Electronic Supplementary Material (ESI) for Chemical Communications

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

Takashi Otani, Takao Saito,* Ryota Sakamoto, Hiroyuki Osada, Akihito Hirahara, Naoki Furukawa, Noriki Kutsumura, Tsukasa Matsuo, and Kohei Tamao

Department of Chemistry, Faculty of Science, Tokyo University of Science, Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan and Functional Elemento-Organic Chemistry Unit, RIKEN Advanced Science Institute, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

E-mail: tsaito@rs.kagu.tus.ac.jp

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Contents

1. Synthesis

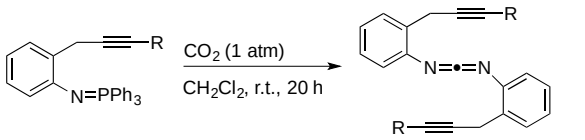
1.1 General Information

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. ^{1}H and ^{13}C 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, $CDCl_3$, or CD_2Cl_2. 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

Scheme S1. **Synthesis of Carbodiimides 1**



S1a: R = Me
S1b: R = Pent

1a: R = Me (92%)
1b: R = Pent (98%)

*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 CO_2, 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}; ^{1}H NMR (600 MHz, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2 × 2), 13.7 (CH_3 × 2); HRMS (ESI) calcd for $C_{21}H_{19}N_2$ $[M + H]^+$: 299.1543, found 299.1550.

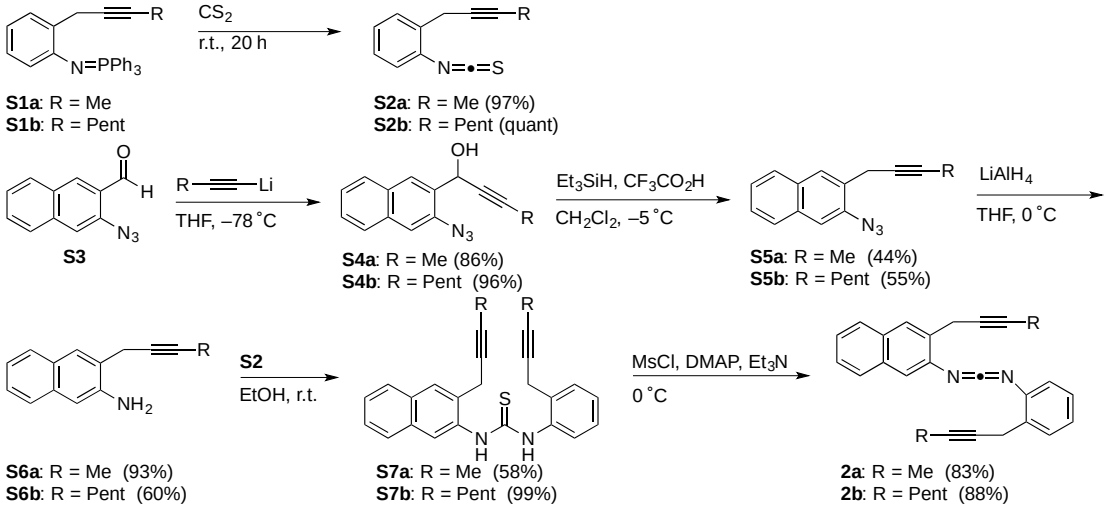
*Bis[2-(2-octyn-1-yl)phenyl]carbodiimide (**1b**).* The title compound (160 mg, 98%) was synthesized from **S1b** (369 mg, 0.80 mmol) using the same procedure described above. Colorless oil: IR (neat): 2931, 2298, 2152, 1581, 1481, 1172, 1087 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, δ): 7.55 (d, J = 7.2 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); ^{13}C NMR (75 MHz, $CDCl_3$, 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.

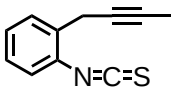
× 2), 127.6 (CH × 2), 125.6 (CH × 2), 124.6 (CH × 2), 83.2 (C × 2), 76.6 (C × 2), 31.1 (CH_2 × 2), 28.7 (CH_2 × 2), 22.2 (CH_2 × 2), 21.6 (CH_2 × 2), 18.8 (CH_2 × 2), 14.0 (CH_3 × 2); HRMS (ESI) calcd for $C_{29}H_{35}N_2$ [M + H]$^+$: 411.2795, found 411.2794.

1.2.2 Synthesis of Carbodiimides 2

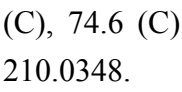
Scheme S2. **Synthesis of Carbodiimides 2**



*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}; ^{1}H NMR (500 MHz, $CDCl_3$, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_2), 3.6 (CH_3); HRMS (ESI) calcd for $C_{11}H_9NSNa$ [M + Na]$^+$: 210.0348, found 210.0348.



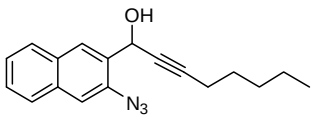
*2-(2-Octyn-1-yl)phenyl isothiocyanate (**S2b**).* The title compound (2.23 g, quant) was obtained from **S1b** (4.14 g, 8.97 mmol) and carbon disulfide (20 mL) using the same procedure described above. Colorless oil: IR (neat): 2931, 2098, 1581, 1481, 1218, 1172, 1095 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$, 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); ^{13}C NMR (76 MHz, $CDCl_3$, 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 (CH_2), 28.6 (CH_2), 22.21 (CH_2), 22.18 (CH_2), 18.8 (CH_2), 14. 0 (CH_3); HRMS (ESI) calcd for $C_{15}H_{17}NSNa$ [M + Na]$^+$: 266.0974, found 266.0978.



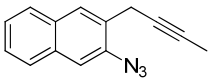
*3-Azido-α-(1-propyn-1-yl)-2-naphthalenemethanol (**S4a**).* To a THF (10 mL) solution of 1-bromo-1-propene (0.68 mL, 7.98 mmol) was added 1.66 M hexane solution of *n*-butyllithium (7.05 mL, 11.7 mmol) at −78 °C. The mixture was stirred for 2 h, and a THF (10 mL) solution of 3-azido-2-naphthalenecarboxaldehyde (**S3**) (1.05 g, 5.32 mmol) was added. The mixture was stirred for 20 min, and the reaction was 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 **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, $CDCl_3$, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_3); HRMS (ESI) calcd for $C_{14}H_{11}N_3NaO$ $[M + Na]^+$: 266.1264, found 266.1267.

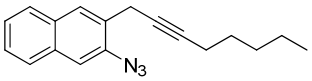
*3-Azido-α-(1-heptyn-1-yl)-2-naphthalenemethanol (**S4b**).* To a THF (10 mL) solution of 1-heptyne (0.94 mL, 7.2 mmol) was added a 1.66 M hexane solution of *n*-butyllithium (4.34 mL, 7.2 mmol) at −78 °C. After being stirred for 1 h, the mixture was warmed to room temperature, and a THF (10 mL) solution 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, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2), 28.2 (CH_2), 22.2 (CH_2), 18.9 (CH_2), 14.0 (CH_3); HRMS (ESI) calcd for $C_{18}H_{19}N_3NaO$ $[M + Na]^+$: 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, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2), 3.7 (CH_3); HRMS (ESI) calcd for $C_{14}H_{12}N_3$ $[M + H]^+$: 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, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2), 28.7 (CH_2), 22.3 (CH_2), 21.1 (CH_2), 18.9 (CH_2), 14.0 (CH_3); HRMS (ESI) calcd for $C_{18}H_{19}N_3Na$ $[M + Na]^+$: 300.1471, found 300.1470.

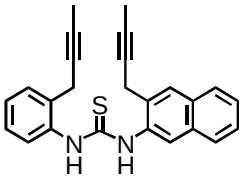
*3-(2-Butyn-1-yl)-2-naphthalenamine (**S6a**).* To a suspension of lithium aluminum hydride (LAH) (214 mg, 5.65 mmol) in THF (30 mL) was added a THF (20 mL) solution of **S5a** (500 mg, 2.26 mmol) at 0 °C. The mixture was stirred for 15 min and quenched by addition of aqueous THF (1:1) followed by 1 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}; ^{1}H NMR (300 MHz, $CDCl_3$, 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), 7.22 (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); ^{13}C NMR (75 MHz, $CDCl_3$, δ): 143.1 (C), 134.0 (C), 128.1 (C), 128.0 (CH), 127.3 (CH), 125.8 (CH), 125.3 (CH), 125.2 (C), 122.6 (CH), 109.9 (CH), 78.7 (C), 75.3 (C), 22.5 (CH_2), 3.6 (CH_3); HRMS (ESI) calcd for $C_{14}H_{14}N$ $[M + H]^+$: 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}; ^{1}H NMR (500 MHz, $CDCl_3$, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_2), 28.6 (CH_2), 22.5 (CH_2), 22.2 (CH_2), 18.8 (CH_2), 14.0 (CH_3); HRMS (ESI) calcd for $C_{18}H_{21}NNa$ $[M + Na]^+$: 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}; ^{1}H NMR (500 MHz, $CDCl_3$, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_2), 30.9 (CH_2), 28.5 (CH_2), 28.3 (CH_2), 22.5 (CH_2), 22.1 (CH_2), 22.1 (CH_2), 22.0 (CH_2),

18.7 (CH_2), 18.3 (CH_2), 13.9 (CH_3), 13.8 (CH_3); HRMS (ESI) calcd for $C_{33}H_{38}N_2SNa$ $[M + Na]^+$: 517.2648, found 517.2648.

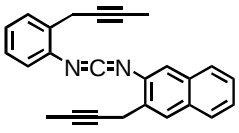
*N-[3-(2-Butyn-1-yl)-2-naphthalenyl]-N'-[2-(2-butyn-1-yl)phenyl]thiourea (**S7a**).* The title compound



(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, $CDCl_3$, 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), 7.58 (d, J = 7.4 Hz, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_2), 22.2 (CH_2), 3.6 (CH_3), 3.0 (CH_3) (one quaternary carbon was not observed); HRMS (ESI) calcd for $C_{25}H_{22}N_2SNa$ $[M + Na]^+$: 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, $CDCl_3$, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_2), 31.0 (CH_2), 28.7 (CH_2), 28.6 (CH_2), 22.2 (CH_2), 22.12 (CH_2), 22.11 (CH_2), 21.6 (CH_2), 18.81 (CH_2), 18.75 (CH_2), 13.94 (CH_3), 13.89 (CH_3); HRMS (ESI) calcd for $C_{33}H_{37}N_2$ $[M + H]^+$: 461.2951, found 461.2951.

*3-(2-Butyn-1-yl)-N-[[2-(2-butyn-1-yl)phenyl]carbonimidoyl]-2-naphthalenamine (**2a**).* The title

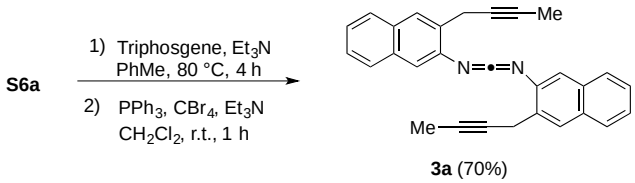


compound (199 mg, 83%) was obtained from **S7a** (262 mg, 0.68 mmol), triethylamine (0.29 mL, 2.05 mmol), DMAP (4.2 mg, 0.03 mmol), methanesulfonyl chloride (0.11 mL, 1.37 mmol), and dichloromethane (10 mL) using the same procedure described above. Colorless solid: Mp 90.9–91.4 °C; IR (KBr): 2908, 2152, 2129, 1573, 1450, 1226, 748 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 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); ^{13}C NMR (75 MHz, $CDCl_3$, 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 (CH_2), 21.7 (CH_2), 3.7 (CH_3), 3.6 (CH_3); HRMS (ESI) calcd for $C_{25}H_{20}N_2Na$ $[M + Na]^+$: 371.1519, found 371.1516.

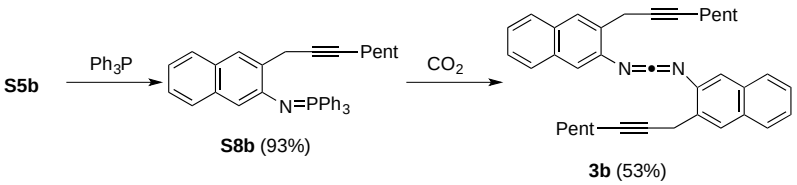
1.2.3 Synthesis of Carbodiimides 3

Scheme S3. **Synthesis of Carbodiimides 3a**



*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, $CDCl_3$, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_2 × 2), 3.7 (CH_3 × 2); HRMS (ESI) calcd for $C_{29}H_{23}N_2$ $[M + H]^+$: 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, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2), 29.0 (CH_2), 22.9 (CH_2), 22.3 (CH_2), 19.0 (CH_2), 14.0 (CH_3); HRMS (ESI) calcd for $C_{36}H_{35}NP$ $[M + H]^+$: 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, $CDCl_3$, 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); ^{13}C NMR (75 MHz, $CDCl_3$, 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 (CH_2 × 2), 28.7 (CH_2 × 2), 22.3 (CH_2 × 2), 22.2 (CH_2 × 2), 18.9 (CH_2 × 2), 14.0 (CH_3 × 2); HRMS (ESI) calcd for $C_{37}H_{39}N_2$ $[M + H]^+$: 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 ($Rh(PPh_3)_3Cl$) (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, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_3), 14.0 (CH_3); HRMS (ESI) calcd for $C_{21}H_{17}N_2$ $[M + H]^+$: 297.1386, found 297.1380; Anal. Calcd for $C_{21}H_{16}N_2$: C, 85.11; H, 5.44; N, 9.34. Found: C, 84.93; H, 5.44; N, 9.34.

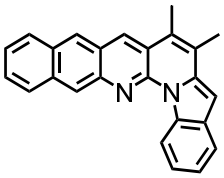
*6,7-Dipentylbenzo[g]indolo[1,2-a][1,8]naphthyridine (**4b**).* The title compound (142 mg, 93%) was obtained from **1b** (155 mg, 0.38 mmol), $Rh(PPh_3)_3Cl$ (35 mg, 0.038 mmol), and toluene (2 mL + 3 mL) using the same procedure described above. Yellow solid: Mp 110.5–110.9 °C; IR (KBr): 3054, 2923, 2854, 1589, 1535, 1457, 1396 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$, 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); ^{13}C NMR (126 MHz, $CDCl_3$, 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 (CH_2), 32.3 (CH_2), 29.7 (CH_2), 29.6 (CH_2), 29.4 (CH_2), 27.7 (CH_2), 22.6 (CH_2), 22.5 (CH_2), 14.1 (CH_3 × 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

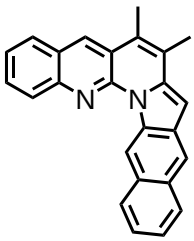
*Synthesis of **5a** and **6a**.* To a heated toluene (2 mL) solution of $Rh(PPh_3)_3Cl$ (17 mg, 0.018 mmol) was added dropwise a toluene (3 mL) solution of carbodiimide **2a** (60.9 mg, 0.175 mmol) at 120 °C. The mixture was heated for 20 min and cooled to room temperature. Manganese(IV) oxide (65 mg, 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 ^{1}H 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 dissolved in toluene by heating and diluted with ethanol. The resulting fine crystals which contain mainly **6a** 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}; ^{1}H NMR (300 MHz, $CDCl_3$, 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). ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_3), 13.8 (CH_3); HRMS (ESI) calcd for $C_{25}H_{19}N_2$ $[M + H]^+$: 347.1543, found 347.1543; Anal. Calcd for $C_{25}H_{18}N_2$: 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}; ^{1}H NMR (600 MHz, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_3), 14.2 (CH_3); HRMS-ESI (*m/z*): $[M + H]^+$: calcd for $C_{25}H_{19}N_2$, 347.1543; found, 347.1540; Anal. Calcd for $C_{25}H_{18}N_2$: 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), $Rh(PPh_3)_3Cl$ (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; ^{1}H NMR (600 MHz, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2), 32.36 (CH_2), 29.6 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 27.8 (CH_2), 22.59 (CH_2), 22.57 (CH_2), 14.12 (CH_3), 14.10 (CH_3); 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.

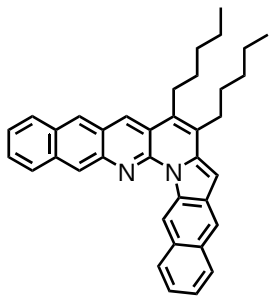
*7,8-Dipentylbenzo[g]benzo[f']indolo[1,2-a][1,8]naphthyridine (**6b**).* Brownish red solid: Mp 174.1–175.9 °C; ^{1}H NMR (600 MHz, $CDCl_3$, δ): 9.78 (d, J = 8.2 Hz, 1H), 8.70 (s, 1H), 8.43 (s, 1H), 8.42 (s, 1H), 8.09 (d, J = 8.3 Hz, 1H), 8.02 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 7.7 Hz, 1H), 7.54–7.50 (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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2), 32.400 (CH_2), 29.64 (CH_2), 29.57 (CH_2), 29.5 (CH_2), 27.7 (CH_2), 22.599 (CH_2), 22.597 (CH_2), 14.13 (CH_3), 14.11 (CH_3); 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 $RhCl(PPh_3)_3$ (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}; ^{1}H NMR (600 MHz, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$,

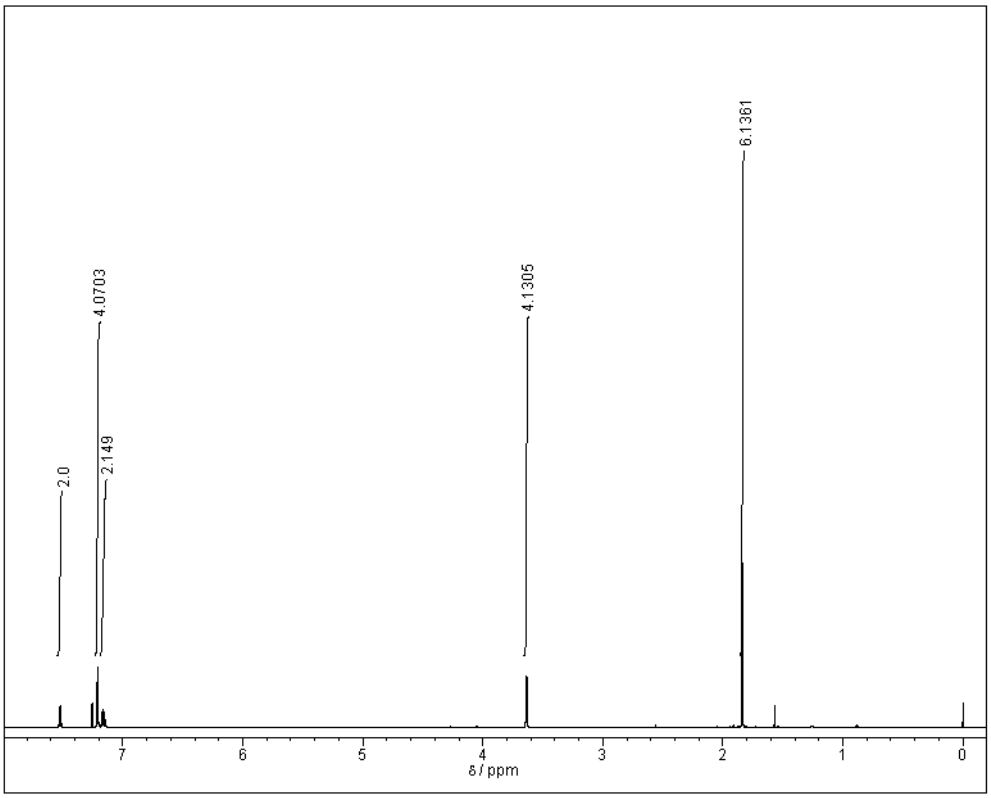
δ): 147.7 (C), 142.7 (C), 140.7 (C), 135.2 (C), 134.5 (C), 131.3 (C), 130.9 (C), 130.8 (CH), 130.6 (C), 130.4 (C), 129.2 (CH), 128.1 (CH), 128.0 (CH), 127.7 (CH), 126.9 (C), 126.6 (CH), 126.2 (CH), 125.1 (C), 125.0 (CH), 124.8 (C), 124.2 (CH), 124.1 (CH), 124.0 (CH), 122.1 (C), 117.7 (CH), 115.1 (CH), 100.3 (CH), 15.1 (CH_3), 14.1 (CH_3); HRMS (ESI) calcd for $C_{29}H_{21}N_2$ $[M + H]^+$: 397.1699, found 397.1699; Anal. Calcd for $C_{29}H_{20}N_2$: C, 87.85; H, 5.08; N, 7.07. Found: C, 87.59; H, 5.13; N, 6.88.

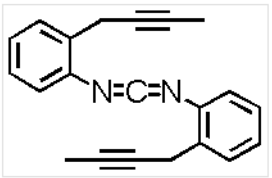
*7,8-Dipentylbenzo[f']indolo[1,2-a]naphtho[2,3-g][1,8]naphthyridine (**7b**).* To a heated toluene (1 mL) solution of $RhCl(PPh_3)_3$ (9.2 mg, 0.01 mmol) was slowly added a toluene (1 mL) solution of carbodiimide **3b** (50.9 mg, 0.10 mmol). After being stirred for 20 min, the mixture was cooled to room 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, $CDCl_3$, 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); ^{13}C NMR (151 MHz, $CDCl_3$, 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 (CH_2 × 2), 29.6 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 27.8 (CH_2), 22.6 (CH_2 × 2), 14.1 (CH_3 × 2); HRMS (ESI) calcd for $C_{37}H_{37}N_2$ $[M + H]^+$: 509.2951, found 509.2952; Anal. Calcd for $C_{37}H_{36}N_2$: C, 87.36; H, 7.13; N, 5.51. Found: C, 87.15; H, 7.36; N, 5.43.



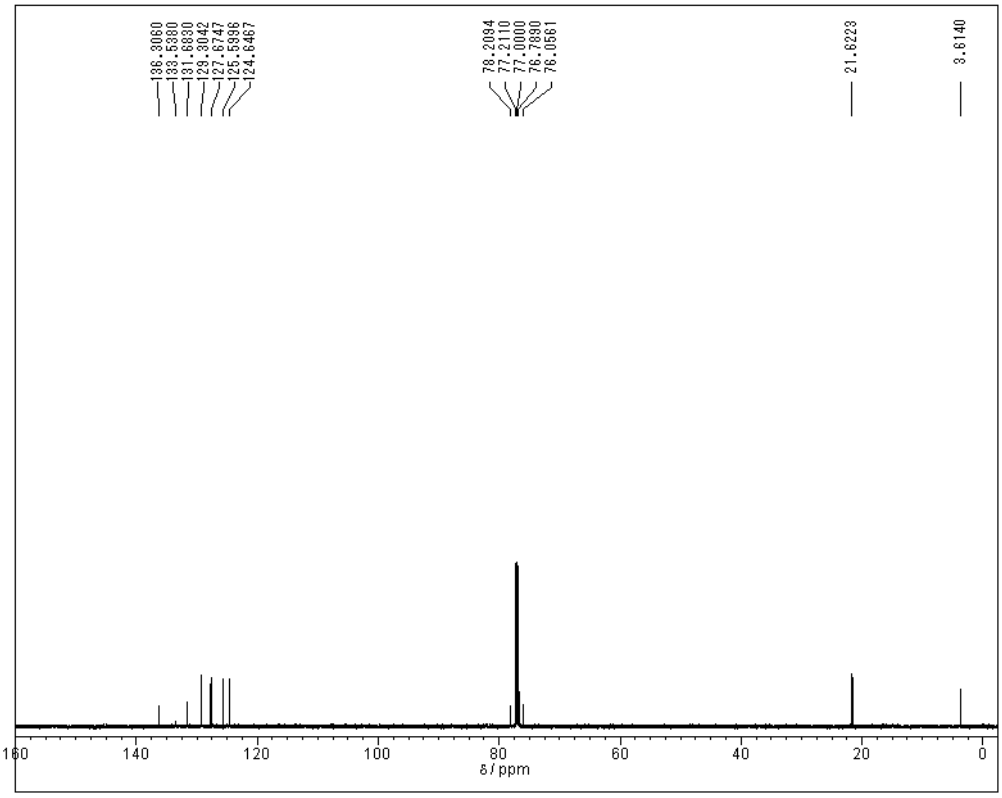
2. NMR Spectra

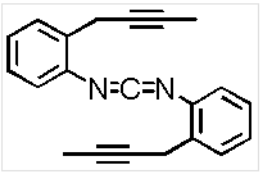
1a





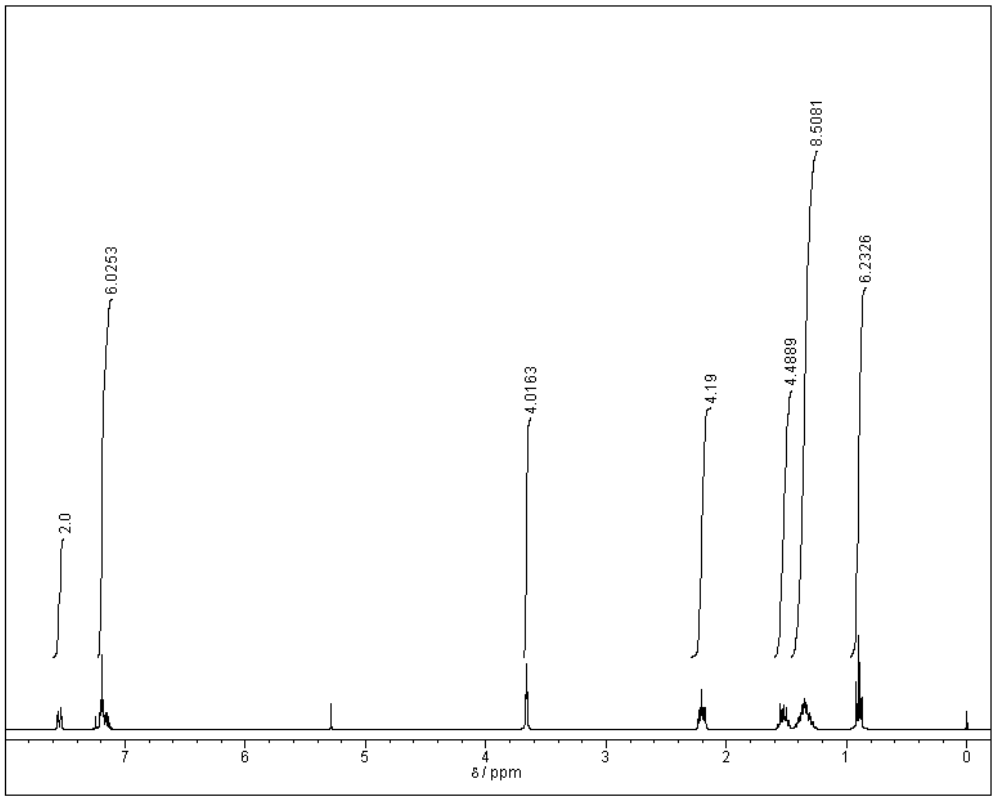
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent CDCL₃

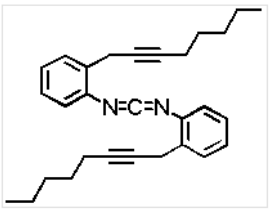




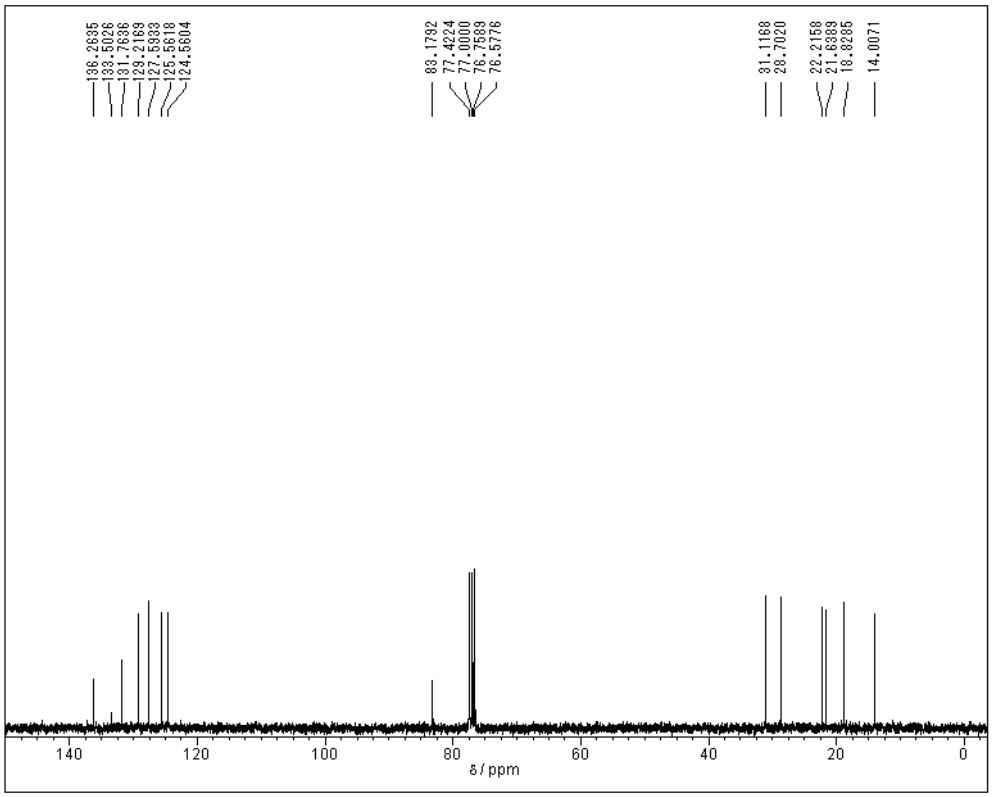
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent CDCL₃

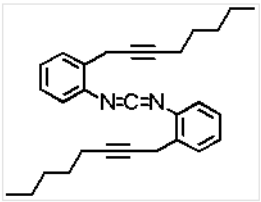
1b





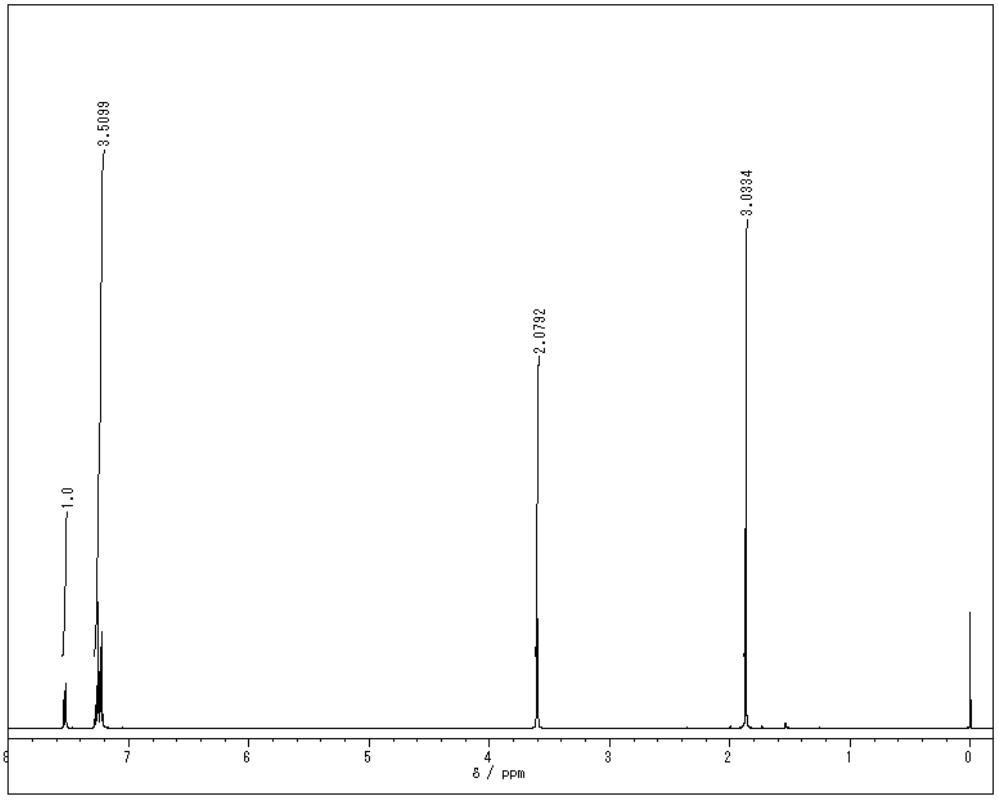
ObsNuc	^{1}H
ObsFreq	300.4 MHz
Solvent	$CDCl_3$

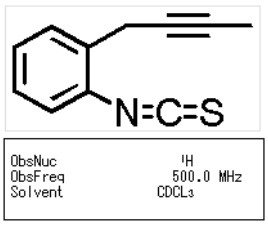




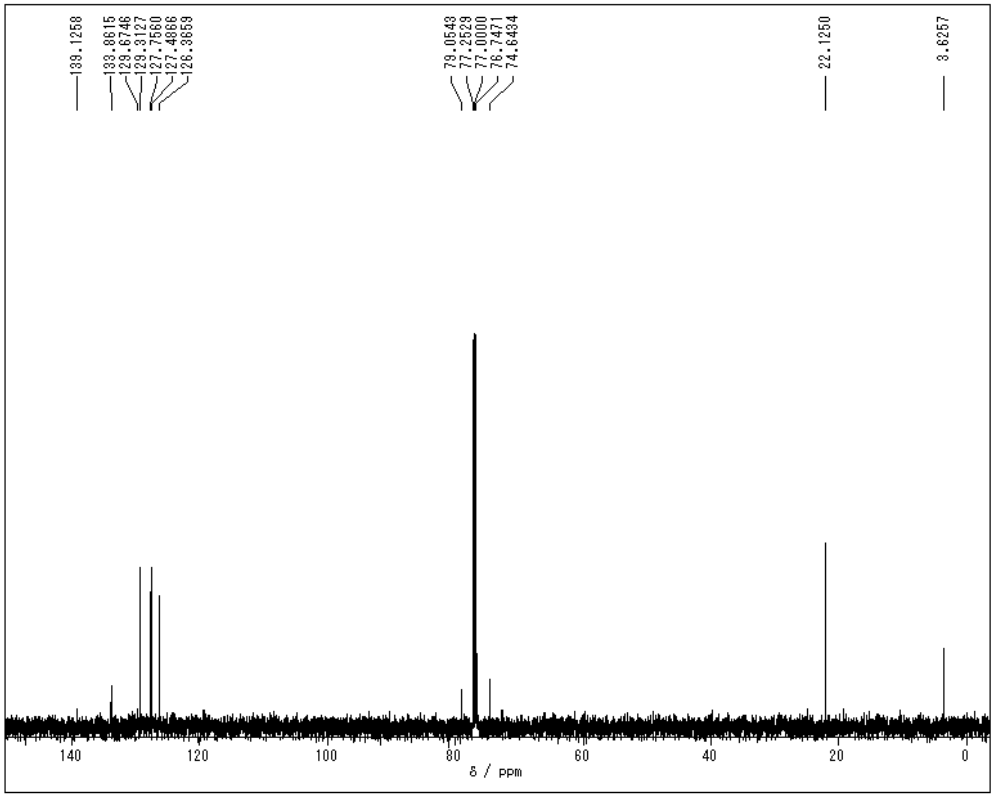
ObsNuc	^{13}C
ObsFreq	75.45 MHz
Solvent	$CDCl_3$

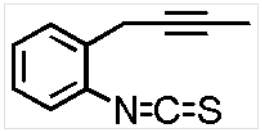
S2a





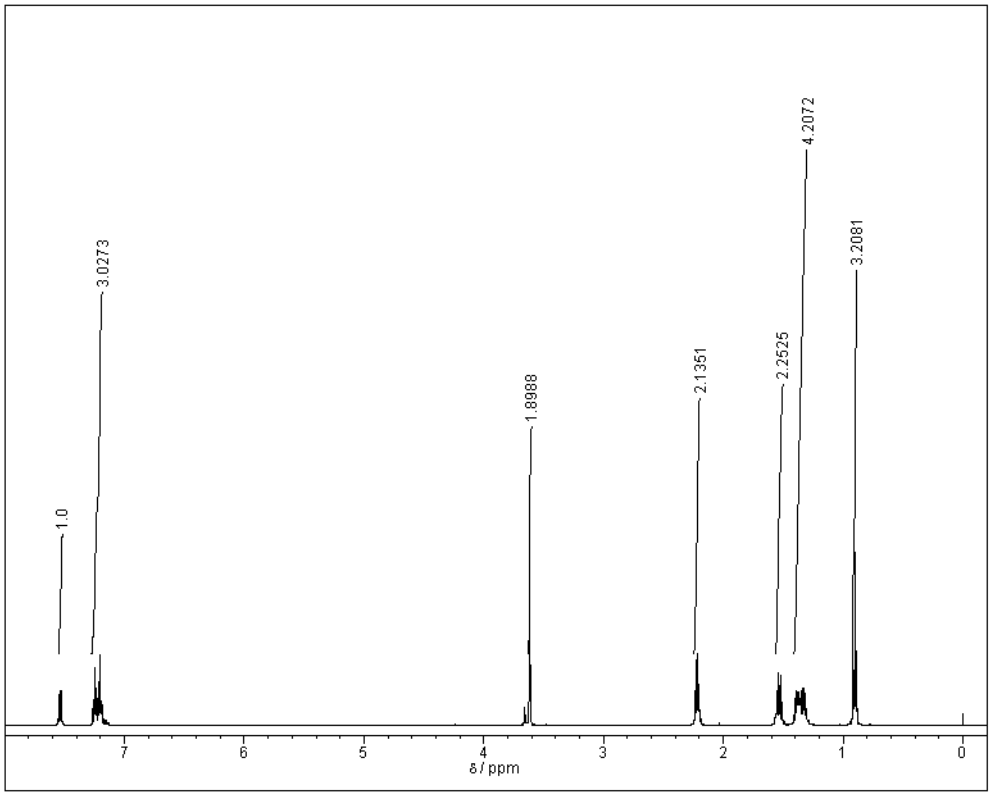
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

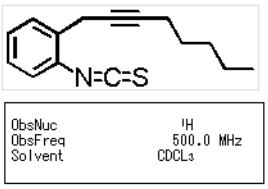


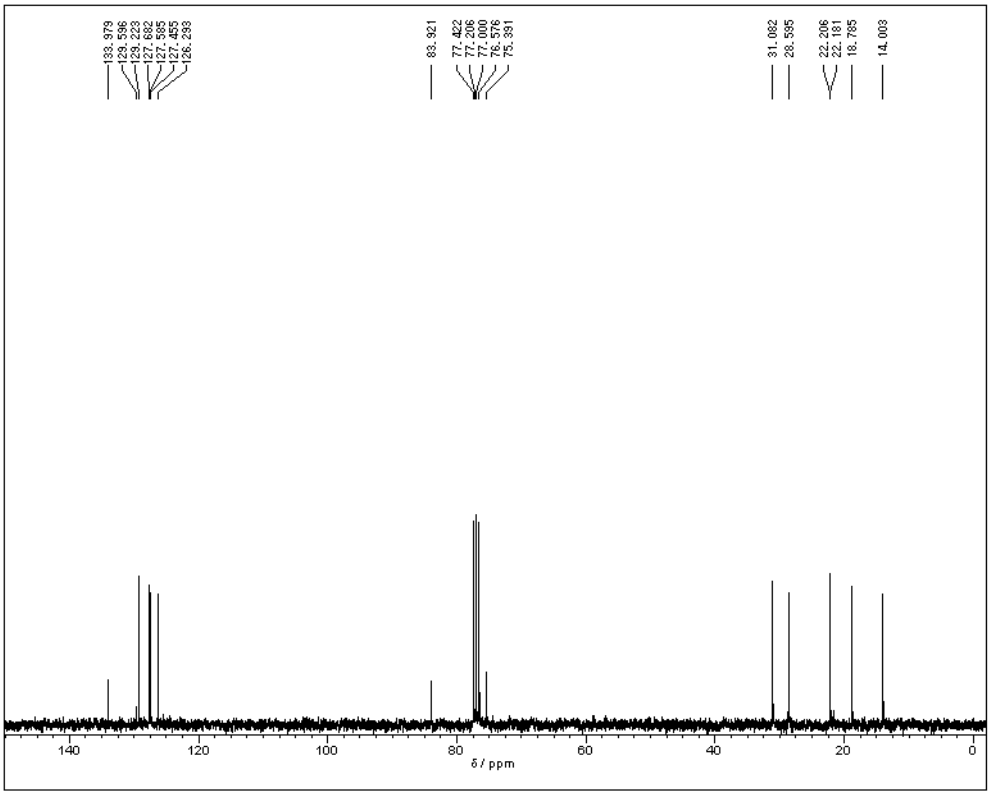


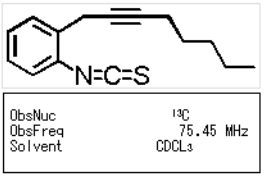
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

S2b

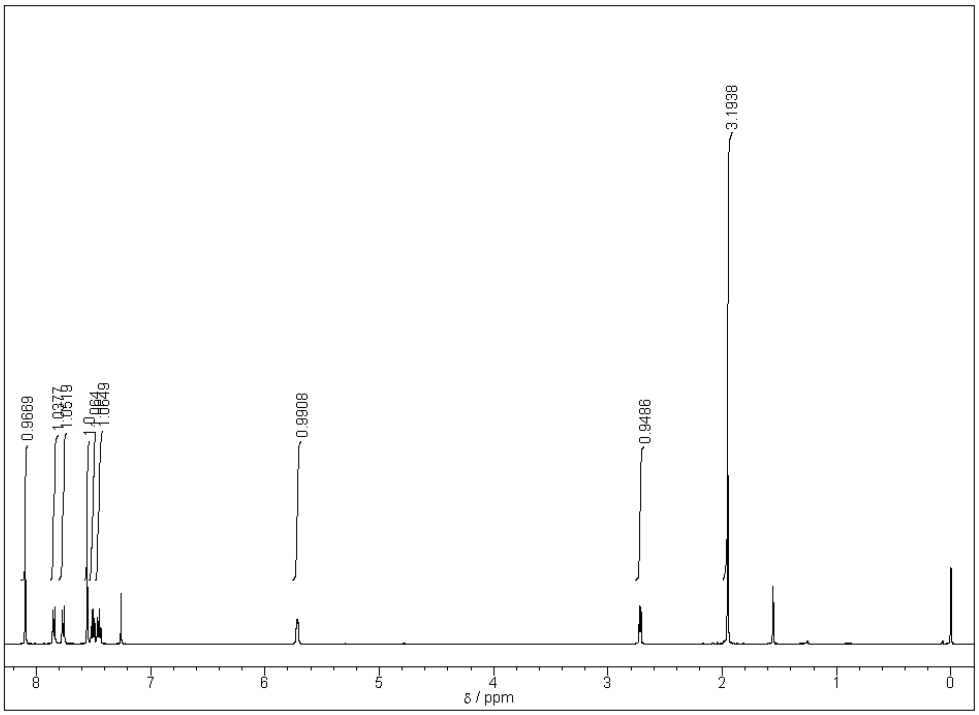

1.0
3.0273
1.8988
2.1351
2.2525
4.2072
3.2081
7
6
5
4
3
2
1
0
δ / ppm

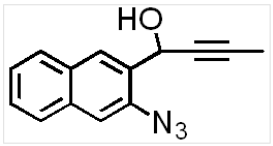

N=C=S
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent CDCL₃


133.979
129.596
129.223
127.682
127.585
127.455
126.293
83.921
77.422
77.206
77.000
76.576
75.391
31.082
28.595
22.206
22.181
18.785
14.003
140
120
100
80
60
40
20
0
δ / ppm

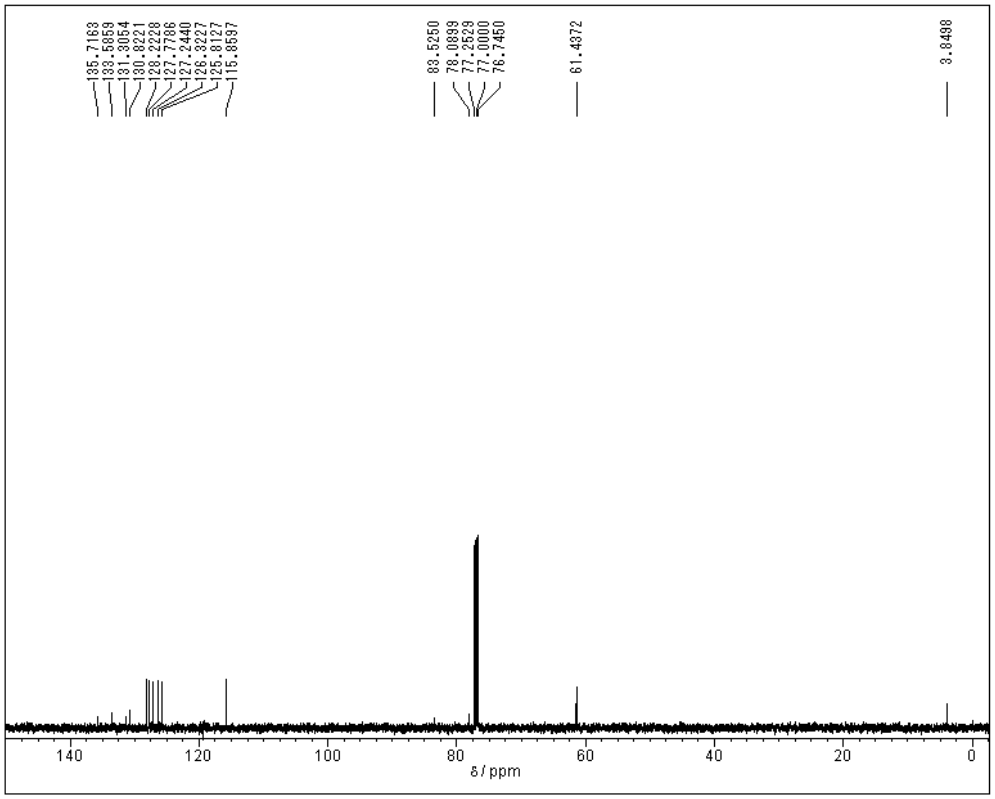

N=C=S
ObsNuc ¹³C
ObsFreq 75.45 MHz
Solvent CDCL₃

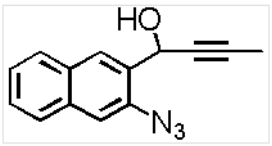
S4a





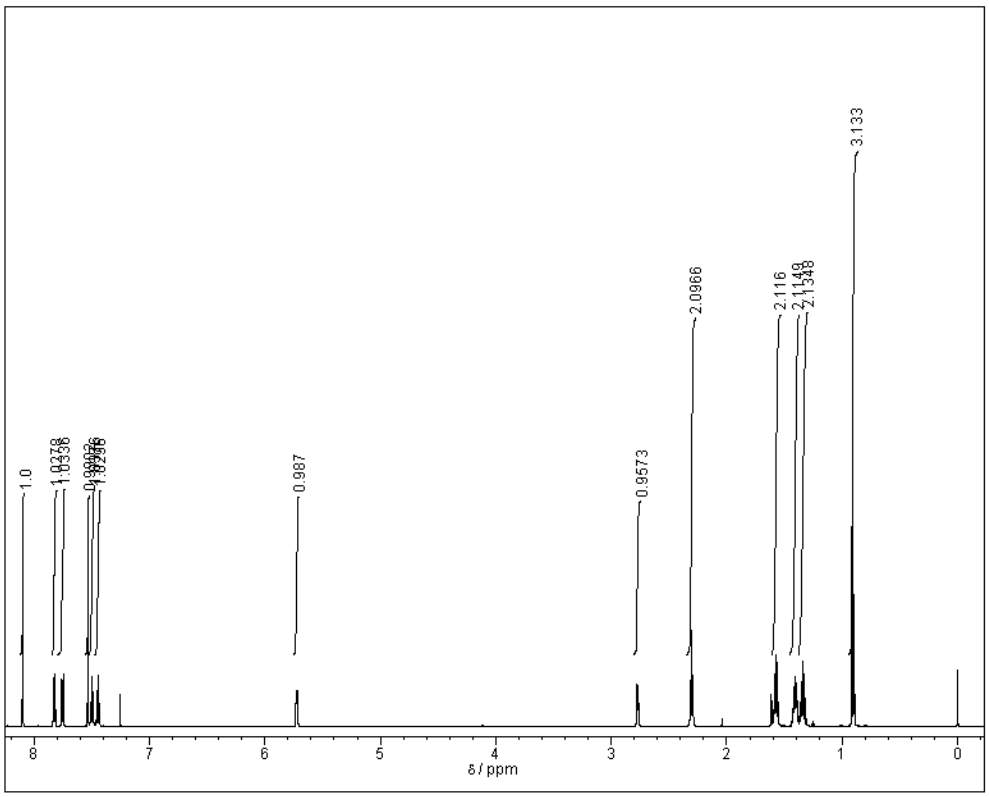
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

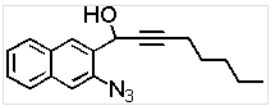




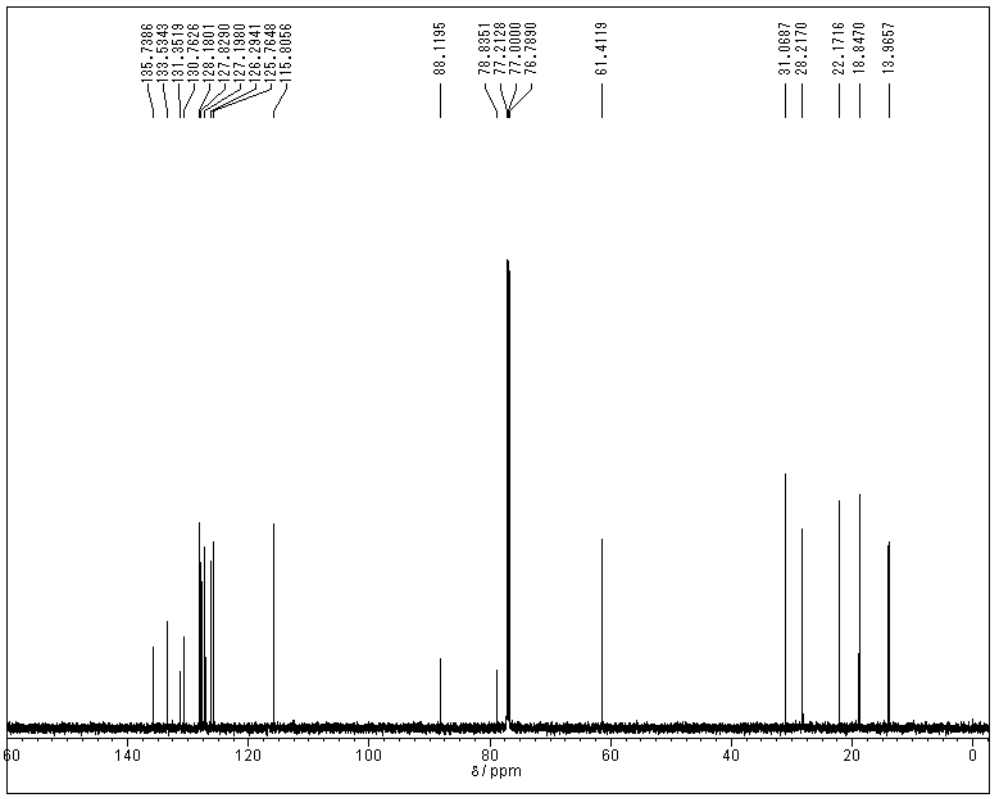
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

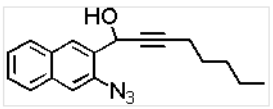
S4b





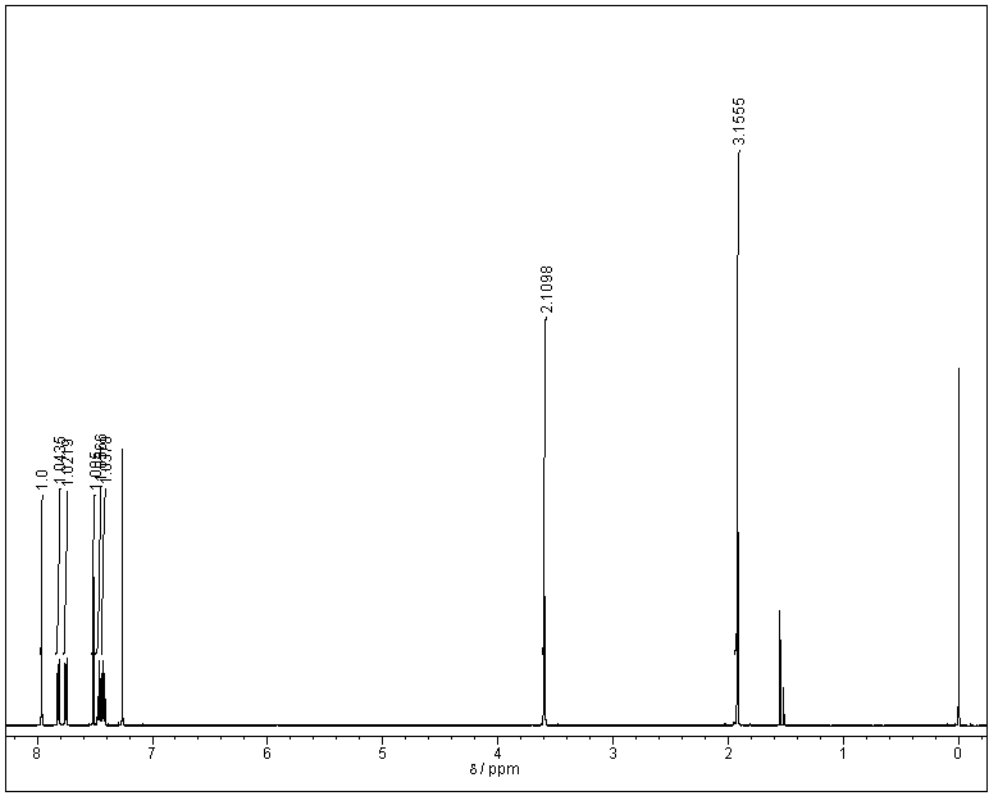
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	$CDCl_3$

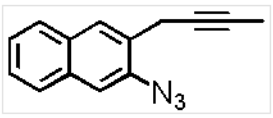




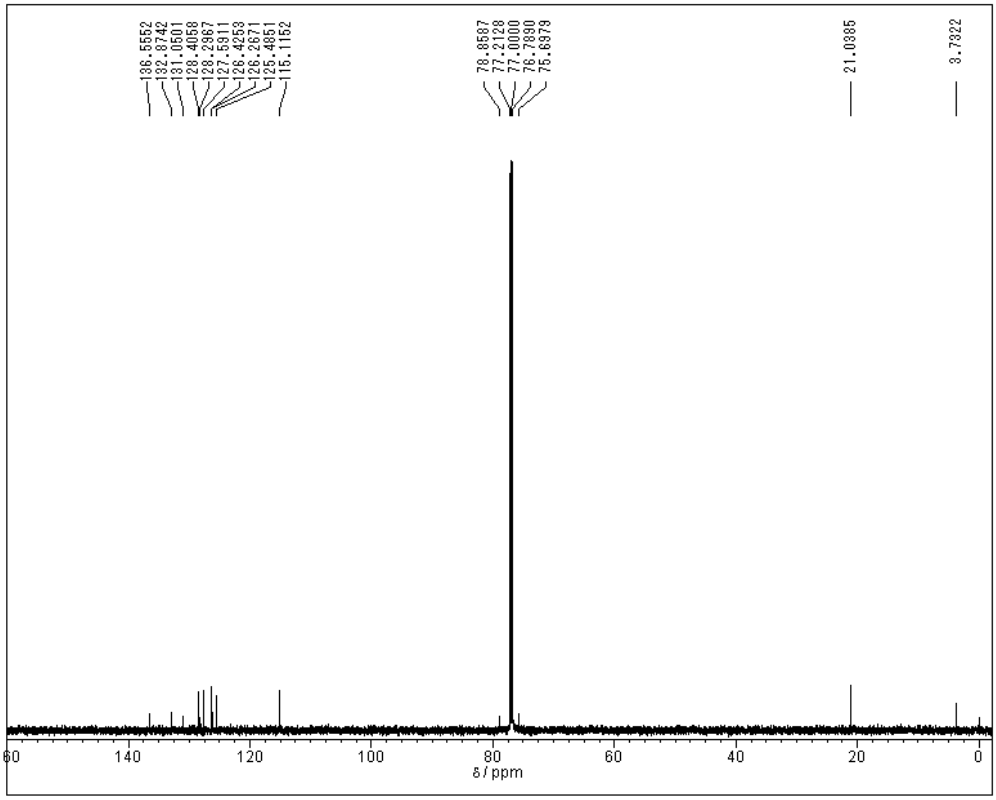
ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	$CDCl_3$

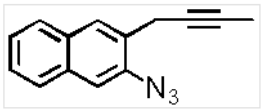
S5a





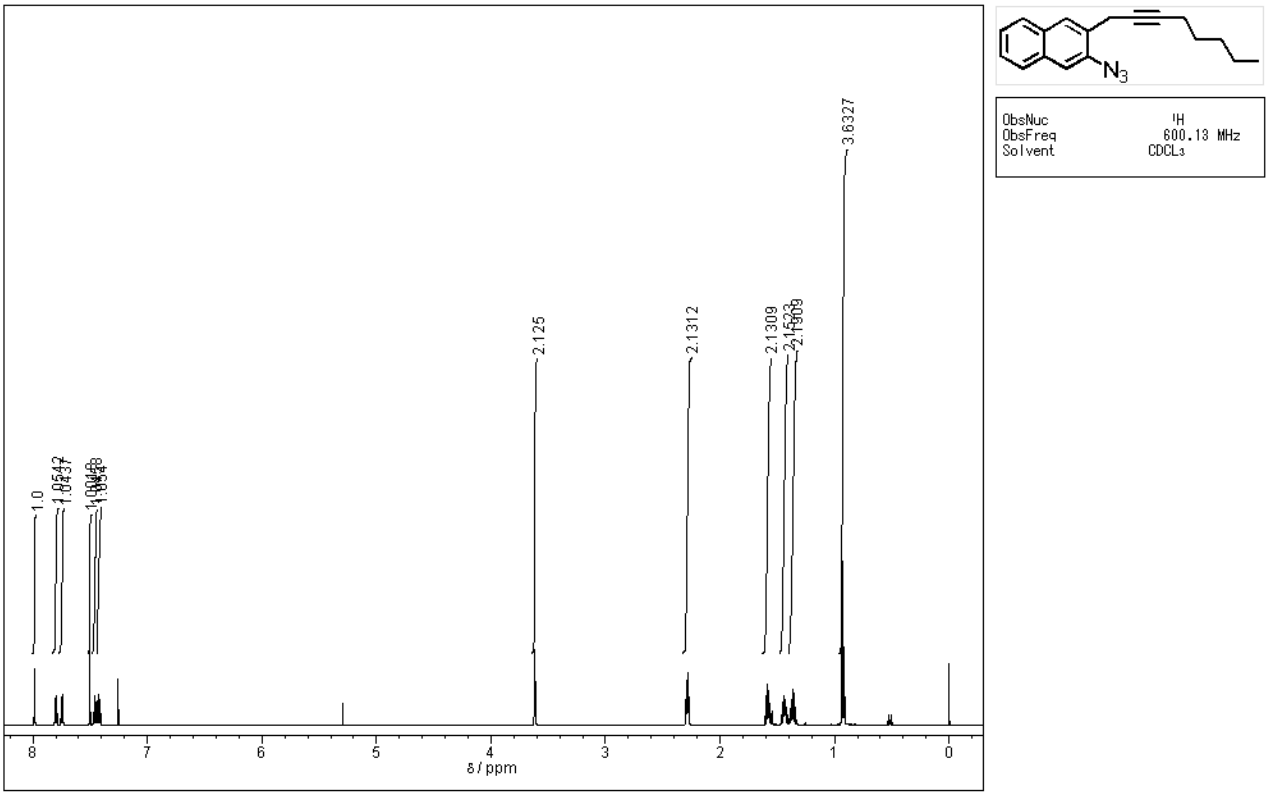
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	$CDCl_3$

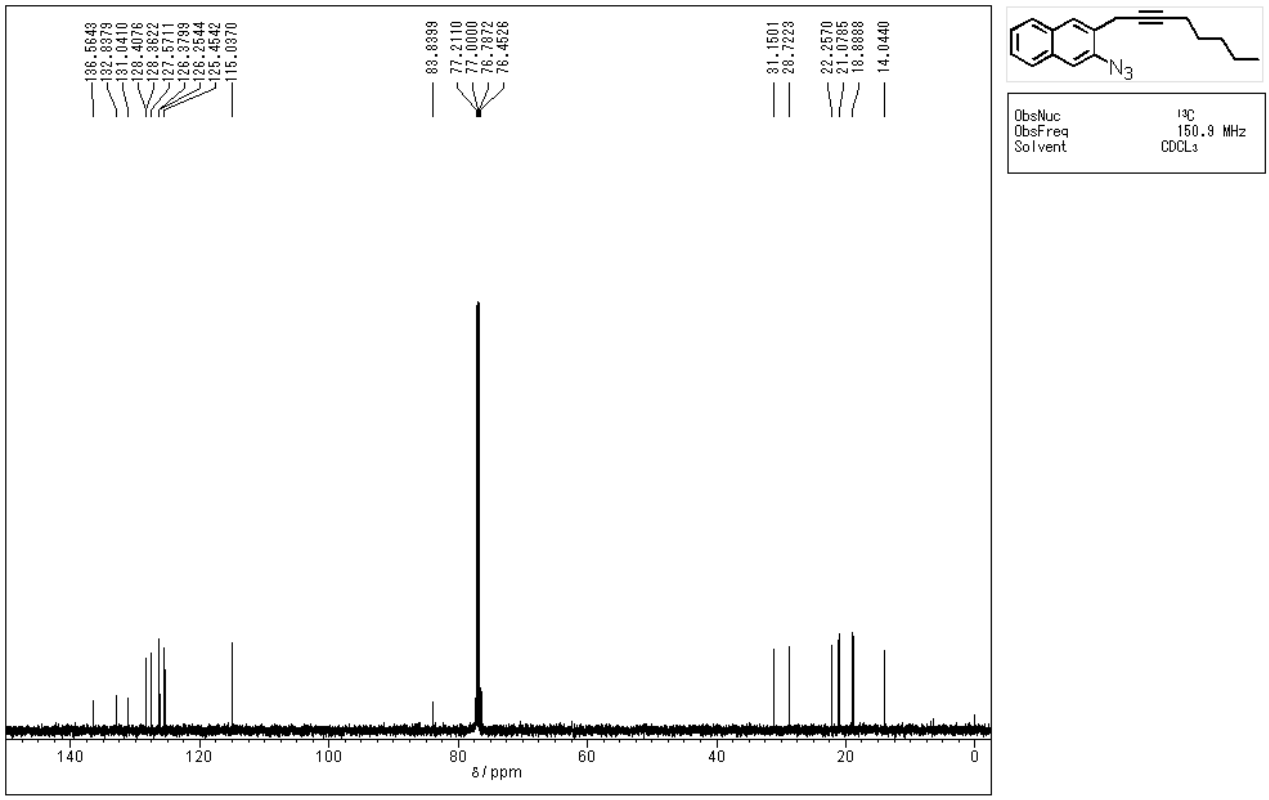




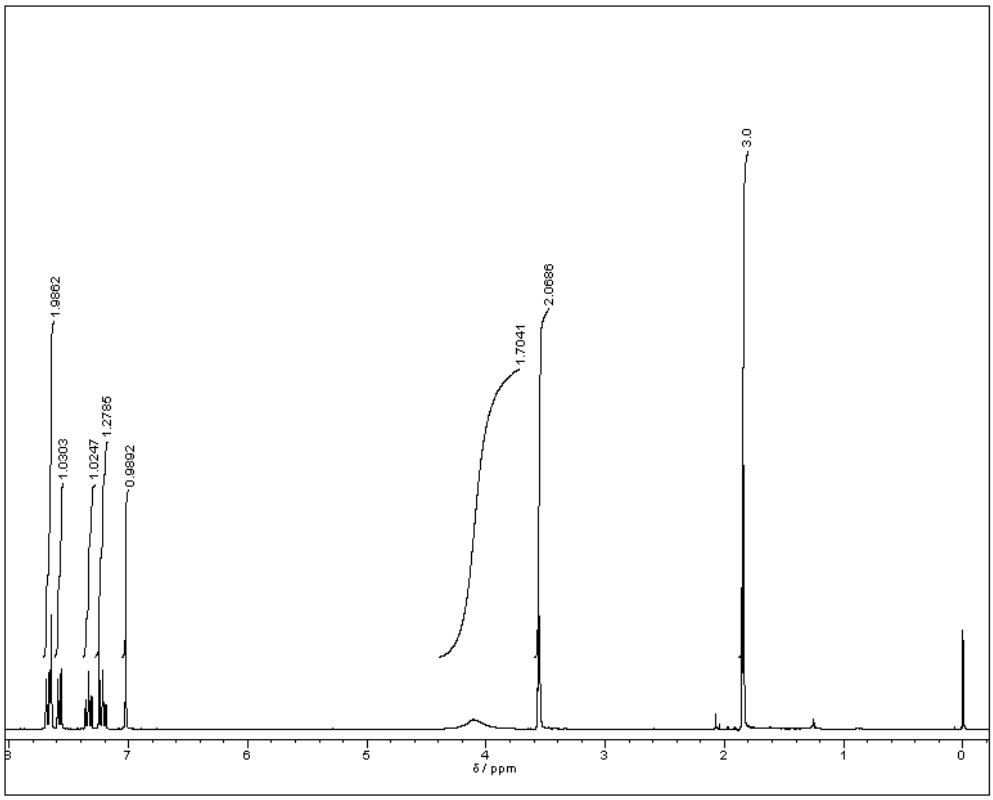
ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	$CDCl_3$

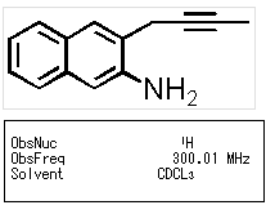
S5b


1.0
2.125
2.1312
2.1309
3.6327
8
7
6
5
4
3
2
1
0
δ / ppm
N3
ObsNuc 1H
ObsFreq 600.13 MHz
Solvent CDCL3

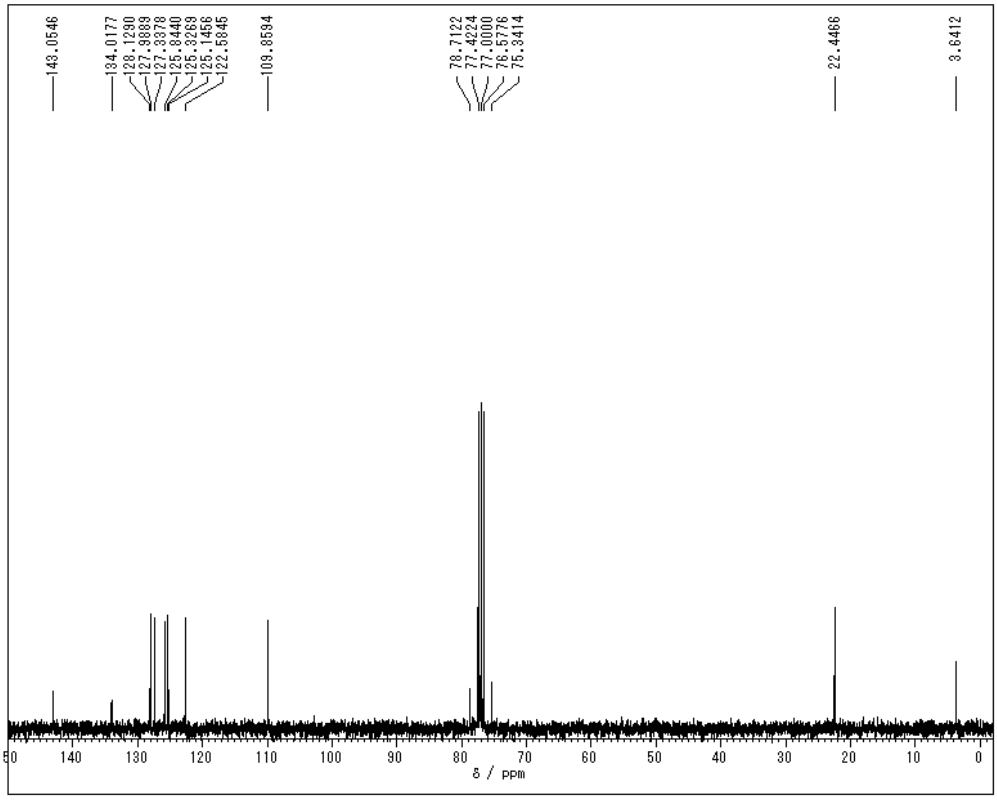

136.5643
132.8379
131.0410
128.4076
128.3622
127.5711
126.3789
126.2544
125.4542
115.0870
83.8389
77.2110
77.0000
76.7872
76.4526
31.1501
28.7223
22.2570
21.0785
18.8888
14.0440
140
120
100
80
60
40
20
0
δ / ppm
N3
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent CDCL3

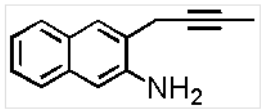
S6a





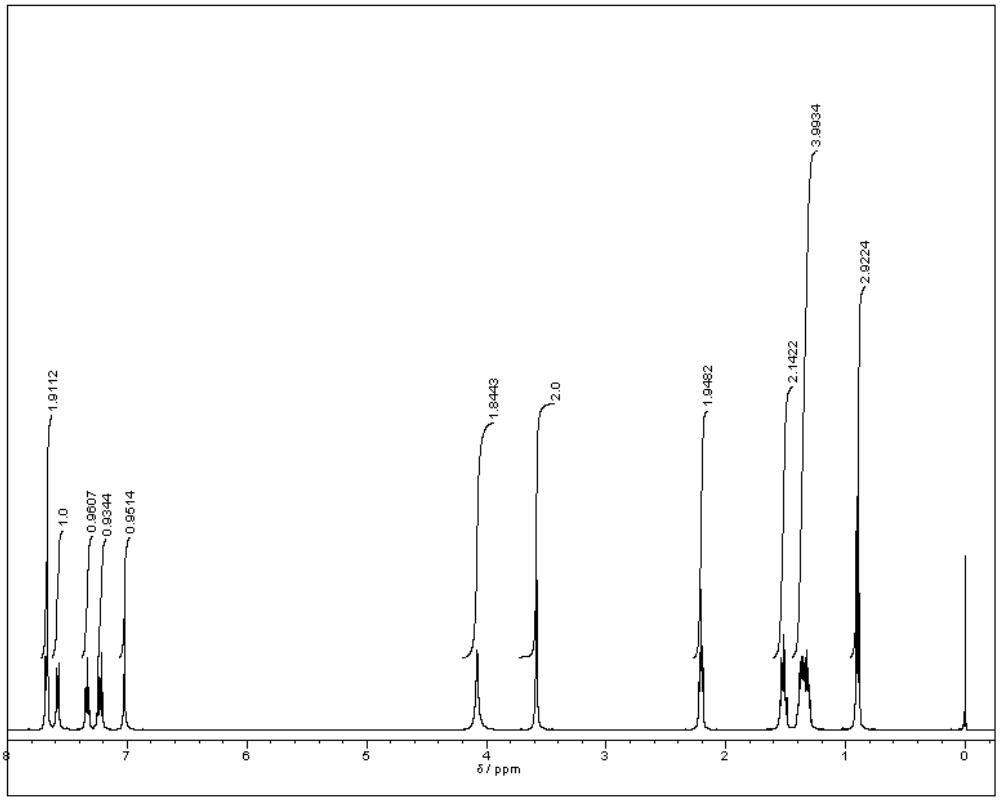
ObsNuc ¹H
ObsFreq 300.01 MHz
Solvent CDCL3

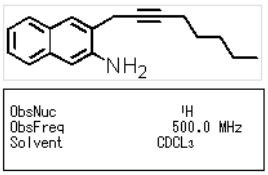




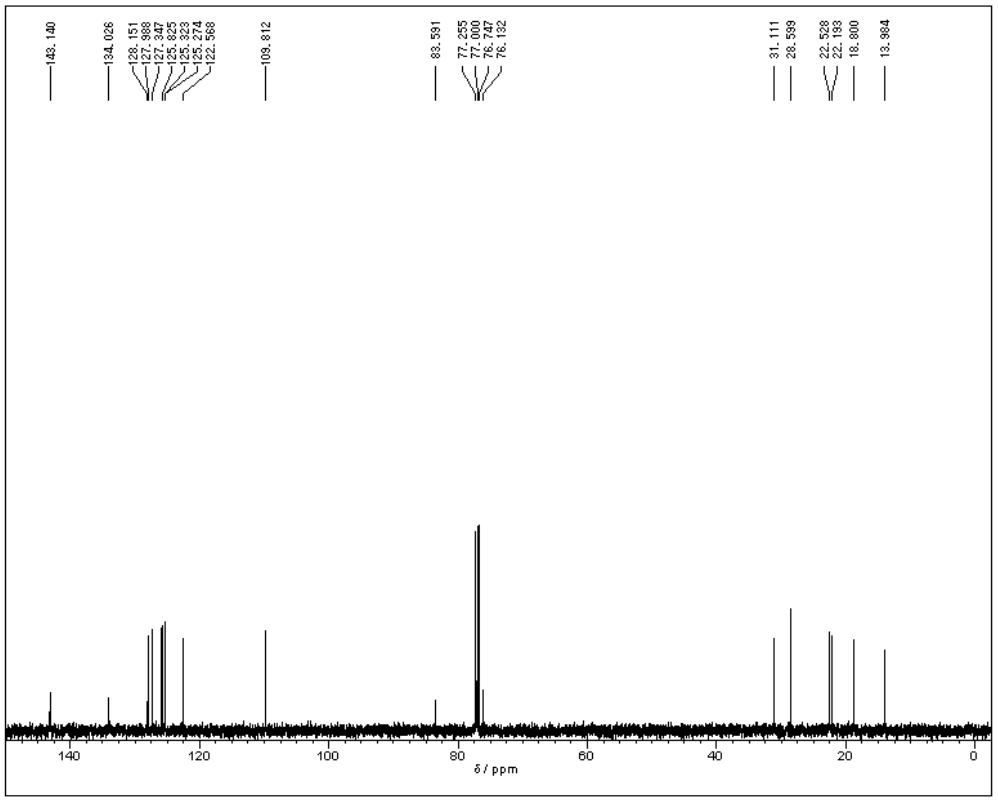
ObsNuc ¹³C
ObsFreq 75.45 MHz
Solvent CDCL3

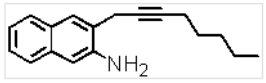
S6b





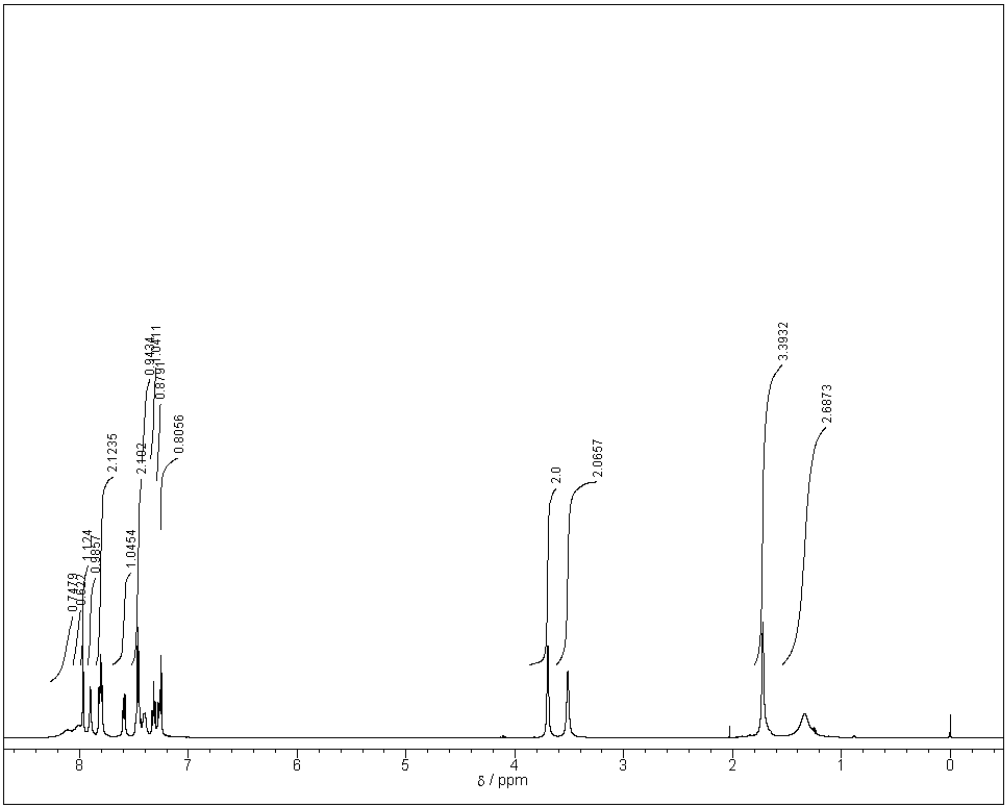
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent CDCL₃

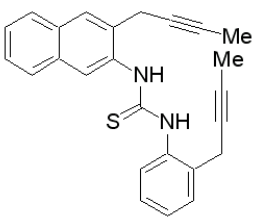




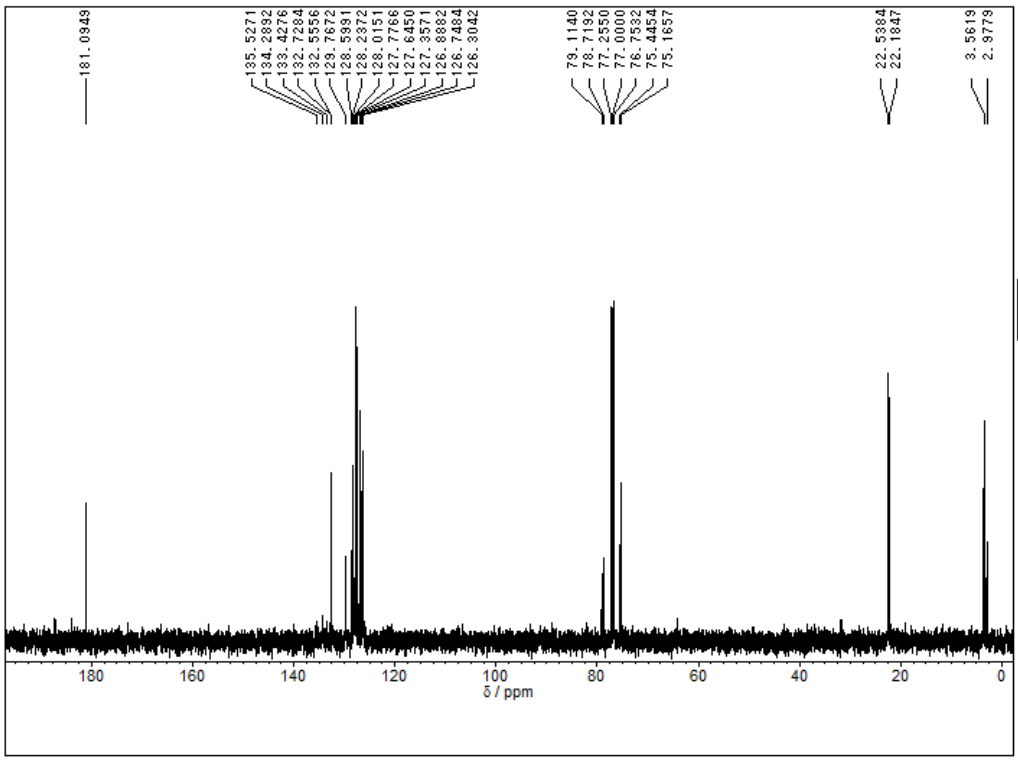
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent CDCL₃

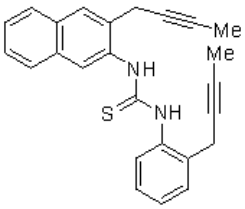
S7a





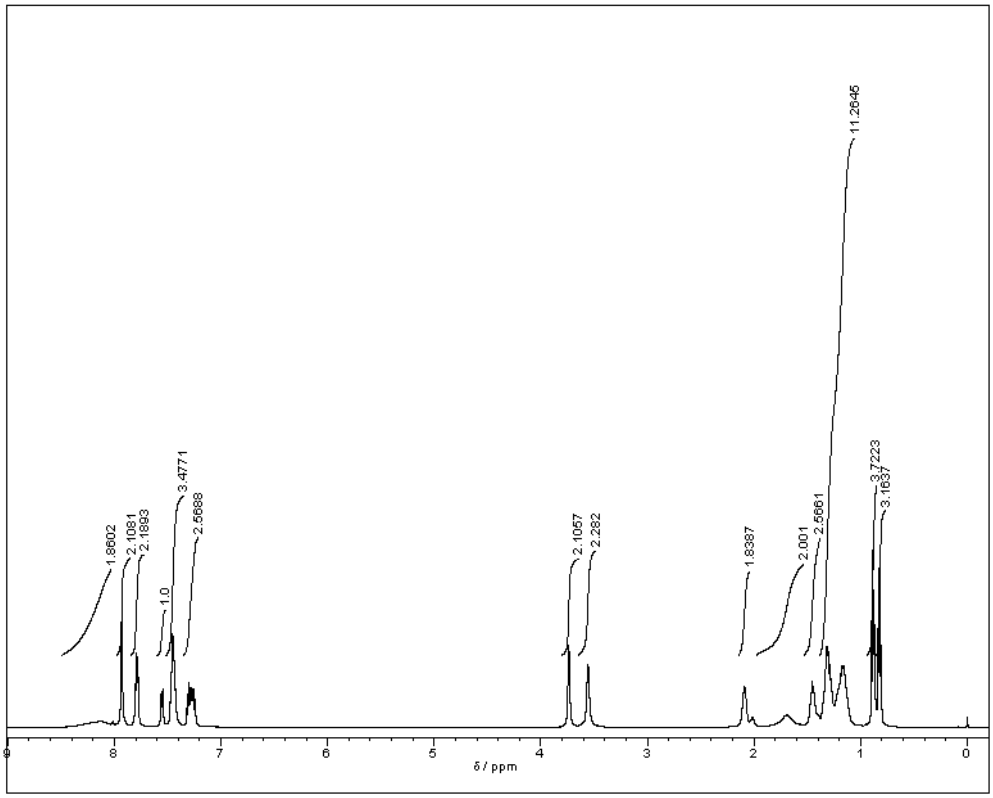
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

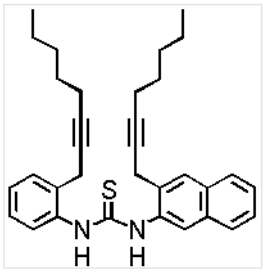




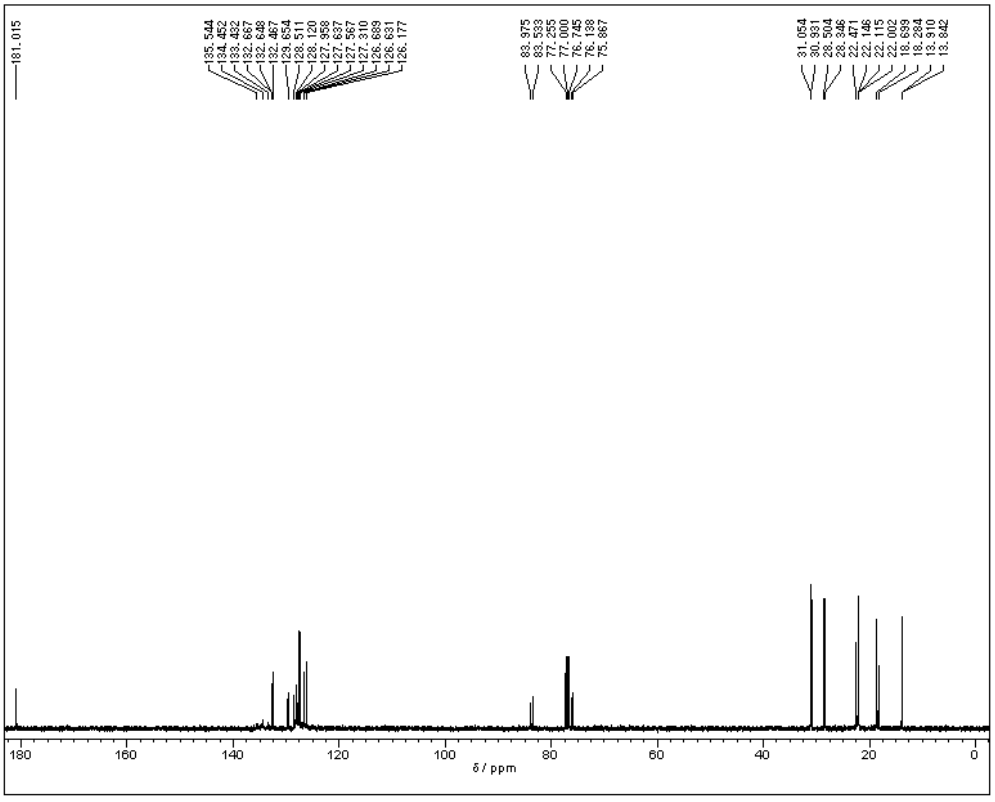
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

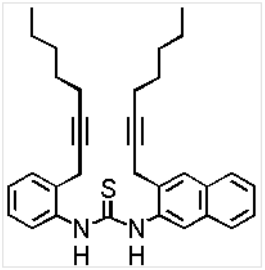
S7b





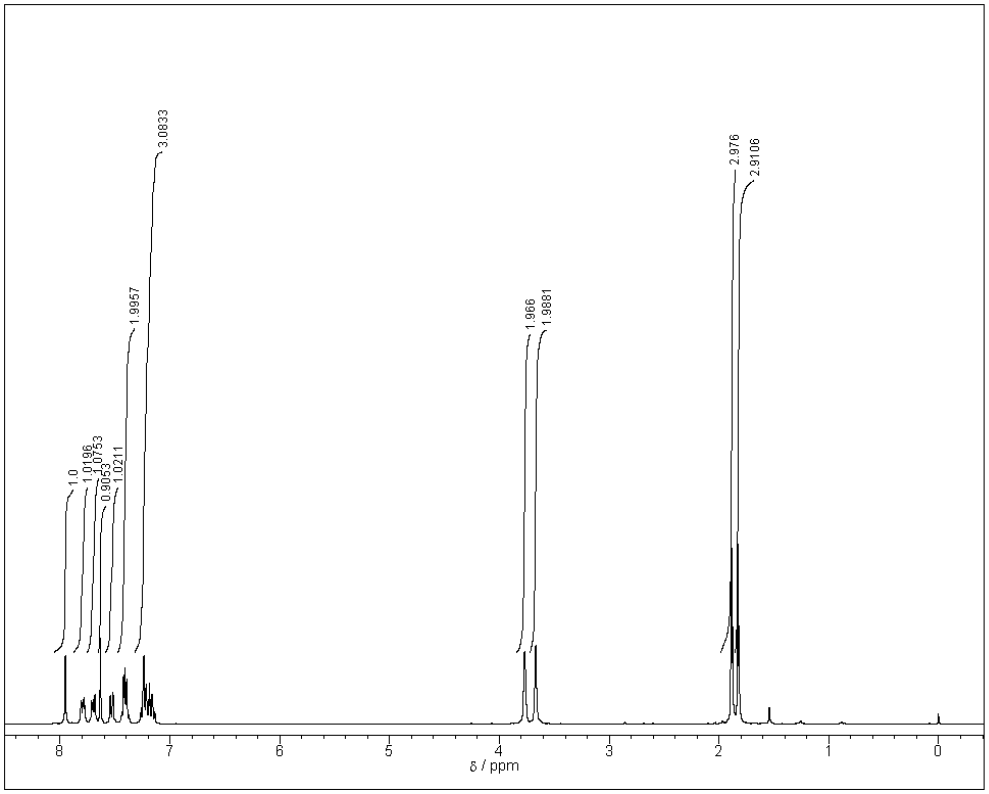
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

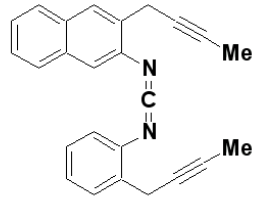




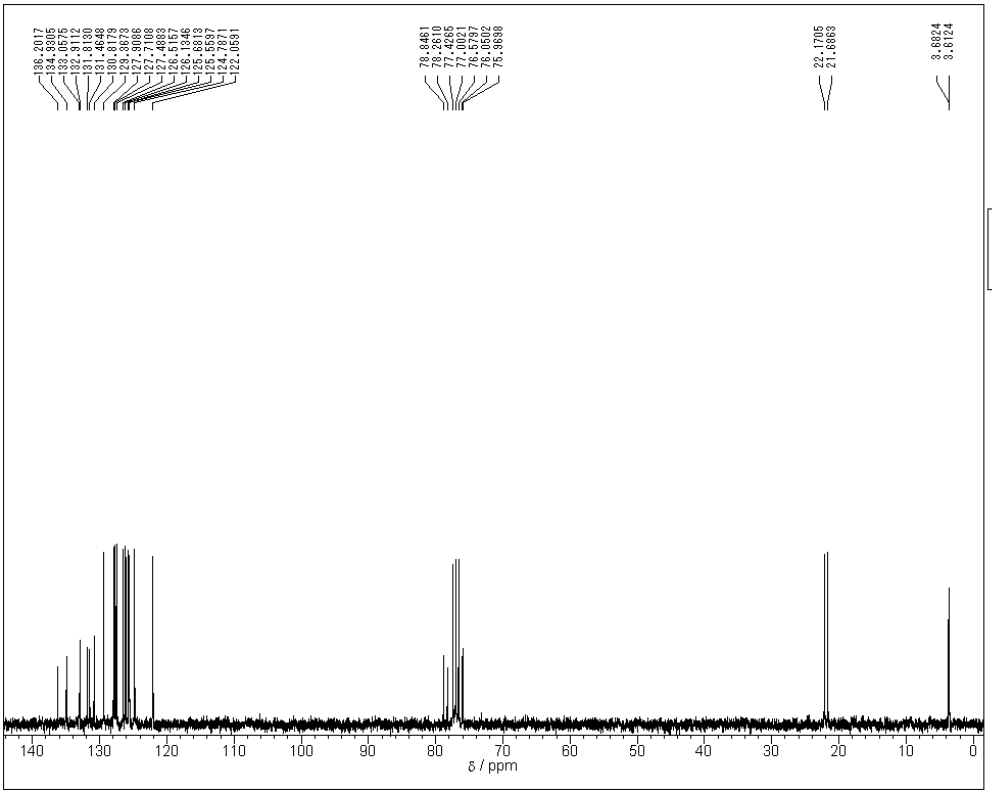
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

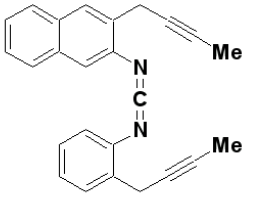
2a





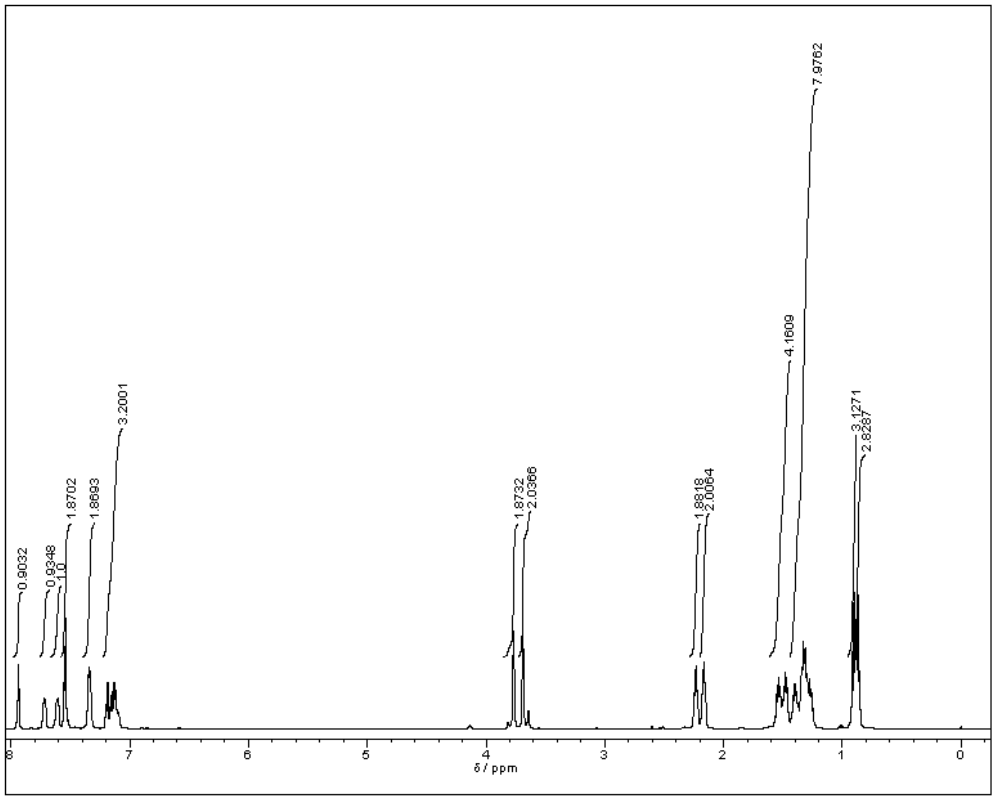
OBNUC	^{1}H
OBFRQ	300.4 MHz
SLVNT	CDCL$_3$

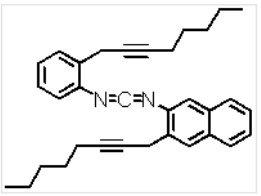




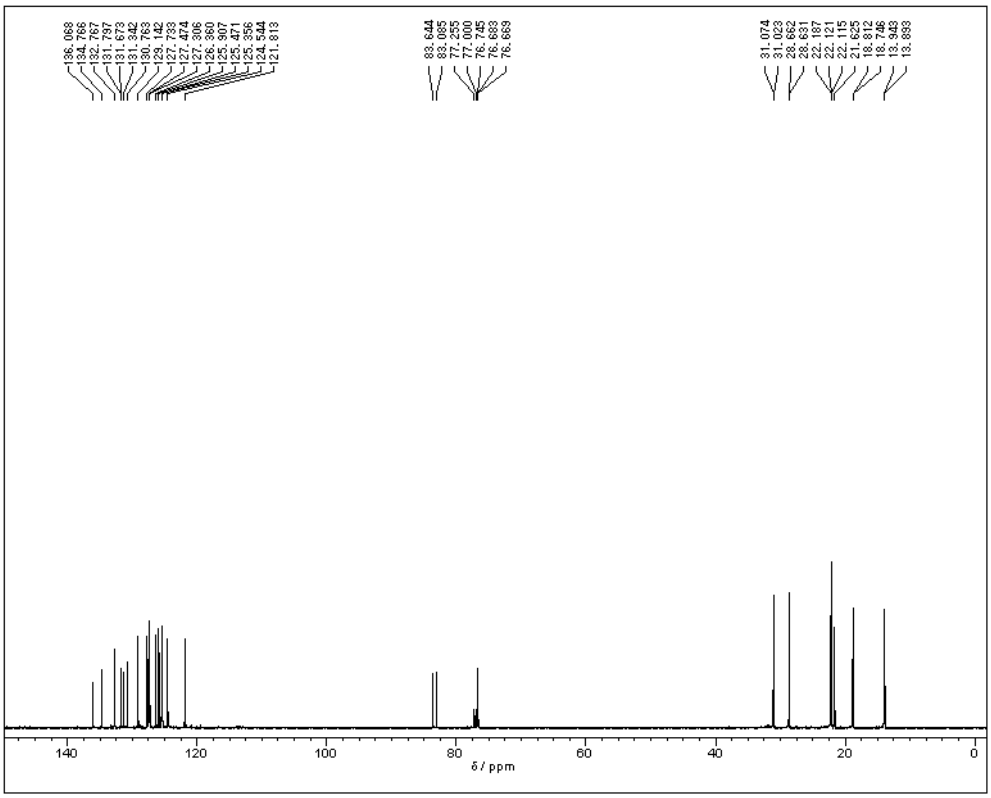
ObsNuc	^{13}C
ObsFreq	75.45 MHz
Solvent	CDCL$_3$

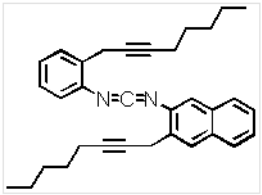
2b





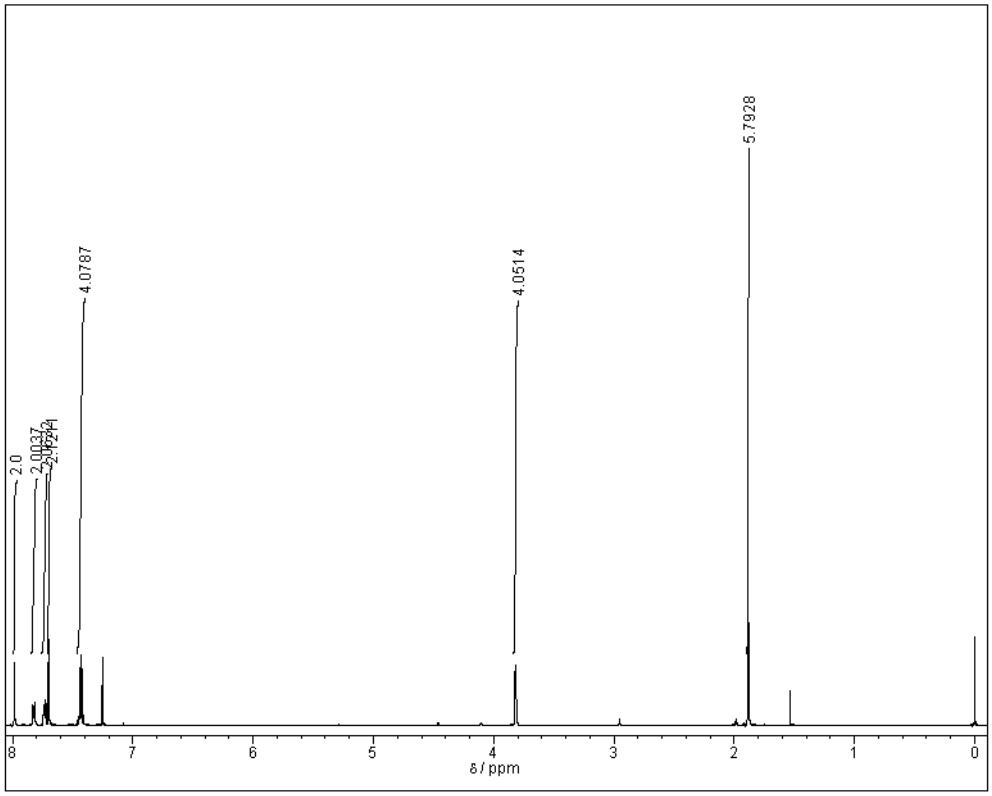
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

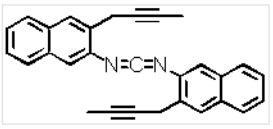




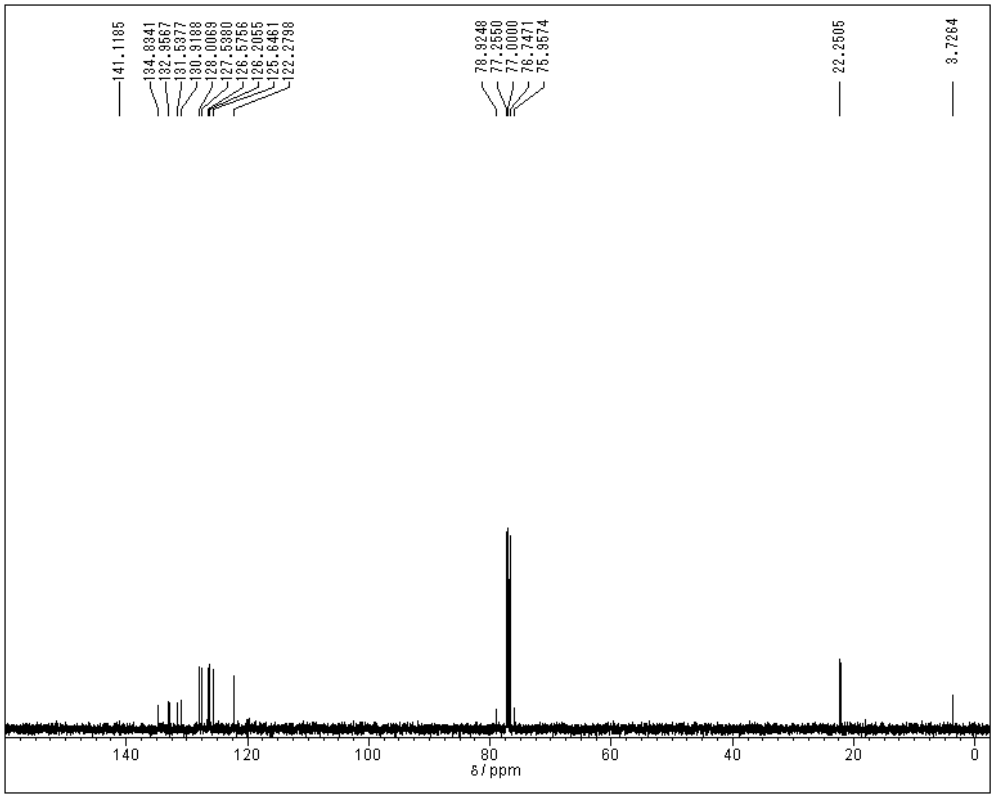
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

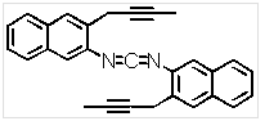
3a





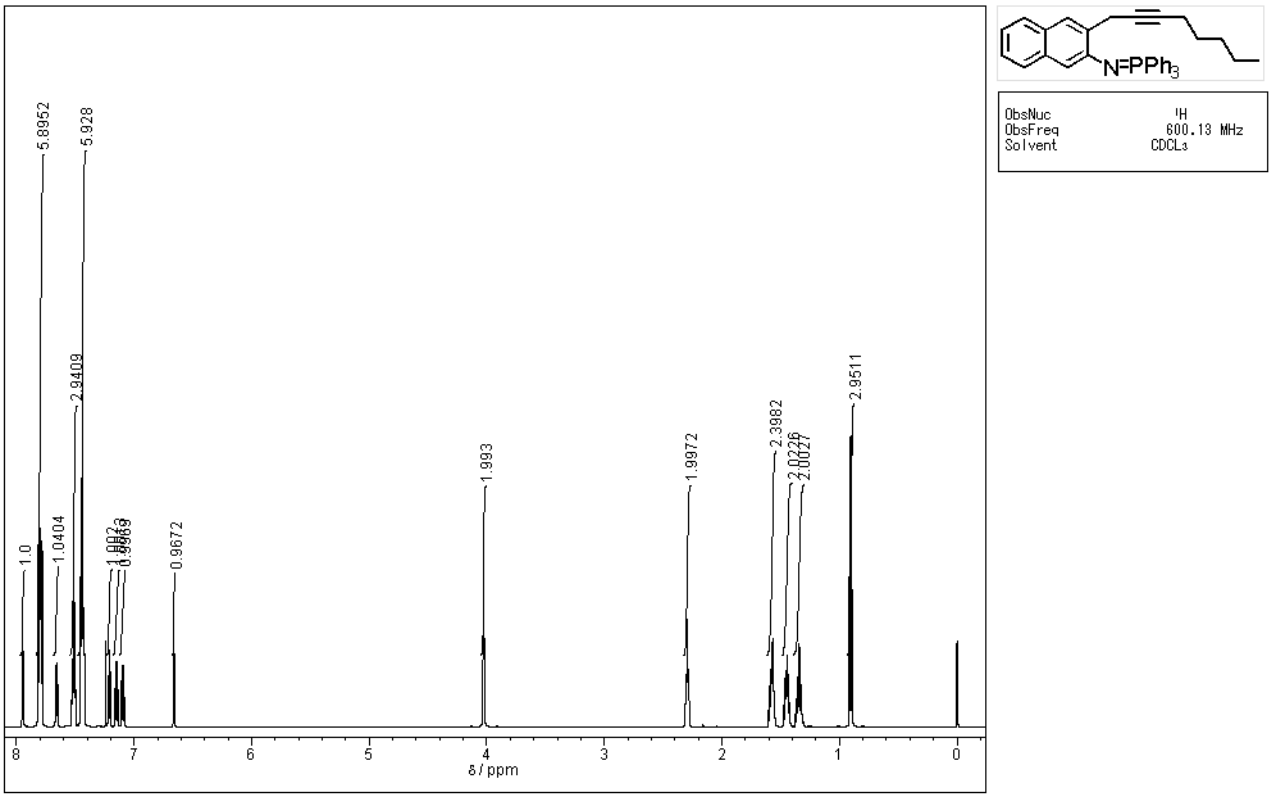
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

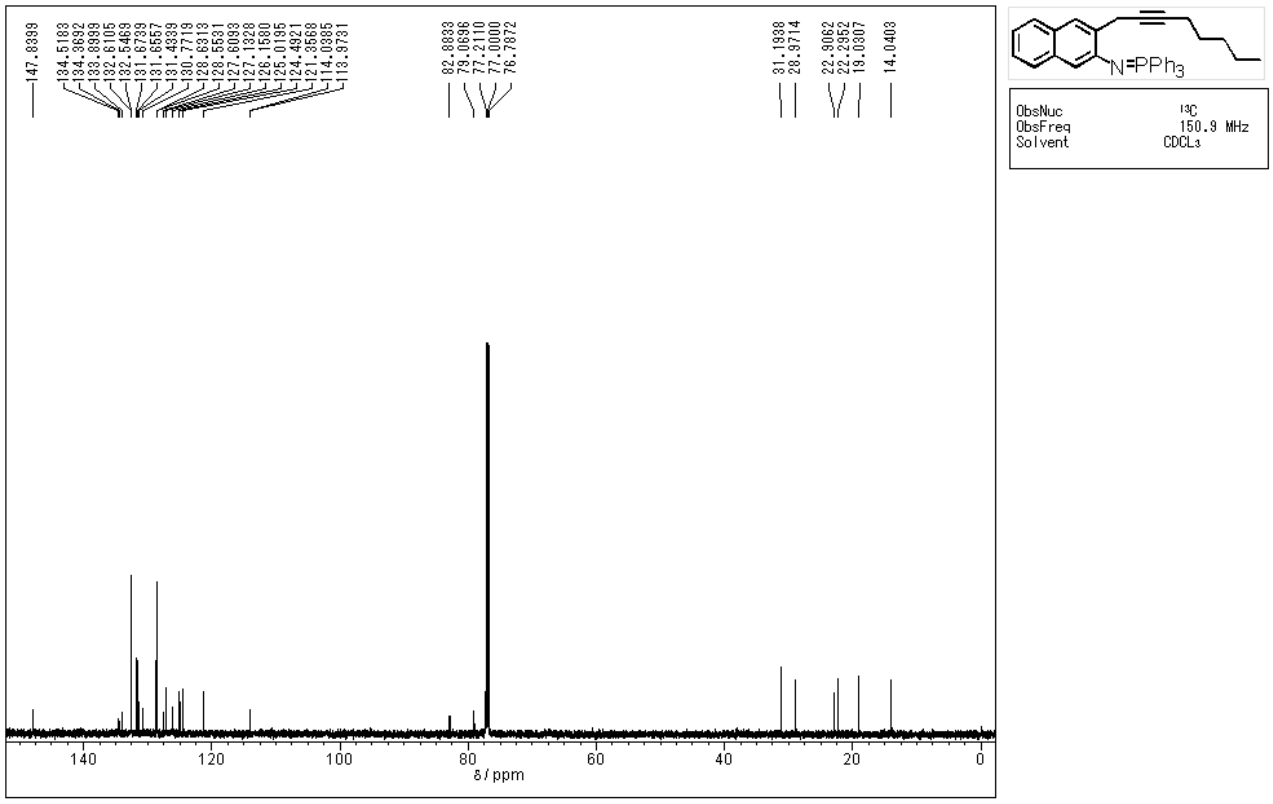




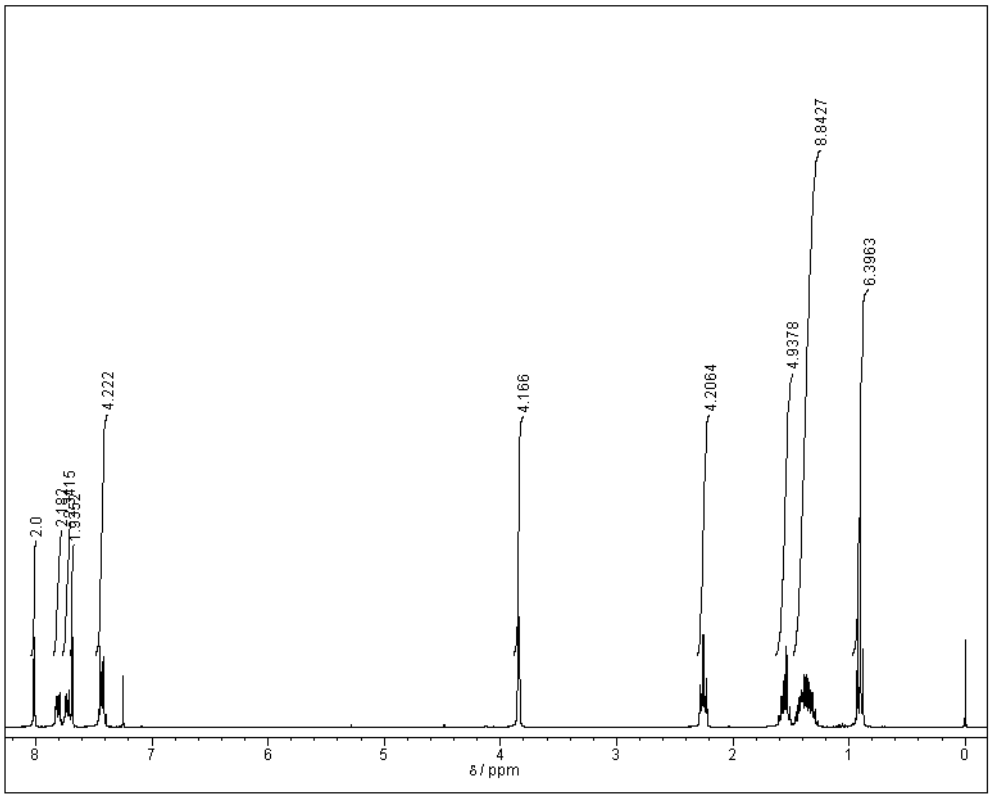
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

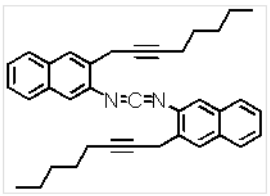
S8b


N=PPh3
ObsNuc 1H
ObsFreq 600.13 MHz
Solvent CDCL3
5.8952
5.928
2.9409
1.0404
1.0
0.9672
1.993
1.9972
2.3982
2.0026
2.0027
2.9511
δ / ppm

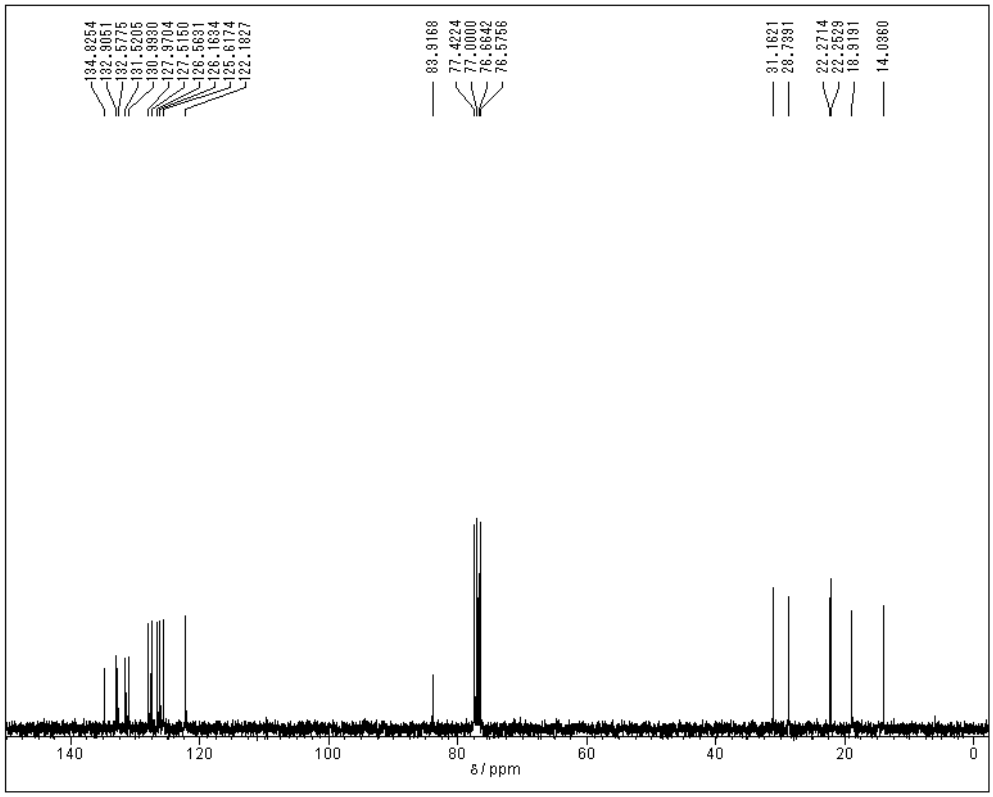

N=PPh3
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent CDCL3
147.8389
134.5183
134.3692
133.8989
132.6105
132.5469
131.6739
131.6557
131.4339
130.7719
128.6313
128.5531
127.6093
127.1328
126.1580
125.0195
124.4921
121.3568
114.0385
113.9731
82.8833
79.0896
77.2110
77.0000
76.7872
31.1838
28.9714
22.9062
22.2852
19.0307
14.0403
δ / ppm

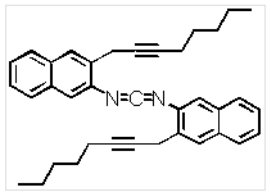
3b





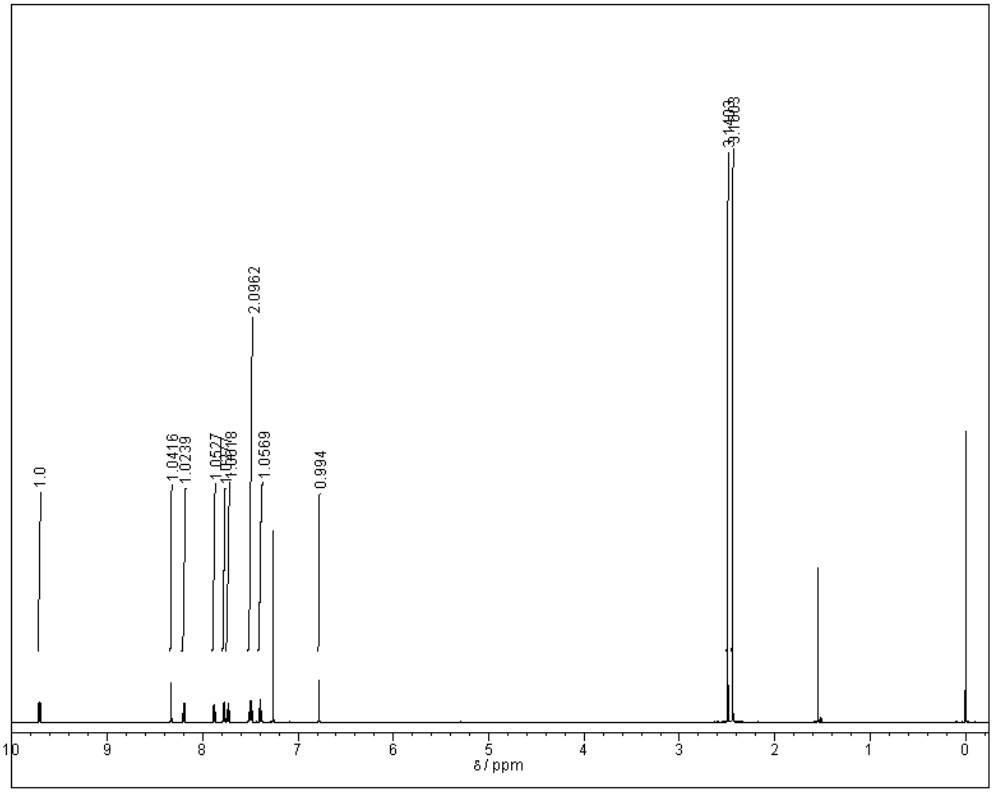
ObsNuc	^{1}H
ObsFreq	300.4 MHz
Solvent	$CDCl_3$

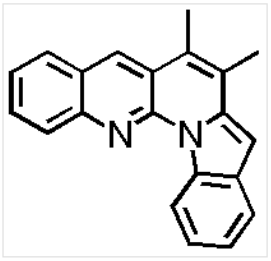




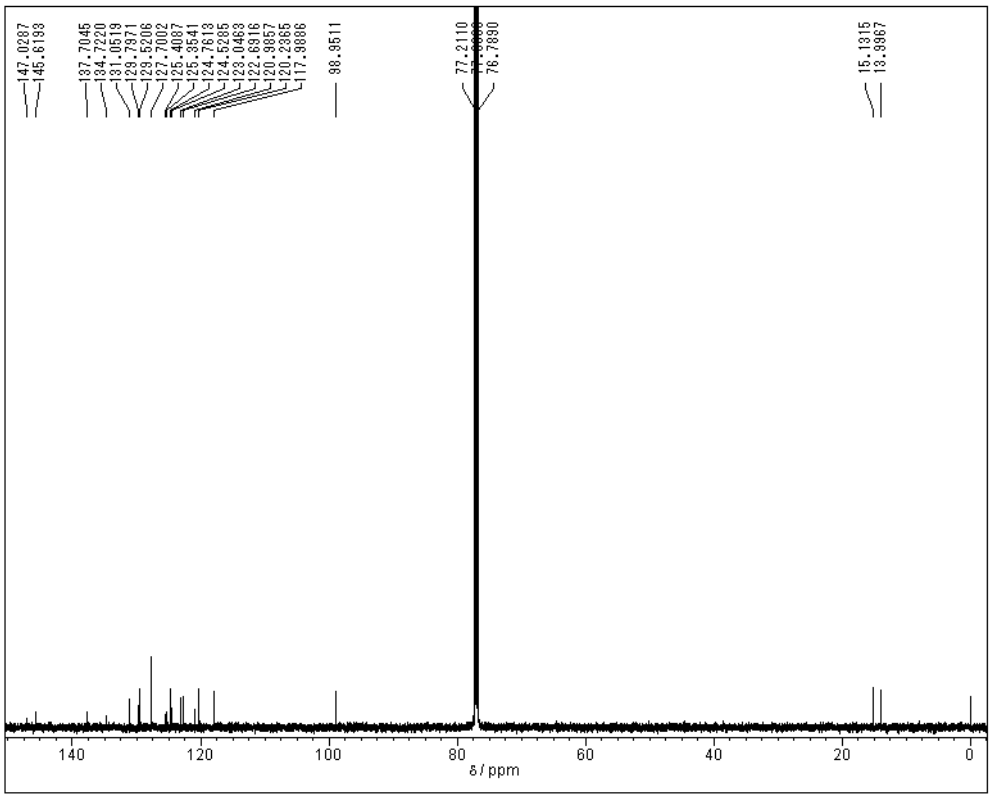
ObsNuc	^{13}C
ObsFreq	75.45 MHz
Solvent	$CDCl_3$

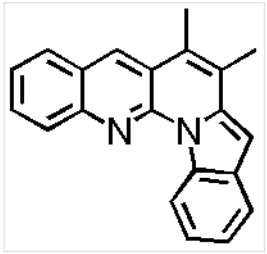
4a





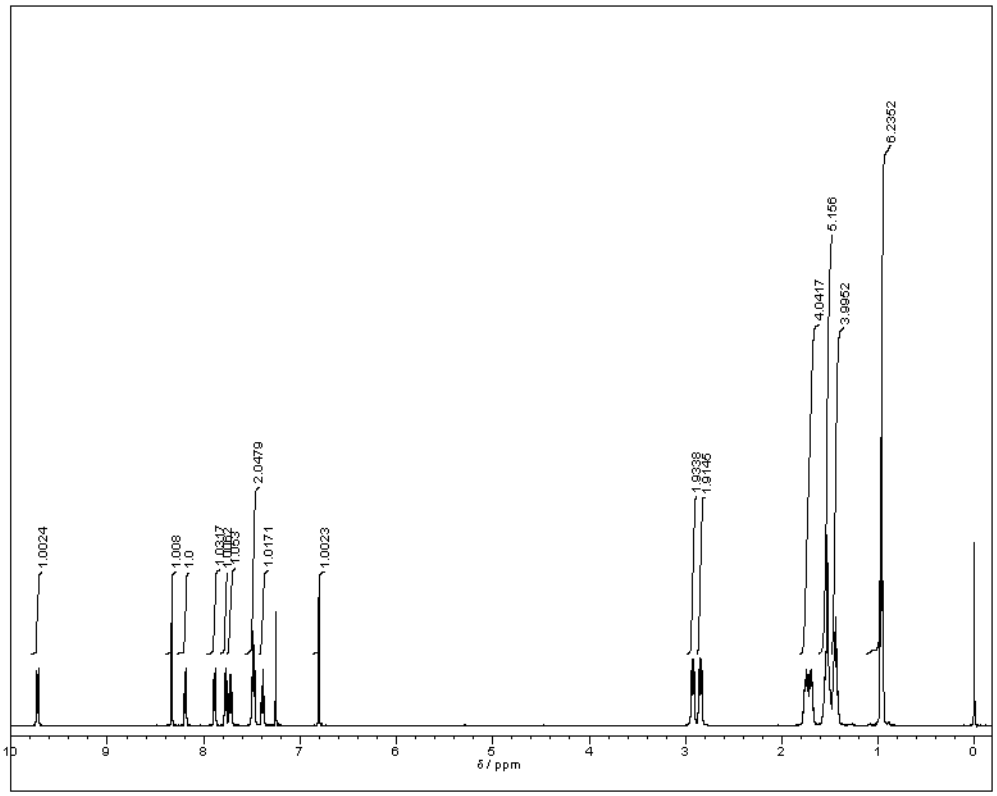
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	$CDCL_3$

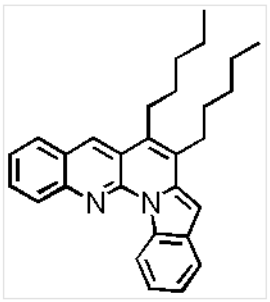




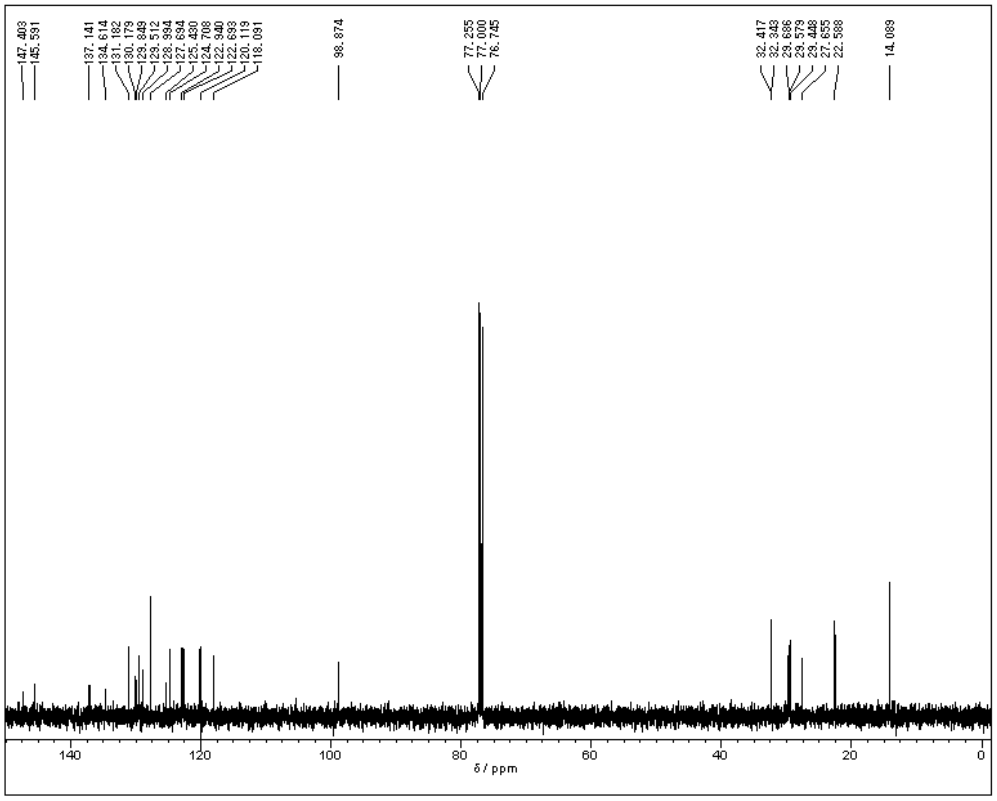
ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	$CDCL_3$

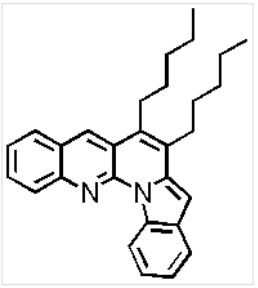
4b





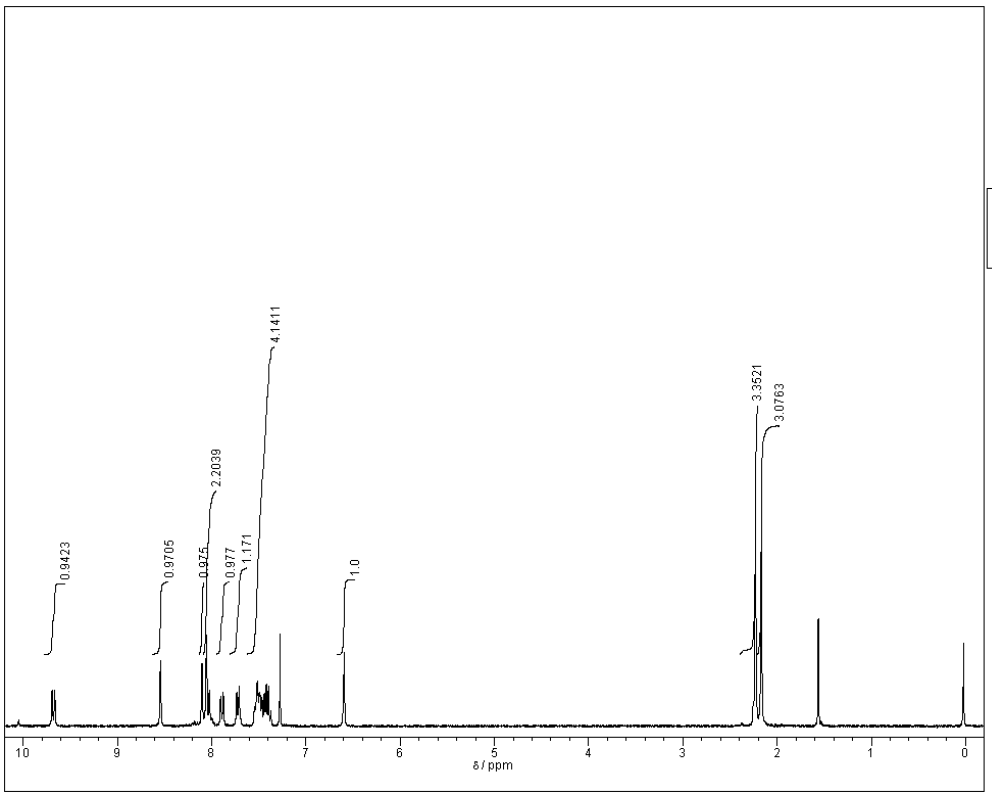
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

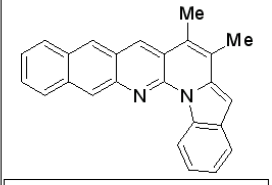




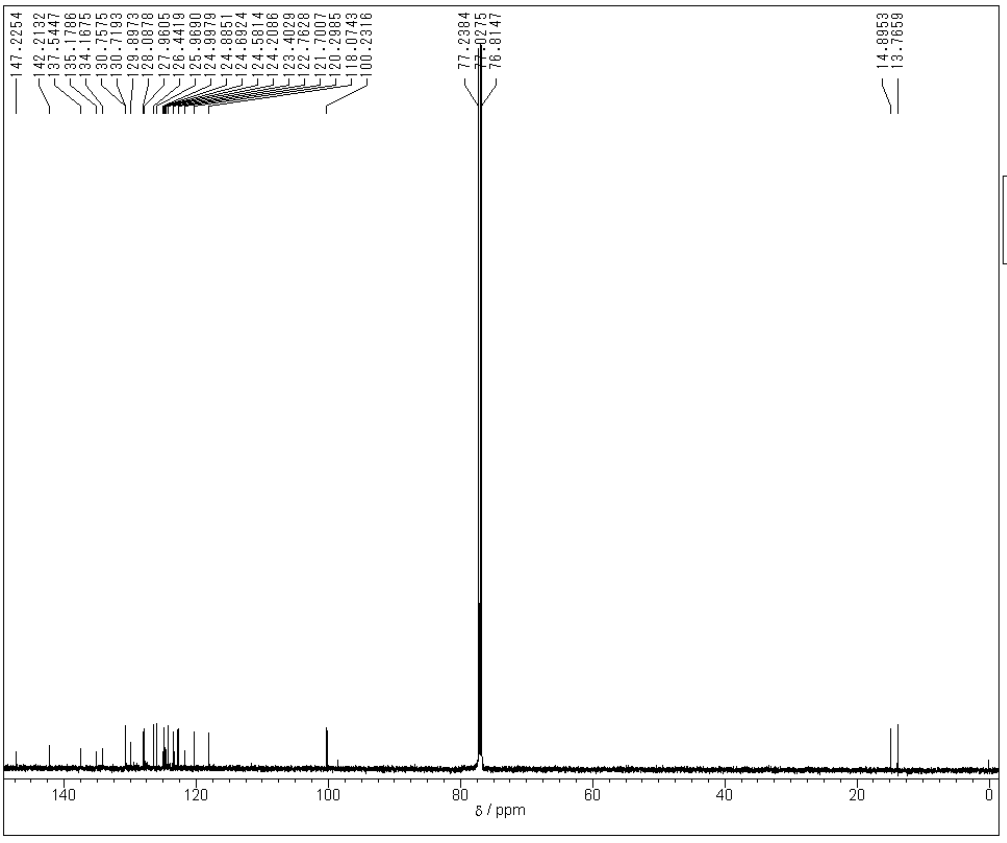
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

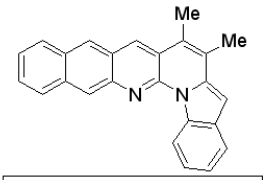
5a





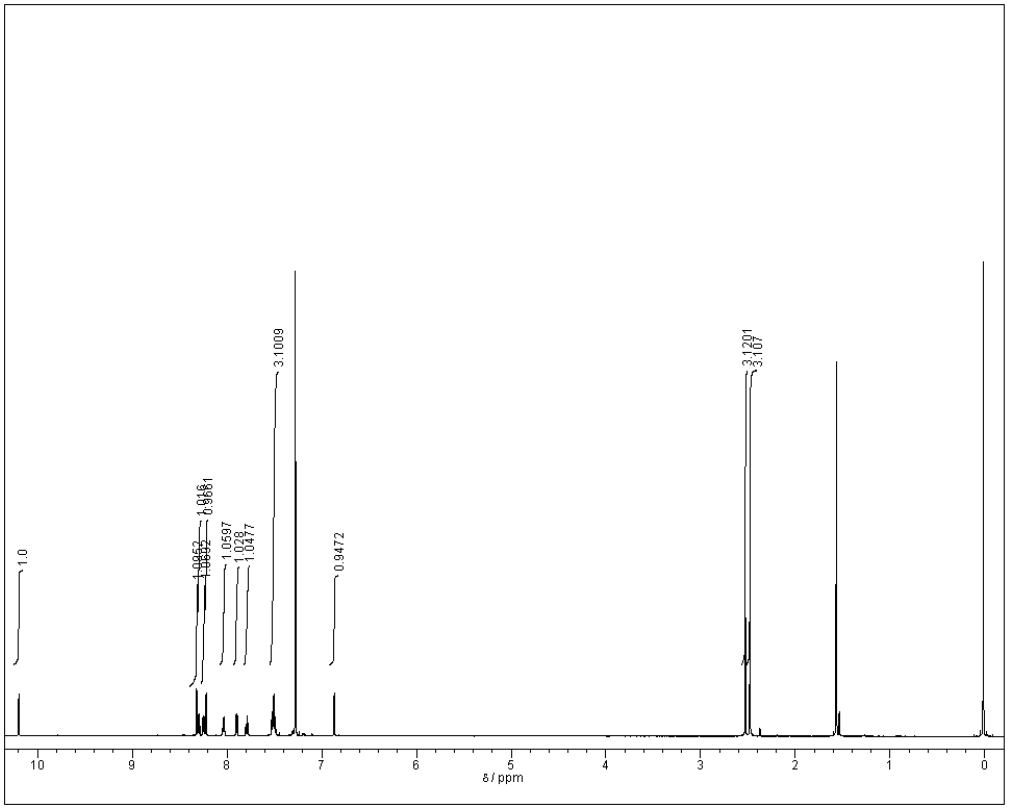
ObsNuc	^{1}H
ObsFreq	300.01 MHz
Solvent	CDCL3

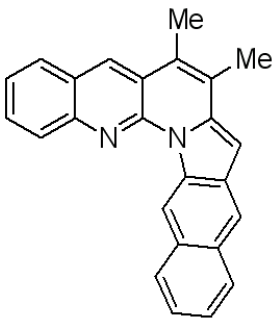




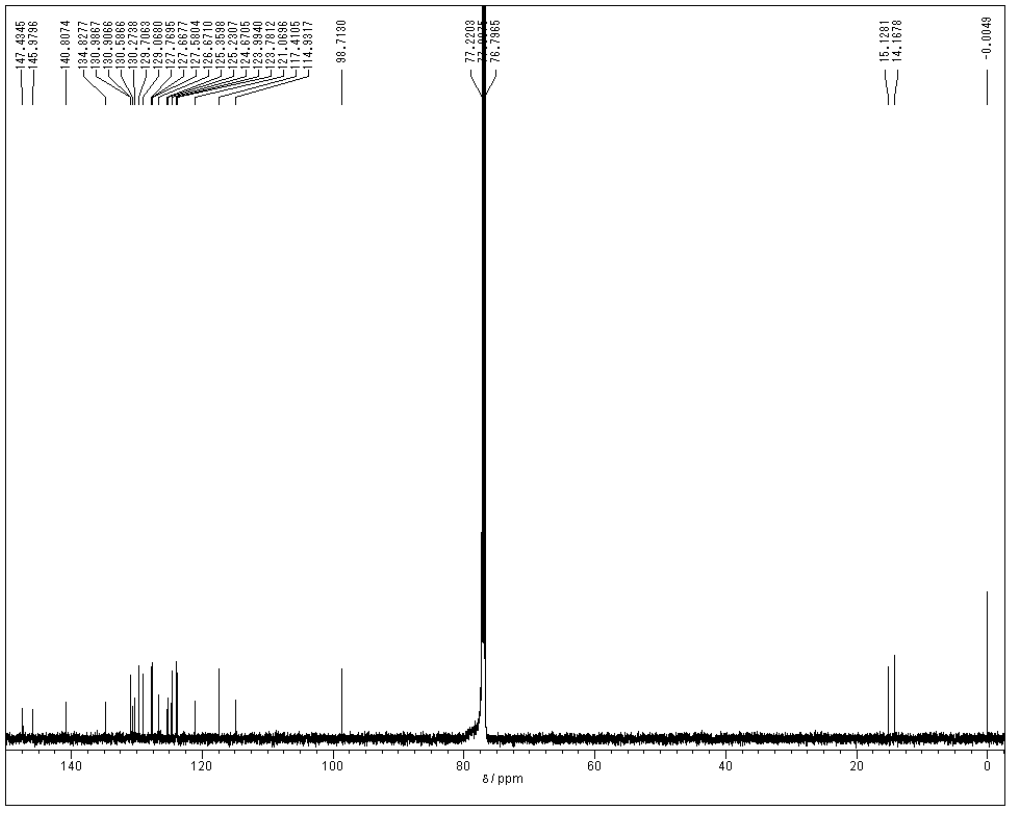
ObsFreq	150.9 MHz
ObsNuo	^{13}C
Solvent	CDCL3

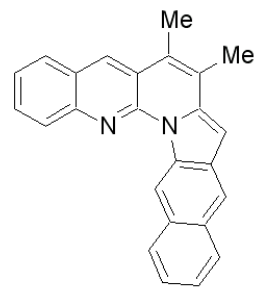
6a





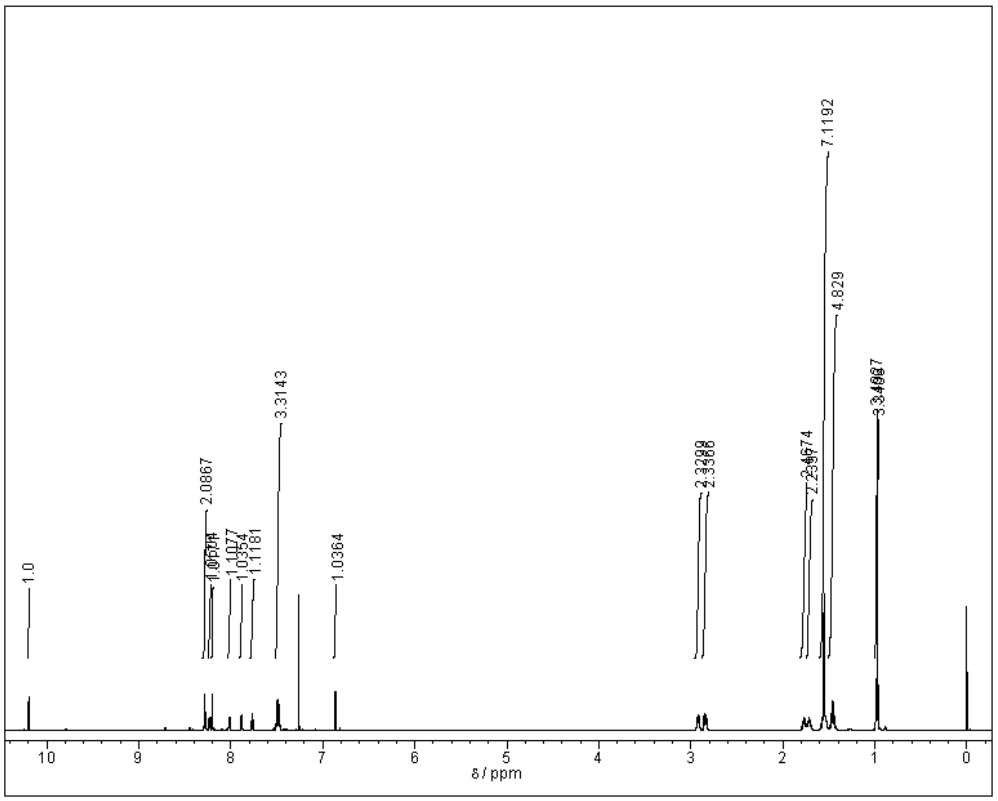
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	CDCL3

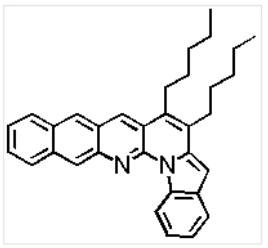




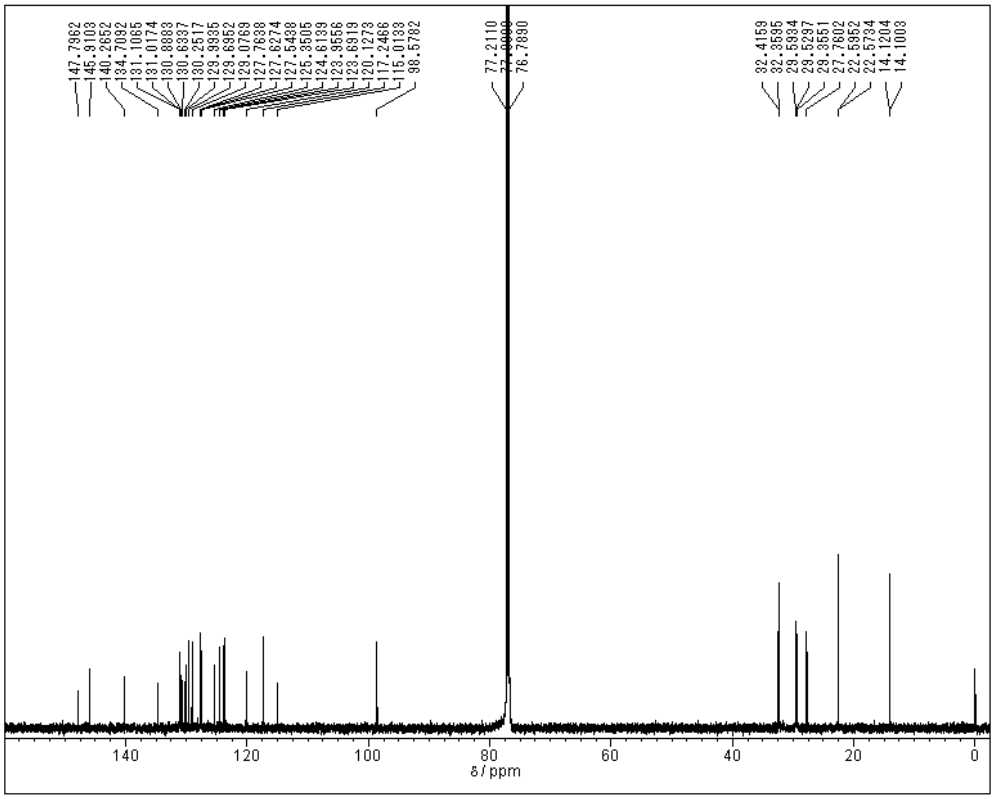
ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	CDCL3

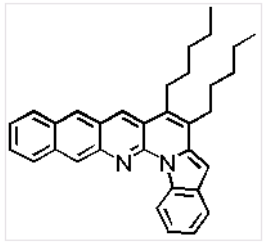
5b





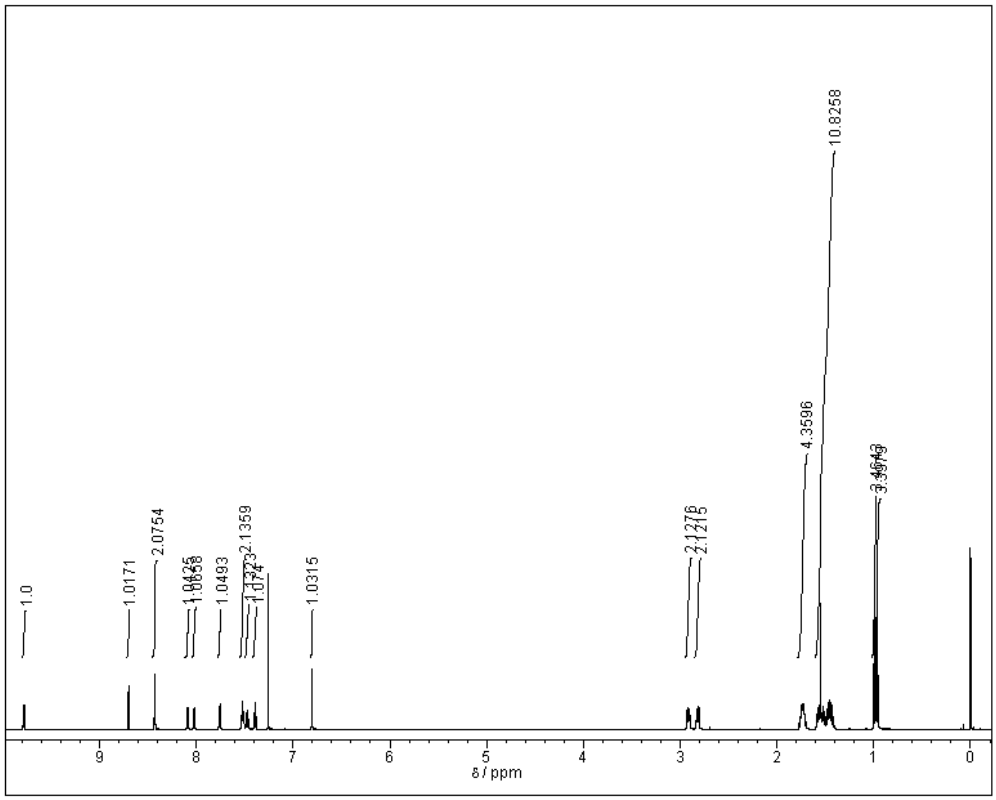
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

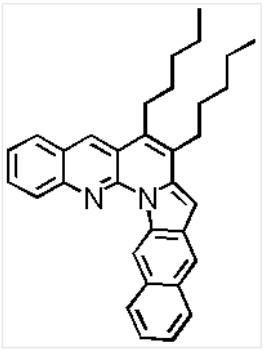




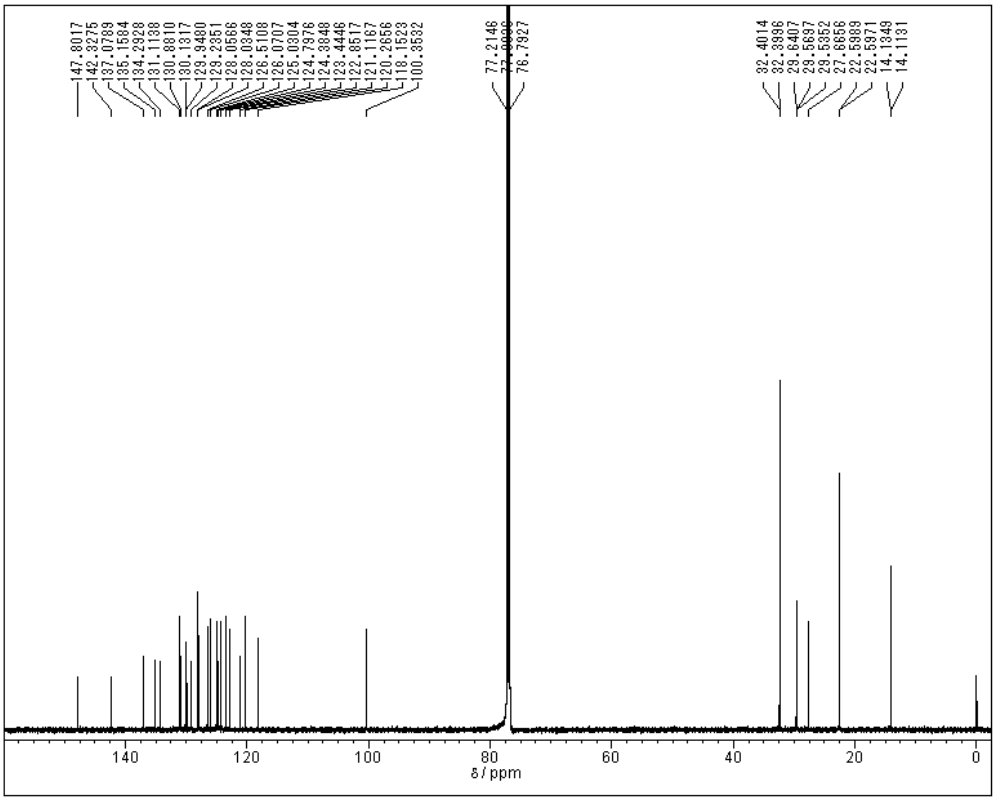
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

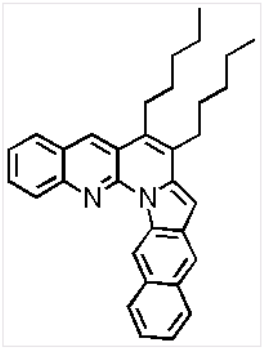
6b





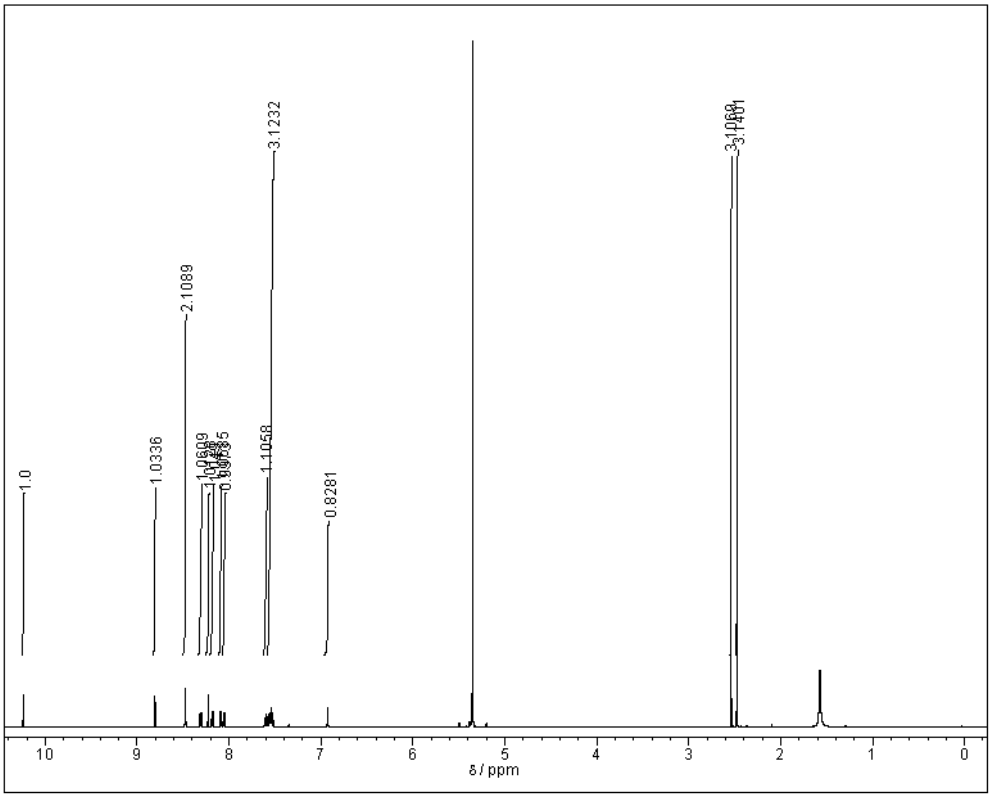
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent CDCL₃

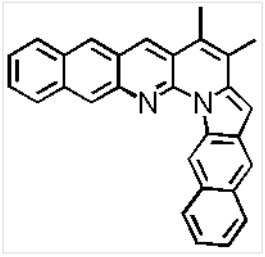




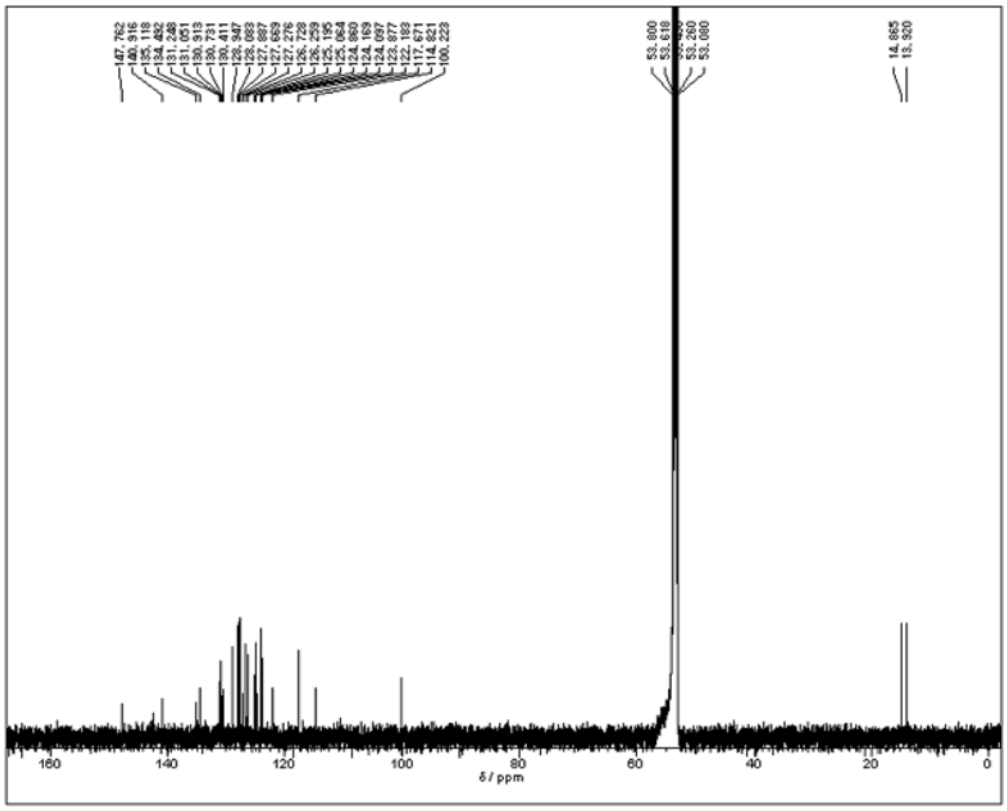
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent CDCL₃

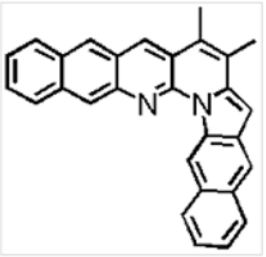
7a





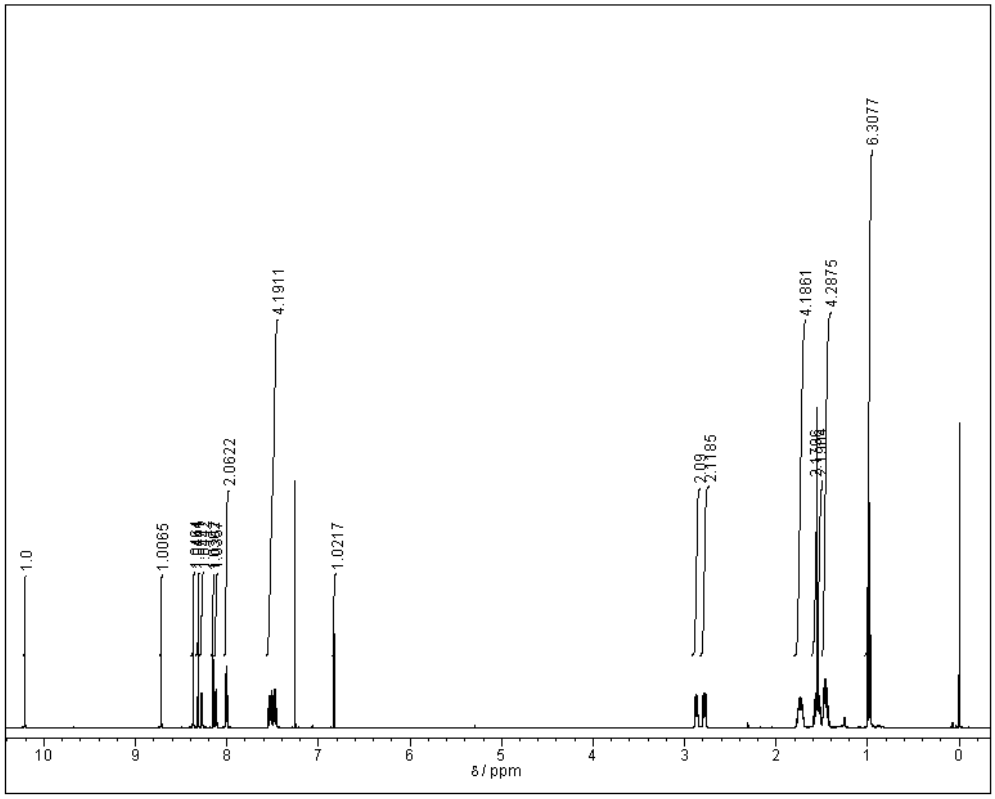
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	CD_2CL_2

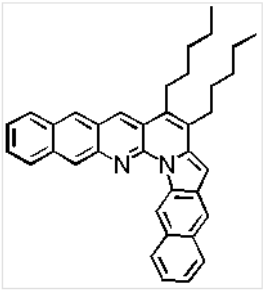




ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	CD_2Cl_2

7b





ObsNuc ¹H
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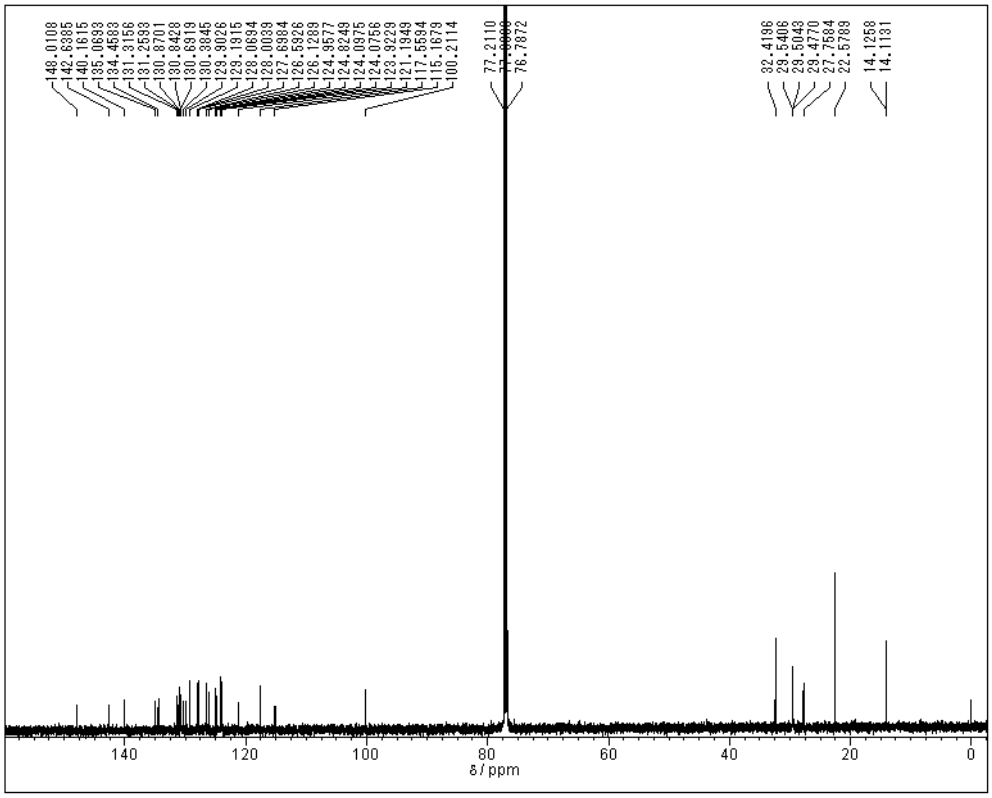
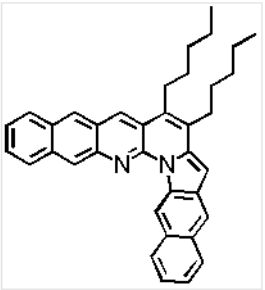
Solvent CDCL₃





ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent CDCL₃

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 MicroMount™ (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 Mo*K*α radiation (λ = 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.

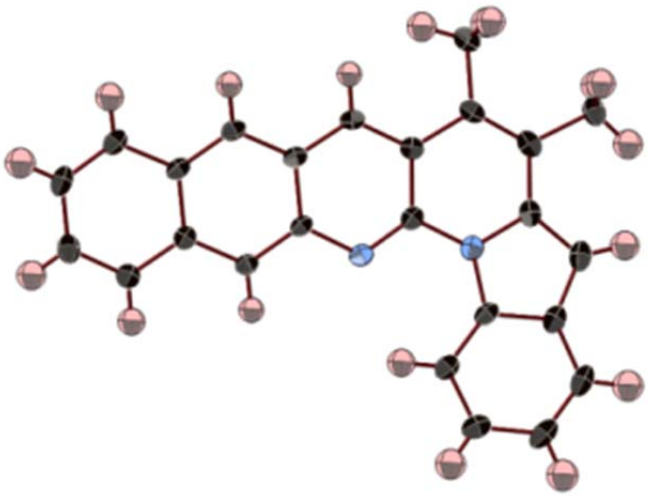


Figure S1. Molecular structure of **5a**. One of the two crystallographically independent molecules is shown.

[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.

Table S1. Crystallographic Data for **5a**.

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	$P\bar{1}$ (#2)
a / Å	8.4955(15)
b / Å	11.1198(19)
c / 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)
Z	4
D_x / g cm^{-3}	1.310
reflections collected	21415
unique reflections	7983
refined parameters	488
GOF on F^2	1.093
$R1$ [$I > 2\sigma(I)$][a]	0.0699
w$R2$ (all data)[b]	0.1899
$\Delta\rho_{min,\ max}$ / e Å^{-3}	− 0.56, 0.57

[a] $R1 = \Sigma\ ||Fo| - |Fc|| / \Sigma\ |Fo|$, [b] $wR2 = [\Sigma\ \{w(Fo^2 - Fc^2)^2 / \Sigma\ w(Fo^2)^2\}]^{1/2}$

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

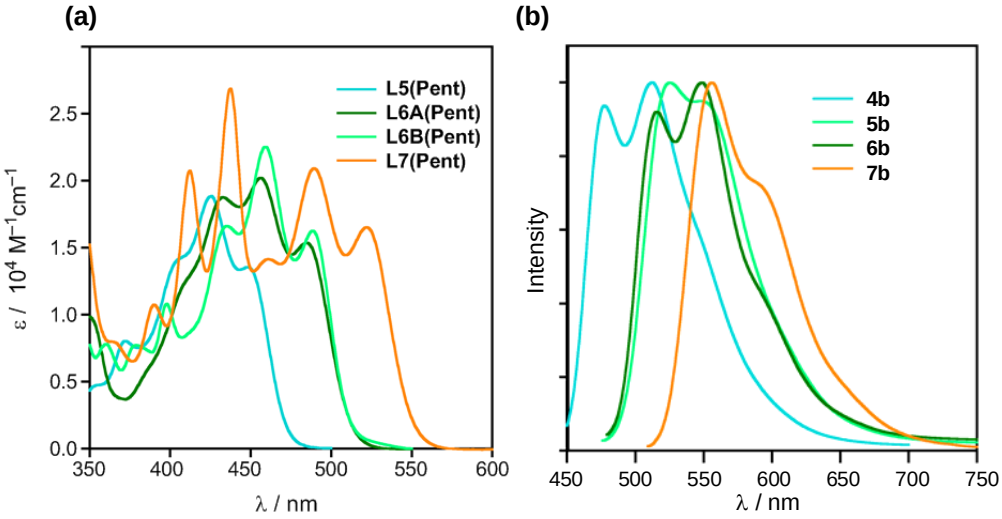


Figure S2. (a) UV–vis spectra of **4b–7b** in CH_2Cl_2. (b) Fluorescence spectra (excited at λ_{max} (abs)) of **4b–7b** in CH_2Cl_2.

Table S2. Photophysical Properties of 4b–7b [a]

Compound	λ_{max} (abs) [nm] (ε [10^4 cm^{-1} M^{-1}])	λ_{max} (em) [nm] [b]	Φ_F [b]	τ_s [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

[a] In CH_2Cl_2. [b] Excitation at λ_{max}(abs).

4.3 Absorption and Emission Spectra of 4–7

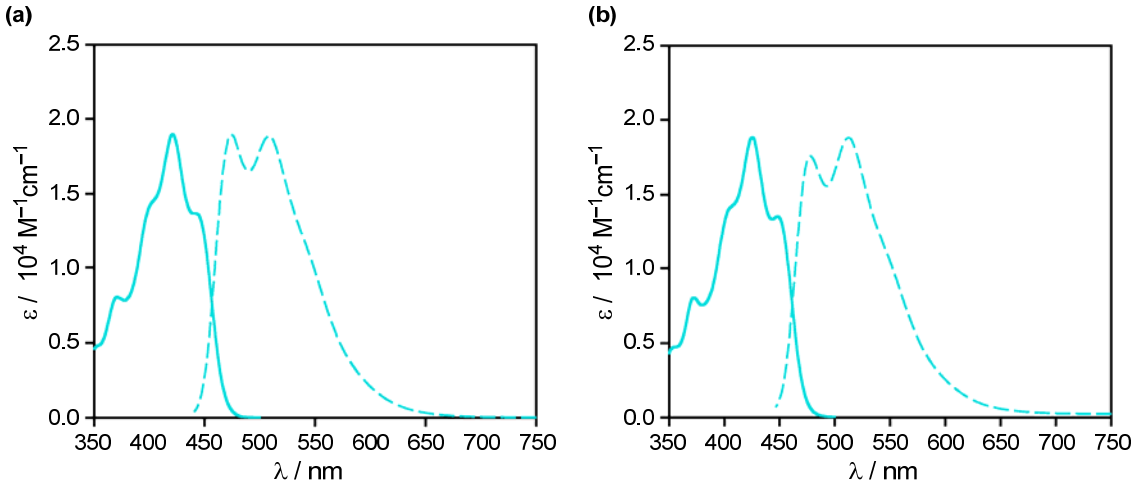


Figure S3. UV–vis spectra (solid line) and fluorescence spectra (dashed line) of **4a** (a) and **4b** (b) in CH_2Cl_2.

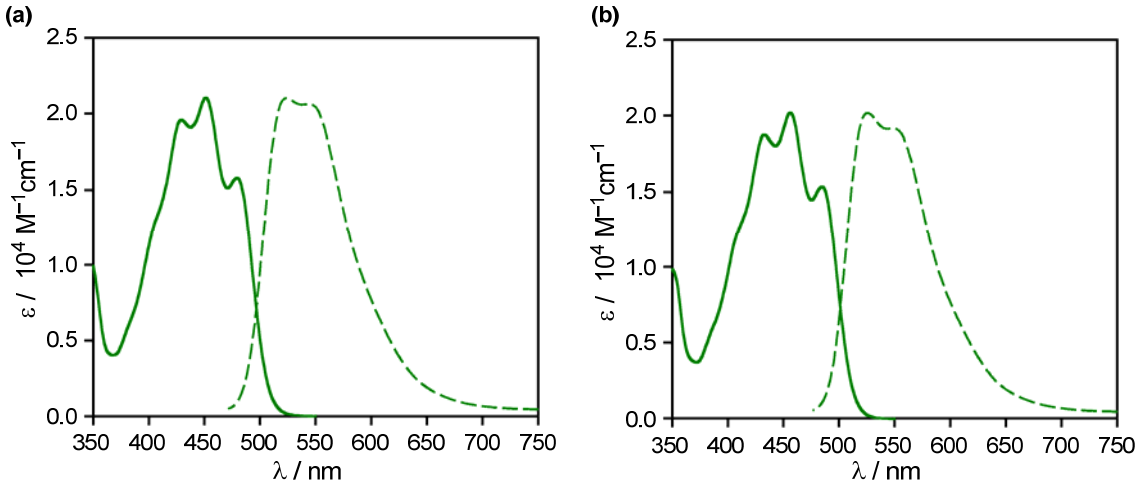


Figure S4. UV–vis spectra (solid line) and fluorescence spectra (dashed line) of **5a** (a) and **5b** (b) in CH_2Cl_2.

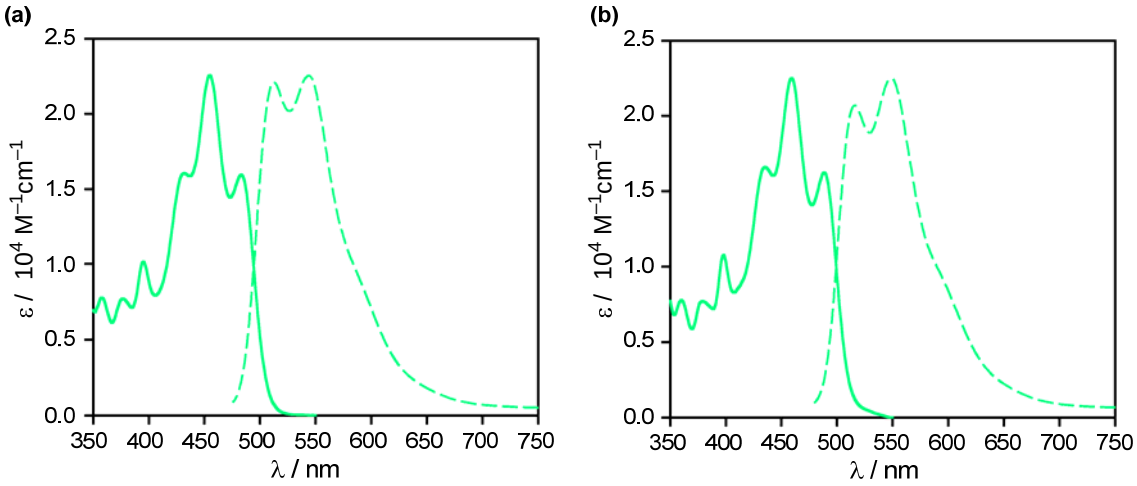


Figure S5. UV–vis spectra (solid line) and fluorescence spectra (dashed line) of **6a** (a) and **6b** (b) in CH_2Cl_2.

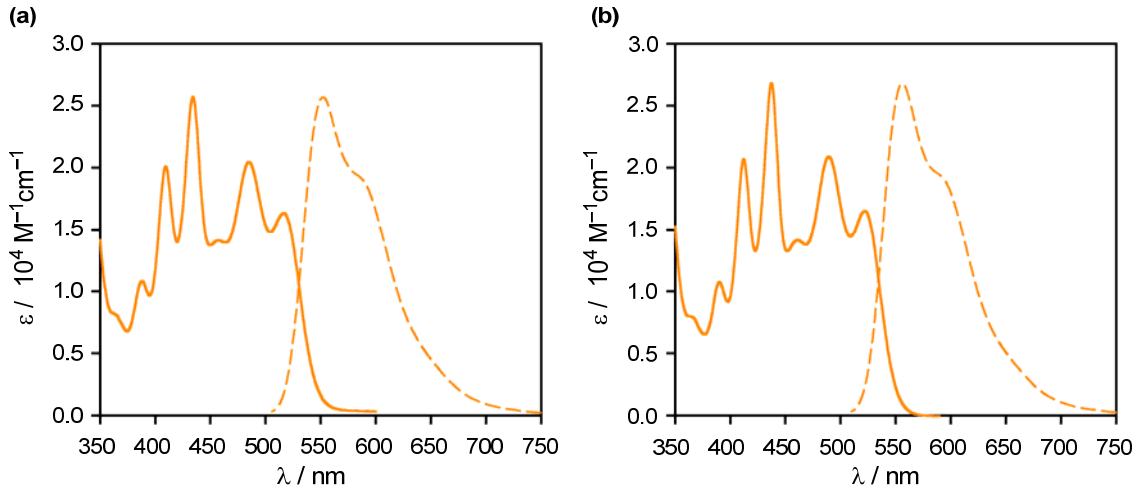


Figure S6. UV–vis spectra (solid line) and fluorescence spectra (dashed line) of **7a** (a) and **7b** (b) in CH_2Cl_2.

4.4 Solvent-dependent Photophysical Properties of 4b

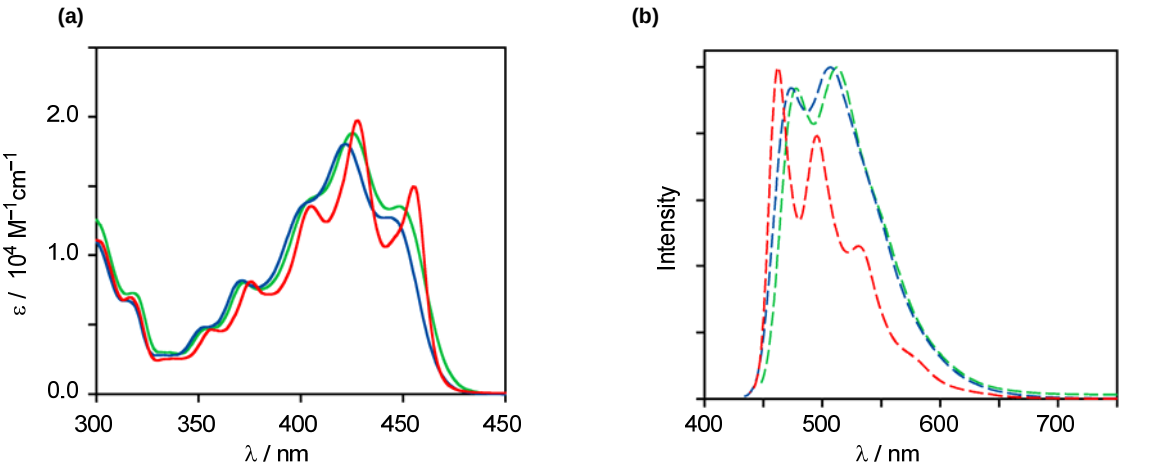


Figure S7. UV-vis spectra (a) and fluorescence spectra (b) of **4b** in methanol (blue), in dichloromethane (green), and in hexane (red).

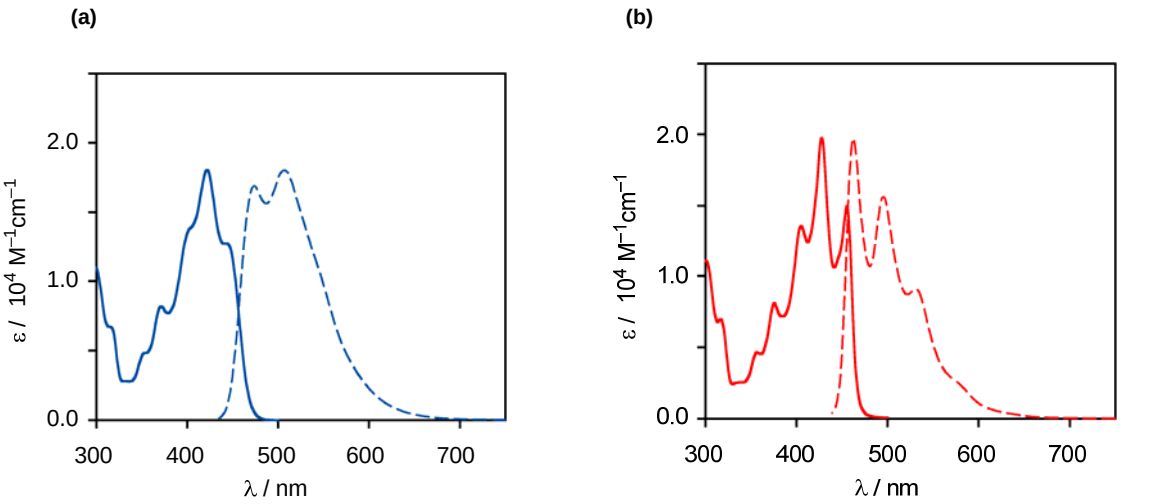


Figure S8. UV-vis spectra (solid line) and fluorescence spectra (dashed line) of **4b** in methanol (a) and in hexane (b). (For the spectra in CH_2Cl_2, see **Figure S2(b)**)

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 $Ag/AgNO_3$ reference electrode ($[AgNO_3]$ = 0.01 mM in 0.1 M $TBAClO_4$-CH_3CN). The measurements were carried out in dry CH_2Cl_2 or THF solution containing 0.1 M $TBAPF_6$ 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

Table S3. Electrochemical properties of 4-7.

Compound	E^{ox} [V vs. Fc^+/Fc] [a]	$E_{1/2}^{red}$ [V vs. Fc^+/Fc] [b,c]
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

[a] In CH_2Cl_2. [b] In THF. [c] Irreversible.

5.3 Cyclic Voltammograms

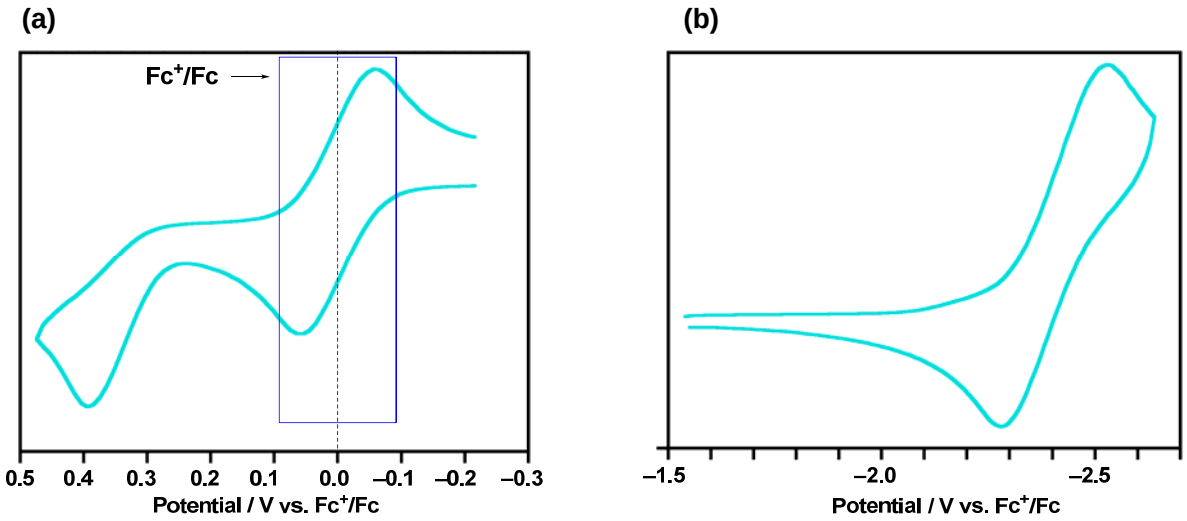


Figure S9. Cyclic voltammograms of **4a** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

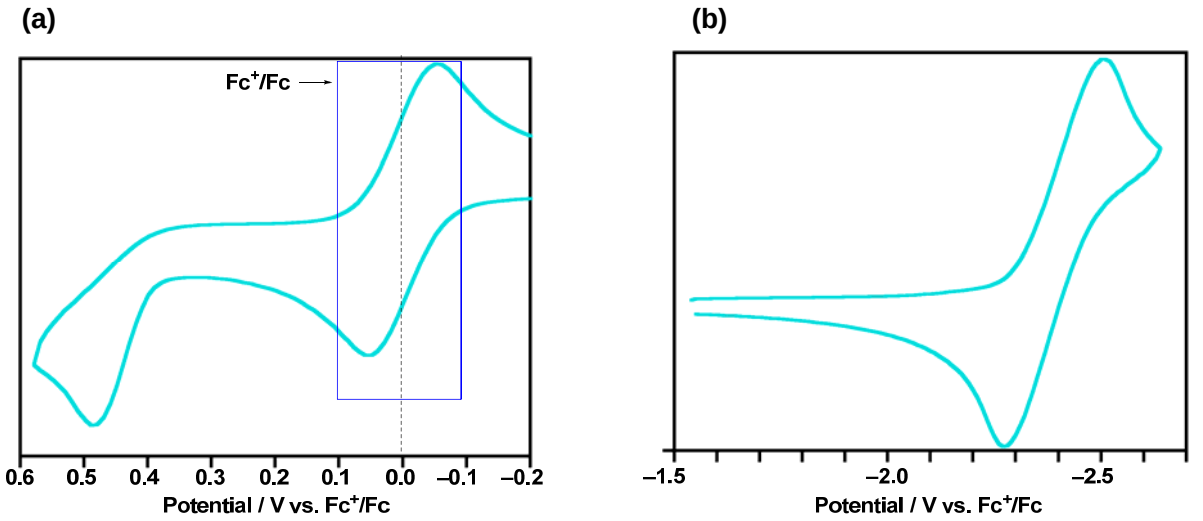


Figure S10. Cyclic voltammograms of **4b** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

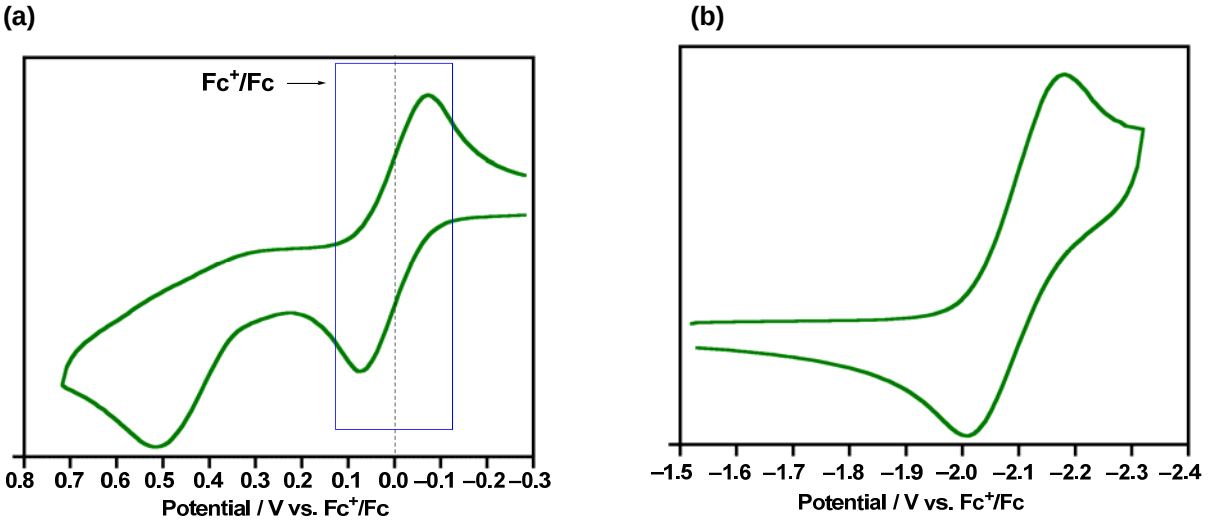


Figure S11. Cyclic voltammograms of **5a** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

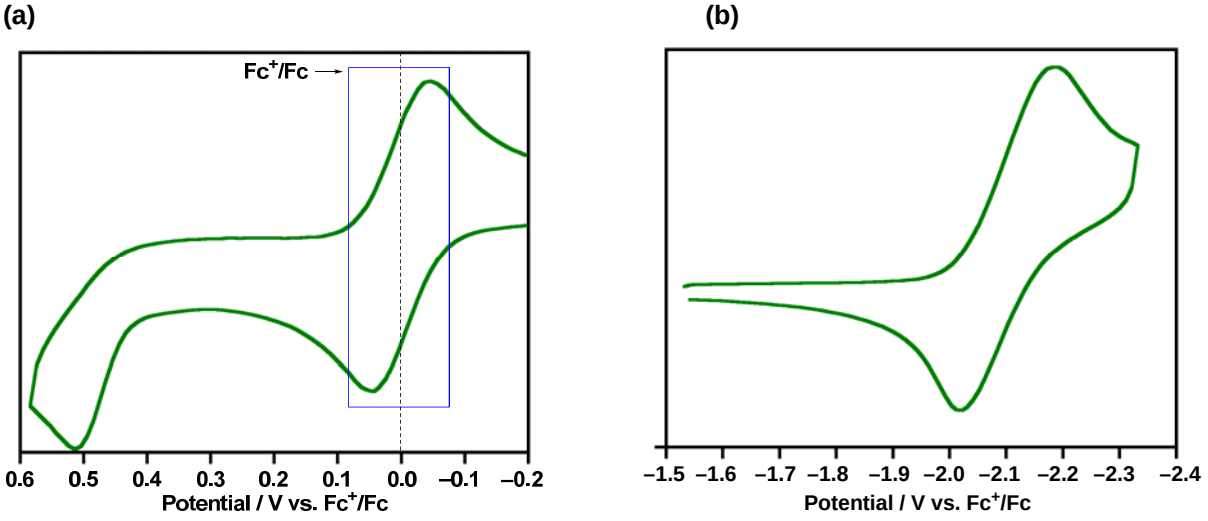


Figure S12. Cyclic voltammograms of **5b** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

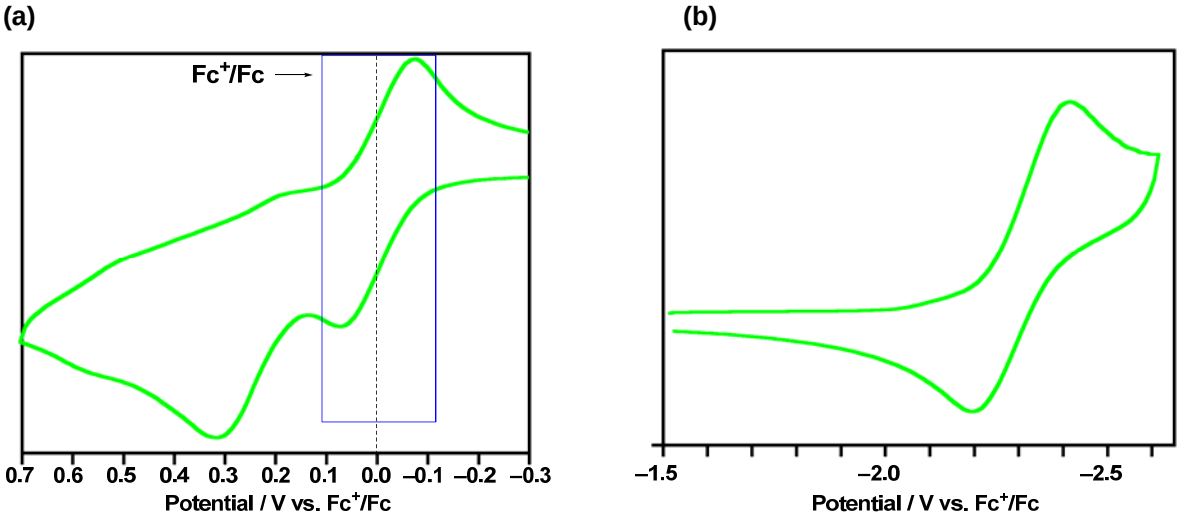


Figure S13. Cyclic voltammograms of **6a** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

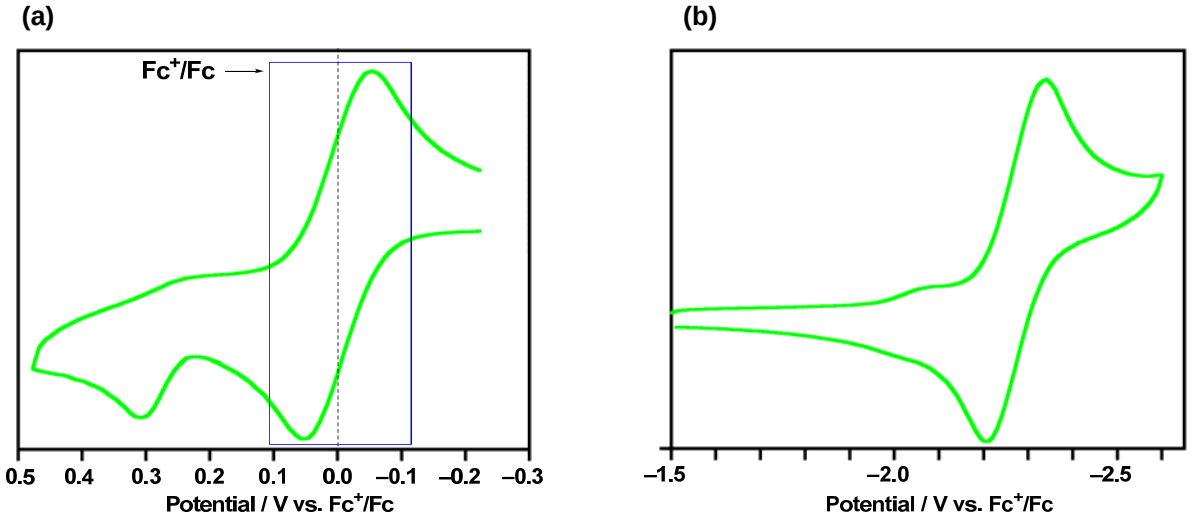


Figure S14. Cyclic voltammograms of **6b** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

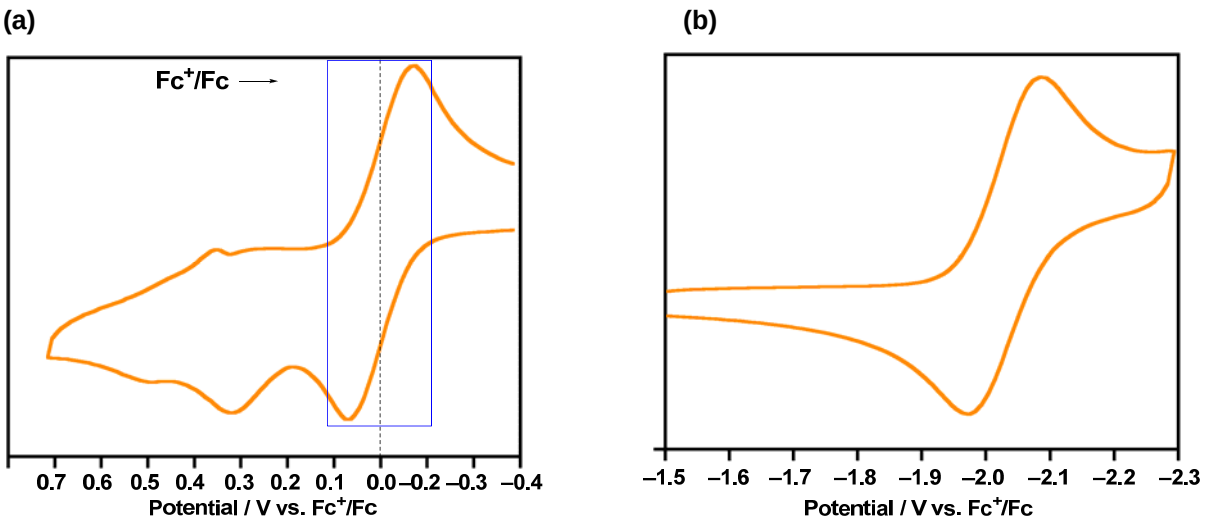


Figure S15. Cyclic voltammograms of **7a** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

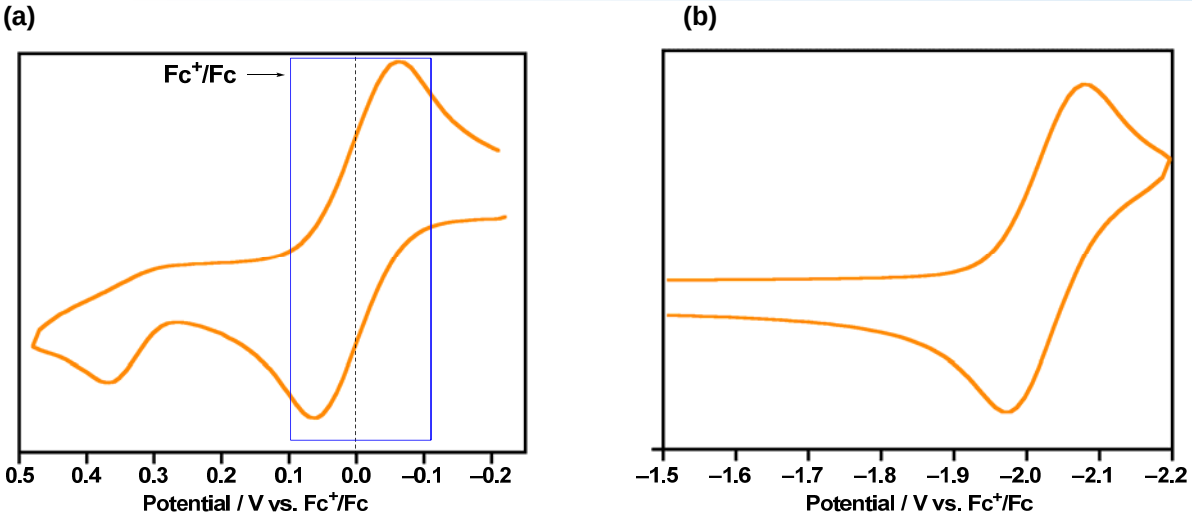


Figure S16. Cyclic voltammograms of **7b** in 0.1 M *n*-Bu_4NPF_6-dichloromethane with ferrocene (a) and in 0.1 M *n*-Bu_4NPF_6-THF (b).

6. Theoretical Calculations

6.1 Molecular Orbitals and Their Levels of L-Shaped Compounds

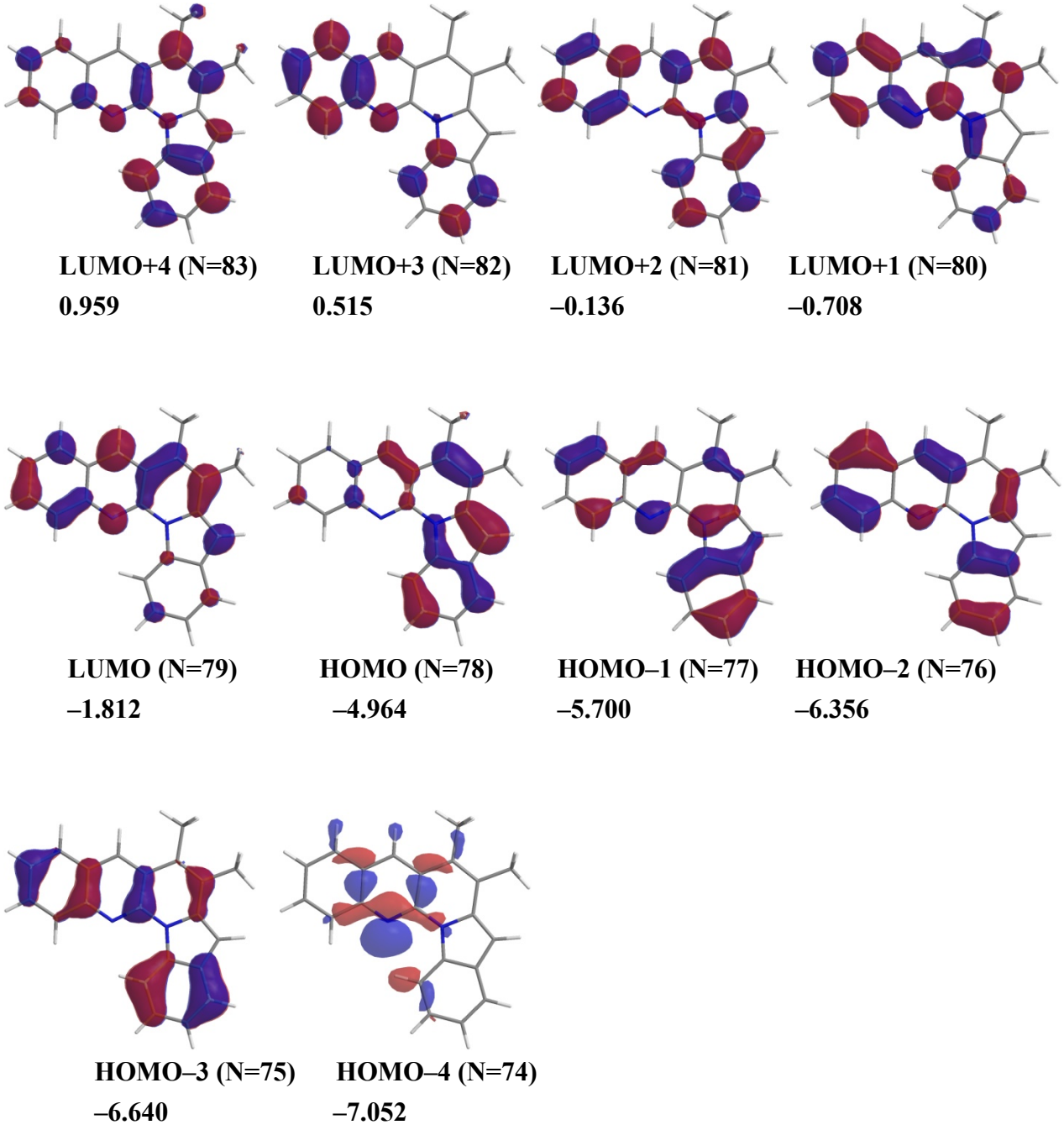


Figure S17. Selected molecular orbitals and their levels (eV) of **4a**.

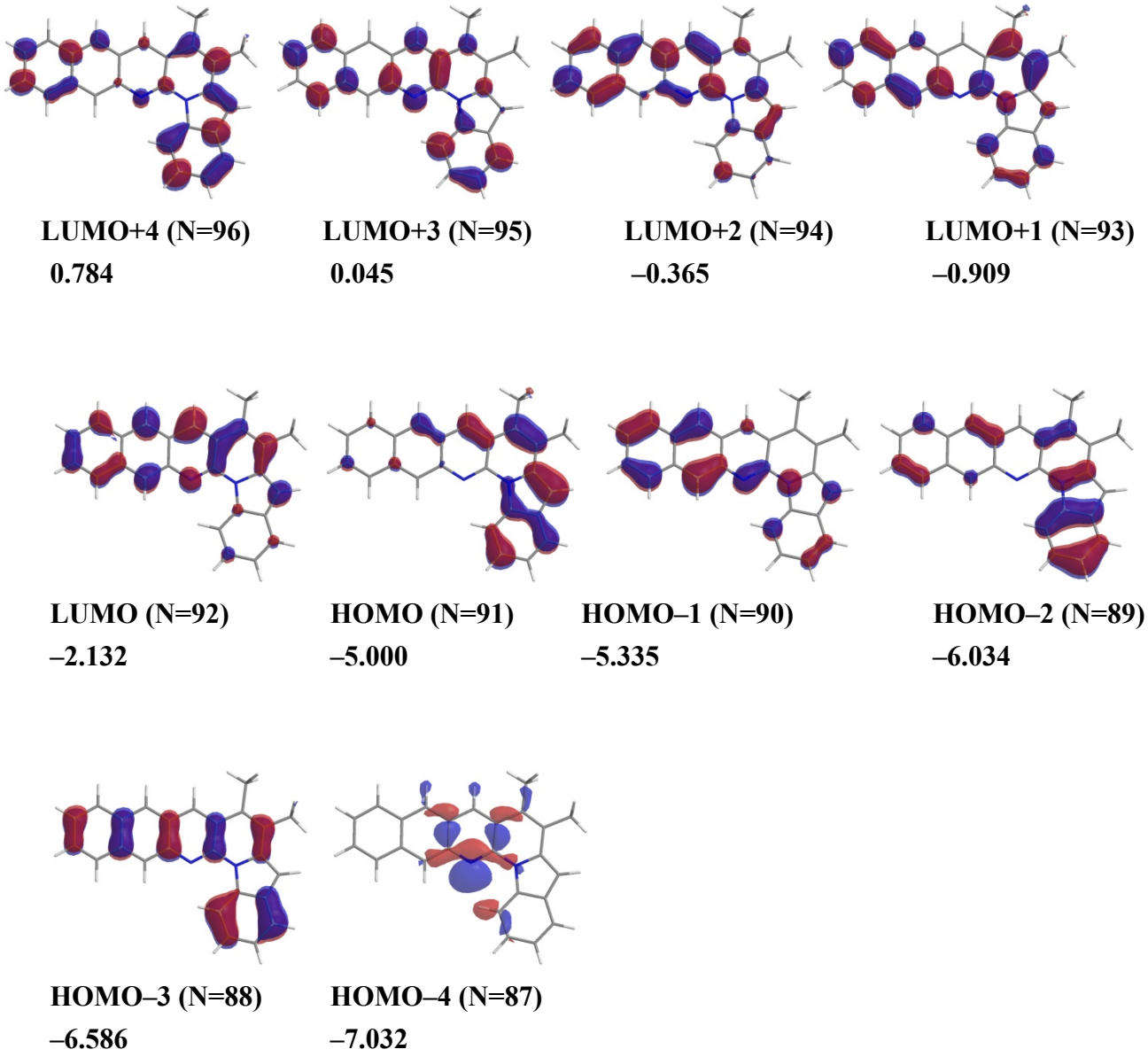
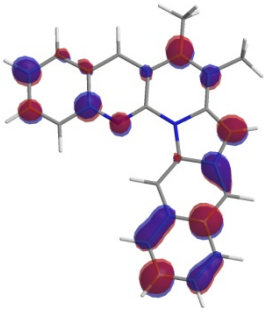
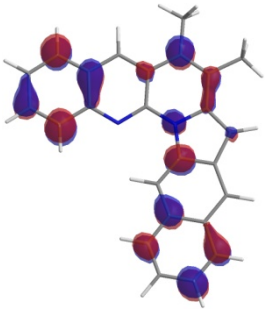


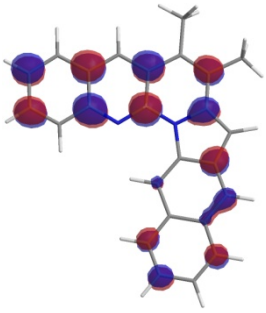
Figure S18. Selected molecular orbitals and their levels (eV) of **5a**.



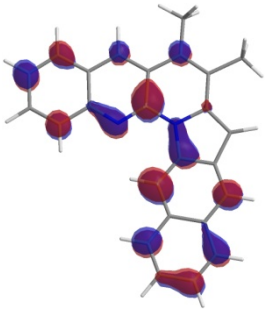
LUMO+4 (N=96)
0.590



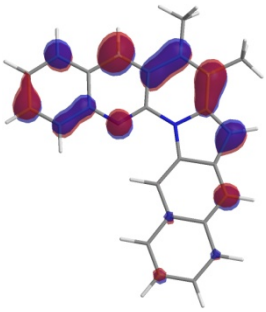
LUMO+3 (N=95)
0.173



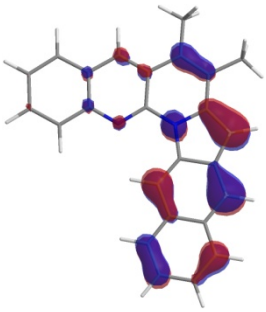
LUMO+2 (N=94)
–0.446



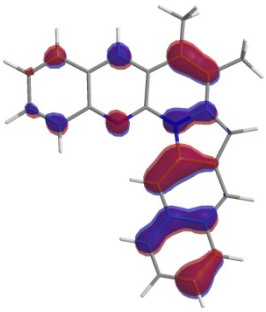
LUMO+1 (N=93)
–1.002



LUMO (N=92)
–1.909



HOMO (N=91)
–4.760



HOMO–1 (N=90)
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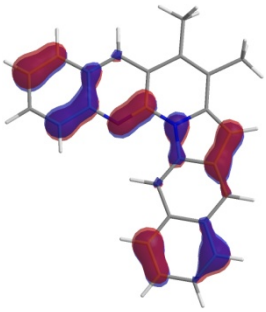
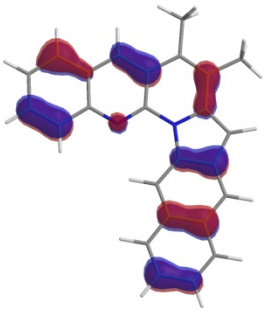
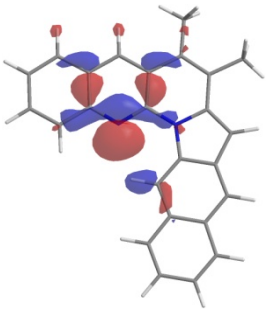


HOMO–2 (N=89)
–6.164



HOMO–3 (N=88)
–6.342



HOMO–4 (N=87)
–7.066

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

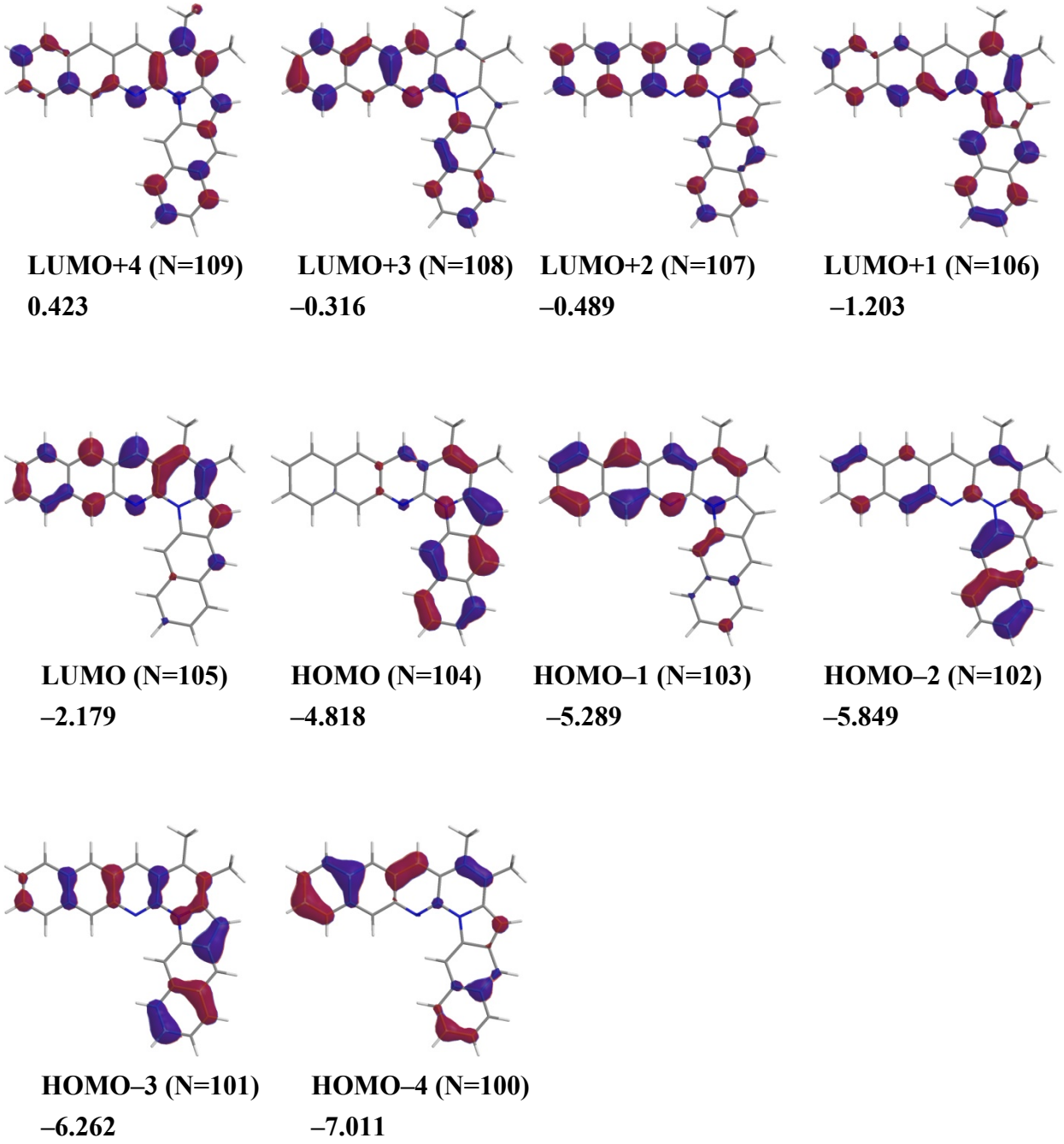


Figure S20. Selected molecular orbitals and their levels (eV) of **7a**.

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 oscillator strengths:
Excited State 1: Singlet-A' 2.8616 eV 433.27 nm f=0.3051
77 -> 80 -0.13499
78 -> 79 0.63738
Excited State 2: Singlet-A' 3.3257 eV 372.81 nm f=0.0189
77 -> 79 0.63829
78 -> 80 0.24744
Excited State 3: Singlet-A' 3.6530 eV 339.41 nm f=0.0082
77 -> 79 -0.21723
78 -> 80 0.63842
Excited State 4: Singlet-A' 4.0677 eV 304.80 nm f=0.0512
76 -> 79 0.63989
78 -> 81 0.11352
Excited State 5: Singlet-A' 4.1713 eV 297.23 nm f=0.0039
75 -> 79 0.56802
77 -> 80 0.21023
78 -> 81 0.33201
Excited State 6: Singlet-A" 4.2556 eV 291.35 nm f=0.0005
74 -> 79 0.69195
Excited State 7: Singlet-A' 4.4572 eV 278.16 nm f=0.1154
75 -> 79 -0.24257
76 -> 79 -0.11611
76 -> 80 0.30423
77 -> 81 -0.18290
78 -> 81 0.50655
Excited State 8: Singlet-A' 4.6155 eV 268.62 nm f=0.6709
75 -> 79 -0.11702
77 -> 80 0.60913
77 -> 81 -0.11513
78 -> 81 -0.13197
Excited State 9: Singlet-A' 4.8534 eV 255.46 nm f=0.0968
73 -> 79 -0.15929
75 -> 79 -0.18043
77 -> 81 0.32150
78 -> 82 0.51066
78 -> 84 0.15533
Excited State 10: Singlet-A' 4.9664 eV 249.65 nm f=0.0398
73 -> 79 0.45443
76 -> 80 0.15774
77 -> 81 -0.17332
78 -> 82 0.38112
78 -> 83 -0.14639
78 -> 84 -0.17094
Excited State 11: Singlet-A' 5.0690 eV 244.59 nm f=0.1033
73 -> 79 0.25608
75 -> 80 -0.16137
76 -> 80 0.33021
77 -> 81 0.45479
78 -> 82 -0.18693
78 -> 84 0.10816
Excited State 12: Singlet-A" 5.2146 eV 237.76 nm f=0.0002
74 -> 80 0.69107
Excited State 13: Singlet-A' 5.2509 eV 236.12 nm f=0.0656
72 -> 79 -0.20325
73 -> 79 -0.10674
76 -> 80 0.24840
76 -> 81 -0.15061
77 -> 82 0.10001
78 -> 83 0.45970
78 -> 84 -0.28411
Excited State 14: Singlet-A' 5.3264 eV 232.77 nm f=0.0955
72 -> 79 0.52608
73 -> 79 -0.21006
75 -> 80 0.19543
76 -> 80 0.26005
Excited State 15: Singlet-A' 5.4293 eV 228.36 nm f=0.0958
72 -> 79 -0.33540
73 -> 79 -0.14911
75 -> 80 0.37894
75 -> 81 -0.11970
76 -> 80 0.17688
78 -> 83 -0.29682
78 -> 84 0.12518
Excited State 16: Singlet-A' 5.4679 eV 226.75 nm f=0.0025
73 -> 79 0.10447
73 -> 80 -0.11818
75 -> 80 0.31319
76 -> 81 0.37051
78 -> 83 0.32267
78 -> 84 0.29257
Excited State 17: Singlet-A' 5.5496 eV 223.41 nm f=0.2347
73 -> 79 -0.13979
73 -> 80 -0.13481
75 -> 80 -0.31116
75 -> 81 -0.10390
76 -> 80 0.10714
77 -> 81 -0.19322
77 -> 82 0.45421
78 -> 84 0.18575
Excited State 18: Singlet-A' 5.8066 eV 213.52 nm f=0.0800
73 -> 79 -0.13221
73 -> 80 -0.14537
75 -> 81 -0.29848
75 -> 82 0.13006
76 -> 81 0.39673
78 -> 84 -0.33219
Excited State 19: Singlet-A' 5.8749 eV 211.04 nm f=0.4528
70 -> 79 0.12259
71 -> 79 -0.11770
72 -> 79 0.13146
73 -> 80 0.13171
75 -> 80 0.12774
75 -> 81 0.17273
76 -> 80 -0.12923
77 -> 81 0.10212
77 -> 82 0.40950
77 -> 83 0.20813
77 -> 84 -0.20005
78 -> 84 -0.16861
Excited State 20: Singlet-A' 5.9739 eV 207.54 nm f=0.2457
73 -> 80 0.24605
75 -> 80 -0.13900
75 -> 81 0.28144
76 -> 80 0.11865
76 -> 81 0.30023
77 -> 83 0.34663
77 -> 84 0.16240
Excited State 21: Singlet-A" 6.0143 eV 206.15 nm f=0.0001
74 -> 81 0.69080
Excited State 22: Singlet-A' 6.0882 eV 203.65 nm f=0.0380
72 -> 80 0.25628
73 -> 80 -0.24300
75 -> 81 -0.25238
75 -> 84 -0.11831
76 -> 81 -0.11045
77 -> 83 0.46197
78 -> 84 0.10107
78 -> 85 -0.12985
Excited State 23: Singlet-A' 6.1810 eV 200.59 nm f=0.1938
71 -> 79 0.23706
73 -> 80 0.33840
75 -> 81 -0.28835
76 -> 82 0.18819
77 -> 82 0.15476
77 -> 84 0.32635
Excited State 24: Singlet-A' 6.2946 eV 196.97 nm f=0.0892
70 -> 79 -0.22413
71 -> 79 0.12613
72 -> 80 0.15807
73 -> 80 0.15162
75 -> 82 0.11570
76 -> 82 0.46926
77 -> 84 -0.30354
Excited State 25: Singlet-A' 6.4032 eV 193.63 nm f=0.0496
71 -> 79 0.44489
72 -> 80 0.23410
73 -> 80 -0.13495
75 -> 81 0.12524
75 -> 82 0.25290
76 -> 82 -0.18128
76 -> 83 0.10342
76 -> 84 -0.10857
78 -> 85 -0.11152
Excited State 26: Singlet-A' 6.4110 eV 193.39 nm f=0.0459
70 -> 79 0.40130
71 -> 79 0.27848
72 -> 80 -0.31801
73 -> 80 -0.12694
76 -> 82 0.14177
76 -> 83 -0.10816
77 -> 84 -0.20575
78 -> 85 -0.15070
Excited State 27: Singlet-A" 6.4650 eV 191.78 nm f=0.0001
69 -> 79 0.68184
Excited State 28: Singlet-A' 6.4843 eV 191.21 nm f=0.0244
70 -> 79 0.30437
71 -> 79 -0.12067
72 -> 80 0.27748
73 -> 80 0.21545
75 -> 82 0.30117
76 -> 83 -0.24892
78 -> 85 -0.16183
Excited State 29: Singlet-A" 6.5192 eV 190.18 nm f=0.0017
74 -> 82 0.65769
74 -> 83 0.13169
74 -> 84 -0.10749
Excited State 30: Singlet-A" 6.5297 eV 189.88 nm f=0.0012
78 -> 86 0.6971

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

Excitation energies and oscillator strengths:
Excited State 1: Singlet-A' 2.6101 eV 475.02 nm f=0.3594
91 -> 92 0.69248
Excited State 2: Singlet-A' 2.7833 eV 445.45 nm f=0.0186
90 -> 92 0.69382
Excited State 3: Singlet-A' 3.3799 eV 366.83 nm f=0.0514
89 -> 92 0.67845
91 -> 93 -0.10638
Excited State 4: Singlet-A' 3.5726 eV 347.04 nm f=0.1051
89 -> 92 0.11973
91 -> 93 0.66794
91 -> 94 -0.12704
Excited State 5: Singlet-A' 3.8005 eV 326.23 nm f=0.0096
88 -> 92 0.54748
90 -> 93 -0.37136
90 -> 94 0.15634
91 -> 94 0.10772
Excited State 6: Singlet-A" 3.9725 eV 312.11 nm f=0.0004
87 -> 92 0.70130
Excited State 7: Singlet-A' 4.0650 eV 305.01 nm f=0.2551
88 -> 92 0.22266
90 -> 93 0.50566
90 -> 94 0.13626
91 -> 93 0.10996
91 -> 94 0.38715
Excited State 8: Singlet-A' 4.1934 eV 295.66 nm f=0.0393
89 -> 93 -0.27140
90 -> 93 -0.23036
90 -> 94 -0.32391
91 -> 94 0.44718
91 -> 95 0.17346
Excited State 9: Singlet-A' 4.4021 eV 281.65 nm f=0.3270
86 -> 92 0.49777
88 -> 92 0.21290
90 -> 94 -0.31238
91 -> 95 -0.19959
91 -> 96 0.11355
Excited State 10: Singlet-A' 4.5419 eV 272.98 nm f=0.1782
85 -> 92 0.21378
88 -> 92 0.18023
89 -> 93 0.25136
90 -> 94 -0.17843
91 -> 94 -0.10349
91 -> 95 0.53712
Excited State 11: Singlet-A' 4.5986 eV 269.61 nm f=0.2715
85 -> 92 -0.32930
86 -> 92 0.38020
90 -> 94 0.31726
91 -> 95 0.30995
Excited State 12: Singlet-A' 4.6945 eV 264.10 nm f=0.3210
85 -> 92 0.47772
86 -> 92 0.14417
89 -> 93 -0.23655
90 -> 94 0.28223
90 -> 95 0.27911
Excited State 13: Singlet-A' 4.7827 eV 259.24 nm f=0.1662
86 -> 92 0.19163
88 -> 92 -0.10584
89 -> 93 0.46689
90 -> 95 0.38436
91 -> 94 0.18632
91 -> 97 0.10541
Excited State 14: Singlet-A' 4.9316 eV 251.41 nm f=0.3597
85 -> 92 -0.21632
88 -> 92 0.13404
89 -> 93 -0.13686
89 -> 94 -0.31746
90 -> 95 0.43180
90 -> 96 -0.11261
91 -> 94 -0.15549
91 -> 97 -0.17247
Excited State 15: Singlet-A" 5.1464 eV 240.91 nm f=0.0000
87 -> 93 0.68402
87 -> 94 -0.15206
Excited State 16: Singlet-A' 5.1509 eV 240.70 nm f=0.0956
84 -> 92 -0.20229
85 -> 92 0.13303
88 -> 93 0.48756
88 -> 94 0.13456
89 -> 94 -0.25115
89 -> 95 0.12453
91 -> 97 -0.18111
91 -> 98 0.10950
Excited State 17: Singlet-A' 5.2046 eV 238.22 nm f=0.0382
84 -> 92 0.60441
88 -> 93 0.15819
89 -> 94 -0.13113
90 -> 97 -0.14597
90 -> 98 -0.13198
91 -> 98 -0.11991
Excited State 18: Singlet-A' 5.2414 eV 236.55 nm f=0.0799
86 -> 93 -0.17896
88 -> 93 -0.13143
89 -> 94 -0.15343
89 -> 95 0.22324
90 -> 95 -0.14040
91 -> 96 0.53575
91 -> 97 0.14525
Excited State 19: Singlet-A' 5.2919 eV 234.29 nm f=0.0342
86 -> 93 0.12857
88 -> 93 0.17843
88 -> 94 -0.12705
89 -> 94 -0.30352
89 -> 95 -0.27148
90 -> 96 0.14715
91 -> 97 0.44417
Excited State 20: Singlet-A' 5.4081 eV 229.25 nm f=0.2081
85 -> 92 -0.10823
86 -> 93 -0.10677
88 -> 93 0.31094
89 -> 94 0.34691
90 -> 95 0.12637
90 -> 96 -0.34477
91 -> 96 0.10915
91 -> 97 0.17808
91 -> 98 -0.12077
Excited State 21: Singlet-A' 5.5041 eV 225.26 nm f=0.0152
83 -> 92 0.19250
84 -> 92 0.11817
86 -> 93 -0.19426
88 -> 93 -0.14783
88 -> 94 0.29001
88 -> 95 0.10117
90 -> 96 -0.14439
91 -> 96 -0.28018
91 -> 97 0.33252
91 -> 98 0.16349
Excited State 22: Singlet-A' 5.6040 eV 221.24 nm f=0.0276
83 -> 92 -0.12714
85 -> 93 -0.10768
86 -> 93 0.36845
88 -> 94 -0.12508
89 -> 95 0.25483
90 -> 96 -0.12361
90 -> 97 -0.21386
91 -> 97 0.12513
91 -> 98 0.37914
Excited State 23: Singlet-A' 5.6540 eV 219.29 nm f=0.1389
86 -> 93 -0.27333
89 -> 95 -0.38639
90 -> 97 -0.11191
91 -> 98 0.42858
Excited State 24: Singlet-A' 5.6708 eV 218.64 nm f=0.0665
83 -> 92 -0.14272
84 -> 92 0.11744
85 -> 93 0.21770
89 -> 95 0.24398
90 -> 96 0.32404
90 -> 97 0.39331
91 -> 97 0.12683
91 -> 98 0.17428
Excited State 25: Singlet-A' 5.7587 eV 215.30 nm f=0.0250
83 -> 92 0.55313
85 -> 93 0.15192
88 -> 94 -0.28770
91 -> 98 0.13637
91 -> 99 -0.12157

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

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A' 2.5726 eV 481.93 nm f=0.2871
91 -> 92 0.69443

Excited State 2: Singlet-A' 3.1211 eV 397.24 nm f=0.0571
90 -> 92 0.55408
91 -> 93 -0.40653
91 -> 94 -0.12201

Excited State 3: Singlet-A' 3.3382 eV 371.41 nm f=0.0608
90 -> 92 0.40483
91 -> 93 0.55915

Excited State 4: Singlet-A' 3.6873 eV 336.25 nm f=0.0279
89 -> 92 0.55460
91 -> 94 -0.40180

Excited State 5: Singlet-A' 3.8334 eV 323.43 nm f=0.1267
88 -> 92 0.16654
88 -> 93 0.11721
89 -> 92 0.39292
90 -> 93 -0.14268
91 -> 94 0.50549

Excited State 6: Singlet-A' 4.0133 eV 308.93 nm f=0.0785
88 -> 92 0.63732
90 -> 93 0.13484
90 -> 94 -0.12232
91 -> 94 -0.11200

Excited State 7: Singlet-A' 4.1068 eV 301.90 nm f=0.2598
90 -> 93 0.59330
91 -> 94 0.17450
91 -> 95 0.27991
91 -> 96 0.11914

Excited State 8: Singlet-A" 4.2251 eV 293.45 nm f=0.0004
87 -> 92 0.69610
87 -> 93 -0.10501

Excited State 9: Singlet-A' 4.3937 eV 282.18 nm f=0.2119
86 -> 92 0.11830
88 -> 93 -0.22763
90 -> 93 -0.23523
90 -> 94 -0.39450
91 -> 95 0.40870

Excited State 10: Singlet-A' 4.5231 eV 274.12 nm f=0.1374
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' 4.6925 eV 264.22 nm f=0.0135
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' 4.7925 eV 258.70 nm f=0.2644
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' 4.8274 eV 256.84 nm f=0.0584
85 -> 92 0.35990
86 -> 92 0.36381
88 -> 94 -0.17472
89 -> 93 0.18574
89 -> 94 -0.11153
90 -> 94 0.13141
91 -> 95 0.11218
91 -> 96 -0.16000
91 -> 97 0.27082

Excited State 14: Singlet-A' 4.9311 eV 251.43 nm f=0.0232
86 -> 92 -0.17366
89 -> 94 -0.11787
91 -> 96 0.43866
91 -> 97 0.47265

Excited State 15: Singlet-A' 4.9721 eV 249.36 nm f=0.0164
85 -> 92 0.51490
88 -> 93 -0.22733
88 -> 94 0.22008
89 -> 93 -0.10490
89 -> 94 0.12674
90 -> 95 -0.14091
90 -> 96 0.11509
91 -> 96 0.15623

Excited State 16: Singlet-A" 5.0599 eV 245.03 nm f=0.0003
87 -> 93 0.65741
87 -> 94 0.22629

Excited State 17: Singlet-A' 5.1541 eV 240.56 nm f=0.3294
88 -> 93 -0.22003
89 -> 94 0.41289
90 -> 94 -0.14154
90 -> 95 0.17732
91 -> 96 -0.19640
91 -> 97 0.37497

Excited State 18: Singlet-A' 5.2719 eV 235.18 nm f=0.1182
85 -> 92 0.12890
86 -> 93 -0.11211
88 -> 94 0.20978
89 -> 94 -0.29381
90 -> 94 -0.10182
90 -> 95 0.53034

Excited State 19: Singlet-A' 5.3292 eV 232.65 nm f=0.1903
84 -> 92 0.41335
86 -> 92 -0.10094
86 -> 93 -0.22198
88 -> 93 -0.11502
88 -> 94 -0.18561
90 -> 95 -0.15850
91 -> 98 0.35634

Excited State 20: Singlet-A' 5.4471 eV 227.62 nm f=0.4501
85 -> 93 -0.18723
86 -> 92 0.22263
86 -> 93 0.15110
88 -> 94 0.28943
89 -> 94 0.16512
89 -> 95 -0.18883
90 -> 94 0.14475
91 -> 98 0.37518

Excited State 21: Singlet-A' 5.4917 eV 225.77 nm f=0.0073
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' 5.5566 eV 223.13 nm f=0.1594
84 -> 92 -0.27718
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' 5.6187 eV 220.66 nm f=0.2488
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" 5.6799 eV 218.29 nm f=0.0001
87 -> 93 -0.21458
87 -> 94 0.65763

Excited State 25: Singlet-A' 5.7320 eV 216.30 nm f=0.0217
83 -> 92 0.21019
85 -> 93 0.39956
86 -> 93 0.27873
88 -> 94 0.11282
89 -> 95 0.13553
90 -> 97 0.35311
91 -> 98 0.14639

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

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A' 2.3847 eV 519.91 nm f=0.3278
103 ->105 -0.16799
104 ->105 0.63012

Excited State 2: Singlet-A' 2.7341 eV 453.47 nm f=0.1691
103 ->105 0.62984
104 ->105 0.13664

Excited State 3: Singlet-A' 3.1484 eV 393.80 nm f=0.0038
102 ->105 0.57608
104 ->106 -0.34924

Excited State 4: Singlet-A' 3.1858 eV 389.18 nm f=0.0046
102 ->105 0.36449
104 ->106 0.55590

Excited State 5: Singlet-A' 3.5679 eV 347.50 nm f=0.0216
101 ->105 0.52096
103 ->106 -0.36020
103 ->107 0.17944
104 ->107 0.16080

Excited State 6: Singlet-A' 3.7099 eV 334.20 nm f=0.2904
101 ->105 0.33222
102 ->106 -0.10504
103 ->106 0.54538
103 ->107 0.17532

Excited State 7: Singlet-A' 3.8315 eV 323.59 nm f=0.1351
101 ->106 0.11712
102 ->106 0.16318
104 ->107 0.62948

Excited State 8: Singlet-A" 3.9635 eV 312.81 nm f=0.0003
99 ->105 0.69335

Excited State 9: Singlet-A' 3.9805 eV 311.48 nm f=0.0548
102 ->106 -0.27057
103 ->106 -0.10549
104 ->107 0.12029
104 ->108 0.59137
104 ->110 0.10642

Excited State 10: Singlet-A' 4.1885 eV 296.01 nm f=0.1841
98 ->105 0.25121
100 ->105 0.23901
101 ->105 -0.13176
101 ->106 -0.15370
102 ->106 0.32756
103 ->107 0.42844

Excited State 11: Singlet-A' 4.2745 eV 290.06 nm f=0.1113
100 ->105 0.43184
101 ->105 -0.11092
102 ->106 -0.36561
103 ->108 -0.20450
104 ->108 -0.23044
104 ->110 0.19667

Excited State 12: Singlet-A' 4.3684 eV 283.82 nm f=0.1078
98 ->105 0.55499
100 ->105 -0.12526
102 ->106 -0.21173
103 ->108 0.27454
104 ->108 -0.11989

Excited State 13: Singlet-A' 4.4885 eV 276.23 nm f=0.0721
98 ->105 -0.21234
101 ->106 -0.22754
102 ->107 -0.14786
103 ->107 0.13841
103 ->108 0.45799
104 ->110 0.28325

Excited State 14: Singlet-A' 4.5350 eV 273.39 nm f=0.0522
98 ->105 -0.11066
100 ->105 0.31656
101 ->106 0.47435
103 ->108 0.28369
104 ->110 -0.12275

Excited State 15: Singlet-A' 4.6394 eV 267.24 nm f=0.5737
100 ->105 -0.14781
101 ->106 0.32022
102 ->107 -0.30795
103 ->107 0.27472
103 ->108 -0.17558
103 ->109 0.10344
104 ->109 0.21948
104 ->110 0.22995

Excited State 16: Singlet-A' 4.7513 eV 260.95 nm f=0.0141
102 ->107 0.22119
104 ->109 0.60838

Excited State 17: Singlet-A' 4.8414 eV 256.09 nm f=0.0446
97 ->105 0.61338
102 ->107 0.17008

Excited State 18: Singlet-A' 4.9304 eV 251.47 nm f=0.4837
97 ->105 -0.23712
98 ->105 -0.12619
100 ->105 -0.19079
100 ->106 -0.14220
101 ->108 0.16828
102 ->106 -0.12197
102 ->107 0.39502
103 ->107 0.21420
103 ->109 0.16652
104 ->109 -0.11082

Excited State 19: Singlet-A" 4.9452 eV 250.71 nm f=0.0001
99 ->106 0.67763
99 ->107 -0.15728

Excited State 20: Singlet-A' 5.0036 eV 247.79 nm f=0.2212
102 ->106 -0.11816
102 ->108 0.53899
103 ->107 0.11749
104 ->110 -0.32056

Excited State 21: Singlet-A' 5.0981 eV 243.20 nm f=0.5377
100 ->106 0.31407
101 ->106 0.10405
101 ->107 -0.21171
102 ->106 0.11630
102 ->107 0.25442
102 ->108 0.25098
103 ->107 -0.10791
103 ->109 0.16065
104 ->110 0.25607

Excited State 22: Singlet-A' 5.1830 eV 239.22 nm f=0.0330
96 ->105 -0.19358
98 ->106 0.20900
101 ->107 0.13319
101 ->108 -0.16635
102 ->108 -0.14107
103 ->109 0.50012
104 ->110 -0.15156
104 ->112 0.15415

Excited State 23: Singlet-A' 5.2457 eV 236.35 nm f=0.0520
96 ->105 0.47586
97 ->105 0.12471
98 ->106 0.17375
103 ->109 0.20033
103 ->110 0.33536
103 ->111 -0.12549

Excited State 24: Singlet-A' 5.3055 eV 233.69 nm f=0.0383
95 ->105 0.18448
96 ->105 -0.22998
98 ->106 0.32371
100 ->106 -0.24476
101 ->107 -0.29310
101 ->108 0.17820
103 ->110 0.22960
104 ->110 0.10472
104 ->112 0.15529

Excited State 25: Singlet-A' 5.3392 eV 232.22 nm f=0.0153
95 ->105 0.15915
96 ->105 -0.20545
98 ->106 -0.30280
101 ->107 0.23433
102 ->108 0.13442
103 ->110 0.40473
103 ->111 0.13857
104 ->111 0.11215
104 ->112 -0.15224

Excited State 26: Singlet-A' 5.3720 eV 230.80 nm f=0.0544
98 ->106 0.15095
100 ->106 0.34459
101 ->107 0.31513
101 ->108 0.29624
104 ->111 -0.17701
104 ->112 0.27988

Excited State 27: Singlet-A' 5.4290 eV 228.37 nm f=0.0307
95 ->105 0.30649
96 ->105 0.13988
98 ->106 0.12437
100 ->106 0.14387
103 ->110 -0.14787
104 ->111 0.52653

Excited State 28: Singlet-A' 5.4428 eV 227.79 nm f=0.0071
95 ->105 0.43057
98 ->106 0.17147
101 ->108 -0.14092
103 ->110 -0.11225
104 ->111 -0.36365
104 ->112 -0.27147

Excited State 29: Singlet-A' 5.4933 eV 225.70 nm f=0.0061
95 ->105 0.22154
96 ->105 0.18286
97 ->106 -0.16043
98 ->106 -0.23895
101 ->108 -0.25067
102 ->109 -0.19098
103 ->112 -0.10211
104 ->112 0.38941

Excited State 30: Singlet-A' 5.6123 eV 220.92 nm f=0.5679
95 ->105 0.10401
100 ->106 0.30745
101 ->107 -0.23644
102 ->108 -0.14878
102 ->109 0.21068
102 ->110 0.24655
103 ->109 -0.10532
103 ->110 0.23060
104 ->110 -0.16258

Excited State 31: Singlet-A" 5.6566 eV 219.19 nm f=0.0000
99 ->106 0.16161
99 ->107 0.66298
99 ->108 -0.13951

Excited State 32: Singlet-A' 5.6703 eV 218.66 nm f=0.0914
97 ->106 0.16797
98 ->106 -0.12622
98 ->107 -0.17522
100 ->107 0.17814
100 ->108 0.11630

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
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
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
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
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
92 ->105 -0.16298
97 ->106 0.31366
100 ->107 0.11127
101 ->109 -0.11095
102 ->109 0.13485
102 ->110 0.33282
103 ->111 0.25795
103 ->112 0.21908
104 ->112 0.10927
Excited State 38: Singlet-A" 5.9934 eV 206.87 nm f=0.0000
91 ->105 -0.17329
94 ->105 0.65866
Excited State 39: Singlet-A' 6.0325 eV 205.53 nm f=0.0941
96 ->106 -0.13360
97 ->106 -0.13296
98 ->107 -0.20724
98 ->108 0.20846
100 ->107 0.36412
101 ->108 -0.15416
102 ->109 0.19760
102 ->110 -0.14579
104 ->113 -0.26055
Excited State 40: Singlet-A' 6.0471 eV 205.03 nm f=0.0785
93 ->105 0.25636
96 ->106 0.11046
98 ->107 -0.16345
100 ->107 0.17645
101 ->109 0.15605
102 ->109 -0.13722
102 ->110 -0.13252
103 ->112 0.44231
104 ->113 0.14590

7. Full Listing for Text Reference (11)

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