

Supporting Information

Recognition of atomic-level difference in porphyrin dyads for self-sorted supramolecular polymer growth

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Materials and Methods

All commercially available reagents were of reagent grade and used without further purification. Dichloromethane (CH_2Cl_2), *n*-hexane, acetonitrile, tetrahydrofuran (THF), and toluene were freshly distilled before each use. ^1H NMR spectra were recorded at 25 °C using a Bruker Advance DPX 250 or DPX 400 spectrometer. ^{13}C NMR spectra were recorded at 25 °C using a Bruker DPX 400 spectrometer. Matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF-MS) was performed using a Bruker Daltonics LRF20 with dithranol (1,8,9-trihydroxyanthracene) as the matrix. Recycling size exclusion chromatography (SEC) was performed using a JAI model LC9201 equipped with JAIGEL-1H, JAIGEL-2H, and JAIGEL-3H columns using THF (DUKSAN Pure Chemicals) as the eluent. UV–vis absorption spectra were measured using a JASCO V-660 spectrometer with a thermostatic cell holder coupled with a controller (ETCS-761, JASCO), and fluorescence spectra were recorded using a JASCO FP-6300 spectrofluorimeter with a temperature controller (ETC-273T, JASCO). All spectral measurements were performed using a quartz cuvette with a path length of 1 cm. Infrared absorption spectra were recorded using a Fourier-transform infrared (FT-IR) (JASCO FT/IR-4700) spectrometer. A transmission electron microscope (TEM) was operated at 120 kV (TEM, JEM-1400, JEOL, Tokyo, Japan) to capture images. For TEM measurements, a drop of each sample in methylcyclohexane was placed on a carbon-coated copper grid and allowed to evaporate under ambient conditions. The sample was stained by placing a drop of uranyl acetate solution (2 wt%) onto the surface of the sample-loaded grid. The deposited sample was allowed to rest for 1 min at minimum, after which the excess solution was wicked off using filter paper.

The images were acquired with Veleta and Tengra CCD cameras (EMSIS, Germany) with 1 and 5.3 MP resolutions, respectively. A scanning electron microscope (SEM, 7610F-Plus, JEOL Ltd.) was used at room temperature, and the samples were prepared by coating on the silicon wafer. Atomic force microscopy (AFM, NX10, Park Systems) images were obtained. Each sample used for AFM measurements was dropped and spin-coated onto a freshly cleaved mica surface.

Non-linear regression for estimating the thermodynamic parameters

The degree of aggregation (α_{agg}) for PD_{Zn} and PD_{Cu} obtained from apparent absorbance changes at the absorption maxima was plotted as a function of absolute temperature (T). The elongation enthalpy (ΔH_e) and equilibrium constant of the nucleation step (K_a) for PD_{Zn} were estimated by the nonlinear least-squares fitting method using eqs (S1) and (S2) from elongation

and nucleation regimes, respectively, where T_e is the critical elongation temperature at a given concentration, R is the ideal gas constant, and α_{SAT} is introduced as a parameter to ensure that $\frac{\alpha_{agg}}{\alpha_{SAT}}$ does not exceed unity.

$$\alpha_{agg} = \alpha_{SAT} \left[1 - \exp \left[\frac{-\Delta H_e}{RT_e^2} (T - T_e) \right] \right] \quad (S1)$$

$$\alpha_{agg} = \alpha_{SAT} \left[K_a^{\frac{1}{3}} \exp \left[\left(\frac{2}{3K_a^{\frac{1}{3}}} - 1 \right) \frac{\Delta H_e}{RT_e^2} (T - T_e) \right] \right] \quad (S2)$$

Estimation of twist angles between adjacent porphyrin units

The transition dipole moment μ was estimated from Soret absorption bands of \mathbf{PD}_{Zn} in MCH at 373 K using eq. S3, where f is oscillator strength, $\Delta\nu_{\frac{1}{2}}$ is full width at half-maximum of the Soret band, ϵ_{max} extinction coefficient at absorption maximum, e is the charge of an electron, $\bar{\nu}$ is the mean absorption frequency of the Soret band in wavenumber, m_e is the mass of an electron, and h is Plank's constant.

$$f = 4.32 \times 10^9 \epsilon_{\max \Delta\nu_{\frac{1}{2}}} = \frac{(8\pi^2 m_e \bar{\nu})}{(3he^2)} |\mu|^2 \quad (S3)$$

The twist angle between adjacent porphyrin units (θ) was estimated using eq. S4, where ΔE is the apparent splitting energy observed from absorption spectra of \mathbf{PD}_{Zn} in MCH at 293 K, $\vec{\mu}_1$ and $\vec{\mu}_2$ are vectors of transition dipole moments, r is the center-to-center distance of porphyrin units, \vec{r}_{12} is the corresponding unit vector, ϕ is the rotation angle of monomer units in helical turns, and ϵ_0 is vacuum permittivity.

$$\Delta E = \frac{[\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \vec{r}_{12})(\vec{\mu}_2 \cdot \vec{r}_{12})]}{4\pi\epsilon_0 r^3} = \frac{\mu^2}{4\pi\epsilon_0 r^3} [\cos \phi - 3\cos \theta \cos (\theta - \phi)] \quad (S4)$$

H, -OCH₂CH₂), 1.44–1.25 (m, 28 H, -(CH₂)₇CH₃), 0.87–0.83 (m, 6 H, -(CH₂)₇CH₃). MALDI-TOF-MS calcd. for C₅₄H₆₂N₄O₄Zn [M]⁺: *m/z* = 894.41; found: 894.05.

2: *N*-bromosuccinimide (264 mg, 1.48 mmol) was added to a solution of **1** (664 mg, 0.74 mmol) in dry CH₂Cl₂ (70 mL), and the mixture was stirred for 30 min at 0 °C. The reaction mixture was quenched with acetone and evaporated to dryness. The crude was chromatographed on silica gel using CH₂Cl₂ as an eluent to obtain **2** (427 mg, 0.41 mmol, 55%) as a purple solid. ¹H NMR (300 MHz, CDCl₃): δ = 9.72–8.84 (m, 8 H, β-pyrrole), 8.42–8.39 (d, *J* = 8.3 Hz, 2 H, *o*-H in C₆H₄), 8.24–8.21 (d, *J* = 8.3 Hz, 2 H, *m*-H in C₆H₄), 7.32–7.31 (d, *J* = 2.2 Hz, 2 H, *o*-H in C₆H₃), 6.89–6.88 (t, *J* = 2.2 Hz, 1 H, *p*-H in C₆H₃), 4.14–4.09 (m, 7 H, overlapped -OCH₂- and -CO₂CH₃), 1.91–1.82 (qui, 4 H, -OCH₂CH₂), 1.25 (m, 28 H, -(CH₂)₇CH₃), 0.87–0.81 (m, 6 H, -(CH₂)₇CH₃). MALDI-TOF-MS calcd. for C₅₄H₆₀Br₂N₄O₄Zn [M]⁺: *m/z* = 1054.22; found: 1054.73

3: Pd(PPh₃)₄ (46.8 mg, 0.041 mmol) was added to the mixture solution of **2** (427 mg, 0.41 mmol), phenylboronic acid (198 mg, 1.62 mmol), and K₃PO₄ (4.48 g, 3.24 mmol) in dried THF (30 mL). The reaction mixture was refluxed for 20 h under N₂ and subsequently evaporated to dryness. The crude fraction was extracted using CH₂Cl₂ and distilled water. The combined organic layer was concentrated and then purified by silica column chromatography using 5% ethyl acetate in *n*-hexane as an eluent. Further purification was performed using recycling SEC, and the first fraction was collected and evaporated to obtain **3** (405 mg, 0.39 mmol, 95%) as a purple solid. ¹H NMR (300 MHz, CDCl₃): δ = 9.08–8.87 (m, 8 H, β-pyrrole), 8.44–8.41 (d, *J* = 8.3 Hz, 2 H, *o*-H in C₆H₄), 8.32–8.29 (d, *J* = 8.3 Hz, 2 H, *m*-H in C₆H₄), 8.23–8.20 (m, 4 H, *o*-H in C₆H₅), 7.81–7.71 (m, 6 H, overlapped *m*- and *p*-H in C₆H₅), 7.38 (d, *J* = 2.2 Hz, 2 H, *o*-H in C₆H₃), 6.89–6.87 (t, *J* = 2.2 Hz, 1 H, *p*-H in C₆H₃), 4.13–4.08 (m, 7 H, overlapped -OCH₂- and -CO₂CH₃), 1.89–1.80 (q, 4 H, -OCH₂CH₂), 1.25 (m, 28 H, -(CH₂)₇CH₃), 0.84 (m, 6 H, -(CH₂)₇CH₃). MALDI-TOF-MS calcd. for C₆₆H₇₀N₄O₄Zn [M]⁺: *m/z* = 1046.47; found: 1046.16.

4: A 10 M NaOH aqueous solution was added to a solution of **1** (1.17 g, 1.31 mmol) in THF (50 mL), and the solution was vigorously stirred for 2 d at 50 °C. The basic solution was neutralized using HCl and extracted with ethyl acetate and distilled water. The combined organic layer was evaporated to dryness and redissolved in 10% MeOH/CH₂Cl₂ (100 mL) with

excess amounts of $\text{Zn}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (3.00 g, 13.68 mmol). Then, the mixture was extracted with ethyl acetate and distilled water. The combined organic layer was purified through column chromatography using 2% MeOH/ CH_2Cl_2 as an eluent. The first fraction was collected and freeze-dried from benzene to obtain **4** (908 mg, 1.03 mmol, 79%) as a reddish powder. ^1H NMR (300 MHz, CDCl_3): δ = 10.34 (s, 2 H, *meso*-H), 9.48–9.10 (m, 8 H, β -pyrrole), 8.58–8.55 (d, J = 8.1 Hz, 2 H, *o*-H in C_6H_4), 8.42–8.40 (d, J = 8.1 Hz, 2 H, *m*-H in C_6H_4), 7.44–7.43 (d, J = 2.1 Hz, 2 H, *o*-H in C_6H_3), 6.94–6.92 (t, J = 2.1 Hz, 1 H, *p*-H in C_6H_3), 4.18–4.14 (t, 4 H, - OCH_2 -), 1.94–1.84 (qui, 4 H, - OCH_2CH_2), 1.25 (m, 28 H, $-(\text{CH}_2)_7\text{CH}_3$), 0.87–0.83 (m, 6 H, $-(\text{CH}_2)_7\text{CH}_3$). MALDI-TOF-MS calcd. for $\text{C}_{53}\text{H}_{60}\text{N}_4\text{O}_4\text{Zn}$ $[\text{M}]^+$: m/z = 880.39; found: 880.74.

$^{\text{D}}\text{PD}_{\text{Zn}}$: To a mixture solution of **4** (405 mg, 0.46 mmol), hexa-2,4-diyne-1,6-diamine (39.5 mg, 0.22 mmol), EDC \cdot HCl (167 mg, 0.87 mmol), and HOBT (118 mg, 0.87 mmol) in CH_2Cl_2 (80 mL), TEA (1.0 mL, 7.18 mmol) were added. The reaction mixture was stirred for 12 h at 25 $^\circ\text{C}$ and subsequently extracted with CH_2Cl_2 and aqueous NH_4Cl . The combined organic layer was collected and evaporated to dryness. The crude product was purified through column chromatography using 2% MeOH/ CH_2Cl_2 as an eluent. Further purification was performed through using recycling SEC, and the first fraction was collected and recrystallized from THF and MeOH to obtain **$^{\text{D}}\text{PD}_{\text{Zn}}$** (66 mg, 0.036 mmol, 16%) as a reddish powder. ^1H NMR (300 MHz, THF- d_8): δ = 10.25 (s, 4 H, *meso*-H), 9.41–9.02 (m, 16 H, β -pyrrole), 8.51 (m, 2 H, CONH), 8.34 (m, 8 H, overlapped *o*-H in C_6H_4 and *m*-H in C_6H_4), 7.40–7.39 (m, 4 H, *o*-H in C_6H_3), 6.94–6.93 (m, 2 H, *p*-H in C_6H_3), 4.54–4.52 (d, 4 H, CONH- CH_2 -), 4.19–4.15 (t, 8 H, - OCH_2 -), 1.92–1.82 (qui, 8 H, - OCH_2CH_2), 1.55–1.29 (m, 56 H, $-(\text{CH}_2)_7\text{CH}_3$), 0.88–0.84 (m, 12 H, $-(\text{CH}_2)_7\text{CH}_3$). MALDI-TOF-MS calcd. for $\text{C}_{112}\text{H}_{124}\text{N}_{10}\text{O}_6\text{Zn}_2$ $[\text{M}]^+$: m/z = 1835.83; found: 1837.12.

5: To a solution of **$^{\text{D}}\text{PD}_{\text{Zn}}$** (54 mg, 0.029 mmol) in CH_2Cl_2 (50 mL), TFA (1 mL) was added, and the solution was stirred for 2 h at 25 $^\circ\text{C}$. Then, the reaction mixture was poured into distilled water and extracted with CH_2Cl_2 . The combined organic layer was collected and dried over Na_2SO_4 and purified via silica column chromatography using 2% MeOH/ CH_2Cl_2 as an eluent to obtain **5** (45 mg, 0.026 mmol, 89%) as a reddish powder. ^1H NMR (300 MHz, THF- d_8): δ = 10.35 (s, 4 H, *meso*-H), 9.44–9.03 (m, 16 H, β -pyrrole), 8.53 (t, 2 H, CONH), 8.38 (m, 8 H, overlapped *o*-H in C_6H_4 and *m*-H in C_6H_4), 7.43–7.42 (d, 4 H, *o*-H in C_6H_3), 6.95 (t, 2 H, *p*-H in C_6H_3), 4.54–4.52 (d, 4 H, CONH- CH_2 -), 4.18–4.14 (t, 8 H, - OCH_2 -), 1.91–1.82 (qui, 8 H, -

OCH₂CH₂), 1.59–1.29 (m, 56 H, -(CH₂)₇CH₃), 0.89–0.83 (m, 12 H, -(CH₂)₇CH₃), -0.34 (s, 4 H, inner H). MALDI-TOF-MS calcd. for C₁₁₂H₁₂₈N₁₀O₆ [M]⁺: *m/z* = 1710.01; found: 1710.31.

^DPD_{Cu}: To the solution of **5** in 10% MeOH/CH₂Cl₂ (50 mL), Cu(OAc)₂•H₂O was added. The reaction mixture was stirred for 12 h at 25 °C and subsequently extracted with CH₂Cl₂ and distilled water. The combined organic layer was collected, evaporated to dryness, and further purified via silica column chromatography using 2% MeOH/ CH₂Cl₂ as eluent. **^DPD_{Cu}** was obtained as reddish power in 97% yield. MALDI-TOF-MS calcd. for C₁₁₂H₁₂₄N₁₀O₆Cu₂ [M]⁺: *m/z* = 1831.83; found: 1832.75.

6: To the solution of **3** (275 mg, 0.262 mmol) in THF (20 mL), aqueous 5 M NaOH (20 mL) was added, and the solution was vigorously stirred for 4 d at 50 °C. The basic solution was neutralized using HCl and extracted using ethyl acetate and distilled water. The combined organic layer was evaporated to dryness over Na₂SO₄. The residue was purified via silica column chromatography using 2% MeOH/CH₂Cl₂ as an eluent to obtain a quantitative yield of **6** (275 mg, 0.266 mmol)%. ¹H NMR (300 MHz, CDCl₃): δ = 9.09–8.89 (m, 8 H, β-pyrrole), 8.52–8.49 (d, *J* = 8.3 Hz, 2 H, *o*-H in C₆H₄), 8.37–8.34 (d, *J* = 8.3 Hz, 2 H, *m*-H in C₆H₄), 8.24–8.21 (m, 4 H, *o*-H in C₆H₅), 7.82–7.72 (m, 6 H, overlapped *m*- and *p*-H in C₆H₅), 7.39–7.38 (d, *J* = 2.2 Hz, 2 H, *o*-H in C₆H₃), 6.89–6.88 (t, *J* = 2.2 Hz, 1 H, *p*-H in C₆H₃), 4.13–4.07 (m, 4 H, -OCH₂-), 1.90–1.81 (q, 4 H, -OCH₂CH₂), 1.25 (m, 28 H, -(CH₂)₇CH₃), 0.84 (m, 6 H, -(CH₂)₇CH₃). MALDI-TOF-MS calcd. for C₆₅H₆₈N₄O₄Zn [M+H]⁺: *m/z* = 1033.46; found: 1034.61.

^TPD_{Zn}: To a mixture solution of **6** (398 mg, 0.398 mmol), HOBt (99 mg, 0.73 mmol), EDC•HCl (140 mg, 0.73), and hexa-2,4-diyne-1,6-diamine (33 mg, 0.183 mmol) in CH₂Cl₂ (20 mL), TEA (1 mL, 7.18 mmol) was added. The reaction mixture was stirred for 2 d at 25 °C and subsequently extracted using ethyl acetate and aqueous NH₄Cl. The combined organic layer was dried over Na₂SO₄, and the crude product was purified via silica column chromatography using 2% MeOH/CH₂Cl₂ as an eluent. Further purification was performed through recyclable SEC using THF as eluent, and the first fraction was collected. After recrystallization using THF/*n*-hexane, **^TPD_{Zn}** (72 mg, 0.034 mmol, 18%) was obtained as a purple powder. ¹H NMR (300 MHz, CDCl₃): δ = 8.96–8.79 (m, 16 H, β-pyrrole), 8.44–8.41 (t, *J* = 5.3 Hz, 2 H, CONH),

8.27 (m, 8 H, overlapped *o*-H in C₆H₄ and *m*-H in C₆H₄), 8.18–8.15 (m, 8 H, *o*-H in C₆H₅), 7.72–7.67 (m, 12 H, overlapped *m*- and *p*-H in C₆H₅), 7.35–7.34 (d, *J* = 2.2 Hz, 4 H, *o*-H in C₆H₃), 6.89–6.88 (t, *J* = 2.2 Hz, 2 H, *p*-H in C₆H₃), 4.48–4.46 (d, *J* = 5.3 Hz, 4 H, CONH-CH₂-), 4.15–4.11 (t, 8 H, -OCH₂-), 1.88–1.79 (qui, 8 H, -OCH₂CH₂), 1.57–1.25 (m, 56 H, -(CH₂)₇CH₃), 0.87–0.82 (m, 12 H, -(CH₂)₇CH₃). MALDI-TOF-MS calcd. for C₁₃₆H₁₄₀N₁₀O₆Zn₂ [M+H]⁺: *m/z* = 2140.96; found: 2141.24.

7: To a solution of **1PD**_{Zn} (72 mg, 0.148 mmol) in CH₂Cl₂ (50 mL), TFA (1.0 mL) was added. The reaction mixture was stirred for 2 h at 25 °C, poured into distilled water, and extracted with CH₂Cl₂. The combined organic layer was collected and dried over Na₂SO₄. The resulting solution was evaporated and purified via silica column chromatography using 2% MeOH/CH₂Cl₂ as an eluent to obtain **7** (45 mg, 0.139 mmol, 94%) as a reddish power. ¹H NMR (300 MHz, CDCl₃): δ = 8.96–8.78 (m, 16 H, β-pyrrole), 8.49–8.45 (t, *J* = 5.3 Hz, 2 H, CONH), 8.30 (m, 8 H, overlapped *o*-H in C₆H₄ and *m*-H in C₆H₄), 8.20–8.17 (m, 8 H, *o*-H in C₆H₅), 7.75–7.73 (m, 12 H, overlapped *m*- and *p*-H in C₆H₅), 7.38–7.37 (d, *J* = 2.2 Hz, 4 H, *o*-H in C₆H₃), 6.92–6.90 (t, *J* = 2.2 Hz, 2 H, *p*-H in C₆H₃), 4.49–4.47 (d, *J* = 5.3 Hz, 4 H, CONH-CH₂-), 4.15–4.11 (t, 8 H, -OCH₂-), 1.89–1.80 (qui, 8 H, -OCH₂CH₂), 1.57–1.25 (m, 56 H, -(CH₂)₇CH₃), 0.86–0.82 (m, 12 H, -(CH₂)₇CH₃) -2.72 (s, 4 H, inner H). MALDI-TOF-MS calcd. for C₁₃₆H₁₄₄N₁₀O₆ [M+H]⁺: *m/z* = 2015.14; found: 2017.66.

1PDCu: Cu(OAc)₂•H₂O was added to a solution of **7** in 10% MeOH/CH₂Cl₂ (50 mL). After being stirred for 12 h at 25 °C, the reaction mixture was extracted with CH₂Cl₂ and distilled water. The combined organic layer was collected and evaporated to dryness, and the residue was purified via silica column chromatography using 2% MeOH/CH₂Cl₂ as an eluent. **1PDCu** was obtained as a reddish power in 94% yield. NMR is not available due to paramagnetism. MALDI-TOF-MS calcd. for C₁₃₆H₁₄₀N₁₀O₆Cu₂ [M+H]⁺: *m/z* = 2137.97; found: 2139.98.

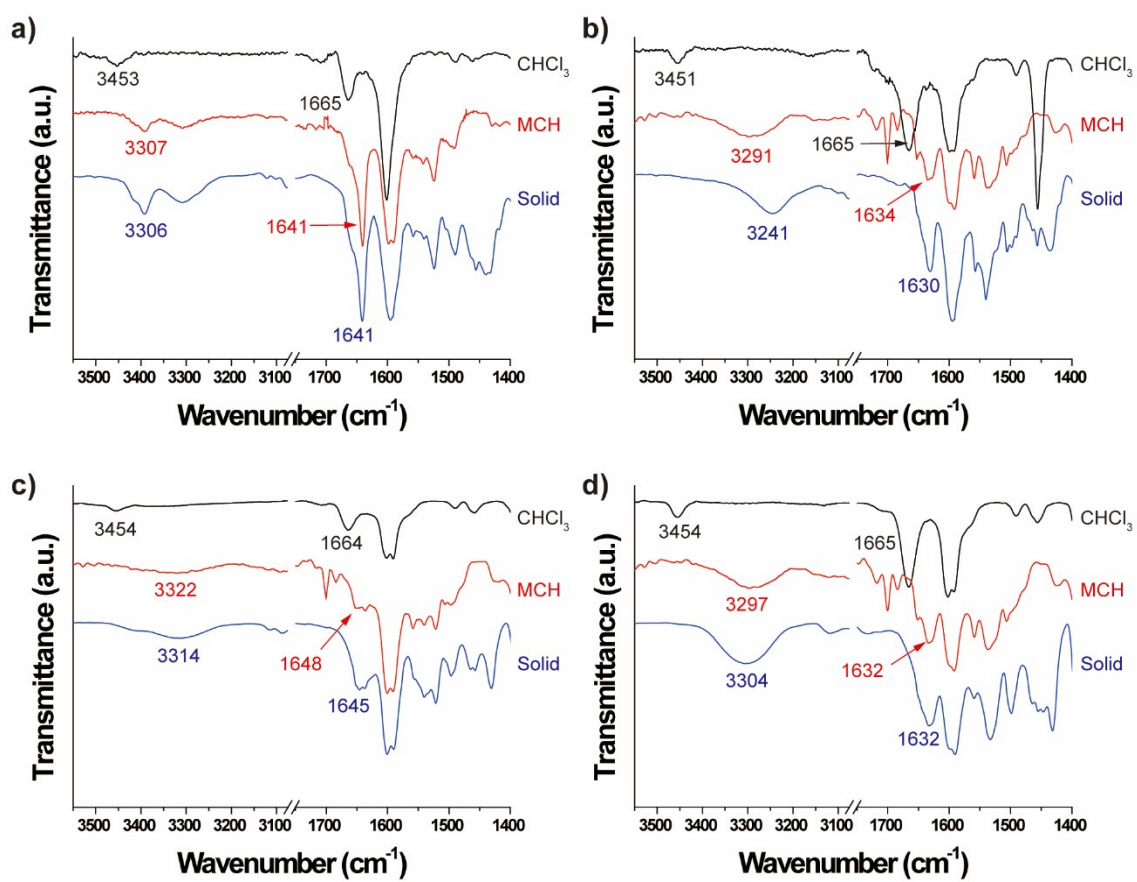


Figure S1. FT-IR spectra of PD_M s in CHCl_3 (Black line), MCH (Red line), and solid film (Blue line of a) ${}^1\text{PD}_{\text{Zn}}$, b) ${}^1\text{PD}_{\text{Cu}}$, c) ${}^2\text{PD}_{\text{Zn}}$, and d) ${}^2\text{PD}_{\text{Cu}}$.

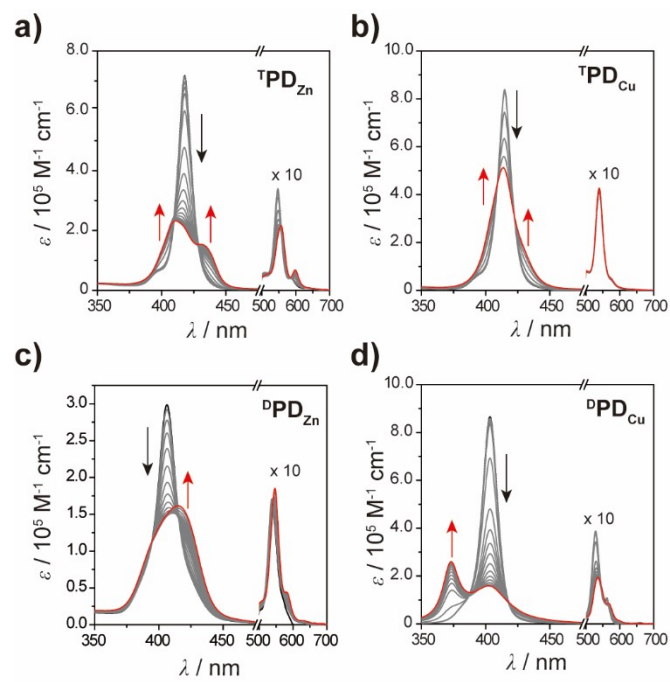


Figure S2. Absorption spectral changes of a) TPD_{Zn} , b) TPD_{Cu} , c) DPD_{Zn} , and d) DPD_{Cu} on cooling from 373 to 293 K at rate of 1.0 K min⁻¹.

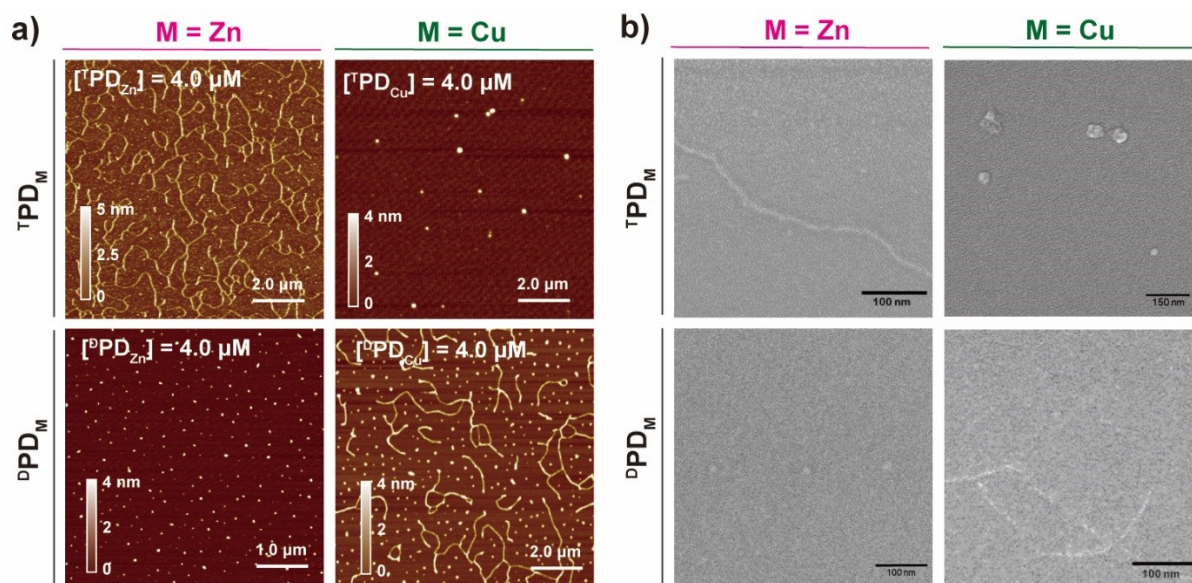
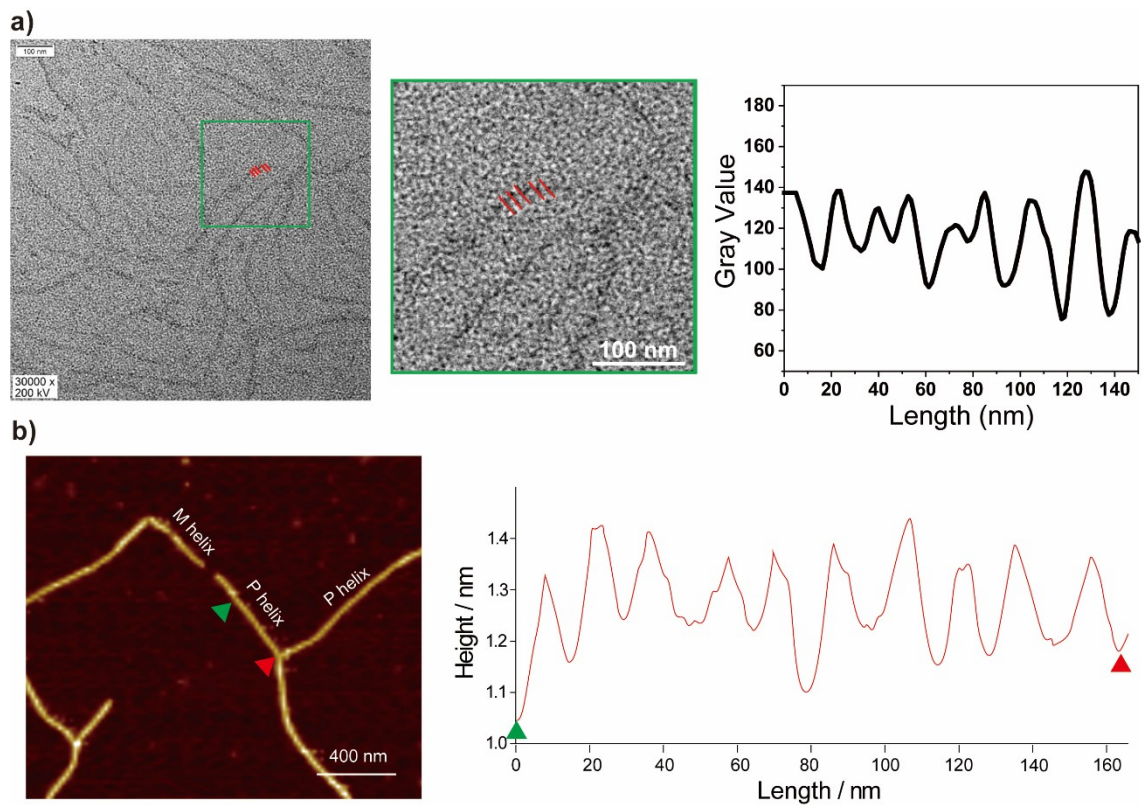


Figure S3. a) AFM and b) SEM images of PD_M s. SEM specimens were prepared from $2.0 \mu M$ PD_M s solutions.



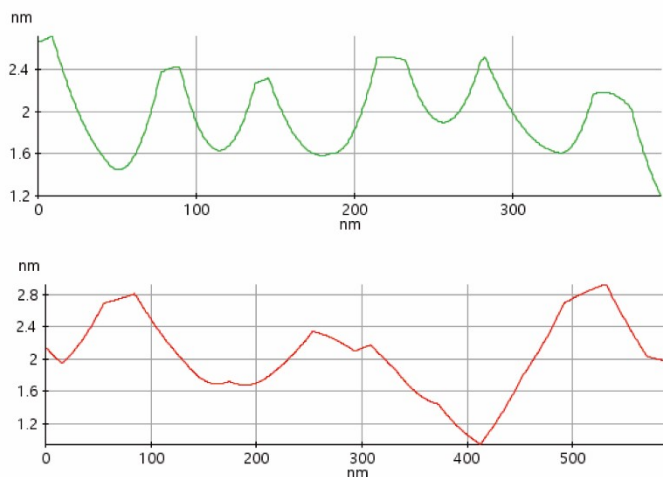
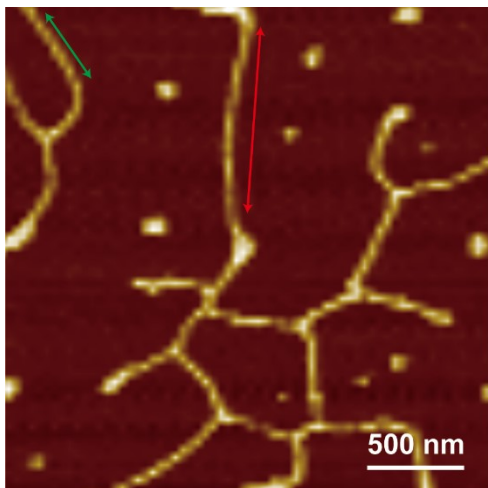


Figure S5. AFM image of DPD_{Cu} with height profiles.

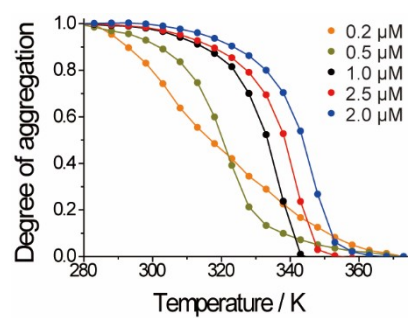


Figure S6. Concentration-dependent degree of aggregation upon heating at a rate of 1.0 K min^{-1} of TPD_{Zn} .

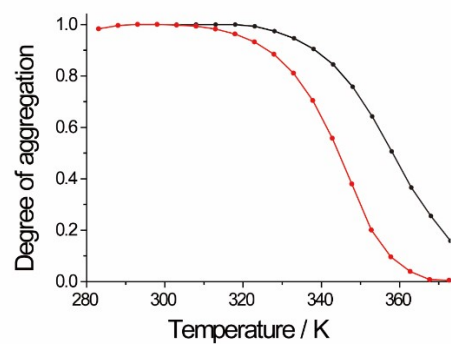


Figure S7. Temperature-dependent absorption change at 406.0 nm for TPD_{zn} ($2.0 \mu\text{M}$) in MCH (black line) and 10% toluene included MCH (red line).

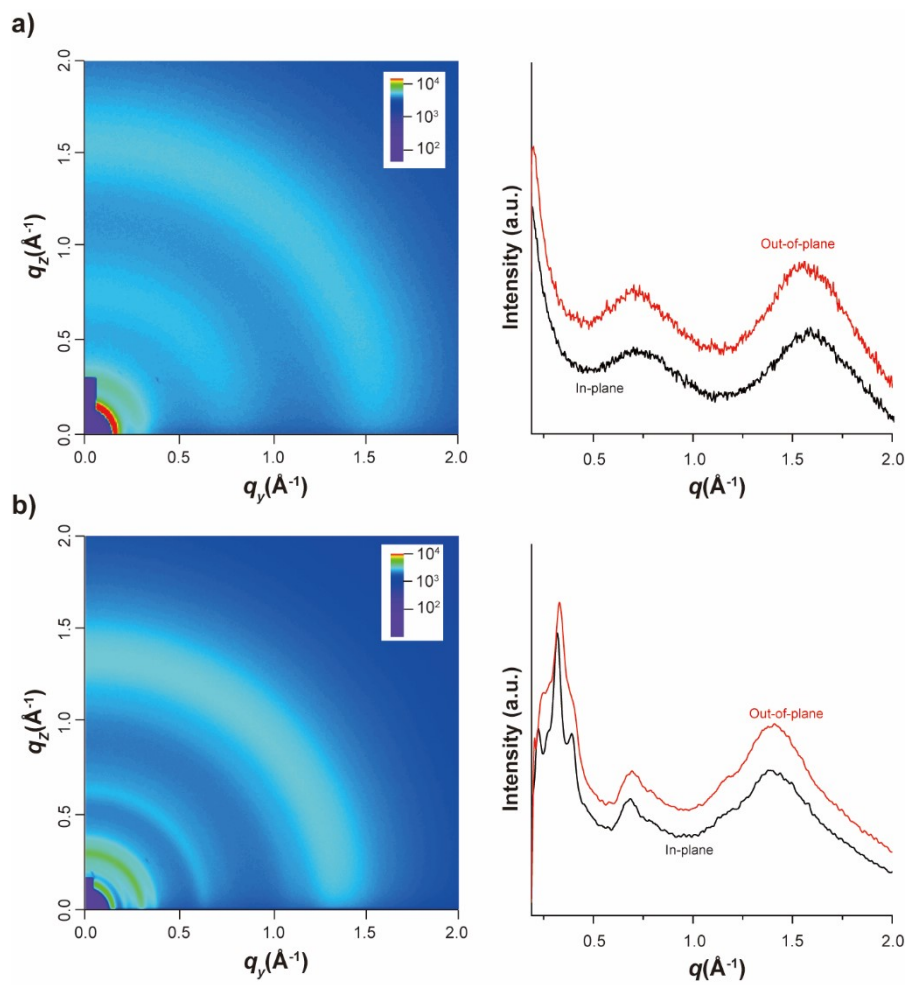


Figure S8. a) GIWAXS scattering of a) DPD_{Zn} and b) TPD_{Cu} .

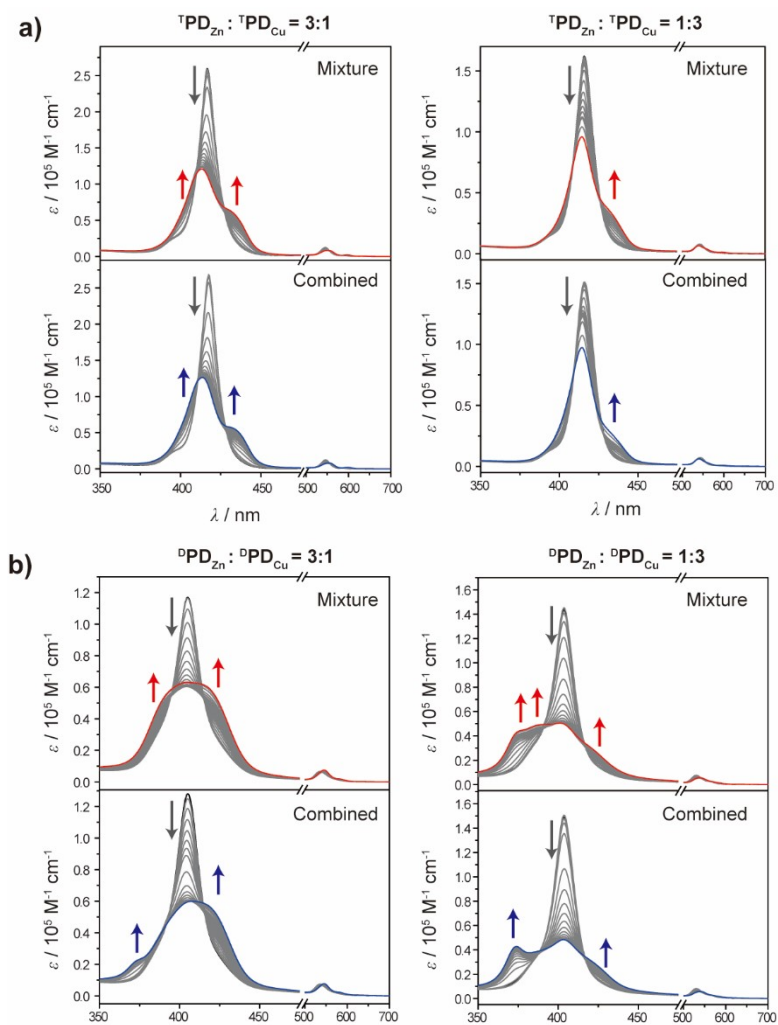


Figure S9. Absorption spectral changes of a) TPD_M mixtures and b) DPD_Ms with various mixing ratios and combined individual absorptions for TPD_Ms and DPD_Ms, respectively, upon cooling from 373 to 293 K at rate of 1.0 K min⁻¹.

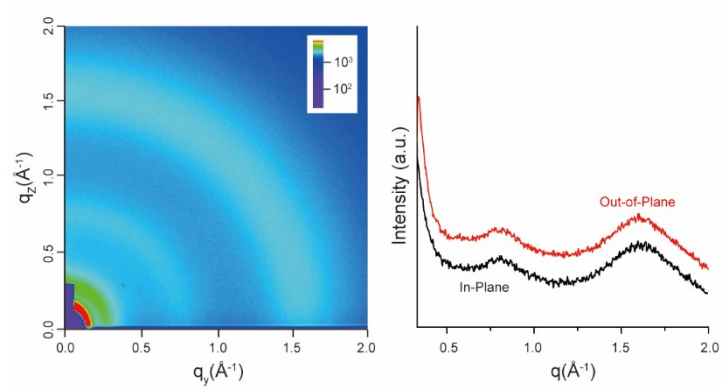


Figure S10. GIWAXS scattering of 1:1 mixture of DPD_{Zn} and DPD_{Cu} .

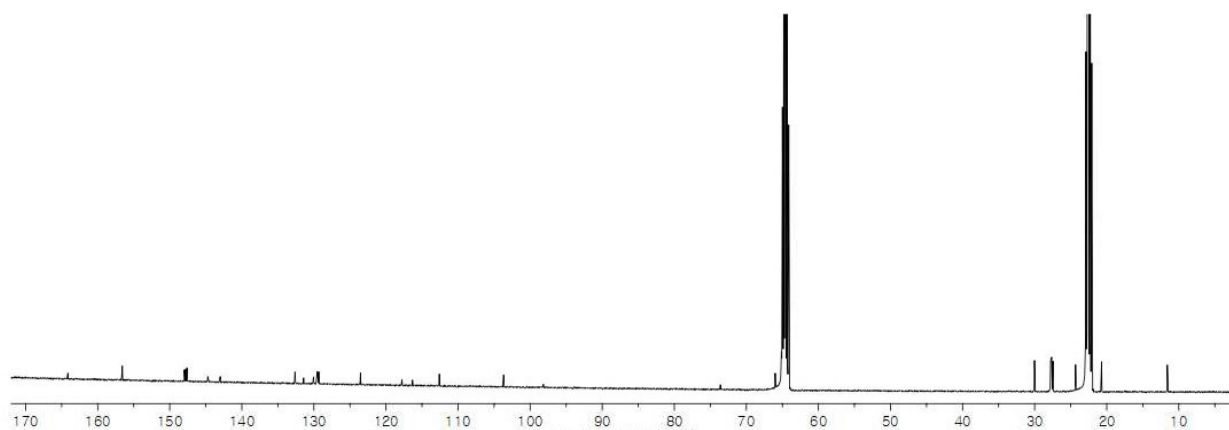
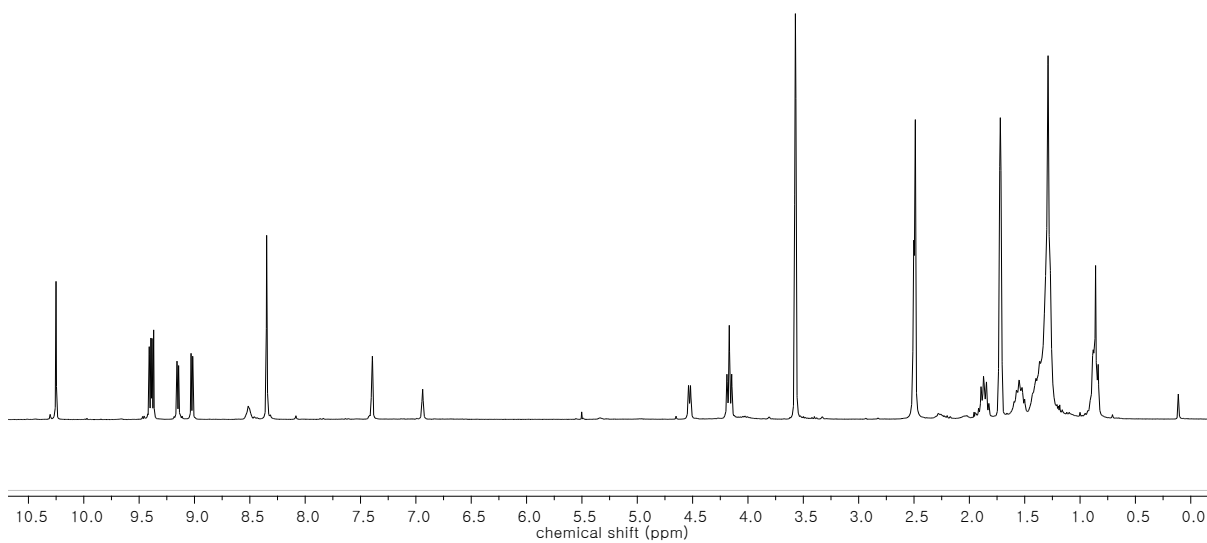


Figure S11. ^1H and ^{13}C NMR spectra of $\text{D}^{\text{PD}}\text{Zn}$ in THF- d_8 at 298 K.

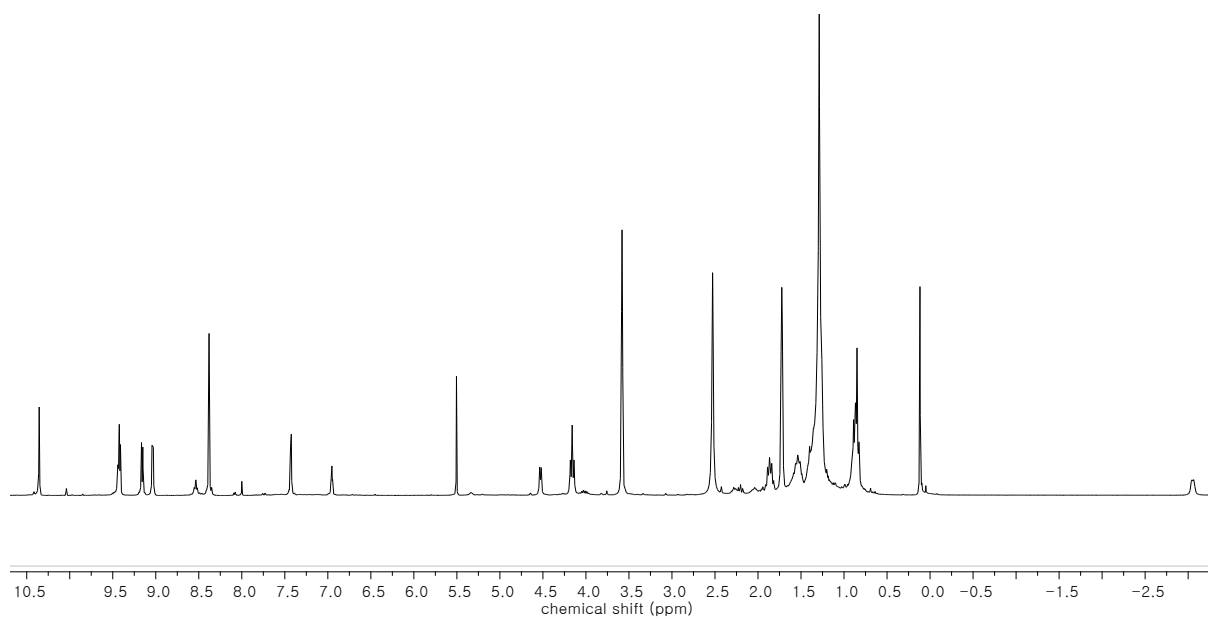


Figure S12. ^1H NMR spectrum of **5** in $\text{THF-}d_8$ at 298 K.

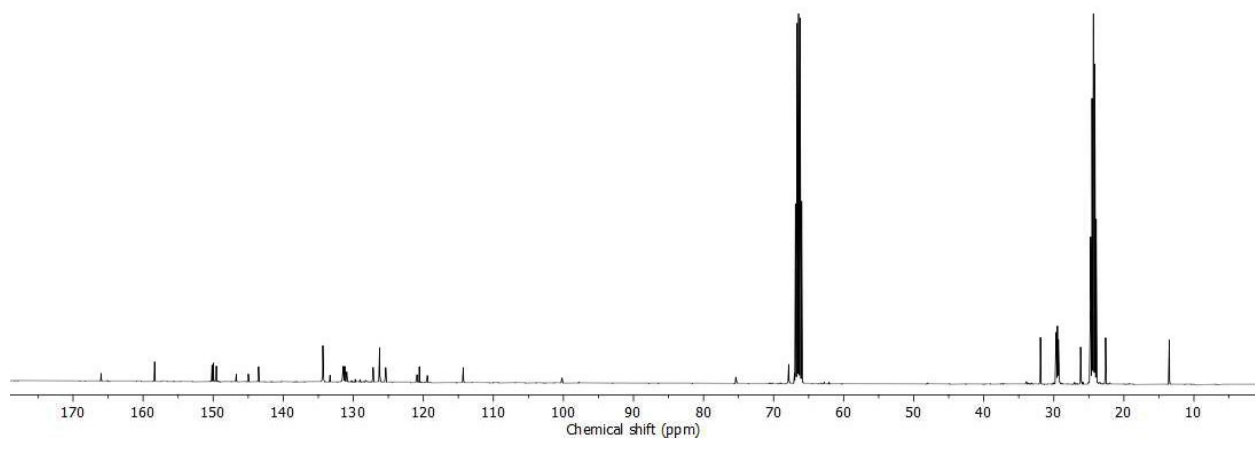
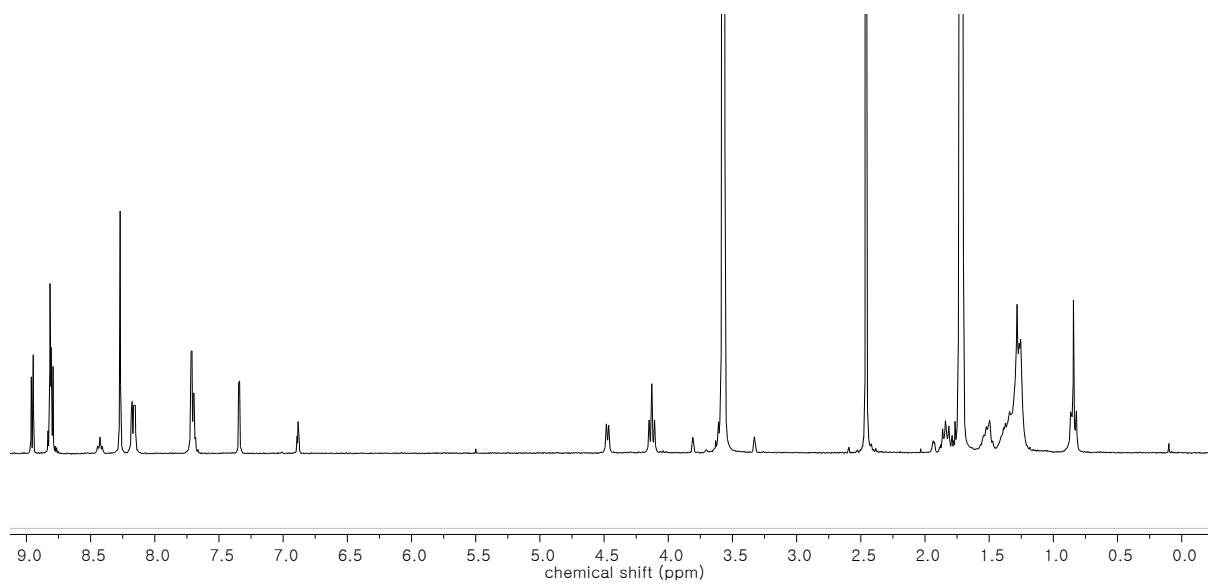


Figure S13. ^1H and ^{13}C NMR spectra of $^1\text{PD}_{\text{Zn}}$ in $\text{THF-}d_8$ at 298 K.

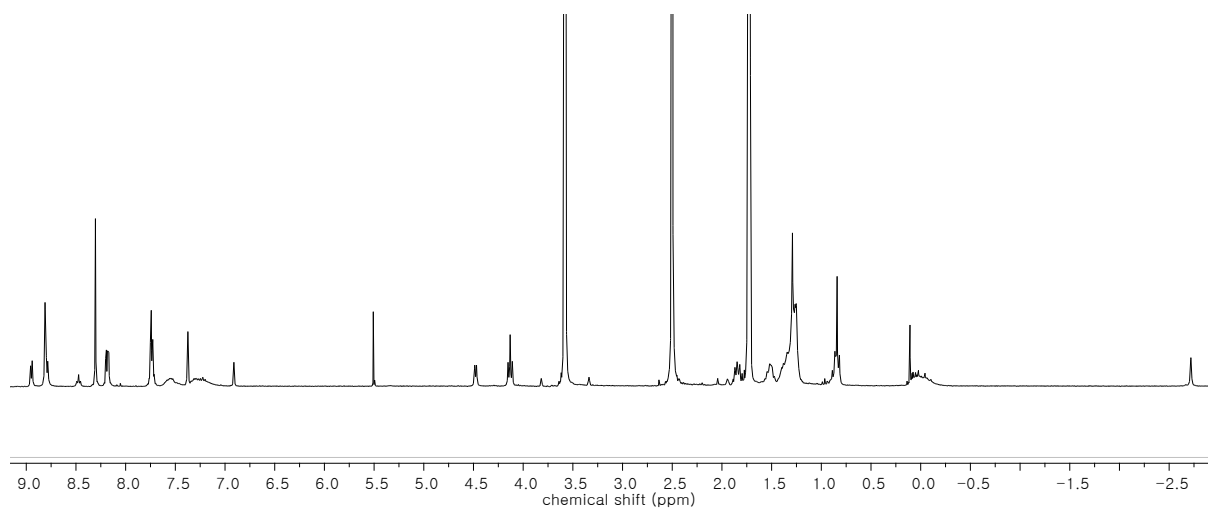


Figure S14. ^1H NMR spectrum of **7** in $\text{THF-}d_8$ at 298 K.

Table S1. Thermodynamic parameters α_{SAT} , T_e , ΔH_e , and K_a , as obtained by fitting curves using equations S1 and S2 from the temperature-dependent degree of aggregation of ${}^{\text{T}}\text{PD}_{\text{Zn}}$ and ${}^{\text{D}}\text{PD}_{\text{Cu}}$ in MCH following a cooperative model.

	Total conc. (M)	α_{SAT}	T_e (K)	ΔH_e (kJ mol $^{-1}$)	K_a
${}^{\text{T}}\text{PD}_{\text{Zn}}$	1.0×10^{-6}	1.020	349.1 ± 0.1	-89.3 ± 1.7	1.00 ± 0.16
	1.5×10^{-6}	1.005	354.1 ± 0.1	-88.8 ± 1.8	0.55 ± 0.10
	2.0×10^{-6}	1.018	357.8 ± 0.2	-89.4 ± 2.0	0.29 ± 0.15
	2.5×10^{-6}	1.004	359.9 ± 0.1	-91.4 ± 1.8	0.41 ± 0.05
${}^{\text{D}}\text{PD}_{\text{Cu}}$	1.0×10^{-6}	1.008	348.8 ± 0.1	-82.2 ± 1.3	1.71 ± 0.44
	1.5×10^{-6}	1.011	353.5 ± 0.2	-75.2 ± 1.3	2.43 ± 0.60
	2.0×10^{-6}	1.012	357.4 ± 0.1	-70.9 ± 1.0	1.56 ± 0.44
	2.5×10^{-6}	1.015	361.2 ± 0.2	-70.4 ± 1.3	3.03 ± 0.57