**Supporting information**

# *Sizeable red-shift of absorption and fluorescence of subporphyrazine induced by peripheral push and pull substitution*

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**Contents:**



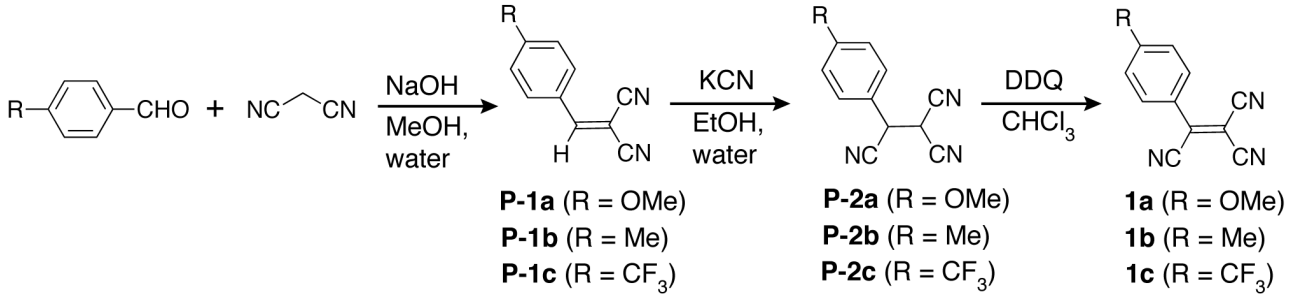
## i. Experimental

**General Procedure:** Electronic absorption spectra were recorded on a JASCO V-570 spectrophotometer. Circular dichroism (CD) and magnetic circular dichroism (MCD) spectra were recorded on a JASCO J-725 spectrodichrometer equipped with a JASCO electromagnet, which produces magnetic fields of up to 1.03 T (1 T = 1 tesla) with both parallel and antiparallel fields. The magnitudes were expressed in terms of molar ellipticity ($[\theta]$/deg dm$^3$ mol$^{-1}$cm$^{-1}$) and molar ellipticity per tesla ($[\theta]_M$/deg dm$^3$ mol$^{-1}$cm$^{-1}$T$^{-1}$), respectively. Fluorescence spectra were measured on a Hitachi F-4500 spectrofluorimeter. Absolute fluorescence quantum yields were measured on a Hamamatsu Photonics C9920-03G calibrated integrating sphere system. $^1$H NMR spectra were recorded on a Bruker AVANCE 500 spectrometer (operating at 500.13 MHz) using the residual solvent as an internal reference for $^1$H ($\delta$ = 7.26 ppm for $CDCl_3$, $\delta$ = 5.32 ppm for $CD_2Cl_2$ and $\delta$ = 2.09 ppm for toluene-$d_8$). High resolution mass spectra were recorded on a Bruker Daltonics solariX 9.4T spectrometer. Preparative separations were performed by silica gel column chromatography (Merck Kieselegel 60H) and recycling preparative GPC-HPLC (JAI LC-9201 with preparative JAIGEL-2H, 2.5H, and 3.0H columns). Separation of all the enantiomers was carried out by high-performance liquid chromatography (HPLC) with a preparative CHIRALPAK IA column by monitoring the absorbance at 580 nm. All reagents and solvents were of commercial reagent grade and were used without further purification except where noted.

**Crystallographic Data Collection and Structure Refinement.** Data collection was carried out at –173(2) ºC on a Bruker APEXII CCD diffractometer with Mo Kα radiation ($\lambda$ = 0.71073 Å) for **2c**. The structure was

solved by a direct method (SHELXS-97)[1] and refined using a full-matrix least squares technique (SHELXL-97). CCDC-1015544 contain the supplementary crystallographic data for **2c** and the data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

**Computational methods**: The Gaussian 09 software package[2] was used to carry out DFT and TDDFT calculations using the B3LYP functional and 6-31G(d) basis sets. Structural optimization was performed on model compounds of **2a**, **2b**, **2c**, **3c**, and unsubstituted subporphyrazine **4** as a reference compound.




***Scheme S1.*** Syntheses of 2-aryl-substituted 1,1,2-tricyanoethylene **1a–c**.

**Synthesis of P-1a:** A 5 mL water solution of NaOH (16 mg, 0.4 mmol) was added to a 30 mL methanol solution of *p*-anisaldehyde (13.6 g, 0.1 mol) and malononitrile (7.92 g, 0.12 mol, 1.2 equiv.). The resultant mixture was stirred at r.t. for 0.5 h. The solid was collected by filtration and further purified by silica gel column chromatography using $CHCl_3$ as an eluent to afford 1,1-dicyano-2-methoxylpnehylethylene **P-1a** in yield 88% (16.2 g). $^1$H NMR (500 MHz, $CDCl_3$, 298K): δ [ppm] = 7.91 (d, 2H, phenyl; *J* = 8.8 Hz), 7.65 (s, 1H, ethylene), 7.01 (d, 2H, phenyl; *J* = 9.0 Hz), 3.92 (s, 3H, -OMe).

**Synthesis of P-1b:** A 5 mL water solution of NaOH (16 mg, 0.4 mmol) was added to a 30 mL methanol mixture of *p*-tolualdehyde (12.0 g, 10 mmol) and malononitrile (7.92g, 12 mmol, 1.2 equiv.). The resultant mixture was stirred at r.t. for 0.5 h. The solid was collected by filtration and further purified by silica gel column chromatography using $CHCl_3$ as an eluent to afford 1,1-dicyano-2-*p*-tolylethylene **P-1b** in 86% yield (14.4 g). $^1$H NMR (500 MHz, $CDCl_3$, 298K): δ [ppm] = 7.81 (d, 2H, phenyl; *J* = 8.3 Hz), 7.72 (s, H, ethylene), 7.34 (d, 2H, phenyl; *J* = 8.2 Hz), 2.45 (s, 1H, -$CH_3$).

**Synthesis of P-1c**: A 5 mL water solution of NaOH (16 mg, 0.4 mmol) was added to a 30 mL methanol mixture of *p*-trifluoromethylbenzaldehyde (17.4 g, 10 mmol) and malononitrile (7.92g, 12 mmol, 1.2 equiv.). The resultant mixture was stirred at r.t. for 0.5 h. The solid was collected by filtration and further purified by silica gel column chromatography using $CHCl_3$ as an eluent to afford 1,1-dicyano-2-*p*-trifluoromethylphenylethylene **P-1c** in 80% yield (17.7 g). $^1$H NMR (500 MHz, $CDCl_3$, 298K): δ [ppm] = 8.01 (d, 2H, phenyl; *J* = 8.8 Hz), 7.84 (s, 1H, ethylene), 7.81 (d, 2H, phenyl; *J* = 8.4 Hz).

**Synthesis of P-2a:** KCN (1.02 g, 15.5 mmol, 1.03 equiv.) was stirred in 20 mL of water and heated at 60 ºC. After KCN was completely dissolved in the water, a 20 mL of EtOH solution of 1,1-dicyano-2-

methoxylpnehylethylene **P-1a** (2.76 g, 15.0 mmol) was slowly added, and the resultant mixture was then continuously stirred at 60 ºC for 15 min. After cooled to room temperature, a solution of acetic acid (2mL) and water (10 mL) was added, and the solvent was removed under vacuum. Further purification was carried out by silica gel column chromatography (eluent: $CHCl_3$:MeOH = 10:1) to afford 1,1,2-tricyano-2-methoxylphenylethane **P-2a** in 65% yield (2.06 g). $^1$H NMR (500 MHz, $CDCl_3$, 298K): δ [ppm] = 7.42 (d, 2H, phenyl; *J* = 8.8 Hz), 7.01 (d, 2H, phenyl; *J* = 8.8 Hz), 4.40 (d, 1H, ethylene; *J* = 6.0 Hz), 4.18 (d, 1H, ethylene; *J* = 6.0 Hz), 3.85 (s, 3H, -OMe).

**Synthesis of P-2b:** KCN (1.02 g, 15.5 mmol, 1.03 equiv.) was stirred in 20 mL of water and heated at 60 ºC. After KCN was completely dissolved in the water, a 20 mL of EtOH solution of 1,1-dicyano-2-*p*-tolylethylene **P-1b** (2.52 g, 15 mmol) was slowly added, and the resultant mixture was then continuously stirred at 60 ºC for 15 min. After cooled to room temperature, a solution of acetic acid (2mL) and water (10 mL) was added, and the solvent was removed under vacuum. Further purification was carried out by silica gel column chromatography (eluent: $CHCl_3$:MeOH = 10:1) to afford 1,1,2-tricyano-2-*p*-tolylethane **P-2b** in 62% yield (1.81 g). $^1$H NMR ($CDCl_3$, 298K): δ [ppm] = 7.38 (d, 2H, phenyl; *J* = 8.2 Hz), 7.32 (d, 2H, phenyl; *J* = 8.2 Hz), 4.41 (d, 1H, ethylene; *J* = 6.0 Hz), 4.20 (d, 1H, ethylene; *J* = 6.0 Hz), 2.41 (s, 3H, -$CH_3$).

**Synthesis of P-2c:** KCN (1.02 g, 15.5 mmol, 1.03 equiv.) was stirred in 20 mL of water and heated at 60 ºC. After KCN was completely dissolved in the water, a 20 mL of EtOH solution of 1,1-dicyano-2-*p*-trifluoromethylphenylethylene **P-1c** (3.4 g, 15 mmol) was slowly added, and the resultant mixture was then continuously stirred at 60 ºC for 15 min. After cooled to room temperature, a solution of acetic acid (2mL) and water (10 mL) was added, and the solvent was removed under vacuum. Further purification was carried out by silica gel column chromatography (eluent: $CHCl_3$:MeOH = 10:1) to afford 1,1,2-tricyano-2-*p*-trifluoromethylphenylethane **P-2c** in yield 42% (1.57 g). $^1$H NMR ($CDCl_3$, 298K): δ [ppm] = 7.82 (d, 2H, phenyl; *J* = 8.2 Hz), 7.68 (d, 2H, phenyl; *J* = 8.2 Hz), 4.53 (d, 1H, ethylene; *J* = 5.7 Hz), 4.31 (d, 1H, ethylene; *J* = 5.7 Hz).

**Synthesis of 1a:** 2,3-Dichloro-5,6-dicyano-*p*-benzoquinone (DDQ; 2.3 g 10.0 mmol, 2.0 equiv.) was added to a 50 mL $CHCl_3$ solution of 1,1,2-tricyano-2-methoxylphenylethane **P-2a** (1.06 g, 5.0 mmol). The resultant mixture was stirred at room temperature for 2 h under air. After removal of the solvent, the mixture was purified by alumina gel column chromatography (eluent: $CHCl_3$) and then by silica gel column chromatography (eluent: $CHCl_3$) to afford 1,1,2-tricyano-2-methoxylphenylethylene **1a** in 95% yield (0.99 g). $^1$H NMR (500 MHz, $CDCl_3$, 298K): δ [ppm] = 8.10 (d, 2H, phenyl; *J* = 9.2 Hz), 7.08 (d, 2H, phenyl; *J* = 9.2 Hz), 3.96 (s, 3H, -OMe).

**Synthesis of 1b:** 2,3-Dichloro-5,6-dicyano-*p*-benzoquinone (DDQ; 2.3 g 10.0 mmol, 2.0 equiv.) was added to a 50 mL $CHCl_3$ solution of 1,1,2-tricyano-2-*p*-tolylethane **P-2b** (0.98 g, 5.0 mmol). The resultant mixture was stirred at room temperature for 2 h under air. After removal of the solvent, the mixture was purified by alumina gel column chromatography (eluent: $CHCl_3$) and then by silica gel column chromatography (eluent: $CHCl_3$) to afford 1,1,2-tricyano-2-*p*-tolylethylene **1b** in 92% yield (0.89 g) $^1$H NMR (500 MHz, $CDCl_3$, 298K): δ

[ppm] = 7.95 (d, 2H, phenyl; $J$ = 8.5 Hz), 7.41 (d, 2H, phenyl; $J$ = 8.5 Hz), 2.50 (s, 3H, -$CH_3$).

**Synthesis of 1c:** 2,3-Dichloro-5,6-dicyano-*p*-benzoquinone (DDQ; 2.3 g 10.0 mmol, 2.0 equiv.) was added to a 50 mL $CHCl_3$ solution of 1,1,2-tricyano-2-*p*-trifluoromethylphenylethane **P-2c** (1.25 g, 5.0 mmol). The resultant mixture was stirred at room temperature for 2 h under air. After removal of the solvent, the mixture was purified by alumina gel column chromatography (eluent: $CHCl_3$) and then by silica gel column chromatography (eluent: $CHCl_3$) to afford 1,1,2-tricyano-2-*p*-trifluorophenylethylene **1c** in 75% yield (0.93 g). $^1$H NMR ($CDCl_3$, 298K): δ [ppm] = 8.10 (d, 2H, phenyl; $J$ = 8.5 Hz), 7.90 (d, 2H, phenyl; $J$ = 8.5 Hz).

**Synthesis of 2a**: Boron trichloride (1.0 M *p*-xylene solution, 0.35 mL, 0.35 equiv.) was added to 1,1,2-tricyano-2-*p*-methoxyphenylethylene **1a** (209 mg, 1.0 mmol) at room temperature. The resulting mixture was gradually heated at 140 ºC, and the temperature maintained for 45 min. After removal of the solvent, the reaction mixture was purified by silica gel column chromatography (eluent: toluene : ethylacetate = 10 : 1) and bio-beads (Sx-1) column (eluent: $CHCl_3$). Recrystallization from toluene and hexane provided compound **2a** in 3.3% yield (7.40 mg). $^1$H NMR (500 MHz, $CDCl_3$): $\delta$ [ppm] = 8.88 (d, $J$ = 9.1 Hz, 6H), 7.24 (d, $J$ = 9.1 Hz, 6H), 4.00 (s, 9H; -OMe); UV/vis (toluene): $\lambda_{max}$ [nm] ($\varepsilon$ [$M^{-1}$ $cm^{-1}$]) = 633 (42300), 435 (17300); HR-MALDI-TOF-MS: $m/z$ = 673.1555 (Calcd. for $C_{36}H_{21}BClN_9O_3$ [$M^-$], 673.1554).

**Synthetic procedure of 2b**: Boron trichloride (1.0 M *p*-xylene solution, 0.35 mL, 0.35 equiv.) was added to 1,1,2-tricyano-2-*p*-tolylethylene **1b** (193 mg, 1.0 mmol) at room temperature. The resulting mixture was gradually heated at 140 ºC, and the temperature maintained for 45 min. After removal of solvents under vacuum, the reaction mixture was purified by silica gel column chromatography (eluent: toluene : ethylacetate = 10 : 1), GPC-HPLC (eluent: $CHCl_3$). Recrystallization from toluene and hexane provided compound **2b** in 5.6% yield (11.7 mg). $^1$H NMR (500 MHz, $CDCl_3$): $\delta$ [ppm] = 8.71 (d, $J$ = 8.3Hz, 6H), 7.55 (d, $J$ = 8.1 Hz, 6H), 2.63 (s, 9H; -$CH_3$); UV/vis (toluene): $\lambda_{max}$ [nm] ($\varepsilon$ [$M^{-1}$ $cm^{-1}$]) = 594 (41200), 419 (15400); HR-MALDI-TOF-MS: $m/z$ = 625.1705 (Calcd. for $C_{36}H_{21}BClN_9$ [$M^-$], 625.1707).

**Synthetic procedure of 2c:** Boron trichloride (1.0 M *p*-xylene solution, 0.35 mL, 0.35 equiv.) was added to 1,1,2-tricyano-2-*p*-trifloromethylphenyl-ethylene **1c** (193 mg, 1.0 mmol) at room temperature. The resulting mixture was gradually heated at 140 ºC, and the temperature maintained for 45 min. After removal of solvents under vacuum, the crude mixture was purified by silica gel column chromatography (eluent: toluene : ethylacetate = 8 : 1) and bio-beads (Sx-1) column (eluent: toluene). Recrystallization from toluene and hexane provided compound **2c** in 7.2% yield (18.9 mg). $^1$H NMR (500 MHz, toluene-$d_8$): $\delta$ [ppm] = 8.68 (d, $J$ = 8.2Hz, 6H), 7.39 (d, $J$ = 8.3Hz, 6H); UV/vis (toluene): $\lambda_{max}$ [nm] ($\varepsilon$ [$M^{-1}$ $cm^{-1}$]) = 571 (41200), 390 (14900); HR-MALDI-TOF-MS: $m/z$ = 787.0857 (Calcd. for $C_{36}H_{12}BClF_9N_9$ [$M^-$], 787.0859).

**Synthetic procedure of 3a**: The subporphyrazine **3a** was isolated from the reaction mixture of the synthesis of **2a**. The reaction mixture was purified by silica gel column chromatography (eluent: toluene : ethylacetate = 10 : 1) and bio-beads (Sx-1) column (eluent: $CHCl_3$). Recrystallization from toluene and hexane provided the target compound in a 0.2% yield (0.45 mg). $^1$H NMR (500 MHz, $CD_2Cl_2$): $\delta$ [ppm] = 8.91 (d, $J$ = 9.0 Hz,

2H); 8.78 (d, $J$ =9.0Hz, 2H), 8.71 (d, $J$ = 9.0Hz, 2H), 7.30 (d, $J$ = 9.1Hz, 2H), 7.23 (d, $J$ = 9.1Hz, 2H), 7.20 (d, $J$ = 9.1 Hz, 2H), 4.01 (s, 3H; -OMe), 3.98 (s, 3H; -OMe), 3.96 (s, 3H; -OMe); UV/vis (toluene): $\lambda_{max}$ [nm] ($\varepsilon$ [$M^{-1}$ $cm^{-1}$]) = 629 (41000), 499 (27100), 435 (22700); HR-MALDI-TOF-MS: $m/z$ = 673.1553 (Calcd. for $C_{36}H_{21}BClN_9O_3$ [$M^-$], 673.1555).

### ii. Crystal packing diagrams of 2c

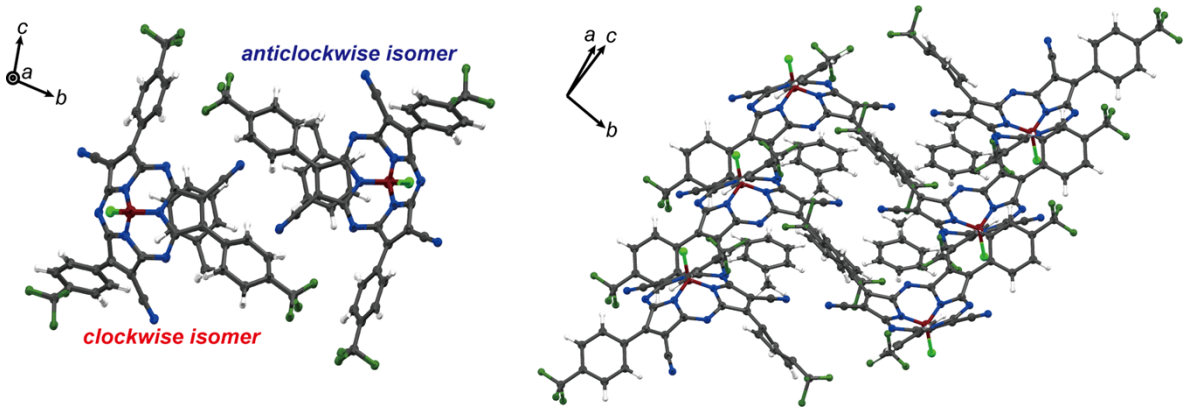



*Fig. S1.* Crystal packing diagram of **2c**.

### iii. $^1$HNMR spectra

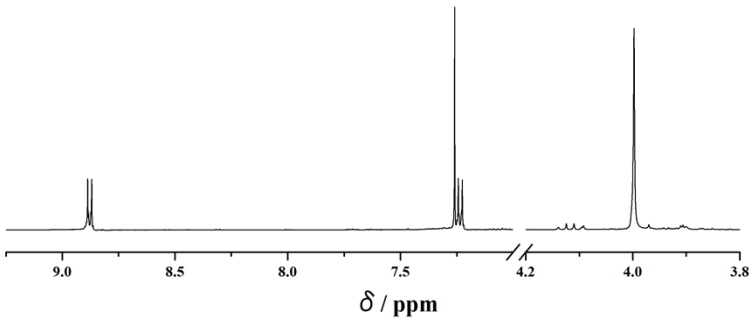



*Fig. S2.* $^1$H NMR spectra of **2a** in $CDCl_3$.

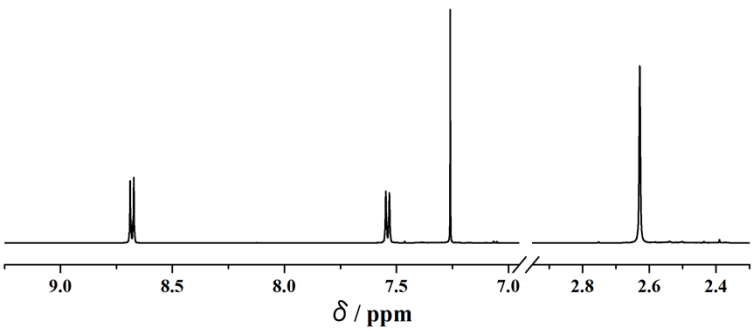



*Fig. S3.* $^1$H NMR spectra of **2b** in $CDCl_3$.

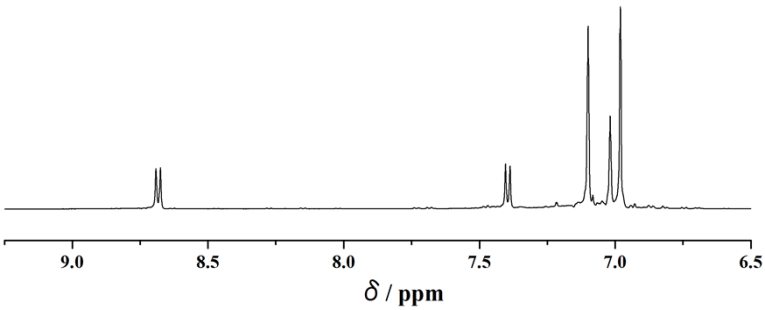



***Fig. S4.*** $^1$H NMR spectra of **2c** in toluene-$d_8$.

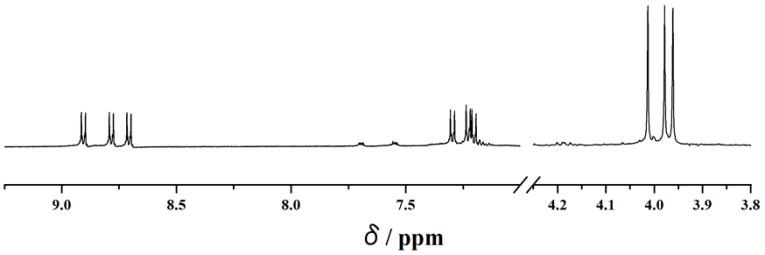



***Fig. S5.*** $^1$H NMR spectra of **3a** in $CD_2Cl_2$.

**iv. Plot of position of the Q bands versus Hammett $\sigma_p$ parameters**

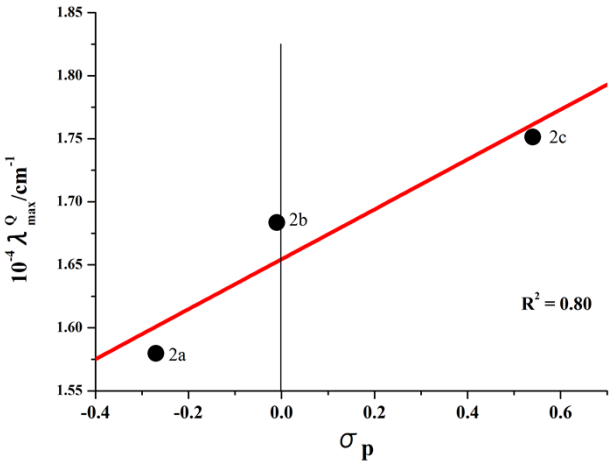



***Fig. S6.*** Plot of position of the Q bands of the push-pull subporphyrazines versus Hammett $\sigma_p$ parameters.

## v. DFT and TDDFT calculations

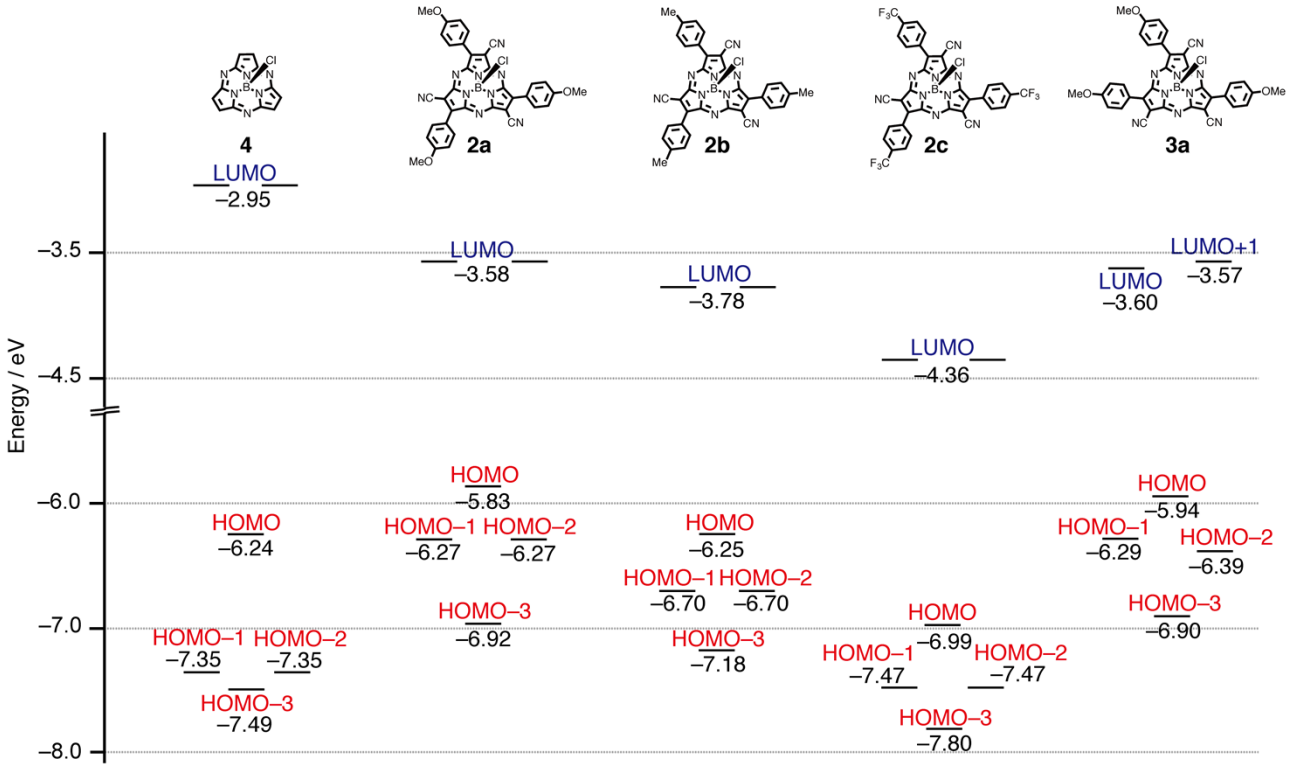



***Fig. S7.*** Frontier MO diagrams of **2a**-**2c**, **3a**, and **4**.

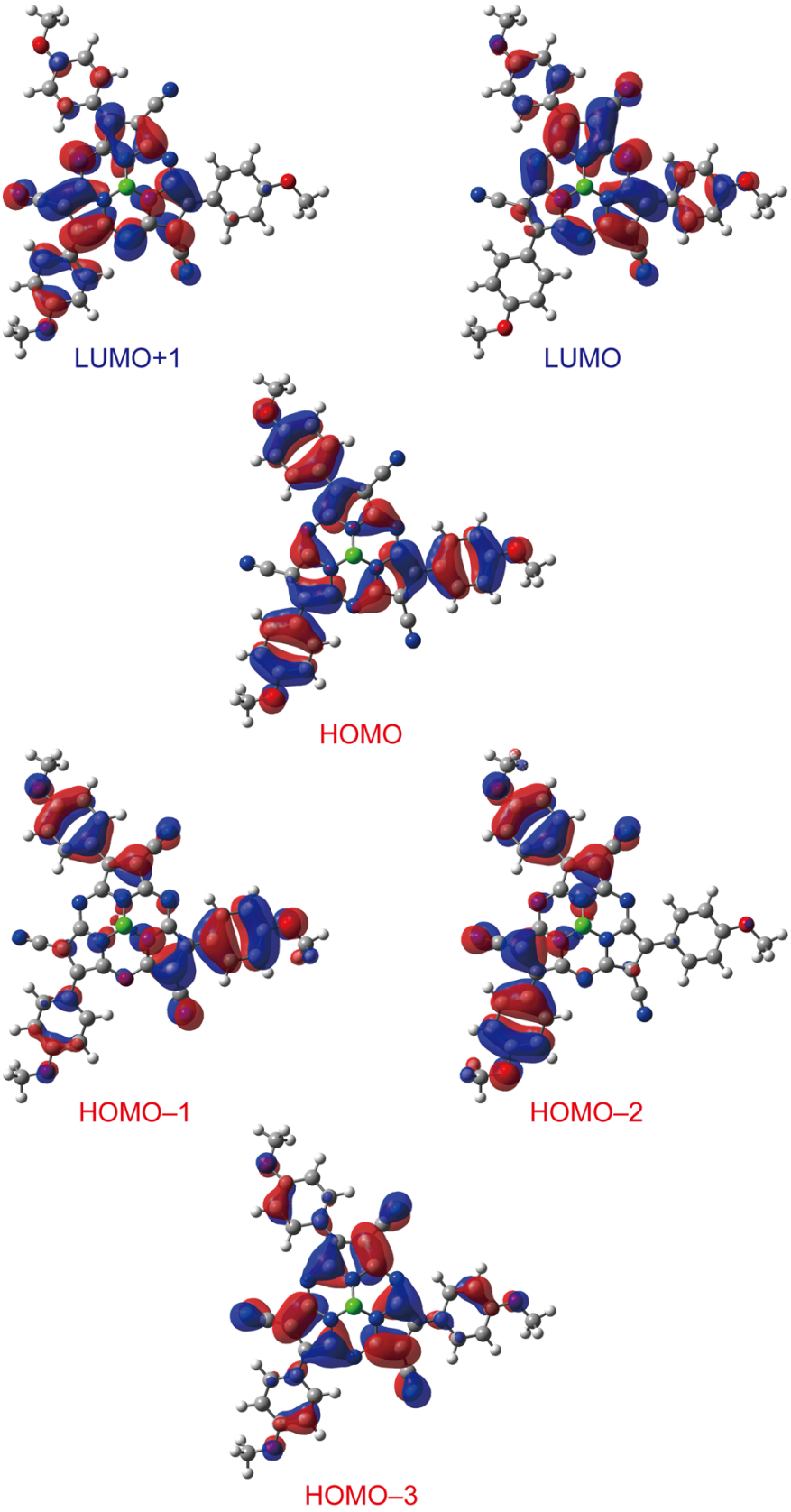



*Fig. S8.* Frontier MOs of **2a**.

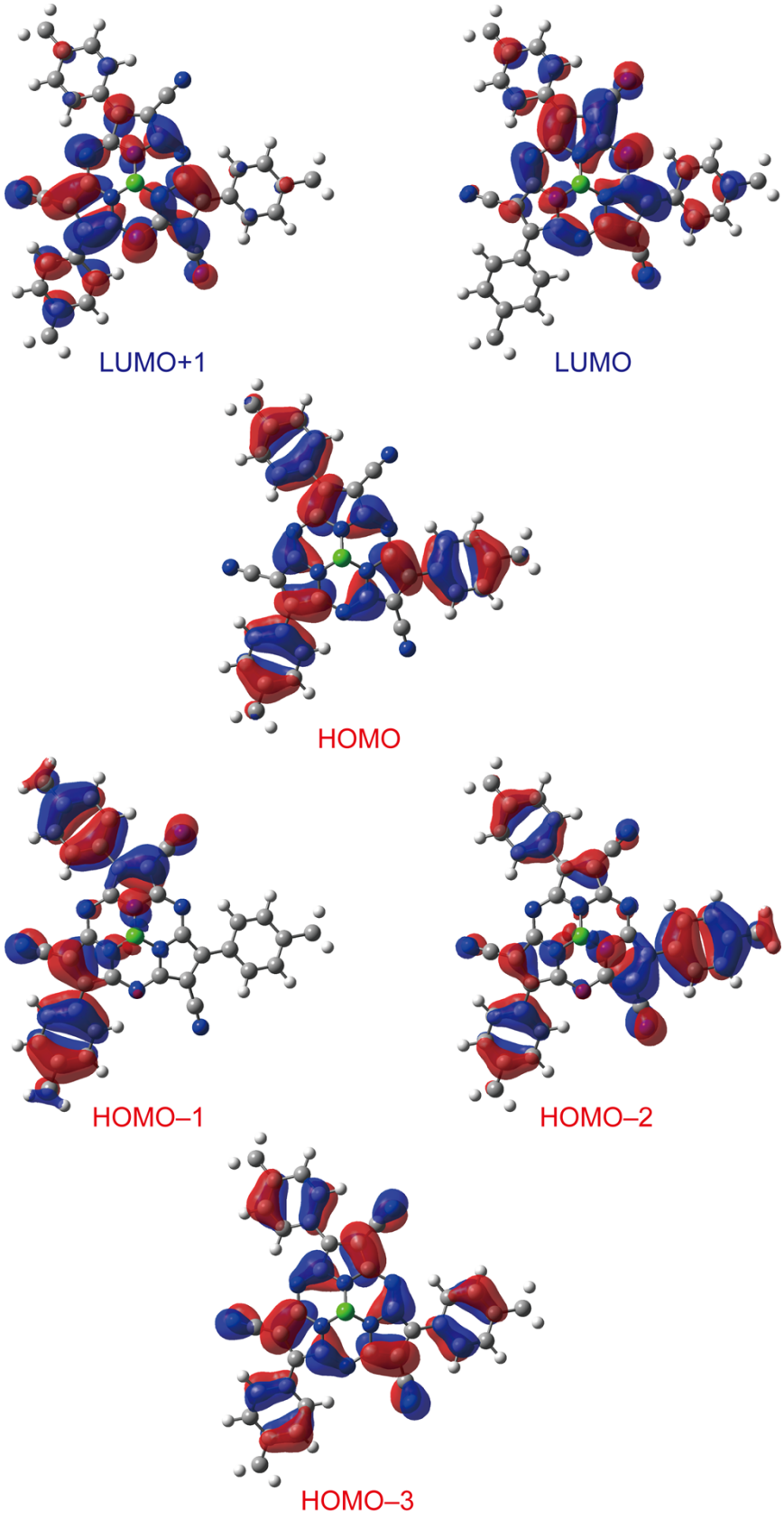



***Fig. S9.*** Frontier MOs of **2b**.

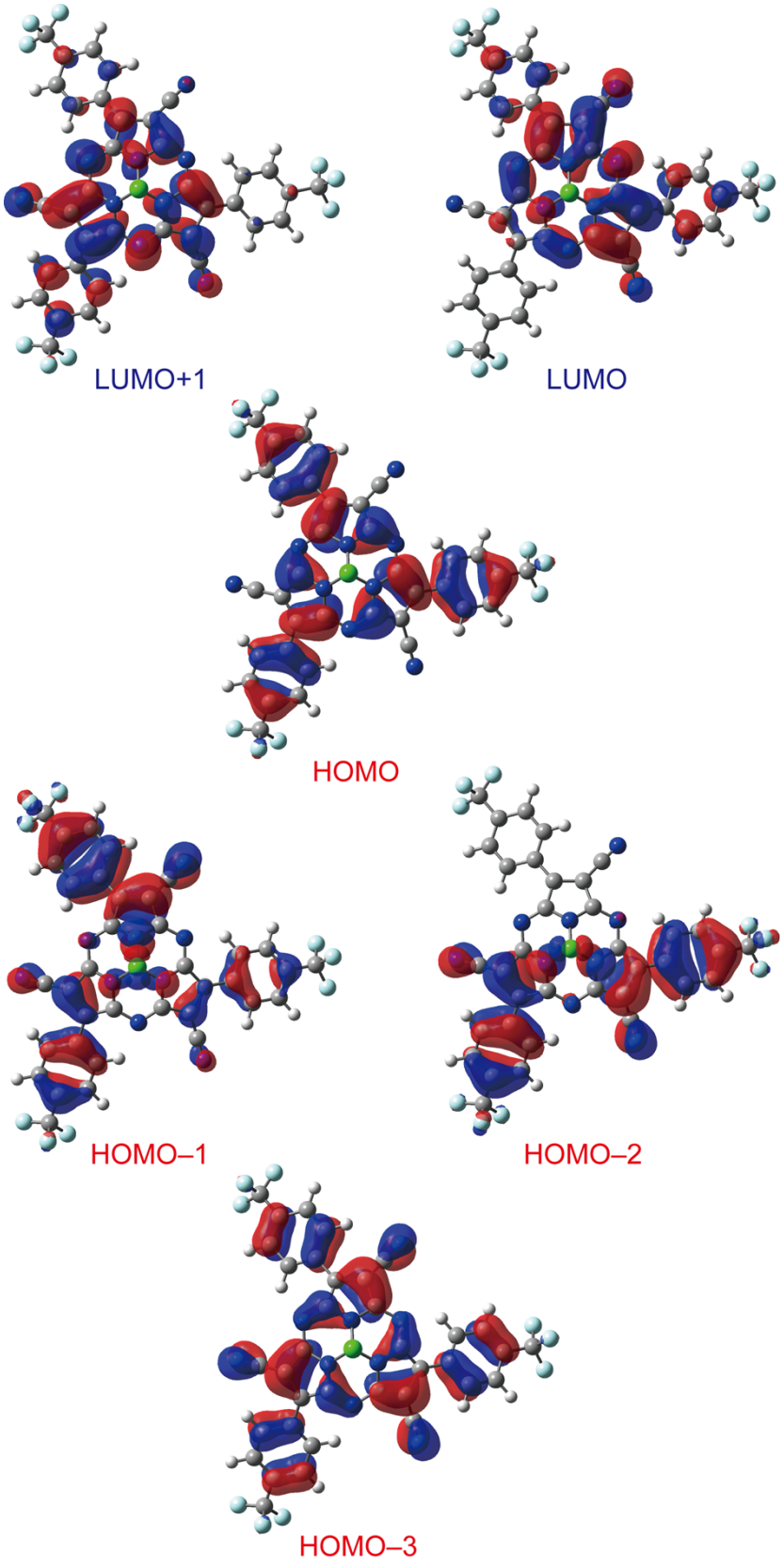



***Fig. S10.*** Frontier MOs of **2c**.

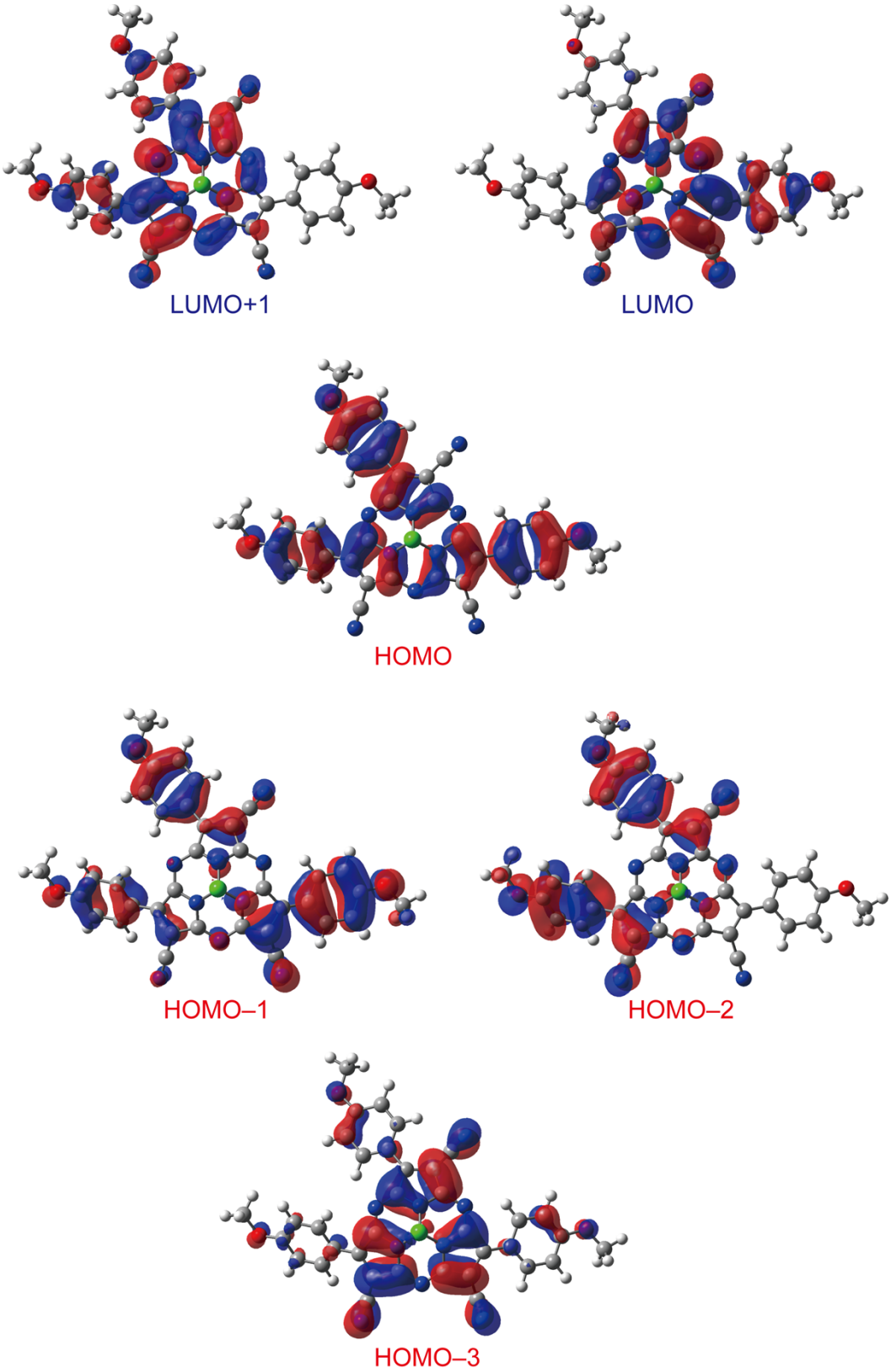



***Fig. S11.*** Frontier MOs of **3a**.

***Table S1.*** Selected transition energies and wave functions of **1a** and **2a** calculated by the TDDFT method (B3LYP/6-31G(d)).

| compd | energy [nm] | $f$ [a] | wave function[b] |
|---|---|---|---|
| **2a** | 614 | 0.376 | + 0.629\|L ← H> + 0.290\|L+1 ← H> +… |
| | 614 | 0.376 | + 0.629\|L+1 ← H> + 0.290\|L ← H> +… |
| | 547 | 0.195 | + 0.472\|L+1 ← H–2> + 0.472\|L ← H–1> – 0.142\|L ← H–2> + 0.142\|L+1 ← H–1> +… |
| | 547 | 0.195 | + 0.472\|L+1 ← H–1> – 0.472\|L ← H–2> – 0.142\|L+1 ← H–2> – 0.142\|L ← H–1> +… |
| | 416 | 0.162 | + 0.606\|L+1 ← H–3> + 0.280\|L ← H–3> – 0.132\|L ← H–9> +… |
| | 416 | 0.162 | + 0.606\|L ← H–3> – 0.280\|L+1 ← H–3> + 0.132\|L+1 ← H–9> +… |
| **2b** | 564 | 0.356 | + 0.687\|L ← H> +… |
| | 564 | 0.356 | + 0.687\|L+1 ← H> +… |
| | 501 | 0.115 | + 0.344\|L ← H–2> + 0.357\|L+1 ← H–2> – 0.357\|L ← H–1> + 0.344\|L+1 ← H–1> +… |
| | 501 | 0.115 | + 0.357\|L ← H–2> – 0.344\|L+1 ← H–2> + 0.344\|L ← H–1> + 0.357\|L+1 ← H–1> +… |
| | 407 | 0.167 | + 0.550\|L+1 ← H–3> – 0.130\|L ← H–8> + 0.199\|L+1 ← H–6> – 0.168\|L ← H–5> + 0.148\|L+1 ← H–5> – 0.148\|L ← H–4> – 0.168\|L+1 ← H–4> – 0.122\|L ← H–3> +… |
| | 407 | 0.167 | + 0.550\|L ← H–3> + 0.130\|L+1 ← H–8> + 0.199\|L ← H–6> – 0.148\|L ← H–5> – 0.168\|L+1 ← H–5> + 0.168\|L ← H–4> – 0.148\|L+1 ← H–4> + 0.122\|L+1 ← H–3> +… |
| **2c** | 528 | 0.341 | + 0.677\|L ← H> – 0.122\|L+1 ← H–3> + 0.109\|L+1 ← H> +… |
| | 528 | 0.341 | + 0.677\|L+1 ← H> + 0.122\|L ← H–3> – 0.109\|L ← H> +… |
| | 403 | 0.190 | + 0.574\|L+1 ← H–3> – 0.118\|L ← H–9> – 0.127\|L+1 ← H–9> – 0.219\|L+1 ← H–6> + 0.153\|L+1 ← H–5> + 0.153\|L ← H–4> – 0.114\|L ← H–3> + 0.112\|L ← H> +… |
| | 403 | 0.190 | + 0.574\|L ← H–3> – 0.127\|L ← H–9> + 0.118\|L+1 ← H–9> – 0.219\|L ← H–6> – 0.153\|L ← H–5> + 0.153\|L+1 ← H–4> + 0.114\|L+1 ← H–3> – 0.112\|L+1 ← H> +… |
| **3a** | 610 | 0.223 | + 0.521\|L ← H> + 0.437\|L+1 ← H> +… |
| | 594 | 0.252 | + 0.535\|L+1 ← H> – 0.445\|L ← H> +… |
| | 496 | 0.283 | + 0.657\|L+1 ← H–2> – 0.107\|L ← H–3> – 0.206\|L ← H–1> +… |
| | 423 | 0.117 | + 0.472\|L+1 ← H–3> – 0.458\|L ← H–3> – 0.125\|L ← H–9> +… |
| | 422 | 0.229 | + 0.487\|L ← H–3> + 0.456\|L+1 ← H–3> – 0.107\|L ← H–9> + 0.107\|L+1 ← H–9> +… |

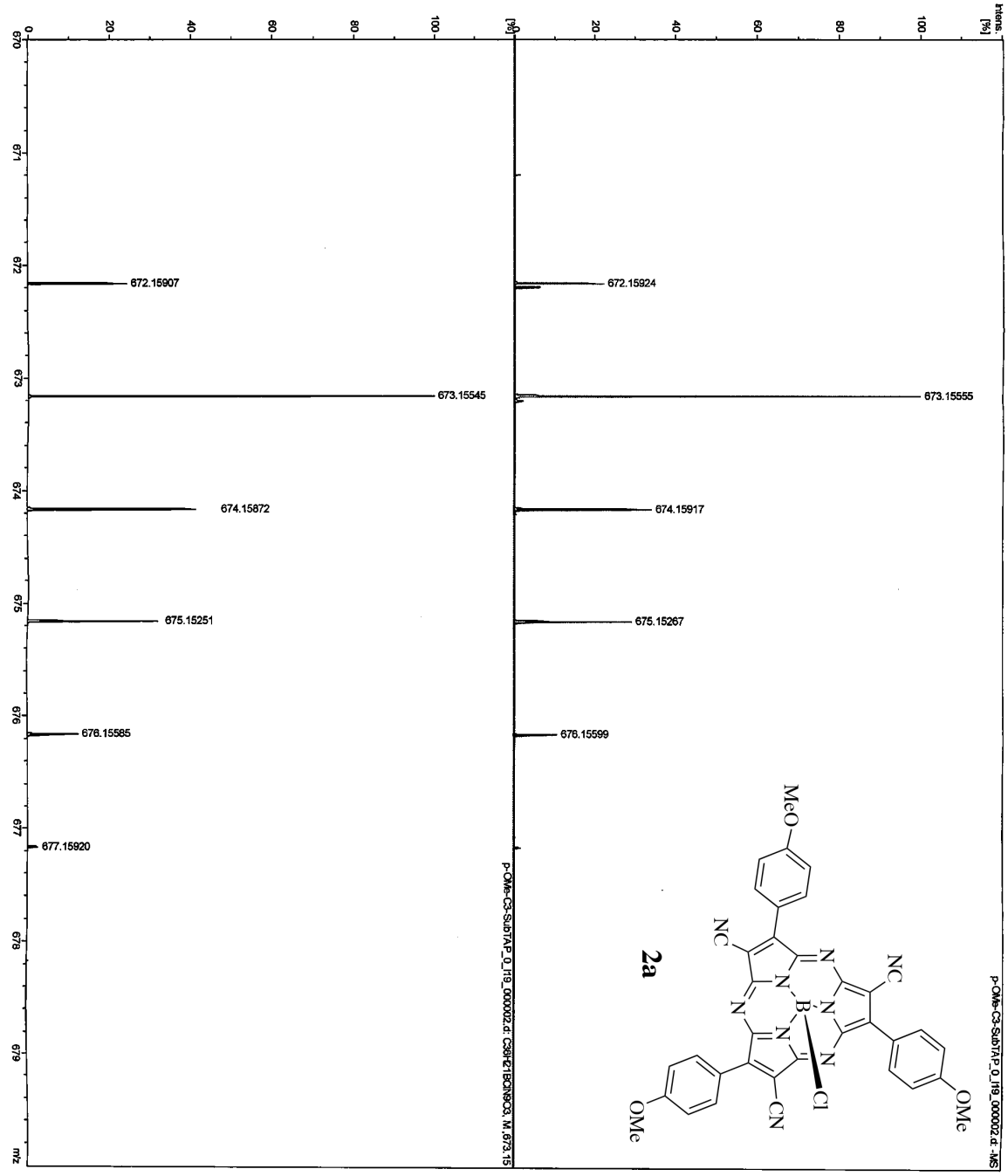
[a] Oscillator strength. [b] Wave functions based on the eigenvectors predicted by TDDFT. H and L represent the HOMO and LUMO, respectively.

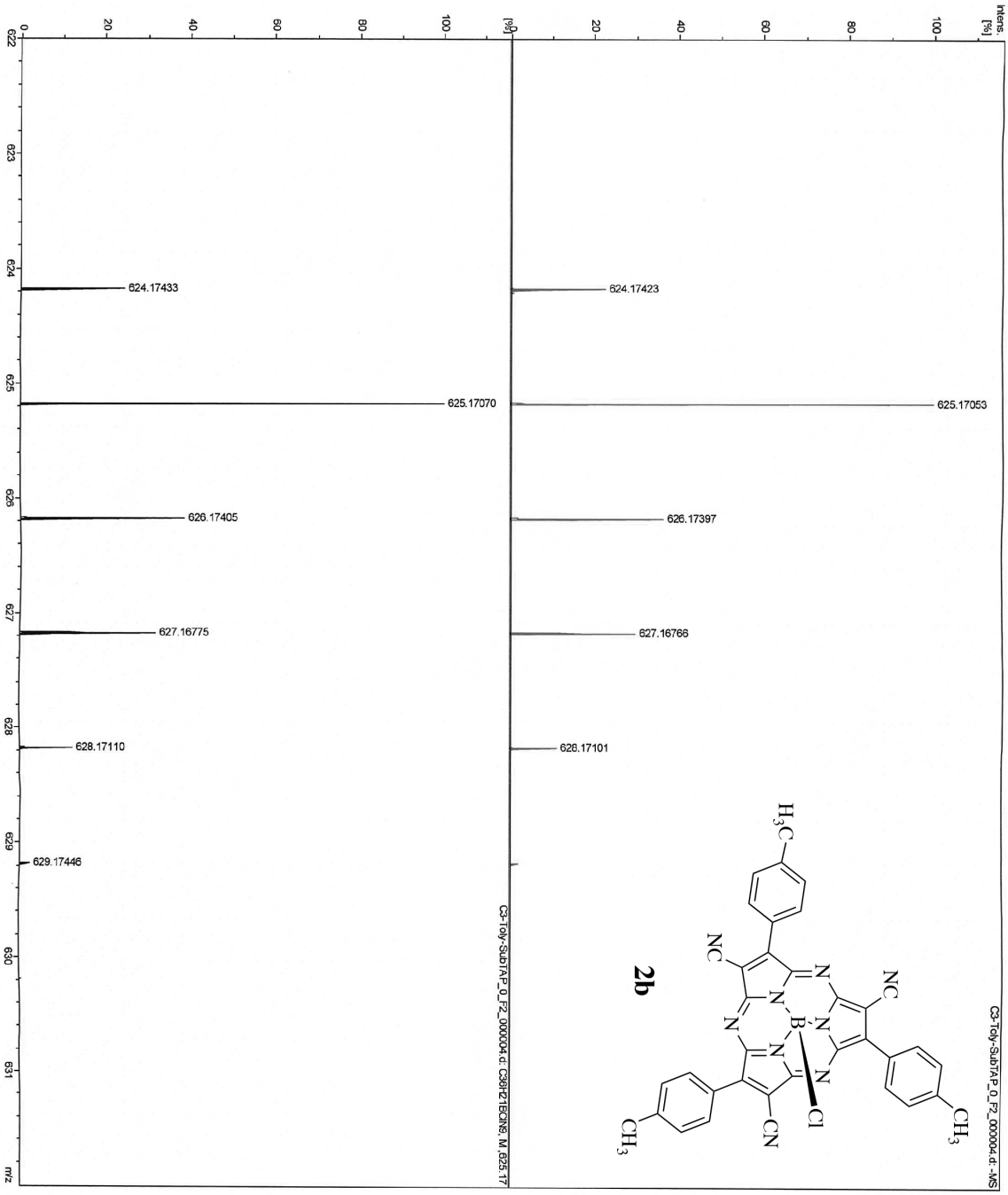
**vi. Reference**

1. G. M. Sheldrick, SHELXL-97, Program for the Solution and Refinement of Crystal Structures, University of Göttingen, Göttingen, Germany, 1997.

2. 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.

## vii. Appendix: HR-MALDI-FT-ICR-MS of 2a–c and 3a and $^{1}$H NMR spectra in a full range




Intens.
[%]
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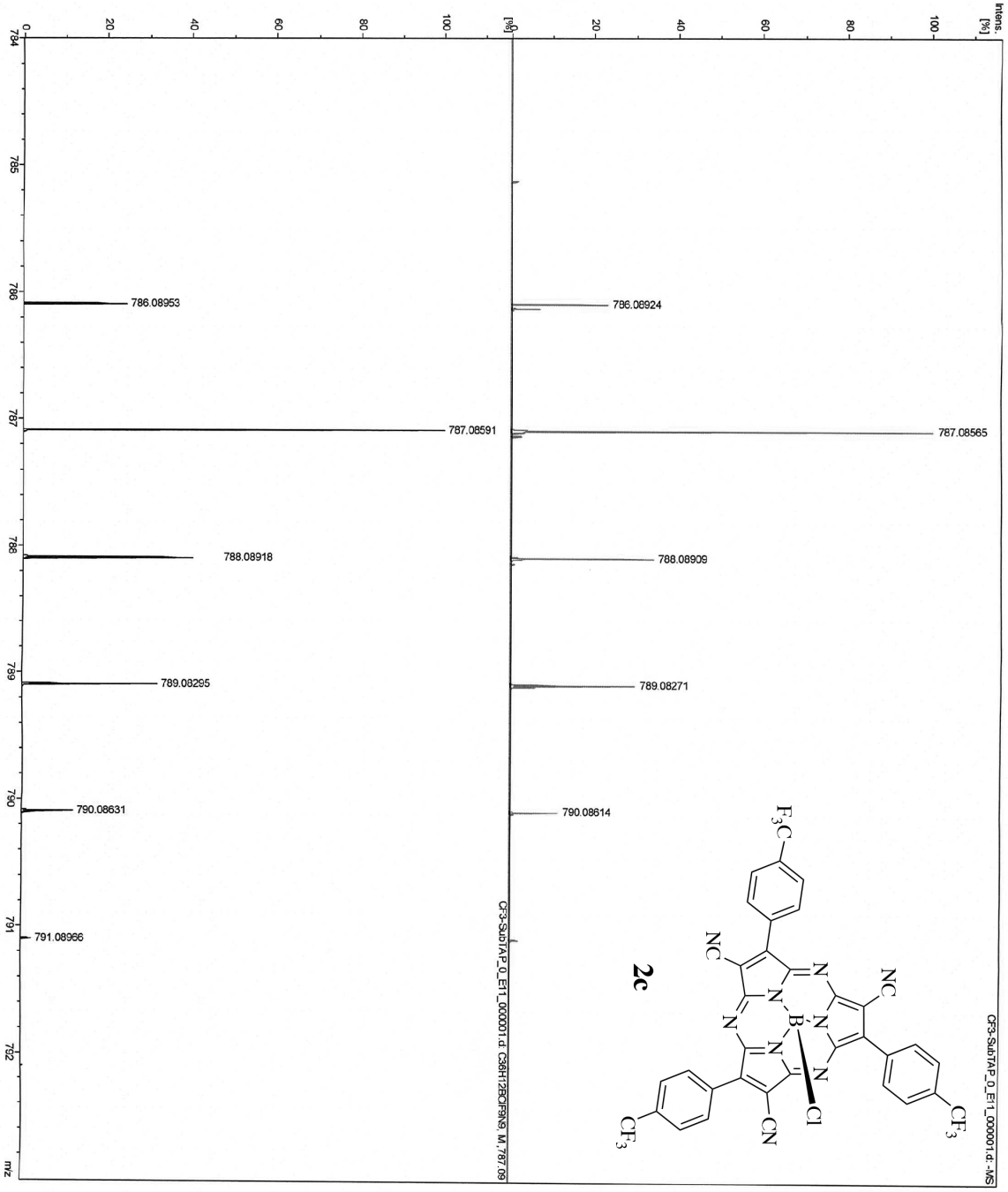
625.17070
626.17405
627.16775
628.17110
629.17446
624.17423
625.17053
626.17397
627.16766
628.17101
C3-Toly-SubTAP_0_F2_000004.d: C38F21ClCN8, M, 625.17
C3-Toly-SubTAP_0_F2_000004.d: -MS
m/z
2b


Intens.
[%]
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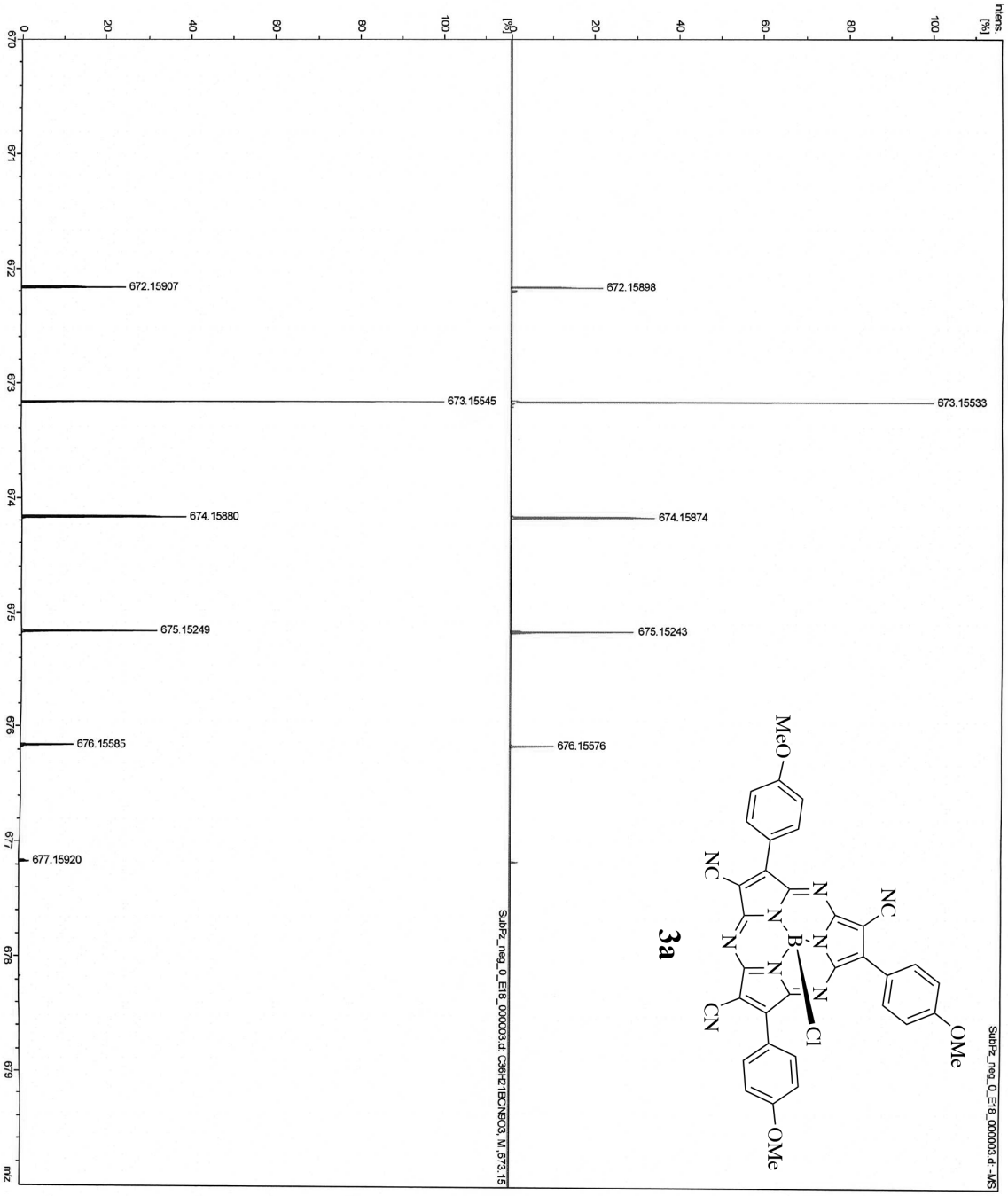
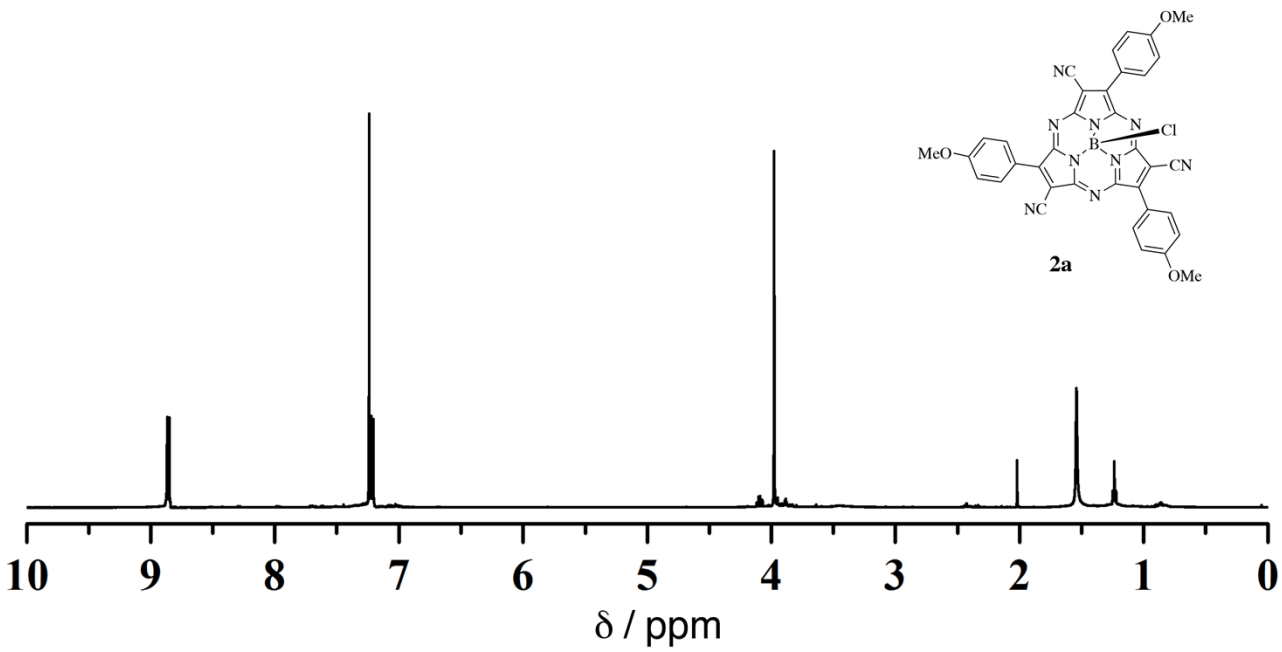
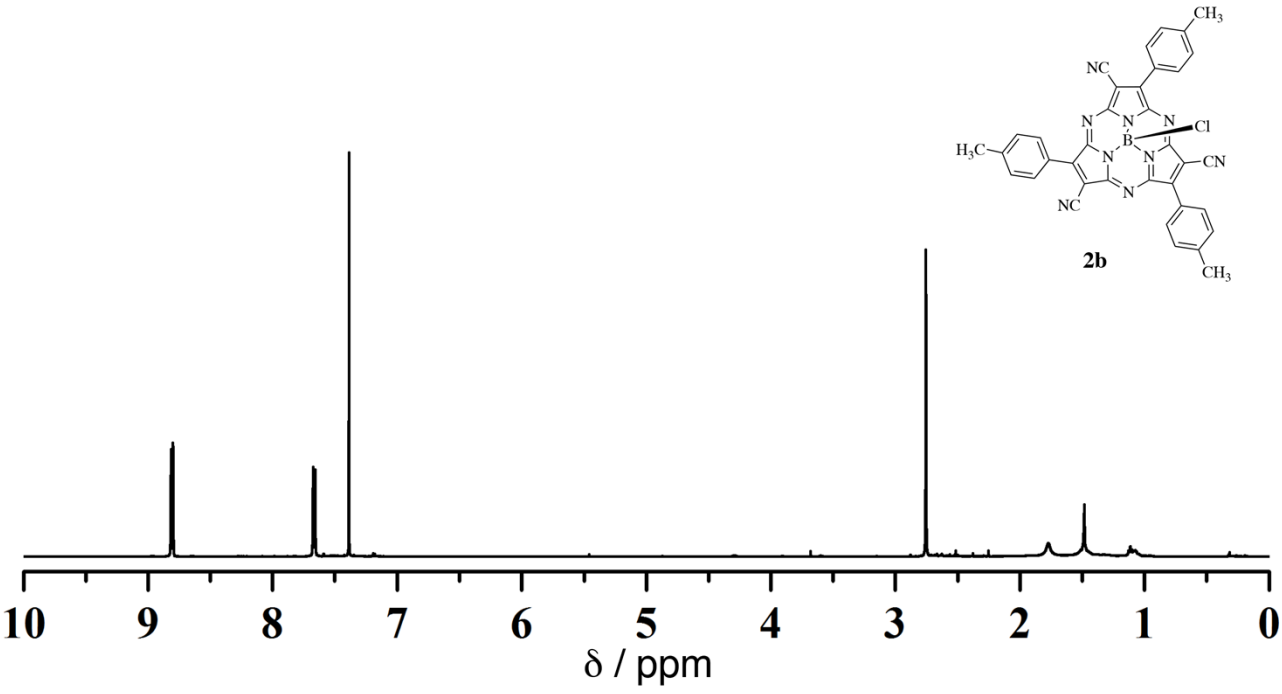
787.08591
788.08918
789.08295
790.08631
791.08966
786.08924
787.08565
788.08909
789.08271
790.08614
m/z
CF3-SubTAP_0_E11_000001.d: -MS
CF3-SubTAP_0_E11_000001.d: C38H17F6N9, M, 787.09
2c

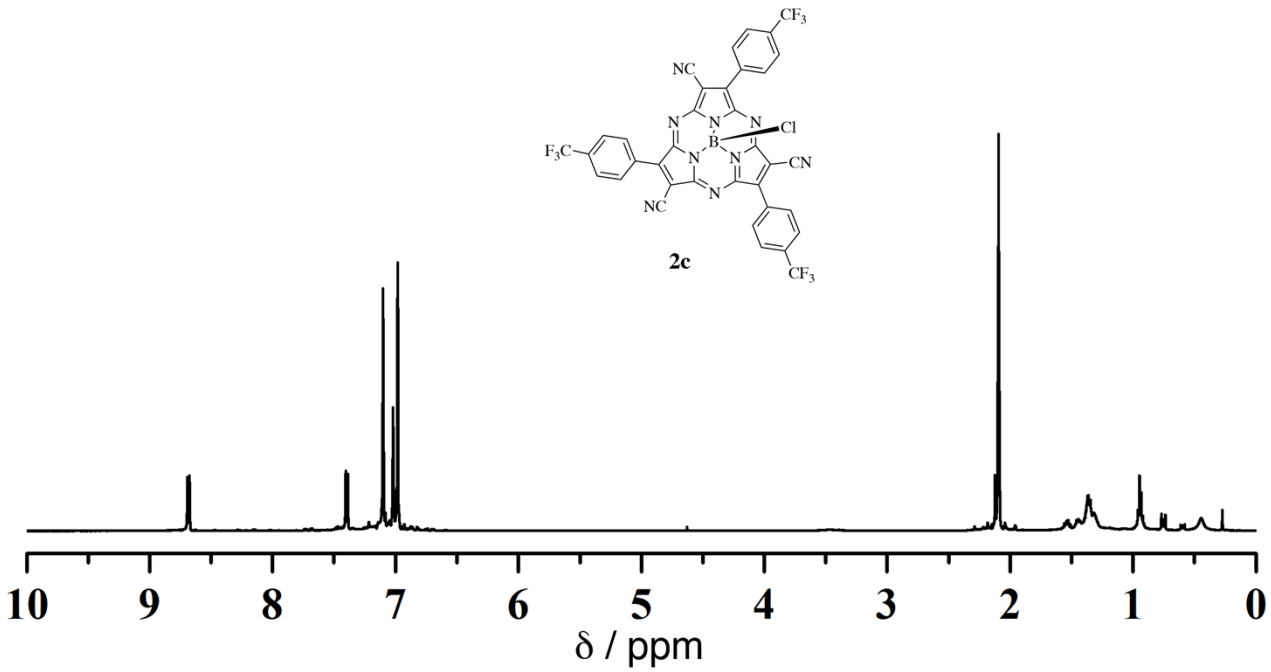

Intens.
[%]
672.15907
673.15545
674.15880
675.15249
676.15585
677.15920
672.15898
673.15533
674.15874
675.15243
676.15576
SubPz_neg_0_E18_000003.d: C36H21BCl2N8O3, M, 673.15
SubPz_neg_0_E18_000003.d: -MS
MeO
NC
CN
OMe
OMe
NC
Cl
3a
m/z


OMe
NC
N
N
N
Cl
B
MeO
N
N
CN
NC
N
OMe
10
9
8
7
6
5
4
3
2
1
0
δ / ppm

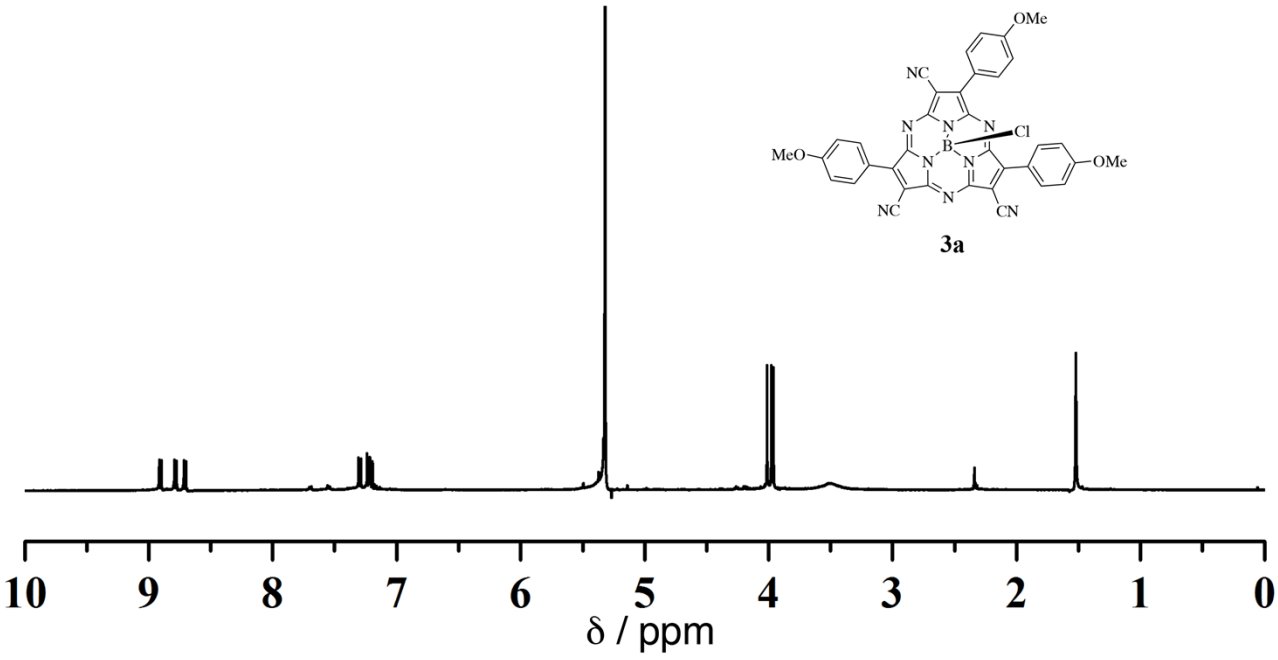
**2a**


CH3
NC
N
N
N
Cl
B
H3C
N
N
CN
NC
N
CH3
10
9
8
7
6
5
4
3
2
1
0
δ / ppm

**2b**


CF3
NC
N
N
N
Cl
F3C
B
N
N
CN
NC
N
CF3
10
9
8
7
6
5
4
3
2
1
0
δ / ppm

**2c**


OMe
NC
N
N
N
Cl
MeO
B
N
N
OMe
NC
N
CN
10
9
8
7
6
5
4
3
2
1
0
δ / ppm

**3a**