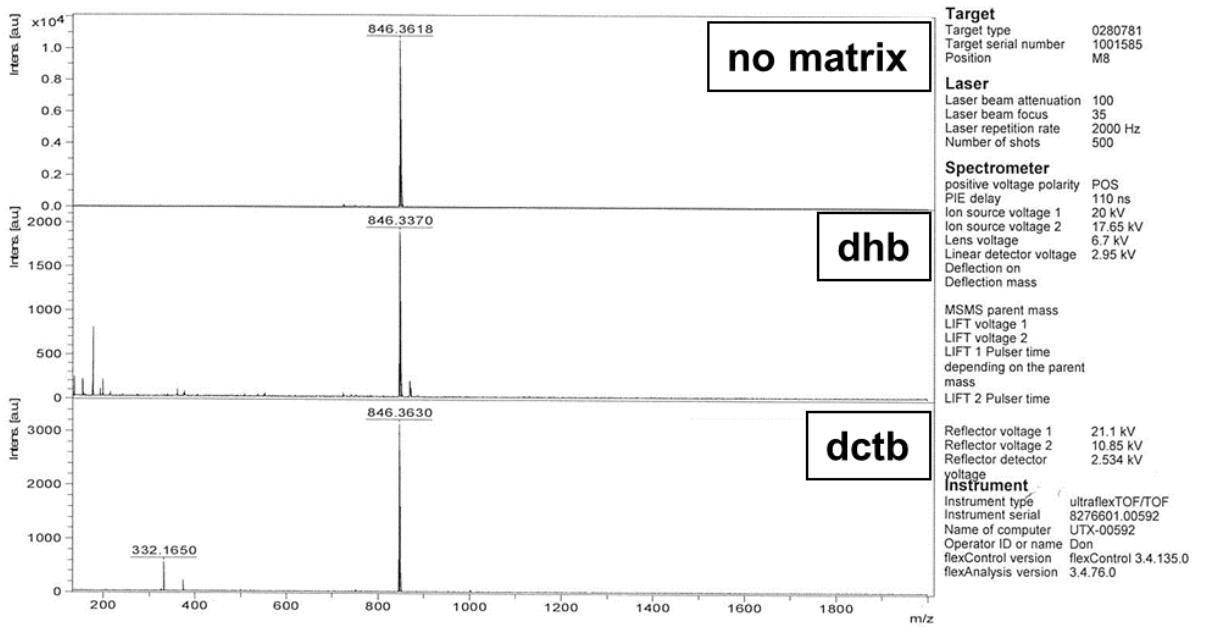
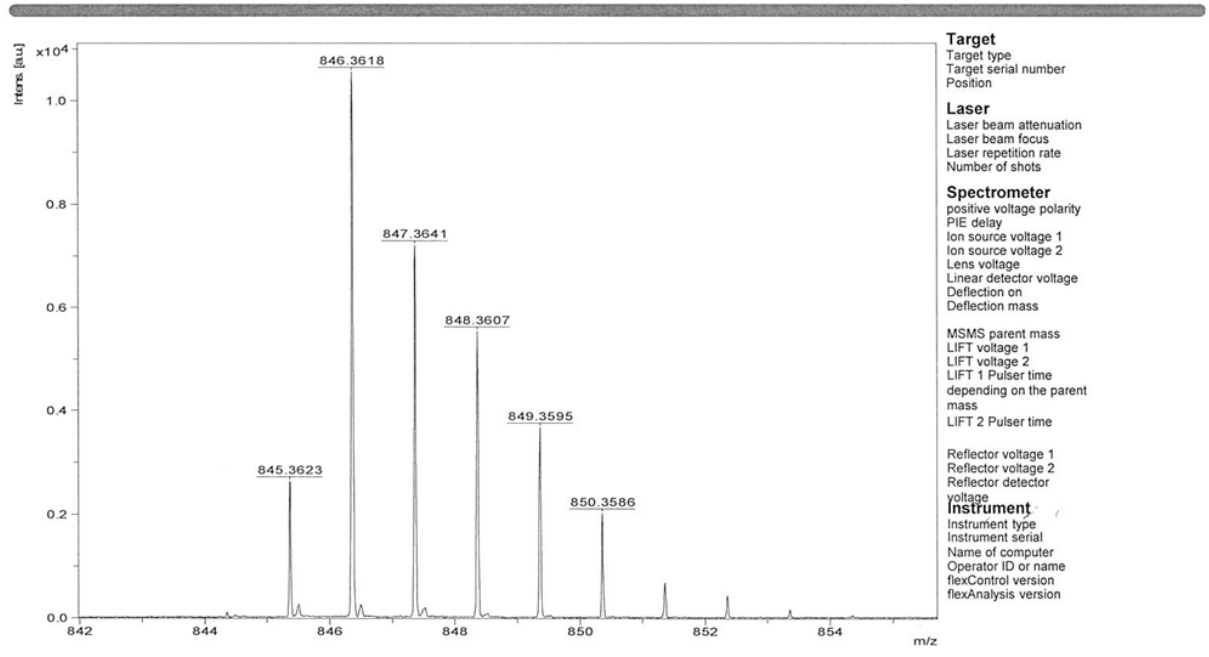


Figure S39. ^{1}H and ^{13}C NMR of **10**.

MS (MALDI)



HRMS (MALDI)

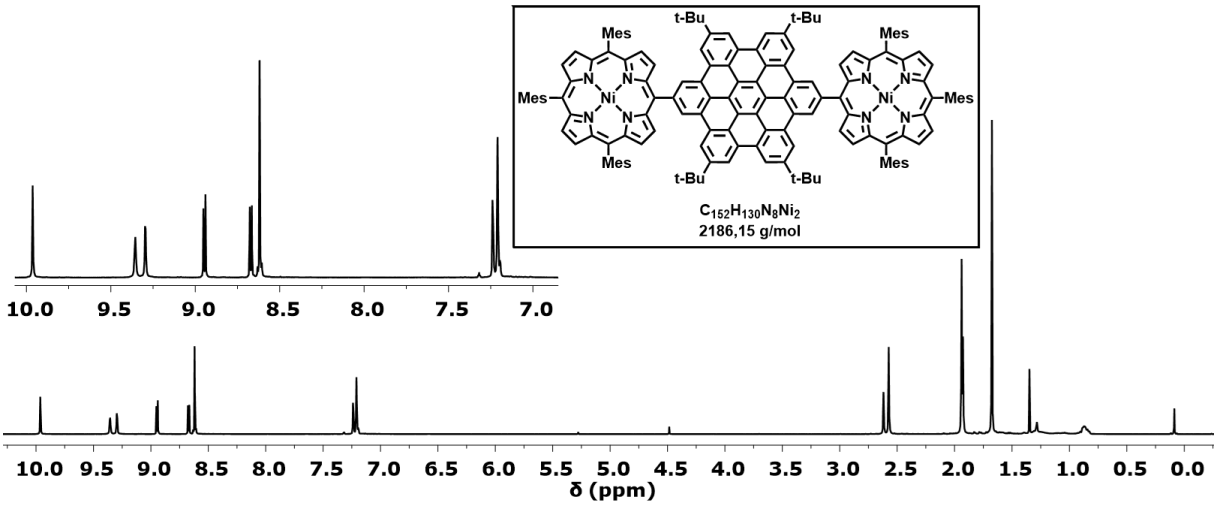


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 53 H 53 B N 4 Ni O 2	846.3610	1.0248	42.1791	30.00	ok	odd

Figure S40. MS/HRMS (MALDI) of **10**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

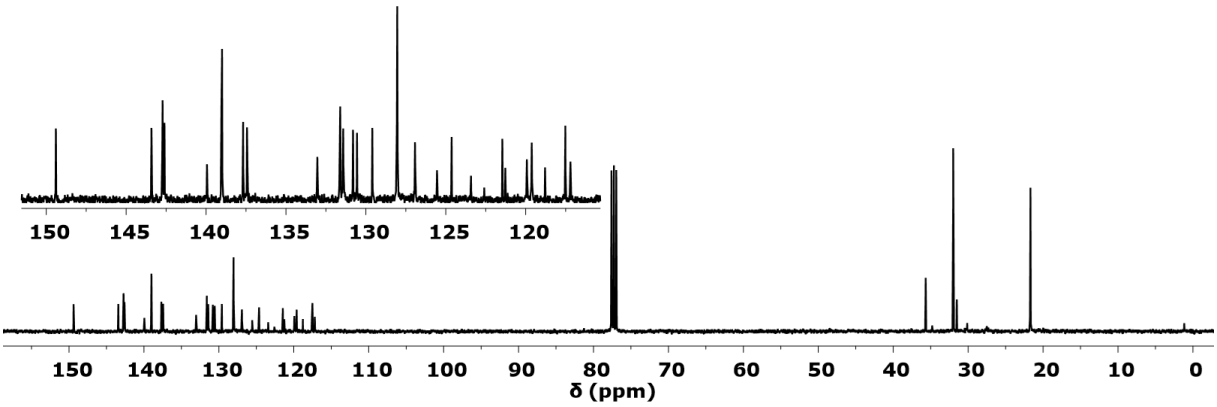
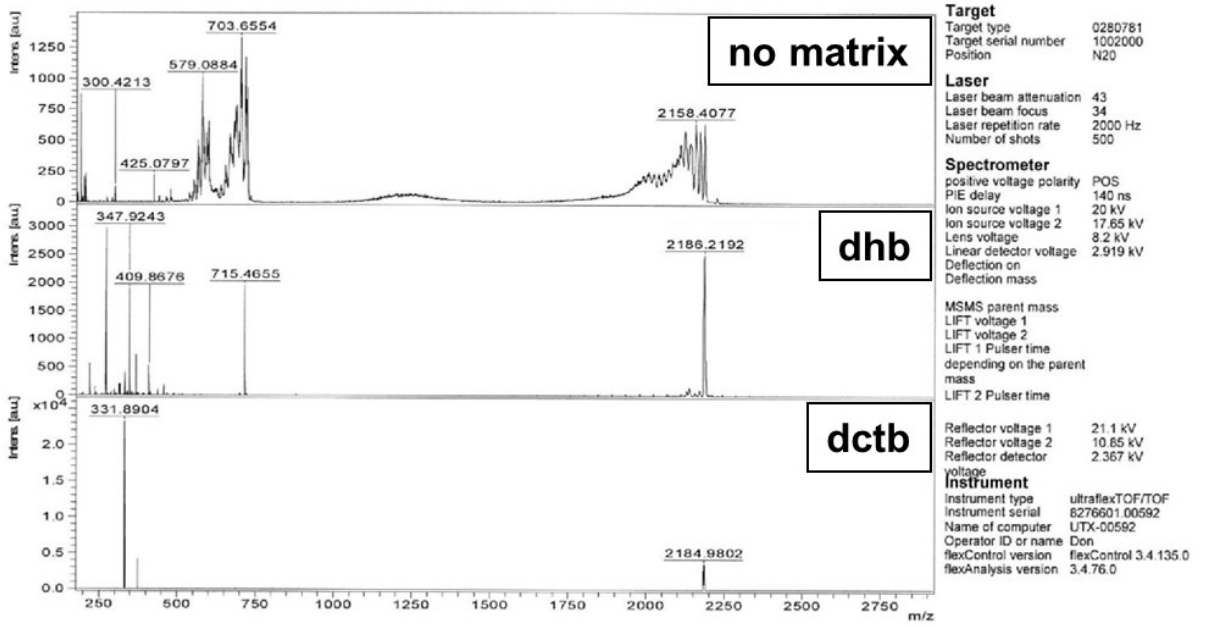
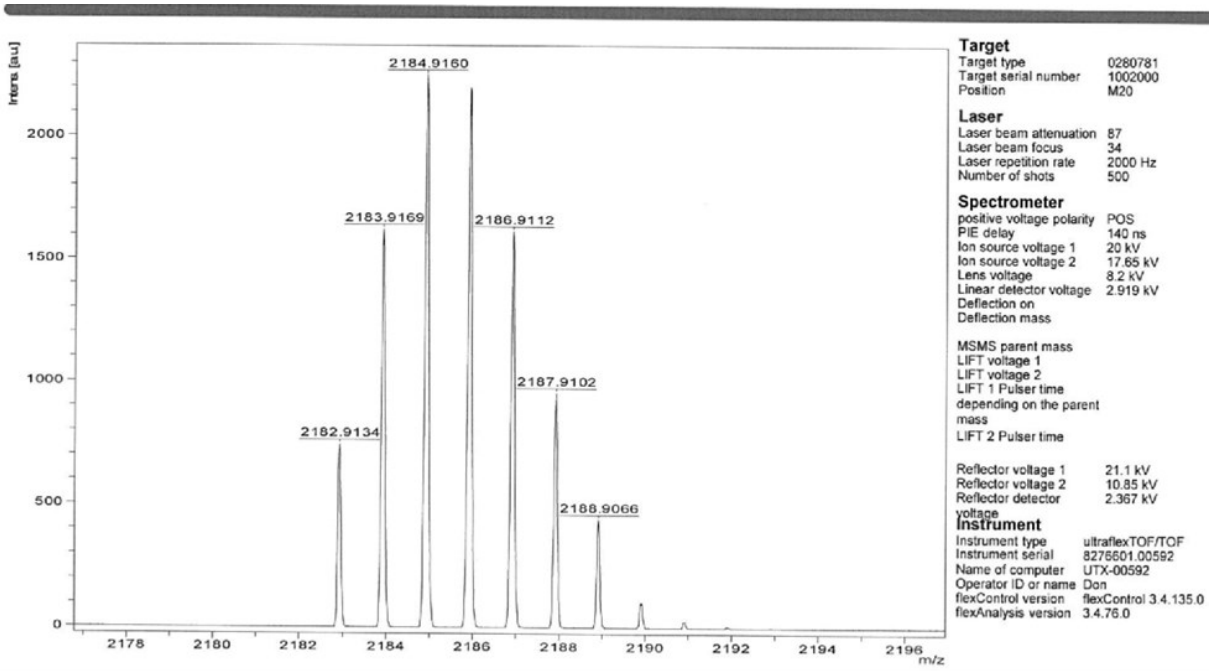


Figure S41. ^{1}H and ^{13}C NMR of **12**.

MS (MALDI)



HRMS (MALDI)

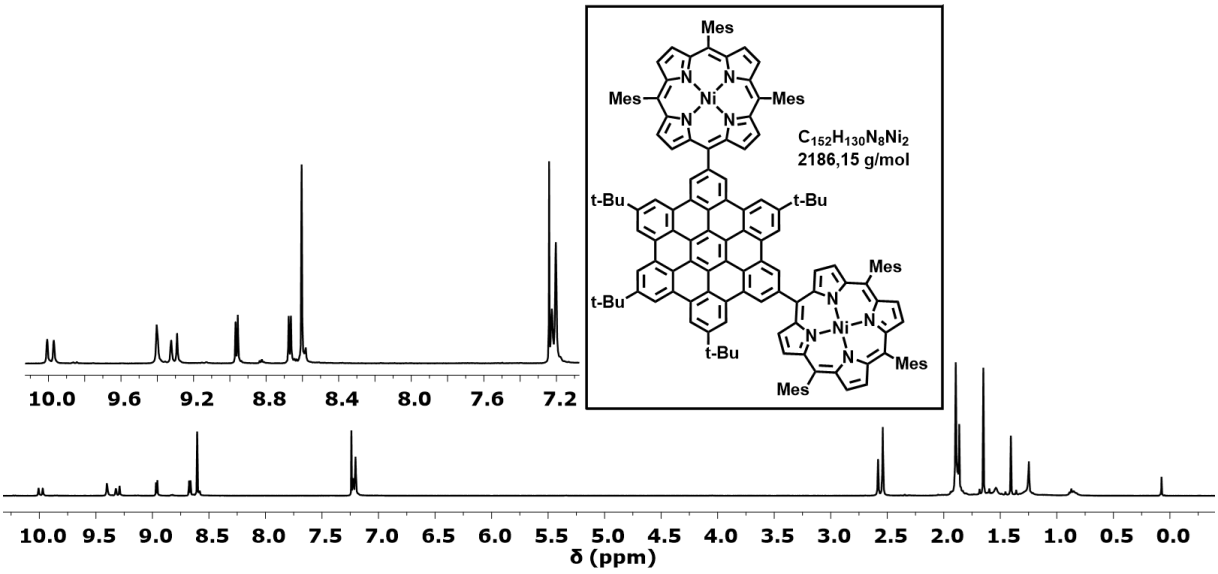


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 152 H 130 N 8 Ni 2	2,182.9120	0.6437	95.6119	92.00	ok	odd

Figure S42. MS/HRMS (MALDI) of **12**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

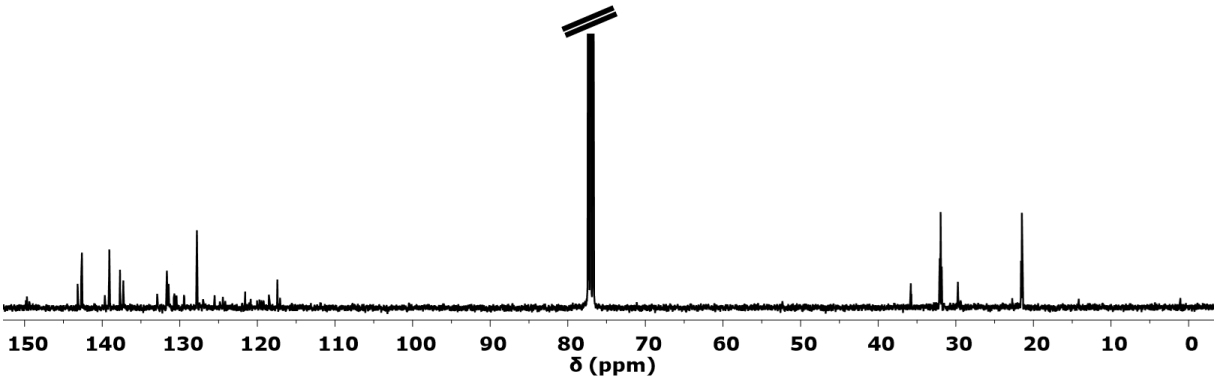
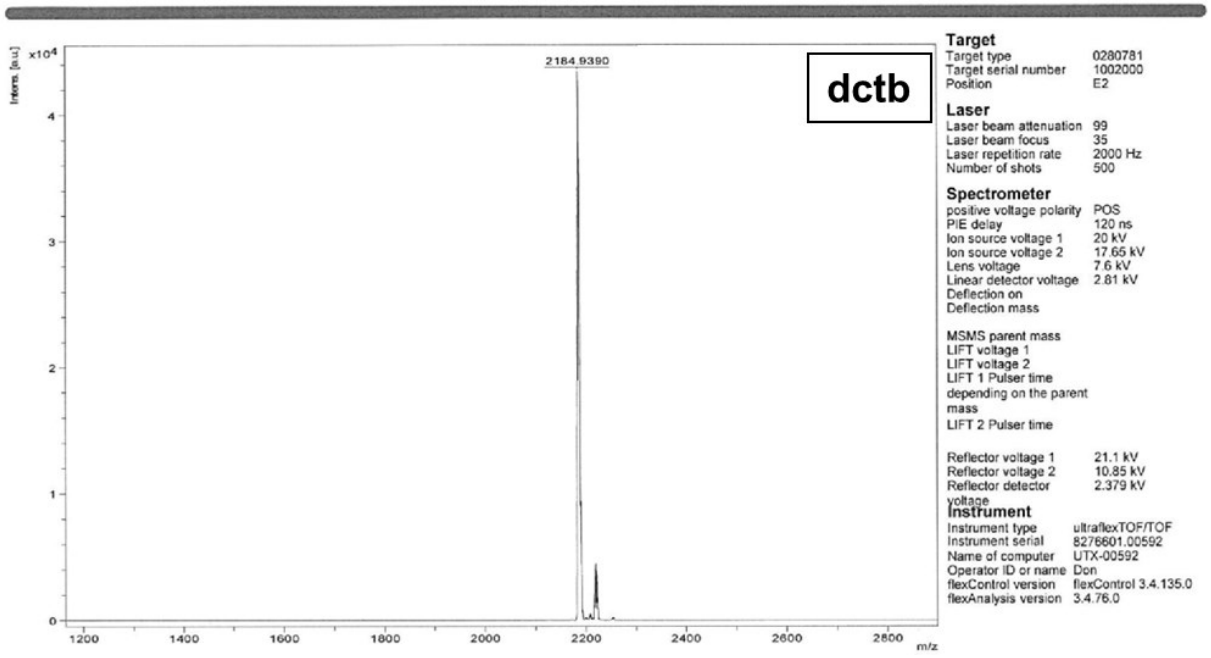
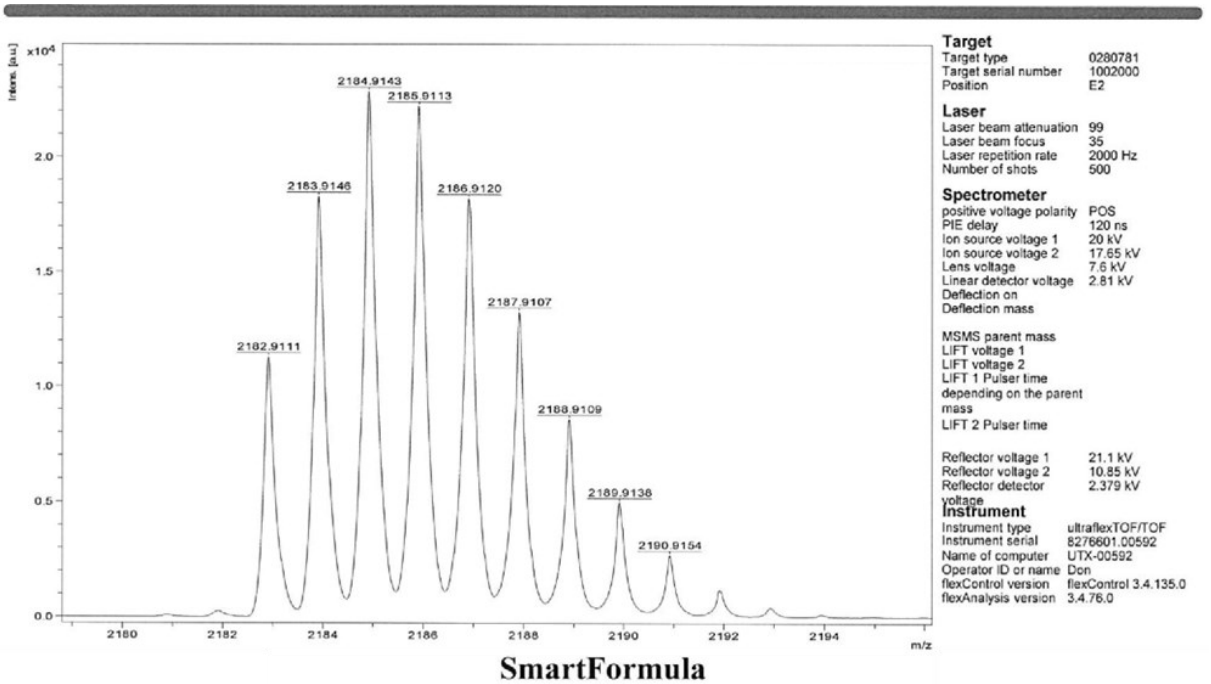


Figure S43. ^{1}H and ^{13}C NMR of **13**.

MS (MALDI)



HRMS (MALDI)

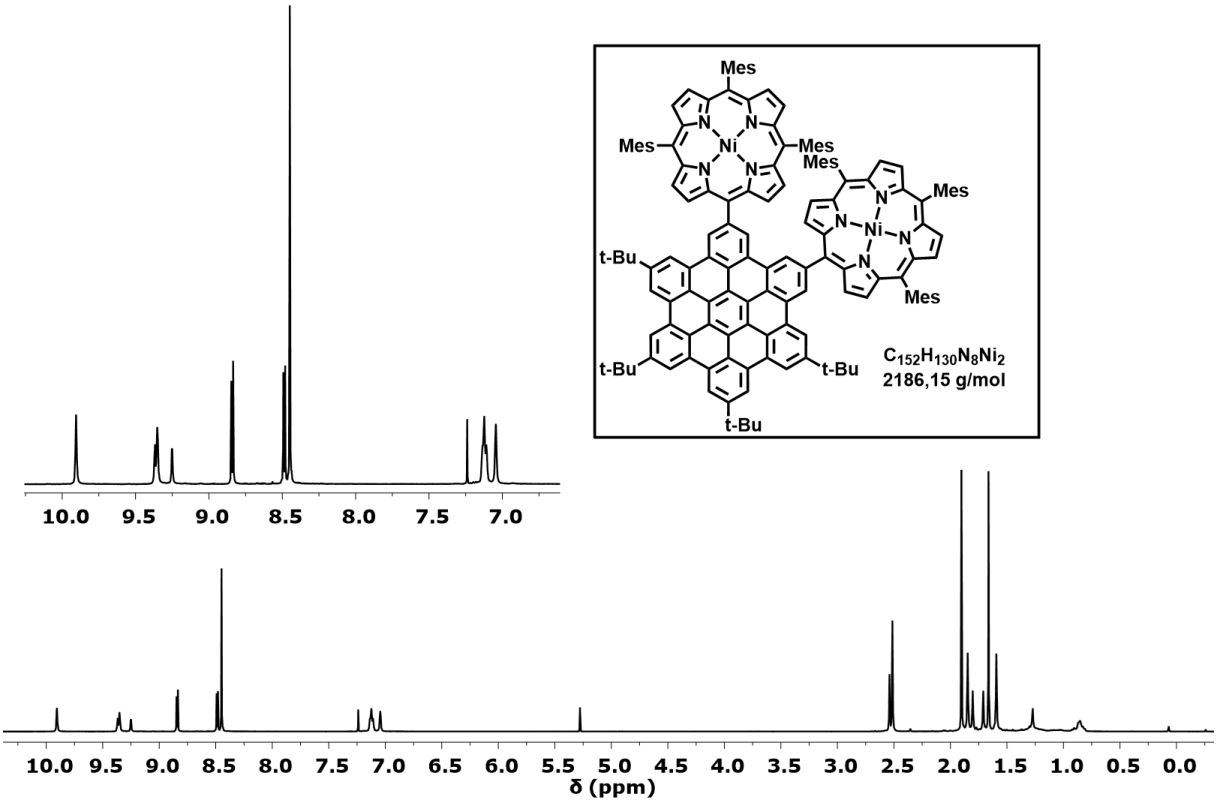


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 152 H 130 N 8 Ni 2	2,182.9120	0.3975	24.5868	92.00	ok	odd

Figure S44. MS/HRMS (MALDI) of **13.**

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

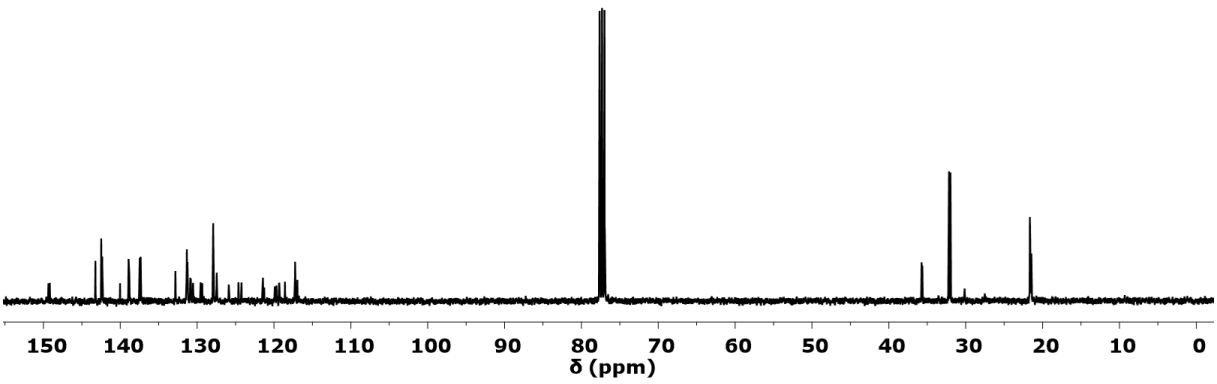
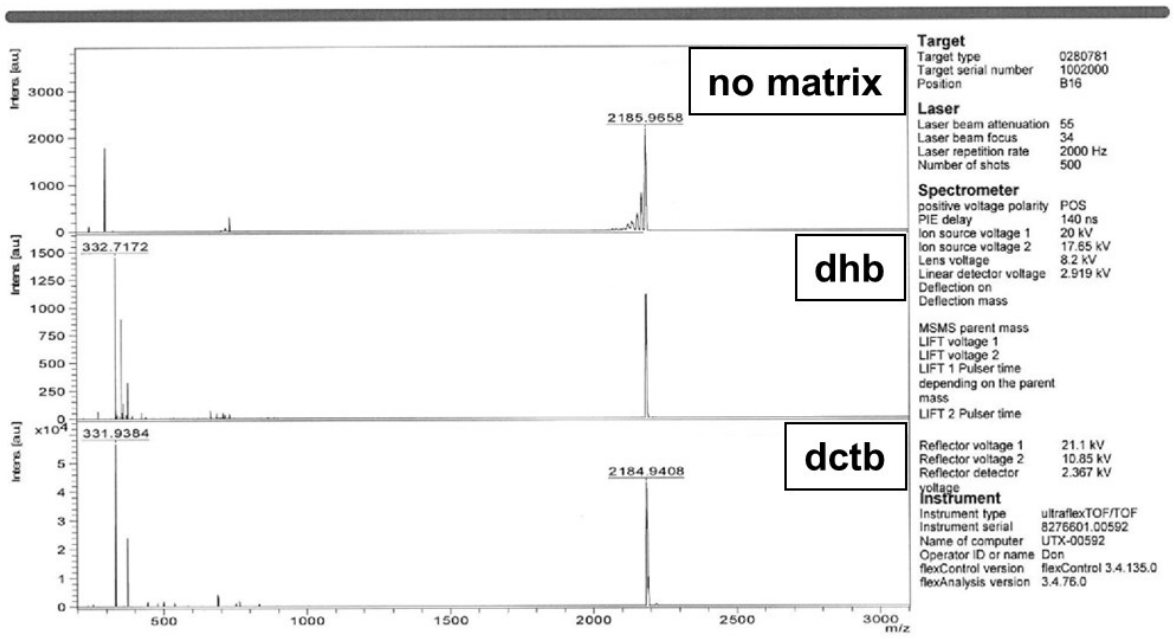
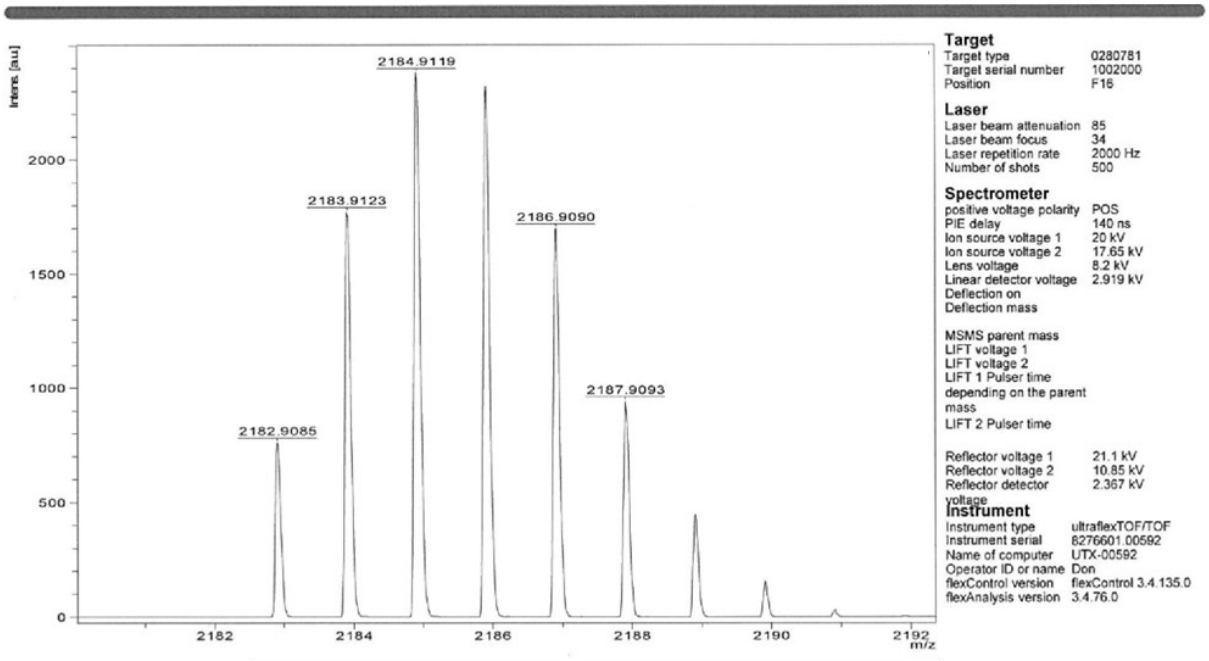


Figure S45. ^{1}H and ^{13}C NMR of **11**.

MS (MALDI)



HRMS (MALDI)

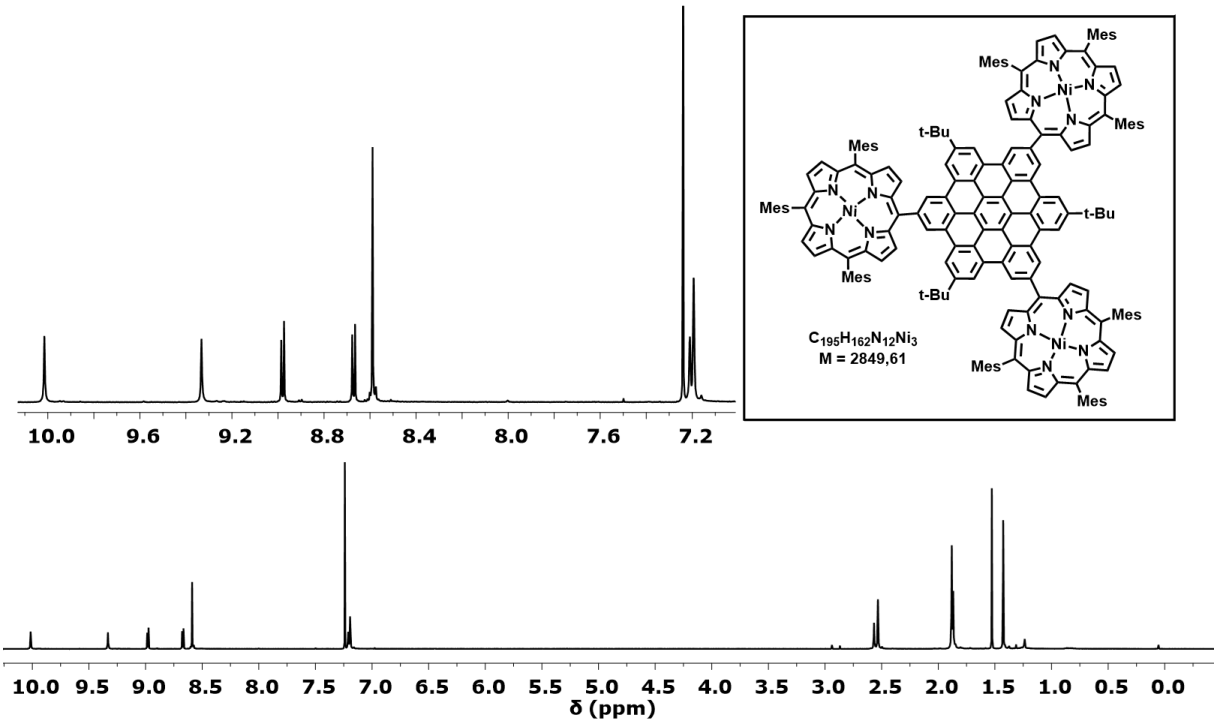


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 152 H 130 N 8 Ni 2	2,182.9120	1.6062	131.5855	92.00	ok	odd

Figure S46. MS/HRMS (MALDI) of **11**.

^{1}H NMR (400 MHz, $CDCl_3$, rt)



^{13}C NMR (101 MHz, $CDCl_3$, rt)

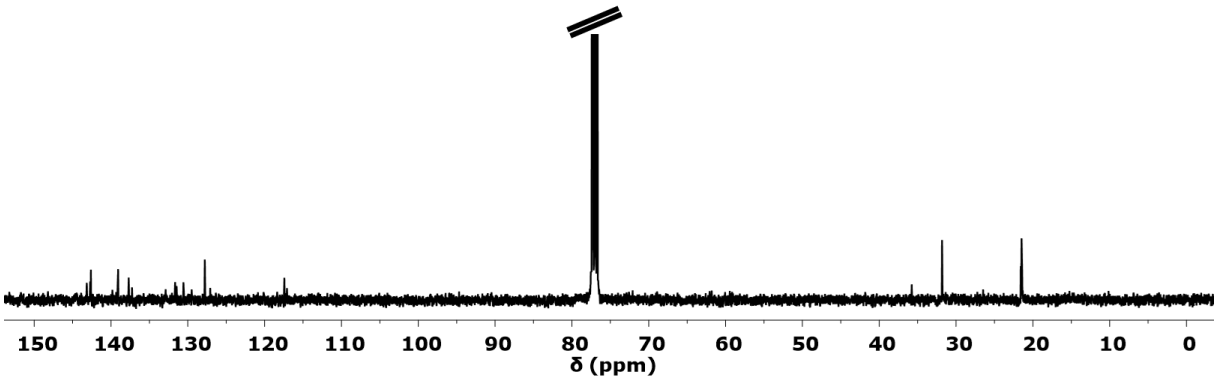
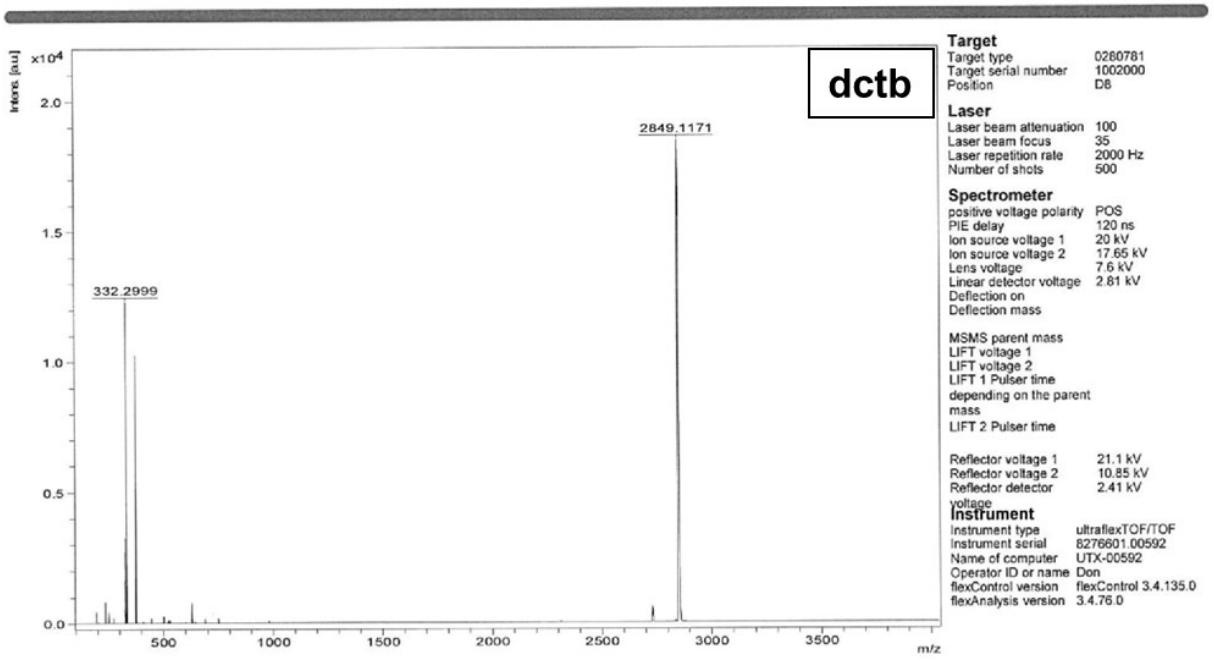
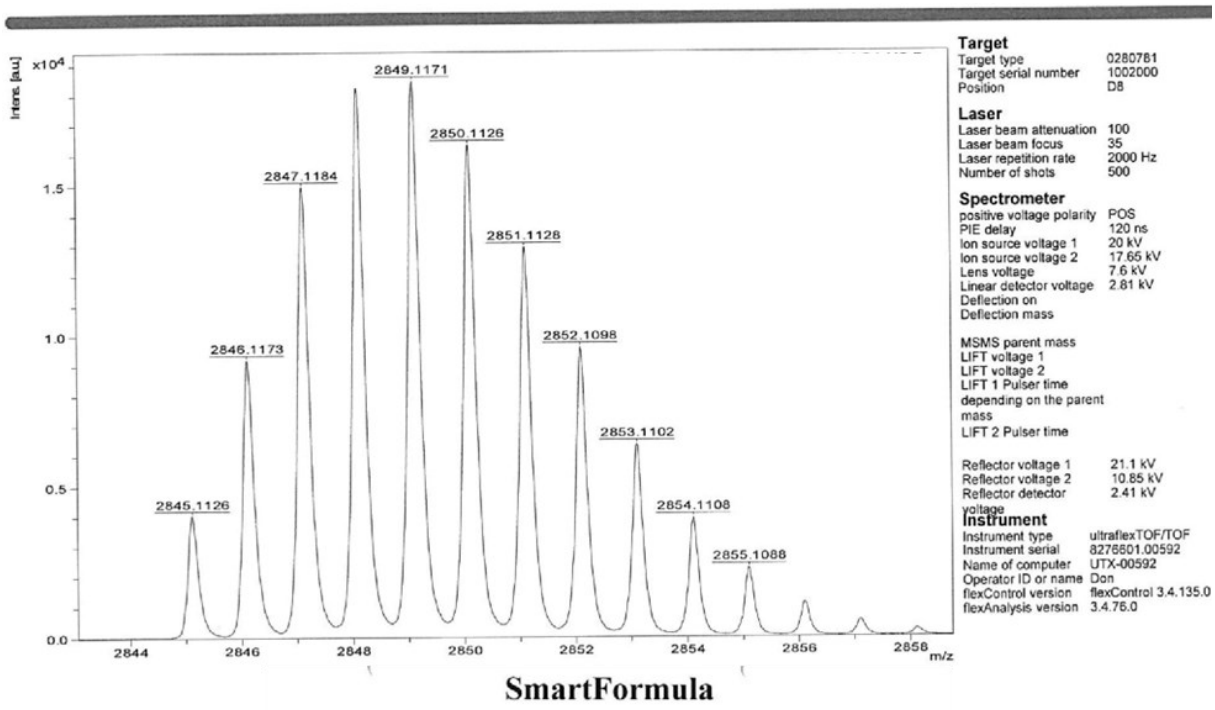


Figure S47. ^{1}H and ^{13}C NMR of **14**.

MS (MALDI)



HRMS (MALDI)

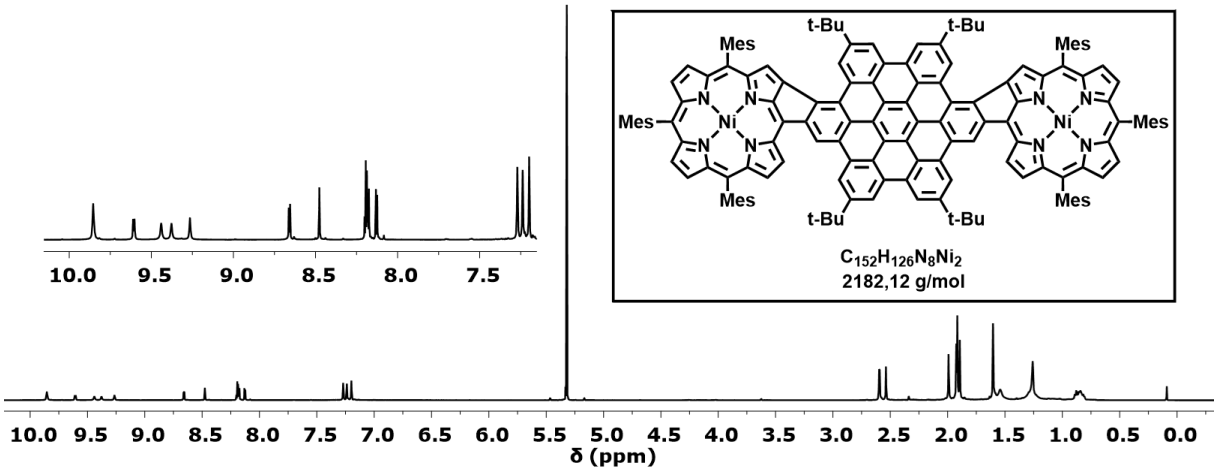


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 195 H 162 N 12 Ni 3	2,845.1100	0.9056	21.7642	121.00	ok	odd

Figure S48. MS/HRMS (MALDI) of **14**.

^{1}H NMR (601 MHz, CD_2Cl_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2, rt)

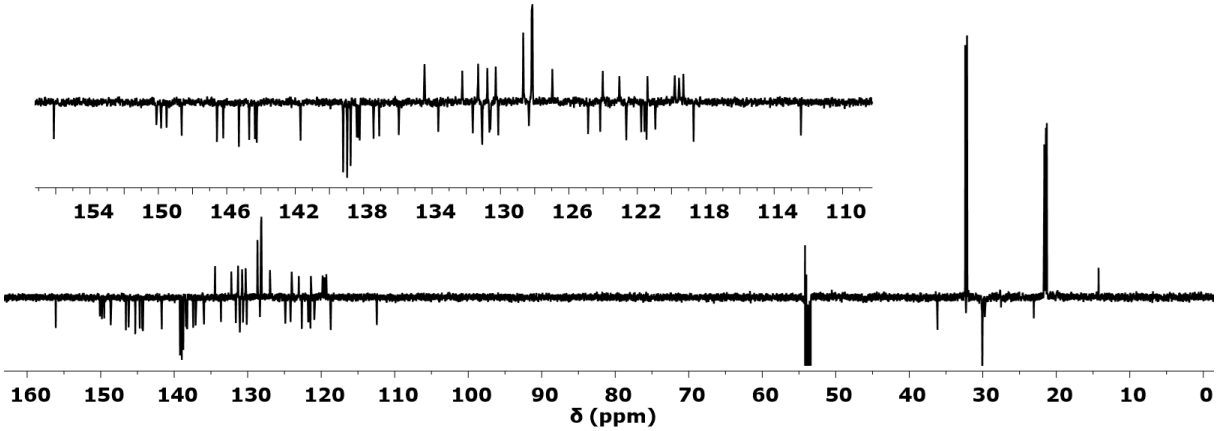


Figure S49. ^{1}H and ^{13}C NMR (DEPTQ135) of ***p*-HBC**.

^{1}H- ^{1}H COSY (601 MHz, CD_2Cl_2, rt)

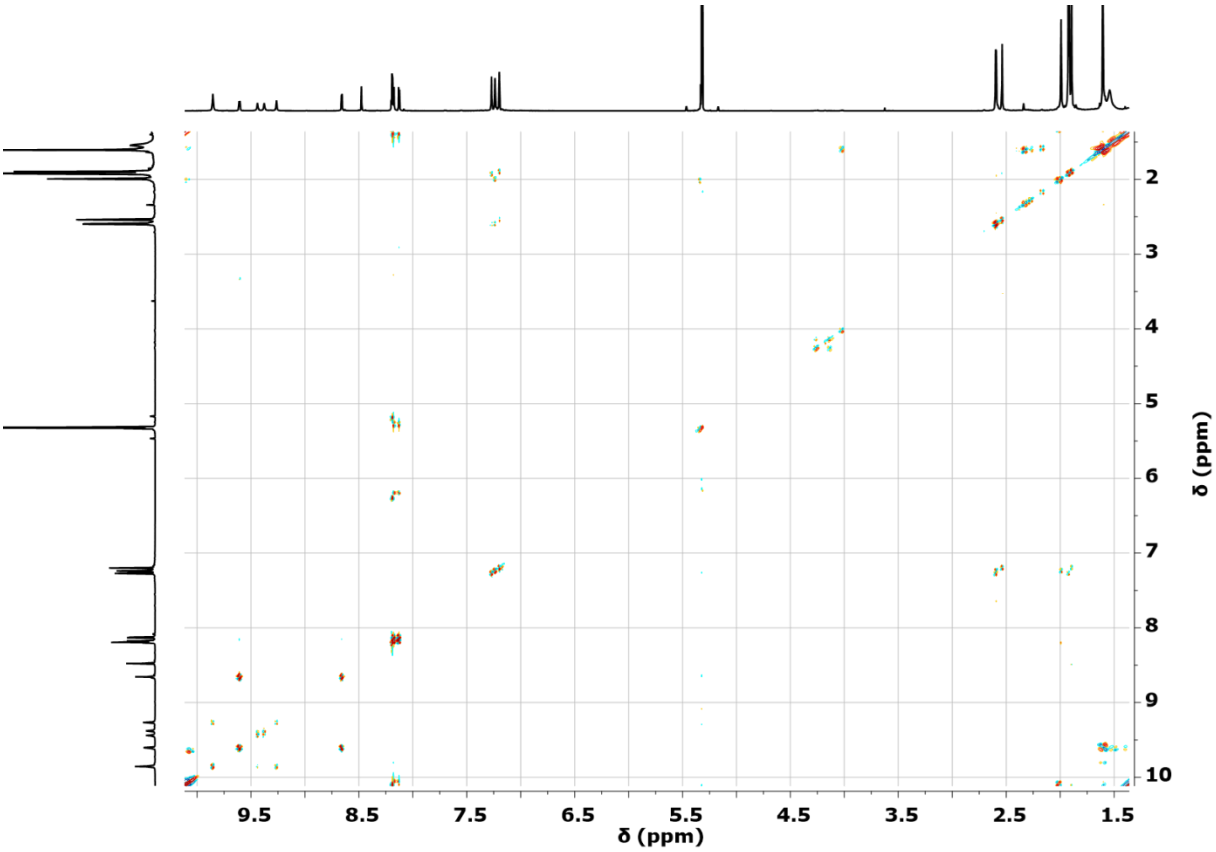


Figure S50. ^{1}H- ^{1}H COSY of ***p*-HBC**.

^{1}H- ^{13}C HSQC (601 MHz, CD_2Cl_2, rt)

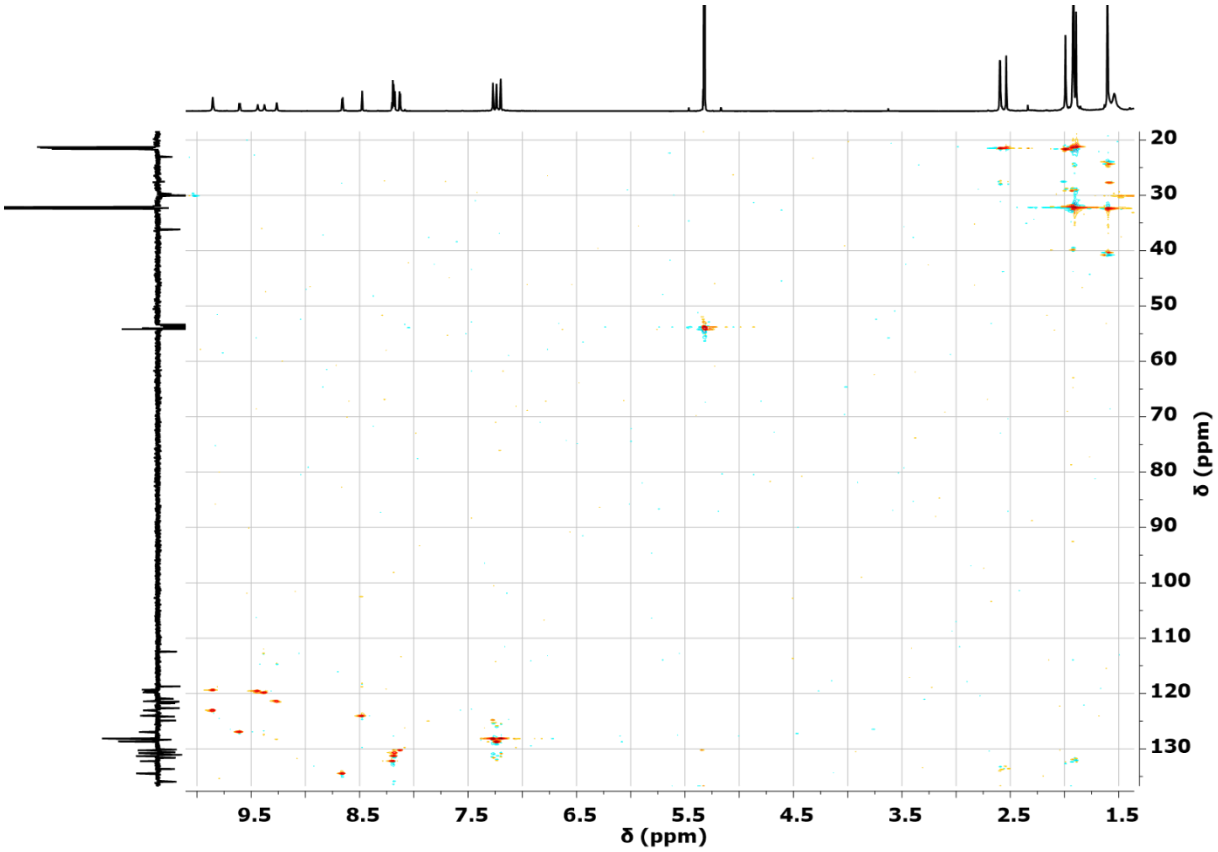


Figure S51. ^{1}H- ^{13}C HSQC of ***p*-HBC**.

^{1}H- ^{13}C HMBC (601 MHz, CD_2Cl_2, rt)

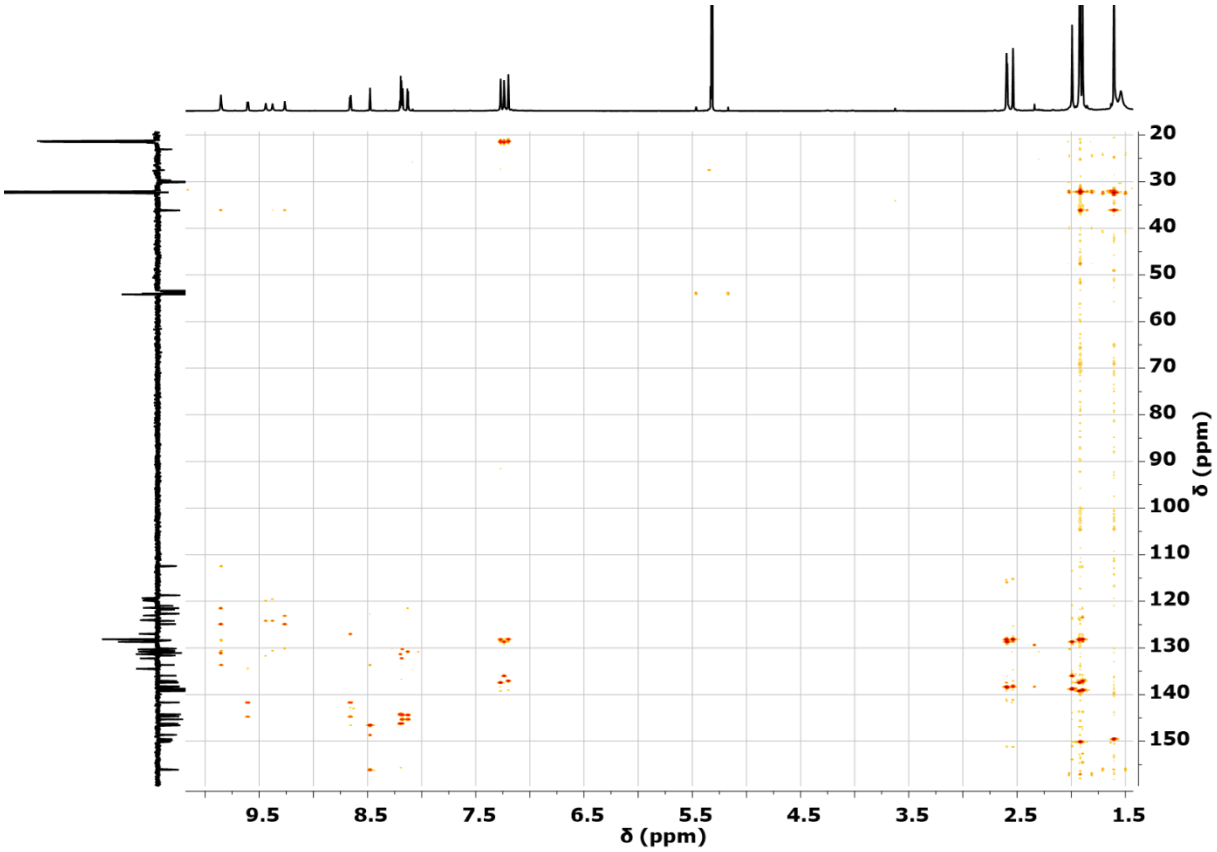


Figure S52. ^{1}H- ^{13}C HMBC of ***p*-HBC**.

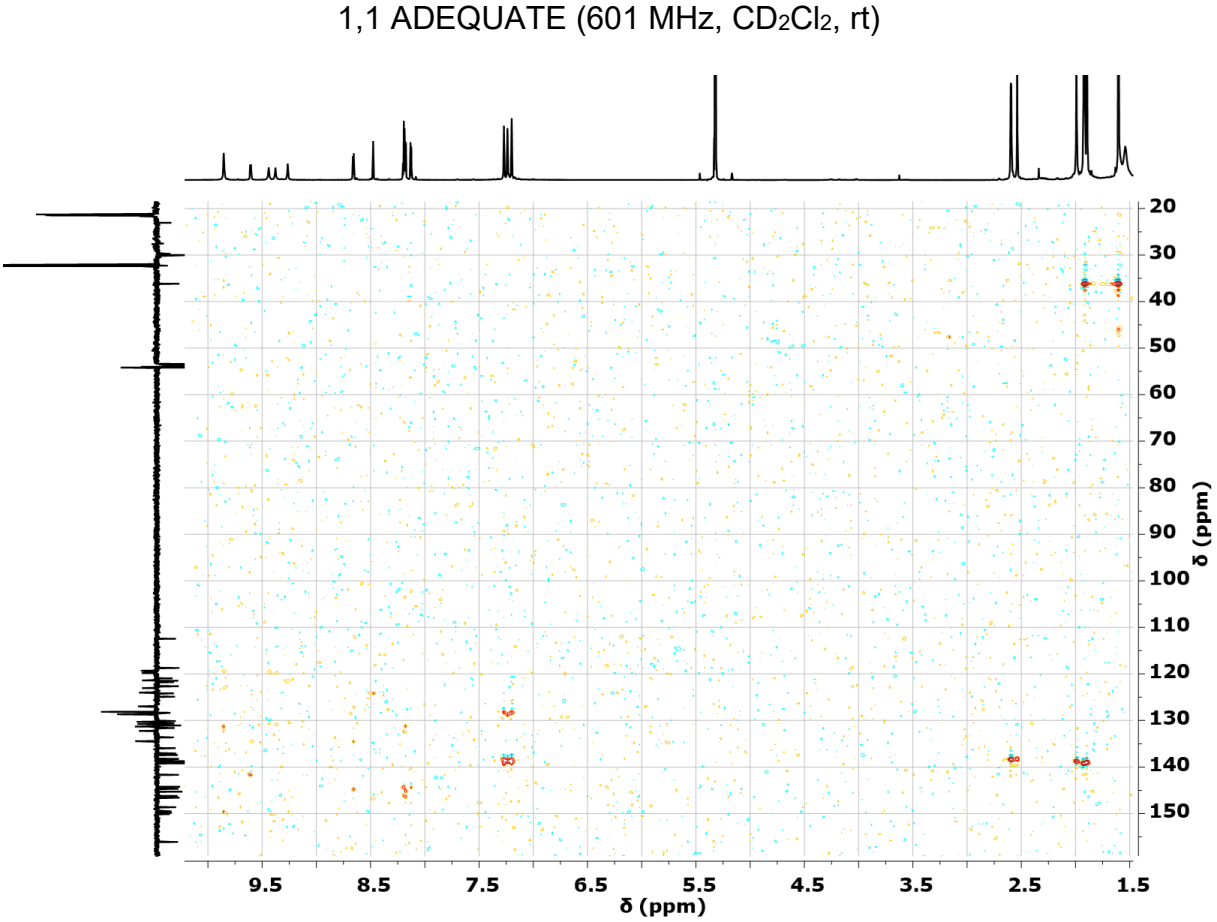
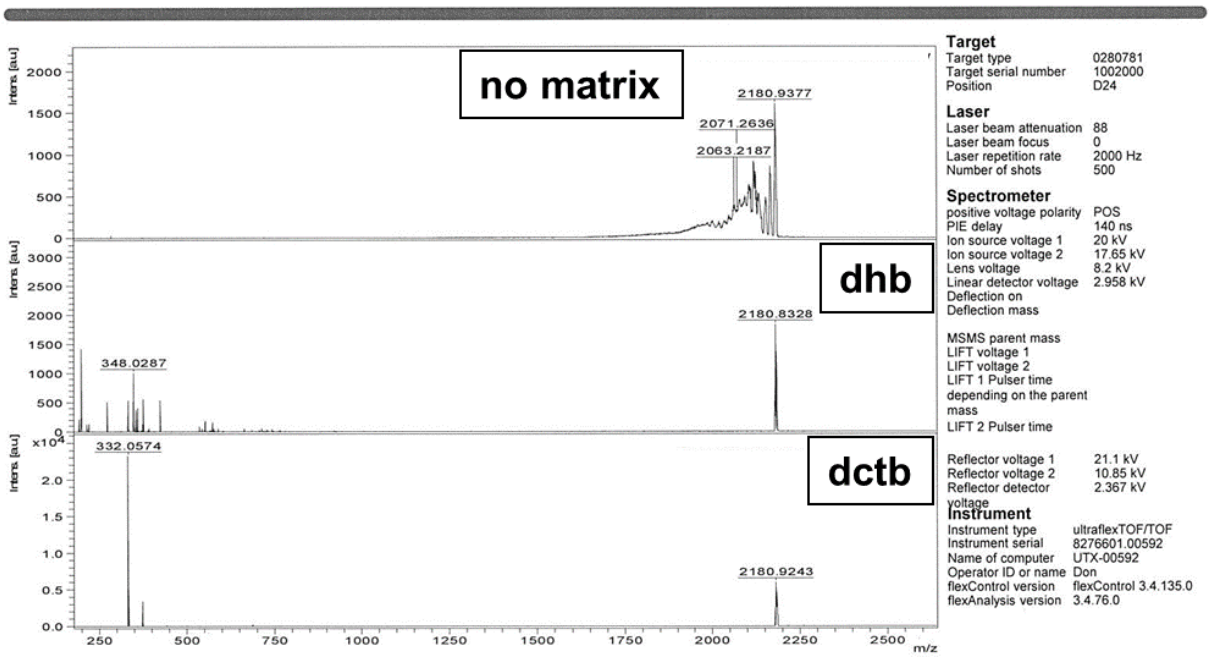
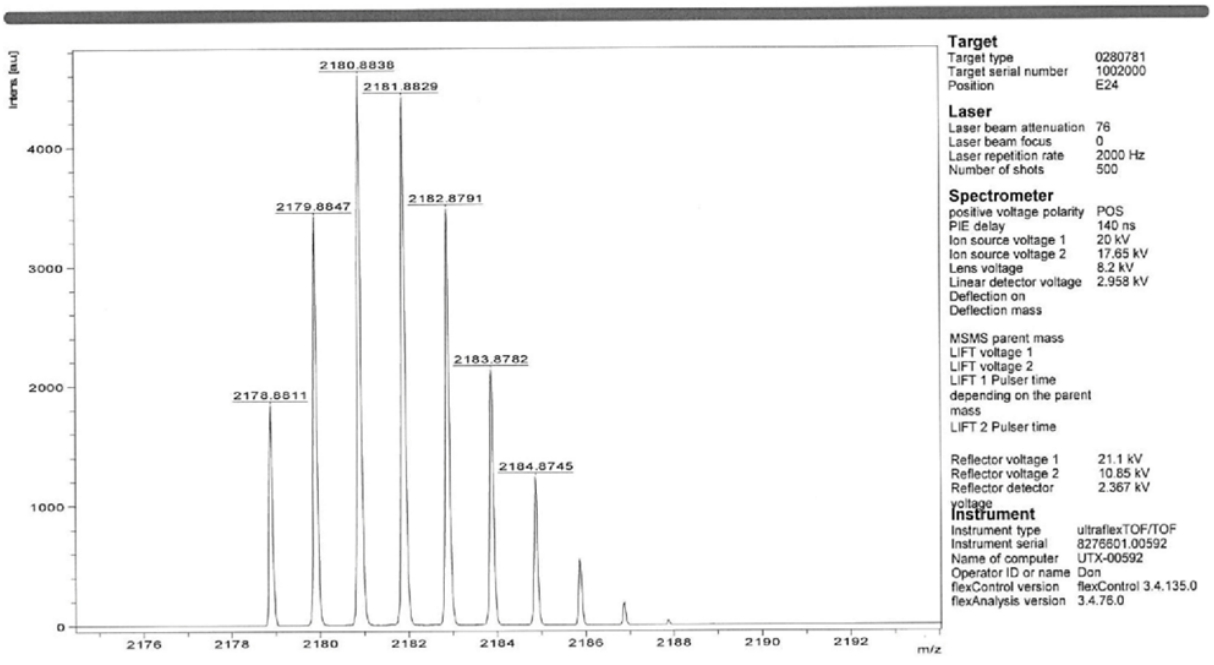


Figure S53. 1,1 ADEQUATE of ***p*-HBC**.

MS (MALDI)



HRMS (MALDI)

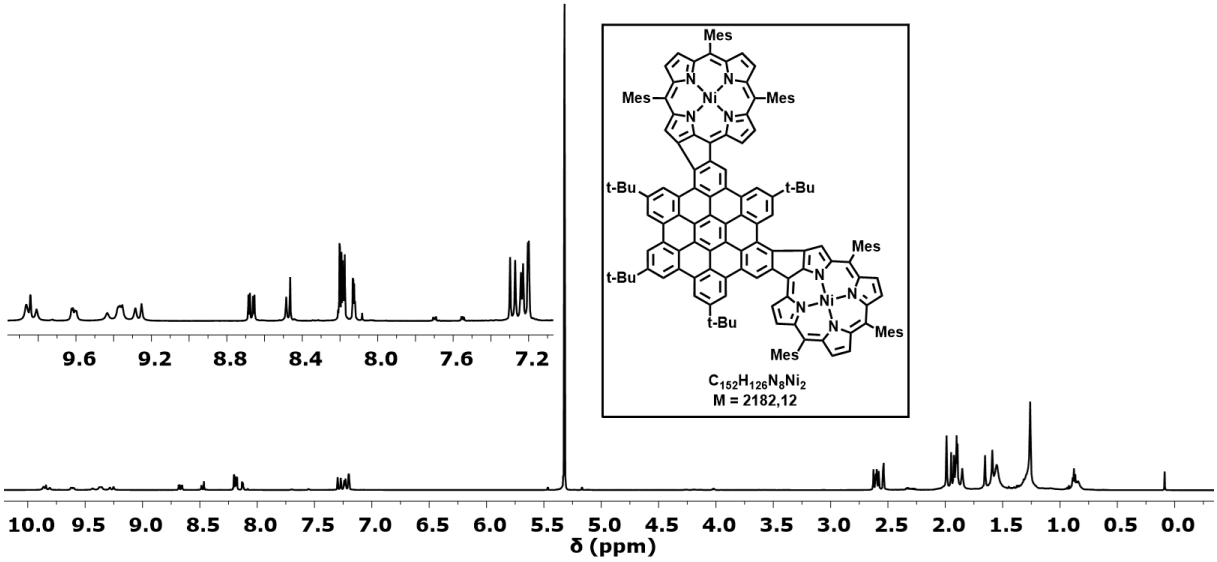


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 152 H 126 N 8 Ni 2	2,178.8807	0.1761	75.5489	94.00	ok	odd

Figure S54. MS/HRMS (MALDI) of ***p*-HBC**.

^{1}H NMR (601 MHz, CD_2Cl_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2, rt)

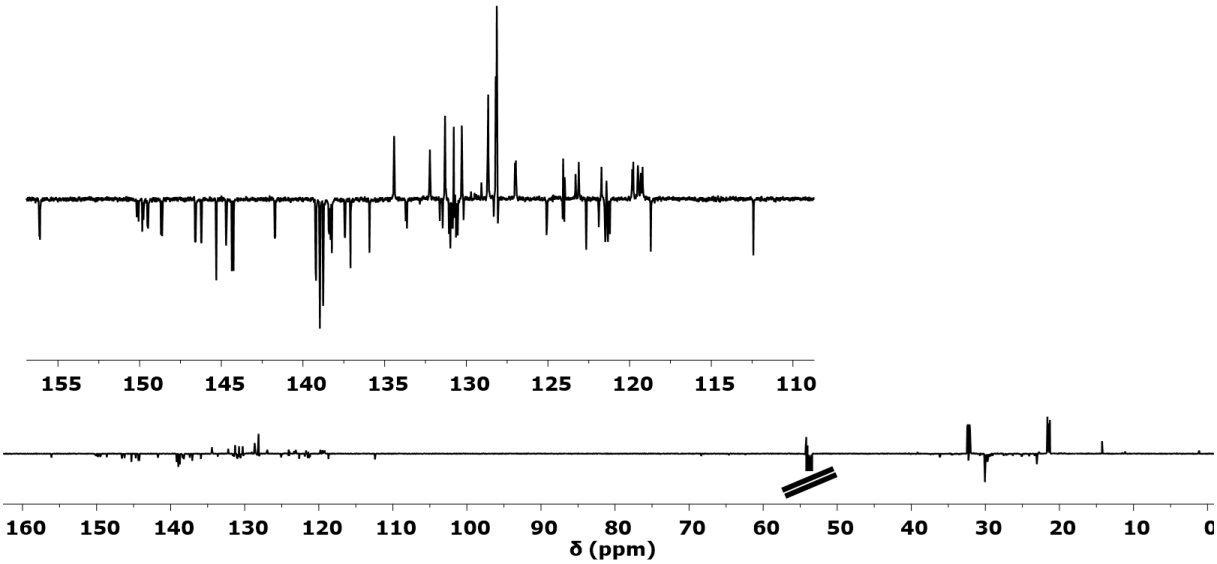


Figure S55. ^{1}H and ^{13}C NMR (DEPTQ135) of ***m*-HBC**.

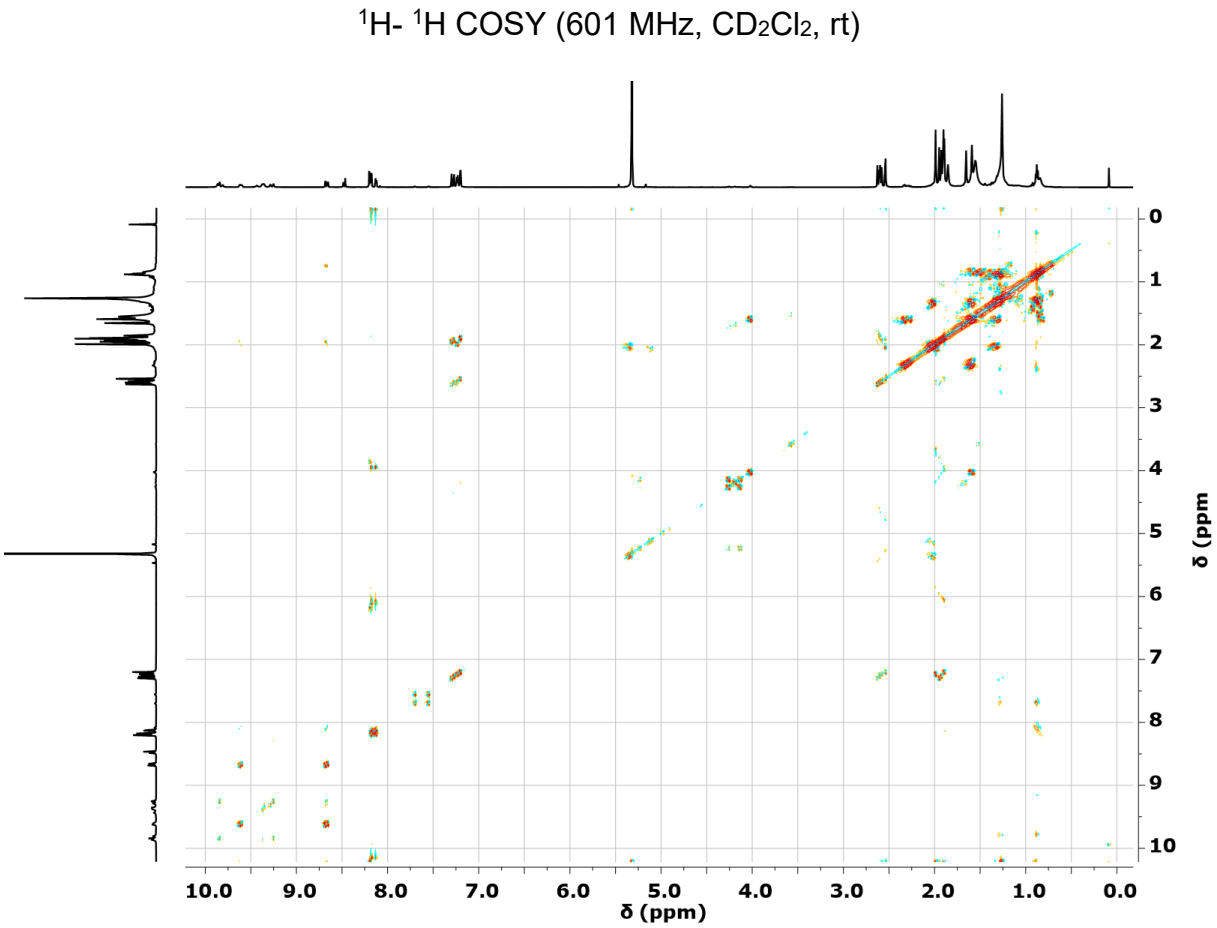


Figure S56. ^{1}H- ^{1}H COSY of ***m*-HBC**.

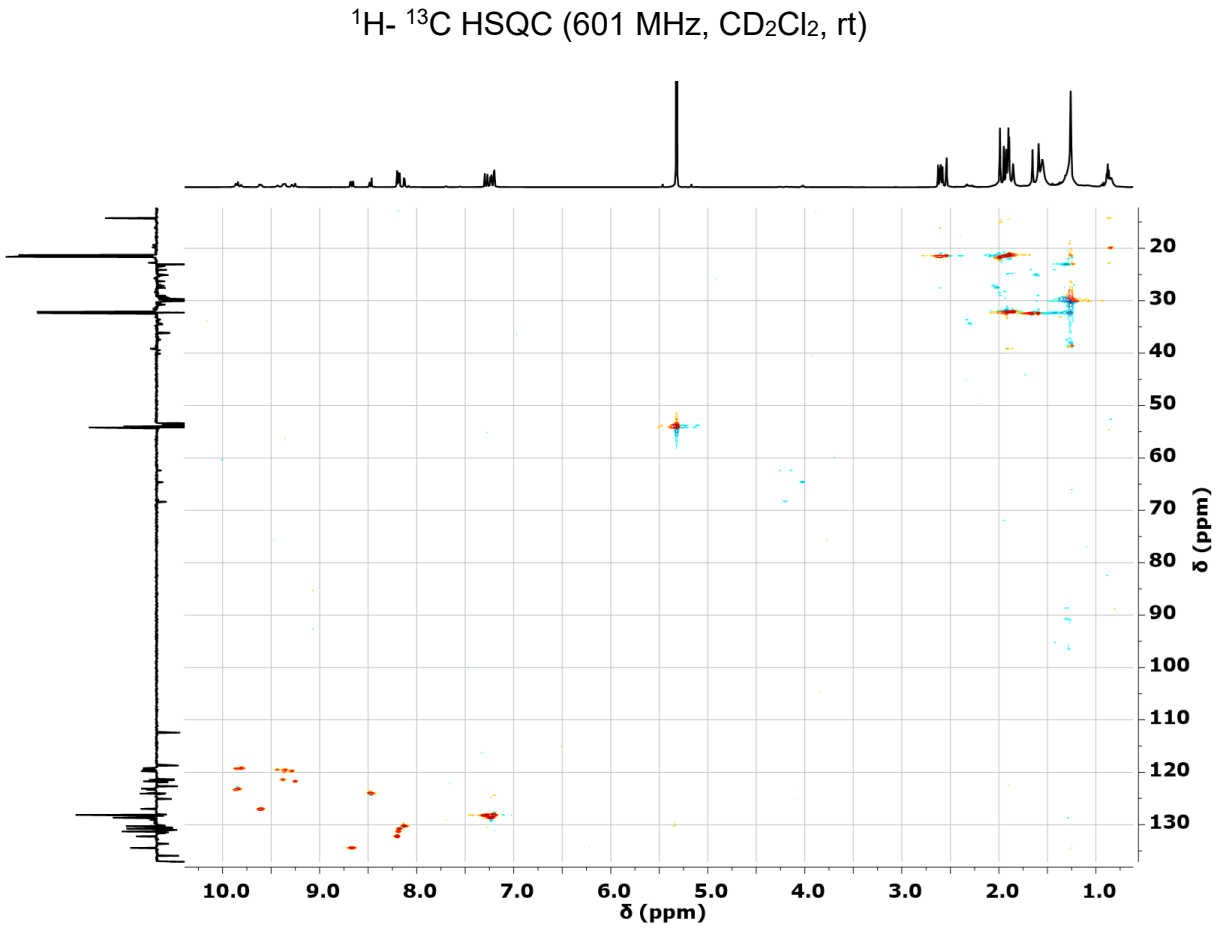


Figure S57. ^{1}H- ^{13}C HSQC of ***m*-HBC**.

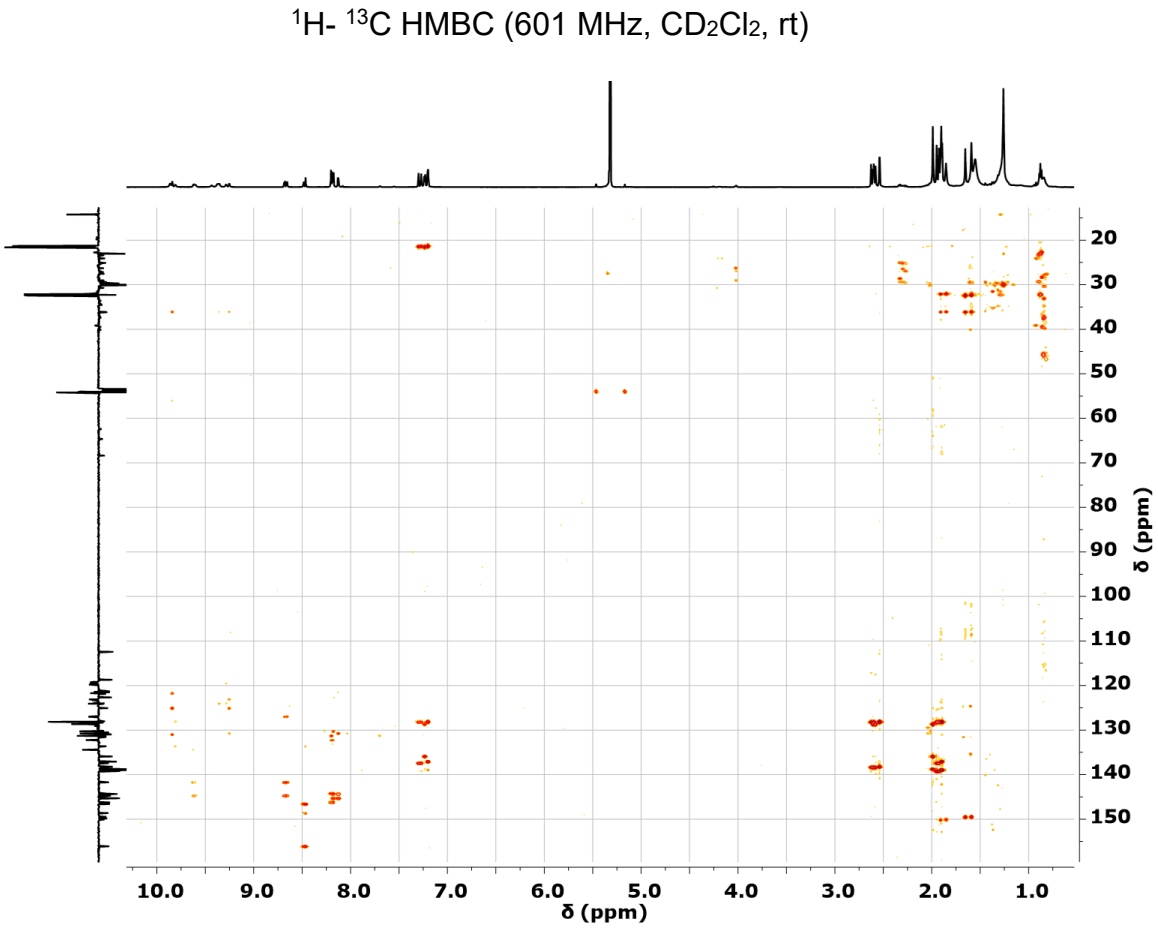


Figure S58. ^{1}H- ^{13}C HMBC of ***m*-HBC**.

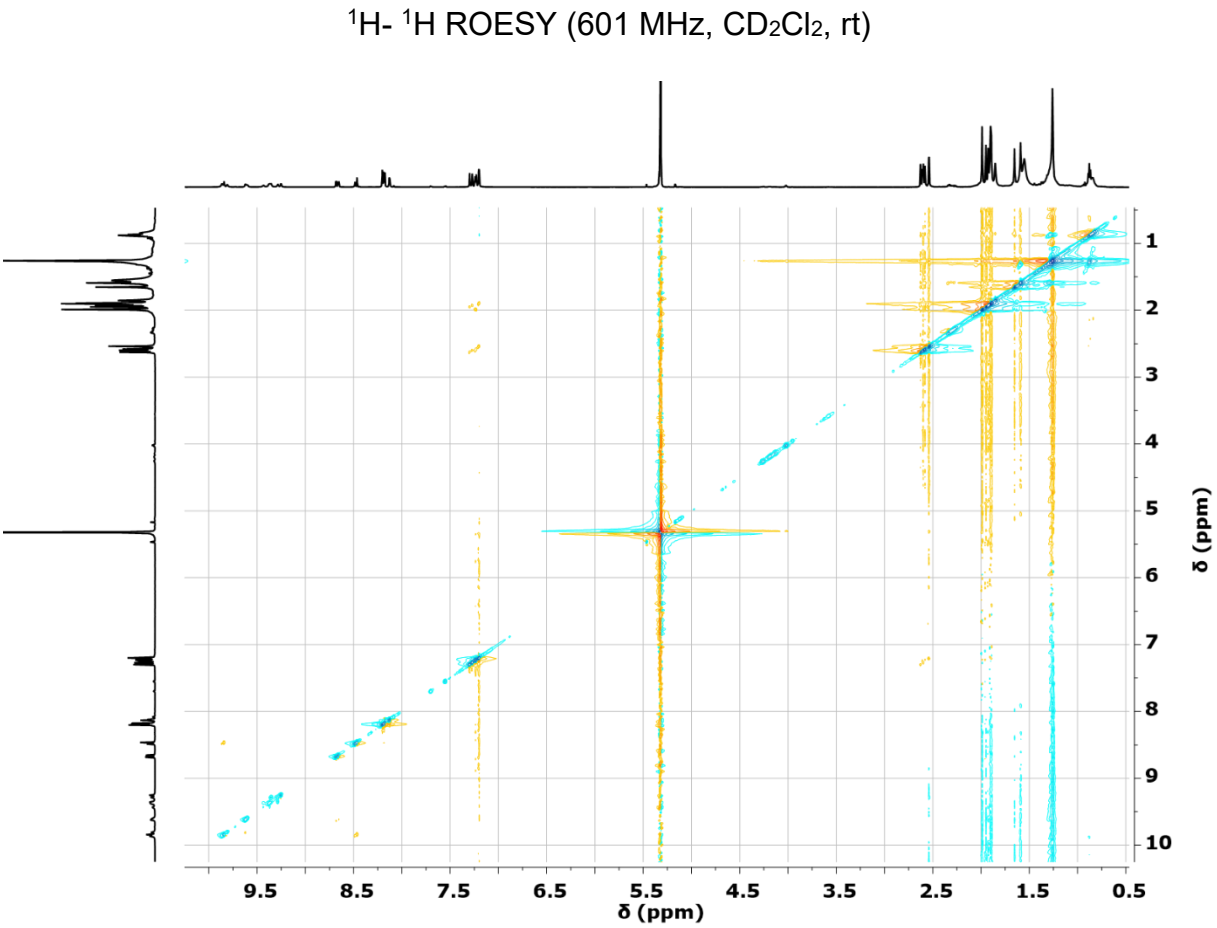
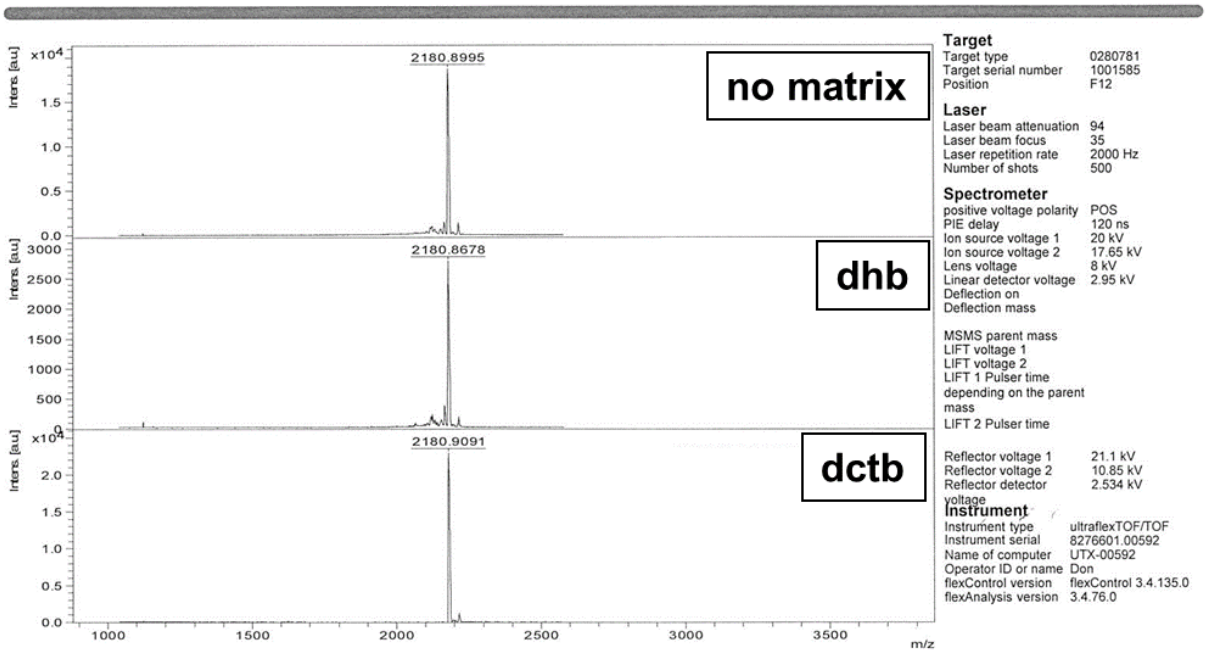
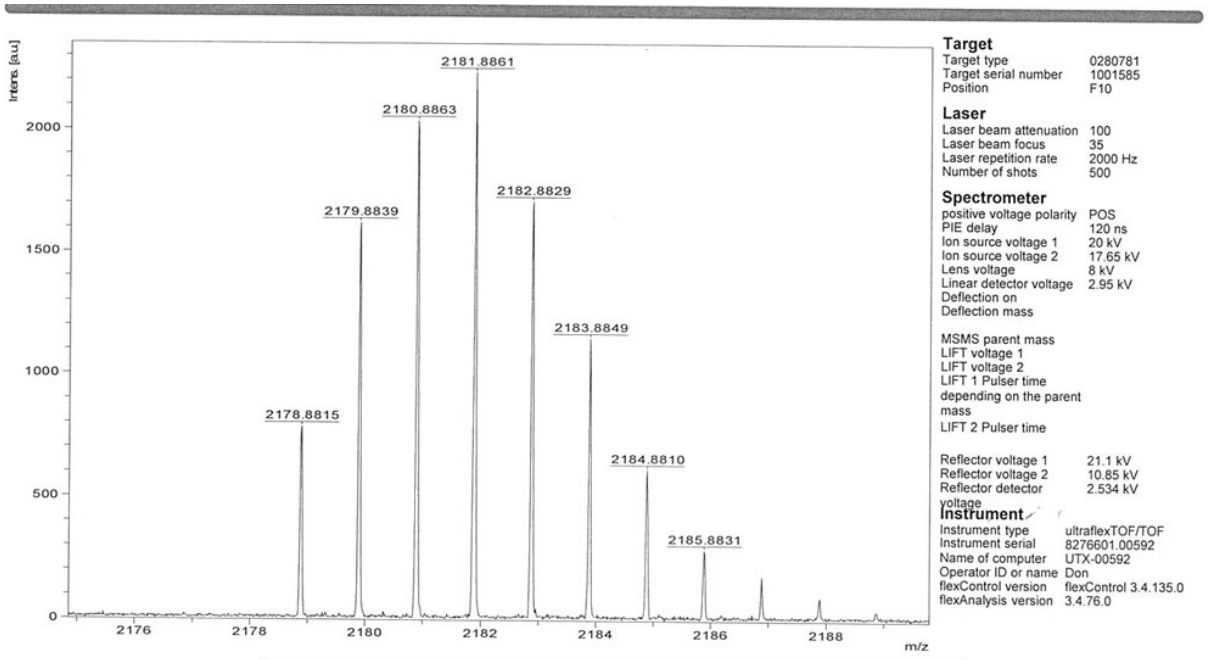


Figure S59. ^{1}H- ^{1}H ROESY of ***m*-HBC**.

MS (MALDI)



HRMS (MALDI)

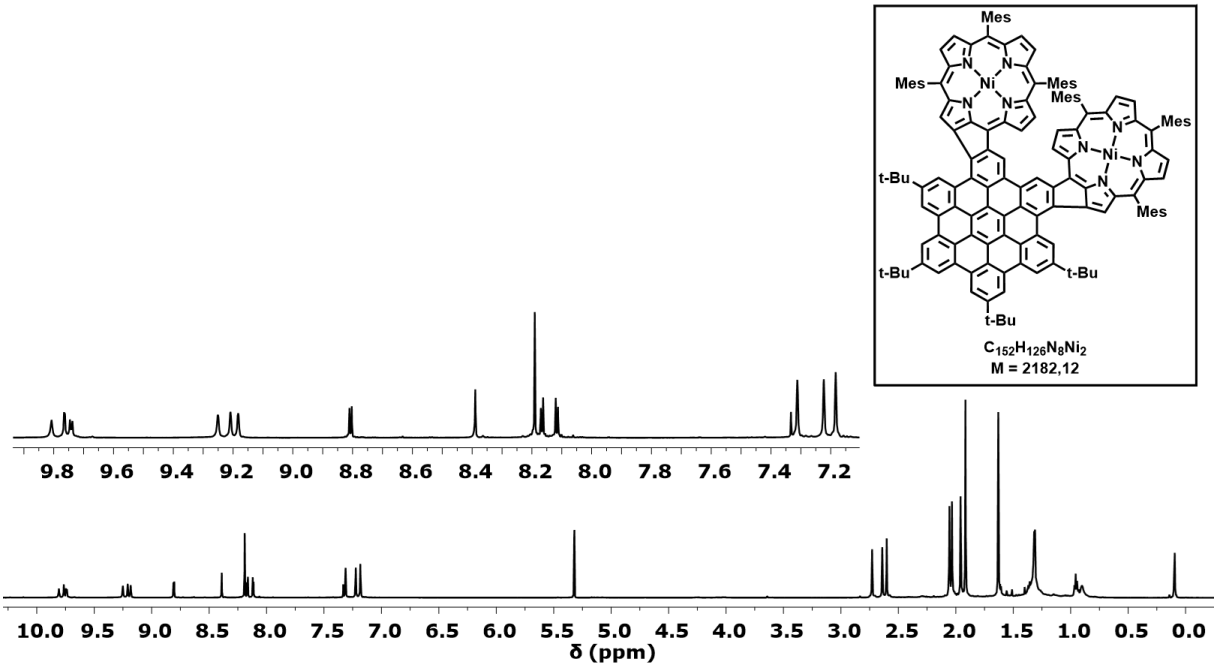


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 152 H 126 N 8 Ni 2	2,178.8807	0.3665	61.5236	94.00	ok	odd

Figure S60. MS/HRMS (MALDI) of ***m*-HBC**.

^{1}H NMR (601 MHz, CD_2Cl_2/CS_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2/CS_2, rt)

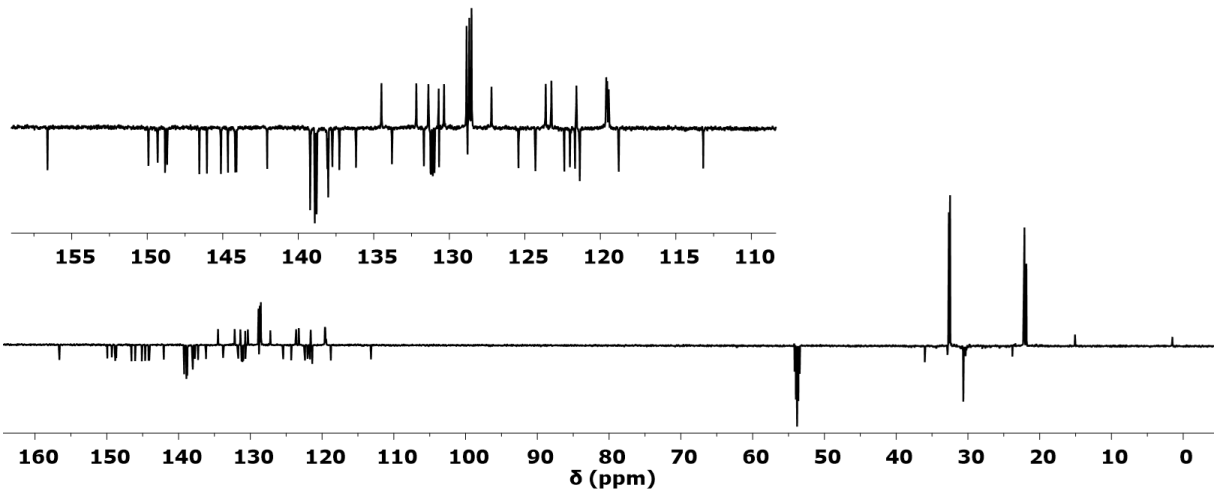


Figure S61. ^{1}H and ^{13}C NMR (DEPTQ135) of ***o*-HBC**.

^{1}H- ^{1}H COSY (601 MHz, CD_2Cl_2/CS_2, rt)

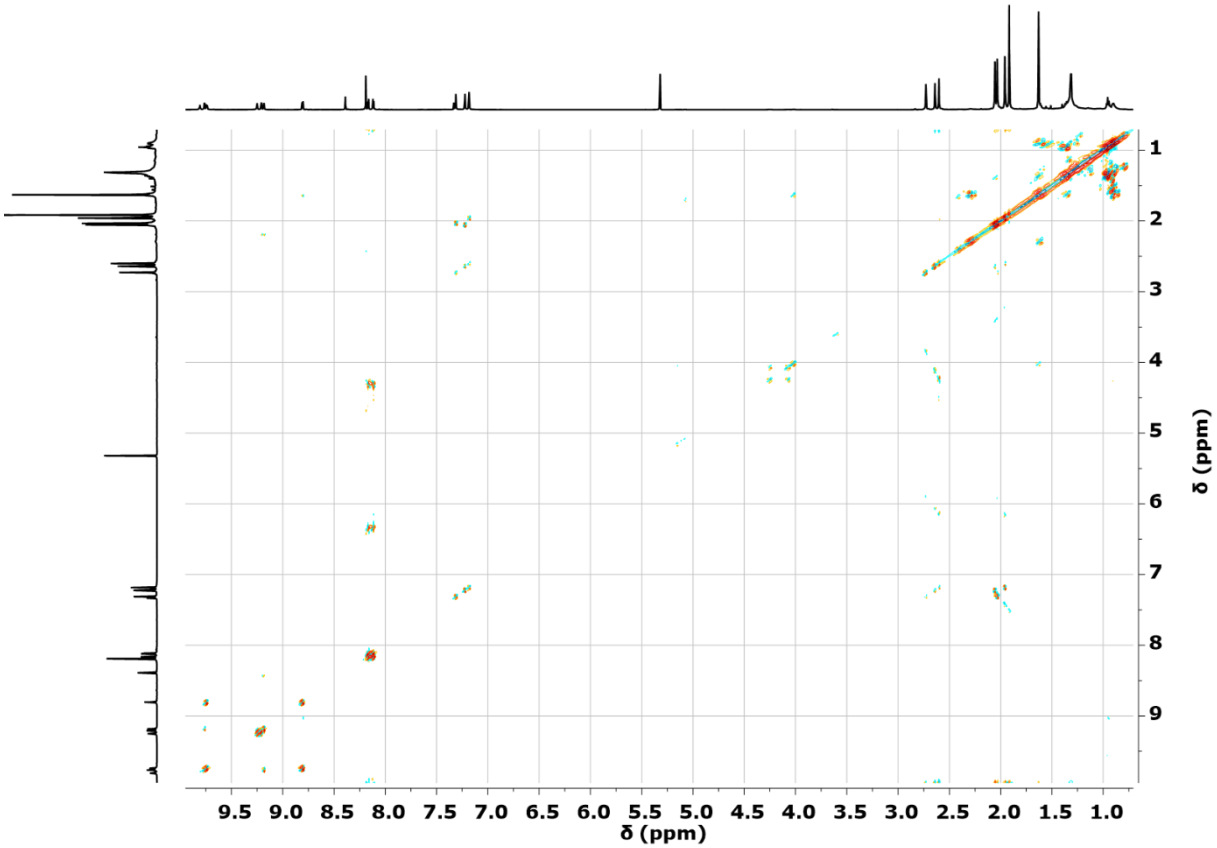


Figure S62. ^{1}H- ^{1}H COSY of ***o*-HBC**.

^{1}H- ^{13}C HSQC (601 MHz, CD_2Cl_2/CS_2, rt)

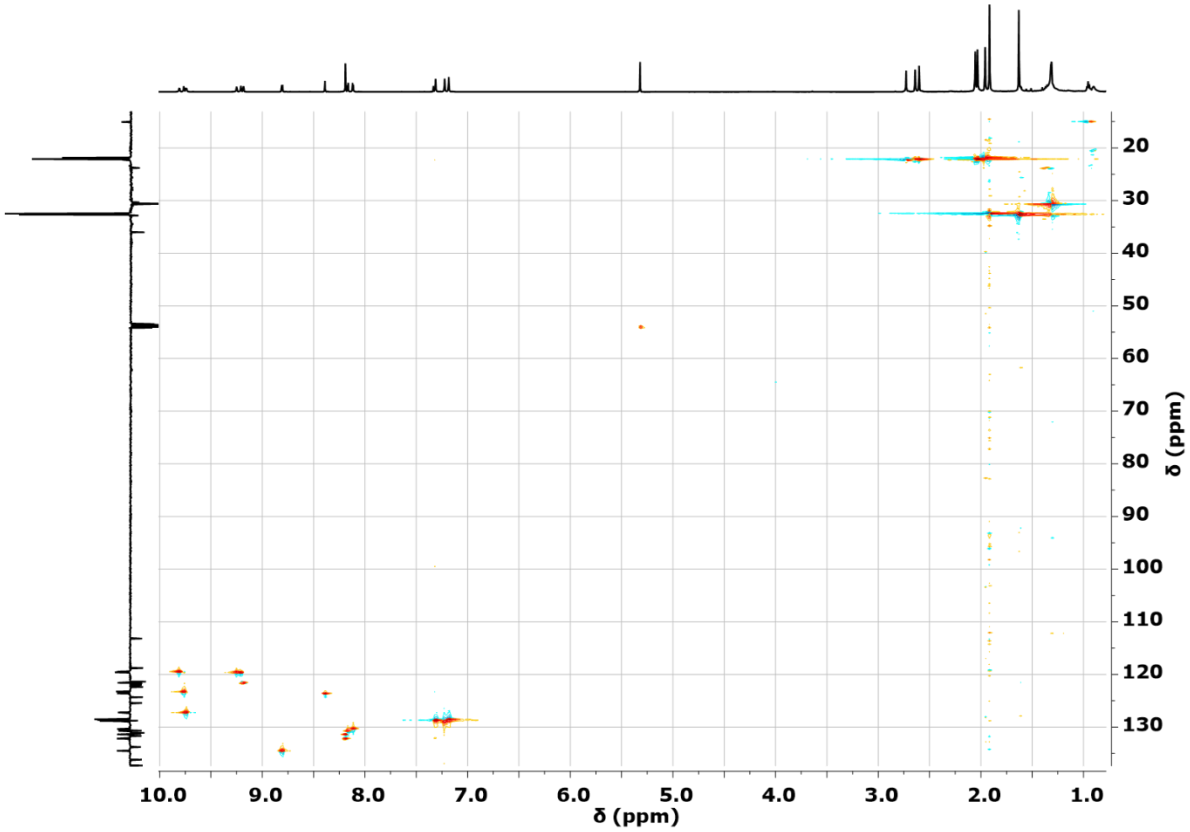


Figure S63. ^{1}H- ^{13}C HSQC of ***o*-HBC**.

^{1}H- ^{13}C HMBC (601 MHz, CD_2Cl_2/CS_2, rt)

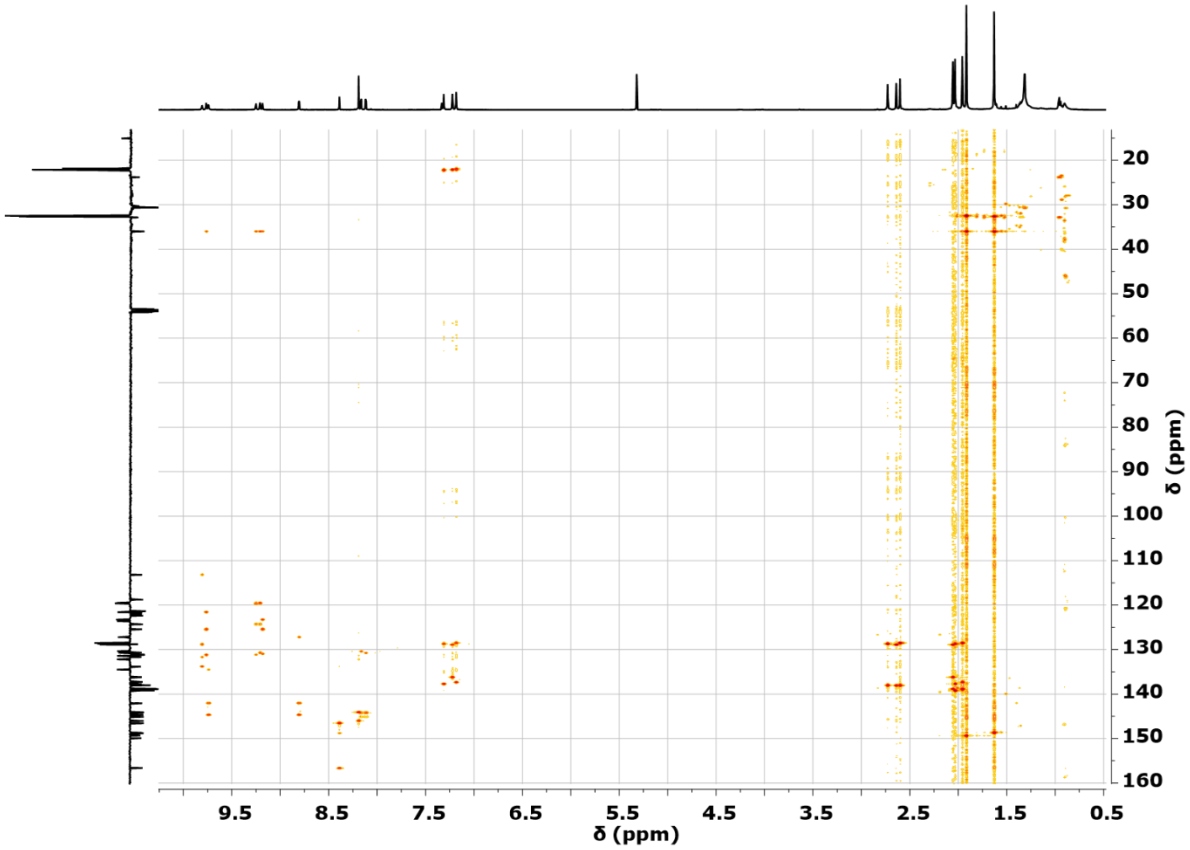
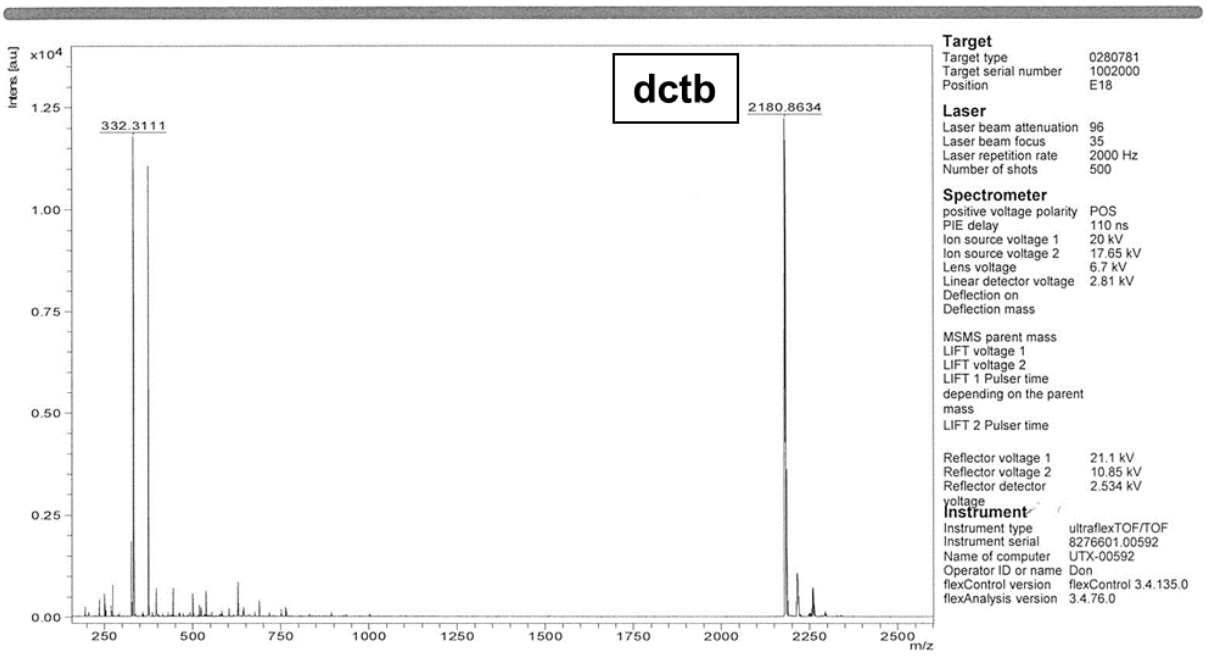
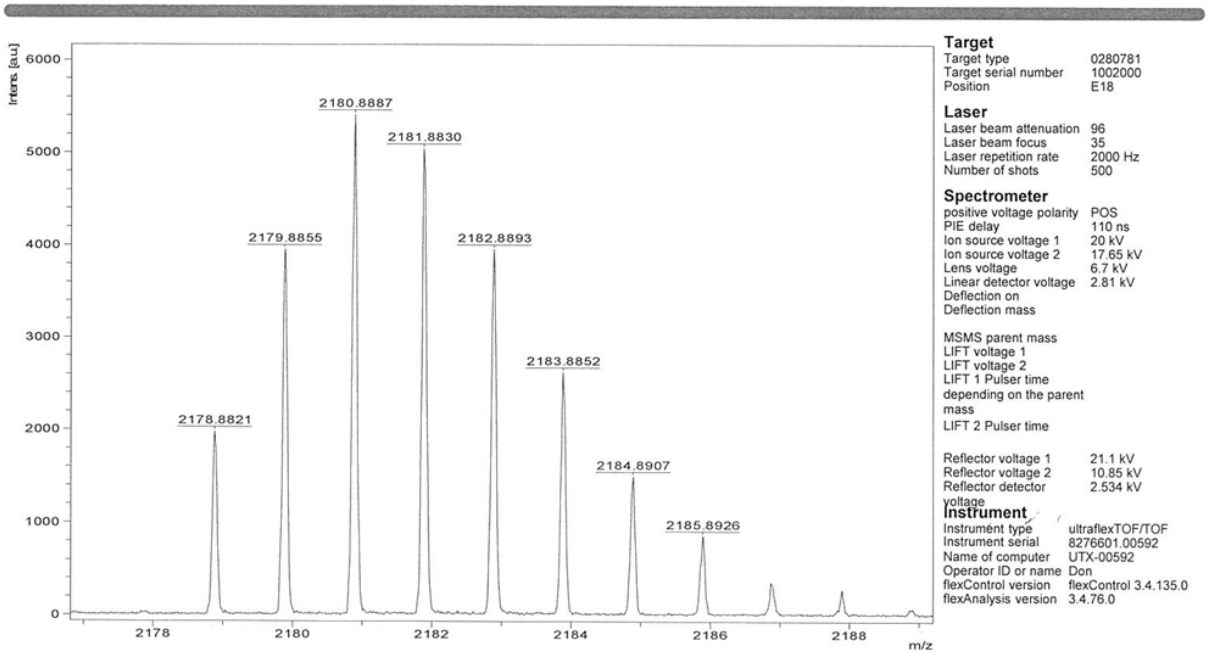


Figure S64. ^{1}H- ^{13}C HMBC of ***o*-HBC**.

MS (MALDI)



HRMS (MALDI)

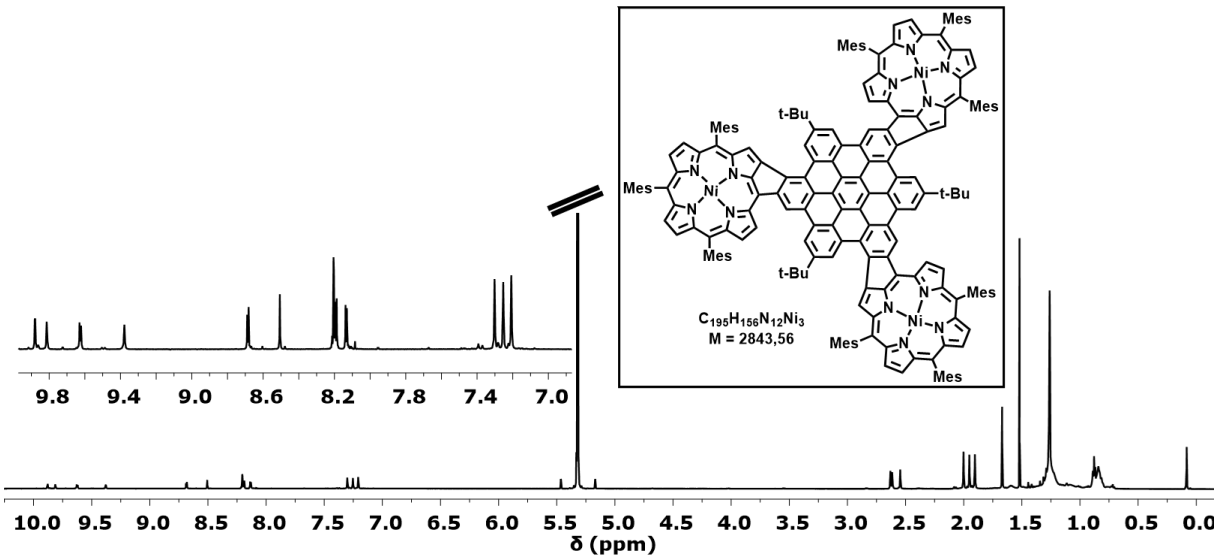


SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 152 H 126 N 8 Ni 2	2,178.8807	0.6712	55.8878	94.00	ok	odd

Figure S65. MS/HRMS (MALDI) of ***o*-HBC**.

^{1}H NMR (601 MHz, CD_2Cl_2, rt)



^{13}C NMR - DEPTQ135 (151 MHz, CD_2Cl_2, rt)

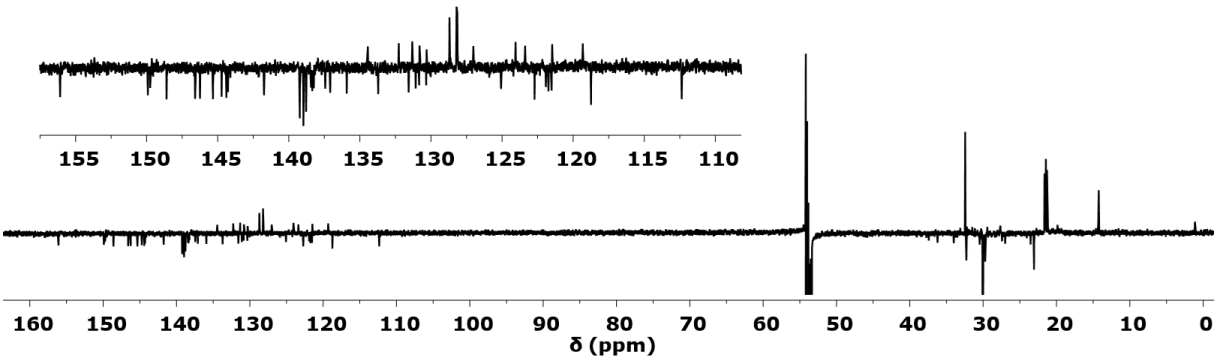


Figure S66. ^{1}H and ^{13}C NMR (DEPTQ135) of ***tri*-HBC**.

^{1}H- ^{1}H COSY (601 MHz, CD_2Cl_2, rt)

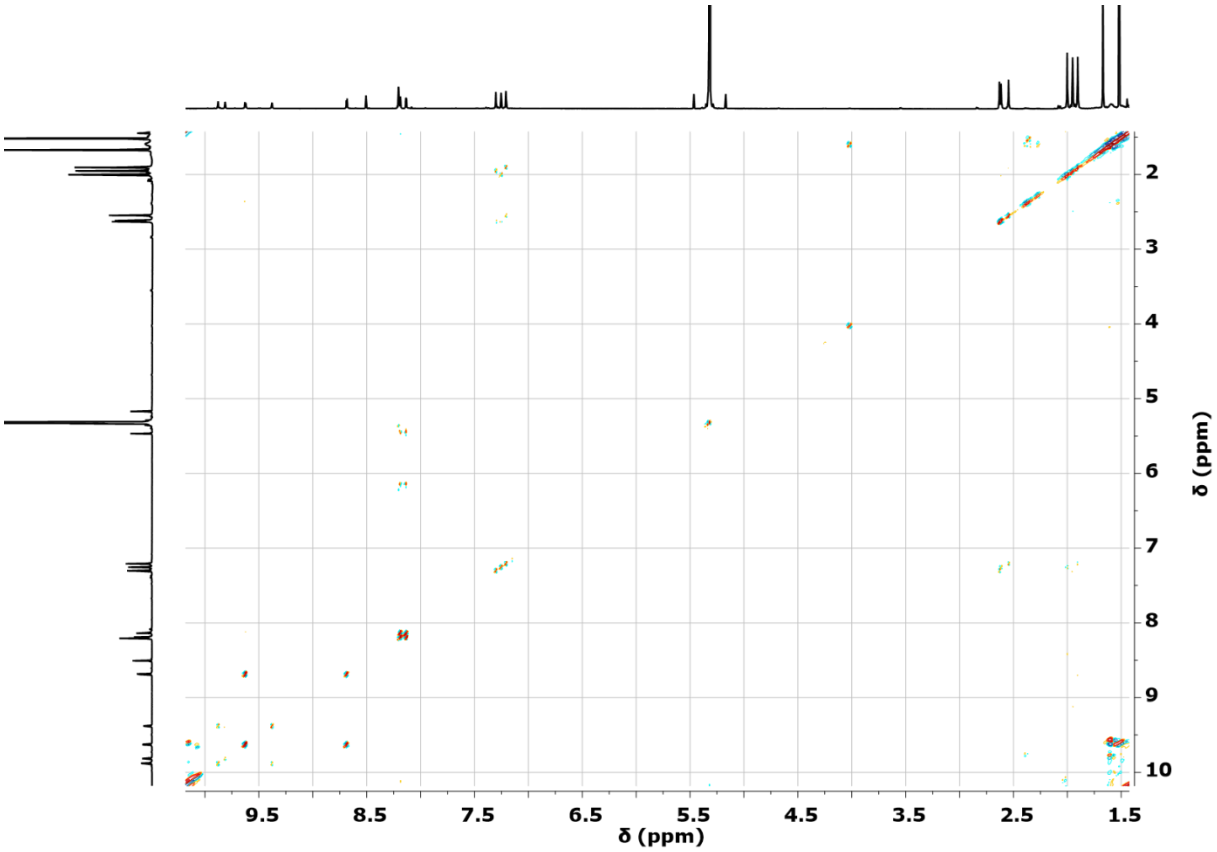


Figure S67. ^{1}H- ^{1}H COSY of ***tri*-HBC**.

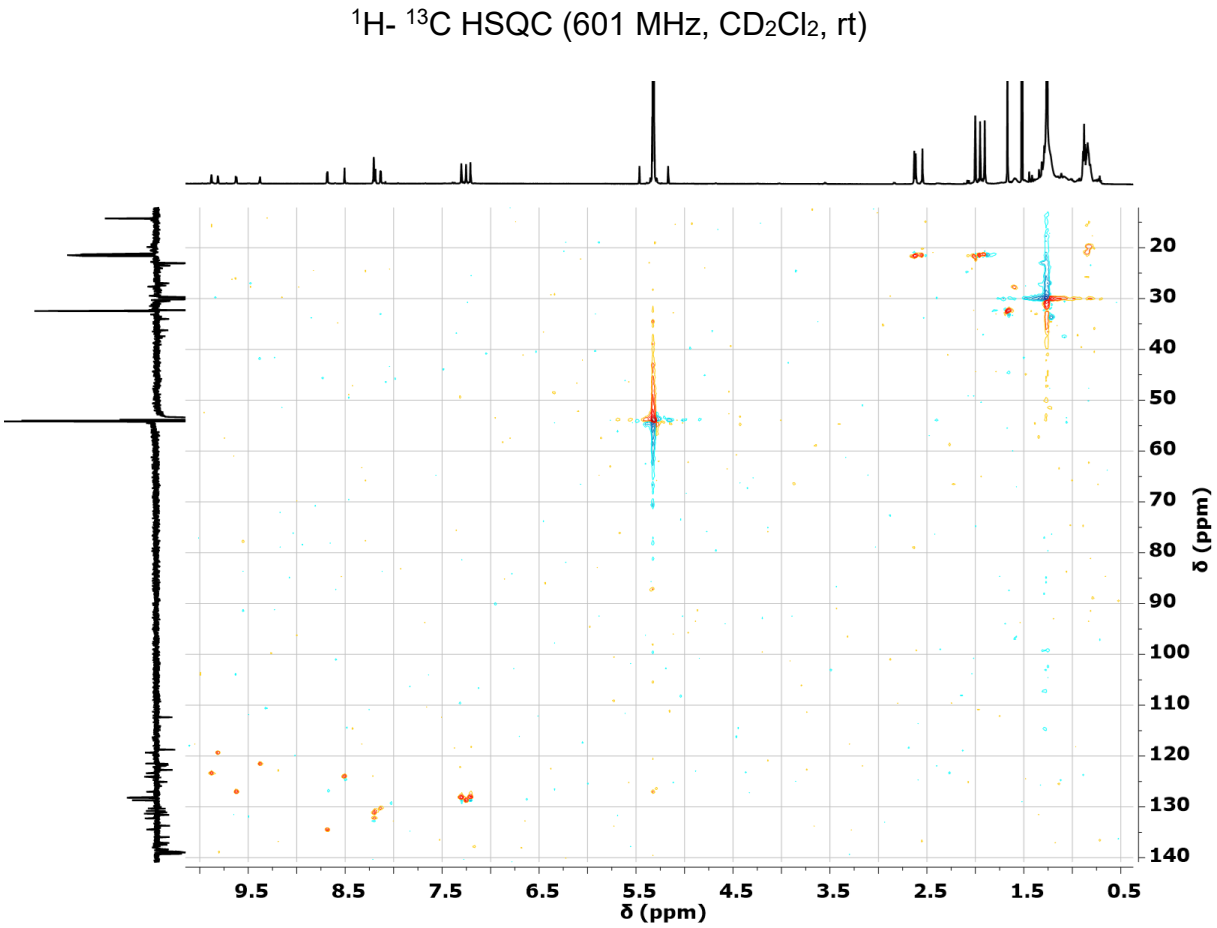


Figure S68. ^{1}H- ^{13}C HSQC of ***tri*-HBC**.

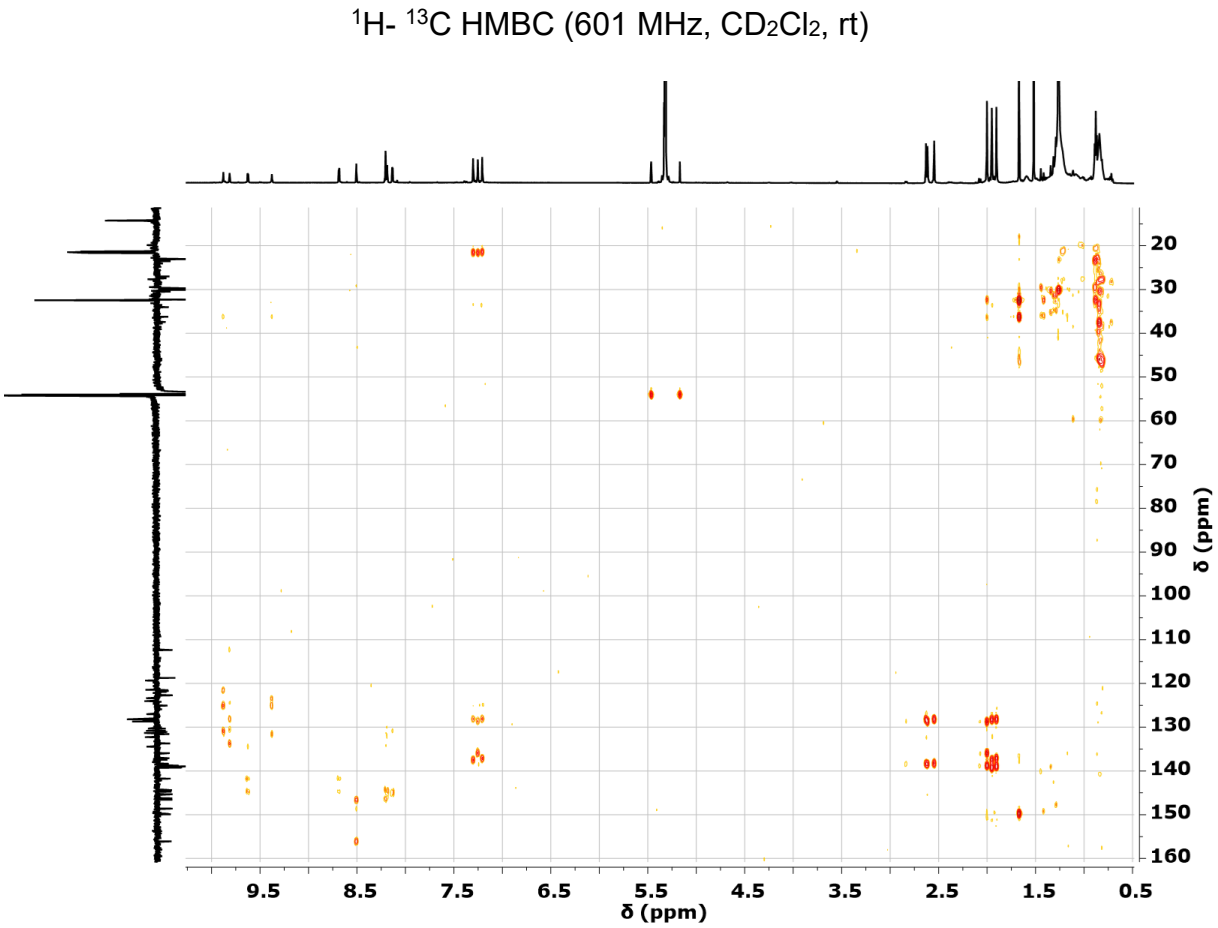
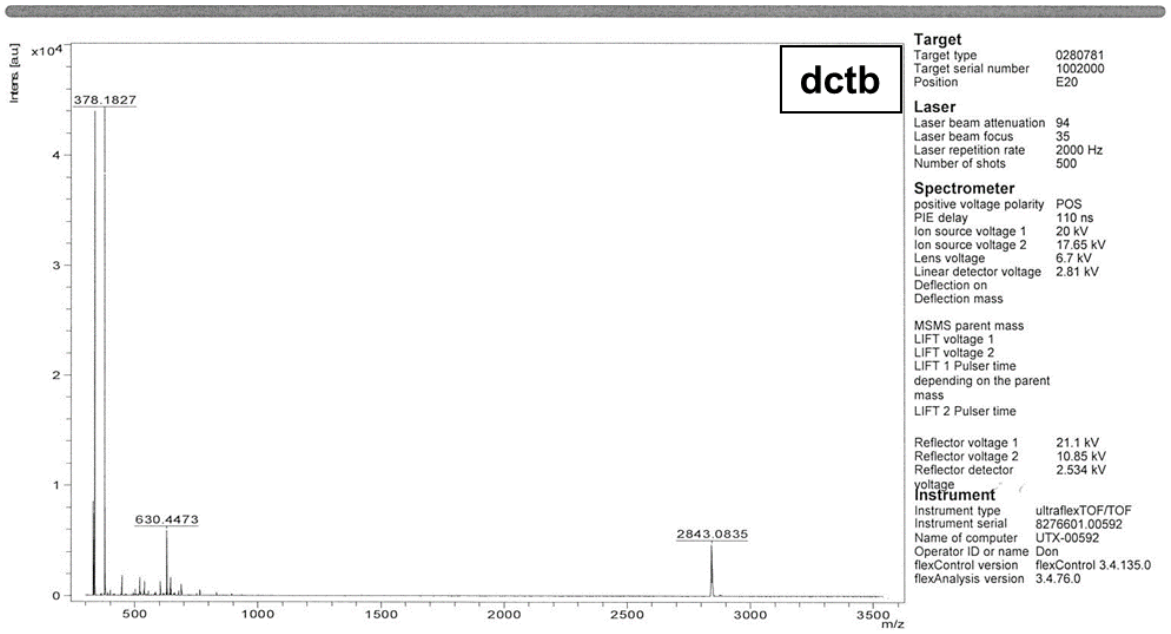
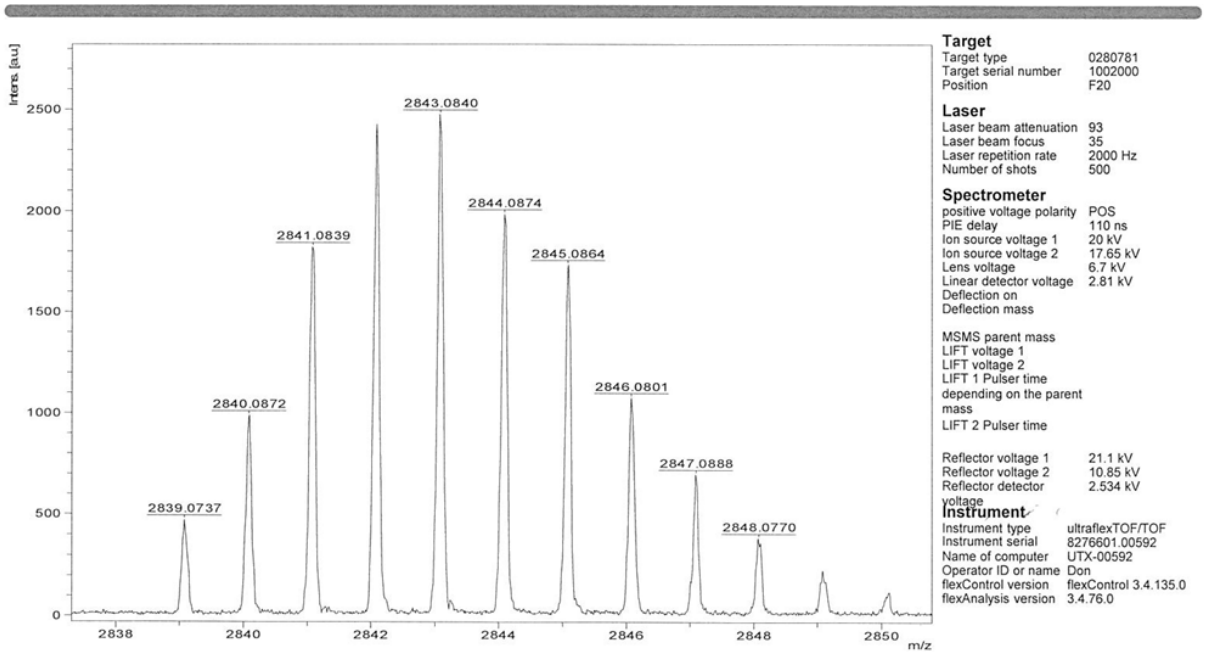


Figure S69. ^{1}H- ^{13}C HMBC of ***tri*-HBC**.

MS (MALDI)



HRMS (MALDI)



SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 195 H 156 N 12 Ni 3	2,839.0631	3.7514	57.9244	124.00	ok	odd

Figure S70. MS/HRMS (MALDI) of ***tri*-HBC**.

4 DFT Calculations

Geometries were relaxed using density-functional theory (DFT). The calculations were carried out with the plane-wave code PWScf of the Quantum Espresso software package,[5] utilizing the gradient-corrected Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional,[6] Grimme D3 dispersion correction with Becke-Johnson damping,[7,8] Vanderbilt ultrasoft pseudopotentials,[9] and a plane-wave basis set with a kinetic energy cutoff of 30 Ry. Structures were assumed to be relaxed when a force convergence threshold of 5 meV/Å was reached. All further analyses (HOMA index, orbitals, absorption spectra, and broken symmetry calculations) were done for the PBE-optimized geometries.

The Harmonic Oscillator Model of Aromaticity (HOMA) index for an *n*-membered ring is defined as:[10,11]

$$\mathrm{HOMA} = 1 - \frac{\alpha}{n}\sum_{i=1}^{n}\left(R_i - R_{\mathrm{opt}}\right)^2 \quad .$$

R_i (in Å) is the length of the *i*-th bond in the analyzed ring. R_{opt} = 1.3976 Å is the C-C bond length in the PBE-optimized benzene reference molecule, which, therefore, has a HOMA index of 1. The empirical constant α = 257.7 Å^{-2} normalizes the index to be unitless, and its value is chosen such that the HOMA index becomes zero for a non-aromatic, hypothetical, perfectly bond alternating Kekulé cyclohexatriene ring.[10,11] The HOMA index is an easily accessible geometric measure for local deviations from global aromaticity. Values much smaller than 1, close to zero, or even with negative sign are indicators of local antiaromatic behavior and increasing biradicaloid character in the ground state.[12]

Electronic properties and absorption spectra of the fused porphyrins were determined with the ORCA code,[13] using the B3LYP hybrid exchange-correlation functional,[14,15] the triple-zeta def2-TZVPP basis set,[16] and the RIJCOSX approximation with def2/J auxiliary basis functions.[17] Time-dependent density functional theory (TD-DFT) was used for the calculation of excitation energies and absorption spectra. The lowest 150 vertical transitions were included in the TD-DFT calculations. Solvation effects in DCM were taken into account by employing the implicit conductor-like continuum polarization model (C-PCM).[13]

The restricted Hartree-Fock (RHF) and the broken symmetry (BS) calculations were also done with the ORCA code using the same basis sets as above. The broken symmetry SCF solution is achieved by first performing an unrestricted Hartree-Fock (UHF) calculation for the triplet state (UHF-T). The orbitals of the triplet state are then used as starting guess for the subsequent unrestricted singlet broken symmetry calculation (UHF-BS). The calculated total energies and the expectation values of the spin operator $\langle S^2 \rangle$ for the building blocks and the final conjugated molecules are listed in Tables S1 and S2. The BS solutions is always lower in energy than both the triplet and the RHF state, indicating biradicaloid character of all molecules.

Table S1. Total energy E_{tot} (in Hartree) and spin expectation value $\langle S^2 \rangle$ of restricted Hartree-Fock (RHF) and unrestricted Hartree-Fock calculations in the triplet (UHF-T) and singlet broken symmetry (UHF-BS) state for the hexabenzocoronene (HBC) and phenyl-fused porphyrin (Ph) building blocks.

	Hexabenzocoronene (HBC)		**Phenyl-fused porphyrin (Ph)**	
	E_{tot}	$\langle S^2 \rangle$	E_{tot}	$\langle S^2 \rangle$
RHF	-2538.79449	0.00	-4070.46301	0.00
UHF-T	-2538.77371	5.99	-4070.50343	5.82
UHF-RS	-2538.89566	5.40	-4070.54653	5.14

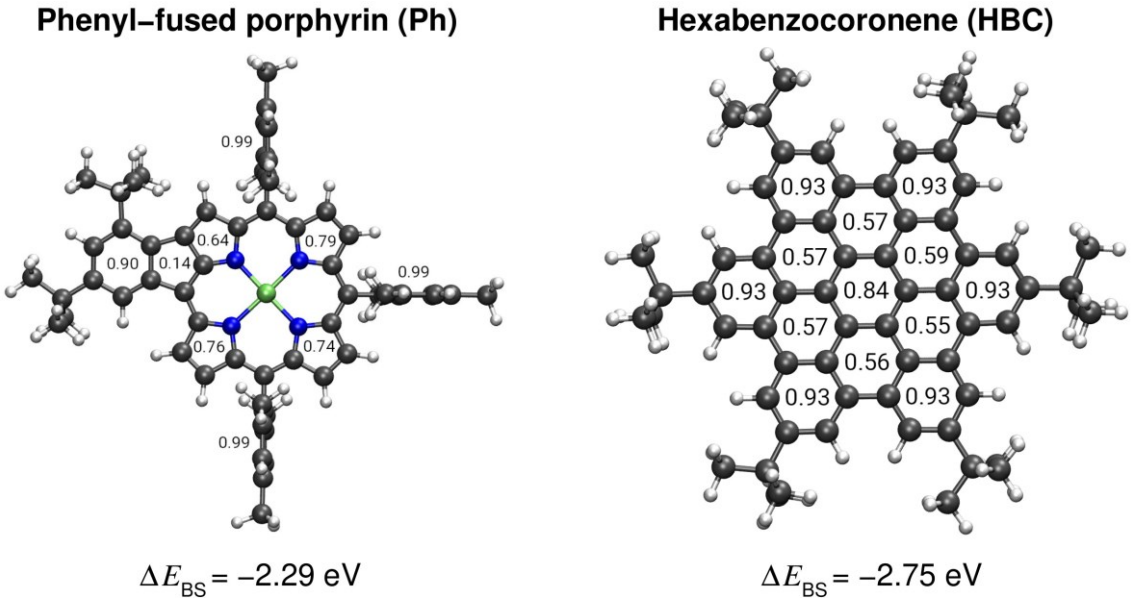


Figure S71. HOMA analysis for the phenyl-fused porphyrin and the HBC building block. The low HOMA value of 0.14 for the fused 5-membered ring and the reduced HOMA index of about 0.57 of the 6-membered rings in HBC indicate a tendency to local antiaromaticity and an increasing biradicaloid character of the ground state. This is confirmed by the negative value of the energy difference ΔE_{BS} between the singlet broken-symmetry and the spin-restricted Hartree-Fock calculation. ΔE_{BS} is positive for the initial tetraphenyl porphyrin molecule without fused 5-membered ring.[12]

Table S2. Total energy E_{tot} (in Hartree) and spin expectation value $\langle S^2 \rangle$ of restricted Hartree-Fock (RHF) and unrestricted Hartree-Fock calculations in the triplet (UHF-T) and singlet broken symmetry (UHF-BS) state for the final conjugated molecules.

	***o*-Ph**		***m*-Ph**		***p*-Ph**		***tri*-Ph**	
	E_{tot}	$\langle S^2 \rangle$	E_{tot}	$\langle S^2 \rangle$	E_{tot}	$\langle S^2 \rangle$	E_{tot}	$\langle S^2 \rangle$
RHF	-9671.47819	0.00	-9671.47881	0.00	-9671.47900	0.00	-13237.82137	0.00
UHF-T	-9671.69730	15.38	-9671.69863	15.40	-9671.69549	15.31	-13238.12005	19.93
UHF-RS	-9671.74194	14.72	-9671.74220	14.72	-9671.74238	14.71	-13238.16657	19.38

	***o*-HBC**		***m*-HBC**		***p*-HBC**		***tri*-HBC**	
	E_{tot}	$\langle S^2 \rangle$	E_{tot}	$\langle S^2 \rangle$	E_{tot}	$\langle S^2 \rangle$	E_{tot}	$\langle S^2 \rangle$
RHF	-9281.00201	0.00	-9281.00465	0.00	-9281.00183	0.00	-12652.10641	0.00
UHF-T	-9281.16149	14.86	-9281.22886	15.28	-9281.21529	15.23	-12652.37945	19.49
UHF-RS	-9281.26967	14.53	-9281.27320	14.54	-9281.27060	14.55	-12652.45824	19.14

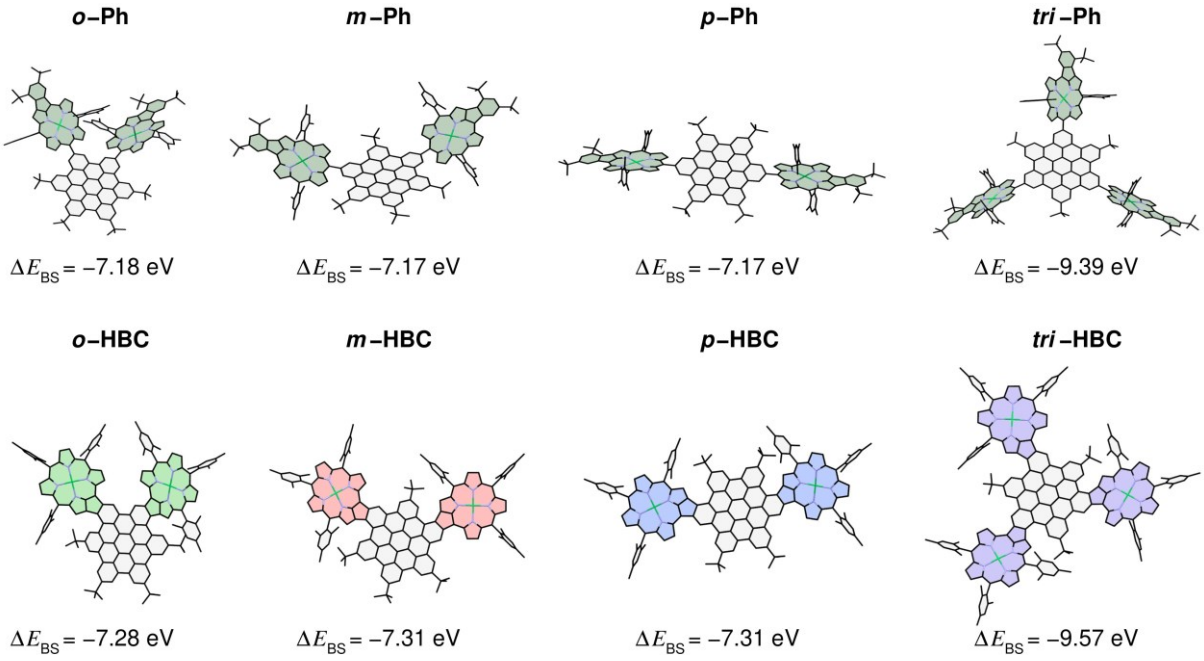


Figure S72. Energy difference ΔE_{BS} between the singlet broken-symmetry and the spin-restricted Hartree-Fock calculation of the final conjugated molecules. ΔE_{BS} is basically independent of the relative position of the porphyrins and is roughly the sum of the ΔE_{BS} values of the building blocks (*bi*-conjugates: -(2×2.29+2.75) eV = -7.33 eV; *tri*-conjugates: -(3×2.29+2.75) eV = -9.62 eV). The small deviations from this sum indicate that the position of the fused 5-membered ring (at the outer periphery of the porphyrin or between porphyrin and HBC) has only a small impact on the biradicaloid character of the fused porphyrin and the HBC.

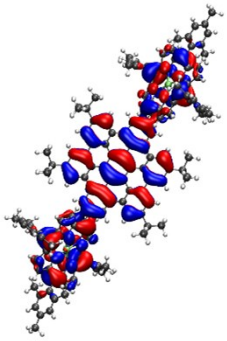
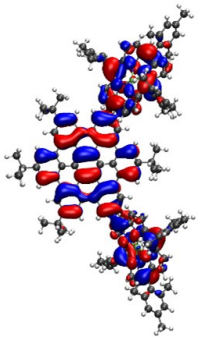
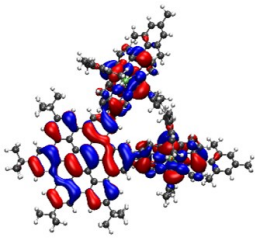
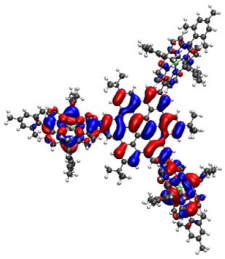
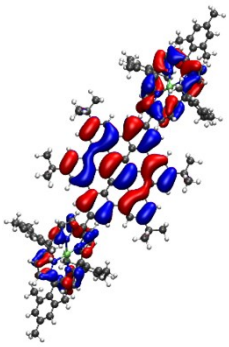
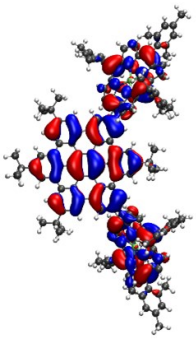
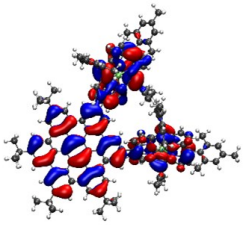
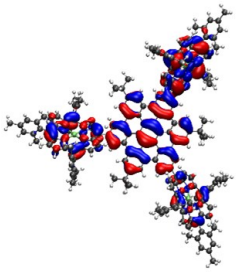
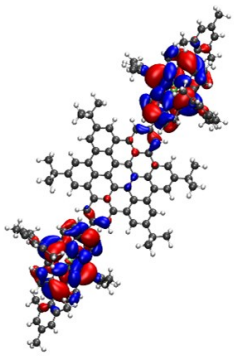
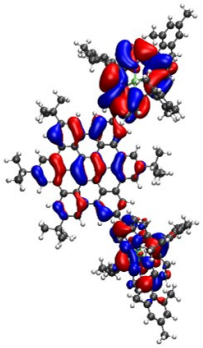
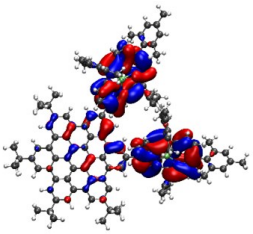
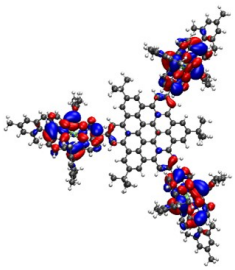
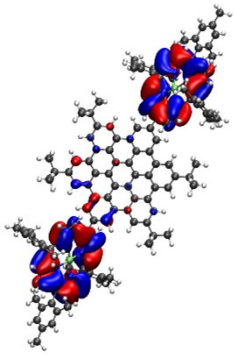
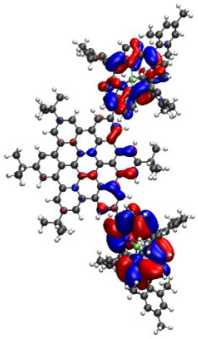
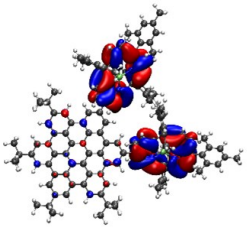
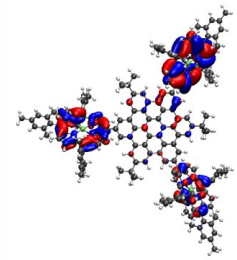
para-Porphyrin-HBC	*meta*-porphyrin-HBC	*ortho*-porphyrin-HBC	*tri*-porphyrin-HBC	
				**HOMO**
				**HOMO-1**
				**HOMO-2**
				**HOMO-3**

Figure S73. Geometry optimized structures of porphyrin-HBCs **11**-**14**.

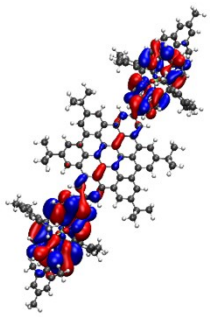
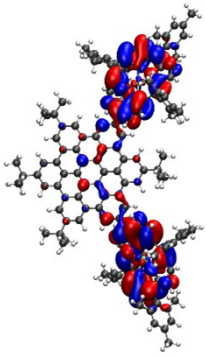
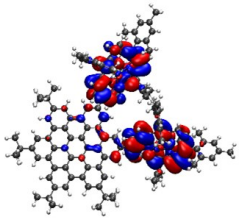
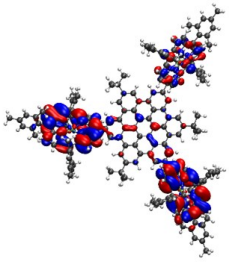
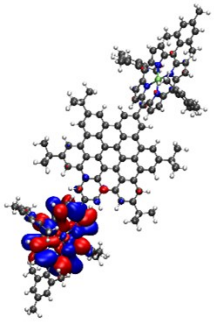
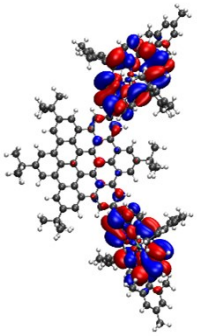
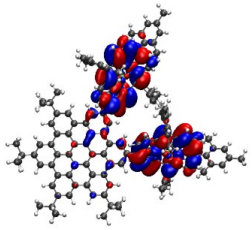
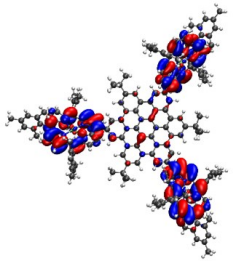
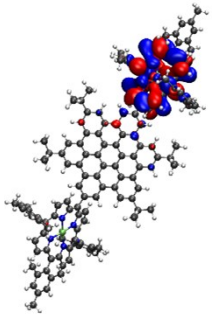
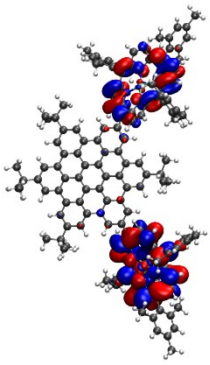
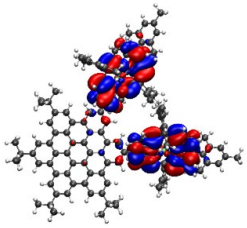
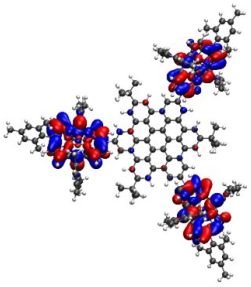
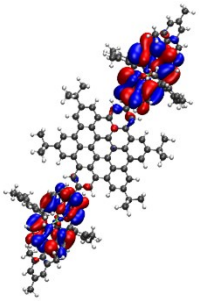
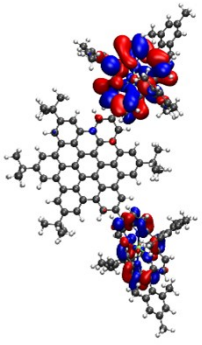
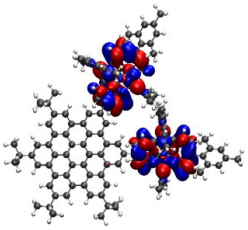
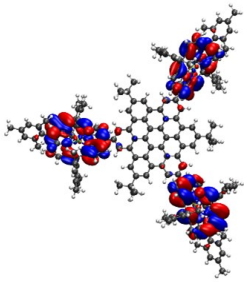
para-Porphyrin-HBC	*meta*-porphyrin-HBC	*ortho*-porphyrin-HBC	*tri*-porphyrin-HBC	
				**LUMO**
				**LUMO+1**
				**LUMO+2**
				**LUMO+3**

Figure S74. Geometry optimized structures of porphyrin-HBCs **11**-**14**.

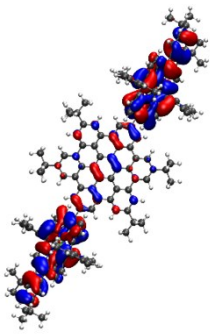
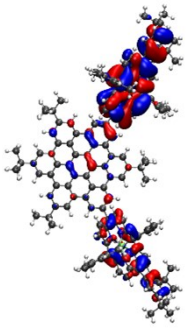
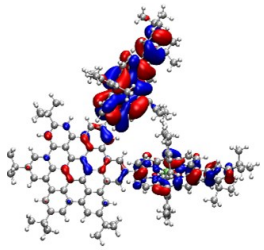
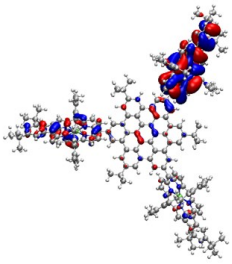
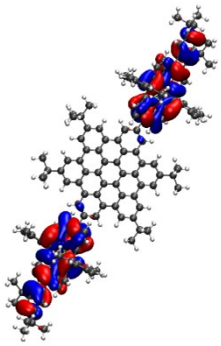
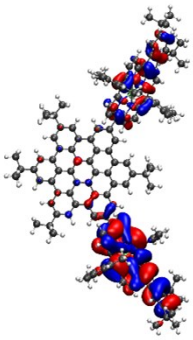
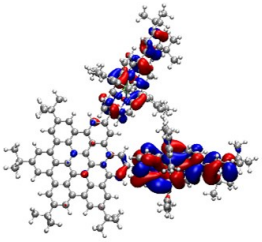
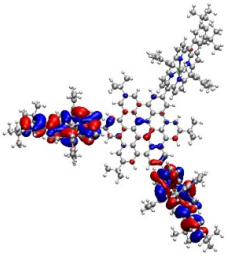
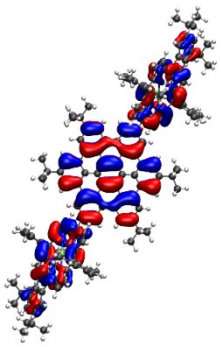
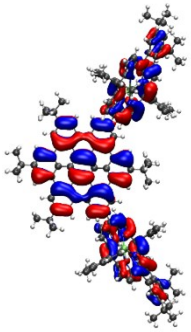
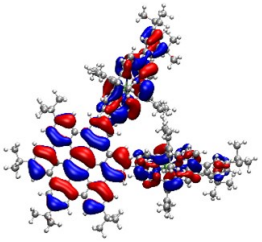
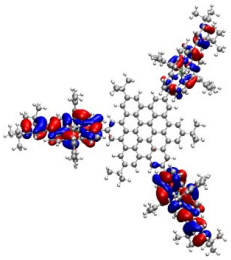
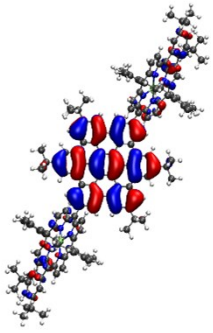
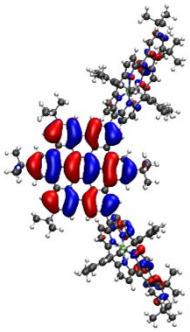
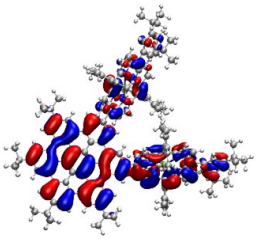
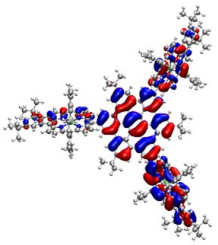
para-phenyl-fused Porphyrin-HBC	*meta*-phenyl-fused Porphyrin-HBC	*ortho*-phenyl-fused Porphyrin-HBC	*tri*-phenyl-fused Porphyrin-HBC	
				**HOMO**
				**HOMO-1**
				**HOMO-2**
				**HOMO-3**

Figure S75. Geometry optimized structures of porphyrin-HBCs ***p*-Ph**, ***m*-Ph**, ***o*-Ph**, ***tri*-Ph**.

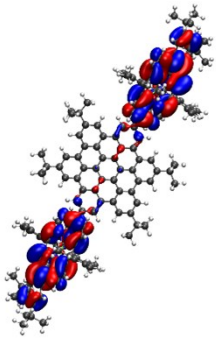
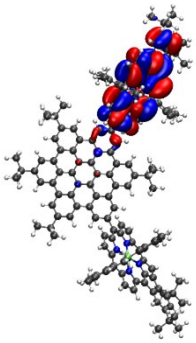
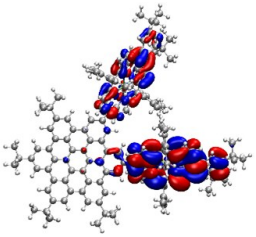
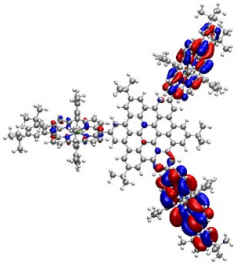
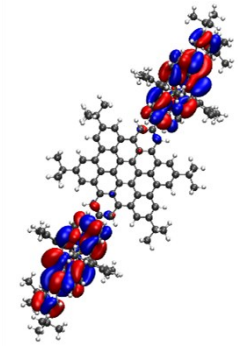
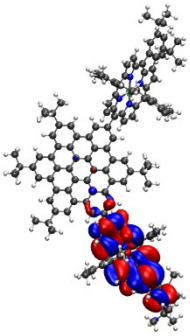
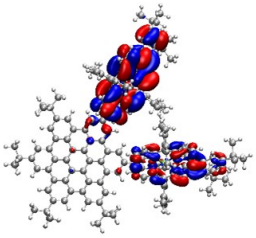
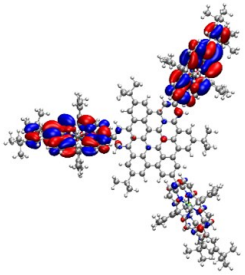
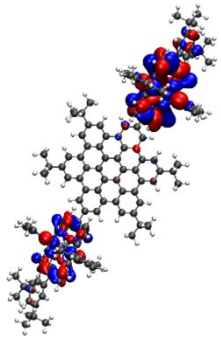
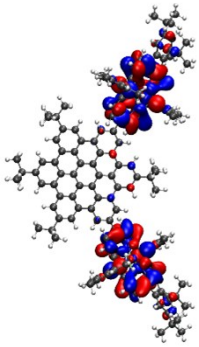
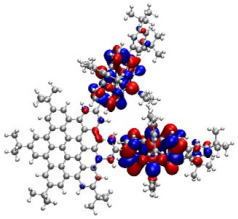
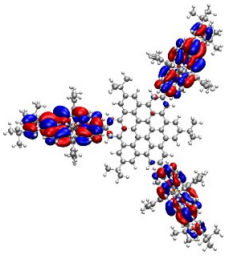
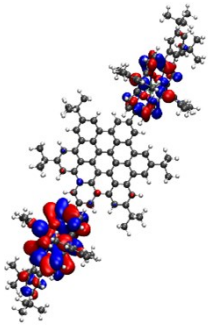
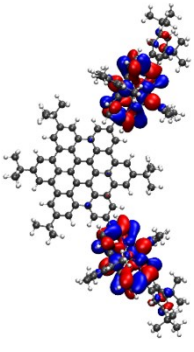
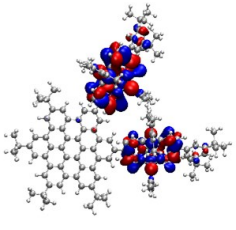
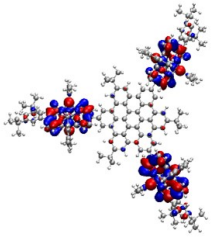
para-phenyl-fused Porphyrin-HBC	*meta*-phenyl-fused Porphyrin-HBC	*ortho*-phenyl-fused Porphyrin-HBC	*tri*-phenyl-fused Porphyrin-HBC	
				**LUMO**
				**LUMO+1**
				**LUMO+2**
				**LUMO+3**

Figure S76. Geometry optimized structures of porphyrin-HBCs ***p*-Ph**, ***m*-Ph**, ***o*-Ph**, ***tri*-Ph**.

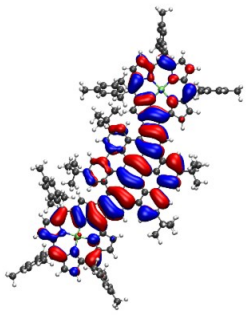
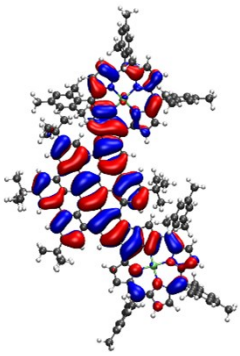
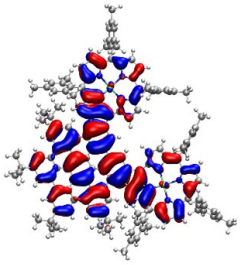
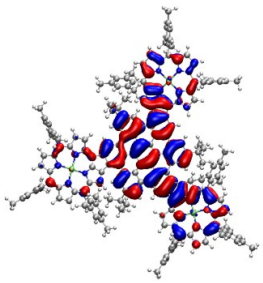
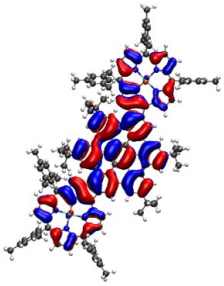
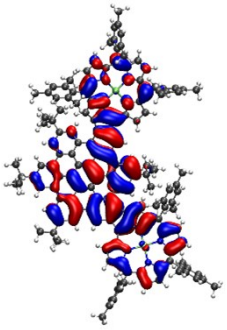
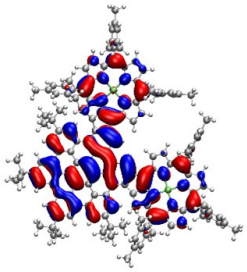
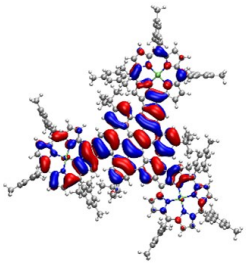
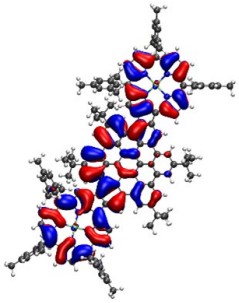
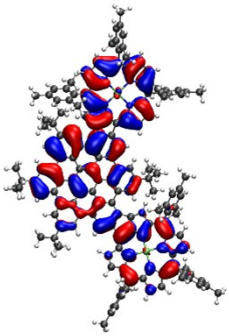
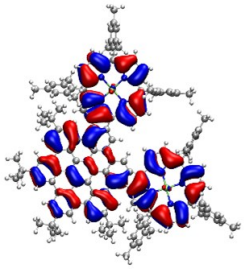
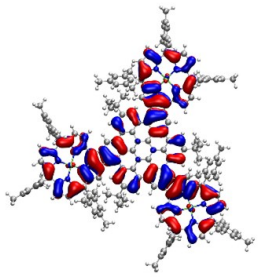
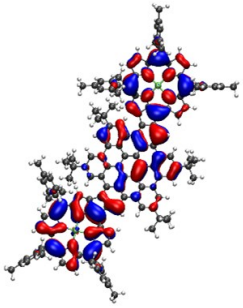
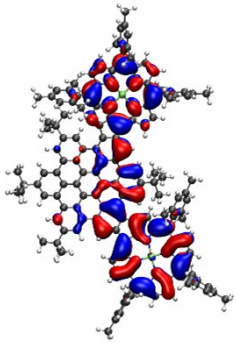
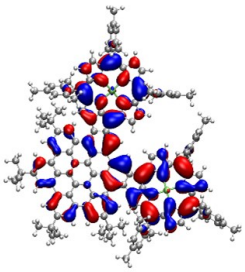
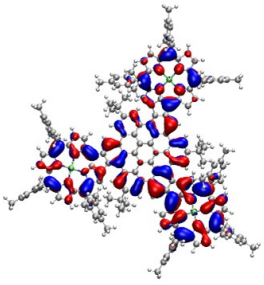
para-HBC-fused Porphyrin-HBC	*meta*-HBC-fused Porphyrin-HBC	*ortho*-HBC-fused Porphyrin-HBC	*tri*-HBC-fused Porphyrin-HBC	
				**HOMO**
				**HOMO-1**
				**HOMO-2**
				**HOMO-3**

Figure S77. Geometry optimized structures of porphyrin-HBCs ***p*-HBC**, ***m*-HBC**, ***o*-HBC**, ***tri*-HBC**.

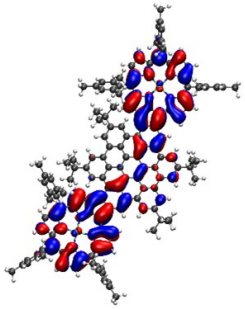
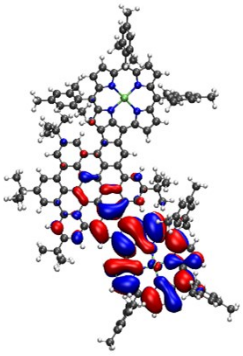
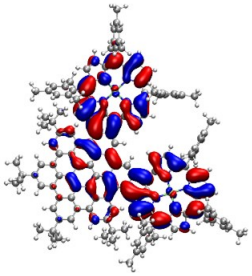
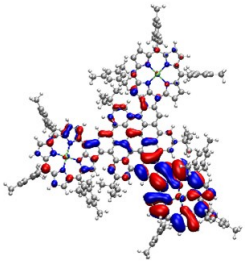
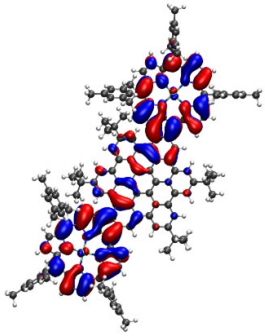
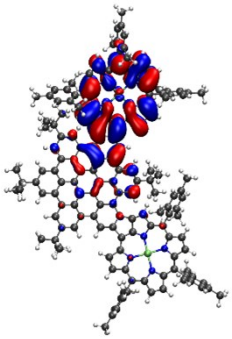
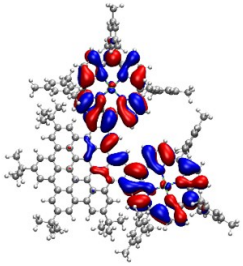
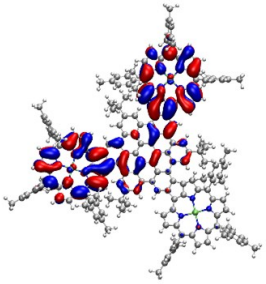
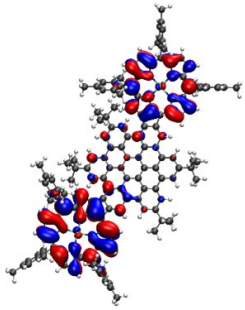
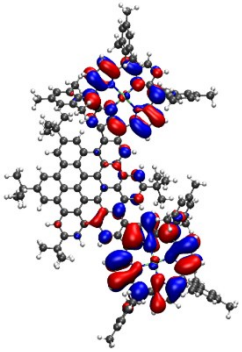
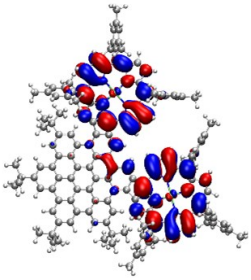
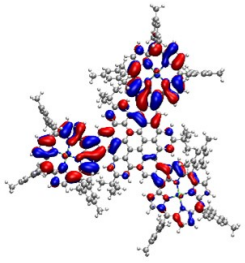
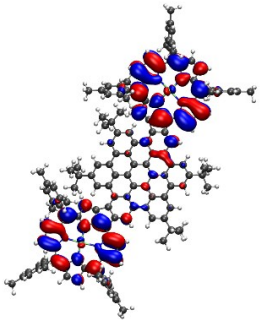
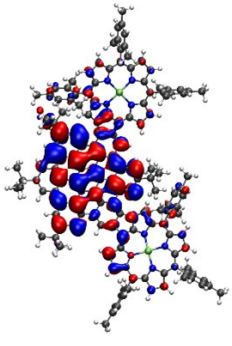
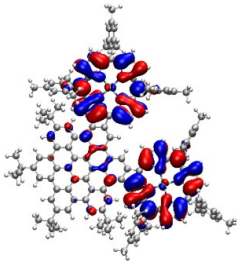
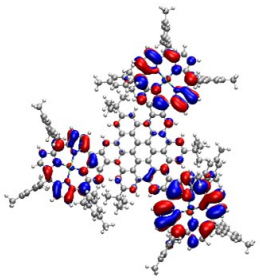
para-HBC-fused Porphyrin-HBC	*meta*-HBC-fused Porphyrin-HBC	*ortho*-HBC-fused Porphyrin-HBC	*tri*-HBC-fused Porphyrin-HBC	
				**LUMO**
				**LUMO+1**
				**LUMO+2**
				**LUMO+3**

Figure S78. Geometry optimized structures of porphyrin-HBCs ***p*-HBC**, ***m*-HBC**, ***o*-HBC**, ***tri*-HBC**.

Table S3. Energy Values of porphyrin-HBCs **11-14.**

***para*-Porphyrin-HBC**		***meta*-porphyrin-HBC**		***ortho*-porphyrin-HBC**		***tri*-porphyrin-HBC**	
Orbital	Energy (eV)	Orbital	Energy (eV)	Orbital	Energy (eV)	Orbital	Energy (eV)
HOMO-3	-5.327	HOMO-3	-5.326	HOMO-3	-5.301	HOMO-3	-5.324
HOMO-2	-5.262	HOMO-2	-5.287	HOMO-2	-5.267	HOMO-2	-5.257
HOMO-1	-5.220	HOMO-1	-5.171	HOMO-1	-5.181	HOMO-1	-5.176
HOMO	-5.135	HOMO	-5.132	HOMO	-5.145	HOMO	-5.160
LUMO	-2.344	LUMO	-2.344	LUMO	-2.304	LUMO	-2.351
LUMO+1	-2.321	LUMO+1	-2.332	LUMO+1	-2.298	LUMO+1	-2.344
LUMO+2	-2.309	LUMO+2	-2.319	LUMO+2	-2.277	LUMO+2	-2.329
LUMO+3	-2.298	LUMO+3	-2.311	LUMO+3	-2.270	LUMO+3	-2.323
GAP	2.791	GAP	2.788	GAP	2.840	GAP	2.810

Table S4. Energy Values for. porphyrin-HBCs ***p*-Ph**, ***m*-Ph**, ***o*-Ph**, ***tri*-Ph**.

***p*-Ph**		***m*-Ph**		***o*-Ph**		***tri*-Ph**	
Orbital	Energy (eV)	Orbital	Energy (eV)	Orbital	Energy (eV)	Orbital	Energy (eV)
HOMO-3	-5.286	HOMO-3	-5.300	HOMO-3	-5.260	HOMO-3	-5.275
HOMO-2	-5.236	HOMO-2	-5.224	HOMO-2	-5.233	HOMO-2	-5.048
HOMO-1	-5.040	HOMO-1	-5.035	HOMO-1	-5.012	HOMO-1	-5.036
HOMO	-5.013	HOMO	-5.020	HOMO	-4.988	HOMO	-5.032
LUMO	-2.639	LUMO	-2.627	LUMO	-2.613	LUMO	-2.641
LUMO+1	-2.617	LUMO+1	-2.626	LUMO+1	-2.594	LUMO+1	-2.638
LUMO+2	-2.351	LUMO+2	-2.350	LUMO+2	-2.332	LUMO+2	-2.632
LUMO+3	-2.347	LUMO+3	-2.342	LUMO+3	-2.308	LUMO+3	-2.360
GAP	2.374	GAP	2.393	GAP	2.375	GAP	2.391

Table S5. Energy Values for porphyrin-HBCs ***p*-HBC**, ***m*-HBC**, ***o*-HBC**, ***tri*-HBC**.

***p*-HBC**		***m*-HBC**		***o*-HBC**		***tri*-HBC**	
Orbital	Energy (eV)	Orbital	Energy (eV)	Orbital	Energy (eV)	Orbital	Energy (eV)
HOMO-3	-5.254	HOMO-3	-5.297	HOMO-3	-5.314	HOMO-3	-5.290
HOMO-2	-5.227	HOMO-2	-5.185	HOMO-2	-5.268	HOMO-2	-5.033
HOMO-1	-4.926	HOMO-1	-4.922	HOMO-1	-4.978	HOMO-1	-4.835
HOMO	-4.839	HOMO	-4.844	HOMO	-4.780	HOMO	-4.834
LUMO	-2.745	LUMO	-2.717	LUMO	-2.788	LUMO	-2.724
LUMO+1	-2.687	LUMO+1	-2.709	LUMO+1	-2.647	LUMO+1	-2.716
LUMO+2	-2.413	LUMO+2	-2.408	LUMO+2	-2.421	LUMO+2	-2.713
LUMO+3	-2.402	LUMO+3	-2.399	LUMO+3	-2.369	LUMO+3	-2.412
GAP	2.094	GAP	2.127	GAP	1.992	GAP	2.111

Calculated Absorption Spectra

ortho-HBC-fused porphyrin-HBC *o*-HBC

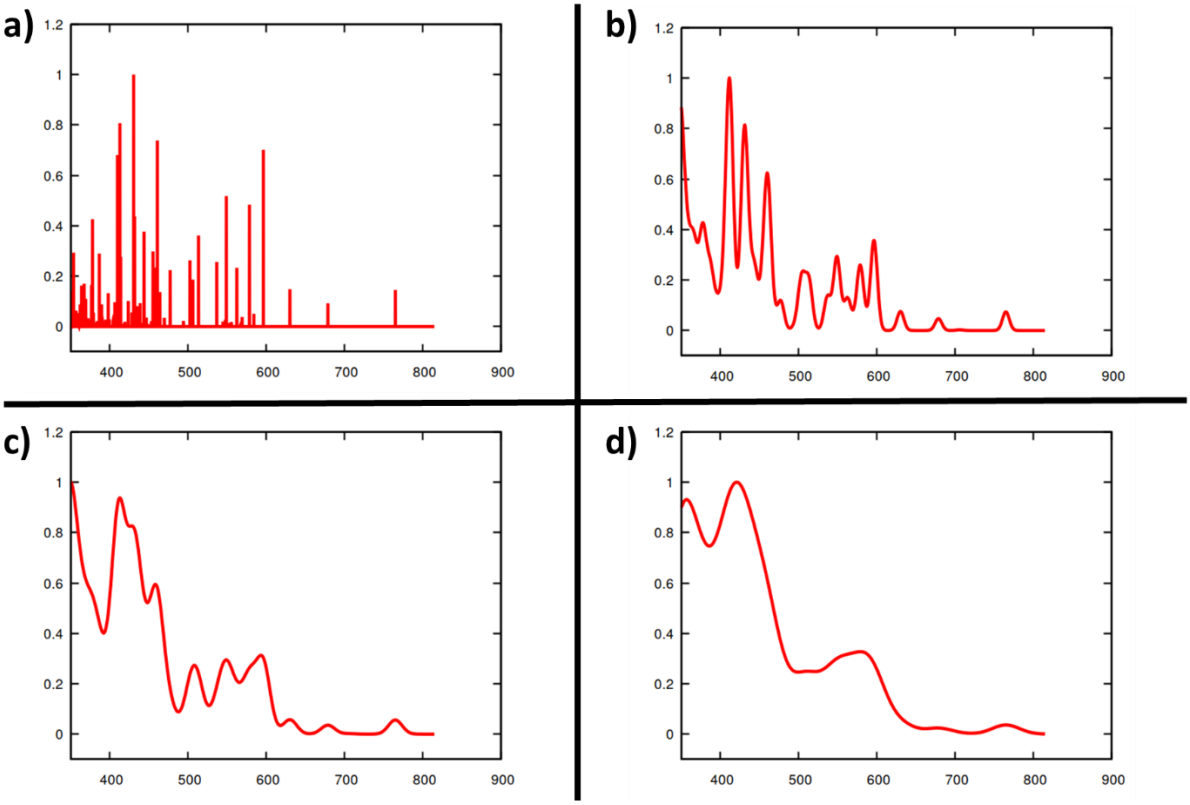


Figure S79. DFT-calculated transitions for ***o*-HBC** with increasing broadening factor σ: a) no broadening, b) 5 nm, c) 10 nm, d) 20 nm.

Table S6. TD-DFT excitation energies and oscillator strengths of ***o*-HBC**.

Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*	Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*
1	764.9	1.621	0.1229	16	544.5	2.277	0.0163
2	705.7	1.757	0.0044	17	536.6	2.311	0.2169
3	678.7	1.827	0.078	18	522.5	2.373	0.0022
4	630.1	1.968	0.1256	19	513.3	2.415	0.3061
5	596.2	2.080	0.5943	20	506.0	2.450	0.1576
6	584.0	2.123	0.0426	21	502.4	2.468	0.2225
7	578.4	2.144	0.4098	22	494.1	2.509	0.0187
8	569.1	2.179	0.0322	23	477.0	2.599	0.1897
9	566.6	2.188	0.0008	24	472.0	2.627	0.0001
10	562.3	2.205	0.1973	25	470.4	2.636	0.0001
11	561.3	2.209	0	26	469.5	2.641	0.0294
12	555.2	2.233	0.0151	27	463.9	2.673	0.1159
13	553.2	2.241	0.0124	28	460.5	2.692	0.6259
14	548.9	2.259	0.439	29	459.2	2.700	0.1987
15	547.4	2.265	0.0228	30	455.1	2.724	0.2526

Table S7. Orbital transitions and their relative contributions to optically active excitations with large oscillator strengths from the TD-DFT calculations of ***o*-HBC**. Only transitions with contributions exceeding 10% are listed.

State	Energy (eV)	Transition	Contribution (%)
1	1.621	HOMO → LUMO	92.1
4	1.968	HOMO-1 → LUMO+1	40.1
		HOMO → LUMO+2	38.9
5	2.080	HOMO-3 → LUMO	16.3
		HOMO-1 → LUMO+1	48.7
		HOMO → LUMO+2	21.2
7	2.144	HOMO-3 → LUMO+1	11.2
		HOMO-1 → LUMO	12.1
		HOMO → LUMO+3	49.5
10	2.205	HOMO-4 → LUMO	16.7
		HOMO-3 → LUMO	10.7
		HOMO-2 → LUMO+1	23.8
		HOMO-1 → LUMO+3	12.4
		HOMO → LUMO+2	19.8
14	2.259	HOMO-4 → LUMO	36.8
		HOMO-3 → LUMO	20.6
		HOMO → LUMO+2	14.3

meta-HBC-fused porphyrin-HBC *m*-HBC

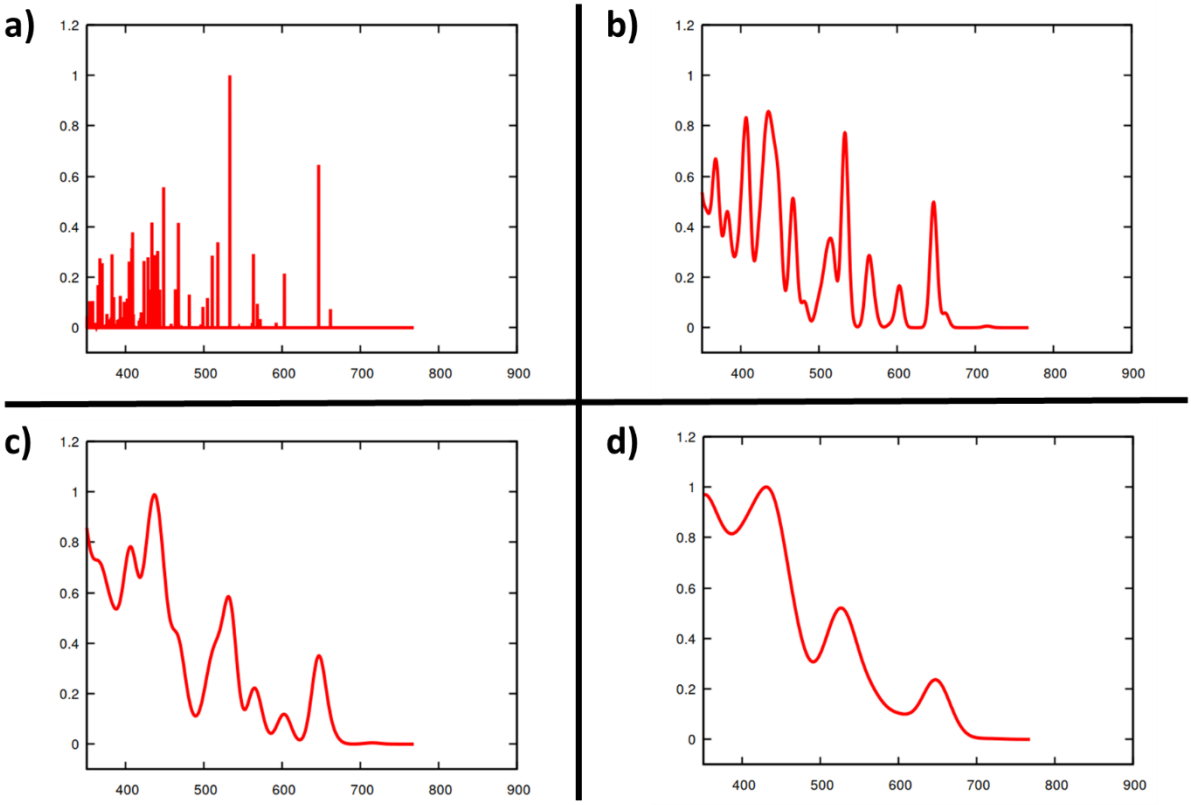


Figure S80. DFT-calculated transitions for ***m*-HBC** with increasing broadening factor σ: a) no broadening, b) 5 nm, c) 10 nm, d) 20 nm.

Table S8. TD-DFT excitation energies and oscillator strengths of ***m*-HBC**.

Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*	Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*
1	718.2	1.726	0.0046	16	540.3	2.295	0.0061
2	712.8	1.739	0.0056	17	532.9	2.327	1.0076
3	661.6	1.874	0.0744	18	517.6	2.395	0.3411
4	646.5	1.918	0.65	19	510.5	2.429	0.2876
5	602.7	2.057	0.2159	20	504.3	2.458	0.1184
6	592.2	2.094	0.02	21	498.6	2.486	0.0835
7	571.7	2.169	0.0345	22	495.9	2.500	0.013
8	569.5	2.177	0.0003	23	481.1	2.577	0.1324
9	568.1	2.182	0.0953	24	471.3	2.631	0.0005
10	563.1	2.202	0.2943	25	467.8	2.65	0.0138
11	562.2	2.205	0.0004	26	467.2	2.654	0.4184
12	561.7	2.207	0.0189	27	466.8	2.656	0.1233
13	558.1	2.221	0.0001	28	463.3	2.676	0.1531
14	553.3	2.241	0.0001	29	457.9	2.708	0.0153
15	544.7	2.276	0.0008	30	455.7	2.721	0.005

Table S9. Orbital transitions and their relative contributions to optically active excitations with large oscillator strengths from the TD-DFT calculations of ***m*-HBC**. Only transitions with contributions exceeding 10% are listed.

State	Energy (eV)	Transition	Contribution (%)
1	1.726	HOMO-1 → LUMO+1	19.9
		HOMO → LUMO	46.2
		HOMO → LUMO+1	18.5
4	1.918	HOMO-1 → LUMO+1	57.6
		HOMO → LUMO	16.2
5	2.057	HOMO-2 → LUMO+1	26.9
		HOMO-1 → LUMO+3	14.2
		HOMO → LUMO+2	23.7
10	2.202	HOMO-3 → LUMO+1	21.7
		HOMO-2 → LUMO+1	21.9
		HOMO → LUMO+3	14.7
17	2.327	HOMO-3 → LUMO	24.1
		HOMO-3 → LUMO+1	20.4
		HOMO → LUMO+2	13.6

para-HBC-fused porphyrin-HBC *p*-HBC

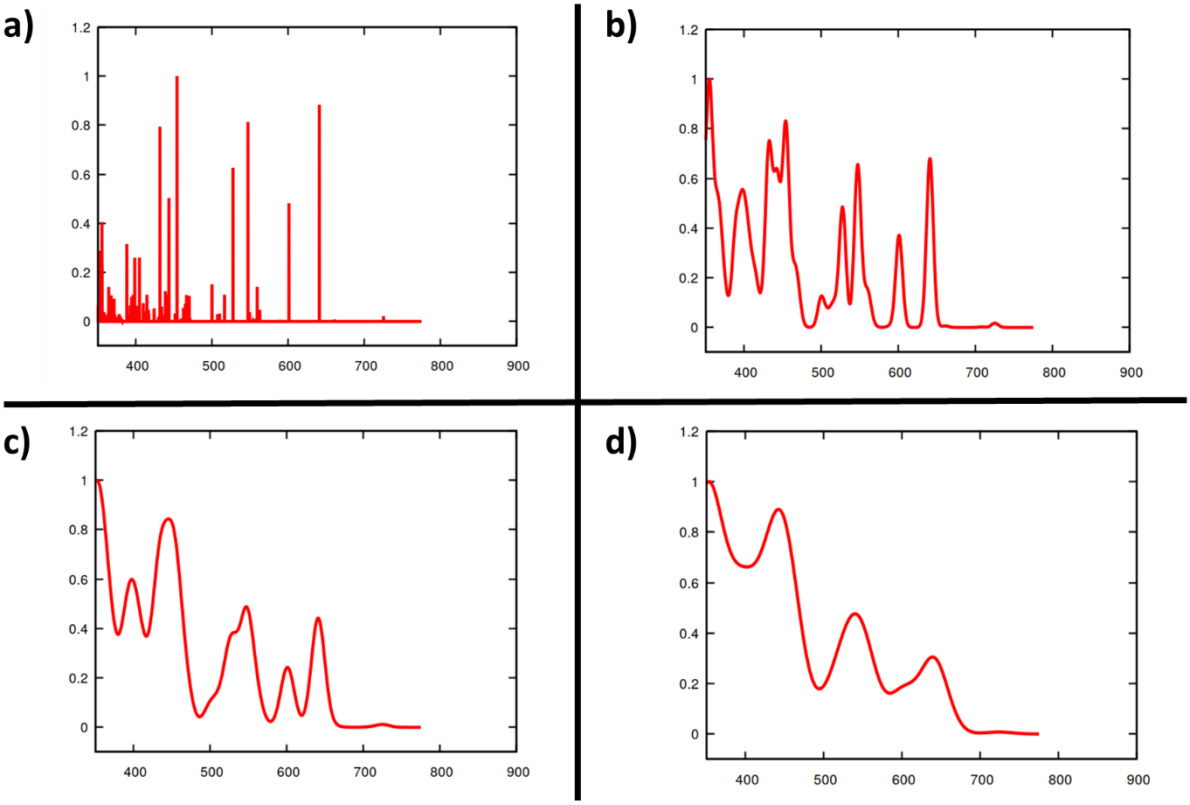


Figure S81. DFT-calculated transitions for ***p*-HBC** with increasing broadening factor σ: a) no broadening, b) 5 nm, c) 10 nm, d) 20 nm.

Table S10. TD-DFT excitation energies and oscillator strengths of ***p*-HBC**.

Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*	Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*
1	725.2	1.710	0.0234	16	539.2	2.299	0.006
2	708.1	1.751	0.0027	17	527.5	2.350	0.6525
3	660.8	1.876	0.0085	18	516.3	2.401	0.1136
4	640.9	1.934	0.9203	19	509.7	2.432	0.0332
5	600.9	2.063	0.5021	20	507.2	2.444	0.0306
6	589.4	2.104	0.0073	21	499.8	2.481	0.1579
7	570.6	2.173	0.002	22	496.8	2.496	0.003
8	568.7	2.180	0	23	471.7	2.628	0.001
9	563.6	2.200	0.0003	24	469.9	2.639	0.1084
10	562.6	2.204	0.05	25	466.9	2.656	0.0212
11	559.3	2.217	0.1468	26	466.4	2.658	0.1122
12	557.3	2.225	0.0122	27	464.7	2.668	0.0757
13	553.5	2.240	0.001	28	462.3	2.682	0.0575
14	549.2	2.258	0.0398	29	459.3	2.700	0.0124
15	547.1	2.266	0.8471	30	453.9	2.732	1.0419

Table S11. Orbital transitions and their relative contributions to optically active excitations with large oscillator strengths from the TD-DFT calculations of ***p*-HBC**. Only transitions with contributions exceeding 10% are listed.

State	Energy (eV)	Transition	Contribution (%)
1	1.710	HOMO-1 → LUMO+1	19.9
		HOMO → LUMO	73.1
4	1.934	HOMO-1 → LUMO+1	58.9
		HOMO → LUMO	15.4
5	2.063	HOMO-2 → LUMO	16.8
		HOMO-1 → LUMO+1	15.6
		HOMO-1 → LUMO+3	12.1
		HOMO → LUMO+2	30.1
11	2.217	HOMO-25 → LUMO+8	10.8
		HOMO-3 → LUMO+1	14.8
		HOMO-2 → LUMO	28.3
		HOMO-1 → LUMO+3	11.5
15	2.266	HOMO-2 → LUMO	22.7
		HOMO → LUMO+2	45.3

tri-HBC-fused porphyrin-HBC *t*-HBC

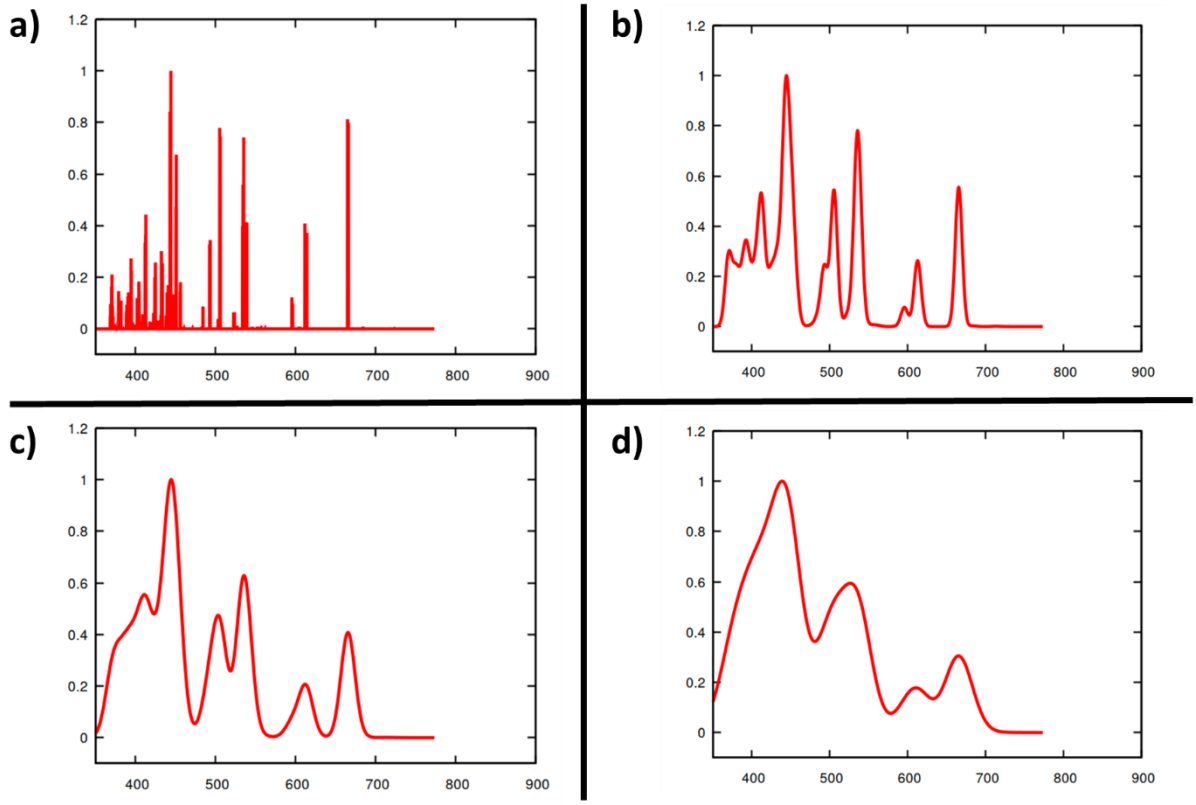


Figure S82. DFT-calculated transitions for ***tri*-HBC** with increasing broadening factor σ: a) no broadening, b) 5 nm, c) 10 nm, d) 20 nm.

Table S12. TD-DFT excitation energies and oscillator strengths of ***tri*-HBC**.

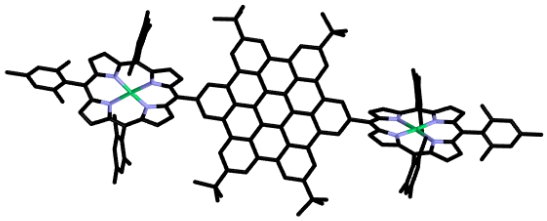
Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*	Excited state	Energy (nm)	Energy (eV)	Oscillator strength *f*
1	723.5	1.714	0.0002	16	558.4	2.221	0.0038
2	714.3	1.736	0.001	17	557.6	2.224	0.0004
3	713.0	1.739	0.0021	18	556.9	2.226	0.0003
4	684.1	1.812	0.0065	19	556.1	2.230	0.0017
5	666.1	1.861	0.6071	20	555.6	2.231	0.0017
6	664.8	1.865	0.6176	21	552.7	2.243	0.0067
7	614.0	2.019	0.2831	22	552.3	2.245	0.001
8	611.6	2.027	0.3104	23	549.1	2.258	0.001
9	604.7	2.050	0.0064	24	545.6	2.272	0.0062
10	596.2	2.080	0.0733	25	539.0	2.300	0.3135
11	595.3	2.083	0.0925	26	538.3	2.303	0.279
12	589.2	2.104	0.0038	27	535.1	2.317	0.5641
13	564.8	2.195	0.0022	28	534.2	2.321	0.4249
14	562.1	2.206	0.0005	29	533.7	2.323	0.3023
15	561.7	2.207	0.0042	30	526.7	2.354	0.0095

Table S13. Orbital transitions and their relative contributions to optically active excitations with large oscillator strengths from the TD-DFT calculations of ***tri*-HBC**. Only transitions with contributions exceeding 10% are listed.

State	Energy (eV)	Transition	Contribution (%)
1	1.714	HOMO-1 → LUMO	21.3
		HOMO-1 → LUMO+1	21.2
		HOMO → LUMO	26.2
		HOMO → LUMO+1	14.6
5	1.861	HOMO-1 → LUMO	23.5
		HOMO-1 → LUMO+2	19.5
		HOMO → LUMO+1	27.1
		HOMO → LUMO+2	14.4
6	1.865	HOMO-1 → LUMO+1	16.9
		HOMO-1 → LUMO+2	28.1
		HOMO → LUMO	13.6
		HOMO → LUMO+2	25.3
7	2.019	HOMO-2 → LUMO	64.4
8	2.027	HOMO-2 → LUMO+1	63.2

Cartesian Coordinates of Calculated Structures

para-porphyrin-HBC 12

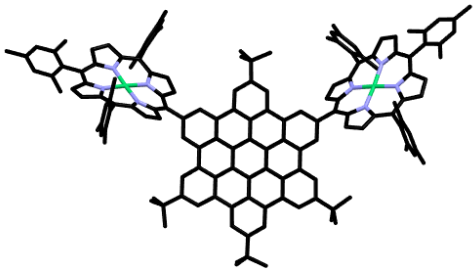


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	32.95467	27.24522	22.41722
C	32.25980	28.45102	22.47657
C	32.20457	26.06640	22.38011
C	30.19061	32.22854	22.70315
C	30.85664	28.51040	22.49135
C	28.72862	29.80818	22.54527
C	30.15499	29.78851	22.56015
C	30.85380	31.00273	22.63897
C	28.79560	32.23905	22.68970
C	28.04686	31.05905	22.60563
H	31.94195	31.01481	22.64515
H	28.29912	33.20483	22.75411
C	26.55948	28.61094	22.45066
C	25.86468	29.87140	22.49641
C	23.68507	28.67162	22.37596
C	26.58900	31.09167	22.57674
C	25.88885	32.30817	22.61861
C	24.49800	32.36944	22.58951
C	23.79874	31.16177	22.51339
C	24.44017	29.91807	22.46261
H	26.44911	33.23680	22.67404
H	22.71099	31.19741	22.49279
C	23.72822	33.69493	22.63829
C	22.81806	33.70732	23.88426
H	23.41406	33.61599	24.80408
H	22.25211	34.65034	23.93188
C	24.66322	34.91101	22.71190
H	25.32304	34.97426	21.83371
H	24.06433	35.83284	22.74511
C	22.86122	33.82591	21.36890
H	23.48854	33.82634	20.46555
H	22.14321	32.99855	21.27962
H	22.29085	34.76703	21.39381
H	25.29051	34.89004	23.61534
C	30.10704	27.30209	22.43986
H	37.37949	44.86903	22.10714
H	37.61406	44.78995	23.86409
H	38.77061	43.99364	22.76763
C	33.85915	41.57528	24.86278
H	33.99109	40.73029	25.55610
H	33.75952	42.49427	25.45495
H	32.90997	41.39995	24.33361
C	36.71965	39.58295	21.18909
H	36.92473	38.65393	21.74269
H	35.87571	39.36498	20.51656
H	37.59793	39.81996	20.57463
Ni	32.60581	36.50186	22.99689
H	38.00511	41.95858	21.42869
H	35.57316	43.65166	24.54353
C	29.96612	34.23290	20.60557
H	29.49896	33.28814	20.34908
C	29.90833	35.41694	19.93565
H	33.02652	33.07763	26.87600
C	34.84711	34.98495	27.10489
C	34.45634	35.53809	28.34027
C	35.09309	35.10343	29.50903
C	36.10568	34.13951	29.48374
C	36.48133	33.61085	28.24373
C	35.86886	34.01413	27.05245
C	36.75874	33.66384	30.75467
H	36.63855	34.39458	31.56624
H	36.31317	32.71519	31.09578
H	37.83356	33.48312	30.60976
C	33.37144	36.58036	28.40682
H	32.44550	36.22497	27.92987
H	33.14488	36.84640	29.44755
H	33.66623	37.49756	27.87361
C	30.80443	26.05930	22.39220
C	28.66753	27.33294	22.43066
C	27.98240	28.57920	22.47398
C	25.82257	27.39661	22.38160
C	26.50776	26.14964	22.34715
C	27.92994	26.11781	22.37249
C	28.62402	24.85591	22.34095
C	25.76076	24.91858	22.29046
C	24.38278	27.43256	22.34369
C	27.89641	23.63075	22.29633
C	28.59908	22.42045	22.26998
C	29.99493	22.35960	22.29337
C	30.69278	23.56463	22.33631
C	30.04584	24.81119	22.35554
C	24.33605	24.94463	22.25370
C	23.63383	23.73470	22.20949
C	24.28613	22.50138	22.21315
C	25.68096	22.48080	22.24162
C	26.43604	23.66252	22.27380
C	22.28161	28.67087	22.32254
C	21.53640	27.49662	22.24269
C	22.23583	26.28751	22.21841
C	23.63303	26.22390	22.26873
H	21.75405	29.62027	22.34163
H	21.66488	25.36306	22.15636
H	22.54672	23.72776	22.16976
H	26.17233	21.50973	22.25015
H	31.77851	23.53498	22.35846
H	32.73814	25.11869	22.33478
H	22.09482	32.87972	23.86746
C	20.00451	27.48737	22.17604
C	19.41027	28.90153	22.24002
H	19.67826	29.41453	23.17581
H	19.74458	29.52234	21.39538
H	18.31307	28.84222	22.19465
C	28.55003	39.17257	16.96876
C	27.98511	39.10350	18.24704
C	28.70446	38.62464	19.34741
C	27.74509	39.66201	15.79383
H	28.39481	40.02852	14.98717
H	27.12516	38.85241	15.37522
H	27.06422	40.47482	16.08426
C	32.05062	37.81578	17.67129
H	32.19757	36.78305	18.02204
H	32.32310	37.86260	16.60890
H	32.75814	38.44198	18.23654
C	28.06177	38.56074	20.70788
H	27.98411	37.52134	21.06359
H	28.65594	39.10419	21.45792
H	27.05217	38.99160	20.68621
H	30.33472	38.79742	15.81879
H	26.95320	39.43432	18.39521
C	20.87258	20.21235	24.34018
C	22.59359	20.98588	23.21212
N	21.67784	19.94148	23.24162
N	22.98601	19.16246	20.94637
C	23.60415	20.39767	21.08285
C	24.39596	20.70247	19.91907
C	24.28914	19.63719	19.07732
C	23.44434	18.67366	19.72850
C	19.75404	19.48846	24.73353
C	23.49266	21.24527	22.18126
C	23.24052	17.39092	19.23771
H	24.95019	21.62420	19.77573
C	19.42983	18.27758	24.13666
C	18.34312	17.44721	24.58377
C	36.30111	33.42296	25.73647
C	19.56127	26.83330	20.85063
H	19.92411	25.79917	20.76758
H	18.46256	26.81282	20.78552
C	19.44648	26.67103	23.36055
H	19.80933	25.63360	23.34788
H	19.74342	27.12002	24.31960
H	18.34691	26.64327	23.31783
H	19.94819	27.39670	19.98895
C	30.69535	20.99545	22.27430
C	30.29148	20.23382	20.99451
H	30.59664	20.78972	20.09586
C	32.22518	21.12401	22.29757
H	32.57795	21.63215	23.20750
H	32.67775	20.12181	22.28004
H	30.53644	20.70758	24.43935
H	32.60225	21.67524	21.42316
H	28.04290	21.48558	22.23098
H	29.20512	20.07606	20.94020
H	30.77701	19.24616	20.97126
C	30.25895	20.18452	23.51248
H	29.17211	20.02239	23.52982
H	30.74797	19.19827	23.51263
C	34.48672	27.17306	22.39655
C	34.97249	26.39542	23.63758
H	34.66446	26.90472	24.56244
H	34.56382	25.37533	23.66283
H	36.07078	26.32062	23.63371
C	34.94665	26.43866	21.11984
H	34.60978	26.97198	20.21896
H	36.04536	26.37667	21.09353
C	35.13849	28.56343	22.41204
H	34.84361	29.16258	21.53780
H	34.88094	29.12692	23.32118
H	36.23277	28.45561	22.38740
H	34.55071	25.41440	21.07309
C	18.29226	13.68826	21.51368
C	17.68575	12.43162	21.62993
C	19.21951	11.80903	23.36757
C	19.85179	13.05408	23.28649
H	22.84992	14.65624	18.66964
H	21.11791	13.47665	20.41894
H	17.61373	17.74651	25.33058
H	17.84310	15.36870	24.01437
C	17.78605	14.68868	20.50841
H	18.56544	14.94718	19.77493
H	16.91844	14.29419	19.96361
H	17.49018	15.63061	20.99503
C	21.01973	13.37796	24.18005
H	21.91494	13.63179	23.59203
H	20.80560	14.25157	24.81490
H	21.26409	12.52935	24.83223
Ni	21.63668	18.36465	22.10188
H	24.74652	19.48920	18.10371
C	23.90377	16.97993	17.96491
C	23.18900	17.03838	16.75275
C	23.82804	16.64536	15.57025
C	25.15135	16.19502	15.56077
C	25.83779	16.13847	16.77932
C	25.23876	16.52448	17.98251
C	25.83027	15.79751	14.27674
H	25.10242	15.64370	13.46853
H	26.53578	16.57653	13.94552
H	26.40828	14.86995	14.40036
C	21.76041	17.51410	16.72545
H	21.66493	18.51953	17.16278
H	21.10872	16.85250	17.31697
H	35.49008	32.83619	25.27717
H	32.82676	29.37711	22.50830
C	30.70445	36.35540	20.67754
C	30.77786	34.45287	21.77483
N	31.27610	35.74966	21.78916
N	32.51894	34.89315	24.09463
C	31.71617	33.77541	23.90981
C	31.80344	32.89132	25.04313
C	32.69050	33.44931	25.91267
C	33.15379	34.66976	25.31081
C	30.82527	37.69219	20.32134
C	30.93617	33.51194	22.78816
C	34.18227	35.43410	25.84555
H	31.24462	31.96701	25.14674
C	31.69760	38.54261	20.98696
C	31.90841	39.91167	20.59826
C	32.96262	40.37095	21.32844
C	33.38061	39.29136	22.18276
N	32.57859	38.17362	21.99604
N	34.04964	37.19004	24.10802
C	34.78458	38.35395	23.91922
C	35.86112	38.43938	24.86996
C	35.75885	37.34960	25.68088
C	34.63115	36.58736	25.21530
C	34.47413	39.37772	23.03447
C	35.30933	40.61540	23.02121
C	35.01179	41.67623	23.89913
C	35.80534	42.82924	23.86104
C	36.88301	42.95506	22.97885
C	37.16207	41.88468	22.12152
C	36.39258	40.71648	22.12478
H	36.37530	37.06843	26.52958
H	36.57712	39.25499	24.90807
H	31.32822	40.42624	19.83802
H	33.43637	41.34781	21.30363
C	37.70629	44.21533	22.93220
C	20.21655	18.48534	27.44204
H	21.19486	18.81579	27.06162
H	20.31102	18.29044	28.51827
H	19.99015	17.53287	26.93821
C	17.68497	21.49078	24.23981
H	18.55787	22.04881	23.86600
H	17.50845	20.67166	23.52668
H	16.81619	22.16181	24.22074
C	18.13232	11.47856	22.55070
C	17.44971	10.14235	22.67922
H	16.74300	10.14038	23.52500
H	16.88029	9.89380	21.77312
H	18.17571	9.33706	22.86212
H	19.58980	11.07596	24.08989
H	16.84052	12.19200	20.97859
H	21.37544	17.54595	15.69781
H	23.27238	16.69177	14.62963
C	22.40856	21.85488	24.34598
H	23.02772	22.71695	24.56971
C	21.32914	21.38645	25.03157
C	17.37250	20.97014	28.01113
C	16.56033	21.51236	29.15752
H	16.59042	20.83844	30.02461
H	16.94544	22.49145	29.48601
H	15.50889	21.65799	28.87061
H	18.54187	19.63436	29.23373
H	16.39160	22.17922	26.51779
H	20.87065	21.78126	25.93308
H	29.38243	35.65515	19.01608
C	30.03810	38.20710	19.16161
C	30.62997	38.26745	17.88381
H	36.56757	34.20807	25.01288

H	37.16864	32.76323	25.86864
H	34.78779	35.53354	30.46693
H	37.27833	32.86320	28.19951
C	18.45972	16.25852	23.92877
C	19.59785	16.37238	23.05597
N	20.17703	17.62947	23.16073
N	21.70580	16.72250	21.05836
C	21.06164	15.52086	21.32505
C	21.47781	14.50101	20.39926
C	22.33941	15.09062	19.52405
C	26.00739	16.44616	19.27516
H	26.16431	17.44693	19.70729
H	25.46100	15.86116	20.03026
H	26.99003	15.98165	19.12020
H	26.87097	15.77993	16.79585
C	18.92589	19.99628	25.86752
C	19.14986	19.51351	27.17260
C	29.87356	38.75031	16.80937
C	22.47059	16.46470	19.92932
C	20.04526	15.33212	22.25181
C	19.38184	13.99837	22.35126
C	18.36700	20.01022	28.22174
C	17.16829	21.43255	26.70620
C	17.92949	20.96523	25.62978

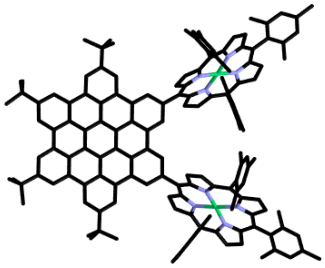
meta-porphyrin-HBC 13



Cartesian Coordinates (Angstroms)

	X	Y	Z
C	28.08794	24.83088	23.11294
C	27.32517	25.99073	22.99534
C	27.42740	23.60548	22.98524
C	25.04315	29.63067	22.65175
C	25.93768	25.95899	22.77872
C	23.74128	27.11568	22.55108
C	25.16019	27.18823	22.67139
C	25.77929	28.44425	22.68914
C	23.65149	29.55156	22.56704
C	22.98440	28.32208	22.48331
H	26.86359	28.52390	22.73509
H	23.08853	30.48236	22.58374
C	21.66073	25.77609	22.41589
C	20.88893	26.98856	22.34481
C	18.79276	25.64332	22.29935
C	21.53396	28.25560	22.34155
C	20.76458	29.41915	22.18130
C	19.37845	29.38282	22.04680
C	18.75384	28.13302	22.10044
C	19.46739	26.93785	22.25285
H	21.26811	30.38103	22.14131
H	17.67085	28.09151	21.99561
C	18.53749	30.64691	21.83179
C	17.52235	30.78736	22.98481
H	18.03967	30.88410	23.95057
H	16.89987	31.68293	22.83566
C	19.39650	31.91904	21.78610
H	20.12825	31.88935	20.96513
H	18.74903	32.79285	21.62306
C	17.78066	30.52684	20.49242
H	18.48565	30.42239	19.65467
H	17.11157	29.65498	20.47987
H	17.16893	31.42557	20.31956
H	19.94027	32.07984	22.72877
C	25.27453	24.70494	22.68871
C	26.04800	23.51191	22.76720
H	29.55557	39.72539	25.10956
H	28.46454	38.67918	24.16385
C	31.53644	36.57379	20.46213
H	31.71223	35.61913	20.98090
H	30.58879	36.46092	19.91273
H	32.34194	36.72407	19.73138
Ni	27.50551	33.86644	22.86308
H	33.05380	38.82085	20.47776
H	31.31679	40.70371	23.92964
C	24.61913	31.74894	20.64477
H	24.13515	30.81810	20.36952
C	24.49144	32.97323	20.06014
H	27.92360	30.50967	26.77973
C	29.90706	32.27902	26.84021
C	29.65822	32.91513	28.07460
C	30.31518	32.45368	29.21939
C	31.21513	31.38239	29.17364
C	31.45263	30.77490	27.93763
C	30.81238	31.20165	26.76714
C	31.89246	30.89232	30.42626
H	32.33040	31.72431	30.99760
H	31.17448	30.38685	31.09167
H	32.69301	30.17675	30.19525
C	28.69604	34.07030	28.16220
H	27.71765	33.80890	27.73195
H	28.54571	34.37855	29.20511
H	29.06417	34.94043	27.59655
C	31.09507	30.51543	25.45643
H	30.20969	29.97090	25.09164
H	31.36144	31.24063	24.67314
H	31.91844	29.79648	25.56001
H	30.11608	32.94589	30.17556
H	32.15931	29.94244	27.87838
C	24.57543	35.80988	19.43610
C	24.99031	35.90420	18.09061
C	29.52402	10.95633	23.22320
C	30.63014	10.41551	22.53752
C	23.84275	24.63981	22.55373
C	23.07920	25.83898	22.50514
C	21.00622	24.51459	22.37334
C	21.77037	23.31564	22.40600
C	23.18850	23.37803	22.49690
C	23.96259	22.16375	22.52702
C	21.10800	22.03938	22.32812
C	19.56890	24.45159	22.31742
C	23.31922	20.89507	22.43089
C	24.09965	19.73127	22.45757
C	25.49183	19.77987	22.54922
C	26.11507	21.02630	22.62632
C	25.38233	22.21903	22.64180
C	19.68999	21.96389	22.24759
C	19.07715	20.70841	22.10391
C	19.80621	19.52167	22.05620
C	21.19598	19.61010	22.17369
C	21.86474	20.83192	22.31183
C	17.39189	25.55046	22.33297
C	16.72550	24.32681	22.36289
C	17.50192	23.16479	22.33157
C	18.90135	23.19238	22.29758
H	16.80542	26.46501	22.35492
H	16.99322	22.20239	22.35223
H	17.99578	20.66007	22.00917
H	21.77581	18.68940	22.14310
H	27.20238	21.04824	22.65728
H	28.01092	22.69130	23.08027
H	16.85342	29.91727	23.04604
C	15.19726	24.21672	22.43440
C	14.51187	25.59048	22.45674
H	14.81435	26.18401	23.33228
H	14.73356	26.17179	21.54934
H	13.42151	25.45555	22.50676
C	14.68269	23.44021	21.20454
H	15.11042	22.42906	21.15317
H	21.49375	36.66017	15.82679
H	21.05349	37.98507	16.92374
C	26.35134	35.41691	17.66892
H	26.51604	34.37456	17.98110
H	26.46896	35.47554	16.57902
H	27.15178	36.01295	18.13422
C	22.83710	36.15017	21.24782
H	22.76508	35.09828	21.56625
H	23.54757	36.63594	21.93350
H	21.85191	36.61641	21.38073
H	24.43591	36.51946	16.10603
H	21.45749	37.15125	19.14095
C	26.51395	16.04177	20.00034
C	26.23088	17.70642	21.41382
N	26.83029	16.46333	21.28656
N	28.03088	17.17116	23.65061
C	27.16210	18.25378	23.59176
C	27.39159	19.14145	24.70375
C	28.46219	18.65021	25.38911
C	28.84992	17.42766	24.74053
C	26.72311	14.76548	19.49085
C	26.29291	18.53011	22.53779
C	29.87946	16.61362	25.20153
H	26.81029	20.03237	24.91575
C	27.28503	13.76100	20.27171
C	27.30369	12.37388	19.88966
C	27.88809	11.68820	20.91305
C	28.27727	12.66162	21.89948
N	27.86751	13.93265	21.51830
N	29.26010	14.71317	23.74904
C	29.62791	13.37663	23.77954
C	30.67554	13.16049	24.74258
C	30.96150	14.37270	25.29666
C	30.05073	15.32315	24.71460
C	29.10500	12.36795	22.97709
C	31.00933	9.09380	22.80168
C	30.32171	8.29769	23.72324
H	13.58717	23.34157	21.24860
C	14.80474	23.45901	23.71997
H	15.23195	22.44662	23.74088
H	15.16175	23.99353	24.61235
H	13.70997	23.36577	23.78801
H	14.94456	23.96492	20.27410
C	19.14674	18.14891	21.87535
C	19.47637	17.26123	23.09346
H	19.08996	17.71009	24.02022
C	17.61982	18.24794	21.74837
H	17.32053	18.85188	20.87872
H	17.19601	17.24174	21.61660
H	19.48275	18.10246	19.71127
H	17.16357	18.68530	22.64906
H	23.63108	18.75023	22.40808
H	20.55993	17.12113	23.21261
H	19.01862	16.26721	22.97385
C	19.69863	17.48549	20.59581
H	20.78707	17.34183	20.64913
H	19.23503	16.49774	20.44990
C	29.59590	24.85498	23.38946
C	29.87380	24.13380	24.72554
H	29.35613	24.63646	25.55573
H	29.53612	23.08798	24.70198
H	30.95352	24.13545	24.94001
C	30.33662	24.12406	22.25024
H	30.16546	24.62528	21.28623
H	31.41965	24.11414	22.44705
C	30.14798	26.28459	23.48765
H	29.99593	26.84616	22.55397
H	29.68207	26.84794	24.30991
H	31.22982	26.24810	23.68172
H	30.00379	23.08125	22.15173
H	27.82002	26.95273	23.09578
C	25.36203	33.86905	20.77033
C	25.52685	31.90627	21.75240
H	31.69388	14.61814	26.06005
H	31.13035	12.19476	24.94250
H	26.90205	11.99371	18.95498
H	28.08244	10.62300	20.99690
C	30.72911	6.86938	23.97236
H	30.11384	6.17443	23.37811
H	31.77856	6.69719	23.69661
H	30.60080	6.59298	25.02872
C	31.40376	11.24646	21.54814
H	31.79060	12.16509	22.01533
H	32.25231	10.68234	21.13970
H	30.76679	11.56682	20.70924
C	27.64602	10.75265	24.91047
H	27.94991	11.61350	25.52602
H	26.87189	11.12122	24.22042
H	27.19269	10.00131	25.57023
Ni	27.99680	15.56972	22.55139
H	28.68213	8.25734	25.12496
H	31.87276	8.67807	22.27476
C	25.57735	18.07967	20.18503
H	25.05831	19.01883	20.02400
C	25.77494	17.05937	19.30360
H	28.94406	19.05161	26.27552
C	30.74499	17.10483	26.31497
C	31.86181	17.91284	26.02397
C	32.66170	18.36991	27.07814
C	32.37864	18.05346	28.41030
C	31.26209	17.25246	28.67450
C	30.43760	16.77260	27.65117
C	33.23171	18.58248	29.53287
H	34.23562	18.85571	29.17996
H	32.78119	19.48462	29.97783
H	33.33924	17.84282	30.33915
C	32.19194	18.28264	24.60194
H	31.39001	18.88879	24.15230
H	33.12566	18.85800	24.55184
H	32.29925	17.38869	23.96923
N	26.03185	33.20057	21.78496
N	27.41242	32.27574	23.97011
C	26.56184	31.19003	23.83036
C	26.64447	30.33163	24.98471
C	27.57851	30.87245	25.81624
C	28.08486	32.04971	25.16567
C	25.48828	35.21815	20.45857
C	25.73965	30.93805	22.73168
C	29.20131	32.74697	25.61063
H	26.04671	29.43846	25.13267
C	26.49271	35.99764	21.01835
C	26.75394	37.35555	20.61983
C	27.94791	37.70738	21.17498
C	28.39863	36.58016	21.94804
N	27.48379	35.53987	21.87779
N	29.09130	34.45069	23.82343
C	29.91572	35.52557	23.51565
C	31.08241	35.52783	24.35836
C	30.94272	34.48908	25.23001
C	29.70605	33.83121	24.90206
C	29.60250	36.56079	22.64327
C	30.54103	37.71230	22.49393
C	30.48592	38.79137	23.40084
C	31.36342	39.86658	23.22721
C	32.29203	39.90084	22.18038
C	32.33166	38.81660	21.29898
C	31.46946	37.72154	21.43481
H	31.60363	34.17934	26.03423
H	31.87898	36.26334	24.29517
H	26.10905	37.93395	19.96481
H	28.49395	38.64169	21.08340
C	33.20200	41.08666	21.99686
H	32.65619	41.93753	21.55802
H	33.61492	41.42866	22.95705
H	34.03956	40.85050	21.32652
C	29.49479	38.79224	24.53444
H	29.67408	37.95131	25.22210
H	33.53257	18.99032	26.84854
H	31.02189	16.99270	29.70943
C	26.25904	14.44241	18.10886
C	24.91863	14.07531	17.87614
C	24.51564	13.77874	16.56818
C	25.40311	13.83910	15.48957
C	26.73080	14.19866	15.74758
C	27.17597	14.50007	17.03877
C	24.94213	13.54776	14.08584
H	23.99397	12.99297	14.08172
H	24.78223	14.48124	13.52238
H	25.68782	12.95951	13.53154
C	23.93312	13.99062	19.01176
H	23.78587	14.97251	19.48773
H	22.95777	13.63060	18.65907
H	24.28973	13.31054	19.80024
C	28.61332	14.87895	17.28065
H	28.69124	15.86089	17.77166
H	29.10970	14.15655	17.94702
H	29.17378	14.91794	16.33742
H	23.47625	13.48911	16.39018
H	27.44414	14.24496	14.91973
H	23.87966	33.26152	19.21070
H	25.43659	16.97439	18.27535
C	21.90223	37.46229	16.46238
H	22.41977	38.16873	15.79690
C	29.22976	8.85930	24.39418
C	28.81876	10.17616	24.16196
H	29.32970	14.91478	27.55094
H	29.11016	15.82751	29.06469
C	24.11233	36.44952	17.14854
C	22.83610	36.90269	17.50293
C	22.44874	36.79908	18.84196
C	23.29484	36.25575	19.81682
H	29.23691	15.92495	27.97864
H	28.31654	16.35929	27.55961

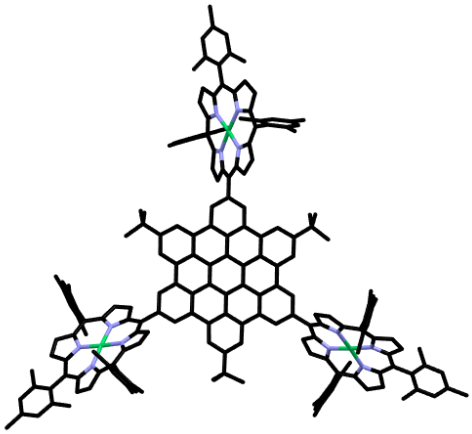
ortho-porphyrin-HBC 11



Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.14023	19.16175	22.53186
C	24.41073	20.34970	22.57058
C	24.45064	17.95122	22.46081
C	22.21929	24.04763	22.68561
C	23.01060	20.35621	22.55087
C	20.83964	21.57763	22.56009
C	22.26402	21.60819	22.59010
C	22.92249	22.84348	22.65789
C	20.82512	24.01292	22.65503
C	20.11572	22.80521	22.60120
H	24.00906	22.89226	22.69357
H	20.29674	24.96410	22.66172
C	18.71781	20.30189	22.45245
C	17.97861	21.53679	22.49302
C	15.84527	20.25754	22.34760
C	18.65751	22.78306	22.57975
C	17.91245	23.97086	22.65122
C	16.51989	23.97914	22.63367
C	15.86625	22.74792	22.53161
C	16.55360	21.53020	22.45557
H	18.43813	24.91798	22.73108
H	14.77776	22.74224	22.52083
C	15.70129	25.27219	22.73047
C	14.81967	25.21792	23.99555
H	15.43935	25.12546	24.89943
H	14.21964	26.13694	24.08043
C	16.59071	26.52126	22.81476
H	17.23162	26.62711	21.92691
H	15.95781	27.41852	22.87729
C	14.80074	25.40228	21.48463
H	15.40535	25.44137	20.56681
H	14.10575	24.55557	21.39442
H	14.20277	26.32457	21.54399
H	17.23483	26.50619	23.70656
C	22.30944	19.11745	22.47932
C	27.31273	18.77554	21.40489
N	28.69178	18.69323	21.27463
N	28.65884	19.96585	23.71880
C	27.29041	19.74182	23.63292
C	26.61583	20.25616	24.79678
C	27.56204	20.86099	25.56647
C	28.82079	20.68565	24.89532
C	30.10588	17.77469	19.46256
C	26.62573	19.20131	22.53735
C	30.01616	21.19248	25.38778
H	25.55026	20.16923	24.98063
C	31.28782	17.88496	20.18279
C	32.54150	17.35170	19.72173
C	33.47524	17.66971	20.66128
C	32.79785	18.41996	21.68528
N	31.44075	18.52247	21.40658
N	31.41663	20.02185	23.71865
C	32.79272	19.85824	23.63410
C	33.46448	20.63947	24.63831
C	32.49827	21.28522	25.34867
C	31.23314	20.87418	24.80049
C	33.46601	19.05321	22.72479
C	34.94932	18.91623	22.82882
C	35.78825	19.81153	22.13399
C	37.17498	19.66399	22.24573
C	37.74985	18.65203	23.02263
C	36.89654	17.78047	23.70680
C	35.50360	17.89494	23.62493
H	32.60612	21.96210	26.19087
H	34.54267	20.67404	24.76312
H	32.66591	16.80610	18.79103
H	34.53831	17.44894	20.66972
C	39.24545	18.49200	23.09576
H	39.62054	17.90495	22.24153
H	39.75462	19.46597	23.06882
H	39.54942	17.96860	24.01277
C	35.20415	20.91335	21.28999
H	34.55736	21.57440	21.88698
C	23.04994	17.90020	22.42610
C	20.86932	19.09899	22.45204
C	20.14014	20.32094	22.48913
C	18.02507	19.06156	22.38513
C	18.75386	17.84026	22.35516
C	20.17581	17.85888	22.38608
C	20.91292	16.62238	22.33433
C	18.05188	16.58403	22.30398
C	16.58603	19.04314	22.33509
C	20.23189	15.37577	22.26598
C	20.97859	14.19016	22.16845
C	22.37170	14.18273	22.14855
C	23.02652	15.41370	22.24088
C	22.33811	16.62856	22.33603
C	16.63012	16.55118	22.27941
C	15.97264	15.31042	22.27602
C	16.66174	14.09974	22.28599
C	18.05826	14.14889	22.28559
H	18.77165	15.35341	22.28541
C	14.44508	20.20826	22.25384
C	13.74447	19.00784	22.15960
C	14.48492	17.82290	22.17204
C	15.88190	17.80562	22.26312
H	13.88546	21.13923	22.24581
H	13.94716	16.87932	22.09884
H	14.88652	15.29021	22.27556
H	18.60724	13.20901	22.29321
H	24.11484	15.42179	22.22761
H	25.03803	17.03532	22.43752
H	14.12832	24.36370	23.97193
C	12.21616	18.94664	22.04839
C	11.57472	20.34154	22.04010
H	11.78789	20.89445	22.96714
H	11.92188	20.94446	21.18776
H	10.48264	20.24286	21.95559
C	22.10440	29.60923	26.86872
C	20.78970	30.09903	26.73188
C	20.06986	30.43774	27.88269
C	20.61615	30.29654	29.16334
C	21.92381	29.81313	29.27255
C	22.68039	29.46679	28.14677
C	19.80769	30.62866	30.38968
H	19.16316	31.50343	30.22259
H	19.14998	29.78875	30.66677
H	20.45456	30.83711	31.25292
C	20.16745	30.25380	25.36930
H	20.05622	29.27878	24.86948
H	19.17509	30.71789	25.44024
H	20.79444	30.87261	24.70995
C	24.08423	28.94509	28.30355
H	24.20044	27.96040	27.82572
H	24.81468	29.61432	27.82310
H	24.35162	28.84871	29.36393
H	19.05185	30.82256	27.77368
H	22.37138	29.69950	30.26395
C	26.92232	27.20654	18.63245
C	27.95216	26.24262	18.60141
C	28.58223	25.96583	17.38365
C	28.21578	26.61292	16.19764
C	27.19110	27.56195	16.25450
C	26.53687	27.87298	17.45281
C	28.89629	26.28071	14.89572
H	29.98743	26.21538	15.01882
H	28.55560	25.30717	14.50791
H	28.68239	27.03679	14.12798
C	28.37397	25.52427	19.85619
H	27.56632	24.88053	20.23835
H	29.25303	24.89337	19.67086
H	28.61719	26.23285	20.66223
C	25.44296	28.90779	17.47525
H	24.52917	28.51533	17.94581
H	30.61034	14.37588	14.16307
H	29.08740	15.21105	13.81990
C	11.82845	18.22807	20.73929
H	12.22692	17.20439	20.70393
H	10.73299	18.16731	20.64932
C	11.65256	18.16047	23.25045
H	12.04437	17.13406	23.28314
H	11.91712	18.65269	24.19776
H	10.55524	18.10163	23.18624
H	12.21714	18.77139	19.86561
C	15.94962	12.74160	22.29752
C	16.34022	11.97523	23.57847
H	16.03260	12.53216	24.47564
C	14.42116	12.88353	22.26534
H	14.08042	13.40746	21.35975
H	13.95956	11.88531	22.26636
H	16.12190	12.45864	20.13328
H	14.04246	13.42604	23.14437
H	20.45240	13.24263	22.09379
H	17.42575	11.81326	23.63843
H	15.84909	10.99016	23.59802
C	16.38474	11.92861	21.06048
H	17.46926	11.75047	21.05127
H	15.88204	10.94938	21.05346
C	23.19379	12.89380	22.02800
C	22.30805	11.64407	21.92329
H	21.67592	11.51558	22.81458
H	21.65639	11.67862	21.03744
H	22.94330	10.75069	21.83480
C	24.07531	12.96927	20.76356
H	24.76668	13.82291	20.79875
H	24.67646	12.05239	20.66486
C	24.09432	12.74765	23.27250
H	24.78240	13.59799	23.37863
H	23.48840	12.68845	24.18848
H	24.69930	11.83090	23.19870
H	23.45574	13.07456	19.86091
H	33.98073	17.47880	25.10422
H	33.92728	16.41376	23.69969
H	35.20485	16.19629	24.92356
Ni	30.05177	19.30051	22.53019
H	37.32526	16.98707	24.32553
H	37.82434	20.36238	21.71010
C	26.65950	18.37240	20.18648
H	25.58543	18.37782	20.03367
C	27.63980	18.01801	19.31052
H	27.44186	21.37820	26.51348
C	29.99119	22.04308	26.61485
C	29.75978	23.42913	26.50199
C	29.73842	24.20863	27.66389
C	29.93299	23.64947	28.93179
C	30.15814	22.27187	29.01736
C	30.19070	21.45582	27.88042
C	29.87342	24.50291	30.17142
H	30.29554	25.50211	29.99257
H	28.83186	24.64426	30.50316
H	30.42272	24.04066	31.00329
C	29.53910	24.06363	25.15414
H	28.63176	23.66847	24.67151
H	29.43098	25.15230	25.24421
H	30.37485	23.85219	24.47000
C	30.42955	19.97486	28.01362
H	29.61590	19.39602	27.55055
H	31.35802	19.67176	27.50534
H	30.50432	19.68250	29.06920
H	29.56457	25.28460	27.57297
H	30.31301	21.81464	29.99873
C	30.12880	17.15066	18.10626
C	29.82791	15.78058	17.95621
C	29.84472	15.22042	16.67470
C	30.14600	15.98171	15.53929
C	30.44818	17.33511	15.71502
C	30.44721	17.93486	16.98054
H	30.62925	15.99883	13.42991
C	29.49433	14.93041	19.15370
H	24.96851	21.28313	22.60565
C	25.21410	26.71992	20.37429
C	23.74634	25.70950	21.65812
N	24.55637	26.83529	21.59355
N	23.29756	27.45941	23.96716
C	22.77576	26.17880	23.83368
C	21.94685	25.84457	24.96262
H	21.90699	26.94528	25.76275
C	22.73123	27.94403	25.13935
C	26.24397	27.53276	19.92203
C	22.94357	25.34474	22.73390
C	22.88320	29.22409	25.65442
H	21.45892	24.88640	25.10635
C	26.67270	28.63272	20.65260
C	27.78403	29.45356	20.25254
C	27.86608	30.47251	21.15219
C	26.79795	30.28148	22.09680
N	26.08223	29.12618	21.80859
N	24.62506	29.88128	24.02622
C	25.42022	31.01711	23.94777
C	25.02412	31.99045	24.93023
C	23.99007	31.44670	25.63025
C	23.76578	30.13321	25.08862
C	26.48949	31.20775	23.08323
C	27.30552	32.45327	23.19437
C	26.94281	33.59771	22.45491
C	27.71782	34.75574	22.57713
C	28.84340	34.80665	23.40735
C	29.18194	33.65893	24.13081
C	28.43155	32.48027	24.03990
H	23.42825	31.86820	26.45846
H	25.49810	32.95968	25.05287
H	28.40325	29.25818	19.38222
H	28.56550	31.30240	21.18288
C	29.67808	36.05689	23.49775
H	30.36985	36.13202	22.64304
H	29.05052	36.95968	23.48642
H	30.28379	36.06980	24.41421
C	25.73893	33.57643	21.55071
H	24.82377	33.32493	22.10818
H	25.59224	34.55119	21.06750
H	25.84516	32.81324	20.76427
C	28.82270	31.26189	24.83379
H	28.01229	30.94918	25.51011
H	29.02708	30.40441	24.17435
H	29.72005	31.45504	25.43602
Ni	24.64024	28.32637	22.84873
H	30.05516	33.67912	24.78899
H	27.43171	35.64424	22.00699
C	23.85538	24.93093	20.45159
H	23.29809	24.02157	20.25343
C	24.76237	25.56036	19.65540
H	21.37721	27.08853	26.69956
H	28.54868	15.25072	19.61864
H	29.39576	13.87453	18.86974
H	30.26835	15.01140	19.93155
C	30.78304	19.39517	17.13110
H	29.99417	19.93385	17.67736
H	31.71185	19.53243	17.70671
H	30.91406	19.87152	16.15061
H	29.61526	14.15699	16.56152
H	30.69169	17.94643	14.84153
H	27.54514	17.65710	18.29081
H	25.11901	25.27591	18.67009
H	35.99630	21.52322	20.83639
H	34.57558	20.50707	20.48258
H	34.61271	16.94325	24.37890
H	29.38550	25.22378	17.36336
H	26.89023	28.07953	15.33938
C	28.89217	18.18710	19.99561
C	30.12236	15.36150	14.16712
H	25.74228	29.79099	18.06116
H	25.19533	29.23985	16.45852

tri-porphyrin-HBC 14

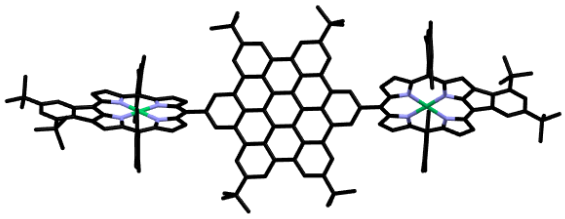


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	36.12622	26.83677	21.96315
C	35.37409	28.00135	22.10248
C	35.44935	25.61575	22.03937
C	33.13625	31.64780	22.64812
C	33.98258	27.97974	22.29296
C	31.79758	29.15530	22.53250
C	33.22000	29.21397	22.44610
C	33.85759	30.46047	22.51740
C	31.74321	31.58593	22.69980
C	31.05430	30.36691	22.64593
H	34.94344	30.52818	22.48564
H	31.19920	32.52497	22.77729
C	29.69776	27.83727	22.57667
C	28.93805	29.05789	22.65124
C	26.82528	27.73729	22.63489
C	29.59685	30.31716	22.69400
C	28.83132	31.49143	22.77658
C	27.43919	31.47391	22.81541
C	26.80507	30.22904	22.76726
C	27.51346	29.02457	22.68555
H	29.34038	32.45033	22.80913
H	25.71729	30.20223	22.79822
C	26.59940	32.75330	22.90663
C	25.74271	32.70707	24.18885
H	26.38085	32.64819	25.08272
H	25.12529	33.61510	24.26482
C	27.46732	34.01922	22.95270
H	28.08723	34.12408	22.04989
H	26.81891	34.90519	23.01509
C	25.67451	32.84264	21.67457
H	26.26292	32.88031	20.74608
H	24.99678	31.97963	21.60983
H	25.05766	33.75266	21.72933
H	28.12936	34.02954	23.83152
C	33.30326	26.73126	22.32684
H	31.79932	38.55025	24.78558
C	35.01565	36.38827	28.33418
H	35.08874	35.41280	27.82959
H	35.77974	37.03565	27.87658
H	35.27144	36.24997	29.39286
H	30.07060	38.49423	27.84172
H	33.33967	37.18375	30.30624
C	37.39241	35.11989	18.36139
C	38.40430	34.16175	18.14727
C	38.89226	33.97194	16.84942
C	38.40190	34.70172	15.76132
C	37.40068	35.64883	16.00035
C	36.88647	35.87241	17.28261
C	38.91972	34.45580	14.36865
H	39.96859	34.12759	14.38250
H	38.33717	33.66725	13.86475
H	38.84937	35.36029	13.74835
C	38.95859	33.35712	19.29332
H	38.18667	32.70684	19.73392
H	39.79149	32.72348	18.96153
H	39.31873	34.00879	20.10369
C	35.81088	36.90286	17.50420
H	34.93367	36.46475	18.00396
H	36.16697	37.71705	18.15443
H	35.48435	37.34166	16.55237
H	39.68191	33.23308	16.68606
H	37.00677	36.23429	15.16478
C	36.79284	19.34365	20.27493
C	35.12596	20.22158	21.41071
N	35.99088	19.13350	21.38844
N	34.74410	18.49088	23.75128
C	34.16231	19.73977	23.58692
C	33.45162	20.12957	24.77775
C	34.06502	25.53158	22.22786
C	31.86870	26.67922	22.43536
C	31.11833	27.88599	22.51167
C	29.02815	26.58210	22.56690
C	29.78010	25.37506	22.51118
C	31.20027	25.42346	22.44476
C	31.96221	24.20095	22.40058
C	29.10421	24.10400	22.53789
C	27.58898	26.53355	22.59929
C	31.30424	22.93727	22.45888
C	32.07425	21.76607	22.44954
C	33.46902	21.80055	22.39876
C	34.10538	23.04135	22.33330
C	33.38459	24.24255	22.31469
C	27.68496	24.04192	22.58951
C	27.05260	22.79070	22.67088
C	27.76534	21.59383	22.67962
C	29.15893	21.66958	22.60046
C	29.84619	22.88727	22.53144
C	25.42608	27.65801	22.61914
C	24.75752	26.43357	22.56236
C	25.51172	25.25958	22.53753
C	26.91210	25.27901	22.57690
H	24.82033	28.56183	22.64421
H	24.97653	24.31526	22.46260
H	25.96925	22.75278	22.74221
H	29.72675	20.74090	22.60080
H	35.19342	23.05307	22.32491
H	36.02464	24.69780	21.93178
H	25.06865	31.83915	24.19739
C	27.08044	20.22472	22.76873
C	27.59982	19.47277	24.01212
H	27.37150	20.03205	24.93123
C	25.55341	20.34405	22.87866
H	25.11843	20.84289	21.99983
H	25.11043	19.33959	22.94295
H	27.04810	19.92406	20.60010
H	25.24977	20.90061	23.77792
H	31.59491	20.78985	22.48941
H	28.68749	19.31937	23.97216
H	27.12291	18.48322	24.08308
C	38.87290	15.19723	20.60644
C	37.79413	15.41248	21.53393
N	37.32307	16.71542	21.44802
N	35.86330	15.97360	23.65542
C	36.38803	14.71722	23.37849
C	35.97329	13.76143	24.37122
C	35.24176	14.44453	25.29580
C	35.17910	15.81154	24.85171
C	37.31433	14.42476	22.38545
C	37.86539	13.04040	22.28096
C	38.97033	12.66043	23.07052
C	39.46676	11.35700	22.95741
C	38.89875	10.42280	22.08441
C	37.80256	10.82320	21.31366
C	37.27597	12.11779	21.39410
H	34.77573	14.07678	26.20519
H	36.24773	12.71071	24.35836
H	39.78336	16.60545	19.16296
H	39.40402	14.25646	20.49639
C	39.46939	9.03452	21.96047
H	40.28882	9.00929	21.22368
H	39.88142	8.68307	22.91706
H	38.70814	8.31529	21.62770
C	39.60898	13.63746	24.02201
H	11.98696	26.23372	21.70037
C	22.36443	27.93980	19.39878
C	19.69982	22.94144	25.88602
C	27.41475	19.41083	21.50110
H	28.49790	19.26258	21.38774
H	26.94071	18.41854	21.55047
C	37.64262	26.85243	21.73576
C	38.33550	26.11589	22.90132
H	38.11671	26.60855	23.85990
H	38.00351	25.07068	22.97544
H	39.42642	26.11413	22.75450
C	37.96711	26.13081	20.41117
H	37.48400	26.63562	19.56187
H	39.05416	26.12797	20.23805
C	38.20627	28.27881	21.65995
H	37.76260	28.85048	20.83103
H	38.03785	28.83516	22.59398
H	39.29207	28.23609	21.49081
H	37.62578	25.08610	20.42187
H	35.88210	28.96007	22.04574
C	35.86791	34.49959	20.22536
C	34.55867	33.37756	21.58882
H	35.33731	34.52317	21.50996
N	34.20519	35.05397	23.96131
C	33.69483	33.76856	23.82472
C	32.88311	33.42111	24.96273
C	32.83272	34.52190	25.76305
C	33.64873	35.52854	25.14140
C	36.85488	35.34496	19.73613
C	33.83648	32.95764	22.70277
C	33.83644	36.79271	25.68623
H	32.40765	32.45722	25.11039
C	37.39341	36.35790	20.51948
C	38.52241	37.15177	20.11386
C	38.75825	38.04487	21.11538
C	37.75319	37.81967	22.12006
N	36.93474	36.75352	21.76829
N	35.61913	37.41976	24.09139
C	36.50140	38.49145	24.08110
C	36.17499	39.43264	25.11931
C	35.08743	38.93839	25.77399
C	34.76984	37.67618	25.16062
C	37.56547	38.66592	23.20510
C	38.48058	39.83132	23.39348
C	32.85188	15.94373	29.43735
C	32.06909	15.85215	28.28160
C	32.58979	16.12716	27.01191
C	32.25841	15.68375	30.79689
H	33.01107	15.29310	31.49600
H	31.85638	16.61216	31.23466
H	31.43011	14.96336	30.74312
C	36.20629	16.98013	27.93214
H	36.32299	17.94540	27.41672
H	36.67137	17.05831	28.92341
H	36.77175	16.24120	27.34352
C	31.71428	16.01576	25.79130
H	31.59523	16.99163	25.29497
H	32.15153	15.33567	25.04448
H	30.71653	15.64281	26.05750
H	34.82680	16.37938	30.18626
H	31.01966	15.55648	28.36797
C	38.67960	18.97461	18.70064
C	38.35407	18.55701	17.39352
C	39.15302	18.98577	16.32803
C	40.26236	19.81592	16.52291
C	40.56591	20.21422	17.82862
C	39.79134	19.81090	18.92272
C	41.08707	20.28773	15.35453
H	20.60736	32.11281	16.99266
C	22.62703	26.96895	21.41487
H	22.56388	25.68780	23.47777
C	38.20480	41.05437	22.74925
C	39.07000	42.13597	22.95082
C	40.20007	42.03567	23.76896
C	40.45112	40.81194	24.39871
C	39.61060	39.70635	24.22608
H	34.54966	39.35831	26.61879
H	36.72255	40.35228	25.30275
H	39.05321	37.02165	19.17555
H	39.52015	38.81608	21.17790
C	41.13266	43.20465	23.94751
H	41.94719	43.17663	23.20544
H	40.60645	44.16082	23.81892
H	41.59864	43.19846	24.94292
C	36.99469	41.20286	21.86561
H	36.06737	40.98734	22.41835
H	36.92677	42.22118	21.46107
H	37.02779	40.49694	21.02139
C	39.90795	38.40470	24.92217
H	39.08568	38.11453	25.59426
H	40.02409	37.58296	24.19909
H	40.82919	38.47632	25.51493
Ni	35.52457	35.93747	22.83329
H	41.32577	40.71285	25.04781
H	38.85030	43.08599	22.45547
C	34.56361	32.67082	20.33376
H	34.00763	31.75984	20.13845
C	35.36226	33.37582	19.48539
H	32.30837	34.65650	26.70429
C	33.07007	37.17336	26.91003
C	31.77649	37.71773	26.78399
C	31.07147	38.06494	27.94215
C	31.61195	37.87910	29.21863
C	32.89712	37.33553	29.31774
C	33.63787	36.97770	28.18583
C	30.82251	38.22539	30.45325
H	30.10556	39.03476	30.25751
H	30.24630	37.35571	30.80900
H	31.48048	38.53817	31.27618
C	31.15950	37.92434	25.42588
H	31.03003	36.96676	24.89770
H	30.17631	38.40570	25.50994
N	21.18964	25.48073	23.47690
C	22.20035	24.22538	25.15176
C	20.96927	24.55586	24.48772
C	19.73910	24.02383	24.85780
C	18.72211	28.18531	20.27679
C	17.51742	28.88429	19.91642
C	16.57829	28.56296	20.85050
C	17.19540	27.63431	21.76042
N	18.52876	27.43378	21.42659
N	18.43735	25.60338	23.47194
C	17.08467	25.91202	23.45980
C	16.35015	25.01403	24.31130
C	17.25391	24.14432	24.84401
C	18.54958	24.53889	24.35751
C	16.48492	26.92642	22.72229
C	15.02676	27.19384	22.90355
C	14.08087	26.51038	22.11277
C	12.71952	26.76994	22.31026
C	12.27344	27.68930	23.26528
C	13.23156	28.35249	24.03937
C	14.60186	28.12070	23.87654
H	17.08557	23.32337	25.53453
H	15.27543	25.05741	24.46065
H	15.54379	28.88631	20.91768
C	23.18301	24.95387	24.55182
C	40.14508	20.26277	20.31495
H	39.33350	20.86083	20.75779

C	33.58078	19.10827	25.66934	H	40.30291	19.40510	20.98639
C	34.34755	18.08111	25.01910	H	41.05844	20.87196	20.31049
C	37.84178	18.53416	19.85574	H	15.17075	25.97557	20.32132
C	34.25712	20.54113	22.45072	C	15.60538	28.84808	24.73165
C	34.52410	16.81301	25.55734	H	41.14745	19.52007	14.57001
H	32.93671	21.07575	24.90586	H	40.64303	21.18640	14.89619
C	38.08003	17.29629	20.43843	H	42.10924	20.54766	15.66250
C	39.06547	16.37172	19.94343	C	37.16481	17.66792	17.14294
C	19.85693	21.59808	25.49104	H	36.23983	18.11925	17.53322
C	19.81935	20.59561	26.46736	H	37.03244	17.48203	16.06904
C	19.63861	20.89120	27.82234	H	37.27750	16.69713	17.64989
C	19.48929	22.23282	28.19000	H	16.21106	28.14377	25.32252
C	19.51758	23.26562	27.24639	H	16.31100	29.42610	24.11556
C	19.63345	19.80111	28.86136	C	10.80543	27.97738	23.43917
H	19.30829	18.84152	28.43598	H	10.49690	28.83885	22.82458
H	20.64213	19.65017	29.27933	H	10.18869	27.12041	23.13463
H	18.96831	20.04992	29.70034	H	10.56537	28.22149	24.48369
C	20.06349	21.24417	24.04189	C	14.52160	25.50891	21.07820
H	21.00251	21.67293	23.65806	H	15.10637	24.69475	21.53321
H	20.10201	20.15569	23.90430	H	13.65666	25.06754	20.56607
H	19.25601	21.64583	23.41130				
C	19.36288	24.69853	27.68296				
H	20.21307	25.31171	27.34715				
H	18.45846	25.15367	27.25045				
H	19.29492	24.77065	28.77631				
H	19.93355	19.55312	26.15728				
H	19.34617	22.48654	29.24418				
C	19.91866	29.02729	18.26307				
C	20.30193	30.38396	18.23667				
C	20.31360	31.05947	17.01099				
C	19.95980	30.42674	15.81459				
C	19.57311	29.08363	15.86889				
C	19.54463	28.37130	17.07306				
C	20.02094	31.16316	14.50248				
H	19.83949	32.23872	14.63687				
H	21.01420	31.05452	14.03687				
H	19.28163	30.77476	13.78804				
C	20.68770	31.10231	19.50316				
H	21.59766	30.66896	19.94702				
H	20.87540	32.16634	19.30825				
H	19.89826	31.02261	20.26592				
C	19.11913	26.92688	17.09386				
H	19.88416	26.29018	17.56320				
H	18.19697	26.79174	17.68027				
H	18.93628	26.55633	16.07679				
H	38.89584	13.96888	24.79260				
H	40.47419	13.18665	24.52539				
H	39.94723	14.54412	23.49740				
C	36.09449	12.51458	20.54889				
H	35.25689	12.86539	21.17087				
H	36.34943	13.34469	19.87198				
H	35.74382	11.67015	19.94123				
Ni	35.97962	17.57771	22.55969				
H	37.33867	10.10697	20.62967				
H	40.32211	11.06365	23.57268				
C	35.34098	21.06203	20.26080				
H	34.76132	21.94886	20.02736				
C	36.39311	20.53387	19.57542				
H	33.18258	19.02860	26.67626				
C	33.94348	16.50394	26.89775				
C	34.75607	16.59122	28.04598				
C	34.19459	16.30984	29.29655				
C	23.27386	26.38541	22.50324				
C	23.31645	27.47920	20.25746				
H	22.27856	23.53645	25.98734				
H	24.23948	24.98873	24.79541				
H	24.39316	27.46229	20.12522				
H	22.49266	28.39621	18.42197				
C	19.90558	28.27667	19.55357				
H	17.42705	29.53859	19.05448				
H	19.28403	28.57155	14.94681				
H	38.89949	18.65997	15.31525				
H	41.43276	20.85742	18.00451				
H	35.61497	33.16178	18.45133				
H	36.86164	20.89324	18.66412				
C	21.09317	27.74512	20.04116				
N	21.25517	27.10406	21.26384				
H	15.10575	29.53825	25.42401				
Ni	19.85249	26.40588	22.40998				
H	12.90460	29.07053	24.79682				

para-phenly-fused porphyrin-HBC *p*-Ph

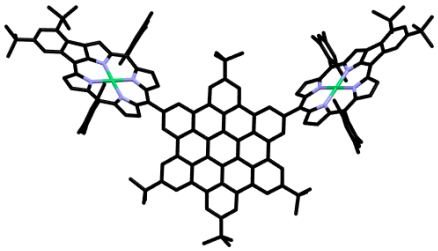


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.19369	18.82298	22.34785
C	24.51776	20.04527	22.38412
C	24.42514	17.66161	22.31852
C	22.53278	23.86710	22.53031
C	23.12110	20.13401	22.39891
C	21.01763	21.47582	22.45367
C	22.44242	21.42595	22.44766
C	23.16591	22.62367	22.49836
C	21.13846	23.91089	22.52851
C	20.36328	22.74225	22.50694
H	24.25341	22.61156	22.52467
H	20.66278	24.88967	22.54231
C	18.82652	20.31726	22.41676
C	18.15750	21.59073	22.47998
C	15.95379	20.42983	22.40394
C	18.90543	22.79885	22.54250
C	18.22741	24.02406	22.65418
C	16.83737	24.10575	22.69801
C	16.11599	22.91198	22.61002
C	16.73375	21.66093	22.49584
H	18.80495	24.94161	22.72197
H	15.02924	22.96271	22.64522
C	22.88298	12.66164	22.16864
C	23.78777	12.54225	23.41247
H	23.19014	12.57625	24.33510
H	24.33719	11.58867	23.39182
C	21.92686	11.46043	22.15053
H	21.27620	11.46957	21.26352
H	22.50959	10.52818	22.12531
C	23.75297	12.60914	20.89532
H	23.13005	12.69191	19.99272
H	24.48911	13.42508	20.87234
H	24.30254	11.65649	20.84937
H	21.29025	11.43077	23.04740
C	23.50346	27.52291	25.21149
C	22.62981	26.54712	25.80618
C	22.45210	25.56008	24.88597
C	23.22880	25.92040	23.72704
C	23.83993	28.71536	25.84320
C	23.31393	28.97673	27.21735
C	22.05475	29.58592	27.38627
C	21.58384	29.81855	28.68408
C	22.32697	29.46322	29.81412
C	23.57159	28.85391	29.62001
C	24.08012	28.60468	28.34070
H	21.86708	24.65124	24.97710
H	22.21276	26.62886	26.80532
H	26.02317	32.68045	25.04578
H	24.51786	31.27199	26.79984
C	21.81527	29.74960	31.20121
H	22.24515	30.68508	31.59477
H	20.72227	29.86061	31.21092
H	22.08659	28.94796	31.90290
C	21.22411	29.97800	26.19306
H	20.98219	29.10286	25.57025
H	20.28307	30.44849	26.50663
H	21.76445	30.68386	25.54383
C	25.42216	27.94393	28.16824
H	25.33694	27.01154	27.58930
H	26.11880	28.59253	27.61508
H	25.87159	27.70628	29.14126
Ni	25.14391	28.00179	22.75820
H	24.16575	28.55976	30.48986
H	20.60516	30.28913	28.81340
H	30.40767	25.00318	17.77718
H	27.63737	27.14980	15.28747
C	27.99450	29.38721	19.96975
H	28.62873	29.22487	19.10369
C	27.83714	30.49222	20.77239
C	27.48127	32.24098	22.26819
C	28.22360	31.87593	21.08869
C	27.60720	33.50433	22.81993
C	28.60786	35.83654	22.87566
C	22.34769	18.93808	22.36334
C	23.02096	17.68594	22.32137
C	20.90875	18.99929	22.36797
C	20.24823	20.25902	22.41215
C	18.06560	19.11632	22.37516
C	18.72596	17.85684	22.33070
C	20.14778	17.79828	22.32857
C	20.81697	16.52383	22.28855
C	17.95622	16.63998	22.29555
C	16.62674	19.17749	22.36627
C	20.06880	15.31497	22.25609
C	20.74625	14.08539	22.22070
C	22.13634	14.00019	22.21282
C	22.85822	15.19626	22.24450
C	22.24076	16.45226	22.28409
C	16.53134	16.68887	22.29798
C	15.80726	15.48949	22.29667
C	16.44250	14.24775	22.26657
C	17.83620	14.20552	22.24416
C	18.61115	15.37353	22.26438
C	14.55061	20.45659	22.34777
C	13.78306	19.29638	22.26969
C	14.45813	18.07299	22.25716
C	15.85362	17.98206	22.30929
H	14.04268	21.41700	22.35466
H	13.86965	17.15937	22.19504
H	14.71982	15.50034	22.33379
H	18.31020	13.22654	22.21112
H	23.94520	15.14048	22.23818
H	24.93457	16.70254	22.29168
H	24.52556	13.35562	23.45829
C	12.25157	19.31622	22.19874
C	11.68318	20.74216	22.21957
H	11.95226	21.27482	23.14389
H	12.03387	21.33499	21.36169
H	10.58543	20.69931	22.16800
C	11.79332	18.63082	20.89447
H	12.13574	17.58786	20.83987
H	10.69425	18.62882	20.83310
C	11.67853	18.55013	23.40935
H	12.01805	17.50514	23.42814
H	30.10321	35.19794	24.34254
H	29.20716	36.67006	24.80361
C	29.58745	36.74276	22.11666
H	29.26482	36.91268	21.07881
H	29.64187	37.72231	22.61411
C	27.22636	36.52426	22.89016
H	26.84277	36.65047	21.86717
H	27.30184	37.51882	23.35624
C	29.09191	32.80191	20.49240
H	30.60320	36.32083	22.09876
H	26.48685	35.94173	23.45735
C	29.90938	32.47227	19.23422
C	30.78068	33.64998	18.76718
H	31.51798	33.94505	19.52834
H	30.17667	34.53149	18.50604
C	30.85915	31.29383	19.53599
H	30.32945	30.41468	19.91989
H	31.39979	30.99872	18.62338
C	28.95018	32.12847	18.07493
H	28.25982	31.31566	18.32728
H	28.34549	33.00854	17.81046
H	29.52407	31.82784	17.18474
H	31.60146	31.59002	20.29189
C	29.19178	34.07375	21.09939
C	28.47726	34.44809	22.23841
H	27.03030	33.77830	23.70155
H	23.84662	23.67379	20.19599
H	29.86190	34.80151	20.65084
C	12.26292	7.96015	21.13619
C	12.09771	9.70236	19.87617
C	29.11616	35.68276	24.32495
H	28.43198	35.07450	24.93321
H	9.78423	6.31880	16.42930
H	7.59771	6.51544	19.45889
C	9.96164	3.99932	20.31147
C	10.62916	3.60251	21.47099
H	12.01731	4.24036	23.00294
H	15.16003	14.53222	19.93460
H	9.30529	3.28296	19.82601
H	9.06315	3.59250	17.67949
H	8.90863	13.00658	19.37486
H	14.92803	8.99663	29.94687
H	31.33601	33.34932	17.86644
H	7.93634	4.79492	17.01952
C	26.72691	18.80450	22.34477
C	27.24384	19.50198	23.62035
H	26.88741	18.98190	24.52151
H	28.34455	19.50244	23.63398
C	27.29464	17.37828	22.31170
H	26.98390	16.83523	21.40665
H	28.39357	17.42119	22.31246
C	27.24234	19.56136	21.10277
H	26.88919	19.08161	20.17821
H	26.90088	20.60606	21.09169
H	28.34314	19.56600	21.09064
H	26.98420	16.79454	23.19124
H	26.90551	20.54595	23.67798
C	16.08915	25.43618	22.84826
C	15.25391	25.40172	24.14545
H	15.90212	25.26650	25.02358
H	14.70103	26.34585	24.26669
C	17.04215	26.63777	22.92131
H	17.65123	26.73350	22.01027
H	16.45782	27.56319	23.02879
C	15.14976	25.63351	21.64036
H	15.72098	25.66476	20.70108
H	14.41323	24.82153	21.56072
H	14.59752	26.58049	21.73977
H	17.71918	26.57043	23.78587
H	14.52274	24.58110	24.13667
C	9.76045	12.41425	16.97358
C	10.26189	12.06059	15.71647
C	11.45880	11.33860	15.66245
C	12.15377	10.97222	16.82058
H	13.23757	13.42628	18.36175
C	9.54679	12.46803	14.45553
H	8.46202	12.54242	14.61537
H	9.89454	13.45405	14.10674
H	9.72773	11.75160	13.64208
C	9.85299	12.45971	19.49428
H	10.55284	13.09684	20.05673
H	9.66342	11.57482	20.12108
C	13.43654	10.18941	16.72422
H	14.25976	10.70476	17.24209
H	13.33858	9.20071	17.19894
H	13.72701	10.03911	15.67633
C	13.24855	7.16936	23.16846
C	13.48362	6.26659	24.25998
C	14.24527	6.93314	25.17076
C	14.49103	8.24566	24.63209
N	13.88405	8.39699	23.39595
N	15.15220	10.89071	23.49153
C	15.54826	10.43343	24.74125
C	16.38479	11.40218	25.39753
C	16.52803	12.44894	24.53966
C	15.76918	12.12942	23.35736
C	15.25045	9.19651	25.30162
C	15.79271	8.86465	26.65392
C	17.07577	8.29634	26.77831
C	17.55668	7.98383	28.05564
C	16.80032	8.22007	29.20769
C	15.53283	8.79418	29.05836
C	15.01381	9.12023	27.80098
C	14.61506	13.60637	20.08414
C	14.79962	12.71913	21.20039
H	11.98991	19.02224	24.35264
H	10.57844	18.54737	23.37063
H	12.18694	19.16156	20.01521
H	20.16864	13.16591	22.19791
H	25.10712	20.96006	22.40278
C	26.86675	30.09597	21.75767
C	27.08833	28.37357	20.47779
N	26.40631	28.83315	21.60469
N	25.09367	26.49338	21.52623
C	25.85823	26.29937	20.37922
C	25.45303	25.10423	19.69850
C	24.42584	24.56403	20.41568
C	24.22919	25.40671	21.56413
C	26.64497	31.09113	22.69407
C	26.85154	27.14797	19.88442
C	23.33596	25.11626	22.59583
C	27.62554	26.75452	18.67090
C	28.78255	25.96201	18.81104
C	29.50652	25.61274	17.66567
C	29.11150	26.02486	16.38855
C	27.96130	26.81290	16.27625
C	27.20881	27.18688	17.39556
H	25.89452	24.75108	18.77136
C	29.88660	25.60806	15.16662
H	30.95176	25.46475	15.39619
H	29.50692	24.65379	14.76632
H	29.80363	26.35449	14.36429
C	29.23878	25.50354	20.17094
H	28.47940	24.86928	20.65387
H	30.17181	24.92949	20.09975
H	29.40744	26.35702	20.84525
C	25.97790	28.03917	17.23461
H	25.10028	27.56694	17.70133
H	26.10244	29.01874	17.72200
H	25.75550	28.21092	16.17343
C	25.84855	30.82493	23.79684
C	25.63007	31.67650	24.93236
C	24.87732	30.97007	25.82072
C	24.61356	29.68762	25.22149
N	25.20801	29.59204	23.97393
N	23.88744	27.12655	23.93746
C	17.92009	8.02857	25.56052
H	18.13511	8.95851	25.01157
H	18.87529	7.56444	25.83888
H	17.40350	7.36093	24.85409
C	13.64584	9.73693	27.67604
H	13.69007	10.70408	27.15232
H	12.97027	9.09488	27.08990
H	13.19553	9.89891	28.66405
Ni	13.94163	10.03845	22.24654
H	18.55302	7.54315	28.15061
H	8.82184	12.97184	17.03856
H	11.86543	11.04754	14.68988
C	11.22328	8.69460	19.30582
H	10.63448	8.86871	18.41047
C	11.33959	7.57954	20.10092
C	11.63762	5.80173	21.57441
C	10.94116	6.19076	20.37494
C	11.48147	4.53106	22.10118
C	10.46504	2.20523	22.08013
C	9.90513	2.33978	23.51209
H	10.57011	2.93462	24.15395
H	8.92084	2.83039	23.50108
H	9.79158	1.34577	23.97160
C	9.50746	1.31922	21.27094
H	9.86701	1.16299	20.24312
H	9.42685	0.33240	21.75004
C	11.84035	1.50737	22.13383
H	12.25880	1.39238	21.12324
H	11.74212	0.50728	22.58354
C	10.09074	5.28058	19.73080
C	12.45986	6.94146	22.05225
C	12.33882	10.94640	19.32543

C	15.65422	12.98757	22.26878
C	11.62909	11.34423	18.07482
C	10.42379	12.06968	18.15653
C	17.32170	7.84566	30.56996
H	16.89769	6.88452	30.90338
H	18.41515	7.73977	30.56641
H	17.05073	8.59795	31.32466
H	7.69180	4.17439	18.66432
C	8.37028	6.81856	18.73680
H	8.89170	7.68689	19.15504
H	7.86708	7.13307	17.80941
C	10.32383	5.99145	17.33142
H	11.01651	6.78875	17.62400
H	10.92475	5.10829	17.06853
N	12.72810	9.22621	21.02614
N	13.98673	11.59970	21.07723
C	13.27149	11.81079	19.90149
C	13.65198	13.05209	19.29312
H	17.08003	13.37123	24.68646
H	16.80141	11.27439	26.39194
H	13.10086	5.25476	24.32845
H	14.62015	6.58625	26.12897
H	8.49640	1.74990	21.22216
H	12.56290	2.07763	22.73442
C	9.32130	5.63734	18.45022
C	8.45749	4.47486	17.93388

meta-phenyl-fused porphyrin-HBC *m*-Ph

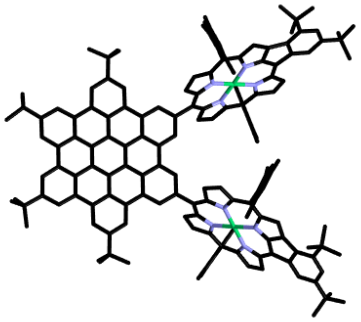


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.23495	18.82494	22.26414
C	24.56191	20.04686	22.34866
C	24.46459	17.66455	22.24017
C	22.58688	23.87042	22.58427
C	23.16635	20.13813	22.39764
C	21.06629	21.48243	22.47701
C	22.49098	21.43036	22.47448
C	23.21721	22.62555	22.54615
C	21.19255	23.91618	22.57455
C	20.41488	22.74962	22.53792
H	24.30446	22.60937	22.58171
H	20.71872	24.89563	22.59287
C	18.87254	20.32924	22.42020
C	18.20617	21.60378	22.48357
C	15.99968	20.44772	22.38833
C	18.95709	22.80946	22.55696
C	18.28148	24.03653	22.65617
C	16.89150	24.12249	22.67457
C	16.16706	22.93089	22.58217
C	16.78226	21.67724	22.48357
H	18.86087	24.95246	22.72844
H	15.08013	22.98762	22.59706
C	26.76714	18.80602	22.20926
C	27.32211	19.40807	23.51737
H	26.99731	18.81720	24.38638
H	28.42269	19.41518	23.49642
C	27.32822	17.38544	22.05352
H	26.96975	16.90320	21.13189
H	28.42587	17.42853	22.00239
C	27.24732	19.65083	21.01068
H	26.85988	19.24344	20.06540
H	26.91733	20.69634	21.08759
H	28.34692	19.64880	20.96249
H	27.06163	16.74425	22.90674
C	22.39004	18.94412	22.35738
H	20.61021	30.32012	28.82388
H	30.44065	25.06539	17.76787
H	27.63071	27.20232	15.31450
C	28.01221	29.41038	19.98837
H	28.64639	29.24614	19.12261
C	27.84872	30.51937	20.78384
C	27.47786	32.27993	22.26219
C	28.22420	31.90855	21.08707
C	27.59386	33.55027	22.80053
C	28.57540	35.89264	22.82689
C	29.06901	35.76350	24.28354
H	28.38138	35.16149	24.89407
H	30.05809	35.28380	24.31896
H	29.15027	36.75841	24.74787
C	29.55928	36.79147	22.06447
H	29.24609	36.94655	21.02144
H	29.60616	37.77793	22.54868
C	27.19077	36.57405	22.81543
H	26.81879	36.68369	21.78625
H	27.25594	37.57566	23.26784
C	29.08622	32.83433	20.48152
H	30.57641	36.37253	22.06153
H	26.44758	35.99569	23.38208
C	29.90808	32.49750	19.22819
C	30.77063	33.67703	18.74964
H	31.50439	33.98627	19.50857
H	30.16009	34.55079	18.47783
C	30.86741	31.33051	19.54408
H	30.34533	30.45185	19.93948
H	31.40974	31.02857	18.63472
C	28.95370	32.13370	18.07107
H	28.26840	31.31912	18.33110
H	28.34347	33.00644	17.79527
H	29.53165	31.82689	17.18565
H	31.60798	31.64245	20.29538
C	29.17542	34.11318	21.07458
C	28.45703	34.49447	22.20873
H	27.01438	33.82896	23.67919
C	23.06092	17.69194	22.29108
C	20.95154	19.00664	22.37076
C	20.29384	20.26796	22.42204
C	18.10833	19.13008	22.36708
C	18.76550	17.86983	22.32048
C	20.18763	17.80765	22.32217
C	20.85408	16.53114	22.27764
C	17.99038	16.65661	22.28091
C	16.66940	19.19343	22.35047
C	20.09584	15.32447	22.24354
C	20.76901	14.09698	22.19777
C	22.16227	14.02013	22.20505
C	22.89986	15.20334	22.24278
C	22.27874	16.46042	22.26871
C	16.56887	16.70400	22.27745
C	15.84234	15.50177	22.27155
C	16.46137	14.25383	22.25648
C	17.85820	14.22459	22.24294
C	18.63694	15.38717	22.25342
C	14.59694	20.47905	22.32920
C	13.82635	19.32151	22.24324
C	14.49809	18.09638	22.22860
C	15.89360	17.99895	22.28620
H	14.09149	21.44054	22.34124
H	13.90646	17.18526	22.16001
H	14.75684	15.54284	22.28701
H	18.35301	13.25538	22.22966
H	23.98496	15.12254	22.25877
H	24.97095	16.70573	22.17270
H	26.97923	20.44188	23.66538
C	12.29512	19.34874	22.15777
C	11.73313	20.77708	22.19661
H	11.99502	21.29293	23.13247
H	12.09701	21.38196	21.35274
H	10.63580	20.74229	22.13164
C	11.85156	18.68938	20.83491
H	12.19152	17.64633	20.76749
H	10.75345	18.69323	20.75645
C	11.70275	18.56289	23.34623
H	12.04095	17.51714	23.35193
H	11.99963	19.01794	24.30250
C	26.22519	9.32368	19.64181
N	25.73850	8.92352	20.88629
N	24.34665	11.21961	20.85655
C	24.92799	11.35844	19.59848
C	24.53353	12.59681	18.99307
C	23.72468	13.23797	19.88471
C	23.61812	12.38727	21.03890
C	26.36576	6.83388	22.14495
C	25.82526	10.47652	18.99360
C	22.84619	12.70030	22.15800
C	26.40166	10.80235	17.65659
C	25.75013	10.36807	16.48569
C	26.32019	10.67017	15.24332
C	27.51470	11.38962	15.13470
C	28.14472	11.80503	16.31293
C	27.60932	11.52515	17.57470
H	24.84949	12.92077	18.00594
C	28.09496	11.73217	13.78792
H	27.78009	11.01268	13.01946
H	27.76350	12.73059	13.45891
H	29.19374	11.74787	13.81672
C	24.46518	9.58737	16.56785
H	23.68049	10.16323	17.08225
H	24.59825	8.65794	17.14260
C	28.31664	11.98220	18.82298
H	27.66256	12.61384	19.44340
H	28.61262	11.12738	19.45066
H	29.21923	12.55615	18.57604
C	25.43165	6.97158	23.15962
C	25.13391	6.02357	24.19630
H	23.91183	23.66511	20.25836
H	29.84018	34.84122	20.61858
H	10.60326	18.56145	23.29113
H	12.26140	19.23346	19.97138
C	15.67702	12.93624	22.25488
C	16.06876	12.11031	23.49814
H	15.83330	12.65913	24.42170
C	14.15844	13.16031	22.28264
H	13.81316	13.72560	21.40412
H	13.64384	12.18840	22.27532
H	15.74949	12.70470	20.07823
H	13.84174	13.69806	23.18878
H	20.21244	13.16346	22.14800
H	17.14255	11.87611	23.50995
H	15.51612	11.15840	23.51136
C	16.02690	12.14000	20.98035
H	17.10175	11.91867	20.92166
H	15.48400	11.18248	20.96944
H	25.15303	20.96060	22.36782
C	26.88170	30.12424	21.77264
C	27.11276	28.39491	20.50409
N	26.42962	28.85703	21.62918
N	25.13482	26.50517	21.56783
C	25.89744	26.31146	20.41931
C	25.50185	25.10845	19.74737
C	24.48243	24.56254	20.47115
C	24.28064	25.41048	21.61497
C	26.64997	31.12704	22.69856
C	26.88104	27.16600	19.91592
C	23.38882	25.12075	22.64862
C	27.64747	26.78118	18.69480
C	28.81302	25.99926	18.82066
C	29.53214	25.66583	17.66732
C	29.12386	26.08344	16.39627
C	27.96483	26.86061	16.29820
C	27.21707	27.21881	17.42557
H	25.94440	24.75409	18.82122
C	29.89495	25.68588	15.16532
H	30.95946	25.53134	15.39045
H	29.50852	24.74255	14.74607
H	29.81585	26.44867	14.37802
C	29.28355	25.53595	20.17399
H	28.54280	24.87370	20.64851
C	21.96513	8.09737	28.56729
C	20.72029	7.46672	28.46361
C	20.19678	7.24820	27.18542
C	20.88378	7.63724	26.02945
H	21.32068	13.00780	24.53346
H	21.26436	10.73323	26.01541
H	25.62488	5.06560	24.32607
H	23.61997	6.12766	25.80396
C	19.97780	7.01553	29.69377
H	20.33180	6.02654	30.02766
H	20.12606	7.71280	30.53066
H	18.89905	6.93062	29.50284
C	24.01855	9.18503	27.58842
H	24.00547	10.18916	27.13719
H	24.29081	9.28674	28.64707
H	24.81651	8.62371	27.07862
C	20.28922	7.38765	24.66872
H	20.16271	8.32729	24.10933
H	20.94397	6.74681	24.05828
H	19.30917	6.89990	24.75113
Ni	24.46470	9.69771	22.06820
H	22.38900	8.28581	29.55777
H	25.81577	10.32905	14.33494
H	29.08368	12.36238	16.25053
C	27.20958	8.38339	19.14032
H	27.70129	8.50621	18.18026
C	27.33871	7.40412	20.09626
C	27.36637	5.79875	21.78226
C	27.96322	6.14096	20.51647
C	27.76575	4.66423	22.46828
H	26.41552	7.77819	21.13397
C	21.79252	10.92563	25.08668
H	30.23236	24.98945	20.09472
H	29.42815	26.38474	20.85956
C	25.97808	28.06213	17.27998
H	25.10800	27.57991	17.75055
H	26.09894	29.03937	17.77299
H	25.74615	28.23930	16.22174
C	25.85131	30.86449	23.80071
C	25.62031	31.72514	24.92680
C	24.87177	31.02010	25.81989
C	24.62256	29.72910	25.23273
N	25.22131	29.62727	23.98774
N	23.92246	27.14791	23.97241
C	23.53321	27.55318	25.24189
C	22.66724	26.57547	25.84477
C	22.49901	25.57817	24.93374
C	23.27475	25.93379	23.77277
C	23.85770	28.75501	25.86231
C	23.32976	29.02182	27.23462
C	22.06615	29.62309	27.40050
C	21.59255	29.85648	28.69697
C	22.33744	29.51010	29.82897
C	23.58658	28.90971	29.63781
C	24.09800	28.65984	28.35959
H	21.92118	24.66545	25.03283
C	22.24804	26.66366	26.84237
H	26.00253	32.73433	25.03084
H	24.50645	31.32830	26.79489
C	21.82178	29.79763	31.21437
H	22.19287	30.76928	31.57922
H	20.72386	29.83818	31.23393
H	22.15164	29.03343	31.93230
C	21.23384	30.00521	26.20522
H	20.99997	29.12661	25.58424
H	20.28859	30.46881	26.51646
H	21.76918	30.71394	25.55495
C	25.44517	28.00878	28.19048
H	25.36790	27.07450	27.61352
H	26.13762	28.66139	27.63673
H	25.89502	27.77671	29.16465
Ni	25.17245	28.02455	22.78749
H	24.18218	28.62290	30.50910
C	28.94454	5.31070	19.95588
H	29.88227	1.39389	20.98697
H	29.03459	3.55823	24.66503
C	29.60775	5.61656	18.60453
C	30.65546	4.56440	18.20531
H	30.21410	3.56296	18.09466
C	28.52971	5.62818	17.50001
H	27.71345	6.32652	17.71669
H	28.97815	5.91162	16.53525
C	30.33589	6.97514	18.68246
H	29.67745	7.78821	19.00814
H	31.17087	6.91701	19.39631
H	30.74737	7.24052	17.69634
H	28.08908	4.62615	17.39088
C	29.30789	4.15929	20.68909
C	28.75305	3.81838	21.92361
H	27.32815	4.42592	23.43654
H	23.22650	14.19553	19.77678
H	30.06667	3.50563	20.26851
H	31.47808	4.50494	18.93318
H	24.09939	9.32458	15.56676
H	19.22204	6.76339	27.08145
H	31.32969	33.37077	17.85314
H	31.09084	4.84423	17.23466
C	16.14689	25.45772	22.79305
C	15.26649	25.43764	24.06001
H	15.88231	25.30044	24.96086
H	14.71905	26.38773	24.15725
C	17.10503	26.65335	22.89094
H	17.74478	26.73808	22.00005
C	21.82023	12.06427	24.34149
C	22.65757	11.79836	23.19977

C	22.87851	8.69818	24.93628
C	22.13742	8.26641	26.16001
C	22.68543	8.50133	27.43772
C	30.24857	1.75059	21.96099
H	31.16822	2.33036	21.79347
H	30.51570	0.86815	22.56073
C	29.76907	3.00293	24.06491
H	30.64690	3.65031	23.92391
H	30.08033	2.11949	24.64345
H	17.75280	26.58630	23.77768
H	14.52792	24.62421	24.02972
C	29.18412	2.57077	22.70356
C	27.95689	1.66552	22.93928
H	27.16971	2.18507	23.50341
H	27.52482	1.33742	21.98260
H	28.24812	0.77155	23.51195
H	16.52416	27.58359	22.97252
C	15.25331	25.65282	21.55048
H	15.86006	25.67876	20.63357
H	14.51925	24.84147	21.44574
H	14.70016	26.60161	21.62540

ortho-phenyl-fused porphyrin-HBC *o*-Ph

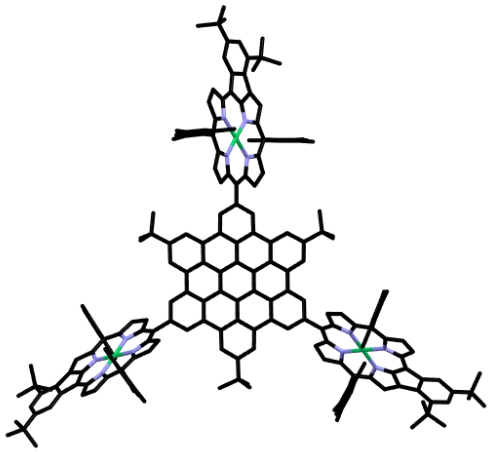


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.17552	18.85680	22.27594
C	24.51489	20.08501	22.31465
C	24.41516	17.68670	22.25609
C	22.53518	23.89758	22.53365
C	23.11657	20.16897	22.35223
C	21.01578	21.50882	22.43765
C	22.44017	21.45923	22.42333
C	23.16722	22.65410	22.48959
C	21.14054	23.94219	22.53545
C	20.36324	22.77505	22.50650
H	24.25470	22.63847	22.51825
H	20.66603	24.92131	22.56025
C	18.82478	20.35090	22.41081
C	18.15679	21.62399	22.48461
C	15.95207	20.46277	22.41616
C	18.90574	22.83156	22.54841
C	18.22894	24.05658	22.66434
C	16.83932	24.13863	22.71303
C	16.11647	22.94519	22.62865
C	16.73293	21.69391	22.50794
H	18.80719	24.97382	22.72944
H	15.02988	22.99728	22.66963
C	16.09394	25.47071	22.86085
C	15.26146	25.44224	24.15974
H	15.91068	25.30245	25.03647
H	14.71538	26.39018	24.28201
C	17.04828	26.67179	22.92610
H	17.65203	26.76423	22.01117
H	16.46460	27.59772	23.03361
C	15.15411	25.66544	21.65289
H	15.72597	25.69342	20.71382
H	14.41694	24.85385	21.57552
H	14.60328	26.61355	21.74910
H	17.73052	26.60719	23.78672
C	22.34497	18.97149	22.31492
H	22.23992	30.67739	31.61019
H	20.71364	29.87039	31.20168
H	22.06277	28.93823	31.89802
C	21.24851	30.00267	26.19135
H	20.99737	29.12629	25.57386
H	20.31215	30.48556	26.50005
H	21.79795	30.69777	25.53835
C	25.43797	27.96814	28.18334
H	25.36022	27.04124	27.59469
H	26.13769	28.62385	27.64252
H	25.87985	27.72224	29.15784
Ni	25.15516	28.02670	22.76119
H	24.16506	28.56991	30.50044
H	20.61368	30.30425	28.80912
H	30.39870	24.99144	17.78609
H	27.63457	27.13638	15.28728
C	28.00244	29.40781	19.96674
H	28.63689	29.24307	19.10134
C	27.84648	30.51409	20.76830
C	27.49514	32.26224	22.26656
C	28.23494	31.89762	21.08518
C	27.62184	33.52521	22.81912
C	28.62563	35.85598	22.87744
C	29.13852	35.69932	24.32481
H	28.45656	35.08950	24.93402
H	30.12627	35.21580	24.33862
H	29.22996	36.68585	24.80489
C	29.60353	36.76298	22.11747
H	29.27705	36.93679	21.08148
H	29.66117	37.74061	22.61817
C	27.24516	36.54554	22.89863
H	26.85925	36.67827	21.87735
H	27.32335	37.53740	23.36996
C	29.10354	32.82382	20.48941
H	30.61863	36.33981	22.09449
H	26.50612	35.96151	23.46488
C	29.92201	32.49436	19.23200
C	30.79305	33.67221	18.76478
C	23.01427	17.71417	22.25578
C	20.90589	19.03243	22.33564
C	20.24638	20.29260	22.39282
C	18.06303	19.15014	22.37110
C	18.72225	17.89082	22.31567
C	20.14348	17.83188	22.29881
C	20.80917	16.55604	22.23332
C	17.95088	16.67479	22.29050
C	16.62424	19.20973	22.37368
C	20.05912	15.34856	22.19353
C	20.73699	14.12265	22.09186
C	22.12661	14.03724	22.04019
C	22.85003	15.23113	22.10009
C	22.23180	16.48294	22.19897
C	16.52940	16.71907	22.31430
C	15.80562	15.51561	22.33691
C	16.42784	14.26903	22.32732
C	17.82389	14.24266	22.27793
C	18.60110	15.40664	22.25192
C	14.54892	20.49090	22.36250
C	13.78097	19.33088	22.28515
C	14.45528	18.10703	22.27532
C	15.85126	18.01276	22.32251
H	14.04143	21.45142	22.36844
H	13.86518	17.19431	22.21541
H	14.72071	15.55477	22.37589
H	18.32097	13.27429	22.27216
H	23.93637	15.17855	22.05801
H	24.94794	16.73801	22.24807
H	14.52476	24.62656	24.15252
C	12.24926	19.35258	22.20746
C	11.68252	20.77931	22.22051
H	11.94865	21.31635	23.14309
H	12.03824	21.36725	21.36138
H	10.58491	20.73843	22.16398
C	11.79751	18.66536	20.90184
H	12.13631	17.62088	20.85437
H	10.69892	18.66803	20.83164
C	11.66700	18.58875	23.41506
H	12.00829	17.54423	23.43760
H	11.96937	19.06232	24.36056
H	30.34325	30.43852	19.92197
H	31.41314	31.02039	18.62410
C	28.96527	32.14815	18.07150
H	28.27472	31.33542	18.32357
H	28.36118	33.02748	17.80320
H	29.54151	31.84576	17.18348
H	31.61504	31.61583	20.29083
C	29.20525	34.09492	21.09790
H	28.49207	34.46888	22.23787
H	27.04500	33.79870	23.70106
H	23.84696	23.70195	20.19789
H	29.87654	34.82215	20.65020
C	32.70932	18.36550	21.11765
C	31.27596	17.35941	19.85900
N	31.37888	18.14278	21.00906
N	28.69237	18.06135	21.06401
C	28.86247	17.34376	19.88286
C	27.59583	17.06944	19.27002
C	26.63828	17.62874	20.06426
C	27.31719	18.21407	21.18855
C	33.49680	19.04418	22.03149
C	30.07446	16.95717	19.30742
C	26.66088	18.80401	22.26876
C	30.07592	16.14021	18.05850
C	30.04489	14.73398	18.14525
C	30.06736	13.98253	16.96503
C	30.11609	14.58808	15.70498
C	30.14640	15.98538	15.64560
C	30.12718	16.77509	16.80104
H	27.47481	16.53226	18.33401
H	31.52955	33.96845	19.52628
H	30.18888	34.55317	18.50201
H	10.56718	18.58375	23.36712
H	12.20080	19.19107	20.02399
C	15.64605	12.95044	22.37715
C	16.05524	12.16739	23.64241
H	15.82880	12.74560	24.55017
C	14.12734	13.17194	22.41718
H	13.76947	13.70621	21.52444
H	13.61509	12.19923	22.45076
H	15.69242	12.64430	20.20888
H	13.82123	13.74016	23.30810
H	20.15814	13.20482	22.04213
H	17.13041	11.93906	23.64798
H	15.50682	11.21420	23.69364
C	15.98007	12.11090	21.12666
H	17.05405	11.88643	21.06300
H	15.43643	11.15413	21.15533
C	22.87322	12.70315	21.91801
C	21.91778	11.50240	21.86692
H	21.30533	11.43037	22.77809
H	21.24419	11.55250	20.99840
H	22.49957	10.57287	21.78338
C	23.71562	12.71003	20.62513
H	24.45382	13.52428	20.62567
H	24.26202	11.75999	20.52215
C	23.80614	12.52881	23.13472
H	24.54099	13.34305	23.20401
H	23.22950	12.51371	24.07118
H	24.36031	11.58103	23.05554
H	23.07415	12.83669	19.74076
H	25.12384	20.98687	22.31278
C	26.87709	30.11882	21.75505
C	27.09635	28.39497	20.47665
N	26.41578	28.85621	21.60376
N	25.09950	26.51886	21.52938
C	25.86302	26.32299	20.38213
C	25.45467	25.12902	19.70128
C	24.42654	24.59161	20.41842
C	24.23300	25.43379	21.56801
C	26.66007	31.11235	22.69419
C	26.85825	27.16830	19.88576
C	23.34090	25.14472	22.60116
C	32.90848	19.61889	23.14698
C	33.57648	20.27833	24.23365
C	32.62153	20.60728	25.14686
C	31.36017	20.16053	24.61542
N	31.52824	19.55677	23.37969
N	28.73422	19.40702	23.48724
C	28.93842	19.97026	24.73984
C	27.68501	20.19616	25.40844
H	26.70304	19.79747	24.55514
C	27.35235	19.31734	23.36171
C	30.16027	20.33676	25.29258
C	30.17633	20.97262	26.64482
C	30.01818	22.36725	26.76714
C	30.03105	22.94005	28.04487
C	30.19459	22.16786	29.19899
C	30.34427	20.78419	29.05102
C	30.33983	20.17151	27.79351
H	25.62985	19.80609	24.71238
H	27.59158	20.61252	26.40672
H	34.64422	20.45494	24.29669
H	32.73788	21.10995	26.10218
C	30.23088	22.80610	30.56278
H	31.26766	22.91321	30.92116
H	29.78141	23.80849	30.54822
H	29.69325	22.19814	31.30490
C	29.83107	23.23064	25.54764
H	28.90956	22.96359	25.00726
H	29.77132	24.29200	25.82148
H	30.66006	23.10256	24.83505
C	30.50092	18.67924	27.67096
C	30.87250	31.31715	19.53612
H	29.10107	14.34625	20.05301
C	27.63051	26.76714	18.67364
C	28.78257	25.96771	18.81715
C	29.50203	25.60710	17.67242
C	29.10676	26.01300	16.39340
C	27.96039	26.80641	16.27780
C	27.21258	27.19218	17.39627
H	25.89576	24.77357	18.77493
C	29.87684	25.58168	15.17313
H	30.94180	25.43490	15.40165
H	29.49171	24.62534	14.78309
H	29.79564	26.32081	14.36379
C	29.23635	25.51176	20.17868
H	28.47359	24.88363	20.66413
H	30.16516	24.93082	20.11084
H	29.41010	26.36697	20.84945
C	25.98214	28.04475	17.23226
H	25.10199	27.56806	17.68997
H	26.10159	29.02122	17.72682
H	25.76599	28.22266	16.17077
C	25.87152	30.84391	23.80229
C	25.66397	31.69233	24.94220
C	24.91249	30.98626	25.83210
C	24.63957	29.70695	25.23044
N	25.22814	29.61262	23.97977
N	23.89943	27.15177	23.94370
C	23.51893	27.54758	25.21884
C	22.64328	26.57389	25.81409
C	22.46214	25.58764	24.89356
C	23.23791	25.94728	23.73375
C	23.86201	28.73757	25.85158
C	23.33298	28.99967	27.22437
C	22.07265	29.60807	27.38821
C	21.59344	29.83464	28.68406
C	22.32912	29.47380	29.81718
C	23.57613	28.86735	29.62810
C	24.09314	28.62482	28.35079
H	21.87588	24.67962	24.98619
H	22.22797	26.65619	26.81390
H	26.06353	32.69364	25.05728
H	24.55955	31.28687	26.81394
C	21.80584	29.74999	31.20229
C	34.90021	18.09798	20.35146
C	36.07520	19.39239	22.07512
C	38.59819	19.66908	22.04787
C	38.76705	19.11438	23.47829
H	37.92328	19.39312	24.12512
H	38.83354	18.01662	23.46580
H	39.68744	19.51136	23.93366
C	39.84098	19.28271	21.23379
H	39.79368	19.67406	20.20680
H	40.73740	19.70486	21.71123
C	38.51798	21.20917	22.10510
H	38.40392	21.63186	21.09618
H	39.43658	21.62117	22.55055
C	36.11163	17.81481	19.70361
H	39.97227	18.19170	21.18295
H	37.66736	21.55076	22.71149
C	36.18314	16.97281	18.42072
C	37.61988	16.80739	17.89824
H	38.26621	16.29205	18.62401
C	35.63675	15.55792	18.70559
H	34.62518	15.57458	19.12667
H	35.61323	14.96648	17.77725
C	35.37148	17.66630	17.30613
H	34.33349	17.85949	17.59964
H	35.83039	18.63243	17.04898
H	35.36134	17.04106	16.39996
H	36.28773	15.03860	19.42441
C	37.28869	18.34024	20.28160
C	37.30330	19.11563	21.44185
H	36.06316	20.00083	22.97770
H	30.86369	14.32329	20.10575
C	30.16340	18.27691	16.69798

H	29.30051	18.73341	17.20640
H	31.06378	18.68943	17.17890
H	30.15598	18.59919	15.64858
H	30.04992	12.89120	17.03459
H	30.18838	16.47933	14.67070
C	32.58405	17.09828	19.28784
H	32.72313	16.50021	18.39262
C	33.49630	17.75242	20.08125
C	34.89376	18.89621	21.55097
H	31.34941	33.37035	17.86508
H	37.59912	16.19905	16.98193
C	30.10740	13.75895	14.44775
H	30.58201	12.78073	14.60846
H	29.07589	13.56998	14.10816
H	30.63321	14.26703	13.62725
C	29.99650	14.04947	19.48554
H	29.64746	18.22660	27.14330
H	31.39997	18.42053	27.09050
H	30.58354	18.20999	28.66002
Ni	30.07368	18.79078	22.23439
H	29.90595	24.02239	28.13823
H	25.56488	17.64910	19.91092
H	38.23541	18.12783	19.79315
H	38.08064	17.77365	17.64504
H	29.98548	12.95781	19.37028
H	30.46531	20.15965	29.94075

tri-phenyl-fused porphyrin-HBC *tri*-Ph

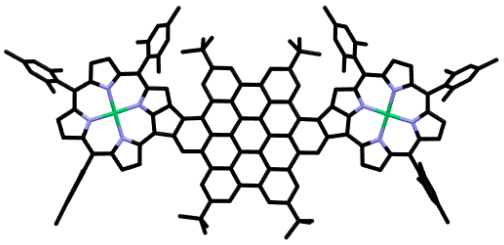


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.20011	18.84671	22.27934
C	24.52341	20.06222	22.34989
C	24.43137	17.68037	22.23872
C	22.52495	23.87224	22.53740
C	23.12141	20.14285	22.37889
C	21.01454	21.47670	22.44959
C	22.43986	21.43093	22.44508
C	23.16062	22.63047	22.50464
C	21.13016	23.91206	22.53141
C	20.35756	22.74167	22.50401
H	24.24803	22.62029	22.53358
H	20.65184	24.88946	22.54687
C	18.82665	20.31073	22.41074
C	18.15506	21.58275	22.47494
C	15.95472	20.41454	22.41635
C	18.89936	22.79372	22.53092
C	18.21612	24.01773	22.62242
C	16.82551	24.09601	22.65337
C	16.10808	22.89861	22.58256
C	16.73163	21.64899	22.49237
H	18.79040	24.93822	22.67805
H	15.02101	22.94776	22.60593
C	16.07131	25.42641	22.76677
C	15.22236	25.41791	24.05559
H	15.86093	25.30226	24.94362
H	14.66718	26.36365	24.15066
C	17.02037	26.63213	22.82102
H	17.63948	26.70579	21.91456
H	16.43249	27.55833	22.89817
C	15.14426	25.59228	21.54429
H	15.72626	25.60519	20.61110
H	14.41164	24.77590	21.47387
H	14.58742	26.53903	21.61679
H	17.68786	26.58852	23.69459
C	22.35273	18.94793	22.33205
H	30.17829	24.99304	20.03209
H	29.42543	26.42677	20.77677
C	25.88172	28.01769	17.22983
H	25.01604	27.51692	17.68953
H	25.98639	28.98952	17.73667
H	25.65179	28.20511	16.17295
C	25.86063	30.82786	23.79701
C	25.65133	31.67730	24.93587
C	24.89060	30.97578	25.82115
C	24.61454	29.69799	25.21746
N	25.21015	29.59961	23.97065
N	23.87757	27.13849	23.93405
C	23.48886	27.54108	25.20463
C	22.61116	26.56954	25.80038
C	22.43770	25.57722	24.88525
C	23.21899	25.93137	23.72762
C	23.82871	28.73317	25.83488
C	23.29052	29.00290	27.20255
C	22.03408	29.62206	27.35403
C	21.54763	29.85899	28.64530
C	22.27276	29.49853	29.78528
C	23.51631	28.88150	29.60834
C	24.03995	28.62782	28.33608
H	21.85259	24.66867	24.97937
H	22.18979	26.65711	26.79717
H	26.05519	32.67652	25.05335
H	24.53400	31.27790	26.80132
C	21.74317	29.78589	31.16544
H	22.19018	30.70594	31.57587
H	20.65339	29.92495	31.15591
H	21.98046	28.97071	31.86408
C	21.22200	30.01871	26.14954
H	20.97022	29.14261	25.53184
C	23.03206	17.69743	22.26390
C	20.91368	19.00046	22.34765
C	20.24850	20.25802	22.40264
C	18.06952	19.10636	22.36515
C	18.73500	17.84954	22.31553
C	20.15724	17.79639	22.30539
C	20.83141	16.52341	22.25331
C	17.96857	16.63090	22.27975
C	16.62962	19.15947	22.36331
C	20.08154	15.31108	22.22900
C	20.76287	14.08727	22.18724
C	22.15621	14.02122	22.15261
C	22.88427	15.21102	22.17081
C	22.25553	16.46192	22.22759
C	16.54698	16.66861	22.28020
C	15.82601	15.46307	22.26337
C	16.45228	14.21929	22.23595
C	17.84955	14.19874	22.22456
C	18.62232	15.36513	22.24686
C	14.55379	20.43748	22.39582
C	13.79934	19.26595	22.32063
C	14.46442	18.04073	22.27755
C	15.86389	17.95765	22.30661
H	14.01559	21.38198	22.44369
H	13.85840	17.13919	22.21326
H	14.74041	15.49828	22.27640
H	18.34954	13.23244	22.19880
H	23.96955	15.13864	22.13843
H	24.94873	16.72441	22.18354
H	14.49165	24.59688	24.05631
C	26.72989	18.75033	22.23411
C	27.40463	20.12651	22.32677
H	27.12280	20.77863	21.48657
H	27.15294	20.64197	23.26564
H	28.49694	20.00179	22.29769
C	27.22321	17.88764	23.41444
H	26.80760	16.87074	23.37979
H	28.32039	17.80337	23.38852
C	27.15199	18.08973	20.90494
H	26.72327	17.08348	20.79794
H	26.81791	18.69145	20.04718
H	20.57091	30.33709	28.76132
H	30.37453	25.06399	17.70449
H	27.51903	27.14495	15.25515
C	27.96867	29.39827	19.94569
H	28.59312	29.23760	19.07211
C	27.82451	30.49960	20.75585
C	27.48848	32.24312	22.26264
C	28.21937	31.88058	21.07519
C	27.62312	33.50363	22.81888
C	28.63129	35.83281	22.87586
C	29.14934	35.67152	24.32084
H	28.46789	35.06273	24.93161
H	30.13510	35.18387	24.32905
H	29.24671	36.65653	24.80293
C	29.60879	36.73870	22.11372
H	29.27997	36.91367	21.07868
H	29.66981	37.71622	22.61440
C	27.25238	36.52530	22.90258
H	26.86394	36.65990	21.88250
H	27.33378	37.51635	23.37510
C	29.08702	32.80598	20.47679
H	30.62305	36.31368	22.08753
H	26.51373	35.94151	23.46957
C	29.89744	32.47856	19.21354
H	-0.79444	18.41410	20.15282
H	-1.75685	18.39701	21.64540
C	0.46728	16.91542	22.08993
H	8.94685	25.18685	19.38499
H	1.41259	21.86120	16.90906
N	7.60272	19.99157	21.02133
C	10.12667	20.81578	19.92726
C	8.91811	21.18507	19.33323
C	8.88529	19.85805	16.72806
H	9.74854	19.41597	17.24853
H	8.91010	19.53312	15.67981
C	6.32299	17.60802	25.19331
C	7.59239	18.01439	24.64859
N	7.43388	18.60101	23.40354
H	6.19857	17.13082	26.16070
H	7.72117	19.78245	27.11443
Ni	8.89937	19.34717	22.25669
N	10.28858	20.08375	21.10076
C	11.39904	21.11724	19.33897
C	12.35199	20.55730	20.13819
C	11.66365	19.94045	21.23938
H	11.52658	21.67189	18.41419
N	10.23107	18.70950	23.50766
C	10.02010	18.13127	24.75215
C	11.61442	18.77594	23.37945
C	8.79205	17.80283	25.31525
C	8.76805	17.16670	26.66714
C	8.84659	15.76505	26.78589
C	8.66566	17.36069	29.07644
C	8.67763	17.97400	27.81906
C	8.60071	19.47304	27.69973
H	9.48132	19.87800	27.17775
H	8.53947	19.94386	28.68957
H	8.60076	17.98979	29.96873
C	8.83037	15.19181	28.06306
C	8.73876	15.97065	29.22093
C	8.69556	15.33258	30.58445
H	7.65743	15.23320	30.94125
H	9.13613	14.32618	30.57075
C	8.95190	14.89461	25.56177
H	9.85575	15.13222	24.97960
H	8.98826	13.83244	25.83697
H	8.09603	15.04819	24.88678
H	8.89510	14.10382	28.15312
C	11.27143	17.85901	25.40733
H	11.35981	17.42089	26.39674
C	12.31243	19.31759	22.30501
C	12.25838	18.25224	24.55704
H	13.33211	18.21557	24.70729
H	9.23710	15.93564	31.32725
H	13.42822	20.55455	20.00271
C	23.91594	8.05368	19.58609
N	24.64809	8.32926	20.74143
N	23.22468	10.60620	20.85995
C	22.67799	10.12346	19.67376
C	21.78752	11.08776	19.09710
C	21.79059	12.17639	19.91884
C	22.65873	11.86467	21.02164
C	26.48427	6.91629	21.73104
C	22.95695	8.89936	19.06275
C	22.85912	12.71142	22.11142
C	22.24647	8.51743	17.80740
C	21.01375	7.83902	17.88221
C	20.36860	7.47559	16.69472
C	20.91213	7.76889	15.43971
C	22.13938	8.43882	15.39243
C	22.81863	8.81982	16.55504
H	21.25091	10.94014	18.16471
H	0.59796	16.47857	21.08908
H	-0.45474	16.50408	22.52893
C	2.88135	20.28911	19.66590
H	28.24781	17.99779	20.85627
H	26.93453	18.33770	24.37562
C	15.67501	12.89779	22.21736
C	16.05710	12.06764	23.46080
H	15.80227	12.60736	24.38459
C	14.15510	13.11420	22.22854
H	13.81629	13.68020	21.34808
H	13.64596	12.13957	22.21295
H	15.77783	12.68108	20.04042
H	13.82440	13.64746	23.13230
H	20.21249	13.14866	22.18864
H	17.13291	11.84418	23.48666
H	15.51392	11.11033	23.45970
C	16.04461	12.11095	20.94234
H	17.12055	11.89104	20.89623
H	15.50343	11.15281	20.91766
H	25.10417	20.97969	22.37893
C	26.86209	30.10218	21.74859
C	27.06459	28.38523	20.45889
N	26.39511	28.84179	21.59442
N	25.07727	26.50268	21.52071
C	25.83442	26.31031	20.36840
C	25.42965	25.11261	19.69205
C	24.40995	24.56895	20.41703
C	24.21708	25.41264	21.56535
C	26.65207	31.09425	22.69087
C	26.82114	27.16131	19.86500
C	23.32679	25.12294	22.60001
C	27.58024	26.77296	18.64050
C	28.75381	26.00278	18.76370
C	29.46099	25.65728	17.60654
C	29.03356	26.05261	16.33473
C	27.86787	26.82035	16.23954
C	27.13114	27.18912	17.37077
H	25.86708	24.76011	18.76274
C	29.79122	25.64052	15.10029
H	30.85828	25.48977	15.31545
H	29.40094	24.69158	14.69763
H	29.70227	26.39300	14.30415
C	29.24441	25.56370	20.11797
H	28.49949	24.93291	20.62726
C	28.19724	11.73710	27.81569
C	27.58945	11.23340	28.97002
C	26.44313	10.44481	28.82111
C	25.90519	10.15399	27.56268
H	23.27273	14.08266	24.55718
H	24.97468	12.75919	26.20722
H	28.24615	6.54354	24.00911
H	27.87647	8.48958	25.85460
C	28.16346	11.51222	30.33413
H	28.80422	10.68078	30.67029
H	28.77977	12.42186	30.33165
H	27.37041	11.63512	31.08557
C	28.36904	12.03621	25.31741
H	27.68586	12.68179	24.74412
H	29.25041	12.62851	25.59602
H	28.69170	11.23665	24.63296
C	24.66622	9.30721	27.43888
H	23.85815	9.85389	26.92885
H	24.85814	8.40350	26.84023
H	24.30209	8.99578	28.42661
Ni	24.56020	9.75485	21.99924
H	29.09060	12.36082	27.90993
H	19.41440	6.94464	16.75460
H	22.58530	8.67234	14.42149
H	-0.99666	19.90836	21.10572
H	1.31192	16.58857	22.71255
C	2.81881	21.11311	18.37102

H	20.28652	30.50834	26.45021	C	1.38631	21.26482	17.83300
H	21.78094	30.70913	25.49951	H	0.73089	21.78647	18.54604
C	25.38047	27.95966	28.18130	C	3.35595	22.53408	18.64321
H	25.29807	27.02797	27.60082	H	4.36472	22.52730	19.07127
H	26.08767	28.60489	27.63766	H	3.38246	23.11492	17.70828
H	25.81570	27.71945	29.16013	C	3.64491	20.40909	17.27374
Ni	25.13505	28.01118	22.75251	C	20.18418	7.39827	14.17470
H	24.09719	28.58494	30.48634	H	19.55033	6.51253	14.32059
C	26.72324	4.09648	19.33233	H	19.52813	8.21955	13.84312
H	28.95785	0.89703	20.74774	H	20.88507	7.18995	13.35420
H	30.74488	4.53248	22.33649	C	20.40359	7.50132	19.21687
C	26.02639	3.64520	18.04003	H	20.21580	8.40861	19.81146
C	26.59552	2.32794	17.48754	H	21.07724	6.86917	19.81567
H	26.47082	1.49552	18.19578	C	24.13954	9.53715	16.46557
C	24.52772	3.41027	18.32369	H	24.10957	10.49798	17.00167
H	24.04040	4.28781	18.76333	H	24.94743	8.94716	16.92558
H	24.00080	3.15477	17.39140	H	24.41012	9.73286	15.41983
C	26.22298	4.71887	16.94896	C	26.68317	7.68007	22.86997
H	25.87773	5.70934	17.26630	C	27.57516	7.39337	23.95817
H	27.28878	4.80511	16.69045	C	27.39042	8.36765	24.89128
H	25.67195	4.43837	16.03803	C	26.39111	9.26362	24.37031
H	24.40273	2.57381	19.02717	N	25.95089	8.84702	23.12428
C	27.76415	3.32307	19.89236	N	24.43910	11.19988	23.28080
C	28.44444	3.66797	21.06109	C	25.04881	11.28619	24.52528
H	28.59649	5.14878	22.63134	C	24.64100	12.48252	25.21186
H	21.25780	13.11338	19.79785	C	23.79313	13.14742	24.38073
H	28.05020	2.40809	19.38170	C	23.67355	12.35681	23.18222
H	27.66245	2.41377	17.23377	C	25.96686	10.39052	25.06201
H	19.45205	6.96854	19.09077	C	26.53670	10.67316	26.41437
H	25.94776	10.04646	29.71107	C	27.69136	11.47120	26.53765
H	31.32335	33.35499	17.84462	H	2.69798	23.05793	19.35235
H	26.05517	2.06367	16.56656	C	1.70067	19.76648	20.23925
C	6.27205	19.76427	21.11829	C	1.67682	19.00660	21.40957
C	7.71394	20.76701	19.86685	H	2.90584	18.14717	22.96939
C	5.47565	19.10446	22.03807	H	0.75832	19.96733	19.73768
C	8.92178	21.99968	18.08286	H	0.93251	20.29315	17.58802
C	8.92527	23.40632	18.16612	C	29.84256	1.54785	20.80939
C	8.90764	24.15401	16.98338	H	30.15806	1.80066	19.78635
C	8.88833	23.54414	15.72464	H	30.65248	0.96667	21.27425
C	8.88143	22.14635	15.66894	C	30.86722	3.63376	21.71573
C	8.89793	21.36046	16.82678	H	31.17624	3.95782	20.71117
C	8.90189	24.36866	14.46448	H	31.68023	3.03157	22.14992
H	8.41358	25.34163	14.61532	H	9.81834	23.80455	20.09675
H	9.93480	24.56873	14.13581	H	8.05433	23.82151	20.10269
H	8.39203	23.85079	13.64004	H	7.98498	19.43384	17.19895
C	8.93713	24.09566	19.50477	H	4.68048	20.22368	17.58074
C	30.77171	33.65474	18.74792	H	3.19286	19.43779	17.02382
H	31.51228	33.94457	19.50793	H	3.66193	21.02326	16.36012
H	30.17019	34.53933	18.49141	H	29.00164	3.21665	23.73492
C	30.84378	31.29541	19.50724	H	28.24880	1.76036	23.04994
H	30.31158	30.41596	19.88708	H	29.97158	1.74262	23.51299
H	31.38176	31.00367	18.59202	C	24.34540	6.80623	18.98204
C	28.93288	32.14288	18.05652	H	23.89555	6.40794	18.07787
H	28.23964	31.33238	18.30845	C	25.36901	6.32468	19.76258
H	28.33155	33.02664	17.79670	C	27.05380	5.64470	21.21831
H	29.50272	31.84248	17.16366	C	26.36648	5.27234	20.00834
H	31.58825	31.58528	20.26349	C	28.07343	4.85560	21.72283
C	29.19556	34.07501	21.08822	C	29.56754	2.80437	21.64758
C	28.49123	34.44722	22.23420	C	29.17225	2.35740	23.07115
H	27.05430	33.77544	23.70647				
H	23.83339	23.67556	20.20297				
H	29.86499	34.80222	20.63783				
C	25.50743	7.28683	20.82304				
C	6.05314	18.55520	23.17144				
C	5.37350	17.93521	24.27391				
H	4.30224	17.78474	24.34339				
H	8.90487	25.24563	17.05013				
H	8.85995	21.64919	14.69509				
C	6.41081	21.01481	19.27813				
H	6.27803	21.60541	18.37694				
C	5.49331	20.36374	20.06767				
C	4.08346	19.24166	21.54201				
C	4.08717	20.02055	20.33016				
C	2.89933	18.74572	22.06015				
C	0.37807	18.45395	22.00835				
C	0.18937	19.03017	23.42779				
H	1.02783	18.76742	24.08812				
H	0.11678	20.12718	23.39681				
H	-0.73363	18.63504	23.87947				
C	-0.85747	18.81930	21.17355				

para-HBC-fused porphyrin-HBC *p*-HBC

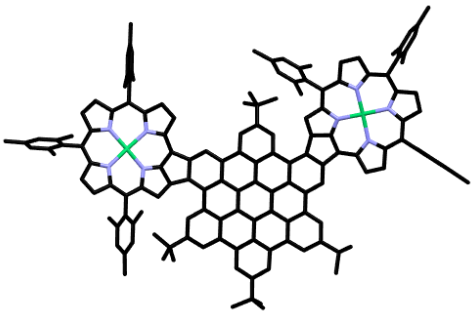


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.22337	19.04454	22.33624
C	24.52248	20.23860	22.15950
C	24.50744	17.85360	22.22227
C	22.44682	23.96348	21.80493
C	23.14483	20.27865	21.89991
C	21.03852	21.54590	21.48013
C	22.43678	21.53964	21.74079
C	23.12358	22.76539	21.85427
C	21.02522	23.98919	21.58666
C	20.33777	22.79293	21.31456
H	24.19325	22.76575	22.03504
C	18.90957	20.29452	21.20061
C	18.23586	21.52564	20.88572
C	16.11040	20.27044	20.55714
C	18.95472	22.75322	20.85467
C	18.34598	23.88667	20.29353
C	17.01585	23.88611	19.87080
C	16.28534	22.70761	20.03803
C	16.86351	21.52099	20.50808
H	18.95220	24.77483	20.14873
H	15.23880	22.70179	19.73963
C	16.34106	25.11772	19.25275
C	15.30899	25.66916	20.25883
H	15.79711	25.99365	21.18926
H	14.78688	26.53958	19.83209
C	17.34766	26.22787	18.91815
H	18.11922	25.87574	18.21739
H	16.82068	27.07053	18.44689
C	15.62077	24.72506	17.94644
H	16.33054	24.30488	17.21896
H	14.83007	23.98099	18.11494
H	15.15093	25.61275	17.49631
H	17.84820	26.61916	19.81353
C	22.42324	19.05292	21.80822
N	13.28195	13.21060	22.42901
C	14.51530	13.67107	22.12315
C	14.57654	15.09435	21.91065
C	13.29519	15.53695	22.16060
C	12.49778	14.36395	22.46289
C	14.66297	8.49692	23.14800
C	15.77462	13.09559	22.14328
C	11.13774	14.35323	22.72937
H	18.13633	11.47433	22.71183
C	13.28613	8.42410	22.95160
C	12.56111	7.18109	22.89045
C	11.25201	7.49399	22.67741
C	11.16402	8.93056	22.64945
N	12.42627	9.49842	22.78261
N	10.99689	11.86694	22.74978
C	9.90723	11.00903	22.76216
C	8.68538	11.74533	22.93323
C	9.02642	13.06363	23.02608
C	10.45253	13.14300	22.87176
C	9.95939	9.62219	22.63619
C	8.67837	8.86001	22.54283
C	8.07995	8.33277	23.70552
C	6.87299	7.63448	23.58801
C	6.24671	7.44410	22.35144
C	6.85819	7.98016	21.21371
C	8.06441	8.68627	21.28631
H	8.37979	13.92548	23.16193
H	7.70017	11.29151	22.98228
H	13.01956	6.20209	22.99390
H	10.39998	6.82848	22.57557
C	4.96303	6.66386	22.24674
H	5.16359	5.58360	22.15893
H	4.33278	6.80610	23.13601
H	4.38364	6.96206	21.36204
C	8.71897	8.52429	25.05546
H	8.86438	9.59183	25.28105
H	8.09983	8.08460	25.84825
C	23.13034	17.82725	21.95240
C	21.00168	19.06443	21.59374
C	20.31708	20.29954	21.41858
C	18.18649	19.07236	21.20594
C	18.86510	17.83750	21.40672
C	20.27923	17.83605	21.57498
C	20.98541	16.59204	21.70532
C	18.12544	16.60235	21.46641
C	16.77422	19.06808	20.93143
C	20.27565	15.36028	21.68404
C	20.99486	14.15160	21.71724
C	22.38354	14.11262	21.80013
C	23.06325	15.33314	21.87401
C	22.40378	16.56687	21.84240
C	16.68695	16.61376	21.37832
C	15.98956	15.42787	21.67864
C	16.71726	14.19935	21.86704
C	18.09237	14.18216	21.80807
C	18.82320	15.37561	21.64331
H	14.75915	20.21594	20.19065
C	14.05406	19.01506	20.09685
C	14.71426	17.84662	20.48278
C	16.03549	17.85028	20.95645
H	14.24624	21.13881	19.92820
H	14.21033	16.89155	20.38111
H	24.14957	15.31636	21.94436
H	18.62075	13.24382	21.94154
H	25.03201	16.91307	22.36624
H	14.55768	24.90773	20.51448
C	12.59941	19.01855	19.60859
C	12.44882	19.91741	18.36431
H	12.68049	20.97008	18.57789
H	13.11180	19.58132	17.55371
H	11.41112	19.87649	17.99997
C	12.11488	17.61202	19.22770
H	12.09735	16.92914	20.08682
H	11.08738	17.66989	18.83997
C	11.70648	19.56784	20.74136
H	11.75754	18.92802	21.63427
H	12.01646	20.58270	21.03105
H	10.65541	19.60511	20.41583
C	15.96513	29.20229	21.32281
C	15.22083	28.74832	22.41631
C	15.91439	28.30731	23.54794
C	17.31295	28.30144	23.60266
C	13.71768	28.69479	22.35928
H	13.31027	29.49131	21.72104
H	13.37809	27.73325	21.93969
H	13.27183	28.79072	23.35908
C	18.12757	29.70430	20.13221
H	18.89983	28.98381	19.82454
H	17.45371	29.87329	19.28216
H	18.64905	30.64955	20.34966
C	18.02300	27.82466	24.84195
H	18.59831	26.90677	24.64564
H	18.74262	28.57481	25.20311
H	17.30765	27.61287	25.64719
H	15.44246	29.55337	20.42850
H	15.35261	27.95768	24.41855
C	27.91897	28.62804	22.63761
C	28.57780	28.59965	23.88317
C	29.97694	28.59038	23.90938
C	30.73736	28.60895	22.73536
C	30.05995	28.64000	21.51175
C	28.66210	28.64761	21.44051
C	32.24206	28.57123	22.78691
H	32.62506	29.05557	23.69616
H	32.61097	27.53251	22.78970
C	15.41958	7.24322	23.44587
C	16.02059	6.51026	22.40175
C	16.72694	5.34301	22.71337
H	12.74904	17.16685	18.44674
C	23.17526	12.79931	21.82047
C	22.26542	11.56624	21.72136
H	21.68393	11.56113	20.78744
C	24.15451	12.77684	20.62858
H	24.86043	13.61835	20.66778
H	24.73984	11.84452	20.63450
H	24.67692	13.54437	23.24574
H	23.61051	12.83753	19.67472
H	20.45151	13.21289	21.65827
H	21.56468	11.50733	22.56779
H	22.88010	10.65434	21.73612
C	23.97239	12.70761	23.13852
H	23.29658	12.72228	24.00612
H	24.55208	11.77216	23.16767
C	26.72295	19.08464	22.65784
C	26.93791	19.85803	23.97605
H	26.56893	20.89103	23.90664
H	26.41003	19.36817	24.80725
H	28.00995	19.89820	24.22329
C	27.32225	17.68035	22.82169
H	27.22427	17.08446	21.90195
H	28.39441	17.76286	23.05274
C	27.47188	19.80257	21.51597
H	27.33943	19.26806	20.56399
H	27.11107	20.83146	21.37657
H	28.54894	19.85061	21.73842
H	26.84624	17.12828	23.64582
H	25.07489	21.17230	22.24270
C	25.74060	27.44061	22.49458
C	24.19062	25.90063	22.23204
N	24.36777	27.27989	22.39118
N	21.60320	27.45530	22.26354
C	21.81600	26.14563	22.00413
C	20.61516	25.38614	21.77184
C	19.59218	26.29087	21.94428
C	20.21071	27.56641	22.24503
C	26.42573	28.64485	22.59025
C	22.94122	25.34007	22.01885
C	19.53228	28.74338	22.50806
C	25.76526	29.86704	22.64594
H	8.08970	9.00943	19.15319
Ni	12.86958	11.37211	22.66154
H	6.38246	7.84909	20.23768
H	6.40716	7.23224	24.49219
C	17.13934	11.05130	22.76366
C	16.79473	9.77677	23.10155
H	12.89482	16.54550	22.16824
C	10.38736	15.64103	22.78134
C	10.43543	16.43388	23.94638
C	9.72795	17.64108	23.97253
C	8.97871	18.08224	22.87727
C	8.94311	17.27620	21.73532
C	9.63582	16.06286	21.66378
C	8.26514	19.40679	22.91026
H	7.97781	19.68367	23.93408
H	8.91489	20.20898	22.52270
H	7.35890	19.39115	22.28869
C	11.22633	15.99133	25.14947
H	12.30770	15.99394	24.94212
H	11.04286	16.65444	26.00493
H	10.96714	14.96322	25.44338
C	9.57167	15.23114	20.40976
H	10.57232	14.90355	20.09225
H	8.97674	14.31754	20.56471
H	9.11647	15.79869	19.58757
H	9.76164	18.25193	24.87887
H	8.36417	17.60360	20.86706
C	16.85529	4.88509	24.02905
C	16.24209	5.62393	25.04575
C	15.52507	6.79590	24.77829
C	26.45951	31.12653	22.71697
C	25.51019	32.09690	22.82111
C	24.23304	31.43405	22.81913
N	24.39137	30.05881	22.68682
N	21.61520	30.08932	22.75228
C	21.80837	31.44398	22.98677
C	20.55286	32.11179	23.18886
C	19.57749	31.16722	23.05831
C	20.23274	29.92180	22.77295
C	23.03163	32.10683	22.99037
C	23.05157	33.58548	23.19905
C	22.88445	34.45309	22.10138
C	22.90156	35.83498	22.32276
C	23.07829	36.37642	23.60047
C	23.23954	35.49380	24.67394
C	23.23118	34.10571	24.49668
H	18.50066	31.28291	23.13799
H	20.45318	33.17245	23.39869
H	27.54021	31.22917	22.69442
H	25.63886	33.17180	22.90465
C	23.11966	37.86709	23.81168
H	24.15138	38.24785	23.73630
H	22.52016	38.39645	23.05789
H	22.74278	38.14186	24.80692
C	22.68736	33.90589	20.71239
H	21.76364	33.31028	20.64543
H	22.62726	34.71701	19.97501
H	23.51288	33.23677	20.42571
C	23.40649	33.18535	25.67550
H	22.57162	32.47264	25.75479
H	24.32340	32.58343	25.57814
H	23.46734	33.75371	26.61271
Ni	22.99243	28.73067	22.52431
H	23.37257	35.89556	25.68245
H	22.77008	36.50661	21.46966
C	25.45374	25.21884	22.26864
H	25.59391	24.14899	22.16410
C	26.41435	26.17018	22.43197
H	18.51781	26.14585	21.90426
C	18.04048	28.75426	22.48327
C	17.36412	29.21217	21.33321
C	14.87906	7.56469	25.90041
H	15.25509	8.59823	25.94550
H	13.78914	7.63403	25.76200
H	15.07305	7.08461	26.86845
H	17.18824	4.77396	21.90124
H	16.32176	5.27995	26.08076
H	17.44226	8.94462	23.36173
H	27.49137	26.04647	22.49279
H	27.29057	29.54718	20.02877
C	28.69381	28.73729	19.28492
H	30.48570	28.57148	24.87732
H	30.63493	28.66280	20.58175
C	15.35898	9.69451	23.02476
C	15.91843	11.76288	22.50443
N	14.81468	10.92560	22.69308
H	17.58723	2.90952	23.53119
H	18.72179	3.89262	24.47241
H	17.31273	3.17221	25.27208
C	15.90003	6.96484	20.97132
H	16.34807	7.95997	20.82741
H	16.40055	6.26132	20.29313
H	14.84569	7.04916	20.66639
H	9.71466	8.05627	25.09632
C	8.69221	9.24974	20.03894
H	8.79372	10.34414	20.10114
H	9.70630	8.84945	19.88691
H	28.45876	28.52303	26.03634
C	17.65483	3.64803	24.34251
H	32.68607	29.07278	21.91567
C	27.79127	28.58501	25.16705

H	27.09689	27.73174	25.20191
H	27.17644	29.49285	25.26830
C	27.96665	28.68202	20.10546
H	27.34518	27.78559	19.95545

meta-HBC-fused porphyrin-HBC *m*-HBC

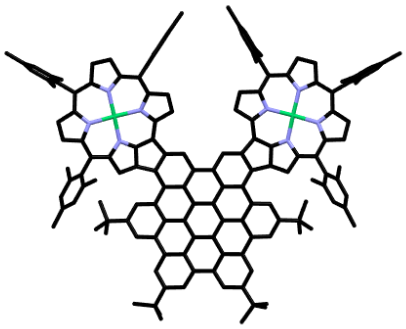


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.03130	19.33920	20.37937
C	24.35005	20.51459	20.70245
C	24.36279	18.12791	20.57632
C	22.33713	24.12435	21.90465
C	23.00684	20.51776	21.10343
C	20.88521	21.74059	21.52368
C	22.30014	21.75411	21.39578
C	23.00430	22.96318	21.57384
C	20.90032	24.13572	21.99442
C	20.16633	22.97205	21.70769
H	24.08900	22.95771	21.51706
C	18.75749	20.46634	21.60542
C	18.02739	21.70362	21.62353
C	15.89380	20.43704	21.76390
C	18.71454	22.94780	21.58063
C	17.98548	24.12006	21.32739
C	16.59298	24.12425	21.22470
C	15.92511	22.91321	21.42677
C	16.60456	21.70265	21.61674
H	18.53830	25.03906	21.16070
H	14.83717	22.90405	21.38014
C	15.78881	25.39452	20.91967
C	14.97289	25.77487	22.17295
H	15.63353	25.98468	23.02658
H	14.37635	26.67964	21.97903
C	16.69008	26.57812	20.54014
H	17.30733	26.34965	19.65858
H	16.06613	27.45131	20.29942
C	14.82626	25.13612	19.74219
H	15.38260	24.84926	18.83784
H	14.10600	24.33640	19.96362
H	14.25298	26.04881	19.51843
H	17.35688	26.87288	21.36120
C	17.26191	29.19171	23.26604
C	15.88265	29.15129	23.49865
C	15.34128	28.52564	24.62567
C	16.22180	27.93816	25.54036
C	17.60808	27.95750	25.34928
C	13.85172	28.44693	24.82630
H	13.33414	29.27990	24.33050
H	13.45089	27.51145	24.40185
H	13.58689	28.46063	25.89289
C	17.80366	29.87034	22.03587
H	18.49646	29.21445	21.48786
H	16.99002	30.15773	21.35723
H	18.37065	30.77778	22.29624
C	18.52504	27.32268	26.36094
H	19.06665	26.46639	25.93031
H	19.28967	28.03406	26.70802
H	17.96094	26.96668	27.23271
H	15.21212	29.61682	22.77095
H	15.82016	27.45077	26.43301
C	27.87670	28.74188	22.61207
C	28.74322	28.56287	23.70882
C	30.12577	28.60186	23.49302
C	30.66905	28.81448	22.22191
C	29.78799	28.99533	21.15009
C	28.39952	28.96190	21.32132
C	32.15966	28.82525	22.00767
H	32.69523	29.10565	22.92526
H	32.52197	27.82855	21.70730
H	32.44601	29.52827	21.21261
C	28.19418	28.34158	25.09347
H	27.51616	27.47510	25.12208
H	29.00386	28.17205	25.81522
H	27.60693	29.20920	25.43266
C	27.48163	29.16853	20.14555
H	26.85588	28.28071	19.96535
H	26.79053	30.00719	20.32061
H	28.05389	29.37684	19.23209
H	30.79648	28.46609	24.34611
C	22.31145	19.27988	21.19920
C	23.03835	18.06888	21.03825
C	20.89063	19.26183	21.39511
C	20.17533	20.48730	21.49557
C	18.06055	19.22995	21.61262
C	18.78007	18.00429	21.52600
C	20.19866	18.01751	21.41330
C	20.93429	16.77911	21.35825
C	18.06804	16.75688	21.53552
C	16.62511	19.21784	21.71785
C	20.23633	15.54067	21.40857
C	20.96869	14.33619	21.46261
C	22.34520	14.34579	21.53561
C	23.06669	15.58912	21.47772
C	22.37238	16.79661	21.28821
C	16.64900	16.72883	21.63928
C	15.98369	15.49387	21.59282
C	16.66269	14.28327	21.45663
C	18.05683	14.32564	21.38887
C	18.78055	15.52545	21.43983
C	14.50267	20.39855	21.94995
C	13.79997	19.20025	22.06295
C	14.52556	18.00960	21.95584
C	15.91373	17.98427	21.77407
H	13.95942	21.33674	22.02940
H	13.98524	17.06729	22.03121
H	14.89867	15.47937	21.64895
H	18.59496	13.38579	21.27987
H	24.86016	17.19579	20.32782
H	14.28647	24.96589	22.46253
C	12.28596	19.14707	22.30285
C	11.65410	20.54529	22.36205
H	12.07078	21.14721	23.18323
H	11.79612	21.09655	21.42043
H	10.57174	20.45213	22.53387
C	11.61217	18.36093	21.15911
H	11.99236	17.33196	21.09241
H	10.52502	18.30808	21.32376
C	12.01324	18.43395	23.64385
H	12.41308	17.41012	23.64654
H	12.47949	18.97916	24.47748
N	24.27355	11.03305	22.13651
N	25.77345	13.35359	22.15847
C	24.54670	13.82023	21.83202
C	24.47289	15.25407	21.72936
C	25.73351	15.69445	22.06587
C	26.53410	14.51312	22.31801
C	24.44980	8.57310	22.35939
C	23.29620	13.23061	21.74238
C	27.87486	14.50799	22.66582
H	20.94578	11.51588	21.94671
C	25.83982	8.54047	22.29843
C	26.59619	7.31722	22.22026
C	27.91227	7.66613	22.17308
C	27.96767	9.10199	22.25653
N	26.68576	9.63904	22.30216
N	28.06267	12.02836	22.54869
C	29.16559	11.18885	22.60068
C	30.35706	11.93299	22.90235
C	29.98500	13.23917	23.03457
C	28.57305	13.30338	22.77948
C	29.15299	9.81146	22.39555
C	30.45336	9.07777	22.37209
C	31.16493	8.96553	21.16077
C	32.39058	8.29026	21.15589
C	32.92757	7.72677	22.31820
C	32.20398	7.85548	23.50855
C	30.97344	8.52041	23.55749
H	30.19153	29.17355	20.14928
C	23.73689	9.76444	22.29017
C	23.16371	11.86605	21.95663
H	10.92995	18.37579	23.83149
H	11.79092	18.84961	20.19025
C	15.94001	12.93234	21.38054
C	16.41913	12.03237	22.53880
H	16.19538	12.49441	23.51147
C	14.41495	13.07864	21.48409
H	14.00675	13.68782	20.66387
H	13.94650	12.08530	21.42582
H	15.93351	12.87453	19.19135
H	14.11247	13.53391	22.43903
H	20.43827	13.39039	21.50734
H	17.50265	11.85305	22.49344
H	15.91357	11.05548	22.49547
C	16.27117	12.25446	20.03464
H	17.35143	12.08855	19.91831
H	15.76953	11.27682	19.96739
C	26.47064	19.41915	19.85495
C	27.38000	19.93273	20.99146
H	27.05744	20.92368	21.34330
H	27.36785	19.24509	21.84947
H	28.42030	20.01447	20.64035
C	26.99492	18.05674	19.38039
H	26.36939	17.64090	18.57658
H	28.01609	18.17292	18.98866
C	26.54157	20.39597	18.66314
H	25.88884	20.06147	17.84356
H	26.23736	21.41416	18.94263
H	27.57309	20.44883	18.28260
H	27.04186	17.32281	20.19575
H	24.86548	21.46642	20.58239
C	25.70525	27.52785	22.63233
C	24.13040	26.01447	22.35706
N	24.33401	27.34863	22.73011
N	21.59476	27.45485	23.13244
C	21.75581	26.21659	22.61222
C	20.53382	25.46620	22.48896
C	19.56153	26.29194	23.00487
C	20.22392	27.51985	23.39460
C	26.39747	28.71712	22.82232
C	22.86312	25.45929	22.26868
C	19.60122	28.61619	23.96391
H	29.23939	8.16105	24.80114
H	30.78854	8.18440	25.68096
Ni	26.20922	11.50967	22.28507
H	32.60992	7.43034	24.43076
H	32.94272	8.20694	20.21549
C	21.94635	11.10830	22.03803
C	22.29798	9.81045	22.25680
H	26.11610	16.70466	22.16640
C	28.58925	15.80423	22.85111
H	29.38571	16.32329	21.80848
C	30.03482	17.54760	22.00039
C	29.91192	18.27202	23.19024
C	29.12090	17.73408	24.21047
C	28.45530	16.51172	24.06332
C	30.57506	19.61360	23.34979
H	31.51826	19.66610	22.78792
H	29.92267	20.41754	22.97014
H	30.78742	19.83497	24.40492
C	29.54072	15.58243	20.50640
H	28.56842	15.25049	20.11380
H	30.02081	16.21759	19.75047
H	30.15438	14.67659	20.63185
C	27.61413	15.96473	25.18647
H	26.54491	15.96665	24.92312
H	27.87878	14.92128	25.41366
H	27.74049	16.56262	26.09842
H	30.64724	17.95125	21.18919
H	23.63093	6.81531	25.86020
H	34.07459	5.91145	22.07450
C	23.16371	11.86605	21.95663
C	25.75592	29.89383	23.19365
C	26.45208	31.14398	23.35535
C	25.53327	32.05856	23.77116
C	24.27387	31.36974	23.87162
N	24.40858	30.03851	23.49212
N	21.68809	29.97387	24.04438
C	21.91530	31.28120	24.45229
C	20.71405	31.86958	24.97573
C	19.73469	30.92560	24.87348
C	20.33293	29.76106	24.28393
C	23.11854	31.97188	24.34900
C	23.17028	33.39973	24.78288
C	22.81620	34.42148	23.87998
C	22.86707	35.75234	24.31111
C	23.25779	36.09327	25.60996
C	23.59999	35.05968	26.48895
C	23.56571	33.71675	26.09837
H	18.68908	30.99357	25.15897
H	20.64895	32.88172	25.36333
H	27.51383	31.27830	23.17160
H	25.67388	33.10937	24.00600
C	23.33383	37.53314	26.04457
H	24.35766	37.92525	25.93093
H	22.67007	38.16990	25.44353
H	23.05766	37.64824	27.10237
C	22.38638	34.09057	22.47518
H	21.46428	33.48861	22.47132
H	22.20266	35.00398	21.89449
H	23.15059	33.49515	21.95286
C	23.94100	32.62949	27.07024
H	23.13114	31.89205	27.17840
H	24.82606	32.07345	26.72375
H	24.16393	33.04743	28.06056
Ni	23.00439	28.71490	23.35192
H	23.90036	35.30375	27.51196
H	22.59044	36.54465	23.60983
H	25.38093	25.37341	22.06242
H	25.49956	24.34068	21.75472
C	26.35701	26.30743	22.23456
H	18.49986	26.11891	23.14535
C	18.12832	28.58742	24.20043
H	25.03656	7.46294	24.97718
C	23.51944	7.24735	19.92235
H	23.05573	8.24104	19.82468
H	24.59844	7.38865	19.75661
H	23.12810	6.60520	19.12258
H	22.55432	5.05699	24.75979
H	22.20194	4.94578	20.47650
H	21.65566	8.94201	22.36853
H	27.42922	26.20442	22.09750
H	34.89918	7.37138	21.49941
H	34.76210	7.04979	23.24645
C	30.62027	9.56748	19.89241
H	30.51484	10.65980	19.98245
H	31.27995	9.35459	19.04111
H	29.61825	9.17519	19.66119
C	30.22618	8.64587	24.85879
H	30.04249	9.70077	25.11415
C	23.24813	6.64717	21.27646
C	21.49224	3.57451	22.72763
H	21.77290	2.99613	23.61895
H	20.41213	3.78256	22.79929
H	21.64379	2.94045	21.84279
H	30.60209	14.10327	23.26230
H	31.34399	11.49176	23.00311
H	26.15224	6.32638	22.20059
H	28.78633	7.02451	22.11323
C	34.23574	6.98153	22.28409
H	29.01791	18.28002	25.15237
C	23.70005	7.28411	22.45000
C	23.45176	6.70843	23.71200

C	22.74515	5.50225	23.77925
C	22.28071	4.85387	22.63004
C	22.54713	5.44108	21.38848
C	23.93883	7.37841	24.96953

ortho-HBC-fused porphyrin-HBC *o*-HBC

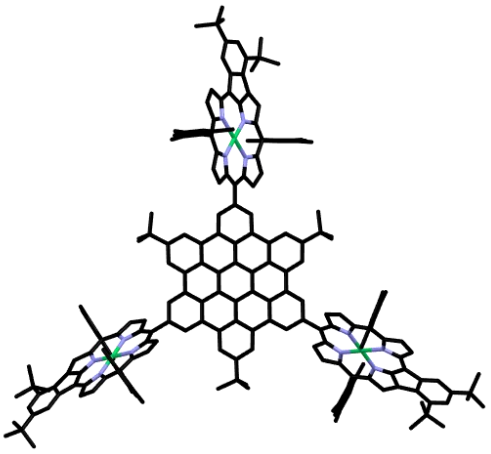


Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.16077	19.11943	21.24430
C	24.48039	20.31274	21.15702
C	24.44248	17.87174	21.26586
C	22.40352	24.02289	21.48930
C	23.06779	20.34762	21.16479
C	20.93673	21.63214	21.26128
C	22.35958	21.61104	21.22360
C	23.06640	22.83223	21.29688
C	20.96446	24.06301	21.51776
C	20.22846	22.88460	21.31127
H	24.15027	22.83233	21.25304
C	18.79501	20.39955	21.43419
C	18.07896	21.64174	21.35265
C	15.93495	20.42797	21.67998
C	18.77826	22.86543	21.17234
C	18.05975	24.01282	20.80185
C	16.66629	24.02013	20.71088
C	15.98738	22.84719	21.05450
C	16.65603	21.65787	21.37064
H	18.62003	24.90429	20.53716
H	14.89865	22.84447	21.02016
C	15.87076	25.25391	20.26704
C	15.04610	25.76963	21.46479
H	15.70048	26.06989	22.29586
H	14.45317	26.64884	21.16900
C	16.78078	26.38584	19.77059
H	17.39790	26.06365	18.91877
H	16.16400	27.23395	19.43898
C	14.91776	24.87160	19.11576
H	15.48220	24.48750	18.25347
H	14.19441	24.10107	19.41645
H	14.34877	25.75550	18.78921
H	17.44819	26.75804	20.55912
C	22.34430	19.12171	21.16419
C	17.35490	29.23511	22.23107
C	15.97626	29.22901	22.46900
C	15.43503	28.75933	23.66981
C	16.31530	28.29504	24.65239
C	17.70141	28.28569	24.45886
C	13.94549	28.71382	23.88013
H	13.43898	29.53150	23.34837
H	13.52689	27.76723	23.49965
H	13.68721	28.78146	24.94606
C	17.89237	29.74233	20.91872
H	18.63141	29.04895	20.49113
H	17.08183	29.87672	20.19058
H	18.40455	30.70934	21.04306
C	18.61651	27.78366	25.54442
H	19.13545	26.86231	25.23791
H	19.39910	28.52062	25.77911
H	18.05457	27.56870	26.46267
H	15.30579	29.59394	21.68571
H	15.91345	27.93004	25.60164
C	27.99652	28.44655	22.79010
C	28.53106	28.47517	24.09472
C	29.91688	28.38730	24.26087
C	30.78509	28.27197	23.16973
C	30.23189	28.25569	21.88542
C	28.84994	28.33967	21.67403
C	32.27012	28.14029	23.37928
H	32.61317	28.75233	24.22569
H	32.54273	27.09554	23.59972
H	32.83151	28.44340	22.48476
C	27.62470	28.59454	25.29132
H	26.87043	27.79315	25.30312
H	28.19770	28.54424	26.22626
H	27.06931	29.54518	25.27817
C	28.29106	28.31792	20.27579
H	27.65395	27.43475	20.11295
H	27.65912	29.19818	20.08325
H	29.09701	28.30049	19.53050
C	23.04445	17.86457	21.12393
C	20.91026	19.14777	21.26041
C	20.21313	20.39122	21.30323
C	18.07794	19.18257	21.56541
C	18.77297	17.94388	21.52844
C	20.18104	17.92815	21.35596
C	20.86467	16.67459	21.19513
C	18.04616	16.70931	21.66437
C	16.64986	19.20074	21.73716
C	20.13777	15.45156	21.18488
C	20.79258	14.27630	20.79827
C	22.13471	14.25945	20.40599
C	22.85698	15.44870	20.51999
C	22.26638	16.64299	20.96337
C	16.64865	16.71615	21.92901
C	15.98427	15.49302	22.11623
C	16.64251	14.26563	22.04706
C	18.00839	14.27595	21.74766
C	18.72061	15.46147	21.53607
H	14.55293	20.43180	21.92705
C	13.84521	19.26279	22.20222
C	14.55446	18.05686	22.20343
C	15.93312	17.99060	21.96947
H	14.02454	21.38206	21.92410
H	14.00657	17.13608	22.39748
H	14.91759	15.50062	22.32362
H	18.53954	13.32632	21.69249
H	23.89927	15.47487	20.21734
H	14.35493	24.99865	21.83508
C	12.34093	19.25671	22.50117
C	11.72590	20.66168	22.42905
H	12.17743	21.34303	23.16540
H	11.84083	21.10555	21.42883
H	10.64937	20.60304	22.64638
C	11.61869	18.35860	21.47530
H	11.99061	17.32485	21.50620
H	10.53826	18.33394	21.68489
C	12.11139	18.69915	23.92158
H	12.49653	17.67447	24.02121
H	12.61819	19.32378	24.67170
H	11.03569	18.68224	24.15553
N	27.74357	16.67881	21.94952
N	29.00692	19.13653	21.75281
C	27.72981	19.66689	21.53600
C	27.78548	21.09884	21.44320
C	29.09057	21.45785	21.59219
C	29.84265	20.24268	21.76584
C	27.79633	14.30111	22.54642
C	26.60651	18.86122	21.42597
C	31.22898	20.22870	21.85332
H	26.93651	21.75118	21.27432
C	29.18313	14.31480	22.70641
C	29.93613	13.14412	23.05965
C	31.25519	13.48844	23.01510
C	31.31080	14.87752	22.65293
N	30.03397	15.39407	22.48138
N	31.41856	17.76934	22.10663
C	32.52716	16.93779	22.22481
C	33.74584	17.69615	22.12169
C	33.38805	19.00200	21.97581
C	31.94878	19.04438	21.97030
C	32.50340	15.57586	22.49133
C	33.79391	14.83884	22.64074
C	34.37101	14.20718	21.52102
C	35.57866	13.51822	21.68016
C	36.22396	13.43625	22.91865
C	35.63191	14.07347	24.01429
C	34.42607	14.77454	23.89871
H	30.32856	28.40796	25.27389
H	30.89379	28.17630	21.01826
C	27.12183	15.44455	22.15516
H	11.76360	18.73831	20.45329
C	15.92860	12.92854	22.28124
C	16.58396	12.20952	23.47888
H	16.49434	12.81364	24.39355
C	14.43442	13.10869	22.58479
H	13.90450	13.59133	21.75011
H	13.97089	12.12489	22.74867
H	15.60401	12.54231	20.15019
H	14.27204	13.70849	23.49263
H	20.22078	13.35073	20.74576
H	17.65257	12.02159	23.30375
H	16.09400	11.23969	23.65579
C	16.06358	12.05017	21.01979
H	17.11611	11.84939	20.77517
H	15.56231	11.08227	21.17399
C	22.75433	12.95711	19.88438
C	21.89545	12.40072	18.72982
H	20.86731	12.17962	19.04843
H	21.84397	13.12037	17.89966
H	22.33666	11.46695	18.34912
C	24.18143	13.15918	19.35611
H	24.87121	13.49527	20.14163
H	24.56751	12.20398	18.97111
C	22.79428	11.92990	21.03523
H	23.41654	12.29126	21.86669
H	21.78652	11.72655	21.42577
H	23.22357	10.97949	20.68232
H	24.20949	13.89048	18.53473
H	25.03940	21.24186	21.14210
C	25.79691	27.33862	22.46412
C	24.21228	25.87851	21.99798
N	24.42980	27.23362	22.26297
N	21.67921	27.46296	22.35282
C	21.83419	26.18503	21.94097
C	20.60314	25.44200	21.86264
C	19.63554	26.32036	22.30034
C	20.30709	27.57306	22.58388
C	26.51564	28.51974	22.61021
C	22.94220	25.37318	21.75680
C	19.69487	28.74511	22.99941
C	25.89822	29.76709	22.55991
H	32.79816	15.07810	25.29141
H	34.42257	15.27173	25.99877
Ni	29.55873	17.23712	22.07183
H	36.12276	14.02599	24.99054
H	36.02807	13.03323	20.80886
C	25.44037	16.83492	21.54218
C	25.69686	15.53401	21.91219
H	29.52896	22.45109	21.57370
C	31.97301	21.52269	21.77873
H	32.33713	22.04887	20.52158
C	33.03721	23.25821	20.47175
C	33.38223	23.96109	21.63209
C	33.01022	23.41916	22.86585
C	32.31121	22.20877	22.96110
C	34.12022	25.27065	21.54392
H	34.95807	25.21046	20.83381
H	33.45515	26.07616	21.19369
H	34.52044	25.57346	22.52100
C	31.98395	21.31974	19.25238
H	30.89337	21.21944	19.13968
H	32.37298	21.84992	18.37338
H	32.39398	20.29822	19.25034
C	31.93245	21.65030	24.30735
H	30.84453	21.50368	24.38821
H	32.39380	20.66448	24.47400
H	32.25151	22.32072	25.11609
H	33.32344	23.66125	19.49613
C	26.72033	17.49238	21.60274
H	37.29807	11.60495	23.31981
H	38.09531	12.66885	22.14710
C	26.62610	31.00856	22.50741
C	25.70260	32.00917	22.44539
C	24.40600	31.38642	22.50650
N	24.53243	30.00201	22.53983
N	21.78443	30.08856	22.82730
C	22.00560	31.45631	22.88755
C	20.79746	32.14856	23.24261
C	19.82929	31.20009	23.40345
C	20.43006	29.92890	23.10883
C	23.22236	32.09721	22.66177
C	23.25628	33.59025	22.66104
C	22.96938	34.29166	21.47307
C	22.98591	35.69104	21.49194
C	23.27607	36.41023	22.65582
C	23.55310	35.69095	23.82345
C	23.54966	34.29177	23.84823
H	18.78589	31.33209	23.67386
H	20.72219	33.22531	23.36002
H	27.70981	31.07963	22.50931
H	25.86232	33.08218	22.39352
C	23.31127	37.91569	22.64908
H	24.33038	38.28586	22.45094
H	22.65546	38.32906	21.87025
H	22.99788	38.32797	23.61859
C	22.64253	33.54959	20.20426
H	21.72399	32.95297	20.31697
H	22.49990	34.24489	19.36680
H	23.44274	32.84316	19.93654
C	23.84213	33.55160	25.12657
H	23.02104	32.86700	25.38870
H	24.74769	32.93254	25.03134
H	23.98983	34.25041	25.96025
Ni	23.10357	28.70742	22.49263
H	23.77304	36.23380	24.74708
H	22.75991	36.23306	20.56939
C	25.44684	25.14750	22.07324
H	25.55338	24.07753	21.93517
C	26.42482	26.04507	22.38059
H	18.57165	26.16785	22.44922
C	18.22214	28.75889	23.23724
H	27.44027	14.11068	25.31109
C	27.71511	12.29979	20.41752
H	27.46270	13.28060	19.98784
H	28.80760	12.28979	20.55579
H	27.45576	11.52438	19.68495
H	25.12868	11.43224	25.07431
H	26.24056	10.14574	21.12662
H	25.01661	14.69936	22.04388
H	27.48663	25.86913	22.52440
H	38.12625	13.06743	23.88356
C	33.70271	14.27442	20.17337
H	33.57653	15.31604	19.84052
H	34.28982	13.73890	19.41603
H	32.69506	13.83217	20.20570
C	33.81715	15.44786	25.10012
H	33.73205	16.53507	24.94893
C	24.77595	9.38772	23.30049
H	24.72425	9.08792	24.35648
H	23.74104	9.54308	22.95276
H	25.19268	8.55073	22.72285
C	26.40533	13.82111	25.07506
H	25.87887	14.74552	24.79099
H	25.93672	13.42870	25.98693
H	34.02347	19.87718	21.87860
H	34.74004	17.26269	22.17516
H	29.49046	12.18224	23.29493
H	32.12814	12.87245	23.20822
C	37.50482	12.65949	23.07407
H	33.27346	23.94934	23.78558
C	27.03755	13.03273	22.75044
C	26.36142	12.80354	23.96593

C	25.64970	11.60951	24.12934
C	25.59019	10.64093	23.12194
C	26.27462	10.88917	21.92793
C	26.99663	12.06956	21.72074

tri-HBC-fused porphyrin-HBC *tri*-HBC



Cartesian Coordinates (Angstroms)

	X	Y	Z
C	25.28757	19.23802	20.21546
C	24.55542	20.41179	20.40064
C	24.60425	18.02330	20.32130
C	22.36156	24.04101	21.10692
C	23.16426	20.41062	20.57776
C	20.99091	21.62256	20.65078
C	22.41112	21.64803	20.71350
C	23.07425	22.87533	20.92116
C	20.92522	24.04011	21.00568
C	20.24339	22.85275	20.68563
H	24.15754	22.88891	20.99335
C	18.88185	20.32183	20.49716
C	18.14471	21.54791	20.40311
C	16.02349	20.26011	20.40409
C	18.81694	22.80090	20.38638
C	18.10330	23.94610	19.99882
C	16.73050	23.91838	19.73794
C	16.05686	22.71009	19.93409
C	16.72910	21.52293	20.25695
H	18.65646	24.86809	19.85064
H	14.98128	22.67508	19.76367
C	15.95252	25.14928	19.25560
C	14.95115	25.56800	20.35220
H	15.47344	25.84869	21.27819
H	14.36405	26.43799	20.01986
C	16.87280	26.33887	18.94952
H	17.61243	26.08969	18.17432
H	16.27070	27.18298	18.58269
C	15.18283	24.80104	17.96445
H	15.87557	24.48566	17.17053
H	14.45702	23.99095	18.12058
H	18.24842	30.63882	20.54128
C	18.08201	27.49183	24.87642
H	18.64241	26.59106	24.58122
H	18.82733	28.22756	25.21373
H	17.44109	27.22954	25.72822
H	15.11601	29.40331	20.79301
H	15.38324	27.54550	24.65990
C	27.73394	28.68279	22.57366
C	28.33431	28.62651	23.84723
C	29.73088	28.63915	23.93909
C	30.54465	28.70799	22.80346
C	29.92469	28.77031	21.55086
C	28.53198	28.75764	21.41399
C	32.04573	28.69056	22.92312
H	32.37720	29.11099	23.88279
H	32.43397	27.66056	22.86474
H	32.51960	29.26317	22.11346
C	27.48832	28.56025	25.09114
H	26.81302	27.69140	25.07041
H	28.11463	28.49028	25.99000
H	26.84785	29.45089	25.18541
C	27.90032	28.83345	20.04915
H	27.29622	27.93773	19.83744
H	27.21967	29.69504	19.97077
H	28.66498	28.92529	19.26677
H	30.19467	28.59771	24.92868
H	30.54224	28.83528	20.65051
C	23.65603	9.65368	22.00091
C	23.17588	11.74301	21.48085
N	24.23647	10.89992	21.82597
N	25.75709	13.19556	22.00106
C	24.59332	13.67713	21.51019
C	24.54348	15.11353	21.42362
C	25.74579	15.53614	21.94829
H	14.62950	25.68326	17.60780
H	17.41079	26.68813	19.84056
C	22.47232	19.16645	20.59239
C	23.22345	17.95731	20.56322
C	21.03868	19.14094	20.57933
C	20.30363	20.35878	20.56643
C	18.19793	19.07765	20.42991
C	18.94183	17.86429	20.42358
C	20.36135	17.89085	20.49922
C	21.10582	16.65742	20.52614
C	18.25385	16.61813	20.25286
C	16.75812	19.04369	20.40426
C	20.41857	15.41885	20.40110
C	21.12628	14.21156	20.56673
C	22.46541	14.22101	20.89431
C	23.19058	15.46334	20.97116
C	22.53520	16.67746	20.69475
C	16.83706	16.57729	20.13786
C	16.22527	15.39564	19.69208
C	16.95127	14.22490	19.45489
C	18.31894	14.24058	19.73831
C	18.98963	15.40691	20.13330
C	14.62296	20.22718	20.56684
C	13.96424	19.02802	20.74907
C	14.68315	17.78317	20.66036
C	16.06436	17.78426	20.40265
H	14.07303	21.16335	20.61255
H	15.16056	15.41876	19.48092
H	18.89315	13.32697	19.58905
H	25.14207	17.09341	20.16749
H	14.25117	24.75297	20.58692
C	16.30664	12.94304	18.91349
C	16.37496	11.85226	20.00252
H	15.81929	12.15513	20.90163
C	14.83892	13.15157	18.51672
H	14.73546	13.92739	17.74376
H	14.43233	12.21371	18.11084
H	17.04851	13.23070	16.87355
H	14.21311	13.43209	19.37420
H	20.59336	13.26773	20.49388
H	17.41429	11.64495	20.29608
C	27.78494	7.47953	22.21592
C	27.86435	8.91617	22.26210
N	26.59086	9.47356	22.24133
N	27.97687	11.83708	22.59148
C	29.06729	10.98598	22.68562
C	30.23783	11.70874	23.10046
C	29.86097	13.00968	23.27155
C	28.47222	13.09779	22.91444
C	29.05196	9.61182	22.45193
C	30.34509	8.86519	22.47380
C	31.10164	8.75909	21.28916
C	32.31956	8.07091	21.32272
C	32.80587	7.48803	22.49766
C	32.03926	7.61185	23.66121
C	30.81473	8.28990	23.67163
H	30.46391	13.85645	23.58580
H	31.21380	11.25734	23.25133
H	26.00155	6.17104	22.22731
H	28.64795	6.82050	22.20865
C	34.10611	6.72815	22.50349
H	33.94299	5.66598	22.25816
H	34.80932	7.12990	21.76046
H	34.58858	6.76496	23.49021
C	30.61232	9.38110	20.00796
H	15.93092	10.91590	19.63090
C	17.07420	12.46573	17.66329
H	18.12761	12.24447	17.88413
H	16.61439	11.54690	17.26844
C	26.79321	19.31970	19.93281
C	27.50795	19.80018	21.21370
H	27.13325	20.78362	21.53343
H	27.35646	19.09169	22.04094
H	28.59151	19.88450	21.03773
C	27.38006	17.96324	19.51846
H	26.88299	17.56539	18.62136
H	28.44948	18.07972	19.28999
C	27.06429	20.32081	18.79110
H	26.54519	20.01595	17.87077
C	26.36909	33.78581	20.44803
H	26.73592	21.33883	19.04214
H	28.14348	20.36365	18.57933
H	27.30009	17.21474	20.31748
H	25.08014	21.36422	20.34847
C	25.58156	27.47548	22.25643
C	24.06860	25.95400	21.75654
N	24.21858	27.31123	22.06340
N	21.45715	27.43303	22.00740
C	21.68736	26.16882	21.58531
C	20.49301	25.39563	21.36501
C	19.46221	26.23539	21.72276
C	20.06602	27.49584	22.10651
C	26.24440	28.68041	22.45658
C	22.83177	25.39851	21.46190
C	19.37625	28.62665	22.50997
C	25.56795	29.89520	22.51126
C	26.24185	31.16531	22.59411
C	25.27635	32.12492	22.63882
C	24.00857	31.44430	22.61146
N	24.19228	30.06989	22.50293
N	21.42588	30.03524	22.63932
C	21.59065	31.39721	22.84906
C	20.33170	32.02280	23.14471
C	19.38454	31.04127	23.11110
C	20.05630	29.81880	22.76920
C	22.79389	32.09431	22.78227
C	22.77776	33.57975	22.93896
H	28.87215	17.47761	24.55665
C	28.22298	16.26545	24.29660
C	30.41980	19.37317	23.92576
H	31.41994	19.43690	23.47460
H	29.81699	20.19413	23.50325
H	30.51427	19.55839	25.00469
C	29.69437	15.44548	20.85226
H	28.77121	15.12253	20.34927
H	30.24545	16.10785	20.17193
H	30.29918	14.53891	21.01057
C	27.25873	15.69082	25.30082
H	26.22585	15.70787	24.91955
H	27.49225	14.63935	25.52498
H	27.28398	16.26082	26.23873
H	30.72471	17.78140	21.73173
H	28.66616	17.99357	25.49851
C	23.55097	7.18888	22.32667
C	23.21379	6.70479	23.60686
C	22.48023	5.51784	23.71070
C	22.07525	4.79917	22.58081
C	22.43077	5.29456	21.32187
C	23.16182	6.47904	21.17284
C	5.43994	14.66051	22.32230
C	4.79914	14.24886	21.13702
C	22.57198	34.39695	21.80923
C	22.55587	35.78666	21.97247
C	22.73691	36.38510	23.22388
C	22.93194	35.55225	24.33076
C	22.95737	34.15783	24.21178
H	18.31489	31.12028	23.28124
H	20.20977	33.08157	23.35268
H	27.32118	31.28234	22.61214
H	25.38872	33.20272	22.70783
C	22.74839	37.88385	23.37036
H	23.76545	38.28509	23.23040
H	22.10251	38.36561	22.62294
H	22.41014	38.19272	24.36928
C	22.36909	33.78581	20.44803
H	21.47262	33.14686	20.42763
H	22.25573	34.56230	19.68031
H	23.21766	33.14306	20.16813
C	23.16630	33.29321	25.42683
H	22.33872	32.57923	25.55696
H	24.08570	32.69404	25.33728
H	23.24180	33.90418	26.33575
Ni	22.82142	28.72291	22.30340
H	23.06557	35.99918	25.31994
H	22.39442	36.41861	21.09455
C	25.33755	25.28301	21.80054
H	25.49463	24.22604	21.61716
C	26.27358	26.22016	22.11963
H	18.39325	26.05330	21.75697
C	17.88758	28.58324	22.59648
C	17.11069	29.08540	21.53129
C	15.71623	29.01894	21.62245
C	15.07317	28.46447	22.73351
C	15.86527	27.97713	23.77830
C	17.26320	28.02618	23.73100
C	13.57296	28.35507	22.78261
H	13.09170	29.16637	22.21878
H	13.23733	27.40323	22.33859
H	13.20015	28.38290	23.81585
C	17.76155	29.67867	20.30970
H	18.54603	29.01784	19.91215
H	17.02145	29.85255	19.51768
C	5.89649	18.87067	22.47964
C	5.51644	17.56606	22.38376
H	5.27797	19.75179	22.62129
C	11.43834	20.98043	21.55345
C	10.18423	21.32235	21.96151
C	7.36385	21.37025	22.62858
C	7.23331	21.82124	23.95735
C	6.56569	23.02687	24.20134
C	6.02562	23.79456	23.16428
C	6.16379	23.32313	21.85443
C	6.82485	22.12366	21.56614
C	7.79942	21.01805	25.09842
H	8.88414	20.87010	24.98353
H	7.61924	21.51769	26.05920
H	7.35016	20.01382	25.14147
C	6.94794	21.64482	20.14387
H	8.00267	21.53581	19.84819
H	6.48327	20.65529	20.01399
H	6.46597	22.34575	19.44990
H	6.46280	23.37293	25.23365
H	5.74137	23.90359	21.02938
H	9.78109	22.30983	22.16523
C	3.59040	13.54922	21.22889
C	3.00325	13.24833	22.46211

C	26.49869	14.34278	22.28350	C	3.66140	13.66414	23.62466
C	24.33302	8.45562	22.20363	C	4.87050	14.36708	23.57810
C	23.36265	13.09869	21.24385	H	9.75387	11.93095	22.54250
C	27.79251	14.31238	22.78066	H	7.11467	12.61991	22.55402
H	20.96169	11.43811	21.26419	H	4.51892	17.14037	22.43711
C	25.72430	8.39241	22.23492	H	20.18126	3.77508	22.76175
C	26.46128	7.15479	22.23053	H	21.41037	2.86905	21.86086
C	1.68718	12.52007	22.53658	C	23.63803	7.45069	24.84432
H	0.84527	13.23036	22.57682	H	23.26158	8.48492	24.83691
H	1.53257	11.87921	21.65741	H	23.26715	6.95416	25.75046
H	1.62598	11.89192	23.43645	H	24.73480	7.51872	24.91254
C	5.40403	14.55342	19.79206	C	23.53175	6.97834	19.80123
H	6.40477	14.10543	19.69303	C	6.71874	16.79052	22.22778
H	4.77243	14.16898	18.98060	N	7.83365	17.61996	22.18060
H	5.53126	15.63722	19.64739	N	9.19950	15.21325	22.11766
C	5.55124	14.79678	24.85063	C	7.92475	14.68051	22.24518
H	6.56524	14.37469	24.92426	C	7.98500	13.25678	22.42780
H	4.97879	14.47481	25.73026	C	9.30552	12.91300	22.42537
Ni	9.66932	17.08681	21.90811	C	10.05476	14.11787	22.20213
H	3.22393	13.43278	24.60001	C	7.33006	18.90168	22.34387
H	3.09620	13.22802	20.30767	C	6.73386	15.40215	22.24175
C	12.20591	12.84966	22.06097	C	21.25764	3.54177	22.71626
C	12.94267	12.53047	23.21974	H	21.51105	2.99475	23.63532
C	12.95251	13.45839	24.40578	N	10.21945	19.00437	21.76245
H	13.46453	14.40412	24.16956	C	11.43685	14.12642	21.99765
H	11.93046	13.72470	24.71400				
H	13.46508	12.99833	25.26057				
C	5.33787	25.10421	23.44677				
H	4.87227	25.10700	24.44221				
H	6.05555	25.94039	23.41912				
H	4.55933	25.31803	22.70106				
C	11.46437	19.54977	21.43016				
N	11.45958	16.54239	21.58364				
C	12.09148	15.30013	21.66304				
C	12.20071	11.97197	20.95657				
C	13.67819	10.44680	22.17071				
C	13.66567	11.33261	23.25311				
H	14.61209	8.81085	23.23684				
H	10.33752	12.24419	19.88787				
H	14.23372	11.08479	24.15410				
C	12.93619	10.78428	21.03447				
H	14.05526	8.39414	21.59580				
C	11.42274	12.29943	19.70940				
H	11.67179	11.60234	18.89870				
H	12.93484	10.10753	20.17543				
C	12.44748	17.37725	21.18835				
C	13.49302	15.41004	21.31038				
C	14.50232	9.18799	22.21052				
H	30.50012	10.47150	20.11102				
H	31.30949	9.18314	19.18336				
H	29.62261	8.99077	19.72587				
C	30.02148	8.40995	24.94589				
H	29.83394	9.46391	25.20208				
H	29.03491	7.93091	24.84936				
H	30.55153	7.93954	25.78427				
Ni	26.15074	11.34722	22.16349				
H	32.40598	7.17230	24.59306				
H	32.90667	7.99300	20.40323				
C	21.93718	11.01496	21.47705				
C	22.22936	9.72759	21.81719				
H	26.11541	16.54124	22.12306				
C	28.48932	15.59550	23.08483				
C	29.39834	16.14245	22.15429				
C	30.02545	17.35595	22.45703				
C	29.77354	18.04254	23.64889				
H	15.51647	9.37372	21.81937				
H	11.63103	13.32250	19.36301				
C	12.54957	18.75565	21.08795				
C	13.71551	16.72839	20.98087				
H	14.18054	14.57144	21.33973				
H	5.66337	15.89117	24.89332				
H	12.27889	21.64056	21.37069				
H	23.08484	7.96424	19.60033				
H	24.62088	7.10285	19.70165				
H	23.19116	6.28194	19.02392				
H	22.22051	5.14378	24.70505				
H	22.13453	4.74186	20.42581				
H	21.55496	8.88281	21.92138				
H	27.34581	26.09680	22.23999				
C	9.42846	20.10116	22.06733				
C	8.06834	20.08155	22.35313				

5 References

[1] Q. Chen, L. Brambilla, L. Daukiya, K. S. Mali, S. de Feyter, M. Tommasini, K. Müllen, A. Narita, *Angew. Chem., Int. Ed. Engl.* **2018**, *57*, 11233-11237.

[2] R. Mishra, R. Regar, R. Singhal, P. Panini, G. D. Sharma, J. Sankar, *J. Mater. Chem. A* **2017**, *5*, 15529-15533.

[3] D. Lungerich, D. Reger, H. Hölzel, R. Riedel, M. M. Martin, F. Hampel, N. Jux, *Angew. Chem., Int. Ed. Engl.* **2016**, *55*, 5602-5605.

[4] K. D. Seo, M. J. Lee, H. M. Song, H. S. Kang, H. K. Kim, *Dyes Pigment.* **2012**, *94*, 143-149.

[5] P. Giannozzi *et al.*, *J. Condens. Matter Phys.* **2009**, *21*, 395502.

[6] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1996**, *77*, 3865-3868.

[7] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456-1465.

[8] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.

[9] D. Vanderbilt, *Phys. Rev. B* **1990**, *41*, 7892-7895.

[10] T. M. Krygowski, *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 70-78.

[11] J. C. Dobrowolski, S. Ostrowski, *J. Chem. Inf. Model.* **2023**, *63*, 7744-7754.

[12] C. Oleszak, P. R. Schol, C. L. Ritterhoff, M. Krug, M. M. Martin, Y. Bo, B. Meyer, T. Clark, D. M. Guldi, N. Jux, *Angew. Chem., Int. Ed. Engl.* **2024,** e202409363.

[13] F. Neese, *WIREs Comput. Mol. Sci.* **2012**, *2*, 73-78.

[14] C. Lee, W. Yang, R. G. Parr, *Phys. Rev B* **1988**, *37*, 785-789.

[15] A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 1372-1377.

[16] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

[17] F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chem. Phys.* **2009**, *356*, 98-109.