Electronic Supplementary Information

Water-supported organized structures based on wedge-shaped amphiphilic derivatives of dipyrrolyldiketone boron complexes

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1. Synthetic procedures and spectroscopic data

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 of the solutions were recorded on a Hitachi U-3500 spectrometer and a System Instruments surface and interface spectrometer SIS-50 was used for the solid-state measurements. Fluorescence spectra of the solutions were recorded on a Hitachi F-4500 fluorescence spectrometer and a Hamamatsu Quantum Yields Measurements System for Organic LED Materials C9920-02 was used for estimation of the quantum yields. NMR spectra used in the characterization of the 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 spectrometry (MALDI-TOF-MS) was recorded on a Shimadzu Axima-CFRplus in the negative 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.

2-(4-Hexadecyloxyphenyl)pyrrole.

To a solution of 4-bromohexadecyloxybenzene[S1] (594.8 mg, 2.0 mmol), 1-*tert*-butoxycarbonylpyrrole-2-boronic acid (464.2 mg, 2.2 mmol), tetrakis(triphenylphosphine)palladium(0) (254.2 mg, 0.22 mmol) in 1,2-dimethoxyethane (20 mL) and water (1 mL) at room temperature under nitrogen was added Na_2CO_3 (699.5 mg, 6.6 mmol). The mixture was heated at reflux for 12 h, cooled, and then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous $MgSO_4$ and evaporated to give an oil. The residue was then chromatographed over flash silica gel column (eluent: CH_2Cl_2/hexane = 1/4) to give 1-*tert*-butoxycarbonyl-2-(4-hexadecyloxyphenyl)pyrrole (822.9 mg, 85%) as a colorless oil. R_f = 0.50 (CH_2Cl_2/hexane = 1/4). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.32 (m, 1H, pyrrole-H), 7.24 (m, 2H, Ar-H), 6.87 (d, J = 8.4 Hz, 2H, Ar-H), 6.20 (m, 1H, pyrrole-H), 6.13 (m, 1H, pyrrole-H), 3.96 (t, J = 6.8 Hz, 2H, OCH_2), 1.78 (m, 2H, $OCH_2\underline{CH_2}$), 1.45–1.26 (m, 26H, $OC_2H_4\underline{C_{13}H_{26}}$), 1.26 (s, 9H, Boc), 0.88 (t, J = 7.2 Hz, 3H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: m/z (% intensity): 482.4 (100), 483.5 (36). Calcd for $C_{31}H_{48}NO_3$ ([M – H]$^-$): 482.36. As a deprotection of Boc moiety, 1-*tert*-butoxycarbonyl-2-(4-hexadecyloxyphenyl)pyrrole (820.0 mg, 1.70 mmol) was heated at 180 °C for 30 min, cooled and then chromatographed over flash silica gel column (eluent: CH_2Cl_2/hexane = 1/1) to give 2-(4-hexadecyloxyphenyl)pyrrole (524.1 mg, 81%) as a colorless oil. R_f = 0.40 (CH_2Cl_2/hexane = 1/1). ^{1}H NMR (600 MHz, CDCl3, 20 °C): δ (ppm) 8.33 (s, 1H, NH), 7.39 (d, J = 8.4 Hz, 2H, Ar-H), 6.91 (d, J = 8.4 Hz, 1H, Ar-H), 6.83 (m, 1H, pyrrole-H), 6.40 (m, 1H, pyrrole-H), 6.28 (m, 1H, pyrrole-H), 3.96 (t, J = 6.8 Hz, 2H, OCH_2), 1.78 (m, 2H, $OCH_2\underline{CH_2}$), 1.45–1.26 (m, 26H, $OC_2H_4\underline{C_{13}H_{26}}$), 1.26 (s, 9H, Boc), 0.87 (t, J = 7.2 Hz, 3H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: m/z (% intensity): 382.3 (100), 383.3 (34). Calcd for $C_{26}H_{40}NO$ ([M – H]$^-$): 382.31.

3-(5-Phenylpyrrol-2-yl)-1-(5-(3,4,5-tris-TEG-phenyl)pyrrol-2-yl)-1,3-propanedione, 3-h´.

A CH_2Cl_2 solution (16 mL) of 2-(3,4,5-tris-TEG-phenyl)pyrrole[S2] (256.0 mg, 0.407 mmol) and 2-phenylpyrrole (58.7 mg, 0.409 mmol) was treated with malonyl chloride (63.4 mg, 0.449 mmol) at room temperature and stirred for 30 min at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 3% MeOH/CH_2Cl_2). Purification on silica gel columns (Wakogel C-300, 5% MeOH/EtOAc) afforded **3-h´** (108.7 mg, 32%) as a pale yellow oil. R_f = 0.45 (5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.70): δ (ppm) keto form 9.92 (br, 1H, NH), 9.60 (br, 1H, NH), 7.58 (m, 2H, Ar-H), 7.42 (m, 2H, Ar-H), 7.33 (m, 1H, Ar-H), 7.15–7.13 (m, 2H, pyrrole-H), 6.85 (s, 2H, Ar-H), 6.59 (m, 1H, pyrrole-H), 6.49 (m, 1H, pyrrole-H), 4.25 (s, 2H, CH_2), 4.22 (m, 4H, OCH_2), 4.18 (m, 2H, OCH_2), 3.86 (m, 4H, OCH_2), 3.78 (m, 2H, OCH_2), 3.76–3.62 (m, 18H, OCH_2), 3.55 (m, 6H, OCH_2), 3.36 (m, 9H, OCH_3); enol form 16.70 (br, 1H, OH), 9.83 (br, 1H, NH), 9.46 (br, 1H, NH), 7.58 (m, 2H, Ar-H), 7.42 (t, 2H, Ar-H), 7.32 (m, 1H, Ar-H), 6.98–6.95 (m, 2H, pyrrole-H), 6.89 (s, 2H, Ar-H), 6.64 (m, 1H, pyrrole-H), 6.53 (m, 1H, pyrrole-H), 6.38 (s, 1H, CH), 4.22 (m, 4H, OCH_2), 4.18 (m, 2H, OCH_2), 3.86 (m, 4H, OCH_2), 3.78 (m, 2H, OCH_2), 3.76–3.62 (m, 18H, OCH_2), 3.55 (m, 6H, OCH_2), 3.36 (m, 9H, OCH_3). MALDI-TOF-MS: m/z (% intensity): 839.4 (100), 840.4 (74). Calcd for $C_{44}H_{59}N_2O_{14}$ ([M – H]$^-$): 840.40.

3-(5-(2-Octyloxyphenyl)pyrrol-2-yl)-1-(5-(3,4,5-tris-TEG-phenyl)pyrrol-2-yl)-1,3-propanedione, 3-o´.

A CH_2Cl_2 solution (50 mL) of 2-(3,4,5-tris-TEG-phenyl)pyrrole[S2] (241.3 mg, 0.542 mmol) and 2-(2-octyloxyphenyl)pyrrole[S3] (138.8 mg, 0.511 mmol) was treated with malonyl chloride (75.4 mg, 0.535 mmol) at room temperature and stirred for 1 h at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 3% MeOH/CH_2Cl_2). Purification using silica gel column flash chromatography (eluent: 1% MeOH/CH_2Cl_2) afforded **3-o´** (160.4 mg, 32%) as a pale yellow oil. R_f = 0.28 (5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.50): δ (ppm) keto form 10.82 (br, 1H, NH), 9.73 (br, 1H, NH), 7.68 (m, 1H, Ar-H), 7.22 (m, 1H, Ar-H), 7.11 (m, 2H, pyrrole-H), 7.01–6.98 (m, 2H, Ar-H), 6.83 (s, 2H, Ar-H), 6.68–6.67 (m, 1H, pyrrole-H), 6.48–6.47 (m, 1H, pyrrole-H), 4.24 (m, 2H, OCH_2), 4.22 (s, 2H, CH_2), 4.21–4.13 (m, 6H, OCH_2), 3.88–3.85 (m, 4H, OCH_2), 3.79–3.74 (m, 2H, OCH_2), 3.73–3.63 (m, 18H, OCH_2), 3.55–3.53 (m, 6H, OCH_2), 3.38–3.35 (m, 9H, OCH_3), 2.06–1.96 (m, 2H, $OCH_2\underline{CH_2}$), 1.55–1.50 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.47–1.24 (m, 4H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.85 (m, 3H, $OC_7H_{14}\underline{CH_3}$); enol form 16.67 (br, 1H, OH), 10.77 (br, 1H, NH), 9.66 (br, 1H, NH), 7.71 (m, 1H, Ar-H), 7.22 (m, 1H, Ar-H), 7.01–6.98 (m, 2H, Ar-H), 6.95–6.92 (m, 2H, pyrrole-H), 6.87 (s, 2H, Ar-H), 6.73–6.71 (m, 1H, pyrrole-H), 6.52–6.51 (m, 1H, pyrrole-H), 6.35 (s, 1H, CH), 4.24 (m, 2H, OCH_2), 4.21–4.13 (m, 6H, OCH_2), 3.88–3.85 (m, 4H, OCH_2), 3.79–3.74 (m, 2H, OCH_2), 3.73–3.63 (m, 18H, OCH_2), 3.55–3.53 (m, 6H, OCH_2), 3.38–3.35 (m, 9H, OCH_3), 2.06–1.96 (m, 2H, $OCH_2\underline{CH_2}$), 1.55–1.50 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.47–1.24 (m, 4H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.85 (m, 3H, $OC_7H_{14}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 967.5 (100), 968.5 (60). Calcd for $C_{52}H_{75}N_2O_{15}$ ($[M - H]^-$): 967.52.

3-(5-(3-Octyloxyphenyl)pyrrol-2-yl)-1-(5-(3,4,5-tris-TEG-phenyl)pyrrol-2-yl)-1,3-propanedione, 3-m´.

A CH_2Cl_2 solution (15 mL) of 2-(3,4,5-tris-TEG-phenyl)pyrrole[S2] (186.9 mg, 0.297 mmol) and 2-(3-octyloxyphenyl)pyrrole[S3] (84.2 mg, 0.310 mmol) was treated with malonyl chloride (43.5 mg, 0.308 mmol) at room temperature and stirred for 2 h at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 5% $MeOH/CH_2Cl_2$), followed by purification using silica gel column flash chromatography (eluent: 1.5% $MeOH/CH_2Cl_2$), which afforded **3-m´** (83.0 mg, 29%) as a pale yellow oil. R_f = 0.47 (5% $MeOH/CH_2Cl_2$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.5): δ (ppm) keto form 9.84 (br, 1H, NH), 9.55 (br, 1H, NH), 7.32 (m, 1H, Ar-H), 7.13 (m, 2H, pyrrole-H), 7.08 (m, 1H, Ar-H), 6.96 (m, 1H, Ar-H), 6.91 (m, 1H, Ar-H), 6.85 (s, 2H, Ar-H), 6.57 (m, 1H, pyrrole-H), 6.49 (m, 1H, pyrrole-H), 4.24 (s, 2H, CH_2), 4.22–4.12 (m, 6H, OCH_2), 3.99 (m, 2H, OCH_2), 3.87–3.83 (m, 2H, OCH_2), 3.80–3.78 (m, 2H, OCH_2), 3.73–3.62 (m, 18H, OCH_2), 3.56–3.53 (m, 6H, OCH_2), 3.38–3.34 (m, 9H, OCH_3), 1.83–1.77 (m, 2H, $OCH_2\underline{CH_2}$), 1.49–1.44 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.37–1.25 (m, 8H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.87 (m, 3H, $OC_7H_{14}\underline{CH_3}$); enol form 16.70 (br, 1H, OH), 9.76 (br, 1H, NH), 9.44 (br, 1H, NH), 7.32 (m, 1H, Ar-H), 7.08 (m, 1H, Ar-H), 6.96 (m, 1H, Ar-H), 6.91 (m, 1H, Ar-H), 6.88–6.86 (m, 2H, pyrrole-H), 6.88 (s, 2H, Ar-H), 6.57 (m, 1H, pyrrole-H), 6.49 (m, 1H, pyrrole-H), 4.24 (s, 2H, CH_2), 4.22–4.12 (m, 6H, OCH_2), 3.99 (m, 2H, OCH_2), 3.87–3.83 (m, 2H, OCH_2), 3.80–3.78 (m, 2H, OCH_2), 3.73–3.62 (m, 18H, OCH_2), 3.56–3.53 (m, 6H, OCH_2), 3.38–3.34 (m, 9H, OCH_3), 1.83–1.77 (m, 2H, $OCH_2\underline{CH_2}$), 1.49–1.44 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.37–1.25 (m, 8H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.87 (m, 3H, $OC_7H_{14}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 967.5 (100), 968.5 (60). Calcd for $C_{52}H_{75}N_2O_{15}$ ($[M - H]^-$): 967.52.

3-(5-(4-Octyloxyphenyl)pyrrol-2-yl)-1-(5-(3,4,5-tris-TEG-phenyl)pyrrol-2-yl)-1,3-propanedione, 3-p´.

A CH_2Cl_2 solution (50 mL) of 2-(3,4,5-tris-TEG-phenyl)pyrrole[S2] (184.1 mg, 0.292 mmol) and 2-(4-octyloxyphenyl)pyrrole[S3] (81.1 mg, 0.299 mmol) was treated with malonyl chloride (43.5 mg, 0.308 mmol) at room temperature and stirred for 1 h at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 3% $MeOH/CH_2Cl_2$). Subsequent purification by silica gel column flash chromatography (eluent: 1% $MeOH/CH_2Cl_2$) afforded **3-p´** (160.4 mg, 32%) as a pale yellow oil. R_f = 0.30 (5% $MeOH/CH_2Cl_2$). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.25): δ (ppm) keto form 9.84 (br, 1H, NH), 9.46 (br, 1H, NH), 7.48 (m, 2H, Ar-H), 7.12 (m, 2H, pyrrole-H), 6.94–6.92 (m, 2H, Ar-H), 6.84 (s, 2H, Ar-H), 6.49–6.48 (m, 2H, pyrrole-H), 4.25–4.17 (m, 6H, OCH_2), 4.22 (s, 2H, CH_2), 3.99–3.97 (m, 2H, OCH_2), 3.87–3.80 (m, 4H, OCH_2), 3.75–3.73 (m, 2H, OCH_2), 3.74–3.62 (m, 18H, OCH_2), 3.56–3.53 (m, 6H, OCH_2), 3.38–3.34 (m, 9H, OCH_3), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.47–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.36–1.25 (m, 24H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.86 (m, 3H, $OC_7H_{14}\underline{CH_3}$); enol form 16.72 (br, 1H, OH), 9.75 (br, 1H, NH), 9.38 (br, 1H, NH), 7.48 (m, 2H, Ar-H), 6.94 (m, 2H, pyrrole-H), 6.94–6.92 (m, 2H, Ar-H), 6.88 (s, 2H, Ar-H), 6.53–6.52 (m, 2H, pyrrole-H), 6.35 (s, 1H, CH), 4.25–4.17 (m, 6H, OCH_2), 3.99–3.97 (m, 2H, OCH_2), 3.87–3.80 (m, 4H, OCH_2), 3.75–3.73 (m, 2H, OCH_2), 3.74–3.62 (m, 18H, OCH_2), 3.56–3.53 (m, 6H, OCH_2), 3.38–3.34 (m, 9H, OCH_3), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.47–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.36–1.25 (m, 24H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.86 (m, 3H, $OC_7H_{14}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 967.5 (100), 968.5 (55). Calcd for $C_{52}H_{75}N_2O_{15}$ ($[M - H]^-$): 967.52.

3-(5-(4-Hexadecyloxyphenyl)pyrrol-2-yl)-1-(5-(3,4,5-tris-TEG-phenyl)pyrrol-2-yl)-1,3-propanedione, 3-pp´.

A CH_2Cl_2 solution (50 mL) of 2-(3,4,5-tris-TEG-phenyl)pyrrole[S2] (1.000 g, 1.589 mmol) and 2-(4-hexadecyloxyphenyl)pyrrole (598.0 g, 1.559 mmol) was treated with malonyl chloride (231.8 mg, 1.644 mmol) at room temperature and stirred for 1 h at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 4% $MeOH/CH_2Cl_2$). Ppurification using silica gel column flash chromatography (eluent: $MeOH/CH_2Cl_2/EtOAc$ = 4/48/48) afforded **3-pp´** (234.7 mg, 25%) as a pale yellow oil. R_f = 0.58 (10% $MeOH/CH_2Cl_2$). ^{1}H NMR

(600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.26): δ (ppm) keto form 9.78 (br, 1H, NH), 9.40 (br, 1H, NH), 7.50 (m, 2H, Ar-H), 7.13 (m, 2H, pyrrole-H), 6.96–6.93 (m, 2H, Ar-H), 6.85 (s, 2H, Ar-H), 6.49–6.48 (m, 2H, pyrrole-H), 4.25–4.17 (m, 6H, OCH_2), 4.22 (s, 2H, CH_2), 3.99–3.97 (m, 2H, $O\underline{CH_2}$), 3.88–3.85 (m, 4H, OCH_2), 3.81–3.75 (m, 2H, OCH_2), 3.79–3.62 (m, 18H, OCH_2), 3.56–3.53 (m, 6H, OCH_2), 3.38–3.34 (m, 9H, OCH_3), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.47–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.36–1.25 (m, 24H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.89–0.86 (m, 3H, $OC_{15}H_{30}\underline{CH_3}$); enol form 16.73 (br, 1H, OH), 9.66 (br, 1H, NH), 9.33 (br, 1H, NH), 7.50 (m, 2H, Ar-H), 6.93 (m, 2H, pyrrole-H), 6.96–6.93 (m, 2H, Ar-H), 6.87 (s, 2H, Ar-H), 6.53–6.52 (m, 2H, pyrrole-H), 6.35 (s, 1H, CH), 4.25–4.17 (m, 6H, OCH_2), 3.99–3.97 (m, 2H, OCH_2), 3.88–3.85 (m, 4H, OCH_2), 3.81–3.75 (m, 2H, OCH_2), 3.79–3.62 (m, 18H, OCH_2), 3.56–3.53 (m, 6H, OCH_2), 3.38–3.34 (m, 9H, OCH_3), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.47–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.36–1.25 (m, 24H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.89–0.86 (m, 3H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 1079.6 (100), 1080.7 (68). Calcd for $C_{60}H_{91}N_2O_{15}$ ($[M - H]^-$): 1080.65.

1-(5-(3,4,5-Tris-HEG-phenyl)pyrrol-2-yl)-3-(5-phenyl pyrrol-2-yl)-1,3-propanedione, 6-h´.

A CH_2Cl_2 solution (50 mL) of 2-(3,4,5-tris-HEG-phenyl)pyrrole[S2] (1.549 g, 1.509 mmol) and 2-phenylpyrrole (218.1 mg, 1.523 mmol) was treated with malonyl chloride (231.8 mg, 1.644 mmol) at room temperature and stirred for 1 h at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 6% $MeOH/CH_2Cl_2$), followed by purification using silica gel column flash chromatography (eluent: $MeOH/CH_2Cl_2/EtOAc$ = 4/48/48), which afforded **6-h´** (488.8 mg, 26%) as a pale yellow oil. R_f = 0.38 (7% $MeOH/CH_2Cl_2$). ^1H NMR (600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.38): δ (ppm) keto form 10.01 (br, 1H, NH), 9.67 (br, 1H, NH), 7.59 (m, 2H, Ar-H), 7.42 (m, 2H, Ar-H), 7.33 (m, 1H, Ar-H), 7.14–7.13 (m, 1H, pyrrole-H), 6.90 (s, 2H, Ar-H), 6.59 (m, 1H, pyrrole-H), 6.49 (m, 1H, pyrrole-H), 4.24 (s, 2H, CH_2), 4.22 (m, 4H, OCH_2), 4.18 (m, 2H, OCH_2), 3.86 (m, 4H, OCH_2), 3.80 (m, 2H, OCH_2), 3.74–3.61 (m, 54H, OCH_2), 3.53 (m, 6H, OCH_2), 3.36 (m, 9H, OCH_3); enol form 16.70 (br, 1H, OH), 9.93 (br, 1H, NH), 9.51 (br, 1H, NH), 7.58 (m, 2H, Ar-H), 7.42 (t, 2H, Ar-H), 7.32 (m, 1H, Ar-H), 6.98–6.96 (m, 2H, pyrrole-H), 6.94 (s, 2H, Ar-H), 6.63 (m, 1H, pyrrole-H), 6.53 (m, 1H, pyrrole-H), 6.42 (s, 1H, CH), 4.22 (m, 4H, OCH_2), 4.18 (m, 2H, OCH_2), 3.86 (m, 4H, OCH_2), 3.80 (m, 2H, OCH_2), 3.74–3.61 (m, 54H, OCH_2), 3.53 (m, 6H, OCH_2), 3.36 (m, 9H, OCH_3). MALDI-TOF-MS: *m/z* (% intensity): 1235.7 (100), 1236.7 (74). Calcd for $C_{62}H_{95}N_2O_{23}$ ($[M - H]^-$): 1235.63.

1-(5-(3,4,5-Tris-HEG-phenyl)pyrrol-2-yl)-3-(5-(4-octy loxyphenyl)pyrrol-2-yl)-1,3-propanedione, 6-p´.

A CH_2Cl_2 solution (50 mL) of 2-(3,4,5-tris-HEG-phenyl)pyrrole[S2] (1.549 g, 1.509 mmol) and 2-(4-octyloxyphenyl)pyrrole[S3] (412.0 mg, 1.518 mmol) was treated with malonyl chloride (217.3 mg, 1.542 mmol) at room temperature and stirred for 30 min at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 10% $MeOH/CH_2Cl_2$). Subsequnt purification by silica gel column flash chromatography (eluent: $MeOH/CHCl_3/EtOAc$ = 6/47/47) afforded **6-p´** (364.0 mg, 18%) as a pale yellow oil. R_f = 0.52 (10% $MeOH/CH_2Cl_2$). ^1H NMR (600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.50. A signal of Ar-H (2H) is overlapped with that of $CHCl_3$): δ (ppm) keto form 10.14 (br, 1H, NH), 9.58 (br, 1H, NH), 7.52 (m, 2H, Ar-H), 7.12 (m, 2H, pyrrole-H), 6.95–6.91 (m, 2H, Ar-H), 6.49–6.48 (m, 2H, pyrrole-H), 4.25–4.17 (m, 6H, OCH_2), 4.21 (s, 2H, CH_2), 3.99–3.96 (m, 2H, OCH_2), 3.87 (m, 4H, OCH_2), 3.80–3.75 (m, 2H, OCH_2), 3.79–3.62 (m, 54H, OCH_2), 3.54–3.52 (m, 6H, OCH_2), 3.38–3.33 (m, 9H, OCH_3), 1.81–1.77 (m, 2H, $OCH_2\underline{CH_2}$), 1.48–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.37–1.25 (m, 8H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.87 (m, 3H, $OC_7H_{14}\underline{CH_3}$); enol form 16.73 (br, 1H, OH), 10.02 (br, 1H, NH), 9.44 (br, 1H, NH), 7.52 (m, 2H, Ar-H), 6.95–6.91 (m, 2H, Ar-H), 6.94 (m, 2H, pyrrole-H), 6.53–6.51 (m, 2H, pyrrole-H), 6.40 (s, 1H, CH), 4.25–4.17 (m, 6H, OCH_2), 3.99–3.96 (m, 2H, OCH_2), 3.87 (m, 4H, OCH_2), 3.80–3.75 (m, 2H, OCH_2), 3.79–3.62 (m, 54H, OCH_2), 3.54–3.52 (m, 6H, OCH_2), 3.38–3.33 (m, 9H, OCH_3), 1.81–1.77 (m, 2H, $OCH_2\underline{CH_2}$), 1.48–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.37–1.25 (m, 8H, $OC_3H_6\underline{C_4H_8}$), 0.89–0.87 (m, 3H, $OC_7H_{14}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 1363.8 (100), 1364.8 (90). Calcd for $C_{70}H_{111}N_2O_{24}$ ($[M - H]^-$): 1363.75.

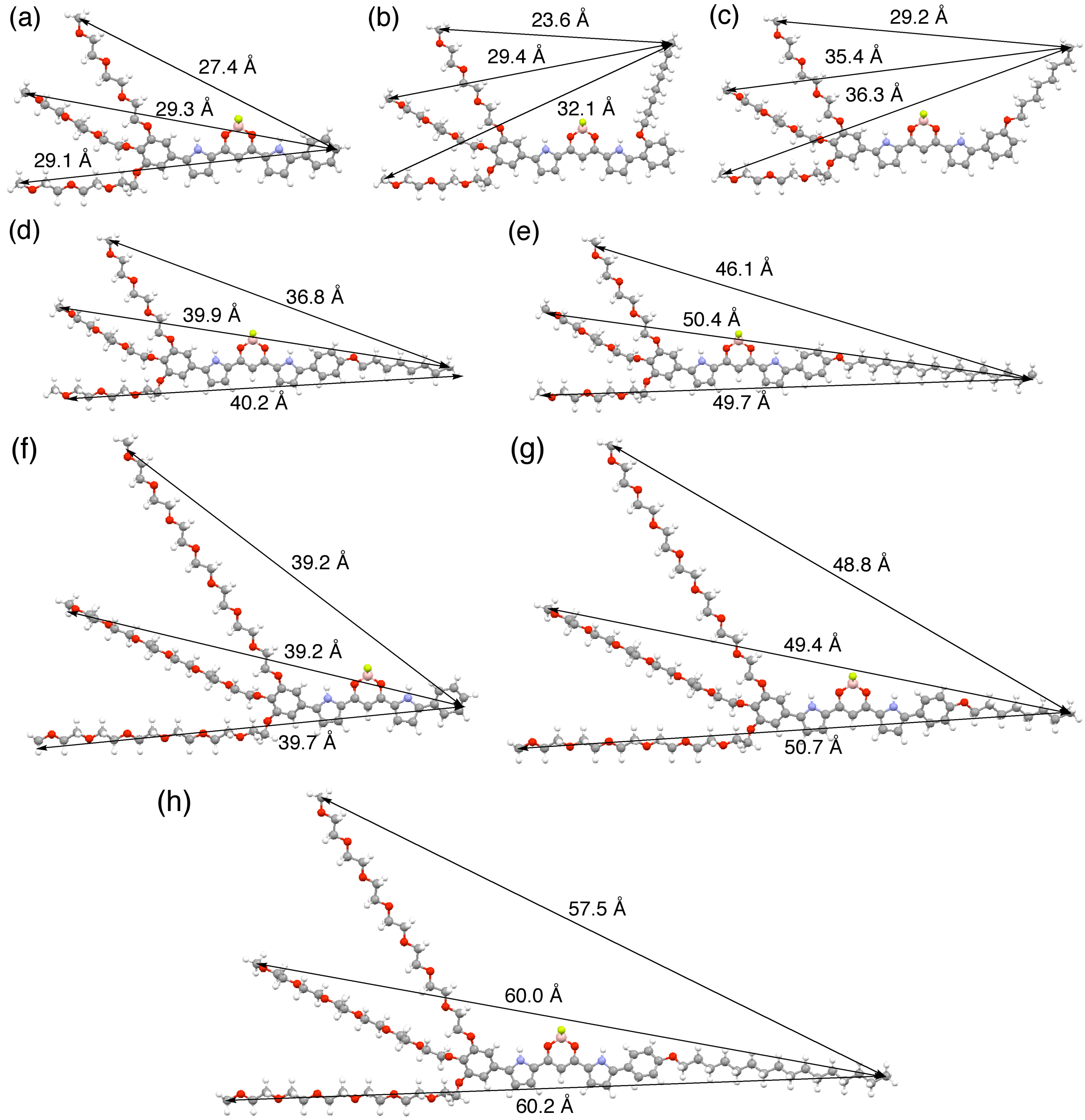
3-(5-(4-Hexadecyloxyphenyl)pyrrol-2-yl)-1-(5-(3,4,5-t ris-HEG-phenyl)pyrrol-2-yl)-1,3-propanedione, 6-pp´.

A CH_2Cl_2 solution (80 mL) of 2-(3,4,5-tris-HEG-phenyl)pyrrole[S2] (1.578 mg, 1.536 mmol) and 2-(4-hexadecyloxyphenyl)pyrrole (583.3 mg, 1.520 mmol) was treated with malonyl chloride (217.4 mg, 1.542 mmol) at room temperature and stirred for 30 min at the same temperature. After confirming the consumption of the starting pyrroles by TLC analysis, the reaction mixture was chromatographed over silica gel columns (Wakogel C-300, 6% $MeOH/CH_2Cl_2$). Subsequent purification by silica gel column flash chromatography (eluent: $MeOH/CHCl_3/EtOAc$ = 4/48/48) afforded **6-pp´** (564.5 mg, 25%) as a pale yellow oil. R_f = 0.30 (5% $MeOH/CH_2Cl_2$). ^1H NMR (600 MHz, $CDCl_3$, 20 °C; the diketone is obtained as a mixture of keto and enol tautomers in the ratio of 1 : 0.34. A signal of Ar-H (2H) is overlapped with that of $CHCl_3$):

δ (ppm) keto form 9.93 (br, 1H, NH), 9.47 (br, 1H, NH), 7.50 (m, 2H, Ar-H), 7.13 (m, 2H, pyrrole-H), 6.97–6.95 (m, 2H, Ar-H), 6.86 (s, 2H, Ar-H), 6.49–6.48 (m, 2H, pyrrole-H), 4.25–4.17 (m, 6H, OCH_2), 4.21 (s, 2H, CH_2), 3.99–3.96 (m, 2H, OCH_2), 3.87 (m, 4H, OCH_2), 3.80–3.75 (m, 2H, OCH_2), 3.79–3.62 (m, 54H, OCH_2), 3.57–3.53 (m, 6H, OCH_2), 3.38–3.33 (m, 9H, OCH_3), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.47–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.36–1.25 (m, 24H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.89–0.86 (m, 3H, $OC_{15}H_{30}\underline{CH_3}$); enol form 16.73 (br, 1H, OH), 9.81 (br, 1H, NH), 9.36 (br, 1H, NH), 7.50 (m, 2H, Ar-H), 6.93 (m, 2H, pyrrole-H), 6.97–6.95 (m, 2H, Ar-H), 6.89 (s, 2H, Ar-H), 6.53–6.52 (m, 2H, pyrrole-H), 6.36 (s, 1H, CH), 4.25–4.17 (m, 6H, OCH_2), 4.25–4.17 (m, 6H, OCH_2), 3.99–3.96 (m, 2H, OCH_2), 3.87 (m, 4H, OCH_2), 3.80–3.75 (m, 2H, OCH_2), 3.79–3.62 (m, 54H, OCH_2), 3.57–3.53 (m, 6H, OCH_2), 3.38–3.33 (m, 9H, OCH_3), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.47–1.43 (m, 2H, $OC_2H_4\underline{CH_2}$), 1.36–1.25 (m, 24H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.89–0.86 (m, 3H, $OC_{15}H_{30}\underline{CH_3}$). MALDI-TOF-MS: *m/z* (% intensity): 1475.8 (100), 1477.8 (98). Calcd for $C_{78}H_{127}N_2O_{24}$ ($[M - H]^-$): 1475.88.

[S1] Y. Zou, T. Yi, S. Xiao, F. Li, C. Li, X. Gao, J. Wu, M. Yu and C. Huang, *J. Am. Chem. Soc.*, 2008, **130**, 15750.
[S2] H. Maeda, Y. Ito, Y. Haketa, N. Eifuku, E. Lee, M. Lee, T. Hashishin and K. Kaneko, *Chem. Eur. J.*, 2009, **15**, 3709.
[S3] H. Maeda and N. Eifuku, *Chem. Lett.*, 2009, **38**, 208.

2. Optimization of wedge-shaped amphiphiles by AM1 calculations [S4]



Supporting Figure 1 Optimized structures of (a) **3-h**, (b) **3-o**, (c) **3-m**, (d) **3-p**, (e) **3-pp**, (f) **6-h**, (g) **6-p**, and (h) **6-pp** at AM1 level. Representative lengths of molecules are described.

Cartesian Coordination of 3-h.

–1.2123397 hartree

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Cartesian Coordination of 3-o.

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H,-2.1686505252,12.4192718915,-5.2331744629
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C,3.3387852669,-8.5897947515,-0.6928973387
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Cartesian Coordination of 3-m

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C,6.1916772013,-5.6271864991,-5.8028980975
C,4.1074316506,-2.6299619584,-5.530204019
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F,-2.929865037,-0.1555481898,4.4593789995
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Cartesian Coordination of 3-p.

–1.3476562hartree

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C,-0.3755611646,6.3959660468,-7.0068003166
C,-0.5326034056,5.8944362478,-5.5740771376
C,4.5355539006,3.6189488016,-15.1704068777
C,-0.7244359056,3.8619438798,-4.3872146019
C,-0.7925716591,2.360033565,-4.6564219919
C,1.3271958493,-2.4736858018,15.6045564823
C,1.4930177659,-1.8757895897,16.9907549153
C,-0.3311858518,-1.8032636466,4.5812545082
C,0.0025701811,-1.1998400583,5.8015128577
C,-0.0859151958,-1.9172035351,7.0515099098
C,-0.5019128366,-3.2556527624,7.2722025956
C,-0.4185776515,-3.4999926218,8.6655445635
C,0.0463808124,-2.3053965742,9.2825260656
C,-0.5440520959,-1.5957216916,2.1142856404
C,-4.6371270247,-2.1763821697,-15.1100555543
C,-0.8234457418,-1.6918669928,-0.1336060438
C,-1.1800467787,-2.9613724062,0.3967857541
C,-1.0065416478,-2.8996701976,1.8029264996
C,0.2902338941,-2.0751738996,10.6944272377
C,-0.8392412604,-1.2771212416,-1.5260116372
C,-1.0001953176,0.065152064,-1.8784829988
C,-1.0163492719,0.4465549067,-3.2324546597
C,-0.8799812215,-0.5239602464,-4.2456708654
C,-0.7160231388,-1.8734263677,-3.8696280172
C,-0.6940955284,-2.2501642047,-2.5250971249
C,-4.1264953678,-2.3872398237,-12.8136943569
C,-3.4638952337,-3.3752556488,-11.8585865814
C,0.6458560746,-3.1550218276,11.5135530345
C,0.8777416257,-2.9717027163,12.8742884115
C,0.7533064305,-1.6901623111,13.4256626571
C,0.3939664046,-0.5951691995,12.6141137221
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C,2.4280879464,1.1022347506,-10.1858311014
C,-0.1410139097,0.3039736749,-7.703034827
C,1.0142334158,1.075961035,-9.6121697842
C,-2.9972353422,-3.6237514982,-9.5569845887
C,-3.2059076736,-2.8835647808,-8.238897135
C,-2.6336778004,-3.0804257335,-5.9509612874
C,-1.5584058341,-3.7271837659,-5.0844161475
C,3.1865417973,-3.3703180696,24.1320331721
C,3.0157762256,-3.9394806037,22.7473534956
C,2.6215161758,-2.8692181041,21.7517422786
F,-0.2839957617,1.8519607171,4.8159662846
F,1.780996282,1.1962271858,4.5816982783
C,-0.2191889733,-1.0445450456,3.4122533174

Cartesian Coordination of 3-pp.

–1.4351886 hartree

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H,-2.6316840802,1.8291372576,-19.778343185
H,-0.8655315555,2.0681025079,-20.065493603
H,-0.3989557428,-0.2063407759,-19.0885236765
H,-2.1651451006,-0.4452777439,-18.8013626174
H,-0.0486401867,-0.6142018616,-5.2536713194
H,0.3171987178,-0.278225605,2.3364101047
H,-2.2019266077,1.5970659657,-17.3276200087
H,-0.4356203712,1.8360779581,-17.614813277
H,0.0310935481,-0.438791308,-16.6379831222
H,-1.7353551352,-0.6778168352,-16.3508063066
H,-1.7727913829,1.3644984952,-14.8777573506
H,-0.0054295285,1.6037885492,-15.1651205326
H,0.4626707093,-0.6744749092,-14.1793250785
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H,0.4435760836,1.3650282419,-12.6882185706
H,-1.3510466559,1.1216355111,-12.3964159187
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H,5.0686557536,-2.9312395484,15.04738742
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H,-5.2342889478,-7.4595944685,11.8983398839
H,-3.7447223275,-5.7386373236,13.0317357633
H,-2.2818386229,-6.7767987896,12.6716070173
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H,3.454364903,-3.0618153138,17.0001237559
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H,-3.884434022,0.4824442947,-28.605477668
H,-3.9211241351,2.5247094065,-27.1313336635
H,-2.1550708663,2.7636418695,-27.4184345536
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C,1.3823190204,2.7718467055,2.5097403427
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H,-0.2848041651,2.1988814988,-10.7088382004
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C,1.2631513801,2.5590916142,1.1127199268
C,0.0570759104,0.3670811248,5.1231231956
C,2.3965557851,3.8328684147,7.8593217378
C,1.2991759748,4.0174996672,8.9019617889
C,1.0867492298,4.3090192549,11.2409006111
C,1.8997117089,4.8197720247,12.4270684593
C,2.2297062855,-1.3428493894,12.6908501552
C,1.4905070581,-0.1078246094,10.819057873
C,3.4125640379,-2.2043020074,13.1238715657
C,1.7398566364,5.0089137025,14.7755903327
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C,1.754061896,1.8040283684,6.8139809733
C,0.8726533324,0.8553090524,7.3729182744
B,-0.2496513421,-1.5122954333,-1.3914321336
C,0.0554549243,0.0693930763,-10.376018513
C,0.3436676231,-0.9334433976,-9.4284027827
C,0.5095247731,-0.5853431227,-8.0958734691
C,0.392193602,0.7531852865,-7.6850372315
C,-3.5083709371,1.4979986009,-31.121580158
C,-3.3913144743,2.2174409052,-29.8028212227
C,-3.0780619588,1.2595896615,-28.6730040395
C,-2.9614166366,1.9864535409,-27.3505689044
C,-2.6482303494,1.0276747282,-26.2219621835
C,-2.5315970163,1.7546945708,-24.8994887048
C,-2.2184052139,0.7958292421,-23.7709533422
C,-2.1017662012,1.5228608614,-22.4484810444
C,-1.7885639604,0.563908347,-21.3200179903
C,-1.6719227854,1.2909715675,-19.9975542332
C,-1.3587098857,0.3318251909,-18.8692485119
C,-0.9288504271,0.0991949097,-16.4190570038
C,-0.8124023683,0.8270984262,-15.0968001617
C,-1.2420875433,1.0590165581,-17.5468245157
C,-0.4992849677,-0.136592062,-13.9734286817
C,-0.3866648733,0.6117046527,-12.6566513911
C,1.9367493297,0.2361993261,9.4001250065

C,-5.0768323459,-9.410731267,13.6746135792
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C,-0.0610554697,1.4078371344,-9.9799770985

Cartesian Coordination of 6-h.

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H,-4.2316975779,9.9377764158,11.3521159325
H,-0.4167950442,-3.6728375357,0.6389222453
H,0.8916905389,-4.3246042828,1.7489259689
H,-3.3884119768,7.1209647416,-4.9543646773
H,-1.6690680832,7.4830018856,-5.4648627891
H,-2.0193752319,0.8885957453,5.85839481
H,-2.9592988893,1.522918365,4.4224598309
H,-2.8080301206,4.796997631,-4.6465967612
H,-1.0883600183,5.1581977625,-5.1566053013
H,-0.2701167682,4.5191281962,-2.8393414866
H,-1.9900912481,4.149202997,-2.3364321718
H,-1.6124700241,3.6741328854,4.4947953858
H,-0.6808669004,3.0400481428,5.9362219103
H,0.3183425087,2.1950674531,-2.5344956253
H,-1.4018391286,1.8272040135,-2.0306266573
H,-1.6767115137,0.3419389859,-4.0740125907
H,0.0510203953,0.6986700441,-4.5607642886
H,-2.5221892838,5.4433814499,5.8648879422
H,-1.5934295882,4.8069303558,7.3071484468
H,-1.1237296552,-1.9888281833,-3.7389005561
H,0.5933399338,-1.6323354614,-4.2627081505
H,1.3290046482,-2.1628281085,-1.8058470421
H,-0.3630005606,-2.8082145674,-1.5319504223
H,-0.0418714337,-12.5783836139,-5.7451978668
H,0.0319939468,-14.6932743655,-6.5382515707
H,-0.5087507974,-16.8279363185,-8.1386101971
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H,4.9894127182,-1.8820556289,6.1338236375
H,-2.2623810319,-18.0128540644,-9.2010916378
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H,-3.8651829839,-18.3432937454,-13.2023083594
H,-3.5455932807,-15.8897283242,-13.5321867384
H,-2.5807331926,-14.4990664499,-11.7228868211
N,-2.0508202616,-14.0349042881,-9.0524145696
N,-0.0985240597,-8.7269076881,-4.243905207
O,-0.0716095338,-1.7647119356,2.2368334265
O,-1.8860990209,6.4104152869,-3.6776203167
O,-1.1812268549,2.9037276456,-3.8151713395
O,-2.7226433984,3.3931436959,6.2498141697
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O,-0.918749601,1.1732104553,4.0977761287
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O,10.6923664102,8.1073136909,12.2638183402
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O,8.1237956342,2.9249179554,8.2247396406
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O,4.1794397117,-5.1798007593,2.6618772823
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H,4.8838238344,-5.9916346414,0.882576209
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H,8.2215369465,5.4392322836,8.985139429
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H,-6.7488315795,20.7279100682,-6.7474295696
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Cartesian Coordination of 6-p.

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Cartesian Coordination of 6-pp.

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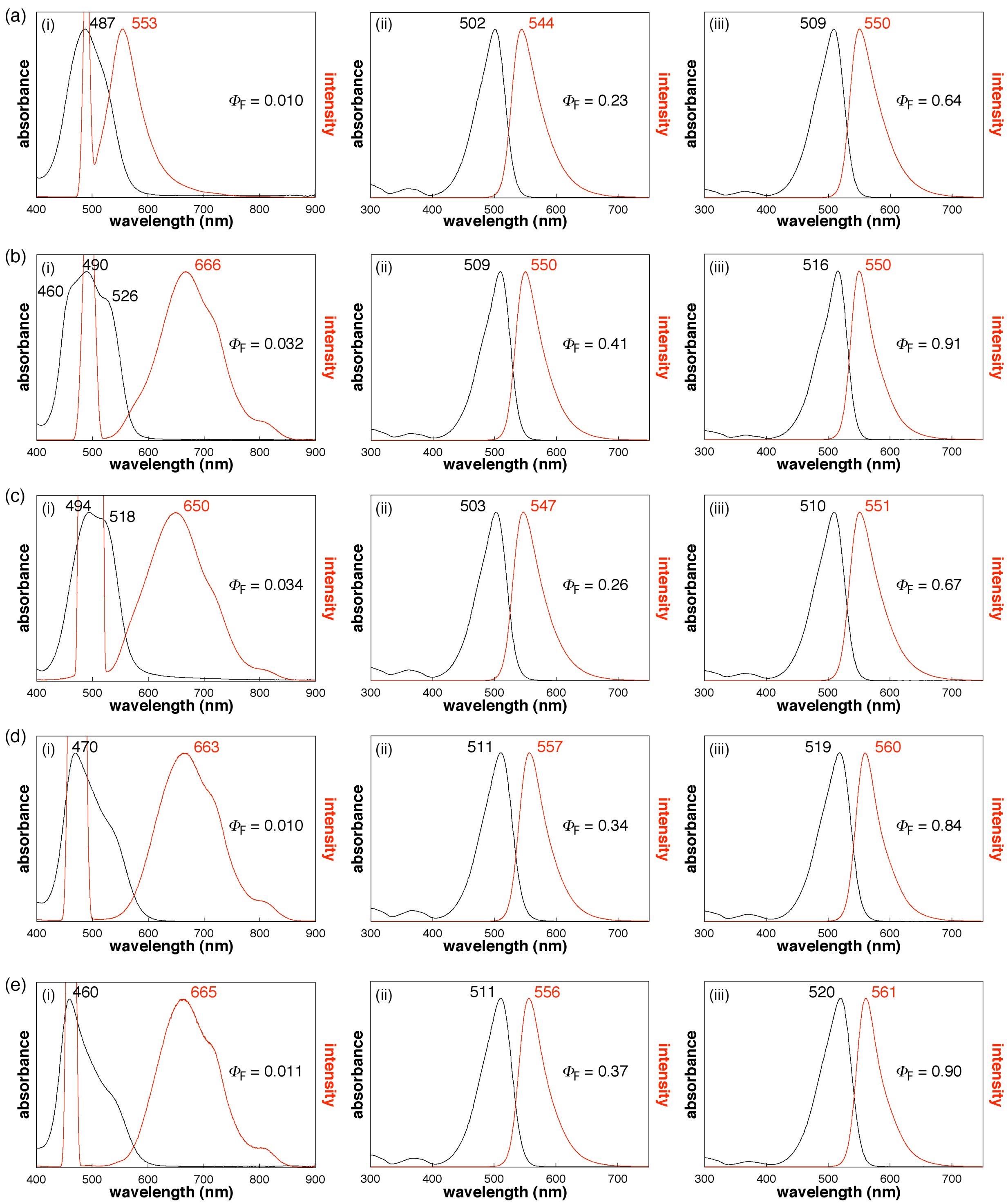
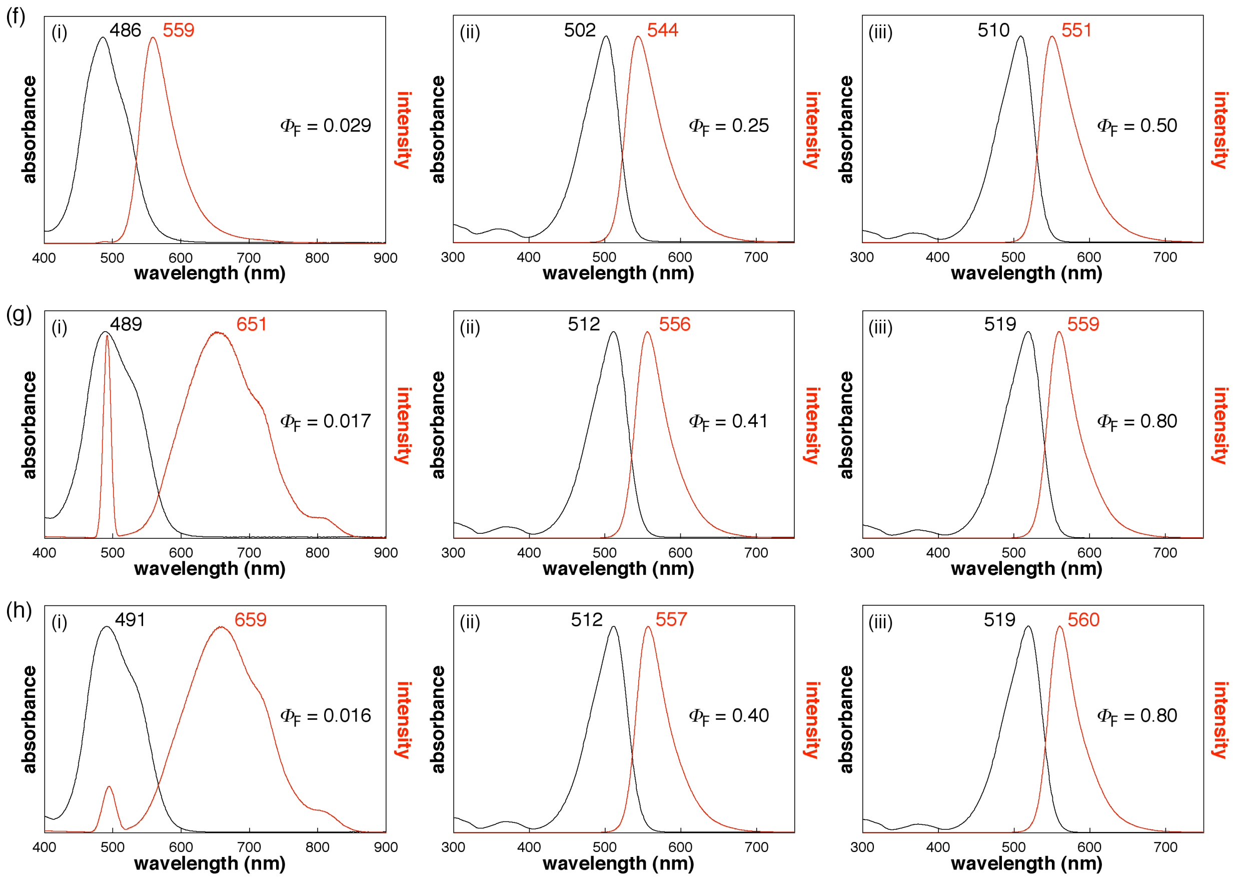
[S4] *Gaussian 03*, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. 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.

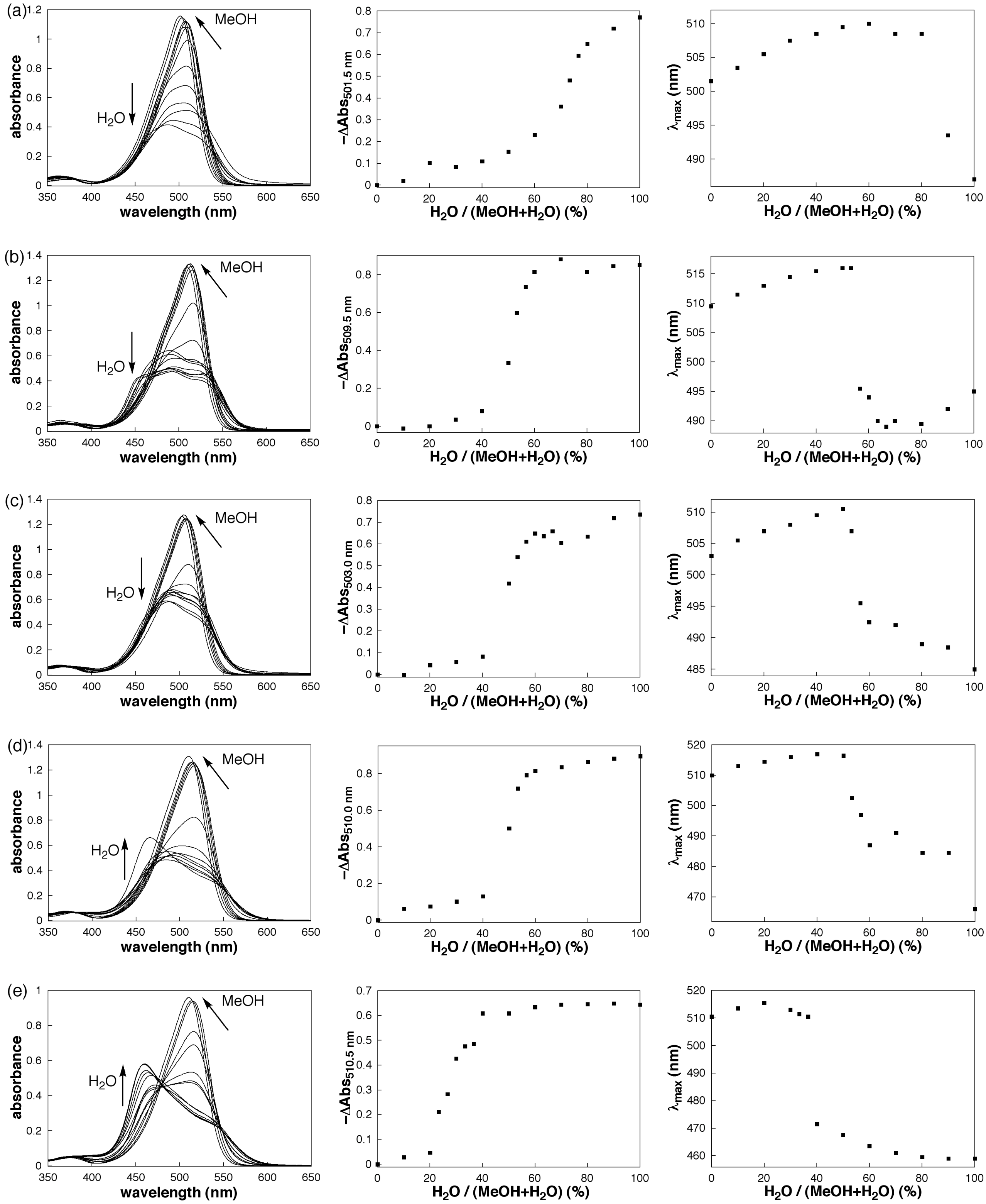
3. Solvent-assisted self-assemblies



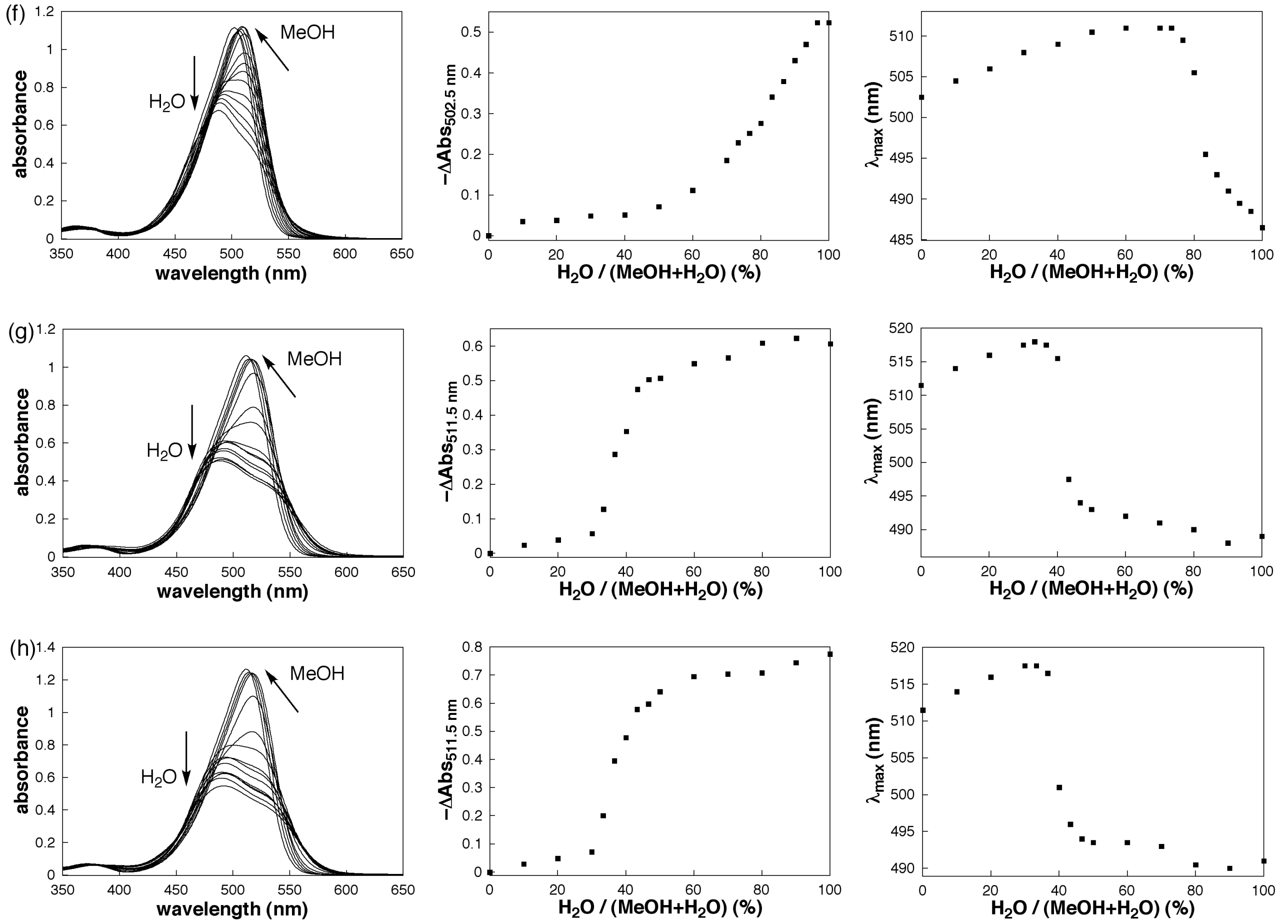
Supporting Figure 2 UV/vis absorption (black line) and fluorescence emission (red line) spectra of (a) **3-o**, (b) **3-m**, (c) **3-p**, (d) **3-h**, (e) **3-pp**, (f) **6-h**, (g) **6-p**, and (h) **6-pp** (1.0×10^{-5} M) in (i) water, (ii) MeOH, and (iii) CH_2Cl_2. Fluorescence was observed by excitation at each absorption maximum (λ_{max}). Each absorbance and emission intensity is normalized. The λ_{max} and λ_{em} along with wavelengths of some shoulders are indicated. In the emission spectra in aqueous solutions, diffraction peaks derived from excitation light are observed due to low emission quantum yields.



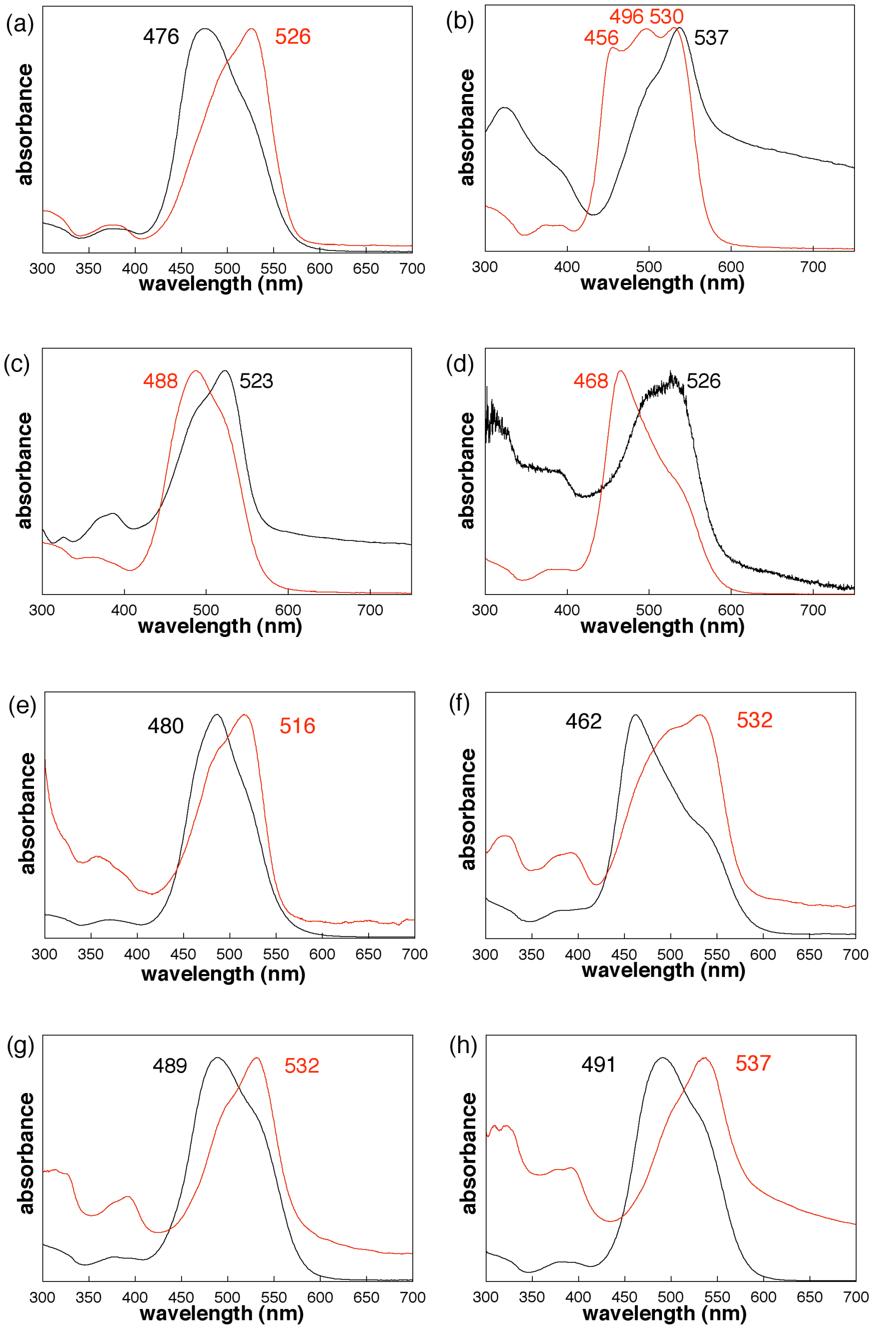
Supporting Figure 2 (Continued).



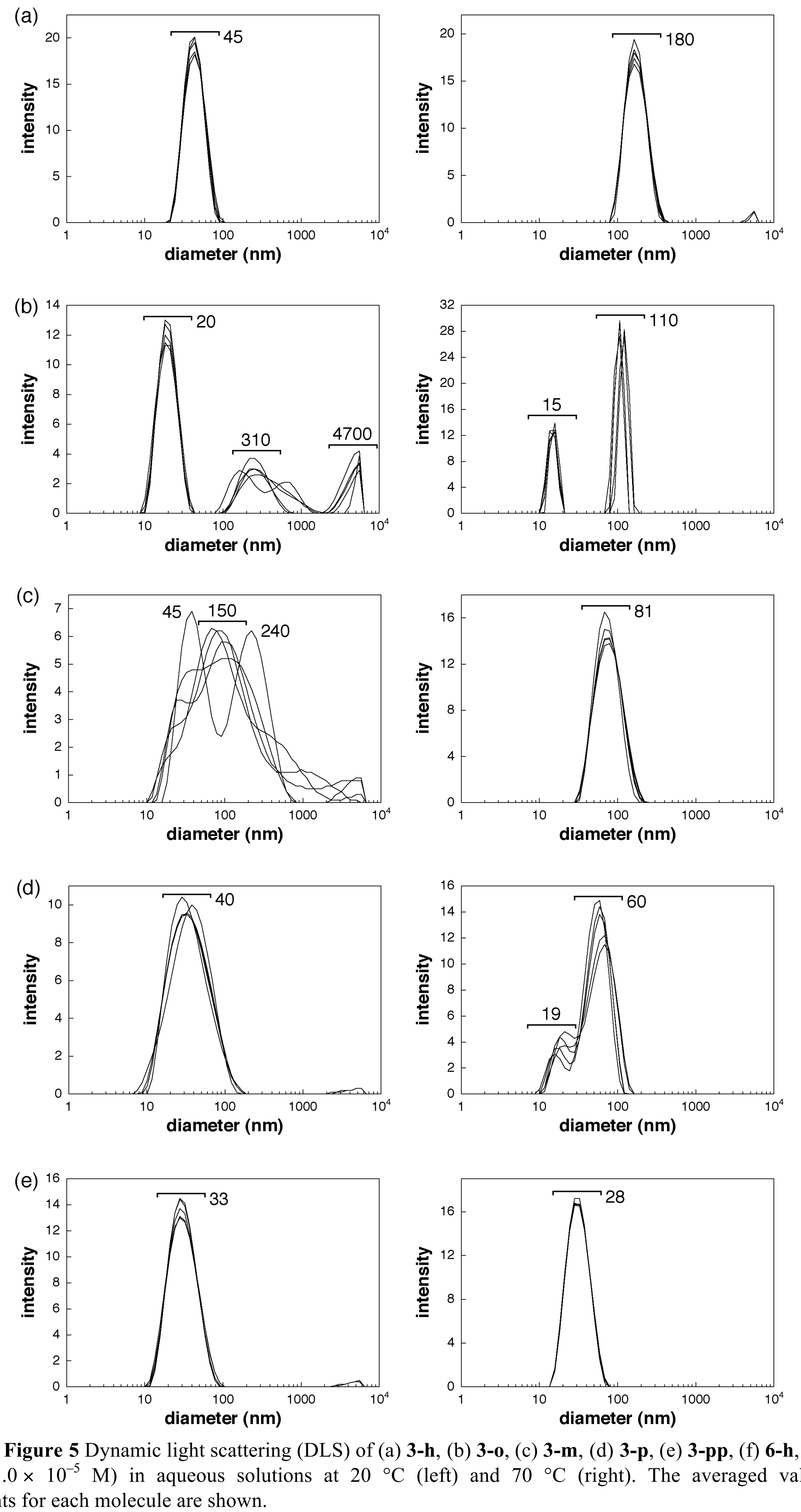
Supporting Figure 3 UV/vis absorption spectral changes in the water-MeOH mixed solvents (1×10^{-5} M) (left), changes in absorbances at the λ_{max} in MeOH according to the ratios (v/v) of water (center), and changes in the λ_{max} values according to the ratios (v/v) of water (right): (a) **3-h**, (b) **3-o**, (c) **3-m**, (d) **3-p**, (e) **3-pp**, (f) **6-h**, (g) **6-p**, and (h) **6-pp**.



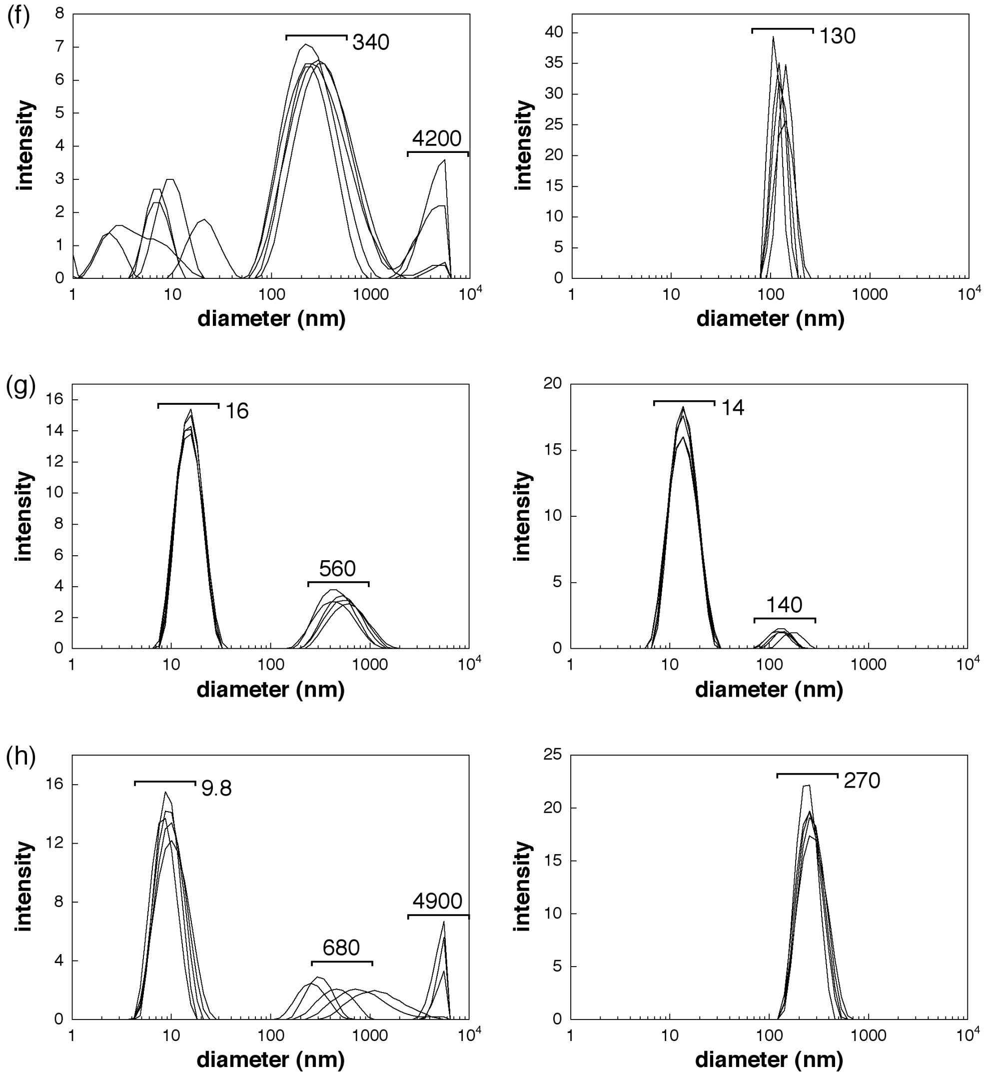
Supporting Figure 3 (Continued).



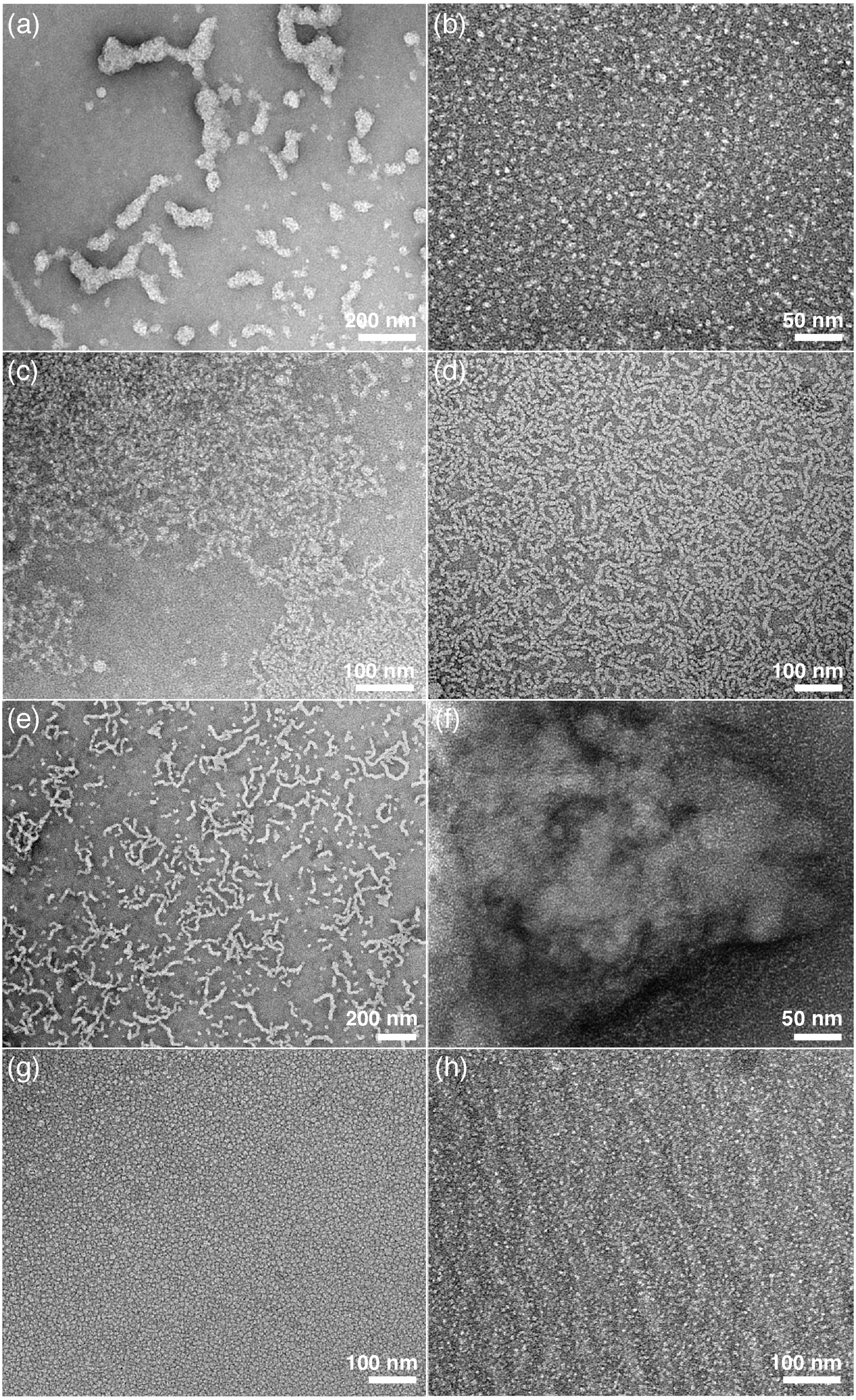
Supporting Figure 4 UV/vis absorption spectra of (a) **3-o**, (b) **3-m**, (c) **3-p**, (d) **3-h**, (e) **3-pp**, (f) **6-h**, (g) **6-p**, and (h) **6-pp** as the solid state cast from aqueous solutions (red line) and those in aqueous solutions (black line, as a reference). The slight differences between the λ_{max} values in aqueous solutions and those in Supporting Figure 2 are within errors and are due to the temperature-dependent spectral changes of H-aggregates of the amphiphiles.



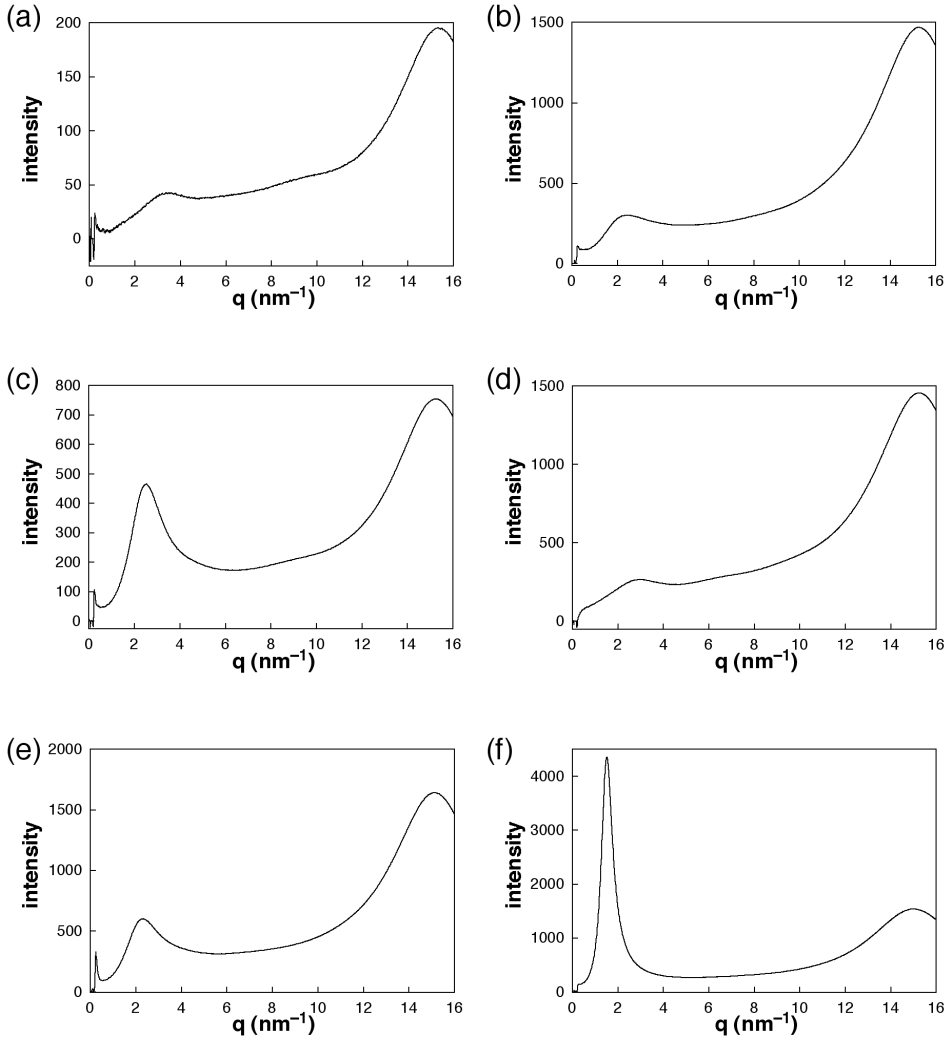
Supporting Figure 5 Dynamic light scattering (DLS) of (a) **3-h**, (b) **3-o**, (c) **3-m**, (d) **3-p**, (e) **3-pp**, (f) **6-h**, (g) **6-p**, and (h) **6-pp** (1.0×10^{-5} M) in aqueous solutions at 20 °C (left) and 70 °C (right). The averaged values of five measurements for each molecule are shown.



Supporting Figure 5 (Continued).



Supporting Figure 6 Images of TEM of (a) **3-h**, (b) **3-o**, (c) **3-m**, (d) **3-p**, (e) **3-pp**, (f) **6-h**, (g) **6-p**, and (h) **6-pp** from aqueous solution (1×10^{-5} M) with $UO_2(OAc)_2$ staining.



Supporting Figure 7 X-ray diffraction (XRD) of (a) **3-h**, (b) **3-o**, (c) **3-m**, (d) **6-h**, (e) **6-p**, and (f) **6-pp** at r.t., suggesting that these amphiphiles are liquid. The detailed properties of the liquid states along with crystalline **3-p** and **3-pp** will be reported elsewhere. Such XRD analyses were carried out using a synchrotron radiation X-ray beam with a wavelength of 1.00 Å on BL40B2 at SPring-8 (Hyogo, Japan). A large Debye-Scherrer camera with a camera length of 543 mm using a quartz capillary was used with an imaging plate as a detector, where the diffraction pattern was obtained with a 0.01° step in 2θ. The exposure time to the X-ray beam was 10 sec.