Supplementary Information

Intramolecular [2+2+2] cycloaddition of dialkynylcarbodiimides: synthesis of L-shaped π -extended compounds with pyrrolo[1,2-*a*][1,8]naphthyridine corner units

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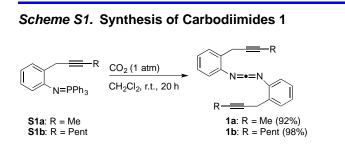
1. Synthesis

1.1 General Information

All melting points were determined on a Yanaco melting point apparatus and are uncorrected. Infrared spectra were recorded on a Horiba FT-710 model spectrophotometer. ¹H and ¹³C NMR spectral data were obtained with a Bruker Avance-600, a JEOL JNM-LA 500, or a JEOL JNM-AL 300 instrument and chemical shifts are reported in ppm down field from tetramethylsilane (TMS) using an internal standard of TMS, CDCl₃, or CD₂Cl₂. Accurate mass was measured by high-resolution electrospray ionization (ESI) mass to determine an elemental formula by comparing calculated exact mass. The elemental analyses (C, H, and N) were performed at the Advanced Technology Support of RIKEN Advanced Science Institute and the Microanalytical Laboratory of the University of Tokyo. Iminophosphoranes **S1a**^{S1} and **S1b**, ^{S1} and 3-azido-2-naphthalenecarboxaldehyde (**S3**)^{S2} were synthesized according to procedures previously described in the literature.

1.2 Synthesis of Carbodiimides

1.2.1 Synthesis of Carbodiimides 1



Bis[2-(2-butyn-1-yl)phenyl]carbodiimide (1a). A dichloromethane (40 mL) solution of iminophosphorane S1a (1.85 g, 4.6 mmol) was degassed, charged with CO₂, and stirred for 20 h at room temperature. The reaction mixture was evaporated, and the residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/10) to give carbodiimide 1a (624 mg, 92%) as a colorless oil: IR (neat): 2915, 2298, 2144, 1589, 1488, 1172, 1087 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ): 7.52 (d, *J* = 7.6 Hz, 2H), 7.22–7.20 (m, 4H), 7.18–7.14 (m, 2H), 3.64 (q, *J* = 2.5 Hz, 4H), 1.84 (t, *J* = 2.5 Hz, 6H); ¹³C NMR (151 MHz, CDCl₃, δ): 136.3 (C × 2), 133.6 (C), 131.7 (C × 2), 129.3 (CH × 2), 127.7 (CH × 2), 125.6 (CH × 2), 124.7 (CH × 2), 84.1 (C × 2), 76.1 (C × 2), 21.6 (CH₂ × 2), 13.7 (CH₃ × 2); HRMS (ESI) calcd for C₂₁H₁₉N₂ [M + H]⁺: 299.1543, found 299.1550.

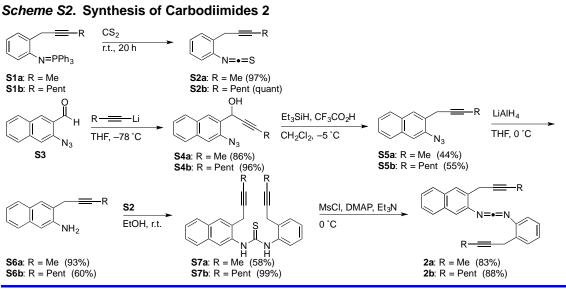
Bis[2-(2-octyn-1-yl)phenyl]carbodiimide (1b). The title compound (160 mg, 98%) was synthesized from **S1b** (369 mg, 0.80 mmol) using the same procedure described above. Colorless oil: IR (neat): 2931, 2298, 2152, 1581, 1481, 1172, 1087 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, δ): 7.55 (d, J = 7.2 Hz, 2H), 7.22–7.12 (m, 6H), 3.66 (t, J = 2.3 Hz, 4H), 2.21 (tt, J = 2.3, 7.1 Hz, 4H), 1.58–1.47 (m, 4H), 1.43–1.25 (m, 8H), 0.90 (t, J = 7.0 Hz, 6H); ¹³C NMR (75 MHz, CDCl₃, δ): 136.3 (C × 2), 133.5 (C), 131.8 (C × 2), 129.2 (CH

^{S1} T. Saito, N. Furukawa and T. Otani, *Org. Biomol. Chem.*, 2010, **8**, 1126–1132.

^{S2} H. Tomioka, N. Nakane and J. Tatsugi, *Bull. Chem. Soc. Jpn.*, 2008, **81**, 1629–1637.

× 2), 127.6 (CH × 2), 125.6 (CH × 2), 124.6 (CH × 2), 83.2 (C × 2), 76.6 (C × 2), 31.1 (CH₂ × 2), 28.7 (CH₂ × 2), 22.2 (CH₂ × 2), 21.6 (CH₂ × 2), 18.8 (CH₂ × 2), 14.0 (CH₃ × 2); HRMS (ESI) calcd for $C_{29}H_{35}N_2$ [M + H]⁺: 411.2795, found 411.2794.

1.2.2 Synthesis of Carbodiimides 2



2-(2-Butyn-1-yl)phenyl isothiocyanate (S2a). Iminophosphorane S1a (810 mg, 2.00 mmol) was dissolved in carbon disulfide (5 mL) and the solution was stirred for 20 h. The reaction mixture was concentrated in vacuo, and the residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/10) to give isothiocyanate S2a (364 mg, 97%) as a

colorless oil: IR (neat): 2915, 2090, 1589, 1481, 1419, 1280, 1095 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, δ): 7.54–7.52 (m, 1H), 7.28–7.22 (m, 3H), 3.61 (q, J = 2.4 Hz, 2H), 1.87 (t, J = 2.4 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃, δ): 139.1 (C), 133.9 (C), 129.7 (C), 129.3 (CH), 127.8 (CH), 127.5 (CH), 126.4 (CH), 79.1 (C), 74.6 (C), 22.1 (CH₂), 3.6 (CH₃); HRMS (ESI) calcd for C₁₁H₉NSNa [M + Na]⁺: 210.0348, found 210.0348.

2-(2-Octyn-1-yl)phenyl isothiocyanate (S2b). The title compound (2.23 g, quant) was obtained from

S N=C=S

S1b (4.14 g, 8.97 mmol) and carbon disulfide (20 mL) using the same procedure described above. Colorless oil: IR (neat): 2931, 2098, 1581, 1481, 1218, 1172, 1095 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, δ): 7.53 (d, J = 7.1 Hz, 1H), 7.27–7.19 (m, 3H), 3.62

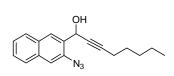
(t, J = 2.4 Hz, 2H), 2.22 (tt, J = 2.4, 7.2 Hz, 2H), 1.57–1.49 (m, 2H), 1.41–1.30 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H); ¹³C NMR (76 MHz, CDCl₃, δ): 134.0 (C), 129.6 (C), 129.2 (CH), 127.7 (CH), 127.6 (C), 127.5 (CH), 126.3 (CH), 83.9 (C), 75.4 (C), 31.1 (CH₂), 28.6 (CH₂), 22.21 (CH₂), 22.18 (CH₂), 18.8 (CH₂), 14. 0 (CH₃); HRMS (ESI) calcd for C₁₅H₁₇NSNa [M + Na]⁺: 266.0974, found 266.0978.

3-Azido- α -(1-propyn-1-yl)-2-naphthalenemethanol (**S4a**). To a THF (10 mL) solution of 1-bromo-1-propene (0.68 mL, 7.98 mmol) was added 1.66 M hexane solution of *n*-butyllithium (7.05 mL, 11.7 mmol) at -78 °C. The mixture was stirred for 2 h, and a THF (10 mL) solution of 3-azido-2-naphthalenecarboxaldehyde (**S3**) (1.05 g, 5.32 mmol) was added. The mixture was stirred for 20 min, and the reaction was guenched by addition of

saturated aqueous ammonium chloride. The mixture was extracted with dichloromethane, washed with brine,

dried over anhydrous magnesium sulfate, and evaporated. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/10) to give alkynyl azide **S4a** (1.08 g, 86%) as a colorless solid: Mp 80.2–80.9 °C; IR (KBr) 3293, 2291, 2113, 1596, 863 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, δ): 8.09 (s, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.55 (s, 1H), 7.51 (dd, *J* = 7.0, 7.9 Hz, 1H), 7.45 (dd, *J* = 7.1, 7.9 Hz, 1H), 5.74–5.70 (m, 1H), 2.72 (d, *J* = 6.2 Hz, 1H), 1.95 (d, *J* = 2.0 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃, δ): 135.7 (C), 133.6 (C), 131.3 (C), 130.8 (C), 128.2 (CH), 127.8 (CH), 127.2 (CH), 126.3 (CH), 125.8 (CH), 115.9 (CH), 83.5 (C), 78.1 (C), 61.4 (CH), 3.9 (CH₃); HRMS (ESI) calcd for C₁₄H₁₁N₃NaO [M + Na]⁺: 266.1264, found 266.1267.

3-Azido-α-(1-heptyn-1-yl)-2-naphthalenemethanol (S4b). To a THF (10 mL) solution of 1-heptyne



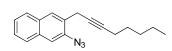
(0.94 mL, 7.2 mmol) was added a 1.66 M hexane solution of *n*-butyllithium (4.34 mL, 7.2 mmol) at -78 °C. After being stirred for 1 h, the mixture was warmed to room temperature, and a THF (10 mL) solution of **S3** (1.18 g, 6.00 mmol) was added. The reaction was quenched by addition of saturated aqueous ammonium chloride. The mixture was extracted with dichloromethane, washed

with brine, dried over anhydrous magnesium sulfate, and evaporated. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/10) to give alkynyl azide **S4b** (1.69 g, 96%) as a colorless solid: Mp 47.7–48.1 °C; IR (KBr): 3309, 2267, 2113, 1596, 863 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ): 8.10 (s, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.53 (s, 1H), 7.50 (dd, *J* = 7.2, 8.2 Hz, 1H), 7.44 (dd, *J* = 7.2, 7.7 Hz, 1H), 5.72 (dd, *J* = 2.0, 6.0 Hz, 1H), 2.77 (d, *J* = 6.1 Hz, 1H), 2.30 (td, *J* = 2.0, 7.2 Hz, 2H), 1.57 (tt, *J* = 7.5, 7.5 Hz, 2H), 1.44–1.38 (m, 2H), 1.37–1.30 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 135.7 (C), 133.5 (C), 131.4 (C), 130.8 (C), 128.2 (CH), 127.8 (CH), 127.2 (CH), 126.3 (CH), 125.8 (CH), 115.8 (CH), 88.1 (C), 78.8 (C), 61.4 (CH), 31.1 (CH₂), 28.2 (CH₂), 22.2 (CH₂), 18.9 (CH₂), 14.0 (CH₃); HRMS (ESI) calcd for C₁₈H₁₉N₃NaO [M + Na]⁺: 316.1420, found 316.1415.

2-Azido-3-(2-butyn-1-yl)naphthalene (S5a). To a dicholomethane (30 mL) solution of alcohol S4a (1.08 g, 4.57 mmol) and triethylsilane (1.46 mL, 9.14 mmol) was added trifluoroacetic acid (0.509 mL, 6.86 mmol) at -5 °C. After being stirred for 16 h at -5 °C, the reaction

was quenched by addition of saturated aqueous sodium hydrogen carbonate. The mixture was extracted with dichloromethane, washed with brine, dried over anhydrous magnesium sulfate, and evaporated. The residue was purified by silica gel column chromatography (hexane) to give **S5a** (440 mg, 44%) as a colorless solid: Mp 82.0–82.4 °C; IR (KBr): 2206, 2113, 1596, 856 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ): 7.96 (s, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.51 (s, 1H), 7.46 (dd, *J* = 1.0, 6.9, 8.0 Hz, 1H), 7.43 (ddd, *J* = 1.0, 7.0, 8.2 Hz, 1H), 3.60 (q, *J* = 2.5 Hz, 2H), 1.92 (t, *J* = 2.5 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 136.6 (C), 132.9 (C), 131.1 (C), 128.4 (CH), 128.3 (C), 127.6 (CH), 126.4 (CH), 126.3 (CH), 125.5 (CH), 115.1 (CH), 78.9 (C), 75.7 (C), 21.0 (CH₂), 3.7 (CH₃); HRMS (ESI) calcd for C₁₄H₁₂N₃ [M + H]⁺: 221.0953, found 221.0950.

2-Azido-3-(2-octyn-1-yl)naphthalene (S5b). The title compound (0.88 g, 55%) was obtained from



S4b (1.69 g, 5.76 mmol), triethylsilane (1.85 mL, 11.5 mmol), trifluoroacetic acid (0.86 mL, 11.5 mmol) and dichloromethane (30 mL) using the same procedure described above. Colorless solid: Mp 142.6–143.1 °C; IR (KBr): 2329, 2105, 1596, 863 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ): 7.99 (s, 1H), 7.80

(d, J = 8.3 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.50 (s, 1H), 7.46 (ddd, J = 1.2, 7.3, 8.3 Hz, 1H), 7.42 (ddd, J = 1.2, 7.3, 8.0 Hz, 1H), 3.62 (s, 2H), 2.28 (tt, J = 2.4, 7.1 Hz, 2H), 1.59 (tt, J = 7.1, 7.5 Hz, 2H), 1.47–1.41 (m, 2H), 1.40–1.33 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 136.6 (C), 132.8 (C), 131.0 (C), 128.4 (C), 128.3 (CH), 127.6 (CH), 126.4 (CH), 126.3 (CH), 125.5 (CH), 115.0 (CH), 83.8 (C), 76.5 (C), 31.2 (CH₂), 28.7 (CH₂), 22.3 (CH₂), 21.1 (CH₂), 18.9 (CH₂), 14.0 (CH₃); HRMS (ESI) calcd for C₁₈H₁₉N₃Na [M + Na]⁺: 300.1471, found 300.1470.

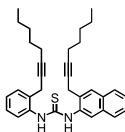
3-(2-Butyn-1-yl)-2-naphthalenamine (S6a). To a suspension of lithium aluminum hydride (LAH) (214 mg, 5.65 mmol) in THF (30 mL) was added a THF (20 mL) solution of S5a (500 mg, 2.26 mmol) at 0 °C. The mixture was stirred for 15 min and quenched by addition of

aqueous THF (1:1) followed by 1 M aqueous HCl (5 mL) at 0 °C. The mixture was extracted with ethyl acetate, dried over anhydrous magnesium sulfate, and evaporated. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/4) to give **S6a** (408 mg, 93%) as a colorless solid: Mp 72.4–72.8 °C; IR (KBr): 3270, 2915, 2291, 1697, 1542, 1049, 879 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, δ): 7.68 (d, *J* = 8.1 Hz, 1H), 7.65 (s, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.34 (ddd, *J* = 1.2, 6.8, 8.1 Hz, 1H), 7.02 (s, 1H), 4.10 (br, 2H), 3.56 (q, *J* = 2.5 Hz, 2H), 1.85 (t, *J* = 2.5 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃, δ): 143.1 (C), 134.0 (C), 128.1 (C), 128.0 (CH), 127.3 (CH), 125.8 (CH), 125.2 (C), 122.6 (CH), 109.9 (CH), 78.7 (C), 75.3 (C), 22.5 (CH₂), 3.6 (CH₃); HRMS (ESI) calcd for C₁₄H₁₄N [M + H]⁺: 196.1121, found 196.1114.

3-(2-Octyn-1-yl)-2-naphthalenamine (S6b). The title compound (529 mg, 60%) was synthesized from S5b (972 mg, 3.50 mmol), lithium aluminum hydride (LAH) (332 mg, 8.76 mmol), and THF (50 mL) using the same procedure described above. Colorless solid: Mp 50.6–51.6 °C; IR (KBr): 3363, 2931, 1635, 1511, 1280, 1018, 871 cm⁻¹;

¹H NMR (500 MHz, CDCl₃, δ): 7.68 (d, *J* = 8.2 Hz, 1H), 7.66 (s, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.33 (ddd, *J* = 1.2, 7.4, 7.6 Hz, 1H), 7.22 (ddd, *J* = 1.2, 7.4, 7.6 Hz, 1H), 7.02 (s, 1H), 4.08 (br, 2H), 3.58 (t, *J* = 1.8 Hz, 2H), 2.21 (tt, *J* = 2.4, 7.1 Hz, 2H), 1.56–1.49 (m, 2H), 1.41–1.28 (m, 4H), 0.90 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃, δ): 143.1 (C), 134.0 (C), 128.2 (C), 128.0 (CH), 127.4 (CH), 125.8 (CH), 125.3 (CH), 125.3 (C), 122.6 (CH), 109.8 (CH), 83.6 (C), 76.1 (C), 31.1 (CH₂), 28.6 (CH₂), 22.5 (CH₂), 22.2 (CH₂), 18.8 (CH₂), 14.0 (CH₃); HRMS (ESI) calcd for C₁₈H₂₁NNa [M + Na]⁺: 274.1566, found 274.1579.

N-[3-(2-Octyn-1-yl)-2-naphthalenyl]-N'-[2-(2-octyn-1-yl)phenyl]thiourea (S7b). A mixture of



isothiocyanate **S2b** (2.23 g, 9.20 mmol) and **S6b** (2.31 g, 9.20 mmol) in ethanol (10 mL) was stirred for 20 h at room temperature and then evaporated. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/10) to give **S7b** (4.38 g, 99%) as a colorless solid: Mp 58.2–58.5 °C; IR (neat): 3301, 2931, 1596, 1457, 1087, 879 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, δ): 8.13 (br, 2H), 7.93 (s, 2H), 7.79 (dd, J = 6.8, 7.0 Hz, 2H), 7.56 (d, J = 7.5 Hz, 1H), 7.48–7.41 (m, 3H), 7.33–7.23

(m, 2H), 3.74 (s, 2H). 3.56 (s, 2H), 2.14–2.04 (m, 2H), 1.80–1.60 (m, 2H), 1.48–1.40 (m, 2H), 1.37–1.10 (m, 10H), 0.89 (t, J = 6.9 Hz, 3H), 0.82 (t, J = 7.0 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃, δ): 181.0 (C), 135.5 (C), 134. 5 (C), 133.4 (C), 132.7 (C), 132.7 (C), 132.5 (C), 129.7 (CH), 128.5 (CH), 128.1 (CH), 128.0 (CH), 127.64 (CH), 127.56 (CH), 127.3 (CH), 126.7 (CH), 126.6 (CH), 126.2 (CH), 84.0 (C), 83.5 (C), 76.1 (C), 75.9 (C), 31.1 (CH₂), 30.9 (CH₂), 28.5 (CH₂), 28.3 (CH₂), 22.5 (CH₂), 22.1 (CH₂), 22.1 (CH₂), 22.0 (CH₂),

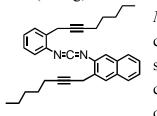
18.7 (CH₂), 18.3 (CH₂), 13.9 (CH₃), 13.8 (CH₃); HRMS (ESI) calcd for $C_{33}H_{38}N_2SNa [M + Na]^+$: 517.2648, found 517.2648.

N-[3-(2-Butyn-1-yl)-2-naphthalenyl]-N'-[2-(2-butyn-1-yl)phenyl]thiourea (S7a). The title compound

(261.7 mg, 58%) was obtained from **S2a** (221 mg, 1.18 mmol), **S6a** (230 mg, 1.18 mmol), and ethanol (10 mL) using the same procedure described above. Colorless solid: Mp 132.8–133.3 °C; IR (KBr): 3332, 3147, 2954, 1527, 1488, 1257, 1203, 755 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, δ): 8.11 (br, 1H), 8.01 (br, 1H), 7.97 (s, 1H), 7.90 (br, 1H), 7.81 (dd, J = 6.0, 7.4 Hz, 1H), 7.81 (d, J = 7.4 Hz, 1H), 7.88 (d, J = 7.4 Hz, 1H), 7.81 (d, J = 7.4 Hz, 1H), 7.88 (d, J = 7.

1H), 7.49–7.44 (m, 2H), 7.40 (br, 1H), 7.32 (dd, J = 7.4, 7.8 Hz, 1H), 7.26 (dd, J = 7.4, 7.8 Hz, 1H), 3.70 (br, 2H), 3.51 (br, 2H), 1.72 (br, 3H), 1.34 (br, 3H); ¹³C NMR (126 MHz, CDCl₃, δ): 181.0 (C), 135.5 (br, C), 134.3 (br, C), 133.4 (br, C), 132.7 (C), 132.6 (C), 129.8 (CH), 128.6 (CH), 128.2 (CH), 128.0 (CH), 127.8 (CH), 127.6 (CH), 127.4 (CH), 126.9 (CH), 126.7 (CH), 126.3 (CH), 79.1 (C), 78.7 (C), 75.4 (C), 75.2 (C), 22.5 (CH₂), 22.2 (CH₂), 3.6 (CH₃), 3.0 (CH₃) (one quaternary carbon was not observed); HRMS (ESI) calcd for C₂₅H₂₂N₂SNa [M + Na]⁺: 405.1393, found 405.1393.

3-(2-Octyn-1-yl)-N-[[2-(2-octyn-1-yl)phenyl]carbonimidoyl]-2-naphthalenamine (2b). Thiourea **S7b** (4.38 g, 8.86 mmol) was dissolved in dichloromethane (10 mL). Triethylamine (3.83 mL, 27.5 mmol),



N,*N*-dimethyl-4-aminopyridine (DMAP) (55 mg, 0.46 mmol), and methanesulfonyl chloride (1.42 mL, 18.3 mmol) were added in this order at 0 °C. The mixture was stirred for 10 min and concentrated in vacuo. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/10) to give **2b** (3.57 g, 88%) as a colorless oil: IR (neat): 2931, 2144, 1581, 1496, 1172, 1087, 871 cm⁻¹; ¹H NMR

(500 MHz, CDCl₃, δ): 7.94 (s, 1H), 7.72 (dd, J = 2.8, 6.9 Hz, 1H), 7.61 (dd, J = 2.8, 6.8 Hz, 1H), 7.54 (s, 2H), 7.36–7.32 (m, 2H), 7.21–7.09 (m, 3H), 3.77 (s, 2H). 3.69 (s, 2H), 2.26–2.21 (m, 2H), 2.19–2.14 (m, 2H), 1.56–1.45 (m, 4H), 1.43–1.23 (m, 8H), 0.90 (t, J = 7.3 Hz, 3H), 0.87 (t, J = 7.2 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃, δ): 136.1 (C), 134.8 (C), 132.8 (C), 131.8 (C), 131.7 (C), 131.3 (C), 130.8 (C), 129.1 (CH), 127.7 (CH), 127.5 (CH), 127.3 (CH), 126.4 (CH), 125.9 (CH), 125.5 (CH), 125.4 (CH), 124.5 (CH), 121.8 (CH), 83.6 (C), 83.1 (C), 76.68 (C), 76.67 (C), 31.1 (CH₂), 31.0 (CH₂), 28.7 (CH₂), 28.6 (CH₂), 22.2 (CH₂), 22.12 (CH₂), 22.11 (CH₂), 21.6 (CH₂), 18.81 (CH₂), 18.75 (CH₂), 13.94 (CH₃), 13.89 (CH₃); HRMS (ESI) calcd for C₃₃H₃₇N₂ [M + H]⁺: 461.2951, found 461.2951.

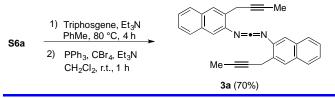
3-(2-Butyn-1-yl)-N-[[2-(2-butyn-1-yl)phenyl]carbonimidoyl]-2-naphthalenamine (2a). The title compound (199 mg, 83%) was obtained from S7a (262 mg, 0.68 mmol), triethylamine (0.29 mL, 2.05 mmol), DMAP (4.2 mg, 0.03 mmol), methanesulfonyl chloride (0.11 mL, 1.37 mmol), and dichloromethane (10 mL) using the same procedure described

above. Colorless solid: Mp 90.9–91.4 °C; IR (KBr): 2908, 2152, 2129, 1573, 1450, 1226, 748 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, δ): 7.95 (s, 1H), 7.79 (dd, J = 2.3, 7.3 Hz, 1H), 7.70 (dd, J = 2.3, 7.3 Hz, 1H), 7.63 (s, 1H), 7.52 (dd, J = 2.2, 7.0 Hz, 1H), 7.41 (m, 2H), 7.24 (m, 3H), 3.77 (q, J = 2.5 Hz, 2H), 3.67 (q, J = 2.5 Hz, 2H), 1.88 (t, J = 2.5 Hz, 3H), 1.82 (t, J = 2.5 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃, δ): 136.2 (C), 134.9 (C), 133.1 (C), 132.9 (C), 131.8 (C), 131.5 (C), 130.8 (C), 129.4 (CH), 127.9 (CH), 127.7 (CH), 127.5 (CH), 126.5 (CH), 126.1 (CH), 125.7 (CH), 125.6 (CH), 124.8 (CH), 122.1 (CH), 78.9 (C), 78.3 (C), 76.1 (C), 76.0

(C), 22.2 (CH₂), 21.7 (CH₂), 3.7 (CH₃), 3.6 (CH₃); HRMS (ESI) calcd for $C_{25}H_{20}N_2Na [M + Na]^+$: 371.1519, found 371.1516.

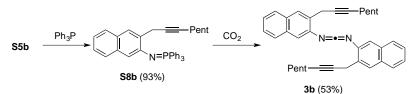
1.2.3 Synthesis of Carbodiimides 3





Bis[3-(2-butyn-1-yl)-2-naphthalenyl]carbodiimide (3a). A mixture of S6a (68 mg, 0.35 mmol), triethylamine (0.11 mL, 0.77 mmol), triphosgene (17 mg, 0.056 mmol), and toluene (3 mL) was heated at 80 °C for 4 h. The mixture was cooled to room temperature and then volatiles were removed under reduced pressure. To the residue were added THF (5 mL), triphenylphosphine (118 mg, 0.46 mmol), and triethylamine (0.10 mL, 0.75 mmol). The mixture was cooled to 0 °C, and carbon tetrabromide (179 mg, 0.54 mmol) was added. After being stirred for 1 h, the mixture was condensed under reduced pressure. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/10) to give **3a** (98 mg, 70%) as a colorless solid: Mp 157.2–157.7 °C; IR (neat): 2375, 2144, 1581, 871 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, δ): 7.98 (s, 2H), 7.84–7.81 (m, 2H), 7.75–7.72 (m, 2H), 7.70 (s, 2H), 7.46–7.41 (m, 4H), 3.82 (q, *J* = 2.5 Hz, 4H), 1.88 (t, *J* = 2.5 Hz, 6H); ¹³C NMR (126 MHz, CDCl₃, δ): 141.1 (C), 134.8 (C × 2), 133.0 (C × 2), 131.5 (C × 2), 130.9 (C × 2), 128.0 (CH × 2), 127.5 (CH × 2), 126.6 (CH × 2), 126.2 (CH × 2), 125.7 (CH × 2), 122.3 (CH × 2), 78.9 (C × 2), 76.0 (C × 2), 22.3 (CH₂ × 2), 3.7 (CH₃ × 2); HRMS (ESI) calcd for C₂₉H₂₃N₂ [M + H]⁺: 399.1856, found 399.1865.

Scheme S4. Synthesis of Carbodiimides 3b



3-(2-Octyn-1-yl)-N-(triphenylphosphoranylidene)-2-naphthalenamine (**S8b**). Triphenyl- phosphine (912 mg, 3.48 mmol) was added to a solution of alkynyl azide **S5b** (877 mg, 3.16 mmol) in dichloromethane (20 mL) at room temperature. After being stirred for 10 h, the mixture was concentrated under reduced pressure. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1/4) to give iminophosphorane **S8b** (1.53 g, 93%) as a colorless solid: Mp 129.5–130.4 °C; IR (KBr): 1589, 1450, 825 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ): 7.95 (s, 1H), 7.82–7.78 (m, 6H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.51 (dd, *J* = 7.4, 7.4 Hz, 3H), 7.44 (ddd, *J* = 2.7, 7.4, 7.7 Hz, 6H), 7.21 (d, *J* = 8.1 Hz, 1H), 7.15 (dd, *J* = 6.8, 8.0 Hz, 1H), 7.09 (dd, *J* = 6.8, 7.9 Hz, 1H), 6.66 (s, 1H), 4.03 (s, 2H), 2.30 (tt, *J* = 2.4, 7.1 Hz, 2H), 1.60–1.55 (m, 2H), 1.47–1.42 (m, 2H), 1.38–1.31 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 147.8 (C), 134.4 (C, d, *J* = 22.5 Hz), 133.9 (C), 132.6 (CH × 6, d, *J* = 9.6 Hz), 131.7 (CH × 3, d, *J* = 2.7 Hz), 131.1 (C × 3, d, *J* = 99.6 Hz), 128.6 (CH × 6, d, *J* = 11.8 Hz), 127.6 (C), 127.1 (CH), 126.2 (CH), 125.0 (CH),

124.5 (CH), 121.4 (CH), 114.0 (CH, d, J = 9.9 Hz), 82.9 (C), 79.1 (C), 31.2 (CH₂), 29.0 (CH₂), 22.9 (CH₂), 22.3 (CH₂), 19.0 (CH₂), 14.0 (CH₃); HRMS (ESI) calcd for C₃₆H₃₅NP [M + H]⁺: 512.2502, found 512.2511.

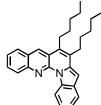
Bis[3-(2-octyn-1-yl)-2-naphthalenyl]carbodiimide (*3b*). A dichloromethane (10 mL) solution of iminophosphorane *S8b* (1.53 g, 3.0 mmol) was degassed, charged with carbon dioxide, and stirred for 20 h at room temperature. The reaction mixture was evaporated, and the residue was purified by silica gel column chromatography (dichloromethane/hexane = 1/2) to give carbodiimide *3b* (405 mg, 53%) as a colorless oil: IR (neat): 2931, 2244, 1573, 1295, 863 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, δ) 8.01 (s, 2H), 7.83–7.79 (m, 2H), 7.75–7.71 (m, 2H), 7.69 (s, 2H), 7.46–7.41 (m, 4H), 3.84 (q, *J* = 2.5 Hz, 4H), 2.25 (tt, *J* = 2.4, 7.1 Hz, 4H), 1.61–1.50 (m, 4H), 1.46–1.28 (m, 8H), 0.90 (t, *J* = 7.2 Hz, 6H); ¹³C NMR (75 MHz, CDCl₃, δ) 134.8 (C × 2), 132.9 (C × 2), 132.6 (C), 131.5 (C × 2), 131.0 (C × 2), 128.0 (CH × 2), 127.5 (CH × 2), 126.6 (CH × 2), 126.2 (CH × 2), 125.6 (CH × 2), 122.3 (CH × 2), 83.9 (C × 2), 76.7 (C × 2), 31.2 (CH₂ × 2), 28.7 (CH₂ × 2), 22.3 (CH₂ × 2), 22.2 (CH₂ × 2), 18.9 (CH₂ × 2), 14.0 (CH₃ × 2); HRMS (ESI) calcd for C₃₇H₃₉N₂ [M + H]⁺: 511.3108, found 511.3104.

1.3 Synthesis of L-Shaped Molecules

1.3.1 Synthesis of 4

6,7-Dimethylbenzo[g]indolo[1,2-a][1,8]naphthyridine (4a). To a heated toluene (2 mL) solution of Wilkinson catalyst (Rh(PPh₃)₃Cl) (23 mg, 0.025 mmol) was added a toluene (3 mL) solution of 1a (75 mg, 0.25 mmol) at 120 °C. After being stirred for 20 min, the mixture was cooled to room temperature. To the mixture was added manganese(IV) oxide (65 mg, 0.75 mmol). After being stirred for 6 h, the suspension was filtered through Celite and the filtrate was evaporated. The residue was purified by silica gel column chromatography (chloroform/hexane = 1/2) to give 4a (67 mg, 90%) as a yellow solid. Mp 221.0–221.7 °C; IR (KBr): 3046, 2923, 2854, 1596, 1542, 1457, 1396 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ) 9.71 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.88 (d, J = 7.9 Hz, 1H), 7.78 (d, J = 7.9 Hz, 1H), 7.74 (ddd, J = 1.3, 6.8, 8.3 Hz, 1H), 7.52–7.48 (m, 2H), 7.39 (ddd, J = 1.0, 7.2, 7.8 Hz, 1H), 6.78 (s, 1H), 2.49 (s, 3H), 2.44 (s, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 147.0 (C), 145.0 (C), 137.7 (C), 134.7 (C), 131.1 (CH), 129.8 (C), 129.5 (CH), 127.7 (CH × 2), 125.4 (C), 125.3 (C), 124.8 (CH), 124.5 (C), 123.1 (CH), 122.7 (CH), 121.0 (C), 120.3 (CH), 118.0 (CH), 99.0 (CH), 15.1 (CH₃), 14.0 (CH₃); HRMS (ESI) calcd for C₂₁H₁₇N₂ [M + H]⁺: 297.1386, found 297.1380; Anal. Calcd for C₂₁H₁₆N₂: C, 85.11; H, 5.44; N, 9.34. Found: C, 84.93; H, 5.44; N, 9.34.

6,7-Dipentylbenzo[g]indolo[1,2-a][1,8]naphthyridine (4b). The title compound (142 mg, 93%) was



obtained from **1b** (155 mg, 0.38 mmol), Rh(PPh₃)₃Cl (35 mg, 0.038 mmol), and toluene (2 mL + 3 mL) using the same procedure described above. Yellow solid: Mp 110.5–110.9 °C; IR (KBr): 3054, 2923, 2854, 1589, 1535, 1457, 1396 cm⁻¹; ¹H NMR (500 MHz, CDCl₃, δ): 9.73 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H), 8.19 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 7.8 Hz, 1H), 7.72 (ddd, J = 1.5, 7.0, 8.3 Hz, 1H), 7.51–7.46

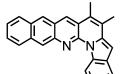
(m, 2H), 7.39 (ddd, J = 1.0, 7.1, 7.8 Hz, 1H), 6.81 (s, 1H), 2.92 (dd, J = 6.6, 9.7 Hz, 2H), 2.84 (dd, J = 6.6, 9.6 Hz, 2H), 1.78–1.66 (m, 4H), 1.57–1.50 (m, 4H), 1.48–1.40 (m, 4H), 0.97 (t, J = 7.3 Hz, 3H), 0.96 (t, J = 7.3 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃, δ): 147.4 (C), 145.6 (C), 137.1 (C), 134.6 (C), 131.2 (CH), 130.2 (C), 129.8 (C), 129.5 (CH), 129.0 (C), 127.7 (CH × 2), 125.4 (C), 124.7 (CH), 122.9 (CH), 122.7 (CH),

121.5 (C), 120.1 (CH), 118.1 (CH), 98.9 (CH), 32.4 (CH₂), 32.3 (CH₂), 29.7 (CH₂), 29.6 (CH₂), 29.4 (CH₂), 27.7 (CH₂), 22.6 (CH₂), 22.5 (CH₂), 14.1 (CH₃ × 2); HRMS (ESI) calcd for $C_{29}H_{33}N_2$ [M + H]⁺: 409.2638, found 409.2631; Anal. Calcd for $C_{29}H_{32}N_2$: C, 85.25; H, 7.89; N, 6.86. Found: C, 85.14; H, 8.10; N, 6.77.

1.3.2 Synthesis of 5 and 6

Synthesis of **5a** and **6a**. To a heated toluene (2 mL) solution of Rh(PPh₃)₃Cl (17 mg, 0.018 mmol) was added dropwise a toluene (3 mL) solution of carbodiimide **2a** (60.9 mg, 0.175 mmol) at 120 °C. The mixture was heated for 20 min and cooled to room temperature. Manganese(IV) oxide (65 mg, 0.75 mmol) was added and the mixture was stirred for 6 h. The suspension was filtrated through Celite and the filtrate was evaporated. The residue was purified by silica gel column chromatography (chloroform/hexane = 1/2) to give a mixture of **5a** and **6a** (31.9 mg, 52%). The ratio of **5a** to **6a** was determined as 51:49 from the integration of ¹H NMR signals. Crystallization of the mixture from toluene at 50 °C afforded almost pure **6a**, which was again recrystallized from toluene to give analytically and spectroscopically pure **6a** as red crystals. The combined filtrate was evaporated and the residue was filtered off and the filtrate was evaporated. Recrystallization of the residue from toluene/ethanol at 50 °C yielded **5a** as cubic crystals together with a small amount of needles. Manual separation of the cubic crystals provided analytically and spectroscopically pure **5a** as brownish red crystals.

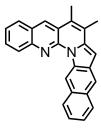
6,7-Dimethylindolo[1,2-a]naphtho[2,3-g][1,8]naphthyridine (5a). Brownish red solid: Mp 217.8-



218.6 °C (dec); IR (KBr): 3046, 2923, 2360, 2337, 1542, 1457, 1403, 1349, 894, 779, 740 cm⁻¹; ¹H NMR (300 MHz, CDCl₃, δ): 9.66 (d, J = 8.4 Hz, 1H), 8.54 (s, 1H), 8.10 (s, 1H), 8.05 (s, 1H), 8.02 (d, J = 8.8 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.71 (d, J = 7.6 Hz, 1H), 7.52 (m, 4H), 6.59 (s, 1H), 2.23 (s, 3H), 2.17 (s, 3H). ¹³C NMR (151 MHz, CDCl₃,

δ): 147.2 (C), 142.2 (C), 137.5 (C), 135.2 (C), 134.2 (C), 130.8 (C), 130.7 (CH), 129.9 (C), 128.1 (CH), 128.0 (CH), 126.4 (CH), 126.0 (CH), 125.0 (C), 124.9 (CH), 124.7 (C), 124.6 (C), 124.2 (CH), 123.4 (CH), 122.8 (CH), 121.7 (C), 120.3 (CH), 118.1 (CH), 100.2 (CH), 14.90 (CH₃), 13.8 (CH₃); HRMS (ESI) calcd for C₂₅H₁₉N₂ [M + H]⁺: 347.1543, found 347.1543; Anal. Calcd for C₂₅H₁₈N₂: C, 86.68; H, 5.24; N, 8.09. Found: C, 86.78; H, 5.31; N, 7.88.

7,8-Dimethylbenzo[g]benzo[f']indolo[1,2-a][1,8]naphthyridine (6a). Brownish red solid: Mp 268.5-

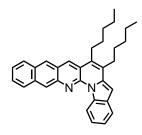


269.0 °C (dec); IR (KBr): 3433, 3047, 2916, 2360, 2337, 1597, 1543, 1442, 1396, 872, 741 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ): 10.20 (s, 1H), 8.32 (s, 1H), 8.29 (d, J = 8.3 Hz, 1H), 8.24 (1H, J = 7.9 Hz, 1H), 8.22 (s, 1H), 8.03 (d, J = 7.9 Hz, 1H), 7.89 (d, J = 7.9 Hz, 1H), 7.79 (dd, J = 7.9, 8.3 Hz, 1H), 7.50 (m, 3H), 6.87 (s, 1H), 2.53 (s, 3H), 2.48 (s, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 147.4 (C), 146.0 (C), 140.8 (C), 134.8 (C), 131.0 (C), 130.9 (CH), 130.6 (C), 130.3 (C), 129.7 (CH), 129.1 (CH), 127.8 (CH), 127.7 (CH), 127.6 (CH),

126.7 (C), 125.4 (C), 125.2 (C), 124.7 (CH), 124.0 (CH), 123.8 (CH), 121.1 (C), 117.4 (CH), 114.9 (C), 98.7 (CH), 15.1 (CH₃), 14.2 (CH₃); HRMS-ESI (*m/z*): $[M + H]^+$: calcd for C₂₅H₁₉N₂, 347.1543; found, 347.1540; Anal. Calcd for C₂₅H₁₈N₂: C, 86.68; H, 5.24; N, 8.09. Found: C, 86.04; H, 5.31; N, 7.96.

Synthesis of **5b** and **6b**. A 53:47 mixture of **5b** and **6b** (48.6 mg, 86%) was obtained from **2b** (56.8 mg, 0.123 mmol), Rh(PPh₃)₃Cl (11.4 mg, 0.012 mmol), and toluene (1 mL + 2 mL) using the same procedure described above.

6,7-Dipentylindolo[1,2-a]naphtho[2,3-g][1,8]naphthyridine (5b). Brownish red solid: Mp 126.3-



126.9 °C; ¹H NMR (600 MHz, CDCl₃, δ): 10.20 (s, 1H), 8.29 (s, 1H), 8.28 (d, J = 8.2 Hz, 1H), 8.23 (dd, J = 1.1, 7.7 Hz, 1H), 8.20 (s, 1H), 8.02 (d, J = 7.7 Hz, 1H), 7.89 (dd, J = 0.9, 8.0 Hz, 1H), 7.77 (ddd, J = 1.4, 6.8, 8.3 Hz, 1H), 7.51–7.45 (m, 3H), 6.86 (s, 1H), 2.92 (dd, J = 6.6, 10.6 Hz, 2H), 2.84 (dd, J = 6.5, 10.5 Hz, 2H), 1.80–1.74 (m, 2H), 1.73–1.68 (m, 2H), 1.59–1.51 (m, 4H), 1.49–1.42 (m, 4H), 0.98 (t, J = 7.3 Hz, 3H), 0.97 (t, J = 7.3 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 147.8 (C), 145.9 (C), 140.3 (C), 134.7 (C), 131.1 (C), 131.0 (CH), 130.9 (C), 130.6 (C), 130.3

(C), 130.0 (C), 129.7 (CH), 129.1 (CH), 127.8 (CH), 127.6 (CH), 127.5 (CH), 125.4 (C), 124.6 (CH), 124.0 (CH), 123.7 (CH), 120.1 (C), 117.3 (CH), 115.0 (CH), 98.6 (CH), 32.42 (CH₂), 32.36 (CH₂), 29.6 (CH₂), 29.5 (CH₂), 29.4 (CH₂), 27.8 (CH₂), 22.59 (CH₂), 22.57 (CH₂), 14.12 (CH₃), 14.10 (CH₃); HRMS (ESI) calcd for $C_{33}H_{35}N_2$ [M + H]⁺: 459.2795, found 459.2796; Anal. Calcd for $C_{33}H_{34}N_2$: C, 86.42; H, 7.47; N, 6.11. Found: C, 86.31; H, 7.53; N, 6.02.

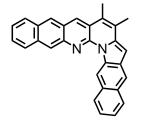
7,8-Dipentylbenzo[g]benzo[f']indolo[1,2-a][1,8]naphthyridine (6b). Brownish red solid: Mp 174.1-

175.9 °C; ¹H NMR (600 MHz, CDCl₃, δ): 9.78 (d, J = 8.2 Hz, 1H), 8.70 (s, 1H), 8.43 (s, 1H), 8.42 (s, 1H), 8.09 (d, J = 8.3 Hz, 1H), 8.02 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 7.7 Hz, 1H), 7.54–7.50 (m, 2H), 7.47 (ddd, J = 1.0, 6.8, 8.3 Hz, 1H), 7.39 (ddd, J = 0.9, 6.8, 7.7 Hz, 1H), 6.81 (s, 1H), 2.92 (dd, J = 6.4, 10.5 Hz, 2H), 2.82 (dd, J =6.5, 10.5 Hz, 2H), 1.77–1.70 (m, 4H), 1.60–1.41 (m, 8H), 0.99 (t, J = 7.2 Hz, 3H), 0.96 (t, J = 7.2 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃, δ): 147.8 (C), 142.3 (C), 137.1 (C), 135.2 (C), 134.3 (C), 131.1 (CH), 130.9 (C), 130.1 (C), 130.0 (C), 129.2

(C), 128.1 (CH), 128.0 (CH), 126.5 (CH), 126.1 (CH), 125.0 (CH), 124.8 (C), 124.4 (CH), 123.4 (CH), 122.9 (CH), 121.1 (C), 120.3 (CH), 118.2 (CH), 100.4 (CH), 32.401 (CH₂), 32.400 (CH₂), 29.64 (CH₂), 29.57 (CH₂), 29.5 (CH₂), 27.7 (CH₂), 22.599 (CH₂), 22.597 (CH₂), 14.13 (CH₃), 14.11 (CH₃); HRMS (ESI) calcd for $C_{33}H_{35}N_2$ [M + H]⁺: 459.2795, found 459.2793; Anal. Calcd for $C_{33}H_{34}N_2$: C, 86.42; H, 7.47; N, 6.11. Found: C, 86.19; H, 7.50; N, 5.99.

1.3.3 Synthesis of 7

7,8-Dimethylbenzo[f']indolo[1,2-a]naphtho[2,3-g][1,8]naphthyridine (7a). To a heated toluene (1



mL) solution of RhCl(PPh₃)₃ (14.1 mg, 0.015 mmol) was slowly added toluene (3 mL) solution of carbodiimide **3a** (60.8 mg, 0.15 mmol) at 120 °C. After being stirred for 20 min at 120 °C, the mixture was cooled to room temperature, and manganese(IV) oxide was added. After being stirred for 38 h, the mixture was extracted with chloroform (100 mL), and the resulting insoluble material was removed by passing through Celite. The filtrate was condensed to ca. 1/5 volume,

and the resulting solid was collected by filtration and washed with ethyl acetate to give red solid of **7a** (30 mg, 50%) as a first crop. The filtrate was evaporated and the residue was purified by silica gel column chromatography (chloroform/hexane = 1/2) to give a second crop of **7a** (9.1 mg, 15%). Mp 296.1 °C (dec); IR (KBr): 3042, 2923, 2854, 1596, 1542, 1457, 1396 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ): 10.19 (s, 1H), 8.72 (s, 1H), 8.35 (s, 1H), 8.31 (s, 1H), 8.27 (d, *J* = 8.2 Hz, 1H), 8.16 (s, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 2H), 7.57–7.47 (m, 4H), 6.81 (s, 1H), 2.45 (s, 3H), 2.39 (s, 3H); ¹³C NMR (151 MHz, CDCl₃,

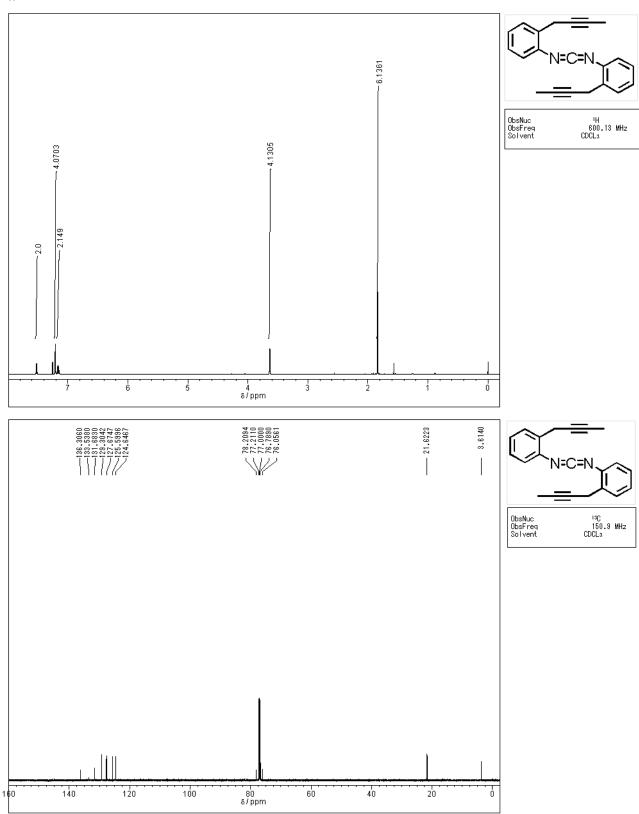
δ): 147.7 (C), 142.7 (C), 140.7 (C), 135.2 (C), 134.5 (C), 131.3 (C), 130.9 (C), 130.8 (CH), 130.6 (C), 130.4 (C), 129.2 (CH), 128.1 (CH), 128.0 (CH), 127.7 (CH), 126.9 (C), 126.6 (CH), 126.2 (CH), 125.1 (C), 125.0 (CH), 124.8 (C), 124.2 (CH), 124.1 (CH), 124.0 (CH), 122.1 (C), 117.7 (CH), 115.1 (CH), 100.3 (CH), 15.1 (CH₃), 14.1 (CH₃); HRMS (ESI) calcd for C₂₉H₂₁N₂ [M + H]⁺: 397.1699, found 397.1699; Anal. Calcd for C₂₉H₂₀N₂: C, 87.85; H, 5.08; N, 7.07. Found: C, 87.59; H, 5.13; N, 6.88.

7,8-Dipentylbenzo[f']indolo[1,2-a]naphtho[2,3-g][1,8]naphthyridine (7b). To a heated toluene (1 mL) solution of RhCl(PPh₃)₃ (9.2 mg, 0.01 mmol) was slowly added a toluene (1 mL) solution of carbodiimide **3b** (50.9 mg, 0.10 mmol). After being stirred for 20 min, the mixture was cooled to room temperature, and manganese(IV) oxide (26.0 mg, 0.30 mmol) was added. The mixture was stirred for 24 h, and the resulting insoluble material was removed by passing through Celite. The filtrate was evaporated and the residue was purified by column chromatography (chloroform/hexane = 1/2) to give **7b** (40.2 mg, 79%) as a red solid: Mp 174.7–

175.1 °C; IR (KBr) 3046, 2923, 2854, 1589, 1535, 1457, 1396 cm⁻¹; ¹H NMR (600 MHz, CDCl₃, δ) 10.21 (s, 1H), 8.72 (s, 1H), 8.37 (s, 1H), 8.32 (s, 1H), 8.27 (d, J = 7.8 Hz, 1H), 8.15 (s, 1H), 8.12 (d, J = 8.3 Hz, 1H), 8.01 (d, J = 8.1 Hz, 2H), 7.55–7.46 (m, 4H), 6.83 (s, 1H), 2.87 (dd, J = 6.8, 9.9 Hz, 2H), 2.78 (dd, J = 6.8, 9.8 Hz, 2H), 1.78–1.69 (m, 4H), 1.60–1.50 (m, 4H), 1.49–1.43 (m, 4H), 0.99 (t, J = 7.3 Hz, 3H), 0.98 (t, J = 7.3 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃, δ) 148.0 (C), 142.6 (C), 140.2 (C), 135.1 (C), 134.5 (C), 131.3 (C), 131.2 (C), 130.9 (CH), 130.8 (C), 130.7 (C), 130.4 (C), 129.9 (C), 129.2 (CH), 128.1 (CH), 128.0 (CH), 127.7 (CH), 126.6 (CH), 126.1 (CH), 125.0 (CH), 124.8 (C), 124.1 (CH), 124.0 (CH), 123.9 (CH), 121.2 (C), 117.6 (CH), 115.2 (CH), 100.2 (CH), 32.4 (CH₂ × 2), 29.6 (CH₂), 29.5 (CH₂), 29.4 (CH₂), 27.8 (CH₂), 22.6 (CH₂ × 2), 14.1 (CH₃ × 2); HRMS (ESI) calcd for C₃₇H₃₇N₂ [M + H]⁺: 509.2951, found 509.2952; Anal. Calcd for C₃₇H₃₆N₂: C, 87.36; H, 7.13; N, 5.51. Found: C, 87.15; H, 7.36; N, 5.43.

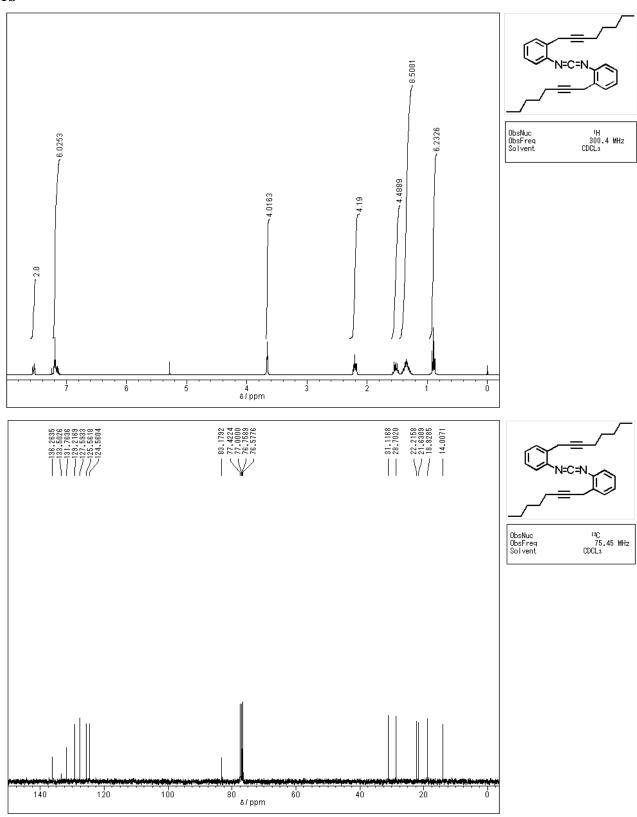
2. NMR Spectra



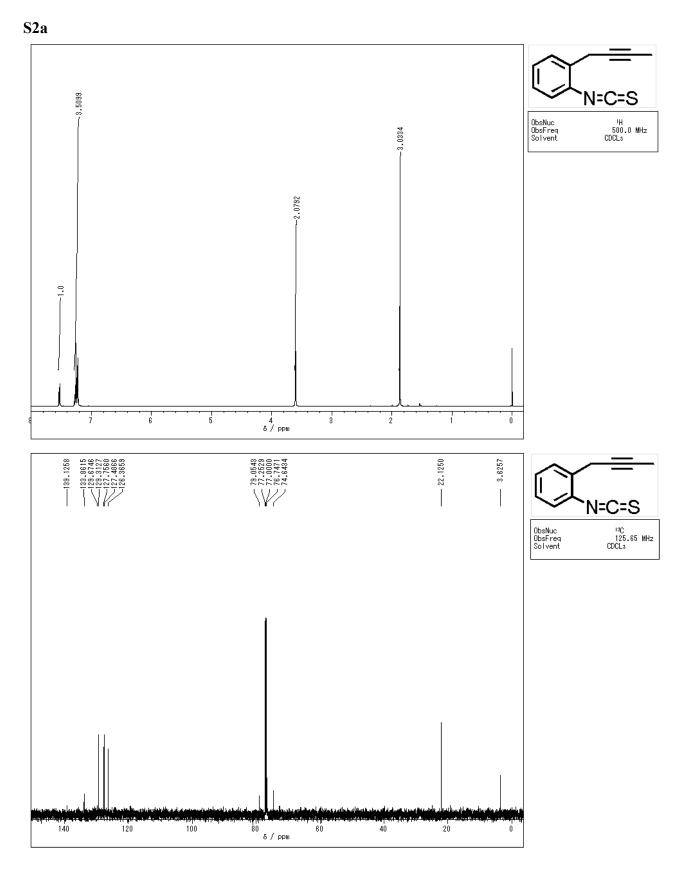


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1b

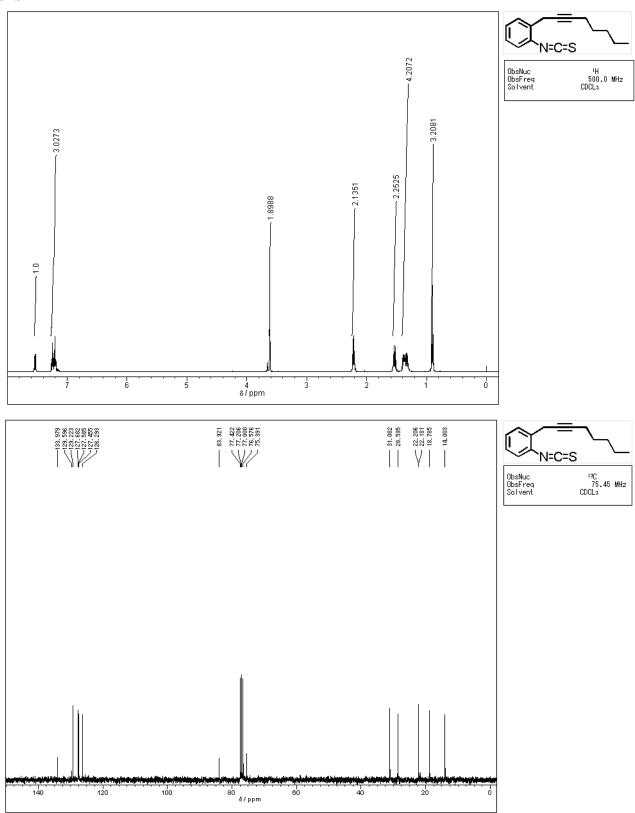


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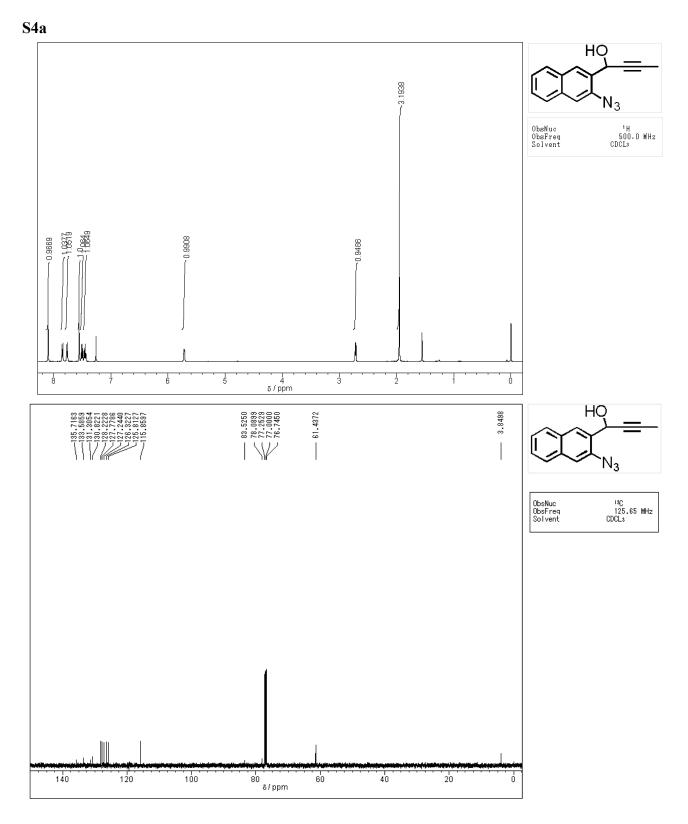


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S2b

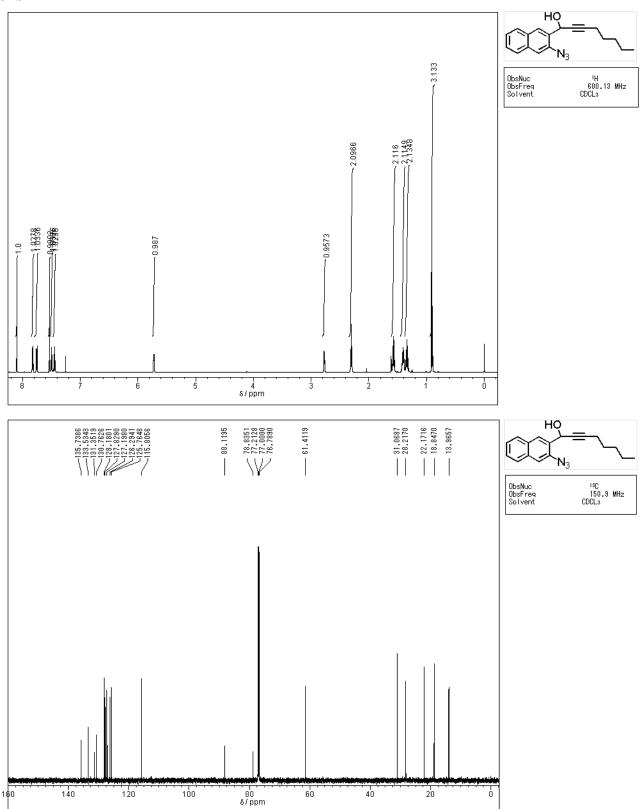


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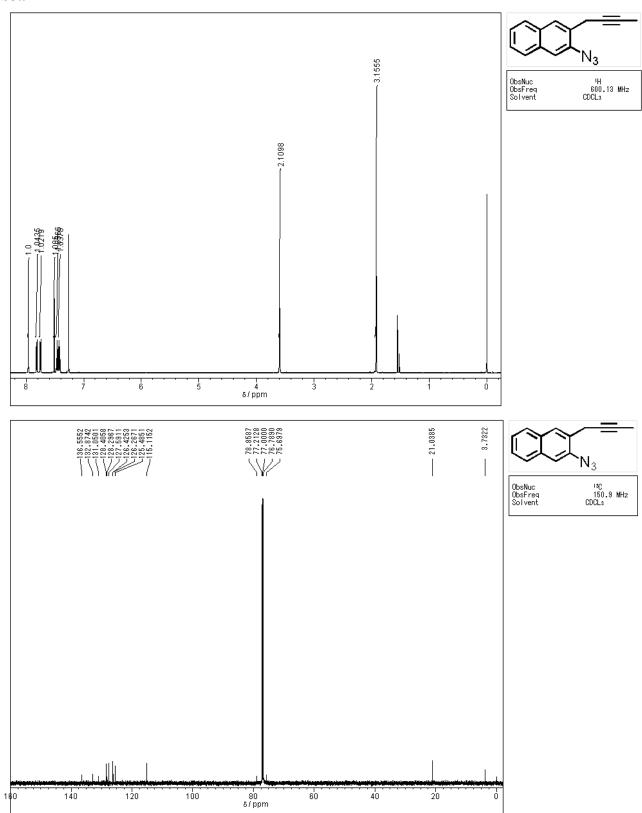


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S4b

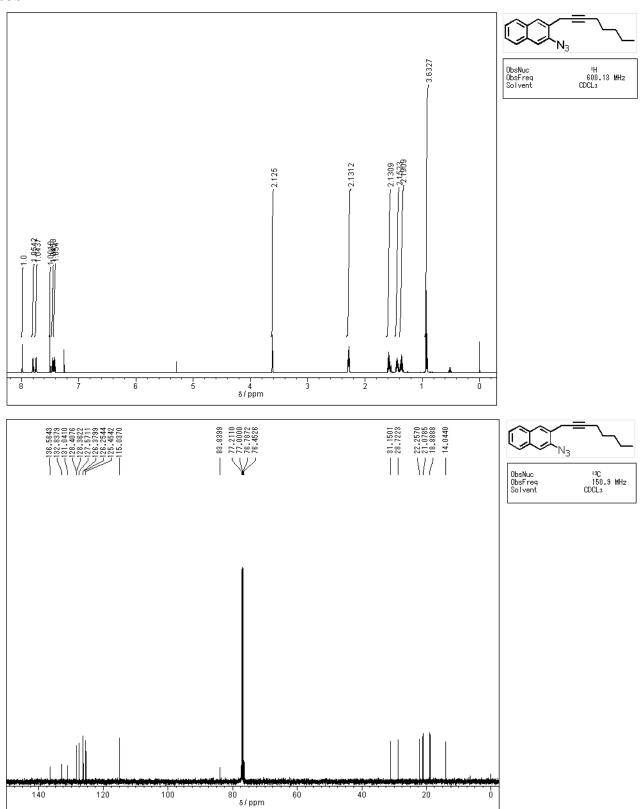


S5a



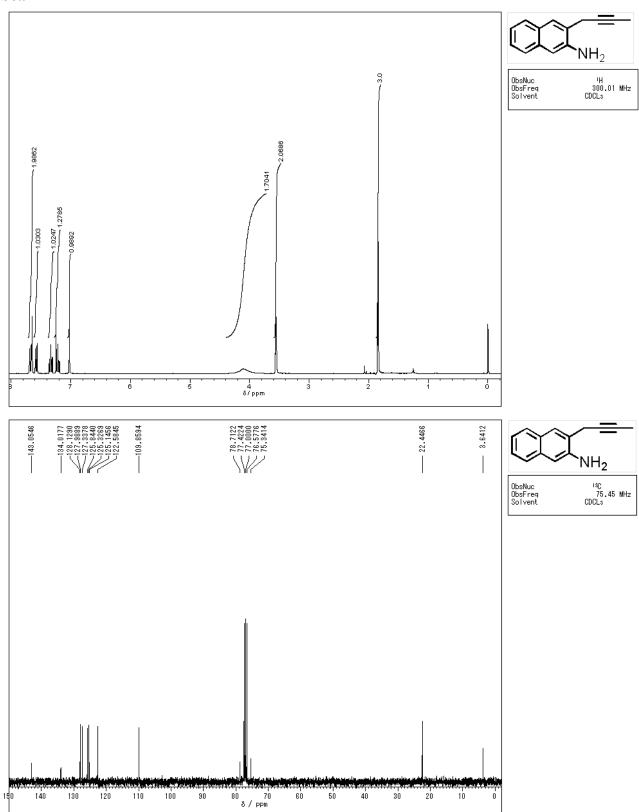
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S5b



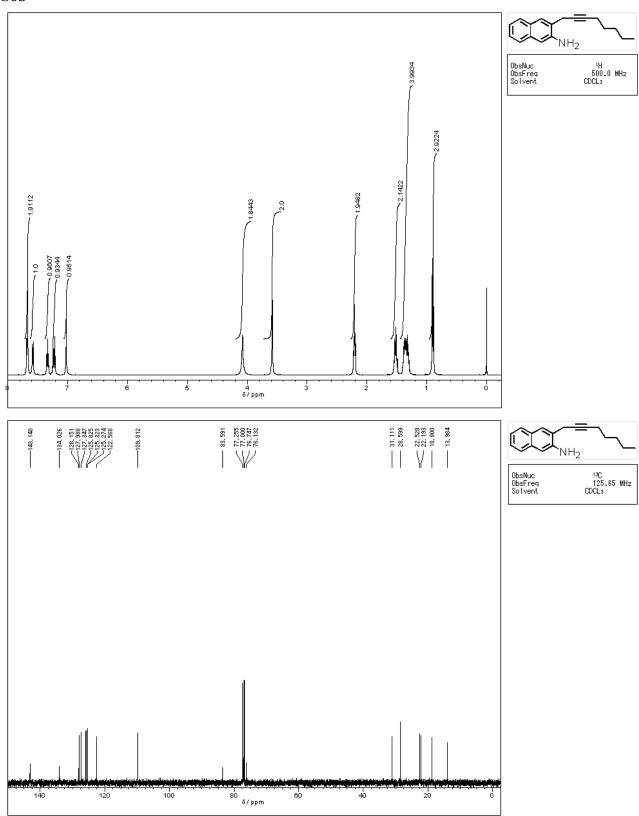
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S6a



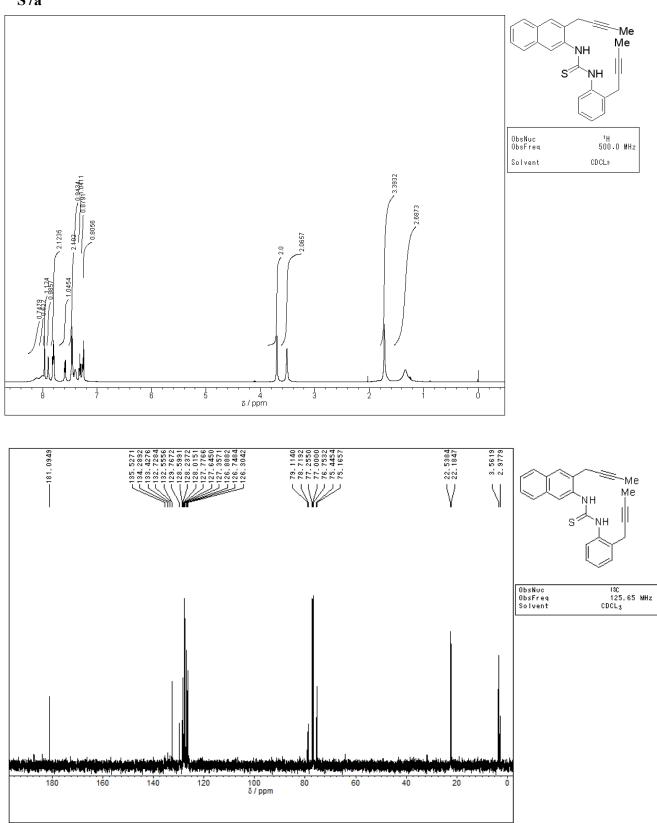
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S6b



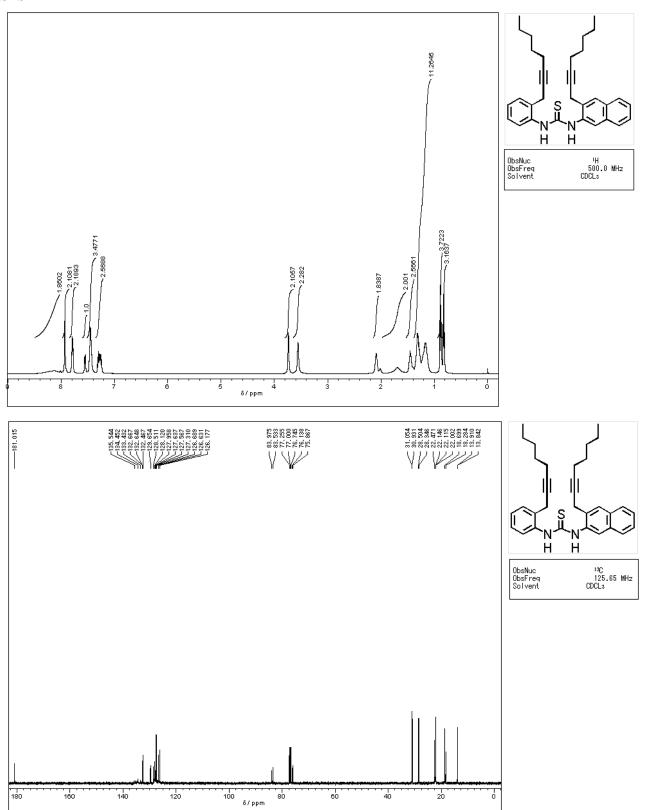
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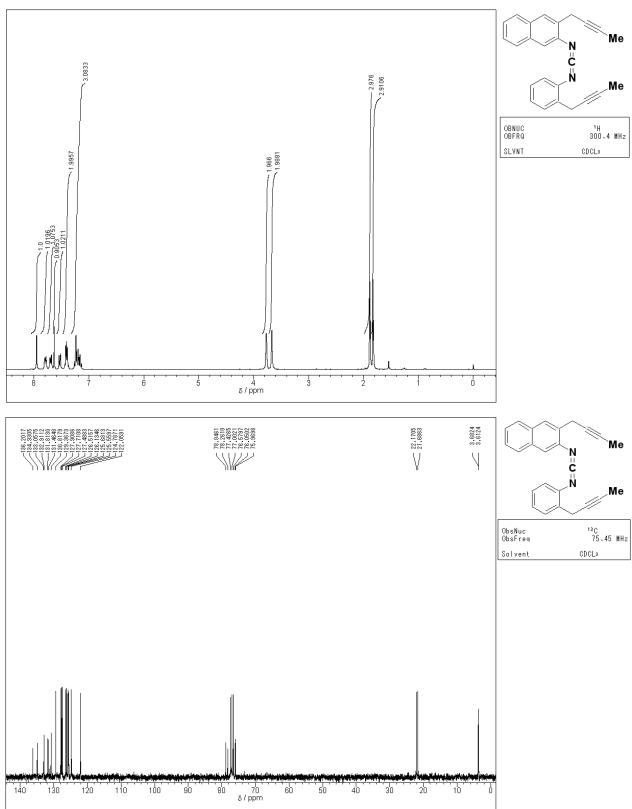
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S7b



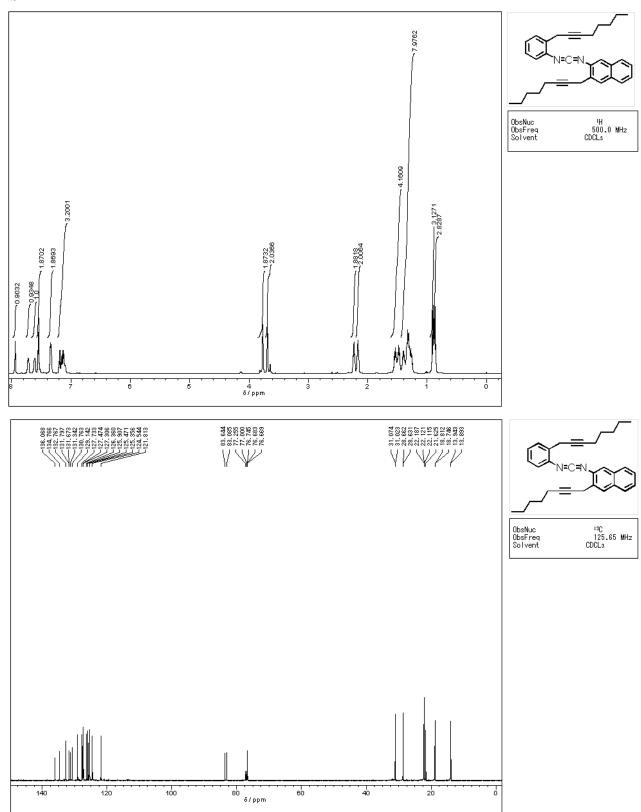
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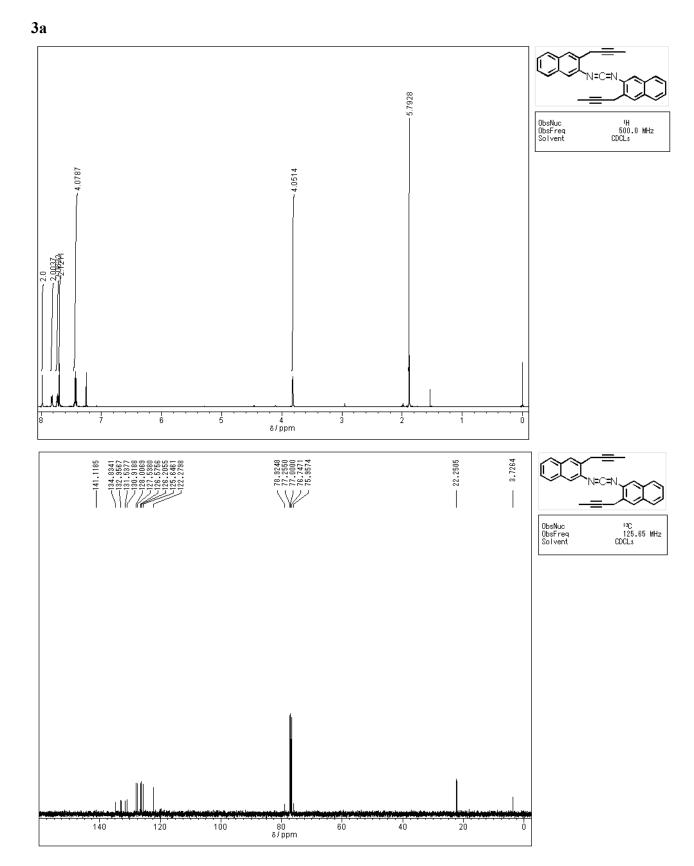




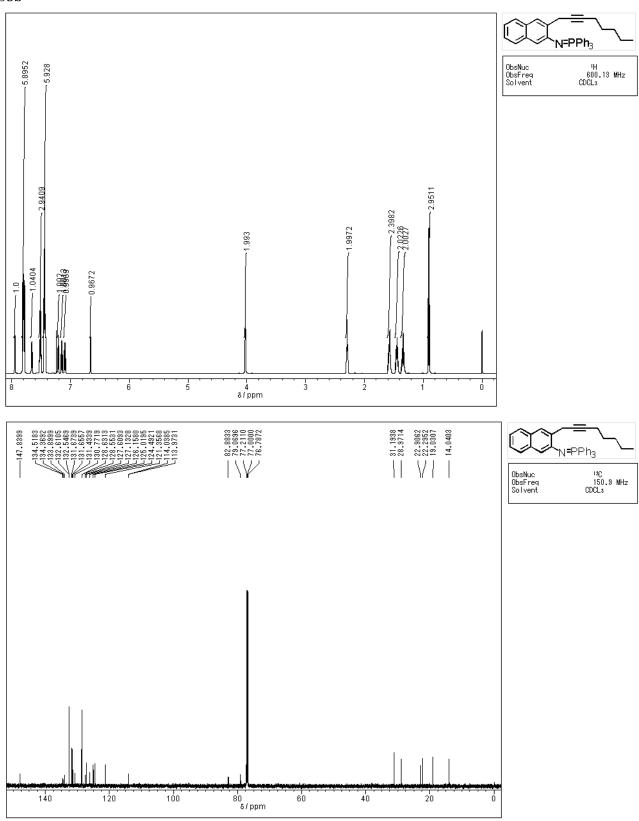
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2b



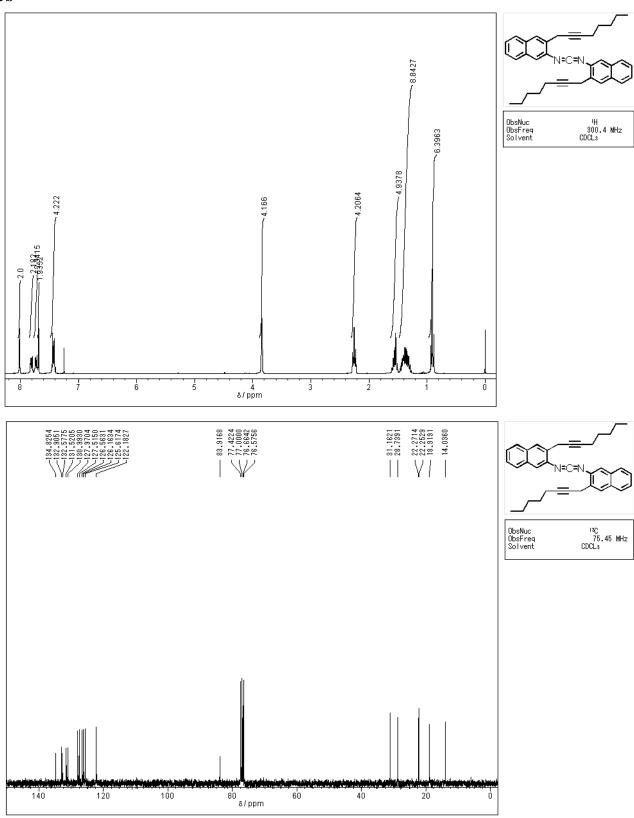


S8b

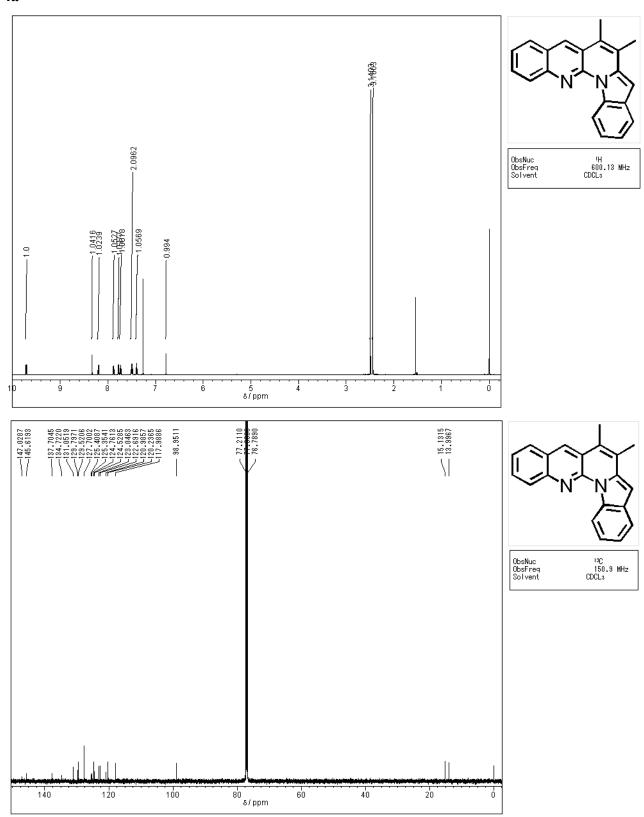


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3b

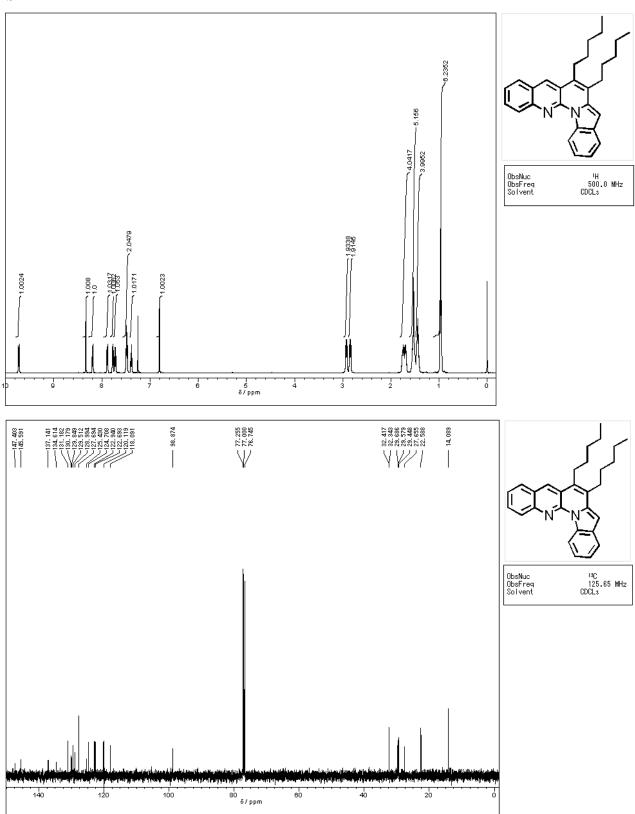


4a

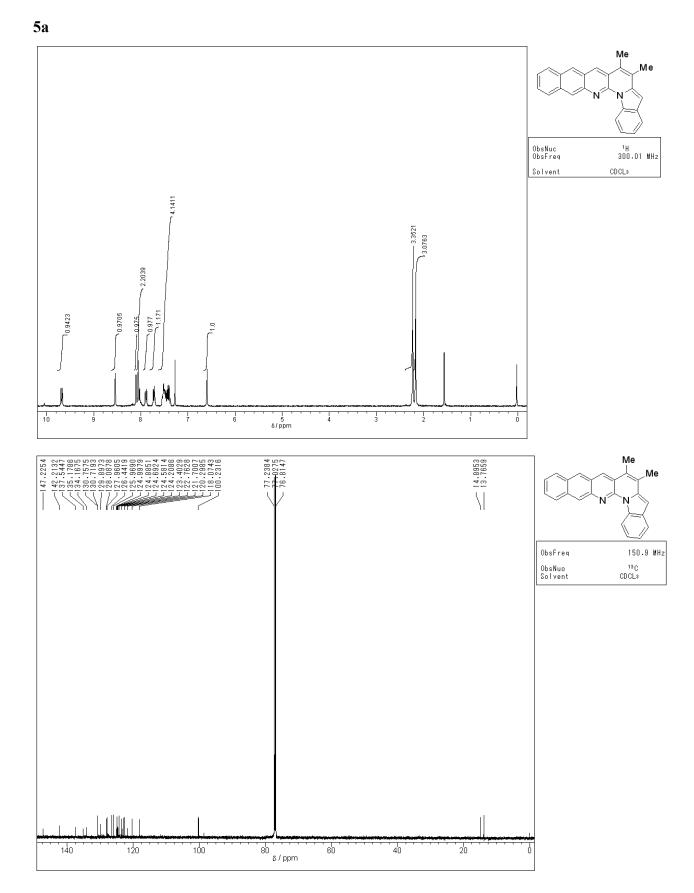


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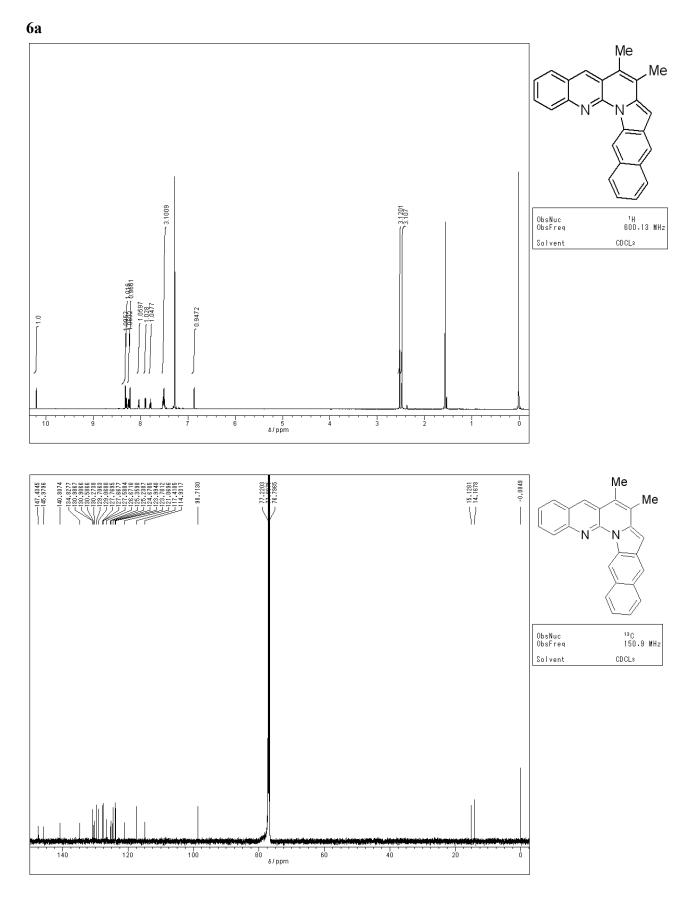
4b



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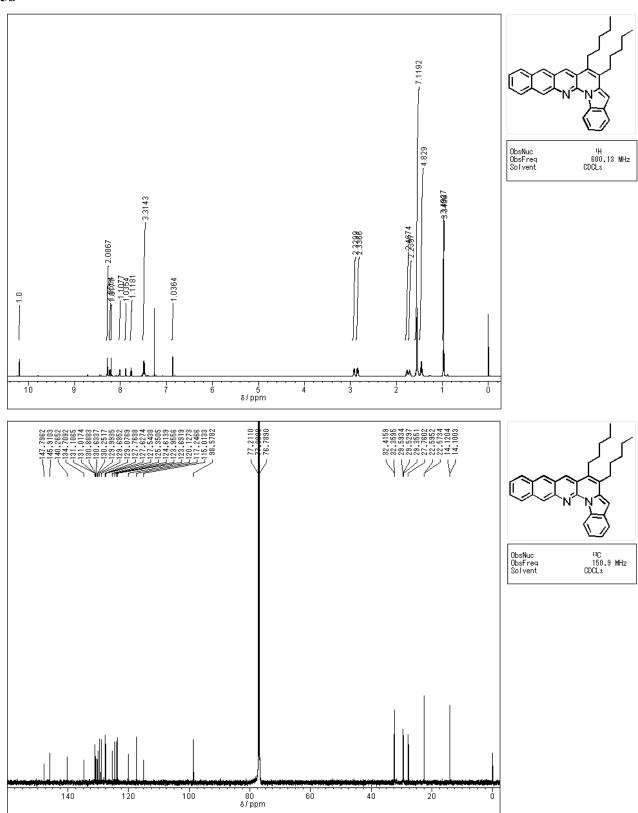


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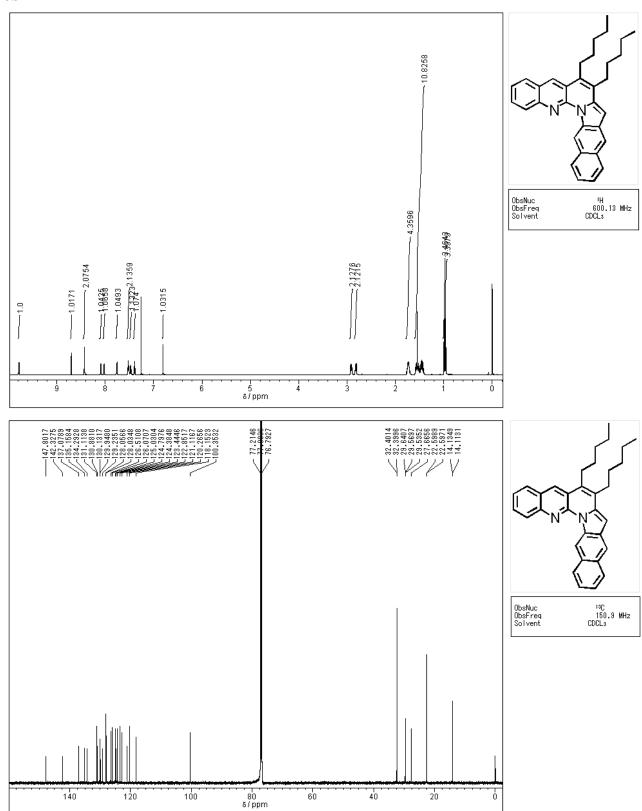
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5b

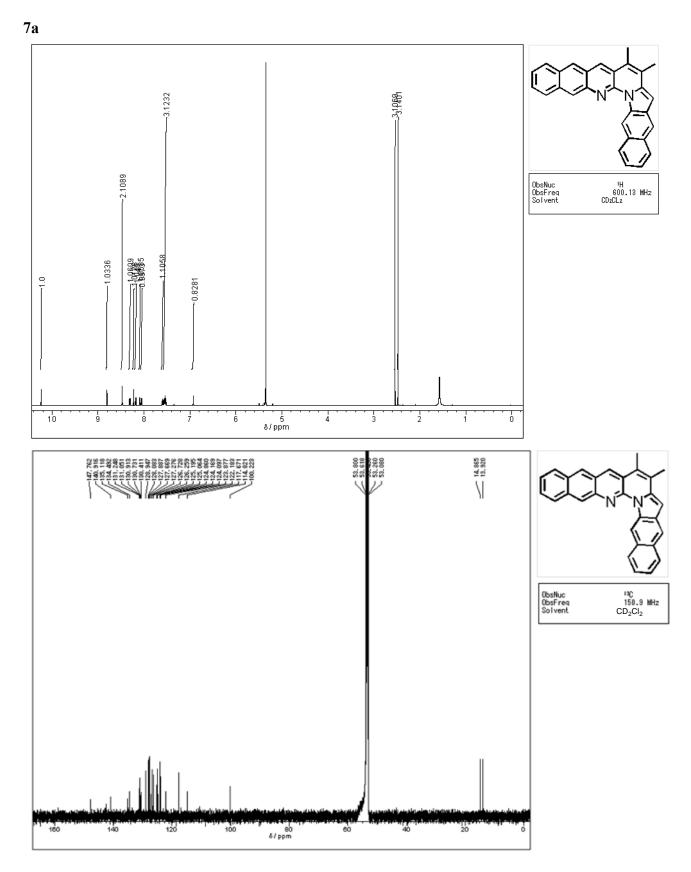


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6b

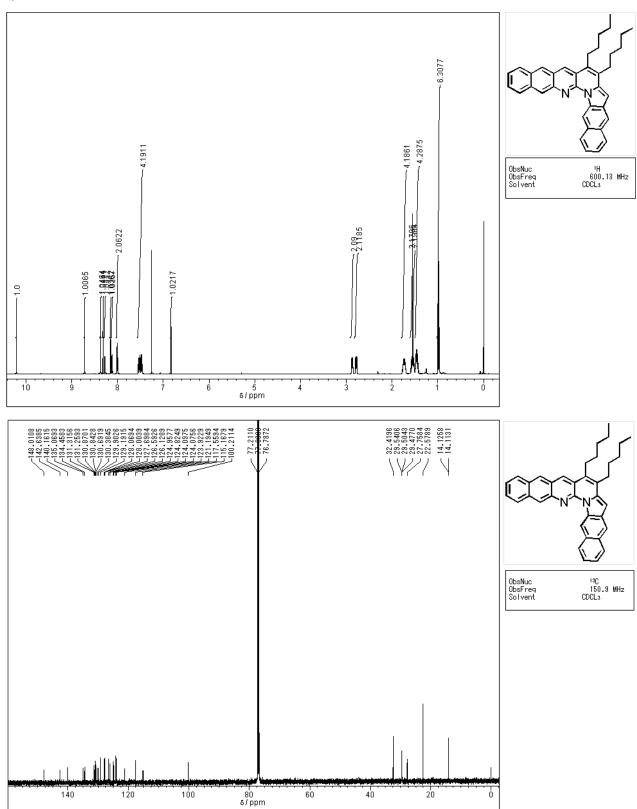


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7b



3. X-ray Crystallographic Analysis

3.1 Measurements

Crystallographic data of **5a** is summarized in Table S1. X-ray quality single crystals of **5a** were obtained from a hexane–dichloromethane solution as brownish red blocks. Single crystals of **5a** were coated with oil (Immersion Oil, type B: Code 1248, Cargille Laboratories, Inc.) and mounted on a MicroMountTM (MiTeGen, LLC). Diffraction data of **5a** were collected at 113 K under a cold nitrogen gas stream on a Rigaku AFC10 diffractometer equipped with a Saturn724+ CCD detector using graphite-monochromated MoK α radiation ($\lambda = 0.71073$ Å). The intensity data were collected by an ω -scan method with 0.5° oscillation for each frame. Bragg spots were integrated using the CrystalClear program package,^{S3} and the empirical absorption corrections (multi-scan) were applied using the REQAB program. The structures were solved by a direct method (SIR97),^{S4} and refined by a full-matrix least squares (SHELXL-97).^{S5} Anisotropic temperature factors were applied to all non-hydrogen atoms. The hydrogen atoms were put at calculated positions, and refined applying riding models.

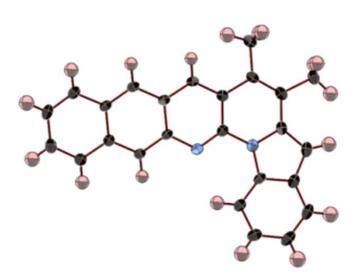


Figure S1. Molecular structure of 5a. One of the two crystallographically independent molecules is shown.

^{S3} CrystalClear: Rigaku/MSC. Inc., 9009 New Trails Drive, The Woodlands TX 77381, USA (2005).

^{S4} A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. J. Spagna, Appl. Cryst., 1999, **32**, 115–119..

^{S5} G. M. Sheldrick, Acta Crystallogr. Sect. A, 2008, 64, 112–122.

formula	$C_{25}H_{18}N_2$
M	346.41
T / K	113
color	brownish red
size, mm	0.20 x 0.15 x 0.05
crystal system	triclinic
space group	P-1 (#2)
<i>a</i> / Å	8.4955(15)
<i>b</i> / Å	11.1198(19)
<i>c</i> / Å	19.241(3)
α / deg.	76.717(4)
β / deg.	87.166(5)
γ/\deg .	83.238(5)
V/Å ³	1756.3(5)
Ζ	4
$D_{\rm x}$ / g cm ⁻³	1.310
reflections collected	21415
unique reflections	7983
refined parameters	488
GOF on F^2	1.093
$R1 \left[I > 2\sigma(I)\right]^{a}$	0.0699
wR2 (all data) ^b	0.1899
$\Delta ho_{ m min}$, max / e Å ⁻³	-0.56, 0.57
	$F_{0} _{,}^{b} wR2 = \left[\sum \left\{w(Fo^{2}-Fc^{2})^{2}/\sum w(Fo^{2})^{2}\right\}\right]^{1/2}$

Table S1. Crystallographic Data for 5a.

4. Photophysical Data

4.1 Measurements

UV-visible spectra of the L-shaped compounds were obtained on Shimadzu UV-3101(PC)S spectrometer. Fluorescence spectra were measured by JASCO FP-6500 spectrofluorometer. Absolute fluorescence quantum yields were measured by a calibrated integrating sphere system C10027 (Hamamatsu Photonics K.K.). Fluorescence lifetimes were measured with a Quantaurus-Tau[®] C1136703 (Hamamatsu Photonics K.K.).

4.2 Photophysical Properties of 4b-7b

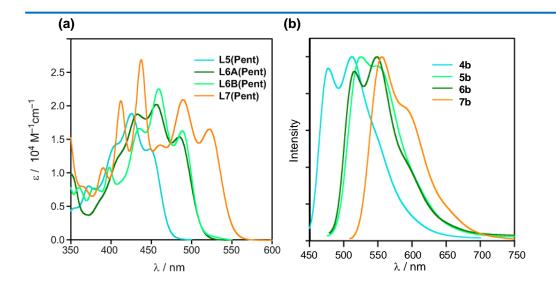


Figure S2. (a) UV-vis spectra of 4b–7b in CH₂Cl₂. (b) Fluorescence spectra (excited at λ_{max} (abs)) of 4b–7b in CH₂Cl₂.

Compound	$\lambda_{\rm max}$ (abs) [nm] (ε [10 ⁴ cm ⁻¹ M ⁻¹])	λ_{\max} (em) [nm] ^b	${\cal P}_{\rm F}{}^b$	$\tau_{\rm s} [{\rm ns}]^{b}$
4b	448 (1.35), 425 (1.88), 406 (1.42)	477, 512	0.82	5.78
5b	485 (1.54), 456 (2.02), 433 (1.87)	525, 547	0.74	6.26
6b	488 (1.62), 459 (2.25), 435 (1.66)	516, 549	0.77	6.29
7b	522 (1.65), 489 (2.09), 437 (2.68)	556, 585 (sh)	0.64	6.31
^{<i>a</i>} In CH ₂ Cl ₂ .	^b Excitation at λ_{max} (abs).			

Table S2. Photophysical Properties of 4b–7b^a

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4.3 Absorption and Emission Spectra of 4-7

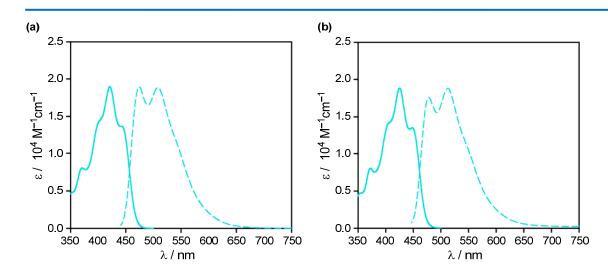


Figure S3. UV-vis spectra (solid line) and fluorescence spectra (dashed line) of 4a (a) and 4b (b) in CH₂Cl₂.

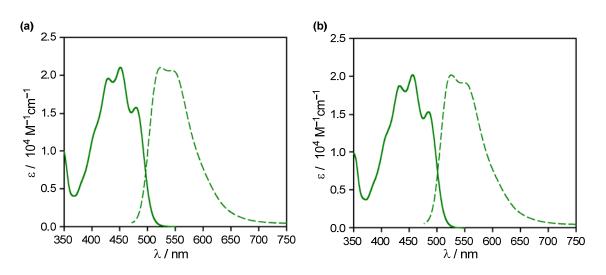


Figure S4. UV-vis spectra (solid line) and fluorescence spectra (dashed line) of 5a (a) and 5b (b) in CH₂Cl₂.

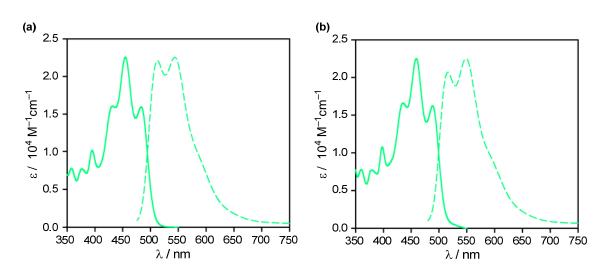


Figure S5. UV-vis spectra (solid line) and fluorescence spectra (dashed line) of 6a (a) and 6b (b) in CH₂Cl₂.

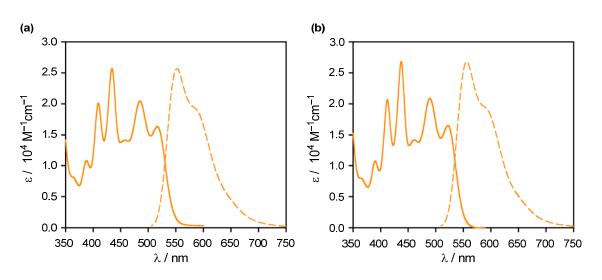


Figure S6. UV-vis spectra (solid line) and fluorescence spectra (dashed line) of 7a (a) and 7b (b) in CH₂Cl₂.

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4.4 Solvent-dependent Photophysical Properties of 4b

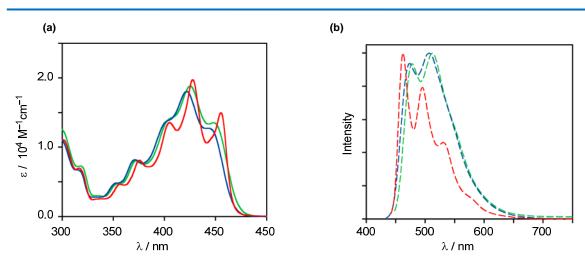


Figure **S7.** UV-vis spectra (a) and fluorescence spectra (b) of **4b** in methanol (blue), in dichloromethane (green), and in hexane (red).

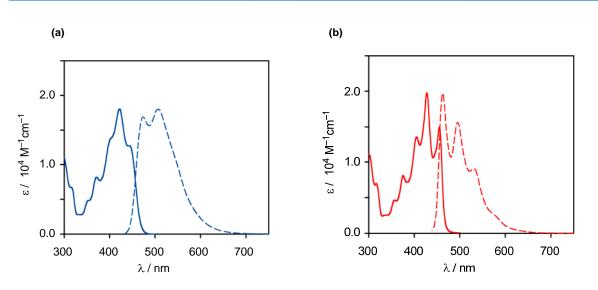


Figure S8. UV-vis spectra (solid line) and fluorescence spectra (dashed line) of **4b** in methanol (a) and in hexane (b). (For the spectra in CH_2Cl_2 , see *Figure S2(b)*)

5. Cyclic Voltammetry

5.1 Measurements

Electrochemical experiments of L-shaped compounds were carried out with an ALS/CHI 624C electrochemical analyzer using a glassy carbon working electrode, a Pt wire counter electrode, and a Ag/AgNO₃ reference electrode ([AgNO₃] = 0.01 mM in 0.1 M TBAClO₄-CH₃CN). The measurements were carried out in dry CH₂Cl₂ or THF solution containing 0.1 M TBAPF₆ a supporting electrolyte with scan rate of 100 mVs⁻¹ in a glove box filled with argon at ambient temperature. The reported value is corrected to the ferrocene couple as an internal standard.

5.2 Electrochemical Properties of L-Shaped Compounds

Compound	E^{ox} [V vs. Fc ⁺ /Fc] ^{<i>a</i>}	$E_{1/2}$ ^{red} [V vs. Fc ⁺ /Fc] ^{<i>b,c</i>}
4a	0.40	-2.40
4b	0.48	-2.36
5a	0.52	-2.10
5b	0.51	-2.11
6a	0.32	-2.30
6b	0.31	-2.27
7a	0.32	-2.04
7b	0.37	-2.13
^{<i>a</i>} In CH ₂ Cl ₂ . ^{<i>b</i>} In	THF. ^c Irreversible.	

Table S3. Electrochemical properties of 4-7.

5.3 Cyclic Voltammograms

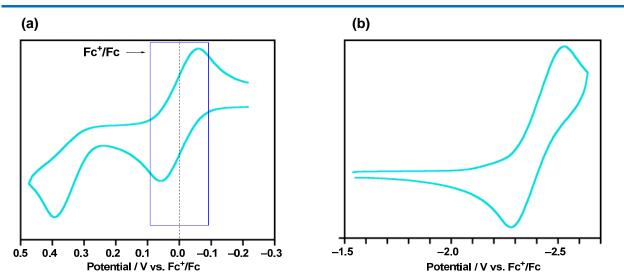


Figure **S9.** Cyclic voltammograms of **4a** in 0.1 M n-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M n-Bu₄NPF₆-THF (b).

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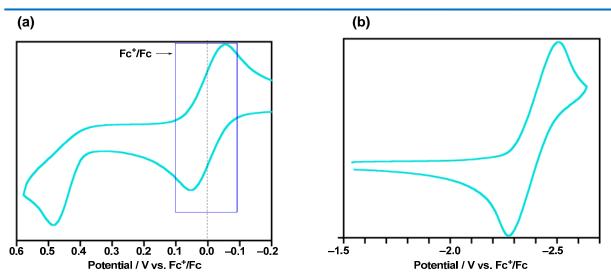


Figure S10. Cyclic voltammograms of **4b** in 0.1 M n-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M n-Bu₄NPF₆-THF (b).

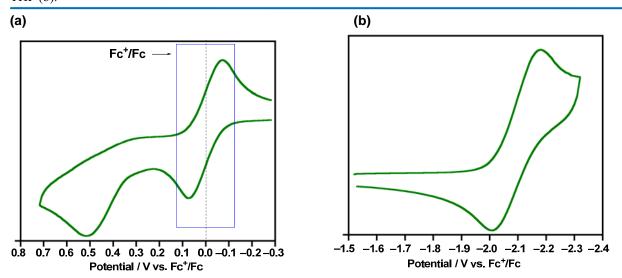


Figure S11. Cyclic voltammograms of **5a** in 0.1 M n-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M n-Bu₄NPF₆-THF (b).

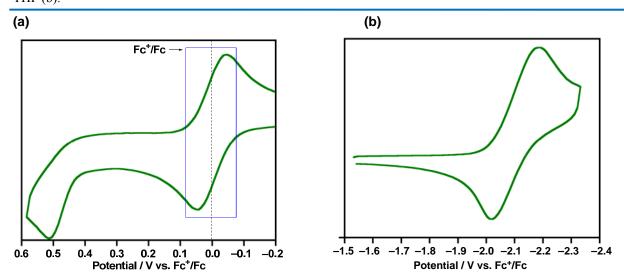


Figure **S12.** Cyclic voltammograms of **5b** in 0.1 M n-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M n-Bu₄NPF₆-THF (b).

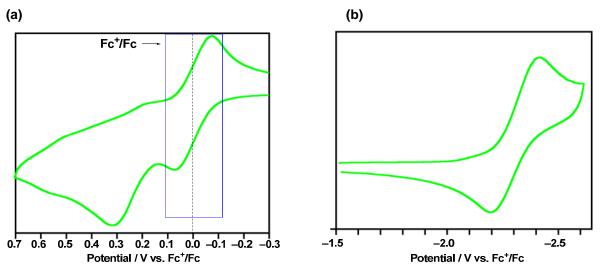


Figure **S13.** Cyclic voltammograms of **6a** in 0.1 M n-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M n-Bu₄NPF₆-THF (b).

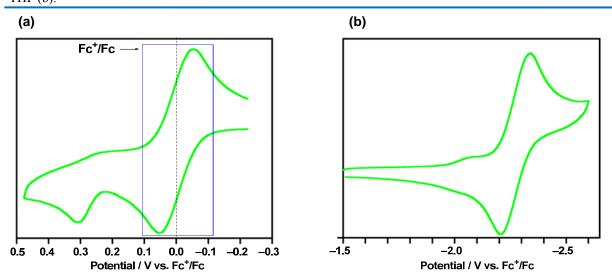


Figure S14. Cyclic voltammograms of **6b** in 0.1 M n-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M n-Bu₄NPF₆-THF (b).

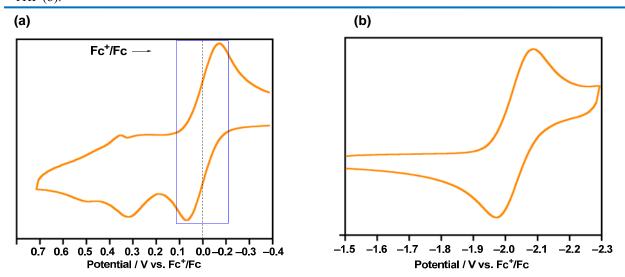


Figure S15. Cyclic voltammograms of 7a in 0.1 M *n*-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu₄NPF₆-THF (b).

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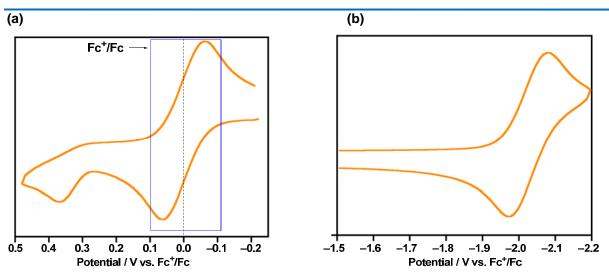
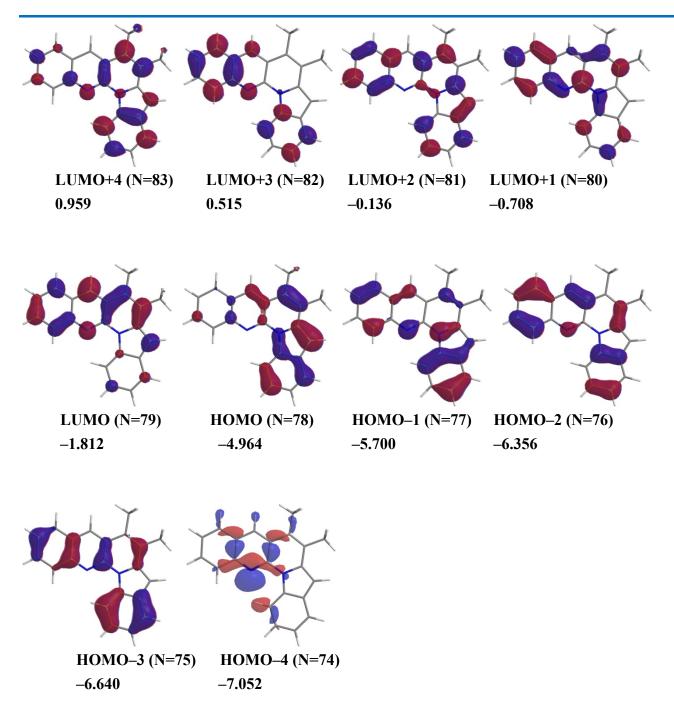


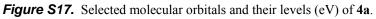
Figure **S16.** Cyclic voltammograms of 7b in 0.1 M n-Bu₄NPF₆-dichloromethane with ferrocene (a) and in 0.1 M n-Bu₄NPF₆-THF (b).

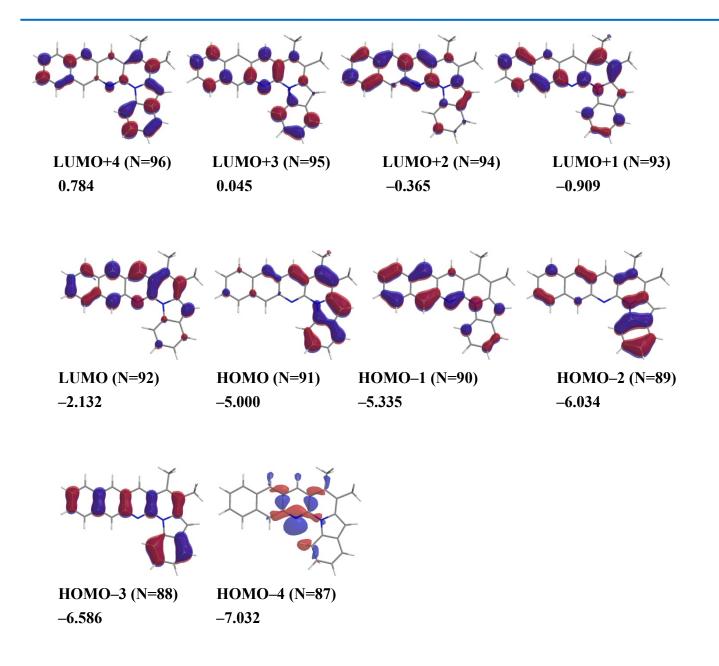
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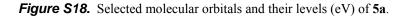
6. Theoretical Calculations

6.1 Molecular Orbitals and Their Levels of L-Shaped Compounds



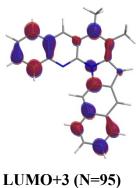


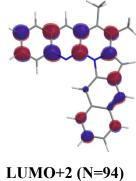






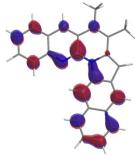
LUMO+4 (N=96) 0.590



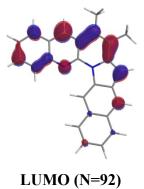


-0.446

-5.586



LUMO+1 (N=93) -1.002

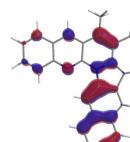


-1.909

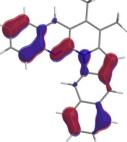
HOMO (N=91)

-4.760

0.173



НОМО–1 (N=90) НОМ



HOMO-2 (N=89) -6.164

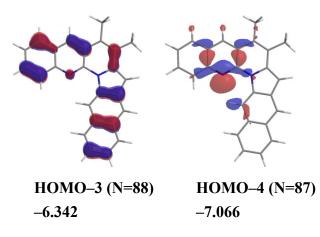


Figure S19. Selected molecular orbitals and their levels (eV) of 6a.

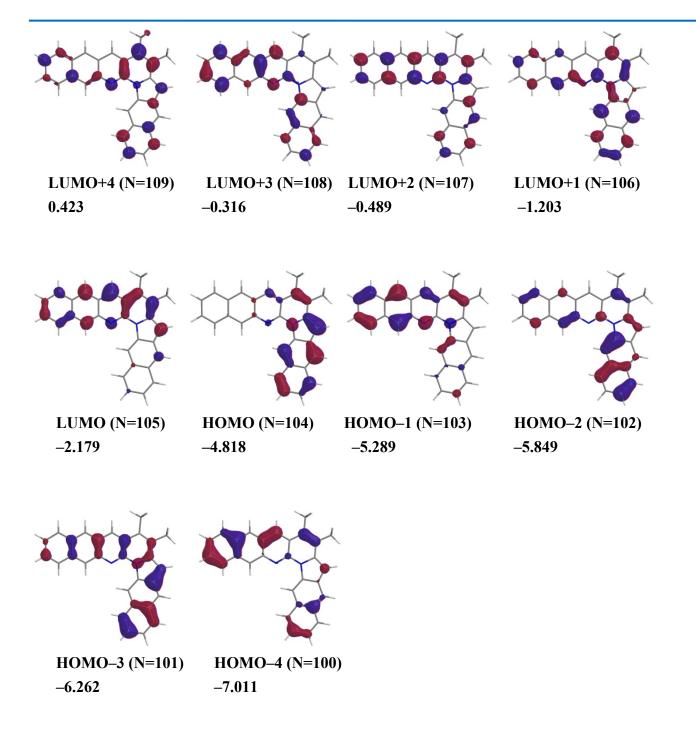


Figure S20. Selected molecular orbitals and their levels (eV) of 7a.

6.2 TDDFT Calculation of L-Shaped Compounds

Transition energy, wavelengths, and oscillator strengths of the electronic transitions of 4a (The 78th orbital is HOMO shown in Figure S16

Excitation energies and oscillato		75 -> 82 0.13006	
Excited State 1: Singlet-A' 2 77 -> 80 -0.13499	2.8616 eV 433.27 nm f=0.3051	$76 \rightarrow 81$ 0.39673 $78 \rightarrow 84$ -0.33219	
77 -> 80 -0.13499 78 -> 79 0.63738			5.8749 eV 211.04 nm f=0.4528
Excited State 2: Singlet-A'	3 3257 eV 372 81 nm f=0 0189	70 -> 79 0.12259	5.8749 EV 211.04 IIII 1=0.4528
77 -> 79 0.63829	5.5207 CT 572.01 IIII T 0.0107	71 -> 79 -0.11770	
78 -> 80 0.24744		72 -> 79 0.13146	
Excited State 3: Singlet-A'	3.6530 eV 339.41 nm f=0.0082	73 -> 80 0.13171	
77 -> 79 -0.21723		75 -> 80 0.12774	
78 -> 80 0.63842		75 -> 81 0.17273	
Excited State 4: Singlet-A'	4.0677 eV 304.80 nm f=0.0512	76 -> 80 -0.12923	
76 -> 79 0.63989 78 -> 81 0.11352		$77 \rightarrow 81 \qquad 0.10212$	
78 -> 81 0.11352 Excited State 5: Singlet-A'	4 1712 oV 207 22 nm f=0 0020	77 -> 82 0.40950 77 -> 83 0.20813	
75 -> 79 0.56802	4.1/13 CV 2/7.25 IIII 1=0.0057	77 -> 84 -0.20005	
77 -> 80 0.21023		78 -> 84 -0.16861	
78 -> 81 0.33201		Excited State 20: Singlet-A'	5.9739 eV 207.54 nm f=0.2457
Excited State 6: Singlet-A"	4.2556 eV 291.35 nm f=0.0005	73 -> 80 0.24605	
74 -> 79 0.69195		75 -> 80 -0.13900	
	4.4572 eV 278.16 nm f=0.1154	$75 \rightarrow 81$ 0.28144	
75 -> 79 -0.24257 76 -> 79 -0.11611		76 -> 80 0.11865 76 -> 81 0.30023	
$76 \rightarrow 80$ 0.30423		77 -> 83 0.34663	
77 -> 81 -0.18290		77 -> 84 0.16240	
78 -> 81 0.50655		Excited State 21: Singlet-A"	6.0143 eV 206.15 nm f=0.0001
Excited State 8: Singlet-A'	4.6155 eV 268.62 nm f=0.6709	74 -> 81 0.69080	
75 -> 79 -0.11702		Excited State 22: Singlet-A'	6.0882 eV 203.65 nm f=0.0380
77 -> 80 0.60913		$72 \rightarrow 80 \qquad 0.25628$	
77 -> 81 -0.11513 78 -> 81 -0.13197		$73 \rightarrow 80 -0.24300$ $75 \rightarrow 81 -0.25238$	
78 -> 81 -0.13197 Excited State 9: Singlet-A'	4 8534 eV 255 46 nm f=0 0068	$75 \rightarrow 81 -0.25238$ $75 \rightarrow 84 -0.11831$	
73 -> 79 -0.15929	4.8554 67 255.40 IIII 1=0.0908	$76 \rightarrow 81 -0.11045$	
75 -> 79 -0.18043		77 -> 83 0.46197	
77 -> 81 0.32150		78 -> 84 0.10107	
78 -> 82 0.51066		78 -> 85 -0.12985	
78 -> 84 0.15533			6.1810 eV 200.59 nm f=0.1938
	4.9664 eV 249.65 nm f=0.0398	71 -> 79 0.23706	
73 -> 79 0.45443		73 -> 80 0.33840	
76 -> 80 0.15774 77 -> 81 -0.17332		$75 \rightarrow 81 -0.28835$ $76 \rightarrow 82 0.18819$	
$78 \rightarrow 82$ 0.38112		$77 \rightarrow 82$ 0.15476	
$78 \rightarrow 83$ -0.14639		$77 \rightarrow 82$ 0.13470 $77 \rightarrow 84$ 0.32635	
78 -> 84 -0.17094			6.2946 eV 196.97 nm f=0.0892
	5.0690 eV 244.59 nm f=0.1033	70 -> 79 -0.22413	
73 -> 79 0.25608		71 -> 79 0.12613	
75 -> 80 -0.16137		72 -> 80 0.15807	
76 -> 80 0.33021		$73 \rightarrow 80 \qquad 0.15162$	
77 -> 81 0.45479 78 -> 82 -0.18693		$75 \rightarrow 82 \qquad 0.11570$	
78 -> 82 -0.18693 78 -> 84 0.10816		$76 \rightarrow 82 \qquad 0.46926 \\ 77 \rightarrow 84 \qquad -0.30354$	
	5.2146 eV 237.76 nm f=0.0002		6.4032 eV 193.63 nm f=0.0496
74 -> 80 0.69107	5.2110 CT 257.70 IIII T 0.0002	71 -> 79 0.44489	0.1052 01 199.05 1111 1 0.0190
Excited State 13: Singlet-A'	5.2509 eV 236.12 nm f=0.0656	72 -> 80 0.23410	
72 -> 79 -0.20325		73 -> 80 -0.13495	
73 -> 79 -0.10674		75 -> 81 0.12524	
$76 \rightarrow 80$ 0.24840		$75 \rightarrow 82$ 0.25290	
76 -> 81 -0.15061 77 -> 82 0.10001		76 -> 82 -0.18128 76 -> 83 0.10342	
$78 \rightarrow 83$ 0.45970		76 -> 84 -0.10857	
$78 \rightarrow 84 -0.28411$		78 -> 85 -0.11152	
	5.3264 eV 232.77 nm f=0.0955	Excited State 26: Singlet-A'	6.4110 eV 193.39 nm f=0.0459
72 -> 79 0.52608		70 -> 79 0.40130	
73 -> 79 -0.21006		71 -> 79 0.27848	
$75 \rightarrow 80$ 0.19543		$72 \rightarrow 80 \qquad -0.31801$	
76 -> 80 0.26005 Excited State 15: Singlet A'	5 4203 eV 228 36 nm f=0.0059	$73 \rightarrow 80 -0.12694$ $76 \rightarrow 82 0.14177$	
72 -> 79 -0.33540	5.4293 eV 228.36 nm f=0.0958	$76 \rightarrow 82 \qquad 0.14177 \\ 76 \rightarrow 83 \qquad -0.10816$	
72 -> 79 -0.33340 73 -> 79 -0.14911		77 -> 84 -0.20575	
75 -> 80 0.37894		78 -> 85 -0.15070	
75 -> 81 -0.11970		Excited State 27: Singlet-A"	6.4650 eV 191.78 nm f=0.0001
$76 \rightarrow 80$ 0.17688		69 -> 79 0.68184	
78 -> 83 -0.29682		Excited State 28: Singlet-A'	6.4843 eV 191.21 nm f=0.0244
78 -> 84 0.12518 Excited State 16: Singlet-A'	5.4679 eV 226.75 nm f=0.0025	$70 \rightarrow 79 \qquad 0.30437$ $71 \rightarrow 79 \qquad -0.12067$	
73 -> 79 0.10447	J. TO / / C Y 220. / J IIII 1=0.0023	72 -> 80 0.27748	
$73 \rightarrow 80 -0.11818$		$73 \rightarrow 80$ 0.21748	
75 -> 80 0.31319		75 -> 82 0.30117	
76 -> 81 0.37051		76 -> 83 -0.24892	
78 -> 83 0.32267		78 -> 85 -0.16183	· · · · · · · · · · · · · · · · · · ·
78 -> 84 0.29257	5 540C - M 202 41 mm 6-0 2247	Excited State 29: Singlet-A"	6.5192 eV 190.18 nm f=0.0017
	5.5496 eV 223.41 nm f=0.2347	$74 \rightarrow 82$ 0.65769 $74 \rightarrow 82$ 0.12160	
73 -> 79 -0.13979 73 -> 80 -0.13481		74 -> 83 0.13169 74 -> 84 -0.10749	
73 -> 80 -0.13481 75 -> 80 -0.31116		Excited State 30: Singlet-A"	6.5297 eV 189.88 nm f=0.0012
$75 \rightarrow 81 -0.10390$		Entered State 50. Singlet-A	
76 -> 80 0.10714		78 -> 86 0.6971	
77 -> 81 -0.19322			
77 -> 82 0.45421			
77 -> 82 0.45421 78 -> 84 0.18575			
77 -> 82 0.45421 78 -> 84 0.18575 Excited State 18: Singlet-A'	5.8066 eV 213.52 nm f=0.0800		
77 -> 82 0.45421 78 -> 84 0.18575 Excited State 18: Singlet-A' 73 -> 79 -0.13221	5.8066 eV 213.52 nm f=0.0800		
77 -> 82 0.45421 78 -> 84 0.18575 Excited State 18: Singlet-A'	5.8066 eV 213.52 nm f=0.0800		

Transition energy, wavelengths, and oscillator strengths of the electronic transitions of 5a (The 91st orbital is HOMO shown in Figure S17).

Excitation energies and oscillato		89 -> 94 -0.25115	
Excited State 1: Singlet-A' 91 -> 92 0.69248	2.6101 eV 475.02 nm f=0.3594	89 -> 95 0.12453 91 -> 97 -0.18111	
Excited State 2: Singlet-A'	2.7833 eV 445.45 nm f=0.0186	91 -> 98 0.10950	
90 -> 92 0.69382			5.2046 eV 238.22 nm f=0.0382
Excited State 3: Singlet-A'	3.3799 eV 366.83 nm f=0.0514	84 -> 92 0.60441	
89 -> 92 0.67845		88 -> 93 0.15819	
91 -> 93 -0.10638	A 556 TA A 5 6 6 6 6 6 6 6	89 -> 94 -0.13113	
Excited State 4: Singlet-A' 89 -> 92 0.11973	3.5726 eV 347.04 nm f=0.1051	$90 \rightarrow 97 -0.14597$	
89 -> 92 0.11973 91 -> 93 0.66794		90 -> 98 -0.13198 91 -> 98 -0.11991	
$91 \rightarrow 94 -0.12704$		Excited State 18: Singlet-A'	5.2414 eV 236.55 nm f=0.0799
Excited State 5: Singlet-A'	3.8005 eV 326.23 nm f=0.0096	86 -> 93 -0.17896	
88 -> 92 0.54748		88 -> 93 -0.13143	
90 -> 93 -0.37136		89 -> 94 -0.15343	
90 -> 94 0.15634		89 -> 95 0.22324	
91 -> 94 0.10772	2 0725 eV 212 11 mm f=0 0004	$90 \rightarrow 95 -0.14040$	
Excited State 6: Singlet-A" 87 -> 92 0.70130	3.9725 eV 312.11 nm f=0.0004	91 -> 96 0.53575 91 -> 97 0.14525	
Excited State 7: Singlet-A'	4.0650 eV 305.01 nm f=0.2551	Excited State 19: Singlet-A'	5.2919 eV 234.29 nm f=0.0342
88 -> 92 0.22266		86 -> 93 0.12857	
90 -> 93 0.50566		88 -> 93 0.17843	
90 -> 94 0.13626		88 -> 94 -0.12705	
91 -> 93 0.10996		89 -> 94 -0.30352	
91 -> 94 0.38715	4 1024 - W 205 (Come 6-0.0202	89 -> 95 -0.27148	
Excited State 8: Singlet-A' 89 -> 93 -0.27140	4.1934 eV 295.66 nm f=0.0393	$90 \rightarrow 96$ 0.14715 $91 \rightarrow 97$ 0.44417	
89 -> 93 -0.27140 90 -> 93 -0.23036		Excited State 20: Singlet-A'	5.4081 eV 229.25 nm f=0.2081
90 -> 94 -0.32391		85 -> 92 -0.10823	5.4001 ev 229.25 mil 1 0.2001
91 -> 94 0.44718		86 -> 93 -0.10677	
91 -> 95 0.17346		88 -> 93 0.31094	
Excited State 9: Singlet-A'	4.4021 eV 281.65 nm f=0.3270	89 -> 94 0.34691	
86 -> 92 0.49777		90 -> 95 0.12637	
$88 \rightarrow 92$ 0.21290		90 > 96 -0.34477	
90 -> 94 -0.31238 91 -> 95 -0.19959		91 -> 96 0.10915 91 -> 97 0.17808	
91 -> 96 0.11355		91 -> 98 -0.12077	
	4.5419 eV 272.98 nm f=0.1782	Excited State 21: Singlet-A'	5.5041 eV 225.26 nm f=0.0152
85 -> 92 0.21378		83 -> 92 0.19250	
88 -> 92 0.18023		84 -> 92 0.11817	
89 -> 93 0.25136		86 -> 93 -0.19426	
$90 \rightarrow 94 -0.17843$		$88 \rightarrow 93 -0.14783$	
91 -> 94 -0.10349 91 -> 95 0.53712		88 -> 94 0.29001 88 -> 95 0.10117	
	4.5986 eV 269.61 nm f=0.2715	90 -> 96 -0.14439	
85 -> 92 -0.32930	1.5500 01 205.01 mil 1 0.2710	91 -> 96 -0.28018	
86 -> 92 0.38020		91->97 0.33252	
90 -> 94 0.31726		91 -> 98 0.16349	
91 -> 95 0.30995		Excited State 22: Singlet-A'	5.6040 eV 221.24 nm f=0.0276
Excited State 12: Singlet-A'	4.6945 eV 264.10 nm f=0.3210	$83 \rightarrow 92 -0.12714$	
85 -> 92 0.47772 86 -> 92 0.14417		85 -> 93 -0.10768 86 -> 93 0.36845	
89 -> 93 -0.23655		88 -> 94 -0.12508	
90 -> 94 0.28223		89 -> 95 0.25483	
90 -> 95 0.27911		90 -> 96 -0.12361	
Excited State 13: Singlet-A'	4.7827 eV 259.24 nm f=0.1662	90 -> 97 -0.21386	
86 -> 92 0.19163		91 -> 97 0.12513	
88 -> 92 -0.10584		91->98 0.37914	
$89 \rightarrow 93$ 0.46689		Excited State 23: Singlet-A'	5.6540 eV 219.29 nm f=0.1389
90 -> 95 0.38436 91 -> 94 0.18632		86 -> 93 -0.27333 89 -> 95 -0.38639	
$91 \rightarrow 97$ 0.10541		90 -> 97 -0.11191	
	4.9316 eV 251.41 nm f=0.3597	91 -> 98 0.42858	
85 -> 92 -0.21632			5.6708 eV 218.64 nm f=0.0665
88 -> 92 0.13404		83 -> 92 -0.14272	
89 -> 93 -0.13686		84 -> 92 0.11744	
$89 \rightarrow 94 -0.31746$		85 -> 93 0.21770	
90 -> 95 0.43180 90 -> 96 -0.11261		89 -> 95 0.24398 90 -> 96 0.32404	
90 -> 96 -0.11261 91 -> 94 -0.15549		$90 \rightarrow 98$ 0.32404 $90 \rightarrow 97$ 0.39331	
$91 \rightarrow 97 -0.17247$		91 -> 97 0.12683	
Excited State 15: Singlet-A"	5.1464 eV 240.91 nm f=0.0000	91 -> 98 0.17428	
87 -> 93 0.68402		Excited State 25: Singlet-A'	5.7587 eV 215.30 nm f=0.0250
87 -> 94 -0.15206		83 -> 92 0.55313	
Excited State 16: Singlet-A'	5.1509 eV 240.70 nm f=0.0956	85 -> 93 0.15192	
84 -> 92 -0.20229 85 -> 92 0.13303		88 -> 94 -0.28770 91 -> 98 0.13637	
85 -> 92 0.13303 88 -> 93 0.48756		91 -> 98 0.13637 91 -> 99 -0.12157	
88 -> 94 0.13456		71 × 77 =0.12137	

Transition energy, wavelengths, and oscillator strengths of the electronic transitions of 6a (The 91st orbital is HOMO shown in Figure S18).

Excitation energies and oscillato		89 -> 94 0.12674	
	2.5726 eV 481.93 nm f=0.2871	90 -> 95 -0.14091	
91 -> 92 0.69443		90 -> 96 0.11509	
Excited State 2: Singlet-A'	3.1211 eV 397.24 nm f=0.0571	91 -> 96 0.15623	
90 -> 92 0.55408		Excited State 16: Singlet-A"	5.0599 eV 245.03 nm f=0.0003
91 -> 93 -0.40653		87 -> 93 0.65741	
91 -> 94 -0.12201		87 -> 94 0.22629	
Excited State 3: Singlet-A'	3.3382 eV 371.41 nm f=0.0608	Excited State 17: Singlet-A'	5.1541 eV 240.56 nm f=0.3294
90 -> 92 0.40483		88 -> 93 -0.22003	
91 -> 93 0.55915		89 -> 94 0.41289	
Excited State 4: Singlet-A'	3.6873 eV 336.25 nm f=0.0279	90 -> 94 -0.14154	
89 -> 92 0.55460		90 -> 95 0.17732	
91 -> 94 -0.40180		91 -> 96 -0.19640	
Excited State 5: Singlet-A'	3.8334 eV 323.43 nm f=0.1267	91 -> 97 0.37497	
88 -> 92 0.16654		Excited State 18: Singlet-A'	5.2719 eV 235.18 nm f=0.1182
88 -> 93 0.11721		85 -> 92 0.12890	
89 -> 92 0.39292		86 -> 93 -0.11211	
90 -> 93 -0.14268		88 -> 94 0.20978	
91 -> 94 0.50549		89 -> 94 -0.29381	
Excited State 6: Singlet-A'	4.0133 eV 308.93 nm f=0.0785	90 -> 94 -0.10182	
88 -> 92 0.63732		90 -> 95 0.53034	
90 -> 93 0.13484		Excited State 19: Singlet-A'	5.3292 eV 232.65 nm f=0.1903
90 -> 94 -0.12232		84 -> 92 0.41335	
91 -> 94 -0.11200		86 -> 92 -0.10094	
Excited State 7: Singlet-A'	4.1068 eV 301.90 nm f=0.2598	86 -> 93 -0.22198	
90 -> 93 0.59330		88 -> 93 -0.11502	
91 -> 94 0.17450		88 -> 94 -0.18561	
91 -> 95 0.27991		90 -> 95 -0.15850	
91 -> 96 0.11914		91 -> 98 0.35634	
Excited State 8: Singlet-A"	4.2251 eV 293.45 nm f=0.0004	Excited State 20: Singlet-A'	5.4471 eV 227.62 nm f=0.4501
87 -> 92 0.69610		85 -> 93 -0.18723	
87 -> 93 -0.10501		86 -> 92 0.22263	
Excited State 9: Singlet-A'	4.3937 eV 282.18 nm f=0.2119	86 -> 93 0.15110	
86 -> 92 0.11830		88 -> 94 0.28943	
88 -> 93 -0.22763		89 -> 94 0.16512	
90 -> 93 -0.23523		89 -> 95 -0.18883	
90 -> 94 -0.39450		90 -> 94 0.14475	
91 -> 95 0.40870		91 -> 98 0.37518	
Excited State 10: Singlet-A'	4.5231 eV 274.12 nm f=0.1374	Excited State 21: Singlet-A'	5.4917 eV 225.77 nm f=0.0073
Excited State 10: Singlet-A' 86 -> 92 -0.21495	4.5231 eV 274.12 nm f=0.1374	Excited State 21: Singlet-A' 84 -> 92 0.43598	5.4917 eV 225.77 nm f=0.0073
Excited State 10: Singlet-A' 86 -> 92 -0.21495 89 -> 93 -0.37035	4.5231 eV 274.12 nm f=0.1374	Excited State 21: Singlet-A' 84 -> 92 0.43598 86 -> 93 0.20135	5.4917 eV 225.77 nm f=0.0073
Excited State 10: Singlet-A' 86 -> 92 -0.21495 89 -> 93 -0.37035 90 -> 94 0.25334	4.5231 eV 274.12 nm f=0.1374	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696	5.4917 eV 225.77 nm f=0.0073
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.5231 eV 274.12 nm f=0.1374	Excited State 21: Singlet-A' 84 > 92 0.43598 86 >> 93 0.20135 88 > 94 0.15696 89 >> 94 -0.16481	5.4917 eV 225.77 nm f=0.0073
Excited State 10: Singlet-A' 86 -> 92 -0.21495 89 -> 93 -0.37035 90 -> 94 0.25334 91 -> 95 0.41678 91 -> 96 -0.21607		Excited State 21: Singlet-A' 84 -> 92 0.43598 86 -> 93 0.20135 88 -> 94 0.15696 89 -> 94 -0.16481 89 -> 95 -0.18220	5.4917 eV 225.77 nm f=0.0073
Excited State 10: Singlet-A' 86 -> 92 -0.21495 89 -> 93 -0.37035 90 -> 94 0.25334 91 -> 95 0.41678 91 -> 96 -0.21607 Excited State 11: Singlet-A'	4.5231 eV 274.12 nm f=0.1374 4.6925 eV 264.22 nm f=0.0135	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.4917 eV 225.77 nm f=0.0073
Excited State 10: Singlet-A' 86 -> 92 -0.21495 89 -> 93 -0.37035 90 -> 94 0.25334 91 -> 95 0.41678 91 -> 96 -0.21607 Excited State 11: Singlet-A' 85 -> 92 0.11087		$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.4917 eV 225.77 nm f=0.0073
Excited State 10: Singlet-A' 86 -> 92 -0.21495 89 -> 93 -0.37035 90 -> 94 0.25334 91 -> 95 0.41678 91 -> 96 -0.21607 Excited State 11: Singlet-A' 85 -> 92 0.11087 86 -> 92 -0.40939		Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603	5.4917 eV 225.77 nm f=0.0073
$\begin{array}{llllllllllllllllllllllllllllllllllll$		$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	
$\begin{array}{llllllllllllllllllllllllllllllllllll$		$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.4917 eV 225.77 nm f=0.0073 5.5566 eV 223.13 nm f=0.1594
$\begin{array}{c cccc} Excited State & 10: & Singlet-A' \\ 86 &> 92 & -0.21495 \\ 89 &> 93 & -0.37035 \\ 90 &> 94 & 0.25334 \\ 91 &> 95 & 0.41678 \\ 91 &> 96 & -0.21607 \\ Excited State & 11: & Singlet-A' \\ 85 &> 92 & 0.11087 \\ 86 &> 92 & -0.40939 \\ 88 &> 93 & 0.14296 \\ 89 &> 93 & 0.45987 \\ 91 &> 96 & -0.22553 \\ \end{array}$	4.6925 eV 264.22 nm f=0.0135	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	
$\begin{array}{llllllllllllllllllllllllllllllllllll$		$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27118 89 > 95 -0.223480 89 > 95 -0.22385 90 > 96 0.22885	
$\begin{array}{c cccc} Excited State 10: Singlet-A'\\ 86 > 92 & -0.21495\\ 89 > 93 & -0.37035\\ 90 > 94 & 0.25334\\ 91 > 95 & 0.41678\\ 91 > 96 & -0.21607\\ \hline Excited State 11: Singlet-A'\\ 85 > 92 & 0.11087\\ 86 > 92 & 0.40939\\ 88 > 93 & 0.14296\\ 89 > 93 & 0.42987\\ 91 > 96 & -0.22553\\ \hline Excited State 12: Singlet-A'\\ 85 > 92 & 0.12962\\ 88 > 93 & 0.50172\\ 89 > 93 & -0.20875\\ 89 > 94 & 0.11460\\ \end{array}$	4.6925 eV 264.22 nm f=0.0135	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 94 -0.23480 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.22585 90 > 96 0.22889 91 > 96 -0.15626	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 94 -0.23480 89 > 95 -0.26937 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22889 91 > 96 -0.15626 91 > 97 0.12818	
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.2718 89 > 95 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.2718 89 > 95 -0.22785 90 > 96 0.29889 91 > 96 -0.15626 91 > 96 0.12818 91 > 97 0.12818 91 > 98 0.18623	5.5566 eV 223.13 nm f=0.1594
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A'	5.5566 eV 223.13 nm f=0.1594
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 0.15696 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 95 -0.26937 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22889 91 > 96 0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 84 > 92 -0.18868	5.5566 eV 223.13 nm f=0.1594
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$ \begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.2718 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 96 0.29889 91 > 96 0.28889 91 > 96 0.28889 91 > 96 0.21818 91 > 98 0.18663 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932	5.5566 eV 223.13 nm f=0.1594
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22889 91 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843	5.5566 eV 223.13 nm f=0.1594
$\begin{array}{c ccccc} Excited State 10: Singlet-A'\\ 86 &> 92 & -0.21495\\ 89 &> 93 & -0.37035\\ 90 &> 94 & 0.25334\\ 91 &> 95 & 0.41678\\ 91 &> 96 & -0.21607\\ \hline Excited State 11: Singlet-A'\\ 85 &> 92 & 0.11087\\ 86 &> 92 & -0.40939\\ 88 &> 93 & 0.14296\\ 89 &> 93 & 0.45987\\ 91 &> 96 & -0.22553\\ \hline Excited State 12: Singlet-A'\\ 85 &> 92 & 0.12962\\ 88 &> 93 & 0.22553\\ \hline Excited State 12: Singlet-A'\\ 85 &> 92 & 0.12962\\ 88 &> 93 & -0.20875\\ 89 &> 94 & 0.11460\\ 90 &> 94 & -0.36762\\ \hline Excited State 13: Singlet-A'\\ 85 &> 92 & 0.36381\\ 88 &> 94 & -0.17472\\ 89 &> 93 & 0.18574\\ 89 &> 94 & 0.11153\\ 90 &> 94 & 0.3141\\ \hline \end{array}$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27118 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.29889 91 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843 90 > 96 0.45412	5.5566 eV 223.13 nm f=0.1594
$\begin{array}{c cccc} Excited State 10: Singlet-A'\\ 86 -> 92 & -0.21495\\ 89 -> 93 & -0.37035\\ 90 -> 94 & 0.25334\\ 91 -> 95 & 0.41678\\ 91 -> 96 & -0.21607\\ Excited State 11: Singlet-A'\\ 85 -> 92 & 0.11087\\ 86 -> 92 & -0.40939\\ 88 -> 93 & 0.14296\\ 89 -> 93 & 0.45987\\ 91 -> 96 & -0.22553\\ Excited State 12: Singlet-A'\\ 85 -> 92 & 0.12962\\ 88 -> 93 & 0.50172\\ 89 -> 93 & 0.20875\\ 89 -> 94 & 0.11460\\ 90 -> 94 & -0.36762\\ Excited State 13: Singlet-A'\\ 85 -> 92 & 0.36381\\ 88 -> 93 & 0.18574\\ 89 -> 94 & 0.11413\\ 90 -> 94 & 0.13141\\ 91 -> 95 & 0.11218\\ \end{array}$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.2718 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 96 0.28889 91 > 96 0.21818 91 > 98 0.186623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843 90 > 96 0.45412 90 > 97 0.17306	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 95 -0.26937 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22889 91 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843 90 > 96 0.45412 90 > 96 0.45412 90 > 96 0.17106 Excited State 24: Singlet-A''	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.2718 89 > 95 -0.26937 90 > 95 -0.26937 90 > 96 0.29889 91 > 96 -0.15626 91 > 97 0.12818 91 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843 90 > 96 0.45412 90 > 97 0.17306 Excited State 24: Singlet-A'' 87 > 93 -0.21458	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.2718 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.18863 Excited State 23: Singlet-A' 85 > 93 -0.18863 Excited State 23: Singlet-A' 85 > 93 -0.18863 Excited State 23: Singlet-A' 85 > 93 -0.18863 Excited State 24: Singlet-A' 85 > 94 -0.33024 90 > 95 0.45412 90 > 97 0.17306 Excited State 24: Singlet-A'' 87 > 93 -0.21458 87 > 94 -0.21458	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488 5.6799 eV 218.29 nm f=0.0001
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 0.15696 89 > 94 0.15696 89 > 95 0.18220 90 > 96 0.12551 90 > 97 0.15462 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.29889 91 > 96 0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843 90 > 96 0.48412 90 > 96 0.48412 90 > 97 0.17306 Excited State 24: Singlet-A'' 87 > 93 -0.21458 87 > 93 -0.21458	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488
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$\begin{array}{c cccc} Excited State 10: Singlet-A'\\ 86 -> 92 & -0.21495\\ 89 -> 93 & -0.37035\\ 90 -> 94 & 0.25334\\ 91 -> 95 & 0.41678\\ 91 -> 96 & -0.21607\\ Excited State 11: Singlet-A'\\ 85 -> 92 & 0.11087\\ 86 -> 92 & -0.40939\\ 88 -> 93 & 0.45987\\ 91 -> 96 & -0.22553\\ Excited State 12: Singlet-A'\\ 85 -> 92 & 0.12962\\ 88 -> 93 & 0.45987\\ 91 -> 96 & -0.22553\\ Excited State 12: Singlet-A'\\ 85 -> 92 & 0.12962\\ 88 -> 93 & 0.50172\\ 89 -> 93 & -0.20875\\ 89 -> 94 & 0.11460\\ 90 -> 94 & -0.36762\\ Excited State 13: Singlet-A'\\ 85 -> 92 & 0.35990\\ 86 -> 92 & 0.36381\\ 88 -> 94 & -0.117472\\ 89 -> 93 & 0.18574\\ 89 -> 94 & -0.11153\\ 90 -> 94 & 0.1218\\ 91 -> 95 & 0.11218\\ 91 -> 95 & 0.1218\\ 91 -> 96 & -0.16000\\ 91 -> 97 & 0.27082\\ Excited State 14: Singlet-A'\\ 86 -> 92 & -0.17366\\ 89 -> 94 & -0.11787\\ 91 -> 96 & 0.43866\\ \end{array}$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 94 -0.23480 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 96 0.29889 91 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843 90 > 96 0.45412 90 > 97 0.17306 Excited State 24: Singlet-A'' 87 > 93 -0.21458 87 > 94 0.65763 Excited State 25: Singlet-A'' 87 > 94 0.65763 Excited State 25: Singlet-A'' 87 > 92 0.21019	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488 5.6799 eV 218.29 nm f=0.0001
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584 4.9311 eV 251.43 nm f=0.0232	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 0.15696 89 > 94 0.15696 89 > 95 0.18220 90 > 96 0.12551 90 > 97 0.15462 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22889 91 > 96 -0.15626 91 > 97 0.12818 91 > 98 0.186623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18843 90 > 96 0.45412 90 > 97 0.17306 Excited State 24: Singlet-A'' 87 > 93 -0.21458 87 > 93 -0.21458 87 > 94 0.65763 Excited State 25: Singlet-A'' 87 > 93 0.21458	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488 5.6799 eV 218.29 nm f=0.0001
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.2718 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 95 -0.26937 90 > 96 0.29889 91 > 96 0.15626 91 > 97 0.12818 91 > 98 0.18623 Excited State 23: Singlet-A' 85 > 93 0.16932 88 > 94 -0.33024 90 > 95 0.18868 86 > 93 0.16932 88 > 94 -0.33024 90 > 96 0.45412 90 > 97 0.17306 Excited State 24: Singlet-A' 87 > 93 -0.21458 87 > 94 0.65763 Excited State 25: Singlet-A' 83 > 92 0.21019 85 > 93 0.39956 86 > 93 0.27873 88 > 94 0.11282	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488 5.6799 eV 218.29 nm f=0.0001
$\begin{array}{c} \mbox{Excited State 10: Singlet-A'}\\ 86 &> 92 & -0.21495\\ 89 &> 93 & -0.37035\\ 90 &> 94 & 0.25334\\ 91 &> 95 & 0.41678\\ 91 &> 96 & -0.21607\\ \mbox{Excited State 11: Singlet-A'}\\ 85 &> 92 & 0.11087\\ 86 &> 92 & -0.40939\\ 88 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 88 &> 93 & 0.12962\\ 88 &> 93 & 0.22553\\ \mbox{Excited State 12: Singlet-A'}\\ 85 &> 92 & 0.12962\\ 88 &> 93 & 0.50172\\ 89 &> 93 & -0.20875\\ 89 &> 94 & 0.11460\\ 90 &> 94 & -0.36762\\ \mbox{Excited State 13: Singlet-A'}\\ 85 &> 92 & 0.35990\\ 86 &> 92 & 0.36381\\ 88 &> 94 & -0.11787\\ 89 &> 93 & 0.18574\\ 89 &> 94 & -0.11153\\ 90 &> 94 & 0.13141\\ 91 &> 95 & 0.11218\\ 91 &> 96 & -0.6000\\ 91 &> 97 & 0.27082\\ \mbox{Excited State 14: Singlet-A'}\\ 86 &> 92 & -0.17366\\ 89 &> 94 & -0.11787\\ 91 &> 96 & 0.43866\\ 91 &> 97 & 0.47265\\ \mbox{Excited State 15: Singlet-A'}\\ 85 &> 92 & 0.51490\\ \end{tabular}$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584 4.9311 eV 251.43 nm f=0.0232	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27118 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.29889 91 > 96 -0.15626 91 - 97 0.12818 91 - 98 0.18623 Excited State 23: Singlet-A' 85 - 93 -0.18868 86 - 93 0.16932 88 - 94 -0.33024 90 - 95 0.18843 90 - 95 0.18843 90 - 96 0.45412 90 - 97 0.17306 Excited State 24: Singlet-A'' 87 - 93 -0.21458 87 - 94 0.65763 Excited State 25: Singlet-A'' 83 - 92 0.21019 85 - 93 0.39956 86 - 93 0.27873 88 - 94 0.11282	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488 5.6799 eV 218.29 nm f=0.0001
$\begin{array}{llllllllllllllllllllllllllllllllllll$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584 4.9311 eV 251.43 nm f=0.0232	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27718 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.22585 90 > 96 0.22585 90 > 96 0.22888 91 > 96 -0.16626 91 > 97 0.12818 91 > 98 0.186623 Excited State 23: Singlet-A' 85 > 93 -0.18868 86 > 93 0.16932 88 > 94 -0.3024 90 > 95 0.18843 90 > 96 0.458412 90 > 96 0.45842 90 > 96 0.45842 90 > 96 0.45843 90 > 96 0.45412 90 > 97 0.17306 Excited State 24: Singlet-A'' 87 > 93 -0.21458 87 > 93 -0.21458 87 > 93 0.21458 87 > 93 0.21730 Excited State 25: Singlet-A'' 83 > 92 0.21019 85 > 93 0.39956 86 > 93 0.17873 88 > 94 0.11282 89 > 95 0.13553 90 > 97 0.73311	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488 5.6799 eV 218.29 nm f=0.0001
$\begin{array}{c} \mbox{Excited State 10: Singlet-A'}\\ 86 &> 92 & -0.21495\\ 89 &> 93 & -0.37035\\ 90 &> 94 & 0.25334\\ 91 &> 95 & 0.41678\\ 91 &> 96 & -0.21607\\ \mbox{Excited State 11: Singlet-A'}\\ 85 &> 92 & 0.11087\\ 86 &> 92 & -0.40939\\ 88 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 89 &> 93 & 0.4296\\ 88 &> 93 & 0.12962\\ 88 &> 93 & 0.22553\\ \mbox{Excited State 12: Singlet-A'}\\ 85 &> 92 & 0.12962\\ 88 &> 93 & 0.50172\\ 89 &> 93 & -0.20875\\ 89 &> 94 & 0.11460\\ 90 &> 94 & -0.36762\\ \mbox{Excited State 13: Singlet-A'}\\ 85 &> 92 & 0.35990\\ 86 &> 92 & 0.36381\\ 88 &> 94 & -0.11787\\ 89 &> 93 & 0.18574\\ 89 &> 94 & -0.11153\\ 90 &> 94 & 0.13141\\ 91 &> 95 & 0.11218\\ 91 &> 96 & -0.6000\\ 91 &> 97 & 0.27082\\ \mbox{Excited State 14: Singlet-A'}\\ 86 &> 92 & -0.17366\\ 89 &> 94 & -0.11787\\ 91 &> 96 & 0.43866\\ 91 &> 97 & 0.47265\\ \mbox{Excited State 15: Singlet-A'}\\ 85 &> 92 & 0.51490\\ \end{tabular}$	4.6925 eV 264.22 nm f=0.0135 4.7925 eV 258.70 nm f=0.2644 4.8274 eV 256.84 nm f=0.0584 4.9311 eV 251.43 nm f=0.0232	Excited State 21: Singlet-A' 84 > 92 0.43598 86 > 93 0.20135 88 > 94 0.15696 89 > 94 -0.16481 89 > 95 -0.18220 90 > 96 0.12551 90 > 97 -0.15462 91 > 96 -0.11603 91 > 98 -0.28836 Excited State 22: Singlet-A' 84 > 92 -0.27118 89 > 94 -0.23480 89 > 94 -0.23480 89 > 95 -0.26937 90 > 95 -0.22585 90 > 96 0.29889 91 > 96 -0.15626 91 - 97 0.12818 91 - 98 0.18623 Excited State 23: Singlet-A' 85 - 93 -0.18868 86 - 93 0.16932 88 - 94 -0.33024 90 - 95 0.18843 90 - 95 0.18843 90 - 96 0.45412 90 - 97 0.17306 Excited State 24: Singlet-A'' 87 - 93 -0.21458 87 - 94 0.65763 Excited State 25: Singlet-A'' 83 - 92 0.21019 85 - 93 0.39956 86 - 93 0.27873 88 - 94 0.11282	5.5566 eV 223.13 nm f=0.1594 5.6187 eV 220.66 nm f=0.2488 5.6799 eV 218.29 nm f=0.0001

Transition energy, wavelengths, and oscillator strengths of the electronic transitions of 7a (The 104th orbital is HOMO shown in Figure S19).

Listing with it support Biol 2008 0.3384 3.388 (*)	``	e ,
Example 10 Subject 2 <	Excitation energies and oscillator strengths:	102 ->108 0 53899
100-510 -1.6799 100-510 -2.0895 100-510 -2.0895 2.08164 5.0814 V 20.20m P4037 100-510 -0.0884 1.1814 V 3520 mm P5030 0.0384 0.0384 100-510 -0.0884 1.1814 V 3520 mm P5030 0.0384 0.0384 100-510 -0.0844 1.0834 V 301 mm P5030 0.0384 0.0384 100-510 -0.0449 1.0834 V 301 mm P5030 0.0384 0.0385 0.0384 100-510 -0.0449 1.0834 V 302 mm P5030 0.0384 0.0384 0.0385 0.0385 100-510 -0.0449 1.0834 V 302 mm P5030 0.0384 0.0385 0.0385 0.0385 100-510 -0.0449 1.0384 V 302 mm P5030 0.0316 0.0316 0.0316 100-510 -0.0584 1.0314 V 102 0.0016 0.0316 0.0316 0.0316 100-510 -0.0584 1.0314 V 102 0.0016 0.0316 0.0316 0.0316 100-510 -0.0584 1.0314 V 102 0.0016 0.0316 0.0316 0.0316 0.0316		
Excited Star 2: Single X: 2014 V: 45.74 mm F-0.1081 100008 8.1.467 000008 0.5.008 100008 8.1.167 Excited Star 3: Single X: 3.18 v: 3.201 mm F-0.008 100007 0.2.141 00018 0.5.008 100017 0.2.141 00018 0.5.008 100017 0.2.141 00018 0.5.004 100017 0.1.141 00018 0.5.004 100017 0.1.141 00018 0.5.004 100017 0.1.141 00018 0.5.004 100017 0.1.141 00017 0.1.141 0.1.141 0.1.141 00017 0.1.141 0.1.141 0.1.141 00017 0.1.141 0.1.141 0.1.141 00017 0.1.141 0.1.141 0.1.141 00017 0.1.141 0.1.141 0.1.141 00017 0.0.1171 0.0.1171 0.0.1171 00017 0.0.1171 0.0.1171 0.0.1171 00016 0.0.1171		
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Bude 100 Bude 40 Bude 40 Bude 400 <		
Faced Star 2 Subject 3 Subject 4 Subject 7		
110 - 308 0.5708 100 - 407 0.2142 110 - 308 0.1570 0.2164 110 - 308 0.1644 1.854 * 39.18 m. Fe0.016 100 - 400 0.1665 110 - 308 0.530 * 50		
104 - 0.0 0.2508 102 - 0.0 0.2508 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2509 0.2509 0.2509 103 - 0.0 0.2502 0.2509 0.2503 103 - 0.0 0.2502 0.2508 0.2509 103 - 0.0 0.2509 0.2503 0.2503 103 - 0.0 0.2503 0.2503 0.2503 103 - 0.0 0.2503 0.2503 0.2503 103 - 0.0 0.2503 0.2503 0.2503 0.2503		
Landson 4: Single A': J.115 av) 3: 0.10791 0.10791 Diamon 2: Single A': J.115 av) 3: 0.10791 0.10791 Daming Mark J. Single A': J.115 av) 3: 0.10791 0.10791 Diamon 2: Single A': J.115 av) 3: 0.10791 0.10791 Diamon 2: Single A': J.115 av) 4: 0.10791 0.10791 Diamon 2: Single A': J.115 av) 4: 0.1079 0.10791 Diamon 2: Single A': J.115 av) 4: 0.1079 0.10791 Diamon 2: Single A': J.115 av) 4: 0.11712 0.11712 Diamon 2: Single A': J.115 av) 4: 0.11712 0.11712 Diamon 3: J.116 av) 4: 0.11712 Diamon 4: 0.11712 Diamon 4: 0.11712 Diamon 4: 0.11712 Diamon 4: Single A': J.116 av) 4: 0.11712 Diamon 4: 0.11712 Diamon 4: 0.11712 Diamon 4: 0.11712 Diamon 4: Single A': J.116 av) 4: 0.11712 Diamon 4: 0.11712 Diamon4		
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1100.30000.30000.30001100.30000.30000.30001100.10140.30000.30001100.10150.30000.30001100.10150.30000.30001100.30000.30000.3000<	Excited State 5: Singlet-A' 3.5679 eV 347.50 nm f=0.0216	Excited State 22: Singlet-A' 5.1830 eV 239.22 nm f=0.0330
183 - 107 0.17344 100 - 107 0.1319 181 - 107 0.1319 100 - 108 0.10157 181 - 108 0.13221 100 - 108 0.10157 181 - 108 0.1319 101 - 1016 0.11514 181 - 108 0.15141 100 - 1017 0.15141 181 - 108 0.15141 100 - 1017 0.15141 181 - 108 0.11712 75.86 0.1217 181 - 108 0.11712 0.15321 65188 0.1548 181 - 108 0.1217 0.15321 67.586 0.1548 181 - 108 0.2548 100 - 108 0.2548 100 - 108 0.2548 181 - 108 0.1217 89.547 11.86 - 108 0.1548 100 - 108 0.2548 182 - 108 0.1649 10.0548 0.16448 100 - 107 0.2549 182 - 108 0.1649 10.0548 100 - 107 0.2549 100 - 107 0.2549 182 - 108 0.1549 100 - 107 0.2544 100 - 107 0.2549		
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Extend Sum 6 Single-A ¹ 3 2009 v/3 34.2 0 m (=0.2904 100 -100 0.01413 100 -100 0.5513 100 -100 0.5513 100 -100 0.5513 100 -100 0.5513 100 -101 0.1542 101 -101 0.1513 100 -100 0.5513 0.7550 0.7550 0.7550 100 -100 0.1513 85 -100 0.7550 0.7550 100 -100 0.65348 100 -100 0.25348 100 -100 0.25349 100 -100 0.65348 100 -100 0.25349 100 -100 0.2548 100 -107 0.2549 0.25347 100 -100 0.2549 100 -100 0.2549 100 -107 0.2511 100 -101 0.2546 0.3371 100 -101 0.2546 100 -100 0.2511 100 -101 0.2546 0.3151 100 -101 0.2546 100 -100 0.2544 100 -101 0.2546 100 -101 0.2546 100 -100 0.2544 100 -101 0.25454 100 -101 0.25454<		
101-105 0.3522 103-106 0.1542 103-107 0.1733 Excert Stars 3. Singlet X 3.015 eV 23.07 eV 216.37 am F-0.050 103-108 0.1712 0.1733 97-108 0.1713 0.1713 0.1714 0.1711 0.1714 0.1711 0.1714 0.1711 0.1714		
101-016 -0.1054 104-110 -0.15156 103-010 -0.5483 104-112 0.15156 2.13747 103-010 0.15112 97-105 0.13711 3.13747 103-010 0.15112 97-105 0.13711 3.13747 103-010 0.15112 97-105 0.13711 3.13747 103-010 0.15118 9.1506 0.03356 103-111 0.15136 103-010 0.04318 8.13864A 3.905 4V 3.1387 10.0316 10.03166 10.0316 103-010 0.15125 10.04108 9.5166 0.33571 10.0416 10.03171 10.05186 10.0518		
103 - 00 0.5453 104 - 112 0.1413 103 - 01 0.1712 2.187 eV 2.267 eV 2.667 state 2.578 eV 102 - 100 0.161 is 89 - 106 0.1273 1.015 eV 1.015 eV 102 - 100 0.61 is 89 - 106 0.1273 1.015 eV 1.015 eV 103 - 100 0.61 is 89 - 106 0.1273 1.015 eV 1.015 eV 103 - 100 0.01 is 3.005 eV 31.05 eV 3.005 eV <td></td> <td></td>		
Iscuel Sume 7Single A7Single A7		
$ \begin{array}{ $	103 ->107 0.17532	Excited State 23: Singlet-A' 5.2457 eV 236.35 nm f=0.0520
101-310 0.6318 96.366 0.1375 101-310 0.6348 905.67 312.81 mm f=0.0031 101.310 0.1319 102-310 0.2373 905.67 31.81 mm f=0.0548 Exceted State 2 Single A' 3.055 eV 233.69 mm f=0.033 102-310 0.14399 90.316 0.13297 0.1318 0.13197 101-310 0.1439 90.316 0.23294 1.00.310 0.23294 101-310 0.1439 90.316 0.23294 1.00.310 0.23294 101-310 0.1431 100.316 0.14312 0.14312 1.01.310 101-310 0.1431 100.310 0.1412 0.13170 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.310 1.01.311 1.01.310 1.01.311 1.01.310 1.01.310 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311 1.01.311	Excited State 7: Singlet-A' 3.8315 eV 323.59 nm f=0.1351	96 ->105 0.47586
104-107 0.62943 8.694-Å 3965 V 31281 um P-0.0033 102-108 6.5694-Å 3965 V 311.88 um P-0.058 100-110 0.353 6 102-108 6.5694-Å 3960 V 311.88 um P-0.058 95-015 0.2357 1 103-108 0.1059 90-105 0.2371 1 103-108 0.1059 90-105 0.2371 1 104-107 0.1059 90-105 0.2371 1 1 104-107 0.1059 90-105 0.2371 <		
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$\begin{array}{l l l l l l l l l l l l l l l l l l l $		
Excited Sine 9 Single A*		
101-2166 4.27057 95.4105 0.16843 103-166 0.10549 93.4106 0.23718 104-167 0.10642 101.2107 0.23910 104-167 0.10642 101.2107 0.23910 104-110 0.1271 103.3101 0.16842 105-101 0.16842 103.3101 0.1271 100-168 0.23910 103.3101 0.1271 101-2166 0.3575 95.5105 0.5192 101-2166 0.32754 4.245 eV 290.06 nm f-0.1113 98106 0.1342 101-2166 0.32754 4.245 eV 290.06 nm f-0.1113 98106 0.1342 101-2166 0.32556 103.3101 0.401743 104.311 0.1342 101-2165 0.3256 103.311 0.3187 1.311 0.1342 101-2165 0.5149 103.311 0.3147 1.311 0.1342 101-2165 0.5149 103.311 0.3147 1.311 0.1342 101-2165 0.5149 103.311 0.3147 1.311 0.1343 101-2165 0.5149		
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104-107 0.12059 98,-106 0.23476 104-108 0.10642 4.185 eV 296.01 nm f=0.1841 101-107 0.2390 100-105 0.2391 100-110 0.2390 100-110 0.2390 100-105 0.2391 100-110 0.1376 3.332 eV 232.22 nm f=0.0137 100-105 0.2391 100-110 0.1376 3.332 eV 232.22 nm f=0.0137 101-106 0.4134 100-4105 0.42344 3.332 eV 232.22 nm f=0.0137 101-106 0.4134 100-4105 0.42344 3.332 eV 232.22 nm f=0.0137 101-106 0.4134 100-4105 0.4344 100-411 0.1132 101-106 0.4134 100-4105 0.4344 100-4105 0.4344 101-108 0.10647 100-4105 0.1356 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105 100-4105		
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Excited State 10 Singlet A' 4.185 eV 296.01 nm f-0.1841 101 -108 0.27820 100 -1015 0.23511 104 -110 0.1072 10532 100 -1015 0.23501 104 -110 0.1072 10532 100 -1015 0.2356 65 -105 0.1951 5.302 eV 232.22 nm f-0.0153 103 -1017 0.42544 65 -105 0.2356 65 -105 0.2356 100 -1015 0.42544 4.275 eV 290.06 nm f-0.1113 101 -107 0.2343 101 -1015 0.11962 102 -108 0.11842 101 -107 0.2343 101 -1015 0.11962 102 -108 0.11842 101 -1017 0.3184 101 -1016 0.11962 102 -1016 103 -101 0.1182 101 -1017 0.3184 104 -110 0.1967 104 -111 0.1195 5.720 eV 23.80 nm f-0.071 104 -111 0.1967 103 -1016 0.1985 5.720 eV 23.80 nm f-0.071 104 -111 0.1967 103 -1016 0.1985 5.720 eV 22.83 nm f-0.071 105 -1016<	104 ->108 0.59137	100 ->106 -0.24476
98-105 0.23501 103-101 0.23960 100-105 0.13170 104-112 0.1537 101-105 0.1376 104-112 0.1537 102-106 0.2376 5.3392 eV 232.22 nm (=0.0153 103-107 0.23543 5.3392 eV 232.22 nm (=0.0153 103-107 0.2344 96-105 0.3043 100-105 0.3144 101-107 0.3343 100-105 0.3144 102-108 0.3447 102-106 0.3447 103-110 0.4473 102-106 0.3447 103-110 0.4473 102-107 0.2343 104-112 0.15224 102-108 0.5490 100-107 0.3473 104-108 0.5590 100-106 0.3445 102-107 0.1504 101-107 0.1514 103-101 0.1504 101-107 0.1514 104-102 0.2173 100-106 0.3445 102-107 103-110 0.4173 101-107 102-107 103-110 0.4187 5.3020 eV 228.37 nm (=0.0071 102-106 0.4287		
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101-1015 -0.1370 104 -112 0.5239 102 -106 0.23756 5.302 eV 32.22 nm F=0.0151 103 -107 0.2344 4.2745 eV 290.06 nm F=0.1113 96 -1163 -23454 100 -1015 0.43144 4.2745 eV 290.06 nm F=0.1113 96 -1163 -23454 101 -1015 0.43144 102 -1016 0.3447 -23434 101 -1015 0.43144 102 -1016 0.3447 - 101 -1015 0.3144 102 -1016 0.3447 - 103 -1016 0.3447 4.3684 eV 28.3.2 nm F=0.1078 Exected Statz 25. Singlet-A' 5.3702 eV 20.00 nm F=0.0544 100 -1015 0.5499 100 -1015 0.3457 5.3702 eV 20.00 nm F=0.0544 100 -1015 0.5494 101 -1016 0.3459 5.3702 eV 20.00 nm F=0.0544 100 -1015 0.5494 101 -1016 0.3459 5.3702 eV 20.00 nm F=0.0544 100 -1015 0.5494 101 -1016 0.3459 5.3702 eV 20.00 nm F=0.0544 100 -1015 0.5145 101 -1016 0.3459 5.3702 eV 20.00 nm F=0.0571		
101-106 -0.1570 Excited State 17. 5.372 eV 32.22 nm f=0.0151 102-106 0.3256 0.595-106 0.1591 103-107 0.4234 96-105 -0.1023 101-106 0.3126 0.3256 0.3256 101-107 0.4234 96-106 0.3024 101-108 0.1197 100-108 0.1142 102-106 0.3156 0.1197 100-108 0.1442 102-106 0.3256 100-108 0.1342 100-108 0.1342 102-106 0.3256 100-108 0.1387 100-108 0.1243 104-108 0.3967 100-108 0.32439 100-108 0.34439 102-106 0.12374 100-108 0.34439 100-108 0.34439 102-106 0.12374 100-108 0.1393 100-108 0.14931 102-106 0.12374 4.885 eV 26.23 m f=0.0721 100+108 0.14931 100-108 0.14931 102-106 0.1234 1.999 100-108 0.14931 1.999 100-108 0.14911 0.12131 10		
102-1016 0.3276 95-1015 0.20545 Excited State 115 Siguel A 2.475 eV 20.00 nm 6.01201 100-2015 0.41384 100-2015 0.22343 100-2015 100-2015 0.41384 100-2015 0.23434 100-2015 100-2015 0.11951 0.13877 100-2015 0.13877 100-2015 0.20507 100-2016 0.14173 0.13877 104-2015 0.13954 100-2016 0.13957 100-2016 0.13957 104-2015 0.19667 100-2016 0.13957 100-2016 0.13957 104-2015 0.15959 98-2015 0.3499 98-2015 0.3499 100-2016 0.5599 98-2015 0.3499 100-2016 0.3499 100-2016 0.21234 100-2016 0.3499 100-2016 0.3499 101-2016 0.22754 100-2016 0.3499 100-2016 0.3499 101-2016 0.22754 98-2016 0.12347 100-2016 0.2497 101-2016 0.22754 4350 eV 27.39 nm f=0.0522 10		
1013-107 0.4234 96-106 -02545 100-105 0.43184 100-2018 0.23433 100-105 0.11092 0.1002 0.1002 0.1002 100-105 0.23433 0.04473 0.1002 0.1002 100-105 0.2363 0.04473 0.1002 0.1002 100-105 0.2569 100-1015 0.1505 100-1015 0.1505 100-105 0.5569 100-1015 0.1505 53720 eV 23.080 nm f=0.0544 100-105 0.2559 100-1015 0.15095 53720 eV 23.080 nm f=0.0514 100-105 0.2554 100-1015 0.15095 53720 eV 23.080 nm f=0.0514 100-105 0.2754 101-1010 0.2563 54200 eV 228.37 nm f=0.0307 100-105 0.2754 101-2010 0.2663 54200 eV 228.37 nm f=0.0307 101-2010 0.2754 101-2010 0.2654 5420 eV 228.37 nm f=0.0307 1012-2010 0.11365 98-5106 0.12837 5420 eV 228.37 nm f=0.0307 1012-2010 0.12437 102-1010 0.21437 5428 eV 227.79 nm f=0.0512 102-2010		
Excited State II. Singlet.** 2474 5 eV 200.06 nm f=0.113 98 >106 >0.03280 100 >105 0.41344 101 >107 0.23443 101 >105 0.3561 103 >110 0.44473 102 >106 0.35641 103 >111 0.44473 104 >106 0.9667 103 >111 0.41843 104 >110 0.9667 100 >106 0.13873 104 >110 0.9667 100 >106 0.13873 104 >101 0.9667 100 >106 0.1599 100 >105 0.2549 100 >106 0.3449 101 >106 0.24624 101 >106 0.3459 102 >106 0.2754 100 >106 0.3459 103 >108 0.27434 4.885 cV 26.23 nm f=0.0721 101 >106 0.3459 101 >106 0.2754 100 >106 0.3985 100 >106 0.3985 101 >106 0.2754 4.885 cV 27.23 nm f=0.0522 100 >106 0.1437 100 >106 0.1437 101 >106 0.4375 100 >106 0.1437 100 >106		
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Excited State 12: Singlet-A' 4 3684 eV 283.82 nm f=0.1078 Excited State Excited State 5 Singlet-A' 5 3720 eV 230.80 nm f=0.0549 100 > 105 -0.12526 100 - 106 0.34459 100 - 1070 0.31513 103 > 108 0.27454 101 - 107 0.31513 101 - 1070 0.2798 89 > 106 -0.1274 104 - 108 0.29624 104 - 111 -0.0371 104 > 108 -0.21234 104 - 111 -0.3988 103 - 107 0.1381 103 - 106 0.12437 102 > 107 0.14784 4.885 eV 276.33 nm f=0.0522 103 - 106 0.12437 103 - 106 0.12437 103 > 108 0.45799 100 > 106 0.1337 104 - 111 -0.1438 5.428 eV 227.79 nm f=0.0071 104 > 101 -0.155 100 > 106 0.12437 100 - 106 0.1747 104 > 101 -0.165 100 > 106 0.1747 104 - 111 -0.3636 104 > 101 0.1225 102 - 106 0.1747 104 - 112 0.3844 101 - 106 0.22144 <td></td> <td></td>		
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Excited State 13:Singlet-A* 98 > 1054.488 eV 276.23 nm f=0.0721104 -112 95 > 1050.27988 $98 > 106$ -0.2273495 > 1050.3064995 > 1050.30649 $102 > 107$ 0.1384198 > 1060.12437 $103 > 108$ 0.4579100 > 1060.14387 $104 > -110$ 0.28325103 > 110-0.14786Excited State 14:Singlet-A*4.550 eV 273.39 nm f=0.0522104 > 1110.55633 $98 > 105$ 0.110660.14387104 > 1110.55633 $98 > 105$ 0.110660.1438798 > 1060.11471 $100 > 105$ 0.3165698 > 1060.114710.12275Excited State 15:Singlet-A*4.6394 eV 267.24 nm f=0.5737104 > 111-0.36365 $100 > 105$ 0.14781104 > 112-0.27147104 > 112-0.27147 $101 > 106$ 0.307295 > 1050.215645.4938 eV 225.70 nm f=0.0061 $102 > 107$ 0.3707595 > 1050.221545.4933 eV 225.70 nm f=0.0061 $102 > 107$ 0.3707595 > 1050.221545.4028 eV 20.92 nm f=0.0061 $102 > 107$ 0.3707595 > 1050.221545.4028 eV 20.92 nm f=0.0061 $102 > 107$ 0.3707595 > 1050.2186108 > 107 $103 > 108$ 0.175895 > 1050.2184108 > 107 $104 > 109$ 0.10344100 > 106 > 0.1634100 > 106 > 0.1634 $104 > 109$ 0.10344100 > 106 > 0.1634100 > 106 > 0.1634 $104 > 109$ 0.10344100 >		
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Excited State14:Singlet-A'4.5350 eV273.39 nmf=0.0522 $104 - 111$ 0.2635 98 -105 0.31656 -0.11664 $5.428 eV$ $227.79 nm$ f=0.0071 $100 -105$ 0.31656 $95 -105$ 0.43057 $98 > 106$ 0.17147 $103 -108$ 0.28369 0.12715 0.13275 0.1492 -0.1492 $104 ->110$ -0.12275 0.3710 -0.14781 -0.3737 $0.04 ->110$ -0.1225 $100 ->105$ 0.14781 -0.3737 $0.04 ->110$ -0.1225 -0.27147 $101 ->106$ 0.3202 -0.27472 $95 ->105$ 0.22154 $5.4933 eV$ $103 ->107$ -0.3775 $95 ->105$ 0.22154 -0.23895 $103 ->108$ -0.17578 $97 ->106$ -0.16043 -0.16043 $103 ->109$ 0.1344 $-0.1531 eV$ $20.95 nm$ f=0.0141 $102 ->107$ -0.1624 $104 ->110$ 0.22995 -0.23995 -0.16043 -0.23895 -0.16043 $104 ->100$ 0.21944 $4.7513 eV$ $20.95 nm$ f=0.0141 $102 ->109$ -0.19098 $104 ->100$ 0.21948 -0.16333 -0.1633 -0.1633 -0.1633 $102 ->107$ 0.3214 $4.513 eV$ $20.95 nm$ f=0.0141 $102 ->109$ -0.19098 $104 ->100$ 0.16937 -0.1632 -0.1633 -0.1633 $102 ->107$ 0.1234 $4.514 eV$ $25.09 nm$ f=0.0446 $95 ->105$ 0.1901 $102 ->107$ 0.12319 -0.1633 <td< td=""><td></td><td></td></td<>		
98 >105 -0.1106 Excited State 28: Singlet-A* 5.4428 eV 227.79 nm f=0.0071 100 >106 0.47435 98 >106 0.17147 103 >108 0.28369 101 >108 0.14092 104 >110 -0.12275 103 >101 -0.14022 100 >105 -0.1471 -0.36365 -0.4303 eV 100 >106 0.32022 Excited State 12: Singlet-A* 4.639 eV 267.24 nm f=0.5737 104 >111 -0.36365 100 >106 0.32022 Excited State 29: Singlet-A* 5.493 eV 225.70 nm f=0.0061 102 >107 -0.30795 96 >105 0.12826 - 103 >108 -0.17558 96 >105 0.12826 - - 103 >108 -0.17578 96 >106 -0.10413 - - 104 >110 0.23995 102 >107 -0.2109 -0.10211 - - 104 >100 0.2995 104 >112 0.3941 - - - - 104 >100 0.2995 104 >112 0.3941 - - - - - - - - - - - <t< td=""><td></td><td></td></t<>		
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Idd = 15: Singlet-A'4.6394 eV 267.24 nm f=0.5737 $104 > 111$ -0.36365 $100 > 105$ -0.14781 -0.3792 $104 > -112$ 0.27147 $101 > 106$ 0.32022 Excited State 29: Singlet-A' 5.4933 eV 225.70 nm f=0.0061 $102 > 107$ -0.37972 $96 > 105$ 0.22154 $103 > 109$ -0.17558 $97 > 106$ -0.16043 $103 > 109$ 0.1948 $101 > 108$ 0.22995 $104 > 110$ 0.22995 $102 > 109$ -0.19098 Excited State 16:Singlet-A' 4.513 eV 260.95 nm f=0.0141 $103 > 112$ 0.38941 $104 > 109$ 0.22199 $104 > 112$ 0.38941 $00 > 114$ $104 > 109$ 0.60838 $103 > 102$ 0.10401 0.23975 Excited State 17:Singlet-A' 4.8414 eV 256.09 nm f=0.0446 $95 > 105$ 0.10401 $97 > 105$ 0.61338 $100 > 106$ 0.30745 0.10401 $97 > 105$ 0.61338 $100 > 106$ 0.30745 $102 > 107$ 0.17008 $100 > 106$ 0.3745 $97 > 105$ 0.01371 0.23061 $102 > 100$ $97 > 105$ 0.01371 0.23061 $102 > 100$ $97 > 106$ 0.10281 $103 > 100$ 0.10532 $100 > 105$ 0.19071 $103 > 100$ 0.10532 $100 > 106$ 0.1628 $104 > 110$ 0.30601 $102 > 100$ 0.1628 $104 > 100$ 0.16161 $102 > 100$ 0.16828 $104 > 100$ 0.16278 $100 > $		
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$ \begin{array}{ccccc} 104 > 109 & 0.21948 \\ 104 > 110 & 0.22995 \\ 104 > 110 & 0.22995 \\ 102 > 107 & 0.22119 \\ 104 > 109 & 0.60838 \\ \\ Excited State 17: Singlet A' 4.8414 eV 256.09 nm f=0.0446 \\ 95 > 105 & 0.10401 \\ 102 > 107 & 0.17008 \\ \\ Excited State 17: Singlet A' 4.9304 eV 251.47 nm f=0.4837 \\ 97 > 105 & 0.02312 \\ 98 > 105 & -0.23712 \\ 98 > 105 & -0.23712 \\ 98 > 105 & -0.23712 \\ 98 > 105 & -0.12619 \\ 100 > 106 & 0.14220 \\ 100 > 106 & 0.14220 \\ 100 > 106 & 0.16828 \\ 100 > 106 & 0.16828 \\ 100 > 106 & 0.16828 \\ 100 > 106 & 0.16828 \\ 102 > 107 & 0.1297 \\ 102 > 107 & 0.1297 \\ 102 > 108 & -0.1297 \\ 102 > 107 & 0.1297 \\ 103 > 109 & 0.16828 \\ 102 > 107 & 0.1297 \\ 103 > 100 & -0.16228 \\ 102 > 107 & 0.1297 \\ 103 > 109 & 0.16828 \\ 102 > 107 & 0.1297 \\ 103 > 100 & 0.16828 \\ 102 > 107 & 0.1297 \\ 103 > 107 & 0.16828 \\ 102 > 107 & 0.1297 \\ 103 > 107 & 0.16828 \\ 102 > 107 & 0.1297 \\ 103 > 100 & -0.16228 \\ 104 > 101 & -0.16228 \\ 104 > 101 & -0.1628 \\ 104 > 101 & -0.1628 \\ 104 > 101 & -0.1628 \\ 104 > 101 & -0.1628 \\ 104 > 101 & -0.1628 \\ 104 > 101 & 0.16828 \\ 104 > 101 & 0.16828 \\ 104 > 101 & 0.16828 \\ 105 & 0.1297 \\ 105 & 0.1297 \\ 105 & 0.1297 \\ 105 & 0.1297 \\ 105 & 0.1665 \\ 106 & 0.1677 \\ 107 & 0.12420 \\ 107 & 0.12420 \\ 108 & 0.1682 \\ 108 & 0.1665 \\ 109 > 108 & 0.16828 \\ 109 > 100 & 0.16651 \\ 109 > 100 & 0.1652 \\ 100 & 0.16797 \\ 100 & 0.1628 \\ 100 & 0.16797 \\ 100 & 0.15728 \\ 100 & 0.1578 \\ 100 & 0.15$	103 ->108 -0.17558	97->106 -0.16043
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103 ->109 0.16652 99 ->108 -0.13951 104 ->109 -0.11082 Excited State 32: Singlet-A' 5.6703 eV 218.66 nm f=0.0914 Excited State 19: Singlet-A' 4.9452 eV 250.71 nm f=0.0001 97 ->106 0.16797 99 ->106 0.67763 98 ->106 -0.12622 99 ->107 -0.15728 98 ->107 -0.15522		99->107 0.66298
Excited State 19: Singlet-A" 4.9452 eV 250.71 nm f=0.0001 97 ->106 0.16797 99 ->106 0.67763 98 ->106 -0.12622 99 ->107 -0.15728 98 ->107 -0.15722	103 ->109 0.16652	99->108 -0.13951
99 ->106 0.67763 98 ->106 -0.12622 99 ->107 -0.15728 98 ->107 -0.17522		
99->107 -0.15728 98->107 -0.17522		
	99 ->107 -0.15728 Excited State 20: Singlet-A' 5.0036 eV 247.79 nm f=0.2212	98 ->107 -0.17522 100 ->107 0.17814
102 > 106 - 0.11816 100 > 108 0.11630		
		0.11000

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101 ->108 0.30996	
101 ->110 -0.16061	
102 ->109 -0.13018	
102 ->110 0.17829	
103 ->109 0.15210	
103 ->111 -0.14145	
103 ->112 -0.10876	
104 ->111 -0.10561	
104 ->113 -0.19918	
Excited State 33: Singlet-A'	5.7378 eV 216.08 nm f=0.1787
95 ->105 0.11340	
96 ->105 0.12283	
98 ->106 -0.13772	
100 ->108 -0.17141	
101 ->108 0.15023	
101 ->110 0.12016	
102 ->107 -0.11066	
102 ->109 0.46214	
102 ->110 -0.11724	
103 ->109 0.15862	
103 ->110 -0.11528	
103 ->111 0.10231	5 7721 - 37 214 80 mm 6-0 0100
Excited State 34: Singlet-A'	5.7721 eV 214.80 nm f=0.0100
92 ->105 -0.15218	
93 ->105 -0.10284	
96 ->105 0.12634	
96 ->106 0.13949 97 ->106 -0.22861	
97 ->106 -0.22861 101 ->107 -0.11690	
101 ->108 0.10429	
102 ->109 -0.16280	
103 ->111 0.46187	
104 ->113 -0.17783	
Excited State 35: Singlet-A"	5.8466 eV 212.06 nm f=0.0008
99 ->107 0.13951	5.0100 CT 212.00 IIII 1 0.0000
99->108 0.65440	
99->111 -0.11881	
Excited State 36: Singlet-A'	5.8582 eV 211.64 nm f=0.0319
93 ->105 0.11109	
95 ->105 -0.12334	
97 ->106 -0.25568	
97 ->106 -0.25568 98 ->108 0.16745	
97 ->106 -0.25568 98 ->108 0.16745 101 ->110 -0.10678	
97 ->106 -0.25568 98 ->108 0.16745 101 ->110 -0.10678 102 ->110 0.18191	
97 ->106 -0.25568 98 ->108 0.16745 101 ->110 -0.10678 102 ->110 0.18191 103 ->112 -0.19109	
97 ->106 -0.25568 98 ->108 0.16745 101 ->110 -0.10678 102 ->110 0.18191 103 ->112 -0.19109 104 ->112 -0.16631	
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5 8768 eV 210 97 nm ⊨0 0212
97->106 -0.25568 98->108 0.16745 101->110 -0.10678 102->110 0.18191 103->112 -0.19109 104->112 -0.16631 104->113 0.44254 Excited State 37: Singlet-A'	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{cccc} 97.{\scriptstyle{>}106} & -0.25568\\ 98.{\scriptstyle{>}101} & 0.16745\\ 101.{\scriptstyle{>}110} & -0.10678\\ 102.{\scriptstyle{>}110} & 0.18191\\ 103.{\scriptstyle{>}112} & -0.19109\\ 104.{\scriptstyle{>}112} & -0.16631\\ 104.{\scriptstyle{>}113} & 0.44254\\ Excited State 37: Singlet-A'\\ 92.{\scriptstyle{>}105} & -0.16298 \end{array}$	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{cccc} 97.{\succ}106 & -0.25568\\ 98.{\succ}108 & 0.16745\\ 101.{\succ}10 & -0.10678\\ 102.{\succ}110 & 0.18191\\ 103.{\succ}112 & -0.19109\\ 104.{\succ}112 & -0.16631\\ 104.{\succ}113 & 0.44254\\ Excited State 37: Singlet-A'\\ 92.{\succ}105 & -0.16298\\ 97.{\succ}106 & 0.31366\\ \end{array}$	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{cccc} 97.{\scriptstyle{>}106} & -0.25568\\ 98.{\scriptstyle{>}101} & 0.16745\\ 101.{\scriptstyle{>}110} & -0.10678\\ 102.{\scriptstyle{>}110} & 0.18191\\ 103.{\scriptstyle{>}112} & -0.19109\\ 104.{\scriptstyle{>}112} & -0.16631\\ 104.{\scriptstyle{>}113} & 0.44254\\ Excited State 37: Singlet-A'\\ 92.{\scriptstyle{>}105} & -0.16298 \end{array}$	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{ccccc} 97 \ {\sim}106 & -0.25568 \\ 98 \ {\sim}108 & 0.16745 \\ 101 \ {\sim}110 & -0.10678 \\ 102 \ {\sim}110 & 0.18191 \\ 103 \ {\sim}112 & -0.19109 \\ 104 \ {\sim}112 & -0.16631 \\ 104 \ {\sim}113 & 0.44254 \\ \text{Excited State } 37: \ \text{Singlet-A'} \\ 92 \ {\sim}105 & -0.16298 \\ 97 \ {\sim}106 & 0.31366 \\ 100 \ {\sim}107 & 0.11127 \\ 101 \ {\sim}109 & -0.11095 \\ \end{array}$	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{cccc} 97.{\succ}106 & -0.25568\\ 98.{\succ}108 & 0.16745\\ 101.{\succ}110 & -0.10678\\ 102.{\succ}110 & 0.10678\\ 103.{\succ}112 & -0.19109\\ 104.{\succ}112 & -0.16631\\ 104.{\succ}112 & -0.16631\\ 104.{\succ}113 & 0.44254\\ Excited State 37: Singlet-A'\\ 92.{\succ}105 & -0.16298\\ 97.{\succ}106 & 0.31366\\ 100.{\succ}107 & 0.11127\\ 101.{\succ}09 & -0.11095\\ 102.{\succ}109 & 0.13485\\ \end{array}$	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{cccc} 97.{\succ}106 & -0.25568\\ 98.{\succ}108 & 0.16745\\ 101.{\succ}110 & -0.10678\\ 102.{\succ}110 & 0.10678\\ 103.{\succ}112 & -0.19109\\ 104.{\succ}112 & -0.16631\\ 104.{\succ}112 & -0.16631\\ 104.{\succ}113 & 0.44254\\ Excited State 37: Singlet-A'\\ 92.{\succ}105 & -0.16298\\ 97.{\succ}106 & 0.31366\\ 100.{\succ}107 & 0.11127\\ 101.{\succ}09 & -0.11095\\ 102.{\succ}109 & 0.13485\\ 102.{\succ}110 & 0.3282\\ 103.{\succ}111 & 0.25795\\ 103.{\succ}112 & 0.21908\\ \end{array}$	5.8768 eV 210.97 nm f=0.0212
$\begin{array}{cccc} 97.{\scriptstyle{>}}106 & -0.25568\\ 98.{\scriptstyle{>}}108 & 0.16745\\ 101.{\scriptstyle{>}}110 & -0.10678\\ 102.{\scriptstyle{>}}110 & 0.10678\\ 102.{\scriptstyle{>}}110 & 0.10678\\ 103.{\scriptstyle{>}}112 & -0.19109\\ 104.{\scriptstyle{>}}112 & -0.16631\\ 104.{\scriptstyle{>}}113 & 0.44254\\ \text{Excited State 37: Singlet-A'}\\ 92.{\scriptstyle{>}}105 & -0.16298\\ 97.{\scriptstyle{>}}106 & 0.31366\\ 100.{\scriptstyle{>}}107 & 0.11127\\ 101.{\scriptstyle{>}}109 & 0.13465\\ 100.{\scriptstyle{>}}109 & 0.13485\\ 102.{\scriptstyle{>}}110 & 0.33282\\ 103.{\scriptstyle{>}}111 & 0.25795\\ 103.{\scriptstyle{>}}112 & 0.21908\\ 104.{\scriptstyle{>}}112 & 0.10927\\ \end{array}$	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	5.8768 eV 210.97 nm f=0.0212 5.9934 eV 206.87 nm f=0.0000
$\begin{array}{cccc} 97.{\succ}106 & -0.25568\\ 98.{\succ}108 & 0.16745\\ 101.{\succ}110 & -0.10678\\ 102.{\succ}110 & 0.10678\\ 102.{\succ}112 & -0.19109\\ 103.{\succ}112 & -0.6631\\ 104.{\succ}113 & 0.44254\\ Excited State 37: Singlet-A'\\ 92.{\succ}105 & -0.16298\\ 97.{\succ}106 & 0.31366\\ 100.{\succ}107 & 0.11127\\ 101.{\succ}09 & -0.11095\\ 102.{\succ}109 & 0.13485\\ 102.{\succ}110 & 0.3282\\ 103.{\succ}111 & 0.25795\\ 103.{\succ}112 & 0.1997\\ Excited State 38: Singlet-A''\\ 91.{\succ}105 & -0.17329\\ \end{array}$	
$\begin{array}{cccc} 97.{\scriptstyle{>}-106} & -0.25568\\ 98.{\scriptstyle{>}-108} & 0.16745\\ 101.{\scriptstyle{>}-110} & -0.10678\\ 102.{\scriptstyle{>}-110} & 0.10678\\ 103.{\scriptstyle{>}-112} & -0.19109\\ 104.{\scriptstyle{>}-112} & -0.16631\\ 104.{\scriptstyle{>}-113} & 0.44254\\ Excited State 37. Singlet-A'\\ 92.{\scriptstyle{>}-105} & -0.16298\\ 97.{\scriptstyle{>}-106} & 0.31366\\ 100.{\scriptstyle{>}-107} & 0.11127\\ 101.{\scriptstyle{>}-109} & -0.11095\\ 102.{\scriptstyle{>}-109} & 0.13485\\ 102.{\scriptstyle{>}-110} & 0.3282\\ 103.{\scriptstyle{>}-111} & 0.25795\\ 103.{\scriptstyle{>}-112} & 0.19921\\ 104.{\scriptstyle{>}-112} & 0.10927\\ Excited State 38: Singlet-A''\\ 91.{\scriptstyle{>}-105} & -0.17329\\ 94.{\scriptstyle{>}-105} & 0.65866\\ \end{array}$	5.9934 eV 206.87 nm f=0.0000
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccc} 97.{}{\sim}106 & -0.25568\\ 98.{}{\sim}108 & 0.16745\\ 101.{}{\sim}110 & -0.10678\\ 102.{}{\sim}110 & 0.18191\\ 103.{}{\sim}112 & -0.19109\\ 104.{}{\sim}112 & -0.6631\\ 104.{}{\sim}113 & 0.44254\\ Excited State 37: Singlet-A'\\ 92.{}{\sim}105 & -0.16298\\ 97.{}{\sim}106 & 0.31366\\ 100.{}{\sim}107 & 0.11127\\ 101.{}{\sim}109 & -0.11095\\ 102.{}{\sim}109 & 0.13485\\ 102.{}{\sim}110 & 0.3282\\ 103.{}{\sim}111 & 0.25795\\ 103.{}{\sim}112 & 0.1927\\ Excited State 38: Singlet-A''\\ 91.{}{\sim}105 & -0.17329\\ 94.{}{\sim}105 & -0.65866\\ Excited State 39: Singlet-A''\\ 96.{}{\sim}106 & -0.13360\\ \end{array}$	5.9934 eV 206.87 nm f=0.0000
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.9934 eV 206.87 nm f=0.0000
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5.9934 eV 206.87 nm f=0.0000
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5.9934 eV 206.87 nm f=0.0000
$\begin{array}{cccc} 97.{->}106 & -0.25568 \\ 98.{->}108 & 0.16745 \\ 101.{->}110 & -0.10678 \\ 102.{->}110 & 0.10678 \\ 103.{->}112 & -0.19109 \\ 104.{->}112 & -0.16631 \\ 104.{->}113 & 0.44254 \\ \mbox{Excited State 37} & \mbox{Singlet-A''} \\ 97.{->}105 & -0.16298 \\ 97.{->}106 & 0.31366 \\ 100.{->}107 & 0.11127 \\ 101.{->}109 & -0.1095 \\ 102.{->}109 & 0.13485 \\ 102.{->}110 & 0.3282 \\ 103.{->}111 & 0.25795 \\ 103.{->}112 & 0.19928 \\ 104.{->}112 & 0.10927 \\ \mbox{Excited State 38} & \mbox{Singlet-A''} \\ 91.{->}105 & -0.17329 \\ 94.{->}105 & -0.13360 \\ 97.{->}106 & -0.13360 \\ 97.{->}106 & -0.13296 \\ 98.{->}107 & -0.20724 \\ 98.{->}108 & 0.20846 \\ 100.{->}107 & 0.36412 \\ \end{array}$	5.9934 eV 206.87 nm f=0.0000
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	5.9934 eV 206.87 nm f=0.0000
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$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.9934 eV 206.87 nm f=0.0000
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $	5.9934 eV 206.87 nm f=0.0000 6.0325 eV 205.53 nm f=0.0941
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $	5.9934 eV 206.87 nm f=0.0000 6.0325 eV 205.53 nm f=0.0941
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	5.9934 eV 206.87 nm f=0.0000 6.0325 eV 205.53 nm f=0.0941
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	5.9934 eV 206.87 nm f=0.0000 6.0325 eV 205.53 nm f=0.0941

7. Full Listing for Text Reference (11)

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.