Electronic Supplementary Information

Two Double Helical Modes of Bidipyrrin–Zn^{II} Complexes

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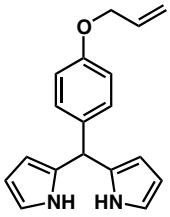
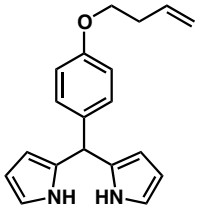
1. Synthetic procedures and spectroscopic data of ligand molecules and metal complexes

General Procedures: Starting materials were purchased from Wako Pure Chemical Industries Ltd., Nacalai Tesque Inc. and Sigma-Aldrich Co., and used without further purification unless otherwise stated. UV-visible spectra were recorded on a Hitachi U-3500 spectrometer. Fluorescence spectra and quantum yields were recorded on a Hitachi F-4500 fluorescence spectrometer for ordinary solution and a Hamamatsu Quantum Yields Measurements System for Organic LED Materials C9920-02, respectively. NMR spectra used in the characterization of products were recorded on a JEOL ECA-600 600 MHz spectrometer. All NMR spectra were referenced to solvent. Matrix-assisted laser desorption ionization time-of-flight mass spectrometries (MALDI-TOF-MS) were recorded on a Shimadzu Axima-CFRplus using a positive mode. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Sumitomo alumina KCG-1525, Wakogel C-200, C-300, and Merck silica gel 60 and 60H.

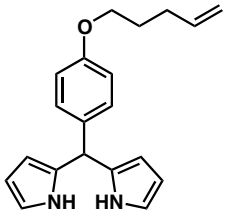
5-(4-(2-Propenyloxy)phenyl)dipyrromethane, s1a. To 4-(2-propenyloxy)benzaldehyde[S1] (1.82 g, 11.22 mmol) in pyrrole (4.0 mL, 63.7 mmol) was added TFA (146 mL, 1.12 mmol) and the solution was stirred at room temperature for 15 min and then quenched with triethylamine (2 mL). The solvent was removed under high vacuum at 130 °C to afford a black oil. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:2) to afford **s1a** (1.15 g, 4.12 mmol, 37%) as a yellow oil. R_f = 0.50 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.94 (s, 2H, pyrrole-NH), 7.12 (m, 2H, phenyl-H), 6.86 (m, 2H, phenyl-H), 6.70 (m, 2H, pyrrole-H), 6.15 (m, 2H, pyrrole-H), 6.08–6.02 (m, 1H, CH), 5.91 (s, 2H, pyrrole-H), 5.43 (s, 1H, CH), 5.41 (m, 2H, CH_2), 5.28 (m, 1H, CH), 4.52 (m, 2H, OCH_2). MALDI-TOF-MS: *m/z* (% intensity): 278.1 (100), 279.1 (14). Calcd for $C_{18}H_{18}N_2O$ ($[M]^+$): 278.14.



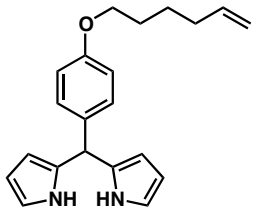
5-(4-(3-Butenyloxy)phenyl)dipyrromethane, s1b. To 4-(3-butenyloxy)benzaldehyde[S1] (4.26 g, 24.2 mmol) in pyrrole (10.0 mL, 144.3 mmol) was added TFA (316 mL, 2.42 mmol) and the solution was stirred at room temperature for 20 min and then quenched with triethylamine (2 mL). The solvent was removed under high vacuum at 130 °C to afford a black oil. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:1) to afford **s1b** (1.98 g, 6.78 mmol, 28%) as a yellow oil. R_f = 0.60 (CH_2Cl_2/hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.92 (s, 2H, pyrrole-H), 7.12 (d, J = 8.4 Hz, 2H, phenyl-H), 6.85 (d, J = 8.4 Hz, 2H, phenyl-H), 6.70 (m, 2H, pyrrole-H), 6.15 (m, 2H, pyrrole-H), 5.88 (m, 1H, CH), 5.14 (m, 2H; CH_2), 3.99 (m, 2H, OCH_2), 2.54 (m, 2H, CH_2). MALDI-TOF-MS: *m/z* (% intensity): 292.2 (100), 293.2 (8). Calcd for $C_{19}H_{20}N_2O$ ($[M]^+$): 292.16.



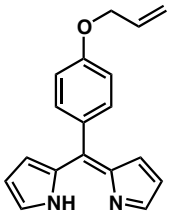
5-(4-(4-Pentenyloxy)phenyl)dipyrromethane, s1c. To 4-(4-pentenyloxy)benzaldehyde[S1] (2.87 g, 15.06 mmol) in pyrrole (4.0 mL, 63.7 mmol) was added TFA (61 mL, 1.51 mmol) and the solution was stirred at room temperature for 20 min and then quenched with triethylamine (2 mL). The solvent removed under high vacuum at 130 °C to afford a black oil. The residue was then chromatographed over silica gel column (Wakogel C-300; eluent: 3% $CHCl_3$/hexane = 1:1) to afford **s1c** (3.28 g, 10.7 mmol, 71%) as a yellow oil. R_f = 0.45 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.92 (s, 2H, pyrrole-NH), 7.12 (d, J = 8.4 Hz, 2H, phenyl-H), 6.84 (d, J = 8.4 Hz, 2H, phenyl-H), 6.69 (m, 2H, pyrrole-H), 6.15 (m, 2H, pyrrole-H), 5.91 (s, 2H, pyrrole-H), 5.88–5.82 (m, 1H, $CHCH_2$), 5.43 (s, 1H, CH), 5.03 (m, 2H, CH_2), 3.95 (m, 2H, OCH_2), 2.21 (m, 2H, CH_2), 1.87 (m, 2H, CH_2). MALDI-TOF-MS: *m/z* (% intensity): 306.2 (100), 307.2 (12). Calcd for $C_{20}H_{22}N_2O$ ($[M]^+$): 306.17.



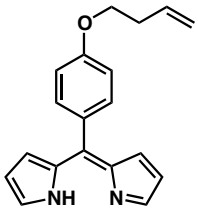
5-(4-(5-Hexenyloxy)phenyl)dipyrromethane, s1d. To 4-(5-hexenyloxy)benzaldehyde[S1] (2.17 g, 10.62 mmol) in pyrrole (4.0 mL, 63.7 mmol) was added TFA (42 mL, 1.06 mmol) and the solution was stirred at room temperature for 20 min and then quenched with triethylamine (1 mL). The solvent was removed under high vacuum at 130 °C to afford a black oil. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2) to afford **s1d** (2.1 g, 2.58 mmol, 62%) as a yellow oil. R_f = 0.60 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.92 (s, 2H, pyrrole-NH), 7.12 (d, J = 8.4 Hz, 2H, phenyl-H), 6.84 (d, J = 8.4 Hz, 2H, phenyl-H), 6.69 (m, 2H, pyrrole-H), 6.15 (m, 2H, pyrrole-H), 5.91 (s, 2H, pyrrole-H), 5.83 (m, 1H, CH), 5.43 (s, 1H, CH), 5.00 (m, 2H, CH_2), 3.94 (m, 2H, OCH_2), 2.12 (m, 2H, CH_2), 1.79 (m, 2H, CH_2), 1.56 (m, 4H, CH_2). MALDI-TOF-MS: *m/z* (% intensity): 320.2 (100), 321.2 (13). Calcd for $C_{21}H_{24}N_2O$ ($[M]^+$): 320.19.



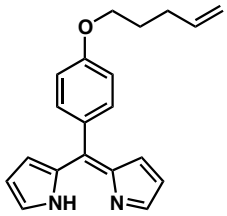
5-(4-(2-Propenyloxy)phenyl)dipyrrin, s2a. To a solution of **s1a** (1.15 g, 4.12 mmol) in THF (20 mL) was added DDQ (1.03 g, 4.53 mmol). After stirring for 30 min at room temperature, the solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/EtOAc = 1:1) to afford **s2a** as an orange oil (631 mg, 2.26 mmol, 50%). R_f = 0.60 (CH_2Cl_2/EtOAc = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.64 (s, 2H, pyrrole-H), 7.44 (d, J = 8.4 Hz, 2H, phenyl-H), 6.98 (d, J = 8.4 Hz, 2H, phenyl-H), 6.65 (m, 2H, pyrrole-H), 6.40 (m, 2H, pyrrole-H), 6.10 (m, 1H, CH), 5.47 (m, 2H, CH_2), 4.62 (m, 2H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 465.0 (0.11). MALDI-TOF-MS: *m/z* (% intensity): 276.1 (100), 277.1 (18). Calcd for $C_{18}H_{16}N_2O$ ($[M]^+$): 276.13.



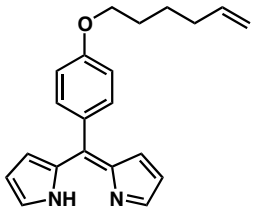
5-(4-(3-Butenyloxy)phenyl)dipyrrin, s2b. To a solution of **s1b** (1.98 g, 6.78 mmol) in THF (25 mL) was added DDQ (1.96 g, 8.14 mmol). After stirring for 30 min at room temperature, the solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: 0.5% MeOH/CH_2Cl_2) to afford **s2b** as an orange oil (1.45 g, 5.01 mmol, 74%). R_f = 0.20 (0.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.64 (s, 2H, pyrrole-H), 7.44 (d, J = 8.4 Hz, 2H, phenyl-H), 6.97 (d, J = 7.8 Hz, 2H, phenyl-H), 6.65 (d, J = 3.6 Hz, 2H, pyrrole-H), 6.40 (m, 2H, pyrrole-H), 5.95 (m, 1H, CH), 5.22 (m, 2H, CH_2), 4.10 (m, 2H, OCH_2), 2.60 (m, 2H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 466.0 (0.19). MALDI-TOF-MS: *m/z* (% intensity): 290.1 (100), 291.1 (23). Calcd for $C_{19}H_{18}N_2O$ ($[M]^+$): 290.14.



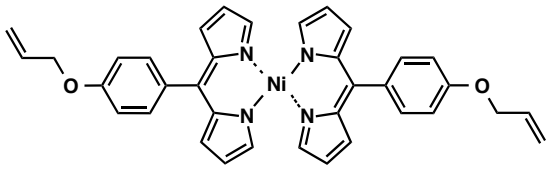
5-(4-(4-Pentenyloxy)phenyl)dipyrrin, s2c. To a solution of **s1c** (3.28 g, 10.7 mmol) in THF (25 mL) was added DDQ (2.66 g, 11.8 mmol) at 0 °C. After stirring for 20 min at room temperature, the solvent was evaporated to dryness and the residue was then chromatographed over silica gel column (Wakogel C-300; eluent: 3% MeOH/CH_2Cl_2) to afford **s2c** as an orange oil (2.31 g, 7.59 mmol, 51%). R_f = 0.20 (3% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.64 (s, 2H, pyrrole-H), 7.43 (d, J = 7.8 Hz, 2H, phenyl-H), 6.96 (d, J = 7.8 Hz, 2H, phenyl-H), 6.66 (m, 2H, pyrrole-H), 6.40 (m, 2H, pyrrole-H), 5.88 (m, 1H, CH), 5.07 (m, 2H, CH_2), 4.04 (m, 2H, OCH_2), 2.28 (m, 2H, CH_2), 1.94 (m, 2H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 466.5 (0.13). MALDI-TOF-MS: *m/z* (% intensity): 304.2 (100), 305.2 (8). Calcd for $C_{20}H_{20}N_2O$ ($[M]^+$): 304.16.



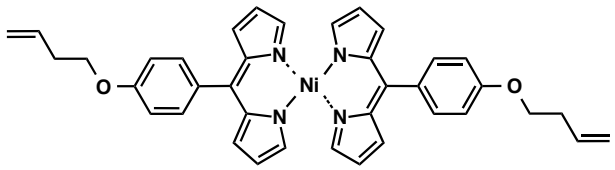
5-(4-(5-Hexenyloxy)phenyl)dipyrrin, s2d. To a solution of **s1d** (2.1 g, 6.58 mmol) in THF (50 mL) was added DDQ (1.64 g, 7.24 mmol) at 0 °C. After stirring for 2.5 h at room temperature, the solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: 2% MeOH/CH_2Cl_2) to afford **s2d** as an orange oil (1.5 g, 4.74 mmol, 72%). R_f = 0.25 (4% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.64 (s, 2H, pyrrole-H), 7.44 (d, J = 8.4 Hz, 2H, phenyl-H), 6.96 (d, J = 8.4 Hz, 2H, phenyl-H), 6.66 (m, 2H, pyrrole-H), 6.40 (m, 2H, pyrrole-H), 5.84 (m, 1H, CH), 5.03 (m, 2H, CH_2), 4.04 (m, 2H, OCH_2), 2.16 (m, 2H, CH_2), 1.85 (m, 2H, CH_2), 1.62 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 466.5 (0.17). MALDI-TOF-MS: *m/z* (% intensity): 318.2 (100), 319.3 (14). Calcd for $C_{21}H_{22}N_2O$ ($[M]^+$): 318.17.



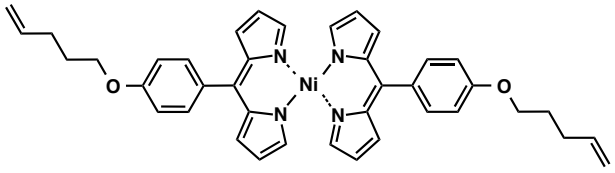
Ni^{II} complex of 5-(4-(2-propenyloxy)phenyl)dipyrrin, s3a. A mixture of **s2a** (1.45 g, 8.53 mmol) and $Ni(OAc)_2 \cdot 4H_2O$ (8.5 g, 34.1 mmol) in $CHCl_3$ (200 mL) was stirred at room temperature overnight. The mixture was washed with brine, extracted with CH_2Cl_2, and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum to give **s3a** (1.84 g, 3.03 mmol, 71%) as a metallic-green solid. R_f = 0.60 (CH_2Cl_2/EtOAc = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.72 (s, 4H, pyrrole-H), 7.39 (d, J = 8.4 Hz, 4H, phenyl-H), 7.15 (m, 4H, pyrrole-H), 6.96 (d, J = 8.4 Hz, 4H, phenyl-H), 6.79 (m, 4H, pyrrole-H), 6.10 (m, 2H, CH), 5.40 (m, 4H, CH_2), 4.61 (m, 4H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 471.5 (0.24). MALDI-TOF-MS: *m/z* (% intensity): 608.2 (100), 609.2 (44), 610.2 (42), 611.3 (16). Calcd for $C_{36}H_{30}N_4NiO_2$ ($[M]^+$): 608.17.



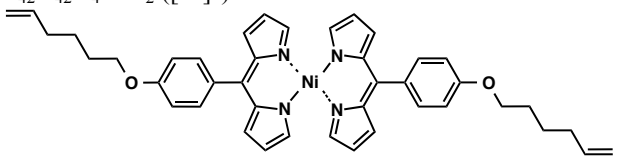
Ni^{II} complex of 5-(4-(3-butenyloxy)phenyl)dipyrrin, s3b. A mixture of **s2b** (1.45 g, 5.01 mmol) and $Ni(OAc)_2 \cdot 4H_2O$ (2.4 g, 9.6 mmol) in $CHCl_3$ (50 mL) was stirred at room temperature overnight. The mixture was washed with brine, extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum to give **s3b** (1.13 g, 1.7 mmol, 68%) as a metallic-green solid. R_f = 0.20 (0.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.59 (s, 4H, pyrrole-H), 7.39 (d, J = 8.4 Hz, 4H, phenyl-H), 7.07 (m, 4H, pyrrole-H), 6.94 (d, J = 8.4 Hz, 4H, phenyl-H), 6.78 (d, J = 3.6 Hz, 4H, pyrrole-H), 5.93 (m, 2H, CH), 5.18 (m, 4H, CH_2), 4.09 (m, 4H, OCH_2), 2.60 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 470.5 (0.36). MALDI-TOF-MS: *m/z* (% intensity): 636.2 (100), 637.2 (62), 638.2 (53), 639.2 (28). Calcd for $C_{38}H_{34}N_4NiO_2$ ($[M]^+$): 636.20.



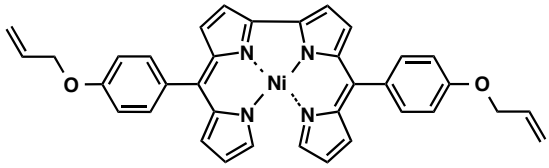
Ni^{II} complex of 5-(4-(4-pentenyloxy)phenyl)dipyrrin, s3c. A mixture of **s2c** (2.31 g, 7.6 mmol) and $Ni(OAc)_2 \cdot 4H_2O$ (400 mg, 30.4 mmol) in $CHCl_3$ (200 mL) was stirred at room temperature overnight. The mixture was washed with brine, extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum to give **s3c** (1.72 g, 2.58 mmol, 68%) as a metallic-green solid. R_f = 0.20 (3% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.56 (s, 4H, pyrrole-H), 7.39 (d, J = 8.4 Hz, 4H, phenyl-H), 7.06 (s, 4H, pyrrole-H), 6.93 (d, J = 8.4 Hz, 4H, phenyl-H), 5.88 (m, 2H, CH), 5.07 (m, 4H, CH_2), 4.04 (m, 4H, OCH_2), 2.28 (m, 4H, CH_2), 1.94 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 470.5 (0.32). MALDI-TOF-MS: *m/z* (% intensity): 664.2 (100), 665.2 (34), 666.2 (44). Calcd for $C_{40}H_{38}N_4NiO_2$ ($[M]^+$): 664.23.



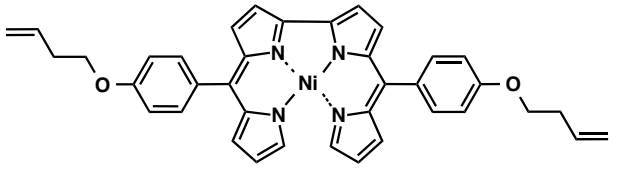
Ni^{II} complex of 5-(4-(5-hexenyloxy)phenyl)dipyrrin, s3d. A mixture of **s2d** (1.5 mg, 4.74 mmol) and $Ni(OAc)_2 \cdot 4H_2O$ (2.36 g, 9.48 mmol) in $CHCl_3$ (100 mL) was stirred at room temperature overnight. The mixture was washed with brine, extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum to afford **s3d** (1.26 g, 1.82 mmol, 77%) as a metallic-green solid. R_f = 0.20 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.56 (s, 4H, pyrrole-H), 7.39 (d, J = 8.4 Hz, 4H, phenyl-H), 7.06 (m, 4H, pyrrole-H), 6.93 (d, J = 8.4 Hz, 4H, phenyl-H), 6.79 (d, J = 4.2 Hz, 4H, pyrrole-H), 5.86 (m, 2H, CH), 5.15 (m, 4H, CH_2), 4.04 (m, 4H, OCH_2), 2.16 (m, 4H, CH_2), 1.85 (m, 4H, CH_2), 1.61 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 470.5 (0.41). MALDI-TOF-MS: *m/z* (% intensity): 692.3 (100), 693.3 (22), 694.3 (8). Calcd for $C_{42}H_{42}N_4NiO_2$ ($[M]^+$): 692.27.



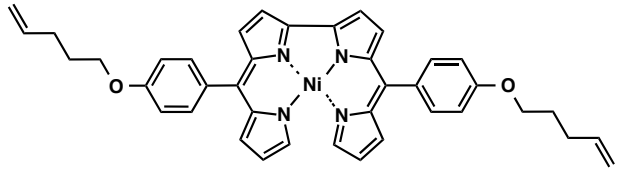
Ni^{II} complex of 5,5′-bis(4-(2-propenyloxy)phenyl)bidipyrrin, s4a. A solution of **s3a** (1.13 g, 3.03 mmol) in toluene (120 mL) was treated with *p*-chloranil (2.6 g, 10.6 mmol) and heated at reflux for 2 days. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:2) to afford **s4a** (397 mg, 0.66 mmol, 22%) as a brown solid. R_f = 0.30 (CH_2Cl_2/hexane = 1:2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.51 (d, J = 8.4 Hz, 4H, phenyl-H), 7.02 (d, J = 8.4 Hz, 4H, phenyl-H), 6.81 (m, 2H, pyrrole-H), 6.79 (d, J = 4.8 Hz, 2H, pyrrole-H), 6.62 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.43 (m, 2H, pyrrole-H), 6.12 (m, 2H, CH), 6.00 (s, 2H, pyrrole-H), 5.48 (m, 4H, CH_2), 4.64 (m, 4H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 413.0 (0.21). MALDI-TOF-MS: *m/z* (% intensity): 606.2 (100), 607.2 (46), 608.2 (80), 609.2 (26). Calcd for $C_{36}H_{28}N_4NiO_2$ ($[M]^+$): 606.16.



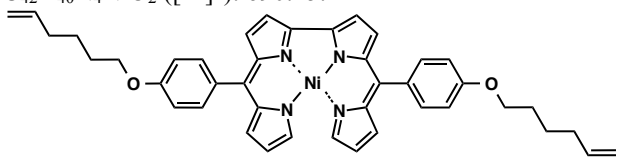
Ni^{II} complex of 5,5′-bis(4-(3-butenyloxy)phenyl)bidipyrrin, s4b. A solution of **s3b** (1.13 g, 1.7 mmol) in toluene (50 mL) was treated with *p*-chloranil (2.1 g, 8.5 mmol) and heated at reflux overnight. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:1) to afford **s4b** (272 mg, 0.41 mmol, 24%) as a brown solid. R_f = 0.60 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.51 (d, J = 8.4 Hz, 4H, phenyl-H), 7.00 (d, J = 8.4 Hz, 4H, phenyl-H), 6.80 (m, 4H, pyrrole-H), 6.62 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.43 (m, 2H, pyrrole-H), 6.00 (s, 2H, pyrrole-H), 5.95 (m, 2H, CH), 5.22 (m, 4H, CH_2), 4.11 (m, 4H, OCH_2), 2.61 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 411.0 (0.37). MALDI-TOF-MS: *m/z* (% intensity): 634.2 (100), 635.2 (38), 636.2 (42), 637.2 (10). Calcd for $C_{38}H_{32}N_4NiO_2$ ($[M]^+$): 634.19.



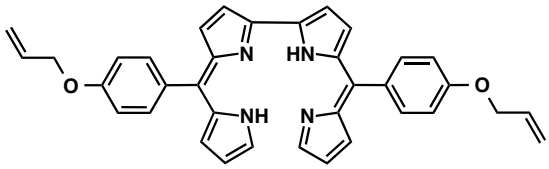
Ni^{II} complex of 5,5′-bis(4-(4-pentenyloxy)phenyl)bidipyrrin, s4c. A solution of **s3c** (1.72 g, 2.58 mmol) in toluene (200 mL) was treated with *p*-chloranil (2.4 g, 9.7 mmol) and heated at reflux overnight. The solvent was evaporated to dryness and the residue was then chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:2) to afford **s4c** (873 mg, 1.32 mmol, 51%) as a brown solid. R_f = 0.60 (CH_2Cl_2/hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.51 (m, 4H, phenyl-H), 6.99 (m, 4H, phenyl-H), 6.80 (m, 4H, pyrrole-H), 6.62 (m, 2H, pyrrole-H), 6.43 (m, 2H, pyrrole-H), 6.00 (s, 2H, pyrrole-H), 5.89 (m, 2H, CH), 5.30 (m, 4H, CH_2), 4.06 (m, 4H, OCH_2), 2.29 (m, 4H, CH_2), 1.95 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 411.0 (0.41). MALDI-TOF-MS: *m/z* (% intensity): 662.2 (100), 663.2 (36), 664.2 (46). Calcd for $C_{40}H_{36}N_4NiO_2$ ($[M]^+$): 662.22.



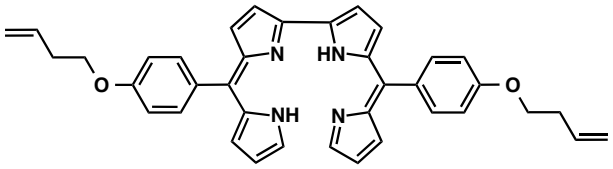
Ni^{II} complex of 5,5′-bis(4-(5-hexenyloxy)phenyl)bidipyrrin, s4d. A solution of **s3d** (1.26 g, 1.82 mmol) in toluene (100 mL) was treated with *p*-chloranil (1.8 mg, 7.28 mmol) and heated at reflux for 16 h. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:2) to afford **s4d** (691 mg, 1.0 mmol, 55%) as a brown solid. R_f = 0.60 (CH_2Cl_2/hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.51 (d, J = 8.4 Hz, 4H, phenyl-H), 6.99 (d, J = 8.4 Hz, 4H, phenyl-H), 6.81 (d, 4H, pyrrole-H), 6.62 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.43 (m, 2H, pyrrole-H), 5.86 (m, 2H, CH), 5.04 (m, 4H, CH_2), 4.06 (m, 4H, OCH_2), 2.16 (m, 4H, CH_2), 1.85 (m, 4H, CH_2), 1.62 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 414.5 (0.48). MALDI-TOF-MS: *m/z* (% intensity): 690.3 (100), 691.3 (52), 692.3 (42), 693.3 (18). Calcd for $C_{42}H_{40}N_4NiO_2$ ($[M]^+$): 690.25.



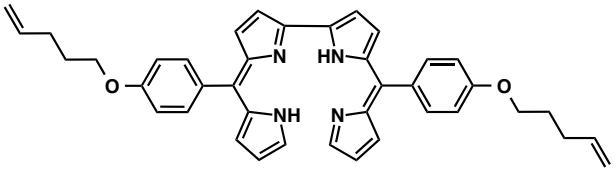
5,5′-Bis(4-(2-propenyloxy)phenyl)bidipyrrin, s5a. 12 M HCl aq. (2 mL) was added to a solution of **s4a** (397 mg, 0.66 mmol) in $CHCl_3$ (60 mL) and was stirred at room temperature for 5 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Merck silica gel 60; eluent: 4% MeOH/CH_2Cl_2) to afford **s5a** (226 mg, 0.41 mmol, 62%) as a green solid. R_f = 0.45 (4% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.59 (s, 2H, pyrrole-H), 7.49 (d, J = 8.4 Hz, 4H, phenyl-H), 7.01 (m, 2H, pyrrole-H), 7.01 (m, 4H, phenyl-H), 6.83 (d, J = 3.6 Hz, 2H, pyrrole-H), 6.63 (m, 2H, pyrrole-H), 6.42 (m, 2H, pyrrole-H), 6.12 (m, 2H, CH), 5.42 (m, 4H, CH_2), 4.64 (m, 4H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 592.0 (0.31). MALDI-TOF-MS: *m/z* (% intensity): 550.2 (100), 551.2 (40). Calcd for $C_{36}H_{30}N_4O_2$ ($[M]^+$): 550.24.



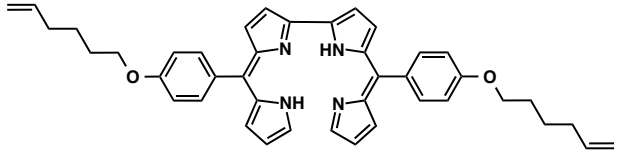
5,5′-Bis(4-(3-butenyloxy)phenyl)bidipyrrin, s5b. 12 M HCl aq. (1 mL) was added to a solution of **s4b** (261 mg, 0.41 mmol) in $CHCl_3$ (50 mL) and was stirred at room temperature for 10 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Merck silica gel 60; eluent: 3% MeOH/CH_2Cl_2) to afford **s5b** (168 mg, 0.29 mmol, 70%) as a green solid. R_f = 0.30 (3% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.59 (s, 2H, pyrrole-H), 7.48 (m, 4H, phenyl-H), 7.01 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.99 (m, 4H, phenyl-H), 6.82 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.41 (m, 4H, pyrrole-H), 5.95 (m, 2H, CH), 5.19 (m, 4H, CH_2), 4.11 (m, 4H, OCH_2), 2.61 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 592.5 (0.24). MALDI-TOF-MS: *m/z* (% intensity): 578.3 (100), 579.3 (68), 580.3 (23). Calcd for $C_{38}H_{36}N_4O_2$ ($[M]^+$): 578.27.



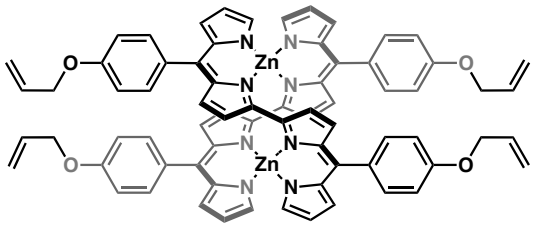
5,5′-Bis(4-(4-pentenyloxy)phenyl)bidipyrrin, s5c. 12 M HCl aq. (2 mL) was added to a solution of **s4c** (42.5 mg, 0.064 mmol) in $CHCl_3$ (50 mL) under nitrogen and was stirred at room temperature for 2 h. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was then chromatographed over silica gel column (Merck silica gel 60; eluent: $CHCl_3$) to afford **s5c** (31 mg, 0.05 mmol, 78%) as a green solid. R_f = 0.20 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.59 (s, 2H, pyrrole-H), 7.48 (d, J = 8.4 Hz, 4H, phenyl-H), 7.01 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.99 (d, J = 8.4 Hz, 4H, phenyl-H), 6.83 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.64 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.41 (m, 2H, pyrrole-H), 5.89 (m, 2H, CH), 5.08 (m, 4H, CH_2), 4.07 (m, 4H, OCH_2), 2.30 (m, 4H, CH_2), 1.95 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 590.5 (0.17). MALDI-TOF-MS: *m/z* (% intensity): 606.3 (100), 607.3 (45). Calcd for $C_{40}H_{38}N_4O_2$ ($[M]^+$): 606.30.



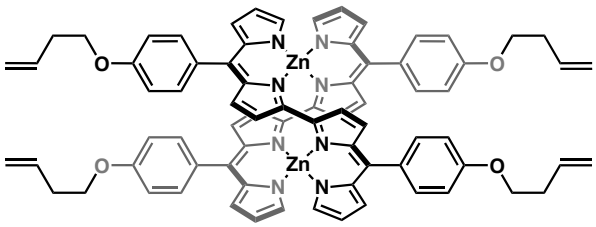
5,5′-Bis(4-(5-hexenyloxy)phenyl)bidipyrrin, s5d. 12 M HCl aq. (5 mL) was added to a solution of **s4d** (691 mg, 1.0 mmol) in $CHCl_3$ (100 mL) and was stirred at room temperature for 15 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Merck silica gel 60; eluent: 2% $MeOH/CH_2Cl_2$) to afford **s5d** (502 mg, 0.79 mmol, 79%) as a green solid. R_f = 0.45 (2% $MeOH/CH_2Cl_2$). ^1H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.59 (s, 2H, pyrrole-H), 7.48 (d, J = 8.4 Hz, 4H, phenyl-H), 7.01 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.98 (d, J = 8.4 Hz, 4H, phenyl-H), 6.83 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.64 (m, 2H, pyrrole-H), 6.41 (m, 2H, pyrrole-H), 5.86 (m, 2H, CH), 5.04 (m, 4H, CH_2), 4.06 (m, 4H, OCH_2), 2.12 (m, 4H, CH_2), 1.87 (m, 4H, CH_2), 1.63 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 592.5 (0.28). MALDI-TOF-MS: m/z (% intensity): 634.3 (100), 635.3 (38). Calcd for $C_{42}H_{42}N_4O_2$ ($[M]^+$): 634.33.



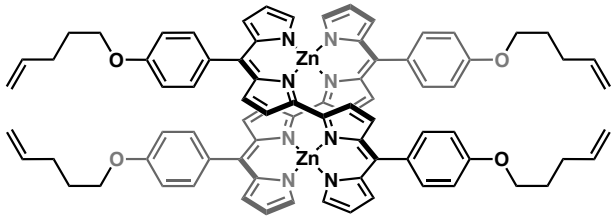
Zn^{II} complex of 5,5′-bis(4-(2-propenyloxy)phenyl)bidipyrrin, s6a. To a $CHCl_3$ solution (20 mL) of **s5a** (226 mg, 0.41 mmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (40 mg, 0.181 mmol) at room temperature and the mixture was stirred for 8 h. The mixture was washed with brine, extracted with $CHCl_3$, dried over anhydrous Na_2SO_4 and evaporated to dryness to afford **s6a** (172 mg, 0.14 mmol, 68%) as a green solid. R_f = 0.70 ($CHCl_3$). ^1H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.39 (m, 4H, phenyl-H), 7.00 (m, 4H, phenyl-H), 6.93 (s, 4H, pyrrole-H), 6.93 (m, 4H, phenyl-H), 6.75 (m, 4H, phenyl-H), 6.61 (m, 4H, pyrrole-H), 6.43 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.39 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.27 (m, 4H, pyrrole-H), 6.14–6.10 (m, 4H, CH), 5.50–5.35 (m, 8H, CH_2), 4.58 (m, 8H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.0 (0.40). MALDI-TOF-MS: m/z (% intensity): 1224.3 (52), 1225.3 (54), 1226.3 (96), 1227.3 (78), 1228.3 (100), 1229.3 (56), 1230.3 (46), 1231.2 (48), 1232.2 (18). Calcd for $C_{72}H_{56}N_8O_4Zn_2$ ($[M]^+$): 1228.30.



Zn^{II} complex of 5,5′-bis(4-(3-butenyloxy)phenyl)bidipyrrin, s6b. To a $CHCl_3$ solution (20 mL) of **s5b** (37 mg, 0.064 mmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (32 mg, 0.145 mmol) at room temperature and the mixture was stirred for 3 h. The mixture was washed with brine, extracted with $CHCl_3$, dried over anhydrous Na_2SO_4 and evaporated to dryness to afford **s6b** (38.2 mg, 0.030 mmol, 93%) as a green solid. R_f = 0.70 (EtOAc/hexane = 1:4). ^1H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.39 (m, 4H, phenyl-H), 6.99 (m, 4H, phenyl-H), 6.92 (s, 4H, pyrrole-H), 6.90 (m, 4H, phenyl-H), 6.73 (m, 4H, phenyl-H), 6.60 (m, 4H, pyrrole-H), 6.43 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.39 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.26 (m, 4H, pyrrole-H), 5.98–5.93 (m, 4H, CH), 5.24–5.15 (m, 8H, CH_2), 4.08 (m, 8H, OCH_2), 2.61 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.0 (0.49). MALDI-TOF-MS: m/z (% intensity): 1280.3 (85), 1281.4 (75), 1282.4 (95), 1283.4 (88), 1284.4 (100), 1285.4 (90), 1286.5 (58), 1287.5 (48). Calcd for $C_{76}H_{64}N_8O_4Zn_2$ ($[M]^+$): 1284.36.

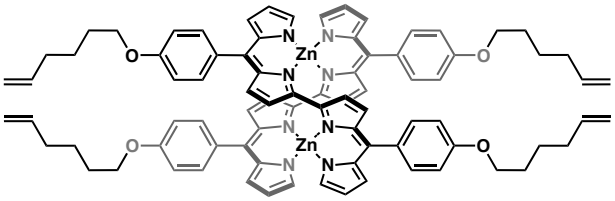


Zn^{II} complex of 5,5′-bis(4-(4-pentenyloxy)phenyl)bidipyrrin, s6c. To a $CHCl_3$ solution (20 mL) of **s5c** (31 mg, 0.05 mmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (32 mg, 0.30 mmol) at room temperature and the mixture was stirred for 6 h. The mixture was washed with brine, extracted with $CHCl_3$, dried over anhydrous Na_2SO_4 and evaporated to dryness. The residue was recrystallized from $CHCl_3$/hexane to afford **s6c** (38 mg, 0.05 mmol, quant.) as a green solid. R_f = 0.75 (EtOAc/hexane = 1:6). ^1H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.39 (m, 4H, phenyl-H), 6.99 (m, 4H, phenyl-H), 6.92 (s, 4H, pyrrole-H), 6.90 (m, 4H, phenyl-H), 6.73 (m, 4H, phenyl-H), 6.61 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.43 (d, J = 3.6 Hz, 4H, pyrrole-H), 6.39 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.26 (m, 4H, pyrrole-H), 5.90 (m, 4H, CH), 5.09 (m, 8H, CH_2), 4.04 (m, 8H, OCH_2), 2.30 (m, 8H, CH_2), 1.95 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 424.5 (0.73). MALDI-TOF-MS: m/z (% intensity): 1336.4 (24), 1337.4 (44), 1338.4 (78), 1339.4 (58), 1340.4 (100), 1341.4 (90), 1342.4 (40), 1343.4 (36), 1344.4 (26). Calcd for $C_{80}H_{72}N_8O_4Zn_2$ ($[M]^+$): 1340.42.

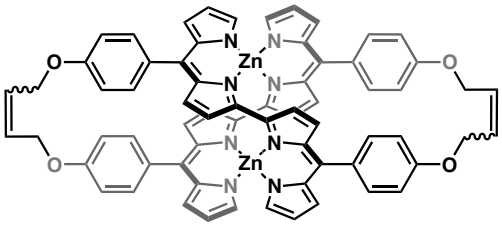


Zn^{II} complex of 5,5′-bis(4-(5-hexenyloxy)phenyl)bidipyrrin, s6d. To a CH_2Cl_2 solution (50 mL) of **s5d** (502 mg, 0.79 mmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (693 mg, 3.16 mmol) at room temperature and the mixture was stirred for 3.5 h. The mixture was washed with brine, extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4, and evaporated to dryness to afford **s6d** (530 mg, 0.38 mmol, 96%) as a green solid. R_f = 0.10 (CH_2Cl_2). ^1H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.38 (m, 4H, phenyl-H), 6.99 (m, 4H, phenyl-H), 6.91 (s, 4H, pyrrole-H), 6.90 (m, 4H, phenyl-H), 6.73 (m, 4H, phenyl-H), 6.61 (m, 4H, pyrrole-

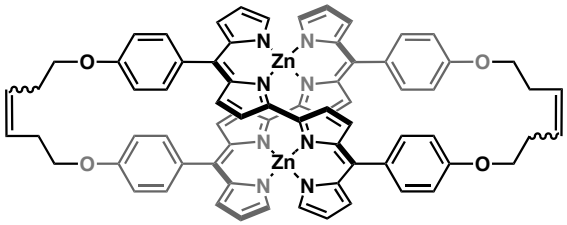
H), 6.43 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.39 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.26 (m, 4H, pyrrole-H), 5.87 (m, 4H, CH), 5.05 (m, 8H, CH_2), 4.03 (m, 8H, OCH_2), 2.18 (m, 8H, CH_2), 1.87 (m, 8H, CH_2), 1.63 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 424.5 (0.49). MALDI-TOF-MS: *m/z* (% intensity): 1392.5 (56), 1393.5 (58), 1394.5 (88), 1395.5 (74), 1396.5 (100), 1397.6 (73), 1398.6 (50). Calcd for $C_{84}H_{80}N_8O_4Zn_2$ ($[M]^+$): 1396.49.



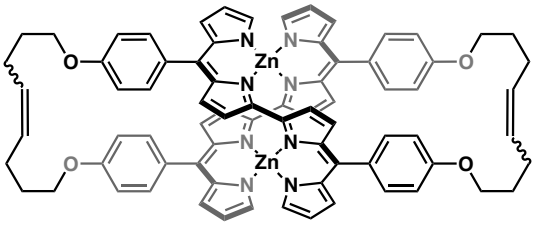
Zn^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(2-butene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 1a. A mixture of **s6a** (5.5 mg, 4.48 mmol) and Grubbs Catalyst 2nd Generation (1.1 mg, 1.34 mmol) in CH_2Cl_2 (18 mL) was stirred at 40 °C for 17 h. The solvent was evaporated to afford a green solid. The residue was chromatographed over silica gel column (Merck silica gel 60; eluent: 3% MeOH/$CHCl_3$) to afford **1a** (4.8 mg, 4.10 mmol, 92%) as a green solid. R_f = 0.80 (3% MeOH/$CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^{1}H NMR suggests the formation of a single product as a *trans*/*trans*-isomer as also determined by single-crystal X-ray diffraction analysis): δ (ppm) 7.40 (m, 4H, phenyl-H), 7.37 (br, 4H, pyrrole-H), 6.93 (m, 4H, phenyl-H), 6.91 (m, 4H, phenyl-H), 6.64 (m, 4H, pyrrole-H), 6.60 (m, 4H, phenyl-H), 6.37 (m, 4H, pyrrole-H), 6.30 (m, 4H, pyrrole-H), 6.20 (m, 4H, pyrrole-H), 6.02 (m, 4H, CH), 4.85–4.78 (m, 8H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 571.0 (0.81). MALDI-TOF-MS: *m/z* (% intensity): 1168.2 (60), 1169.2 (56), 1170.2 (96), 1171.2 (74), 1172.2 (100), 1173.3 (82), 1174.3 (42), 1175.3 (34). Calcd for $C_{68}H_{48}N_8O_4Zn_2$ ($[M]^+$): 1172.24. This compound was further characterized by single-crystal X-ray diffraction analysis.



Zn^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(3-hexene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 1b. A mixture of **s6b** (4.4 mg, 3.4 mmol) and Grubbs Catalyst 2nd Generation (0.7 mg, 0.086 mmol) in CH_2Cl_2 (12 mL) was stirred at 40 °C for 19 h. The solvent was evaporated to afford a green solid. The residue was chromatographed over silica gel column (Merck silica gel 60; eluent: EtOAc/hexane = 1:4) to afford **1b** (2.9 mg, 2.36 mmol, 69%) as a green solid. R_f = 0.65 (EtOAc/hexane = 1:4). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of more than one isomer): δ (ppm) 7.43–7.36 (m, 8H, phenyl-H), 7.06–6.87 (m, 8H, phenyl-H and pyrrole-H), 6.78–6.46 (m, 8H, phenyl-H and pyrrole-H), 6.44–6.27 (m, 8H, pyrrole-H), 6.23 (m, 4H, pyrrole-H), 5.79–5.71 (m, 4H, CH), 4.30–4.11 (m, 8H, OCH_2), 2.54 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 571.5 (0.41). MALDI-TOF-MS: *m/z* (% intensity): 1224.5 (40), 1225.3 (50), 1226.3 (90), 1227.3 (84), 1228.3 (100), 1229.3 (80), 1230.3 (62), 1231.3 (38). Calcd for $C_{72}H_{56}N_8O_4Zn_2$ ($[M]^+$): 1228.30.

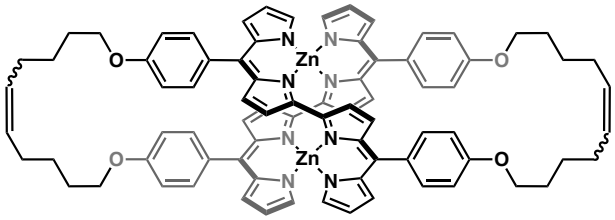


Zn^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(4-octene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 1c. A mixture of **s6c** (38 mg, 0.028 mmol) and Grubbs Catalyst 2nd Generation (12 mg, 0.014 mmol) in CH_2Cl_2 (110 mL) was stirred at 40 °C for 25 h. The solvent was evaporated to afford a green solid. The residue was then chromatographed over silica gel column (Merck silica gel 60, eluent: CH_2Cl_2) to afford **1c** (14.8 mg, 11.6 mmol, 41%) as a green solid. R_f = 0.70 (EtOAc/hexane = 1:6). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^{1}H NMR suggests the formation of a single product possibly as a *trans*/*trans*-isomer as also speculated by theoretical study): δ (ppm) 7.40 (m, 4H, phenyl-H), 7.14 (s, 4H, pyrrole-H), 6.94 (d, J = 2.4 Hz, 4H, phenyl-H), 6.93 (d, J = 2.4 Hz, 4H, phenyl-H), 6.63 (m, 4H, pyrrole-H), 6.60 (m, 4H, phenyl-H), 6.40 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.30 (m, 4H, pyrrole-H), 6.29 (m, 4H, pyrrole-H), 5.53 (m, 4H, CH), 3.96 (m, 8H, OCH_2), 2.27 (m, 8H, CH_2), 2.01 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.5 (0.42). MALDI-TOF-MS: *m/z* (% intensity): 1280.4 (42), 1281.4 (46), 1282.4 (83), 1283.4 (76), 1284.4 (100), 1285.4 (70), 1286.4 (58), 1287.4 (34). Calcd for $C_{76}H_{64}N_8O_4Zn_2$ ($[M]^+$): 1284.36.

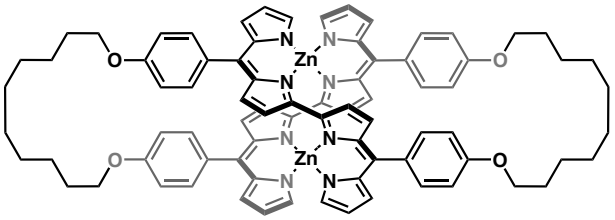


Zn^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(5-decene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 1d. A mixture of **s6d** (44 mg, 31.5 mmol) and Grubbs Catalyst 2nd Generation (13 mg, 15.7 mmol) in CH_2Cl_2 (125 mL) was stirred at 40 °C for 24 h. The solvent was evaporated to afford a green solid. The residue was chromatographed over silica gel column (Merck silica gel 60, eluent: EtOAc/hexane = 1:5) to afford **1d** (28.3 mg, 21.1 mmol, 67%) as a green solid. R_f = 0.50 (EtOAc/hexane = 1:5). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of more than one isomer): δ (ppm)

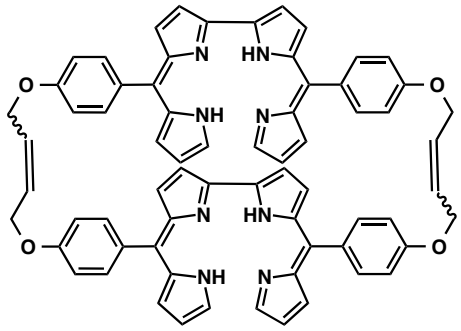
7.41 (m, 4H, phenyl-H), 7.20–7.08 (m, 4H, pyrrole-H), 6.93–6.88 (m, 8H, phenyl-H), 6.69–6.66 (m, 8H, phenyl-H and pyrrole-H), 6.42 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.32–6.27 (m, 8H, pyrrole-H), 5.57–5.48 (m, 4H, CH), 4.07 (m, 8H, OCH_2), 2.16 (m, 8H, CH_2), 1.89 (m, 8H, CH_2), 1.67 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.5 (0.48). MALDI-TOF-MS: *m/z* (% intensity): 1336.4 (38), 1337.4 (50), 1338.4 (80), 1339.4 (80), 1340.4 (100), 1341.5 (80), 1342.5 (56). Calcd for $C_{80}H_{72}N_8O_4Zn_2$ ($[M]^+$): 1340.42.



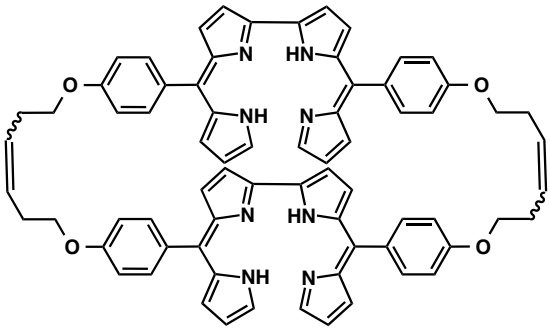
Zn^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(5-decane)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 1d′. A mixture of **1d** (1.8 mg, 1.34 mmol) and 10% Pd/C (3.6 mg) in EtOAc/MeOH (3:1, 8 mL) was stirred at room temperature for 32 h. The reaction mixture was filtered through and evaporated to dryness to afford **1d′** (1.6 mg, 1.23 mmol, 92%) as a green solid. R_f = 0.35 (EtOAc/hexane = 1:5). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.41 (m, 4H, phenyl-H), 7.02 (s, 4H, pyrrole-H), 6.98 (m, 4H, phenyl-H), 6.91 (m, 4H, phenyl-H), 6.70 (m, 4H, phenyl-H), 6.66 (m, 4H, pyrrole-H), 6.42 (d, J = 3.6 Hz, 4H, pyrrole-H), 6.34 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.28 (m, 4H, pyrrole-H), 4.04 (m, 8H, OCH_2), 1.88 (m, 8H, CH_2), 1.44 (s, 24H, CH_2), 1.67 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.0 (0.53). MALDI-TOF-MS: *m/z* (% intensity): 1340.5 (32), 1341.5 (40), 1342.5 (75), 1343.5 (72), 1344.5 (100), 1345.5 (54), 1346.5 (40). Calcd for $C_{80}H_{76}N_8O_4Zn_2$ ($[M]^+$): 1344.45.



5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(2-butene)-strapped 4,4′,4′′,4′′′-oxaphenyl)bisbidipyrrin, 2a. 12 M HCl aq. (100 mL) was added to a solution of **1a** (5.3 mg, 4.5 mmol) in $CHCl_3$ (10 mL) and was stirred at room temperature for 5 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Merck silica gel 60; eluent: 3% $MeOH/CH_2Cl_2$) to afford **2a** (4.7 mg, 4.5 mmol, quant.) as a green solid. R_f = 0.20 (3% $MeOH/CH_2Cl_2$). ^{1}H NMR (600 MHz, $CDCl_3$, 60 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^{1}H NMR suggests the formation of a single product possibly as a *trans*/*trans*-isomer): δ (ppm) 7.52 (s, 4H, pyrrole-H), 7.31 (d, J = 8.4 Hz, 8H, phenyl-H), 6.88 (d, J = 8.4 Hz, 8H, phenyl-H), 6.65 (m, 4H, pyrrole-H), 6.56 (m, 4H, pyrrole-H), 6.51 (m, 4H, pyrrole-H), 6.33 (m, 4H, pyrrole-H), 6.02 (m, 4H, CH), 4.82 (s, 8H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 589.0 (0.43). MALDI-TOF-MS: *m/z* (% intensity): 1044.4 (100), 1045.4 (64), 1046.4 (35). Calcd for $C_{68}H_{52}N_8O_4$ ($[M]^+$): 1044.41.

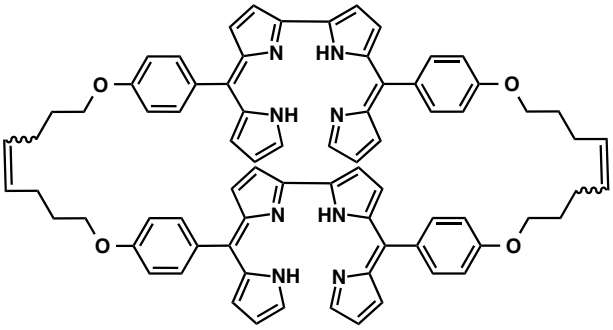


5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(3-hexene)-strapped 4,4′,4′′,4′′′-oxaphenyl)bisbidipyrrin, 2b. 12 M HCl aq. (10 mL) was added to a solution of **1b** (1.4 mg, 1.09 mmol) in $CHCl_3$ (5 mL) and was stirred at room temperature for 5 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Merck silica gel 60; eluent: $CHCl_3$) to afford **2b** (1.2 mg, 1.09 mmol, quant.) as a green solid. R_f = 0.25 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 60 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of more than one isomer): δ (ppm) 7.50 (br, 4H, pyrrole-H), 7.31 (m, 8H, phenyl-H), 6.88 (m, 8H, phenyl-H), 6.72 (br, 4H, pyrrole-H), 6.59 (m, 4H, pyrrole-H), 6.53 (m, 4H, pyrrole-H), 6.34 (br, 4H, pyrrole-H), 5.55 (m, 4H, CH), 4.03 (m, 8H, OCH_2), 2.28 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 571.5 (0.41). MALDI-TOF-MS: *m/z* (% intensity): 1100.5 (100), 1101.5 (86). Calcd for $C_{72}H_{60}N_8O_4$ ($[M]^+$): 1100.47.

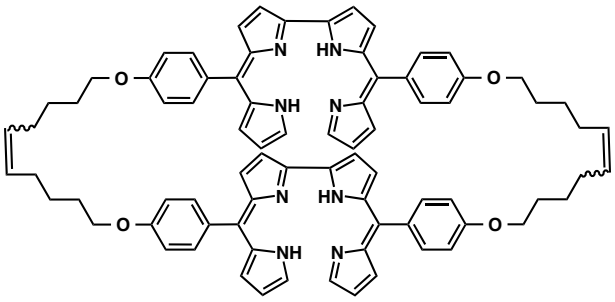


5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(4-octene)-strapped 4,4′,4′′,4′′′-oxaphenyl)bisbidipyrrin, 2c. 12 M HCl aq. (1 mL) was added to a solution of **1c** (2.2 mg, 1.7 mmol) in $CHCl_3$ (5 mL) and was stirred at room temperature for 2 h. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was then chromatographed over silica gel column (Merck silica gel 60; eluent: 2% $MeOH/CHCl_3$) to afford **2c** (1.4 mg, 1.17 mmol, 69%) as a green solid. R_f = 0.15 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 60 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^{1}H NMR

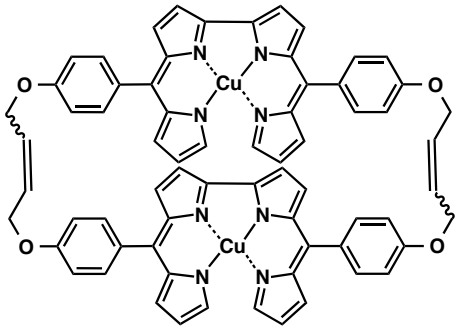
suggests the formation of a single product possibly as a *trans*/*trans*-isomer): δ (ppm) 7.51 (s, 4H, pyrrole-H), 7.33 (d, J = 8.4 Hz, 8H, phenyl-H), 6.90 (d, J = 8.4 Hz, 8H, phenyl-H), 6.70 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.58 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.54 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.33 (d, J = 4.2 Hz, 4H, pyrrole-H), 5.57 (m, 4H, CH), 4.06 (m, 8H, OCH_2), 2.30 (m, 8H, CH_2), 1.96 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 591.0 nm (0.47). MALDI-TOF-MS: *m*/*z* (% intensity): 1156.5 (100), 1157.5 (68), 1158.5 (50). Calcd for $C_{76}H_{68}N_8O_4$ ($[M]^+$): 1156.54.



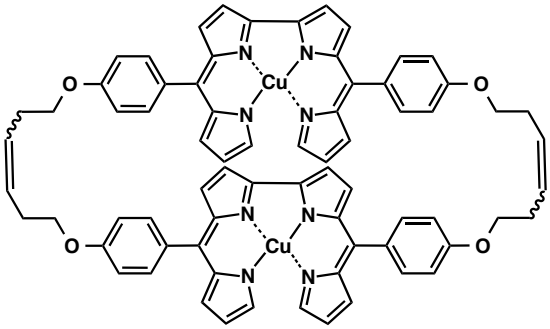
5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(5-decene)-strapped 4,4′,4′′,4′′′-oxaphenyl)bisbidipyrrin, 2d. 12 M HCl aq. (30 mL) was added to a solution of **1d** (2.1 mg, 1.57 mmol) in $CHCl_3$ (5 mL) and was stirred at room temperature for 1 h. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Merck silica gel 60; eluent: 5% $MeOH/CH_2Cl_2$) to afford **2d** (1.9 mg, 1.57 mmol, quant.) as a green solid. R_f = 0.50 (5% $MeOH/CH_2Cl_2$). ^1H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*/*cis*-, *cis*/*trans*-, and *trans*/*trans*-isomers at C=C, ^1H NMR suggests the formation of a mixture of more than one isomer): δ (ppm) 7.52 (s, 4H, pyrrole-H), 7.38 (m, 8H, phenyl-H), 6.92 (m, 8H, phenyl-H), 6.80–6.75 (m, 4H, pyrrole-H), 6.67–6.58 (m, 4H, pyrrole-H), 6.33 (m, 4H, pyrrole-H), 5.51–5.48 (m, 4H, CH), 4.03 (m, 8H, OCH_2), 2.15 (m, 8H, CH_2), 1.86 (m, 8H, CH_2), 1.60 (m, 8H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 593.5 (0.48). MALDI-TOF-MS: *m*/*z* (% intensity): 1212.6 (100), 1213.6 (99), 1214.6 (58). Calcd for $C_{80}H_{76}N_8O_4$ ($[M]^+$): 1212.60.



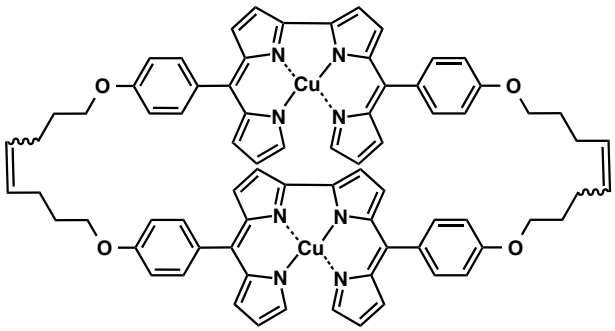
Cu^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(2-butene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 2a·Cu^{II}_2. To a $CHCl_3$ solution (5 mL) of **2a** (3.3 mg, 3.0 mmol) was added $Cu(OAc)_2·H_2O$ (7 mg, 38.5 mmol) at room temperature and the mixture was stirred for 5 h. The mixture was washed with brine, extracted with $CHCl_3$, dried over anhydrous Na_2SO_4 and evaporated to dryness to afford **2a**·Cu^{II}_2 (2.7 mg, 2.34 mmol, 78%) as a green solid. R_f = 0.60 ($CHCl_3$). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 375.5 (0.31). MALDI-TOF-MS: *m*/*z* (% intensity): 1166.2 (75), 1167.2 (74), 1168.2 (100), 1169.2 (76), 1170.2 (50), 1171.2 (26). Calcd for $C_{68}H_{48}Cu_2N_8O_4$ ($[M]^+$): 1168.24.



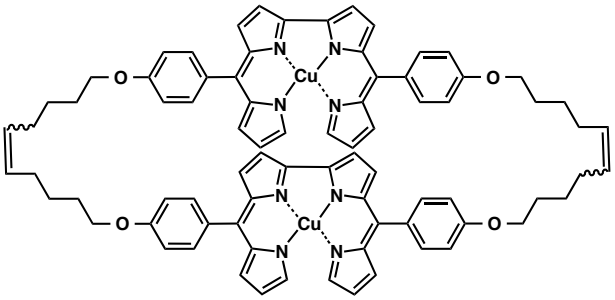
Cu^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(3-hexene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 2b·Cu^{II}_2. To a $CHCl_3$ solution (5 mL) of **2b** (1.30 mg, 1.2 mmol) was added $Cu(OAc)_2·H_2O$ (32 mg, 7.2 mmol) at room temperature and the mixture was stirred for 5 h. The mixture was washed with brine, extracted with $CHCl_3$, dried over anhydrous Na_2SO_4 and evaporated to dryness to afford **2b**·Cu^{II}_2 (1.47 mg, 1.2 mmol, quant.) as a green solid. R_f = 0.60 ($CHCl_3$). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 464.0 (0.26). MALDI-TOF-MS: *m*/*z* (% intensity): 1222.3 (74), 1223.3 (70), 1224.3 (100), 1225.3 (70), 1226.3 (58), 1227.4 (24). Calcd for $C_{72}H_{56}Cu_2N_8O_4$ ($[M]^+$): 1224.30.



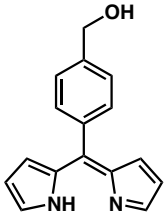
Cu^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(4-octene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 2c·Cu^{II}_2. To a $CHCl_3$ solution (8 mL) of **2c** (2.45 mg, 2.12 mmol) was added $Cu(OAc)_2·H_2O$ (6.1 mg, 0.03 mmol) at room temperature and the mixture was stirred for 9 h. The mixture was washed with brine, extracted with $CHCl_3$, dried over anhydrous Na_2SO_4 and evaporated to dryness to afford **2c**·Cu^{II}_2 (2.2 mg, 1.74 mmol, 82%) as a green solid. R_f = 0.60 ($CHCl_3$). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 464.0 (0.29). MALDI-TOF-MS: *m*/*z* (% intensity): 1278.4 (78), 1279.4 (72), 1280.4 (100), 1281.4 (80), 1282.4 (56). Calcd for $C_{76}H_{64}Cu_2N_8O_4$ ($[M]^+$): 1280.36.



Cu^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(5-decene)-strapped 4,4′,4′′,4′′′-oxaphenyl)-bisbidipyrrin, 2d·Cu^{II}_2. To a $CHCl_3$ solution (3 mL) of **2d** (2.4 mg, 1.98 mmol) was added $Cu(OAc)_2·H_2O$ (8.3 mg, 0.042 mmol) at room temperature and the mixture was stirred overnight. The mixture was washed with brine, extracted with $CHCl_3$, dried over anhydrous Na_2SO_4 and evaporated to dryness to afford **2d**·Cu^{II}_2 (2.6 mg, 1.98 mmol, quant.) as a yellow solid. R_f = 0.65 ($CHCl_3$). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 462.0 (0.21). MALDI-TOF-MS: *m/z* (% intensity): 1334.4 (69), 1375.9 (74), 1336.4 (100), 1337.5 (81), 1338.4 (52). Calcd for $C_{80}H_{72}Cu_2N_8O_4$ ($[M]^+$): 1336.42.

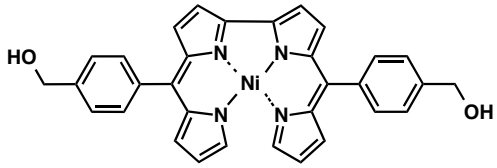


5-(4-Hydroxymethylphenyl)dipyrrin, s2e. To a solution of 5-(4-hydroxymethylphenyl)dipyrromethane **s1e**[S2] (4.92 g, 19.5 mmol) in THF (25 mL) was added *p*-chloranil (5.27 g, 21.5 mmol). After stirring for 30 min at room temperature, the solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: $CHCl_3$/EtOAc = 3:1) and recrystallized from CH_2Cl_2/hexane to afford **s2e** as an orange solid (1.05 g, 4.18 mmol, 21%). R_f = 0.40 ($CHCl_3$/EtOAc = 3:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.67 (s, 2H, pyrrole-H), 7.50 (d, J = 7.8 Hz, 2H, phenyl-H), 7.45 (d, J = 7.8 Hz, 2H, phenyl-H), 6.61 (m, 2H, pyrrole-H), 6.41 (m, 2H, pyrrole-H), 4.81 (s, 2H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 466.0 (0.15). MALDI-TOF-MS: *m/z* (% intensity): 250.1 (100), 251.1 (15). Calcd for $C_{16}H_{14}N_2O$ ($[M]^+$): 250.11.



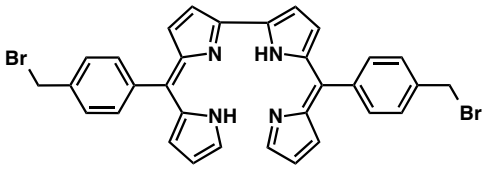
Ni^{II} complex of 5-(4-hydroxymethylphenyl)dipyrrin, s3e. A mixture of **s2e** (201.5 mg, 0.80 mmol) and $Ni(OAc)_2·4H_2O$ (400 mg, 1.60 mmol) and Na_2CO_3 (335 mg, 3.20 mmol) in $CHCl_3$ (15 mL) was stirred at room temperature for 6 h. The mixture was washed with brine, extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum to afford **s3e** (135.7 mg, 0.244 mmol, 61%) as a metallic-green solid. R_f = 0.40 ($CHCl_3$/EtOAc = 3:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.32 (s, 4H, pyrrole-H), 7.45 (d, J = 3.6 Hz, 4H, pyrrole-H), 7.42 (s, 8H, phenyl-H), 6.74 (d, J = 4.2 Hz, 4H, pyrrole-H), 4.80 (s, 4H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 468.0 (0.19). MALDI-TOF-MS: *m/z* (% intensity): 556.1 (100), 557.2 (33), 558.2 (37). Calcd for $C_{32}H_{26}N_4NiO_2$ ($[M]^+$): 556.14.

Ni^{II} complex of 5,5′-bis(4-hydroxymethylphenyl)bidipyrrin, s4e. A solution of **s3e** (353 mg, 0.633 mmol) in toluene (25 mL) was treated with *p*-chloranil (934 mg, 3.80 mmol) and heated at reflux overnight. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Wakogel C-300; eluent: 4% MeOH/CH_2Cl_2) and recrystallized from $CHCl_3$/hexane to afford **s4e** as a brown solid (192 mg, 0.346 mmol, 55%). R_f = 0.45 (4% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.58 (d, J = 7.8 Hz, 4H, phenyl-H), 7.49 (d, J = 7.8 Hz, 4H, phenyl-H), 6.79 (m, 2H, pyrrole-H), 6.74 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.62 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.44 (m, 2H, pyrrole-H), 5.98 (s, 2H, pyrrole-H), 4.83 (s, 4H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 414.0 (0.21). MALDI-TOF-MS: *m/z* (% intensity): 554.1 (100), 555.1 (66), 556.1 (68), 557.2 (42). Calcd for $C_{32}H_{24}N_4NiO_2$ ($[M]^+$): 554.12.

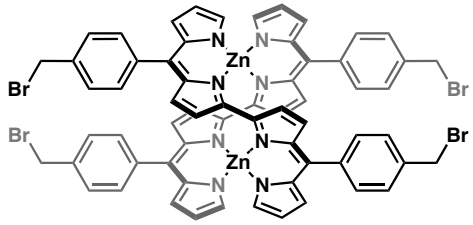


5,5′-Bis(4-bromomethylphenyl)bidipyrrin, s5e. PBr_3 (15 μL, 0.16 mmol) was added to a solution of **s4e** (15 mg, 0.027 mmol) in $CHCl_3$ (3 mL) under nitrogen and was stirred at room temperature for 10 h. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was chromatographed over silica gel column (Merck silica gel 60; eluent: 2% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to afford **s5e** (6.1 mg, 9.76 μmol, 36%) as a green solid. R_f = 0.45 (2% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.62 (s, 2H, pyrrole-H), 7.53 (d, J = 7.8 Hz, 4H, phenyl-H), 7.50 (d, J = 7.8 Hz, 4H, phenyl-H), 7.00 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.77 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.58 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.42 (d, J = 4.2 Hz, 2H, pyrrole-H), 4.59 (s, 4H, CH_2Br). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 431.5 (0.13). MALDI-TOF-MS: *m/z* (% intensity):

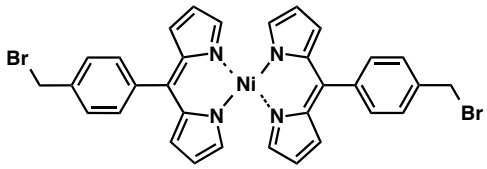
622.0 (46), 623.0 (14), 624.0 (100), 625.0 (28), 626.0 (50). Calcd for $C_{32}H_{24}Br_2N_4$ ([M]$^+$): 624.04.



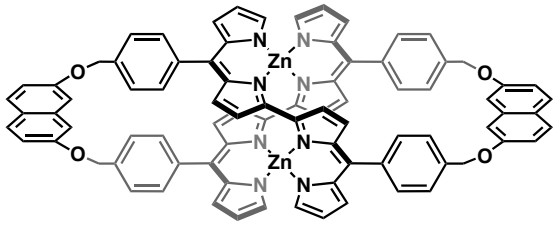
Zn^{II} complex of 5,5′-bis(4-bromomethylphenyl)bidipyrrin, s6e. To a $CHCl_3$ solution (5 mL) of **s5e** (22.7 mg, 0.0363 mmol) was added $Zn(OAc)_2 \cdot 2H_2O$ (32 mg, 0.145 mmol) at room temperature and the mixture was stirred for 5 h. The mixture was washed with brine, extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4, and evaporated to dryness. The residue was recrystallized from $CHCl_3$/hexane to afford **s6e** (8.1 mg, 5.88 μmol, 32%) as a green solid. R_f = 0.85 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.45 (m, 4H, phenyl-H), 7.44 (m, 4H, phenyl-H), 7.30 (d, J = 7.8 Hz, 4H, phenyl-H), 7.12 (s, 4H, pyrrole-H), 7.02 (m, 4H, phenyl-H), 6.57 (m, 4H, pyrrole-H), 6.40 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.34 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.31 (m, 4H, pyrrole-H), 4.62 (d, J = 3.0 Hz, 8H, CH_2Br). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 427.5 (0.58). MALDI-TOF-MS: *m/z* (% intensity): 1370.0 (25), 1370.9 (23), 1371.9 (62), 1372.9 (56), 1374.0 (90), 1374.9 (81), 1375.9 (100), 1376.9 (72), 1377.9 (66), 1379.0 (48), 1379.9 (30). Calcd for $C_{64}H_{44}Br_4N_8Zn_2$ ([M]$^+$): 1375.89.



Ni^{II} complex of 5-(4-bromomethylphenyl)dipyrrin, s4e′. PBr_3 (275 μL, 2.90 mmol) was added to a solution of **s3e** (363.3 mg, 1.45 mmol) in dry $CHCl_3$ (5 mL) and the mixture was stirred at room temperature for 1 h. The mixture was washed with Na_2CO_3 aq., extracted with CH_2Cl_2, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness. After the addition of $Ni(OAc)_2 \cdot 4H_2O$ (722 mg, 2.90 mmol), the reaction mixture in $CHCl_3$ (15 mL) was stirred at room temperature for 30 min. The residue was chromatographed over silica gel column (EtOAc/hexane = 1:5) and recrystallized from CH_2Cl_2/hexane to give **s4e′** (43.9 mg, 0.064 mmol, 9%) as a red-orange solid. R_f = 0.50 (EtOAc/hexane = 1:5). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.40 (s, 4H, pyrrole-H), 7.50 (d, J = 3.0 Hz, 4H, pyrrole-H), 7.44 (d, J = 7.8 Hz, 4H, phenyl-H), 7.39 (d, J = 7.8 Hz, 4H, phenyl-H), 6.73 (d, J = 4.2 Hz, 4H, pyrrole-H), 4.56 (s, 4H, CH_2Br). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 474.5 (0.48). MALDI-TOF-MS: *m/z* (% intensity): 681.1 (58), 682.0 (100), 683.1 (82), 684.0 (94), 685.0 (51), 686.0 (54). Calcd for $C_{32}H_{24}Br_2N_4Ni$ ([M]$^+$): 681.97. This compound was further characterized by single-crystal X-ray diffraction analysis. It is difficult to convert **s4e′** to the Ni^{II} complex of **s5e** as a precursor due to less stability.

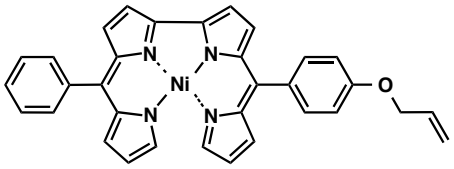


Zn^{II} complex of 5,5′,5′′,5′′′-(4,4′′′- and 4′,4′′-(2,7-naphtyl)-strapped 4,4′,4′′,4′′′-oxamethylphenyl)-bisbidipyrrin, 1e. A mixture of **s6e** (49 mg, 0.0356 mmol) and 2,7-dihydroxynaphthalene (13.7 mg, 0.085 mmol) and K_2CO_3 (50 mg, 0.356 mmol) in dry DMF (150 mL) was stirred at 80 °C for 16 h. The solvent was removed under high vacuum at 130 °C to afford a green solid. The residue was chromatographed over silica gel column (Merck silica gel 60; eluent: CH_2Cl_2) to afford **1e** (5.3 mg, 3.86 μmol, 11%) as a green solid. R_f = 0.70 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.65 (d, J = 9.0 Hz, 4H, naphthalene-H), 7.46 (m, 4H, phenyl-H), 7.40 (m, 4H, phenyl-H), 7.33 (m, 4H naphthalene-H), 7.05 (m, 4H, naphthalene-H), 7.05 (m, 4H, pyrrole-H), 6.88 (d, J = 2.4 Hz, 4H, pyrrole-H), 6.75 (s, 4H, pyrrole-H), 6.53 (m, 4H, phenyl-H), 6.49 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.46 (d, J = 4.2 Hz, 4H, pyrrole-H), 6.21 (m, 4H, phenyl-H), 5.38 (s, 8H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 429.0 (0.41). MALDI-TOF-MS: *m/z* (% intensity): 1368.3 (45), 1369.3 (46), 1370.3 (72), 1371.3 (90), 1372.3 (100), 1373.3 (82), 1374.3 (34), 1375.3 (34). Calcd for $C_{84}H_{56}N_8O_4Zn_2$ ([M]$^+$): 1372.30.

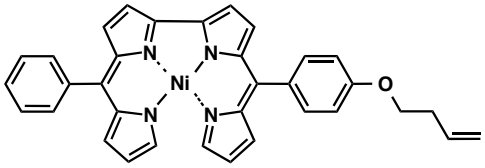


Ni^{II} complex of 5-(4-(2-propenyloxy)phenyl)-5′-phenylbidipyrrin, s7a. A mixture of **s2a** (120 mg, 0.43 mmol), 5-phenyldipyrrin[S3] (94.6 mg, 0.43 mmol), and $Ni(OAc)_2 \cdot 4H_2O$ (0.85 g, 3.44 mmol) in $CHCl_3$ (80 mL) was stirred at room temperature for 2 h. The solvent was evaporated to dryness. After the addition of *p*-chloranil (845 mg, 3.44 mmol), the reaction mixture in toluene (85 mL) was heated at reflux overnight. The solvent was evaporated to dryness. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:2) to afford **s7a** as a brown solid (62.4 mg, 0.113 mmol, 26%). R_f = 0.35 (CH_2Cl_2/hexane = 1:3). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.56 (d, J = 7.2 Hz, 2H, phenyl-H), 7.52 (d, J = 8.4 Hz, 2H, phenyl-H), 7.48 (m, 3H, phenyl-H), 7.02 (d, J = 8.4 Hz, 2H, phenyl-H), 6.82–6.80 (m, 3H, pyrrole-H), 6.78 (d, J = 4.2 Hz, 1H, pyrrole-H), 6.62 (m, 2H, pyrrole-H), 6.44 (m, 2H, pyrrole-H), 6.15–6.08 (m, 1H, CH), 6.01 (s, 1H, pyrrole-H), 5.98 (s, 1H, pyrrole-H), 5.50–5.47 (m, 2H, CH_2), 4.63 (m, 2H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-}$

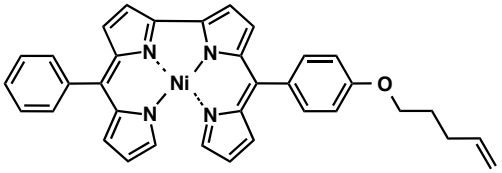
[1])): 413.0 (0.32). MALDI-TOF-MS: *m/z* (% intensity): 550.1 (100), 551.1 (30), 552.1 (44). Calcd for $C_{33}H_{24}N_4NiO$ ([M]$^+$): 550.13.



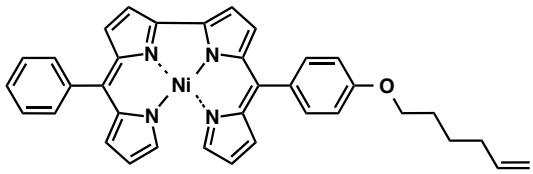
Ni^{II} complex of 5-(4-(3-butenyloxy)phenyl)-5′-phenylbidipyrrin, s7b. A mixture of **s2b** (612 mg, 2.11 mmol), 5-phenyldipyrrin[S3] (465 mg, 2.11 mmol), and $Ni(OAc)_2{\cdot}4H_2O$ (3.15 g, 12.68 mmol) in $CHCl_3$ (150 mL) was stirred at room temperature for 8 h. The solvent was evaporated to dryness. After the addition of *p*-chloranil (2.08 g, 8.44 mmol), the reaction mixture in toluene (150 mL) was heated at reflux overnight. The solvent was evaporated to dryness. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 2:3) to afford **s7b** as a brown solid (208.1 mg, 0.367 mmol, 17%). R_f = 0.40 (CH_2Cl_2/hexane = 2:3). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.57 (m, 2H, phenyl-H), 7.52 (d, J = 8.4 Hz, 2H, phenyl-H), 7.48 (m, 3H, phenyl-H), 7.00 (d, J = 9.0 Hz, 2H, phenyl-H), 6.82–6.78 (m, 3H, pyrrole-H), 6.74 (d, J = 4.2 Hz, 1H, pyrrole-H), 6.62 (m, 2H, pyrrole-H), 6.43 (m, 2H, pyrrole-H), 6.01 (s, 1H, pyrrole-H), 5.99 (s, 1H, pyrrole-H), 5.98–5.92 (m, 1H, CH), 5.24–5.14 (m, 2H, CH_2), 4.12 (m, 2H, OCH_2), 2.62 (m, 2H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 412.5 (0.22). MALDI-TOF-MS: *m/z* (% intensity): 566.2 (100), 567.2 (48), 568.2 (50), 569.2 (25). Calcd for $C_{34}H_{28}N_4NiO$ ([M]$^+$): 566.16.



Ni^{II} complex of 5-(4-(4-pentenyloxy)phenyl)-5′-phenylbidipyrrin, s7c. A mixture of **s2c** (201.5 mg, 0.44 mmol), 5-phenyldipyrrin[S3] (96.7 mg, 0.44 mmol), and $Ni(OAc)_2{\cdot}4H_2O$ (1.31 g, 5.27 mmol) in $CHCl_3$ (175 mL) was stirred at room temperature for 24 h. The solvent was evaporated to dryness. After the addition of *p*-chloranil (1.3 g, 5.27 mmol), the reaction mixture in toluene (180 mL) was heated at reflux overnight. The solvent was evaporated to dryness. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:3) to afford **s7c** as a brown solid (107 mg, 0.185 mmol, 42%). R_f = 0.35 (CH_2Cl_2/hexane = 1:3). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.57 (m, 2H, phenyl-H), 7.52–7.47 (m, 5H, phenyl-H), 6.99 (m, 2H, phenyl-H), 6.82 (m, 1H, pyrrole-H), 6.80 (m, 1H, pyrrole-H), 6.78 (m, 1H, pyrrole-H), 6.73 (m, 1H, pyrrole-H), 6.60 (m, 2H, pyrrole-H), 6.43 (m, 2H, pyrrole-H), 6.01–5.98 (m, 2H, pyrrole-H), 5.89 (m, 1H, CH), 5.12–5.03 (m, 2H, CH_2), 4.07 (m, 2H, OCH_2), 2.29 (m, 2H, CH_2), 1.96 (m, 2H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 412.5 (0.34). MALDI-TOF-MS: *m/z* (% intensity): 578.2 (100), 579.2 (48), 580.2 (53). Calcd for $C_{35}H_{28}N_4NiO$ ([M]$^+$): 578.16.

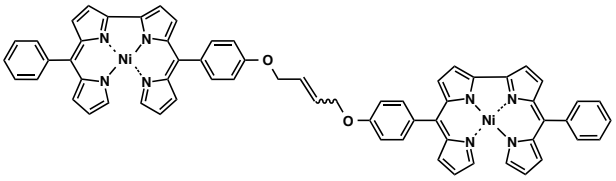


Ni^{II} complex of 5-(4-(5-hexeneyloxy)phenyl)-5′-phenylbidipyrrin, s7d. A mixture of **s2d** (246.3 mg, 0.774 mmol), 5-phenyldipyrrin[S3] (170.1 mg, 0.774 mmol), and $Ni(OAc)_2{\cdot}4H_2O$ (1.52 g, 6.19 mmol) in $CHCl_3$ (50 mL) was stirred at room temperature for 18 h. The solvent was evaporated to dryness. After the addition of *p*-chloranil (1.14 g, 4.64 mmol), the reaction mixture in toluene (150 mL) was heated at reflux for 24 h. The solvent was evaporated to dryness. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:2) to afford **s7d** as a brown solid (175.8 mg, 0.296 mmol, 38%). R_f = 0.55 (CH_2Cl_2/hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.57 (d, J = 7.2 Hz, 2H, phenyl-H), 7.51 (d, J = 8.4 Hz, 2H, phenyl-H), 7.47 (m, 3H, phenyl-H), 6.99 (d, J = 8.4 Hz, 2H, phenyl-H), 6.82–6.80 (m, 2H, pyrrole-H), 6.78 (d, J = 4.2 Hz, 1H, pyrrole-H), 6.74 (d, J = 4.2 Hz, 1H, pyrrole-H), 6.62 (m, 2H, pyrrole-H), 6.43 (m, 2H, pyrrole-H), 6.01 (s, 1H, pyrrole-H), 5.99 (s, 1H, pyrrole-H), 5.86 (m, 1H, CH), 5.08–4.99 (m, 2H, CH_2), 4.06 (m, 2H, OCH_2), 2.17 (m, 2H, CH_2), 1.87 (m, 2H, CH_2), 1.61 (m, 2H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 413.0 (0.34). MALDI-TOF-MS: *m/z* (% intensity): 594.2 (100), 595.2 (77), 596.2 (82), 597.2 (40), 598.2 (16). Calcd for $C_{36}H_{32}N_4NiO$ ([M]$^+$): 594.19.

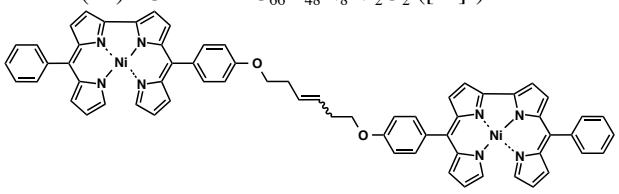


Ni^{II} complex of dimer of 5-(4-(2-propenyloxy)phenyl)-5′-phenylbidipyrrin, s8a. A mixture of **s7a** (12.5 mg, 0.023 mmol) and Grubbs Catalyst 2nd Generation (5.8 mg, 6.8 μmol) in CH_2Cl_2 (5 mL) was stirred at 40 °C for 24 h. The solvent was evaporated to afford a green solid. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:1) to afford **s8a** (3.1 mg, 2.89 μmol, 25%) as a green solid. R_f = 0.30 (CH_2Cl_2/hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.57–7.44 (m, 14H, phenyl-H), 7.08–7.00 (m, 4H, phenyl-H), 6.83–6.77 (m, 6H, pyrrole-H), 6.74–6.72 (m, 2H, pyrrole-H), 6.64–6.60 (m, 4H, pyrrole-H), 6.46–6.42 (m, 4H, pyrrole-H), 6.20 (m, 1H, CH), 6.01 (m, 1H, CH), 6.01–5.98 (m, 4H, pyrrole-H), 4.81–

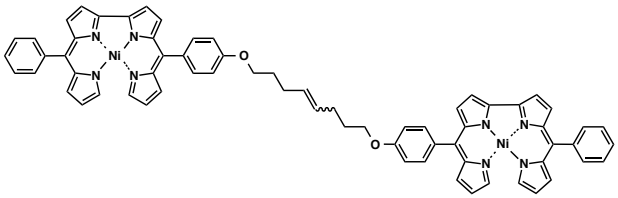
4.64 (m, 4H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 412.0 (0.58). MALDI-TOF-MS: *m/z* (% intensity): 1072.2 (98), 1073.2 (78), 1074.2 (100), 1075.2 (68), 1076.2 (46), 1077.2 (26). Calcd for $C_{64}H_{44}N_8Ni_2O_2$ ($[M]^+$): 1074.23.



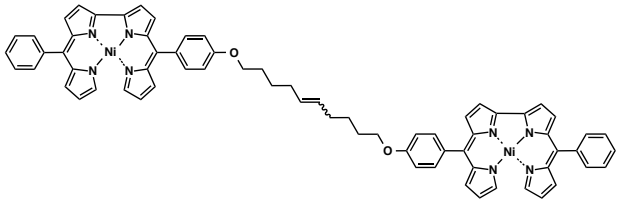
Ni^{II} complex of dimer of 5-(4-(3-butenyloxy)phenyl)-5′-phenylbidipyrrin, s8b. A mixture of **s7b** (123.9 mg, 0.218 mmol) and Grubbs Catalyst 2nd Generation (60 mg, 0.065 mmol) in CH_2Cl_2 (15 mL) was stirred at 40 °C for 11 h. The solvent was evaporated to afford a brown solid. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:1) to afford **s8b** (41.3 mg, 0.037 mmol, 34%) as a brown solid. R_f = 0.55 (CH_2Cl_2/hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a single product possibly as a *trans*-isomer): δ (ppm) 7.57–7.47 (m, 14H, phenyl-H), 7.02 (d, *J* = 9.0 Hz, 4H, phenyl-H), 6.82–6.73 (m, 8H, pyrrole-H), 6.62 (m, 4H, pyrrole-H), 6.45–6.42 (m, 4H, pyrrole-H), 6.39–6.32 (m, 2H, CH), 6.01 (m, 2H, pyrrole-H), 5.99 (m, 2H, pyrrole-H), 4.19 (m, 4H, OCH_2), 2.17 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 411.5 (0.26). MALDI-TOF-MS: *m/z* (% intensity): 1101.2 (10), 1102.3 (100), 1103.3 (74), 1104.3 (34), 1105.3 (12). Calcd for $C_{66}H_{48}N_8Ni_2O_2$ ($[M]^+$): 1102.26.



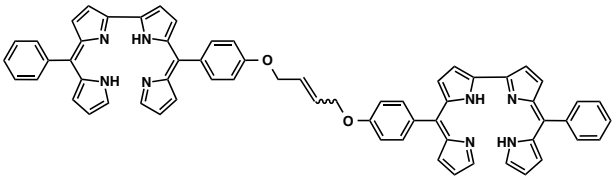
Ni^{II} complex of dimer of 5-(4-(4-pentenyloxy)phenyl)-5′-phenylbidipyrrin, s8c. A mixture of **s7c** (22 mg, 0.038 mmol) and Grubbs Catalyst 2nd Generation (13.7 mg, 0.085 mmol) in CH_2Cl_2 (5 mL) was stirred at 40 °C for 24 h. The solvent was evaporated to afford a green solid. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 1:2) to afford **s8c** (13.1 mg, 0.012 mmol, 61%) as a brown solid. R_f = 0.30 (CH_2Cl_2/hexane = 1:2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.54–7.43 (m, 14H, phenyl-H), 6.98 (m, 4H, phenyl-H), 6.78–6.71 (m, 8H, pyrrole-H), 6.60–6.57 (m, 4H, pyrrole-H), 6.42–6.40 (m, 4H, pyrrole-H), 6.00–5.97 (m, 4H, pyrrole-H), 5.67–5.52 (m, 2H, CH), 4.06 (m, 4H, OCH_2), 2.36–2.25 (m, 4H, CH_2), 1.97–1.92 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 412.0 (0.60). MALDI-TOF-MS: *m/z* (% intensity): 1128.3 (78), 1129.3 (78), 1130.3 (100), 1131.3 (74), 1132.3 (42). Calcd for $C_{68}H_{52}N_8Ni_2O_2$ ($[M]^+$): 1130.29.



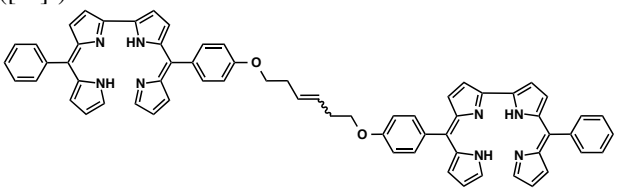
Ni^{II} complex of dimer of 5-(4-(5-hexenyloxy)phenyl)-5′-phenylbidipyrrin, s8d. A mixture of **s7d** (90.0 mg, 0.152 mmol) and Grubbs Catalyst 2nd Generation (12.9 mg, 15.2 μmol) in CH_2Cl_2 (50 mL) was stirred at 40 °C for 16 h. The solvent was evaporated to afford a green solid. The residue was chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2/hexane = 2:3) to afford **s8d** (57.1 mg, 0.049 mmol, 65%) as a brown solid. R_f = 0.55 (CH_2Cl_2/hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.56–7.46 (m, 14H, phenyl-H), 6.99 (m, 4H, phenyl-H), 6.78 (m, 6H, pyrrole-H), 6.73 (m, 2H, pyrrole-H), 6.61 (m, 4H, pyrrole-H), 6.41 (m, 4H, pyrrole-H), 5.99 (m, 4H, pyrrole-H), 5.54 (s, 1H, CH), 5.51 (s, 1H, CH), 4.06 (m, 4H, OCH_2), 2.19 (m, 4H, CH_2), 1.90 (m, 4H, CH_2), 1.59 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 412.5 (0.54). MALDI-TOF-MS: *m/z* (% intensity): 1160.3 (82), 1161.3 (92), 1162.4 (100), 1163.3 (80), 1164.3 (50), 1165.4 (28). Calcd for $C_{70}H_{60}N_8Ni_2O_2$ ($[M]^+$): 1162.35.



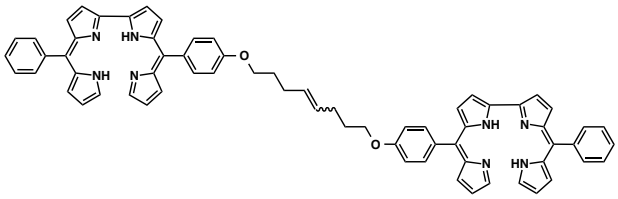
Dimer of 5-(4-(2-propenyloxy)phenyl)-5′-phenylbidipyrrin, s9a. 12 M HCl aq. (100 μL) was added to a solution of **s8a** (2.2 mg, 2.2 μmol) in $CHCl_3$ (10 mL) and was stirred at room temperature for 15 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was the chromatographed over silica gel column (Merck silica gel 60; eluent: 3% MeOH/CH_2Cl_2) to afford **s9a** (1.6 mg, 1.67 μmol, 73%) as a green solid. R_f = 0.35 (3% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.60 (s, 4H, pyrrole-H), 7.55–7.46 (m, 14H, phenyl-H), 7.05–6.99 (m, 4H, phenyl-H), 7.01–6.99 (m, 4H, pyrrole-H), 6.83–6.76 (m, 4H, pyrrole-H), 6.64–6.57 (m, 4H, pyrrole-H), 6.43–6.40 (m, 4H, pyrrole-H), 6.22 (m, 1H, CH), 6.01–5.98 (m, 1H, CH), 4.72 (m, 4H, OCH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 588.5 (0.49). MALDI-TOF-MS: *m/z* (% intensity): 960.4 (100), 961.4 (66), 962.4 (28). Calcd for $C_{64}H_{48}N_8O_2$ ($[M]^+$): 960.39.



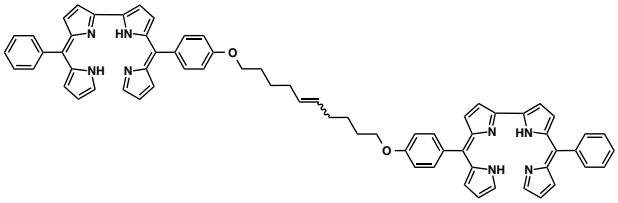
Dimer of 5-(4-(3-butenyloxy)phenyl)-5′-phenylbidipyrrin, s9b. 12 M HCl aq. (30 μL) was added to a solution of **s8b** (41.3 mg, 0.037 mmol) in $CHCl_3$ (25 mL) and was stirred at room temperature for 10 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was the chromatographed over silica gel column (Merck silica gel 60; eluent: $CHCl_3$/EtOAc = 5:1) to afford **s9b** (24.7 mg, 0.025 mmol, 68%) as a green solid. R_f = 0.35 ($CHCl_3$/EtOAc = 5:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a single product possibly as a *trans*-isomer): δ (ppm) 7.60 (s, 4H, pyrrole-H), 7.55–7.45 (m, 14H, phenyl-H), 7.02 (m, 4H, phenyl-H), 6.99 (m, 2H, pyrrole-H), 6.82 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.77 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.64 (m, 2H, pyrrole-H), 6.57 (m, 4H, pyrrole-H), 6.43–6.40 (m, 4H, pyrrole-H), 6.35–6.33 (m, 2H, CH), 4.19 (m, 4H, OCH_2), 2.77 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 590.0 (0.26). MALDI-TOF-MS: *m/z* (% intensity): 988.4 (100), 989.4 (98), 990.4 (40). Calcd for $C_{66}H_{52}N_8O_2$ ([M]$^+$): 988.42.



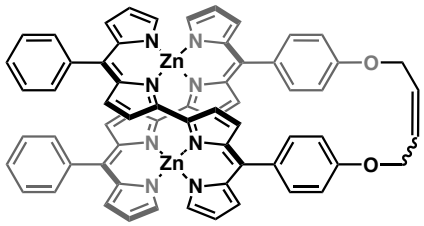
Dimer of 5-(4-(4-pentenyloxy)phenyl)-5′-phenylbidipyrrin, s9c. 12 M HCl aq. (100 μL) was added to a solution of **s8c** (11 mg, 9.73 μmol) in $CHCl_3$ (5 mL) and was stirred at room temperature for 15 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was the chromatographed over silica gel column (Merck silica gel 60; eluent: $CHCl_3$) to afford **s9c** (8.0 mg, 7.88 μmol, 36%) as a green solid. R_f = 0.25 ($CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a single product possibly as a *trans*-isomer): δ (ppm) 7.60 (s, 4H, pyrrole-H), 7.54 (m, 4H, phenyl-H), 7.48 (m, 10H, phenyl-H), 7.00 (m, 4H, phenyl-H), 6.99 (m, 4H, pyrrole-H), 6.82 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.76 (d, J = 4.2 Hz, 2H, pyrrole-H), 6.64 (m, 2H, pyrrole-H), 6.57 (m, 2H, pyrrole-H), 6.41 (m, 4H, pyrrole-H), 5.58 (m, 2H, CH), 4.07 (m, 4H, OCH_2), 2.26 (m, 4H, CH_2), 1.93 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 589.0 (0.24). MALDI-TOF-MS: *m/z* (% intensity): 1016.5 (100), 1017.4 (70). Calcd for $C_{68}H_{56}N_8O_2$ ([M]$^+$): 1016.45.



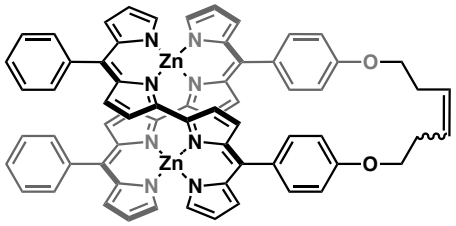
Dimer of 5-(4-(5-hexenyloxy)phenyl)-5′-phenylbidipyrrin, s9d. 12 M HCl aq. (200 μL) was added to a solution of **s8d** (57 mg, 0.049 mmol) in $CHCl_3$ (20 mL) and was stirred at room temperature for 20 min. The mixture was washed with Na_2CO_3 aq., extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4. The solvent was evaporated to dryness and the residue was the chromatographed over silica gel column (Merck silica gel 60; eluent: 1% MeOH/CH_2Cl_2) to afford **s9d** (31.8 mg, 0.03 mmol, 62%) as a green solid. R_f = 0.35 (3% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.60 (s, 4H, pyrrole-H), 7.54–7.43 (m, 14H, phenyl-H), 7.00–6.97 (m, 4H, phenyl-H), 7.00–6.97 (m, 4H, pyrrole-H), 6.82 (m, 2H, pyrrole-H), 6.76 (m, 2H, pyrrole-H), 6.64 (m, 2H, pyrrole-H), 6.57 (m, 2H, pyrrole-H), 6.42–6.39 (m, 4H, pyrrole-H), 5.55–5.49 (m, 2H, CH), 4.06 (m, 4H, OCH_2), 2.27–2.10 (m, 8H, CH_2), 1.96–1.83 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 590.0 (0.62). MALDI-TOF-MS: *m/z* (% intensity): 1044.5 (100), 1045.4 (58), 1046.4 (24), 1047.4 (8). Calcd for $C_{70}H_{60}N_8O_2$ ([M]$^+$): 1044.48.



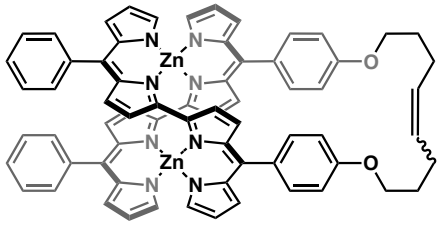
Zn^{II} complex of 5,5′′′-(4,4′′′-(2-butene)-strapped 4,4′′′-oxaphenyl)-5′,5′′-diphenylbisbidipyrrin, 3a. To a $CHCl_3$ solution (0.5 mL) of **s9a** (1.49 mg, 1.55 μmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (1.9 mg, 0.016 mmol) at room temperature and the mixture was stirred for 9 h. The mixture was washed with brine, extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4, and evaporated to dryness and the residue was chromatographed over GPC column (Bio-Beads S-X1, THF) to afford **3a** (1.3 mg, 1.18 μmol, 76%) as a green solid. R_f = 0.80 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.48–7.38 (m, 8H, phenyl-H), 7.20 (m, 2H, phenyl-H), 7.11 (m, 4H, pyrrole-H), 7.06 (m, 2H, phenyl-H), 6.98–6.93 (m, 4H, phenyl-H), 6.64–6.62 (m, 2H, phenyl-H), 6.62–6.60 (m, 4H, pyrrole-H), 6.42–6.35 (m, 6H, pyrrole-H), 6.30–6.29 (m, 6H, pyrrole-H), 5.53 (br, 2H, CH), 4.01–3.90 (m, 4H, CH). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.0 (0.55). MALDI-TOF-MS: *m/z* (% intensity): 1084.2 (54), 1085.2 (61), 1086.2 (84), 1087.2 (86), 1088.2 (100), 1089.2 (80), 1090.2 (58), 1091.1 (37). Calcd for $C_{64}H_{44}N_8O_2Zn_2$ ([M]$^+$): 1088.21.



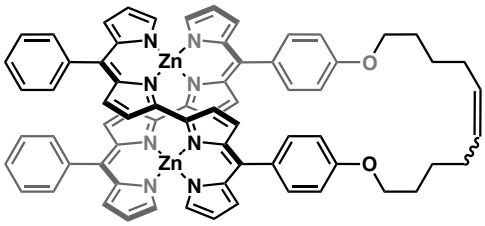
Zn^{II} complex of 5,5′′′-(4,4′′′-(3-hexene)-strapped 4,4′′′-oxaphenyl)-5′,5′′-diphenylbisbidipyrrin, 3b. To a $CHCl_3$ solution (5 mL) of **s9b** (24.7 mg, 0.025 mmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (11.8 mg, 0.1 mmol) at room temperature and the mixture was stirred for 12 h. The mixture was washed with brine, extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4, and evaporated to dryness and the residue was chromatographed over GPC column (Bio-Beads S-X1, THF) to afford **3b** (22.8 mg, 0.02 mmol, 82%) as a green solid. R_f = 0.80 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.46–7.31 (m, 12H, phenyl-H), 7.11–6.92 (m, 6H, phenyl-H), 7.00 (s, 4H, pyrrole-H), 6.78–6.54 (m, 6H, pyrrole-H), 6.47–6.25 (m, 10H, pyrrole-H), 6.27 (m, 2H, CH), 4.16 (m, 4H, OCH_2), 2.76 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.0 (0.37). MALDI-TOF-MS: *m/z* (% intensity): 1114.1 (36), 1115.2 (50), 1116.2 (100), 1117.2 (88), 1118.3 (75), 1119.3 (50), 1120.4 (38). Calcd for $C_{66}H_{48}N_8O_2Zn_2$ ([M]$^+$): 1116.25.



Zn^{II} complex of 5,5′′′-(4,4′′′-(4-octene)-strapped 4,4′′′-oxaphenyl)-5′,5′′-diphenylbisbidipyrrin, 3c. To a $CHCl_3$ solution (0.66 mL) of **s9c** (2.0 mg, 1.96 μmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (2.4 mg, 0.02 mmol) at room temperature and the mixture was stirred for 5 h. The mixture was washed with brine, extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4, and evaporated to dryness and the residue was chromatographed over GPC column (Bio-Beads S-X1, THF) to afford **3c** (1.88 mg, 1.64 μmol, 84%) as a green solid. R_f = 0.85 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a single product possibly as a *trans*-isomer): δ (ppm) 7.48 (d, J = 7.2 Hz, 2H, phenyl-H), 7.44–7.38 (m, 6H, phenyl-H), 7.20 (m, 2H, phenyl-H), 7.13 (s, 2H, pyrrole-H), 7.09 (s, 2H, pyrrole-H), 7.09–7.05 (m, 2H, phenyl-H), 6.98–6.93 (m, 4H, phenyl-H), 6.78 (m, 2H, phenyl-H), 6.61 (m, 4H, pyrrole-H), 6.42 (d, J = 3.6 Hz, 2H, pyrrole-H), 6.37 (m, 4H, pyrrole-H), 6.30 (m, 6H, pyrrole-H), 5.53 (br, 2H, CH), 3.95 (m, 4H, OCH_2), 2.28 (br, 4H, CH_2), 2.02 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.5 (0.56). MALDI-TOF-MS: *m/z* (% intensity): 1140.3 (44), 1141.3 (54), 1142.3 (83), 1143.3 (73), 1144.3 (100), 1145.3 (78), 1146.3 (62), 1147.3 (34). Calcd for $C_{68}H_{52}N_8O_2Zn_2$ ([M]$^+$): 1144.28.



Zn^{II} complex of 5,5′′′-(4,4′′′-(5-decene)-strapped 4,4′′′-oxaphenyl)-5′,5′′-diphenylbisbidipyrrin, 3d. To a $CHCl_3$ solution (30 mL) of **s9d** (31.8 mg, 0.03 mmol) was added $Zn(OAc)_2{\cdot}2H_2O$ (10.2 mg, 0.08 mmol) at room temperature and the mixture was stirred for 2 h. The mixture was washed with brine, extracted with $CHCl_3$, and dried over anhydrous Na_2SO_4, and evaporated to dryness and the residue was chromatographed over GPC column (Bio-Beads S-X1, THF) to afford **3a** (23.9 mg, 0.02 mmol, 68%) as a green solid. R_f = 0.80 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; as for the *cis*- and *trans*-isomers at C=C, ^{1}H NMR suggests the formation of a mixture of *cis*- and *trans*-isomers): δ (ppm) 7.48–7.38 (m, 8H, phenyl-H), 7.24–6.87 (m, 10H, phenyl-H), 7.08 (s, 4H, pyrrole-H), 6.68–6.58 (m, 6H, pyrrole-H), 6.46–6.26 (m, 10H, pyrrole-H), 5.61–5.46 (m, 2H, CH), 4.09–4.03 (m, 4H, OCH_2), 2.10 (m, 8H, CH_2), 1.89 (m, 4H, CH_2). UV/vis ($CHCl_3$, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 425.0 (0.71). MALDI-TOF-MS: *m/z* (% intensity): 1168.3 (54), 1169.3 (64), 1170.3 (83), 1171.3 (94), 1172.3 (100), 1173.3 (86), 1174.3 (80), 1175.3 (56), 1176.3 (40), 1177.3 (34), 1178.3 (20). Calcd for $C_{70}H_{56}N_8O_2Zn_2$ ([M]$^+$): 1172.31.



[S1] R. Wakabayashi, T. Ikeda, Y. Kubo, S. Shinkai and M. Takeuchi, *Angew. Chem. Int. Ed.*, 2009, **48**, 6667–6670.

[S2] S. H. H. Zaidi, R. S. Loewe, B. A. Clark, M. J. Jacob and J. S. Lindsey, *Org. Process Res. Dev.*, 2006, **10**, 304–314.

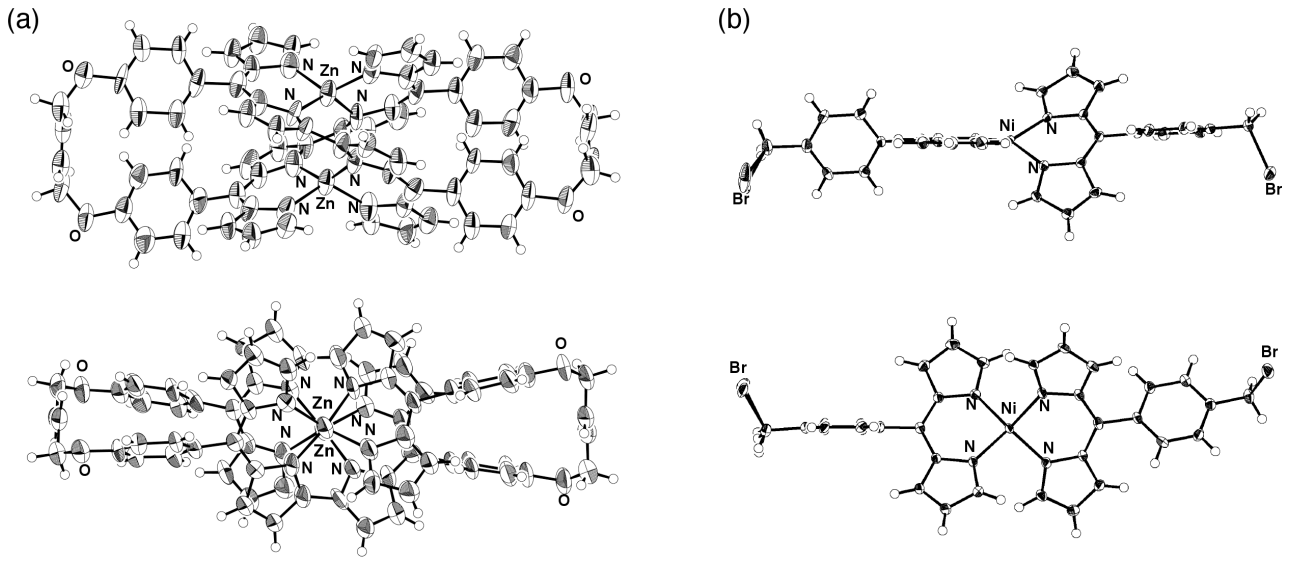
[S3] L. Yu, K. Muthukumaran, I. V. Sazanovich, C. Kirmaier, E. Hinden, J. R. Diers, P. D. Boyle, D. F. Bocian, D. Holten and J. S. Lindsey, *Inorg. Chem.*, 2003, **42**, 6629–6647.

2. X-ray crystallographic data for dipyrrin metal complexes

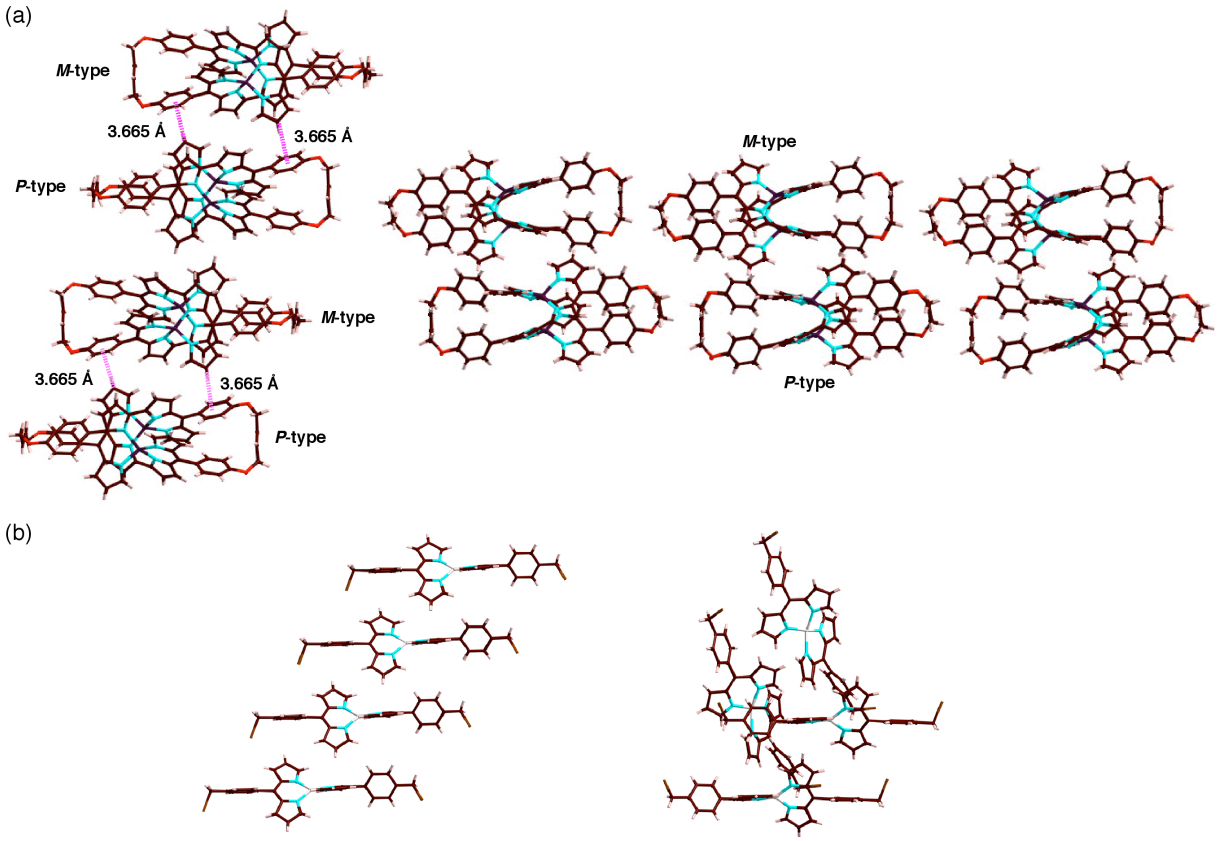
Single-Crystal X-ray Analysis. Crystallographic data are summarized in Supporting Table 1. A single crystal of **1a** was obtained by vapor diffusion of EtOH into a $CHCl_3$ solution of **1a** with a small amount of toluene. The data crystal was a dark-purple-colored prism of approximate dimensions 0.30 mm × 0.20 mm × 0.10 mm. Data was collected at 93 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å), structure was solved by direct method. A single crystal of **s4e´** was obtained by vapor diffusion of hexane into a $CHCl_3$ solution of **s4e´**. The data crystal was a purple-colored prism of approximate dimensions 0.40 mm × 0.30 mm × 0.10 mm. Data was collected at 123 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), structure was solved by direct method. In each case, the non-hydrogen atoms were refined anisotropically. The hydrogen atoms were calculated in ideal positions. Solutions of the structures were performed by using the Crystal Structure crystallographic software package (Molecular Structure Corporation)[S4] and SIR97[S5] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[S6] CIF files (CCDC-851580 and 851581) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Supporting Table 1 Crystallographic details for the compounds **1a** and **s4e´**.

	1a	**s4e´**
formula	$C_{68}H_{48}N_8O_4Zn_2 \cdot 1.63CHCl_3 \cdot 0.24C_2H_5OH$	$C_{32}H_{24}Br_2N_4Ni$
fw	1376.88	683.08
crystal size, mm	0.30 × 0.20 × 0.10	0.40 × 0.30 × 0.10
crystal system	triclinic	monoclinic
space group	*P*-1 (no. 2)	$P2_1/n$ (no. 14)
a, Å	11.1564(2)	12.324(5)
b, Å	16.8638(4)	8.833(3)
c, Å	17.2397(4)	25.104(11)
α, °	94.3150(14)	90
β, °	93.4125(18)	94.105(14)
γ, °	108.6451(12)	90
V, Å^3	3052.51(12)	2725.7(17)
ρ_{calcd}, gcm^{-3}	1.498	1.665
Z	2	4
T, K	93(2)	123(2)
μ, mm^{-1}	3.407 (Cu-Kα)	3.673 (Mo-Kα)
no. of reflns	27771	24630
no. of unique reflns	8915	6228
variables	826	362
λ, Å	1.54187 (Cu-Kα)	0.71075 (Mo-Kα)
R_1 ($I > 2\sigma(I)$)	0.1033	0.0429
wR_2 ($I > 2\sigma(I)$)	0.2520	0.0796
GOF	1.126	1.047



Supporting Figure 1 ORTEP drawings of single-crystal X-ray structures of (a) **1a** (side and top view) and (b) **s4e´** (side and perspective view). Thermal ellipsoids are scaled to the 50% probability level. Solvent molecules ($CHCl_3$ and C_2H_5OH) are omitted for clarity for **1a**, whose single crystal prepared by vapor diffusion of EtOH into a $CHCl_3$ solution with a small amount of toluene contains $CHCl_3$ and C_2H_5OH with the occupancies of 0.76:0.24 in a disordered form at one site and $CHCl_3$ with the occupancy of 0.87 at another site. Single-crystal X-ray analysis of **1a** suggests the formation of a *trans*/*trans*-isomer with a short Zn···Zn distance of 3.258 Å, suggesting that the minor mode (*S* mode) of double helices of **1a** is stabilized in the solid state (Supporting Figure 18 and 19).

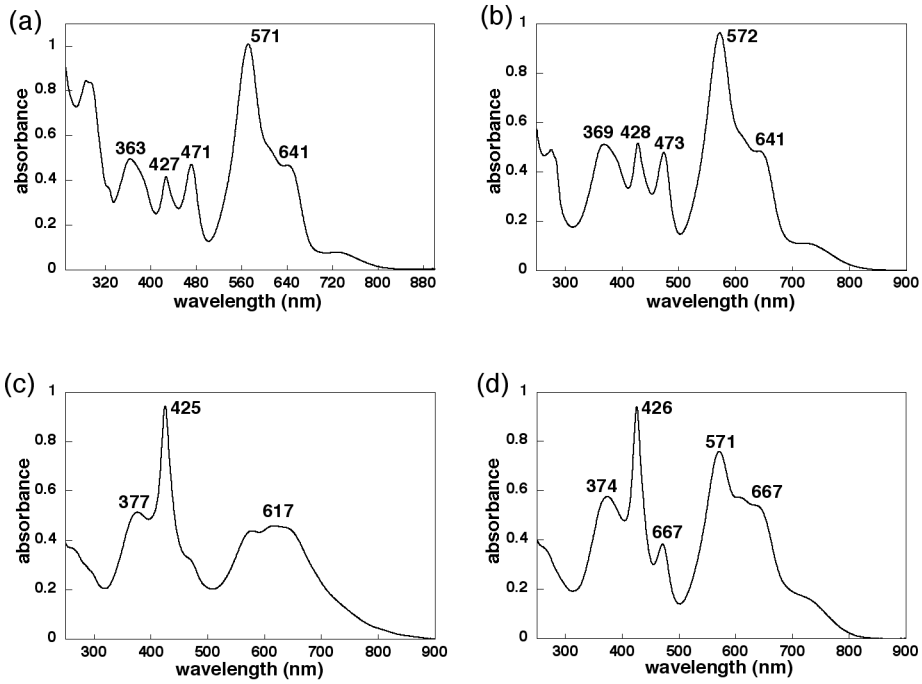


Supporting Figure 2 Solid-state assembled structures of (a) **1a** and (b) **s4e´**. Atom color code: brown, pink, blue, light brown, gray, and purple represent carbon, hydrogen, nitrogen, bromine, nickel, and zinc, respectively. As seen in the left figure of (a), *M*- and *P*-type double helices are alternately arranged in columns.

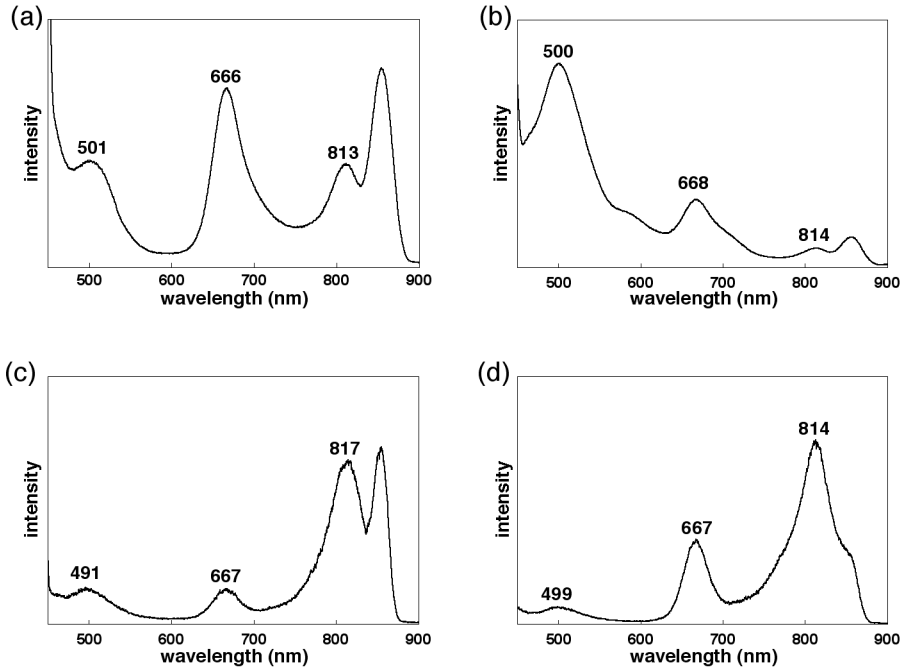
[S4] *CrystalStructure: Crystal Structure Analysis Package* Rigaku and Rigaku/MSC, The Woodlands, 2000.

[S5] *SIR97: A program for crystal structure solution*, A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, *J. Appl. Crystallogr.*, 1999, **32**, 115–119.
[S6] *SHELXL-97: Programs for Crystal Structure Analysis*, G. M. Sheldrick, University of Göttingen, Germany, 1998.

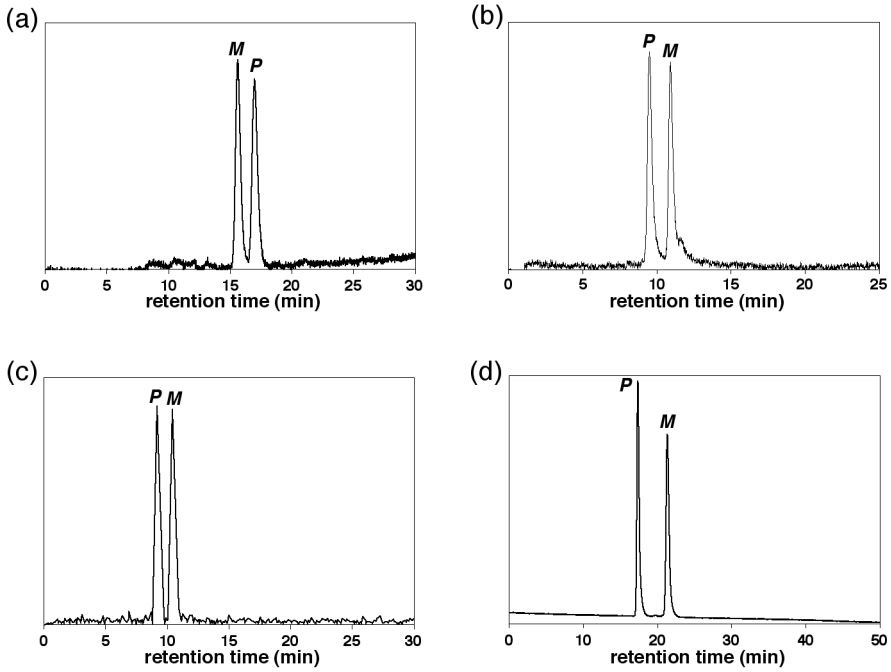
3. Spectral changes of double helices



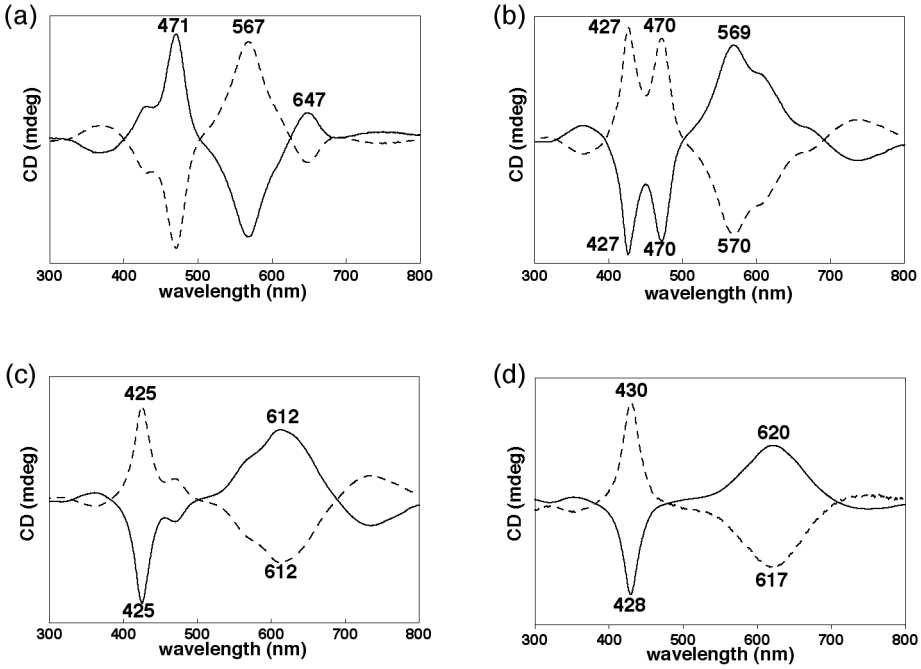
Supporting Figure 3 UV/vis absorption spectra of strapped Zn^{II}-bridged bidipyrrin double helices (a) **1a**, (b) **1b**, (c) **1c**, and (d) **1d** in $CHCl_3$. The relative absorbance intensities at the long and short wavelengths (ca. 570 and 430 nm, respectively) are depending on the pitch lengths of double helices as suggested by theoretical study (see also Supporting Figure 18 and 19). Under the conditions for measurements of UV/vis absorption spectra, the larger absorbances at ca. 570 nm in **1a** and **1b** suggest the extended Zn···Zn distances, whereas the larger ones at ca. 430 nm in **1c** and **1d** are derived from the shorter Zn···Zn distances (see also Supporting Figure 12).



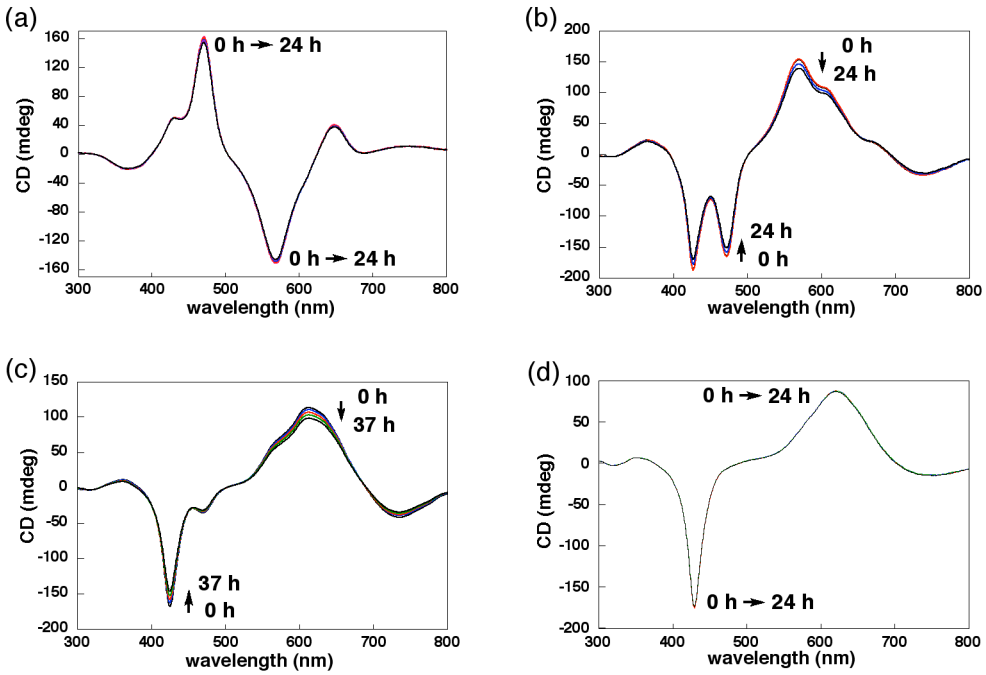
Supporting Figure 4 Fluorescence spectra (excited at each absorption maximum: 426, 427, 426, and 425 nm, respectively) of strapped Zn^{II}-bridged bidipyrrin double helices (a) **1a** (emission quantum yield (Φ_F): 0.010), (b) **1b** (Φ_F: 0.010), (c) **1c** (Φ_F: 0.002), and (d) **1d** (Φ_F: 0.002) in $CHCl_3$. As also observed in other Zn^{II}-bridged bidipyrrin double helices, emissions from higher excited states are observed. The details will be discussed elsewhere.



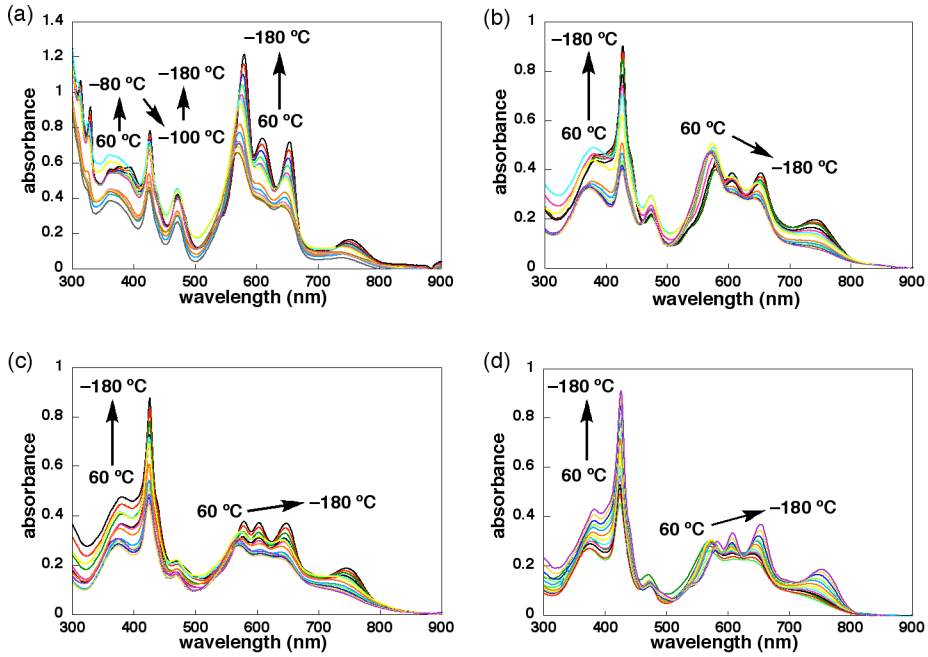
Supporting Figure 5 Chiral HPLC profiles of strapped Zn^{II}-bridged bidipyrrin double helices (Daicel CHIRALPAK IA, flow rate: 0.5 mL/min): (a) **1a** using CH_2Cl_2/hexane = 1:2 as an eluent (monitored at 570 nm), (b) **1d** using CH_2Cl_2/hexane = 1:2 as an eluent (monitored at 425 nm), (c) **1d´** using CH_2Cl_2/hexane = 1:2 as an eluent (monitored at 425 nm), and (d) **1e**, a naphthyl-bridged double helix prepared by Williamson ether synthesis, using CH_2Cl_2/hexane = 1:1 as an eluent (monitored at 425 nm). Optical resolutions of **1b**,**c** are not easy due to low solubility in the eluent solvent. The double helices with the longer straps are more soluble, although **1a** shows the fairly good solubility because the conformation (the main mode of double helix) are different from **1b**–**d**.



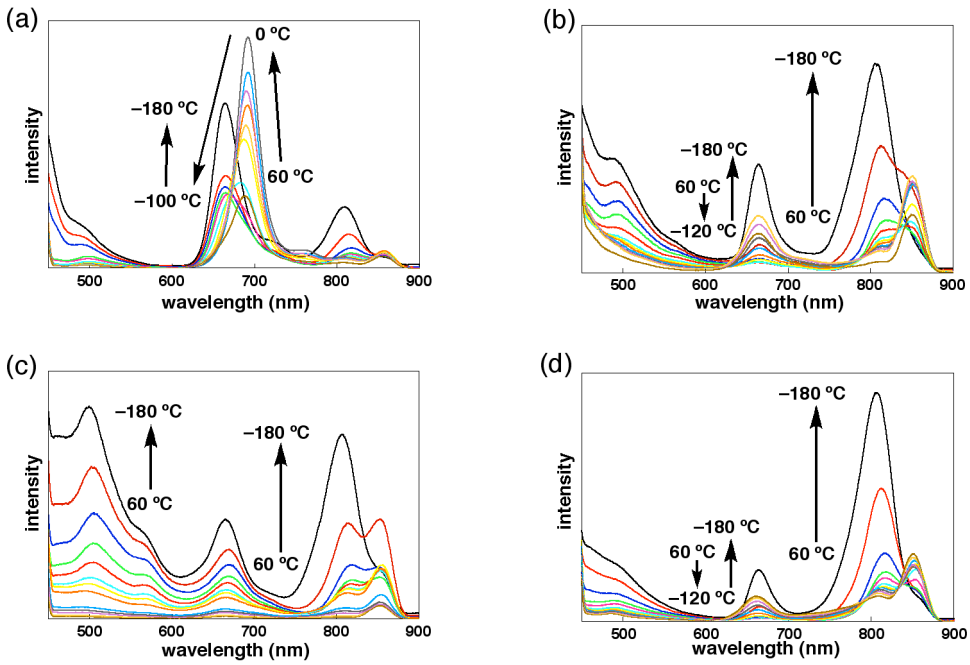
Supporting Figure 6 CD spectra of strapped Zn^{II}-bridged bidipyrrin double helices in $CHCl_3$ (first fraction isolated by chiral HPLC (Supporting Figure 5): solid line; second fraction: broken line): (a) **1a**, (b) **1d**, (c) **1d´**, and (d) **1e**. Based on the theoretical studies (see also Supporting Figure 18 and 19), the first fraction of **1a** is an *M*-type double helix, whereas those of **1d**, **1d´**, and **1e** are *P*-type double helices.



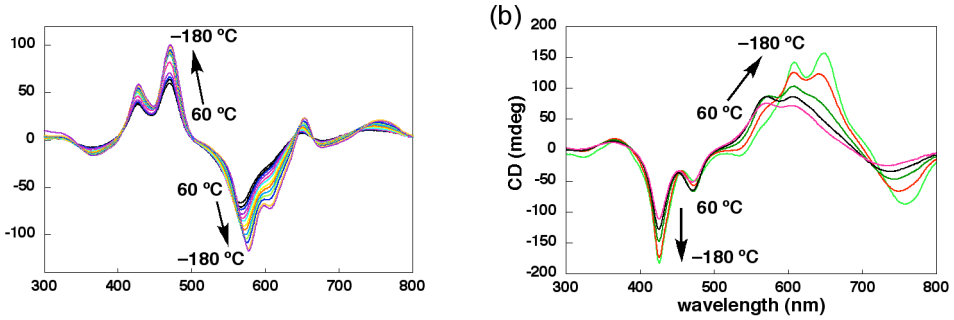
Supporting Figure 7 Time-dependent CD spectral changes of (a) **1a**, (b) **1d**, (c) **1d′**, and (d) **1e** in $CHCl_3$. This figure suggests that the strapped double helices are stable without significant racemization in solution state.



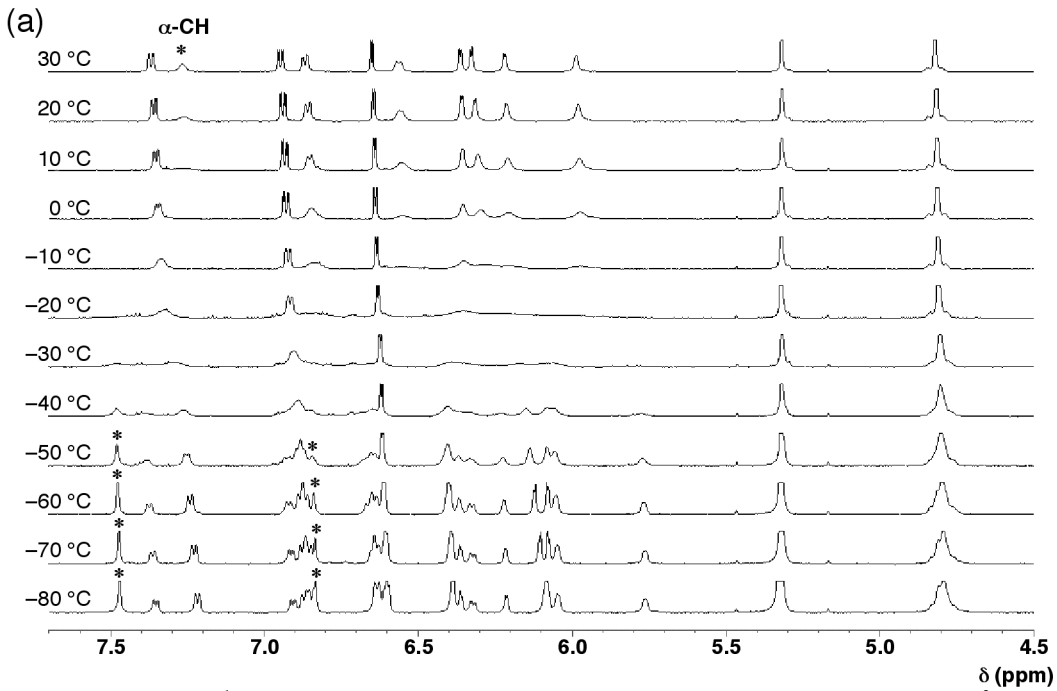
Supporting Figure 8 VT UV/vis absorption spectral changes of (a) **1a**, (b) **1b**, (c) **1c**, and (d) **1d** at each 20 °C from 60 to –180 °C in 2-methyl-THF (1×10^{-5} M). Based on theoretical studies (see also Supporting Figure 18 and the caption of Supporting Figure 3), at lower temperature, **1a** provides a longer Zn···Zn distance with an extended double helix, in contrast to **1b**–**d**, which have shorter Zn···Zn distances with shrunk double helices. The existence of two modes of double helices and the corresponding stretching behaviors are discussed in the manuscript and also Supporting Figure 18. In particular, **1a** exists as a mixture of two modes of double helices, although the mode with a longer Zn···Zn distance is predominant even at r.t. (see also VT ^{1}H NMR in Supporting Figure 11).



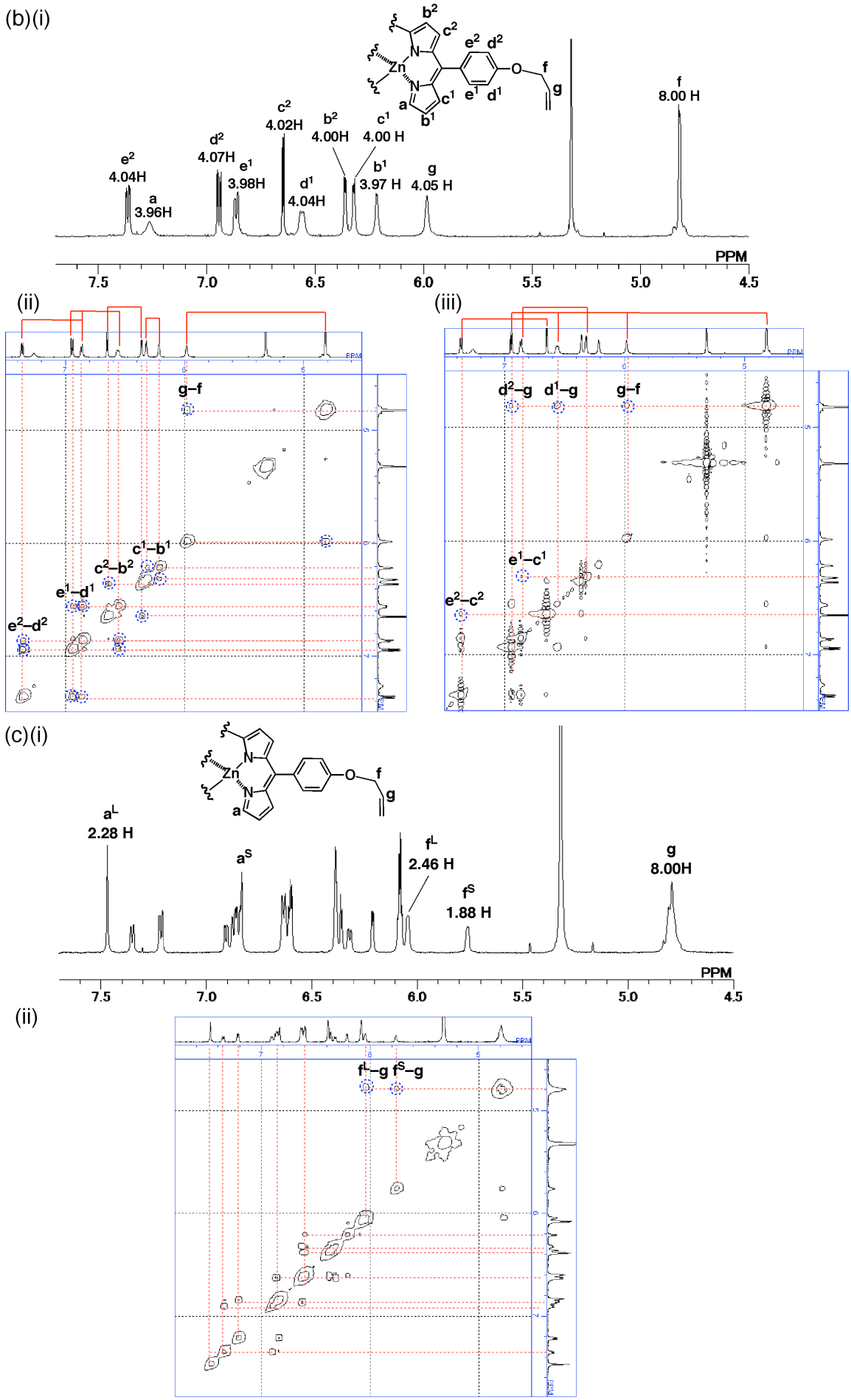
Supporting Figure 9 VT FL spectral changes of (a) **1a** (emission quantum yield (Φ_F) at r.t.: 0.019), (b) **1b** (Φ_F at r.t.: 0.009), (c) **1c** (Φ_F at r.t.: 0.009), and (d) **1d** (Φ_F at r.t.: 0.013) at each 20 °C from 60 to –180 °C in 2-methyl-THF (1×10^{-5} M). In each derivative, much higher emission was observed at lower temperatures, even though changes of solvent volumes may be slightly changed. Basically, the emissions at ca. 800 nm are increased at lower temperatures due to the formation of rigid double helical structures. In **1a**, the complicated behavior with two-step transitions at 600–750 nm was observed. The details will be discussed elsewhere.



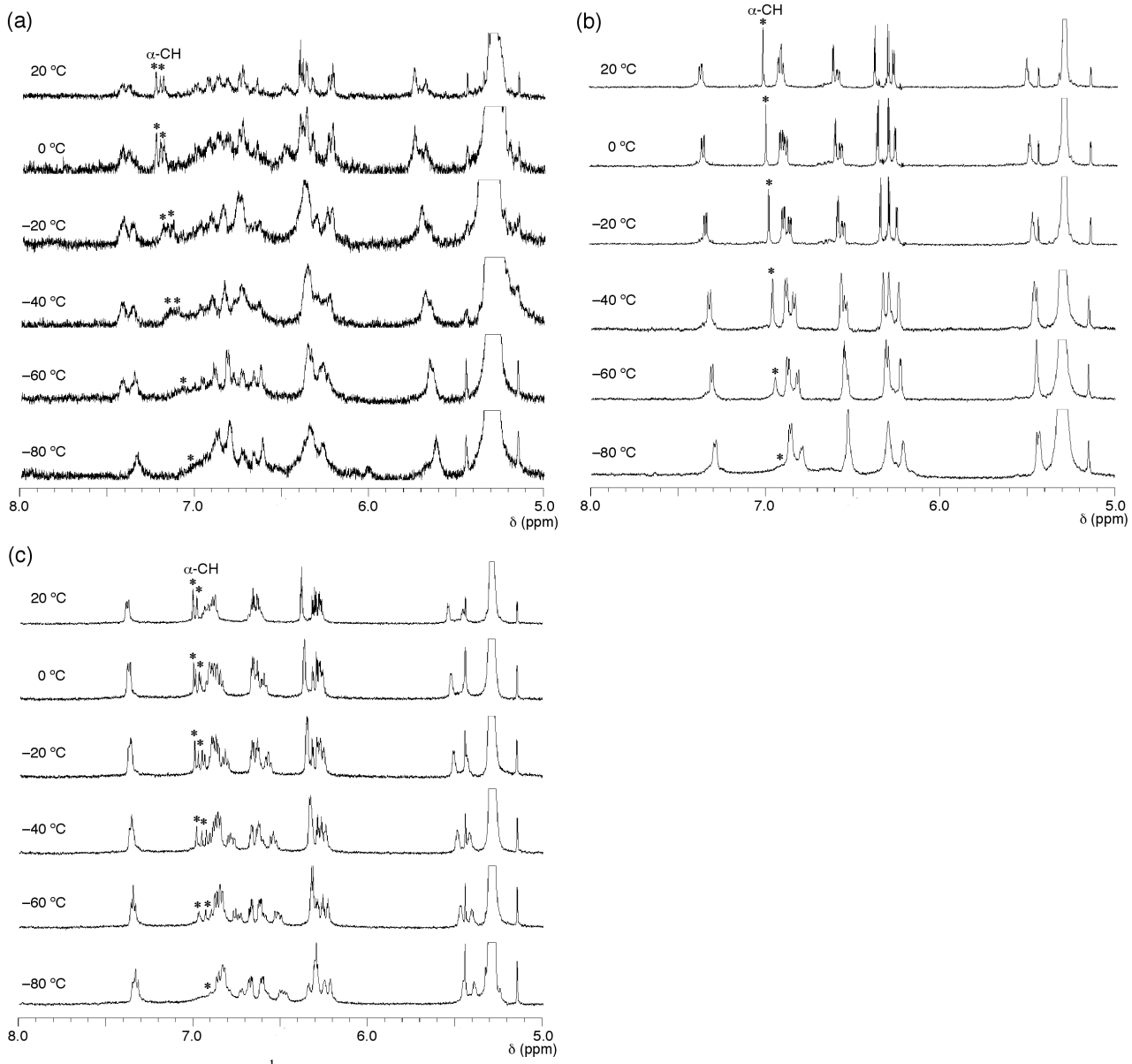
Supporting Figure 10 VT CD spectral changes of (a) **1a** and (b) **1d** as first fractions at each 20 °C from 60 to –180 °C in 2-methyl-THF (1×10^{-5} M). As related with the UV/vis spectral changes (Supporting Figure 9), double helices in **1a** and **1d** are stretching depending on the temperatures according to the corresponding modes (see also Supporting Figure 18 and 19).



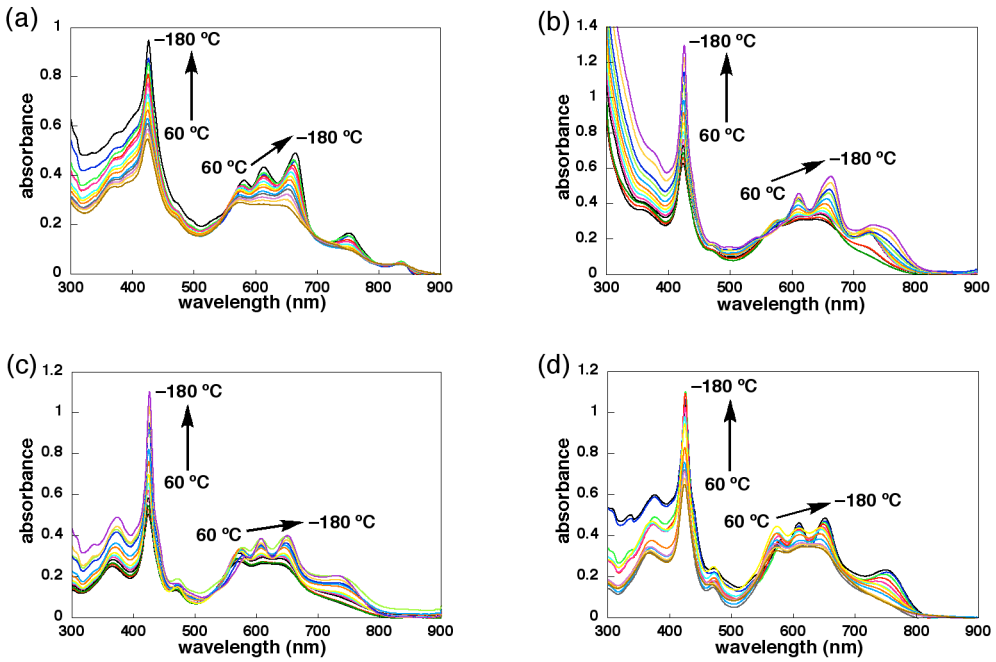
Supporting Figure 11 (a) VT ^{1}H NMR spectral changes of **1a** from 30 to –80 °C in CD_2Cl_2 (1×10^{-3} M), wherein the signals assignable to α-H are labeled by asterisk, (b) ^{1}H NMR (i) 1D, (ii) COSY, and (iii) ROESY spectra of **1a** at 20 °C, and (c) ^{1}H NMR (i) 1D and (ii) COSY spectra of **1a** at –80 °C. Based on the theoretical studies for ^{1}H NMR of the Zn-bridged double helices with various Zn···Zn distances (see also Supporting Figure 21), as seen in (a) and (b), **1a** mainly forms an *L* mode with a long Zn···Zn distance (due to ca. 7.2 ppm for pyrrole α-H) in an equilibrium between two modes of double helices at 20 °C. After coalescence at –20 °C, as seen in (a) and (c), **1a** exhibits independent signals including a downfield shift of pyrrole α-H at ca. 7.9 ppm derived from the *L* mode with a long Zn···Zn distance and an upfield shift of pyrrole α-H at ca. 6.8 ppm derived from the *S* mode with a short Zn···Zn distance. At r.t. in (b), the assignment of pyrrole α-H as the averaged signal of the *L* and *S* modes was achieved by 2D NMR. Although the details should be examined, pyrrole α-H showed no significant correlations with other ^{1}H signals and can be assigned by the correlations of the other ^{1}H signals. On the other hand, at –80 °C, two sets of independent signals, derived from main *L* and minor *S* modes, were observed. Assignment of pyrrole α-H in both the *L* and *S* modes was conducted by the signal shapes and correlations (no significant correlations as observed at 20 °C), also supported by the theoretical study (Supporting Figure 21) and the results of **1b**–**d** (Supporting Figure 12). Furthermore, the ratios (ca. 11:9) of the *L* and *S* modes were derived from the integrals of f^L and f^S as methylene units of the linkers. In particular, the chemical shift of f^S at 5.77 ppm is very close to the corresponding signals of **1b**–**d** as mainly *S* modes. From these observations, the VT ^{1}H NMR suggests that there are the transitions between two modes of double helices, and the preferable stretching modes are different at lower temperatures in **1a** and **1b**–**d** (Supporting Figure 12). Short straps in **1a** can behave as jacks that extend the double helix, resulting in the formation of the main *L* mode along with the minor *S* mode. These results are consistent with the VT UV/vis spectral changes in 2-methyl-THF (Supporting Figure 8).



Supporting Figure 11 (Continued)



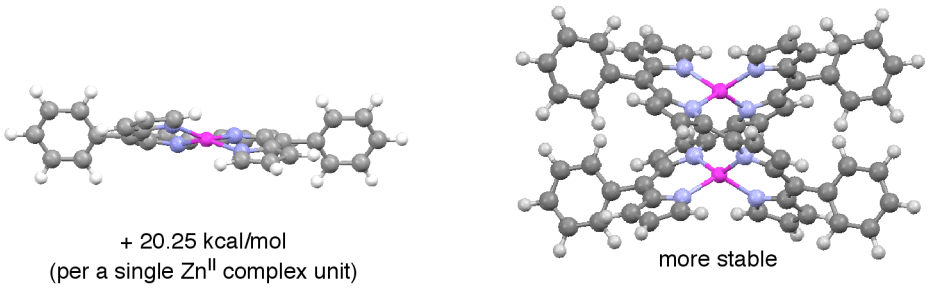
Supporting Figure 12 VT ^{1}H NMR spectral changes of (a) **1b**, (b) **1c**, and (c) **1d** from 20 to –80 °C in CD_2Cl_2. The less fine spectra in (a) are ascribable to the low solubility of **1b**. Based on the theoretical studies for ^{1}H NMR of the Zn-bridged double helices with various Zn···Zn distances (see also Supporting Figure 21), **1b–d** mainly exist as *S* modes with short Zn···Zn distances. At r.t., the downfield-shifted signals of pyrrole α-H in **1b** (ca. 7.1–7.2 ppm) compared to those of **1c**,**d** (ca. 6.9–7.0 ppm) are derived from the partial contribution of the *L* mode in **1b** (Supporting Figure 3). The upfield shifts of pyrrole α-H in **1b–d** at lower temperatures suggest the transition to the double helices with shorter Zn···Zn distances (as more shrunk double helices in the *S* modes).



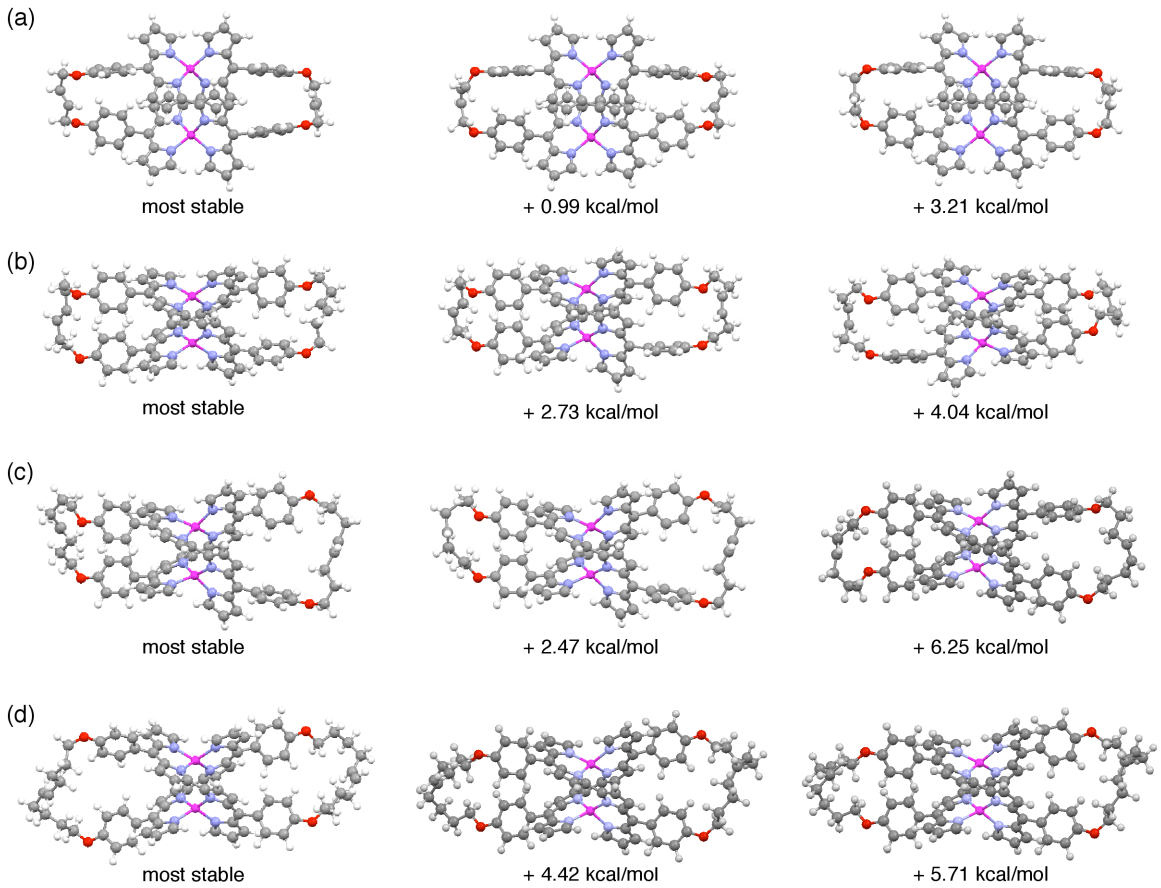
Supporting Figure 13 VT UV/vis absorption spectral changes of (a) **3a**, (b) **3b**, (c) **3c**, and (d) **3d** at each 20 °C from 60 to –180 °C in 2-methyl-THF (1×10^{-5} M). In contrast to the behaviors in Supporting Figure 8, singly strapped species show the stretching as the *S* mode of double helices with short Zn···Zn distances. It is not easy to optically resolve these singly strapped double helices due to their low solubilities.

4. Computational and theoretical studies of double helical metal complexes

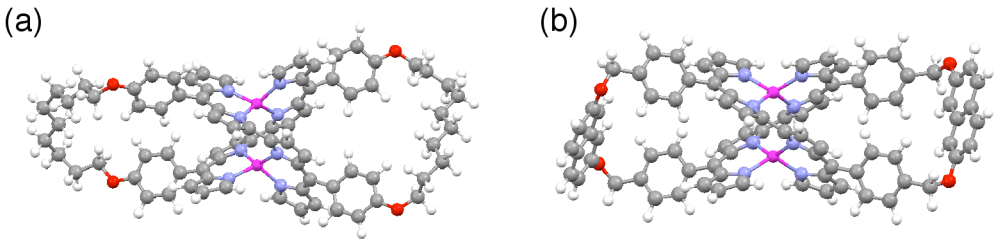
DFT and semi-empirical calculations. Ab initio and semi-empirical calculations of metal complexes in Supporting Figure 14–17 were carried out by using Gaussian 03 program[S7] and DELL optiplex 960 and HP Compaq dc5100 SFF computers. The structures were optimized, and the total electronic energies were calculated at the B3LYP level using a 6-31G(d,p) basis set and AM1 level. Ab initio and semi-empirical calculations of model *M*-type helices in Supporting Figure 18–21 were carried out by using Gaussian 09 program[S8] and the RIKEN Integrated Cluster of Clusters (RICC) facility. The structures were optimized by constraining the Zn···Zn distance under D_2 or C_1 symmetry, and the total electronic energies were calculated at the B3LYP or M06 level using 6-31G(d,p) basis sets. Electronic absorption and CD spectra were calculated by the ZINDO/S method. The transition length form was used to calculate rotational strengths. ^{1}H NMR spectra were calculated at B3LYP/6-31G(d,p) level. Chemical shifts were calculated from $\delta = \sigma_{ref} - \sigma$. TMS was used as the reference compound with the σ_{ref} values: ^{1}H: 31.7551.



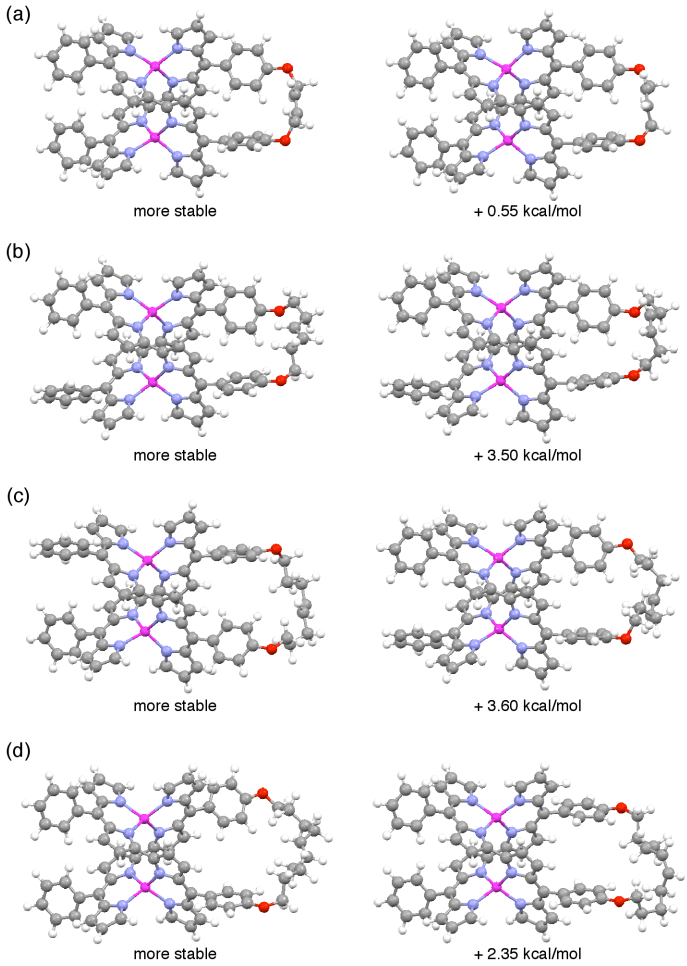
Supporting Figure 14 Optimized structures of Zn^{II} complexes of *meso*-phenyl-substituted bidipyrrin as a [1 + 1]-type single helix (left) and a [2 + 2]-type double helix (**BDPR-Zn**)[S9] (right) at B3LYP/6-31G(d,p) level, suggesting that the [2 + 2]-type double helix is more stable at 20.25 kcal/mol per a single Zn^{II} complex unit.



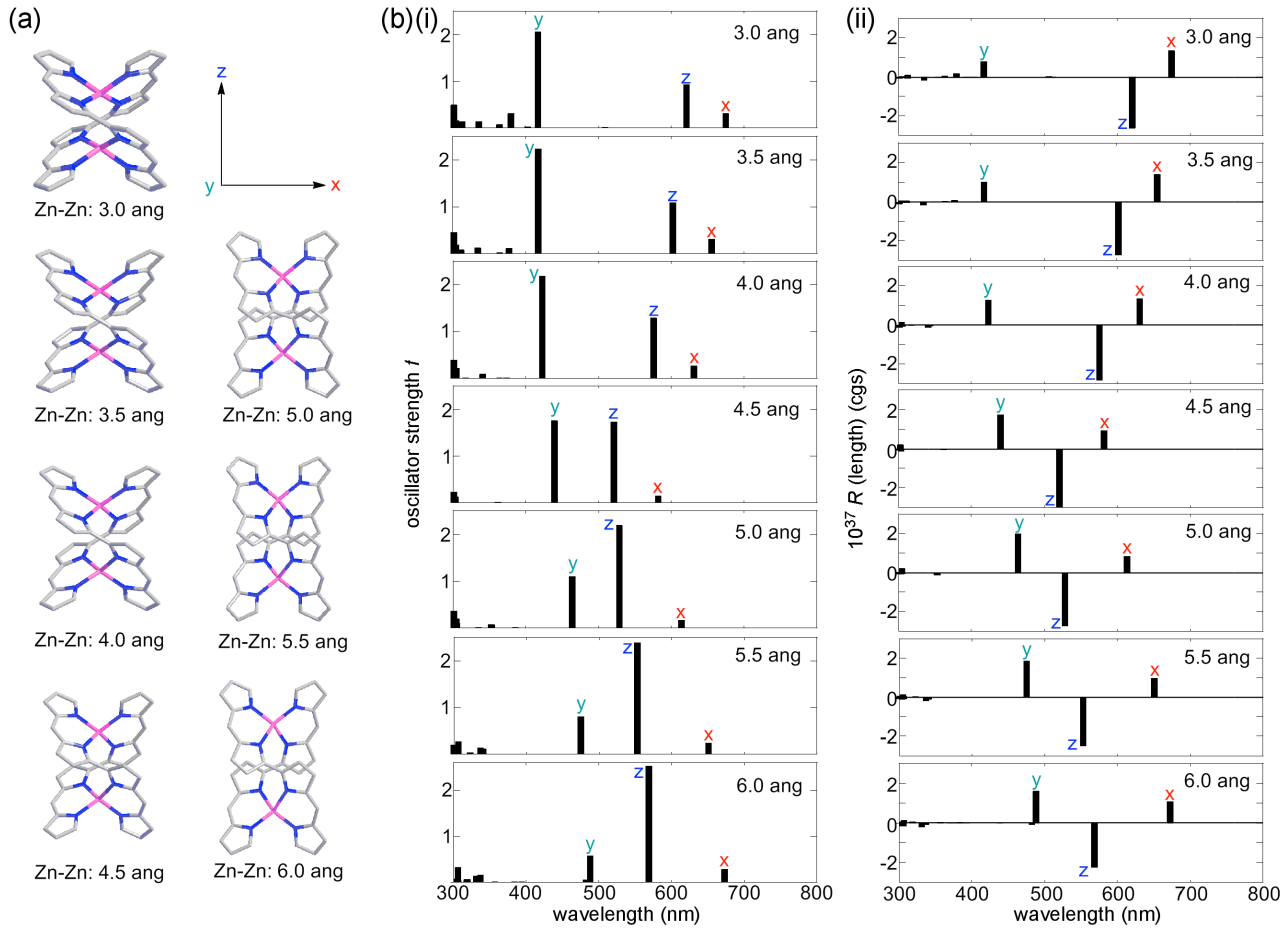
Supporting Figure 15 Optimized structures (three isomers *trans*/*trans*-, *cis*/*trans*-, and *cis*/*cis*-isomers from left to right) of (a) **1a**, (b) **1b**, (c) **1c**, and (d) **1d** at B3LYP/6-31G(d,p) level. Single-crystal X-ray analysis of **1a** suggests the formation of a *trans*/*trans*-isomer. Although it is not easy to completely determine the streoisomers of C=C, theoretical study along with ^{1}H NMR provides the speculation that *trans*/*trans*-isomers are often preferable.



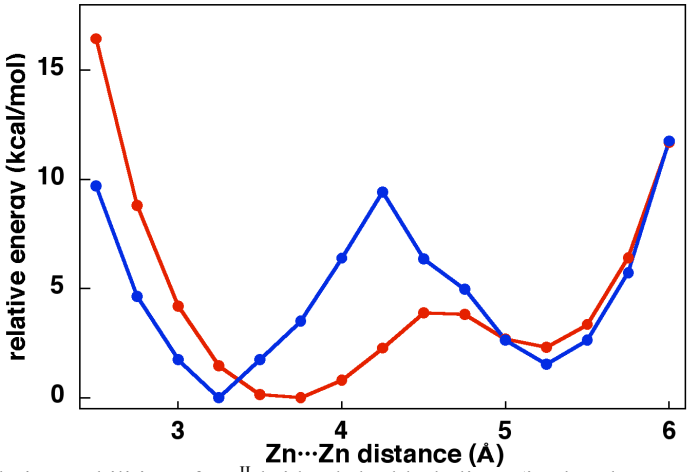
Supporting Figure 16 Optimized structures of (a) **1d´** and (b) **1e** at B3LYP/6-31G(d,p) level. It is not easy to treat the alkyl-strapped **1d´** in several procedures, resulting in choosing alkenyl-strapped **1a**–**d** as the double helices in this study, even though they have several problems for stereoisomers (see also the caption of Supporting Figure 15).



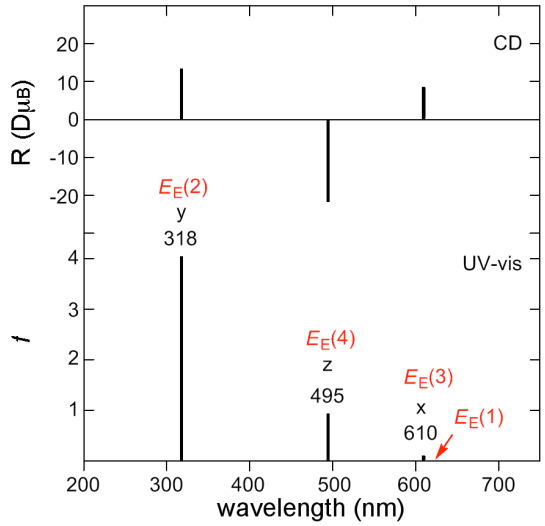
Supporting Figure 17 Optimized structures of (a) **3a**, (b) **3b**, (c) **3c**, and (b) **3d** as *trans*-isomers (left) and *cis*-isomers (right) at AM1 level. Compared to the optimized structures by DFT, the AM1 calculations of the Zn^{II}-bridged double helices afford the longer Zn···Zn distances. Preferable *trans*- and *cis*-geometries in singly strapped double helices are estimated by the calculations in this figure. Although it is not easy to completely determine the streoisomers of C=C, theoretical study along with ^{1}H NMR provides the speculation that *trans*-isomers are often preferable.



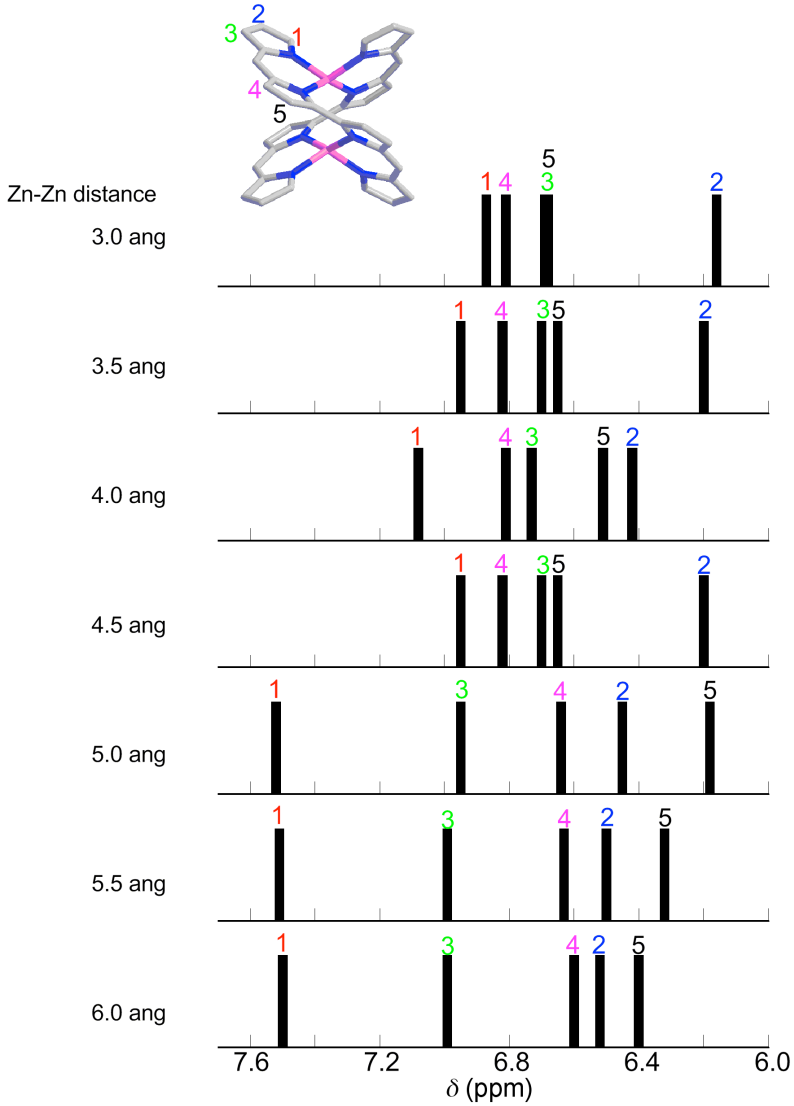
Supporting Figure 18 (a) Optimized structures of Zn^{II}-bridged *M*-type double helices (in the absence of *meso*-phenyl moieties) with Zn···Zn distances of 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, and 6.0 Å estimated by B3LYP/6-31G(d,p) and (b) corresponding calculated (i) electronic absorption and (ii) CD spectra by ZINDO. Hydrogen atoms are omitted for clarity in (a). The relative intensity for the electronic transition along the z-axis increases with increasing the Zn···Zn distance. The CD sign for the z-axis transition is negative, independent of the Zn···Zn distance. There are no significant differences between the double helices with (not shown) and without *meso*-phenyl moieties.



Supporting Figure 19 Relative stabilities of Zn^{II}-bridged double helices (in the absence of *meso*-phenyl moieties as seen in Supporting Figure 18) with Zn···Zn distances of 2.5–6.0 Å (with each 0.25 Å unit) estimated by B3LYP/6-31G(d,p) (red) and M06/6-31G(d,p) (blue). Both DFT calculations show the similar features. The minima at 3.75 and 5.25 Å (B3LYP) and 3.25 and 5.25 Å (M06) suggest the existence of two stable modes of double helices. The energy barrier at 4.5 Å (B3LYP) and 4.25 Å (M06) is derived from the orthogonally arranged two dipyrrin moieties in a bidipyrrin unit. In fact, the N–αC–αC–N dihedral angles between two dipyrrin units are arranged at 22.2° (26.7°), 24.9° (29.7°), 27.9° (32.8°), 31.8° (36.5°), 36.3° (40.2°), 41.5° (42.5°), 48.2° (49.8°), 58.1° (58.7°), 76.7° (102.6°), 102.7° (114.2°), 116.4° (124.4°), 125.9° (132.8°), 133.0° (137.9°), 138.5° (142.2°), and 142.9° (144.5°) by B3LYP (M06) for the Zn···Zn distances of 2.5, 2.75, 3.0, 3.25, 3.5, 3.75, 4.0, 4.25, 4.5, 4.75, 5.0, 5.25, 5.5, 5.75, and 6.0 Å, respectively.



Supporting Figure 20 Calculated absorption and CD spectra of the double helix using exciton coupling theory. Geometrical parameters of the B3LYP-optimized structure of the *M*-form of **BDPR-Zn** (Zn···Zn distance: 3.51 Å)[S6] and spectral parameters of a dipyrrin anion by the ZINDO calculations were used to simulate the spectra.



Supporting Figure 21 ^{1}H NMR chemical shifts of Zn^{II}-bridged double helices (in the absence of *meso*-phenyl moieties) with Zn···Zn distances of 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, and 6.0 Å estimated by B3LYP/6-31G(d,p). Two modes of double helices according to the Zn···Zn distances exhibit the dramatic chemical shifts such as, in particular, pyrrole α-H, which are shifted to upfield and downfield at shorter and longer Zn···Zn distances, respectively.

Cartesian Coordination of Optimized Structures

Zn^{II} complexes of *meso*-phenyl-substituted bidipyrrin as a [1 + 1]-type single helix (DFT)

–3153.4681514 hartree

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1a (*cis/cis*) (DFT)

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1a (*cis*/*trans*) (DFT)

–6917.468336 hartree
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3a (*trans*) (AM1)

0.9231927 hartree

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3b (*cis*) (AM1)
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N,-1.7321002037,-0.26986237,-0.9403024486
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C,-1.1660061841,2.8043095922,-7.9744022611
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3c (*trans*) (AM1)

0.8752639 hartree

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C,0.8442928381,-2.250927515,-4.7192850159
C,-1.6792004875,-2.3786651115,-4.7063017525
C,-2.9477822269,-2.289678971,-4.1254024267
C,1.8089798511,-1.8930089115,-3.7883032836
C,2.5795195314,-2.1434783672,-0.5891965666
C,5.6234714553,-0.1149240222,4.5047892039
C,-1.5336197241,-3.4898888555,-8.8305811107
C,-2.0659107422,-4.3697761844,-7.8882970775
C,-2.1187139559,-4.0085806929,-6.5431498356
C,-1.6254447993,-2.763232077,-6.1300854669
C,-1.0478992762,-2.2469190187,-8.4247908461
C,-1.086375073,-1.8840643293,-7.079616352
C,2.7525303071,-0.0500819939,0.323292941
C,2.7393391714,2.3151781324,1.1386412329
C,3.0588242636,3.3496338587,2.1173520363
C,3.1197942694,0.9716314532,1.2190176659
C,3.1708651966,-1.4375526522,0.449794404
C,1.8063089081,-1.1792948413,-1.3501420798
C,1.7895959403,4.2065419333,0.4398927177
C,-5.2290050484,-2.2881863803,-3.8878936119
C,-4.5730178456,-1.9598959248,-2.636988917
C,6.1296132602,-1.3025619747,6.5316594486
C,-1.37086932,3.4568981446,-6.4052443156
C,-0.4968751006,4.1161790795,-5.5296317466
C,-0.1188238763,5.4391699497,-5.7969525011
C,-0.6161937782,6.0941979494,-6.9223005703
C,-1.4814576424,5.4329025781,-7.793691545
C,2.3174237781,-0.9975531526,8.7746710389
C,-2.452785356,-1.5507306302,5.7323246195
C,-3.7343732508,-1.0972967951,6.068444243
C,-4.6446633413,-0.7233496235,5.0595690596
C,-2.4940514053,2.1072686456,0.8531191094
C,-2.2980950762,-2.6324146144,1.4655137073
C,-2.495390551,-0.1474981804,1.2520906674
C,-2.7232230052,1.1624830343,1.843552708
C,-2.5772198934,-1.3564446983,1.9653938414
C,-2.9806474383,-1.2673084655,3.3809166033
C,-4.2594332153,-0.8039559045,3.7283374331
C,-1.8550543256,4.1141535775,-7.5348978227
C,1.1507865423,-1.2560280212,9.3722102312

[S7] *Gaussian 03* (Revision C.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

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