Electronic Supplementary Information

Dipyrrolylpyrimidines as anion-responsive π-electronic systems

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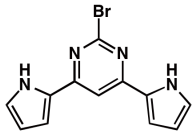
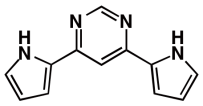
1. Synthetic procedures and spectroscopic data

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. 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. 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 and a Hamamatsu Quantum Yields Measurements System for Organic LED Materials C9920-02, respectively. Matrix-assisted laser desorption ionization time-of-flight mass spectrometries (MALDI-TOF-MS) were recorded on a Shimadzu Axima-CFRplus using positive mode. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Wakogel C-300, Merck silica gel 60, and activated alumina.

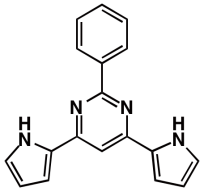
2-Bromo-4,6-di(pyrrol-2-yl)pyrimidine, 3a. To a two-necked flask under N_2, a mixture of 2,4,6-tribromopyrimidine (882 mg, 2.78 mmol), 1-*tert*-butoxycarbonylpyrrole-2-boronic acid[S1] (1.16 g, 5.50 mmol), and Na_2CO_3 (1.76 g, 16.6 mmol) in degassed 1,4-dioxane (20 mL) and water (8.0 mL) was stirred at r.t. After that, $Pd(PPh_3)_4$ (231 mg, 0.20 mmol) was added and stirred at reflux for 48 h and cooled to r.t. The solvent was evaporated under vacuum, and to the mixture was added water, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After the evaporation of solvent, the residue was then chromatographed over silica gel column in twice (Wakogel C-300; first eluent: 2% MeOH/CH_2Cl_2, second eluent: EtOAc:*n*-hexane = 1:2) and recrystallized from CH_2Cl_2/*n*-hexane to give **3a** (313 mg, 1.08 mmol, 38%) as a yellow solid. R_f = 0.55 (EtOAc:*n*-hexane = 1:2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.62 (s, 2H, NH), 7.43 (s, 1H, pyrimidine-H), 7.01–7.00 (m, 2H, pyrrole-H), 6.94–6.93 (m, 2H, pyrrole-H), 6.36–6.35 (m, 2H, pyrrole-H). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 158.15, 152.71, 128.35, 122.48, 111.47, 111.43, 105.38. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$): 368.5 (5.1). MALDI-TOF-MS: *m/z* (% intensity): 286.9 (48), 287.9 (100), 288.9 (65), 289.9 (99), 291.0 (13). Calcd for $C_{12}H_9BrN_4$ ([M – H]$^-$): 286.99. This compound was further characterized by single-crystal X-ray analysis.



4,6-Di(pyrrol-2-yl)pyrimidine, 3b. To **3a** (30.0 mg, 0.104 mmol) in dry THF (2 mL) at –80 °C under N_2 was added *n*-butyllithium in *n*-hexane (1.6 M, 0.22 mL) and stirred for 10 min at the same temperature. Water (5 mL) was added to the reaction mixture at r.t. and extracted with CH_2Cl_2. The organic phase was dried over $MgSO_4$ and the solvent was evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300; eluent: 4% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **3b** (21.4 mg, 0.102 mmol, 98%) as a yellow solid. R_f = 0.45 (4% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.66 (s, 2H, NH), 8.83 (d, *J* = 1.2 Hz, 1H, pyrimidine-H), 7.55 (d, *J* = 1.2 Hz, 1H, pyrimidine-H), 7.00–6.99 (m, 2H, pyrrole-H), 6.94–6.92 (m, 2H, pyrrole-H), 6.37–6.35 (m, 2H, pyrrole-H). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 158.36, 156.17, 129.69, 121.51, 111.15, 110.21, 107.07. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 352.5 (3.8). MALDI-TOF-MS: *m/z* (% intensity): 209.1 (100), 210.1 (54). Calcd for $C_{12}H_9N_4$ ([M – H]$^-$): 209.08. This compound was further characterized by single-crystal X-ray analysis.

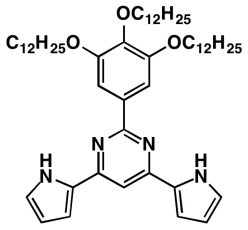


2-Phenyl-4,6-di(pyrrol-2-yl)pyrimidine, 3c. To a two-necked flask under N_2, a mixture of **3a** (57.6 mg, 0.199 mmol), phenylboronic acid (57.6 mg, 0.473 mmol), and Na_2CO_3 (125.1 mg, 1.18 mmol) in degassed 1,4-dioxane (4.2 mL) and water (0.3 mL) was stirred at r.t. After that, $Pd(PPh_3)_4$ (46.5 mg, 40.2 μmol) was added and stirred at reflux for 24 h and cooled to r.t. The solvent was evaporated under vacuum, and to the mixture was added water, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After the evaporation of solvent, the residue was then chromatographed over flash silica gel column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **3c** (16.9 mg, 0.059 mmol, 29%) as a yellow solid. R_f = 0.70 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.80 (s, 2H, NH), 8.54–8.51 (m, 2H, Ar-H), 7.53–7.51 (m, 3H, Ar-H), 7.49 (s, 1H, pyrimidine-H), 7.04–7.03 (m, 2H, pyrrole-H), 6.97–6.96 (m, 2H, pyrrole-H), 6.39–6.38 (m, 2H, pyrrole-H). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 163.58, 156.34, 138.05, 130.46, 129.98, 128.31, 128.08, 121.15, 111.0, 109.99, 105.12. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 358.0 (3.3). MALDI-TOF-MS: *m/z* (% intensity): 285.0 (100), 286.0 (34). Calcd for $C_{18}H_{13}N_4$ ([M – H]$^-$): 285.12.

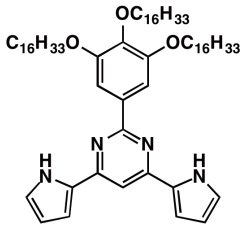


2-(3,4,5-Tridodecyloxyphenyl)-4,6-di(pyrrol-2-yl)pyri

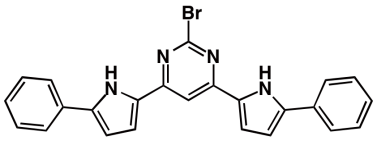
midine, 3d. To a two-necked flask under N_2, a mixture of **3a** (59.2 mg, 0.204 mmol), 3,4,5-tridodecyloxyphenylpinacolborane[S2] (311 mg, 0.411 mmol), and Na_2CO_3 (130 mg, 1.23 mmol) in degassed 1,4-dioxane (1.8 mL) and water (0.1 mL) was stirred at r.t. After that, $Pd(PPh_3)_4$ (17.2 mg, 14.9 μmol) was added and stirred at reflux for 32 h and cooled to r.t. The solvent was evaporated under vacuum, and to the mixture was added water, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After the evaporation of solvent, the residue was then chromatographed over silica gel column in twice (Wakogel C-300; first eluent: CH_2Cl_2, second eluent: CH_2Cl_2:*n*-hexane = 1:1) and recrystallized from CH_2Cl_2/MeOH to give **3d** (65.2 mg, 0.077 mmol, 38%) as a yellow solid. R_f = 0.30 (CH_2Cl_2:*n*-hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.73 (s, 2H, NH), 7.71 (s, 2H, Ar-H), 7.46 (s, 1H, pyrimidine-H), 7.04–7.03 (m, 2H, pyrrole-H), 6.96–6.95 (m, 2H, pyrrole-H), 6.39–6.38 (m, 2H, pyrrole-H), 4.14 (t, J = 6.6 Hz, 4H, OCH_2), 4.05 (t, J = 6.6 Hz, 2H, OCH_2), 1.89–1.84 (m, 4H, $OCH_2\underline{CH_2}$), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.54–1.48 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.41–1.26 (m, 48H, $OC_3H_6\underline{C_8H_{16}}$), 0.88 (t, J = 7.2 Hz, 3H, CH_3), 0.87 (t, J = 7.2 Hz, 6H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 163.72, 156.33, 153.13, 140.99, 133.09, 129.86, 121.20, 111.03, 110.15, 107.39, 104.96, 73.52, 69.47, 31.94, 31.92, 30.38, 29.76, 29.74, 29.72, 29.69, 29.67, 29.63, 29.55, 29.50, 29.39, 29.37, 26.18, 26.14, 22.69, 14.11 (some of the signals for dodecyl chains were overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 313.0 (4.8). MALDI-TOF- MS: *m/z* (% intensity): 837.6 (100), 838.6 (40). Calcd for $C_{54}H_{85}N_4O_3$ ([M – H]$^-$): 837.66.



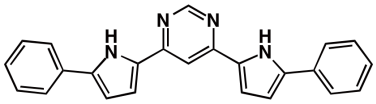
2-(3,4,5-Trihexadecyloxyphenyl)-4,6-di(pyrrol-2-yl)py rimidine, 3e. To a two-necked flask under N_2, a mixture of **3a** (60.5 mg, 0.208 mmol), 3,4,5-trihexadecyloxyphenylpinacolborane[S2] (557 mg, 0.602 mmol), and Na_2CO_3 (135 mg, 1.27 mmol) in degassed 1,4-dioxane (2.8 mL) and water (0.1 mL) was stirred at r.t. After that, $Pd(PPh_3)_4$ (17.2 mg, 14.9 μmol) was added and stirred at reflux for 32 h and cooled to r.t. The solvent was evaporated under vacuum, and to the mixture was added water, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After the evaporation of solvent, the residue was then chromatographed over silica gel column in twice (Wakogel C-300; first eluent: CH_2Cl_2, second eluent: CH_2Cl_2:*n*-hexane = 1:1) and recrystallized from CH_2Cl_2/MeOH to give **3e** (74.2 mg, 0.073 mmol, 35%) as a yellow solid. R_f = 0.30 (CH_2Cl_2:*n*-hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.73 (s, 2H, NH), 7.71 (s, 2H, Ar-H), 7.46 (s, 1H, pyrimidine-H), 7.04–7.03 (m, 2H, pyrrole-H), 6.96–6.94 (m, 2H, pyrrole-H), 6.39–6.38 (m, 2H, pyrrole-H), 4.14 (t, J = 6.6 Hz, 4H, OCH_2), 4.05 (t, J = 6.6 Hz, 2H, OCH_2), 1.89–1.84 (m, 4H, $OCH_2\underline{CH_2}$), 1.81–1.76 (m, 2H, $OCH_2\underline{CH_2}$), 1.54–1.48 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.40–1.26 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.88 (t, J = 7.2 Hz, 9H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 163.73, 156.34, 153.15, 141.01, 133.12, 129.89, 121.19, 111.05, 110.14, 107.42, 104.96, 73.54, 69.50, 31.94, 30.39, 29.77, 29.74, 29.71, 29.69, 29.65, 29.56, 29.52, 29.38, 26.20, 26.16, 22.70, 14.12 (some of the signals for hexadecyl chains were overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 313.0 (4.6). MALDI-TOF-MS: *m/z* (% intensity): 1005.8 (100), 1006.8 (74). Calcd for $C_{66}H_{109}BrN_4O_3$ ([M – H]$^-$): 1005.85.



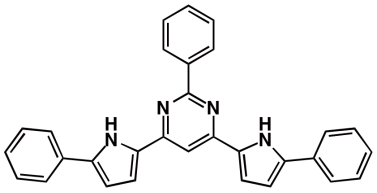
2-Bromo-4,6-di(5-phenylpyrrol-2-yl)pyrimidine, 4a. Schlenk flask was charged with 5-phenyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyrrole[S3] (2.33 mmol, 627.1 mg), 2,4,6-tribromopyrimidine (369.3 mg, 1.17 mmol), $Pd(PPh_3)_4$ (77.0 mg, 0.07 mmol), and Na_2CO_3 (987.8 mg, 9.32 mmol) and flushed with N_2. Degassed 1,4-dioxane (8 mL) and water (0.3 mL) were added and mixture was stirred at 90 °C for 18 h and cooled to r.t. The solvent was evaporated under vacuum, and to the mixture was added water, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After the evaporation of solvent, the residue was then chromatographed over silica gel column (first eluent: 0.5% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4a** (202.0 mg, 45.8 μmol, 39%) as a yellow solid. R_f = 0.40 (0.5% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.75 (s, 2H, NH), 7.64 (dd, J = 8.4 and 1.2 Hz, 4H, Ar-H), 7.46 (s, 1H, pyrimidine-H), 7.44 (t, J = 7.8 Hz, 4H, Ar-H), 7.32 (t, J = 7.2 Hz, 2H, Ar–H), 7.00 (dd, J = 2.4 and 1.8 Hz, 2H, pyrrole-H), 6.66 (dd, J = 3.0 and 0.6 Hz, 2H, pyrrole-H). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 157.72, 152.96, 136.72, 131.38, 129.06, 127.69, 124.71, 113.32, 109.22, 105.43 (one of the peaks was overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 416.5 (7.4). MALDI-TOF-MS: *m/z* (% intensity): 439.1 (22), 440.1 (80), 441.1 (64), 442.1 (100), 443.1 (17). Calcd for $C_{24}H_{16}BrN_4$ ([M – H]$^-$): 439.06. This compound was further characterized by single-crystal X-ray analysis.



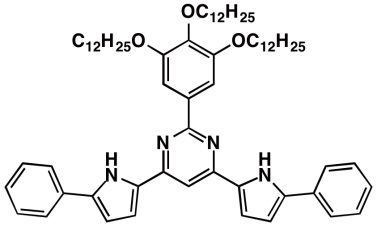
4,6-Di(5-phenylpyrrol-2-yl)pyrimidine, 4b. To **4a** (40.0 mg, 9.06 μmol) in dry THF (2 mL) at –80 °C under N_2 was added *n*-butyllithium in *n*-hexane (1.6 M, 0.17 mL) and stirred for 10 min at the same temperature. Water (5 mL) was added to the reaction mixture at r.t. and extracted with CH_2Cl_2. The organic phase was dried over $MgSO_4$ and the solvent was evaporated. The residue was then chromatographed over flash silica gel column (eluent: 2% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4b** (26.9 mg, 7.40 μmol, 82%) as a yellow solid. R_f = 0.45 (3% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.85 (s, 2H, NH), 8.87 (d, *J* = 1.8 Hz, 1H, pyrimidine-H), 7.63 (dd, *J* = 7.8 and 1.2 Hz, 4H, Ar-H), 7.58 (d, *J* = 1.8 H, 1H, pyrimidine-H), 7.43 (t, *J* = 7.8 Hz, 4H, Ar-H), 7.30 (t, *J* = 7.8 Hz, 2H, Ar-H), 7.00 (dd, *J* = 2.4 and 1.2 Hz, 2H, pyrrole-H), 6.66 (dd, *J* = 3.6, 0.6 Hz, 2H, pyrrole- H). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 158.38, 155.69, 135.67, 131.79, 130.31, 129.04, 127.36, 124.49, 111.99, 108.90, 107.03. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 398.0 (6.9). MALDI-TOF-MS: *m/z* (% intensity): 361.2 (100), 362.2 (31). Calcd for $C_{24}H_{17}N_4$ ($[M - H]^-$): 361.15.



2-Phenyl-4,6-di(5-phenylpyrrol-2-yl)pyrimidine, 4c. To a dried two-necked flask under N_2, a mixture of **4a** (38.1 mg, 86.3 μmol), phenylboronic acid (24.8 mg, 0.203 mmol), and Na_2CO_3 (54.8 mg, 0.517 mmol) in degassed 1,4-dioxane (1.8 mL) and water (0.12 mL) was stirred at r.t. After that, $Pd(PPh_3)_4$ (18.8 mg, 16.3 μmol) was added and stirred for reflux for 24 h and cooled to r.t. The solvent was evaporated under vacuum, and to the mixture was added water, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After the evaporation of solvent, the residue was then chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/*n*-hexane to give **4c** (32.7 mg, 0.074 mmol, 86%) as a yellow solid. R_f = 0.70 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): *δ* (ppm) 9.94 (s, 2H, NH), 8.57–8.55 (m, 2H, Ar-H), 7.66 (dd, *J* = 8.4 and 1.2 Hz, 4H, Ar-H), 7.60–7.54 (m, 3H, Ar-H), 7.52 (s, 1H, pyrimidine-H), 7.46 (t, *J* = 7.2 Hz, 4H, Ar-H), 7.32 (t, *J* = 7.2 Hz, 2H, Ar-H), 7.03 (dd, *J* = 2.4 and 1.8 Hz, 2H, pyrrole-H), 6.69 (dd, *J* = 3.0 and 0.6 Hz, 2H, pyrrole-H). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 163.82, 155.98, 138.11, 135.21, 131.85, 130.68, 130.55, 129.03, 128.41, 128.20, 127.28, 124.47, 111.84, 108.81, 105.20. UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 400.0 (6.6). MALDI-TOF- MS: *m/z* (% intensity): 437.1 (100), 438.1 (36). Calcd for $C_{30}H_{21}N_4$ ($[M - H]^-$): 437.18.

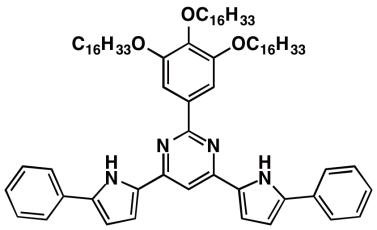


2-(3,4,5-Tridodecyloxyphenyl)-4,6-di(5-phenylpyrrol-2-yl)pyrimidine, 4d. To a dried two-necked flask under N_2, a mixture of **4a** (19.0 mg, 43.1 μmol), 3,4,5-tridodecyloxyphenylpinacolborane[S2] (78.3 mg, 0.103 mmol), Na_2CO_3 (27.7 mg, 0.261 mmol) in degassed 1,4-dioxane (0.94 mL) and water (0.06 mL) was stirred at r.t. After that, $Pd(PPh_3)_4$ (9.20 mg, 7.96 μmol) was added and stirred at reflux for 24 h and cooled to r.t. The solvent was evaporated under vacuum, and water was added to the mixture, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After that, the solvent was evaporated, and the residue was then chromatographed over silica gel column (Wakogel C-300; eluent: $CHCl_3$:*n*-hexane = 2:1) and recrystallized from CH_2Cl_2/MeOH to give **4d** (40.4 mg, 40.7 μmol, 94%) as a yellow solid. R_f = 0.33 ($CHCl_3$:*n*-hexane = 2:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): *δ* (ppm) 9.91 (s, 2H, NH), 7.74 (s, 2H, Ar-H), 7.62 (dd, *J* = 8.4 and 1.2 Hz, 4H, Ar-H), 7.48 (s, 1H, pyrimidine-H), 7.44 (t, *J* = 7.2 Hz, 4H, Ar-H), 7.31 (t, *J* = 7.8 Hz, 2H, Ar-H), 7.02 (dd, *J* = 2.4 and 1.8 Hz, 2H, pyrrole-H), 6.69 (dd, *J* = 3.0 and 0.6 Hz, 2H, pyrrole-H), 4.18 (t, *J* = 6.6 Hz, 4H, OCH_2), 4.07 (t, *J* = 6.6 Hz, 2H, OCH_2), 1.92–1.86 (m, 4H, $OCH_2\underline{CH_2}$), 1.82–1.78 (m, 2H, $OCH_2\underline{CH_2}$), 1.55–1.49 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.42–1.25 (m, 48H, $OC_3H_6\underline{C_8H_{16}}$), 0.88 (t, *J* = 7.2 Hz, 3H, CH_3), 0.87 (t, *J* = 7.2 Hz, 6H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 163.88, 155.90, 153.09, 141.0, 135.11, 133.16, 131.81, 130.60, 129.03, 127.25, 124.33, 111.89, 108.84, 107.43, 104.93, 73.60, 69.50, 31.95, 31.93, 30.39, 29.78, 29.77, 29.73, 29.70, 29.67, 29.64, 29.52, 29.50, 29.41, 29.37, 26.16, 22.71, 22.69, 14.12 (some of the signals for dodecyl chains were overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 402.0 (6.5). MALDI-TOF-MS: *m/z* (% intensity): 989.7 (100), 990.7 (73). Calcd for $C_{66}H_{93}N_4O_3$ ($[M - H]^-$): 989.73.



2-(3,4,5-Trihexadecyloxyphenyl)-4,6-di(5-phenylpyrrol-2-yl)pyrimidine, 4e. To a dried two-necked flask under N_2, a mixture of **4a** (37.8 mg, 85.7 μmol), 3,4,5-trihexadecyloxyphenylpinacolborane[S2] (185 mg, 0.20 mmol), Na_2CO_3 (54.5 mg, 0.514 mmol) in degassed

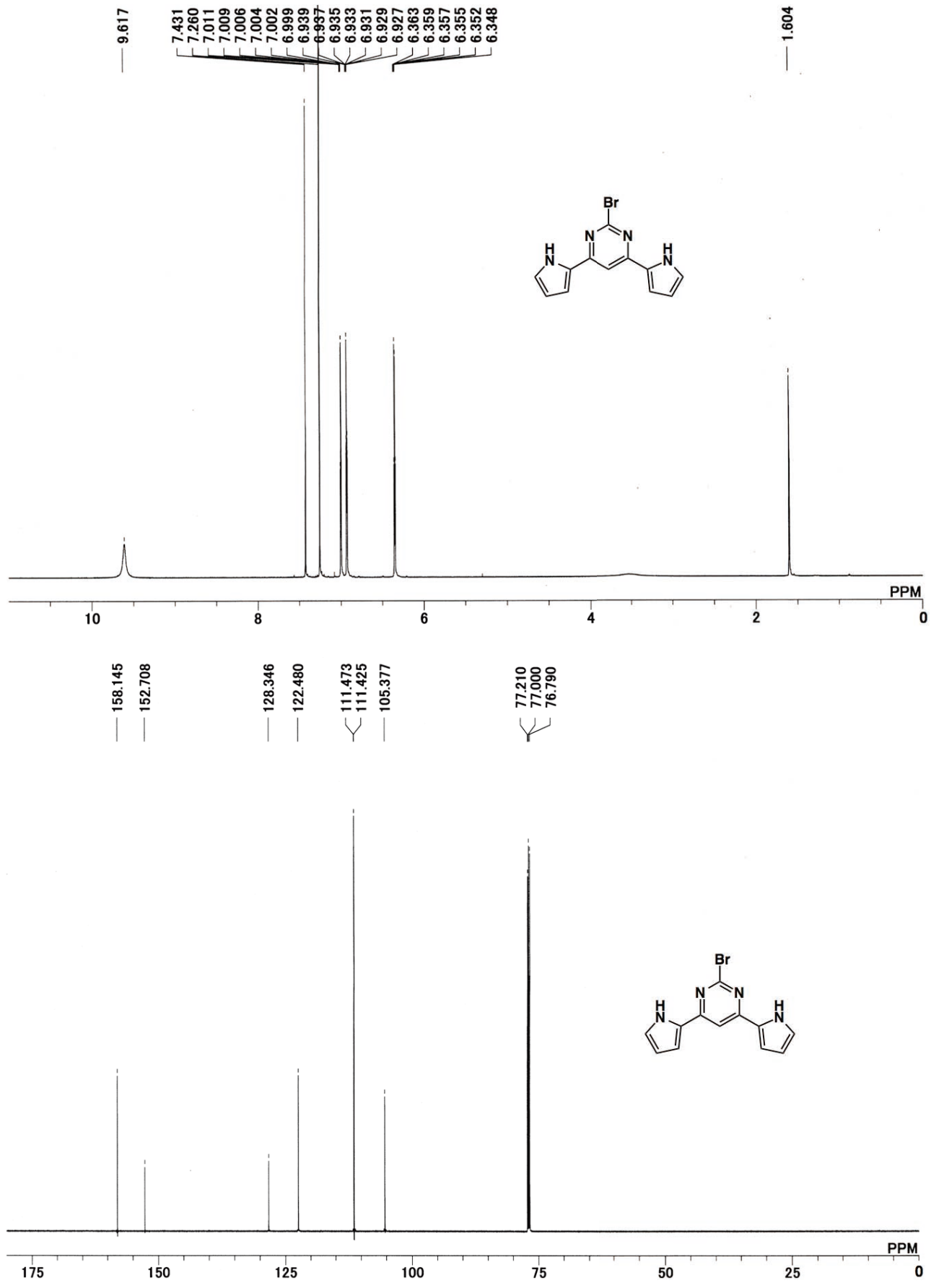
1,4-dioxane (1.8 mL) and water (0.12 mL) was stirred at r.t. After that, $Pd(PPh_3)_4$ (18.4 mg, 15.9 μmol) was added and stirred at reflux for 15 h and cooled to r.t. The solvent was evaporated under vacuum, and water was added to the mixture, followed by the extraction with CH_2Cl_2. The organic phase was washed with brine and dried over Na_2SO_4. After that, the solvent was evaporated, and the residue was then chromatographed over silica gel column twice (Wakogel C-300; first eluent: $CHCl_3$, second eluent: $CHCl_3$:*n*-hexane = 2:1) and recrystallized from CH_2Cl_2/MeOH to give **4e** (82.7 mg, 71.3 μmol, 84%) as a yellow solid. R_f = 0.42 (CH_2Cl_2:*n*-hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 9.91 (s, 2H, NH), 7.74 (s, 2H, Ar-H), 7.62 (dd, J = 8.4 and 1.2 Hz, 4H, Ar-H), 7.48 (s, 1H, pyrimidine-H), 7.44 (t, J = 7.2 Hz, 4H, Ar-H), 7.31 (t, J = 7.2 Hz, 2H, Ar–H), 7.02 (dd, J = 2.4 and 1.2 Hz, 2H, pyrrole-H), 6.69–6.68 (m, 2H pyrrole-H), 4.18 (t, J = 7.2 Hz, 4H, OCH_2), 4.08 (t, J = 6.6 Hz, 2H, OCH_2), 1.92–1.88 (m, 4H, $OCH_2\underline{CH_2}$), 1.82–1.78 (m, 2H, $OCH_2\underline{CH_2}$), 1.56–1.49 (m, 6H, $OC_2H_4\underline{CH_2}$), 1.42–1.25 (m, 72H, $OC_3H_6\underline{C_{12}H_{24}}$), 0.89–0.86 (m, 9H, CH_3). ^{13}C NMR (151 MHz, $CDCl_3$, 20 °C): δ (ppm) 163.89, 155.92, 153.11, 141.03, 135.10, 133.18, 131.82, 130.62, 129.05, 127.27, 124.33, 111.88, 108.85, 107.47, 104.93, 73.60, 69.54, 31.93, 30.39, 29.79, 29.77, 29.73, 29.70, 29.68, 29.65, 29.52, 29.50, 29.37, 26.16, 22.70, 14.12 (some of the signals for hexadecyl chains were overlapped). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^4 $M^{-1}cm^{-1}$)): 402.0 (5.8). MALDI-TOF-MS: *m/z* (% intensity): 1157.8 (100), 1158.8 (90), 1159.8 (44). Calcd for $C_{78}H_{117}N_4O_3$ ([M – H]$^-$): 1157.91.



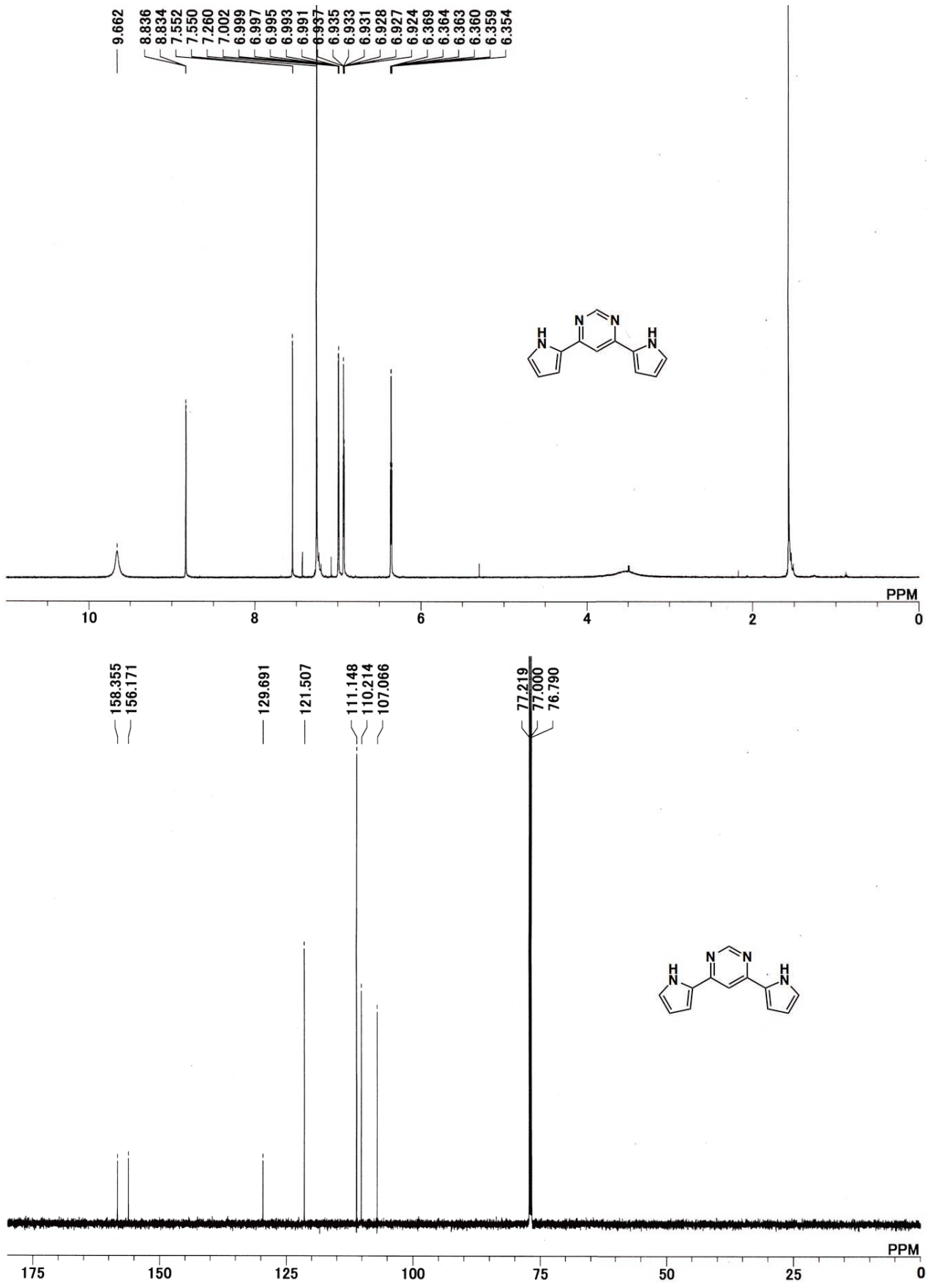
[S1] A. T. Kelly, U. V. Fuchs, W. C. Perry and J. R. Snow, *Tetrahedron*, 1993, **49**, 1009–1016.

[S2] Y. Haketa, S. Sakamoto, K. Chigusa, T. Nakanishi and H. Maeda, *J. Org. Chem.*, 2011, **76**, 5177–5184.

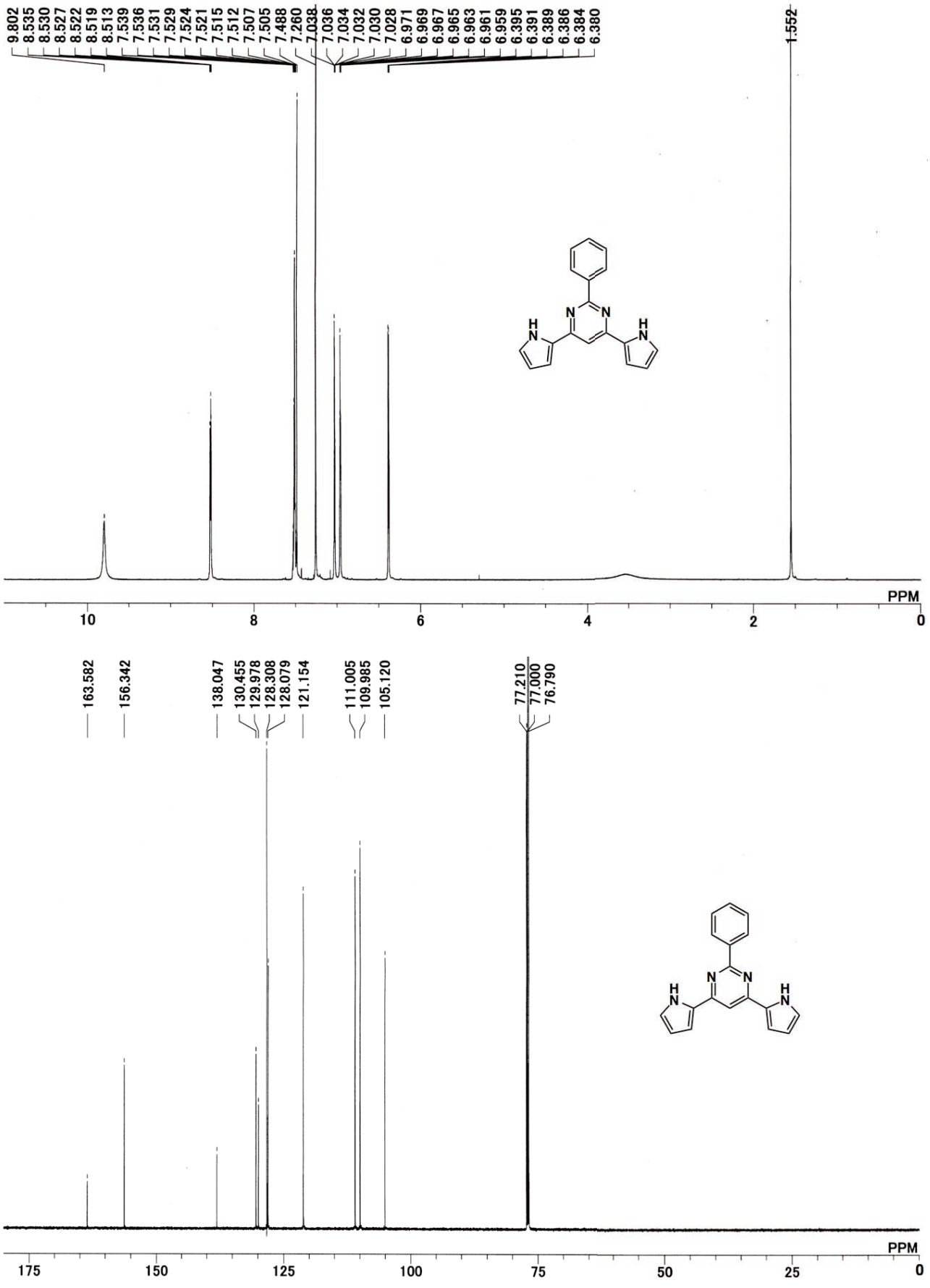
[S3] H. Maeda and Y. Takeda, manuscript in preparation.



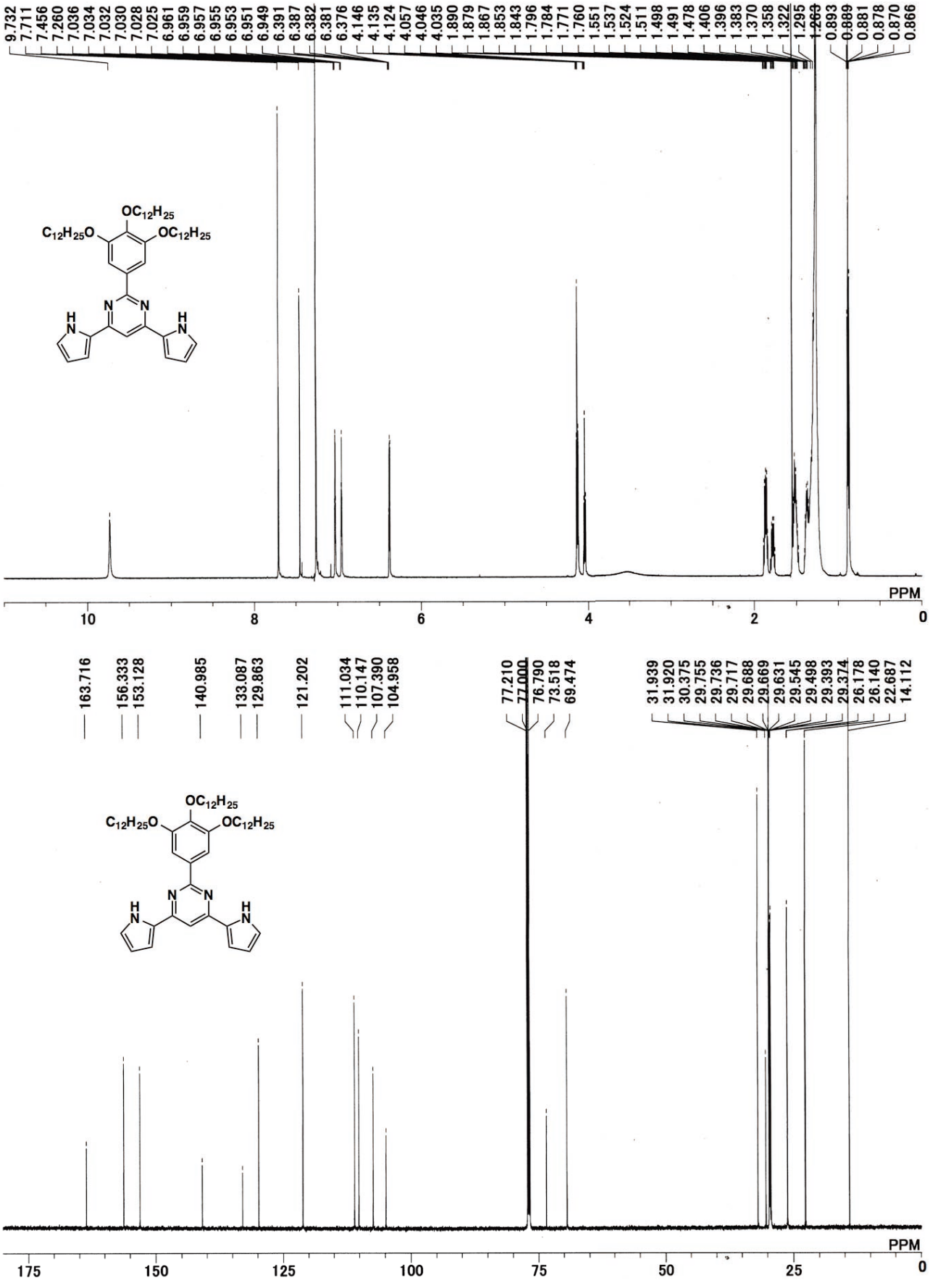
Supporting Figure 1 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3a** in $CDCl_3$ at 20 °C.



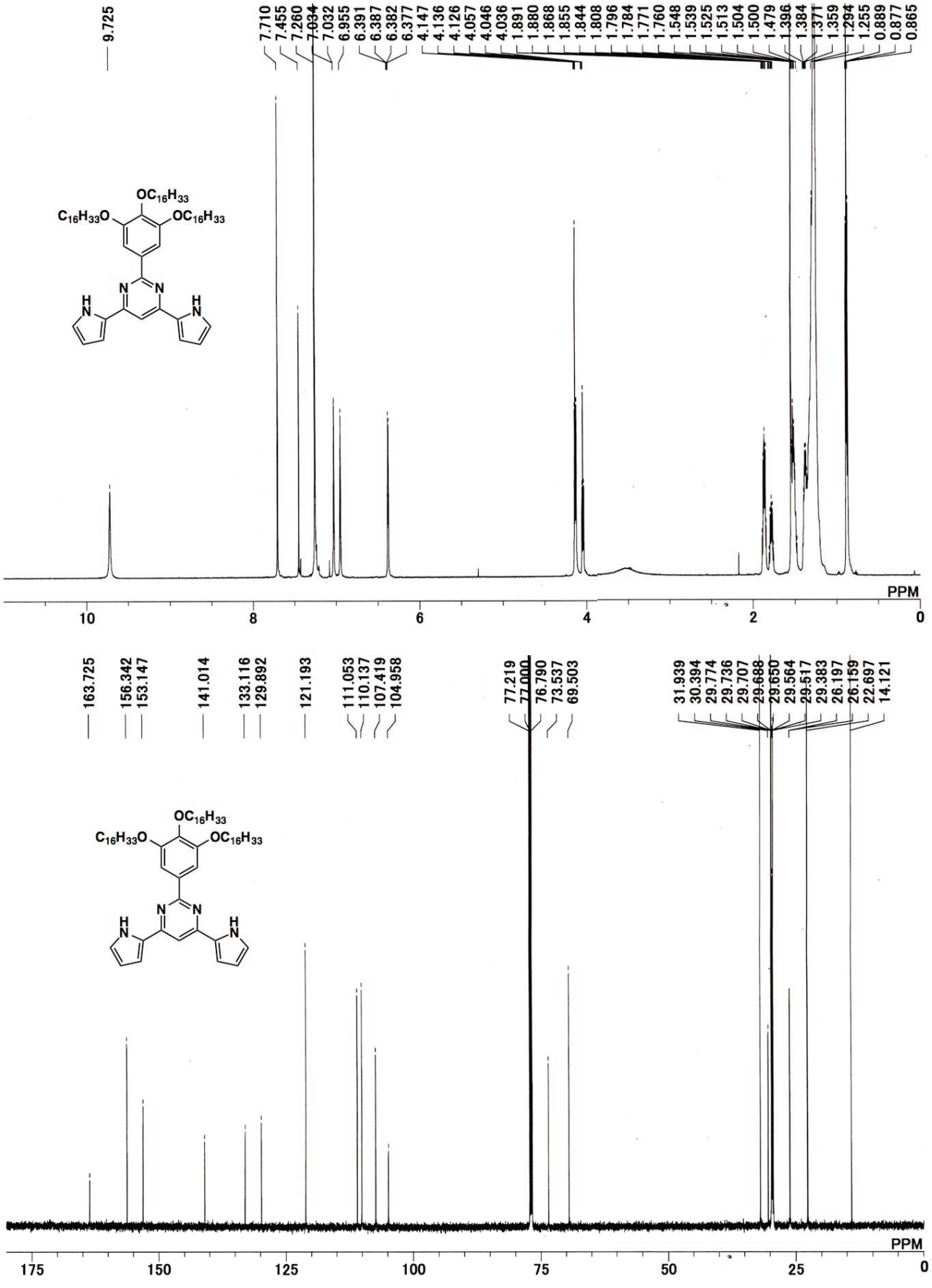
Supporting Figure 2 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3b** in $CDCl_3$ at 20 °C.



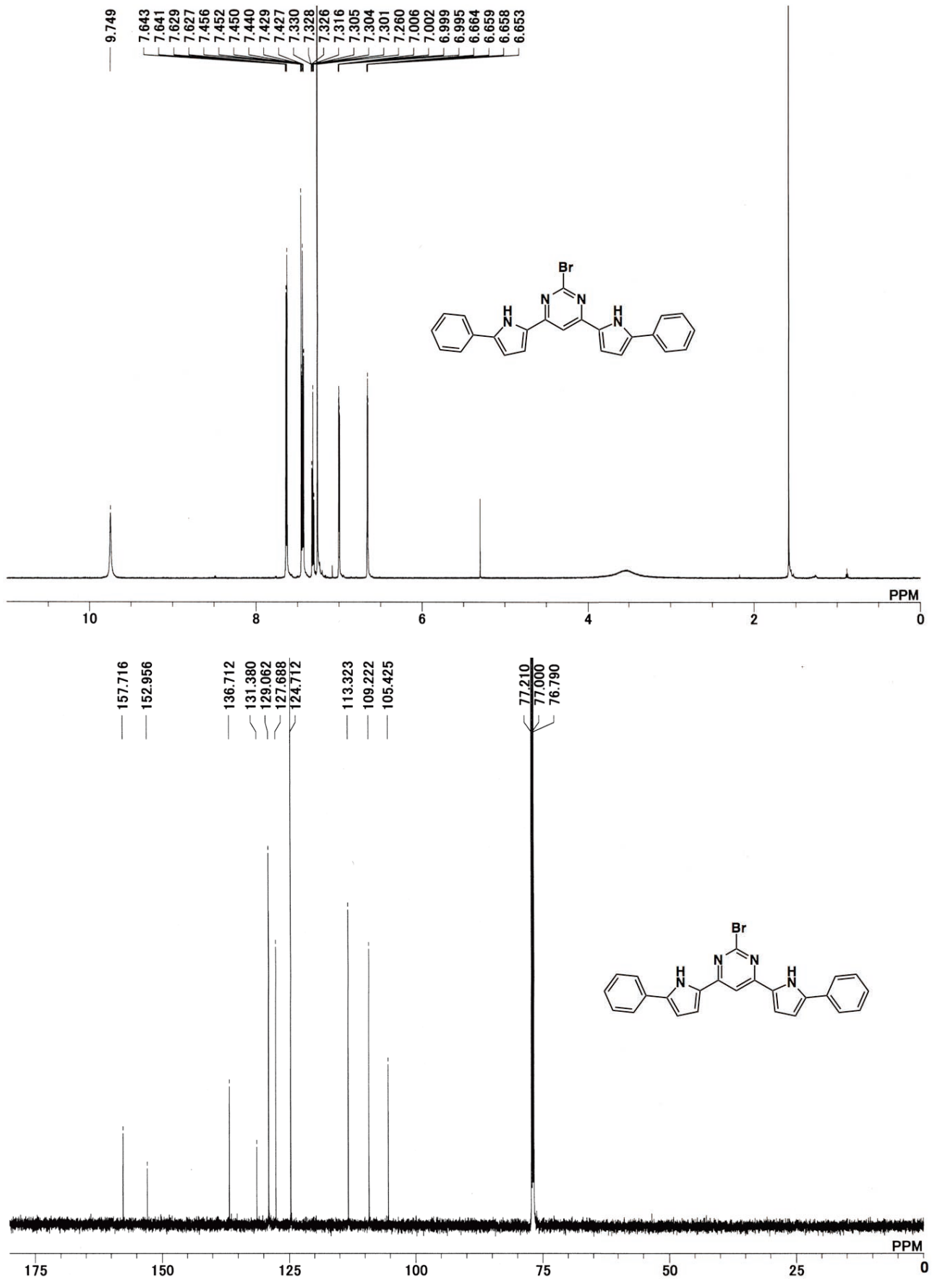
Supporting Figure 3 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3c** in $CDCl_3$ at 20 °C.



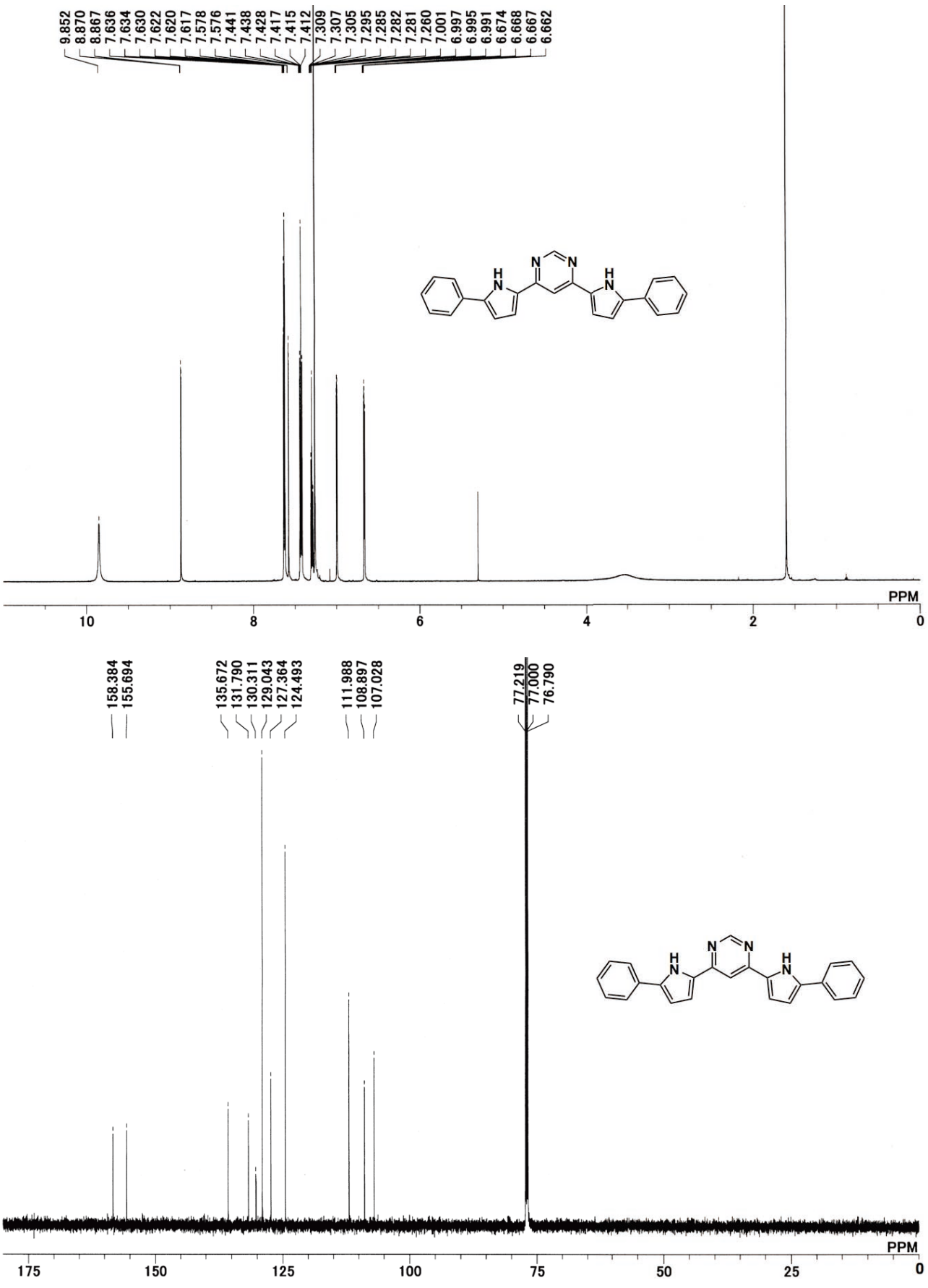
Supporting Figure 4 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3d** in $CDCl_3$ at 20 °C.



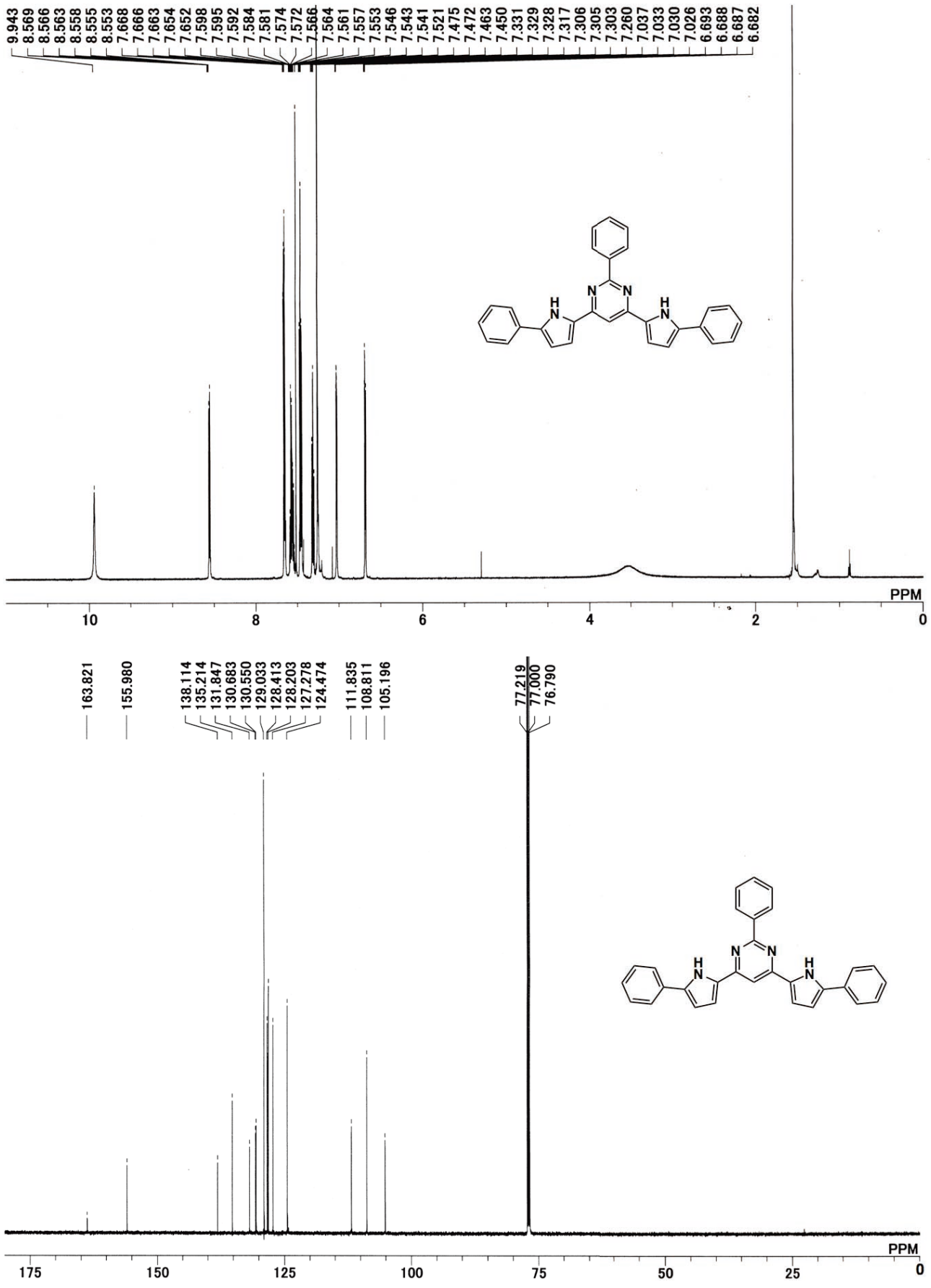
Supporting Figure 5 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3e** in $CDCl_3$ at 20 °C.



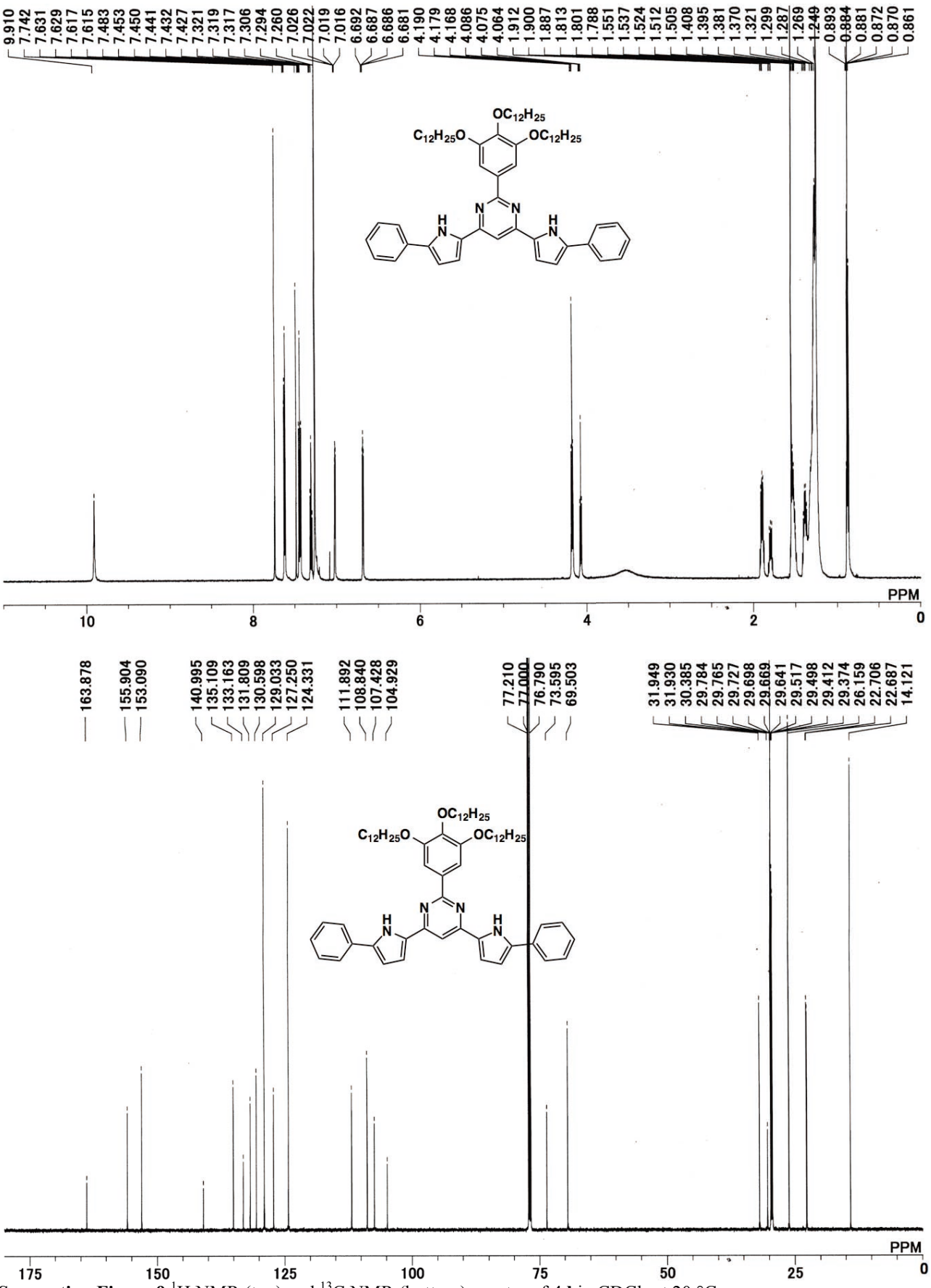
Supporting Figure 6 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4a** in $CDCl_3$ at 20 °C.



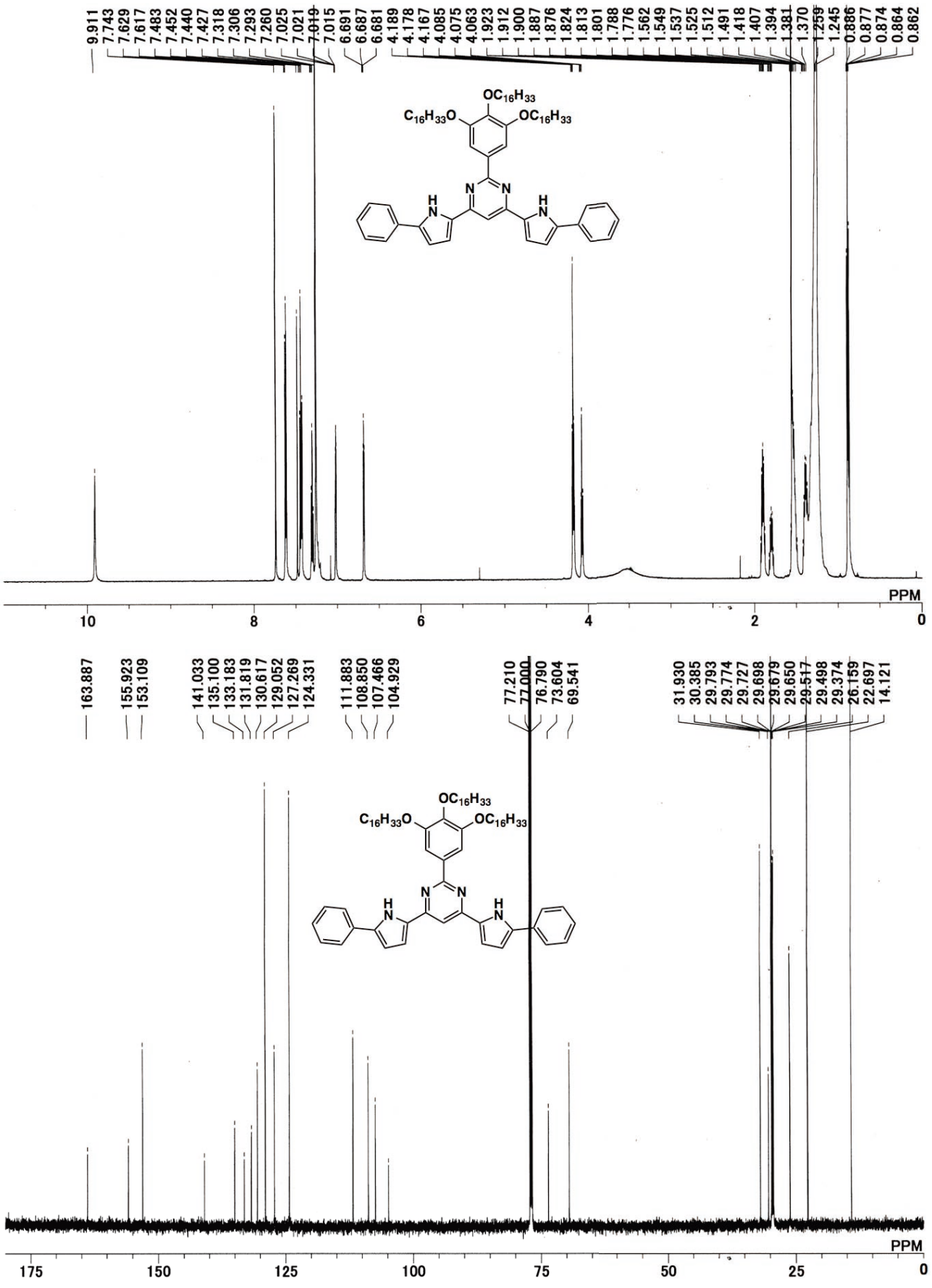
Supporting Figure 7 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4b** in $CDCl_3$ at 20 °C.



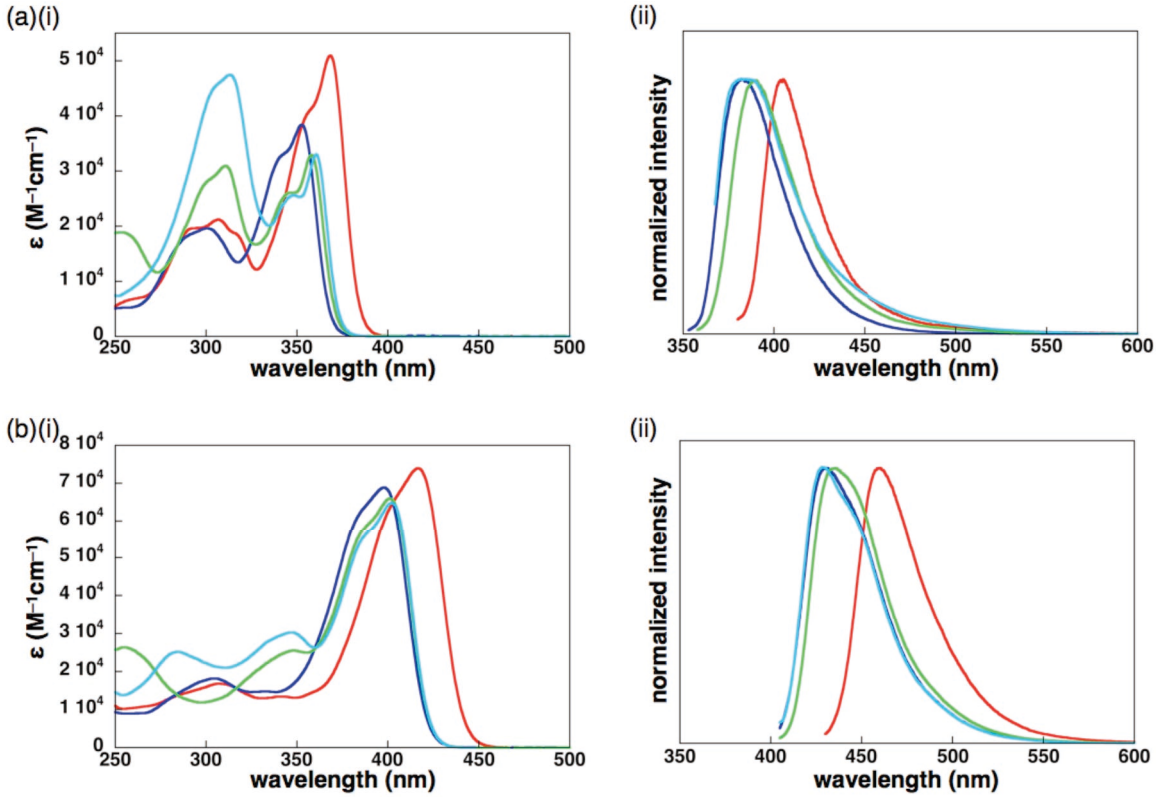
Supporting Figure 8 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4c** in $CDCl_3$ at 20 °C.



Supporting Figure 9 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4d** in $CDCl_3$ at 20 °C.



Supporting Figure 10 ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4e** in $CDCl_3$ at 20 °C.



Supporting Figure 11 (i) UV/vis absorption and (ii) fluorescence spectra ($\lambda_{ex} = \lambda_{max}$) and their quantum yields (Φ_F) in CH_2Cl_2 of (a) **3a** (λ_{max} = 368.5 nm, λ_{em} = 404.0 nm (Φ_F = 0.04), red), **3b** (λ_{max} = 352.5 nm, λ_{em} = 382.2 nm (Φ_F = 0.45), blue), **3c** (λ_{max} = 358.0 nm, λ_{em} = 390.2 nm (Φ_F = 0.24), green), and **3d** (λ_{max} = 313.0 nm, λ_{em} = 384.2 nm (Φ_F = 0.13), cyan) and (b) **4a** (λ_{max} = 416.5 nm, λ_{em} = 459.8 nm (Φ_F = 0.12), red), **4b** (λ_{max} = 398.0 nm, λ_{em} = 430.8 (Φ_F = 0.75) nm, blue), **4c** (λ_{max} = 400.0 nm, λ_{em} = 435.4 nm (Φ_F = 0.69), green), and **4d** (λ_{max} = 402.0 nm, λ_{em} = 429.0 nm (Φ_F = 0.66), cyan).

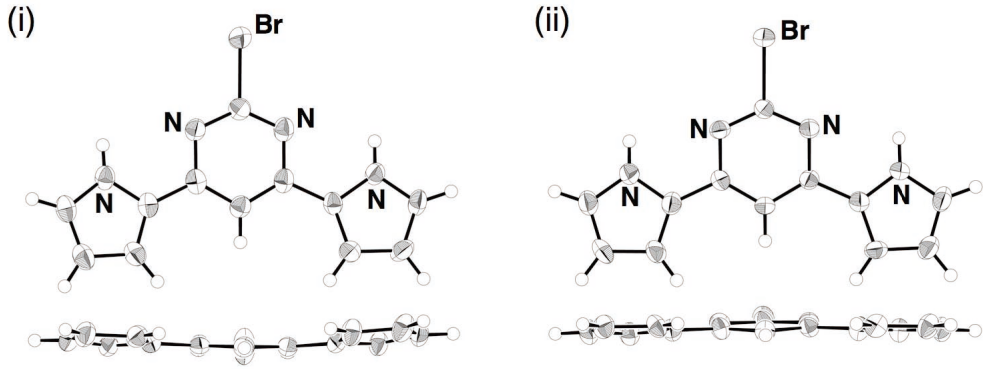
2. X-ray crystallographic data

Single-Crystal X-ray Analysis. Crystallographic data of dipyrrolylpyrimidines and anion complexes are summarized in Supporting Table 1. Single crystal of **3a** was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 solution of **3a**. The data crystal was a colorless prism of approximate dimensions 0.40 mm × 0.20 mm × 0.10 mm. Single crystal of **3a**·Cl^--TBA^+ was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 solution including **3a** and tetrabutylammonium chloride (TBACl) as a mixture with the 1:1 molar ratio. The data crystal was a colorless prism of approximate dimensions 0.24 mm × 0.10 mm × 0.10 mm. Single crystal of **3b** was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 and small amount of toluene solution of **3b**. The data crystal was a yellow prism of approximate dimensions 0.01 mm × 0.01 mm × 0.01 mm. Single crystal of **4a** was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 solution of **4a**. Single crystal of **3a**·Cl^--$TATA^+$ was obtained by vapor diffusion of *n*-hexane into a CH_2Cl_2 solution including **3a** and 4,8,12-tripropyl-4,8,12-triazatriangulenium chloride (TATACl)[S4,5] as a mixture with the 1:1 molar ratio. The data crystal was a colorless prism of approximate dimensions 0.29 mm × 0.27 mm × 0.02 mm. The data crystal was a yellow prism of approximate dimensions 0.23 mm × 0.10 mm × 0.10 mm. Data were collected at 93 K on a Rigaku RAXIS-RAPID II diffractometer for **3a**, **3a**·Cl^--TBA^+, and **3a**·Cl^--$TATA^+$ and a Rigaku XtaLAB P200 diffractometer for **4a** with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å) and at 100(2) K on a Rigaku Saturn 724 diffractometer for **3b** with Si (111) monochromated synchrotron radiation (λ = 0.78201 Å) at BL40XU (SPring-8).[S6] In each compound, structures were solved by direct method and the non-hydrogen atoms were refined anisotropically. The calculations were performed using the Crystal Structure crystallographic software package of Molecular Structure Corporation.[S7] CIF files (CCDC 1485805–1485809) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

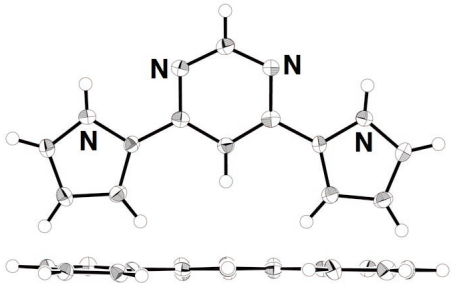
Supporting Table 1 Crystallographic details for compounds **3a**, **3b**, **4a**, **3a**·Cl^--TBA^+, and **3a**·Cl^--$TATA^+$.

	3a	**3b**	**4a**	**3a**·Cl^--TBA^+	**3a**·Cl^--$TATA^+$
formula	$C_{12}H_9BrN_4$	$C_{12}H_{10}N_4$	$C_{24}H_{17}BrN_4$	$C_{12}H_9BrN_4Cl·C_{16}H_{36}N·$water	$C_{12}H_9BrN_4Cl·C_{28}H_{30}N_3·$water
fw	289.14	210.24	441.33	583.05	733.15
crystal size, mm	0.40 × 0.20 × 0.10	0.160 × 0.008 × 0.008	0.23 × 0.10 × 0.10	0.24 × 0.10 × 0.10	0.29 × 0.27 × 0.02
crystal system	monoclinic	monoclinic	monoclinic	orthorhombic	triclinic
space group	$P2_1$ (no. 4)	$P2_1/n$ (no. 14)	$P2_1/n$ (no. 14)	$Pna2_1$ (no. 33)	$P\bar{1}$ (no. 1)
a, Å	10.8827(2)	13.250(7)	13.262(5)	18.4725(3)	11.2758(2)
b, Å	7.0798(2)	4.9503(3)	5.685(2)	8.38730(10)	13.2794(2)
c, Å	15.4121(3)	15.2995(8)	25.480(9)	19.5557(4)	14.0394(3)
α, °	90	90	90	90	65.8676(7)
β, °	100.5296(12)	102.893(4)	101.5060(10)	90	83.1022(9)
γ, °	90	90	90	90	65.9622(7)
V, Å^3	1167.47(5)	978.22(10)	1882.4(12)	3029.85(9)	1749.38(6)
ρ_{calcd}, gcm^{-3}	1.645	1.428	1.557	1.278	1.407
Z	4	4	4	4	1
T, K	93(2)	100(2)	93(2)	93(2)	93(2)
μ(Cu-Kα), mm^{-1}	4.652	0.111[a]	3.115	2.872	2.632
no. of reflns	11758	4932	12125	30843	16737
no. of unique reflns	3739	1728	3228	5487	8979
variables	307	145	262	325	892
$\lambda_{Cu\text{-}K\alpha}$, Å	1.54187	0.78201[a]	1.54187	1.54187	1.54187
R_1 ($I > 2\sigma(I)$)	0.0522	0.0546	0.0215	0.0372	0.0756
wR_2 ($I > 2\sigma(I)$)	0.1052	0.1233	0.0569	0.0987	0.1888
GOF	1.039	1.153	1.061	1.047	1.019

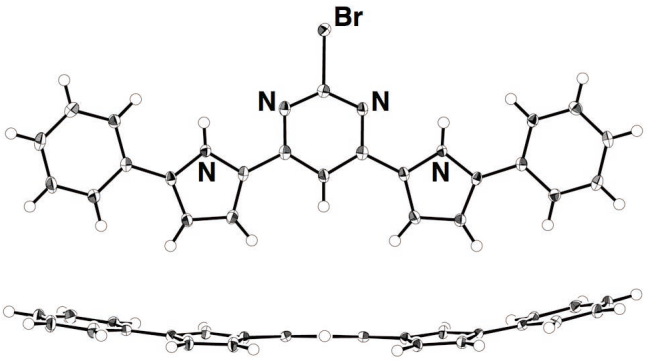
[a] The values under the synchrotron radiation.



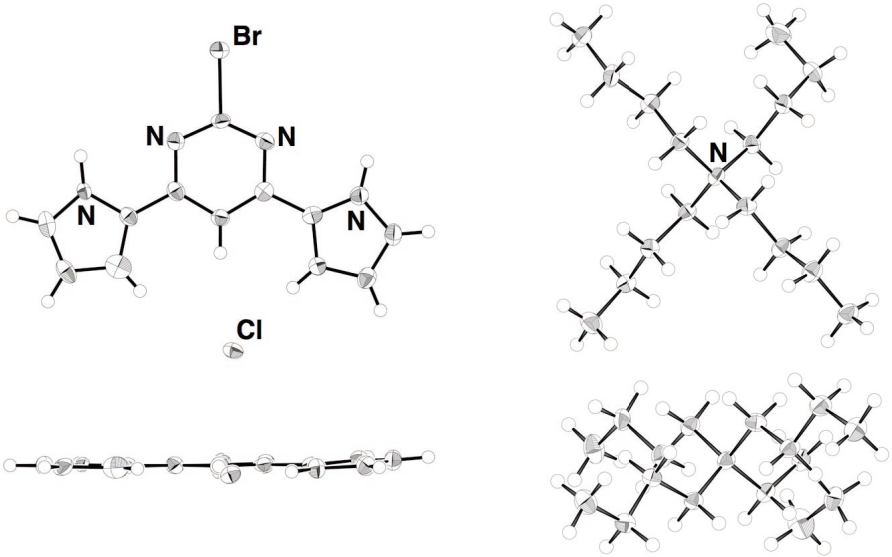
Supporting Figure 12 Ortep drawing of single-crystal X-ray structure of **3a** (top and side view) with two independent structures ((i) and (ii)). Thermal ellipsoids are scaled to the 50% probability level.



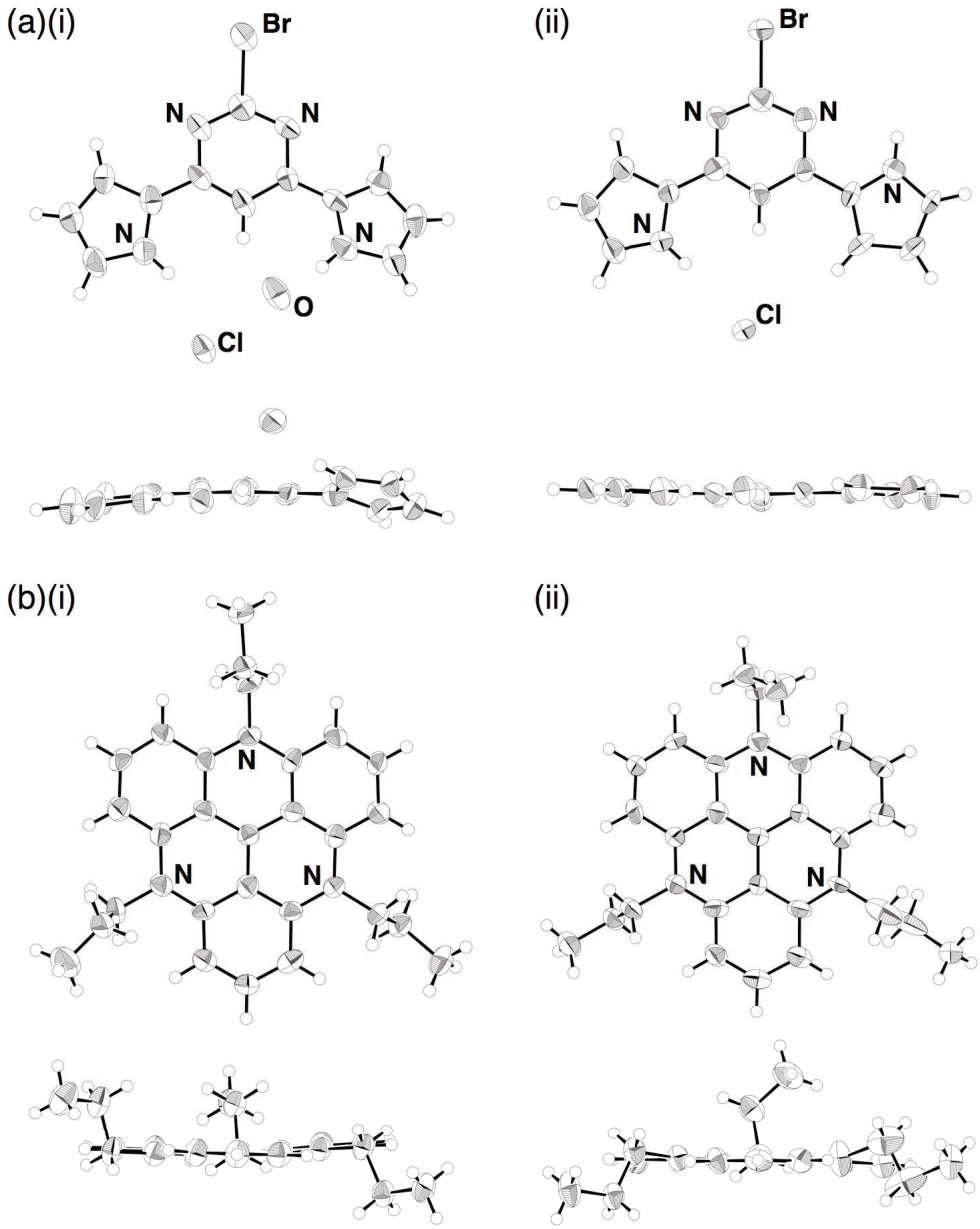
Supporting Figure 13 Ortep drawing of single-crystal X-ray structure of **3b** (top and side view). Thermal ellipsoids are scaled to the 50% probability level.



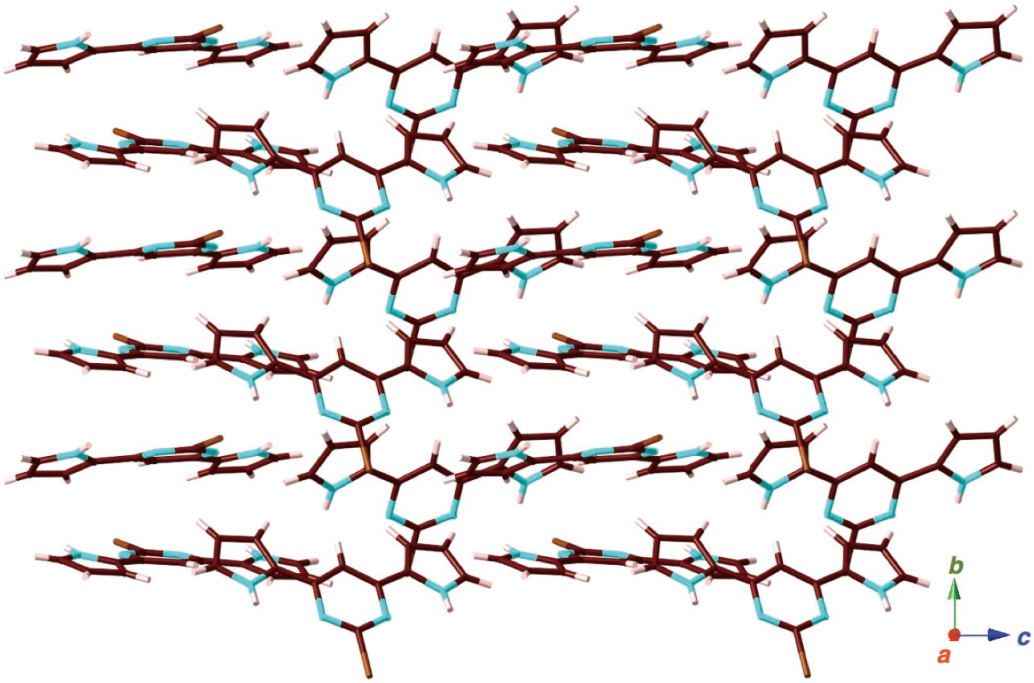
Supporting Figure 14 Ortep drawing of single-crystal X-ray structure of **4a** (top and side view). Thermal ellipsoids are scaled to the 50% probability level.



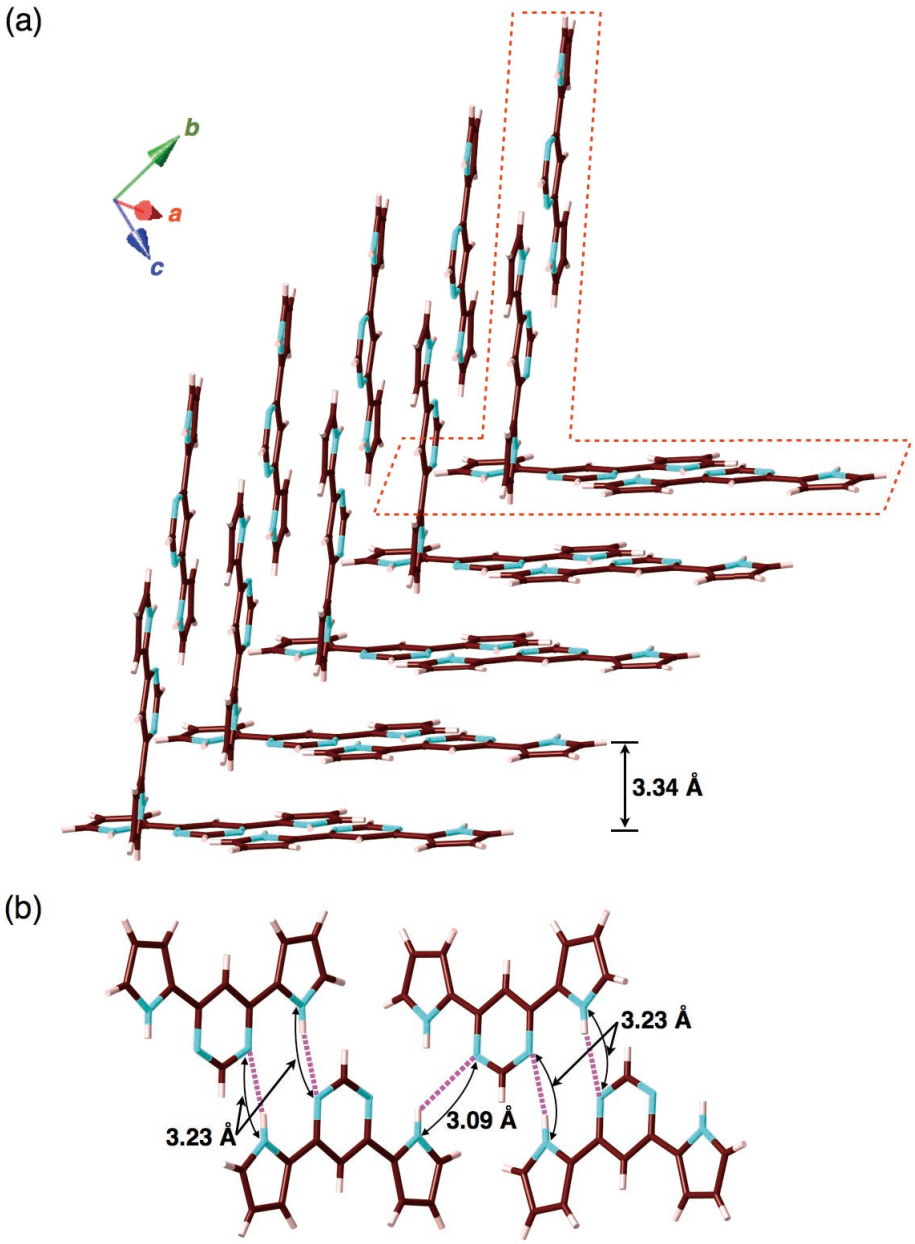
Supporting Figure 15 Ortep drawing of single-crystal X-ray structure of **3a**·Cl^--TBA^+, wherein **3a**·Cl^- and TBA^+ are drawn separately. Thermal ellipsoids are scaled to the 50% probability level. Water molecule included in the crystal is omitted for clarity.



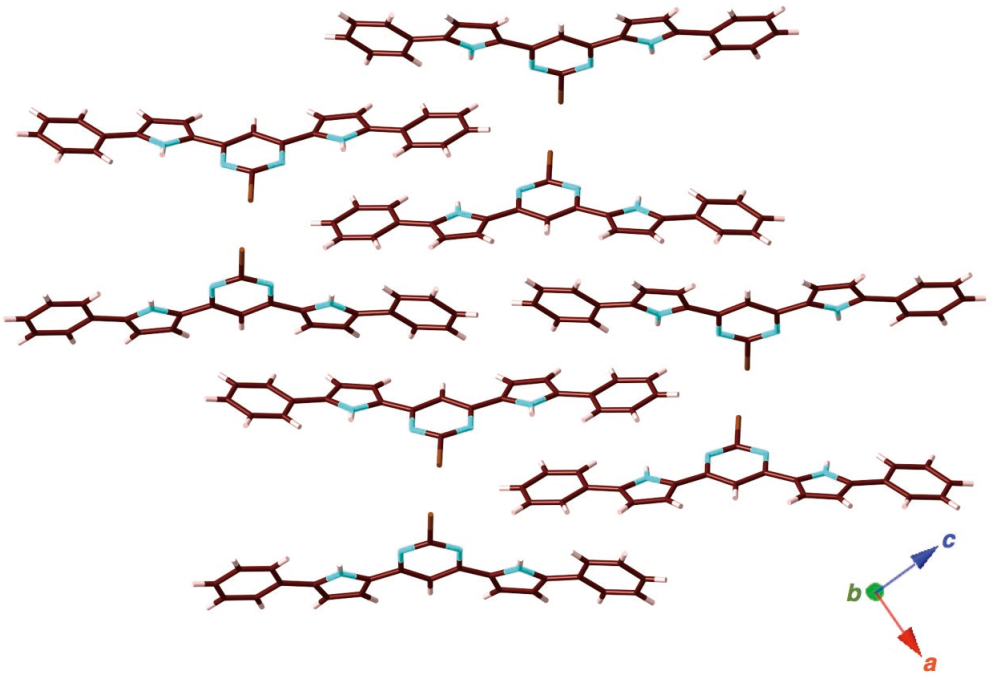
Supporting Figure 16 Ortep drawing of single-crystal X-ray structure of **3a**·Cl^--$TATA^+$ with two independent structures ((i) and (ii)), wherein (a) **3a**·Cl^- and (b) $TATA^+$ are drawn separately. Thermal ellipsoids are scaled to the 50% probability level.



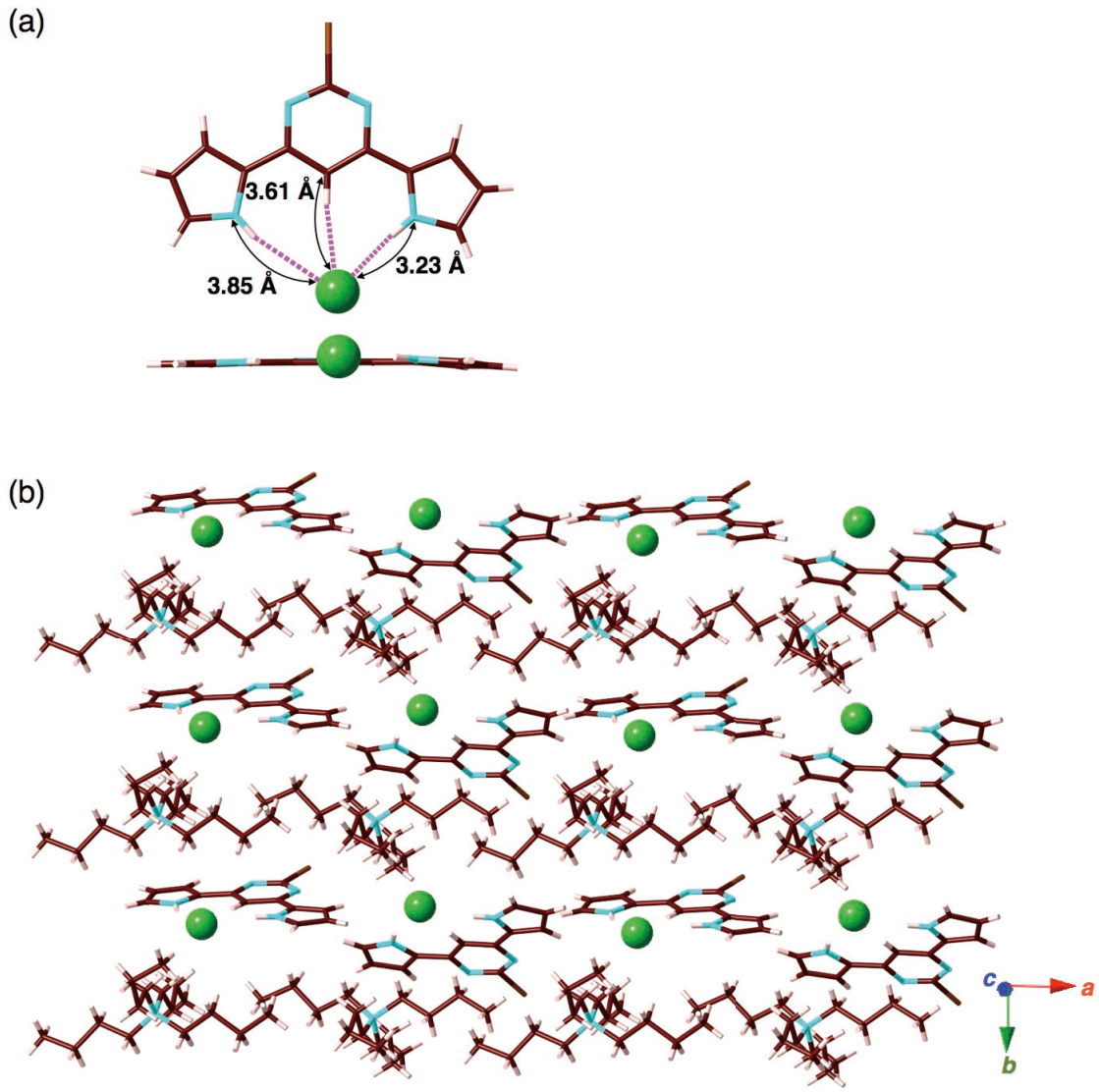
Supporting Figure 17 Packing diagram of **3a**. Atom color code: brown, pink, light brown, and blue refer to carbon, hydrogen, bromine, and nitrogen, respectively.



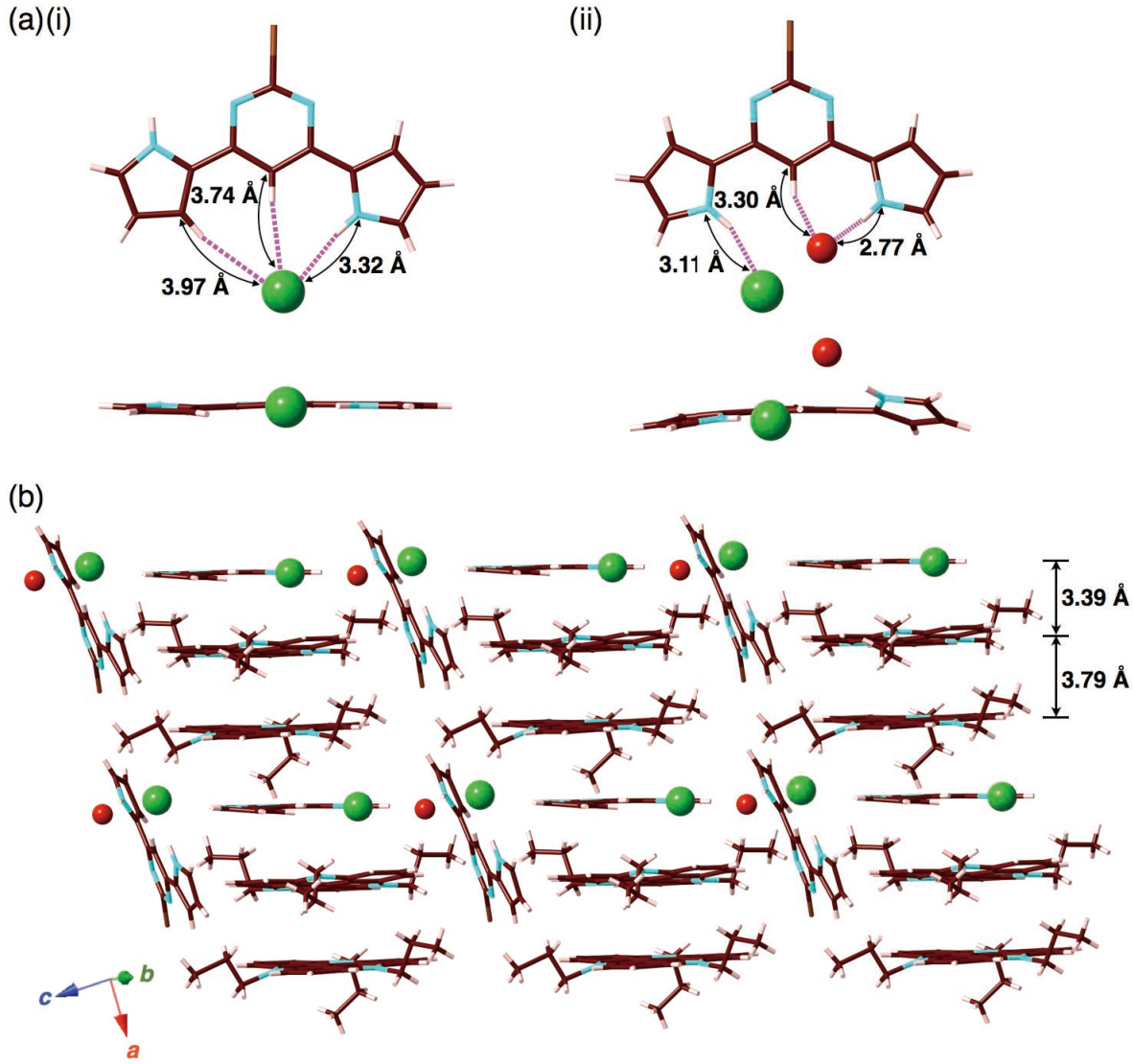
Supporting Figure 18 (a) Packing diagram and (b) a pair of hydrogen-bonding dimers of **3b** shown in the red dotted part in (a), including a hydrogen bonding with the pyrrole-N(–H)···pyrimidine–N distance of 3.23 Å in the dimer and that with the pyrrole-N(–H)···pyrimidine–N distance of 3.09 Å in the pair, and resulting assemblies with the stacking distance of 3.34 Å through the alternate stacking of pyrrole and pyrimidine moieties with appropriate dipole orientations. Atom color code: brown, pink, and blue refer to carbon, hydrogen, and nitrogen, respectively.



Supporting Figure 19 Packing diagrams of **4a**. Atom color code: brown, pink, light brown, and blue refer to carbon, hydrogen, bromine, and nitrogen, respectively.



Supporting Figure 20 (a) Top and side view of **3a**·Cl^- and (b) packing diagram of **3a**·Cl^--TBA^+. **3a** forms a [1+1]-type Cl^- complex with the hydrogen-bonding distances of N(H)···Cl^- and C(H)···Cl^- for 3.23, 3.85, and 3.61 Å, respectively. Atom color code: brown, pink, light brown, yellow green, and blue refer to carbon, hydrogen, bromine, chlorine, and nitrogen, respectively.



Supporting Figure 21 (a) Top and side view of **3a**·Cl^- and (b) packing diagram of **3a**·Cl^--$TATA^+$. Two types of [1+1]-type complexes **3a**·Cl^- are formed as seen in (i) with the hydrogen-bonding distances of 3.32 and 3.74/3.97 Å for N(–H)···Cl^- and C(–H)···Cl^-, respectively, and (ii) with the hydrogen-bonding distances of 3.11 and 2.77/3.30 Å for N(–H)···Cl^- and N/C(–H)···O, respectively. The stacking distance between **3a**·Cl^- and $TATA^+$ and that between two $TATA^+$ are 3.39 and 3.79 Å, respectively. The distances between two planes are calculated as the average distance of each atom and mean plane consisted of core structure. Atom color code: brown, pink, light brown, yellow green, blue, and red refer to carbon, hydrogen, bromine, chlorine, nitrogen, and oxygen, respectively.

[S4] (a) B. W. Laursen and F. C. Krebs, *Angew. Chem., Int. Ed.*, 2000, **39**, 3432–3434; (b) B. W. Laursen and F. C. Krebs, *Chem. Eur. J.*, 2001, **7**, 1773–1783.

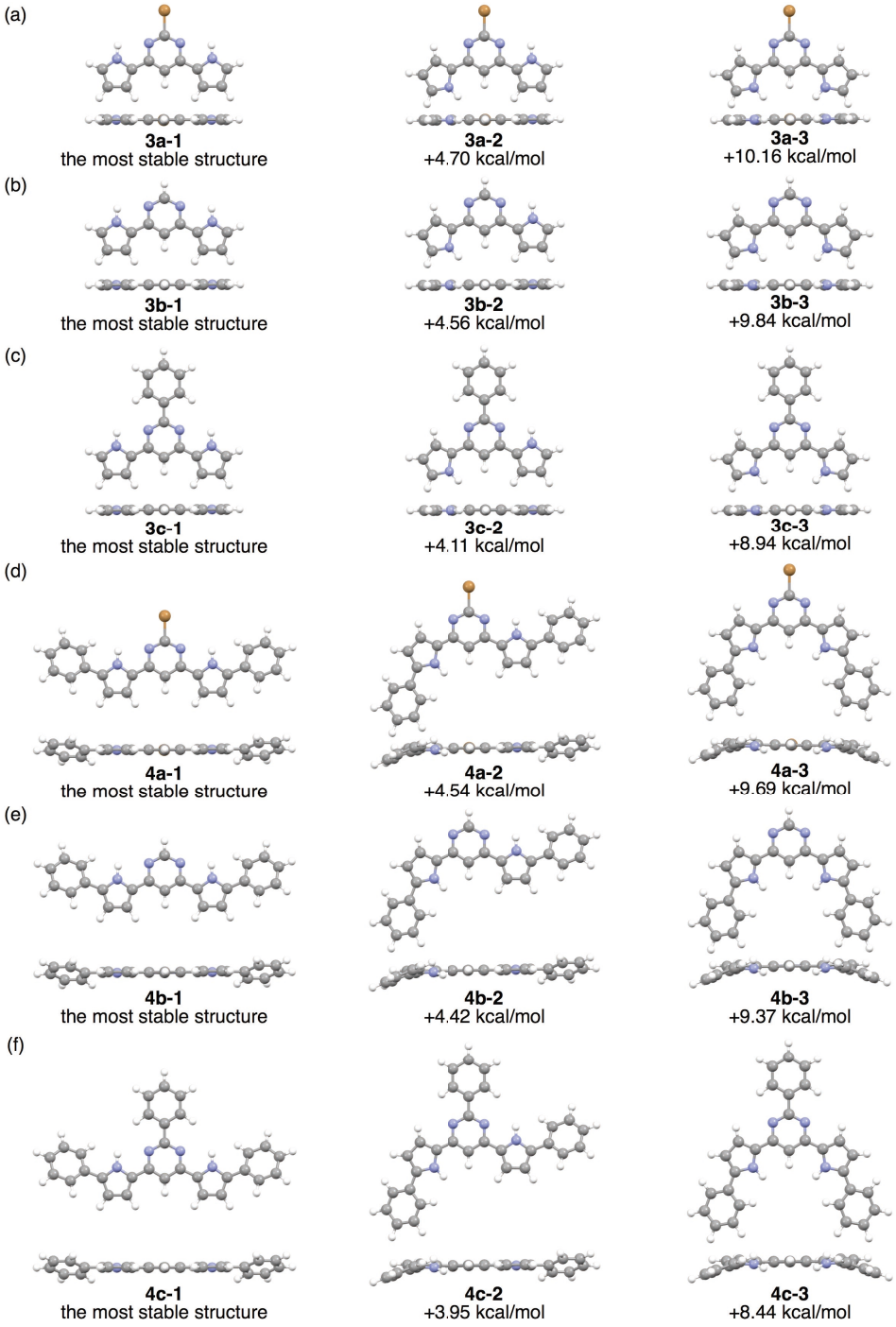
[S5] Y. Haketa, S. Sasaki, N. Ohta, H. Masunaga, H. Ogawa, N. Mizuno, F. Araoka, H. Takezoe and H. Maeda, *Angew. Chem., Int. Ed.*, 2010, **49**, 10079–10083.

[S6] (a) N. Yasuda, H. Murayama, Y. Fukuyama, J. E. Kim, S. Kimura, K. Toriumi, Y. Tanaka, Y. Moritomo, Y. Kuroiwa, K. Kato, H. Tanaka and M. Takata, *J. Synchrotron Rad.*, 2009, **16**, 352–357; (b) N. Yasuda, Y. Fukuyama, K. Toriumi, S. Kimura and M. Takata, *AIP Conf. Proc.*, 2010, **1234**, 147–150.

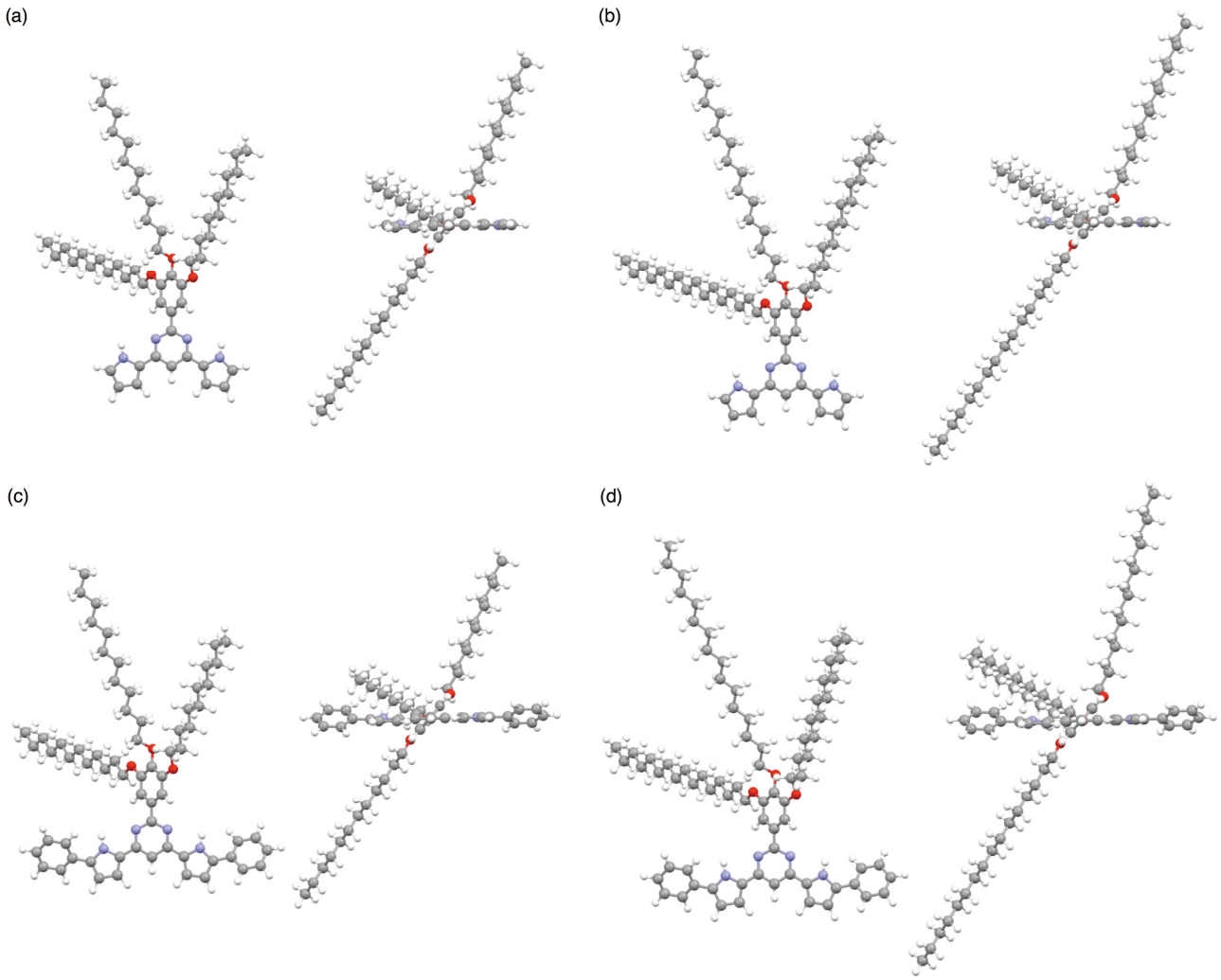
[S7] *CrystalStructure (Ver. 3.8), Single Crystal Structure Analysis Software,* Rigaku/MSC and Rigaku Corporation, 2006.

3. Theoretical studies

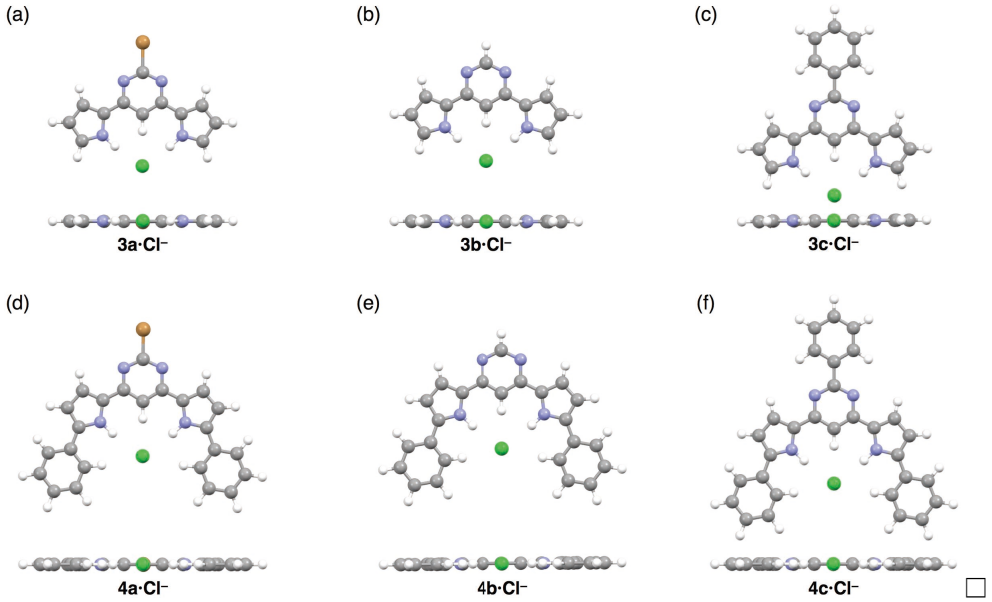
DFT and semi-empirical calculations. DFT and semi-empirical calculations for dipyrrolylpyrimidines and their anion complexes were carried out using Gaussian 09 program[S8].



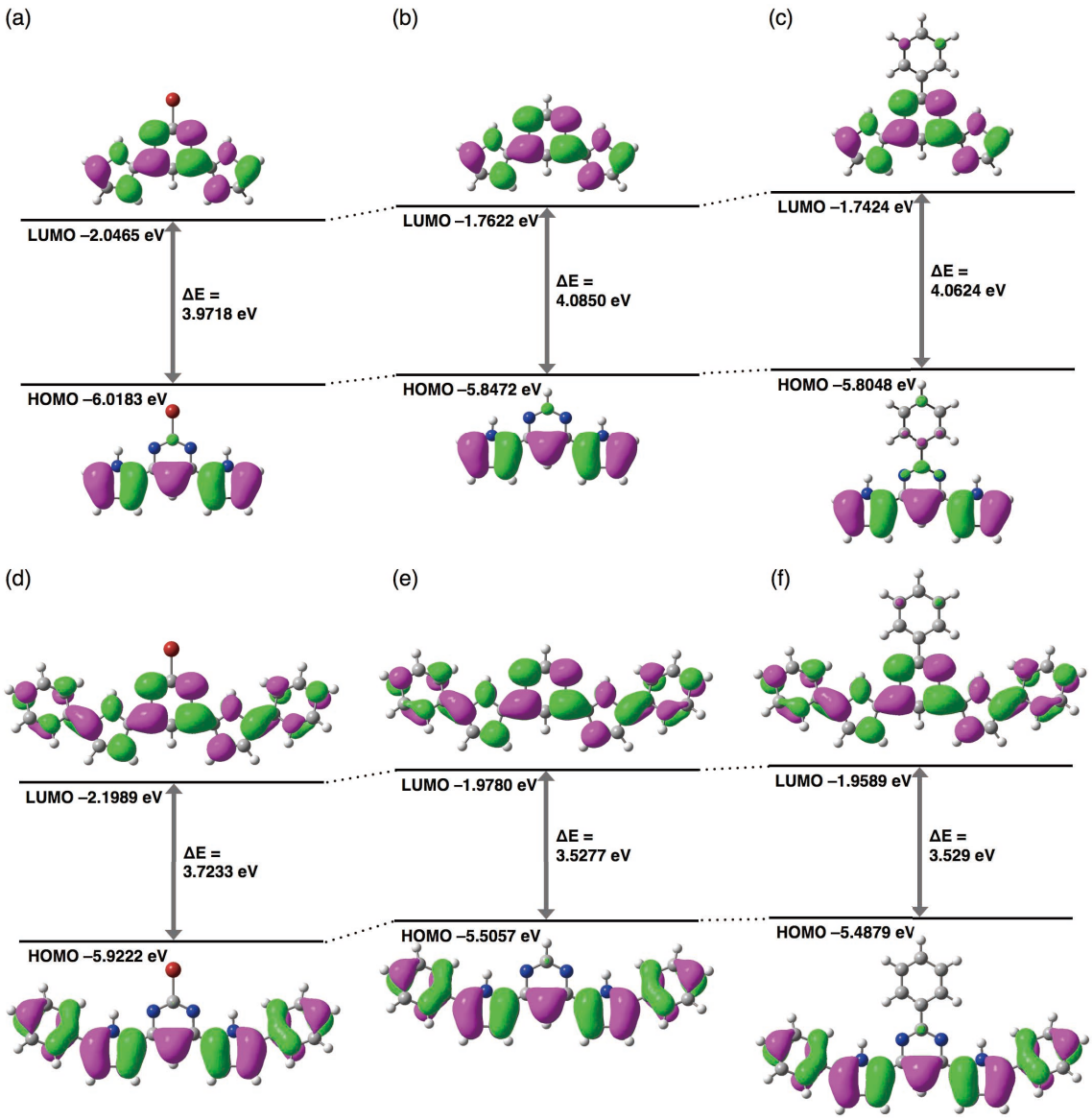
Supporting Figure 22 Optimized structures of (a) **3a**, (b) **3b**, (c) **3c**, (d) **4a**, (e) **4b**, and (f) **4c** (three conformations for each molecule) at B3LYP/6-31G(d,p) level. Relative energies according to pyrrole-inverted states show the orders of **3a** > **3b** > **3c** and **4a** > **4b** > **4c**, which are partially derived from the electron-withdrawing/donating characters of the substituents at the pyrimidine 2-position. Compared to hydrogen (**3b** and **4b**) and phenyl (**3c** and **4c**) moieties, the electron-withdrawing bromo moiety in **3a** and **4a** at the pyrimidine 2-position more effectively induces the orientation of the pyrrole NH facing the pyrimidine N site through canceling their dipoles (pyrimidine and pyrroles). Furthermore, the dipole moments, calculated at B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p), for the central units of DPPs, such as 2-Br-pyrimidine, 2-H-pyrimidine, and 2-Ph-pyrimidine, were 3.91, 2.48, and 1.64 D, respectively, clearly suggesting the electron-withdrawing moiety at 2-position induces larger dipole moment.



Supporting Figure 23 Optimized structures of (a) **3d**, (b) **3e** (c) **4d**, and (d) **4e** at AM1 level.



Supporting Figure 24 Optimized structures of (a) **3a**·Cl^-, (b) **3b**·Cl^-, (c) **3c**·Cl^-, (d) **4a**·Cl^-, (e) **4b**·Cl^-, and (f) **4c**·Cl^- at B3LYP/6-31+G(d,p) level.



Supporting Figure 25 Molecular orbitals (HOMO/LUMO) of (a) **3a**, (b) **3b**, (c) **3c**, (d) **4a**, (e) **4b**, and (f) **4c** at B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) level. Electron-withdrawing bromo moiety at the 2-position in **3a** and **4a** provided lower HOMO and LUMO levels than those of 2-unsubstituted derivatives (**3b** and **4b**) and 2-phenyl derivatives (**3c** and **4c**), wherein 2-phenyl derivatives (**3c** and **4c**) showed slightly higher HOMO and LUMO levels than the 2-unsubstituted derivatives (**3b** and **4b**).

Cartesian Coordination of 3a-1 (DFT)

-3253.4307196 hartree

H,-2.2910582926,-3.4497947125,0.0000460495
H,-4.9964463028,-3.4311292744,0.0003278566
H,-5.7379048854,-0.8109503183,-0.0000017475
H,3.5754108101,0.5452721546,-0.0002154554
H,4.9964333516,-3.4311481878,0.0002135072
H,-0.0000046727,-2.4365017554,-0.0001029241
H,5.7379017838,-0.8109720307,-0.0000668769
H,2.2910452036,-3.4498034201,0.00003548
H,-3.5754088086,0.5452857123,-0.0002355125
N,-3.6336323591,-0.4632019685,-0.0001467165
N,3.6336305742,-0.4632157478,-0.0001450083
N,-1.1926992263,0.7304964437,-0.0002793661
N,1.1927019746,0.7304918894,-0.0002909043
C,-4.7484776601,-1.2435105475,0.0000031642
C,-4.3430680053,-2.5706129711,0.0001723755
C,-1.1967169007,-0.6307835231,-0.0001384804
C,4.3430582749,-2.5706294348,0.0000947667
C,-0.0000025791,-1.3538138276,-0.0001510925
C,1.196714493,-0.6307881461,-0.0001515005
C,-2.5040872316,-1.2517462664,-0.0000687915
C,-2.9303384956,-2.578350026,0.0000168159
C,4.7484729274,-1.2435285391,-0.0000501047
C,0.0000024704,1.2942046848,-0.0005561324
C,2.9303287164,-2.5783611587,-0.0000033354
C,2.5040824648,-1.2517557985,-0.000090458
Br,0.0000061207,3.2184514525,0.000330578

Cartesian Coordination of 3a-2 (DFT)

-3253.4232271 hartree

H,-2.1078570072,-3.5617772353,0.0000846634
H,-4.8092871271,-3.6861353278,-0.0002868408
H,-5.6885827634,-1.1086968145,-0.0006319738

H,2.173036843,-3.1959064912,0.0006612204
H,5.8849733886,-1.2274427661,0.0009685919
H,0.1092097658,-2.4211548439,0.0002819547
H,4.630006692,-3.6430033117,0.0010264705
H,3.8992307112,0.6400982274,0.0005202267
H,-3.5995946836,0.360007195,-0.0004805387
N,-3.6056202669,-0.6503578672,-0.0003901267
N,2.8556420304,-2.4561343128,0.0006782416
N,-1.2361334814,0.6722321747,-0.0001804697
N,1.1484369708,0.8037451267,0.0001374831
C,-4.6777542924,-1.4884944608,-0.000459141
C,-4.2026260888,-2.7920685197,-0.0002810482
C,-1.164510174,-0.6831977769,-0.0000525637
C,4.8194817647,-1.4063420136,0.0008411011
C,0.0721365894,-1.3381177445,0.0001790964
C,1.2322933189,-0.5531982491,0.0002674337
C,-2.4359740252,-1.3772661555,-0.0001633465
C,-2.7911643127,-2.7243482194,-0.0000867465
C,4.2086087542,-2.6486286975,0.0008747635
C,-0.0710321335,1.2989454153,-0.0000683999
C,3.7947801561,-0.434130026,0.0006090716
C,2.5739159338,-1.1003949872,0.0005050573
Br,-0.1839235628,3.2194586819,-0.0002851805

Cartesian Coordination of 3a-3 (DFT)

-3253.4145262 hartree
H,3.9238829572,0.5274602018,0.0001165712
H,5.8164578574,-1.4350538375,0.0000506859
H,4.4449564909,-3.7863754169,-0.0000946867
H,-2.0139468517,-3.2198177359,-0.0001792489
H,-5.8164578572,-1.4350538379,0.0000602559
H,-0.0000000015,-2.3308267648,-0.0001322194
H,-4.4449564912,-3.7863754161,-0.0001077185
H,-3.9238829568,0.527460201,0.0001329314
H,2.0139468511,-3.2198177376,-0.0001578488
N,2.7304162342,-2.5134073289,-0.0000927977
N,-2.7304162344,-2.5134073281,-0.0001016257
N,1.1953288378,0.8291361314,0.0000214277
N,-1.1953288377,0.8291361314,0.0000218224
C,4.0730485582,-2.7724338544,-0.0000539079
C,4.7435068786,-1.5618568208,0.0000189029
C,1.2038590136,-0.5266187956,0.0000062861
C,-4.7435068784,-1.5618568209,0.0000233649
C,-0.0000000009,-1.2459776505,-0.0000717102
C,-1.2038590136,-0.5266187955,0.0000061662
C,2.515524222,-1.1453376353,-0.0000020347
C,3.7675035334,-0.5404344743,0.0000532971
C,-4.0730485583,-2.7724338539,-0.0000604601
C,0.0000000005,1.3884718621,-0.0001686222
C,-3.7675035332,-0.5404344746,0.000061216
C,-2.515524222,-1.1453376351,-0.0000026885
Br,0.0000000015,3.3122126869,0.0009016415

Cartesian Coordination of 3b-1 (DFT)

-682.3269266 hartree
H,2.2844665718,2.4859171627,0.0002497432
H,4.9908174481,2.4746328473,0.0002428422
H,5.7394014363,-0.1437291747,0.0000227803
H,-3.5728285459,-1.5038592106,-0.0001572921
H,-4.9908174026,2.4746329522,0.0001910442
H,0.0000000126,1.4637725781,0.0001399715
H,-5.7394014432,-0.1437290544,-0.0000387149
H,-2.2844665265,2.4859172111,0.0002251667
H,3.5728285129,-1.5038592864,-0.0001201822
N,3.6344317911,-0.4957483807,-0.0000276349
N,-3.634431805,-0.4957483042,-0.0000651763
N,1.1958866589,-1.700470158,-0.0001492765
N,-1.1958866978,-1.7004701328,-0.0001616514
C,4.74909923,0.2868952269,0.0000557703
C,4.3399733644,1.6120358525,0.0001659924
C,1.1969844863,-0.3424207663,-0.0000260754
C,-4.3399733362,1.6120359437,0.0001206632
C,0.0000000017,0.3802918688,0.0000379076
C,-1.1969844972,-0.3424207408,-0.0000384315
C,2.5032176505,0.2891430435,0.0000399102
C,2.9258255936,1.6159549455,0.0001703778
C,-4.7490992284,0.2868953267,0.0000050095
C,-0.0000000251,-2.2865122819,-0.0001959205
C,-2.9258255656,1.6159550073,0.0001392041
C,-2.5032176489,0.2891430962,0.0000138568
H,-0.000000036,-3.3757745718,-0.0003288842

Cartesian Coordination of 3b-2 (DFT)

-682.3196571 hartree
H,-2.1105925185,-2.1620361041,0.0002166133
H,-4.5597162187,-2.6575715563,0.0002922753
H,-5.8597822271,-0.2655705258,0.0000437028
H,3.6033739882,1.4517550329,-0.0001519722
H,4.8534269177,-2.5830684401,0.0002344944
H,-0.0697617315,-1.3575124606,0.0001050621
H,5.7115439844,0.0020610147,-0.0000296723
H,2.1501105273,-2.4805696851,0.0002036713
H,-3.9072399479,1.6387601309,-0.0001373313
N,3.6232542141,0.4417893706,-0.0000609188
N,-1.1522532589,1.8520295988,-0.000166253
N,1.2406123305,1.7493094664,-0.0001705769
C,-4.791049344,-0.4248921058,0.0000588941
C,-4.1577508051,-1.6551831267,0.0001876242
C,-1.2163289932,0.4971840626,-0.0000404666
C,4.2397602532,-1.6936278726,0.0001453164
C,-0.0463641425,-0.2730981138,0.0000147003
C,1.1826086486,0.3960342542,-0.0000456261
C,-2.5509311581,-0.076017206,0.0000212268
C,4.7042326318,-0.3869987728,0.0000102131
C,0.0659528448,2.3836896411,-0.0002412382
C,2.8264124931,-1.6373839624,0.0001278612
C,2.4602551192,-0.2940666491,0.0000112218
H,0.1125009112,3.4719349361,-0.0002959834
C,-3.7834540294,0.5666823495,-0.0000345781
N,-2.807821489,-1.4361032765,0.0001477397

Cartesian Coordination of 3b-3 (DFT)

-682.3112477 hartree
H,1.9979551257,2.1549458769,0.0002471542
H,4.4258593374,2.7418975038,0.0002765125
H,5.814516854,0.4005505494,0.0000591556
H,-3.9348321415,-1.5758645409,-0.0001689394
H,-4.4258593396,2.7418975059,0.0002132081
H,-0.0000000003,1.2609536318,0.0001067441
H,-5.814516854,0.4005505488,0.0000112221

H,-1.9979551274,2.1549458806,0.000194547
H,3.9348321435,-1.5758645389,-0.0001537583
N,1.1988637155,-1.8965235262,-0.0001613162
N,-1.1988637137,-1.896523526,-0.0001727346
C,4.7405707833,0.5197696882,0.0000678153
C,4.0619688095,1.7250481887,0.0001775446
C,1.2043808692,-0.5435368996,-0.000047894
C,-4.0619688107,1.72504819,0.0001269702
C,0.0000000001,0.1749964404,0.0000140201
C,-1.2043808684,-0.5435368994,-0.0000602554
C,2.5149636365,0.0857392263,0.0000173696
C,-4.7405707834,0.5197696881,0.0000244869
C,0.0000000011,-2.4773706156,-0.0001860432
C,-2.5149636361,0.0857392268,-0.0000092621
H,0.0000000015,-3.5665961283,-0.0003655456
C,3.7707889584,-0.5092492278,-0.0000435058
N,2.7205796772,1.4548019918,0.0001633424
N,-2.7205796782,1.4548019937,0.000121
C,-3.7707889574,-0.5092492286,-0.000069838

Cartesian Coordination of 3c-1 (DFT)
-913.3957532 hartree
H,3.8923612659,2.2519661861,-0.0004137974
H,3.9162056523,4.9576949675,-0.0001614226
H,1.3068931519,5.7395529638,0.0003709473
H,-0.0791045369,-3.5949650824,-0.0004779345
H,3.9161357414,-4.9577528203,0.0001775766
H,2.868382997,-0.0000213722,-0.000001274
H,1.3068121278,-5.7395740217,-0.0003912865
H,3.8923292903,-2.252024051,0.000374827
H,-0.079053764,3.5949636344,0.0004836628
N,0.9290784784,3.6387898833,0.0002618383
N,0.9290270639,-3.6388055572,-0.0002594295
N,-0.2937613774,1.1915507516,0.0000119411
N,-0.2937786075,-1.1915486376,-0.0000119754
C,1.7257982181,4.7442555971,0.000206222
C,3.0451122694,4.3182845952,-0.0000567862
C,1.0589157871,1.1937680676,-0.0000033883
C,3.0450513226,-4.3183302208,0.0000613922
C,1.7855305981,-0.0000138801,-0.0000014694
C,1.0588988528,-1.1937854423,0.0000008612
C,1.6987284194,2.4977137999,0.0000133813
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C,1.7257312553,-4.7442825692,-0.0002238243
C,-0.9082876475,0.000005463,0.0000012714
C,3.0304484811,-2.9040811232,0.0001552582
C,1.6986929648,-2.4977402825,-0.0000193383
C,-2.3986591473,0.0000174373,0.0000018189
C,-3.1140943836,-1.2070543248,0.0011289957
C,-3.1140739112,1.2071006749,-0.0011248528
C,-4.5068453385,-1.2066417208,0.0011405922
H,-2.5624412035,-2.1392483098,0.0020265054
C,-4.5068252603,1.2067118879,-0.0011349883
H,-2.5624054297,2.1392856049,-0.0020232056
C,-5.2093385855,0.0000411919,0.0000031891
H,-5.0457390857,-2.149812382,0.0020545251
H,-5.0457024981,2.1498919765,-0.0020485788
H,-6.2955721791,0.0000500201,0.0000037626

Cartesian Coordination of 3c-2 (DFT)
-913.3891943 hartree
H,3.7094252184,1.9429916806,-0.0003521712
H,4.3531633999,4.3571200578,-0.0001951027
H,2.0445044211,5.7999577451,0.0003173354
H,-0.200435908,-3.5673355251,-0.0004211865
H,3.7724820285,-4.9952451651,0.0000946191
H,2.7960373138,-0.0402112895,0.000107331
H,1.1516308648,-5.7355909306,-0.0004491677
H,3.7922319531,-2.2904226581,0.0004732467
H,0.026373123,3.9699583256,0.0004414097
N,0.8069917055,-3.6290150853,-0.0002208208
N,-0.3449618382,1.2167125855,-0.0000091986
N,-0.3791364447,-1.1684897953,0.000004884
C,2.138906916,4.723540277,0.0001898385
C,3.328207039,4.0168457791,-0.0000634212
C,1.0053134206,1.2068541814,0.0000289427
C,2.9116525818,-4.3420757749,0.0000255018
C,1.7128643678,-0.0015324714,0.0000648956
C,0.9703345587,-1.1873220418,0.0000455078
C,1.6540060481,2.5082099342,0.0000401006
C,1.5858807811,-4.7469189438,-0.0002452873
C,-0.9742493085,0.036051808,-0.0000279109
C,2.9191168906,-2.9274822001,0.0002175673
C,1.5940405326,-2.5002019391,0.0000232052
C,-2.4636364908,0.0641146176,-0.0000065781
C,-3.2055601139,-1.1265166992,0.0011577566
C,-3.148437915,1.2891222919,-0.0011659823
C,-4.5981098708,-1.0932417749,0.001158647
H,-2.6763427369,-2.0717991804,0.0020861026
C,-4.5408650614,1.320321887,-0.0011991629
H,-2.5708429231,2.2057351174,-0.0020436374
C,-5.2713231252,0.1300887057,-0.0000350478
H,-5.1595399786,-2.0232470252,0.0020983928
H,-5.0578124732,2.2756967338,-0.0021371953
H,-6.3573456065,0.155475758,-0.0000496712
C,1.0881199922,3.777649105,0.0002437689
N,3.0270376382,2.682879909,-0.0001375116

Cartesian Coordination of 3c-3 (DFT)
-913.381491 hartree
H,3.6143938047,1.9850750304,-0.000400541
H,4.2153683286,4.4097558118,-0.0003739873
H,1.8812747418,5.811216477,0.0000837757
H,-0.1042155884,-3.9457460065,-0.0002063147
H,4.2153435034,-4.4097793474,0.0002859453
H,2.725626382,-0.0000074,0.0000178043
H,1.881242089,-5.8112267907,-0.0000225137
H,3.6143826258,-1.9850950607,0.0003144761
H,-0.1041933954,3.9457467787,0.0003082566
N,-0.4302216149,1.19376023,0.000037084
N,-0.4302283018,-1.1937574811,-0.0000118192
C,1.995013019,4.7366683588,0.0000117547
C,3.1964973399,4.0515784079,-0.0002174138
C,0.9169836875,1.2011477402,0.0000044758
C,3.1964745616,-4.0515961008,0.000175579
C,1.6404981549,-0.0000044757,0.000010568
C,0.916977179,-1.2011525642,0.0000129287
C,1.5484088618,2.5128641847,-0.000026186
C,1.9949863639,-4.7366793076,0.000021822
C,-1.0401587698,0.0000029254,0.0000213385

C,1.5483947163,-2.5128726171,0.0000357072
C,-2.5288181467,0.0000072944,0.0000096249
C,-3.2410003263,-1.2090038529,0.0005591728
C,-3.2409936354,1.2090212651,-0.0005511155
C,-4.6338771215,-1.2074580399,0.0005578011
H,-2.6861260203,-2.1397532886,0.0009777845
C,-4.6338713801,1.2074828544,-0.0005689675
H,-2.6861157825,2.1397685895,-0.0009622313
C,-5.3357265479,0.0000146561,-0.0000104251
H,-5.1729763881,-2.1505220058,0.001010726
H,-5.1729642649,2.1505504546,-0.0010295399
H,-6.4220549379,0.0000165945,-0.0000180206
C,0.9606903475,3.7720023694,0.0001206969
N,2.9184458006,2.7118408173,-0.0002282644
N,2.9184305856,-2.7118569927,0.0001861391
C,0.9606691288,-3.7720075082,-0.0000671212

Cartesian Coordination of 4a-1 (DFT)

-3715.5675487 hartree
H,2.288411771,-3.5344617966,0.4028797171
H,4.982252715,-3.520677302,0.3980357743
H,-3.5727449446,0.4120836567,-0.2018995966
H,-4.9821484085,-3.5207433144,0.3989880575
H,0.0000306394,-2.529878542,0.2621617707
H,-2.2883028685,-3.5344616346,0.4035339209
H,3.5726881857,0.4121756599,-0.2021988013
N,3.6320082409,-0.5781679188,-0.0115405454
N,-3.6320138128,-0.5782836073,-0.0113379164
N,1.1928332954,0.6061734889,-0.1877319625
N,-1.192891112,0.606144823,-0.1876077052
C,4.7602945606,-1.3471763942,0.0764536474
C,4.3343154354,-2.6678615325,0.2567442107
C,1.1967772025,-0.7419503188,0.0067457574
C,-4.3342432286,-2.6679374659,0.2574786865
C,0.0000112289,-1.4580678175,0.1085547863
C,-1.1967829829,-0.7419757889,0.0068746938
C,2.5025696399,-1.3560578858,0.095737769
C,2.9276245978,-2.6730099593,0.2711442778
C,-4.7602707826,-1.3472930185,0.0769915453
C,-0.0000382174,1.1636101599,-0.268826863
C,-2.9275532276,-2.6730491743,0.2717281147
C,-2.5025488559,-1.3561148907,0.0960181575
Br,-0.0000792595,3.0677211438,-0.5463177767
C,-6.1097021746,-0.7872669872,0.0034846535
C,-7.1960045835,-1.6028273176,-0.3622285096
C,-6.360526177,0.5656213653,0.2963118345
C,-8.4856511957,-1.0836729594,-0.4291992119
H,-7.0195216997,-2.6439192588,-0.6135660976
C,-7.6509757462,1.0843205981,0.2185170169
H,-5.5478305549,1.2121842197,0.6150807182
C,-8.7202194386,0.2631162205,-0.1427595944
H,-9.3095971797,-1.7304784641,-0.7162082523
H,-7.822315023,2.1311535514,0.4514295998
H,-9.7260231941,0.6679262893,-0.1999266378
C,6.1097074155,-0.7871025855,0.0029100638
C,7.196025124,-1.6026362038,-0.3628235057
C,6.3604913158,0.5657980755,0.295701424
C,8.485650474,-1.083438912,-0.4298488664
H,7.0195707451,-2.6437366616,-0.6141417284
C,7.6509225968,1.0845378017,0.2178616784
H,5.5477857775,1.2123395881,0.6144862987
C,8.7201811267,0.2633647875,-0.1434362133
H,9.3096158653,-1.7302060845,-0.7168880033
H,7.8222411027,2.1313767464,0.4507624159
H,9.725970612,0.6682066211,-0.2006458027

Cartesian Coordination of 4a-2 (DFT)

-3715.5603114 hartree
H,3.4581138989,2.9375808054,-0.0605923587
H,5.932941978,1.8188110147,-0.0949284892
H,-3.5371236786,0.2338565209,0.0718676421
H,-3.3589145929,-3.9787296245,-0.1272070077
H,0.8712801189,-1.1833946865,-0.0891765679
H,-0.8559376925,-2.9849303256,-0.1219332978
H,3.0749844987,-1.2372058019,0.2025103745
N,3.4740083789,-0.3287034699,0.0297338757
N,-3.215984457,-0.724137531,0.0596589433
N,0.8041889949,2.1974511639,0.1351807649
N,-1.4076792542,1.296277954,0.1354132118
C,4.8265684317,-0.0835151637,0.0156173241
C,4.9867339061,1.3019315221,-0.025447137
C,1.3239539396,0.9428667654,0.0550896516
C,-3.081428237,-2.9351500297,-0.0944972518
C,0.4826793418,-0.1758459614,0.0012008609
C,-0.8996271442,0.0397121662,0.05007235
C,2.7688380183,0.8613655221,0.0275404284
C,3.7073287991,1.8882534515,-0.0186322218
C,-3.9739964494,-1.8610907761,-0.0078816044
C,-0.5097104596,2.267340656,0.164273515
C,-1.7737163291,-2.4156042352,-0.0802071504
C,-1.8756040112,-1.0276144174,0.0110520367
Br,-1.2412549872,4.0440192152,0.2681284985
C,-5.4363786419,-1.8416628611,0.0309521428
C,-6.1736077431,-2.9225226917,-0.4857191088
C,-6.1415677136,-0.7561858971,0.5818049657
C,-7.5649598607,-2.9175975172,-0.4497096598
H,-5.6484797573,-3.7593568798,-0.9352878629
C,-7.5342454484,-0.7499228026,0.6069716236
H,-5.6000008935,0.0776781635,1.0195260997
C,-8.2533495899,-1.8302602079,0.0932395747
H,-8.114628965,-3.7612585194,-0.8568138681
H,-8.0581434967,0.0976302733,1.0389644287
H,-9.3388124387,-1.8255499455,0.1160792787
C,5.8164925237,-1.1597775731,0.0270290149
C,7.1141496321,-0.9234334018,0.5163322562
C,5.5072748904,-2.4480424935,-0.4467716886
C,8.0659671886,-1.9388180439,0.5288677285
H,7.3644728085,0.0581344786,0.9061334749
C,6.4586583222,-3.4654165777,-0.4214845675
H,4.5273622597,-2.6480140933,-0.8720018375
C,7.7428369832,-3.2162804267,0.0650464205
H,9.0612456969,-1.7354794141,0.9130378634
H,6.1996597485,-4.4514988187,-0.795857859
H,8.4851304831,-4.0083854848,0.080663189

Cartesian Coordination of 4a-3 (DFT)

-3715.552098 hartree
H,3.953895365,2.4731236565,-0.1997813688
H,5.7995620191,0.4814886844,-0.2828653889
H,-2.0339302453,-1.1635622697,0.2483262811

H,-5.7990700754,0.6482211863,-0.0955386318
H,-0.0120813071,-0.3071394049,-0.1764152205
H,-3.895222052,2.5859595752,-0.0728163727
H,1.9969702354,-1.2215054812,0.1832497261
N,2.7063675319,-0.5424892488,-0.0399841714
N,-2.7303462715,-0.4643359117,0.0477479509
N,1.2335719105,2.819814658,0.124392518
N,-1.1569966472,2.8541810068,0.1630076382
C,4.0479219653,-0.8413660697,-0.0968905483
C,4.7302385288,0.372536817,-0.1732012017
C,1.2199858757,1.4676625162,0.0192312666
C,-4.7303361147,0.5085273744,-0.0204154955
C,0.0057152621,0.767580043,-0.030904603
C,-1.1856794113,1.5022388131,0.0580921223
C,2.5183699486,0.8283228728,-0.0452562578
C,3.77871963,1.4097249817,-0.1407524661
C,-4.0810741426,-0.7245203069,0.0342703514
C,0.0468296299,3.3955467519,0.1757602719
C,-3.7488572122,1.5179351108,-0.0190699376
C,-2.5033058736,0.9005111111,0.0358744496
Br,0.0763877033,5.3148061404,0.2969138781
C,-4.6143381145,-2.0858228577,0.0590193782
C,-5.9096899913,-2.3310425202,0.5501667359
C,-3.8591073272,-3.179155645,-0.4037009192
C,-6.4284328225,-3.6223136357,0.5754022552
H,-6.4991843978,-1.50297315,0.9307325128
C,-4.3767031065,-4.4720070246,-0.3657507961
H,-2.8735605808,-3.0135575689,-0.830810436
C,-5.6639147581,-4.7004191766,0.1228316773
H,-7.42991413,-3.7899122905,0.960662849
H,-3.7780457502,-5.3009498214,-0.7319663338
H,-6.0686682037,-5.7074754129,0.1484652129
C,4.5423814263,-2.2174379017,-0.0886253207
C,5.8453260691,-2.4999605039,0.3606002981
C,3.7415182178,-3.2884418994,-0.5261559843
C,6.3273082929,-3.8056123274,0.3697751708
H,6.4703379822,-1.689319526,0.7215071005
C,4.2227173387,-4.5956413665,-0.504236657
H,2.7478686324,-3.0944286081,-0.9213356582
C,5.5179328316,-4.8611302242,-0.0573164698
H,7.3354726633,-4.0020624723,0.722609168
H,3.5889954732,-5.4069039821,-0.8505027154
H,5.8942040023,-5.8794096916,-0.0442188583

Cartesian Coordination of 4b-1 (DFT)

-1144.4638156 hartree

C,-4.7608418918,0.6759663312,-0.0856804219
C,-4.3324530201,1.9940555767,-0.2724021871
C,-1.1969185962,0.0582873469,-0.0012022548
C,4.3324682835,1.994019563,-0.272375049
C,0.0000020516,0.7733646166,-0.1098314009
C,1.1969160626,0.0582776828,-0.0011930781
C,-2.5020744431,0.6811658131,-0.0988910808
C,-2.9243992424,1.9969372915,-0.2831527303
C,4.7608450251,0.675926615,-0.0856515118
C,-0.0000101609,-1.863467852,0.2956491262
C,2.9244146011,1.9969131842,-0.2831333793
C,2.5020777067,0.6811450651,-0.098875355
C,7.651259223,-1.7572924139,-0.2215013844
C,6.3604283313,-1.2388682197,-0.2955884149
C,6.1105440521,0.1168293495,-0.0143967641
C,7.2000684901,0.9350083927,0.336321729
C,8.4901173096,0.4163433157,0.3991419834
C,8.7233183524,-0.9332087646,0.1243458865
C,-6.3604399882,-1.2388151919,-0.2956254848
C,-7.6512755606,-1.757228639,-0.2215454552
C,-8.7233298175,-0.9331358631,0.1242952743
C,-8.4901191393,0.4164144212,0.3990918978
C,-7.2000656454,0.9350687906,0.3362787158
C,-6.1105460511,0.1168804975,-0.0144331008
H,-2.2838139574,2.8569356638,-0.4176681646
H,-4.9786904225,2.8471113087,-0.420733154
H,3.5690979259,-1.0825407034,0.2068469579
H,4.9787135902,2.8470701031,-0.420701435
H,0.000007013,1.8442213633,-0.2751020944
H,2.2838373387,2.8569172057,-0.4176508834
H,-3.5691114153,-1.0825107615,0.2068265498
H,-0.0000151356,-2.9397709364,0.4627768051
H,7.8207570551,-2.8064220025,-0.4457648373
H,5.5453920211,-1.8878904838,-0.6032417783
H,7.0254911645,1.9785457314,0.578728614
H,9.3159636335,1.0660530729,0.6741670978
H,9.7295539312,-1.3374057,0.1785242875
H,-5.5454072301,-1.8878442005,-0.6032740146
H,-7.8207808642,-2.8063569452,-0.4458092665
H,-9.7295690502,-1.3373244283,0.1784682484
H,-9.3159616531,1.0661311955,0.674111884
H,-7.0254810222,1.9786047929,0.5786860828
N,-3.6322911696,-0.0937960175,0.009598879
N,3.632287251,-0.0938262748,0.0096207508
N,-1.1959019353,-1.2844574742,0.2057028187
N,1.1958869972,-1.284467418,0.2057100927

Cartesian Coordination of 4b-2 (DFT)

-1144.4567739 hartree

C,4.8992288445,1.8800853947,-0.1546119086
C,4.6696645307,0.5094282495,-0.0389585719
C,1.2184744206,1.7126149237,-0.0743676835
C,-3.3426196489,-1.9840373495,-0.026381917
C,0.3274874183,0.6317270295,-0.0683973807
C,-1.0439134508,0.9108155189,-0.0377534992
C,2.6609141113,1.5556206128,-0.0908461267
C,-4.1917247745,-0.8733968154,-0.0010214938
C,-0.5609041689,3.1395749977,-0.048179628
C,-2.0142472455,-1.516008229,-0.0359692202
C,-2.0611430137,-0.1229873399,-0.0205011287
C,3.6498445149,2.529247013,-0.1876199038
C,6.1313625234,-2.9690136528,-0.2831289283
C,5.2319327499,-1.9084296495,-0.3677500891
C,5.6039965219,-0.6127616282,0.0357886814
C,6.9115934024,-0.4155138471,0.5164446887
C,7.8116373697,-1.4746555621,0.5880421858
C,7.4259919011,-2.7581491764,0.1936595474
C,-6.4320657485,-1.8735536523,-0.4203080802
C,-7.8221146291,-1.8120577334,-0.3875527696
C,-8.4678277947,-0.6681883981,0.0875933114
C,-7.7063750082,0.4117313573,0.5370392199
C,-6.3149459371,0.3491354846,0.5155540331
C,-5.6519213027,-0.7938905513,0.0325308215
H,2.8589836902,-0.5421907497,0.197591265

H,5.8706387973,2.3442059165,-0.2466494792
H,-3.6658185309,1.2054182808,-0.0336799057
H,-3.6609712528,-3.0162574209,-0.0030826425
H,0.6708991738,-0.3965700122,-0.0987717445
H,-1.1197475953,-2.1226633013,-0.0442431323
H,3.4531634361,3.5856770858,-0.2875837325
H,-0.9254098329,4.1659659267,-0.0472345218
H,5.8235807369,-3.9600783201,-0.6037319807
H,4.2435182695,-2.0825206089,-0.7845818173
H,7.2100520829,0.5723654699,0.8528056569
H,8.8154267114,-1.3001593295,0.9643758199
H,8.1278044265,-3.5842029265,0.2555240581
H,-5.9403658805,-2.7558288094,-0.8177669489
H,-8.4043224835,-2.6566600793,-0.7445776511
H,-9.55228964,-0.6197047449,0.1077580362
H,-8.1965020125,1.3035987098,0.9165189668
H,-5.7408009913,1.185668072,0.9039869154
N,-3.3876760663,0.2350579673,0.0077907
N,0.7596048907,2.9896458496,-0.068007178
N,-1.4968846729,2.1877596981,-0.0261715512
N,3.3052901576,0.3343413296,-0.0192552923

Cartesian Coordination of 4b-3 (DFT)

-1144.4488772 hartree

C,4.7301576438,-1.3767088832,-0.1843808644
C,4.0522582307,-0.1614265075,-0.1037464315
C,1.2130014271,-2.4637158296,0.0141005568
C,-4.053866356,-0.1942191312,0.0369769928
C,0.005485524,-1.752083382,-0.0377719179
C,-1.193705045,-2.4734234127,0.0557674074
C,2.5165350086,-1.8272177214,-0.0534605208
C,-4.7243118968,-1.4149588706,-0.020093431
C,0.0199274366,-4.3976377944,0.1784502169
C,-2.5038948625,-1.8475045549,0.0335029212
C,3.7744258952,-2.4115115215,-0.1530145434
C,-3.7597309004,-2.4419873049,-0.0221528712
C,-5.8532555471,1.4453969308,0.5537050261
C,-4.5617916492,1.1764573635,0.0642432582
C,-3.7859468996,2.2573170724,-0.3941458637
C,-4.2793937662,3.5595606923,-0.3536654836
C,-5.563015968,3.8111276545,0.1328760014
C,-6.3480659344,2.7459645158,0.5810872844
C,4.5497602653,1.2133070981,-0.0937154376
C,5.855468311,1.4925691789,0.3500177138
C,6.3403918234,2.7971040738,0.360638507
C,5.5314211754,3.8559763645,-0.0590067442
C,4.2335034862,3.5941486053,-0.5001055834
C,3.749495904,2.2879642855,-0.5238675646
H,2.0014392782,0.2219745927,0.1814520591
H,5.798990399,-1.4887346349,-0.2968056115
H,-3.9245641692,-3.5070862332,-0.0780828861
H,-0.0013781417,-0.6767483432,-0.1874282728
H,-5.7954741837,-1.535701121,-0.095095798
H,-1.9974814722,0.2059014603,0.2499872119
H,3.9457961104,-3.4752505606,-0.214892719
H,0.0255896911,-5.4843147126,0.2518940001
H,-6.458746472,0.6275976111,0.9314343621
H,-2.8026467973,2.0746894181,-0.8194937197
H,-3.6643187351,4.3780277141,-0.7164144405
H,-5.9489245169,4.8255305827,0.1604782535
H,-7.3470800039,2.9309928392,0.9649878427
H,6.480504737,0.6796064459,0.7057011754
H,7.3507976278,2.9901406675,0.7091508462
H,5.9098386028,4.8734693153,-0.0444613516
H,3.5994329353,4.4077181136,-0.8404733212
H,2.7533200144,2.0974584853,-0.9143660072
N,1.2158555836,-3.8128223339,0.1224523414
N,-1.1818842543,-3.8225169572,0.1639370418
N,2.7091776664,-0.4576650558,-0.0449833358
N,-2.7072062059,-0.479581215,0.0488157007

Cartesian Coordination of 4c-1 (DFT)

-1375.5326132 hartree

H,2.2479601907,-3.7041899125,0.1094363874
H,4.9424535627,-3.7334004287,0.1039652355
H,-3.5934376828,0.2614548985,-0.0413611261
H,-4.9424569223,-3.7334033346,0.1037503376
H,-0.0000009778,-2.6795730523,0.090137051
H,-2.2479636224,-3.7041952655,0.1092313115
H,3.5934387889,0.2614493884,-0.0413991749
N,3.6373255181,-0.7436323144,0.0396709372
N,-3.6373263286,-0.7436326896,0.0396340819
N,1.1916049748,0.482254385,-0.0050750196
N,-1.1916062613,0.4822536432,-0.0051084003
C,4.7553630028,-1.5353046119,0.0356182644
C,4.3084821206,-2.8595144383,0.0621611043
C,1.1935627942,-0.8701814926,0.0364574958
C,-4.3084847237,-2.8595151801,0.0620027611
C,-0.0000007728,-1.5972567674,0.0575940537
C,-1.1935642045,-0.8701824816,0.0364189815
C,2.4960841166,-1.5093418599,0.0560590722
C,2.900343646,-2.8431947133,0.0775512887
C,-4.7553645219,-1.5353033125,0.0355345176
C,-0.0000004917,1.0966335108,-0.024738535
C,-2.9003463856,-2.8431975453,0.0774002405
C,-2.496085721,-1.5093436714,0.0559854679
C,-6.1124840698,-0.9900611642,0.025861495
C,-7.1865351279,-1.7686648384,-0.4428497468
C,-6.3848434575,0.3125816558,0.4823466451
C,-8.4833406945,-1.2632877066,-0.4512289105
H,-6.9940084869,-2.768142201,-0.8199306069
C,-7.6823377329,0.8192870568,0.4626302291
H,-5.5823022997,0.9248102617,0.8841847572
C,-8.7387682579,0.0345638123,-0.0024143603
H,-9.2969078614,-1.8813730227,-0.8197793792
H,-7.8696423348,1.8267207108,0.8227976176
H,-9.7501493458,0.4292581993,-0.0141491755
C,6.1124832425,-0.9900647857,0.0259225443
C,7.1865364975,-1.7686955737,-0.4427385436
C,6.3848413914,0.3126020624,0.4823397202
C,8.4833431866,-1.2633214895,-0.4511334563
H,6.9940108844,-2.7681927652,-0.8197674006
C,7.6823367587,0.8193039105,0.4626073235
H,5.5822975551,0.9248531175,0.8841381538
C,8.7387696448,0.0345534181,-0.0023859303
H,9.2969123082,-1.881428143,-0.8196438235
H,7.8696403834,1.8267564749,0.8227223097
H,9.7501517303,0.4292448751,-0.0141328765
C,0.0000001534,2.5859654931,-0.0724768053
C,1.2071293755,3.3009073981,-0.095301779

C,-1.2071280297,3.3008925775,-0.0958059588
C,1.2066924504,4.6929490821,-0.140525003
H,2.1396201847,2.7501629104,-0.0773483259
C,-1.2066896213,4.6929341694,-0.1410335253
H,-2.1396195755,2.7501365692,-0.0782535184
C,0.0000018353,5.3950506896,-0.1635259797
H,2.1498514268,5.2314989546,-0.1581850032
H,-2.1498479238,5.2314716845,-0.1591004099
H,0.0000027112,6.4806778527,-0.1989536109

Cartesian Coordination of 4c-2 (DFT)

-1375.5263057 hartree

H,3.5429610494,2.8316196538,-0.3588866772
H,6.0354709477,1.757349608,-0.3102936031
H,-3.3995945628,-0.0976801261,-0.0297508277
H,-3.0254196097,-4.2988351406,-0.1551794655
H,1.056597854,-1.3370630241,-0.1797548798
H,-0.572140891,-3.185878536,-0.1793788574
H,3.2300426146,-1.3091230596,0.2489169814
N,3.6141015626,-0.41453223,-0.0095412085
N,-3.034640544,-1.0388587802,-0.0226352744
N,0.8812561221,2.0383045503,-0.0333560587
N,-1.2988750088,1.0696384716,-0.0076684567
C,4.9636234484,-0.1484895019,-0.0445564499
C,5.0988490669,1.2307859648,-0.1959650062
C,1.435806862,0.8075254536,-0.0787061933
C,-2.7982402547,-3.2426108679,-0.1416636688
C,0.6354795093,-0.3411036461,-0.1063242396
C,-0.7518477506,-0.1635130954,-0.0613235976
C,2.8876199349,0.7583983865,-0.1018902049
C,3.8075668479,1.7932995191,-0.2310162043
C,-3.7399508122,-2.2123195997,-0.0684748123
C,-0.4543814217,2.1148338705,-0.0051411543
C,-1.5156474718,-2.6600657644,-0.1418587324
C,-1.6825189411,-1.2779713634,-0.0736783378
C,-5.2011312775,-2.2603115493,-0.0215384306
C,-5.8913637488,-3.3768513383,-0.5277302478
C,-5.9537193947,-1.2060327602,0.5275171666
C,-7.2812283176,-3.436314206,-0.4831167918
H,-5.3303491893,-4.1908230117,-0.9759737768
C,-7.3451743363,-1.2637462528,0.5606509099
H,-5.4482796055,-0.3469078562,0.959621555
C,-8.0167597597,-2.378953101,0.0573698525
H,-7.793320452,-4.3071188472,-0.8821484676
H,-7.9053501331,-0.4391399504,0.9918384245
H,-9.1011392216,-2.4244677773,0.0866347582
C,5.9713194749,-1.2034232082,0.0527187222
C,7.2671139041,-0.9062808798,0.5135041085
C,5.6822734384,-2.5324270392,-0.3082876443
C,8.2357346956,-1.901319208,0.6067132891
H,7.5026029037,0.1086915576,0.817680288
C,6.6503640668,-3.5286195495,-0.2016323363
H,4.7038093636,-2.7836545434,-0.7088782712
C,7.9323276402,-3.2188205443,0.2548607
H,9.2290395117,-1.6498643534,0.9670010229
H,6.4057612273,-4.5470375738,-0.4892539027
H,8.6876618692,-3.9946799168,0.3338684832
C,-1.0524051939,3.4782646777,0.0376265917
C,-0.2268176014,4.6120385314,0.0886343543
C,-2.4442299464,3.6535992655,0.0267273844
C,-0.7817950439,5.8888776708,0.127752605
H,0.8473848295,4.4712220934,0.0982498751
C,-2.9972958243,4.9314468404,0.0649153071
H,-3.0810218437,2.778115273,-0.0134081428
C,-2.1684478611,6.0540502247,0.115758033
H,-0.1309426238,6.7576181624,0.1680493139
H,-4.0768128132,5.0520994268,0.0542951112
H,-2.6001752888,7.0504190005,0.1458010839

Cartesian Coordination of 4c-3 (DFT)

-1375.5191585 hartree

H,4.0723520561,1.925199877,-0.4235887031
H,5.7839600612,-0.1823118711,-0.4334924384
H,-2.0783758645,-1.3452827503,0.2387076469
H,-5.7675737256,0.5736386194,-0.2896147149
H,-0.0435609209,-0.6086552249,-0.2941246819
H,-3.7962022756,2.4401330606,-0.3252407775
H,1.890483909,-1.604852001,0.1899486313
N,2.6374137546,-0.9887172587,-0.0870244031
N,-2.7453191049,-0.6365230422,-0.0202899084
N,1.3567029843,2.4503192166,-0.024264747
N,-1.0262784622,2.6062279618,0.005427786
C,3.9565780723,-1.3778241862,-0.1492943651
C,4.7123312567,-0.2166140421,-0.2992723284
C,1.2736523814,1.1078154417,-0.107187302
C,-4.7065499747,0.3997477284,-0.1820450298
C,0.0284094273,0.4645886235,-0.1523390993
C,-1.1209220569,1.2644767554,-0.0773847446
C,2.5362484117,0.3888436561,-0.1584716268
C,3.8282261886,0.880894263,-0.3039849682
C,-4.1050688211,-0.8503173372,-0.0492252527
C,0.205330279,3.1368784201,0.0149891541
C,-3.6873684967,1.3726982199,-0.2102948882
C,-2.4673063753,0.7162277266,-0.0962280887
C,-4.687658131,-2.1886156873,0.0342103889
C,-6.0044662289,-2.361856854,0.4988597972
C,-3.9606421979,-3.33214341,-0.3452959264
C,-6.570733555,-3.6307317274,0.5780874915
H,-6.5739042992,-1.4939879539,0.8161546166
C,-4.5259121679,-4.6021262134,-0.2526519956
H,-2.9578648663,-3.2250840011,-0.7503606654
C,-5.8339352299,-4.7585712657,0.2081362843
H,-7.588263721,-3.7414778262,0.9414300344
H,-3.9473940497,-5.4703612178,-0.5547824297
H,-6.275727386,-5.7479607627,0.2761943201
C,4.3617028491,-2.780747497,-0.0778817585
C,5.6558159593,-3.1247635605,0.3543456584
C,3.4827011857,-3.8192385362,-0.4372078667
C,6.0537083283,-4.456719673,0.4218206908
H,6.3411643442,-2.3389487763,0.6558826714
C,3.8797920196,-5.1521842382,-0.3562891604
H,2.4926944991,-3.5818340047,-0.817506937
C,5.167291901,-5.4784001917,0.0722574745
H,7.0568210876,-4.6996338925,0.7600627039
H,3.1857682211,-5.9371995149,-0.6424364687
H,5.4779437369,-6.517020224,0.1311450644
C,0.3032902927,4.6205527478,0.0857255345
C,1.5567331769,5.2511147135,0.1040787652
C,-0.8564745465,5.4090317533,0.1338107498
C,1.6466852866,6.6396275726,0.1675241437

H,2.4484578418,4.6365326557,0.0692374528
C,-0.7631536889,6.797324082,0.1972116563
H,-1.8212621087,4.9159405402,0.121847098
C,0.4879180733,7.4178194627,0.2138576386
H,2.6228073834,7.1161255839,0.1811832423
H,-1.6682348247,7.3969272451,0.2340337371
H,0.5593891111,8.5007228155,0.2632648434

Cartesian Coordination of 3d (AM1)

-0.2787948 hartree

C,-6.4755482729,8.7356046855,5.4801037248
C,-7.7092142571,9.2008446183,4.9854815073
C,-6.7903458345,6.5317293948,2.5742941243
C,-10.5509264436,5.3878315641,-1.6856171836
C,-7.8062543759,6.3920893768,1.6011247784
C,-7.6211412064,5.4168562558,0.5950507512
C,-6.9485574093,7.5247106043,3.6278575978
C,-8.0096822963,8.4390652194,3.8178584943
C,-9.6659645981,4.4771116373,-2.2932731853
C,-5.5787091597,4.8423899744,1.5387222862
C,-9.9108488409,5.8763346256,-0.5080126777
C,-8.6471231441,5.2491949692,-0.4255656436
C,-4.354430494,3.9924827419,1.5065214536
C,-4.4836529902,2.6080922488,1.3390060769
C,-3.1037126817,4.5840893267,1.6404158407
C,-3.3366848399,1.8124699864,1.3186270931
C,-1.9432756519,3.7822649118,1.6074509144
C,-2.0482234363,2.3888016461,1.4527874569
C,-4.6405435148,-0.1845191726,1.232386622
C,0.4471701376,3.879773052,1.3959809438
C,-4.370595356,-1.6789568435,1.2001178188
C,-0.6353729065,0.8254546822,0.3667328466
C,1.473876665,4.9988610189,1.3613309646
C,-5.6732514043,-2.4466194397,1.2486068187
C,0.8008684052,0.3546386573,0.512109174
C,2.8349958846,4.4435772025,1.0036235382
C,-5.4248307593,-3.9396707004,1.2205384067
C,1.1954240734,-0.503400735,-0.6693954809
C,3.8733811906,5.5434088822,0.9458137285
C,-6.7255622765,-4.7123304038,1.2690169888
C,2.6254187354,-0.9830496743,-0.5406641723
C,5.2373744699,4.9914744023,0.5906760841
C,-6.4780137906,-6.2053586475,1.2408007587
C,3.0242936795,-1.8414449593,-1.7218777594
C,6.2760666649,6.0909645077,0.5322294953
C,-7.7783753788,-6.9785737175,1.2892798181
C,4.4541507949,-2.3212847836,-1.5936731807
C,7.640270786,5.539580548,0.1771859499
C,-7.5310362772,-8.4716091936,1.260985551
C,4.853564791,-3.1795377205,-2.7747761533
C,8.6789872856,6.6390167803,0.1186361767
C,-8.8312854661,-9.2449939246,1.3094619693
C,6.2834070083,-3.659389106,-2.6466462153
C,10.0432542512,6.0878302808,-0.2364452844
C,-8.5841611912,-10.737962305,1.2812083458
C,6.6830017228,-4.5176315075,-3.8276884638
C,11.0820383951,7.1870738337,-0.2948188552
C,-9.8839371833,-11.5128139119,1.3294197112
C,8.1128058196,-4.9973384119,-3.6997978198
C,12.4469585689,6.6373277805,-0.65106271
C,-9.6426933678,-12.9999188351,1.3020049691
C,8.5135007275,-5.8568982941,-4.8799426837
C,13.4850000805,7.7280497018,-0.7078163046
C,9.9373061369,-6.3347595786,-4.7580617172
H,-8.8894638395,8.5430760483,3.1903615186
H,-8.3150501857,9.9918655783,5.4153962121
H,-5.9079461789,9.0602797023,6.3530067532
H,-7.724823626,3.836226693,-1.7162361368
H,-11.5356365722,5.6643336787,-2.0483192275
H,-8.704547626,7.0193215483,1.6247166967
H,-9.7844211531,3.8954258707,-3.2081027692
H,-10.3199780239,6.5941537556,0.1962894887
H,-5.1794094822,7.213327291,4.7629827194
H,-5.4819431214,2.1625102895,1.2287642361
H,-2.9915637719,5.6696222985,1.7788904056
H,-5.1461473498,0.1152163152,2.1871590586
H,-5.2655125333,0.1326892217,0.3565116832
H,0.321254847,3.4095517849,0.3861757115
H,0.7256195265,3.0888919776,2.1421638052
H,-3.7218532994,-1.9584059574,2.0708406728
H,-3.8030430761,-1.9347446815,0.2676656941
H,-0.7645009288,1.4586143035,-0.5485819359
H,-1.3473789203,-0.0401297541,0.3291589469
H,1.1606248073,5.772400059,0.6130663011
H,1.5106347802,5.5014429034,2.3628948568
H,-6.2364834759,-2.176634566,2.1808438167
H,-6.3166323357,-2.1560221094,0.3764136194
H,1.4776175884,1.2463309608,0.5895676031
H,0.9063213143,-0.2254415053,1.4657887862
H,2.7816279439,3.9231896506,0.0108219743
H,3.1408983063,3.6761493587,1.7631022763
H,-4.7814768999,-4.2302248926,2.092639507
H,-4.8608320049,-4.2097437528,0.2889881301
H,1.0794842991,0.0835707638,-1.6186642516
H,0.5072272055,-1.386876169,-0.7401663138
H,3.5676888924,6.3098491431,0.1855747954
H,3.9246045461,6.0643068947,1.9382341635
H,-7.2892860776,-4.4421121014,2.2007201549
H,-7.3691097872,-4.4212428139,0.3972651428
H,3.3134636535,-0.0998232499,-0.4678755407
H,2.7407297801,-1.5708603329,0.4080444114
H,5.1856978921,4.4698647327,-0.4013346747
H,5.5430266618,4.2254109688,1.3513204512
H,-5.8345808142,-6.4964682367,2.1126397341
H,-5.9141316292,-6.4757024849,0.3092527904
H,2.908441689,-1.2536583903,-2.6705207665
H,2.3362490392,-2.7247218381,-1.7944081743
H,5.9704247817,6.8571213501,-0.2283103257
H,6.3277282959,6.6126140612,1.5242250344
H,-8.3421605633,-6.7083440689,2.2209257709
H,-8.4219572192,-6.6873749754,0.4175976001
H,5.1422302656,-1.4380721978,-1.5207788044
H,4.569920985,-2.9093099154,-0.6451647217
H,7.5886099944,5.017809001,-0.8147356199
H,7.9459464092,4.7735237953,0.9378110401
H,-6.8875299408,-8.7628286137,2.1327223382
H,-6.967179499,-8.7419123171,0.329415346
H,4.737747475,-2.5915586023,-3.7232978676
H,4.165551056,-4.0628021381,-2.8476434385
H,8.3732915738,7.4051450816,-0.6419051138

H,8.7307020475,7.1607639106,1.1105708415
H,-9.3951131252,-8.9746607251,2.2410564186
H,-9.4748526975,-8.9537224467,0.4377850219
H,6.9714556898,-2.7761599605,-2.5737080321
H,6.3992254212,-4.2474114617,-1.6981500996
H,9.9915568294,5.5661500797,-1.2284199415
H,10.3488328501,5.3215872886,0.5240396076
H,-7.9409200466,-11.0295533517,2.1529808253
H,-8.0202921366,-11.0086055812,0.3497748323
H,6.5669763571,-3.9296532915,-4.7761932912
H,5.9950340339,-5.4009387686,-3.9005425194
H,10.7763582492,7.953841003,-1.0546829362
H,11.134655889,7.7082561412,0.6973337465
H,-10.4473037671,-11.2394483977,2.2606393869
H,-10.5263716843,-11.2190308643,0.4574986625
H,8.8010860683,-4.1142389081,-3.6278923742
H,8.2292904577,-5.584766203,-2.7510469328
H,12.3923953439,6.1168990113,-1.643764503
H,12.7494770173,5.8681542291,0.1079667511
H,-9.0245318436,-13.3154222659,2.177171686
H,-9.1039657754,-13.2949824023,0.3691190613
H,8.3930607209,-5.2689519654,-5.8281434983
H,7.8243039986,-6.7397299648,-4.9499156017
H,13.2134664809,8.4912802745,-1.4767379538
H,13.5710978701,8.2424089684,0.2798971714
H,10.6413737689,-5.4689152268,-4.7115815536
H,10.0709157296,-6.9439164658,-3.8314666411
H,-10.6129282269,-13.5515455723,1.3384211201
H,14.4828103594,7.301412427,-0.9712880556
H,10.2119694658,-6.9656681256,-5.6376040734
N,-6.0192144341,7.7236505928,4.657032214
N,-8.5177645712,4.3944623259,-1.5277250471
N,-5.6689523744,5.7594440949,2.5489355242
N,-6.5077411623,4.6335403274,0.5569346818
O,-3.3531168797,0.4433066137,1.144282198
O,-0.7814018724,4.4919957591,1.8133486
O,-0.9148191939,1.6034162338,1.5468478497

Cartesian Coordination of 3e (AM1)

-0.4100797 hartree

H,-1.3741883882,-3.0962279774,-0.8442793558
H,-2.8784650012,-4.0505044102,1.2066258862
H,-3.2950006097,-1.9417278562,2.9156214424
H,1.9982449707,1.720438817,-4.4514453973
H,2.3720054906,-2.1595569409,-6.1189208253
H,-0.1837436205,-1.7001283429,-2.0447003591
H,2.9779752936,0.4975949771,-6.4554133914
H,0.9859617406,-2.3460396887,-3.7898072517
H,-2.1053522565,0.0613378252,1.89452338
N,-2.1158272046,-0.8357656661,1.4797674037
N,1.9272142605,0.7436992635,-4.5812593839
N,-0.6399262807,1.0834398215,-0.1211803483
N,0.7257873284,1.5907493363,-2.0748331362
C,-2.7391454612,-1.9642454896,1.9775043202
C,-2.5153949439,-3.0345390193,1.0901291908
C,-0.7294012936,-0.2122617953,-0.5307283726
C,2.1114214981,-1.3413579829,-5.4553640871
C,-0.1047299907,-0.656951936,-1.7184380392
C,0.6229360454,0.2920553251,-2.4717019436
C,-1.4853654329,-1.1633014119,0.2724220273
C,-1.7252037785,-2.5322492639,0.0143838734
C,2.4317568762,0.0165365802,-5.6432980247
C,0.0862939502,1.9283179185,-0.913921655
C,1.3824869625,-1.4376639202,-4.2328810534
C,1.2760765574,-0.1319136622,-3.70298139
C,0.1895300652,3.3477026975,-0.4701692021
C,1.4423495501,3.973437048,-0.4559743351
C,-0.9565574761,4.0304688501,-0.0796106987
H,2.334211132,3.41655265,-0.774946819
C,1.5386814983,5.2997439281,-0.0310491846
C,-0.8619577746,5.3747780208,0.338135511
H,-1.9443500871,3.5463200598,-0.0809317763
O,2.7205871845,6.0117340526,0.0062067425
C,0.3864245865,6.0205179659,0.3727361974
O,-2.0629314181,5.9046829664,0.7539669505
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C,0.9899893459,8.2789019351,-0.0207314713
H,-1.7189225214,7.7853969319,-0.1228894463
H,-1.6234200581,7.7084507649,1.7032464102
C,-3.6590314104,7.6316903443,0.8859423504
C,6.391803964,5.5086438872,-0.1138498356
H,4.9869164655,6.5903386311,1.1425747309
H,4.9801474818,7.089932089,-0.5920596762
H,0.4980148224,8.1574015769,-1.020013427
H,2.0972655525,8.1362579247,-0.1265045775
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H,-4.174818535,7.2385437336,-0.0282725311
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H,7.4760830764,7.3371037419,-0.5268504738
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C,-10.4795144797,14.8889883802,1.6984167752
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C,1.4535709307,19.5263314165,-0.5229618852
H,-10.9929601334,14.5095912397,0.7757807903
H,-10.9390225931,14.3585430116,2.5738069125
C,-10.7093154953,16.3792465796,1.8305086459
C,17.4906819769,7.4374255446,0.4117444657
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C,1.9677921398,20.6481144609,-1.3994929234
H,1.9145145107,19.6045038223,0.4969635791
H,-10.249785402,16.9097060714,0.9551414899
H,-10.1959045653,16.7586344662,2.7531673268
C,-12.1861144308,16.7033989836,1.9019993377
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H,1.506849155,20.5699594639,-2.4194183118
H,3.0774001973,20.54512015,-1.5298249468
C,1.6506462609,22.0020965793,-0.8017699316
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C,-12.416002628,18.1936411253,2.034101405
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H,18.8864273682,6.3592715637,-0.8443962043
H,0.5410423985,22.105098118,-0.6714091217
C,2.1648154533,23.1239374781,-1.6782543628
H,2.1115977678,22.0802709417,0.2181502159
H,-11.9564096329,18.7240922972,1.1587539982
H,-11.9025474772,18.5730131998,2.9567494012
C,-13.8926718818,18.517887204,2.10558384
C,21.3081686845,6.9931921706,0.2714941051
H,19.9117670022,8.0702814979,1.5272968652
H,19.9065058116,8.5724235995,-0.2065076861
H,1.7038775932,23.045727259,-2.698184696
H,3.2744198988,23.0208993115,-1.8086361072
C,1.8477495096,24.4778787171,-1.0806670213
H,-14.4063504086,18.1387524521,1.1830021389
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C,-14.1240715634,20.0082289174,2.2377496541
C,22.4619733033,7.9249945265,0.5378501685
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H,0.7382060043,24.5812447961,-0.9503027558
C,2.3615002508,25.6009582289,-1.9563873183
H,2.3086859685,24.5564202464,-0.0607967955
H,-13.6622063785,20.5368920583,1.3622681067
H,-13.6083545375,20.3858152116,3.1601041105
C,-15.5931131798,20.3357475828,2.3092766741
H,23.4327720686,7.3956862051,0.3816178189
H,22.4305779442,8.3012460456,1.5890182046
H,22.4253109114,8.8047035981,-0.1493694946
H,1.9006093323,25.5198499476,-2.9763256002
H,3.47101718,25.4950266248,-2.0868619783
C,2.0480095684,26.9510364769,-1.3652193251
H,-16.119876829,19.9890533217,1.3874156838
H,-16.0658749638,19.8375681467,3.1900824292
H,-15.7409980424,21.438348055,2.406363824
H,0.9450959373,27.0849632387,-1.2505473036
H,2.4351107344,27.7637871927,-2.0259869839
H,2.5197228898,27.0600713769,-0.3586894178

Cartesian Coordination of 4d (AM1)

-0.2009167 hartree

H,-1.4834143057,-3.1955538082,-0.3443992494
H,-3.3327252128,-4.0163149235,1.4657649555
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H,3.0440026371,-2.6045082925,-5.0020936128
H,-0.1183928546,-1.8772629481,-1.430186884
H,1.2863166465,-2.6336436592,-2.9327671668
H,-2.6505342157,0.1354295277,2.0160252433
N,-0.8140423033,1.0145473439,0.2465185591
N,0.8622239652,1.3930444168,-1.4811657655
C,-3.3133059608,-1.8827900542,2.1230004878
C,-2.94590343,-3.0090715448,1.3462874994
C,-0.8666352832,-0.300020074,-0.1046411916
C,2.7064790439,-1.7478483162,-4.42698629
C,-0.068298102,-0.8191193419,-1.1496273985

C,0.7944669144,0.076280908,-1.8214632709
C,-1.7652404402,-1.1948083509,0.6126815146
C,3.10186742,-0.4037268342,-4.63313252
C,0.0511994099,1.8039711817,-0.4592766692
C,1.629760262,-0.4249597604,-2.9055533991
C,0.1156723986,3.243653792,-0.0783017918
C,1.3648518697,3.8521312839,0.0972850788
C,-1.0616805573,3.9620549895,0.0948834828
H,2.2828490824,3.2666450167,-0.050485136
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C,-1.0030077415,5.3254988182,0.4530448806
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C,-2.3251767127,7.3248781882,0.6032742215
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H,3.9740184777,4.6733421281,-0.3514800984
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H,-1.7261597533,7.7186496706,-0.2585738949
H,-1.9146957223,7.7402549686,1.5618059045
C,-3.8013832941,7.646035223,0.4441049253
C,6.242864387,5.3448062,1.0669089709
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H,0.6140231295,8.0116465428,-0.818660952
H,2.0531938007,8.0181118257,0.3150446919
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H,-4.1784554954,7.2109212617,-0.5176054628
H,-4.3789346764,7.1641175992,1.2755371223
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C,1.226940314,10.6270489314,-0.1190710525
H,0.850404119,9.6784844887,1.7988175004
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C,8.6987590184,5.566731953,1.4672455974
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H,-6.0737666328,9.0143666152,1.1058337482
C,-5.6890132218,10.9889216203,0.3037119148
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H,-7.5250535995,10.9139612175,-0.8417454677
H,-7.7520851684,10.8597291623,0.9483183562
C,-7.367156851,12.834058669,0.1467129562
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H,11.3598220564,5.3527709226,0.8539225683
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C,1.8102680374,15.5348626672,-0.8603050938
H,1.4378667569,14.5960521387,1.0550749778
H,-6.7669004105,13.3102602669,-0.6728892458
H,-6.9941591735,13.2559448563,1.1171338709
C,-8.8300311965,13.1811003272,-0.028489145
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C,-9.0454694124,14.6792274772,-0.0104084921
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H,1.7294887903,17.0502723731,0.684224606
H,-8.4451323364,15.155424381,-0.8299623672
H,-8.6724283535,15.1011195759,0.9599977037
C,-10.50820645,15.0263631851,-0.1856222559
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C,-10.7251936568,16.5246055177,-0.1677293929
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H,2.3299737704,21.9857738291,-0.0756011623
H,-12.317747665,17.9829963578,-0.3257233117
H,2.5229518176,22.5994552274,-1.7692427887
H,18.1657176743,6.6157642716,3.0560940811
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N,-2.5871481871,-0.7876548388,1.666662184
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C,1.7823605891,-1.7604708321,-3.3458605978
C,-4.2712963326,-1.8261839422,3.211797579
C,-4.166884213,-0.8701192651,4.2328061196
C,-5.3209237474,-2.7578220031,3.2494525434
C,-5.0984617761,-0.8470378057,5.2690699613
H,-3.344157127,-0.1399620937,4.233436854
C,-6.2464884553,-2.7301494892,4.2895263491
H,-5.4102326823,-3.5087338638,2.449867493
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H,-5.0088102735,-0.0940440662,6.0661288964
H,-7.0657984382,-3.4639296558,4.3110831417
H,-6.8723576274,-1.7536481378,6.1195495632
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C,5.0406867258,-0.7291580524,-6.1164659756
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H,3.1340938476,2.0922374,-5.7540627091
C,5.9351243314,-0.2617305764,-7.0760161118
H,5.1248193477,-1.7588306581,-5.7370533024
C,5.8336070598,1.0450092483,-7.5537570875
H,4.7441268404,2.9131431338,-7.4478582429
H,6.7249202057,-0.9265104032,-7.4561941348
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Cartesian Coordination of 4e (AM1)

-0.3321704 hartree

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H,-3.100210362,-3.9531042937,1.2177552845
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H,2.4215363646,-1.9160510688,-5.8426504828
H,-0.2647726001,-1.5378855267,-1.8515982363
H,0.9406253822,-2.1458397611,-3.578444808
H,-2.3315188629,0.1348533941,2.0561067811
N,-2.3178828365,-0.7518485577,1.6182220875
N,1.9963481039,0.9434920048,-4.2107421689
N,-0.7278090897,1.1836774903,0.1574381915
N,0.7191815776,1.7293642837,-1.7256530067
C,-2.9866516514,-1.8886726609,2.060085803
C,-2.7260841069,-2.936770079,1.1433567508
C,-0.831486921,-0.0933467925,-0.3033932322
C,2.1623656958,-1.1174059131,-5.1545118219
C,-0.1739610945,-0.5096402467,-1.4837349578
C,0.6021045508,0.4489368745,-2.1738281517
C,-1.6374463607,-1.0556390982,0.4363133616
C,-1.8793463835,-2.4149035352,0.1272275331
C,2.5325073822,0.2430637766,-5.2869764536
C,0.0458269524,2.0402290318,-0.5761999104
C,1.3828738567,-1.2349267817,-3.9706093509
C,1.2914927393,0.0542500963,-3.3958401285
C,0.1653862454,3.4386507371,-0.0757834874
C,1.4264209752,4.0447325669,-0.0224828724
C,-0.9757767536,4.125771725,0.3269703067
H,2.3142466317,3.4885459107,-0.3547255717
C,1.5410304344,5.3504542433,0.4592460627
C,-0.8630898341,5.4473981804,0.7986751821
H,-1.971585295,3.6593298273,0.2928696262
O,2.7364999313,6.0397988254,0.5325861927
C,0.3966589928,6.0700928922,0.8817878703
O,-2.0460572629,5.9977524313,1.2437227553
C,3.923676408,5.2518211859,0.3625567973
O,0.4701698017,7.3212052375,1.4597483259
C,-2.1832833708,7.4197896671,1.0945866845
C,5.0813207858,6.1753745019,0.7006524198
H,3.896816488,4.367431698,1.0511876824
H,3.9831619611,4.9022052806,-0.7016817247
C,1.2738863213,8.2789535286,0.745325341
H,-1.6876601216,7.764396364,0.1507449371
H,-1.6879671439,7.9129631532,1.9732505549
C,-3.6767592412,7.6944903632,1.0693393853
C,6.396750319,5.4470353055,0.5338883786
H,4.9698886079,6.5406363945,1.754835704
H,5.0479497548,7.0747818734,0.0321796515
H,1.2635174219,8.0628690485,-0.3528832328
H,2.3246764813,8.1951552899,1.1309174418
C,0.6795434657,9.642727056,1.0497894785
H,-4.1359497792,7.1892816299,0.1803264912
H,-4.1513670518,7.2523935645,1.983973399
C,-3.9322596738,9.1846266539,1.0154261965
C,7.5641100742,6.3515931152,0.8666707849
H,6.4170528167,4.5457750877,1.2020994008
H,6.4946989259,5.0796128713,-0.5218275773
H,-0.3837562866,9.6742811421,0.6933535553
C,1.4899869878,10.7310205427,0.3815743998
H,0.6602950211,9.7992570488,2.1599826528
H,-3.4309083754,9.6213587842,0.1114462928
H,-3.4793088136,9.6779522277,1.9158182881
C,-5.4158309409,9.481146224,0.9664880949
C,8.8827800836,5.6269761055,0.7013961548
H,7.4660717048,6.7191123698,1.9222250324
H,7.5436409953,7.2532063882,0.1992142767
H,1.5078964655,10.5618383184,-0.7275501436
H,2.5520074955,10.684548652,0.7409049235
C,0.9135758575,12.0991706115,0.677181866
H,-5.8682751048,8.9892951654,0.0652576587
H,-5.9166959123,9.0417728783,1.8692287514
C,-5.6757940038,10.9714805692,0.9160693013
C,10.0506519248,6.5307819019,1.0336990542
H,8.9030314601,4.7254506181,1.369014687
H,8.9803929774,5.2588964789,-0.3539896339
H,-0.148640321,12.1453806415,0.3189103675
C,1.7223984852,13.1907961625,0.0098118039
H,0.8960149994,12.2681150347,1.7862416484
H,-5.173951482,11.4107636159,0.0138425226
H,-5.2238357984,11.4630113948,1.8177254177
C,-7.159208682,11.2684513756,0.8664194611
C,11.3695927354,5.8067033672,0.8685598736
H,9.9531277011,6.8987285678,2.0891403421
H,10.0304121865,7.4324435044,0.3662951307
H,1.7403418585,13.0214254024,-1.0991642291
H,2.7845556521,13.1446177786,0.3683307229

C,1.1463167587,14.5590891483,0.3049016336
H,-7.6112430077,10.776899777,-0.0351776343
H,-7.6610744865,10.8290733748,1.7685951287
C,-7.4197628883,12.7586594157,0.8161269584
C,12.5376211911,6.7103367744,1.2006833541
H,11.389888044,4.9051297431,1.5360897841
H,11.4670851375,5.4385346843,-0.1867965215
H,0.0840678694,14.6052598833,-0.0533272788
C,1.9547352187,15.651031247,-0.362381489
H,1.1285617557,14.7285186927,1.4138764724
H,-6.9178171947,13.1980696441,-0.0859770861
H,-6.967818453,13.250168587,1.717789861
C,-8.9031570201,13.055659197,0.7664202658
C,13.8566187192,5.9863763023,1.0355586248
H,12.4401809145,7.078420412,2.2560770212
H,12.5173398301,7.611974966,0.5332541652
H,1.9725813636,15.4815971275,-1.471345204
H,3.0169674327,15.6049467024,-0.0040936942
C,1.3786825347,17.019340445,-0.0673663211
H,-9.3551382346,12.5641156553,-0.1352039053
H,-9.4051093447,12.6162495296,1.6685260647
C,-9.1638680111,14.5458367826,0.7161345404
C,15.024709221,6.8899529513,1.3675927379
H,13.8769411288,5.0847958796,1.7030713929
H,13.9540577685,5.6181725543,-0.0197879725
H,0.3164145835,17.0654356612,-0.4255424854
C,2.1869691213,18.111369632,-0.7346570924
H,1.3609128189,17.1888184432,1.0415948537
H,-8.6618944729,14.9852680423,-0.1859434569
H,-8.711934679,15.037365112,1.6177898054
C,-10.647260547,14.8428220892,0.6664019996
C,16.3437268039,6.1660339369,1.2024747155
H,14.9273002293,7.258106476,2.422962133
H,15.0044000182,7.7915687589,0.7001354362
H,2.2047699142,17.941910768,-1.8436167749
H,3.2492310936,18.0653203112,-0.3764589929
C,1.6109158492,19.4796773724,-0.4396570606
H,-11.0992119168,14.3512799347,-0.2352365301
H,-11.1492372058,14.4033868824,1.5684795056
C,-10.9080460104,16.3329857275,0.6161253459
C,17.5118471783,7.0695825151,1.5344638985
H,16.3640586412,5.2644532574,1.8699835568
H,16.4411394437,5.7978095813,0.1471337132
H,0.5486374284,19.5257373668,-0.7978040485
C,2.4191375898,20.5717502715,-1.1069507949
H,1.593147595,19.6491627404,0.6693008257
H,-10.4060633827,16.7724321842,-0.2859401242
H,-10.4561166055,16.8245209059,1.5177778453
C,-12.3914375594,16.6299596175,0.5663853868
C,18.8308973893,6.3457229248,1.3693683942
H,17.4144534747,7.4377804449,2.5898173663
H,17.4915285542,7.9711864255,0.8669920514
H,2.4369198269,20.402280142,-2.2159086017
H,3.4814134416,20.5257148798,-0.7487947029
C,1.843084921,21.9400558292,-0.8119557191
H,-12.8433807637,16.1384157487,-0.3352550016
H,-12.8934246375,16.1905081683,1.4684474288
C,-12.6523162893,18.1201054713,0.5161138242
C,19.9990287681,7.2491024443,1.7012905038
H,18.8511851475,5.4441176991,2.0368545956
H,18.9282534389,5.9774558448,0.3140304118
H,0.7807993519,21.9861018224,-1.170080198
C,2.6512376712,23.032188977,-1.4792301006
H,1.8253148169,22.1095446412,0.2970000838
H,-12.1502817423,18.5595467255,-0.3859333926
H,-12.2003355179,18.6116288638,1.4177546536
C,-14.1355809316,18.4171678314,0.4663752769
C,21.3190843676,6.5262913176,1.5365759127
H,19.9020074928,7.6173801899,2.756622694
H,19.9790760903,8.1507257454,1.033876673
H,2.6690323733,22.8626646372,-2.5881857967
H,3.7135316323,22.9861083436,-1.1211144037
C,2.0753129802,24.4004485666,-1.1843211362
H,-14.5877918933,17.9258767571,-0.4352365868
H,-14.6378368392,17.9779611314,1.3683746304
C,-14.3979772078,19.9073849486,0.4160626111
C,22.4850995028,7.4220209372,1.8660353401
H,21.336554746,5.6240988379,2.2036731005
H,21.4136212252,6.1573843959,0.4809990889
H,1.0130711592,24.4468584954,-1.5424476728
C,2.8827278062,25.4938414384,-1.851183618
H,2.0575386651,24.5702994216,-0.075447072
H,-13.8936423299,20.3450818985,-0.4857905832
H,-13.9436907026,20.3971577353,1.3177382917
C,-15.8736847903,20.2078710865,0.3664365185
H,23.4473126915,6.8699147054,1.7381667841
H,22.421482959,7.7799249465,2.922142822
H,22.4987622197,8.3146665297,1.1948424742
H,2.9006432563,25.3214320661,-2.9598885622
H,3.945057976,25.4448684448,-1.492952521
C,2.3128628128,26.8580542549,-1.5602476878
H,-16.3395144872,19.7485910448,-0.5388637161
H,-16.3896913711,19.8008115891,1.2695117998
H,-16.0445079271,21.3108233419,0.3298489921
H,1.2624855164,26.9343017016,-1.9322663623
H,2.9224996682,27.6485033317,-2.0608050948
H,2.3097117445,27.058068154,-0.4613895942
C,3.3273919796,0.8520049595,-6.3374317411
C,4.2660423261,0.0686002512,-7.0275561219
C,3.1716229336,2.2013282849,-6.6873308192
C,5.032804479,0.6279225999,-8.0466123322
H,4.3943530585,-0.9903310162,-6.7565201242
C,3.944245137,2.7546735285,-7.7066490597
H,2.4301254196,2.8300128627,-6.1727750363
C,4.8756435867,1.9714878302,-8.3875609229
H,5.7657148752,0.0066349148,-8.5824208723
H,3.8144947504,3.8133973377,-7.9759524365
H,5.4832615591,2.4111797254,-9.191760818
C,-3.799635302,-1.9379552364,3.2613647434
C,-4.8406093339,-2.8762310615,3.3456472528
C,-3.5629878129,-1.0781355138,4.344017938
C,-5.6277492779,-2.949641445,4.492037039
H,-5.0334589627,-3.5517957315,2.4985367904
C,-4.3566175448,-1.1557875919,5.4869686628
H,-2.7433098926,-0.345449118,4.307749295
C,-5.3894491304,-2.0894931869,5.5641527862
H,-6.4413192491,-3.6878604635,4.5494778841
H,-4.163821494,-0.4778225164,6.3316838788
H,-6.0136665842,-2.1480325363,6.46757596

Cartesian Coordination of 3a·Cl⁻ (DFT)

-3713.8106073 hartree

Br,-3.8803419137,-0.0007895529,0.000055261
C,2.3791136272,-3.9037328229,-0.0000279267
C,1.2196495087,-4.6741310057,-0.0000811406
C,-0.0315639804,-1.2010079737,-0.0000214427
C,1.2176682974,4.674727183,-0.0001626517
C,0.6806813552,0.0001856532,-0.0000456689
C,-0.0320763659,1.201075948,-0.000058183
C,0.6484624245,-2.4823514625,-0.0000424311
C,0.1267540736,-3.775978081,-0.0000760385
C,2.3774579471,3.9048196707,-0.0001917935
C,-1.9400321823,-0.0003733937,0.0000150351
C,0.1251504835,3.7761137748,0.0000046679
C,0.6474047622,2.482707831,-0.0000645193
Cl,4.1165765801,0.0008727022,-0.0003538497
H,-0.9277922672,-4.0106387622,-0.0000876055
H,1.1764253206,-5.7549784126,-0.0000937064
H,3.4199020195,-4.193922527,-0.0000079708
H,2.704645693,1.8124929405,-0.0000077566
H,1.1739872824,5.7555590282,-0.0002226296
H,1.7649182265,0.0004149698,-0.0000655887
H,3.4181197568,4.1954491438,-0.0002644941
H,-0.9294943524,4.0103311584,0.0000884222
H,2.7054246371,-1.8112692184,-0.0001290069
N,2.0281109693,-2.5897077494,-0.0001044497
N,2.0270083359,2.5906471704,-0.0000461767
N,-1.3938253634,-1.199336954,0.0000055729
N,-1.3943348753,1.1988207419,-0.0000139283

Cartesian Coordination of 3b·Cl⁻ (DFT)

-1142.6763222 hartree

H,-1.7968048472,-1.6813232028,0.0004479557
H,-4.1708685802,-2.4170640976,0.0003018461
H,-5.7520594827,-0.1868786668,0.0001160852
H,4.0244175102,1.9326284419,0.000082267
H,4.1709468294,-2.4167931228,0.0001683515
H,-0.000018568,-0.7313916228,0.0002117647
H,5.7519907471,-0.1865022294,-0.0000257048
H,1.7968340781,-1.6812209828,0.0004791447
H,-4.0246281428,1.9323673865,0.0000916839
N,-1.2041265848,2.4228672042,-0.0000695812
N,1.2038900284,2.4229422723,-0.0000948627
C,-4.6706899016,-0.2213088269,0.000151229
C,-3.8910113911,-1.3734345629,0.0002404585
C,-1.2022675902,1.0648570275,0.0000815255
C,3.8910202069,-1.3731821152,0.0001381647
C,-0.0000530328,0.3526467956,0.0001102501
C,1.202118236,1.0649307527,0.0000495786
C,-2.4822729124,0.3707877386,0.0001502889
C,4.6706233834,-0.2210042631,0.0000475894
C,-0.000135584,3.0005195657,-0.0002656304
C,2.4821668958,0.3709440729,0.0001035329
H,-0.0001699487,4.0905982179,-0.0000522756
C,-3.7802992551,0.8800309208,0.0001455343
N,-2.5791995845,-1.0092684623,0.0003212956
N,2.5791848129,-1.009105504,0.0003113046
C,3.7801597935,0.8802754242,0.0001141055
Cl,0.0001318845,-3.1152461614,0.0000000982

Cartesian Coordination of 3c·Cl⁻ (DFT)

-1373.7535848 hartree

H,0.4897396242,-4.0258967332,0.0000515659
H,-1.6286535948,-5.7502699299,0.0002052245
H,-3.8585596795,-4.1685169189,0.0003046656
H,-3.1231039303,1.795056086,-0.0001106714
H,-1.6286287646,5.7502811373,-0.0000169811
H,-2.1785487378,0.0000067164,-0.0000151662
H,-3.8585416917,4.1685376764,0.0000955895
H,0.4897570712,4.0258987945,-0.0001844968
H,-3.123112259,-1.7950385268,0.0000324874
N,-2.4505978928,-2.5773782105,0.0000836205
N,-2.4505866393,2.5773928466,-0.0000743753
N,0.9750459294,-1.1987195252,-0.0001143883
N,0.9750511924,1.1987192994,-0.0001716184
C,-2.8149065027,-3.8888666994,0.0002285599
C,-1.6630936906,-4.6689766911,0.0001675455
C,-0.3785048464,-1.1991166398,-0.0000614312
C,-1.6630735303,4.6689880341,-0.0000318597
C,-1.0948485558,0.0000044146,-0.0000631815
C,-0.3784995721,1.1991222403,-0.0001161911
C,-1.0705013935,-2.4805235624,0.0000352514
C,-0.5618914823,-3.7789025229,0.000088224
C,-2.8148897123,3.8888829869,0.0000331146
C,1.5759115618,-0.0000014383,-0.0001921429
C,-0.5618750907,3.7789090739,-0.0001230325
C,-1.0704905382,2.4805322615,-0.0000881754
Cl,-4.5534632495,0.000008425,0.0005008997
C,3.0722962263,-0.0000047286,-0.0001571181
C,3.7886742055,1.208086423,-0.0001681952
C,3.7886688886,-1.2080990298,-0.0001107805
C,5.1845748623,1.2074732307,-0.000136947
H,3.231383256,2.1379008274,-0.0002038448
C,5.1845695531,-1.207491975,-0.0000796993
H,3.2313738516,-2.1379109879,-0.0001017891
C,5.890448249,-0.0000109263,-0.0000924932
H,5.722592238,2.1522492383,-0.0001478183
H,5.7225827678,-2.1522703523,-0.0000454289
H,6.9776248767,-0.0000133144,-0.0000679222

Cartesian Coordination of 4a·Cl⁻ (DFT)

-4175.9655777 hartree

C,-0.00009611,3.5727415746,-0.0066791266
N,-1.1971114479,3.024283878,-0.0060035513
C,-1.1998720065,1.6617372383,-0.0043059823
C,-0.0000226486,0.9449193358,-0.0034329248
C,1.199786688,1.6618043115,-0.0043141687
N,1.196949902,3.0243507656,-0.0060117154
H,0.0000076668,-0.1396274167,-0.0021190801
C,-2.4935840981,1.0069157725,-0.0035465597
C,-3.7654609278,1.5802817839,-0.0043214077
N,-2.6548419683,-0.3648388842,-0.0018455201
C,-4.6996846621,0.5299545085,-0.0031128953
H,-3.9573963493,2.6430165664,-0.0056410565
C,-3.9905694413,-0.6805696595,-0.0015517955
H,-1.8855377029,-1.045466544,-0.0009351938
H,-5.7755852428,0.6318820193,-0.0033153553
C,2.4935353601,1.0070550857,-0.0035631591
C,3.7653800156,1.5804925361,-0.0043463272
N,2.6548702955,-0.3646905698,-0.0018603375

C,4.6996626988,0.5302176857,-0.0031485762
H,3.9572558118,2.6432380843,-0.0056679113
C,3.9906155332,-0.6803463488,-0.0015758955
H,1.8856041252,-1.0453613618,-0.0009422002
H,5.7755575546,0.632205657,-0.0033621046
Br,-0.0001503096,5.5093605043,-0.0092316883
C,-4.4962344568,-2.0562365865,0.0001320786
C,-3.6344775485,-3.1721130336,0.0016405404
C,-5.8870342948,-2.2936860446,0.0002892299
C,-4.1525986969,-4.468073565,0.0032303368
H,-2.5547183304,-3.0447811883,0.0016121304
C,-6.3969925484,-3.5900416456,0.001873954
H,-6.5754488238,-1.4545000928,-0.0008478489
C,-5.5323495815,-4.6901839696,0.0033620249
H,-3.4627728591,-5.3076033854,0.0043774397
H,-7.4736926199,-3.741488741,0.0019512059
H,-5.9287254049,-5.7020520344,0.0046058207
C,4.4963582743,-2.0559847335,0.0001077887
C,3.634664574,-3.171910018,0.0016247568
C,5.8871715441,-2.2933554182,0.0002560019
C,4.1528591381,-4.467841188,0.0032138619
H,2.55489816,-3.0446393703,0.001603957
C,6.3972032379,-3.5896821325,0.0018398677
H,6.5755385411,-1.4541304757,-0.0008875634
C,5.5326226079,-4.6898734183,0.0033363438
H,3.4630808563,-5.3074100728,0.0043677783
H,7.473911889,-3.7410682502,0.0019100225
H,5.9290557984,-5.7017190102,0.0045796057
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Cartesian Coordination of 4b·Cl⁻ (DFT)

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Cartesian Coordination of 4c·Cl⁻ (DFT)

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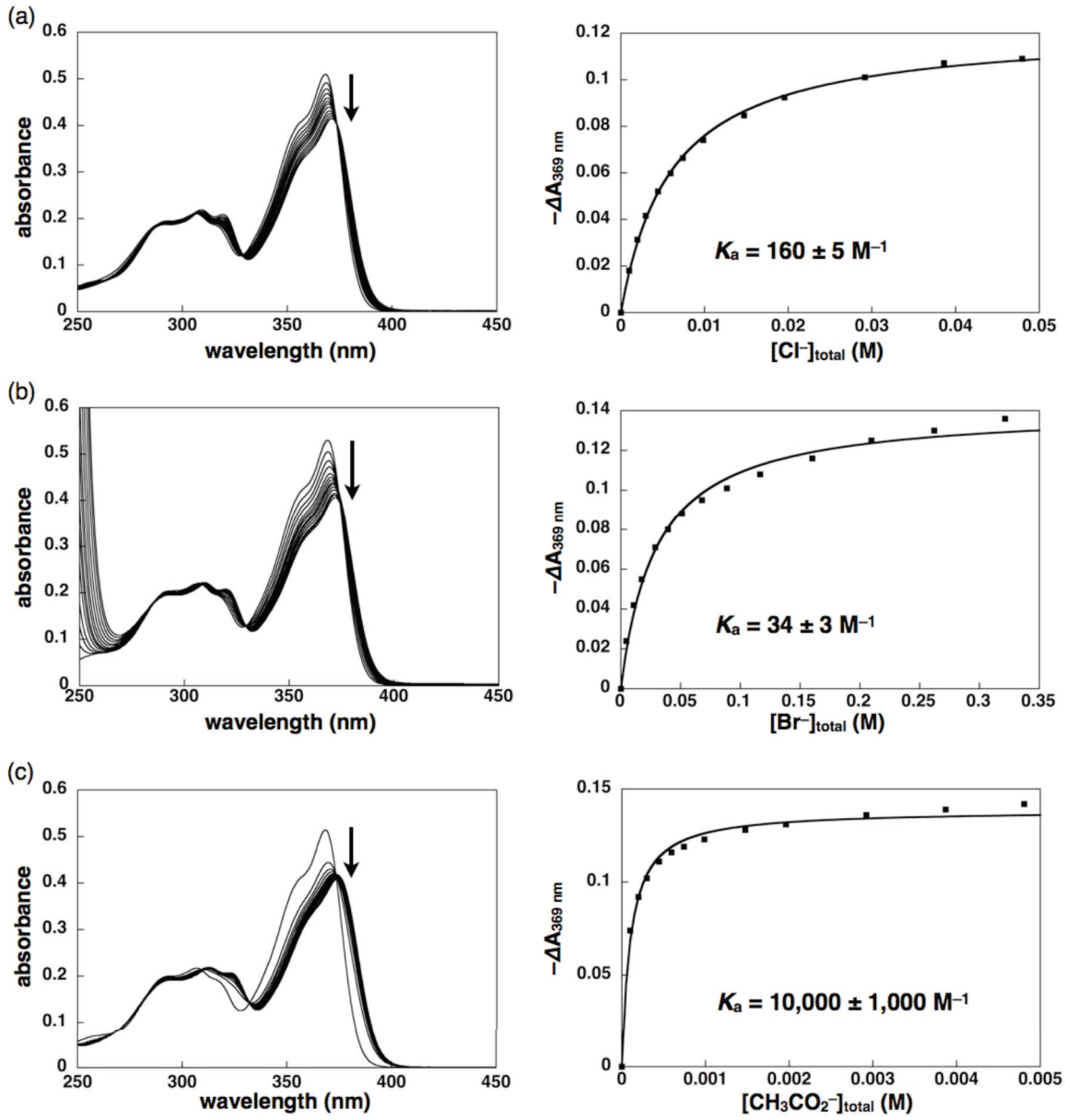
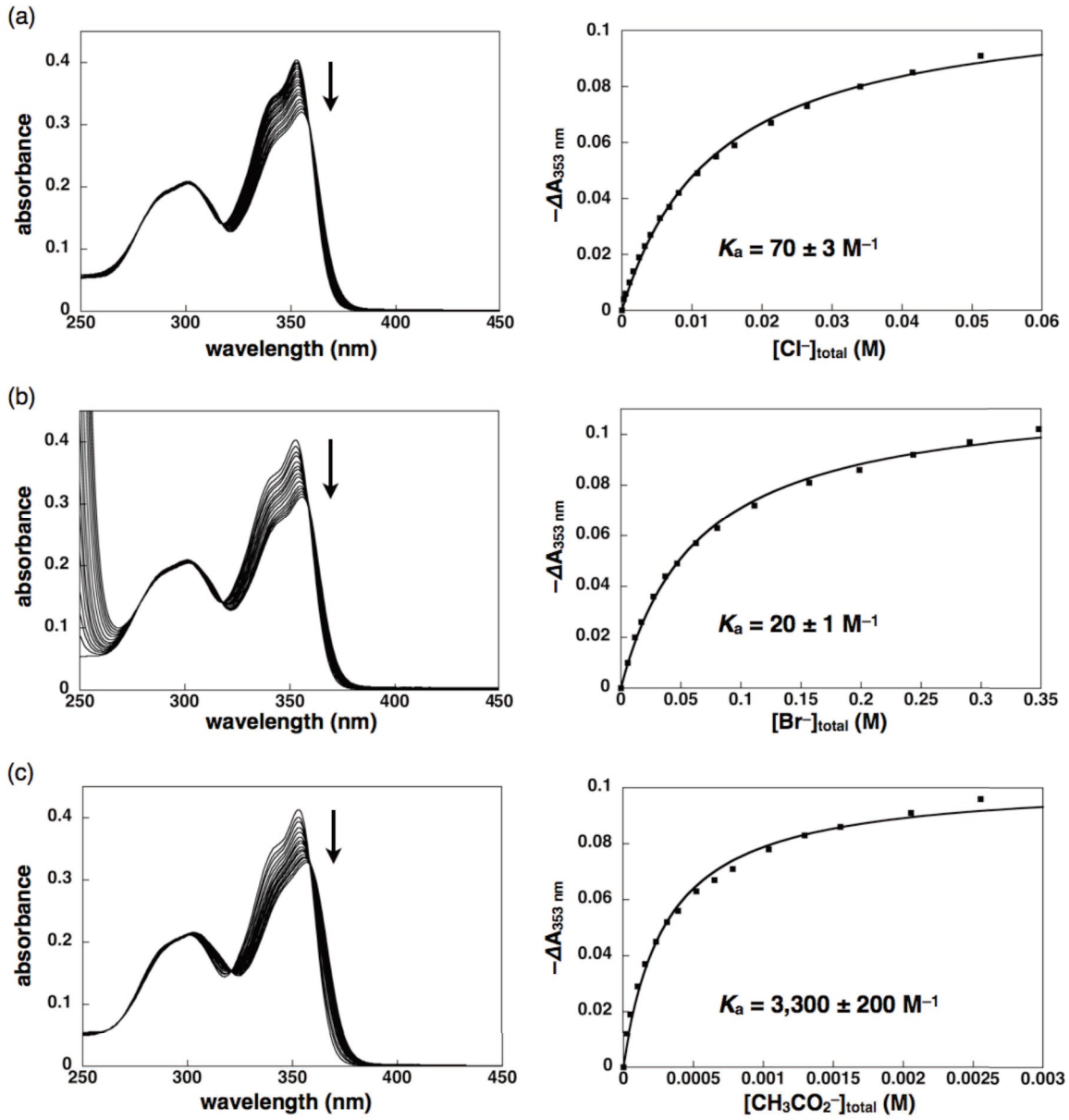
[S8 (complete ref. 11)] *Gaussian 09*, (Revision D.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

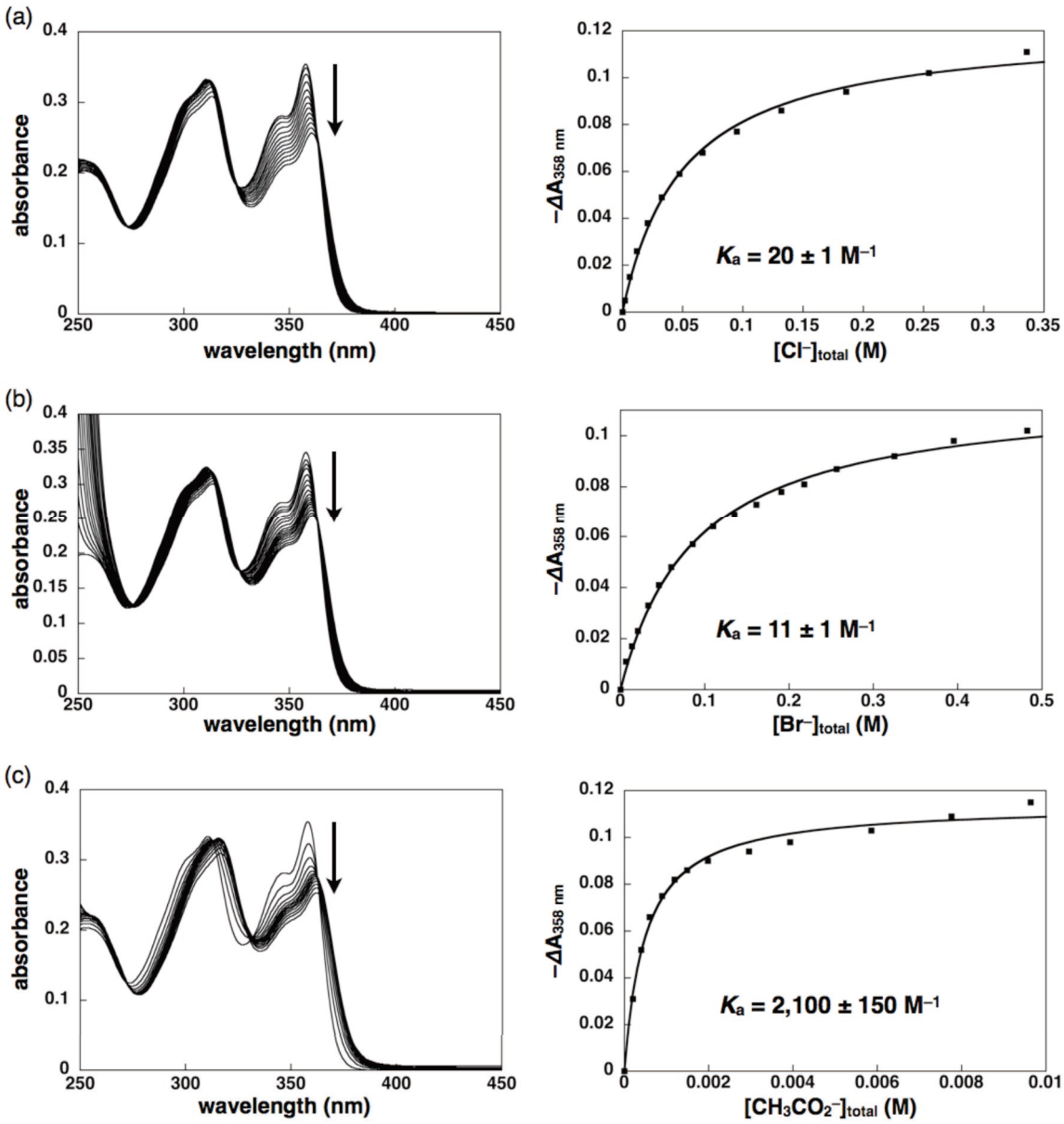
4. Anion-binding behaviors



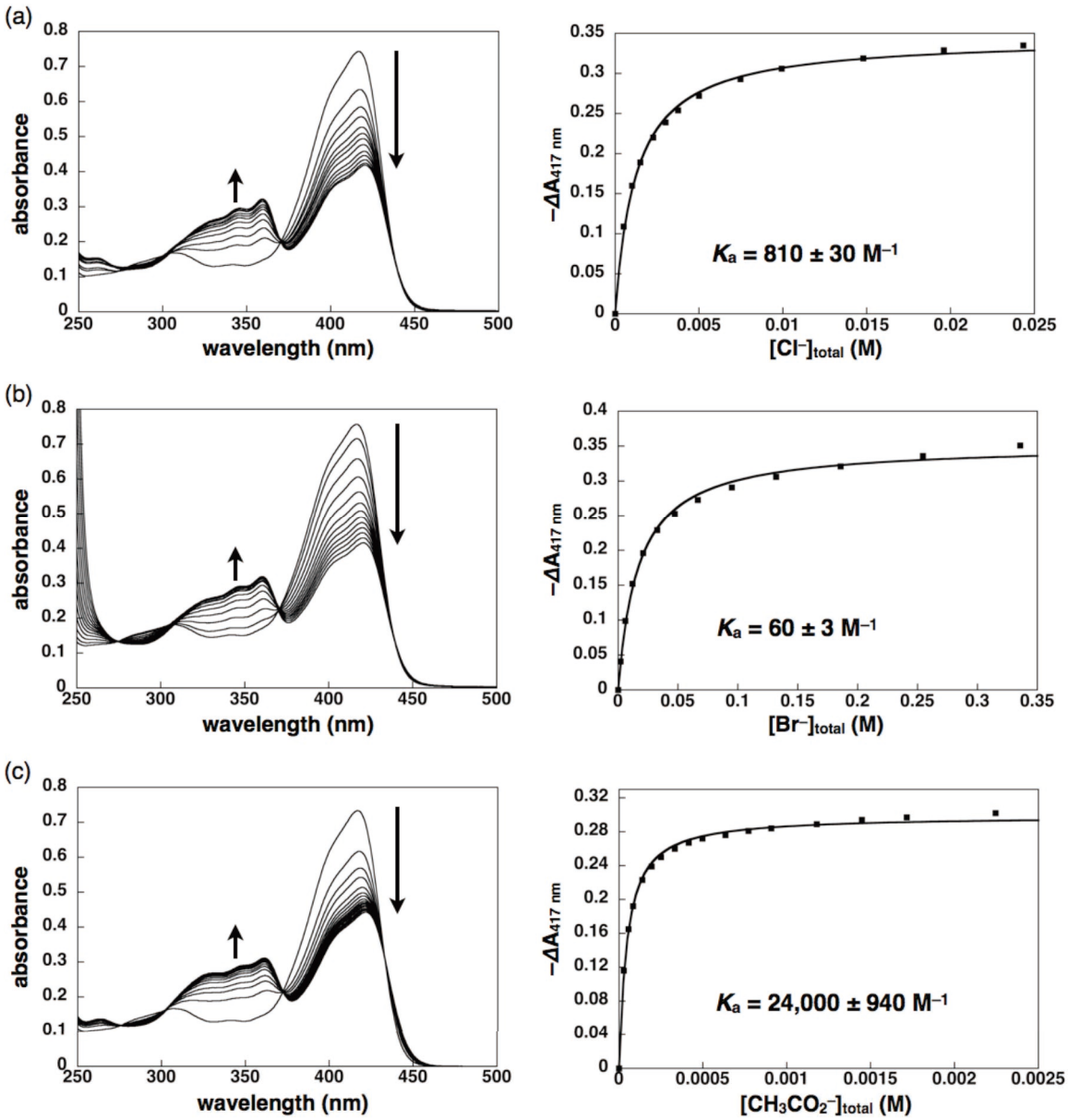
Supporting Figure 26 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **3a** (1.0×10^{-5} M) upon the addition of (a) Cl^- (a) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



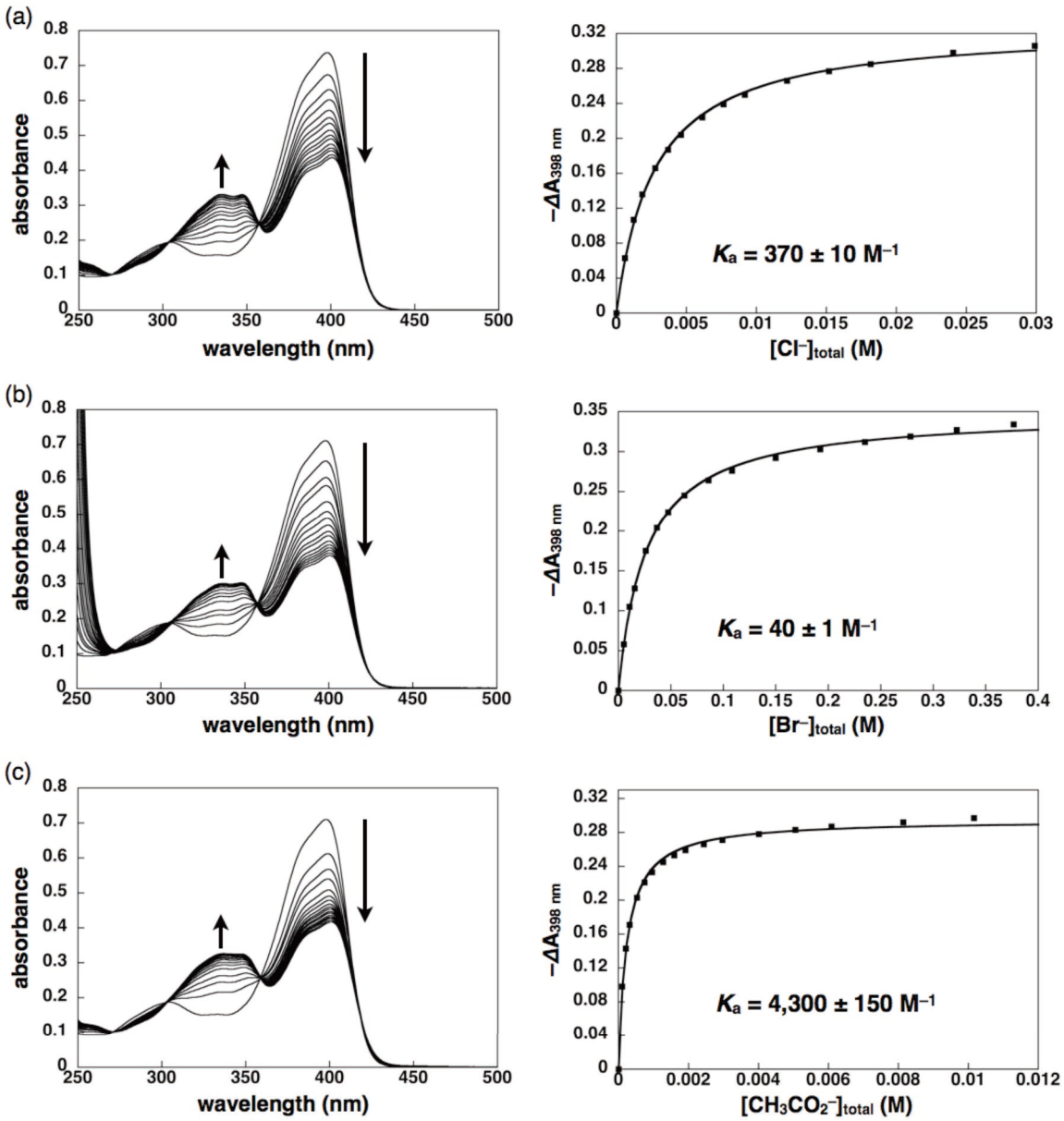
Supporting Figure 27 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **3b** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



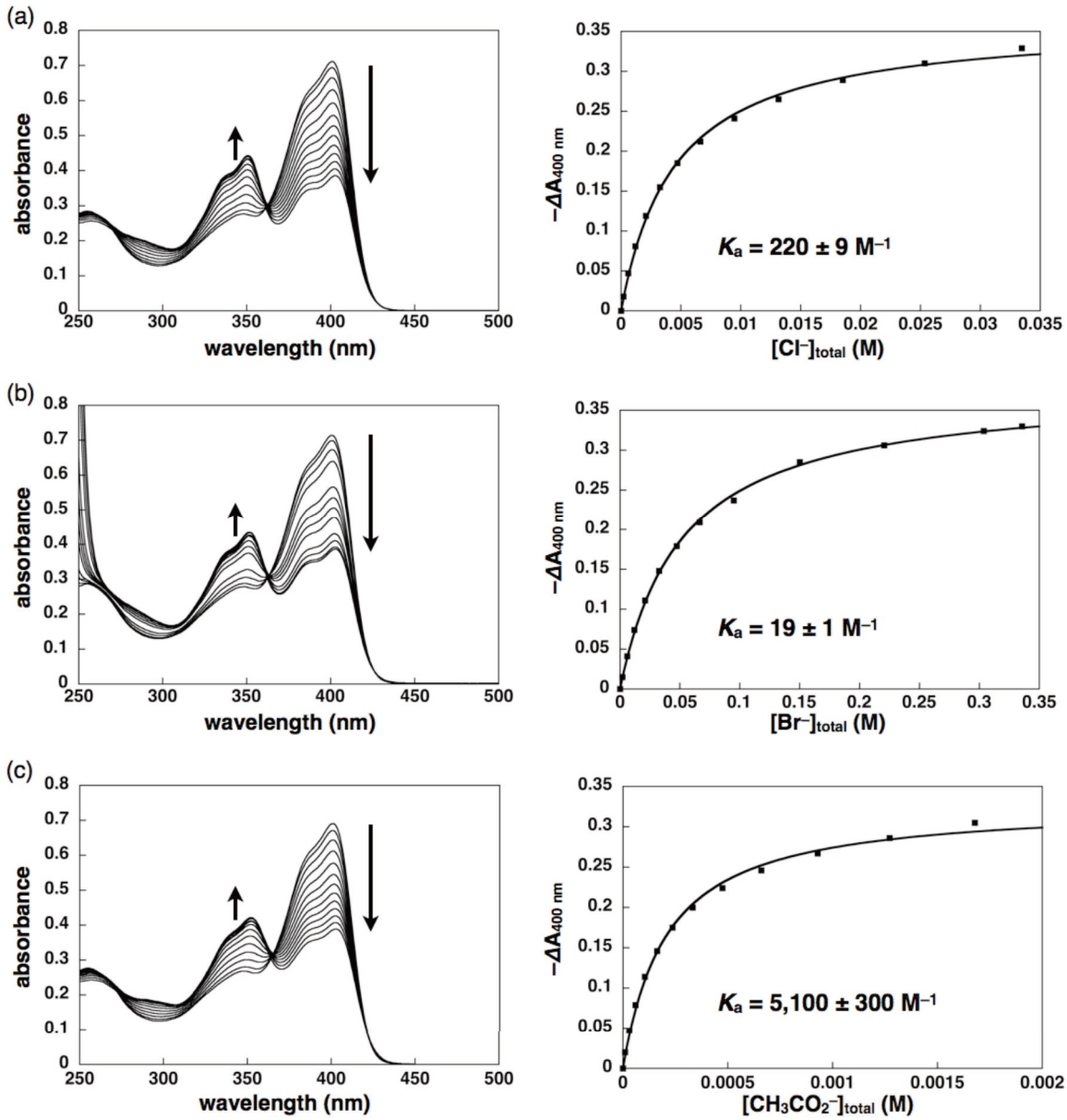
Supporting Figure 28 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **3c** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



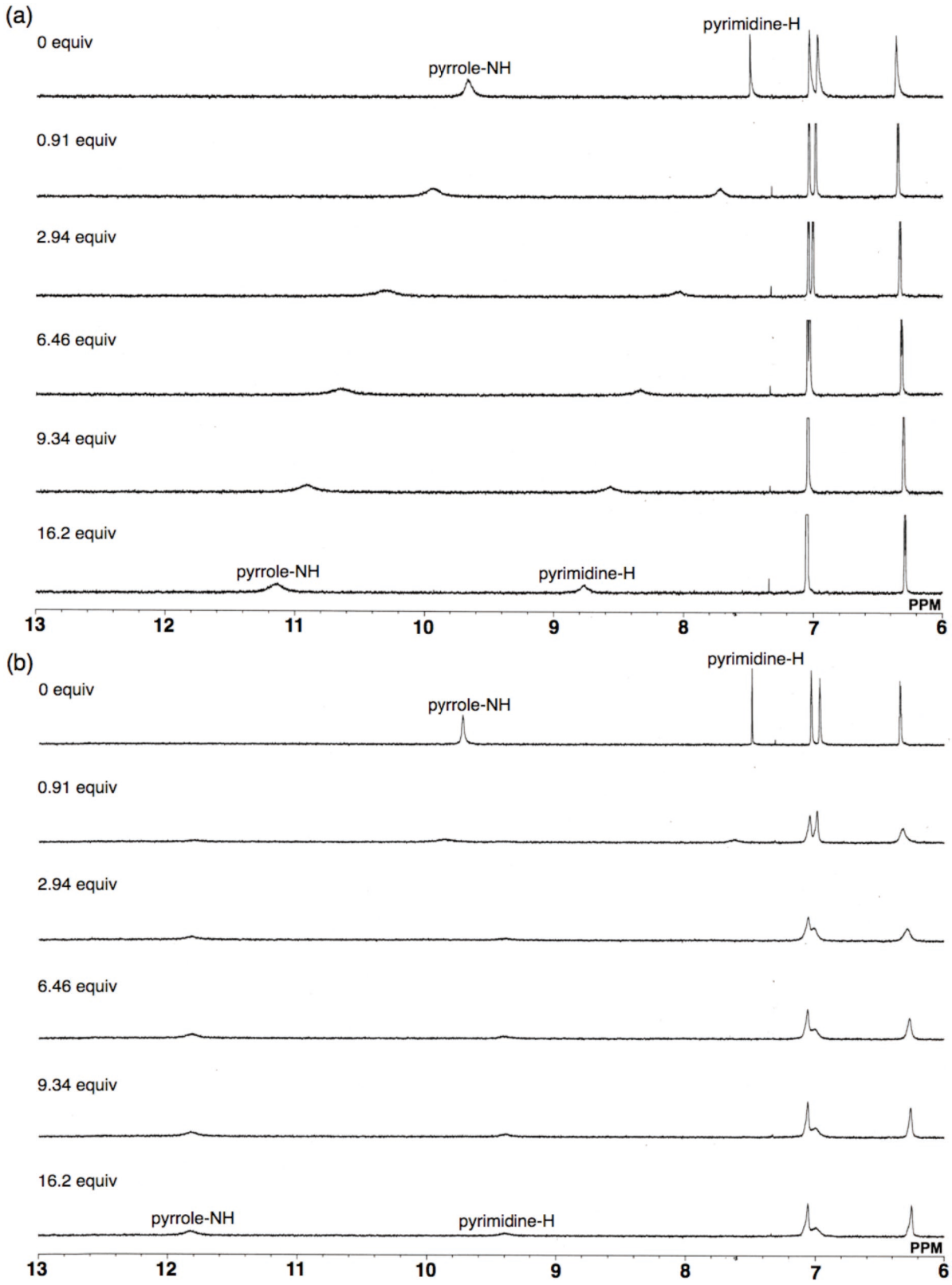
Supporting Figure 29 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **4a** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



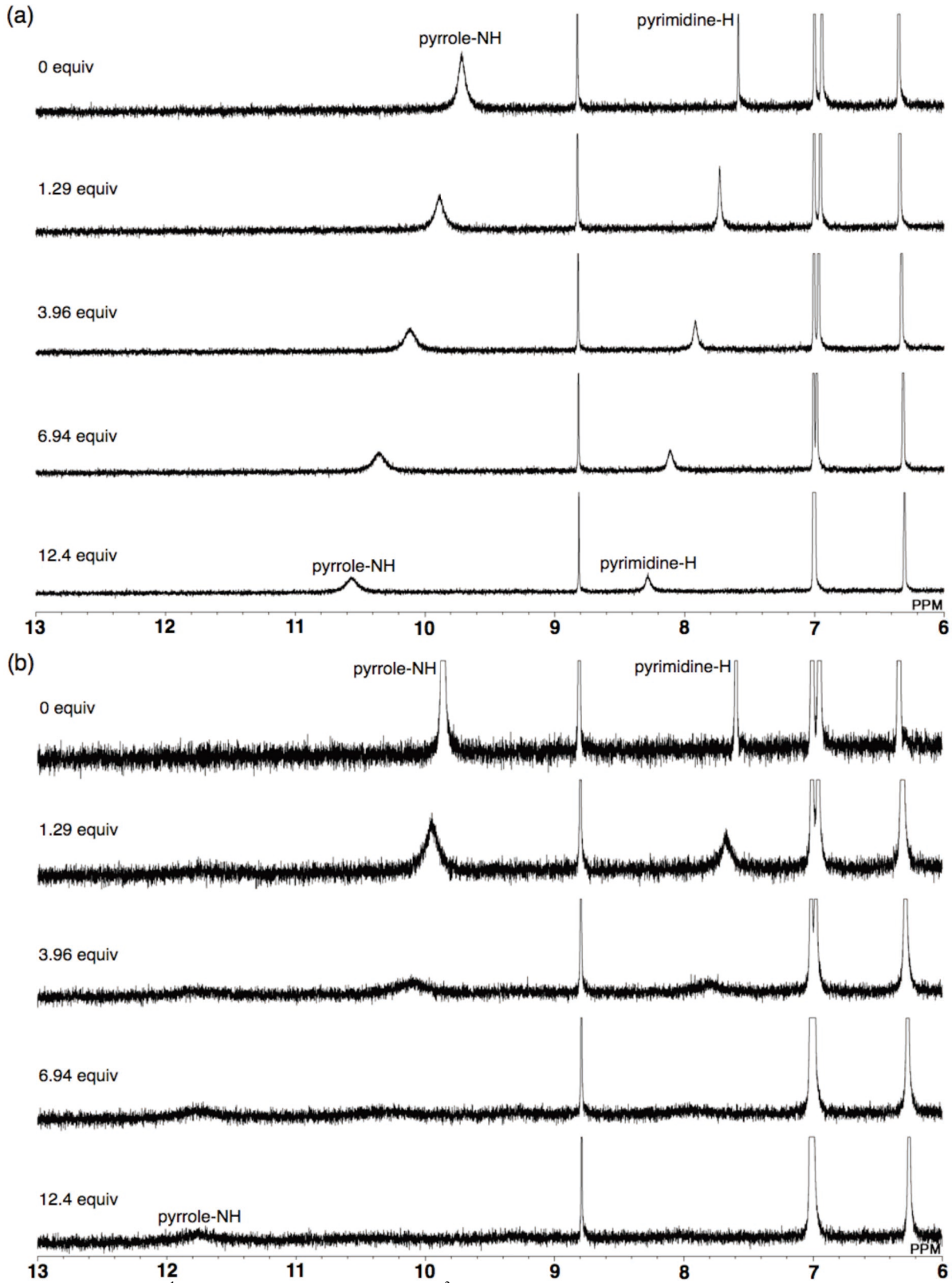
Supporting Figure 30 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **4b** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



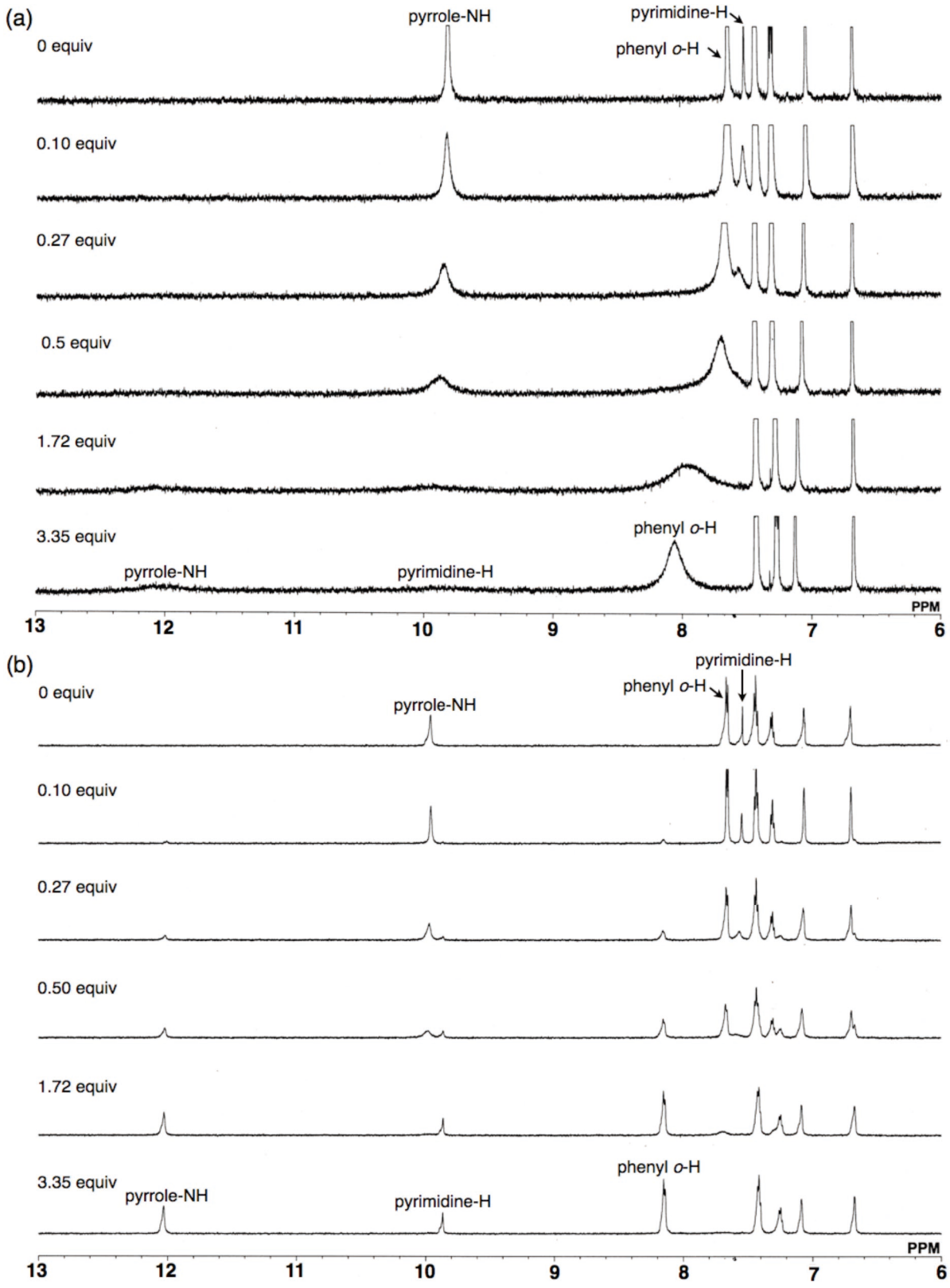
Supporting Figure 31 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 binding fitting curves (right) of **4c** (1.0×10^{-5} M) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.



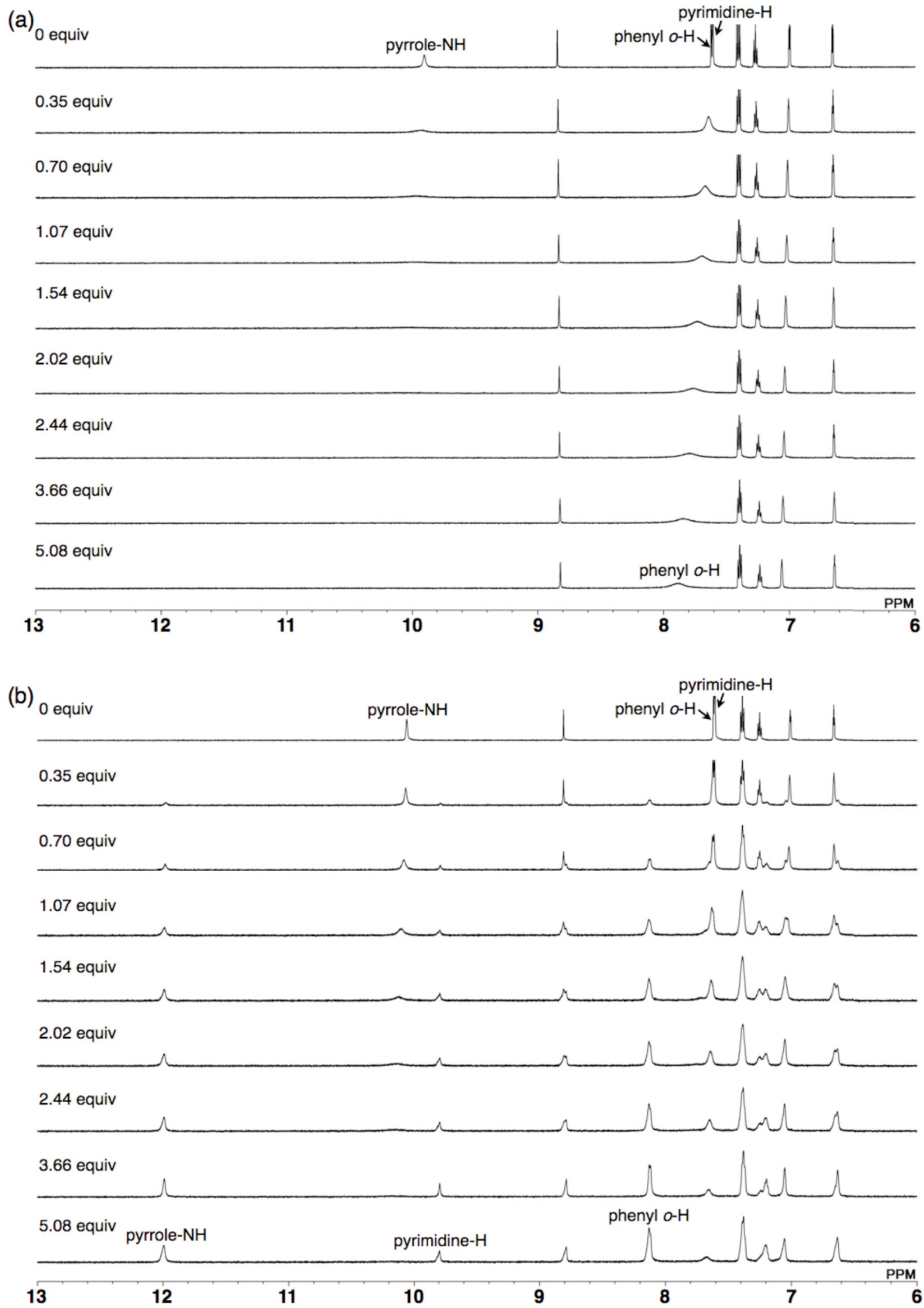
Supporting Figure 32 ^{1}H NMR titration of **3a** (1×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- as a TBA salt. Gradual downfield shift of pyrrole-NH and pyrimidine-H signals was observed at 20 °C, whereas disappearance and concurrent appearance of those peaks were observed at –50 °C due to the slow equilibrium at low temperature. The signal shift upon the addition of Cl^- suggests the formation of a [1+1]-type receptor–anion complex.



Supporting Figure 33 ^{1}H NMR titration of **3b** (1×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- as a TBA salt. The signal shift at 20 °C upon the addition of Cl^- suggests the formation of a [1+1]-type receptor–anion complex, whereas disappearance and concurrent appearance of pyrrole-NH and pyrimidine-H signals were observed at –50 °C upon the addition of Cl^-, also suggesting the formation of a [1+1]-type receptor–anion complex.



Supporting Figure 34 ^{1}H NMR titration of **4a** (1×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- as a TBA salt. Disappearance and concurrent appearance of pyrrole-NH and pyrimidine-H signals were observed upon the addition of Cl^-, suggesting the formation of a [1+1]-type receptor–anion complex.



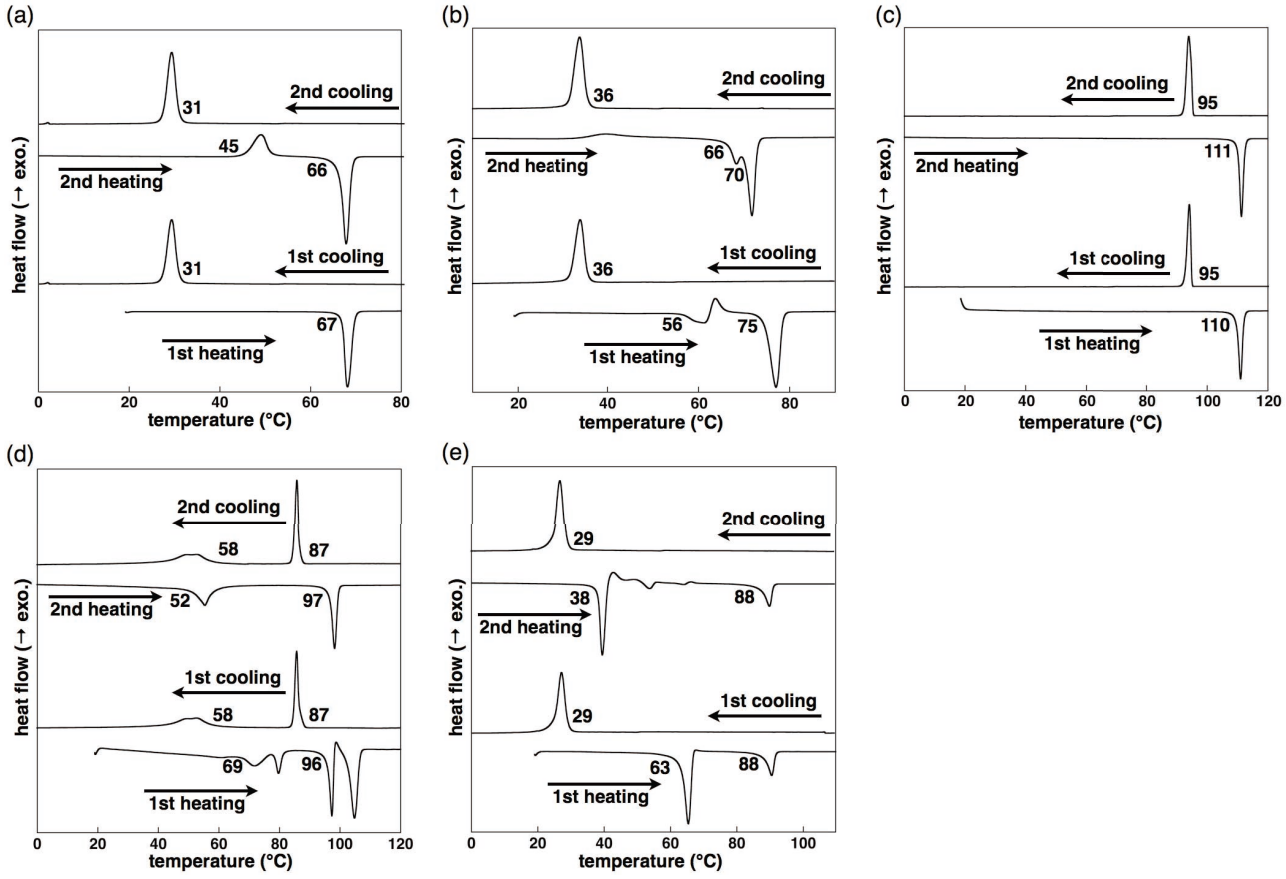
Supporting Figure 35 ^{1}H NMR titration of **4b** (1×10^{-3} M) in CD_2Cl_2 at (a) 20 °C and (b) –50 °C upon the addition of Cl^- as a TBA salt. Broad or disappeared signals were observed upon the addition of Cl^- at 20 °C due to the fast equilibrium process. At – 50 °C, disappearance and concurrent appearance of pyrrole-NH and pyrimidine-H signals were observed upon the addition of Cl^-, suggesting the formation of a [1+1]-type receptor–anion complex.

5. Assembled behaviors

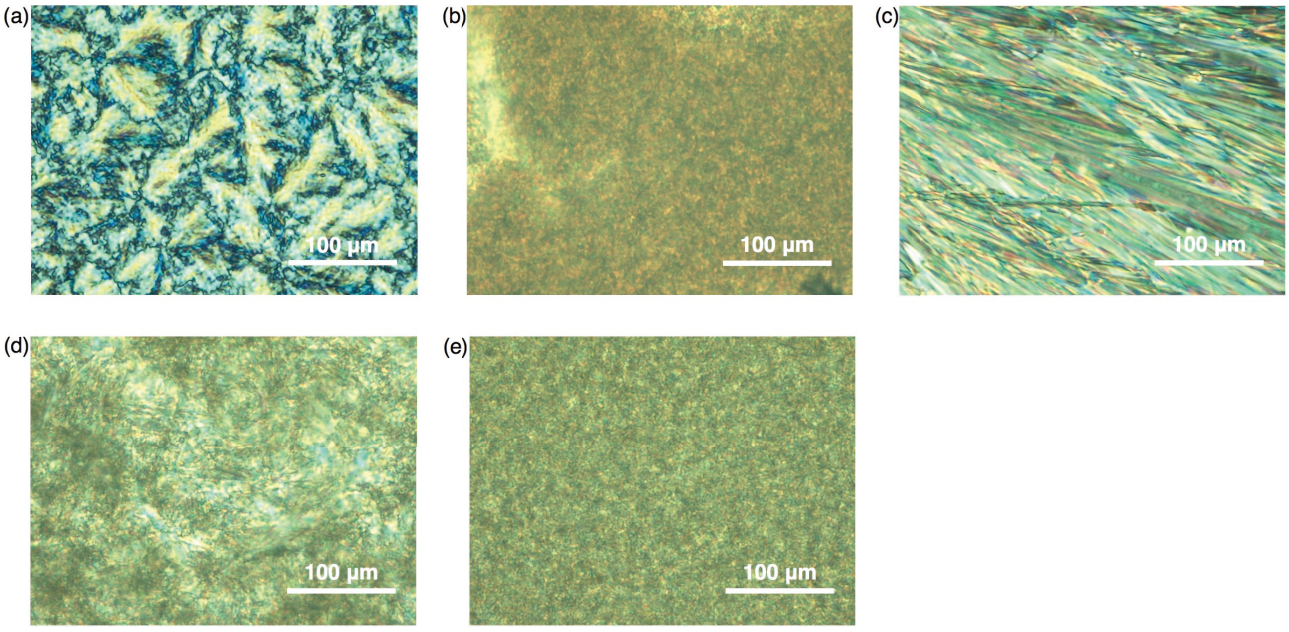
Differential scanning calorimetry (DSC). The phase transitions were measured on a differential scanning calorimetry (Shimadzu DSC-60).

Polarizing optical microscopy (POM). POM measurements were carried out with a Nikon OPTIPHOT-POL polarizing optical microscope equipped with a Mettler FP82 HT hot stage.

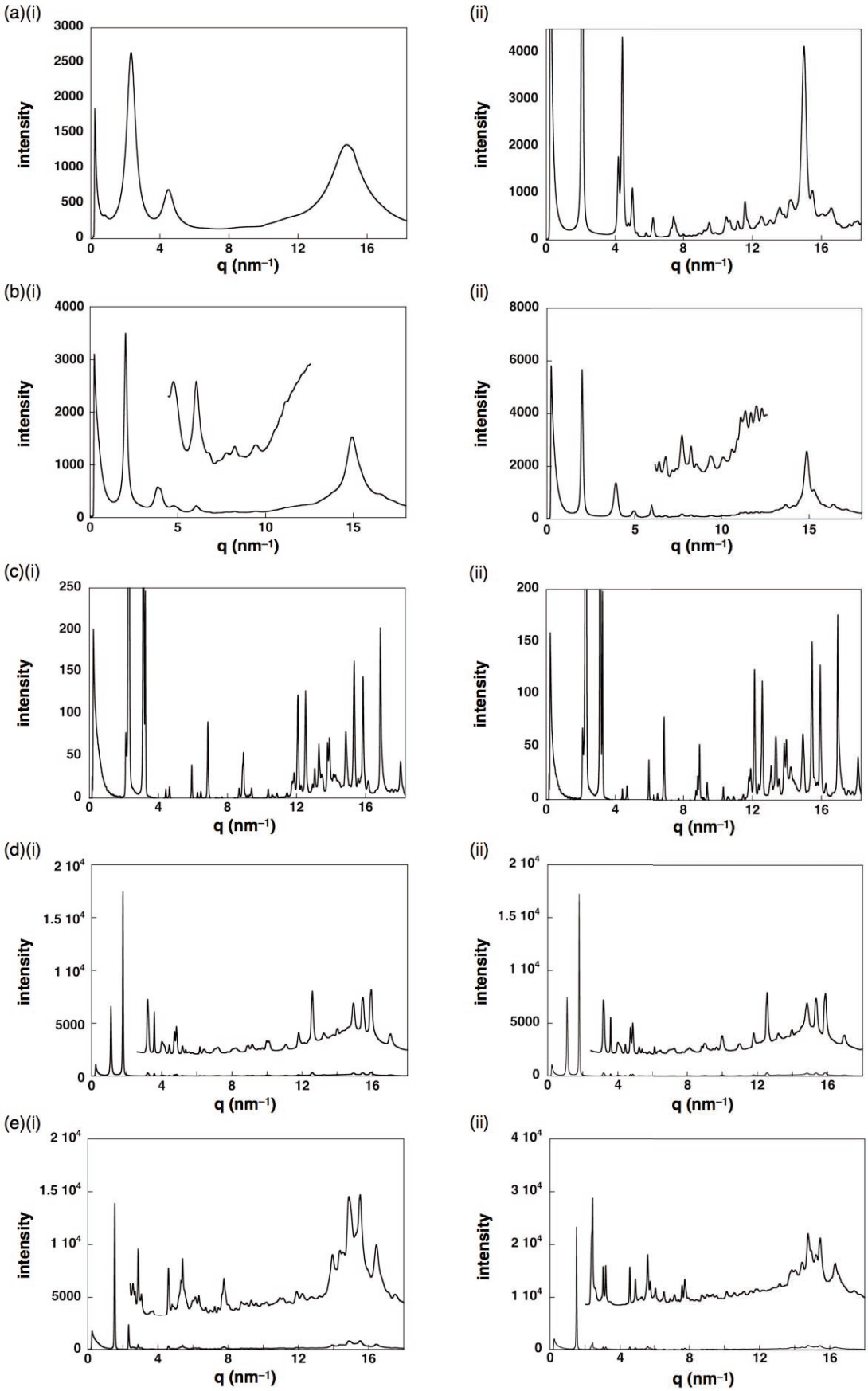
Synchrotron X-ray diffraction analysis (XRD). High-resolution XRD analyses were carried out using a synchrotron radiation X-ray beam with a wavelength of 1.00 Å on BL40B2 at SPring-8 (Hyogo, Japan). A large Debye-Scherrer camera with a camera length of 531.527 nm for **3d**,**e**, **4d**,**e**, and **4e**·Cl^--TBA^+ 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 30 sec for the solid state of **3d**,**e**, **4d**,**e** prepared from CH_2Cl_2/MeOH and of **4e**·Cl^--TBA^+ prepared from *n*-octane.



Supporting Figure 36 DSC thermograms (5 °C/min) of (a) **3d**, (b) **3e**, (c) **4d**, (d) **4e**, and (e) **4e**·Cl^--TBA^+. Onset temperatures (°C) of phase transitions are labeled. Alkoxy-substituted DPPs showed crystal–crystal transitions rather than liquid crystalline mesophase transitions as supported by the complicated XRD diffraction patterns (Supporting Figure 38).



Supporting Figure 37 POM images of (a) **3d** at 20 °C, (b) **3e** at 25 °C, (c) **4d** at 70 °C, (d) **4e** at 75 °C, and (e) **4e**·Cl^{-}-TBA^{+} at 35 °C upon 1st cooling from isotropic state. All samples showed highly crystalline POM textures, which were also supported by the observations of complicated XRD diffraction patterns (Supporting Figure 38).



Supporting Figure 38 XRD patterns of (a) **3d** at (i) 20 °C (first cooling) and (ii) 55 °C (second heating), (b) **3e** at (i) 25 °C (first cooling) and (ii) 50 °C (second heating), (c) **4d** at (i) 70 °C (first cooling) and (ii) 60 °C (second heating), (d) **4e** at (i) 75 °C (first cooling) and (ii) 85 °C (second heating), and (e) **4e**·Cl^--TBA^+ at (i) 35 °C (first cooling) and (ii) 70 °C (second heating). All XRD data showed many unidentified peaks with highly ordered structures derived from crystalline states.