Supplementary Information

Star-shaped Magnesium Tetraethynylporphyrin Bearing Four Peripheral Electron-accepting Diketopyrrolopyrrole Functionalities for Organic Solar Cells

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1. Experimental Section

1.1. General

Materials were purchased from Tokyo Kasei (TCI) Co., Sigma-Aldrich Inc., and other commercial suppliers and used after appropriate purification. Anhydrous solvents (stabilizer-free) were purchased from WAKO Pure Chemical. Compound **7** was synthesized as according to previous literature.[1] Compounds **11**, **DPP**, **DPP-Br** were prepared according to previous papers.[2–4] Compounds **DPP-CHO**, **Br-DPP-CHO** were synthesized according to previously reported procedures.[5–6] All reactions dealing with air- or moisture-sensitive compounds were carried out in a dry reaction vessel under nitrogen or argon. All reactions were monitored by thin layer chromatography (TLC, eluent, $CHCl_3/CH_2Cl_2$). The NMR spectra were measured on a Bruker US400 for ^1H NMR and ^{13}C NMR, respectively, reported in parts per million from tetramethylsilane. High-resolution mass spectra were acquired by MALDI using a time-of-flight mass analyzer on Bruker Ultra exTOF/TOF spectrometer. Elemental analyses were carried out using a Vario EL cube&III elemental analyzer. UV-vis absorption was recorded on Shimadzu UV-3600. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were performed using a HOKUTO DENKO HZ-5000 voltammetric analyzer. All CV measurements were carried out in a one-compartment cell under argon gas, equipped with a glassy-carbon working electrode, a platinum wire counter electrode, and an Ag/Ag^+ reference electrode. The solvent with supporting electrolyte was a 0.1 mol L^{-1} acetonitrile solution of tetrabutylammonium hexafluorophosphate ($TBAPF_6$). Ionization potential was measured by a RIKEN KEIKI AC-3 photoemission yield spectroscopy in air. Current–voltage (*J–V*) characteristics were measured using a source meter (Keithley 2400) under sun AM 1.5G simulated sunlight irradiation (100 mW/cm^2) from a solar simulator (EMS-35AAA, Ushio Spax Inc.), which was calibrated using a silicon diode (BS-520BK, Bunkoukeiki).

Mobility Measurements: Hole-only and electron-only devices were fabricated by using hole-only devices with a configuration of ITO/PEDOT:PSS/**3a**:$PC_{61}BM/MoO_3$/Ag and electron-only devices with a configuration of ITO/ZnO/**3a**:$PC_{61}BM$/PFN/Al, The mobility was extracted by fitting the current density–voltage curves using space charge limited current (SCLC). The equation is as follows (Figure S11)**:**

$$J = 9\varepsilon_0\varepsilon_r\mu V^2/8d^3$$

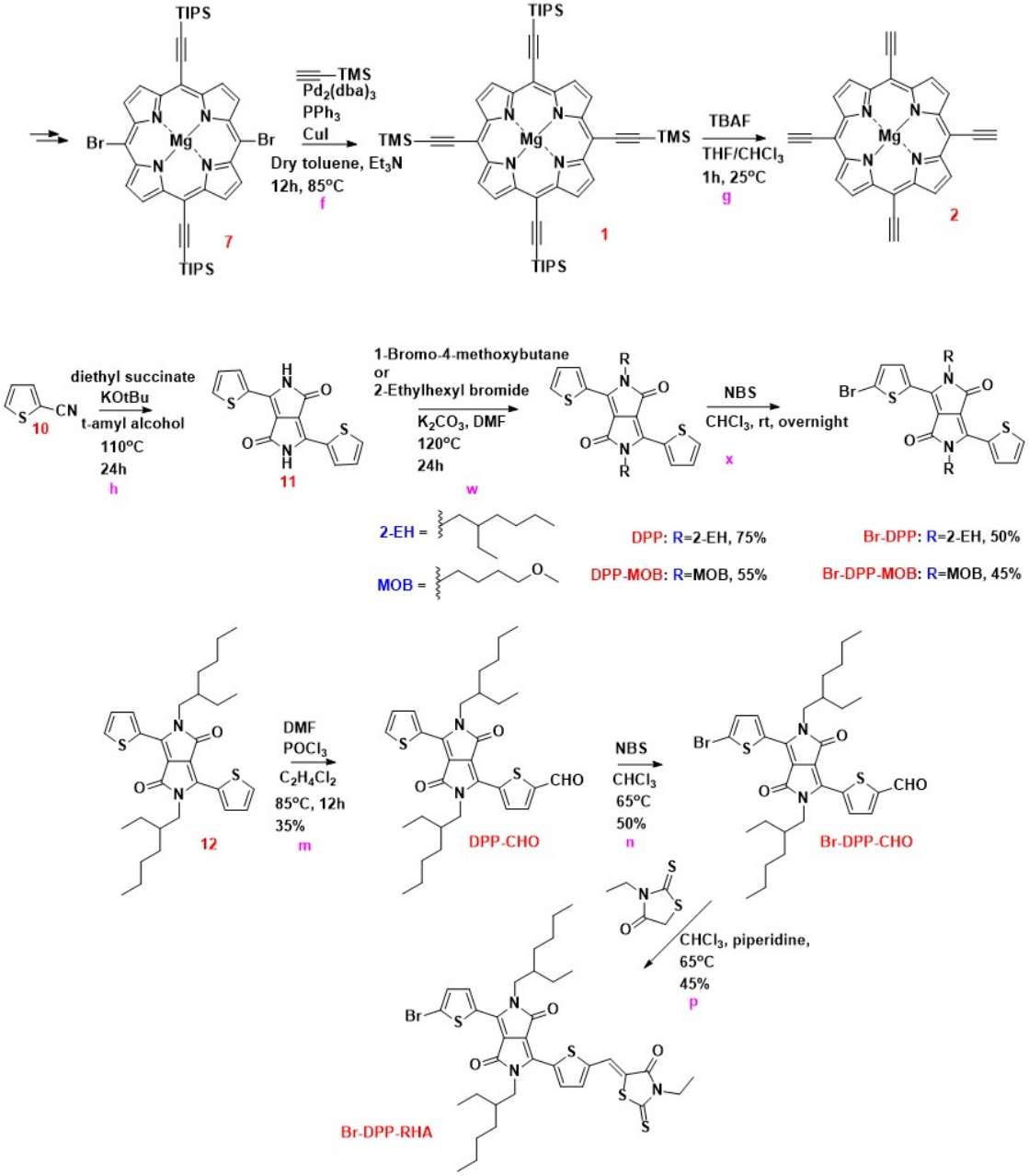
By the plots of $J^{0.5}$ vs V, hole and electron mobilities can be calculated.

Where μ is the mobility, J is the current, ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material, V is the effective voltage, and d is the thickness of the active layer.

Theoretically J_{SC} calculation: According to the following equation, the theoretically estimated J_{SC}^{cal} values were also obtained by integrating the EQE spectra with the AM1.5G solar spectra (Table S4):

$$J_{SC}^{cal} = q \int \mathrm{EQE}\,(\lambda)\,\mathrm{AM1.5G}\,(\lambda)\,d\lambda$$

1.2. Synthesis of the Starting Materials



Scheme S1. Synthetic routes of the starting materials.

1.3. Synthetic procedures

Magnesium(II) 5,15-bis(triisopropylsilylethynyl)-10,20-bis(trimethylsilylethynyl) porphyrinate (1). Porphyrin **7** (500 mg, 0.59 mmol) was dissolved in dry THF (40 mL) and dry triethylamine (20 mL) was added. The mixture was purged with Argon for 30 min. Then $Pd_2(dba)_3$ (54.0 mg, 0.059 mmol), PPh_3 (15.0 mg, 0.059 mmol), CuI (5.5 mg, 0.029 mmol), and trimethylsilylacetylene (578 mg, 5.88 mmol) were added. The mixture was stirred at 80 °C for 12 h under argon, the reaction was quenched with saturated brine. After the mixture was extracted with chloroform (50 mL × 2), the combined organic layers were dried with anhydrous $MgSO_4$ and concentrated. Finally, the residue was purified with silica gel column by using ethyl acetate/petroleum ether (1/10) to afford compound **1** as a dark green powder (411 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (d, J = 4.4 Hz, 4H), 9.59 (d, J = 4.4 Hz, 4H), 1.52–1.41 (m, 42H), 0.62 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.86, 151.60, 131.57, 131.42, 109.08, 107.26, 103.21, 102.79, 101.15, 98.03, 60.22, 18.93, 11.47, 0.66. MALDI-TOF-HRMS (+) (*m*/*z*): calcd for $C_{52}H_{68}MgN_4Si_4$ (M^+): 884.4371, found 884.4355. Anal. Calc. for $C_{52}H_{68}MgN_4Si_4$: C, 70.51; H, 7.74; Mg, 2.74; N, 6.33; Si, 12.68. Found: C, 70.29; H, 7.63; N, 6.27.

Magnesium(II) 5,10,15,20-tetraethynylporphyrin (2). To a solution of porphyrin **9** (200 mg, 0.23 mmol) in a mixture of CH_2Cl_2 (30 mL) and THF (15 mL) was added TBAF (1.5 mL, 1M in THF). After the mixture was stirred at room temperature for 1 h under nitrogen, water (20 mL) was added. Then the mixture was extracted with chloroform (50 mL × 2), the combined organic layers were dried with anhydrous $MgSO_4$ and concentrated, the residue was purified with silica gel column by using ethyl acetate/DCM/petroleum ether (1/5/10) to afford compound **2** as dark green solid, and washed with petroleum ether and methanol (62.6 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (d, J = 1.3 Hz, 8H), 4.67 (d, J = 0.9 Hz, 4H). MALDI-TOF-HRMS (+) (*m*/*z*): calcd for $C_{28}H_{12}MgN_4$ (M^+): 428.0912, found 428.0901. Anal. Calc. for $C_{28}H_{12}MgN_4$: C, 78.44; H, 2.82; Mg, 5.67; N, 13.07. Found: C, 77.74; H, 2.91; N, 12.68.

3-(5-Bromothiophen-2-yl)-6-(5-((3-ethyl-4-oxo-2-thioxothiazolidin-5 ylidene)methyl) thiophen-2-yl)-2,5-bis(2-ethylhexyl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (Br-DPP-RHA). 3-Ethylrhodanine (123 mg, 0.76 mmol) was added to a solution of compound **Br-DPP-CHO** (300 mg, 0.48 mmol) in dry chloroform (30 mL) in a two-necked 100-mL round-bottomed flask under an Ar atmosphere. Piperidine (1.5 mL) was then added and the reaction mixture was stirred at 50 °C overnight. The reaction was quenched with water and extracted with chloroform (30 mL × 2). The organic phase was dried with Na_2SO_4 and the solvent removed under reduce pressure. The crude mixture was purified by column chromatography (silica gel; eluent: ethyl acetate/CH_2Cl_2 = 1:20) and washed with methanol to give a copper-color solid (276 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.08 (d, J = 4.3 Hz, 1H), 8.78 (d, J = 4.2 Hz, 1H), 7.88 (s, 1H), 7.49 (d, J = 4.3 Hz, 1H), 7.24 (d, J = 4.2 Hz, 1H), 4.20 (q, J = 7.1 Hz, 2H), 4.11–3.89 (m, 4H), 1.93–1.79 (m, 2H), 1.46–1.20 (m, 19H),

0.97–0.82 (m, 12H). ^{13}C NMR (100 MHz, CDCl3): δ190.83, 166.99, 161.27, 161.08, 141.88, 140.28, 138.37, 136.40, 136.37, 135.57, 134.33, 131.67, 130.98, 123.53, 123.49, 120.02, 109.84, 108.31, 46.08, 40.09, 39.61, 39.08, 30.25, 30.10, 28.47, 28.26, 28.23, 23.51, 23.47, 23.42, 23.40, 23.18, 23.04, 14.13, 14.04, 12.30, 10.47, 10.42. MALDI-TOF-HRMS (+) (*m*/*z*): calcd for $C_{28}H_{12}MgN_4$ (M^+): 773.1449, found 773.1438. Anal. Calc. for $C_{36}H_{44}BrN_3O_3S_4$: C, 55.80; H, 5.72; Br, 10.31; N, 5.42; O, 6.19; S, 16.55. Found: C, 55.81; H, 5.80; N, 5.33; O, 7.00; S, 16.57.

2,5-Bis(4-methoxybutyl)-3,6-di(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (DPP-MOB). Potassium carbonate (4.84 g, 35.0 mmol) was added to a solution of **11** (3.01 g, 10.0 mmol) in dry DMF (60 mL), and the mixture was heated at 120 °C for 1 h. Then 1-Bromo-4-methoxybutane (5.35 g, 32.0 mmol) was added and the mixture was stirred for 24 h at the same temperature. The suspension was then filtered and the solvent removed under reduce pressure. The crude mixture was washed with methanol to give a copper-color solid, the solid was dried under vacuum and used for next step without further purification (3.31g, 70% yield). MALDI-TOF-HRMS (+) (*m*/*z*): calcd for $C_{24}H_{28}N_2O_4S_2$ (M^+): 472.1490, found 472.1475. Anal. Calc. for $C_{24}H_{28}N_2O_4S_2$: C, 60.99; H, 5.97; N, 5.93; O, 13.54; S, 13.57. Found: C, 70.68; H, 4.96; N, 5.58; O, 12.28; S, 14.23.

3-(5-Bromothiophen-2-yl)-2,5-bis(4-methoxybutyl)-6-(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione (Br-DPP-MOB). DPP-MOB (0.76 g, 1.60 mmol) and N-bromosuccinimide (0.28 g, 1.60 mmol) were dissolved in $CHCl_3$ (50 mL), then the solution was protected from light and stirred at room temperature for 24 h. Water (25 mL) was added and the mixture was extracted with chloroform (50 mL × 2). The organic layer was separated and dried over magnesium sulfate. After the solvent was removed under reduced pressure, the crude product was purified by column chromatography on silica gel with dichloromethane:ethyl acetate from 50:1 to 20:1 (v/v) to afford a red powder (0.49 g, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ8.90 (dd, J = 3.9 Hz, 1.1 Hz, 1H), 8.64 (d, J = 4.2 Hz, 1H), 7.65 (dd, J = 5.0, 1.1 Hz, 1H), 7.29–7.27 (m, 1H), 7.22 (d, J = 4.2 Hz, 1H), 4.13–4.01 (m, 4H), 3.41 (m, 4H), 3.33 (s, 3H), 3.32 (s, 3H), 1.88–1.60 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ161.24, 161.08, 140.36, 138.46, 135.49, 135.06, 131.56, 131.12, 131.06, 129.61, 128.70, 118.90, 107.82, 107.53, 72.14, 72.07, 58.62, 58.59, 41.94, 41.91, 26.95, 26.93, 26.91, 26.84. MALDI-TOF-HRMS (+) (*m*/*z*): calcd for $C_{24}H_{27}BrN_2O_4S_2$ (M^+): 550.0596, found 550.0582. Anal. Calc. for $C_{24}H_{27}BrN_2O_4S_2$: C, 52.27; H, 4.93; Br, 14.49; N, 5.08; O, 11.60; S, 11.63. Found: C, 52.65; H, 4.96; N, 4.77; O, 12.01; S, 11.99.

2. Thermal Properties of the Porphyrin Derivatives

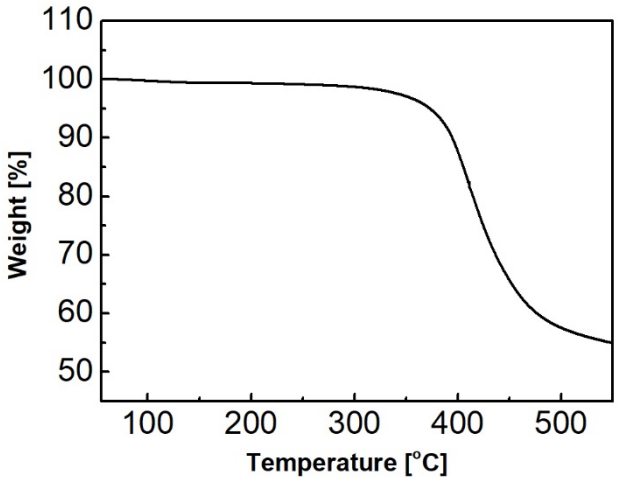


Figure S1. TGA data for **3b** under a N_2 gas flow with temperature ramp rate of 10 °C/min until 550 °C. Temperature with 5% weight loss is 211.71 °C.

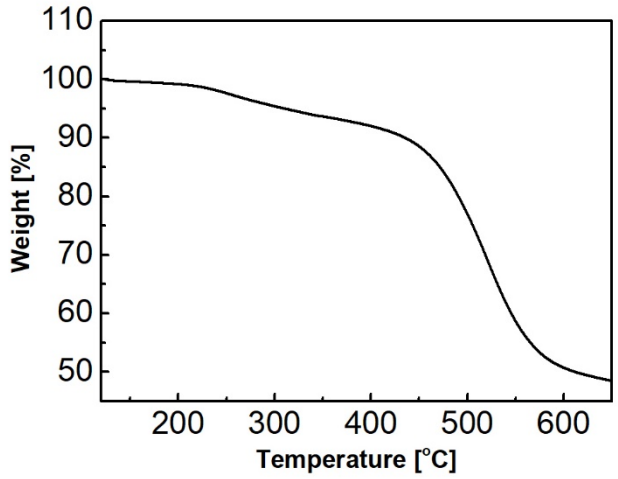


Figure S2. TGA data for **3c** under a N_2 gas flow with temperature ramp rate of 10 °C/min until 650 °C. Temperature with 5% weight loss is 210.26 °C.

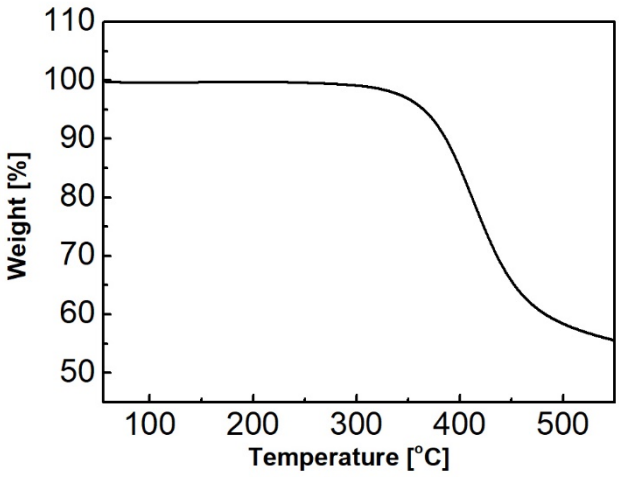


Figure S3. TGA data for **3d** under a N_2 gas flow with temperature ramp rate of 10 °C/min until 550 °C. Temperature with 5% weight loss is 242.44 °C.

3. Absorption Spectra and Electrochemical Data

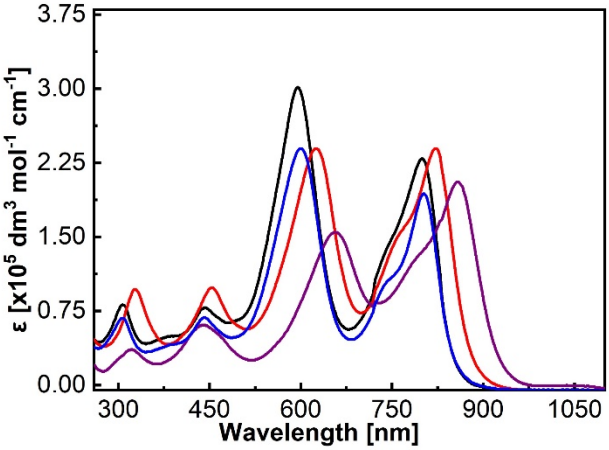


Figure S4. UV-vis absorption spectra of **3a** (black), **3b** (red), **3c** (purple), and **3d** (blue) in DCM.

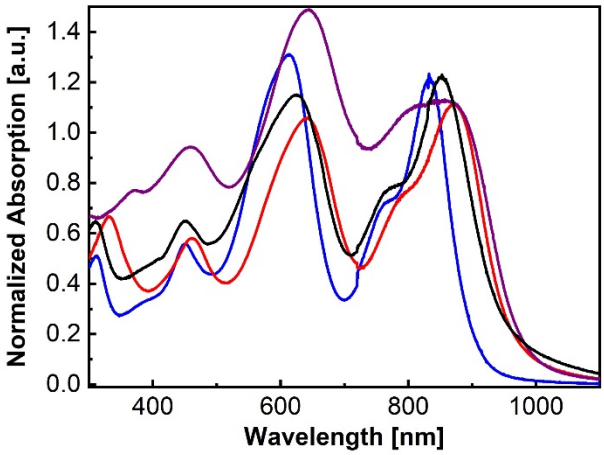


Figure S5. UV-vis absorption spectra of **3a** (black), **3b** (red), **3c** (purple), and **3d** (blue) as solid thin films, respectively.

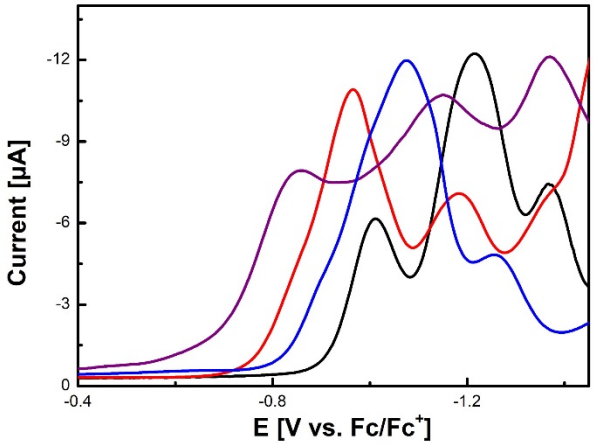


Figure S6. DPV of the reduction range for **3a** (black), **3b** (red), **3c** (purple), and **3d** (blue) in THF.

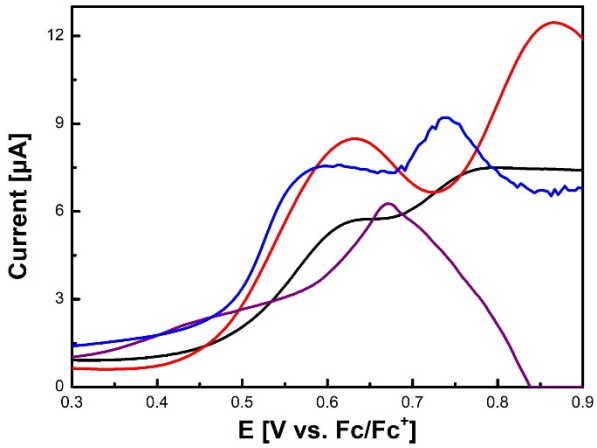


Figure S7. Differential pulse voltammetry (DPV) of the oxidation range for **3a** (black), **3b** (red), **3c** (purple), and **3d** (blue) in THF.

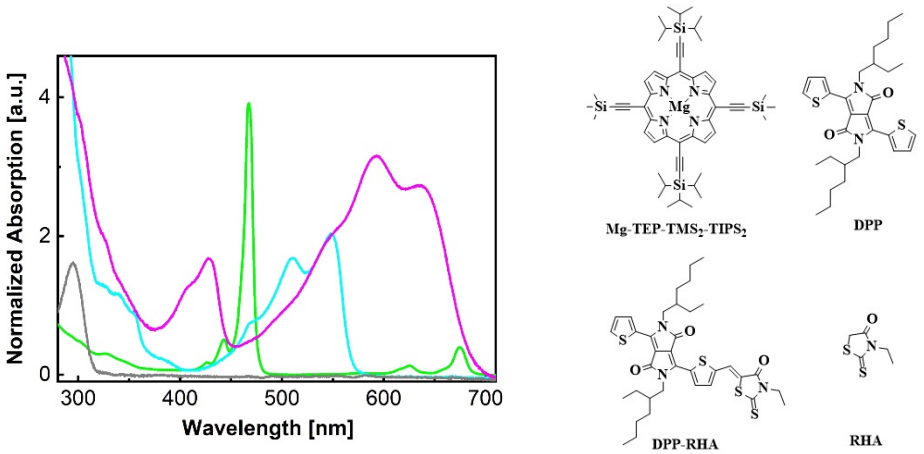


Figure S8. UV-vis absorption spectra of **Mg-TEP-TMS$_2$-TIPS$_2$** (green), **DPP** (cyan), **DPP-RHA** (magenta), and **RHA** (gray) in THF.

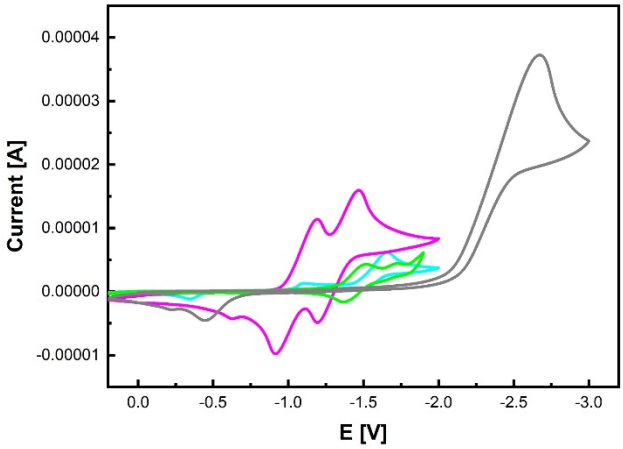


Figure S9. Cyclic voltammetry of the reduction range of **Mg-TEP-TMS$_2$-TIPS$_2$** (green), **DPP** (cyan), **DPP-RHA** (magenta), and **RHA** (gray) in THF containing $TBAPF_6$ (0.1 M) as a supporting electrolyte.

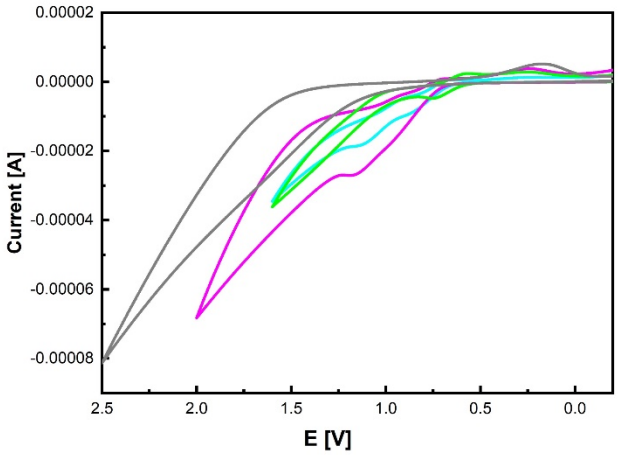


Figure S10. Cyclic voltammetry of the oxidation range of **Mg-TEP-TMS$_2$-TIPS$_2$** (green), **DPP** (cyan), **DPP-RHA** (magenta), and **RHA** (gray) in THF containing $TBAPF_6$ (0.1 M) as a supporting electrolyte.

4. Photovoltaic Data

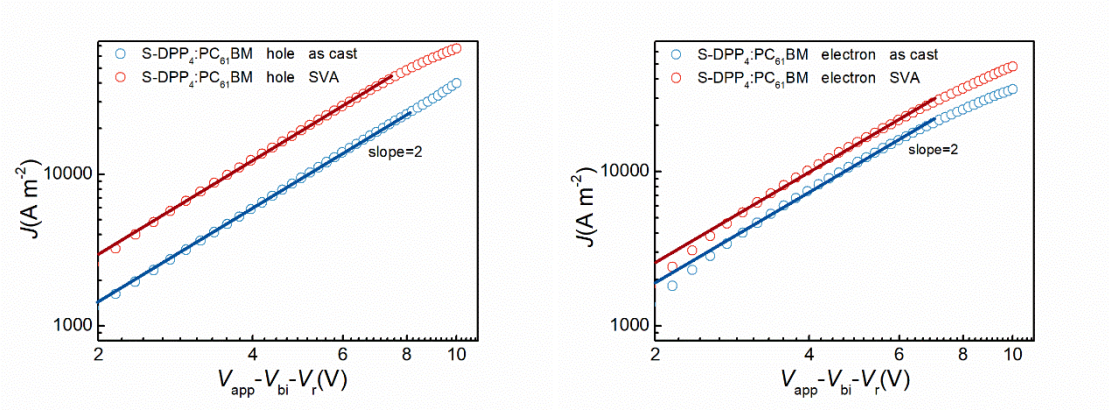


Figure S11. The hole mobility and electron mobility of **3a**:$PC_{61}BM$ before and after SVA at the best optimized device condition measured by SCLC method.

Table S1. Photovoltaic performance of **3a** in conventional BHJ devices with different D/A ratio.

D:A	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
1:1	0.74	14.07	63.21	6.56
1:1.5	0.72	16.42	62.24	7.40
1:2	0.72	15.26	60.41	6.70

Table S2. Thickness influence on photovoltaic performance of **3a** in BHJ devices after SVA for 20s.

Thickness [nm]	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
90	0.73	15.21	63.23	7.04
110	0.72	16.42	62.24	7.40
130	0.72	16.54	56.56	6.80

Table S3. Photovoltaic performance of the **3a** in the BHJ devices with different SVA time.

SVA	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
as-cast	0.75	16.35	47.45	5.80
THF 10s	0.74	16.78	51.14	6.37
THF 20s	0.72	16.42	62.24	7.40
THF 30s	0.73	15.08	60.84	6.69
THF 40s	0.72	13.75	59.96	6.00

Table S4. Photovoltaic performance of the devices under 100 mW/cm^2 simulated solar irradiation.

3a:$PC_{61}BM$	**J_{SC} [mA/cm^2]**	**J_{SC}^{cal} [mA/cm^2]**	**error**	**J_{SAT} [mA cm^{-2}]**	**P(E,T)[a]**	**P(E,T)[b]**
as cast	16.35	15.74	–3.7%	19.25	84.9%	57.6%
SVA	16.42	15.88	–3.3%	17.25	95.2%	77.9%

[a] Exciton dissociation probability under short-circuit condition. [b] Exciton dissociation probability under maximum power output condition.

Table S5. Photovoltaic performance of the devices under 100 mW/cm^2 simulated solar irradiation.

donor	**acceptor**	**Conc. [mg/mL]**	**additive**	**TA [°C]**	**SVA [s]**	**V_{OC} [V]**	**J_{SC} [mA/cm^2]**	**FF [%]**	**PCE [%]**
3d	$PC_{61}BM$	30	1%Py	–	–	0.67	9.40	43.0	2.71
3b	$PC_{61}BM$	30	–	–	–	0.63	0.92	37.0	0.22
3c	$PC_{61}BM$	30	–	–	–	0.59	1.58	28.9	0.27

Table S6. Photovoltaic performance of **3a** in conventional BHJ devices under 100 mW/cm^2 simulated solar irradiation.

donor	**acceptor**	**Conc. [mg/mL]**	**D:A**	**TA [°C]**	**SVA [s]**	**V_{OC} [V]**	**J_{SC} [mA/cm^2]**	**FF [%]**	**PCE [%]**
3a	$PC_{71}BM$	30	1:1	–	–	0.73	6.23	49.34	2.23
3a	$PC_{71}BM$	30	1:1	–	THF 20s	0.73	8.49	59.61	3.70
3a	$PC_{71}BM$	30	1:1.5	–	–	0.72	4.59	52.45	1.73
3a	$PC_{71}BM$	30	1:1.5	–	THF 20s	0.73	3.81	56.20	1.57
3a	$PC_{71}BM$	30	1:2	–	–	0.71	4.29	54.20	1.66
3a	$PC_{71}BM$	30	1:2	–	THF 20s	0.71	3.60	55.81	1.43

5. Spectroelectrochemistry, Fluorescence, and Time-resolved Photophysics Data

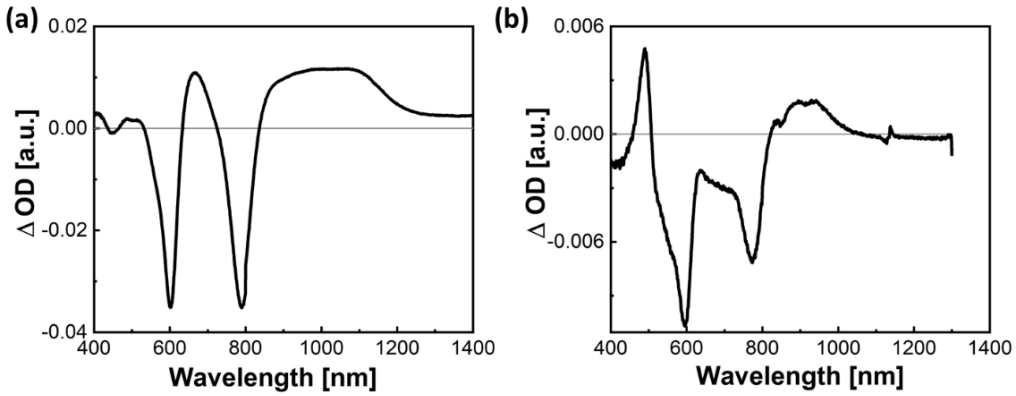


Figure S12. The spectroelectrochemical spectra of **3a** in *o*-dichlorobenzene upon application of (a) +0.8 V and (b) −1.2V versus Ag/Ag^{+}, with tetrabutylammonium perchloride used as the electrolyte.

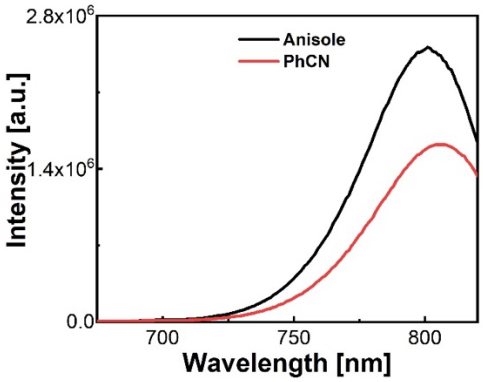


Figure S13. Room-temperature fluorescence spectra of **3a** in anisole and PhCN upon 480 nm excitation with matching optical density of 0.05.

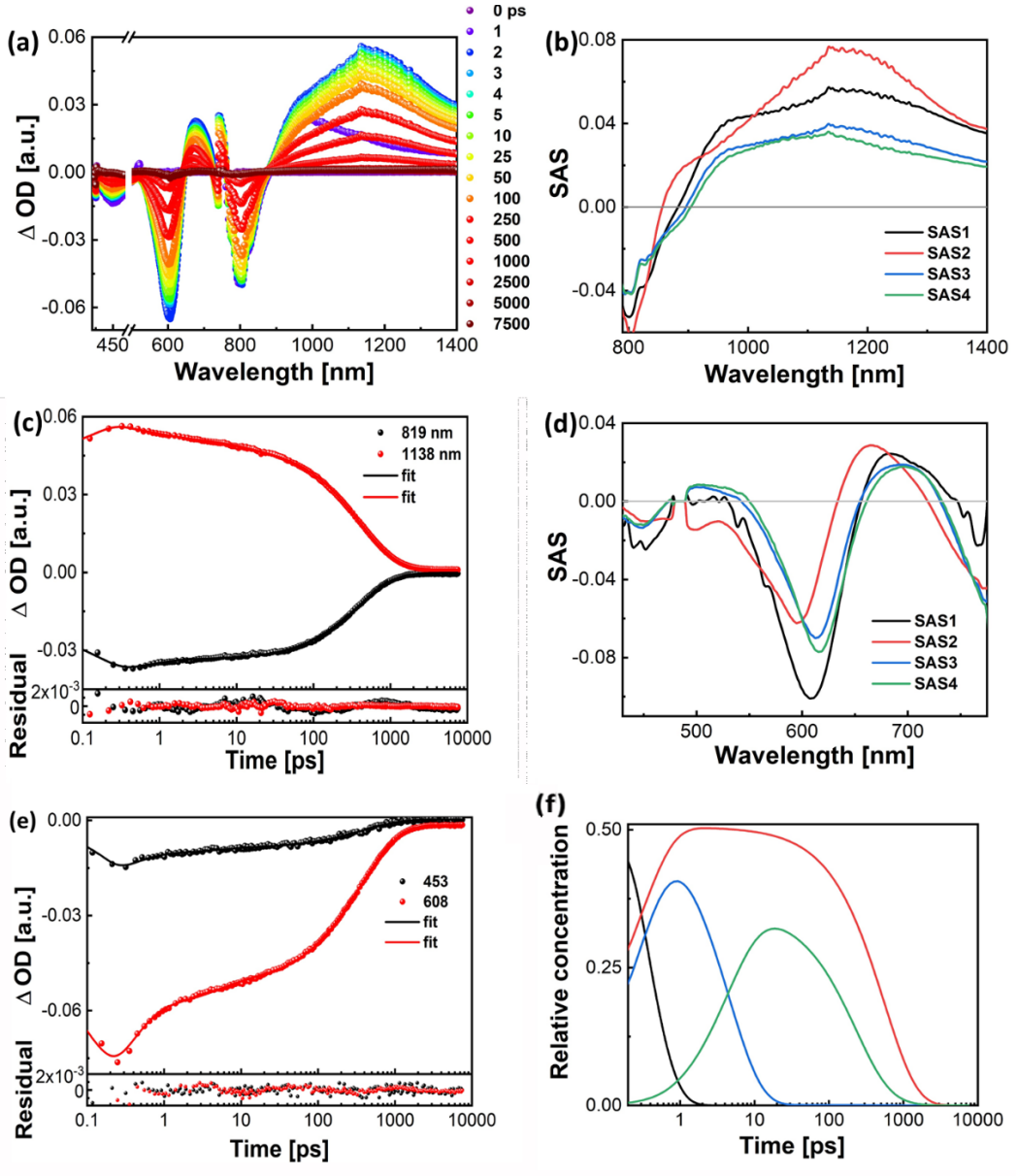


Figure S14. (a) Differential absorption spectra (visible and near-infrared) obtained upon femtosecond flash photolysis (480 nm) of **3a** in argon-saturated PhCN with several time delays between 0 and 7500 ps at room temperature. (b) Deconvoluted transient absorption spectra of $MgP^{\delta+}$-$(DPP_4)^{\delta-}$ (black), $\{MgP^{\delta+}\text{-}(DPP_4)^{\delta-}\}_{relaxed}$ (red), $MgP^{\bullet+}\text{-}(DPP)^{\bullet-}(DPP_3)$ (blue), and $MgP^{\bullet+}\text{-}(DPP_4)^{\bullet-}$ (green) as obtained by global target analysis (NIR). (c) Time absorption profiles of **3a** and the corresponding fits (NIR). (d) Deconvoluted transient absorption spectra of $MgP^{\delta+}\text{-}(DPP_4)^{\delta-}$ (black), $\{MgP^{\delta+}\text{-}(DPP_4)^{\delta-}\}_{relaxed}$ (red), $MgP^{\bullet+}\text{-}(DPP)^{\bullet-}(DPP_3)$ (blue), and $MgP^{\bullet+}\text{-}(DPP_4)^{\bullet-}$ (green) as obtained by global target analysis (Vis). (e) Time absorption profiles of **3a** and the corresponding fits (Vis). (f) Evolution of the population of the involved states.

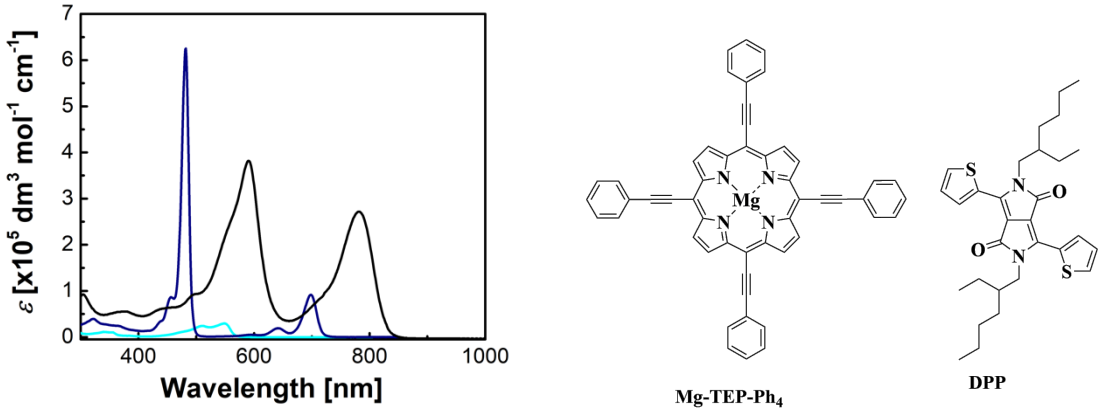


Figure S15. UV-Vis absorption spectra of **3a** (black), **Mg-TEP-Ph$_4$** (navy), and **DPP** (cyan) in THF.

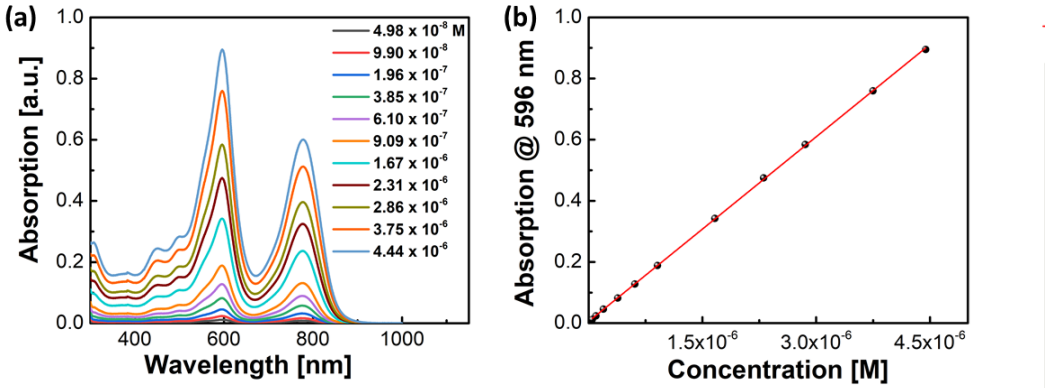


Figure S16. a) Concentration-dependent UV-Vis absorption spectra of **3a** in PhCN. b) Correlation of the absorption intensity as a function of concentration detected at 596 nm in PhCN.

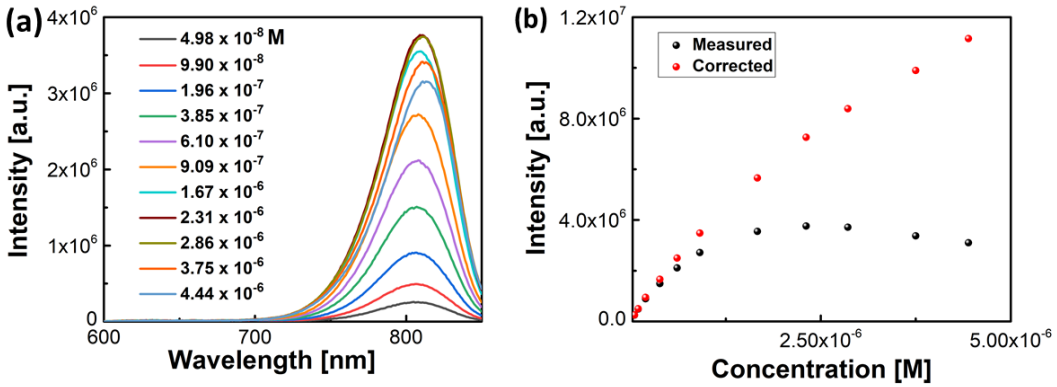


Figure S17. a) Concentration-dependent fluorescence spectra of **3a** in PhCN upon 575 nm excitation. b) Correlation of the fluorescence intensity detected at 809 nm as a function of concentration in PhCN. The spectra was corrected for the primary inner-filter effect using equation:

$$F_{corr.} = F_{obs.} \times 10^{\frac{A_{exc.}+A_{em.}}{2}},$$

where $F_{corr.}$ is the corrected fluorescence value, $F_{obs.}$ is the measured fluorescence value, $A_{exc.}$ the absorption value at the excitation wavelength, $A_{em.}$ is the absorption value at the emission wavelength. Owing to the overlap of the absorption and fluorescence spectra, the non-linearity of the corrected values stems from the secondary inner filter-effect.[7–8]

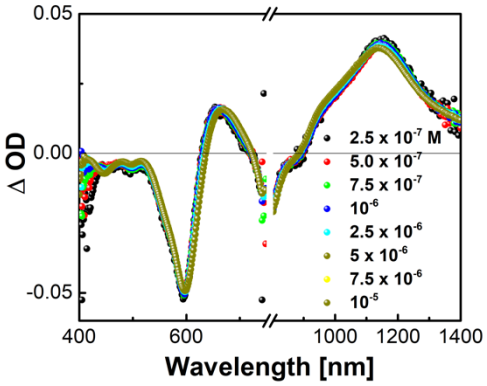


Figure S18. Differential absorption spectra with the time delay of 5 ps with increasing concentration of **3a**. The spectra were obtained upon femtosecond pump-probe experiment (775 nm) in argon-saturated benzonitrile.

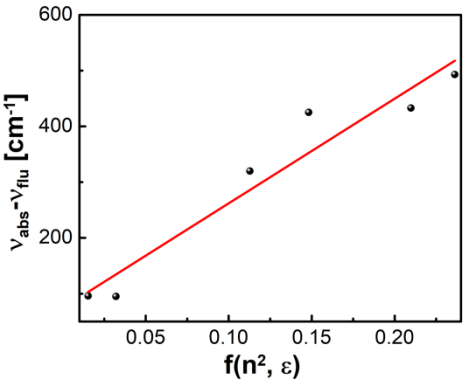


Figure S19. Lippert-Mataga plot showing Stokes shift as a function of solvent orientation polarizability $f(n^2, \varepsilon)$:

$$f(n^2, \varepsilon) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1},$$

Where ε stands for the dielectric constant and n is the refractive index. The Stokes shifts were measured in toluene, chlorobenzene, anisole, chloroform, tetrahydrofuran, and benzonitrile.

7. ^{1}H and ^{13}C NMR Spectra

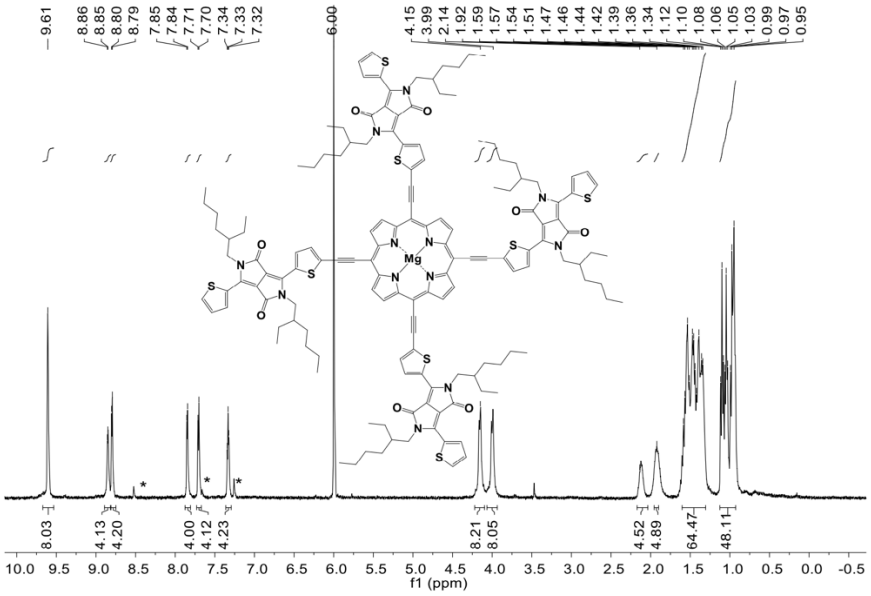


Figure S20. ^{1}H NMR spectrum for **3a**.

^{1}H NMR (400 MHz, tetrachloroethane-d_2 with 1% pyridine-d_5*, 100 °C): δ 9.61 (s, 8H, porphyrin), 8.85 (s, 4H, Th), 8.80 (d, J = 3.6 Hz, 4H, Th), 7.85 (d, J = 4.1 Hz, 4H, Th), 7.71 (d, J = 4.7 Hz, 4H, Th), 7.33 (t, J = 4.0 Hz, 4H, Th), 4.15 (d, J = 6.8 Hz, 8H, NCH_2), 4.00 (d, J = 6.9 Hz, 8H, NCH_2), 2.13 (m, 4H, CH), 1.92 (m, 4H, CH), 1.61–1.28 (m, 64H, CH_2), 1.15–0.88 (m, 48H, CH_3).

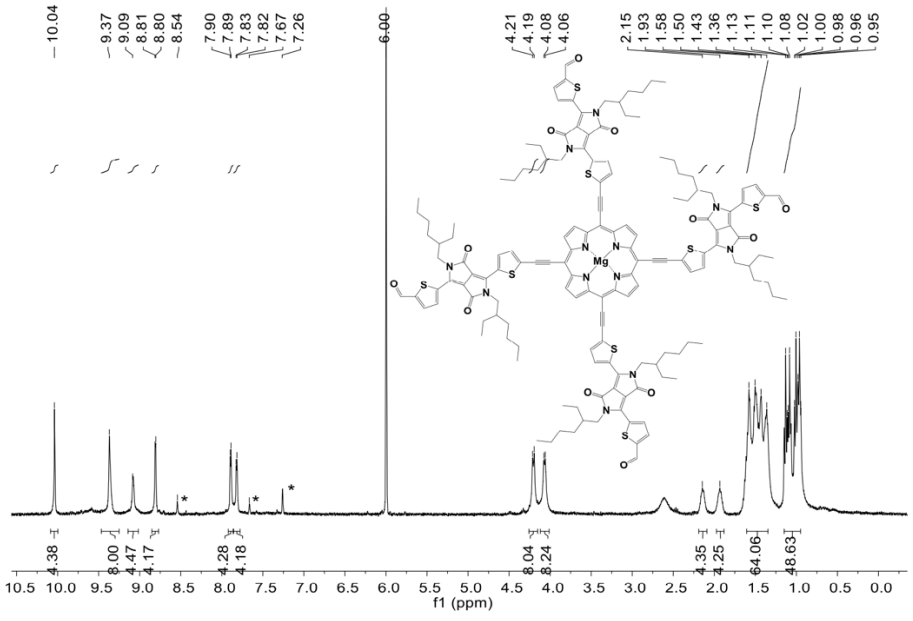


Figure S21. ^{1}H NMR spectrum for **3b**.

^{1}H NMR (400 MHz, tetrachloroethane-d_2 with 1% pyridine-d_5*, 100 °C): δ 10.04 (s, 4H, CHO), 9.37 (s, 8H, porphyrin), 9.08 (m, 4H, Th), 8.81 (d, J = 3.9 Hz, 4H, Th), 7.89 (d, J = 3.4 Hz, 4H, Th), 7.82 (m, 4H, Th), 4.20 (d, J = 7.6 Hz, 8H, NCH_2), 4.07 (d, J = 6.3 Hz, 8H, NCH_2), 2.15 (m, 4H, CH), 1.93

(m, 4H, CH), 1.75–1.47 (m, 64H, CH_2), 1.18–0.92 (m, 48H, CH_3).

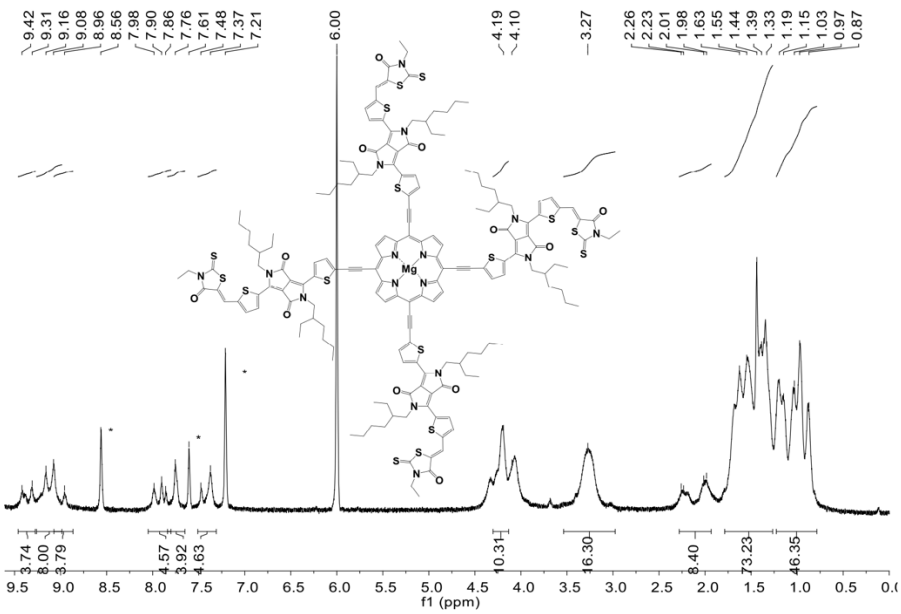


Figure S22. ^{1}H NMR spectrum for **3c**.

^{1}H NMR (400 MHz, tetrachloroethane-d_2 with 5% pyridine-d_5*, 100°C): δ 9.36 (m, 4H, Th), 9.12 (m, 8H, porphyrin), 8.96 (s, 4H, Th), 8.01–7.82 (m, 4H, Th), 7.75 (s, 4H, Th), 7.42 (m, 4H, Th), 4.13 (m, 8H, $CSNCH_2$), 3.26 (m, 16H, NCH_2), 2.12 (m, 8H, CH), 1.72–1.29 (m, 76H, CH_2 and CH_3), 1.24–0.82 (m, 48H, CH_2).

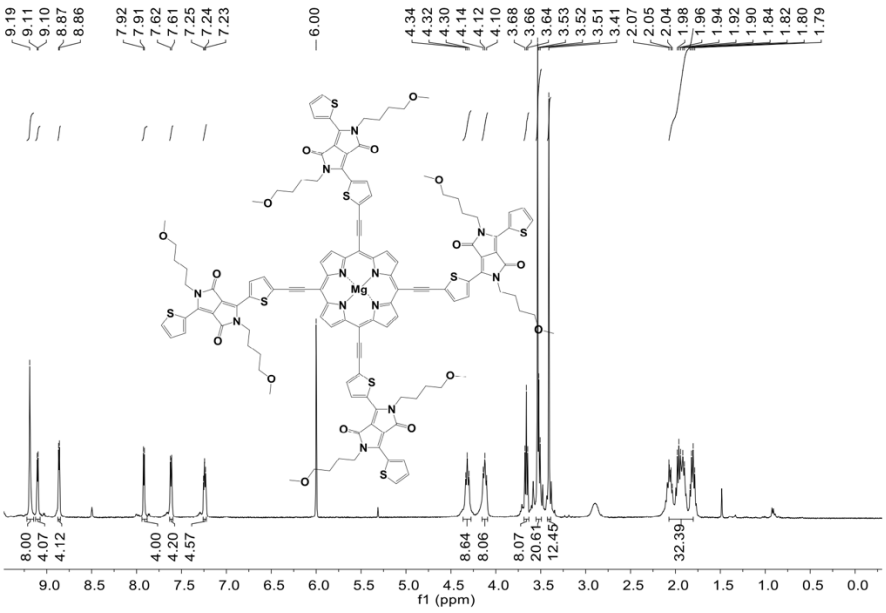


Figure S23. ^{1}H NMR spectrum for **3d**.

^{1}H NMR (400 MHz, tetrachloroethane-d_2 with 1% pyridine-d_5, 100 °C): δ 9.19 (s, 8H, porphyrin), 9.10 (d, J = 3.7 Hz, 4H, Th), 8.86 (d, J = 3.7 Hz, 4H, Th), 7.92 (d, J = 4.0 Hz, 4H, Th), 7.62 (d, J = 5.6 Hz, 4H, Th), 7.27–7.21 (br, 4H, Th), 4.37–4.26 (br, 8H, NCH_2), 4.20–4.06 (br, 8H, NCH_2), 3.66

(t, J = 6.3 Hz, 8H, OCH_2), 3.55–3.50 (m, 20H, OCH_2 and OCH_3), 3.41 (m, 12H, OCH_3), 2.11–1.77 (m, 32H, CH_2).

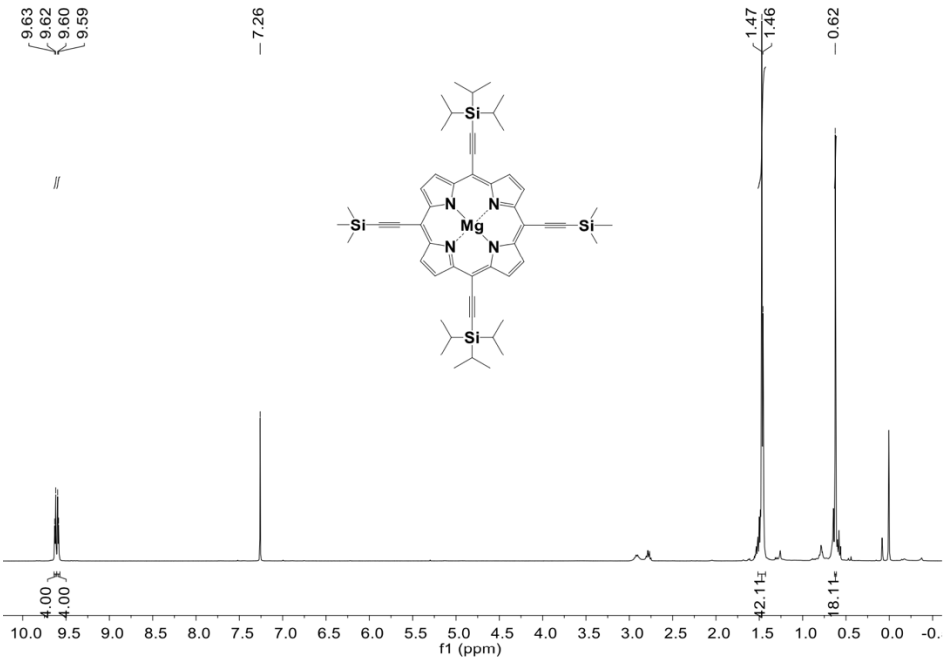


Figure S24. ^{1}H NMR spectrum for **1**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (d, J = 4.4 Hz, 4H, porphyrin), 9.59 (d, J = 4.4 Hz, 4H, porphyrin), 1.52–1.41 (m, 42H, TIPS), 0.62 (s, 18H, TMS).

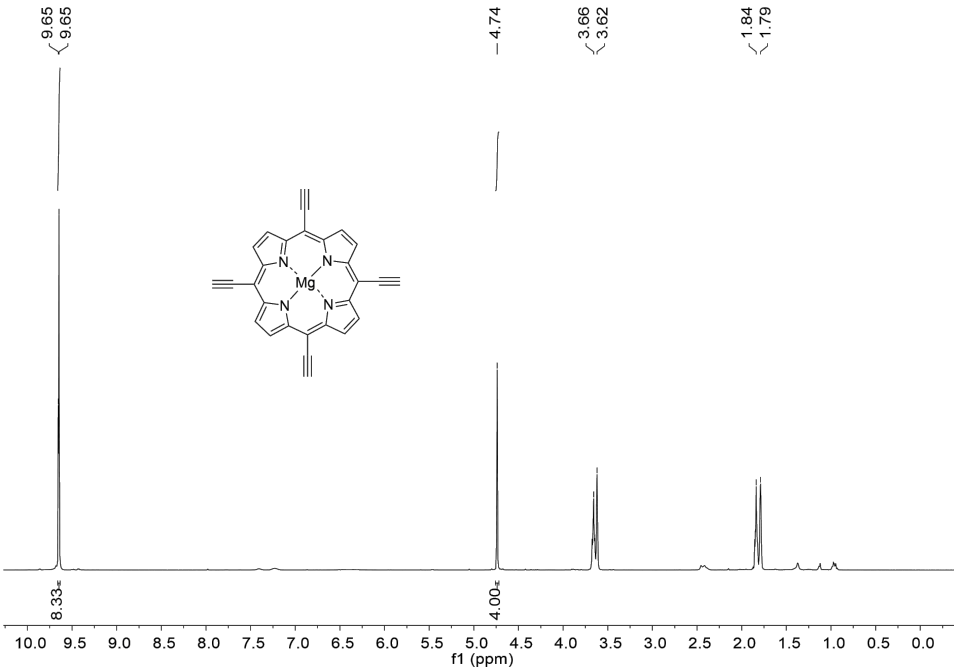


Figure S25. ^{1}H NMR spectrum for **2**.

^{1}H NMR (400 MHz, THF-d_8): δ 9.65 (d, J = 1.3 Hz, 8H, porphyrin), 4.74 (s, 4H, Ethynyl).

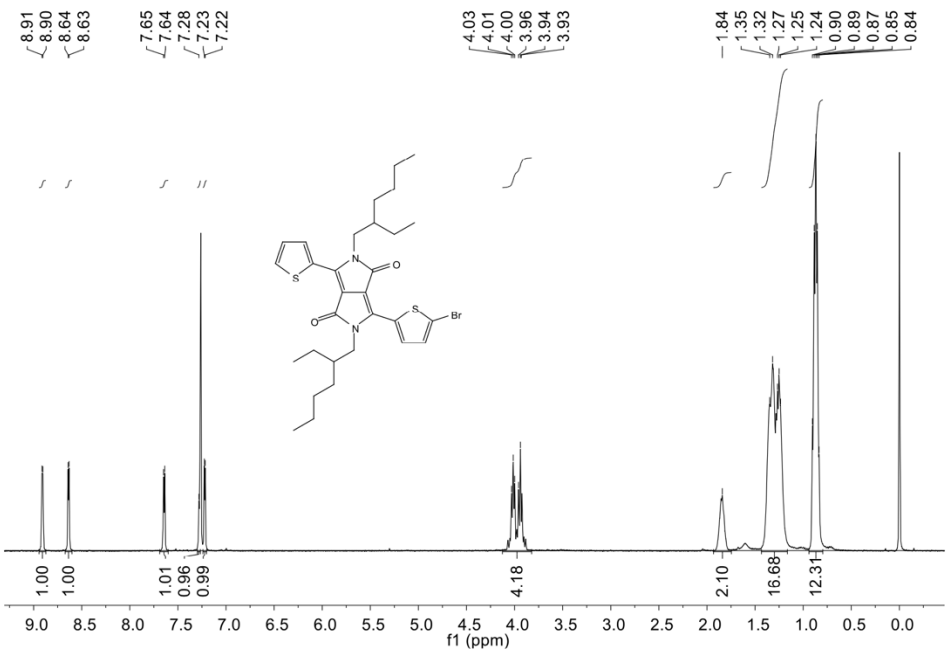


Figure S26. ^{1}H NMR spectrum for **Br-DPP**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.91 (d, J = 3.7 Hz, 1H, Th), 8.63 (d, J = 3.7 Hz, 1H, Th), 7.64 (d, J = 4.9 Hz, 1H, Th), 7.27 (d, J = 3.6 Hz, 1H, Th), 7.22 (d, J = 3.6 Hz, 1H, Th), 4.05–3.90 (m, 4H, NCH_2), 1.84 (s, 2H, CH), 1.39–1.20 (m, 16H, CH_2), 0.93–0.81 (m, 12H, CH_3).

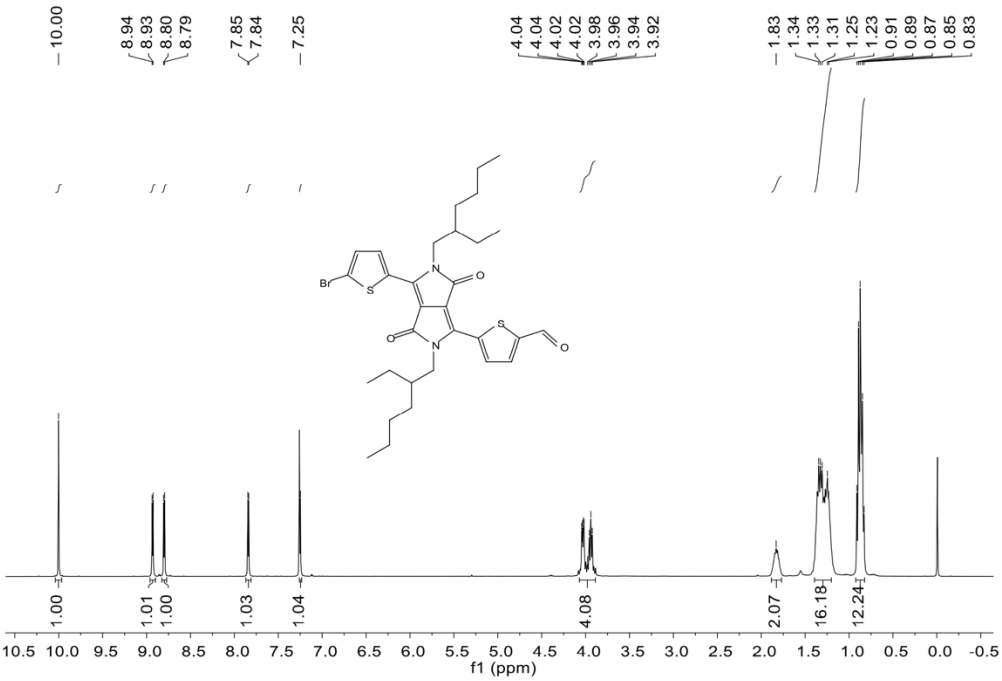


Figure S27. ^{1}H NMR spectrum for **Br-DPP-CHO**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.00 (s, 1H, CHO), 8.93 (d, J = 4.1 Hz, 1H, Th), 8.80 (d, J = 4.2 Hz, 1H, Th), 7.84 (d, J = 4.2 Hz, 1H, Th), 7.25 (d, J = 4.7 Hz, 1H, Th), 4.09–3.88 (m, 4H, NCH_2), 1.82 (m, 2H, CH), 1.42–1.17 (m, 16H, CH_2), 0.87 (m, 12H, CH_3).

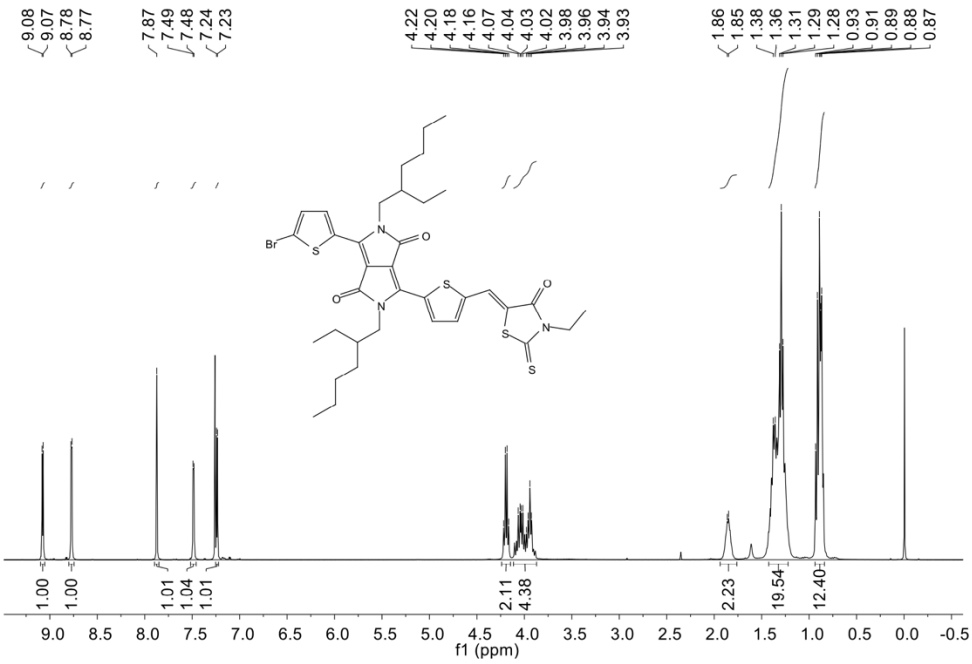


Figure S28. ^{1}H NMR spectrum for **Br-DPP-RHA**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.08 (d, J = 4.3 Hz, 1H, Th), 8.78 (d, J = 4.2 Hz, 1H, Th), 7.88 (s, 1H, Vinyl), 7.49 (d, J = 4.3 Hz, 1H, Th), 7.24 (d, J = 4.2 Hz, 1H, Th), 4.20 (q, J = 7.1 Hz, 2H, $CSNCH_2$), 4.11–3.89 (m, 4H, NCH_2), 1.93–1.79 (m, 2H, CH), 1.46–1.20 (m, 19H, CH_2 and CH_3), 0.97–0.82 (m, 12H, CH_2).

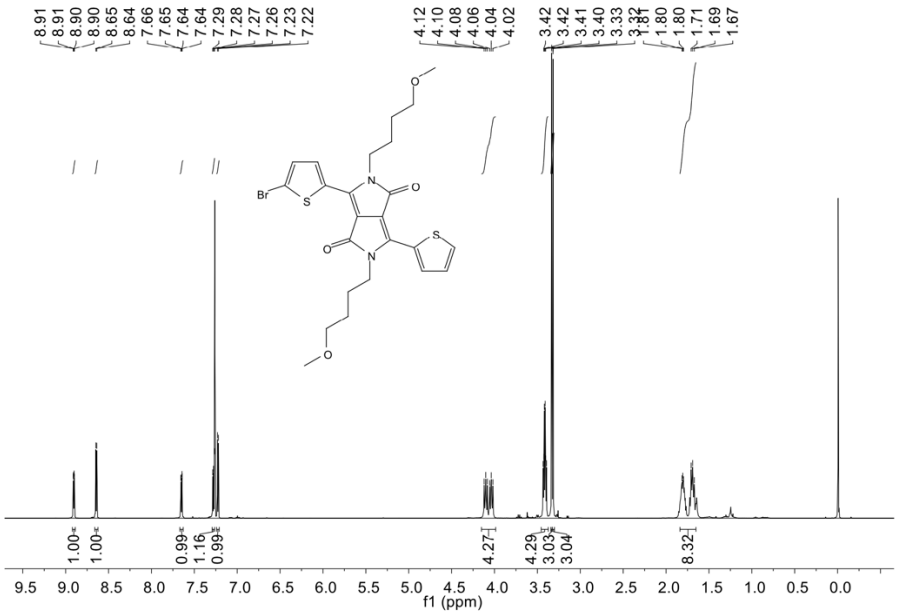


Figure S29. ^{1}H NMR spectrum for **Br-DPP-MOB**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.90 (dd, J = 3.9 Hz, 1.1 Hz, 1H, Th), 8.64 (d, J = 4.2 Hz, 1H, Th), 7.65 (dd, J = 5.0 Hz, 1.1 Hz, 1H, Th), 7.29–7.27 (m, 1H, Th), 7.22 (d, J = 4.2 Hz, 1H, Th), 4.13–4.01 (m, 4H, NCH_2), 3.41 (m, 4H, OCH_2), 3.33 (s, 3H, OCH_3), 3.32 (s, 3H, OCH_3), 1.86–1.60 (m, 8H,

CH_2).

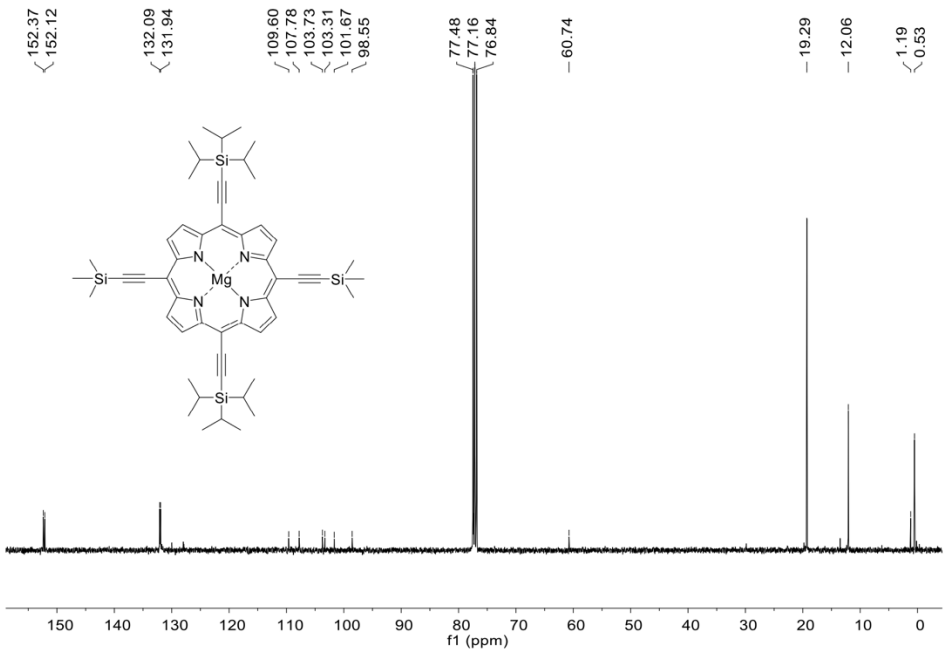


Figure S30. ^{13}C NMR spectrum for **1**.

^{13}C NMR (100 MHz, $CDCl_3$): δ 152.37, 152.12, 132.09, 131.94, 109.60, 107.78, 103.73, 103.31, 101.67, 98.55, 60.74, 19.29, 12.06, 1.19, 0.53.

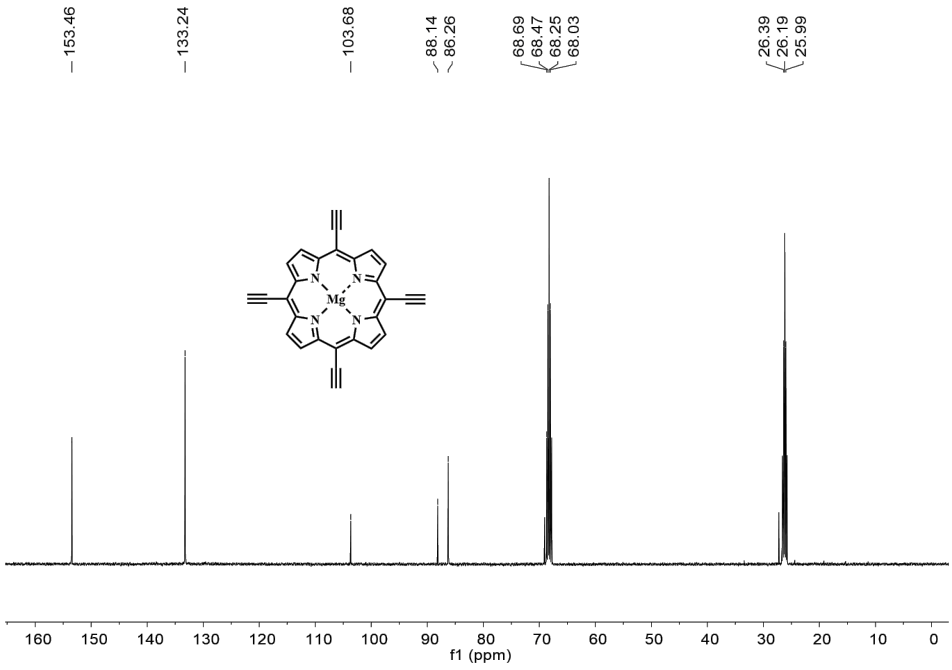


Figure S31. ^{13}C NMR spectrum for **1**.

^{13}C NMR (100 MHz, THF-d_8): δ 153.46, 133.24, 103.68, 88.14, 86.26.

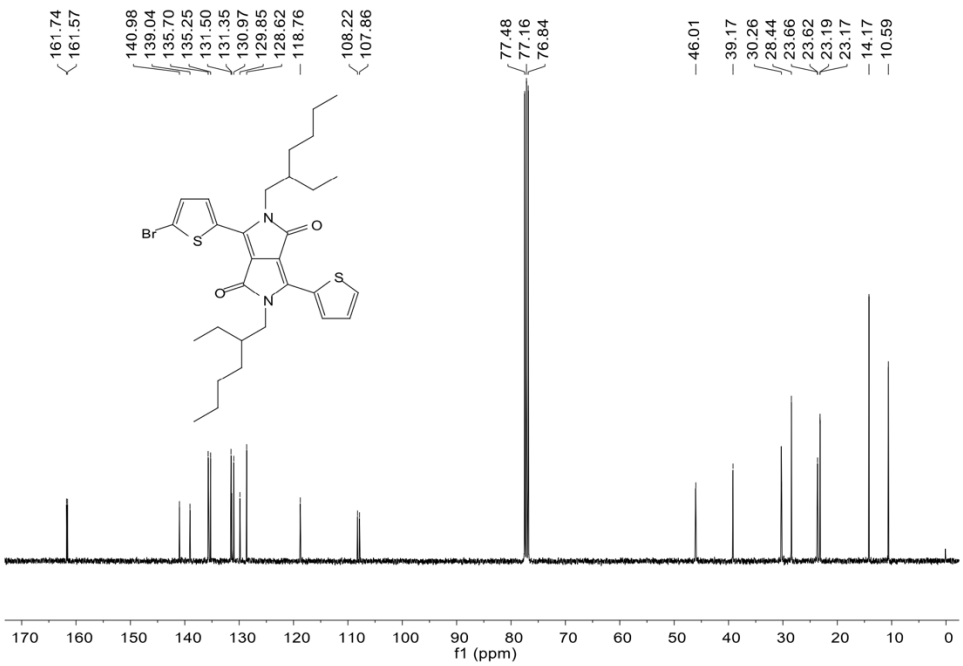


Figure S32. ^{13}C NMR spectrum for **Br-DPP**.

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.74, 161.57, 140.98, 139.04, 135.70, 135.25, 131.50, 131.35, 130.97, 129.85, 128.61, 118.76, 108.22, 107.86, 46.01, 39.17, 30.26, 28.44, 23.66, 23.62, 23.19, 23.17, 14.17, 10.59.

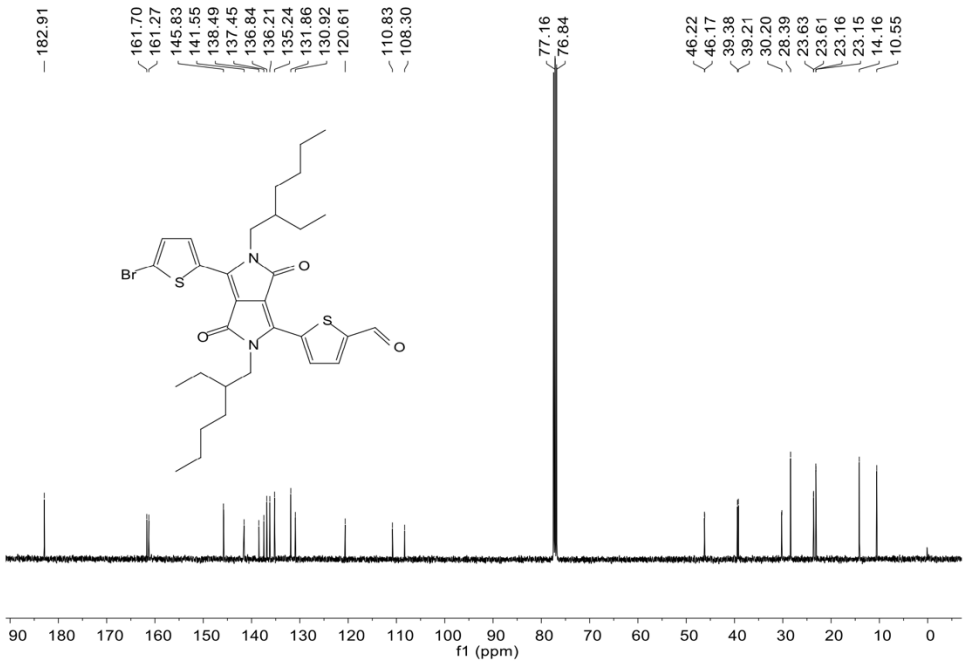


Figure S33. ^{13}C NMR spectrum for **Br-DPP-CHO**.

^{13}C NMR (100 MHz, $CDCl_3$): δ 182.91, 161.70, 161.27, 145.83, 141.55, 138.49, 137.45, 136.84, 136.21, 135.24, 131.86, 130.92, 120.61, 110.83, 108.30, 46.22, 46.17, 39.38, 39.21, 30.20, 28.39, 23.63, 23.61, 23.16, 23.15, 14.16, 10.55.

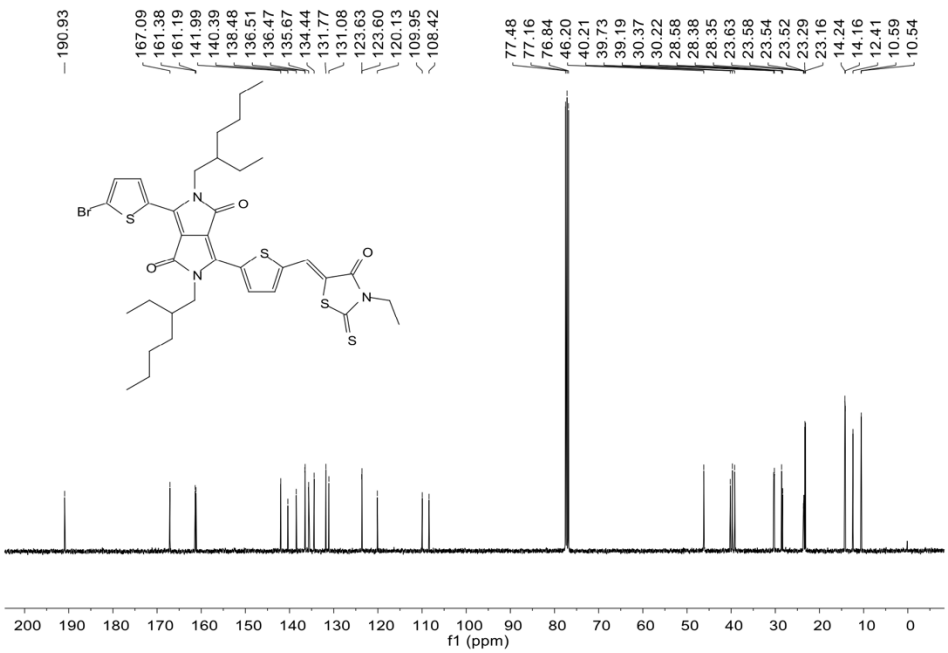


Figure S34. ^{13}C NMR spectrum for **Br-DPP-RHA**.

^{13}C NMR (100 MHz, $CDCl_3$): δ 190.93, 167.09, 161.38, 161.19, 141.99, 140.39, 138.48, 136.51, 136.47, 135.67, 134.44, 131.77, 131.08, 123.63, 123.60, 120.13, 109.95, 108.42, 46.20, 40.21, 39.73, 39.19, 30.37, 30.22, 28.58, 28.38, 28.35, 23.63, 23.58, 23.54, 23.52, 23.29, 23.16, 14.24, 14.16, 12.41, 10.59, 10.54.

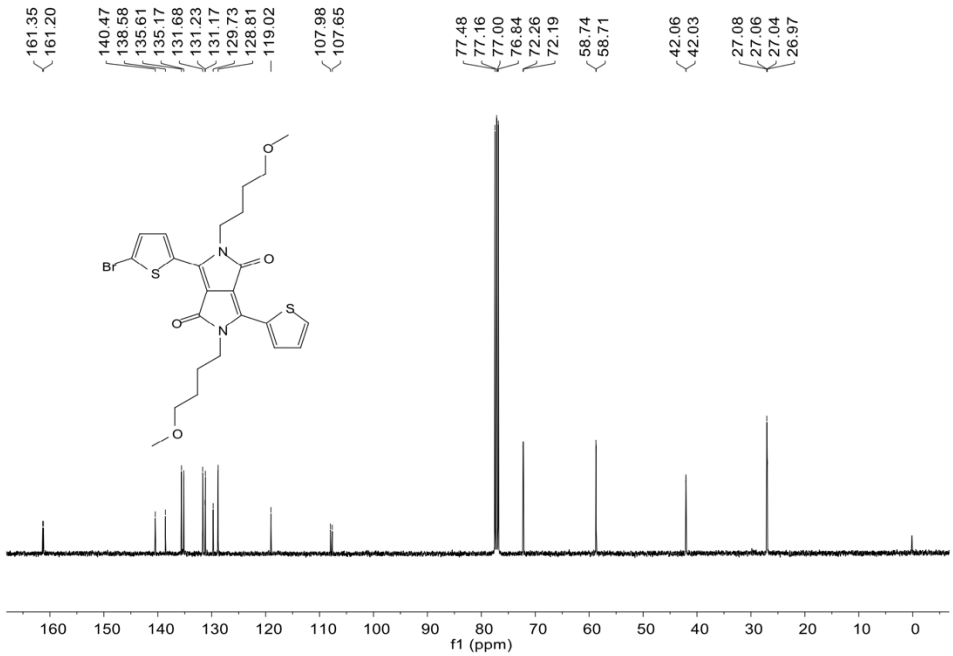


Figure S35. ^{13}C NMR spectrum for **Br-DPP-MOB**.

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.35, 161.20, 140.47, 138.58, 135.61, 135.17, 131.68, 131.23, 131.17, 129.73, 128.81, 119.02, 107.98, 107.65, 72.26, 72.19, 58.74, 58.71, 42.06, 42.03, 27.08, 27.06, 27.04, 26.97.

8. MALDI-TOF HRMS Data

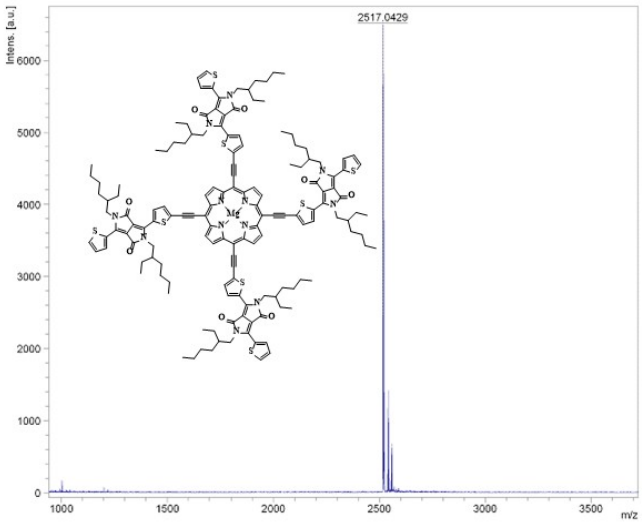


Figure S36. HRMS spectrum for **3a**.

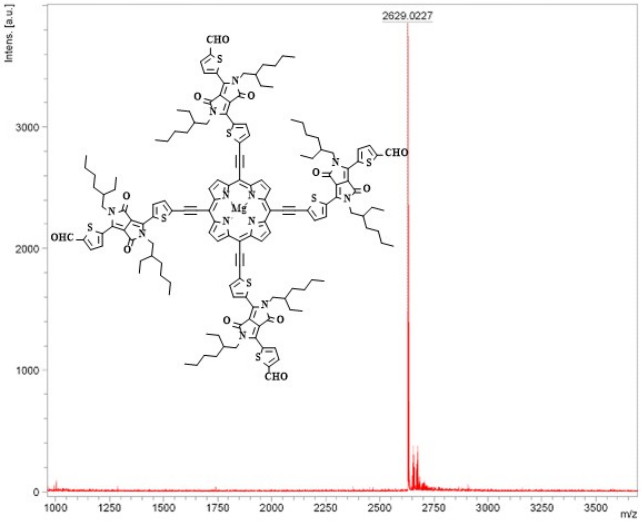


Figure S37. HRMS spectrum for **3b**.

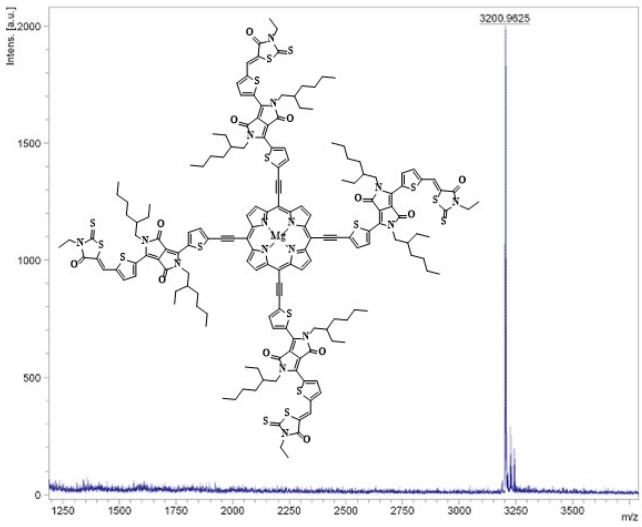


Figure S38. HRMS spectrum for **3c**.

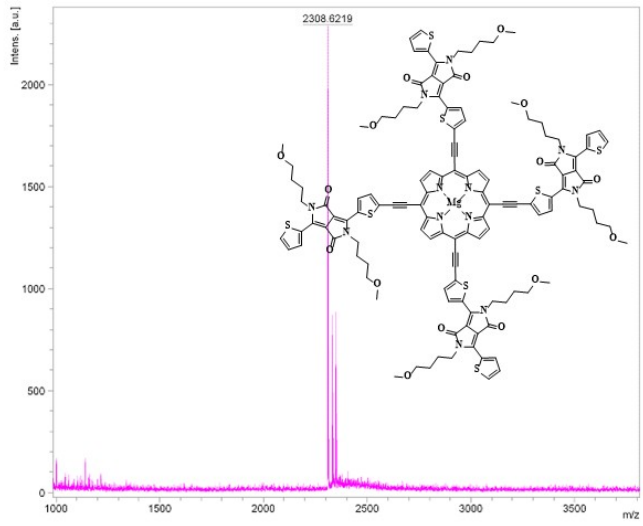


Figure S39. HRMS spectrum for **3d**.

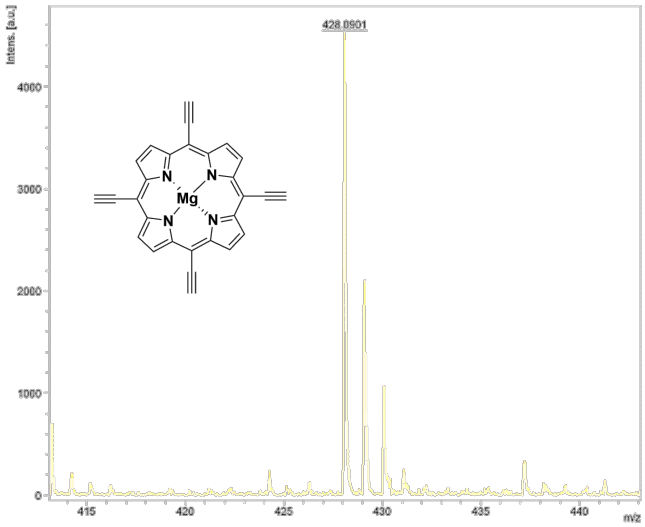


Figure S40. HRMS spectrum for **2**.

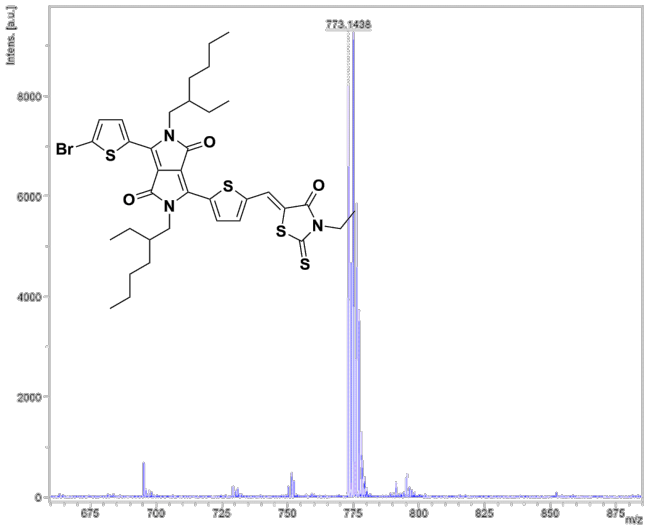


Figure S41. HRMS spectrum for **Br-DPP-RHA**.

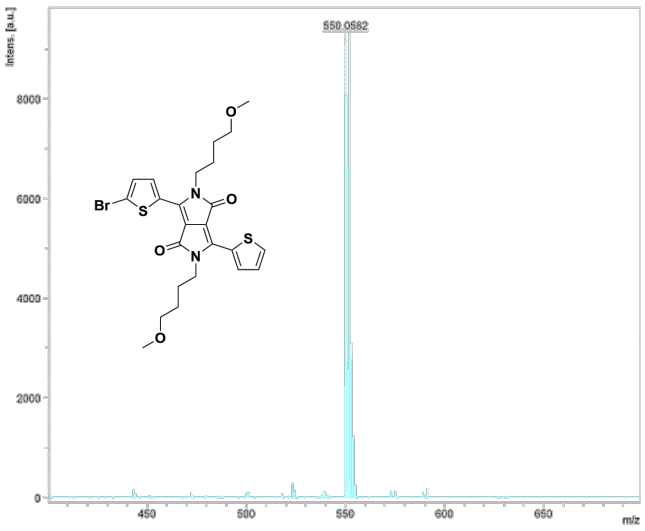


Figure S42. HRMS spectrum for **Br-DPP-MOB**.

9. Computational Calculation

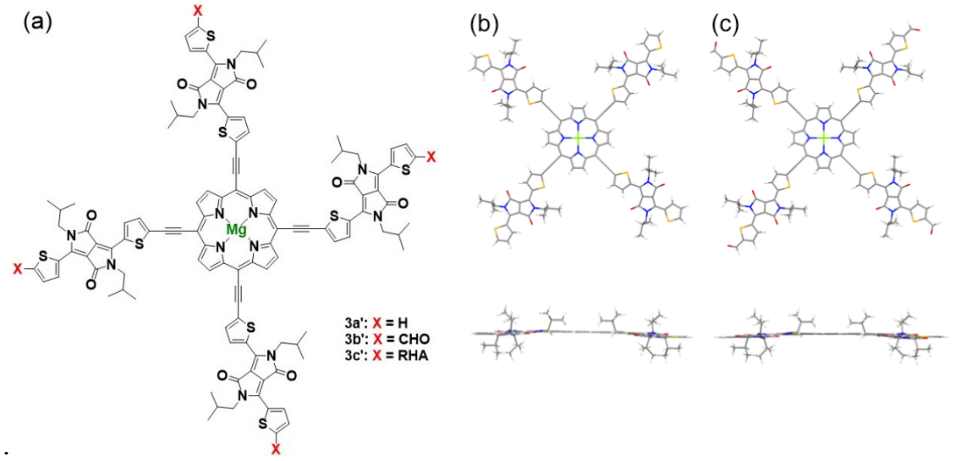


Figure S43. Calculated structures for **3a'–c'** (a) and optimized structures for **3a'** (b) and **3b'** (c) as top and side view (for **3c'**, see Figure 8). Calculations were carried out by using Gaussian09[9] package at the B3LYP/6-31G(d) level.

Table S7. Calculated energies and the numbers of imaginary frequency for the optimized structures.

	Number of imaginary frequencies	free energy[a]/ Hartree	HOMO/ Hartree	LUMO/ Hartree
3a'	0	–9123.294193	–0.17242	–0.11533
3b'	0	–9576.573404	–0.18481	–0.12892
3c'	0	–13755.062886	–0.18335	–0.13028

[a] in standard conditions.

Table S8. Cartesian coordinates for the optimized structures.

3a'

Symbol	X	Y	Z
C	0.023381	–0.001906	–0.022580
C	0.023091	–0.000785	1.342415
C	1.400569	–0.002224	1.760065
N	2.221664	–0.004499	0.660357
C	1.400923	–0.003860	–0.439661
C	4.974621	–0.004940	–3.607263
C	3.609624	–0.005215	–3.607552
C	3.191979	–0.005676	–2.230068
N	4.291684	–0.006046	–1.408971
C	5.391697	–0.005126	–2.229715
C	1.839287	–0.004119	–1.792213
C	8.559294	–0.001185	1.343985
C	8.559591	–0.002235	–0.021011
C	7.182108	–0.004093	–0.438662
N	6.361009	–0.004538	0.661045
C	7.181750	–0.002290	1.761059
C	6.744242	–0.003752	–1.791361
C	3.608055	0.001904	4.928664
C	4.973050	0.001527	4.928962
C	5.390705	–0.001266	3.551482
N	4.290998	–0.002963	2.730386
C	3.190980	–0.000594	3.551120

C	1.838440	0.000161	3.112763
C	6.743405	–0.000429	3.113602
C	7.745909	0.000893	–2.792093
C	0.836759	0.006574	4.113471
C	8.603554	0.007453	–3.662485
C	–0.021076	0.014689	4.983661
C	9.594842	0.019829	–4.647371
C	–1.013084	0.028040	5.967811
C	0.838556	0.000197	–2.793881
Mg	4.291339	–0.004633	0.660708
C	7.744158	0.005499	4.115241
C	8.614631	0.013114	4.972794
C	–0.031707	0.006386	–3.651661
C	9.599429	0.026059	5.964163
C	–7.184700	0.494757	–13.96530
C	–5.823628	0.453334	–14.11992
C	–5.127166	0.430314	–12.88789
C	–5.959152	0.459137	–11.77509
S	–7.642862	0.513135	–12.30024
C	–5.486591	0.410086	–10.41126
C	–4.153257	0.257655	–10.01143
C	–4.083972	0.213432	–8.594920
C	–5.426795	0.340639	–8.076360
N	–6.248447	0.470770	–9.243617
C	–2.808597	0.136258	–10.53127
N	–1.987213	0.010871	–9.361614
C	–2.751452	0.070075	–8.194934
O	–2.338325	0.133977	–11.66751
O	–5.900873	0.342286	–6.941096
C	–7.684920	0.664146	–9.037820
C	–0.549123	–0.186918	–9.527729
C	–2.270976	0.032563	–6.839723
C	–3.095430	0.050577	–5.714388
C	–2.398584	0.039560	–4.497148
C	–1.016277	0.017489	–4.643280
S	–0.582042	0.006114	–6.343504
C	–8.074780	2.092727	–8.600619
C	–7.688818	3.167479	–9.624226
C	–9.578431	2.128078	–8.291435
H	–6.618142	3.144191	–9.854673
H	–9.850010	1.389595	–7.527919
C	–0.067900	–1.648766	–9.399417
C	–0.743371	–2.572909	–10.42141
C	1.460886	–1.680056	–9.541100
H	–1.829372	–2.601164	–10.28484
H	1.950776	–1.053597	–8.785773
C	10.981707	0.047913	5.817836
C	11.678687	0.061144	7.034982
C	10.854373	0.044940	8.160442
S	9.165386	0.017664	7.664470
C	11.335068	0.084659	9.515519
C	12.667634	0.228932	9.914989
C	12.737230	0.275256	11.331411
C	11.392714	0.154383	11.851753
N	10.571086	0.027067	10.682473
C	14.010413	0.354794	9.395958
N	14.832363	0.486250	10.562862
C	14.070701	0.427616	11.730746
O	14.484212	0.354881	8.260582
O	10.922731	0.153847	12.988109
C	9.133081	–0.170786	10.849234
C	16.268667	0.680209	10.356446
C	14.543555	0.478144	13.094429
C	13.711709	0.452502	14.207395
C	14.408425	0.476053	15.439280

C	15.769547	0.514640	15.284370
S	16.227454	0.529625	13.619200
C	8.652248	–1.632911	10.723019
C	9.328403	–2.555404	11.746069
C	7.123526	–1.664577	10.865310
H	10.414358	–2.583572	11.609095
H	6.633122	–1.039292	10.109345
C	16.657678	2.108639	9.918002
C	16.271695	3.183926	10.941044
C	18.161182	2.144435	9.608134
H	15.201069	3.160589	11.171719
H	18.432733	1.405540	8.845010
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H	–0.828565	0.001161	2.007646
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H	2.944374	–0.004736	–4.459198
H	9.409997	0.000492	2.010252
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H	2.941782	0.003921	5.779361
H	5.638287	0.003328	5.780614
H	–5.331910	0.439135	–15.08619
H	–4.046526	0.384960	–12.79574
H	–8.224929	0.369421	–9.938296
H	–7.972146	–0.033289	–8.245052
H	–0.331310	0.175822	–10.53664
H	–0.012434	0.461602	–8.828123
H	–4.177453	0.080145	–5.799734
H	–7.530737	2.289380	–7.668710
H	–8.238834	3.042587	–10.56479
H	–7.920102	4.165436	–9.234199
H	–9.874924	3.115584	–7.920841
H	–10.17452	1.919704	–9.189800
H	–0.322753	–2.008274	–8.393303
H	–0.546901	–2.240560	–11.44701
H	–0.367994	–3.597257	–10.31464
H	1.840816	–2.701059	–9.426166
H	1.771426	–1.318883	–10.52992
H	12.760722	0.090853	7.120157
H	8.915503	0.193221	11.857742
H	8.596009	0.476718	10.148978
H	16.809153	0.386535	11.256970
H	16.555934	–0.017741	9.564160
H	12.630984	0.408765	14.115483
H	13.916850	0.464250	16.405658
H	8.906876	–1.993701	9.717304
H	9.132255	–2.221594	12.771255
H	8.953261	–3.580012	11.640973
H	6.743968	–2.685884	10.751842
H	6.813195	–1.302237	11.853767
H	16.113164	2.304409	8.986174
H	16.821920	3.059665	11.881577
H	16.502715	4.181705	10.550404
H	18.457078	3.131816	9.236732
H	18.757770	1.936943	10.506375
H	16.534657	0.538693	16.049165
H	11.460738	0.054720	4.845731
H	–2.877708	0.048134	–3.525104
H	–7.949637	0.519108	–14.73026
C	–0.867819	0.051545	7.350169
S	–2.713071	0.018079	5.532497
C	–2.085502	0.064804	8.046216
C	–3.210335	0.047060	7.221072
C	–4.565807	0.086750	7.700645
C	–4.966458	0.232638	9.032680
N	–5.732096	0.027664	6.935768

C	–6.382955	0.278567	9.101024
C	–4.448581	0.360791	10.375688
C	–6.902110	0.155698	7.756227
C	–6.783441	0.432961	10.433927
C	–5.897533	–0.172381	5.497904
N	–5.616196	0.493202	11.196445
C	–5.411107	0.688818	12.632707
C	–8.147526	0.484069	10.905546
C	–5.770110	–1.635138	5.019333
C	–4.972831	2.117646	13.020449
C	–9.259772	0.456170	10.072803
S	–8.673787	0.539467	12.588871
C	–10.49226	0.481040	10.768387
C	–10.33854	0.522920	12.129546
C	–6.793452	–2.557160	5.695707
C	–5.910682	–1.669158	3.490507
C	–5.995161	3.192675	12.631870
C	–4.664761	2.155280	14.524279
O	–3.313606	0.361819	10.850451
O	–8.038074	0.153989	7.285289
H	0.103914	0.059551	7.829935
H	–2.171510	0.095771	9.128148
H	–4.764497	–1.995063	5.275578
H	–5.197131	0.474705	4.960520
H	–5.154472	–1.044240	3.000015
H	–5.796282	–2.690980	3.112621
H	–6.906033	0.190809	5.278914
H	–6.898971	–1.307786	3.178517
H	–6.657797	–2.583553	6.781868
H	–6.687313	–3.582292	5.322294
H	–7.818592	–2.224254	5.497783
H	–4.040327	2.312525	12.476785
H	–4.619197	–0.008891	12.921614
H	–6.224485	3.168035	11.560983
H	–9.166924	0.410005	8.992257
H	–6.312195	0.395910	13.172667
H	–5.604572	4.190651	12.862127
H	–3.902361	1.416341	14.797753
H	–6.936407	3.069337	13.181077
H	–4.293169	3.142849	14.819304
H	–5.563835	1.949063	15.120049
H	–11.45821	0.467803	10.275998
H	–11.10401	0.548594	12.893935
C	9.448470	0.041333	–6.029645
S	11.295180	0.010972	–4.213390
C	10.665600	0.053945	–6.726682
C	11.791075	0.037635	–5.902402
C	13.146160	0.077025	–6.383102
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N	14.313061	0.018770	–5.619102
C	14.962142	0.267888	–7.785101
C	13.026720	0.348968	–9.058252
C	15.482410	0.146071	–6.440630
C	15.361527	0.421370	–9.118435
C	14.479716	–0.181081	–4.181357
N	14.193665	0.480962	–9.880059
C	13.987311	0.675772	–11.31626
C	16.725227	0.472023	–9.591241
C	14.352313	–1.643719	–3.702426
C	13.548714	2.104388	–11.70442
C	17.838199	0.444766	–8.759451
S	17.249995	0.525865	–11.27507
C	19.070078	0.468905	–9.456151
C	18.915163	0.509588	–10.81721
C	15.374677	–2.566167	–4.379681

C	14.494460	–1.677503	–2.173732
C	14.571570	3.179573	–11.31767
C	13.238987	2.141080	–13.20793
O	11.891357	0.349551	–9.532074
O	16.618756	0.144767	–5.970623
H	8.476352	0.048331	–6.508647
H	10.750742	0.083516	–7.808720
H	13.346324	–2.003374	–3.957576
H	13.780043	0.466309	–3.643381
H	13.739069	–1.052116	–1.682570
H	14.379951	–2.699192	–1.795520
H	15.488532	0.181846	–3.963406
H	15.483249	–1.316547	–1.862849
H	15.237737	–2.592902	–5.465679
H	15.268769	–3.591155	–4.005812
H	16.400114	–2.233403	–4.183058
H	12.616798	2.299692	–11.15989
H	13.195126	–0.022099	–11.60400
H	14.802218	3.155561	–10.24705
H	17.746287	0.399551	–7.678786
H	14.887917	0.382522	–11.85684
H	14.180794	4.177449	–11.54803
H	12.475888	1.402347	–13.47998
H	15.512141	3.055811	–11.86794
H	12.867618	3.128640	–13.50327
H	14.137279	1.933947	–13.80457
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H	19.679957	0.534491	–11.58229

3b'

Symbol	X	Y	Z
C	0.003425	0.121497	0.001300
C	0.003737	0.125951	1.366094
C	1.381621	0.117169	1.783077
N	2.202179	0.107135	0.683257
C	1.381021	0.110138	–0.416208
C	4.953182	0.078569	–3.585712
C	3.588413	0.087236	–3.585426
C	3.171464	0.092960	–2.207521
N	4.271284	0.087620	–1.386916
C	5.370719	0.079205	–2.208078
C	1.819151	0.103991	–1.768754
C	8.540265	0.072897	1.364160
C	8.539949	0.067981	–0.000630
C	7.162052	0.073639	–0.417592
N	6.341476	0.081598	0.682237
C	7.162651	0.081616	1.781691
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C	4.955293	0.106751	4.950924
C	5.372219	0.097939	3.573028
N	4.272384	0.101094	2.752429
C	3.172968	0.112421	3.573577
C	1.820433	0.120424	3.135415
C	6.724533	0.089401	3.134250
C	7.724354	0.067158	–2.771117
C	0.819335	0.135698	4.136484
C	8.581387	0.064325	–3.642055
C	–0.037961	0.151496	5.007024
C	9.571337	0.064769	–4.628116
C	–1.028593	0.173764	5.992148
C	0.818146	0.112086	–2.770002
Mg	4.271828	0.094282	0.682755
C	7.725766	0.091198	4.135303
C	8.596828	0.094958	4.992206

C	–0.052139	0.121549	–3.627649
C	9.583162	0.103223	5.981849
C	–7.221175	0.572499	–13.92120
C	–5.846784	0.556720	–14.07041
C	–5.152215	0.546927	–12.84841
C	–5.995628	0.559447	–11.73575
S	–7.677821	0.580858	–12.24264
C	–5.518478	0.520667	–10.37258
C	–4.182509	0.374979	–9.977587
C	–4.108990	0.332700	–8.563891
C	–5.451257	0.457055	–8.039840
N	–6.277146	0.580138	–9.202824
C	–2.834694	0.254254	–10.50011
N	–2.011035	0.129906	–9.333037
C	–2.773247	0.190341	–8.166657
O	–2.368049	0.254248	–11.63595
O	–5.917130	0.462039	–6.901585
C	–7.713749	0.778458	–8.990058
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C	–2.291363	0.154337	–6.813526
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C	–2.419192	0.168152	–4.471251
C	–1.036665	0.136338	–4.619016
S	–0.602213	0.117136	–6.318172
C	–8.098285	2.212959	–8.568257
C	–7.725432	3.273374	–9.611621
C	–9.598703	2.251098	–8.243485
H	–6.657305	3.248868	–9.854550
H	–9.860829	1.524447	–7.465505
C	–0.087482	–1.525377	–9.376722
C	–0.760496	–2.448928	–10.40092
C	1.441401	–1.552032	–9.518810
H	–1.846451	–2.481681	–10.26449
H	1.929960	–0.926085	–8.762187
C	10.965631	0.120393	5.831121
C	11.665172	0.130297	7.045931
C	10.842594	0.115959	8.173656
S	9.152093	0.094394	7.681959
C	11.327743	0.151729	9.525624
C	12.665544	0.283632	9.919488
C	12.742590	0.329635	11.332874
C	11.394947	0.221969	11.858725
N	10.567629	0.101378	10.693817
C	14.007633	0.394930	9.392074
N	14.837134	0.514717	10.552826
C	14.080626	0.465350	11.724452
O	14.471003	0.392135	8.252791
O	10.930890	0.229021	12.995603
C	9.127316	–0.081365	10.866115
C	16.274916	0.699866	10.336207
C	14.561138	0.504490	13.086428
C	13.720144	0.502111	14.200993
C	14.417497	0.510367	15.421414
C	15.791631	0.514898	15.269104
S	16.244568	0.514302	13.589528
C	8.631486	–1.538917	10.745256
C	9.300761	–2.465677	11.769010
C	7.102924	–1.553425	10.892357
H	10.385956	–2.507146	11.628893
H	6.616758	–0.925411	10.135908
C	16.670804	2.129565	9.908644
C	16.310116	3.196620	10.949534
C	18.170598	2.153586	9.579697
H	15.242600	3.181952	11.195970
H	18.424266	1.422309	8.803251

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H	–0.847723	0.134699	2.031465
H	5.618841	0.072576	–4.436824
H	2.923043	0.089847	–4.436925
H	9.391384	0.071037	2.029833
H	9.391414	0.061552	–0.666018
H	2.924868	0.124036	5.802308
H	5.620697	0.106535	5.802404
H	–5.360563	0.552225	–15.04069
H	–4.071543	0.521306	–12.75562
H	–8.260548	0.472997	–9.882441
H	–7.994152	0.090680	–8.186834
H	–0.355472	0.301438	–10.50963
H	–0.037064	0.584873	–8.801261
H	–4.198150	0.216645	–5.772878
H	–7.544105	2.423247	–7.645166
H	–8.287626	3.135744	–10.54303
H	–7.952846	4.276266	–9.232444
H	–9.891719	3.244060	–7.885165
H	–10.20398	2.028433	–9.131872
H	–0.341418	–1.888010	–8.371484
H	–0.564478	–2.114152	–11.42581
H	–0.382094	–3.472232	–10.29644
H	1.823641	–2.572343	–9.406397
H	1.750761	–1.187920	–10.50683
H	12.747714	0.155612	7.128846
H	8.916283	0.287924	11.873947
H	8.595867	0.570610	10.165852
H	16.821105	0.392694	11.228379
H	16.547583	0.007019	9.534675
H	12.639097	0.484684	14.110695
H	13.933432	0.512799	16.392771
H	8.879469	–1.905211	9.739862
H	9.110904	–2.127319	12.793887
H	8.914064	–3.486212	11.667918
H	6.712311	–2.570957	10.783592
H	6.799766	–1.184564	11.880545
H	16.115926	2.341611	8.986377
H	16.874136	3.057431	11.879607
H	16.544786	4.196255	10.566192
H	18.471306	3.142850	9.217535
H	18.776301	1.928361	10.467153
C	16.809529	0.523637	16.311317
H	11.441994	0.126578	4.857804
H	–2.897500	0.182604	–3.498974
C	–8.236669	0.585880	–14.96570
C	–0.879571	0.202244	7.374616
S	–2.728160	0.170635	5.558873
C	–2.095234	0.225041	8.072395
C	–3.221944	0.209811	7.248439
C	–4.574342	0.257474	7.731339
C	–4.969328	0.402855	9.067416
N	–5.741749	0.207556	6.969954
C	–6.382529	0.457636	9.141979
C	–4.443189	0.522126	10.409329
C	–6.907090	0.341846	7.794513
C	–6.775232	0.606450	10.478289
C	–5.913071	0.013952	5.530940
N	–5.604418	0.655318	11.236100
C	–5.388940	0.851197	12.672611
C	–8.137649	0.657190	10.956472
C	–5.799726	–1.448284	5.047322
C	–4.954513	2.281819	13.057538
C	–9.250966	0.654883	10.113834
S	–8.643174	0.682403	12.639033

C	–10.47235	0.675276	10.809250
C	–10.32205	0.689167	12.183542
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C	–5.943154	–1.474558	3.518557
C	–5.988546	3.351472	12.685050
C	–4.629418	2.316657	14.557966
O	–3.304600	0.516704	10.874374
O	–8.043249	0.351733	7.328737
H	0.093139	0.207186	7.852234
H	–2.179464	0.260242	9.154563
H	–4.797152	–1.818533	5.300803
H	–5.208386	0.657586	4.995177
H	–5.181758	–0.855118	3.029116
H	–5.839532	–2.495942	3.136714
H	–6.918499	0.387212	5.315458
H	–6.928362	–1.102372	3.209822
H	–6.693664	–2.396831	6.807390
H	–6.734568	–3.387716	5.343484
H	–7.853011	–2.020666	5.526094
H	–4.029614	2.484214	12.503410
H	–4.591522	0.156364	12.952204
H	–6.231116	3.330029	11.616769
H	–9.159152	0.628785	9.033090
H	–6.283589	0.553217	13.219839
H	–5.600909	4.350866	12.913601
H	–3.858119	1.582872	14.819959
H	–6.921375	3.221271	13.246642
H	–4.262024	3.306234	14.851189
H	–5.519815	2.101997	15.163191
H	–11.44296	0.679628	10.323702
C	–11.36572	0.711344	13.199743
C	9.421233	0.084678	–6.010615
S	11.271151	0.040100	–4.196518
C	10.636315	0.084225	–6.709754
C	11.763609	0.058956	–5.886836
C	13.116004	0.082766	–6.371551
C	13.511425	0.210685	–7.709290
N	14.283494	0.022401	–5.611074
C	14.925199	0.244041	–7.785935
C	12.985463	0.326018	–9.051609
C	15.449663	0.132417	–6.438087
C	15.318394	0.375465	–9.123913
C	14.453774	–0.159699	–4.170430
N	14.147506	0.434899	–9.880827
C	13.932905	0.621435	–11.31875
C	16.680817	0.402071	–9.604012
C	14.321859	–1.615589	–3.672587
C	13.518117	2.054746	–11.71517
C	17.795100	0.390362	–8.762723
S	17.184390	0.406146	–11.28731
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C	18.863794	0.392056	–10.83395
C	15.338571	–2.551118	–4.340390
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C	14.568766	3.112532	–11.35550
C	13.188652	2.080994	–13.21481
O	11.846338	0.333405	–9.515327
O	16.586406	0.129927	–5.973652
H	8.448173	0.100132	–6.487296
H	10.719783	0.109584	–7.792253
H	13.313746	–1.974601	–3.920174
H	13.758016	0.498143	–3.640316
H	13.717116	–0.994299	–1.658849
H	14.351432	–2.645162	–1.751962
H	15.464193	0.202425	–3.959307

H	15.459638	–1.267863	–1.841089
H	15.198317	–2.592971	–5.425547
H	15.229507	–3.570311	–3.952322
H	16.366000	–2.220438	–4.150852
H	12.598081	2.275314	–11.15993
H	13.125293	–0.064345	–11.59132
H	14.816255	3.095485	–10.28826
H	17.704381	0.374593	–7.681687
H	14.822407	0.306166	–11.86467
H	14.193967	4.115550	–11.58953
H	12.405193	1.356942	–13.46764
H	15.496968	2.965329	–11.92058
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H	14.073637	1.847010	–13.82080
H	19.986938	0.381266	–8.975465
C	19.906271	0.390809	–11.85161
O	19.701595	0.398809	–13.05421
H	20.938202	0.381574	–11.44042
O	18.012081	0.530535	16.106318
H	16.398564	0.523408	17.343379
O	–11.16249	0.725922	14.402528
H	–12.39714	0.713969	12.787196
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3c'

Symbol	X	Y	Z
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N	2.204104	0.149120	0.661055
C	1.389103	0.151087	–0.442996
C	4.979246	0.148844	–3.592483
C	3.614422	0.149733	–3.599864
C	3.189698	0.148715	–2.224373
N	4.284908	0.146849	–1.397593
C	5.388959	0.147416	–2.212596
C	1.834770	0.151312	–1.793108
C	8.538447	0.147897	1.377544
C	8.545827	0.147211	0.012720
C	7.170336	0.146278	–0.412001
N	6.343556	0.146012	0.683210
C	7.158559	0.147500	1.787260
C	6.739073	0.147520	–1.766930
C	3.568422	0.152933	4.936747
C	4.933246	0.151674	4.944128
C	5.357966	0.149027	3.568639
N	4.262754	0.148282	2.741860
C	3.158706	0.151166	3.556861
C	1.808593	0.153069	3.111194
C	6.712894	0.149283	3.137374
C	7.746150	0.152184	–2.761854
C	0.801522	0.160164	4.106106
C	8.610668	0.159075	–3.625480
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C	9.613442	0.171526	–4.598106
C	–1.065806	0.184219	5.942265
C	0.839868	0.157634	–2.800197
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C	7.707828	0.154726	4.144435
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C	–7.039838	0.673117	–14.08750
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C	–5.846431	0.635196	–11.85190
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C	–5.393780	0.587292	–10.48648
C	–4.063538	0.435084	–10.06995
C	–4.012534	0.386478	–8.656366
C	–5.362772	0.511926	–8.152427
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C	–0.996151	0.180189	–4.667681
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C	–7.600403	3.344177	–9.723377
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C	–0.649118	–2.399602	–10.44791
C	1.542432	–1.516282	–9.527378
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C	10.769452	0.195397	8.223037
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C	11.231675	0.235253	9.582310
C	12.562019	0.379363	9.999302
C	12.613523	0.428250	11.412857
C	11.259049	0.308549	11.916067
N	10.452753	0.179634	10.737845
C	13.912235	0.503205	9.494908
N	14.719848	0.634280	10.669209
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C	9.196156	–2.402526	11.792308
C	7.005148	–1.516791	10.872770
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H	–0.838138	0.155643	–0.703775
H	–0.853413	0.156469	1.992063
H	5.649737	0.149369	–4.439841
H	2.953902	0.151334	–4.455116

H	9.385806	0.148842	2.048032
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C	–3.277458	0.206947	7.167099
C	–4.636784	0.248329	7.629032
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C	–4.549679	0.518923	10.309337
C	–6.970487	0.323494	7.655882
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C	–5.535235	0.848832	12.555750
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C	–9.353896	0.623707	9.937650
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H	–5.232364	0.637105	4.881112
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C	–11.47891	0.717591	13.014231
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S	11.306767	0.157672	–4.140769
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C	19.136146	0.614484	–9.256510
C	19.032452	0.650912	–10.64415
C	15.391844	–2.412101	–4.249327
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O	16.647936	0.300022	–5.829984
H	8.518733	0.207999	–6.474342
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H	14.991374	0.529714	–11.74176
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H	12.991131	3.275719	–13.41136
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H	20.080851	0.602690	–8.726473
C	20.026945	0.679570	–11.67136
C	16.500391	0.696482	17.778919
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C	17.709798	0.728416	18.630683
C	16.010203	0.695669	20.289545
N	17.347848	0.716647	19.993823
C	18.401812	0.758533	21.021106
C	18.784890	2.188646	21.400097
O	18.867229	0.759034	18.249743
S	15.300983	0.688072	21.777711
H	17.650434	0.717311	16.076320
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O	–13.30526	0.786219	15.262388
S	–16.83261	0.714770	11.695546
H	–11.13164	0.741739	14.046045
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S	–6.502951	0.677256	–17.44070
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S	22.385757	0.652913	–10.10794
C	22.234021	0.712076	–12.76224
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C	25.004713	2.169870	–13.83727
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S	25.380729	0.669551	–10.35304
H	19.679641	0.703203	–12.70317
H	24.197613	0.209966	–14.30788
H	24.134251	2.714281	–14.21585
H	25.487557	0.187775	–13.07799
H	25.419479	2.708508	–12.98019
H	25.763394	2.146336	–14.62701

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