Supplementary Information Material

for Organic & Biomolecular Chemistry

A facile synthesis of pyrrolo[2,3-*b*]quinolines via a Rh(I)-catalyzed carbodiimide-Pauson–Khand reaction

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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-EX 500, or a JEOL JNM-EX 300 instrument and chemical shifts are reported in ppm down field from tetramethylsilane (TMS) using an internal standard of TMS or $CDCl_3$. HRMS analysis were performed on a Bruker Daltonics microTOF. 2-Azidobenzaldehyde[17] and 1-(2-azidophenyl)-ethanone[18] were prepared according to the reported method.

Typical procedure for preparation of alcohols 7 and 8: 1-(2-Azidophenyl)-4,4-dimethylpent-2-yn-1-ol (7c).

Typical procedure for preparation of 9 and 10: 1-Azido-2-(but-2-ynyl)benzene (9b).

Typical procedure for preparation of 11: 1-Azido-2-(2-methoxypent-3-yn-2-yl)benzene (11a).

Typical procedure for preparation of iminophosphoranes 12–14: 2-(But-2-ynyl)-*N*-(triphenylphosphonylidene)-benzen-amine (12b).

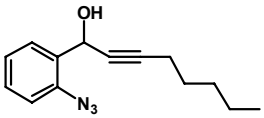
Typical procedure for preparation of carbodiimides 4, 5, and 6: (2-But-2-ynyl)propylcarbodiimide (4e).

Typical procedure for the catalytic Pauson–Khand reaction using $[Rh(CO)_2Cl]_2$-dppp to produce 15: 3-Pentyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15a) (Table 2, Entry 1).

Typical procedure for the catalytic Pauson–Khand reaction using $[Rh(CO)_2Cl]_2$ to produce 17 and 18 (Table 3, Entry 3), and 19a and 20.

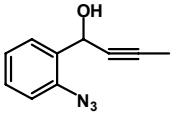
Typical procedure for preparation of alcohols 7 and 8: 1-(2-Azidophenyl)-4,4-dimethylpent-2-yn-1-ol (7c).
n-Butyllithium/*n*-hexane solution (1.6 M, 9.6 mL, 15.1 mmol) was added to a solution of 3,3-dimethyl-1-butyne (1.80 mL, 15.1 mmol) in THF (5 mL) at −78 °C. After stirring for 2 h, a solution of 2-azidobenzaldehyde (1.50 g, 10.1 mmol) in THF (10 mL) was added, and the mixture was stirred for a further 2 h. The mixture was quenched with saturated aqueous ammonium chloride and extracted with dichloromethane. The organic extracts were washed with brine, dried over anhydrous magnesium sulfate, and evaporated. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1:4) to give alcohol **7c** (2.18 g, 8.97 mmol, 89%) as a yellow oil.

1-(2-Azidophenyl)oct-2-yn-1-ol (7a). 99%



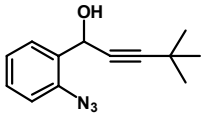
Brown oil.
IR (neat/ cm^{-1}): 3394, 2931, 2229, 2129, 1589, 1295.
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.66 (dd, J = 1.7, 7.8 Hz, 1H), 7.36 (ddd, J = 1.5, 7.3, 8.1 Hz, 1H), 7.19–7.15 (m, 2H), 5.64 (dt, J = 2.0, 6.0 Hz, 1H), 2.61–2.57 (m, 1H), 2.26 (dt, J = 2.0, 7.2 Hz, 2H), 1.58–1.50 (m, 2H), 1.27–1.41 (m, 4H), 0.90 (t, J = 7.1 Hz, 3H).
^{13}C NMR (125 MHz, $CDCl_3$, δ): 137.32 (C), 132.17 (C), 129.55 (CH), 128.35 (CH), 125.01 (CH), 118.23 (CH), 87.81 (C), 78.93 (C), 60.78 (CH), 31.04 (CH_2), 28.21 (CH_2), 22.14 (CH_2), 18.79 (CH_2), 13.93 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{14}H_{17}N_3NaO$, 266.1264; found, 266.1267.

1-(2-Azidophenyl)but-2-yn-1-ol (7b). 99%



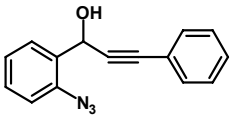
Yellow solid; mp: 50.0–51.5 °C.
IR (KBr/ cm^{-1}): 3301, 2291, 2129, 1581, 1303, 748.
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.65 (dd, J = 1.7, 8.0 Hz, 1H), 7.36 (ddd, J = 1.5, 7.2, 7.8 Hz, 1H), 7.20–7.12 (m, 2H), 5.64–5.56 (m, 1H), 2.80–2.68 (br, 1H), 1.90 (d, J = 2.2 Hz, 3H).
^{13}C-NMR (75 MHz, $CDCl_3$, δ): 137.15 (C), 132.05 (C), 129.50 (CH), 128.22 (CH), 124.99 (CH), 118.16 (CH), 83.03 (C), 78.17 (C), 60.60 (CH), 3.70 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{10}H_9N_3NaO$, 210.0638; found, 210.0633.
Anal calcd for $C_{10}H_9N_3O$: C 64.16, H 4.85, N 22.45, found: C 64.20, H 5.23, N 22.06.

1-(2-Azidophenyl)-4,4-dimethylpent-2-yn-1-ol (7c). 89%



Yellow oil.
IR (neat/ cm^{-1}): 2970, 2129, 1589, 1481, 1296, 987, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.68 (dd, J = 1.4, 7.9 Hz, 1H), 7.37 (ddd, J = 1.5, 7.8, 7.8 Hz, 1H), 7.20–7.14 (m, 2H), 5.65 (d, J = 5.8 Hz, 1H), 2.49 (dd, J = 2.4, 5.8 Hz, 1H), 1.26 (d, J = 0.5 Hz, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.53 (C), 132.23 (C), 129.62 (CH), 128.49 (CH), 125.03 (CH), 118.26 (CH), 95.99 (C), 77.30 (C), 60.65 (CH), 38.89 (CH_3×3), 27.51 (C).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{13}H_{15}N_3NaO$, 252.1107; found, 252.1105.

1-(2-Azidophenyl)-3-phenylprop-2-yn-1-ol (7d). 96%



Yellow oil.

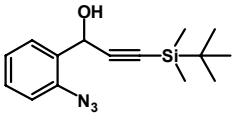
IR (neat/ cm^{-1}): 3016, 2237, 2114, 1589, 1489, 1296, 1026, 910, 756.

^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.73 (d, J = 7.8 Hz, 1H), 7.50–7.43 (m, 2H), 7.39 (ddd, J = 1.1, 7.8, 7.8 Hz, 1H), 7.34–7.27 (m, 3H), 7.20 (dd, J = 7.6 Hz, 1H), 7.19 (dd, J = 6.7, 6.7 Hz, 1H), 5.87 (d, J = 6.3 Hz, 1H), 2.79–2.71 (br, 1H),.

^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.46 (C), 131.77 (CH×2), 131.55 (C), 129.83 (CH), 128.60 (CH), 128.51 (CH), 128.27 (CH×2), 125.14 (CH), 122.35 (C), 118.37 (CH), 87.84 (C), 86.61 (C), 61.16 (CH).

HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{11}N_3NaO$, 272.0794; found, 272.0786.

1-(2-Azidophenyl)-3-(*tert*-butyldimethylsilanyl)prop-2-yn-1-ol (7e). 78%



Yellow oil.

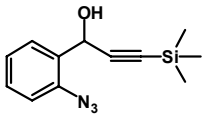
IR (neat/ cm^{-1}): 2954, 2854, 2129, 1728, 1466, 1296, 1041, 833, 756.

^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.67 (dd, J = 1.4, 7.8 Hz, 1H), 7.38 (ddd, J = 1.3, 7.7, 7.7 Hz, 1H), 7.18 (dd, J = 7.7, 7.7 Hz, 1H), 7.18 (d, J = 7.8 Hz, 1H), 5.65 (s, 1H), 2.68– 2.56 (br, 1H), 0.94 (s, 9H), 0.13 (d, J = 4.3 Hz, 6H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.53 (C), 131.41 (C), 129.79 (CH), 128.29 (CH), 125.06 (CH), 118.29 (CH), 104.67 (C), 90.04 (C), 61.03 (CH), 26.00 (CH_3×3), 16.53 (C), –4.73 (CH_3), –4.75 (CH_3).

HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{21}N_3NaOSi$, 310.1346; found, 310.1339.

1-(2-Azidophenyl)-3-(trimethylsilanyl)prop-2-yn-1-ol (7f). 80%



Yellow oil.

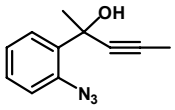
IR (neat/ cm^{-1}): 2962, 2129, 1589, 1489, 1296, 1041, 849, 756.

^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.67 (d, J = 7.9 Hz, 1H), 7.41-7.36 (m, 1H), 7.21–7.16. (m, 2H), 5.56 (dd, J = 1.8, 6.1 Hz, 1H), 2.66–2.57 (br, 1H), 0.20 (s, 9H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.55 (C), 131.31 (C), 129.82 (CH), 128.52 (CH), 125.10 (CH), 118.32 (CH), 103.90 (C), 91.71 (C), 60.94 (CH), –0.20 (CH_3×3).

HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{12}H_{15}N_3NaOSi$; 268.0877; found, 268.0874.

2-(2-Azidophenyl)pent-3-yn-2-ol (8a). 55%



Yellow oil.

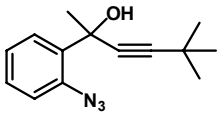
IR (neat/ cm^{-1}): 3055, 2129, 1473, 1265, 741.

^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.67(dd, J = 1.4, 7.8 Hz, 1H), 7.34 (ddd, J = 1.4, 7.7, 7.7 Hz, 1H), 7.19 (d, J = 7.9 Hz, 1H), 7.14 (ddd, J = 1.2, 7.6, 7.6 Hz, 1H), 3.82 (s, 1H), 1.90 (s, 3H), 1.86 (s, 3H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ): 136.58 (C), 135.67 (C), 128.96 (CH), 127.05 (CH), 124.91 (CH), 119.12 (CH), 82.21 (C), 80.83 (C), 69.14 (C), 30.44 (CH_3), 3.75 (CH_3).

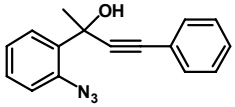
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{11}N_{11}N_3NaO$, 224.0794; found, 224.0789.

2-(2-Azidophenyl)-5,5-dimethylhex-3-yn-2-ol (8b). 80%



Yellow oil.
IR (neat/ cm^{-1}): 2970, 1805, 1627, 1473, 1365, 1196, 1119, 941, 748.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.69 (d, J = 7.9 Hz, 1H), 7.33 (dd, J = 7.6, 7.6 Hz, 1H), 7.19 (d, J = 7.8 Hz, 1H), 7.14 (dd, J = 7.6, 7.6 Hz, 1H), 3.71–3.67 (br, 1H), 1.84 (s, 3H), 1.25 (s, 9H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 136.66 (C), 136.10 (C), 128.88 (CH), 127.15 (CH), 124.89 (CH), 119.24 (CH), 93.58 (C), 81.56 (C), 69.25 (C), 30.96 (CH_3), 30.78 (CH_3×3), 27.39 (C).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{14}H_{17}N_3NaO$, 266.1264; found, 266.1254.

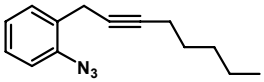
2-(2-Azidophenyl)-4-phenylbut-3-yn-2-ol (8c). 53%



Yellow oil.
IR (neat/ cm^{-1}): 3062, 2978, 2121, 1612, 1466, 1103, 995, 941, 725.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.70 (dd, J = 1.5, 7.9 Hz, 1H), 7.47–7.43 (m, 2H), 7.39–7.35 (m, 1H), 7.32–7.28 (m, 3H), 7.22 (dd, J = 1.1, 7.9 Hz, 1H), 7.17 (ddd, J = 1.2, 7.7, 7.7 Hz, 1H), 3.94 (s, 1H), 1.97 (s, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 136.80 (C), 135.24 (C), 131.71 (CH×2), 129.13 (CH), 128.36 (CH), 128.20 (CH×2), 126.86 (CH), 125.00 (CH), 122.63 (C), 119.22 (CH), 91.94 (C), 84.36 (C), 69.14 (C), 30.12 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{13}N_3NaO$, 286.0951; found, 286.0948.

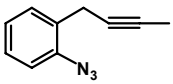
Typical procedure for preparation of 9 and 10: 1-Azido-2-(but-2-ynyl)benzene (9b).
Trifluoroacetic acid (0.22 mL, 3.0 mmol) was added to a mixture of alcohol **7b** (374 mg, 2.0 mmol) and triethylsilane (0.48 mL, 3.00 mmol) in dichloromethane (7 mL) at 0 °C. After stirring for 10 h at 0 °C, the mixture 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 alkyne **9b** (142 mg, 0.83 mmol, 41%) as a yellow solid.

1-Azido-2-(oct-2-ynyl)benzene (9a). 61%



Brown oil.
IR (neat/ cm^{-1}): 2931, 2121, 1581, 1288.
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.54 (d, J = 7.6 Hz, 1H), 7.28 (dd, J = 7.7, 7.7 Hz, 1H), 7.13 (dd, J = 7.7, 7.7 Hz, 1H), 7.12 (d, J = 7.8 Hz, 1H), 3.48 (t, J = 2.2 Hz, 2H), 2.22 (tt, J = 2.3, 7.1 Hz, 2H), 1.57–1.50 (m, 2H), 1.42–1.28 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H).
^{13}C NMR (125 MHz, $CDCl_3$, δ): 137.51 (C), 129.57 (CH), 128.93 (C), 127.82 (CH), 124.80 (CH), 117.74 (CH), 83.17 (C), 76.57 (C), 31.11 (CH_2), 28.70 (CH_2), 22.22 (CH_2), 20.59 (CH_2), 18.82 (CH_2), 14.0 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{14}H_{17}N_3Na$, 250.1315; found, 250.1312.

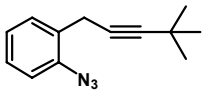
1-Azido-2-(but-2-ynyl)benzene (9b). 41%



Yellow solid; mp: 49.5–50.5 °C.
IR (KBr/ cm^{-1}): 2916, 2283, 2121, 1581, 1288, 748.

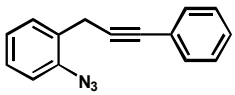
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.51 (d, J = 7.3 Hz, 1H), 7.26 (dd, J = 7.3, 7.5 Hz, 1H), 7.20–7.04 (m, 2H), 3.44 (s, 2H), 1.84 (d, J = 1.5 Hz, 3H).
^{13}C-NMR (75 MHz, $CDCl_3$, δ): 137.45 (C), 129.57 (CH), 128.75 (C), 127.81 (CH), 124.75 (CH), 117.69 (CH), 78.14 (C), 75.79 (C), 20.49 (CH_2), 3.52 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{10}H_9N_3Na$, 194.0689; found, 194.0691.

1-Azido-2-(4,4-dimethylpent-2-ynyl)benzene (9c). 85%



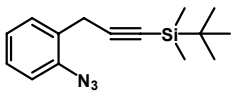
Yellow oil.
IR (neat/ cm^{-1}): 2970, 2121, 1705, 1581, 1489, 1288, 748.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.56 (d, J= 7.6 Hz, 1H), 7.28 (dd, J= 7.6, 7.6 Hz, 1H), 7.14 (dd, J= 7.6, 7.6 Hz, 1H), 7.11 (d, J= 7.7 Hz, 1H), 3.48 (s, 2H), 1.26 (s, 9H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 137.45 (C), 129.30 (CH), 128.95 (C), 127.71 (CH), 124.79 (CH), 117.63 (CH), 91.98 (C), 74.91 (C), 31.28 (CH_3×3), 27.50 (C), 20.39 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{13}H_{15}N_3Na$, 236.1158; found, 236.1159.

1-azido-2-(3-phenylprop-2-ynyl)benzene (9d). 51%



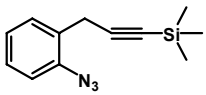
Colorless oil.
IR (neat/ cm^{-1}): 2954, 2121, 1589, 1489, 1288, 1072, 741.
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.58 (d, J = 7.4 Hz, 1H), 7.52–7.39 (m, 2H), 7.34–7.20 (m, 4H), 7.09 (dd, J = 7.7, 7.7 Hz, 2H), 3.71 (s, 2H).
^{13}C-NMR (75 MHz, $CDCl_3$, δ): 137.53 (C), 131.59 (CH×2), 129.55 (CH), 128.10 (CH×2), 128.01 (CH), 127.92 (C), 127.79 (CH), 124.82 (CH), 123.52 (C), 117.75 (CH), 86.61 (C), 83.01 (C), 21.12 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{11}N_3Na$, 256.0845, found 256.0842.

(3-(2-Azidophenyl)prop-1-ynyl)(*tert*-butyl)dimethylsilane (9e). 87%



Yellow oil.
IR (neat/ cm^{-1}): 2129, 1643, 1265, 833, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.57 (d, J = 7.6 Hz, 1H), 7.29 (dd, J = 7.6, 7.6 Hz, 1H), 7.14 (dd, J = 7.5, 7.5 Hz, 1H), 7.12 (d, J = 7.7 Hz, 1H), 3.57 (s, 2H), 0.95 (s, 9H), 0.13 (s, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.53 (C), 129.44 (CH), 127.97 (CH), 127.81 (C), 124.87 (CH), 117.74 (CH), 103.83 (C), 85.68 (C), 26.08 (CH_3×3), 21.64 (CH_2), 16.57 (C), -4.48 (CH_3×2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{21}N_3NaSi$, 294.1397; found, 294.1394.

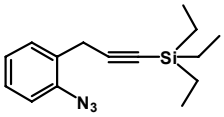
(3-(2-Azidophenyl)prop-1-ynyl)trimethylsilane (9f). 58%



Yellow oil.
IR (neat/ cm^{-1}): 2962, 2129, 1265, 849, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.54 (d, J = 7.6 Hz, 1H), 7.29 (dd, J = 7.6, 7.6 Hz, 1H), 7.14 (dd, J = 7.6, 7.6 Hz, 1H), 7.12 (d,

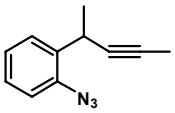
J = 7.6 Hz, 1H), 3.56 (s, 2H), 0.19 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.54 (C), 129.48 (CH), 128.01 (CH), 127.67 (C), 124.89 (CH), 117.77 (CH), 103.36 (C), 87.46 (C), 21.58 (CH_2), 0.07 (CH_3×3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{12}H_{16}N_3Si$, 230.1108; found, 230.1111.

(3-(2-Azidophenyl)prop-1-ynyl)triethylsilane (9g). 20%



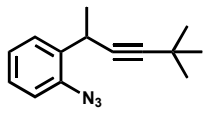
Yellow oil.
IR (neat/ cm^{-1}): 2952, 2120, 1254, 850, 746.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.59 (d, *J* = 7.7 Hz, 1H), 7.29 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.14 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.12 (d, *J* = 7.7 Hz, 1H), 3.58 (s, 2H), 1.01 (t, *J* = 7.9 Hz, 9H), 0.62 (q, *J* = 7.9 Hz, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.53 (C), 129.44 (CH), 127.95 (CH), 127.87 (C), 124.86 (CH), 117.72 (CH), 104.34 (C), 84.83 (C), 21.68 (CH_2), 7.47 (CH_2×3), 4.50 (CH_3×3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{15}H_{22}N_3Si$, 272.1578; found, 272.1575.

1-Azido-2-(pent-3-yn-2-yl)benzene (10a). 40%



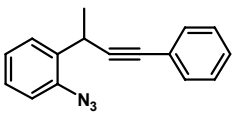
Yellow oil.
IR (neat/ cm^{-1}): 3054, 2121, 1265, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.59 (dd, *J* = 1.5, 7.7 Hz, 1H), 7.27 (ddd, *J* = 1.5, 7.7, 7.7 Hz, 1H), 7.14 (ddd, *J* = 1.2, 7.7, 7.7 Hz, 1H), 7.11 (dd, *J* = 1.2, 7.7 Hz, 1H), 3.99 (dq, *J* = 2.3, 2.4 Hz, 1H), 1.85 (d, *J* = 2.4 Hz, 3H), 1.37 (d, *J* = 7.1 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 136.57 (C), 135.23 (C), 128.40 (CH), 127.83 (CH), 125.02 (CH), 117.95 (CH), 81.58 (C), 77.25 (C), 26.62 (CH_3), 23.36 (CH), 3.60 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{11}H_{11}N_3Na$, 208.0845; found, 208.0841.

1-Azido-2-(1,4,4-trimethylpent-2-ynyl)benzene (10b). 47%



Yellow oil.
IR (neat/ cm^{-1}): 3055, 2970, 2129, 1265, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.61 (dd, *J* = 1.3, 7.7 Hz, 1H), 7.26 (ddd, *J* = 1.4, 7.6, 7.6 Hz, 1H), 7.13 (ddd, *J* = 1.1, 7.5, 7.5 Hz, 1H), 7.10 (dd, *J* = 1.1, 7.8 Hz, 1H), 3.99 (q, *J* = 7.0 Hz, 1H), 1.34 (d, *J* = 7.0 Hz, 3H), 1.24 (d, *J* = 0.5 Hz, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 136.55 (C), 135.64 (C), 128.43 (CH), 127.70 (CH), 124.99 (CH), 117.86 (CH), 90.88 (C), 80.77 (C), 31.33 (CH_3×3), 27.39 (C), 26.70 (CH_3), 23.94 (CH).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{14}H_{17}N_3Na$, 250.1315; found, 250.1307.

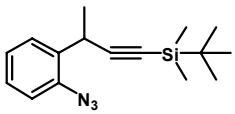
1-Azido-2-(4-phenylbut-3-yn-2-yl)benzene (10c). 35%



Yellow oil.
IR (neat/ cm^{-1}): 2978, 2129, 1581, 1489, 1296, 741.
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.67 (d, *J* = 7.6 Hz, 1H), 7.47–7.40 (m, 2H), 7.33–7.25 (m, 4H), 7.16 (dd, *J* = 7.7, 7.7 Hz, 2H), 4.26 (q, *J* = 7.0 Hz, 1H), 1.50 (d, *J* = 7.0 Hz, 3H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ): 136.66 (C), 134.59 (C), 131.63 (CH×2), 128.52 (CH), 128.20 (CH×2), 128.04 (CH), 127.79 (CH), 125.13 (CH), 123.62 (C), 118.03 (CH), 92.18 (C), 82.11 (C), 27.29 (CH), 23.25 (CH_3)
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{13}N_3Na$, 270.1002; found, 270.1002.

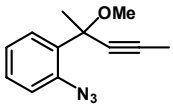
(3-(2-Azidophenyl)but-1-ynyl)(tert-butyl)dimethylsilane (10d). 39%



Yellow oil.
IR (neat/ cm^{-1}): 2931, 2121, 1458, 1288, 833, 771.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.61 (d, J = 7.7 Hz, 1H), 7.28 (dd, J = 7.7, 7.7 Hz, 1H), 7.14 (dd, J = 7.7, 7.7 Hz, 1H), 7.12 (d, J = 8.0 Hz, 1H), 4.07 (q, J = 7.0 Hz, 1H), 1.40 (d, J = 7.1 Hz, 3H), 0.95 (s, 9H), 0.11 (d, J = 3.4 Hz, 6H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 136.59 (C), 134.42 (C), 128.45 (CH), 127.96 (CH), 125.05 (CH), 117.94 (CH), 109.62 (C), 84.27 (C), 27.78 (CH_3), 26.08 (CH_3×3), 23.50 (CH), 16.59 (C), −4.49 (CH_3×2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{23}N_3NaSi$, 308.1553; found, 308.1560.

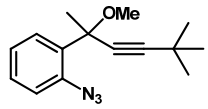
Typical procedure for preparation of 11: 1-Azido-2-(2-methoxypent-3-yn-2-yl)benzene (11a).
A solution of azide alcohol **8a** (2.44 g, 12.1 mmol) in THF (5 mL) was added to a cold (–50 °C) stirred suspension of 60% NaH (726 mg, 18.1 mmol) in THF (15 mL). After stirring for 10 min, methyl iodide (1.1 mL, 18.1 mmol) was added. The mixture was allowed to warm to room temperature, stirred for a further 3 h then quenched with water. The resulting mixture was extracted with dichloromethane, dried over anhydrous magnesium sulfate, and evaporated. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1:4) to provide methyl ether **11a** as a yellow oil (2.30 g, 88%).

1-Azido-2-(2-methoxypent-3-yn-2-yl)benzene (11a).



Yellow oil.
IR (neat/ cm^{-1}): 2931, 2121, 1481, 1296, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.80(dd, J = 1.5, 7.8 Hz, 1H), 7.34 (ddd, J = 1.6, 7.8, 7.8 Hz, 1H), 7.20 (dd, J = 1.1, 7.9 Hz, 1H), 7.13 (ddd, J = 1.0, 7.6, 7.6 Hz, 1H), 3.22 (s, 3H), 1.98 (s, 3H), 1.83 (s, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.18 (C), 132.55 (C), 129.64 (CH), 129.13 (CH), 124.39 (CH), 119.58 (CH), 83.39 (C), 79.30 (C), 76.26 (C), 52.18 (CH_3), 29.11 (CH_3), 3.63 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{12}N_{13}N_3NaO$, 238.0951; found, 238.0949.

1-Azido-2-(2-methoxy-5,5-dimethylhex-3-yn-2-yl)benzene (11b).



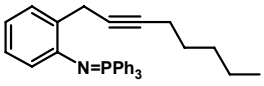
Yellow oil.
IR (neat/ cm^{-1}): 2970, 2121, 1473, 1219, 1126, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.70 (dd, J = 1.6, 7.8 Hz, 1H), 7.34 (ddd, J = 1.5, 7.6, 7.6 Hz, 1H), 7.20 (dd, J = 1.2, 7.9 Hz, 1H), 7.13 (ddd, J = 1.2, 7.6, 7.6 Hz, 1H), 3.21 (s, 3H), 1.81 (s, 3H), 1.30 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.33 (C), 133.02 (C), 129.57 (CH), 129.05 (CH), 124.40 (CH), 119.72 (CH), 96.49 (C), 78.59 (C), 76.10 (C), 52.11 (CH_3), 31.03 (CH_3×3), 29.38 (CH_3), 27.57 (C).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{19}N_3NaO$, 280.1420; Found, 280.1413.

Typical procedure for preparation of iminophosphoranes 12–14: 2-(But-2-ynyl)-*N*-(triphenylphosphonylidene)-

benzen-amine (12b).

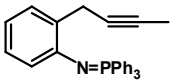
Triphenylphosphine (228.7 mg, 0.82 mmol) was added to a solution of alkynyl azide **9b** (135.7 mg, 0.79 mmol) in dichloromethane (5 mL) at room temperature. After stirring for 10 h, the mixture was concentrated under reduced pressure. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1:4) to give iminophosphorane **12b** (318.8 mg, 0.78 mmol, 99%) as a yellow solid.

2-(Oct-2-ynyl)-*N*-(triphenylphosphonylidene)benzenamine (12a). 87%



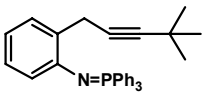
Yellow solid; mp: 78.6–80.3 °C.
IR (KBr/ cm^{-1}): 2923, 1581, 1481, 1311.
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.74 (dd, J = 8.0, 11.5 Hz, 6H), 7.49 (dd, J = 7.4, 7.4 Hz, 3H), 7.45–7.35 (m, 7H), 6.78 (dd, J = 7.5, 7.5 Hz, 1H), 6.68 (dd, J = 7.2, 7.2 Hz, 1H), 6.42 (d, J = 7.6 Hz, 1H), 3.88 (s, 2H), 2.28–2.14 (m, 2H), 1.52 (tt, J = 7.0, 7.0 Hz, 2H), 1.44–1.23 (m, 4H), 0.87 (t, J = 7.2 Hz, 3H).
^{13}C NMR (125 MHz, $CDCl_3$, δ): 148.54 (C), 132.52 (CH×6, d, J = 9.6 Hz), 131.70 (C, d, J = 22.2 Hz), 131.62 (C×3, d, J = 99.8 Hz), 131.50 (CH×3, d, J = 2.6 Hz), 128.50 (CH×6, d, J = 11.6 Hz), 127.90 (CH), 126.35 (CH), 120.28 (CH, d, J = 10.3 Hz), 117.20 (CH), 82.11 (C), 79.33 (C), 31.15 (CH_2), 28.96 (CH_2), 22.34 (CH_2), 22.23 (CH_2), 18.98 (CH_2), 13.98 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{32}H_{33}NP$, 462.2345; found, 462.2349.

2-(But-2-ynyl)-*N*-(triphenylphosphonylidene)benzenamine (12b).



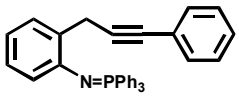
Yellow solid; mp: 139.6–141.0 °C.
IR (KBr/ cm^{-1}): 3047, 1589, 1481, 1442, 1342, 1103, 748.
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.84–7.68 (m, 6H), 7.55–7.35 (m, 10H), 6.78 (dd, J = 7.1, 7.1 Hz, 1H), 6.67 (dd, J = 7.1, 7.1 Hz, 1H), 6.49–6.38 (m, 1H), 3.85 (s, 2H), 1.83 (dd, J = 2.1, 2.1 Hz, 3H).
^{13}C-NMR (75 MHz, $CDCl_3$, δ): 148.54 (C), 132.49 (CH×6, d, J = 9.7 Hz), 131.63 (C×3, d, J = 100.0 Hz), 131.59 (C, d, J = 21.7 Hz), 131.50 (CH×3, d, J = 2.6 Hz), 128.49 (CH×6, d, J = 11.9 Hz), 127.92 (CH), 126.39 (CH), 120.36 (CH, d, J = 9.5 Hz), 117.23 (CH), 78.61 (C), 77.00 (C), 22.24 (CH_2), 3.67 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{28}H_{25}NP$, 406.1719; found, 406.1718.
Anal calcd for $C_{28}H_{24}NP$: C 82.94, H 5.97, N 3.45, found: C 82.56, H 6.05, N 3.43.

2-(4,4-Dimethylpent-2-ynyl)-*N*-(triphenylphosphonylidene)benzenamine (12c). 97%



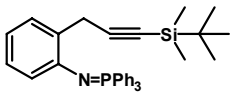
White solid; mp: 143–145 °C.
IR (KBr/ cm^{-1}): 3054, 2962, 1897, 1589, 1481, 1349, 717.
^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.69–7.79 (m, 6H), 7.36–7.52 (m, 10H), 6.77 (t, J= 7.31 Hz, 1H), 6.67 (t, J= 7.2 Hz, 1H), 6.41 (d, J= 8.3 Hz, 1H), 3.88 (s, 2H), 1.25 (s, 9H).
^{13}C NMR (125 MHz, $CDCl_3$, δ): 148.60 (C), 132.51 (CH×6, d, J = 9.5 Hz), 131.71 (C, d, J = 22.5 Hz), 131.57 (C×3, d, J = 99.8 Hz), 131.53 (CH×3), 128.51 (CH×6, d, J = 12.2 Hz), 127.70 (CH), 126.27 (CH), 120.10 (CH , d, J = 9.8 Hz), 117.08 (CH), 90.86 (C), 77.77 (C), 31.50 (CH_3×3), 27.51 (C), 22.25 (CH_2).
HRMS-ESI (*m/z*): $[M+H^+]$ calcd for $C_{31}H_{31}NP$, 448.2189; found, 448.2194.

2-(3-Phenylprop-2-ynyl)-*N*-(triphenylphosphonylidene)benzenamine (12d). 99%



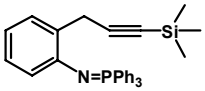
Brown solid; mp: 121.3–123.6 °C.
IR (KBr/ cm^{-1}): 3055, 2222, 1589, 1481, 1442, 1349, 1111, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.81–7.73 (m, 6H), 7.54–7.48 (m, 4H), 7.46–7.36 (m, 8H), 7.26–7.20 (m, 3H), 6.81 (ddd, J = 1.5, 7.4, 7.4 Hz, 1H), 6.67 (dd, J = 7.4, 7.4 Hz, 1H), 6.45 (d, J = 7.8 Hz, 1H), 4.12 (s, 2H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 148.78 (C), 132.54 (CH×6, d, J = 9.3 Hz), 131.60 (CH×2), 131.56 (CH×3, d, J = 2.6 Hz), 131.51 (C, d, J = 99.6 Hz), 130.90 (C×3, d, J = 22.5 Hz), 128.55 (CH×6, d, J = 12.1 Hz), 128.17 (CH), 128.06 (CH×2), 127.23 (CH), 126.67 (CH), 124.48 (C), 120.42 (CH, d, J = 9.8 Hz), 117.26 (CH), 90.13 (C), 82.00 (C), 23.11 (CH_2).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{33}H_{27}NP$, 468.1876; found, 468.1875.
Anal calcd for $C_{33}H_{26}NP$: C 84.77, H 5.61, N 3.00, found: C 84.37, H 5.95, N 2.93.

2-(3-(*tert*-Butyldimethylsilyl)prop-2-ynyl)-*N*-(triphenylphosphonylidene)benzenamine (12e). 94%



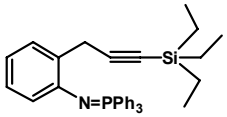
Yellow solid; mp: 159.9–160.3 °C.
IR (KBr/ cm^{-1}): 3055, 2947, 2854, 2168, 1589, 1481, 1342, 1111, 1018, 833, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.74 (dd, J = 9.4, 9.4 Hz, 6H), 7.60–7.33 (m, 10H), 6.79 (dd, J = 6.8, 6.8 Hz, 1H), 6.68 (dd, J = 6.6, 6.6 Hz, 1H), 6.41 (d, J = 6.9 Hz, 1H), 3.98 (s, 2H), 0.96 (s, 9H), 0.11 (s, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 148.61 (C), 132.49 (CH×6, d, J = 9.3 Hz), 131.54 (CH×3, d, J = 1.8 Hz), 131.47 (C×3, d, J = 99.6 Hz), 130.54 (C), 128.53 (CH×6, d, J = 11.9 Hz), 127.88 (CH), 126.50 (CH), 120.14 (CH, d, J = 10.1 Hz), 117.10 (CH), 107.48 (C), 84.07 (C), 26.19 (CH_3×3), 23.53 (CH_2), 16.59 (C), –4.29 (CH_3×2).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{33}H_{37}NPSi$, 506.2427; found, 506.2424.

2-(3-(Trimethylsilyl)prop-2-ynyl)-*N*-(triphenylphosphonylidene)benzenamine (12f). 94%



Yellow solid; mp: 105.6–107.3 °C.
IR (KBr/ cm^{-1}): 3055, 2954, 2175, 1589, 1481, 1358, 1103, 841, 748, 694.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.78–7.72 (m, 6H), 7.51 (dd, J = 7.4 Hz, 3H), 7.46 (d, J = 7.5 Hz, 1H), 7.43 (dd, J = 7.4, 7.4 Hz, 6H), 6.79 (ddd, J = 1.2, 7.5, 7.5 Hz, 1H), 6.68 (dd, J = 7.4, 7.4 Hz, 1H), 6.41 (d, J = 7.7 Hz, 1H), 3.95 (s, 2H), 0.15 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 148.68 (C), 132.53 (CH×6, d, J = 9.8 Hz), 131.55 (C×3, d, J = 2.6 Hz), 131.48 (C×3, d, J = 99.3 Hz), 130.45 (C, d, J = 22.5 Hz), 128.53 (CH×6, d, J = 12.4 Hz), 127.97 (CH, d, J = 2.1 Hz), 126.60 (CH), 120.28 (CH, d, J = 9.8 Hz), 117.18 (CH), 107.09 (C), 85.74 (C), 23.59 (CH_2), 0.25 (CH_3×3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{30}H_{31}NPSi$, 464.1958; found, 464.1964.

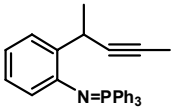
2-(3-(Triethylsilyl)prop-2-ynyl)-*N*-(triphenylphosphonylidene)benzenamine (12g). 92%



Yellow solid; mp: 96.3–99.5 °C.
IR (KBr/ cm^{-1}): 2946, 2869, 2168, 1589, 1481, 1358, 1103, 1018, 709.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.78–7.71 (m, 6H), 7.56–7.47 (m, 4H), 7.46–7.39 (m, 6H), 6.79 (ddd, J = 1.3, 7.5, 7.5 Hz, 1H), 6.68 (dd, J = 7.4, 7.4 Hz, 1H), 6.41 (d, J = 7.7 Hz, 1H), 3.98 (s, 2H), 1.01 (t, J = 7.9 Hz, 9H), 0.61 (q, J = 7.9 Hz, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 132.51 (CH×6, d, J = 9.6 Hz), 131.57 (CH×3, d, J = 1.6 Hz), 131.48 (C×3, d, J = 96.7 Hz),

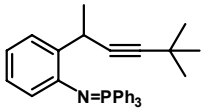
130.69 (C), 130.52 (C), 128.56 (CH×6, d, J = 12.4 Hz), 127.88 (CH, d, J = 1.6 Hz), 126.48 (CH), 120.20 (CH), 117.17 (CH), 107.91 (C), 83.33(C), 23.54 (CH_2), 7.55 (CH_2×3), 4.66 (CH_3×3).
HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{33}H_{37}NPSi$, 506.2427; found, 506.2427.

2-(Pent-3-yn-2-yl)-*N*-(triphenylphosphonylidene)benzenamine (13a). 99%



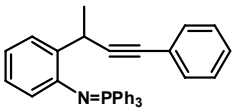
Yellow solid; mp: 144.0–144.3 °C.
IR (KBr/ cm^{-1}): 3062, 2916, 1589, 1481, 1350, 1103, 694.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.80–7.67 (m, 6H), 7.55–7.47 (m, 4H), 7.45–7.35 (m, 6H), 6.79–6.72 (m, 1H), 6.70–6.64 (m, 1H), 6.45–6.37 (m, 1H), 4.81–4.69 (m, 1H), 1.85 (dd, J = 2.4, 2.4 Hz, 3H), 1.49 (s, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 147.61 (C), 137.78 (C, d, J = 22.0 Hz), 132.48 (CH×6, d, J = 9.31 Hz), 131.63 (C×3, d, J = 99.3 Hz), 131.47 (CH×3, d, J = 2.6 Hz), 128.50 (CH×6, d, J = 12.2 Hz), 126.84 (CH), 126.36 (CH), 120.73 (CH, d, J = 10.1 Hz), 117.32 (CH), 84.26 (C), 75.87 (C), 27.42 (CH_3), 22.89 (CH), 3.70 (CH_3).
HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{29}H_{27}NP$, 420.1876; found, 420.1867.

2-(5,5-Dimethylhex-3-yn-2-yl)-*N*-(triphenylphosphonylidene)benzenamine (13b). 66%



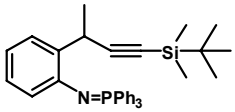
Yellow solid; mp: 162.8–163.0 °C.
IR (KBr/cm^{-1}): 3055, 2962, 1589, 1481, 1350, 1110, 1018, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.80–7.69 (m, 6H), 7.56–7.47 (m, 4H), 7.47–7.38 (m, 6H), 6.76 (dd, J = 7.7, 7.4 Hz, 1H), 6.68 (dd, J = 7.3, 7.3 Hz, 1H), 6.39 (d, J = 7.9 Hz, 1H), 4.72 (q, J = 7.0 Hz, 1H), 1.49 (d, J = 6.9 Hz, 3H), 1.26 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 147.62 (C), 138.03 (C), 132.50 (CH×6, d, J = 9.8 Hz), 131.60 (C×3, d, J = 99.6 Hz), 131.47 (CH×3, J = 2.6 Hz), 128.51 (CH×6, J = 12.2 Hz), 126.88 (CH), 126.25 (CH), 126.58 (CH, J = 10.4 Hz), 117.19 (CH), 89.76 (C), 83.39 (C), 31.59 (CH_3×3), 27.49 (CH), 27.45 (C), 23.25 (CH_3).
HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{32}H_{33}NP$, 462.2345; found, 462.2350.

2-(4-Phenylbut-3-yn-2-yl)-*N*-(triphenylphosphonylidene)benzenamine (13c). 98%



Yellow solid; mp: 56.2–56.7 °C.
IR (KBr/ cm^{-1}): 3055, 2970, 2222, 1589, 1481, 1342, 1111, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.86–7.15 (m, 21H), 6.73 (d, J = 4.3 Hz, 2H), 6.44 (s, 1H), 5.01 (s, 1H), 1.63 (s, 3H)
^{13}C-NMR (125 MHz, $CDCl_3$,δ): 147.77 (C), 137.06 (C, d, J = 22.5 Hz), 132.46 (CH×6, d, J = 9.3 Hz), 131.55 (CH×3, d, J = 7.2), 131.52 (CH×2), 131.46 (C×3, d, J = 99.3 Hz), 128.53 (CH×6, d, J = 11.9 Hz), 128.02 (CH×2), 127.15 (CH), 126.94 (CH), 126.57 (CH), 124.52 (C), 120.74 (CH, d, J = 10.1 Hz), 117.35 (CH), 95.43 (C), 81.09 (C), 28.11 (CH), 25.56 (CH_3).
HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{34}H_{29}NP$, 482.2032; found, 482.2032.

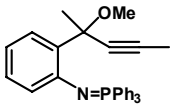
2-(4-(*tert*-Butyldimethylsilyl)but-3-yn-2-yl)-*N*-(triphenylphosphonylidene)benzenamine (13d). 80%



Yellow solid; mp: 45.2–46.0 °C.
IR (KBr/ cm^{-1}): 3055, 2954, 2854, 2160, 1589, 1481, 1350, 1111, 833, 687.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.82–7.73 (m, 6H), 7.62–7.57 (m, 1H), 7.53–7.49 (m, 3H), 7.47–7.41 (m, 6H), 6.79 (dd, J =

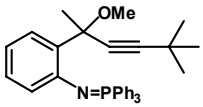
7.5, 7.5 Hz, 1H), 6.71 (dd, *J* = 7.4, 7.4 Hz, 1H), 6.49 (d, *J* = 7.8 Hz, 1H), 4.90-4.83 (m, 1H), 1.58 (d, *J* = 6.8 Hz, 3H), 1.01 (s, 9H), 0.15 (s, 6H).
^{13}C-NMR (150 MHz, $CDCl_3$, *δ*): 147.62 (C), 136.90 (C, d, *J* = 22.2 Hz), 132.43 (CH×6, d, *J* = 9.6 Hz), 131.52 (CH×3, d, *J* = 2.7 Hz), 131.40 (C×3, d, *J* = 100.2 Hz), 128.52 (CH×6, d, *J* = 12.1 Hz), 126.92 (CH), 126.47 (CH), 120.60 (CH, d, *J* = 10.2 Hz), 117.25 (CH), 113.05 (C), 82.62 (C), 28.64 (CH), 26.20 (CH_3×3), 22.92 (CH_3), 16.64 (C), –4.28 (CH_3×2).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{34}H_{39}NPSi$, 520.2584; found, 520.2592.

2-(2-Methoxypent-3-yn-2-yl)-*N*-(triphenylphosphonylidene)benzenamine (14a).



Yellow solid; mp: 140.9–141.3 C.
IR (KBr/ cm^{-1}): 3055, 2977, 2931, 2245, 1913, 1581, 1473, 1342, 1111, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, *δ*): 7.91–7.80 (m, 6H), 7.65–7.59 (m, 1H), 7.50–7.36 (m, 9H), 6.84–6.77 (m, 1H), 6.67–6.60 (m, 1H), 6.46–6.40 (m, 1H), 3.37 (s, 3H), 2.09 (s, 3H), 1.70 (s, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, *δ*): 134.11 (C, d, *J* = 22.2), 132.57 (CH×6, d, *J* = 9.8 Hz), 132.00 (C, d, *J* = 9.8 Hz), 131.80 (C×3, d, *J* = 99.8 Hz), 131.28 (CH×3), 128.39 (CH×6, d, *J* = 11.9 Hz), 127.49 (CH), 127.47 (CH), 122.29 (CH, d, *J* = 11.6 Hz), 116.29 (CH), 81.72 (C), 80.46 (C), 77.07 (C), 51.80 (CH_3), 27.56 (CH_3), 3.55 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{30}H_{29}NOP$, 450.1981; found, 450.1986.

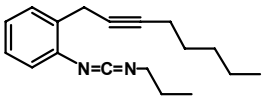
2-(2-Methoxy-5,5-dimethylhex-3-yn-2-yl)-*N*-(triphenylphosphonylidene)benzenamine (14b).



Yellow solid; mp: 94.9–96.0 °C.
IR (KBr/cm^{-1}): 3055, 2970, 1589, 1473, 1442, 1342, 1111, 856, 748, 717.
^{1}H-NMR (500 MHz, $CDCl_3$, *δ*): 7.88–7.82 (m, 6H), 7.63 (ddd, *J* = 2.0, 2.0, 7.0 Hz, 1H), 7.52–7.47 (m, 3H), 7.46–7.40 (m, 6H), 6.80 (ddd, *J* = 1.6, 7.5, 7.5 Hz, 1H), 6.63 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.40 (d, *J* = 7.7 Hz, 1H), 3.33 (s, 3H), 2.07 (s, 3H), 1.16 (d, *J* = 0.5 Hz, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, *δ*): 135.96 (C), 133.95 (C), 132.74 (CH×6, d, *J* = 10.3 Hz), 131.78 (C×3, d, *J* = 99.6 Hz), 131.35 (CH), 131.33 (CH×3, *J* = 2.3 Hz), 128.46 (CH×6, *J* = 12.4 Hz), 127.96 (CH), 127.51 (CH), 116.11 (CH), 100.56 (C), 93.50 (C), 77.34 (C), 51.77 (CH_3), 31.18 (CH_3×3), 27.76 (CH_3), 27.46 (C).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{33}H_{35}NOP$, 492.2451; Found, 492.2450.

Typical procedure for preparation of carbodiimides 4, 5, and 6: (2-But-2-ynyl)propylcarbodiimide (4e).
Propyl isocyanate (0.16 mL, 1.66 mmol) was added to a solution of iminophosphorane **12b** (446.0 mg, 1.10 mmol) in dichloromethane (5 mL) at room temperature. After stirring 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 carbodiimide **4e** (220.3 mg, 1.03 mmol, 94%) as a colorless oil.

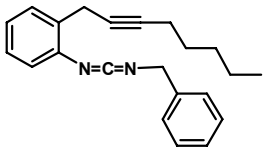
(2-Oct-2-ynylphenyl)propylcarbodiimide (4a). 95%



Colorless oil.
IR (neat/ cm^{-1}): 2314, 2136, 1265, 740.
^{1}H-NMR (500 MHz, $CDCl_3$, *δ*): 7.52 (d, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 7.14–7.07 (m, 2H), 3.60 (dd, *J* = 2.3, 2.3 Hz,

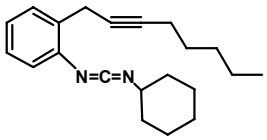
2H), 3.38 (t, J = 6.8 Hz, 2H), 2.22 (tt, J = 2.4, 7.2 Hz, 2H), 1.70 (tq, J = 7.1, 7.4 Hz, 2H), 1.53 (tq, J = 7.2, 7.6 Hz, 2H), 1.42–1.28 (m, 4H), 1.01 (t, J = 7.4 Hz, 3H), 0.90 (t, J = 7.2 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.36 (C), 135.31 (C), 131.30 (C), 129.01 (CH), 127.37 (CH), 124.58 (CH), 123.57 (CH), 82.86 (C), 77.18 (C), 48.59 (CH_2), 31.13 (CH_2), 28.76 (CH_2), 24.73 (CH_2), 22.22 (CH_2), 21.27 (CH_2), 18.86 (CH_2), 14.00 (CH_3), 11.45 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{24}N_2Na$, 291.1832; found, 291.1842.

Benzyl-(2-oct-2-ynylphenyl)carbodiimide (4b). 67%



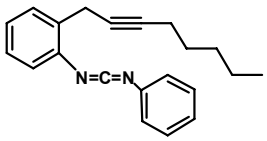
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2137, 1219, 771.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.50 (d, J = 7.3 Hz, 1H), 7.39–7.34 (m, 4H), 7.33–7.28 (m, 1H), 7.12 (dddd, J = 1.7, 7.4, 7.4, 7.4 Hz, 1H), 7.09 (dddd, J = 1.4, 7.5, 7.5, 7.5 Hz, 1H), 6.97 (dd, J = 1.5, 7.5 Hz, 1H), 4.56 (s, 2H), 3.54 (t, J = 2.4 Hz, 2H), 2.21 (tt, J = 2.4, 7.1 Hz, 2H), 1.53 (tt, J = 7.4, 7.4 Hz, 2H), 1.42-1.28 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.85 (C), 137.60 (C), 136.46 (C), 131.38 (C), 128.98 (CH), 128.76 (CH×2), 127.77 (CH), 127.37 (CH×3), 124.90 (CH), 123.86 (CH), 82.94 (C), 77.02 (C), 50.47 (CH_2), 31.11 (CH_2), 28.73 (CH_2), 22.21 (CH_2), 21.29 (CH_2), 18.84 (CH_2), 13.99 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{24}N_2Na$, 339.1832; found, 339.1830.

Cyclohexyl-(2-oct-2-ynylphenyl)carbodiimide (4c). 85%



Colorless oil.
IR (neat/ cm^{-1}): 2854, 2129, 1643, 1265, 741.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.53 (d, J = 7.6 Hz, 1H), 7.18 (ddd, J = 1.5, 7.5, 7.5 Hz, 1H), 7.13 (dd, J = 1.3, 7.7 Hz, 1H), 7.10 (ddd, J = 1.5, 7.5, 7.5 Hz, 1H), 3.60 (dd, J = 2.4, 2.4 Hz, 2H), 3.50–3.44 (m, 1H), 2.22 (tt, J = 2.4, 7.2 Hz, 2H), 2.04–1.97 (m, 2H), 1.80–1.74 (m, 2H), 1.60–1.44 (m, 6H), 1.41–1.30 (m, 6H), 0.90 (t, J = 7.3 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.55 (C), 135.48 (C), 131.25 (C), 128.98 (CH), 127.37 (CH), 124.53 (CH), 123.34 (CH), 82.84 (C), 77.21 (C), 56.58 (CH), 34.93 (CH_2×2), 31.12 (CH_2), 28.76 (CH_2), 25.32 (CH_2×2), 24.39 (CH_2), 22.22 (CH_2), 21.23 (CH_2), 18.86 (CH_2), 14.00 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{28}N_2Na$, 331.2145; found, 331.2150.

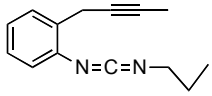
(2-Oct-2-ynylphenyl)phenylcarbodiimide (4d). 83%



Colorless oil.
IR (neat/ cm^{-1}): 2924, 2144, 1643, 1265, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.55 (d, J = 7.6 Hz, 1H), 7.35–7.30 (m, 2H), 7.22–7.14 (m, 6H), 3.67 (dd, J = 2.3, 2.3 Hz, 2H), 2.21 (tt, J = 2.4, 7.2 Hz, 2H), 1.52 (tq, J = 7.4, 7.4 Hz, 2H), 1.42–1.28 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.62 (C), 136.13 (C), 131.86 (C), 129.48 (CH×2), 129.28 (CH), 127.63 (CH), 125.73 (CH), 125.60 (C), 125.43 (CH,), 124.64 (CH), 124.12 (CH×2), 83.21 (C), 76.75 (C), 31.13 (CH_2), 28.71 (CH_2), 22.22 (CH_2), 21.67 (CH_2), 18.85 (CH_2), 14.00 (CH_3).

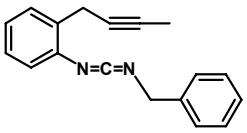
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{21}H_{23}N_2$, 303.1856; found, 303.1858.

(2-But-2-ynyl)propylcarbodiimide (4e). 94%



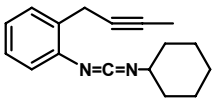
Colorless oil.
IR (neat/ cm^{-1}): 2970, 2877, 2144, 1496, 1265, 1088, 740.
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.49 (d, J = 7.4 Hz, 1H), 7.25–7.04 (m, 3H), 3.61–3.54 (m, 2H), 3.36 (t, J = 6.8 Hz, 2H), 1.84 (dd, J = 2.6, 2.6 Hz, 3H), 1.69 (tq, J = 7.1, 7.1 Hz, 2H), 1.00 (t, J = 7.3 Hz, 3H).
^{13}C-NMR (75 MHz, $CDCl_3$, δ): 138.33 (C), 135.20 (C), 131.11 (C), 129.02 (CH), 127.38 (CH), 124.52 (CH), 123.54 (CH), 77.75 (C), 76.38 (C), 48.48 (CH_2), 24.65 (CH_2), 21.17 (CH_2), 11.37 (CH_3), 3.56 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{14}H_{17}N_2$, 213.1386; found, 213.1385.

Benzyl-((2-but-2-ynyl)phenyl)carbodiimide (4f). 85%



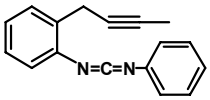
Colorless oil.
IR (neat/ cm^{-1}): 3055, 2923, 2136, 1589, 1496, 1450, 1265, 746.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.47 (d, J = 7.2 Hz, 1H), 7.37 (d, J = 4.4 Hz, 4H), 7.31 (dt, J = 4.0, 4.4 Hz, 1H), 7.13 (ddd, J = 1.4, 7.3, 7.3 Hz, 1H), 7.08 (ddd, J = 1.3, 7.4, 7.4 Hz, 1H), 6.97 (d, J = 7.6 Hz, 1H), 4.57 (s, 2H), 3.51 (dd, J = 2.5, 5.0 Hz, 2H), 1.84 (t, J = 2.5 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 137.86 (C), 137.65 (C), 136.46 (C), 131.28 (C), 129.08 (CH), 128.77 (CH×2), 127.78 (CH), 127.46 (CH), 127.38 (CH×2), 124.94 (CH), 123.93 (CH), 77.92 (C), 76.31 (C), 50.47 (CH_2), 21.26 (CH_2), 3.64 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{16}N_2Na$, 283.1206; found, 283.1207.

((2-But-2-ynyl)phenyl)cyclohexylcarbodiimide (4g). 74%



Colorless oil.
IR (neat/ cm^{-1}): 2931, 2306, 2129, 1736, 1265, 741.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.50 (d, J = 7.5 Hz, 1H), 7.18 (dd, J = 7.8, 7.8 Hz, 1H), 7.13 (dd, J = 1.2, 7.8 Hz, 1H), 7.09 (ddd, J = 1.1, 7.5, 7.5 Hz, 1H), 3.57 (dd, J = 2.4, 5.0 Hz, 2H), 3.52–3.42 (m, 1H), 2.06–1.97 (m, 2H), 1.86 (dd, J = 2.6, 2.6 Hz, 3H), 1.81–1.73 (m, 2H), 1.60–1.54 (m, 1H), 1.53–1.44 (m, 2H), 1.38–1.30 (m, 2H), 1.30–1.21 (m, 1H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.57 (C), 135.48 (C), 131.14 (C), 129.06 (CH), 127.44 (CH), 124.56 (CH), 123.40 (CH), 77.82 (C), 76.49 (C), 56.58 (CH), 34.94 (CH_2×2), 25.32 (CH_2×2), 24.38 (CH_2), 21.21(CH_2), 3.65(CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{20}N_2Na$, 275.1519; found, 275.1521.

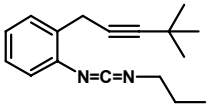
((2-But-2-ynyl)phenyl)phenylcarbodiimide (4h). 71%



Colorless oil.
IR (neat/ cm^{-1}): 2924, 2144, 1643, 910, 733.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.53 (d, J = 7.5 Hz, 1H), 7.37–7.29 (m, 2H), 7.24–7.14 (m, 6H), 3.64 (dd, J = 2.5, 5.1 Hz, 2H), 1.84 (dd, J = 2.6, 2.6 Hz, 3H).

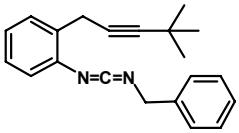
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.57 (C), 136.15 (C), 134.34 (C), 131.74 (C), 129.47 (CH×2), 129.34 (CH), 127.71 (CH), 125.75 (CH), 125.44 (CH), 124.70 (CH), 124.12 (CH×2), 78.22 (C), 76.03 (C), 21.64 (CH_2), 3.62 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{17}H_{15}N_2$, 247.1230; found, 247.1224.

(2-(4,4-Dimethylpent-2-ynyl)phenyl)propylcarbodiimide (4i). 92%



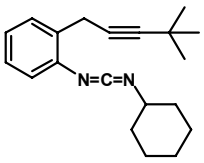
Yellow oil.
IR (neat/ cm^{-1}): 2970, 2137, 1643, 910, 733.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.54 (d, *J*= 8.0 Hz, 1H), 7.16 (dd, *J*= 7.6, 7.6 Hz, 1H), 7.13–7.06 (m, 2H), 3.59 (s, 2H), 3.55 (t, *J*= 6.8 Hz, 2H), 1.68 (tq, *J*= 6.8, 7.2 Hz, 2H), 1.25 (s, 9H), 1.00 (dt, *J*= 7.4, 1.5 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.28 (C), 135.25 (C), 131.26 (C), 128.73 (CH), 127.22 (CH), 124.50 (CH), 123.40 (CH), 91.53 (C), 75.53 (C), 48.49 (CH_2), 31.28 (CH_3×3), 27.45 (C), 24.69 (CH_2), 21.04 (CH_2), 11.39 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{22}N_2Na$, 277.1675; found, 277.1680.

Benzyl-(2-(4,4-dimethylpent-2-ynyl)phenyl)carbodiimide (4j). 88%



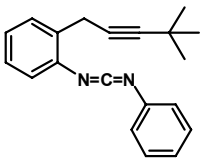
Colorless oil.
IR (neat/ cm^{-1}): 2970, 2137, 1705, 1450, 1265, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.52 (d, *J* = 7.1 Hz, 1H), 7.40–7.35 (m, 4H), 7.34–7.29 (m, 1H), 7.12 (ddt, *J* = 1.6, 7.3, 7.3 Hz, 1H), 7.10 (ddt, *J* = 1.6, 7.3, 7.3 Hz, 1H), 6.96 (dd, *J* = 1.6, 7.3 Hz, 1H), 4.57 (s, 2H), 3.53 (s, 2H), 1.25 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.87 (C), 137.57 (C), 136.49 (C), 131.44 (C), 128.78 (CH×3), 127.79 (CH), 127.40 (CH×2), 127.28 (CH), 124.90 (CH), 123.76 (CH), 91.72 (C), 75.41 (C), 50.50 (CH_2), 31.32 (CH_3×3), 27.50 (C), 21.12 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{22}N_2Na$, 325.1675; found, 325.1675.

Cyclohexyl-(2-(4,4-dimethylpent-2-ynyl)phenyl)carbodiimide (4k). 70%



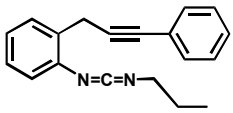
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2129, 1666, 1265, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.54 (dd, *J* = 0.8, 7.6 Hz, 1H), 7.17 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.12 (dd, *J* = 1.4, 7.6 Hz, 1H), 7.10 (ddd, *J* = 1.3, 7.6, 7.6 Hz, 1H), 3.59 (s, 2H), 3.47 (tt, 7.12 *J* = 3.9, 9.7 Hz, 1H), 2.04–1.96 (m, 2H), 1.81–1.72 (m, 2H), 1.52–1.43 (m, 2H), 1.39–1.23 (m, 4H), 1.26 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.52 (C), 135.49 (C), 131.32 (C), 128.77 (CH), 127.26 (CH), 124.51 (CH), 123.24 (CH), 91.63 (C), 75.61 (C), 56.56 (CH), 34.44 (CH_2×2), 31.34 (CH_3×3), 25.34 (C), 24.38 (CH_2×2), 21.07 (CH_2), 21.07 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{26}N_2Na$, 317.1988; found, 317.1985.

(2-(4,4-Dimethylpent-2-ynyl)phenyl)phenylcarbodiimide (4l). 78%



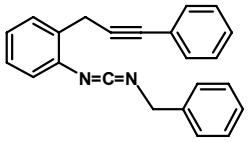
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2144, 1589, 1265, 1211, 748.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.58 (d, J = 7.1 Hz, 1H), 7.35–7.30 (m, 2H), 7.22–7.15 (m, 6H), 3.67 (s, 2H), 1.26 (s, 9H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 137.36 (C), 136.06 (C), 135.33 (C), 129.50 (CH×2), 129.07 (CH), 127.52 (CH), 125.72 (CH), 125.42 (CH), 124.54 (CH), 124.19 (C), 124.09 (CH×2), 91.95 (C), 75.13 (C), 31.29 (CH_3×3), 27.52 (C), 2.48 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{20}N_2Na$, 311.1519; found, 311.1529.

(2-(3-Phenylprop-2-ynyl)phenyl)propylcarbodiimide (4m). 80%



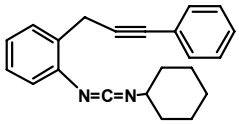
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2854, 2129, 1581, 1496, 1450, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.58 (dd, J = 0.9, 7.5 Hz, 1H), 7.49–7.42 (m, 2H), 7.34–7.27 (m, 3H), 7.25–7.08 (m, 3H), 3.85 (s, 2H), 3.39 (t, J = 6.8 Hz, 2H), 1.71 (tq, J = 0.7, 7.4 Hz, 2H), 1.01 (t, J = 7.4 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.55 (C), 135.22 (C), 131.64 (CH×2), 130.40 (C), 129.12 (CH), 128.18 (CH×2), 127.72 (CH), 127.65 (CH), 124.67 (CH), 123.76 (C), 123.68 (CH), 87.42 (C), 82.69 (C), 48.58 (CH_2), 24.72 (CH_2), 21.88 (CH_2), 11.43 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{18}N_2Na$, 297.1362; found, 297.1371.

Benzyl-(2-(3-phenylprop-2-ynyl)phenyl)carbodiimide (4n). 80%



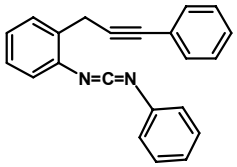
Colorless oil.
IR (neat/ cm^{-1}): 3055, 2137, 1497, 1265, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.55 (d, J = 7.6 Hz, 1H), 7.47–7.42 (m, 2H), 7.37 (d, J = 4.5 Hz, 4H), 7.34–7.27 (m, 4H), 7.16 (ddd, J = 1.4, 7.4, 7.4 Hz, 1H), 7.11 (ddd, J = 1.3, 7.4, 7.4 Hz, 1H), 7.00 (dd, J = 1.3, 7.7 Hz, 1H), 4.58 (s, 2H), 3.79 (s, 2H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.81 (C), 136.41 (C), 131.65 (CH×2), 130.52 (C), 129.11 (CH), 128.80 (CH×2), 128.58 (C), 128.20 (CH×2), 127.82 (CH), 127.75 (CH), 127.66 (CH), 127.40 (CH×2), 125.01 (CH), 123.99 (CH), 123.74 (C), 87.27 (C), 82.77 (C), 50.51 (CH_2), 21.91 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{23}H_{18}N_2Na$, 345.1362; found, 345.1353.

Cyclohexyl-(2-(3-phenylprop-2-ynyl)phenyl)carbodiimide (4o). 72%



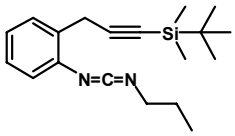
Colorless oil.
IR (neat/ cm^{-1}): 2962, 2129, 1589, 1489, 1296, 1041, 849, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.58 (d, J = 7.4 Hz, 1H), 7.47–7.43 (m, 2H), 7.31–7.27 (m, 3H), 7.21 (ddd, J = 1.4, 7.4, 7.4 Hz, 1H), 7.17 (ddd, J = 1.4, 7.9, 7.9 Hz, 1H), 7.11 (ddd, J = 1.5, 7.4, 7.4 Hz, 1H), 3.85 (s, 2H), 3.48 (tt, J = 3.7, 9.7 Hz, 1H), 2.05–1.98 (m, 2H), 1.80–1.72 (m, 2H),1.60-1.45 (m, 3H), 1.38–1.20 (m, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.77 (C), 131.66 (CH×2), 130.41 (C), 129.12 (CH), 128.18 (CH×2), 127.71 (CH), 127.66 (CH), 124.63 (CH), 123.81 (C), 123.48 (CH), 120.37 (C), 87.50 (C), 82.68 (C), 56.63 (CH), 34.95 (CH_2×2), 25.32 (CH_2×2), 24.38 (CH_2), 21.90 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{22}N_2Na$, 337.1675; found, 338.1685.

Phenyl-(2-(3-phenylprop-2-ynyl)phenyl)carbodiimide (4p). 80%



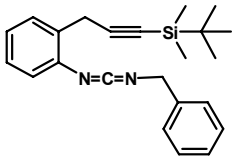
Colorless oil.
IR (neat/ cm^{-1}): 3016, 2893, 2276, 2144, 1589, 1489, 1211, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.61 (d, J = 7.7 Hz, 1H), 7.47–7.43 (m, 2H), 7.31–7.28 (m, 4H), 7.27–7.24 (m, 2H), 7.20–7.14 (m, 5H), 3.93 (s, 2H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.45 (C), 137.89 (C), 136.36 (C), 131.70 (CH×2), 130.97 (C), 129.52 (CH×2), 129.43 (CH), 129.05 (CH×2), 128.24 (CH), 127.95 (CH), 125.85 (CH), 125.54 (CH), 124.80 (CH), 124.18 (CH×2), 123.62 (C), 86.95 (C), 82.94 (C), 22.32 (CH_2).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{22}H_{17}N_2$, 309.1386; found, 309.1395.

(2-(3-(*tert*-Butyldimethylsilanyl)prop-2-ynyl)phenyl)propylcarbodiimide (4q). 72%



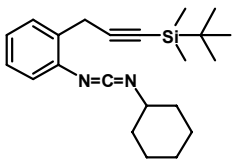
Colorless oil.
IR (neat/ cm^{-1}): 3055, 2954, 2854, 2137, 1581, 1496, 1265, 833, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.54 (d, J = 7.6 Hz, 1H), 7.19 (dd, J = 7.7, 7.4 Hz, 1H), 7.12 (d, J = 7.7 Hz, 1H), 7.10 (dd, J = 7.6, 7.6 Hz, 1H), 3.68 (s, 2H), 3.38 (t, J = 6.7 Hz, 2H), 1.70 (tq, J = 6.8, 7.3 Hz, 2H), 1.01 (t, J = 7.3 Hz, 3H), 0.95 (s, 9H), 0.12 (s, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.41 (C), 135.21 (C), 130.17 (C), 128.89 (CH), 127.53 (CH), 124.62 (CH), 123.54 (CH), 104.66 (C), 85.23 (C), 48.59 (CH_2), 26.12 (CH_3×3), 24.74 (CH_2), 22.32 (CH_2), 16.59 (C), 11.45 (CH_3), –4.44 (CH_3×2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{28}N_2NaSi$, 335.1914; found, 335.1917.

Benzyl-(2-(3-(*tert*-butyldimethylsilanyl)prop-2-ynyl)phenyl)carbodiimide (4r). 75%



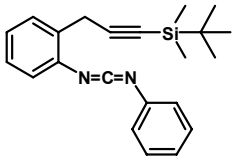
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2854, 2137, 1350, 1026, 833, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.52 (d, J = 7.6 Hz, 1H), 7.39–7.35 (m, 4H), 7.34–7.28 (m, 1H), 7.13 (dd, J = 7.5, 7.5 Hz, 1H), 7.09 (dd, J = 7.4, 7.4 Hz, 1H), 6.97 (d, J = 7.6 Hz, 1H), 4.56 (s, 2H), 3.62 (s, 2H), 0.95 (s, 9H), 0.12 (s, 6H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 137.88 (C), 137.72 (C), 136.38 (C), 130.32 (C), 128.91 (CH), 128.81 (CH×2), 127.83 (CH), 127.54 (CH), 127.41 (CH×2), 124.96 (CH), 123.85 (CH), 104.53 (C), 85.36 (C), 50.53 (CH_2), 26.14 (CH_3×3), 22.34 (CH_2), 16.57 (C), -4.43 (CH_3×2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{23}H_{28}N_2NaSi$, 383.1914; found, 383.1912.

(2-(3-(*tert*-Butyldimethylsilanyl)prop-2-ynyl)phenyl)cyclohexylcarbodiimide (4s). 84%



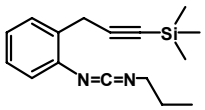
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2137, 1697, 1527, 1234, 1018, 833, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.55 (d, J = 7.7 Hz, 1H), 7.19 (ddd, J = 1.5, 7.7, 7.7 Hz, 1H), 7.14 (dd, J = 1.5, 7.7 Hz, 1H), 7.10 (ddd, J = 1.4, 7.7, 7.7 Hz, 1H), 3.69 (s, 2H), 3.47 (tt, J = 3.9, 9.7 Hz, 1H), 2.04–1.94 (m, 2H), 1.80–1.72 (m, 2H), 1.60–1.53 (m, 1H), 1.52–1.43 (m, 2H), 1.39–1.21 (m, 3H), 0.96 (s, 9H), 0.13 (s, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.60 (C), 135.37 (C), 130.13 (C), 128.87 (CH), 127.51 (CH), 124.56 (CH), 123.30 (CH), 104.72 (C), 85.20 (C), 56.59 (CH), 34.94 (CH_2×2), 26.12 (CH_3×3), 25.33 (CH_2), 24.37 (CH_2), 22.29 (CH_2×2), 16.58 (C), –4.43 (CH_3×2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{32}N_2NaSi$, 375.2227; found, 375.2228.

(2-(3-(*tert*-Butyldimethylsilanyl)prop-2-ynyl)phenyl)phenylcarbodiimide (4t). 82%



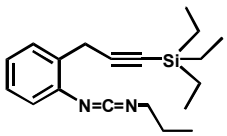
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2854, 2144, 1658, 1489, 1250, 1026, 833, 756, 687.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.59 (d, J = 7.4 Hz, 1H), 7.36 (m, 2H), 7.24 (m, 6H), 3.76 (s, 2H), 0.96 (s, 9H), 0.13 (s, 6H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.46 (C), 136.17 (C), 134.39 (C), 130.72 (C), 129.52 (CH×2), 129.16 (CH), 127.79 (CH), 125.79 (CH), 125.53 (CH), 124.65 (CH), 124.14 (CH×2), 104.08 (C), 85.66 (C), 26.13 (CH_3×3), 22.64 (CH_2), 16.59 (C), –4.45 (CH_3×2).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{22}H_{27}N_2Si$, 347.1938; found, 347.1944.

Propyl-(2-(3-trimethylsilanylprop-2-ynyl)phenyl)carbodiimide (4u). 94%



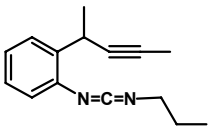
Colorless oil.
IR (neat/ cm^{-1}): 3055, 2144, 1265, 849, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.52 (d, J = 1.0, 7.6 Hz, 1H), 7.19 (ddd, J = 1.6, 7.3, 7.3 Hz, 1H), 7.14–7.08 (m, 2H), 3.67 (s, 2H), 3.38 (t, J = 6.8 Hz, 2H), 1.71 (tq, J = 6.9, 7.3 Hz, 2H), 1.01 (t, J = 7.4 Hz, 3H), 0.19 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.45 (C), 135.20 (C), 130.02 (C), 128.94 (CH), 127.58 (CH), 124.63 (CH), 123.57 (CH), 104.19 (C), 86.99 (C), 48.58 (CH_2), 24.73 (CH_2), 22.28 (CH_2), 11.44 (CH_3), 0.12 (CH_3×3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{22}N_2NaSi$, 293.1444; found, 293.1453.

Propyl-(2-(3-triethylsilanylprop-2-ynyl)phenyl)carbodiimide (4v). 85%



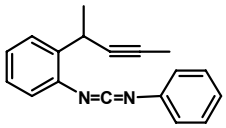
Colorless oil.
IR (neat/ cm^{-1}): 2962, 2137, 1643, 1265, 1018, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.51 (d, J = 7.6 Hz, 1H), 7.19 (dd, J = 7.5, 7.5 Hz, 1H), 7.13 (d, J = 7.3 Hz, 1H), 7.10 (dd, J = 7.6, 7.6 Hz, 1H), 3.70 (s, 2H), 3.38 (t, J = 6.8 Hz, 2H), 1.70 (tq, J = 7.1, 7.1 Hz, 2H), 1.01 (t, J = 7.8 Hz, 12H), 0.62 (q, J = 7.8 Hz, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.40 (C), 135.21 (C), 130.21 (C), 128.89 (CH), 127.50 (CH), 124.60 (CH), 123.51 (CH), 105.16 (C), 84.58 (C), 48.58 (CH_2), 24.73 (CH_2), 22.34 (CH_2), 11.43 (CH_3), 7.49 (CH_3×3), 4.53 (CH_2×3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{19}H_{29}N_2Si$, 313.2095; found, 313.2088.

(2-(1-Methylbut-2-ynyl)phenyl)propylcarbodiimide (5a). 90%



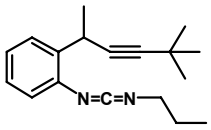
Colorless oil.
IR (neat/ cm^{-1}): 2970, 2137, 1589, 1496, 1265, 741.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.56 (dd, J = 1.5, 7.6 Hz, 1H), 7.20–7.08 (m, 3H), 4.20–4.14 (m, 1H), 3.38 (t, J = 6.8 Hz, 2H), 1.85 (d, J = 2.4 Hz, 3H), 1.71 (dt, J = 7.2, 7.2 Hz, 2H), 1.39 (d, J = 7.0 Hz, 3H), 1.02 (t, J = 7.3 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 137.50 (C), 137.46 (C), 135.62 (C), 127.82 (CH), 127.36 (CH), 124.82 (CH), 123.84 (CH), 82.18 (C), 76.88 (C), 48.61 (CH_2), 27.09 (CH_3), 24.76 (CH_2), 23.50 (CH), 11.45 (CH_3), 3.64 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{15}H_{18}N_2Na$, 249.1362; found, 249.1361.

(2-(1-Methylbut-2-ynyl)phenyl)phenylcarbodiimide (5b). 63%



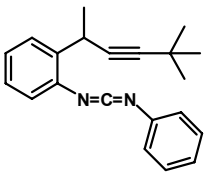
Colorless oil.
IR (neat/ cm^{-1}): 2970, 2306, 1589, 1411, 1265, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.63–7.58 (m, 1H), 7.35–7.30 (m, 2H), 7.21–7.15 (m, 6H), 4.25–4.17 (m, 1H), 1.85 (d, J = 2.4 Hz, 3H), 1.45 (d, J = 7.1 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.63 (C), 137.94 (C), 135.27 (C), 129.50 (CH×2), 128.03 (CH), 127.60 (CH), 125.96 (CH), 125.44 (CH), 124.96 (CH), 124.19 (C), 124.10 (CH×2), 81.78 (C), 77.26 (C), 27.56 (CH_3), 23.47 (CH), 3.63 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{18}H_{17}N_2$: 261.1386, found 261.1374.

Propyl-(2-(1,4,4-trimethylpent-2-ynyl)phenyl)carbodiimide (5c). 91%



Colorless oil.
IR (neat/ cm^{-1}): 2970, 2137, 1643, 1257, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.58 (dd, J = 1.4, 7.6 Hz, 1H), 7.18–7.14 (m, 1H), 7.13–7.08 (m, 2H), 4.16 (q, J = 7.0 Hz, 1H), 3.37 (t, J = 6.8 Hz, 2H), 1.71 (tq, J = 7.1, 7.2 Hz, 2H), 1.36 (d, J = 7.1 Hz, 3H), 1.24 (s, 9H), 1.01 (t, J = 7.4 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 137.90 (C), 137.41 (C), 135.67 (C), 127.87 (CH), 127.23 (CH), 124.78 (CH), 123.77 (CH), 90.58 (C), 81.34 (C), 48.62 (CH_2), 31.37 (CH_3×3), 27.39 (C), 27.16 (CH_3), 24.77 (CH_2), 24.07 (CH), 11.45 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{24}N_2Na$, 291.1832; found, 291.1843.

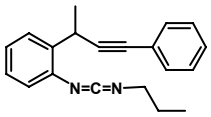
Phenyl-(2-(1,4,4-trimethylpent-2-ynyl)phenyl)carbodiimide (5d). 80%



Colorless oil.
IR (neat/ cm^{-1}): 3062, 2970, 2144, 1651, 1589, 1489, 1211, 748.

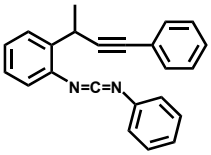
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.64–7.61 (m, 1H), 7.35–7.31 (m, 3H), 7.21–7.15 (m, 5H), 4.21 (q, J = 7.0 Hz, 1H), 1.42 (d, J = 7.1 Hz, 3H), 1.25 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.68 (C), 138.36 (C), 135.19 (C), 129.53 (CH×2), 128.10 (CH), 127.51 (CH), 125.97 (CH), 125.62 (C), 125.45 (CH), 124.92 (CH), 124.10 (CH×2), 90.34 (C), 80.96 (C), 31.37 (CH_3×3), 27.60 (CH_3), 27.43 (C), 24.11 (CH).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{21}H_{23}N_2$, 303.1856; found, 303.1856.

(2-(1-Methyl-3-phenylprop-2-ynyl)phenyl)propylcarbodiimide (5e). 90%



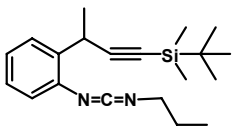
Colorless oil.
IR (neat/ cm^{-1}): 2970, 2924, 2138, 1581, 1496, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.65 (d, J = 7.7 Hz, 1H), 7.46–7.43 (m, 2H), 7.32–7.26 (m, 3H), 7.20 (dd, J = 7.8, 7.8, 1H), 7.17 (dd, J = 7.7, 7.7 Hz, 1H), 7.13 (dd, J = 7.8, 7.8 Hz, 1H), 4.45 (q, J = 7.0 Hz, 1H), 3.39 (t, J = 0.9 Hz, 2H), 1.72 (tq, J = 6.8, 7.2 Hz, 2H), 1.52 (d, J = 7.1 Hz, 3H), 1.02 (t, J = 7.2 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 137.60 (C), 136.86 (C), 135.54 (C), 131.63 (CH×2), 128.15 (CH×2), 127.93 (CH), 127.64 (CH), 127.57 (CH), 124.90 (CH), 123.91 (CH), 123.83 (C), 92.93 (C), 81.80 (C), 48.62 (CH_2), 27.77 (CH), 24.78 (CH_2), 23.37 (CH_3), 11.46 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{20}H_{21}N_2$, 289.1699; found, 289.1694.

(2-(1-Methyl-3-phenylprop-2-ynyl)phenyl)phenylcarbodiimide (5f). 37%



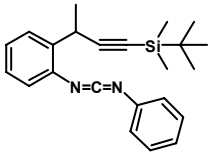
Colorless oil.
IR (neat/ cm^{-1}): 3062, 2924, 2854, 1650, 1404, 1211, 903, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.68 (d, J = 7.2 Hz, 1H), 7.47–7.43 (m, 2H), 7.33–7.27 (m, 5H), 7.25–7.15 (m, 6H), 4.49 (q, J = 7.1 Hz, 1H), 1.58 (d, J = 7.0 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.44 (C), 137.24 (C), 135.39 (C), 134.79 (C), 131.64 (CH×2), 129.51 (CH×2), 128.18 (CH×2), 128.11 (CH), 127.82 (CH), 127.74 (CH), 126.04 (CH), 125.51 (CH), 125.04 (CH), 124.12 (CH×2), 123.65 (C), 92.42 (C), 82.08 (C), 28.19 (CH), 23.29 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{23}H_{19}N_2$, 323.1543; found, 323.1540.

(2-(3-(*tert*-Butyldimethylsilanyl)-1-methylprop-2-ynyl)phenyl)propylcarbodiimide (5g). 39%



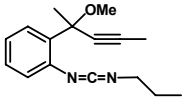
Colorless oil.
IR (neat/ cm^{-1}): 2954, 2862, 2144, 1496, 1250, 1080, 833, 764.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.59 (dd, J = 1.4, 7.6 Hz, 1H), 7.17 (ddd, J = 1.6, 7.0, 7.1 Hz, 1H), 7.14–7.08 (m, 2H), 4.25 (q, J = 7.0 Hz, 1H), 3.38 (t, J = 6.8 Hz, 2H), 1.71 (tq, J = 7.0, 7.3 Hz, 2H), 1.41 (d, J = 7.0 Hz, 3H), 1.02 (t, J = 7.3 Hz, 3H), 0.95 (s, 9H), 0.11 (d, J = 3.1 Hz, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 146.57 (C), 137.51 (C), 136.73 (C), 127.88 (CH), 127.47 (CH), 124.82 (CH), 123.81 (CH), 110.44 (C), 83.84 (C), 48.60 (CH_2), 28.26 (CH), 26.12 (CH_3×3), 24.77 (CH_2), 23.67 (CH_3), 15.60 (C), 11.44 (CH_3), –4.44 (CH_3×2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{30}N_2NaSi$, 349.2070; found, 349.2077.

(2-(3-(*tert*-Butyldimethylsilanyl)-1-methylprop-2-ynyl)phenyl)phenylcarbodiimide (5h). 27%



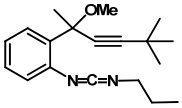
Colorless oil.
IR (neat/ cm^{-1}): 2931, 2144, 1589, 1489, 1211, 833, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.65–7.62 (m, 1H), 7.32 (dd, J = 7.9, 7.9 Hz, 2H), 7.21–7.15 (m, 6H), 4.30 (q, J = 7.0 Hz, 1H), 1.47 (d, J = 7.0 Hz, 3H), 0.96 (s, 9H), 0.13 (s, 3H), 0.12 (s, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 138.51 (C), 137.18 (C), 135.30 (C), 134.70 (C), 129.52 (CH×2), 128.10 (CH), 127.74 (CH), 125.98 (CH), 125.51 (CH), 124.95 (CH), 124.11 (CH×2), 109.89 (C), 84.29 (C), 28.65 (CH_3), 26.12 (CH_3×3), 23.70 (CH), 16.00 (C), -4.45 (CH_3×2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for calcd for $C_{23}H_{28}N_2NaSi$, 383.1914; found, 383.1918.

Propyl -(2-(2-methoxypent-3-yn-2-yl))carbodiimide (6a). 51%



Colorless oil.
IR (neat/ cm^{-1}): 2970, 2939, 2144, 1496, 1095, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.74 (d, J = 7.4 Hz, 1H), 7.24 (ddd, J = 1.5, 7.7, 7.7 Hz, 1H), 7.15 (dd, J = 1.3 7.8 Hz, 1H), 7.09 (ddd, J = 1.3, 7.4, 7.7 Hz, 1H), 3.38 (t, J = 6.8 Hz, 2H), 3.23 (s, 3H), 1.98 (s, 3H), 1.87 (s, 3H), 1.70 (tq, J = 7.1, 7.3 Hz, 2H), 1.01 (t, J = 7.4 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.07 (C), 134.33 (C), 134.30 (C), 128.97 (CH), 128.69 (CH), 125.61 (CH), 124.02 (CH), 82.93 (C), 79.77 (C), 76.61 (C), 52.13 (CH_3), 48.50 (CH_2), 29.00 (CH_3), 24.74 (CH_2), 11.47 (CH_3), 3.72 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{20}N_2NaO$, 279.1468; found, 279.1462.

(2-(1-Methoxy-1,4,4-trimethylpent-2-ynyl)phenyl)propylcarbodiimide (6b). 66%

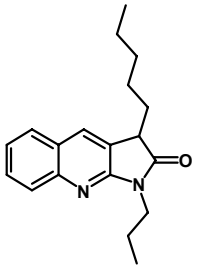


Colorless oil.
IR (neat/ cm^{-1}): 2970, 2144, 1219, 1095, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.74 (dd, J = 1.5, 7.8 Hz, 1H), 7.23 (ddd, J = 1.5, 7.5, 7.5 Hz, 1H), 7.14 (dd, J = 1.3, 7.7 Hz, 1H), 7.08 (ddd, J = 1.3, 7.6, 7.6 Hz, 1H), 3.38 (dt, J = 1.2, 6.8 Hz, 2H), 3.21 (s, 3H), 1.85 (s, 3H), 1.69 (tq, J = 7.0, 7.3 Hz, 2H), 1.31 (s, 9H), 1.00 (t, J = 7.3 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 138.10 (C), 134.55 (C), 134.30 (C), 129.07 (CH), 128.61 (CH), 125.68 (CH), 123.97 (CH), 96.06 (C), 78.92 (C), 76.54 (C), 52.02 (CH_3), 48.46 (CH_2), 31.06 (CH_3×3), 29.25 (CH_3), 27.57 (C), 24.77 (CH_2), 11.48 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{19}H_{27}N_2O$, 299.2122; found, 299.2118.

Typical procedure for the catalytic Pauson–Khand reaction using $[Rh(CO)_2Cl]_2$-dppp to produce 15: 3-Pentyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15a) (Table 2, Entry 1).
1,2-Bis(diphenylphosphino)propane (dppp) (28.4 mg, 0.069 mmol) was added to a stirred solution of $[Rh(CO)_2Cl]_2$ (12.5 mg, 0.032 mmol) in *p*-xylene (5 mL), and the mixture was degassed and charged with carbon monoxide. The resulting pale yellow suspension was heated at 130 °C, and a solution of carbodiimide **4a** (123.7 mg, 0.462 mmol) in *p*-xylene (1 mL) was added slowly. After heating at the same temperature for 2.5 h, the mixture was evaporated. The residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1:10) to provide pyrroloquinoline **15a** (109.6 mg, 0.370 mmol, 80%) as a

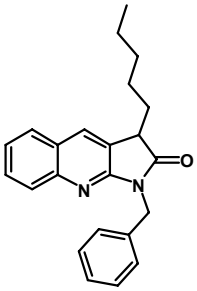
yellow oil.

3-Pentyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15a).



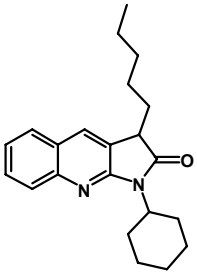
Yellow oil.
IR (neat/ cm^{-1}): 2931, 2862, 1728, 1643, 1581, 1450, 1219, 1088, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.92 (d, J = 8.3 Hz, 1H), 7.81 (s, 1H), 7.73 (dd, J = 0.9, 8.0 Hz, 1H), 7.62 (ddd, J = 1.4, 7.2, 8.4 Hz, 1H), 7.40 (ddd, J = 0.9, 7.4, 8.0 Hz, 1H), 3.95–3.85 (m, 2H), 3.55 (ddd, J = 1.1, 5.5, 6.7 Hz, 1H), 2.09–2.01 (m, 1H), 1.99–1.91 (m, 1H), 1.84 (tq, J = 7.4, 7.4 Hz, 2H), 1.48–1.24 (m, 6H), 0.99 (t, J = 7.5 Hz, 3H), 0.86 (t, J = 7.1 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.48 (C), 156.94 (C), 146.91 (C), 130.23 (CH), 129.19 (CH), 127.75 (CH×2), 125.95 (C), 124.63 (C), 124.34 (CH), 44.15 (CH), 40.88 (CH_2), 31.66 (CH_2), 30.58 (CH_2), 25.44 (CH_2), 22.35 (CH_2), 20.85 (CH_2), 13.93 (CH_3), 11.35 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{24}N_2NaO$, 319.1781; found, 319.1775.

1-Benzyl-3-pentyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15b).



Yellow oil.
IR (neat/ cm^{-1}): 2931, 1720, 1643, 1442, 1219, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.94 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.71 (dd, J = 1.2, 7.9 Hz, 1H,), 7.62 (ddd, J = 1.5, 7.0, 8.3 Hz, 1H), 7.54 (d, J = 7.3 Hz, 2H), 7.39 (ddd, J = 1.2, 7.0, 7.9 Hz, 2H), 7.28 (dd, J = 7.3, 7.3 Hz, 1H), 7.22 (dd, J = 7.3, 7.3 Hz, 1H), 5.15–5.07 (m, 2H), 3.56 (t, J = 6.0 Hz, 1H), 2.10–1.90 (m, 2H), 1.42–1.21 (m, 6H), 0.82 (t, J = 7.1 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.25 (C), 156.44 (C), 146.83 (C), 136.75 (C), 130.45 (CH), 129.23 (CH), 128.71 (CH×2), 128.41 (CH×2), 127.91 (CH), 127.74 (CH), 127.50 (CH), 126.12 (C), 124.52 (C), 124.44 (CH), 44.22 (CH), 42.73 (CH_2), 31.62 (CH_2), 30.62 (CH_2), 25.43 (CH_2), 22.32 (CH_2), 13.91 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{23}H_{24}N_2NaO$, 364.1781; found, 367.1791.

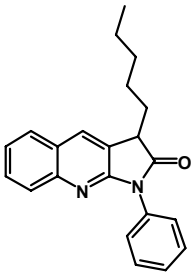
1-Cyclohexyl-3-pentyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15c).



Brownish solid; mp: 67.8–69.0 °C.
IR (KBr/ cm^{-1}): 2931, 1720, 1635, 1581, 1435, 1219, 895, 748.

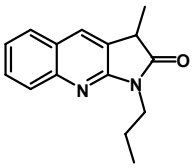
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.92 (d, J = 8.3 Hz, 1H), 7.78 (s, 1H), 7.71 (d, J = 7.5 Hz, 1H), 7.61 (ddd, J = 1.3, 7.2, 8.3 Hz, 1H), 7.38 (ddd, J = 0.8, 7.4, 7.4 Hz, 1H), 4.48 (tt, J = 3.8, 12.2 Hz, 1H), 3.48 (t, J = 5.6 Hz, 1H), 2.61–2.49 (m, 2H), 2.06–1.84 (m, 4H), 1.76–1.69 (m, 2H), 1.51–1.22 (m, 10H), 0.85 (t, J = 6.6 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.35 (C), 157.04 (C), 146.69 (C), 129.99 (CH), 129.03 (CH), 127.85 (CH), 127.59 (CH), 125.57 (C), 124.59 (C), 124.25 (CH), 51.98 (CH), 44.00 (CH), 31.64 (CH_2), 30.65 (CH_2), 28.83 (CH_2), 28.71 (CH_2), 26.01 (CH_2), 25.99 (CH_2), 25.29 (CH_2), 25.14 (CH_2), 22.32 (CH_2), 13.91 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{28}N_2NaO$, 359.2094; found, 359.2097.

3-Pentyl-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15d).



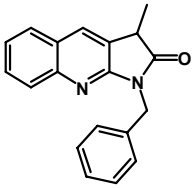
Yellow solid; mp: 103.4–106.3 °C.
IR (KBr/ cm^{-1}): 2924, 1736, 1581, 1427, 1219, 910, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.91 (s, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.75 (d, J = 7.9 Hz, 1H), 7.63 (d, J = 8.1 Hz, 2H), 7.40 (dd, J = 7.8, 7.8 Hz, 1H), 7.54 (dd, J = 7.7, 7.7 Hz, 2H), 7.41 (dd, J = 7.5, 7.5 Hz, 2H), 3.73 (t, J = 6.1 Hz, 1H), 2.18–2.03 (m, 2H), 1.57–1.37 (m, 2H), 1.37–1.27 (m, 4H), 0.87 (t, J = 6.8 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 176.69 (C), 156.56 (C), 146.59 (C), 133.33 (C), 130.89 (CH), 129.29 (CH), 128.96 (CH×2), 128.16 (CH), 127.91 (CH), 127.58 (CH), 126.70 (CH×2), 126.22 (C), 124.74 (CH), 124.15 (C), 44.21 (CH), 31.65 (CH_2), 30.94 (CH_2), 25.42 (CH_2), 22.35 (CH_2), 13.94 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{22}N_2NaO$, 353.1624; found, 353.1621.

3-Methyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15e).



Yellow solid; mp: 105.0–105.8 °C.
IR (KBr/ cm^{-1}): 2939, 2360, 1712, 1635, 1442, 1373, 1219, 957, 756.
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.92 (d, J = 8.3 Hz, 1H), 7.77 (s, 1H), 7.70 (d, J = 7.8 Hz, 1H), 7.61 (ddd, J = 1.4, 7.0, 8.3 Hz, 1H), 7.38 (ddd, J = 1.0, 7.5, 7.5 Hz, 1H), 3.89 (t, J = 7.3 Hz, 2H), 3.53 (q, J = 7.2 Hz, 1H), 1.84 (tq, J = 7.4, 7.4 Hz, 2H), 1.54 (d, J = 7.5 Hz, 3H), 0.99 (t, J = 7.4 Hz, 3H).
^{13}C-NMR (75 MHz, $CDCl_3$, δ): 177.97 (C), 156.44 (C), 146.84 (C), 129.88 (CH), 129.10 (CH), 127.67 (CH), 127.61 (CH), 125.92 (C), 125.74 (C), 124.26 (CH), 40.76 (CH_2), 38.97 (CH), 20.76 (CH_2), 15.33 (CH_3), 11.24 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{15}H_{17}N_2O$, 241.1335; found, 241.1343.

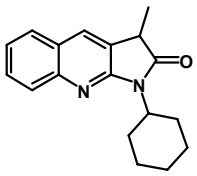
1-Benzyl-3-methyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15f).



Yellow solid; mp: 135.0–135.2 °C.
IR (KBr/ cm^{-1}): 2978, 1813, 1720, 1643, 1581, 1442, 1211, 957, 733.

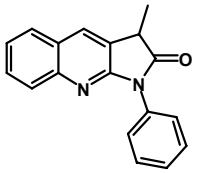
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.94 (d, J = 8.4 Hz, 1H), 7.78 (s, 1H), 7.70 (dd, J = 1.1, 8.0 Hz, 1H), 7.62 (ddd, J = 1.3, 7.1, 7.2 Hz, 1H), 7.56 (d, J = 7.9 Hz, 2H), 7.39 (ddd, J = 1.1, 7.1, 8.0 Hz, 1H), 7.29 (dd, J = 7.5, 7.5 Hz, 2H), 7.23 (dd, J = 7.3, 7.3 Hz, 1H), 5.14–5.06 (m, 2H), 3.55 (dq, J = 1.3, 7.7 Hz, 1H), 1.54 (d, J = 7.6 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.80 (C), 156.08 (C), 146.87 (C), 136.69 (C), 130.19 (CH), 129.24 (CH), 128.74 (CH×2), 128.44 (CH×2), 127.93 (CH), 127.69 (CH), 127.53 (CH), 126.17 (C), 125.70 (C), 124.47 (CH), 42.73 (CH_2), 39.20 (CH), 15.32 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{16}N_2NaO$, 311.1155; found, 311.1149.

1-Cyclohexyl-3-methyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15g).



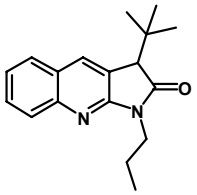
Yellow solid; mp: 135.0–137.8 °C.
IR (KBr/ cm^{-1}): 2924, 2854, 1720, 1635, 1581, 1427, 1219, 949, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.92 (d, J = 8.4 Hz, 1H), 7.76 (s, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.60 (ddd, J = 1.3, 8.3, 8.3 Hz, 1H), 7.38 (ddd, J = 1.1, 8.1, 8.1 Hz, 1H), 4.47 (tt, J = 3.8, 12.8 Hz, 1H), 3.47 (q, J = 7.6 Hz, 1H), 2.55 (ddt, J = 3.6, 12.3, 21.8 Hz, 2H), 1.89 (d, J = 13.1 Hz, 2H), 1.78 –1.68 (m, 3H), 1.52 (d, J = 7.6 Hz, 3H), 1.50–1.30 (m, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.89 (C), 156.61 (C), 146.69 (C), 129.73 (CH), 129.00 (CH), 127.84 (CH), 127.50 (CH), 125.79 (C), 125.25 (C), 124.25 (CH), 51.90 (CH), 38.99 (CH), 28.72 (CH_2×2), 25.95 (CH_2×2), 25.23 (CH_2), 15.42 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{20}N_2NaO$, 303.1568; found, 303.1463.

3-Methyl-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15h).



Yellow solid; mp: 155.0–156.3 °C.
IR (KBr/ cm^{-1}): 3055, 1720, 1643, 1435, 1227, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.91 (s, 1H), 7.87 (d, J = 8.3 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.66–7.63 (m, 2H), 7.60 (ddd, J = 1.4, 7.1, 8.2 Hz, 1H), 7.57–7.52 (m, 2H), 7.45–7.39 (m, 2H), 3.76 (q, J = 7.6 Hz, 1H), 1.67 (d, J = 7.6 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.25 (C), 156.22 (C), 146.65 (C), 133.29 (C), 130.70 (CH), 129.34 (CH), 129.00 (CH×2), 128.20 (CH), 127.95 (CH), 127.55 (CH), 126.67 (CH×2), 126.31 (C), 125.38 (C), 124.81 (CH), 39.24 (CH), 15.68 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{14}N_2NaO$, 297.0998; found, 297.1001.

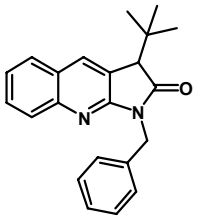
3-*tert*-Butyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15i).



Yellow oil.
IR (KBr/ cm^{-1}): 2962, 1720, 1635, 1365, 1219, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.90 (d, J = 8.4 Hz, 1H), 7.82 (s, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.60 (dd, J = 7.5, 7.5 Hz, 1H), 7.37 (dd, J = 7.4, 7.4 Hz, 1H), 3.94–3.81 (m, 2H), 3.19 (s, 1H), 1.87–1.75 (m, 2H), 1.13 (s, 9H), 0.99 (t, J = 7.4 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 175.96 (C), 157.02 (C), 146.70 (C), 132.14 (CH), 129.14 (CH), 127.78 (CH), 127.43 (CH), 125.45 (C), 124.07 (CH), 122.87 (C), 53.79 (CH), 40.54 (CH_2), 35.04 (C), 27.30 (CH_3×3), 20.80 (CH_2), 11.35 (CH_3).

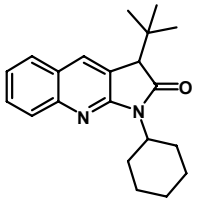
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{22}N_2NaO$, 305.1624; found, 305.1633.

1-Benzyl-3-*tert*-butyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15j).



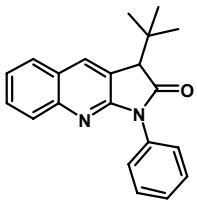
Yellow solid; mp: 115.2–115.7 °C.
IR (KBr/ cm^{-1}): 2954, 1720, 1635, 1442, 1219, 1157, 887, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.93 (d, J = 8.3 Hz, 1H), 7.86 (s, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.61 (dd, J = 7.1, 7.1 Hz, 1H), 7.55 (d, J = 7.8 Hz, 2H), 7.38 (dd, J = 7.5, 7.5 Hz, 1H), 7.27 (dd, J = 7.6, 7.6 Hz, 2H), 7.23–7.18 (m, 1H), 5.12 (d, J = 14.5 Hz, 1H), 5.06 (d, J = 14.5 Hz, 1H), 3.25 (s, 1H), 1.10 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 175.92 (C), 156.70 (C), 146.75 (C), 136.83 (C), 132.50 (CH), 129.32 (CH), 128.76 (CH×2), 128.32 (CH×2), 127.88 (CH), 127.69 (CH), 127.42 (CH), 125.75 (C), 124.31 (CH), 122.93 (C), 54.03 (CH), 42.57 (CH_2), 35.40 (C), 27.42 (CH_3×3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{22}N_2NaO$, 353.1624; found, 353.1628.

3-*tert*-Butyl-1-cyclohexyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15k).



Yellow solid: mp: 139.1–139.4 °C.
IR (KBr/ cm^{-1}): 2931, 2862, 1720, 1628, 1581, 1427, 1350, 1219, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.90 (d, J = 8.3 Hz, 1H), 7.86 (s, 1H), 7.71 (dd, J = 0.9, 8.0 Hz, 1H), 7.62 (ddd, J = 1.4, 7.1, 8.3 Hz, 1H), 7.39 (ddd, J = 1.0, 7.0, 8.0 Hz, 1H), 4.48 (tt, J = 3.7, 12.3 Hz, 1H), 3.19 (s, 1H), 2.60–2.47 (m, 2H), 1.92-1.85 (m, 2H), 1.75–1.67 (m, 3H), 1.51–1.29 (m, 3H), 1.13 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 176.17 (C), 157.33 (C), 146.70 (C), 132.17 (CH), 129.20 (CH), 127.81 (CH), 127.70 (CH), 125.27 (C), 124.20 (CH), 123.06 (C), 53.81 (CH), 51.91 (CH), 35.38 (C), 28.85 (CH_2), 28.58 (CH_2), 27.35 (CH_3×3), 26.09 (CH_2), 26.06 (CH_2), 25.36 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{26}N_2NaO$, 345.1937; found, 345.1931.

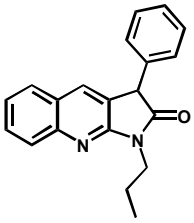
3-*tert*-Butyl-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15l).



Yellow solid; mp: 90.4–91.1 °C.
IR (KBr/ cm^{-1}): 3055, 2947, 1728, 1635, 1589, 1496, 1427, 1358, 1227, 1165, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.98 (s, 1H), 7.85 (d, J = 8.3 Hz, 1H), 7.75 (dd, J = 8.0, 1.2 Hz, 1H), 7.62–7.52 (m, 5H), 7.44–7.38 (m, 2H), 3.43 (d, J = 1.2 Hz, 1H), 1.22 (s, 9H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 175.48 (C), 156.92 (C), 146.58 (C), 133.35 (C), 132.97 (CH), 129.42 (CH), 129.00 (CH×2), 128.02 (CH), 127.97 (CH), 127.76 (CH), 126.92 (CH×2), 125.87 (C), 124.65 (CH), 122.59 (C), 54.07 (CH), 35.85 (C), 27.39

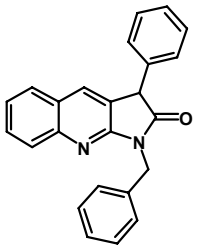
(CH_3×3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{20}N_2NaO$, 339.1468; found, 339.1462.

3-Phenyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15m).



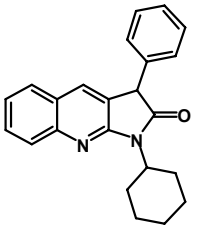
Yellow solid; mp: 102.1–103.7 °C.
IR (KBr/ cm^{-1}): 2962, 1720, 1643, 1442, 1365, 1211, 1095, 725.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.96 (d, J = 8.4 Hz, 1H), 7.74 (s, 1H), 7.66 (d, J = 7.9 Hz, 1H), 7.64 (dd, J = 7.1, 7.1 Hz, 1H), 7.42–7.28 (m, 4H), 7.24–7.20 (m, 2H), 4.71 (s, 1H), 1.84 (t, J = 7.3 Hz, 2H), 1.54 (tq, J = 7.4, 7.4 Hz, 2H), 1.00 (t, J = 7.5 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 175.45 (C), 156.81 (C), 147.18 (C), 136.03 (C), 131.75 (CH), 129.55 (CH), 129.06 (CH×2), 128.29 (CH×2), 127.93 (CH), 127.88 (CH), 127.83 (CH), 126.13 (C), 124.53 (CH) 124.43 (C), 50.60 (CH), 41.19 (CH_2), 20.87 (CH_2), 11.35 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{18}N_2NaO$, 325.1311; found, 325.1327.
Anal calcd for $C_{20}H_{18}N_2O$: C 79.44, H 6.00, N 9.26, found: C 79.82, H 6.04, N 8.97.

1-Benzyl-3-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15n).



Brown solid; mp: 135.0–135.8 °C.
IR (KBr/ cm^{-1}): 3032, 1728, 1635, 1581, 1442, 1358, 1173, 1026, 849, 725.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.98 (d, J = 8.4 Hz, 1H), 7.73 (s, 1H), 7.66–7.61 (m, 2H), 7.58 (d, J = 7.6 Hz, 2H), 7.38 (dd, J = 7.5, 7.5 Hz, 1H), 7.35–7.26 (m, 5H), 7.25–7.21 (m, 1H), 7.18 (d, J = 7.5 Hz, 2H), 5.19 (d, J = 14.3 Hz, 1H), 5.11 (d, J = 14.4 Hz, 1H), 4.72 (s, 1H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 175.21 (C), 156.31 (C), 147.11 (C), 136.62 (C), 135.82 (C), 131.96 (CH), 129.59 (CH), 129.06 (CH×2), 128.81 (CH×2), 128.48 (CH×2), 128.31 (CH×2), 127.99 (CH), 127.91 (CH), 127.91 (CH), 127.61 (CH), 124.47 (C), 124.63 (CH), 124.26 (C), 50.66 (CH), 43.07 (CH_2).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{18}N_2NaO$, 373.1311; found, 373.1316.

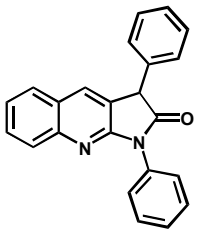
1-Cyclohexyl-3-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15o).



Yellow solid; mp: 185.0–187.2 °C.
IR (KBr/ cm^{-1}): 2924, 2854, 1720, 1643, 1581, 1427, 1211, 1072, 756, 663.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.96 (d, J = 8.3 Hz, 1H), 7.74 (s, 1H), 7.67–7.62 (m, 2H), 7.41–7.28 (m, 4H), 7.21 (d, J = 6.9

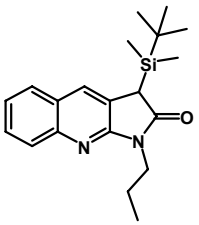
Hz, 2H), 4.67 (s, 1H), 4.53 (tt, *J* = 3.9, 12.3 Hz, 1H), 2.60 (ddt, *J* = 3.6, 12.6, 12.6 Hz, 1H), 2.55 (ddt, *J* = 3.6, 12.6, 12.6 Hz, 1H), 1.95–1.87 (m, 2H), 1.83-1.70 (m, 3H), 1.52–1.41 (m, 2H), 1.36 (tt, *J* = 3.2, 12.5 Hz, 1H).
^{13}C-NMR (125 MHz, $CDCl_3$, *δ*): 175.36 (C), 156.97 (C), 147.03 (C), 136.42(C), 131.61 (CH), 129.45 (CH), 129.06 (CH×2), 128.26 (CH×2), 128.26 (C), 128.20 (CH), 127.83 (CH×2), 125.80 (C), 124.51 (CH), 52.38 (CH), 50.63 (CH), 28.91 (CH_2), 28.79 (CH_2), 26.05 (CH_2), 26.01 (CH_2), 25.31 (CH_2).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{23}H_{23}N_2O$, 343.1805; found, 343.1817.

1,3-Diphenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15p).



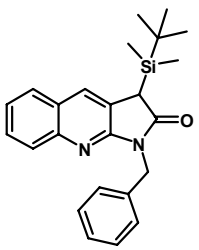
Yellow solid; mp: 227.3–228.1 °C.
IR (KBr/ cm^{-1}): 3062, 1728, 1643, 1496, 1427, 1219, 756, 694.
^{1}H-NMR (500 MHz, $CDCl_3$, *δ*): 7.91 (d, *J* = 8.6 Hz, 1H), 7.89 (s, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.63 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.56 (dd, *J* = 7.9, 7.9 Hz, 2H), 7.46–7.32 (m, 7H), 4.92 (s, 1H).
^{13}C-NMR (125 MHz, $CDCl_3$, *δ*): 174.62 (C), 156.49 (C), 146.92 (C), 135.95 (C), 133.31 (C), 132.51 (CH), 129.70 (CH), 129.17 (CH×2), 129.02 (CH×2), 128.41 (CH×2), 128.29 (CH), 128.07 (CH), 128.07 (CH), 127.79 (CH), 126.76 (CH×2), 126.44 (C), 124.96 (CH), 123.91 (C), 50.69 (CH).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{23}H_{16}N_2NaO$, 359.1155; found, 359.1155.
Anal calcd for $C_{23}H_{16}N_2O$: C 82.12, H 4.79, N 8.33, found: C 81.74, H 4.88, N 8.22.

3-(*tert*-Butyldimethylsilyl)-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15q).



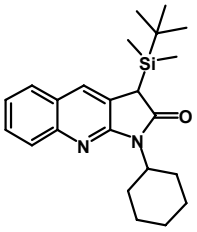
Brown oil.
IR (neat/ cm^{-1}): 2954, 2862, 1705, 1635, 1358, 1219, 1049, 833, 733.
^{1}H-NMR (600 MHz, $CDCl_3$, *δ*): 7.92 (d, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 7.0 Hz, 1H), 7.69 (s, 1H), 7.60 (dd, *J* = 7.0, 8.1 Hz, 1H), 7.38 (dd, *J* = 7.0, 8.0 Hz, 1H), 3.98–3.83 (m, 2H), 3.50 (s, 1H), 1.90–1.76 (m, 2H), 1.02 (t, *J* = 7.5 Hz, 3H), 0.90 (s, 9H), 0.26 (s, 3H), 0.15 (s, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, *δ*): 176.84 (C), 156.55 (C), 146.17 (C), 128.74 (CH), 128.64 (CH), 127.61 (CH), 127.49 (CH), 125.75 (C), 124.07 (CH), 124.05(C), 41.07 (CH_2), 38.27(CH), 26.95 (CH_3×3), 21.04 (CH_2), 18.22 (C), 11.51 (CH_3), –5.55 (CH_3), –6.28 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{28}N_2NaOSi$, 363.1863; found, 363.1860.

1-Benzyl-3-(*tert*-butyldimethylsilyl)-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15r).



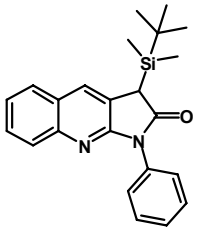
Brown solid; mp: 112.5–113.1 °C.
IR (KBr/ cm^{-1}): 2947, 2854, 1697, 1628, 1581, 1435, 1358, 1072, 910, 841, 741.
^{1}H-NMR (600MHz, $CDCl_3$, δ): 7.96 (d, J = 8.4 Hz, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.68 (s, 1H), 7.63–7.59 (m, 3H), 7.38 (dd, J = 7.6,. 7.6 Hz, 1H), 7.27 (dd, J = 7.7, 7.7 Hz, 2H), 7.24–7.20 (m, 1H), 5.12 (s, 2H), 3.49 (d, J = 1.0 Hz, 1H), 0.80 (s, 9H), 0.20 (s, 3H), 0.06 (s, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 176.47 (C), 156.11 (C), 146.15 (C), 136.89 (C), 129.20 (CH×2), 128.89 (CH), 128.66 (CH), 128.33 (CH×2), 127.79 (CH), 127.49 (CH×2), 125.93 (C), 124.16 (CH), 124.02 (C), 42.92 (CH_2), 38.38 (CH), 26.87 (CH_3×3), 18.15 (C), –5.54 (CH_3), –6.32 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{28}N_2NaOSi$, 411.1863; found, 411.1873.

3-(*tert*-Butyldimethylsilyl)-1-cyclohexyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15s).



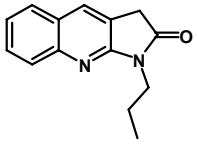
Brown oil.
IR (neat/ cm^{-1}): 2978, 2129, 1736, 1612, 1466, 1196, 748.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.97 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 7.9 Hz, 1H), 7.73 (s, 1H), 7.65 (ddd, J = 1.5, 7.0, 7.0 Hz, 1H), 7.44 (ddd, J = 1.0, 7.0, 7.0 Hz, 1H), 4.57 (tt, J = 4.0, 12.5 Hz, 1H), 3.52 (d, J = 1.2 Hz, 1H), 2.67–2.55 (m, 2H), 1.98–1.92 (m, 2H), 1.82–1.75 (m, 2H), 1.57–1.47 (m, 2H), 1.45–1.35 (m, 2H), 0.95 (s, 9H), 0.30 (s, 3H), 0.21 (s, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 176.81 (C), 156.56 (C), 145.95 (C), 128.52 (CH), 128.50 (CH), 127.72 (CH), 127.36 (CH), 125.38 (C), 124.02 (CH), 124.02 (C), 52.05 (CH), 38.51 (CH), 28.89 (CH_2), 28.68 (CH_2), 27.00 (CH_3×3), 26.10 (CH_2), 26.07 (CH_2), 25.33 (CH_2), 18.28 (C), –5.54 (CH_3), –6.26 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{28}N_2NaOSi$, 411.1863; found, 411.1873.

3-(*tert*-Butyldimethylsilyl)-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15t).



Brown oil.
IR (neat/ cm^{-1}): 3016, 1712, 1635, 1427, 1219, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.87 (d, J = 8.4 Hz, 1H), 7.80 (s, 1H), 7.73 (dd, J = 1.0, 7.9 Hz, 1H), 7.62 (d, J = 8.2 Hz, 2H), 7.60–7.53 (m, 3H), 7.44–7.39 (m, 2H), 3.70 (d, J = 1.2 Hz, 1H), 0.91 (s, 9H), 0.32 (s, 3H), 0.26 (s, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 176.00 (C), 156.08 (C), 145.87 (C), 133.65 (C), 129.24 (CH), 129.03 (CH×2), 128.73 (CH), 128.08 (CH), 127.83 (CH), 127.33 (CH), 126.74 (CH×2), 126.03 (C), 124.52 (CH), 123.57 (C), 38.72 (CH), 27.03 (CH_3×3), 18.39 (C), –5.55 (CH_3), –6.08 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{23}H_{26}N_2NaOSi$, 397.1707; found, 397.1698.

1-Propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (15u).

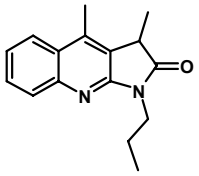


Brown oil.

IR (neat/ cm^{-1}): 2946, 1712, 1643, 1581, 1365, 1219, 1103, 849, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.92 (d, J = 8.2 Hz, 1H), 7.82 (s, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.63 (dd, J = 7.6, 7.6 Hz, 1H), 7.40 (dd, J = 7.4, 7.4 Hz, 1H), 3.91 (t, J = 7.4 Hz, 2H), 3.62 (s, 2H), 1.84 (tq, J = 7.5, 7.5 Hz, 2H), 1.01 (t, J = 7.5 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 174.41 (C), 157.42 (C), 146.90 (C), 130.76 (CH), 129.27 (CH), 127.80 (CH), 127.68 (CH), 125.95 (C), 124.44 (CH), 119.81 (C), 41.01 (CH_2), 34.09 (CH_2), 20.80 (CH_2), 11.38 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{14}H_{14}N_2NaO$, 249.0998; found, 249.1002.

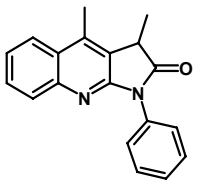
Typical procedure for the catalytic Pauson–Khand reaction using $[Rh(CO)_2Cl]_2$ to produce 17 and 18 (Table 3, Entry 3), and 19a and 20. A solution of $[Rh(CO)_2Cl]_2$ (14.0 mg, 0.036 mmol) in *p*-xylene (5 mL) was degassed, charged with carbon monoxide, and was heated to 130 °C. A solution of carbodiimide **5c** (138.4 mg, 0.516 mmol) in *p*-xylene (1 mL) was added, and the mixture was heated at the same temperature for 2.0 h. The mixture was evaporated, and the residue was purified by silica gel column chromatography (ethyl acetate/hexane = 1:10) to give pyrroloquinoline **17c** (13.1 mg, 0.041 mmol, 8% as a yellow oil) and **18a** (94.9 mg, 0.299 mmol, 58%).

3,4-Dimethyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17a).



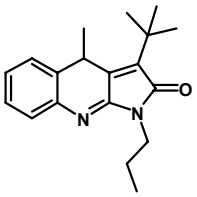
Brown solid; mp: 89.7–90.3 °C.
IR (KBr/ cm^{-1}): 3070, 2962, 1720, 1635, 1581, 1465, 1265, 1119, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.92–7.86 (m, 2H), 7.61 (ddd, J = 1.4, 7.0, 8.2 Hz, 1H), 7.42 (ddd, J = 1.2, 6.9, 8.2 Hz, 1H), 3.94–3.83 (m, 2H), 3.57 (q, J = 7.7 Hz, 1H), 2.60 (s, 3H), 1.83 (tq, J = 7.4, 7.4 Hz, 2H), 1.56 (d, J = 7.7 Hz, 3H), 0.98 (t, J = 7.5 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 178.21 (C), 156.07 (C), 146.69 (C), 138.56 (C), 128.92 (CH), 128.28 (CH), 126.24 (C), 124.12 (CH), 123.43 (CH), 123.43 (C), 40.73 (CH_2), 38.99 (CH), 20.86 (CH_2), 15.81 (CH_3), 14.52 (CH_3), 11.30 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{18}N_2NaO$, 277.1311; found, 277.1312.

3,4-Dimethyl-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17b).



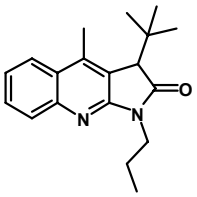
Brown solid; mp: 185.2–186.7 °C.
IR (KBr/ cm^{-1}): 3062, 2969, 1720, 1635, 1589, 1435, 1227, 748.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.91 (d, J = 8.3 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.63 (d, J = 8.1 Hz, 2H), 7.59 (dd, J = 7.6, 7.6 Hz, 1H), 7.53 (dd, J = 7.7, 7.7 Hz, 2H), 7.46–7.38 (m, 2H), 3.76 (dt, J = 7.4, 7.4 Hz, 1H), 2.66 (s, 3H), 1.68 (d, J = 7.4 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.40 (C), 155.77 (C), 146.36 (C), 139.42 (C), 133.30 (C), 129.03 (CH), 128.93 (CH×2), 128.71 (CH), 127.86 (CH), 126.76 (CH×2), 126.48 (C), 124.53 (CH), 123.29 (CH), 122.98 (C), 39.14 (CH), 16.11 (CH_3), 14.67 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{16}N_2NaO$, 311.1155; found, 311.1145.

3-*tert*-butyl-4-methyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(4*H*)-one (18a).



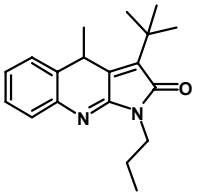
Yellow oil.
IR (neat/ cm^{-1}): 3062, 2962, 1712, 1635, 1450, 1365, 1088, 941, 764.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.42 (dd, J = 1.1, 7.8 Hz, 1H), 7.26 (ddd, J = 1.6, 7.5, 7.6 Hz, 1H), 7.18 (dd, J = 1.5, 7.6 Hz, 1H), 7.13 (ddd, 1.2, 7.4, 7.4 Hz, 1H), 4.31 (q, J = 7.3 Hz, 1H), 3.75–3.65 (m, 2H), 1.73 (dtq, J = 1.2, 7.4, 7.4 Hz, 2H), 1.45 (s, 9H), 1.39 (d, J = 7.4 Hz, 3H), 0.94 (t, J = 7.5 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 170.32 (C), 155.57 (C), 141.87 (C), 141.64 (C), 134.08 (C), 132.00 (C), 128.16 (CH), 127.87 (CH), 127.62 (CH), 125.91 (CH), 40.10 (CH_2), 34.51 (C), 33.11 (CH), 29.27 (CH_3×3), 28.16 (CH_3), 21.91 (CH_2), 11.36 (CH_3)
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{24}N_2NaO$, 319.1781; found, 319.1782.

3-*tert*-Butyl-4-methyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17c).



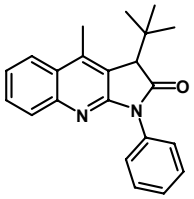
Yellow oil.
IR (KBr/ cm^{-1}): 3070, 2962, 1720, 1628, 1466, 1358, 1288, 1219, 1103, 756.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.89 (d, J = 8.8 Hz, 2H), 7.62 (ddd, J = 1.4, 7.0, 8.3 Hz, 1H), 7.42 (ddd, J = 1.2, 6.9, 8.3 Hz, 1H), 3.90–3.84 (m, 1H), 3.81–3.74 (m, 1H), 3.33 (s, 1H), 2.60 (s, 3H), 1.88–1.74 (m, 2H), 1.08 (s, 9H), 1.01 (t, J = 7.6 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 177.04 (C), 157.19 (C), 146.39 (C), 139.58 (C), 128.98 (CH), 128.00 (CH), 126.29 (C), 124.03 (CH), 123.82 (CH), 122.10 (C), 53.87 (CH), 40.58 (CH_2), 37.84 (C), 28.07 (CH_3×3), 21.00 (CH_2), 17.91 (CH_3), 11.61 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{24}N_2NaO$, 319.1781; found, 319.1775.

3-*tert*-butyl-4-methyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(4*H*)-one (18a).



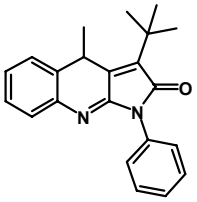
Yellow oil.
IR (neat/ cm^{-1}): 3062, 2962, 1712, 1635, 1450, 1365, 1088, 941, 764.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.42 (dd, J = 1.1, 7.8 Hz, 1H), 7.26 (ddd, J = 1.6, 7.5, 7.6 Hz, 1H), 7.18 (dd, J = 1.5, 7.6 Hz, 1H), 7.13 (ddd, 1.2, 7.4, 7.4 Hz, 1H), 4.31 (q, J = 7.3 Hz, 1H), 3.75–3.65 (m, 2H), 1.73 (dtq, J = 1.2, 7.4, 7.4 Hz, 2H), 1.45 (s, 9H), 1.39 (d, J = 7.4 Hz, 3H), 0.94 (t, J = 7.5 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 170.32 (C), 155.57 (C), 141.87 (C), 141.64 (C), 134.08 (C), 132.00 (C), 128.16 (CH), 127.87 (CH), 127.62 (CH), 125.91 (CH), 40.10 (CH_2), 34.51 (C), 33.11 (CH), 29.27 (CH_3×3), 28.16 (CH_3), 21.91 (CH_2), 11.36 (CH_3)
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{24}N_2NaO$, 319.1781; found, 319.1782.

3-*tert*-Butyl-4-methyl-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17d).



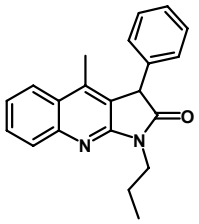
Yellow solid; mp: 157.8–158.8 °C.
IR (KBr/ cm^{-1}): 3054, 2954, 1727, 1427, 1288, 1227, 1173, 918, 764.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.91 (dd, J = 1.0, 8.2 Hz, 1H), 7.83 (d, J = 8.3 Hz, 1H), 7.61–7.56 (m, 3H), 7.55–7.51 (m, 2H), 7.45–7.39 (m, 2H), 3.52 (s, 1H), 2.66 (s, 3H), 1.16 (s, 9H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 176.17 (C), 156.84 (C), 146.03 (C), 140.40 (C), 133.27 (C), 129.05 (CH), 128.98 (CH×2), 128.46 (CH), 127.88 (CH), 126.90 (CH×2), 126.47 (C), 124.42 (CH), 123.66 (CH), 121.47 (C), 53.02 (CH), 38.57 (C), 27.95 (CH_3×3), 17.96 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{22}N_2NaO$, 353.1624; found, 353.1634.

3-*tert*-Butyl-4-methyl-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(4*H*)-one (18b).



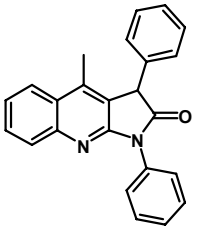
Yellow oil.
IR (neat/ cm^{-1}): 3062, 2954, 1720, 1627, 1589, 1496, 1427, 1227, 918, 764.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.54 (d, J = 8.0 Hz, 2H), 7.48 (dd, J = 7.9, 7.9 Hz, 2H), 7.40 (d, J = 7.7 Hz, 1H), 7.35 (dd, J = 7.4, 7.4 Hz, 1H), 7.27–7.19 (m, 2H), 7.16 (dd, J = 7.4, 7.4 Hz, 1H), 4.43 (q, J = 7.2 Hz, 1H), 1.51 (s, 9H), 1.47 (d, J = 7.2 Hz, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 169.23 (C), 155.01 (C), 141.47 (C), 141.37 (C), 134.96 (C), 133.07 (C), 131.92 (C), 128.67 (CH), 128.67 (CH×2), 127.68 (CH), 127.66 (CH), 127.07 (CH), 127.03 (CH×2), 126.40 (CH), 34.76 (C), 33.28 (CH), 29.31 (CH_3×3), 28.35 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{22}N_2NaO$, 353.1624; found, 353.1624.

4-Methyl-3-phenyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17e).



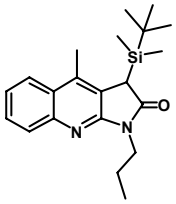
Yellow solid; mp: 193.3–194.2 °C.
IR (KBr/ cm^{-1}): 3062, 2962, 1720, 1635, 1589, 1442, 1080, 763.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.97 (d, J = 8.3 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.66 (dd, J = 7.7, 7.7 Hz, 1H), 7.43 (dd, J = 7.6, 7.6 Hz, 1H), 7.35–7.27 (m, 3H), 7.18 (d, J = 7.5 Hz, 2H), 4.69 (s, 1H), 3.94–3.88 (m, 2H), 2.31 (s, 3H), 1.85 (tq, J = 7.5, 7.5 Hz, 2H), 0.97 (t, J = 7.5 Hz, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 175.42 (C), 156.67 (C), 147.12 (C), 140.07 (C), 135.70 (C), 129.29 (CH), 129.06 (CH×2), 128.43 (CH), 128.07 (CH×2), 127.78 (CH), 126.39 (C), 124.28 (CH), 123.68 (CH) 121.96 (C), 50.44 (CH), 41.04 (CH_2), 20.88 (CH_2), 14.86 (CH_3), 11.33 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{21}H_{21}N_2O$, 317.1648; found, 317.1646.

4-Methyl-1,3-diphenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17f).



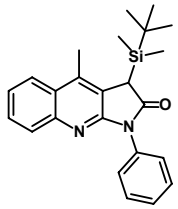
Yellow solid; mp: 218.8–219.5 °C.
IR (KBr/ cm^{-1}): 3055, 2985, 2306, 1581, 1489, 1412, 1265, 740.
^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.92 (d, J = 8.3 Hz, 2H), 7.66–7.62 (m, 3H), 7.53 (dd, J = 7.9, 7.9 Hz, 2H), 7.46 (ddd, J = 1.2, 7.0, 8.1 Hz, 1H), 7.41 (dd, J = 7.4, 7.4 Hz, 1H), 7.38–7.31 (m, 3H), 7.29–7.26 (m, 2H), 4.90 (s, 1H), 2.39 (s, 3H).
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 174.58 (C), 156.36 (C), 146.82 (C), 140.97 (C), 135.57 (C), 133.20 (C), 129.42 (CH), 129.16 (2CH), 128.96 (2CH), 128.90 (CH), 128.19 (2CH), 127.98 (CH), 127.95 (CH), 126.81 (2CH), 126.65 (C), 124.70 (CH), 123.55 (CH), 121.46 (C), 50.50 (CH), 15.04 (CH_3).
HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{24}H_{18}N_2O$, 373.1311; found, 373.1321.

3-(*tert*-Butyldimethylsilyl)-4-methyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17g).



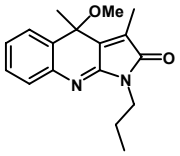
Brown solid; mp: 99.8–100.1 °C.
IR (KBr/ cm^{-1}): 3062, 2931, 2854, 1712, 1628, 1581, 1442, 1219, 1049, 841, 756.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.91 (dd, J = 1.0, 8.3 Hz, 1H), 7.85 (dd, J = 1.2, 8.2 Hz, 1H), 7.59 (ddd, J = 1.3, 6.9, 8.3 Hz, 1H), 7.40 (ddd, J = 1.3, 6.9, 8.2 Hz, 1H), 3.93–3.86 (m, 1H), 3.85–3.78 (m, 1H), 3.64 (s, 1H), 2.52 (s, 3H), 1.90–1.75 (m, 2H), 1.09 (s, 9H), 1.01 (t, J = 7.5 Hz, 3H), 0.01 (d, J = 3.2 Hz, 6H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 177.45 (C), 156.06 (C), 145.93 (C), 135.48 (C), 128.30 (CH), 128.07 (CH), 126.08 (C), 123.82 (CH), 123.30 (CH), 122.72 (C), 40.92 (CH_2), 37.44 (CH), 26.80 (CH_3×3), 21.17 (CH_2), 18.10 (C), 16.68 (CH_3), 11.56 (CH_3), –5.00 (CH_3), –6.04 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{30}N_2NaOSi$, 377.2020; found, 377.2016.

3-(*tert*-Butyldimethylsilyl)-4-methyl-1-phenyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(3*H*)-one (17h).



Brown solid: mp: 153.0–154.0 °C.
IR (KBr/ cm^{-1}): 3062, 2931, 2854, 1720, 1589, 1496, 1396, 1219, 1041, 818, 764.
^{1}H-NMR (500 MHz, $CDCl_3$, δ): 7.86 (dd, J = 8.3, 12.6 Hz, 2H), 7.61–7.48 (m, 5H), 7.45–7.37 (m, 2H), 3.84 (s, 1H), 2.58 (s, 3H), 1.08 (s, 9H), 0.14 (s, 3H), 0.06 (s, 3H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ): 176.62 (C), 155.64 (C), 145.64 (C), 136.13 (C), 133.71 (C), 128.96 (CH×2), 128.56 (CH), 128.38 (CH), 127.71 (CH), 126.85 (CH×2), 126.33 (C), 124.25 (CH), 123.17 (CH), 122.22 (C), 37.85 (CH), 26.85 (CH_3×3), 18.23 (C), 16.75 (CH_3), –5.06 (CH_3), –5.87 (CH_3).
HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{28}N_2NaOSi$, 411.1863; found, 411.1874.

4-Methoxy-3,4-dimethyl-1-propyl-1*H*-pyrrolo[2,3-*b*]quinolin-2(4*H*)-one (19a).



Yellow oil.

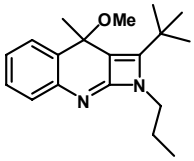
IR (neat/ cm^{-1}): 2970, 2931, 1720, 1635, 1442, 1103, 756.

^{1}H-NMR (600 MHz, $CDCl_3$, δ): 7.54 (dd, J = 1.5, 7.6 Hz, 1H), 7.44 (dd, J = 1.1, 7.7 Hz, 1H), 7.33 (ddd, J = 1.4, 7.7, 7.7 Hz, 1H), 7.25 (ddd, J = 1.3, 7.5, 7.5 Hz, 1H), 3.76–3.67 (m, 2H), 2.94 (s, 3H), 2.22 (s, 3H), 1.76 (tq, J = 7.3, 7.5 Hz, 2H), 1.64 (s, 3H), 0.96 (t, J = 7.5 Hz, 3H).

^{13}C-NMR (150 MHz, $CDCl_3$, δ): 170.74 (C), 156.46 (C), 143.75 (C), 135.83 (C), 133.31 (C), 131.33 (C), 129.04 (CH), 128.51 (CH), 126.75 (CH), 125.97 (CH), 74.40 (C), 52.47 (CH_3), 40.36 (CH_2), 31.01 (CH_3), 21.98 (CH_2), 11.32 (CH_3), 9.12 (CH_3).

HRMS-ESI (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{20}N_2NaO_2$, 307.1417; found, 307.1415.

2-*tert*-Butyl-3-methoxy-3-methyl-1-propyl-1,3-dihydro-1,8-diaza-cyclobuta[*b*]naphthalene (20).



Yellow oil.

IR (neat/ cm^{-1}): 2962, 1643, 1219, 1111, 756.

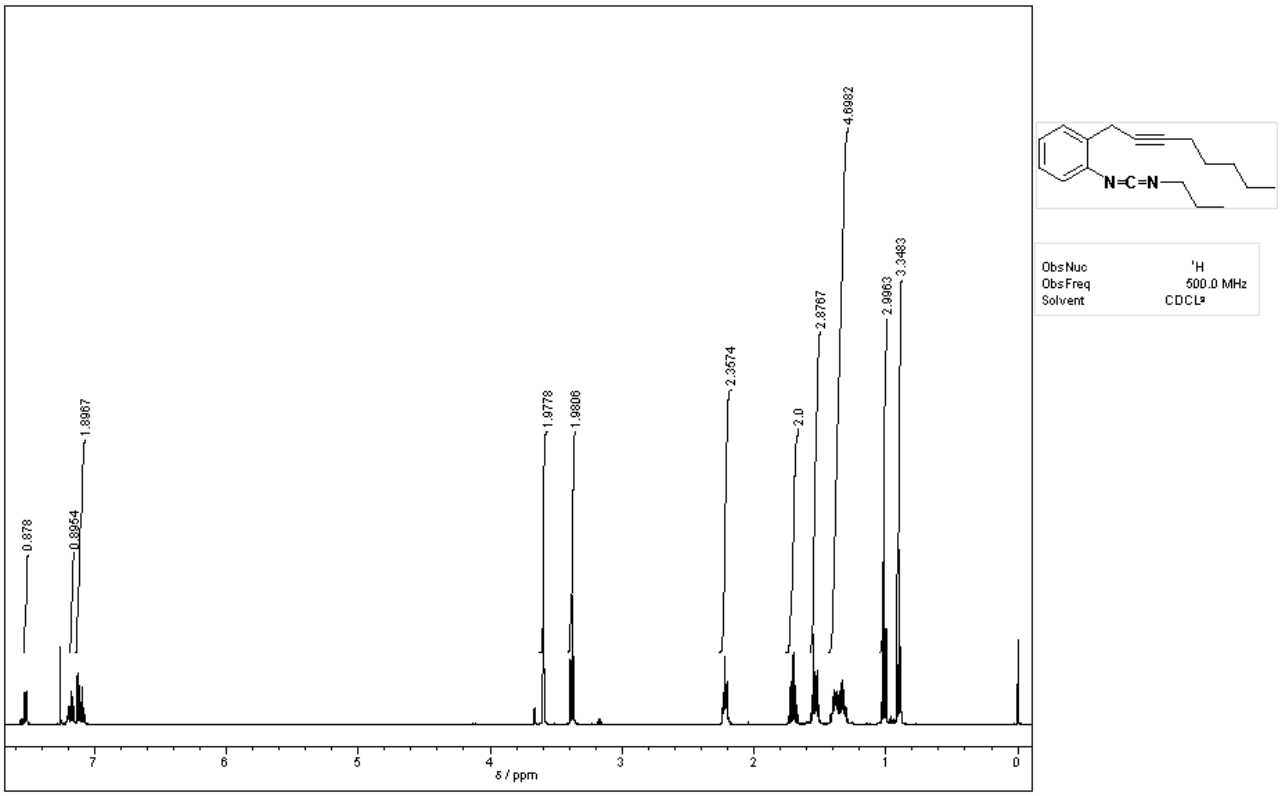
^{1}H-NMR (300 MHz, $CDCl_3$, δ): 7.70 (dd, J = 1.3, 8.0 Hz, 1H), 7.64 (dd, J = 1.2, 8.1 Hz, 1H), 7.45 (ddd, J = 1.5, 7.0, 8.2 Hz, 1H), 7.20 (ddd, J = 1.4, 7.0, 8.1 Hz, 1H), 3.45-3.25 (m, 2H), 3.21 (s, 3H), 2.40 (s, 3H), 1.95-1.78 (m, 2H), 1.13 (s, 9H), 1.01 (t, J = 7.4 Hz, 3H).

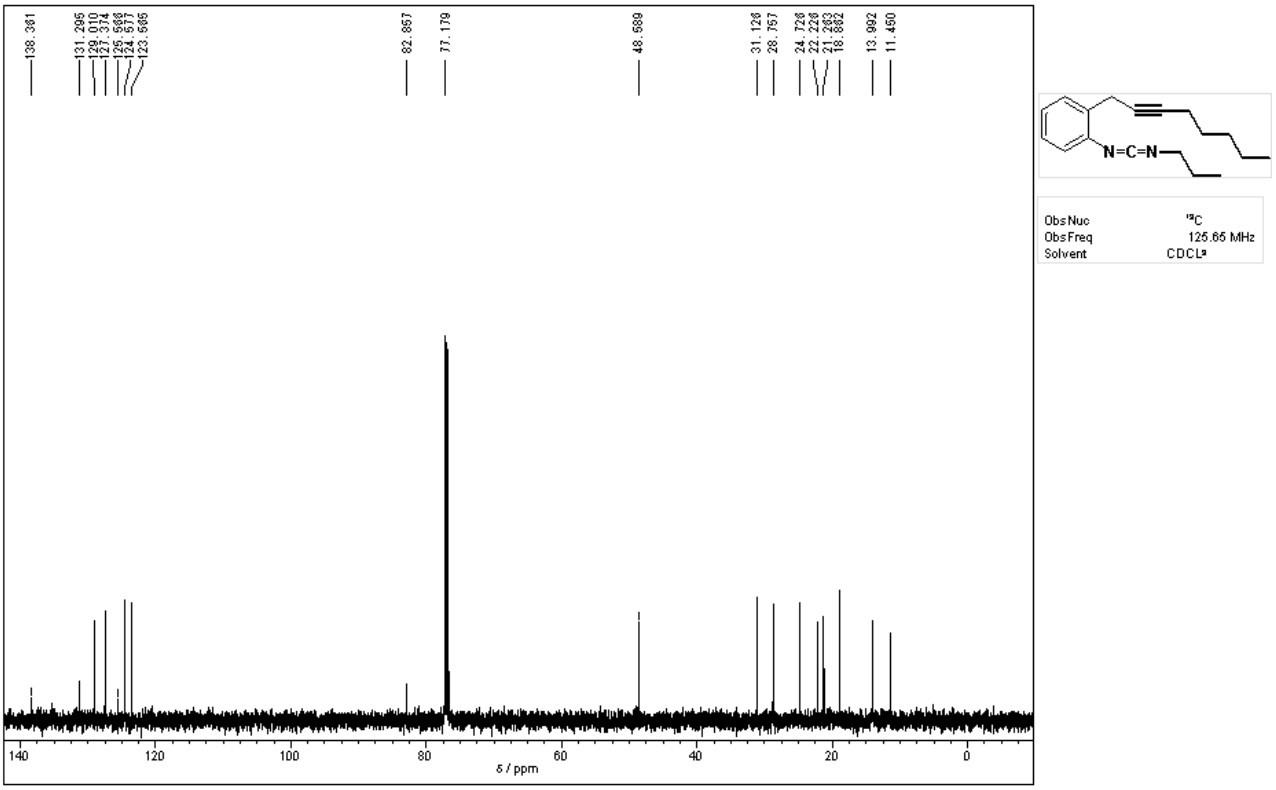
^{13}C-NMR (150 MHz, $CDCl_3$, δ): 163.90 (C), 149.88 (C), 132.53 (C), 129.20 (C), 128.44 (CH), 126.28 (CH), 126.11 (C), 123.95 (CH), 121.63 (CH), 110.41 (C), 52.43 (CH_3), 45.12 (CH_2), 38.10 (C), 26.27 ($CH_3\times3$), 22.62 (CH_2), 14.84 (CH_3), 11.84 (CH_3).

HRMS-ESI (*m/z*): $[M+H]^+$ calcd for $C_{19}H_{27}N_2O$, 299.2118; found, 299.2104.

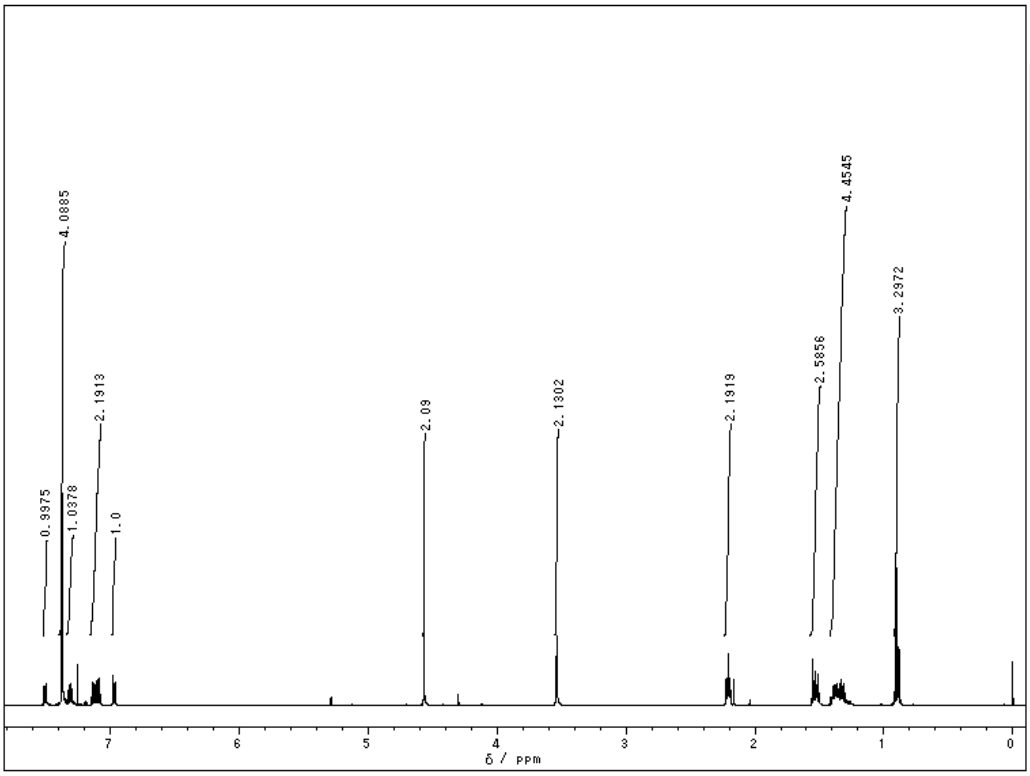
Copies of ^{1}H- and ^{13}C NMRspectra for compounds

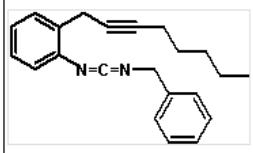
4a



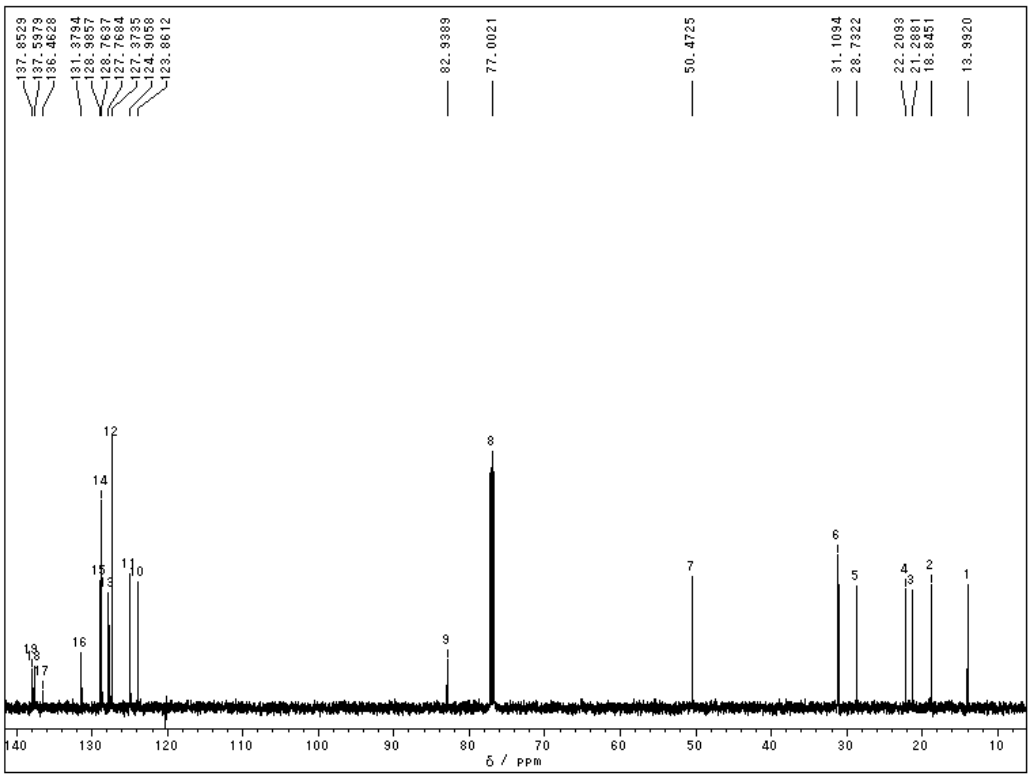


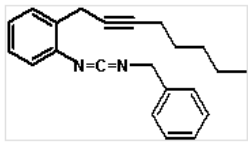
4b





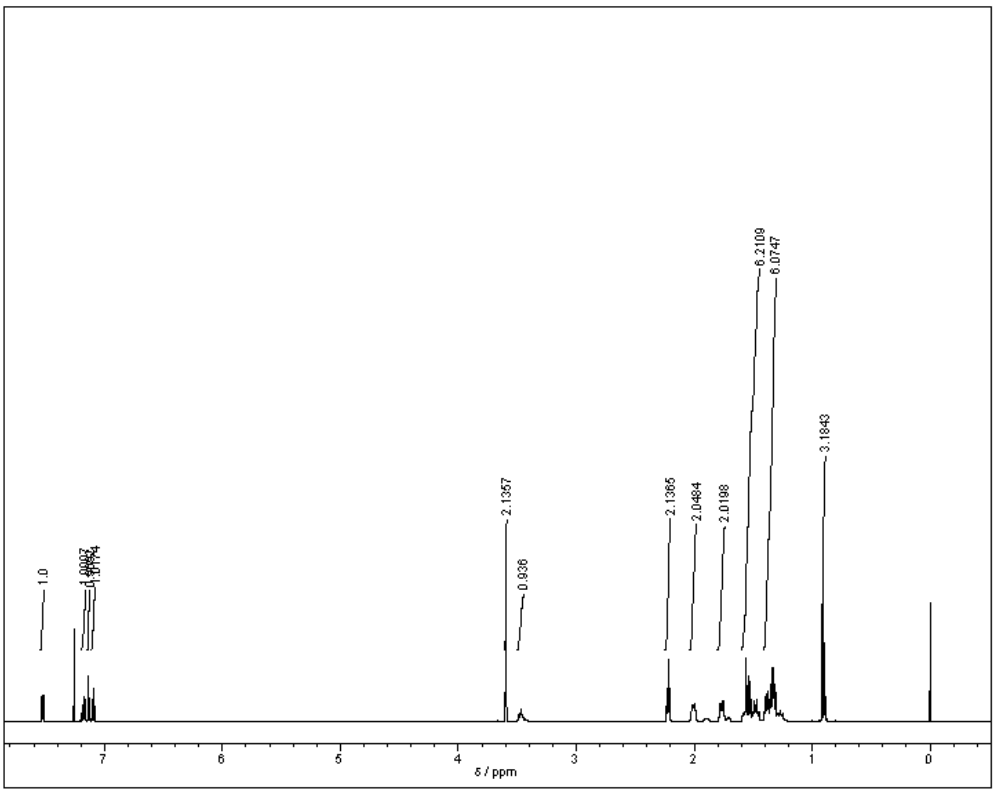
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCL^{3}$

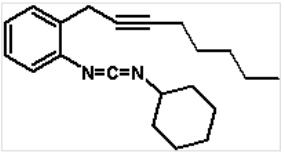




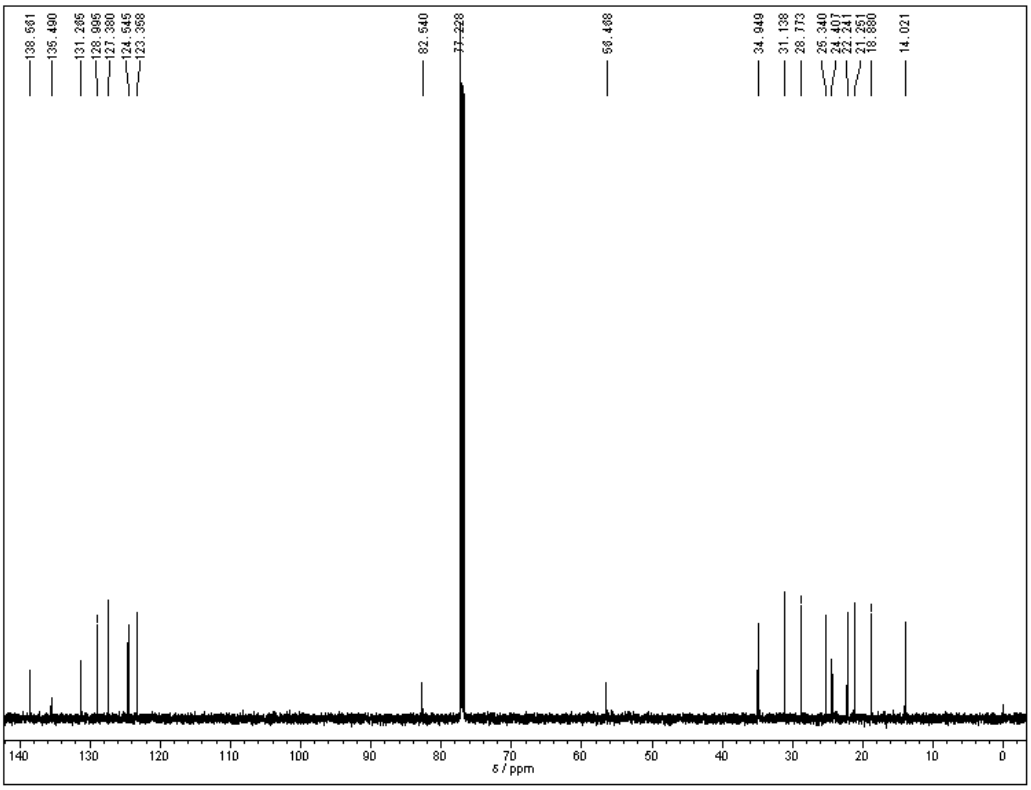
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCL^{3}$

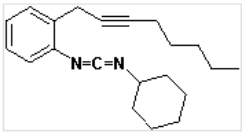
4c





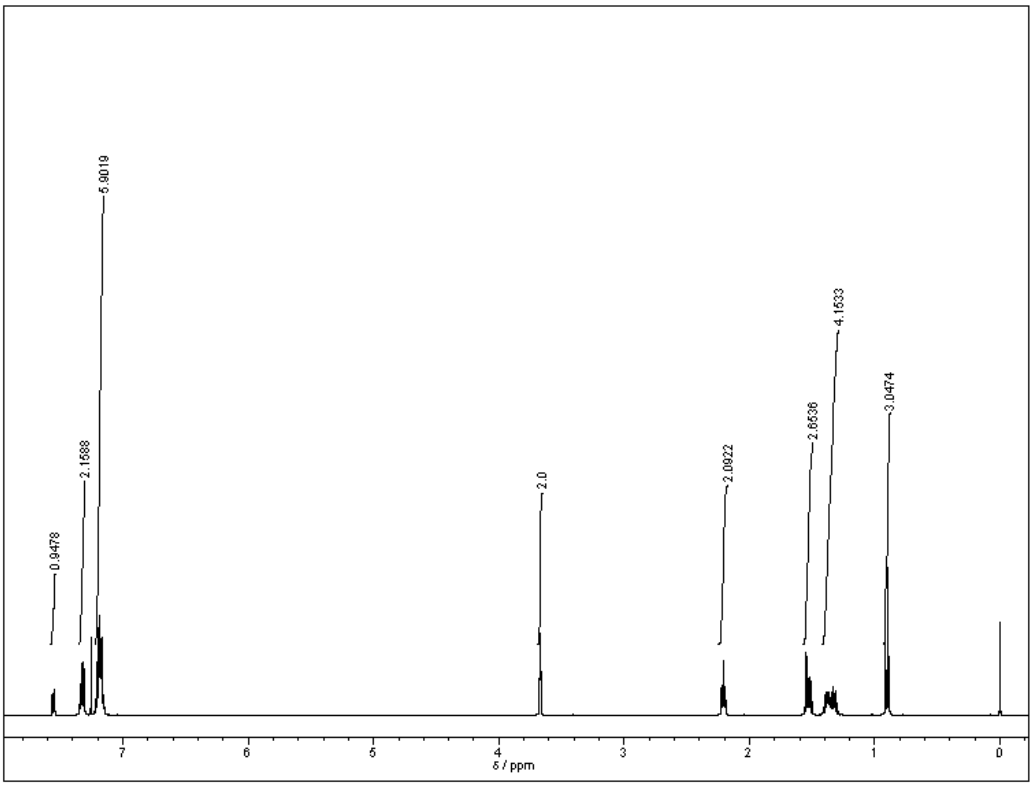
Obs Nuc	^{1}H
Obs Freq	600.13 MHz
Solvent	$CDCl_3$

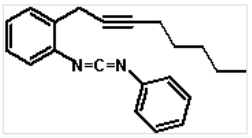




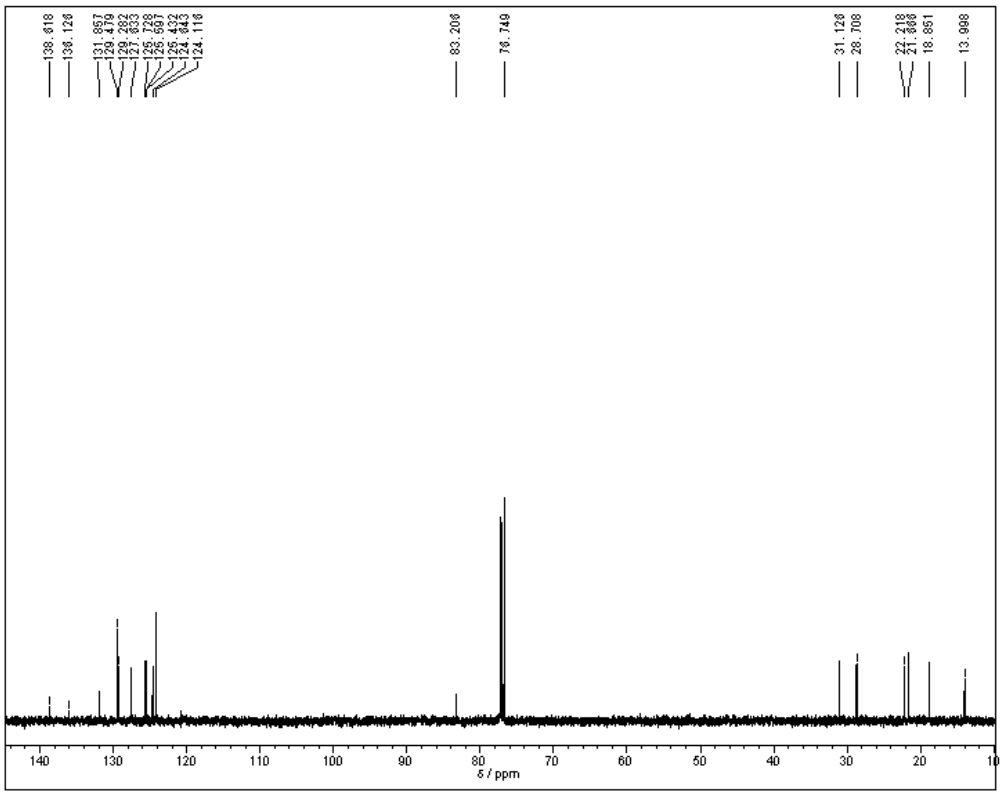
Obs Nuc	^{13}C
Obs Freq	150.9 MHz
Solvent	$CDCl_3$

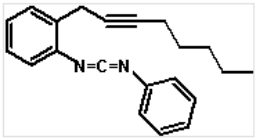
4d





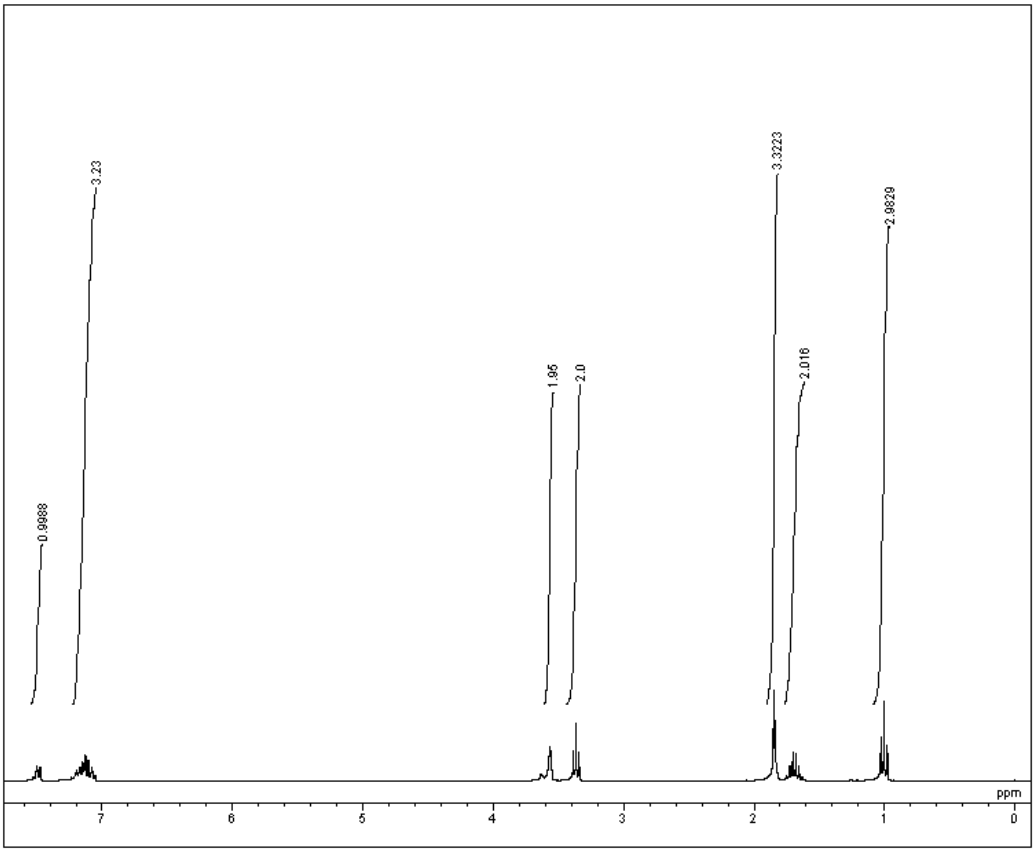
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

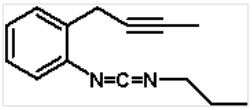




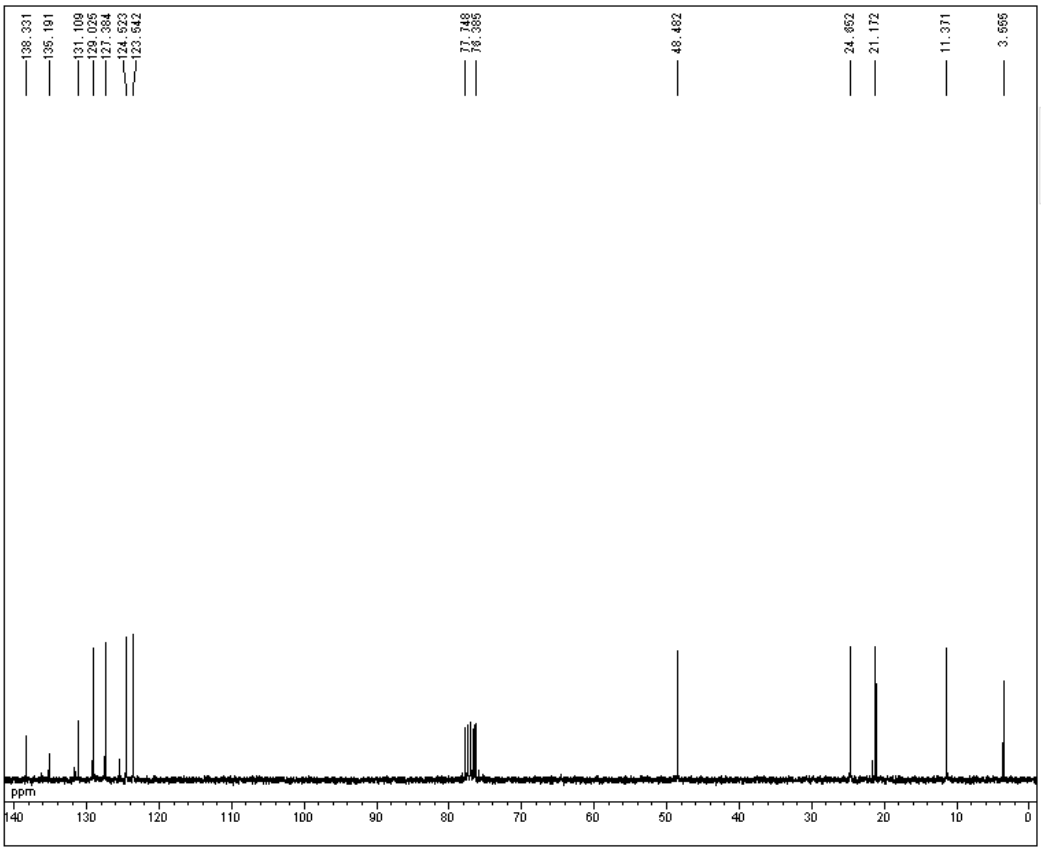
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

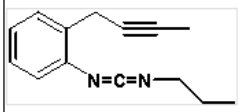
4e





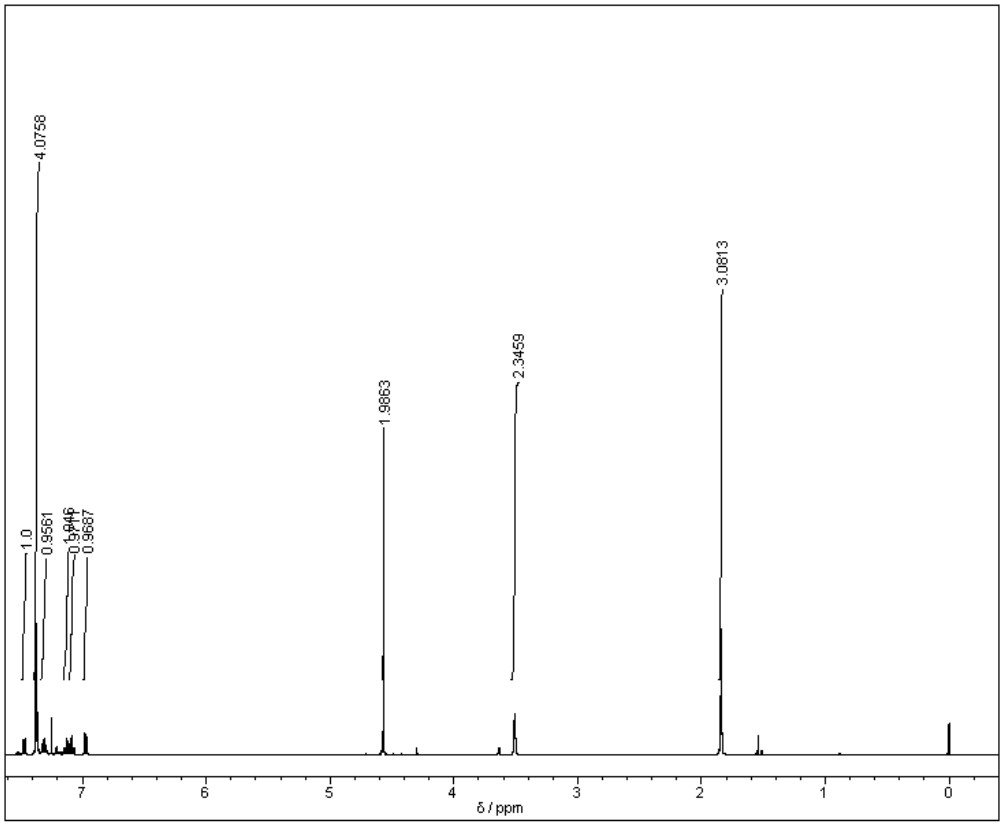
ObsNuc	^{1}H
ObsFreq	300.01 MHz
Solvent	$CDCl_3$

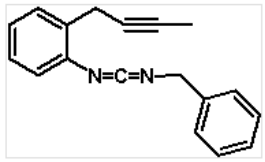




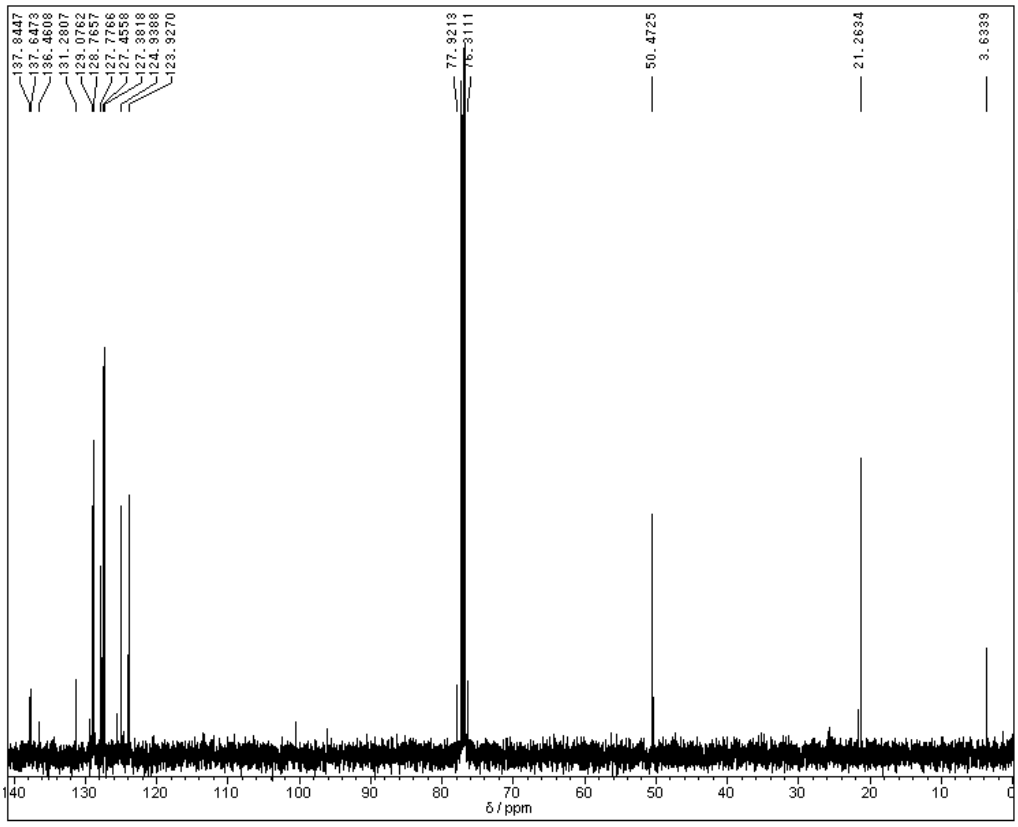
ObsNuc	^{13}C
ObsFreq	75.44 MHz
Solvent	$CDCl_3$

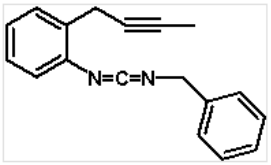
4f





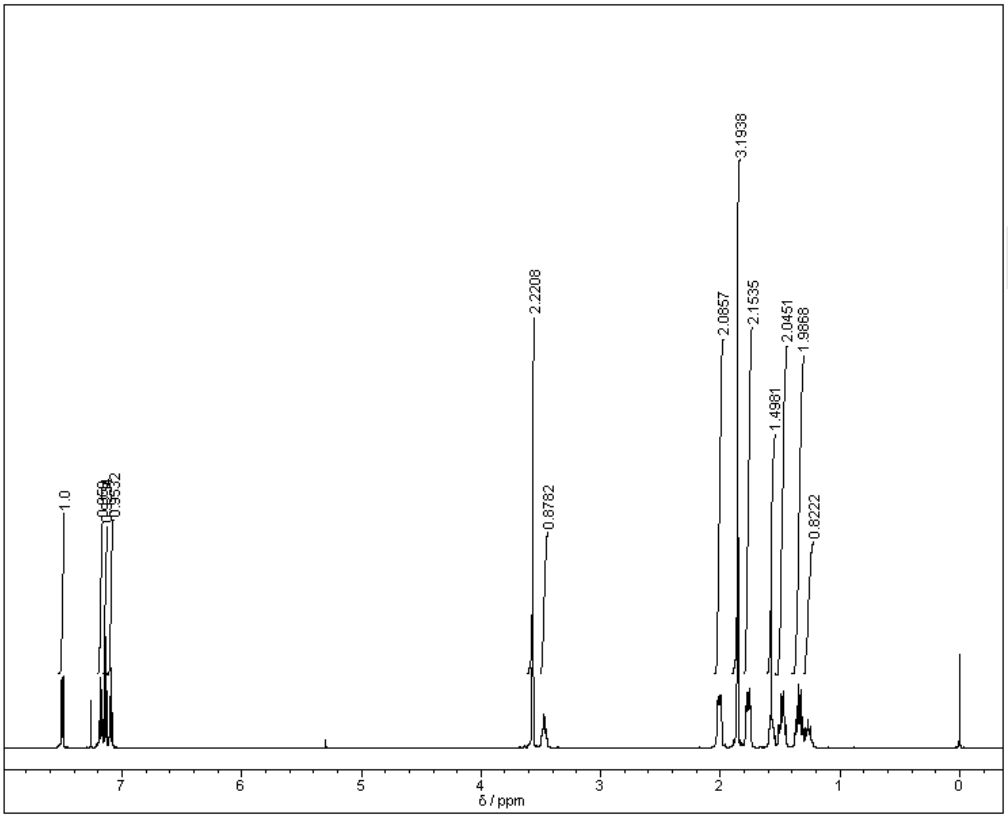
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

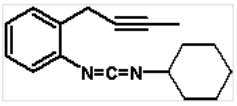




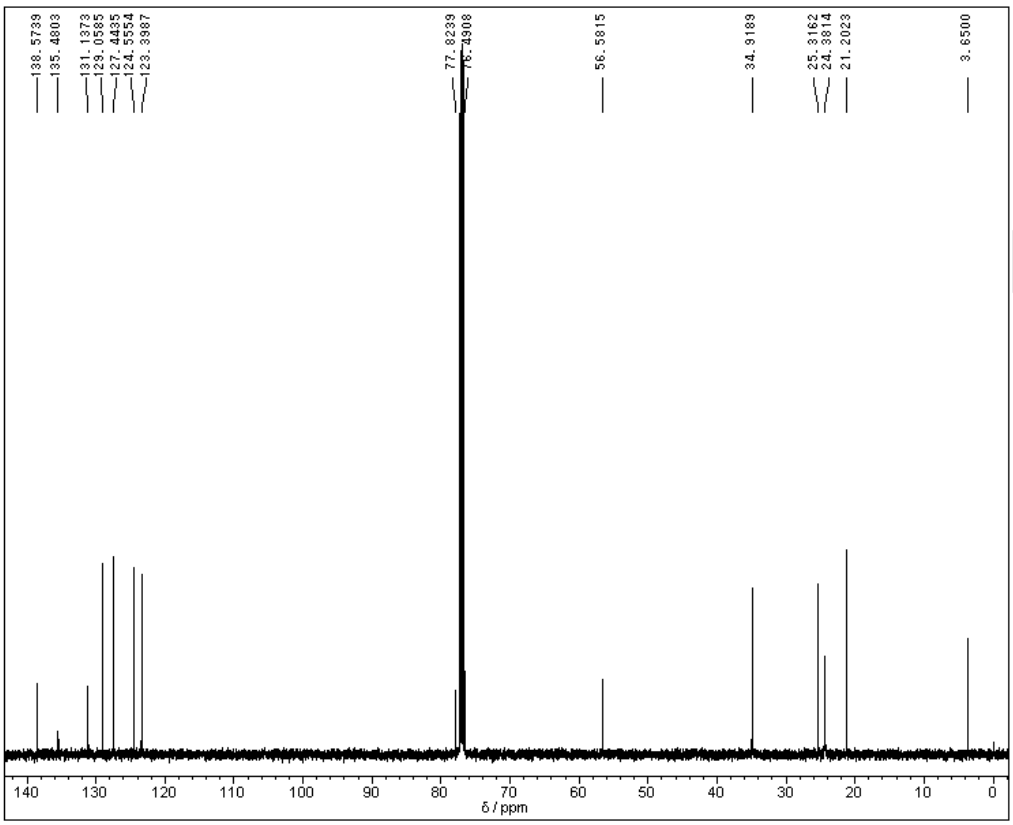
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

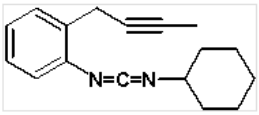
4g





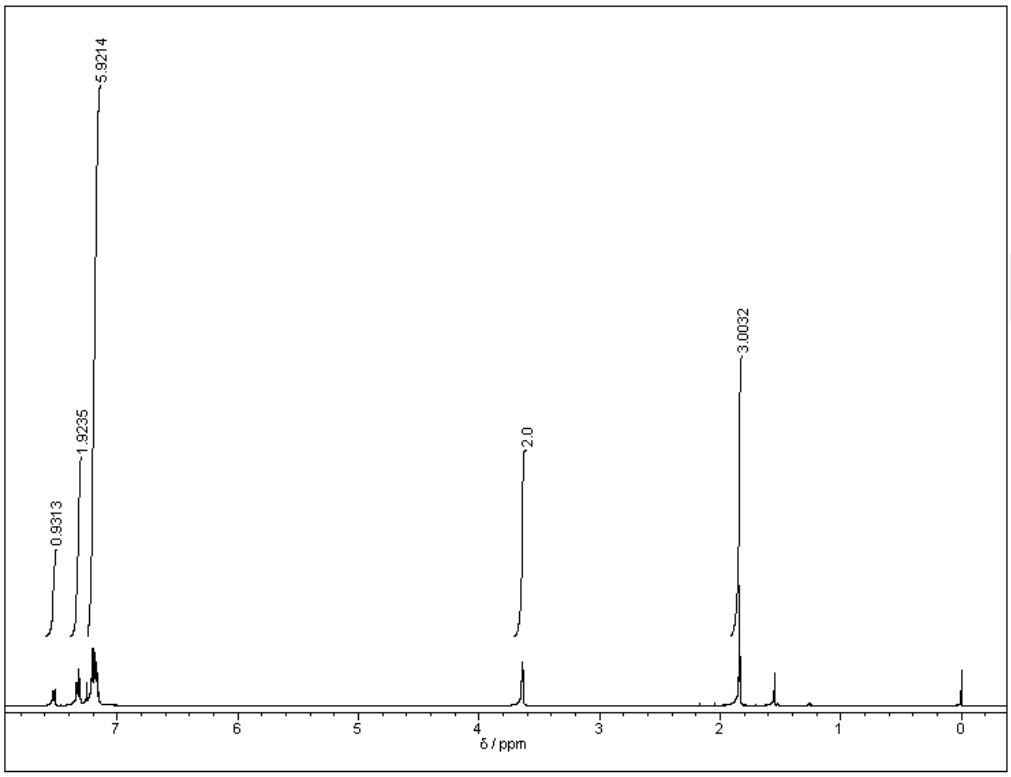
ObsNuc 1H
ObsFreq 600.13 MHz
Solvent $CDCL_3$

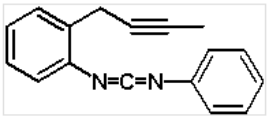




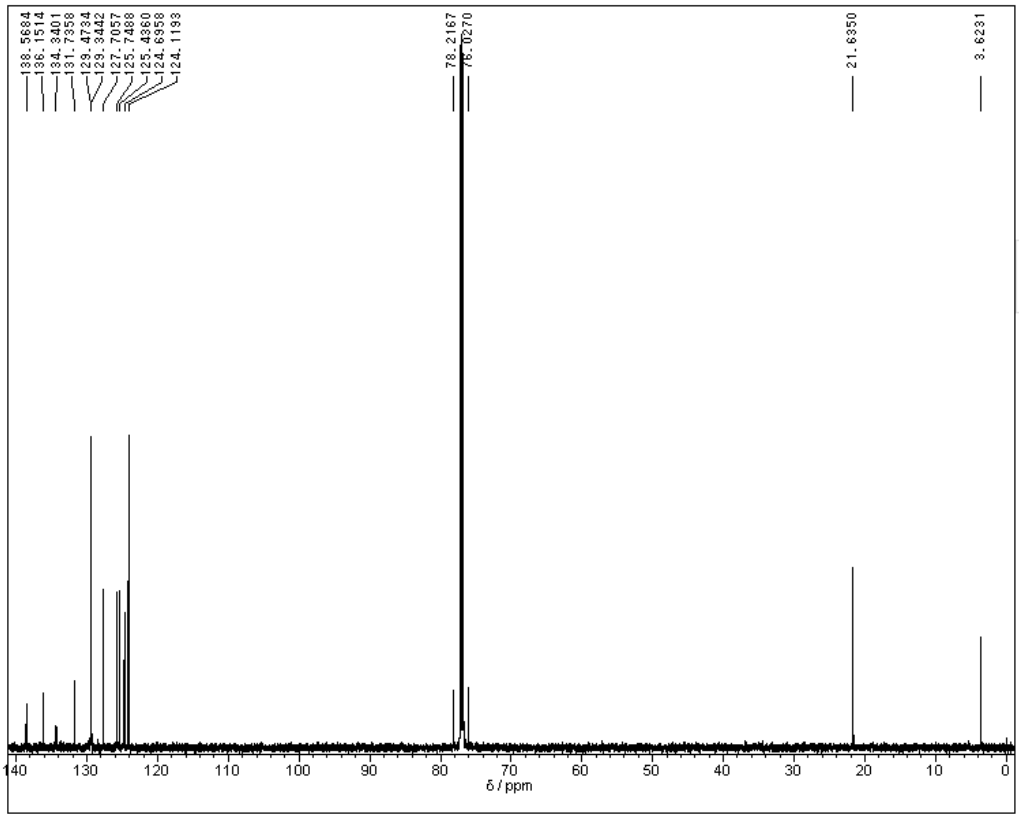
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent $CDCL_3$

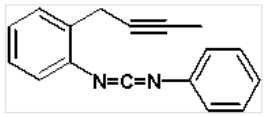
4h





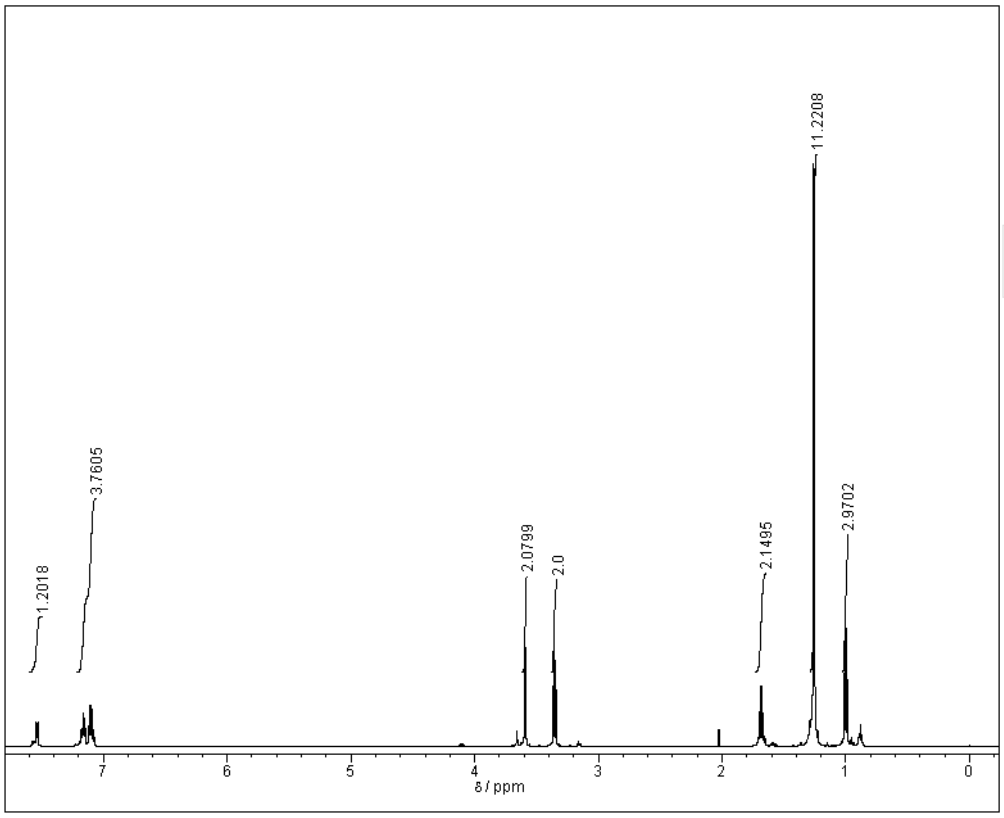
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

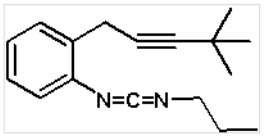




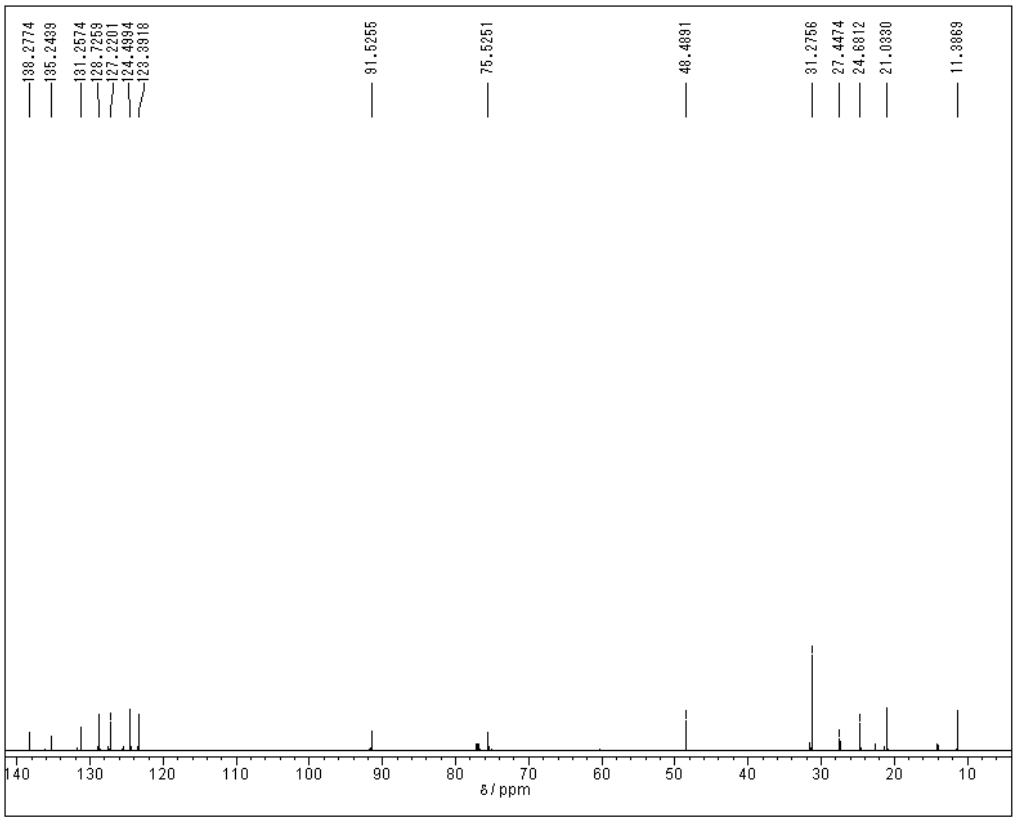
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

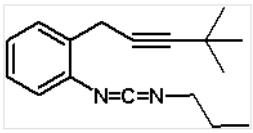
4i





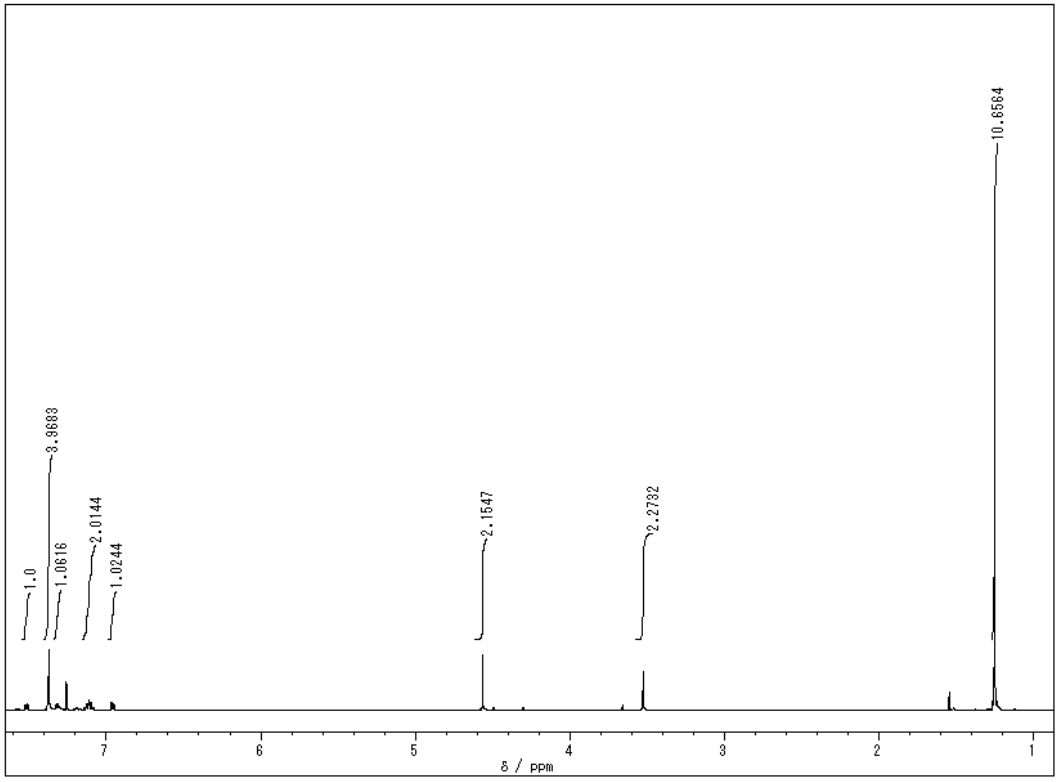
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	$CDCl_3$

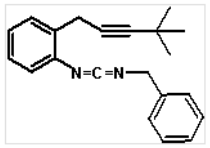




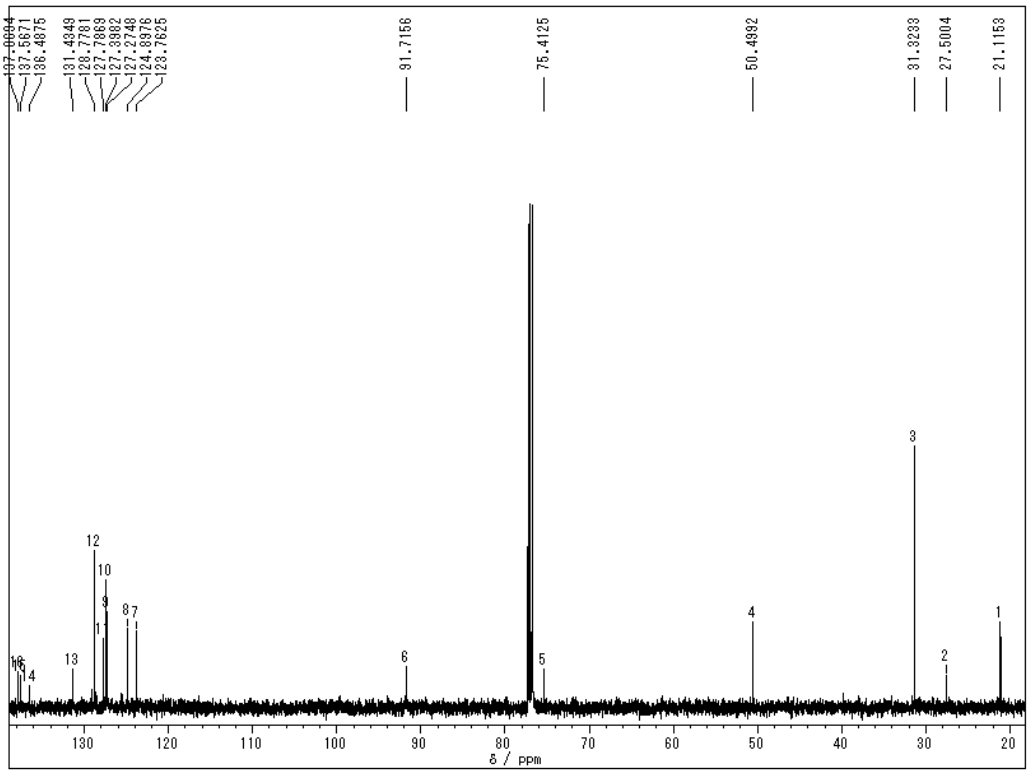
ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	$CDCl_3$

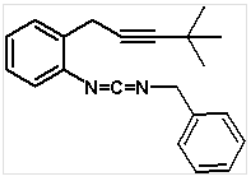
4j





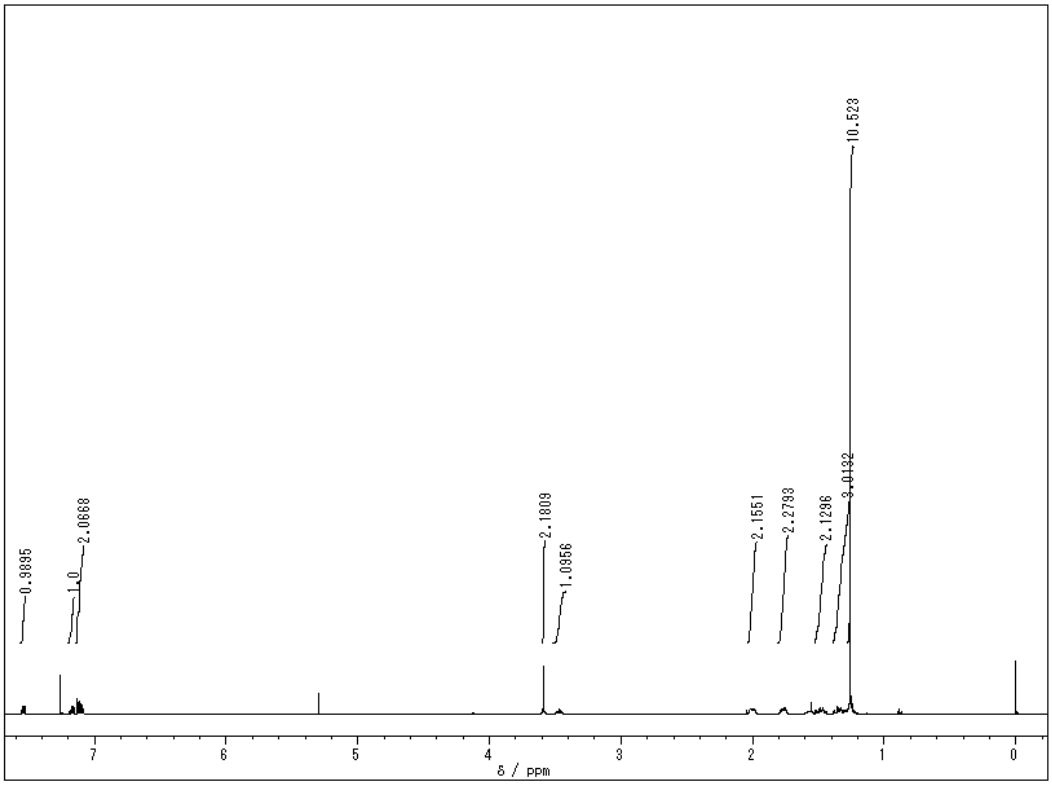
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

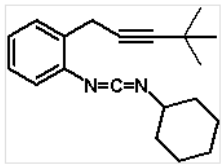




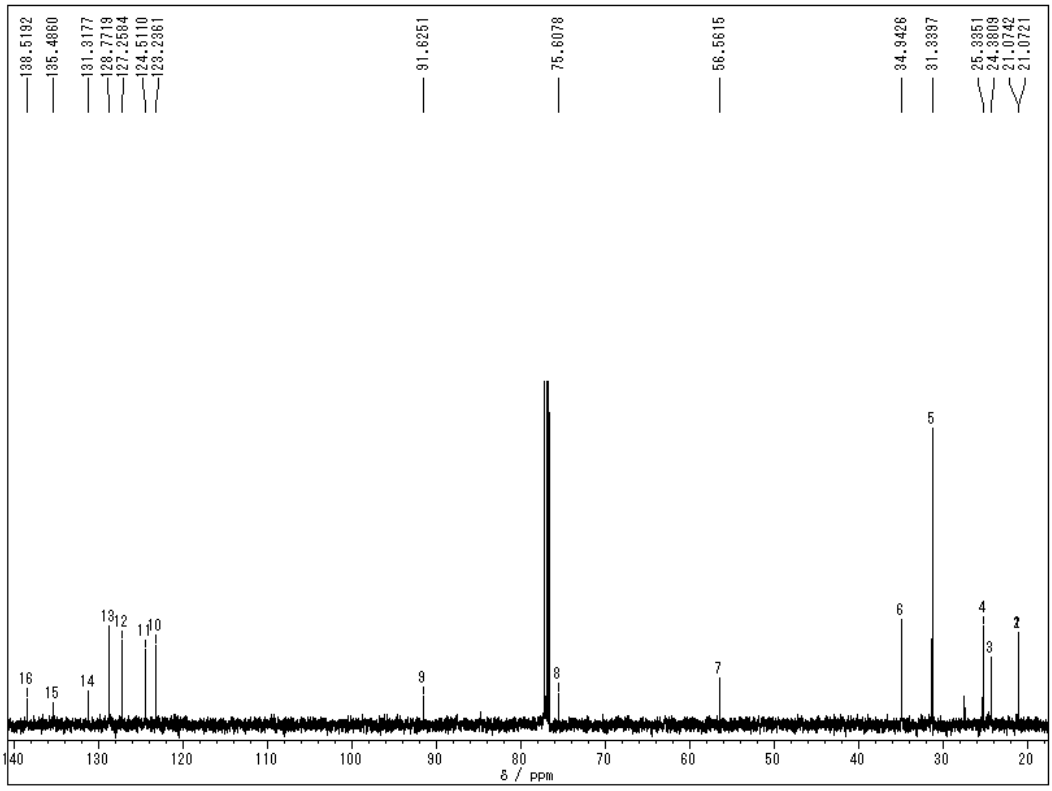
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

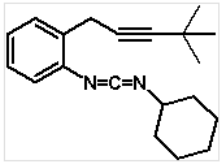
4k





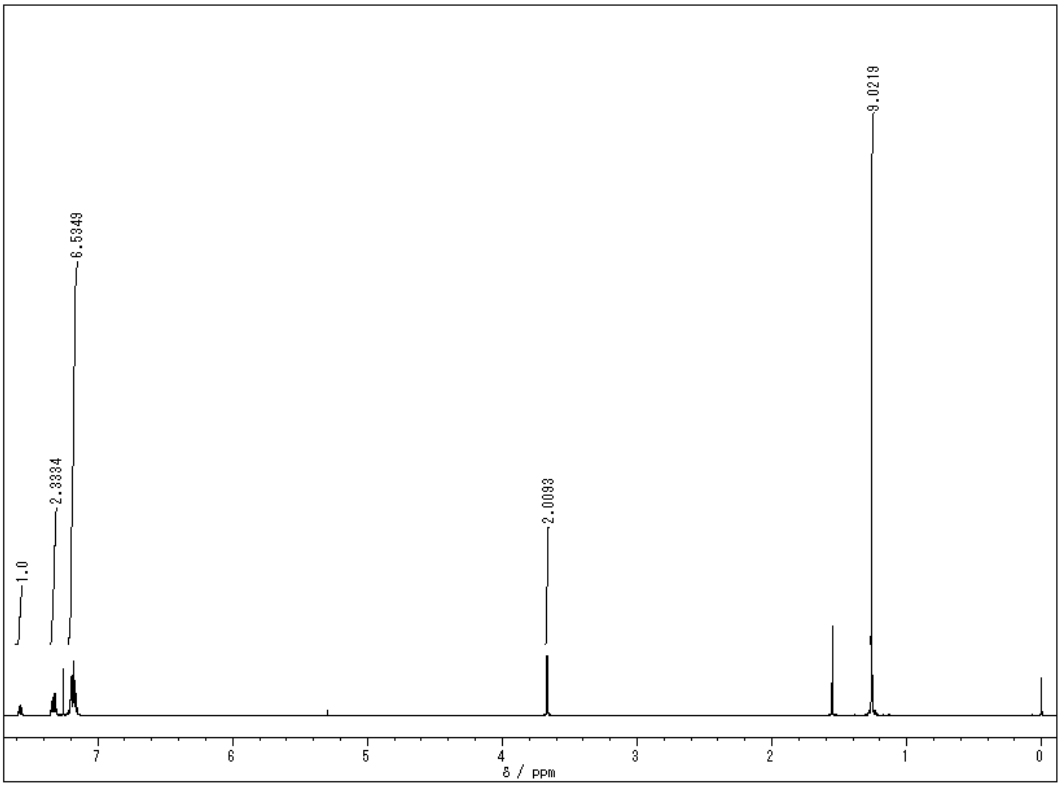
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

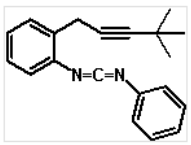




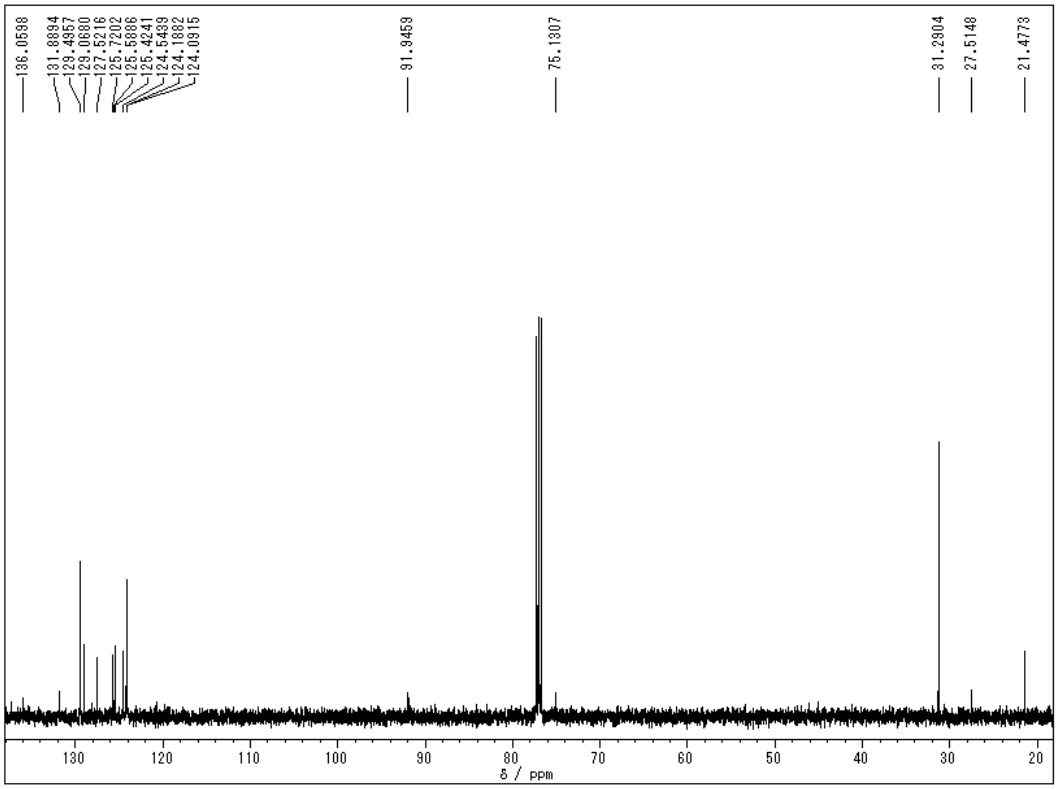
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

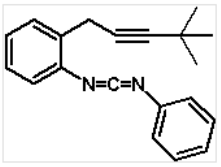
4l





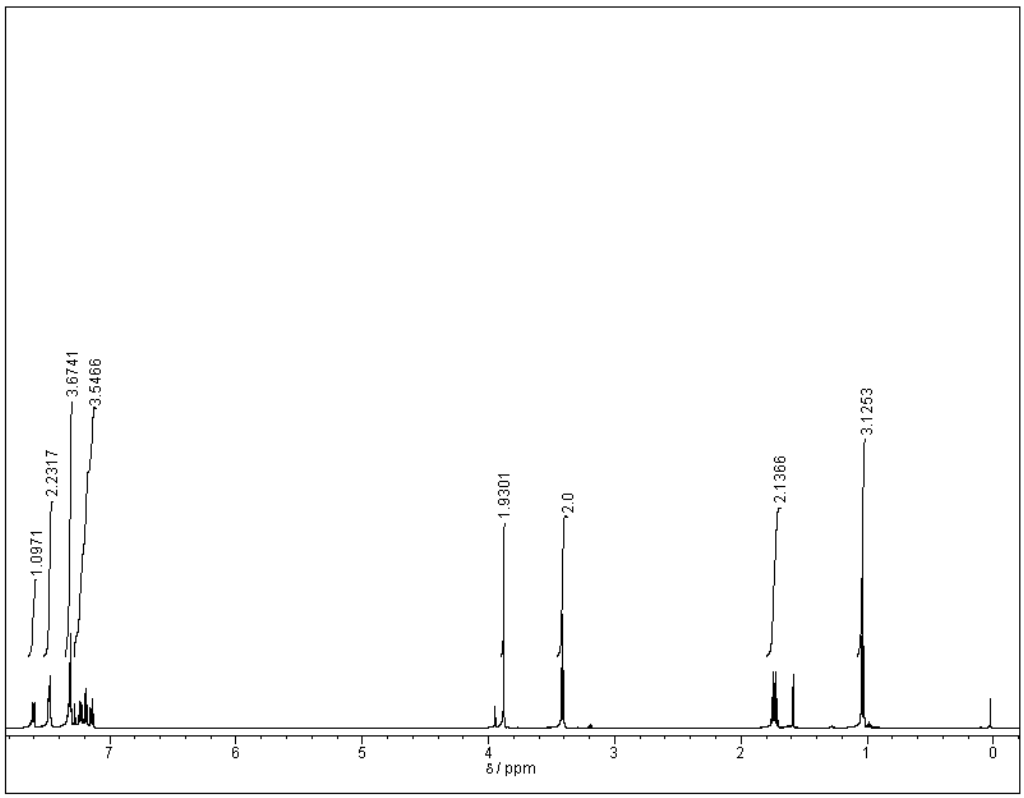
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent CDCL₃

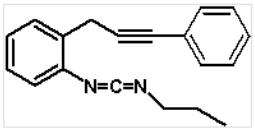




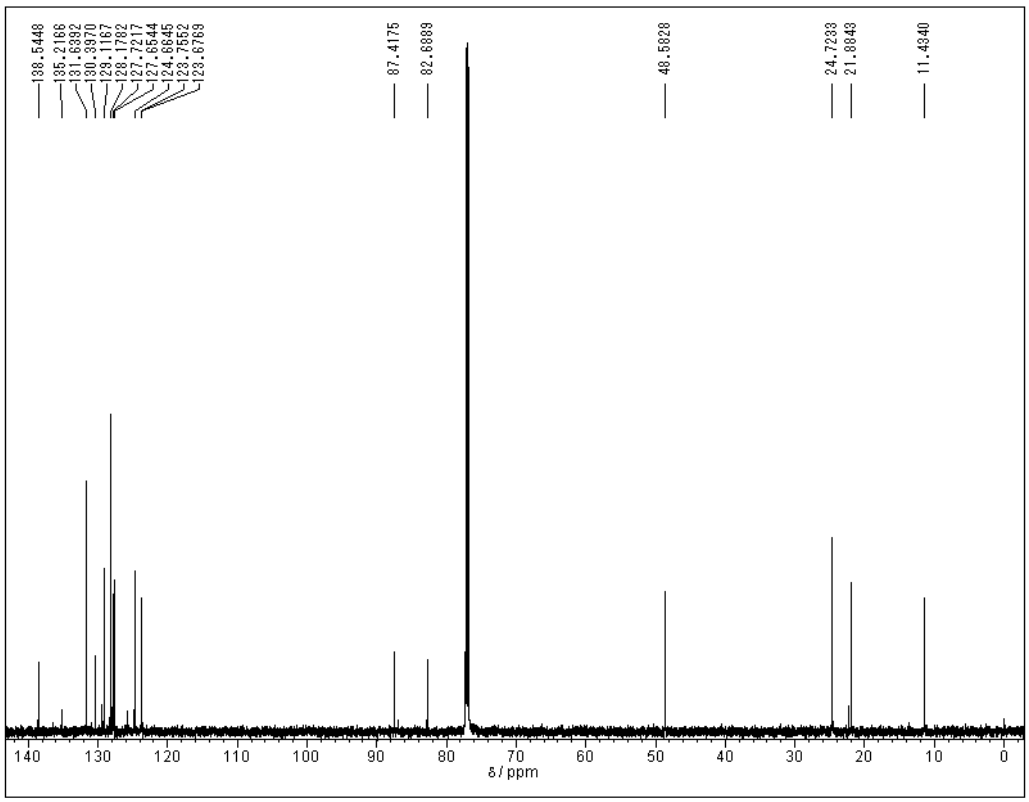
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent CDCL₃

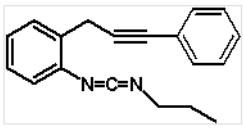
4m





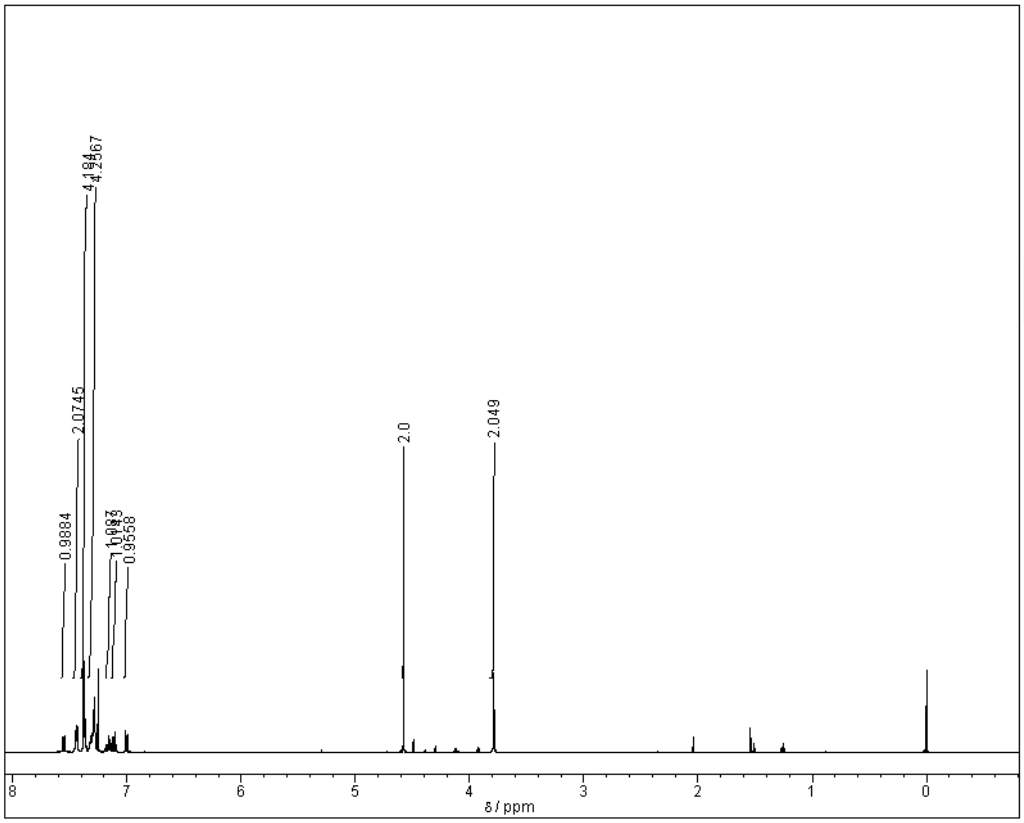
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent CDCL₃

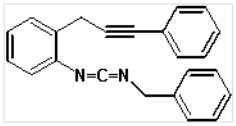




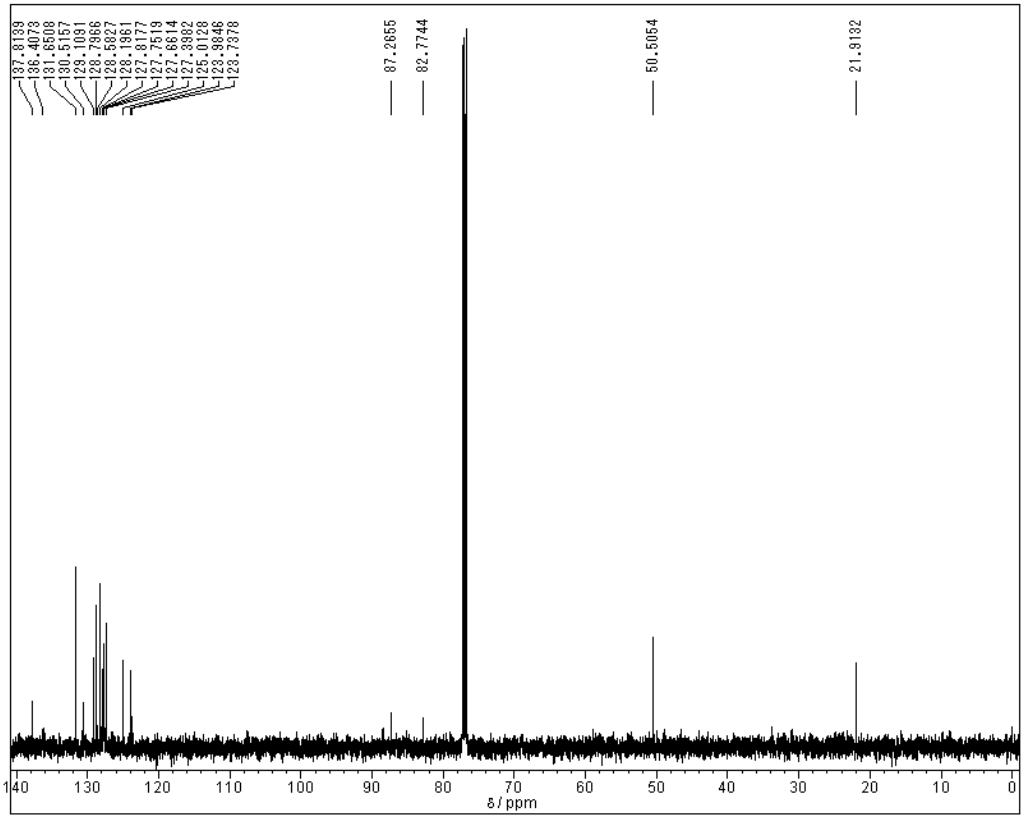
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent CDCL₃

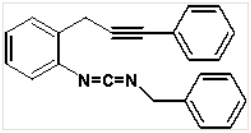
4n





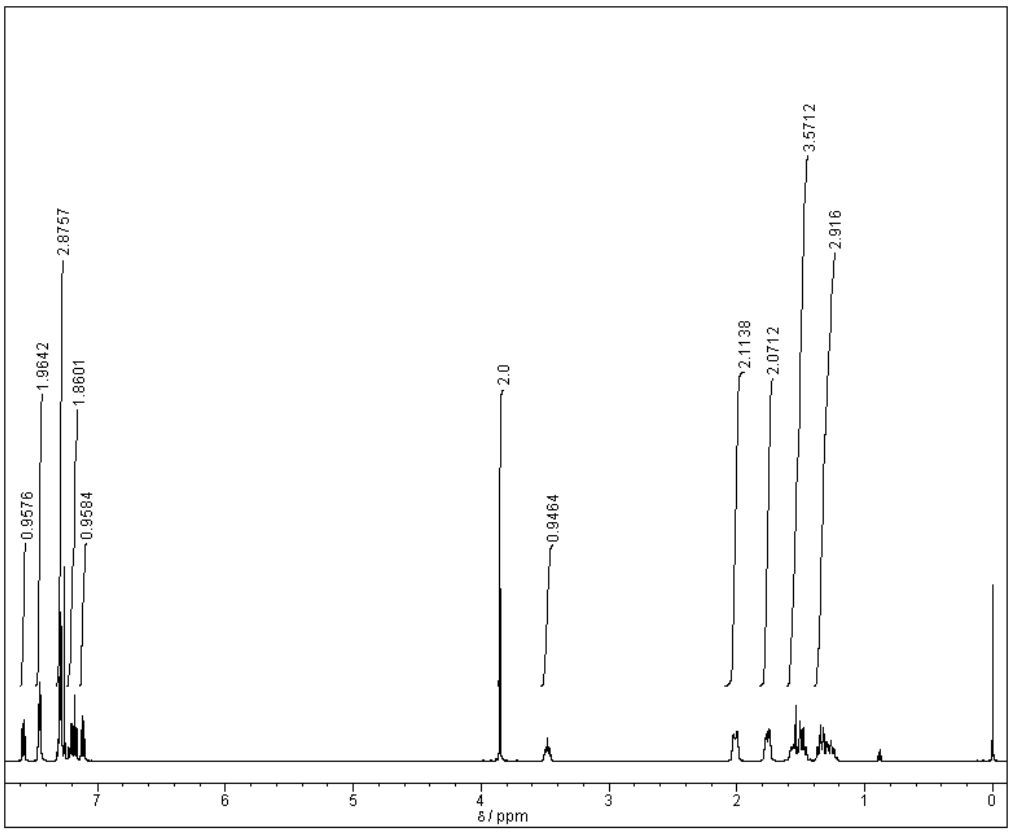
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

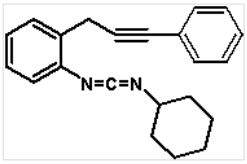




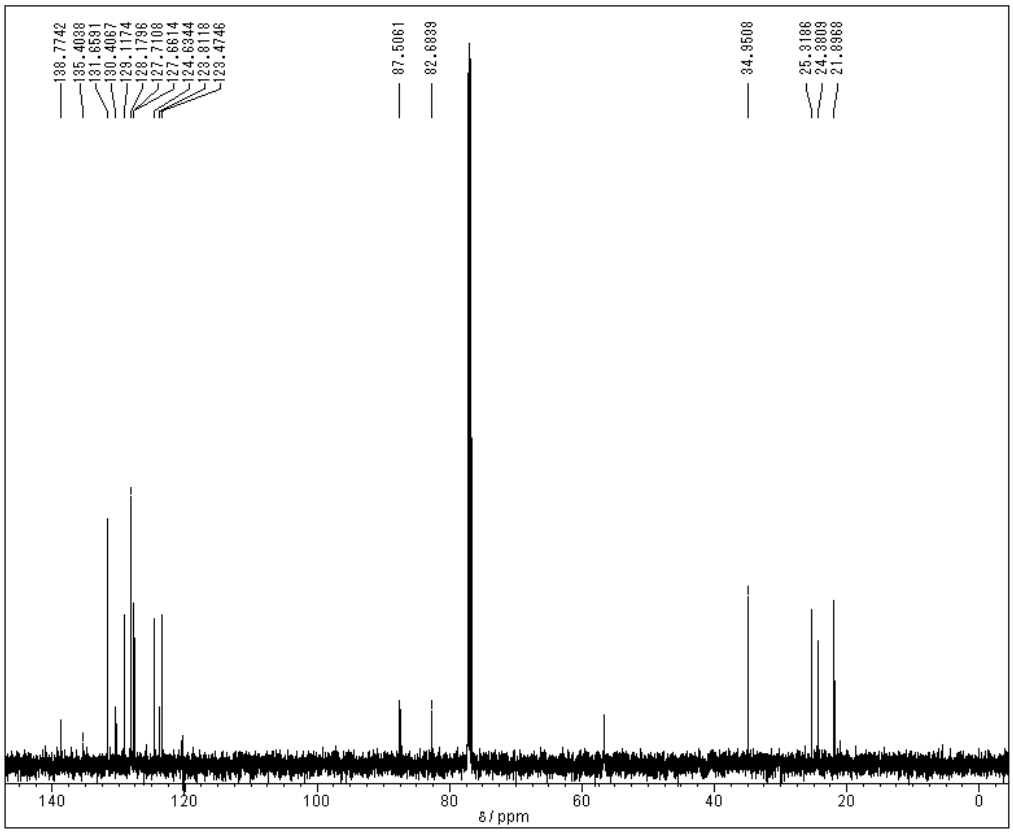
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

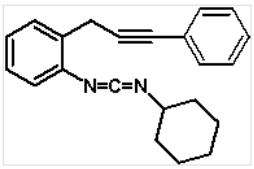
4o





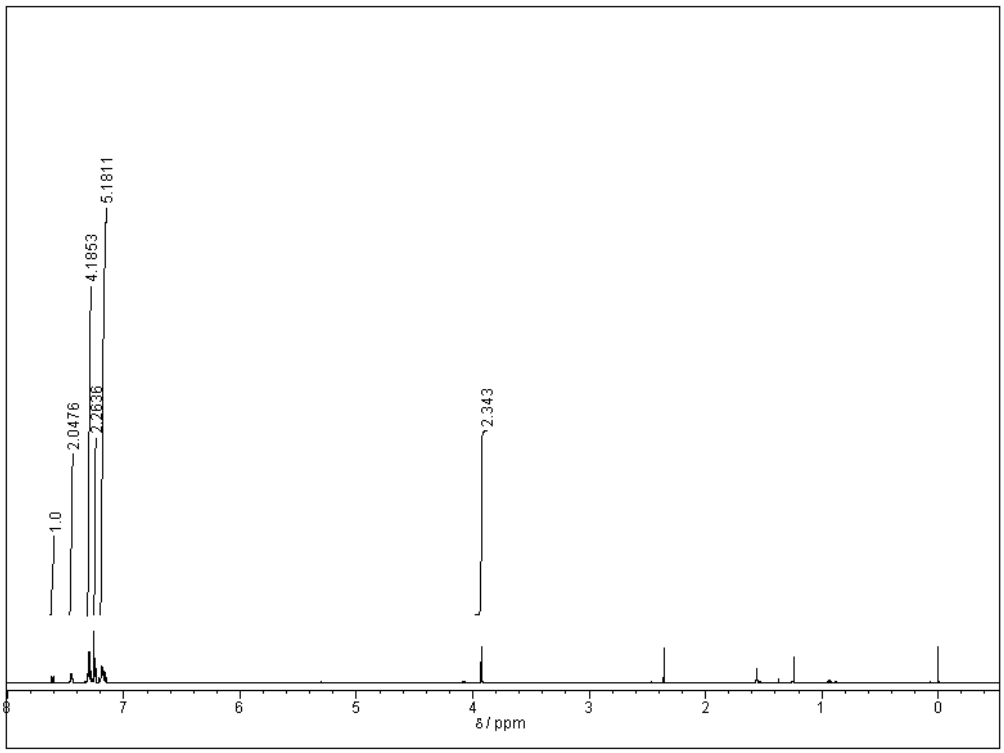
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

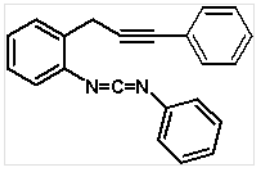




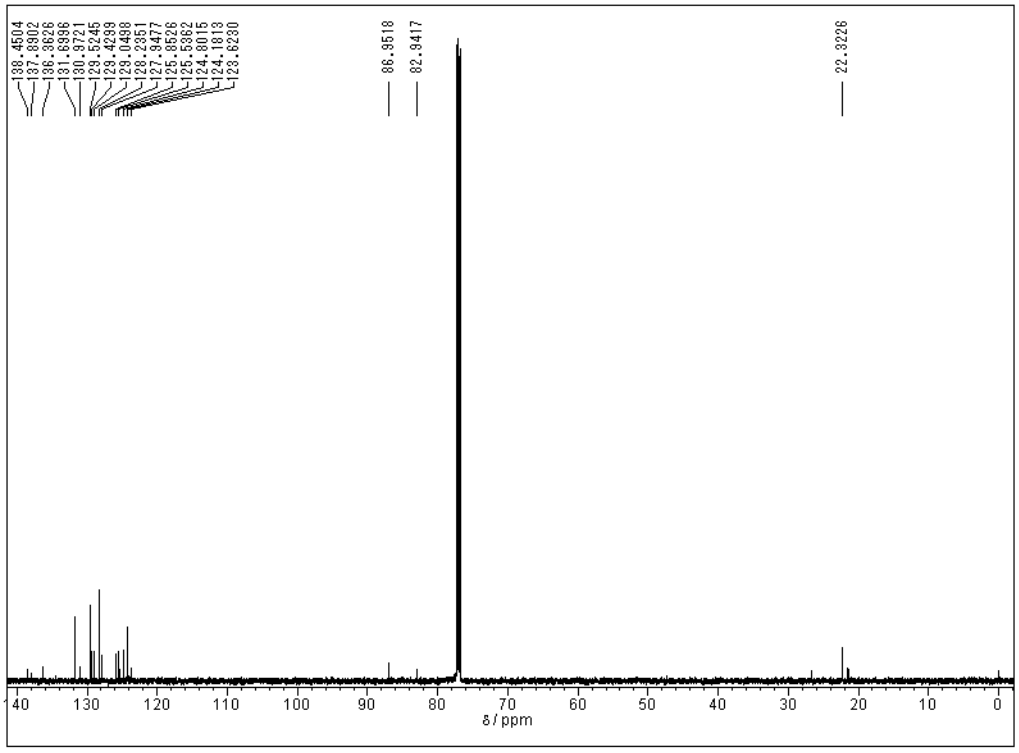
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

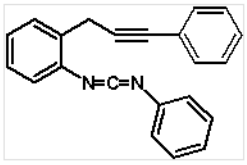
4p





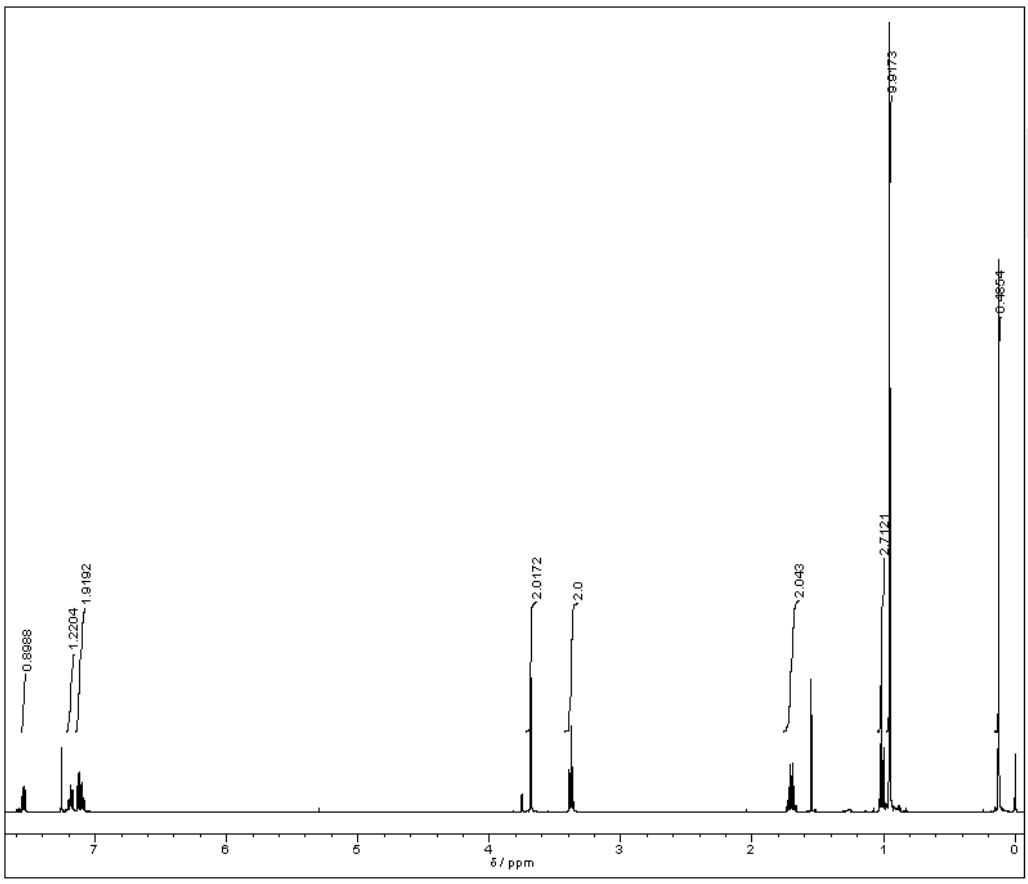
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

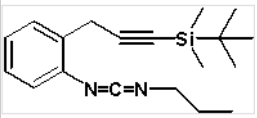




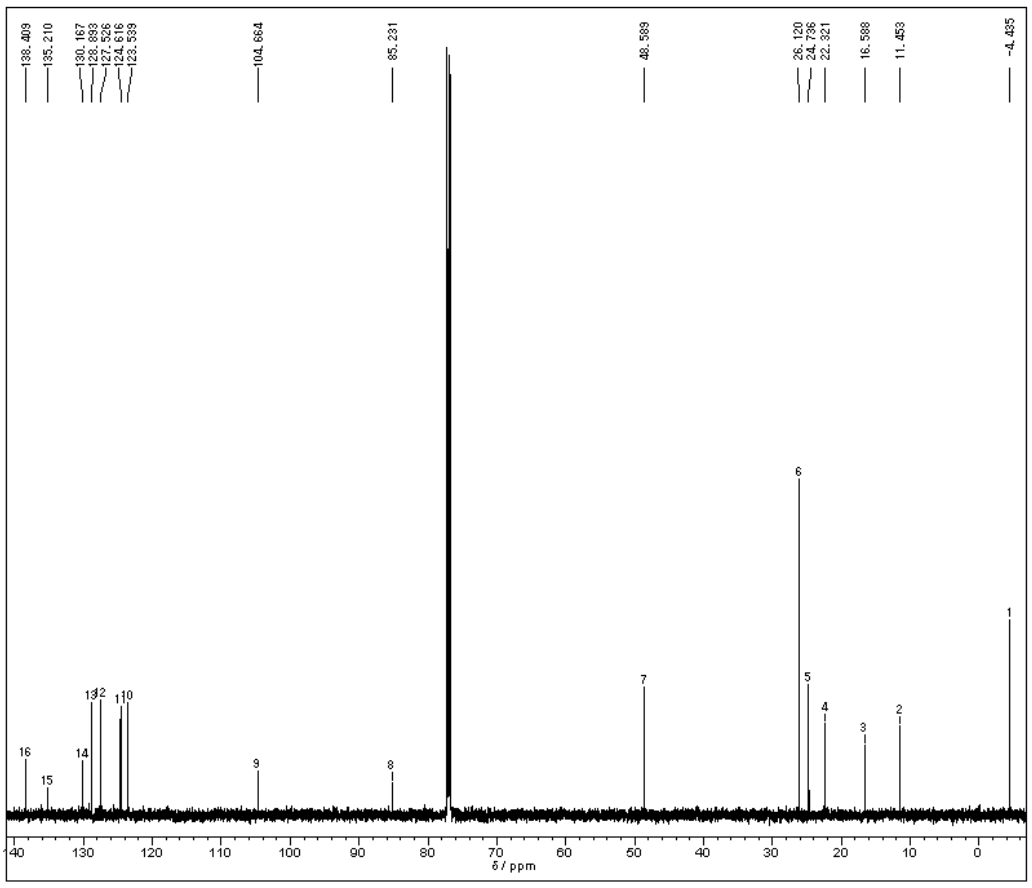
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

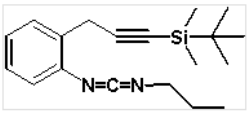
4q





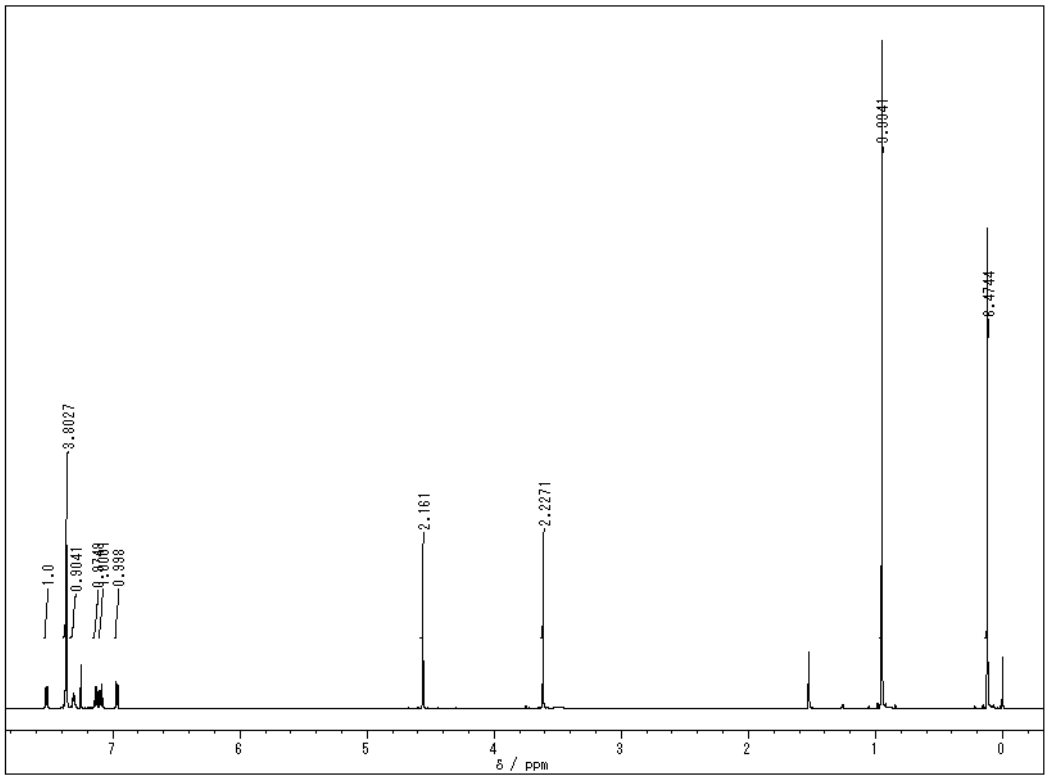
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

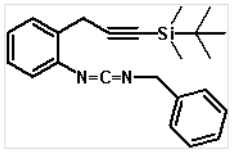




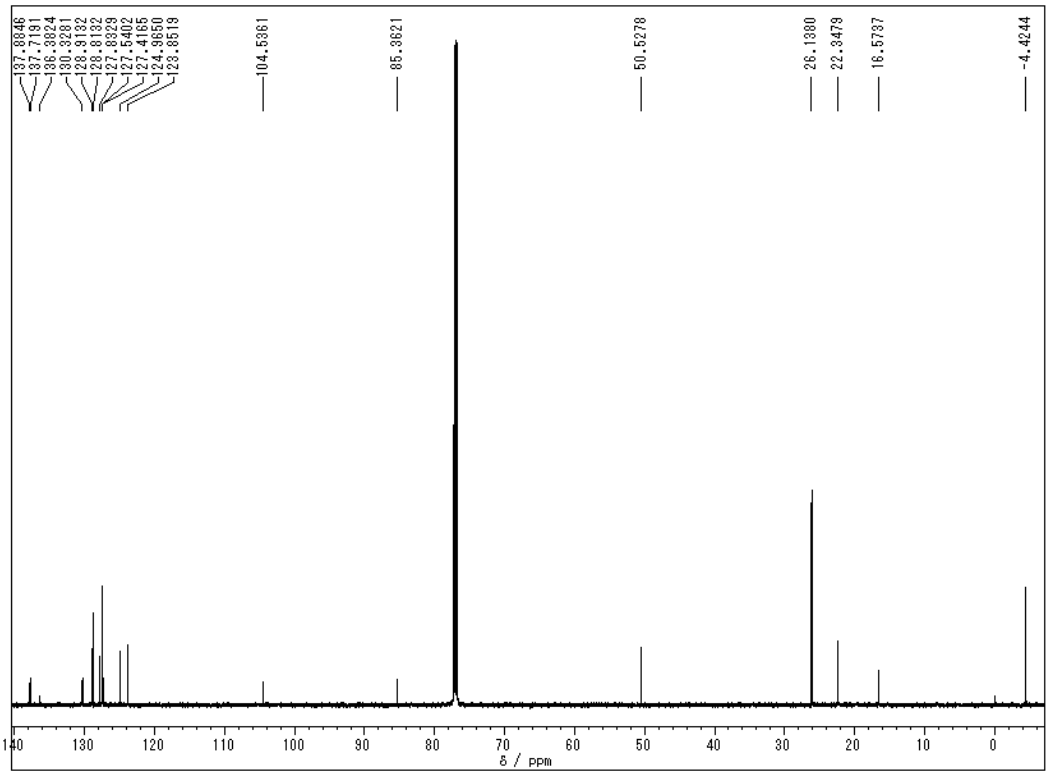
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

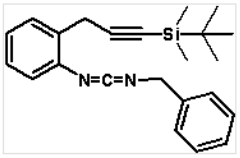
4r





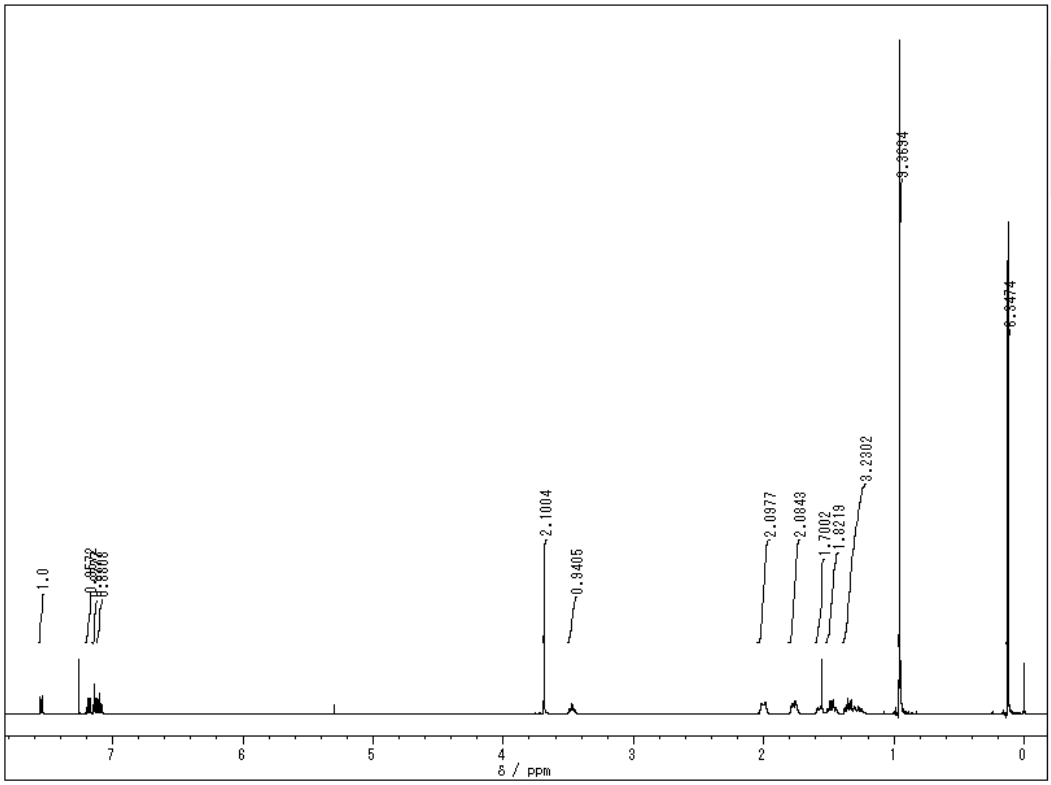
ObsNuc 1H
ObsFreq 600.13 MHz
Solvent CDCL3

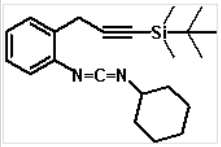




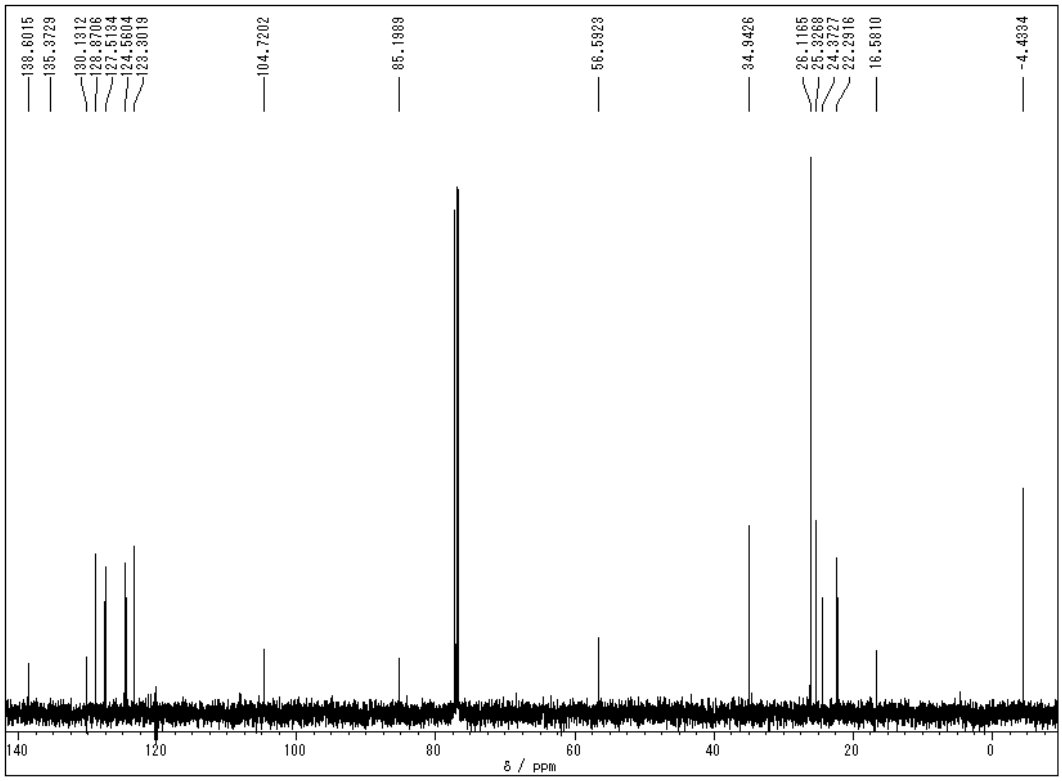
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent CDCL3

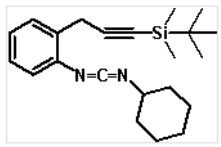
4s





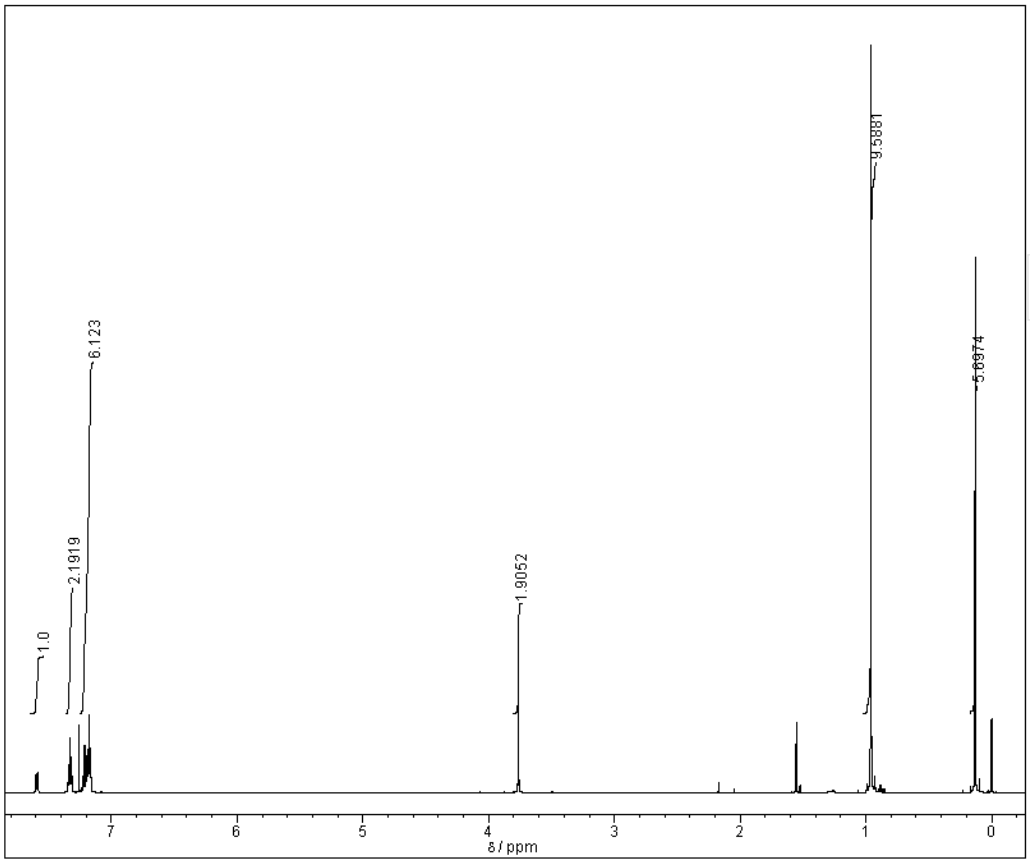
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

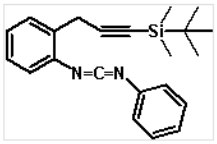




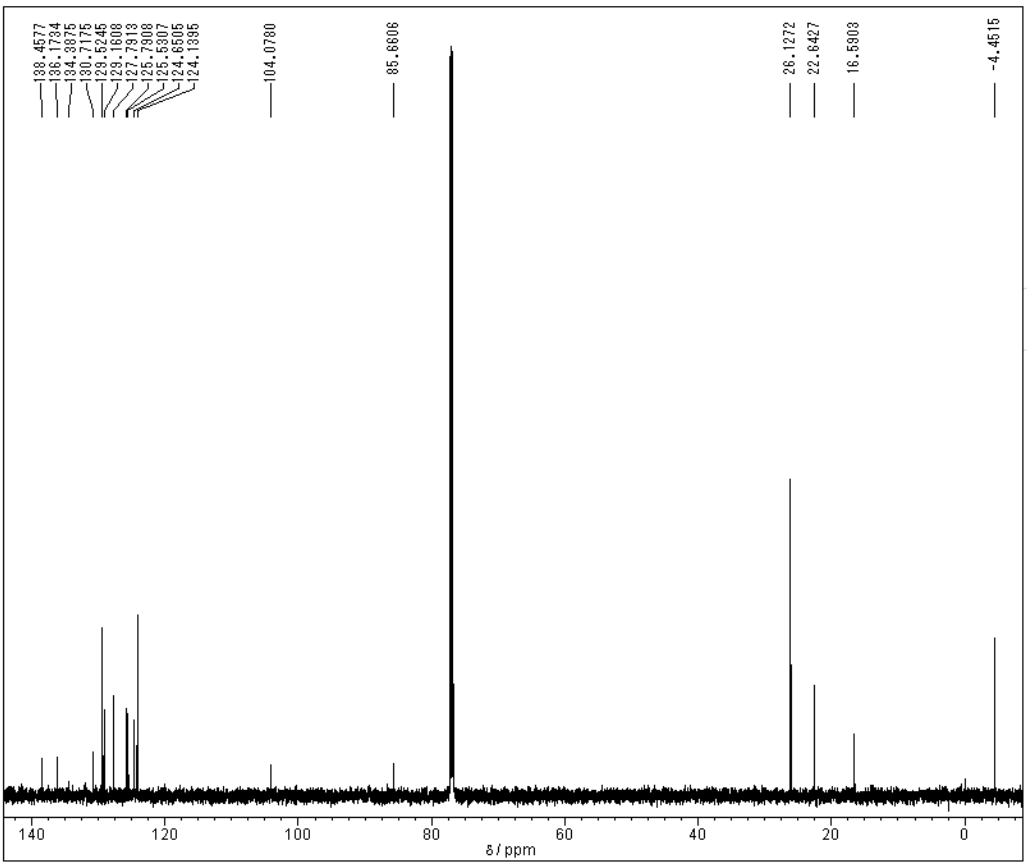
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

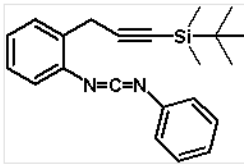
4t





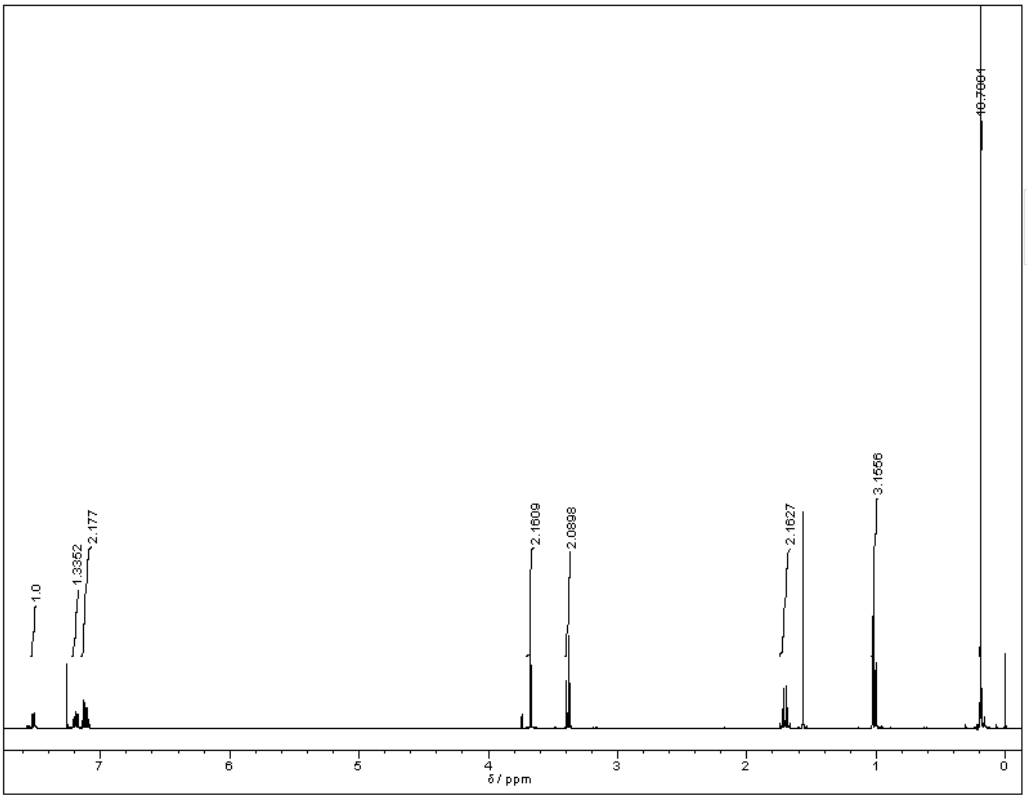
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

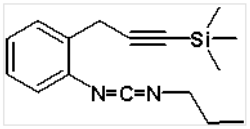




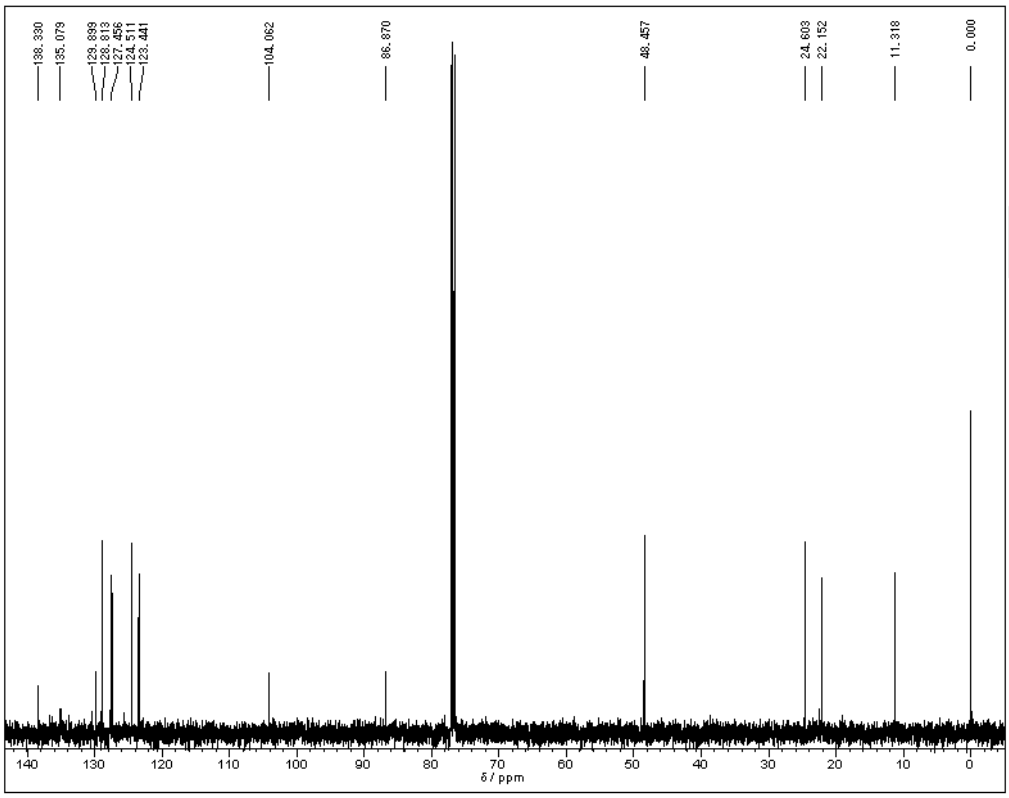
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

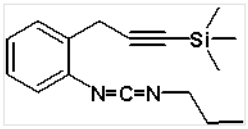
4u





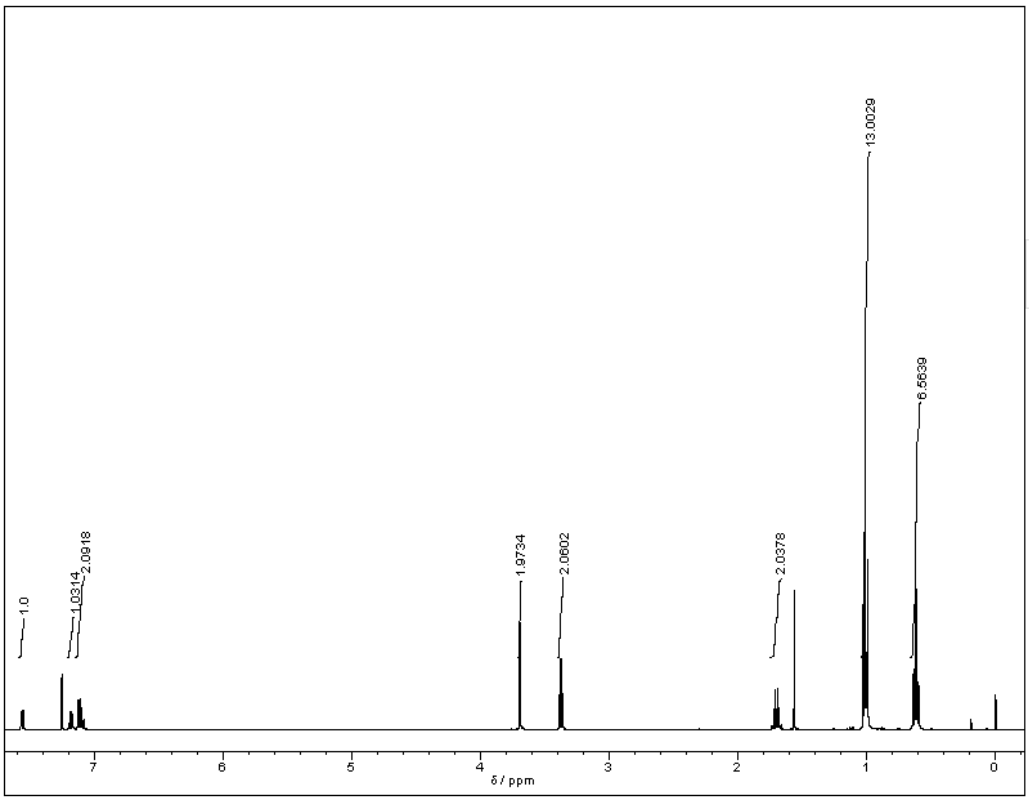
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent CDCL3

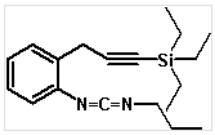




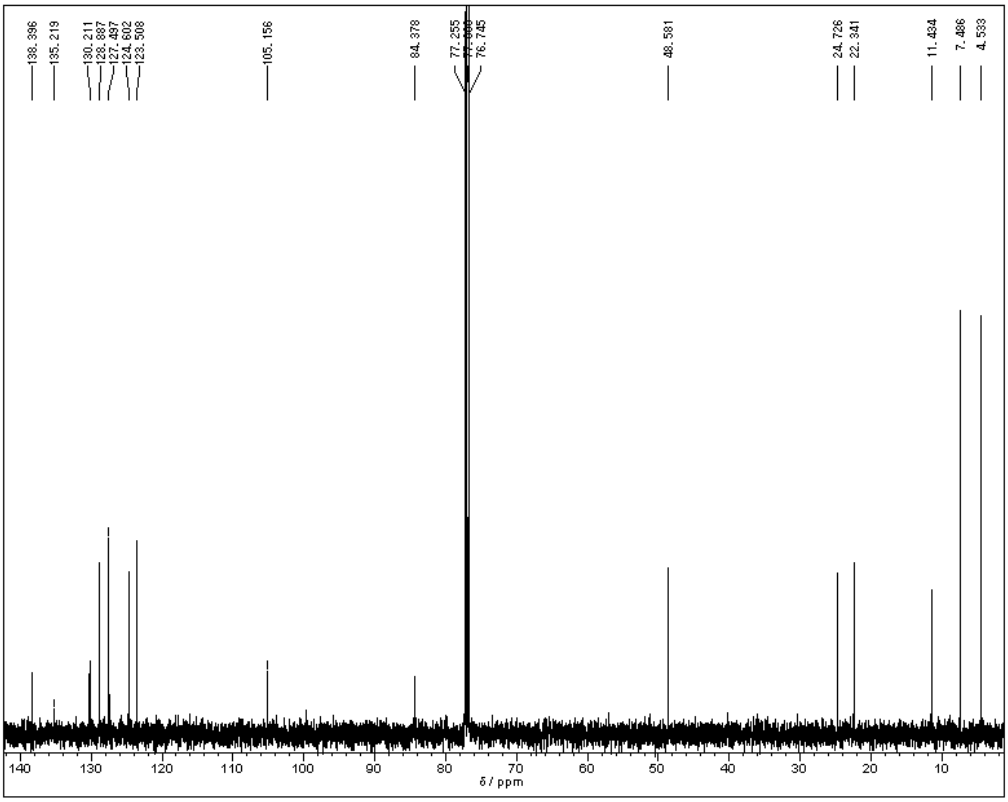
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent CDCL3

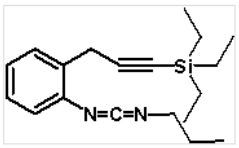
4v





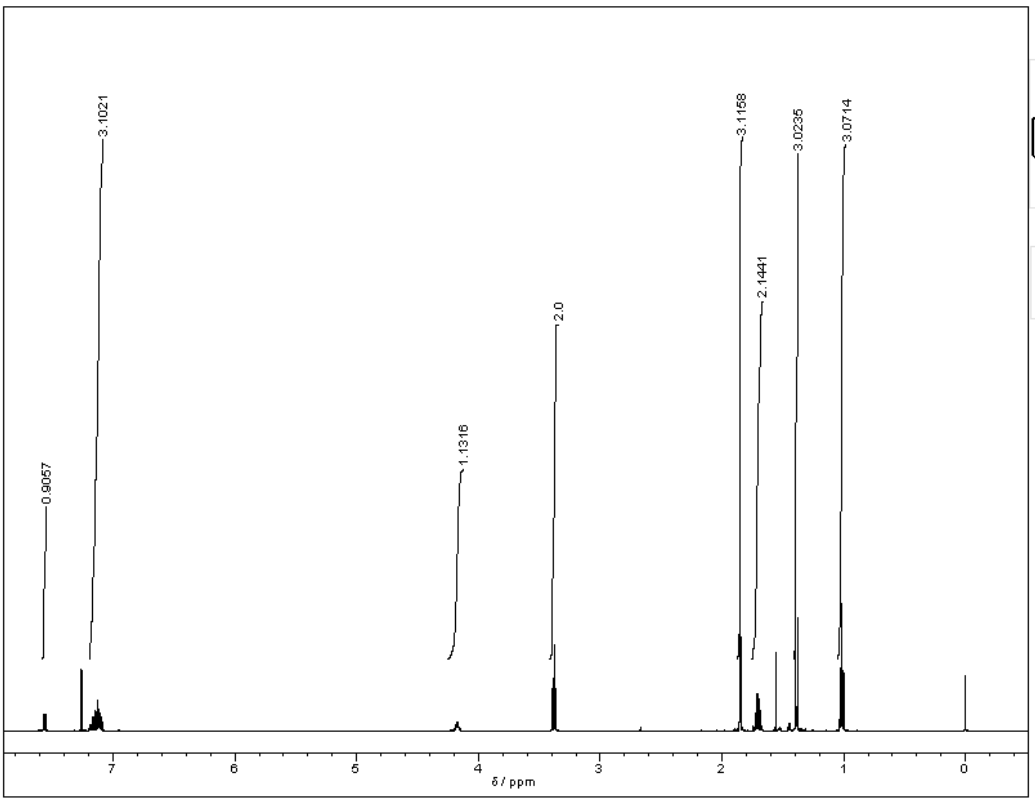
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

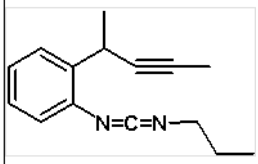




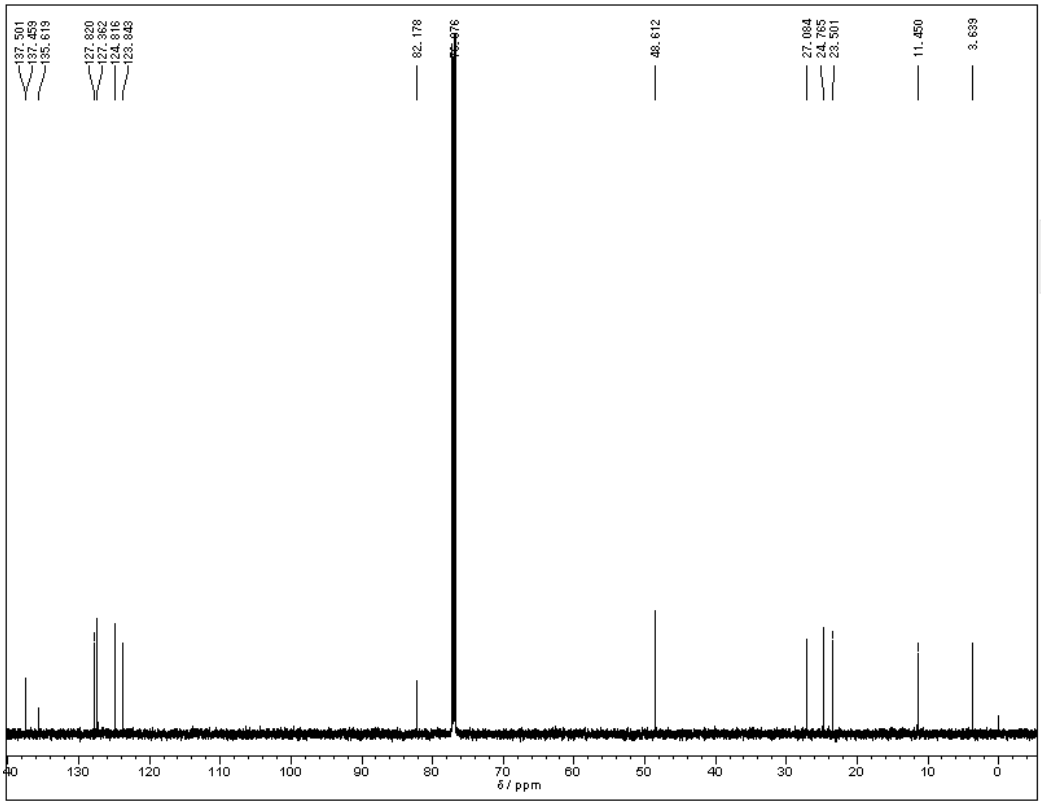
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

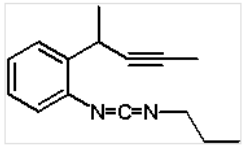
5a





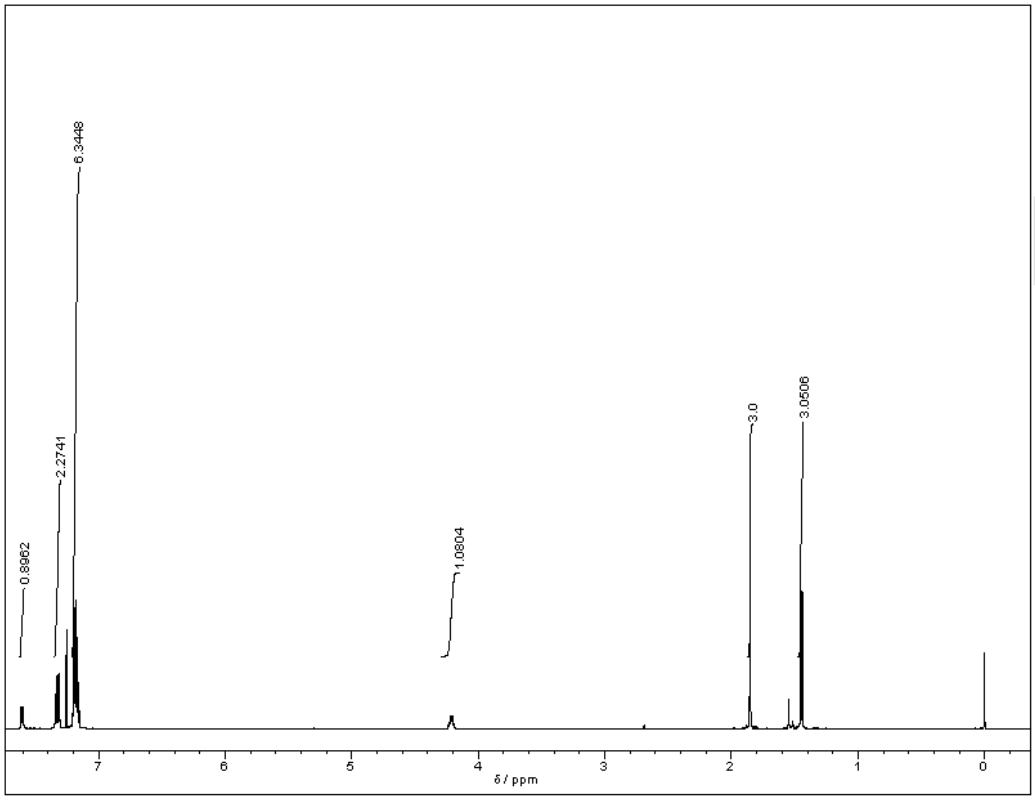
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

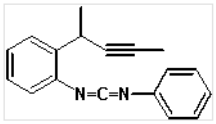




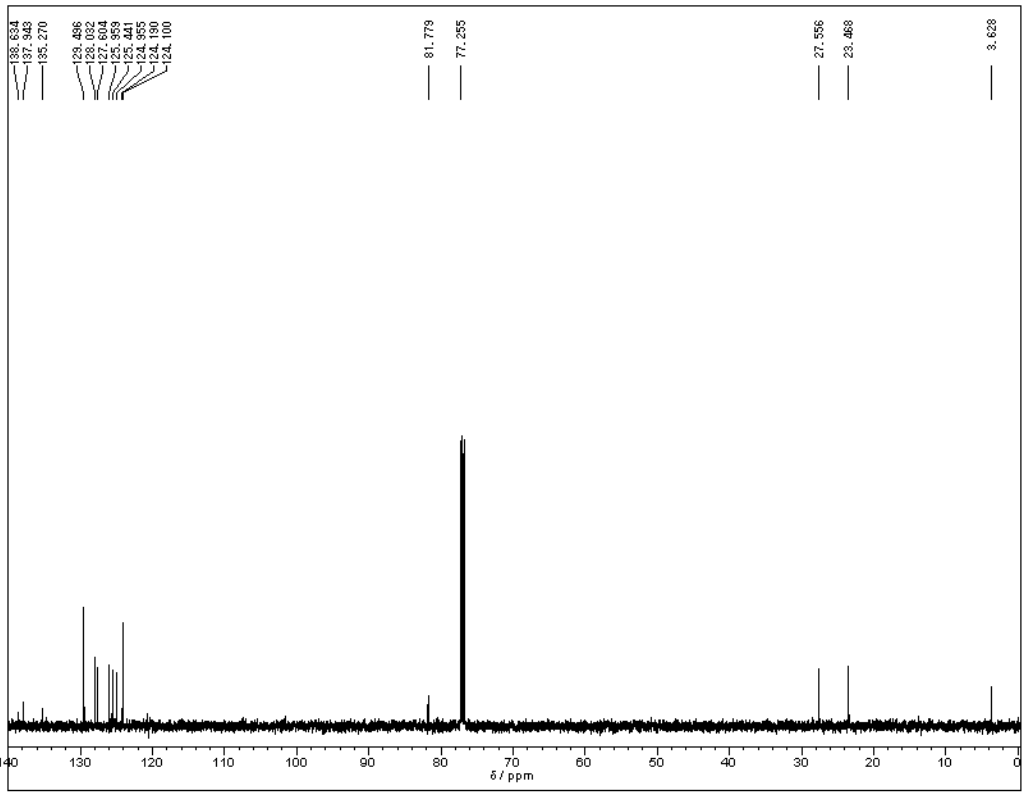
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

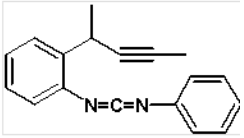
5b





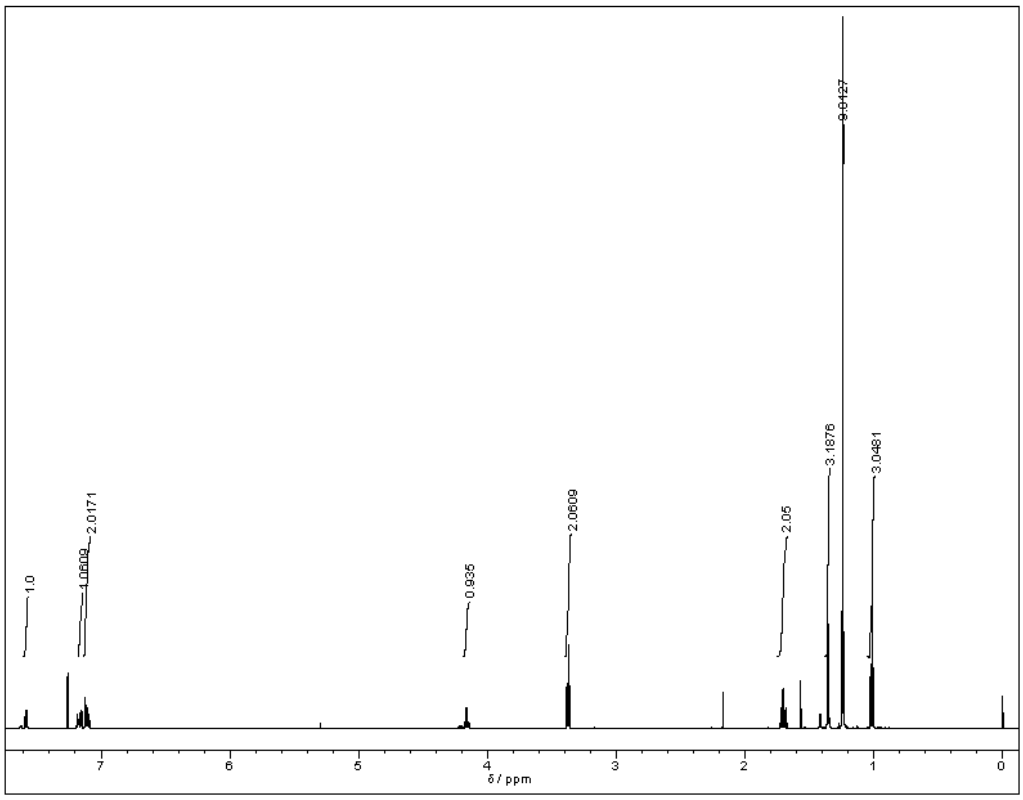
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

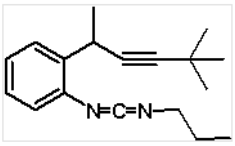




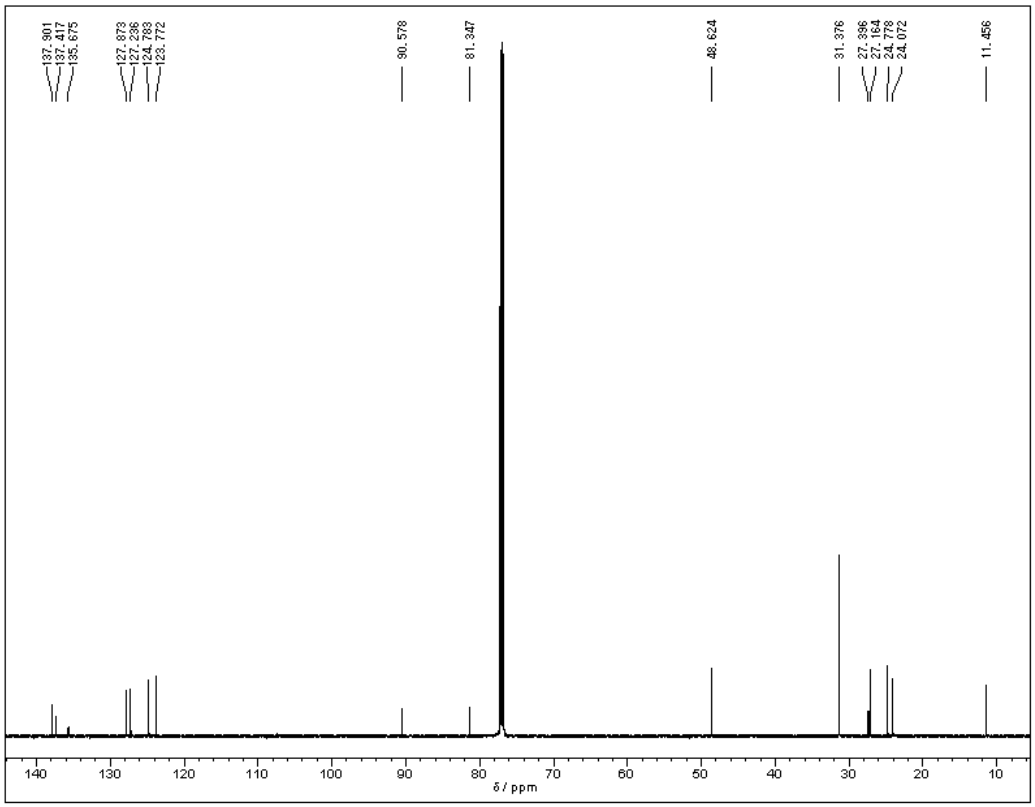
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

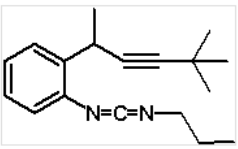
5c





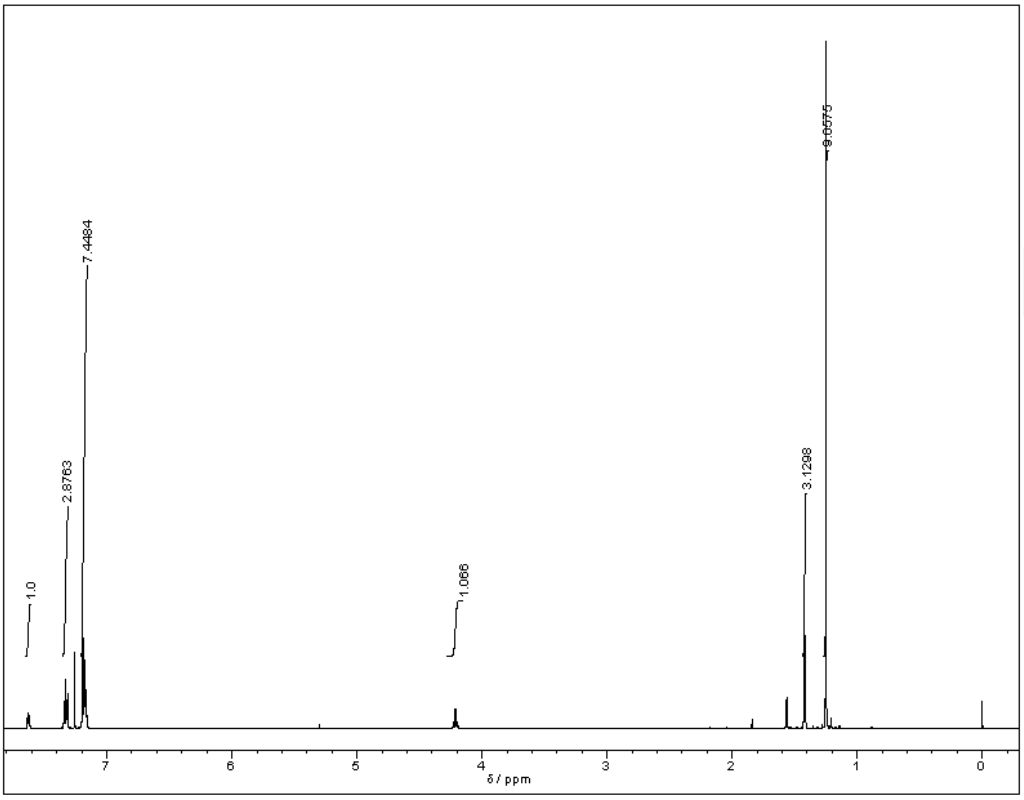
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent CDCL3

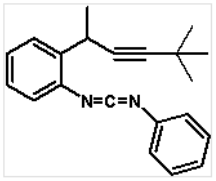




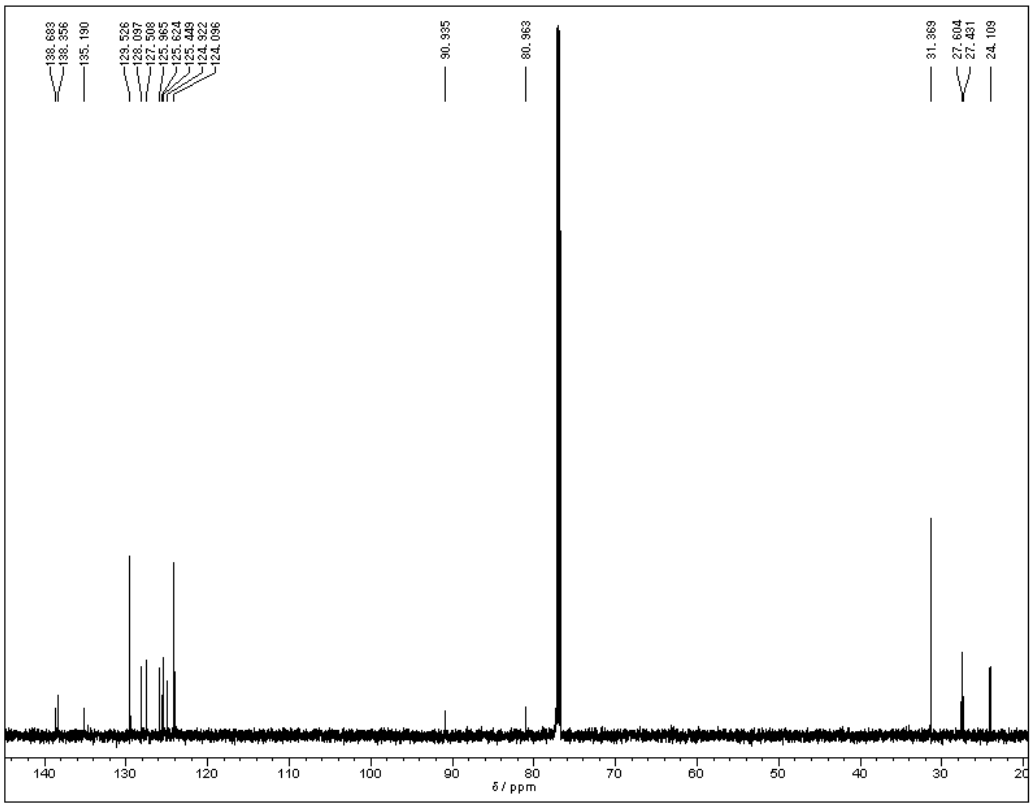
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent CDCL3

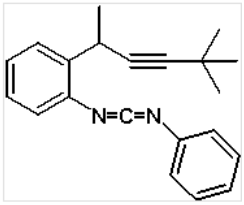
5d





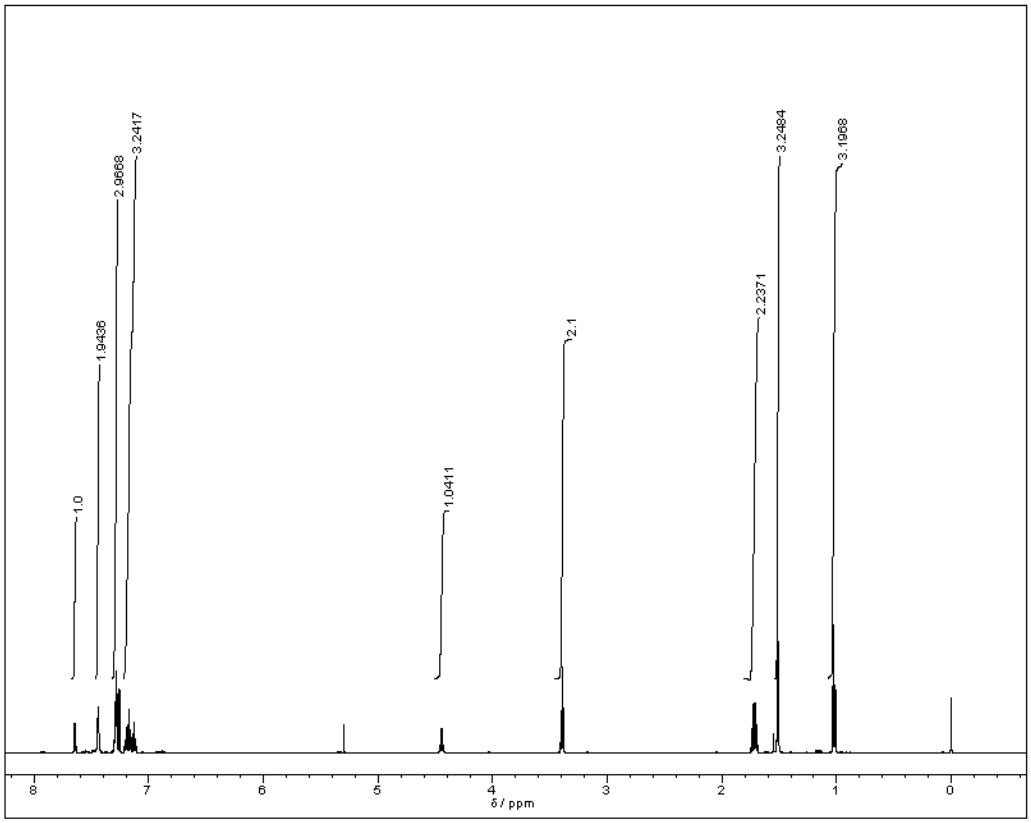
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

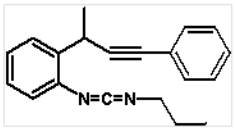




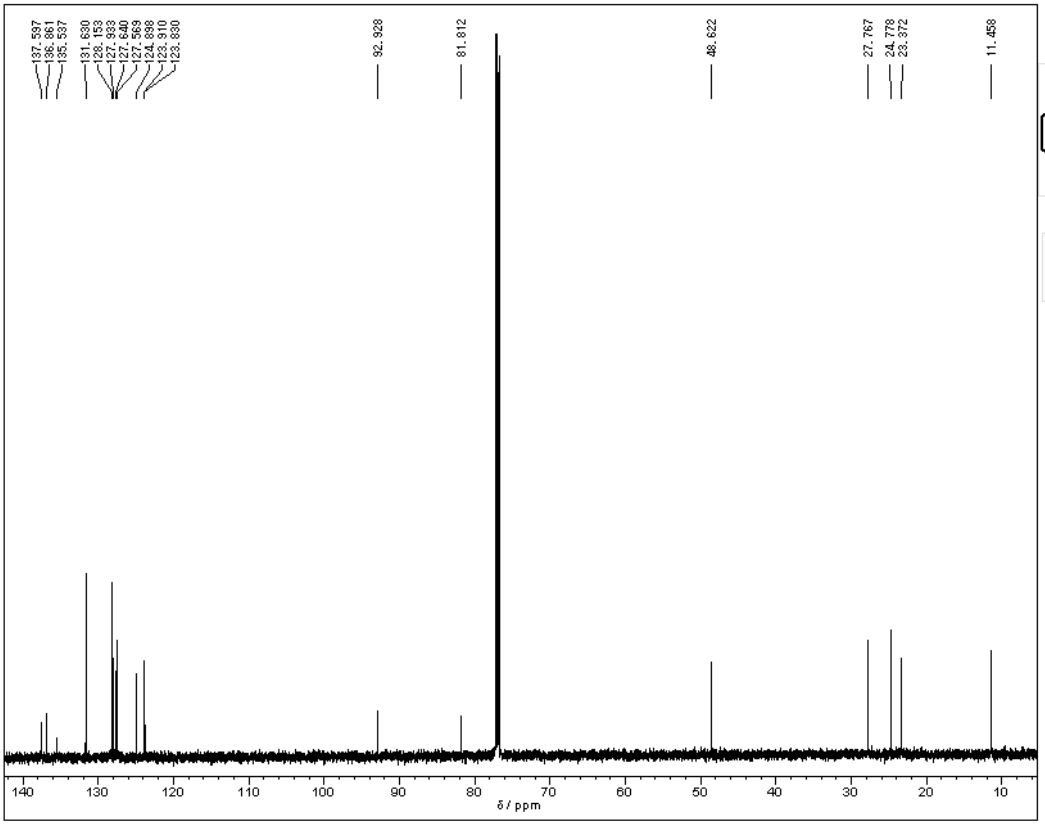
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

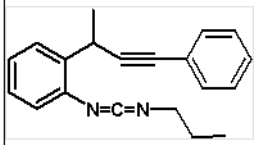
5e





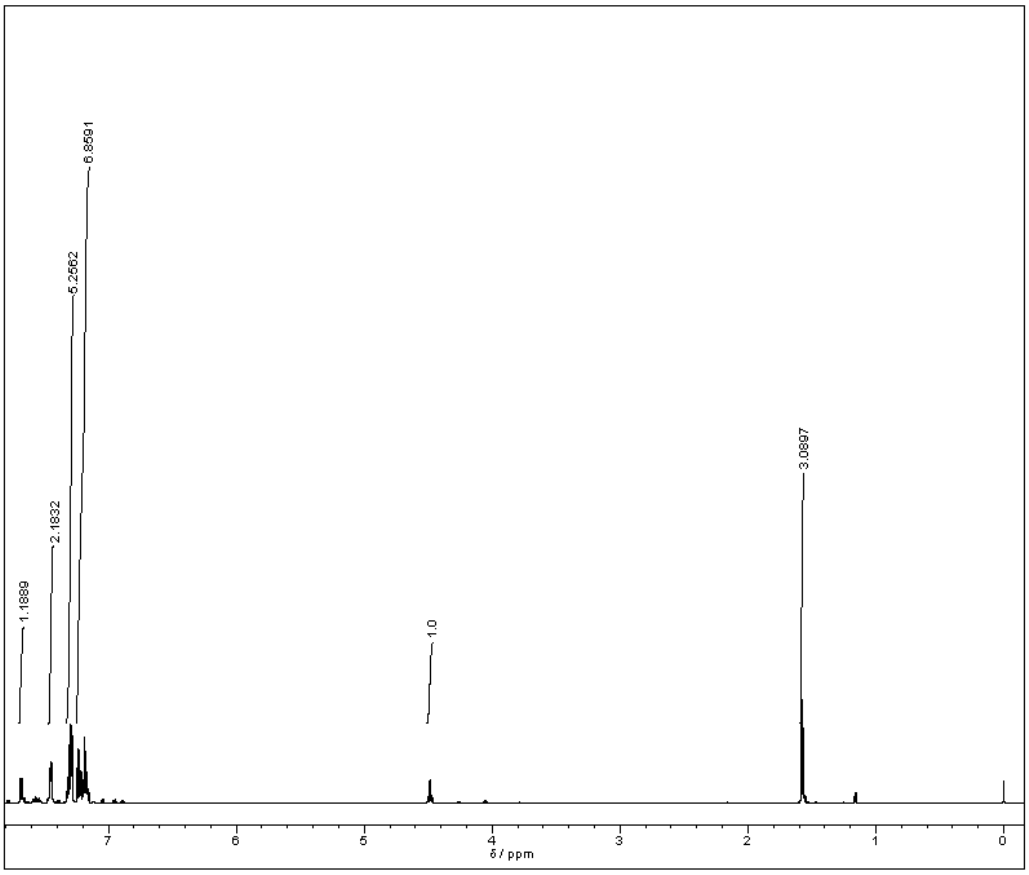
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

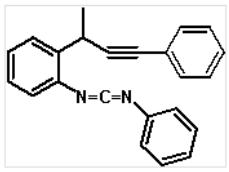




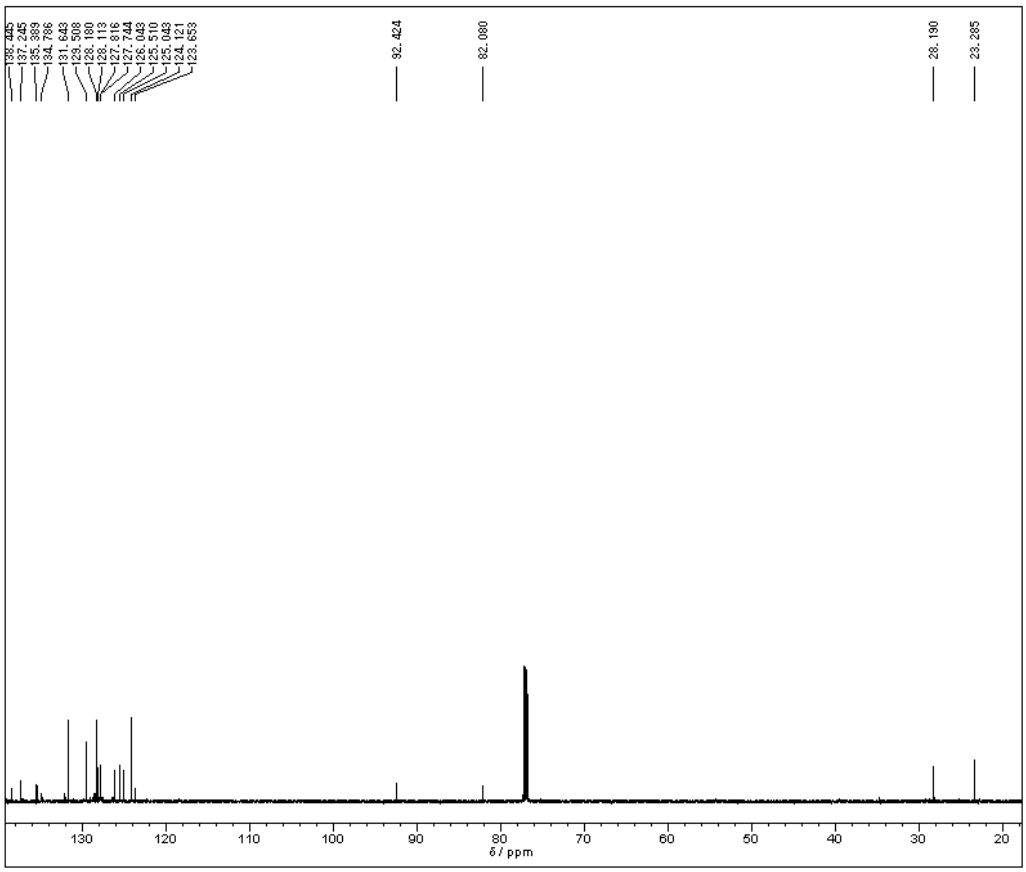
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

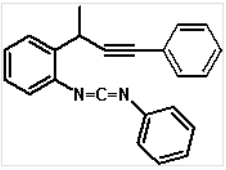
5f





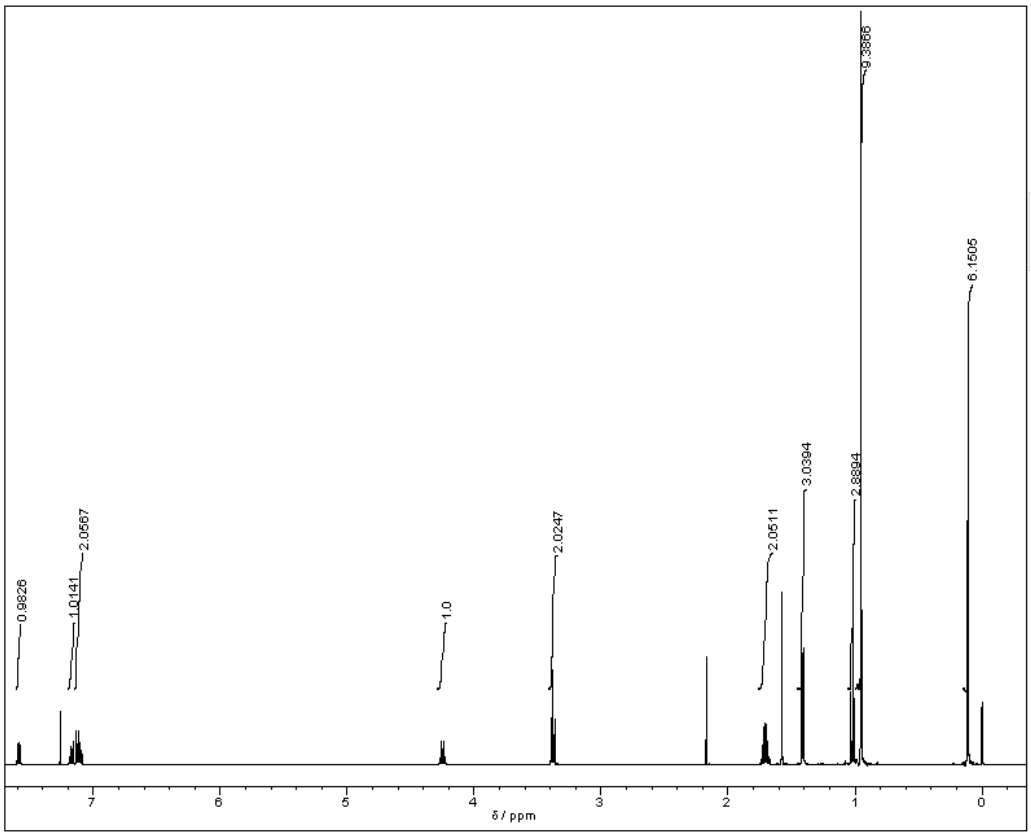
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	CDCL3

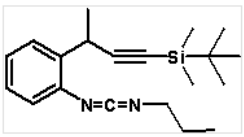




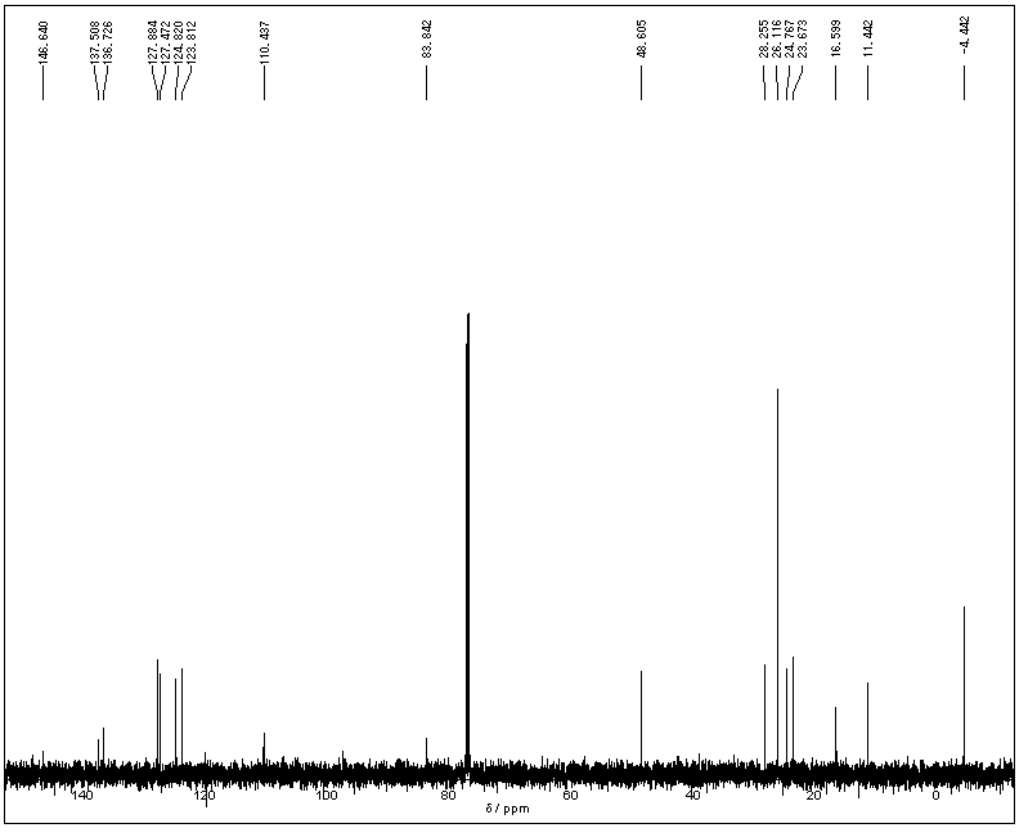
ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	CDCL3

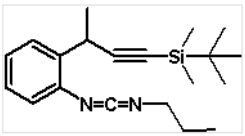
5g





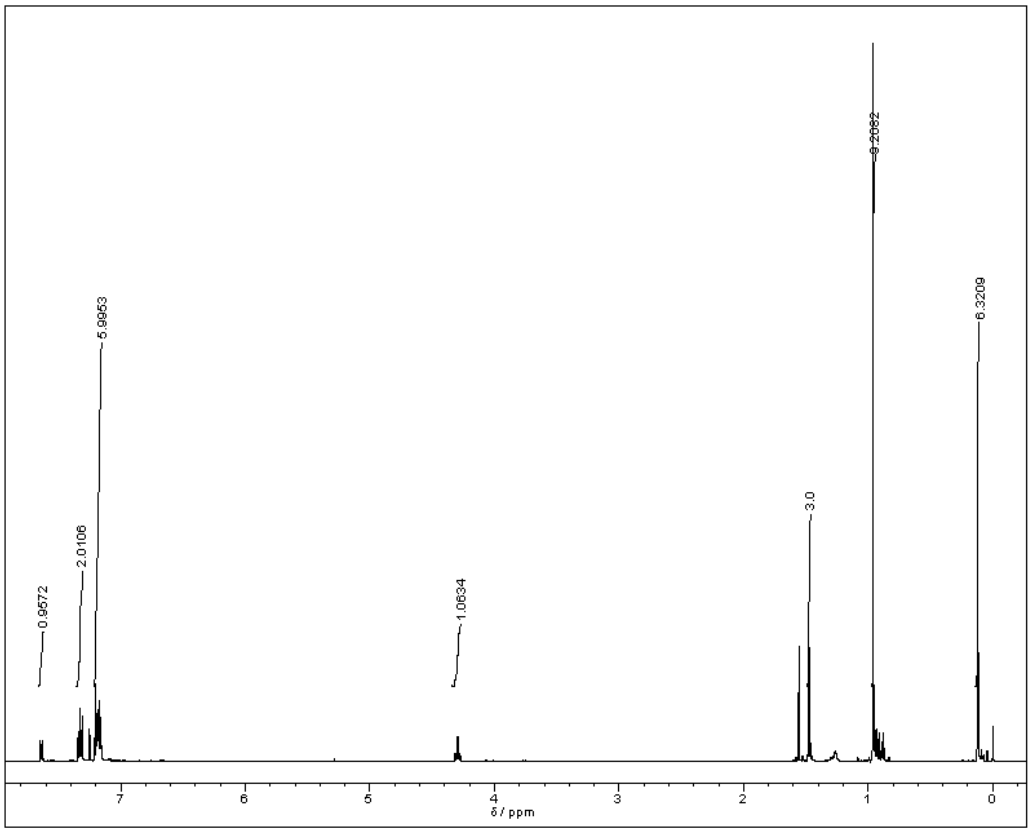
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent CDCL3

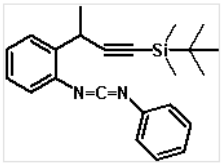




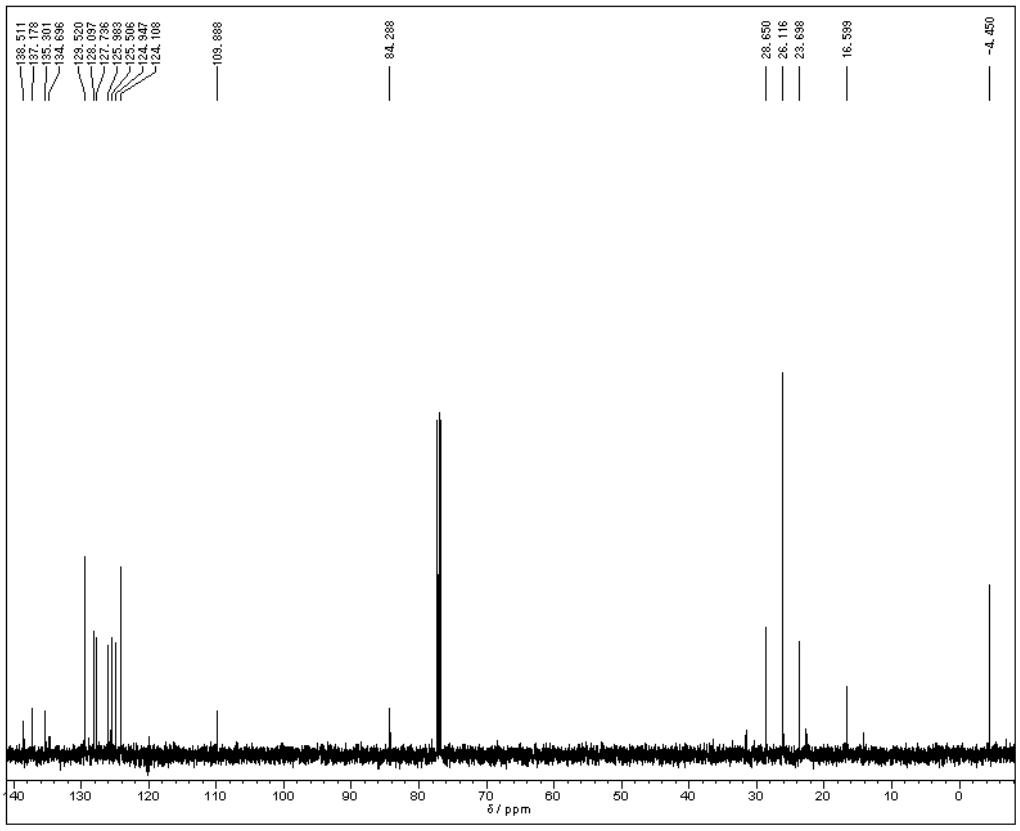
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent CDCL3

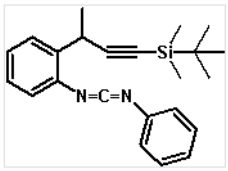
5h





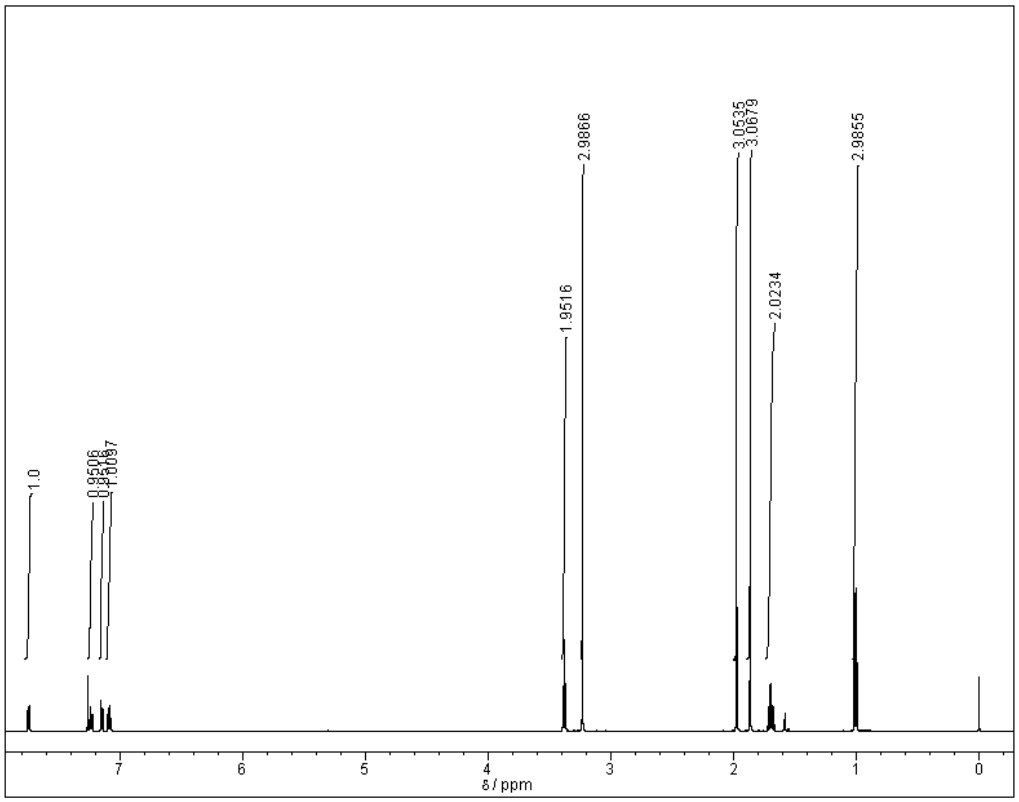
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	CDCL3

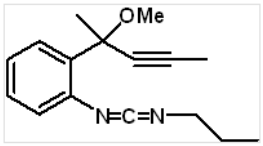




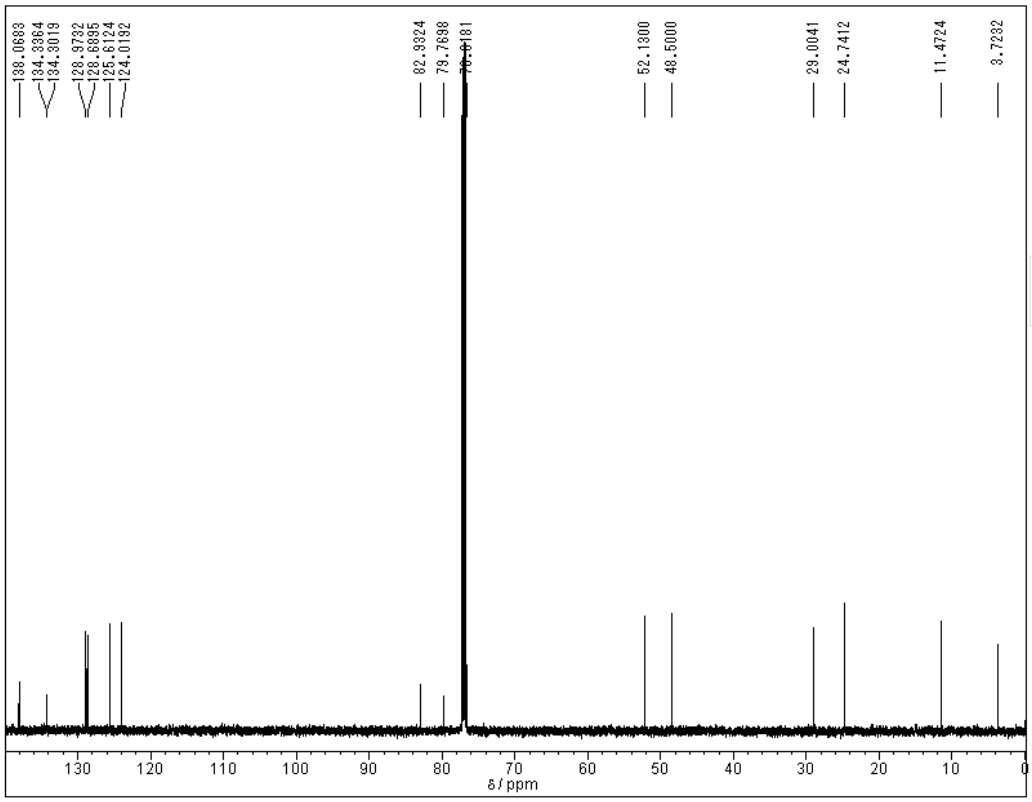
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	CDCL3

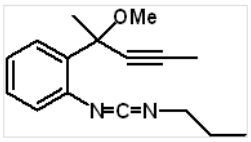
6a





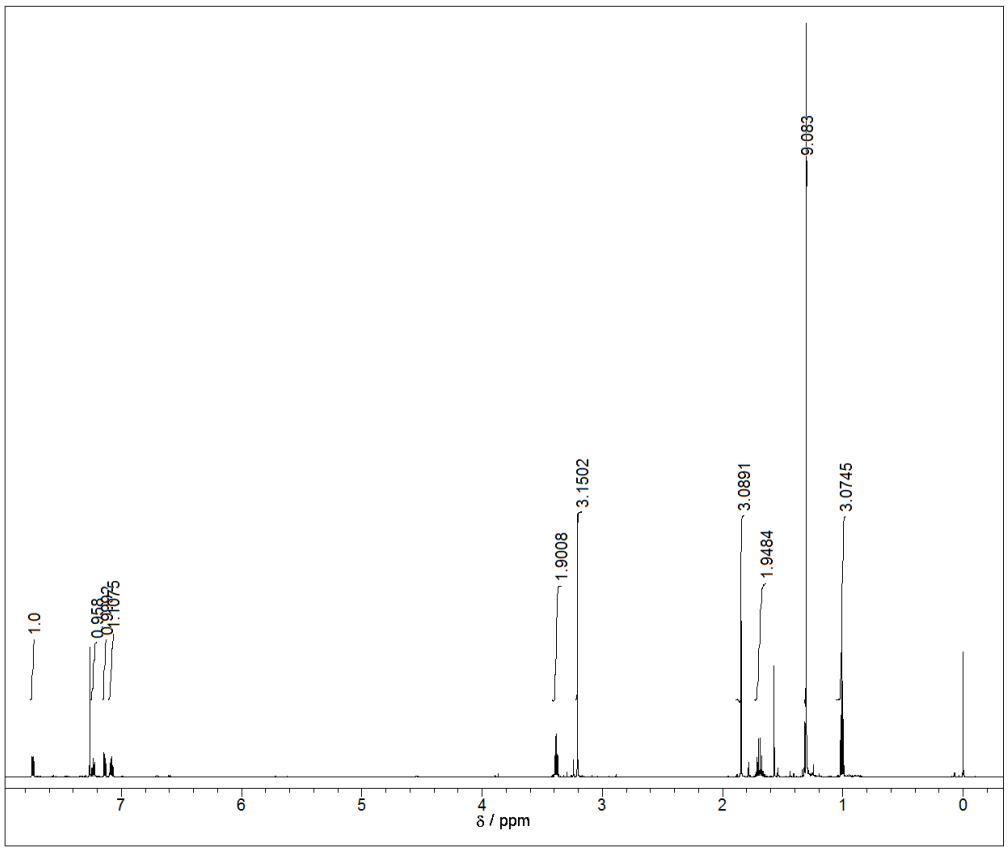
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	$CDCl_3$

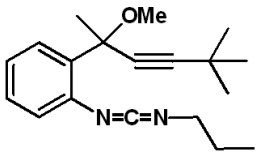




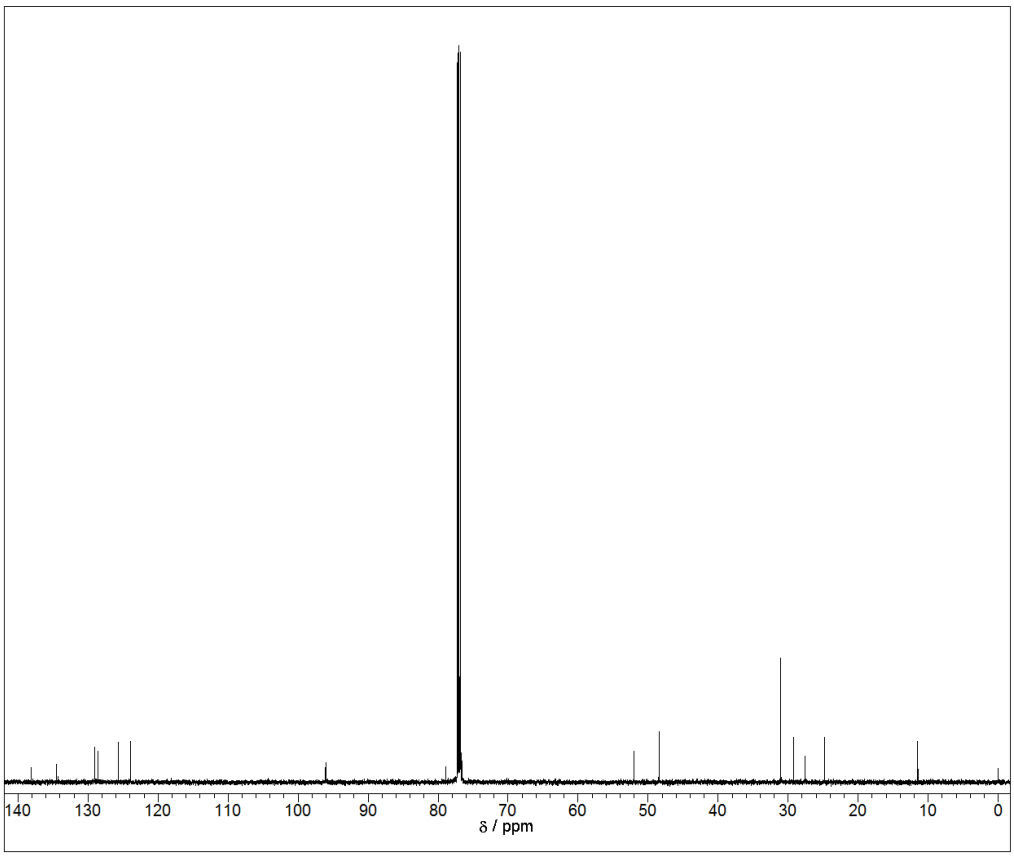
ObsFreq	150.9 MHz
ObsNuo	^{13}C
Solvent	$CDCl_3$

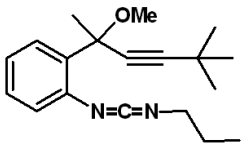
6b





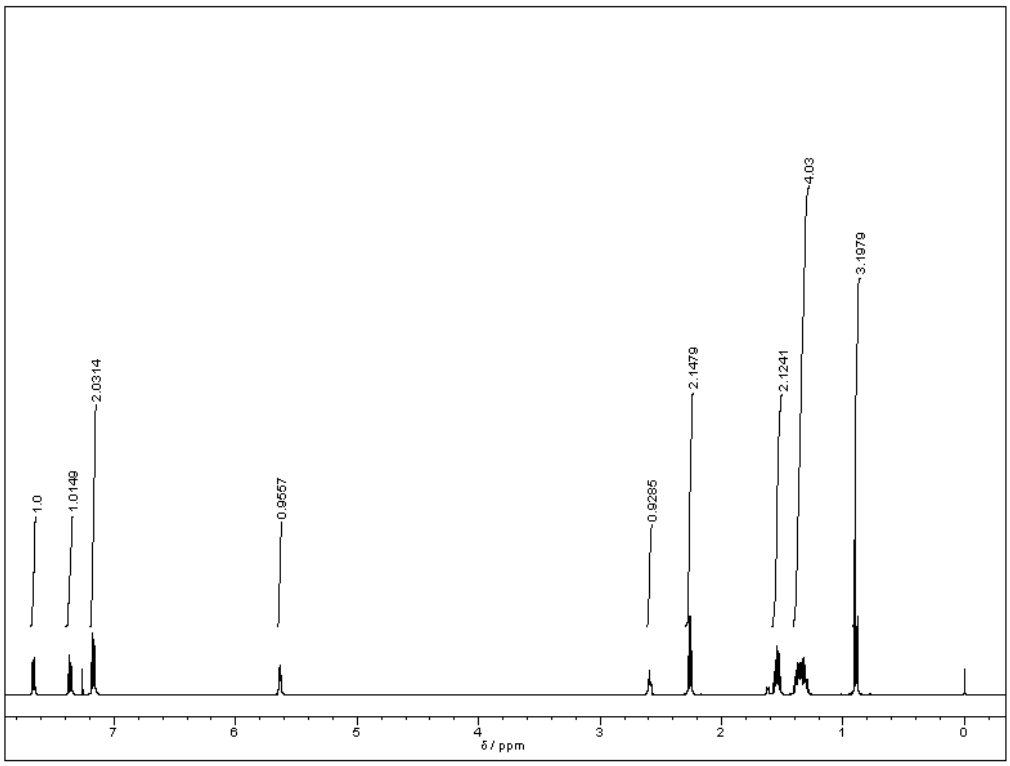
ObsNuc 1H
ObsFreq 600.13 MHz
Solvent $CDCL_3$

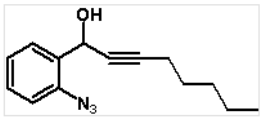




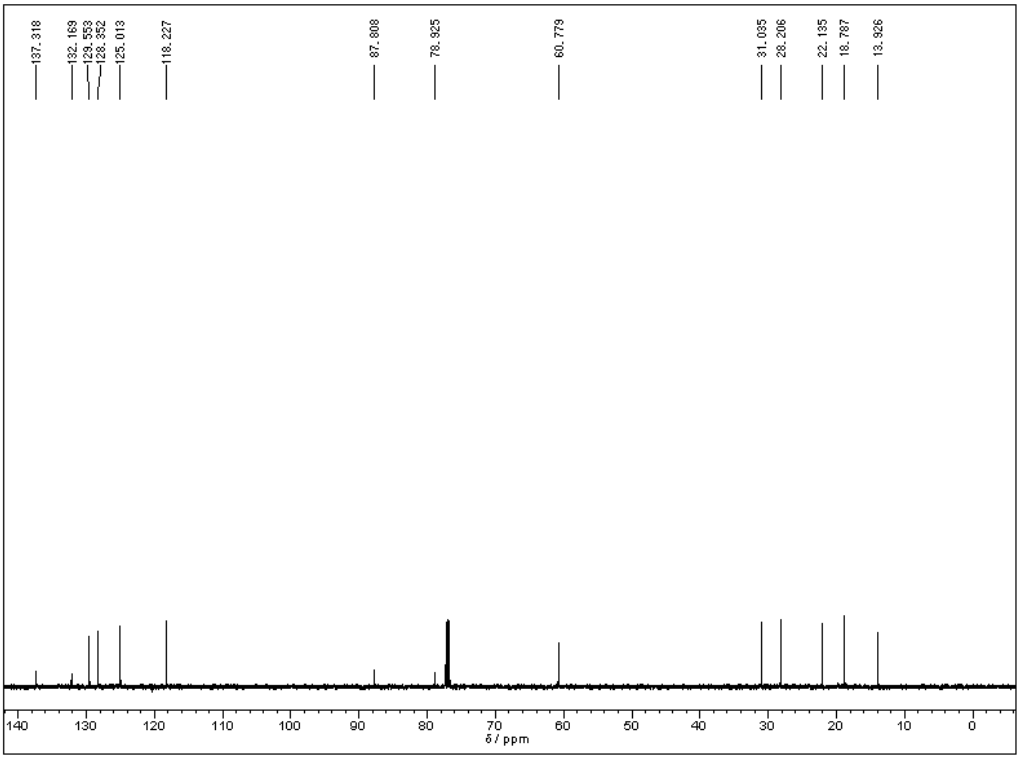
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent $CDCL_3$

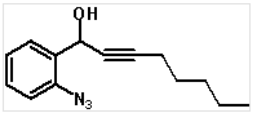
7a





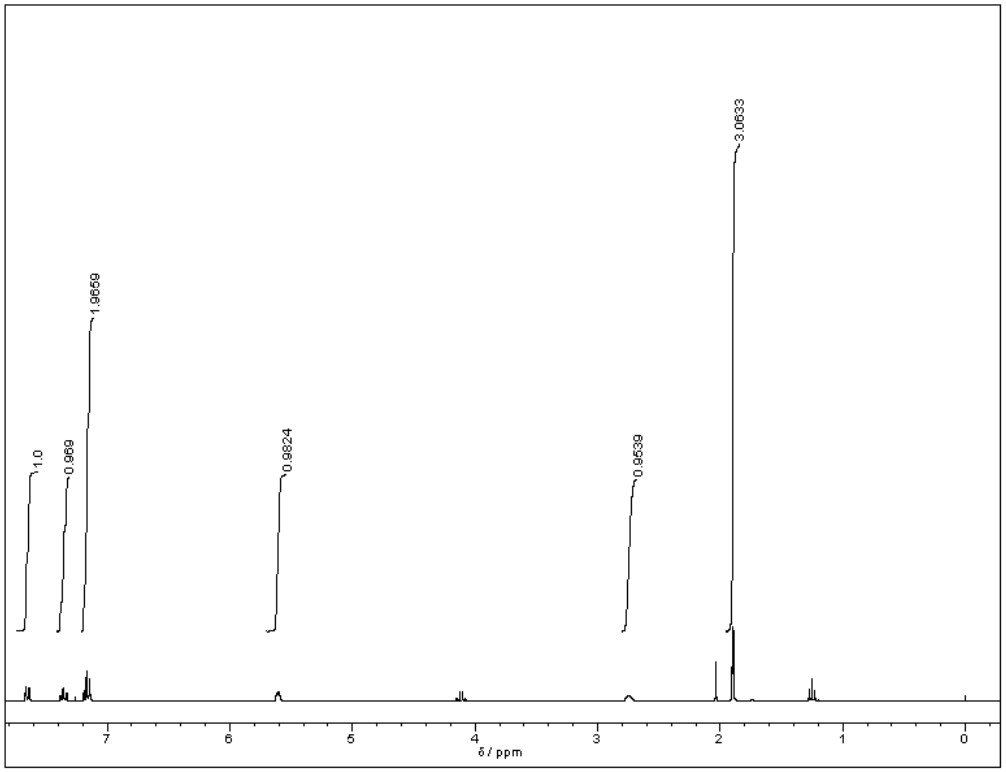
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCL_3$

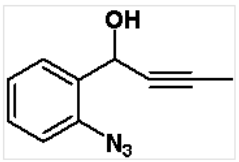




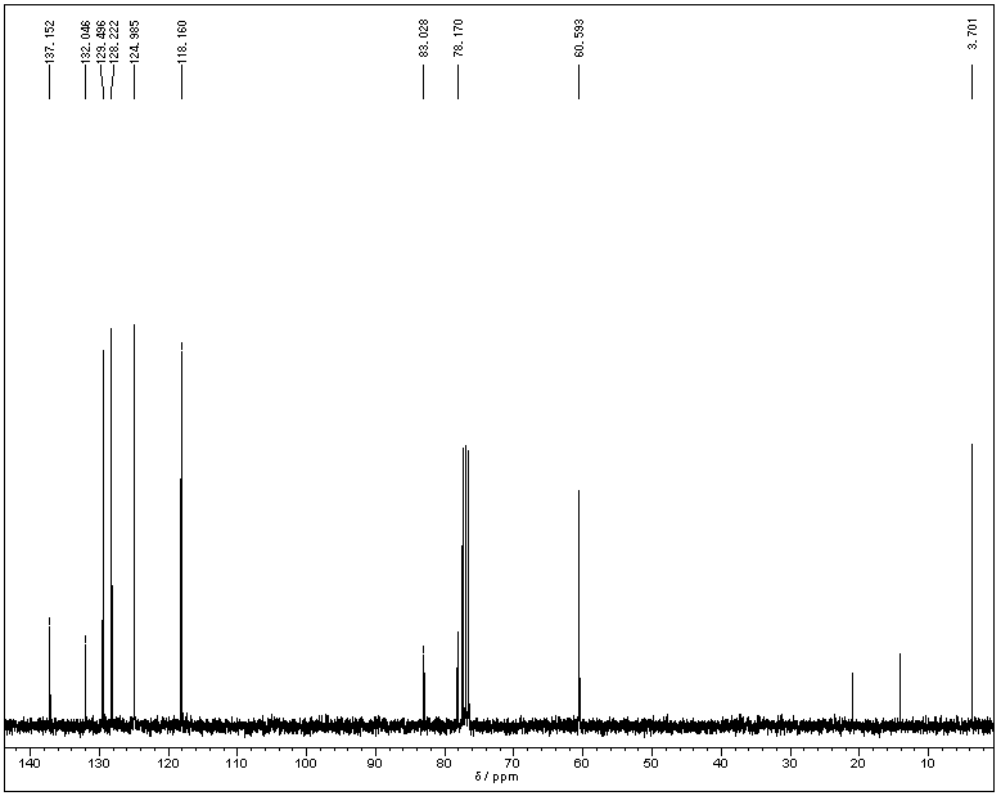
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCL_3$

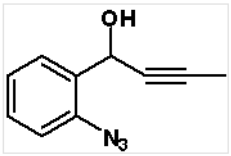
7b





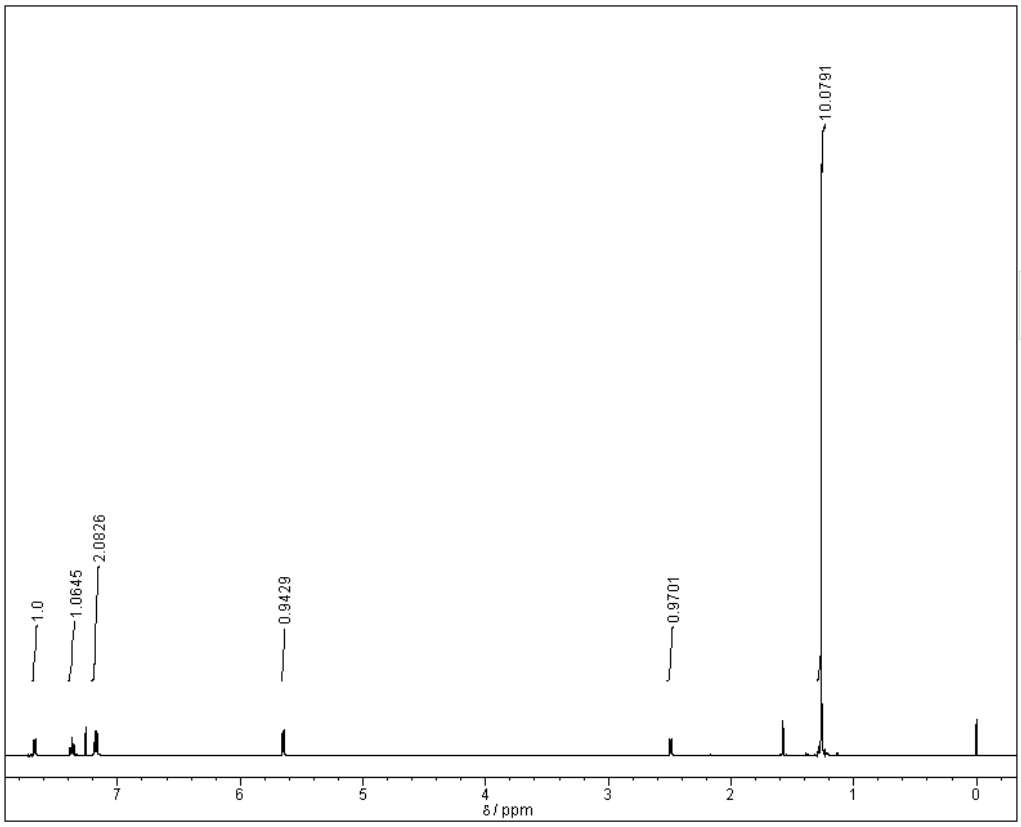
ObsNuc ^{1}H
ObsFreq 300.01 MHz
Solvent $CDCl_3$

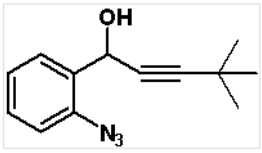




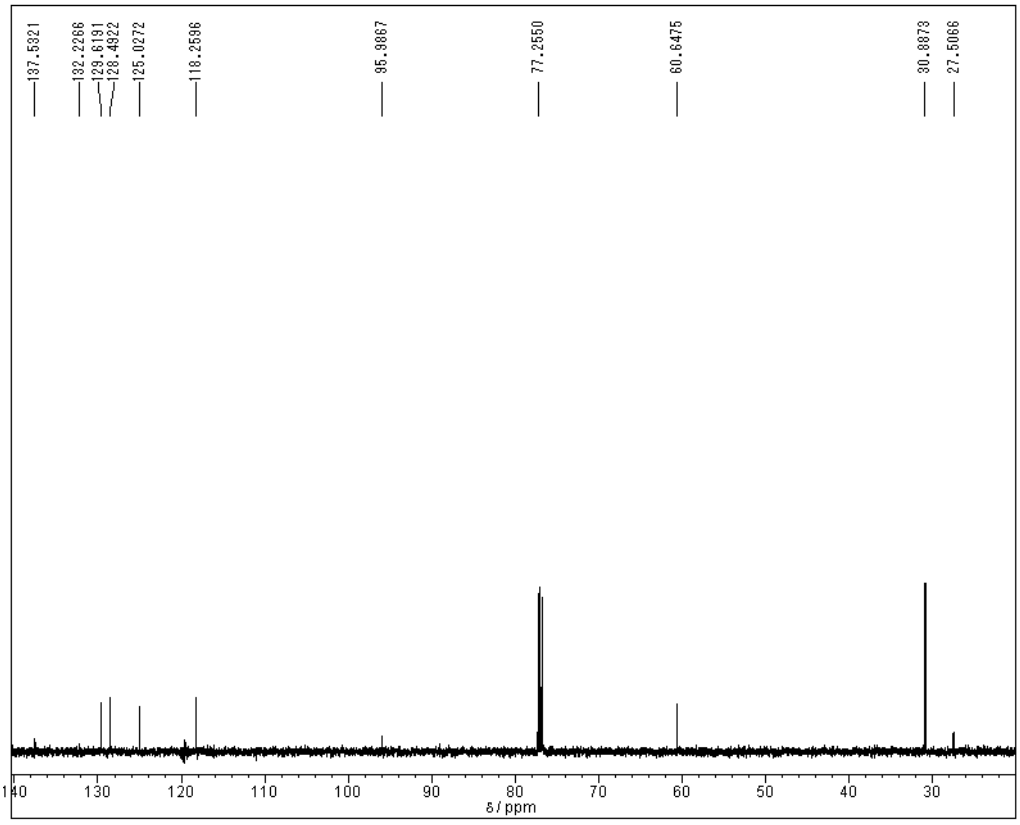
ObsNuc ^{13}C
ObsFreq 75.44 MHz
Solvent $CDCl_3$

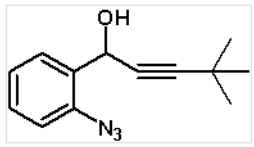
7c





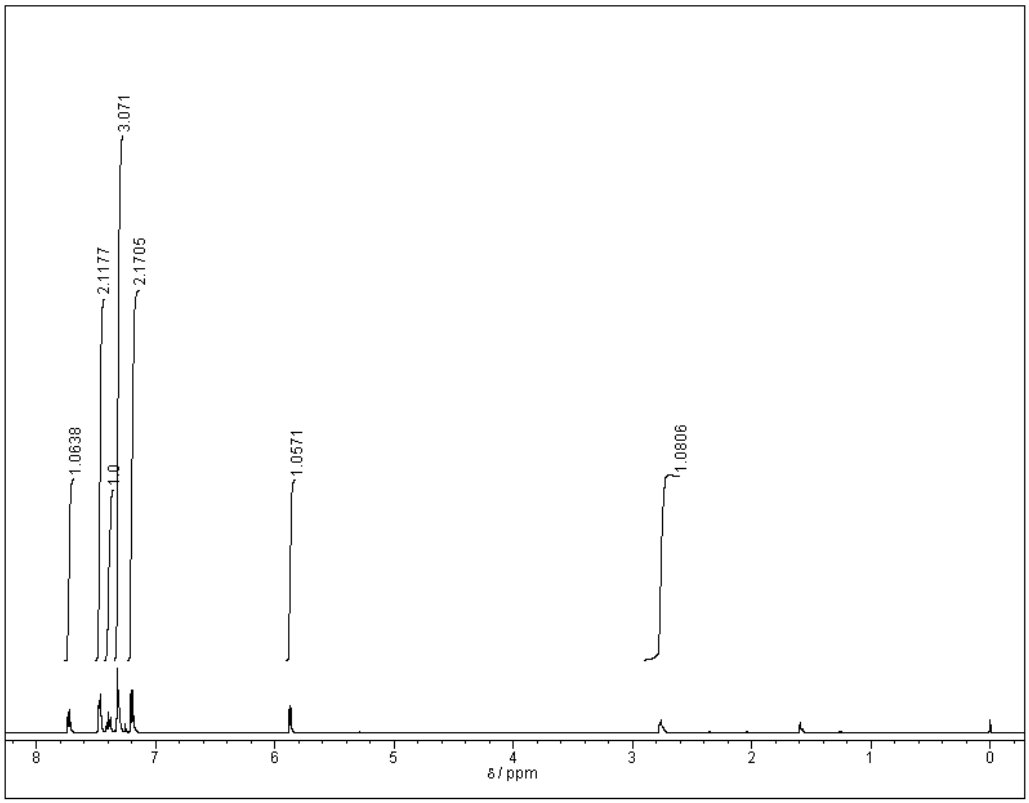
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

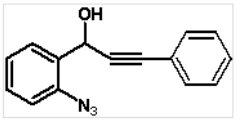




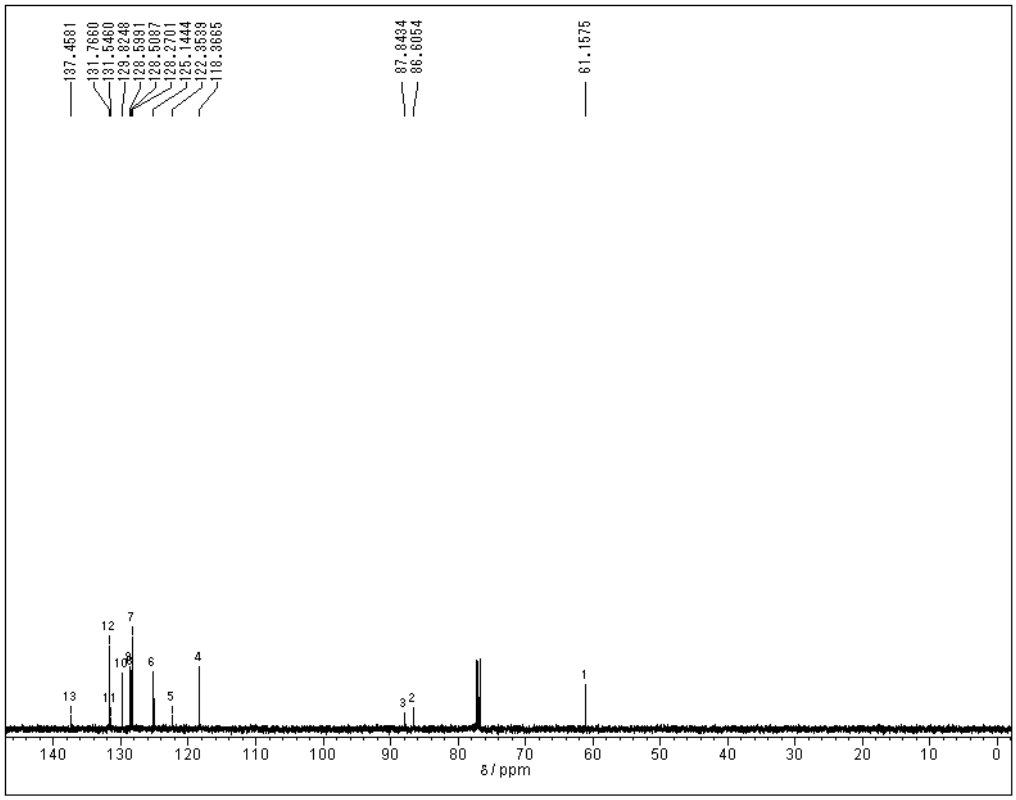
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

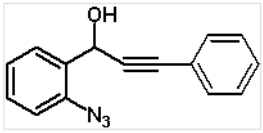
7d





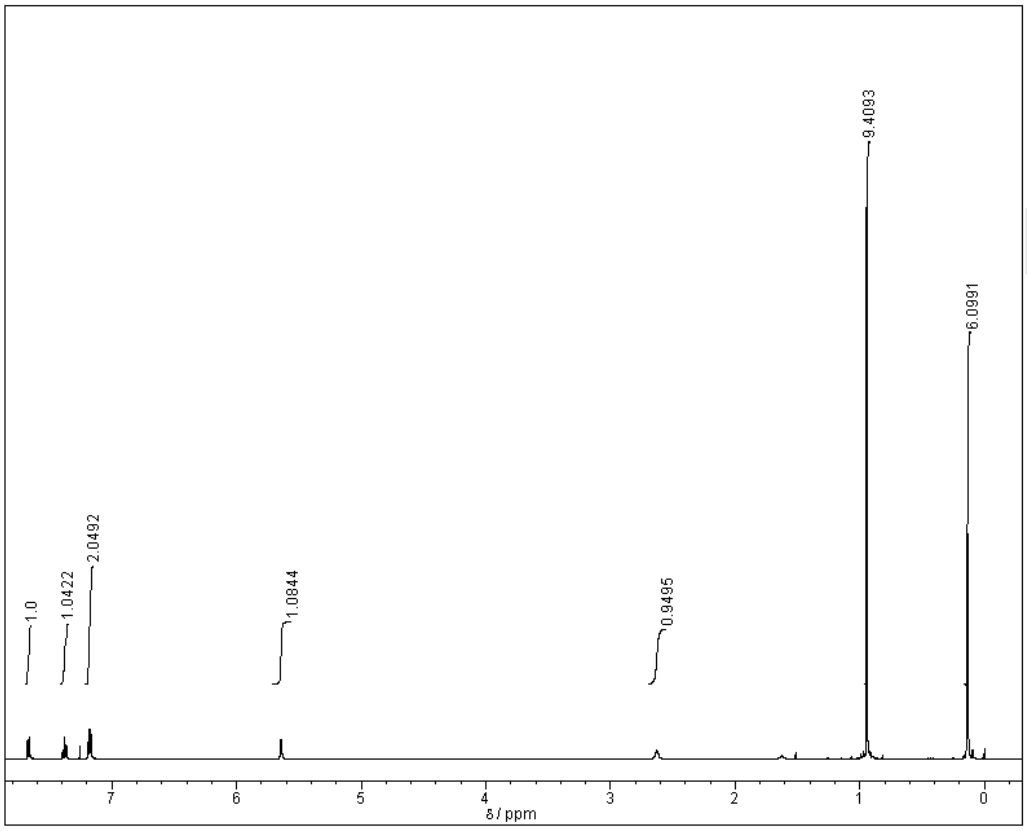
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent CDCL₃

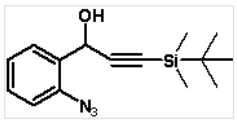




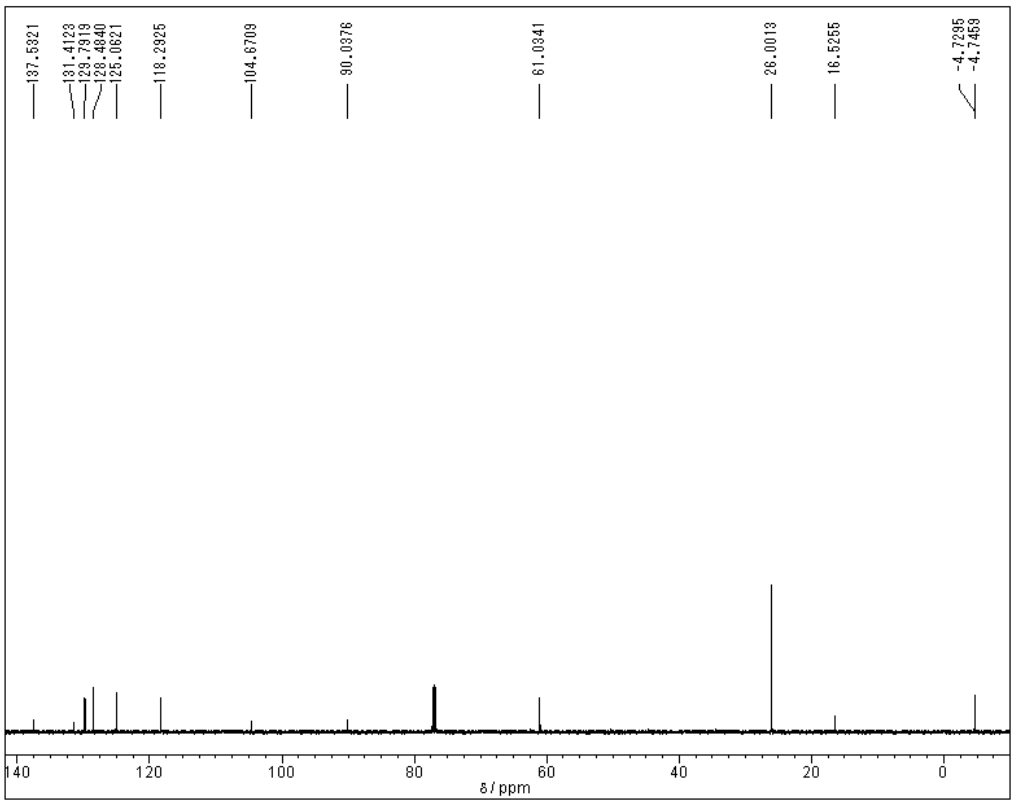
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent CDCL₃

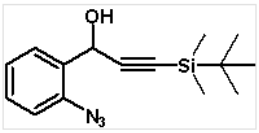
7e





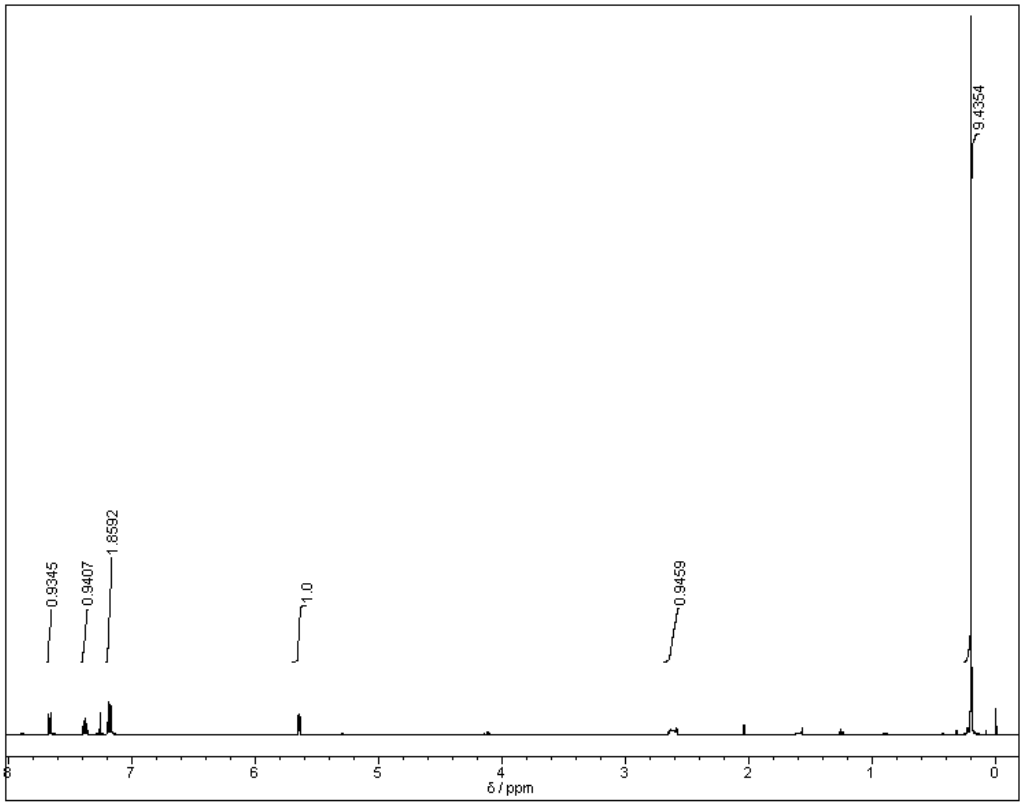
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent CDCL₃

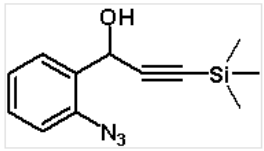




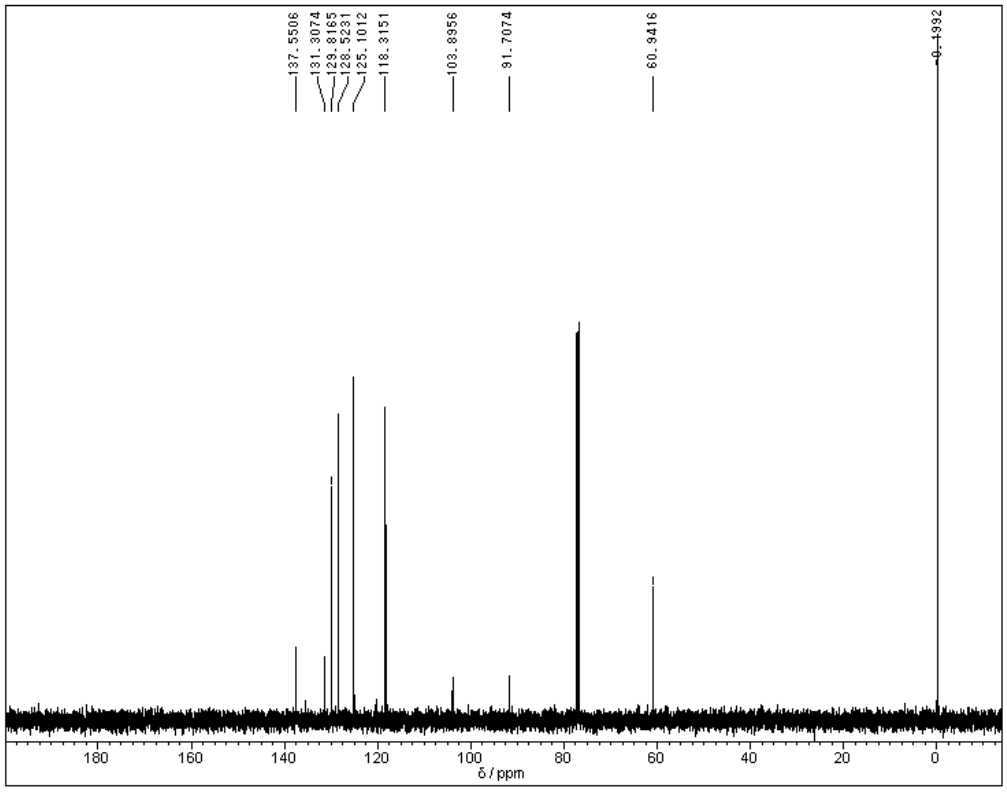
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent CDCL₃

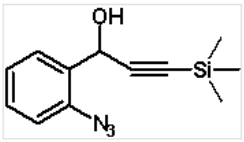
7f





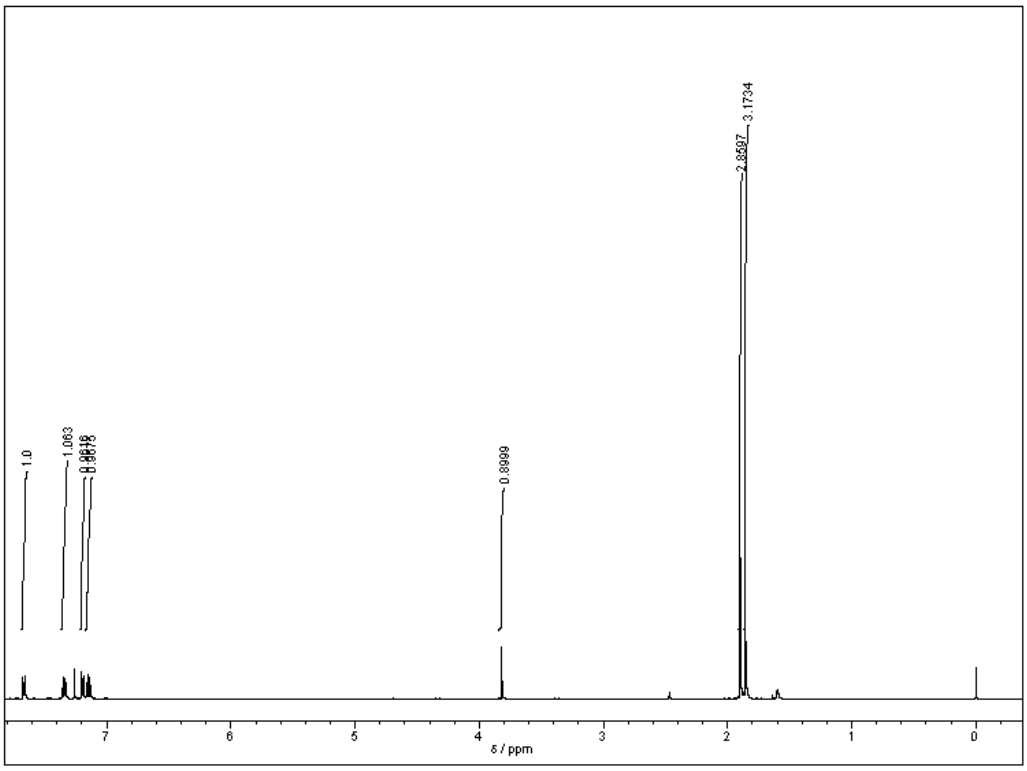
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

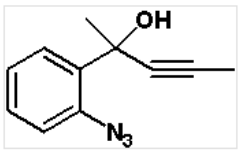




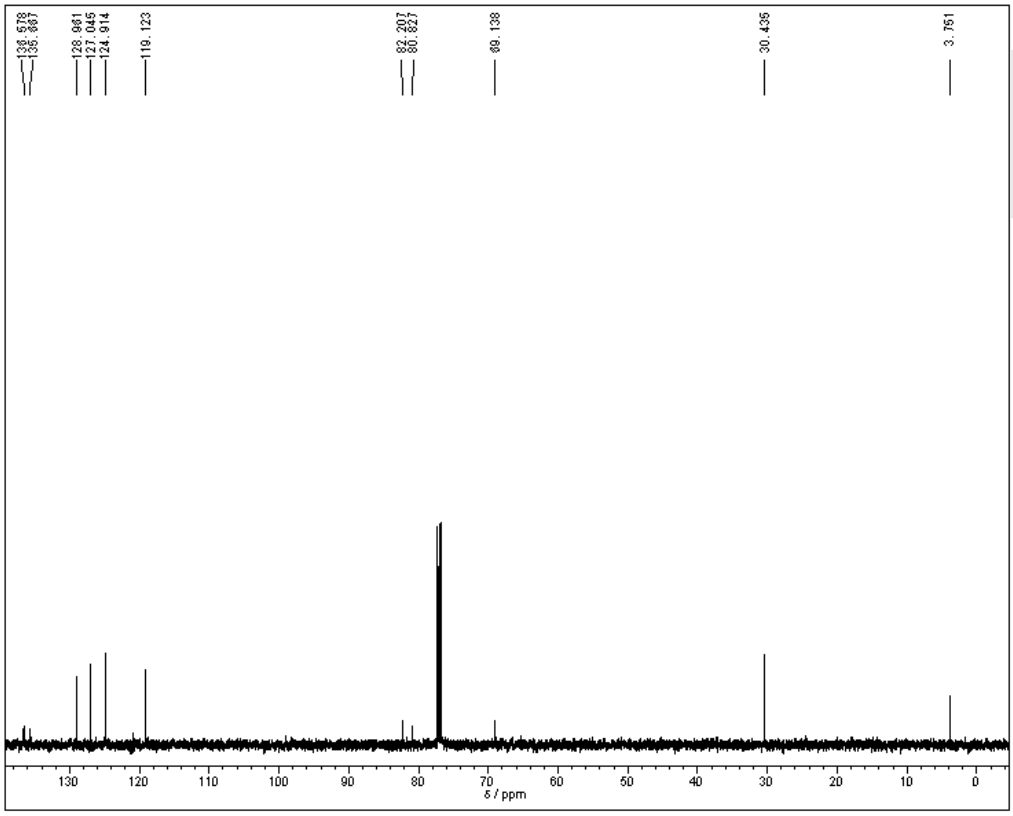
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

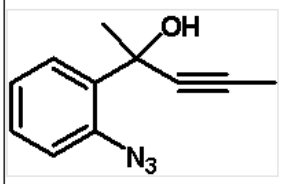
8a





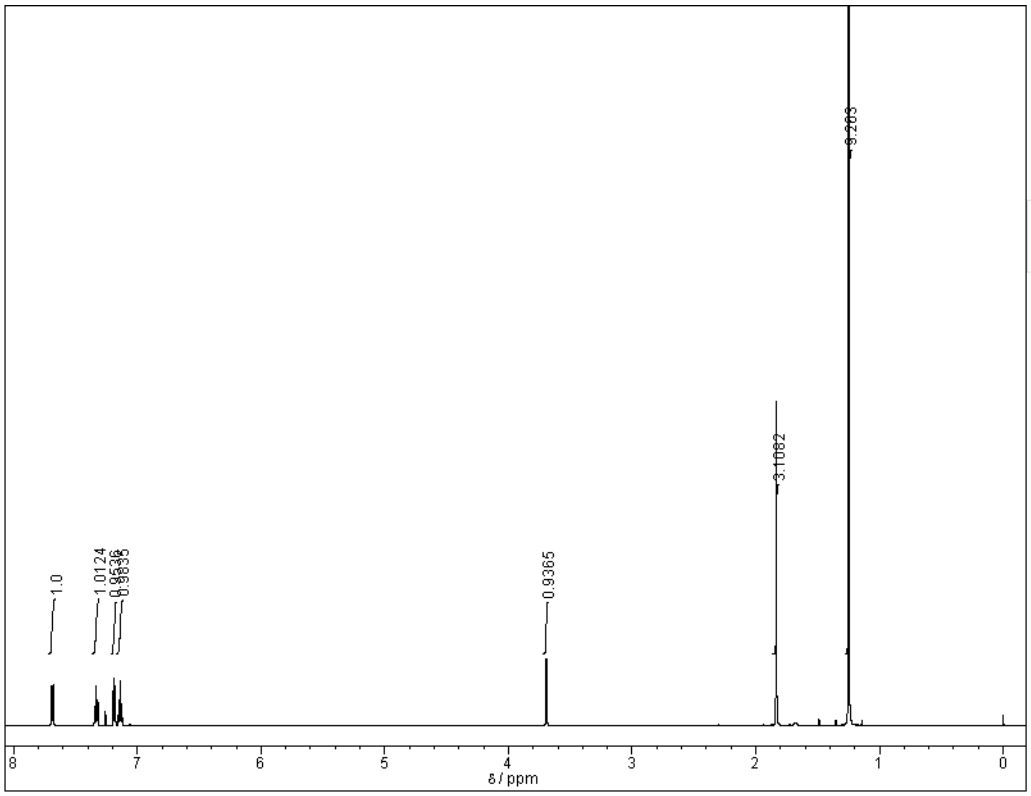
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

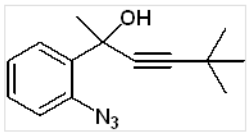




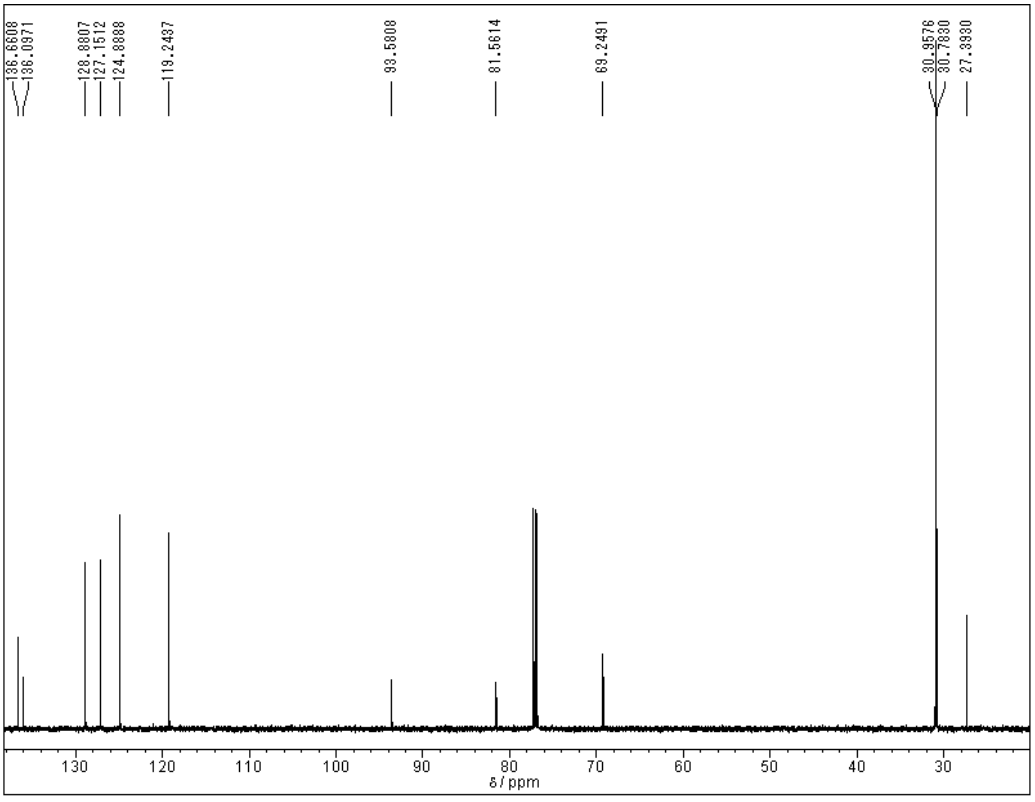
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

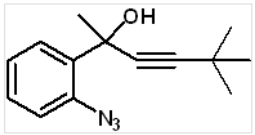
8b





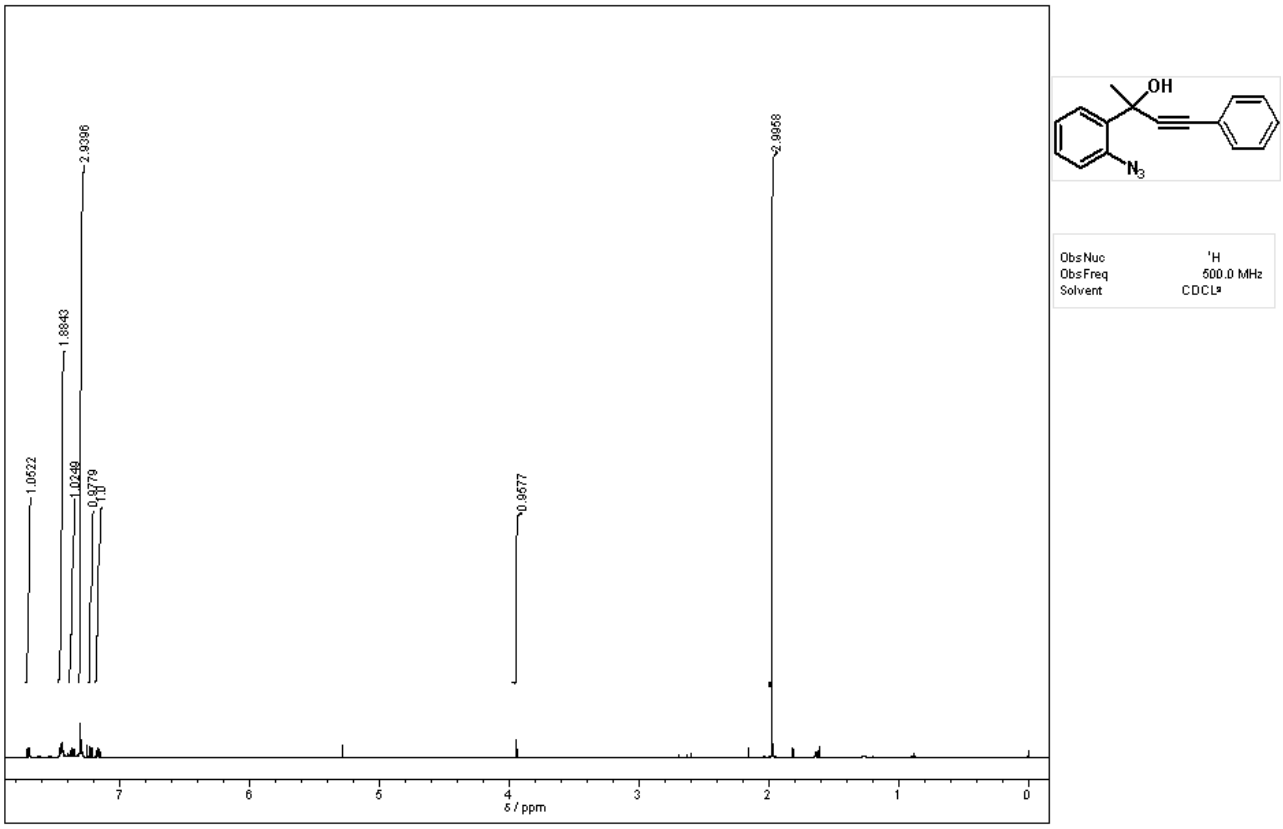
ObsFreq 600.13 MHz
ObsNuc ^{1}H
Solvent $CDCl_3$

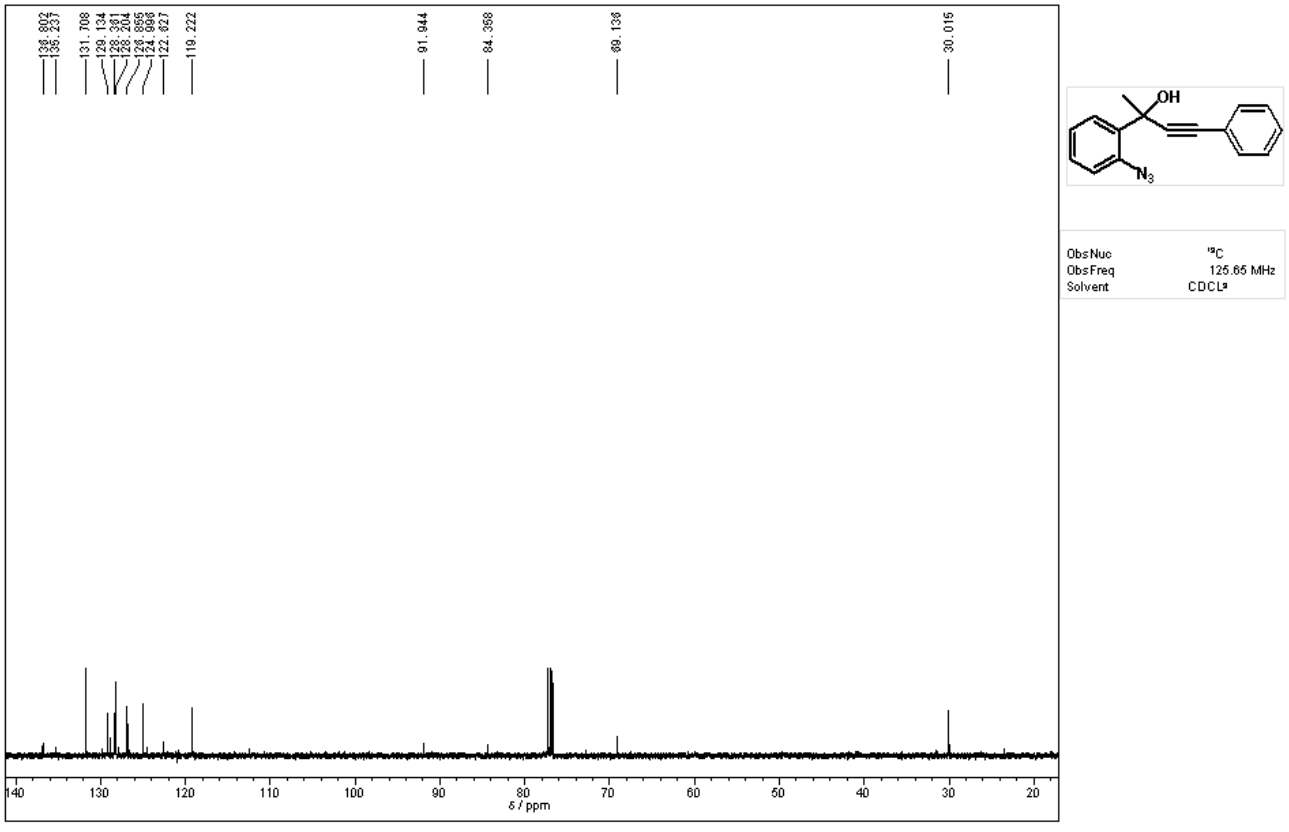




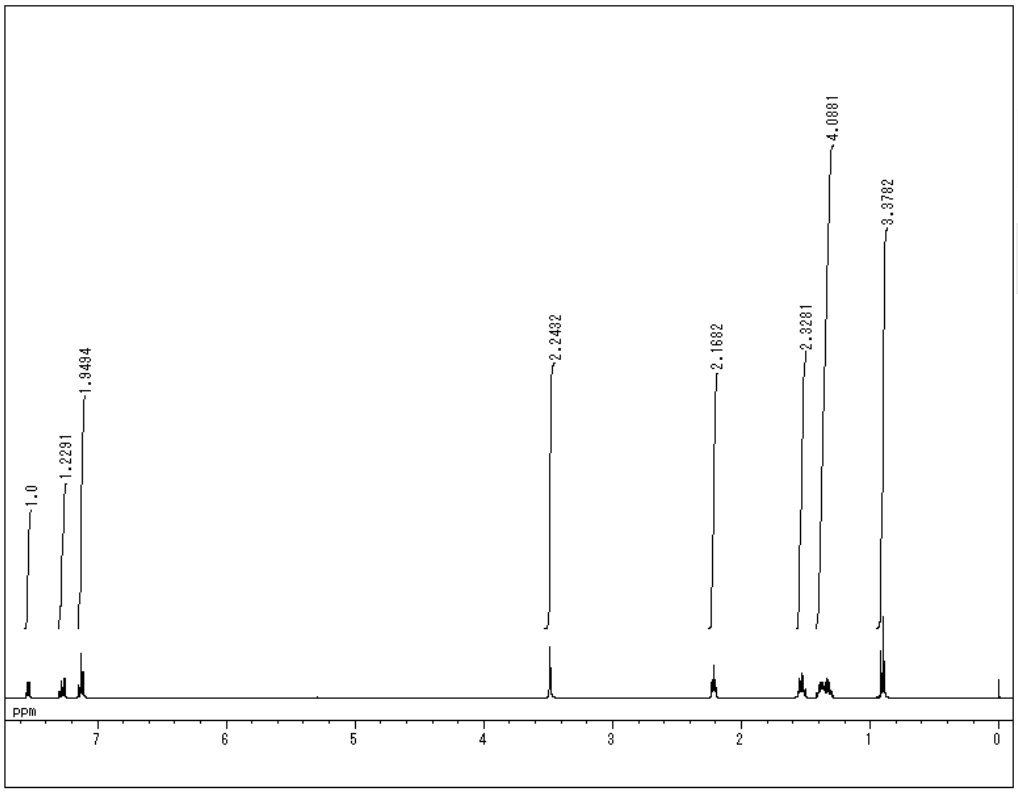
ObsFreq 150.9 MHz
ObsNuc ^{13}C
Solvent $CDCl_3$

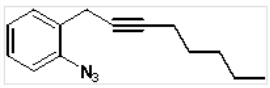
8c


2.9396
1.8843
1.0522
1.0249
0.9779
1.0
0.9577
2.9958
OH
N3
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3
7
6
5
4
3
2
1
0
δ / ppm

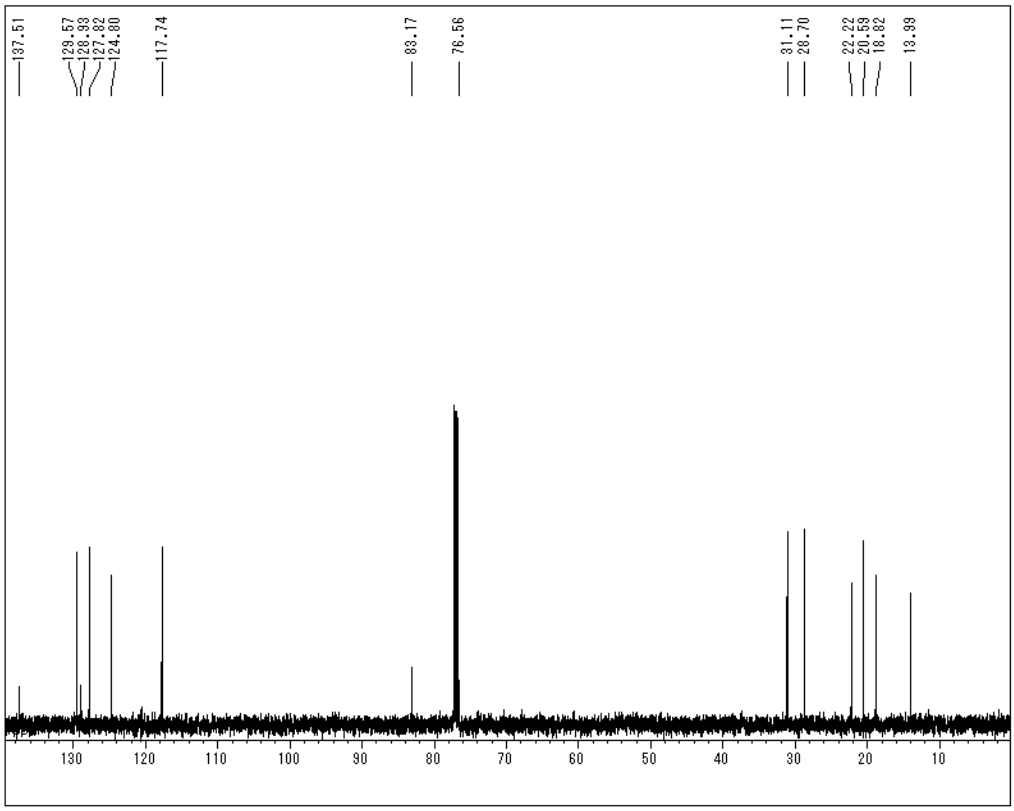

138.802
135.237
131.708
129.134
128.381
128.204
126.855
124.998
122.627
119.222
91.944
84.358
89.136
30.015
OH
N3
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3
140
130
120
110
100
90
80
70
60
50
40
30
20
δ / ppm

9a



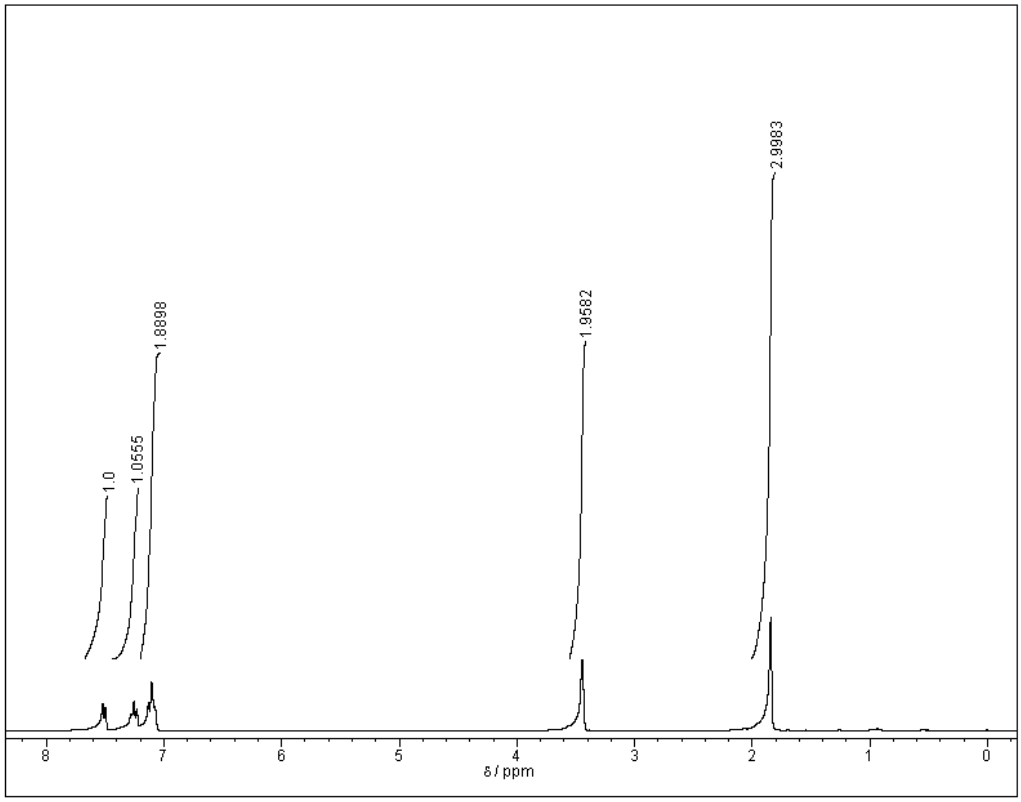


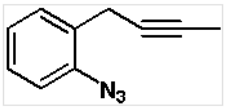
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent CDCL3



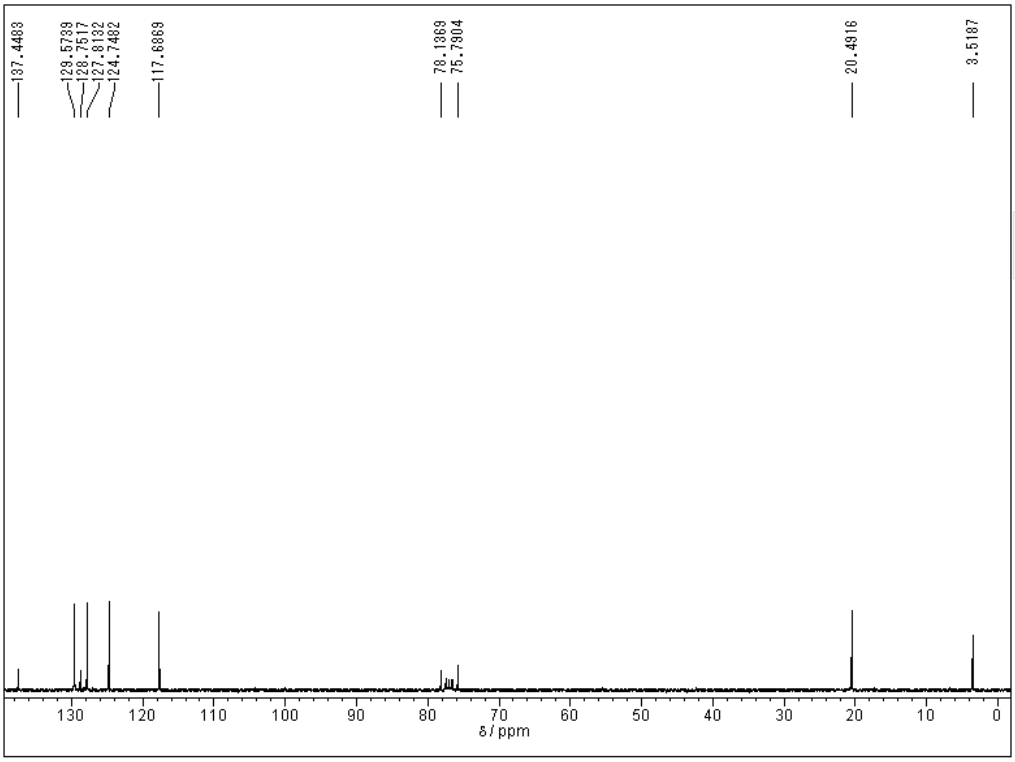
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent CDCL3

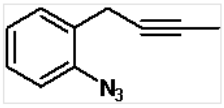
9b





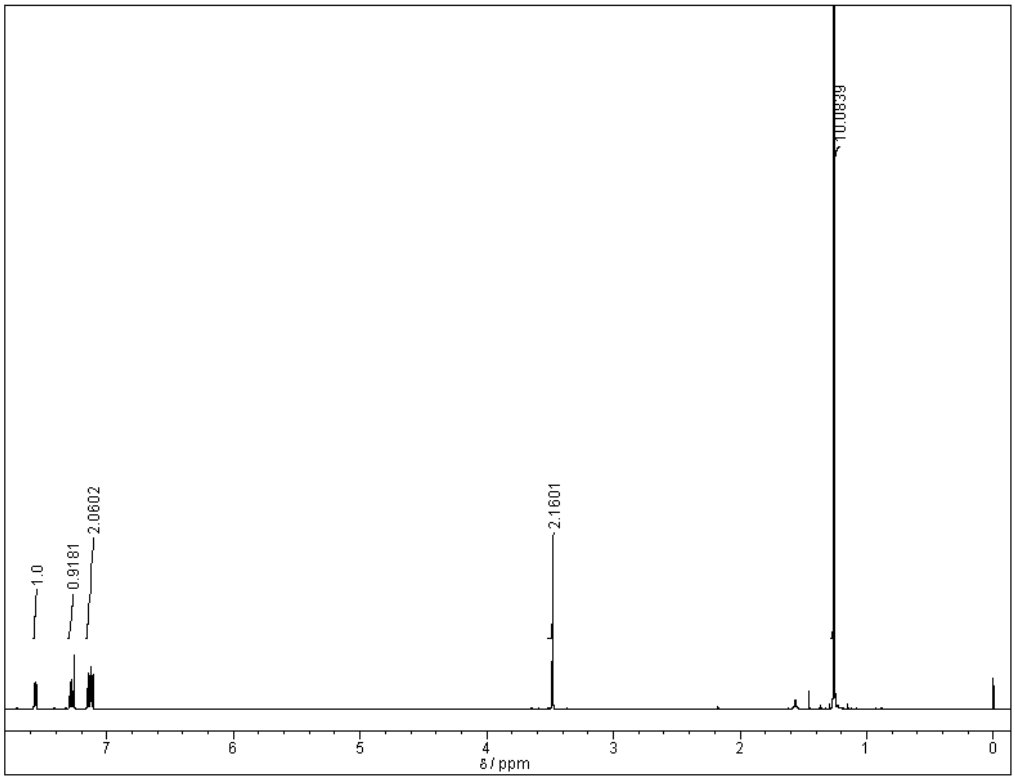
ObsNuc ¹H
ObsFreq 300.01 MHz
Solvent CDCL₃

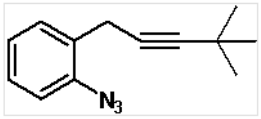




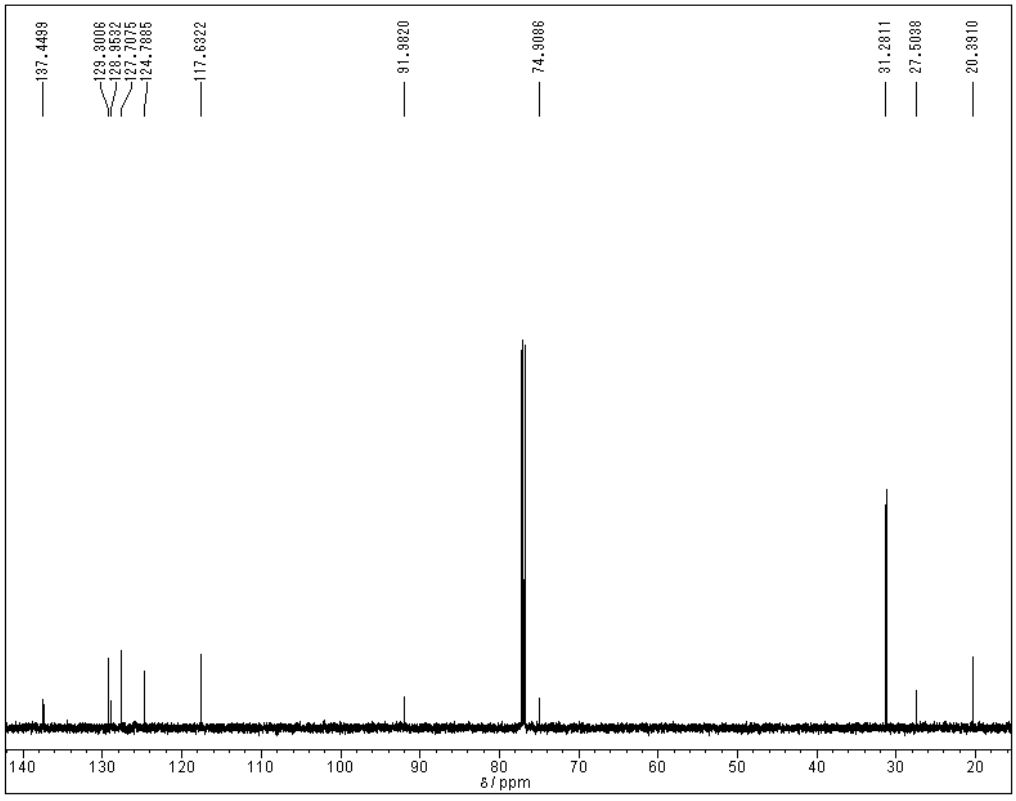
ObsNuc ¹³C
ObsFreq 75.44 MHz
Solvent CDCL₃

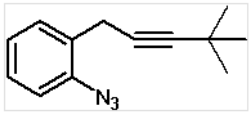
9c





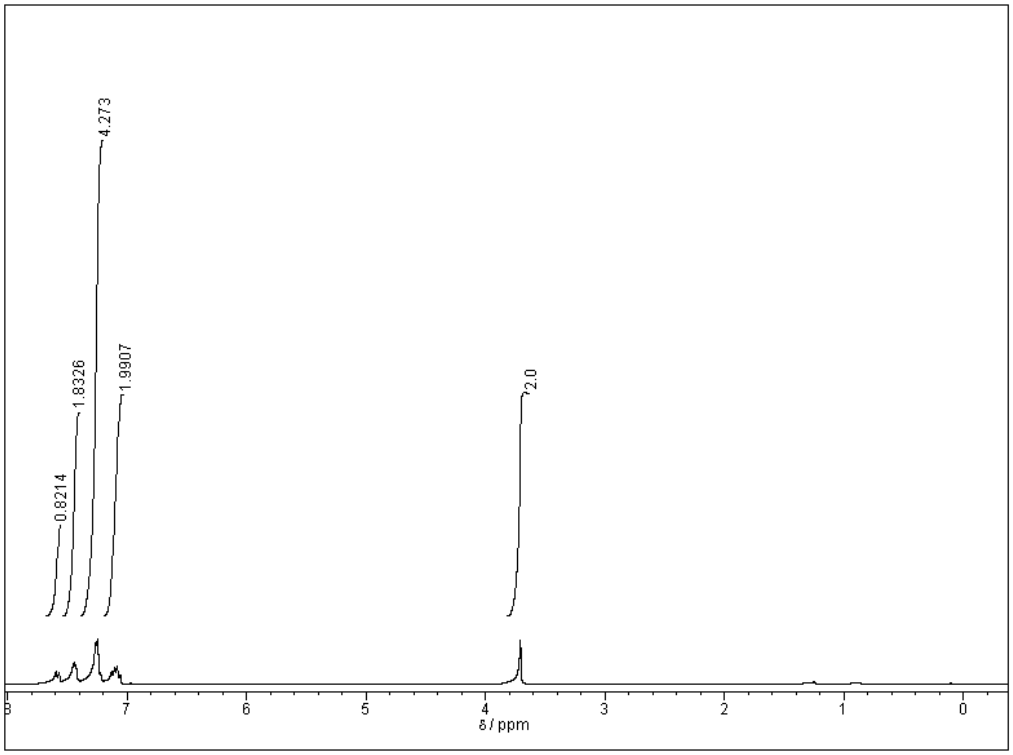
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

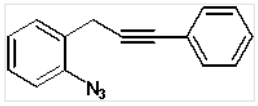




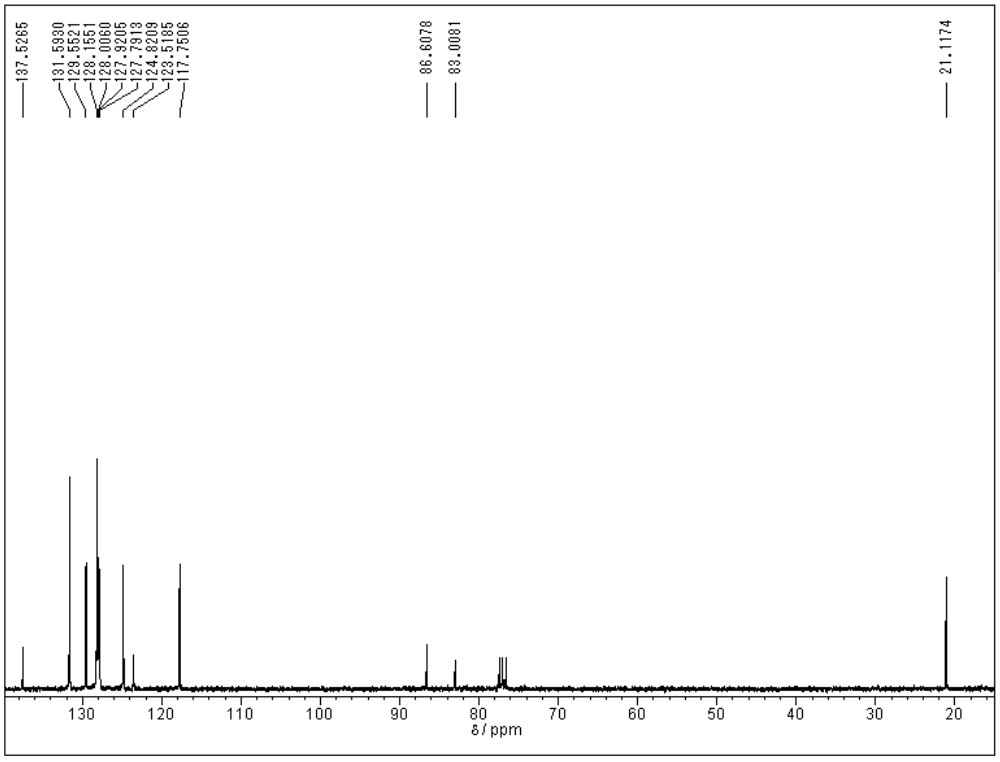
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

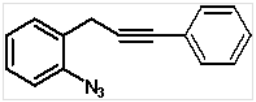
9d





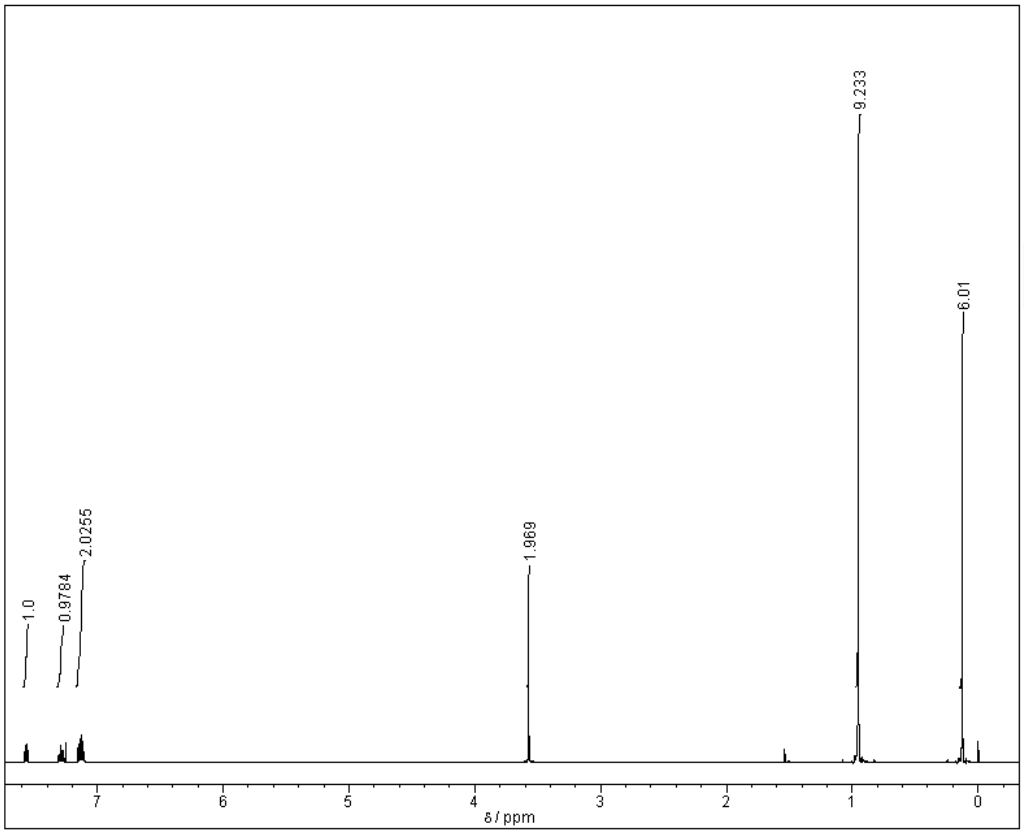
ObsNuc ¹H
ObsFreq 300.01 MHz
Solvent CDCL₃

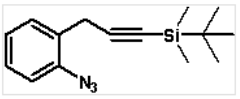




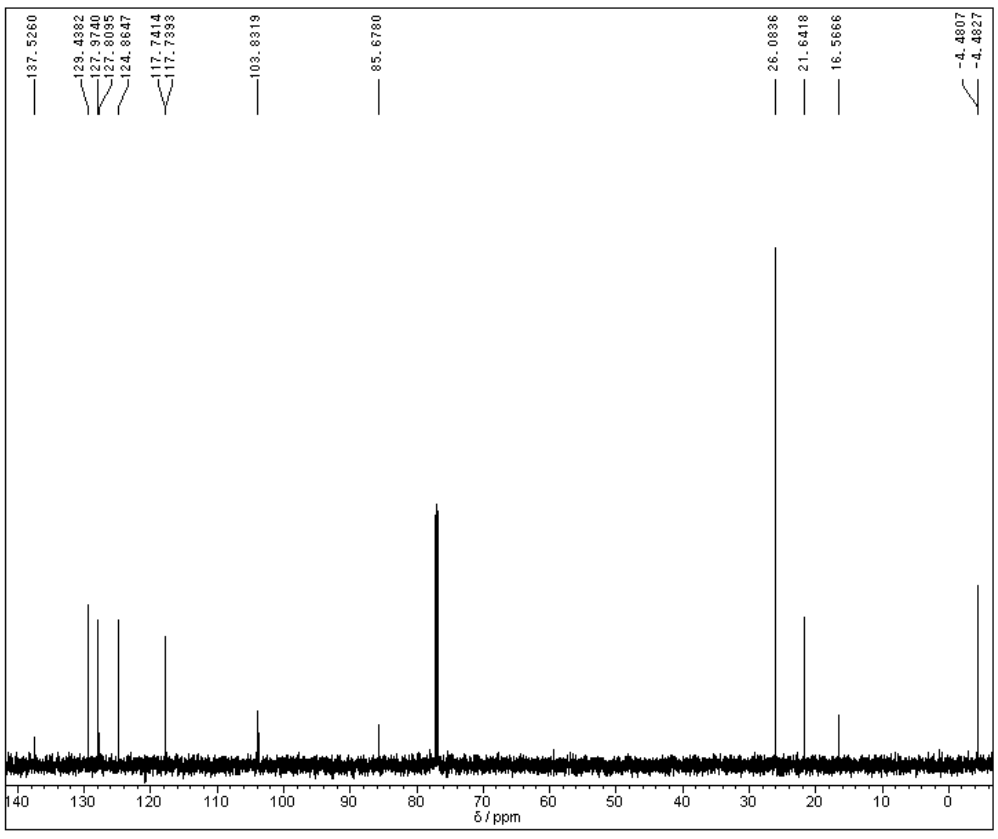
ObsNuc ¹³C
ObsFreq 75.44 MHz
Solvent CDCL₃

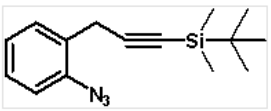
9e





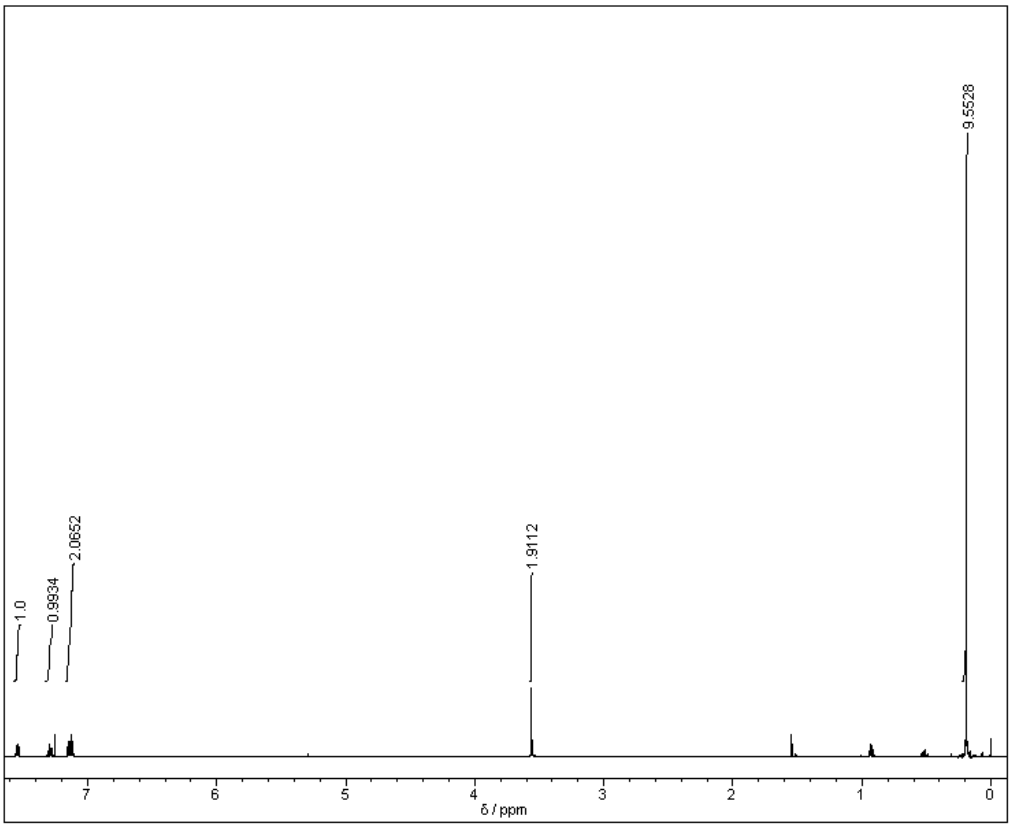
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

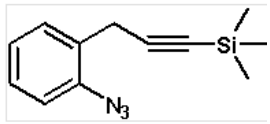




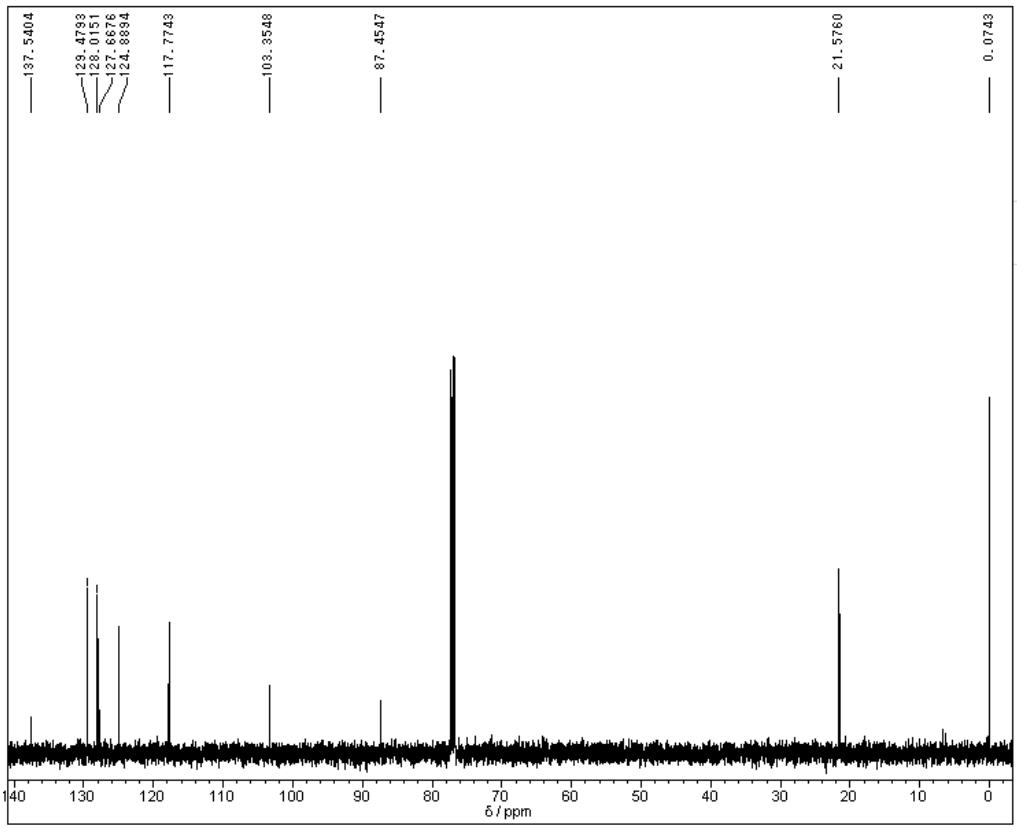
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

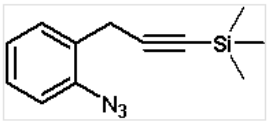
9f





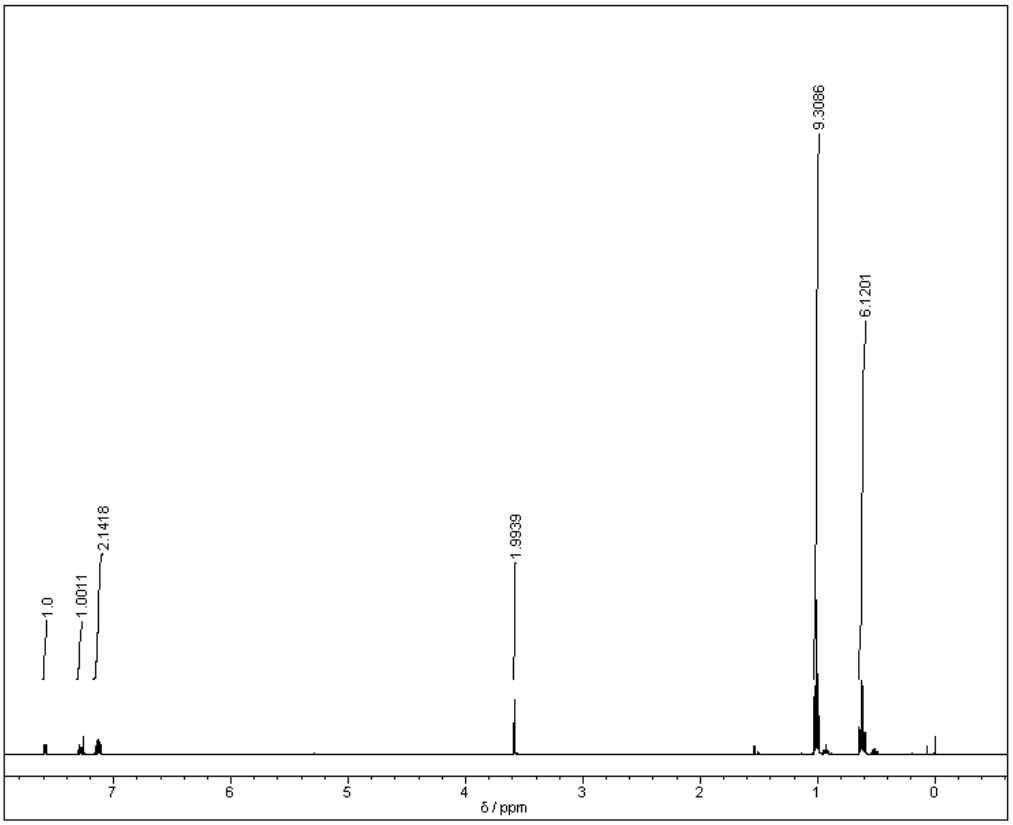
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCL_3$

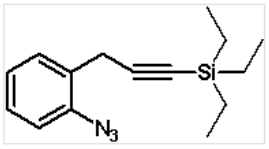




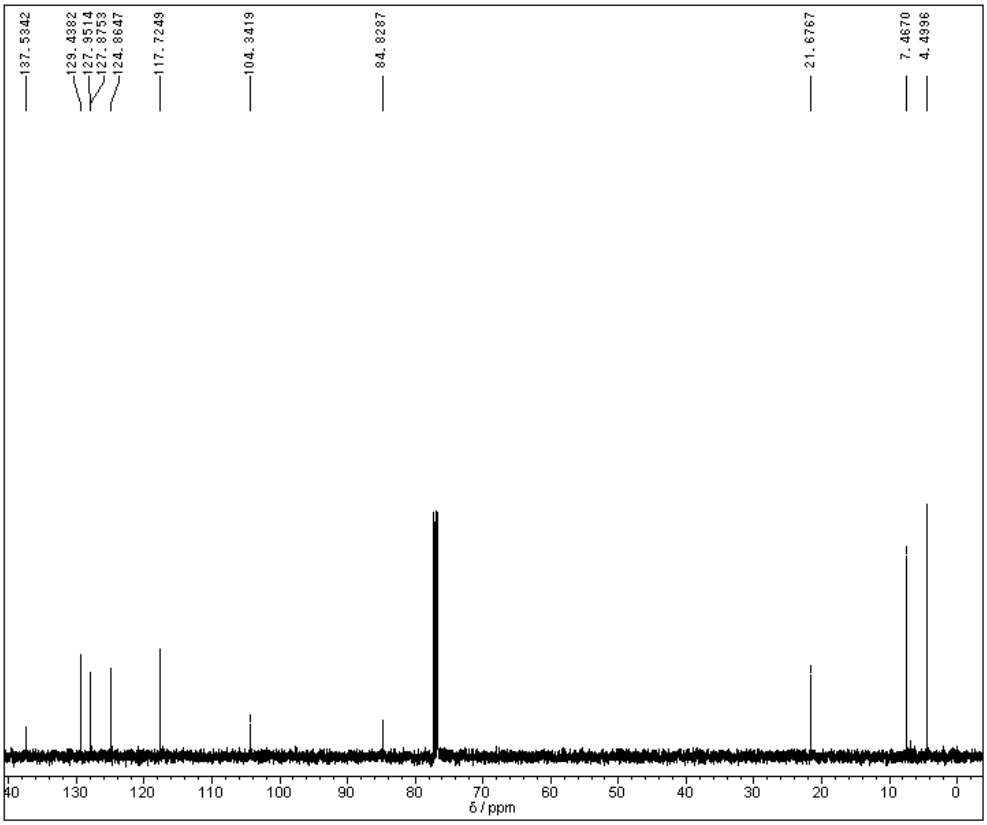
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCL_3$

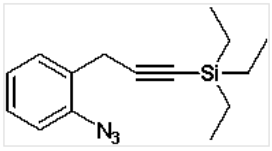
9g





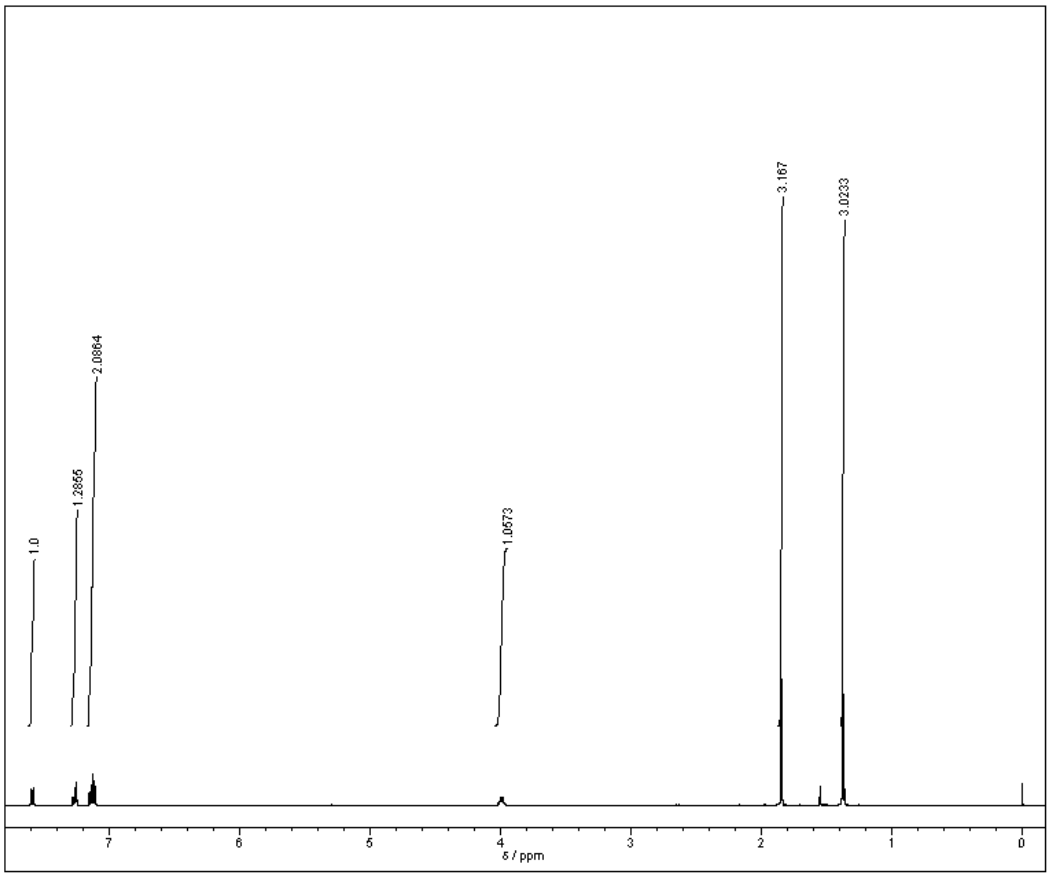
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCL_3$

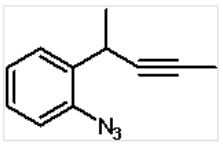




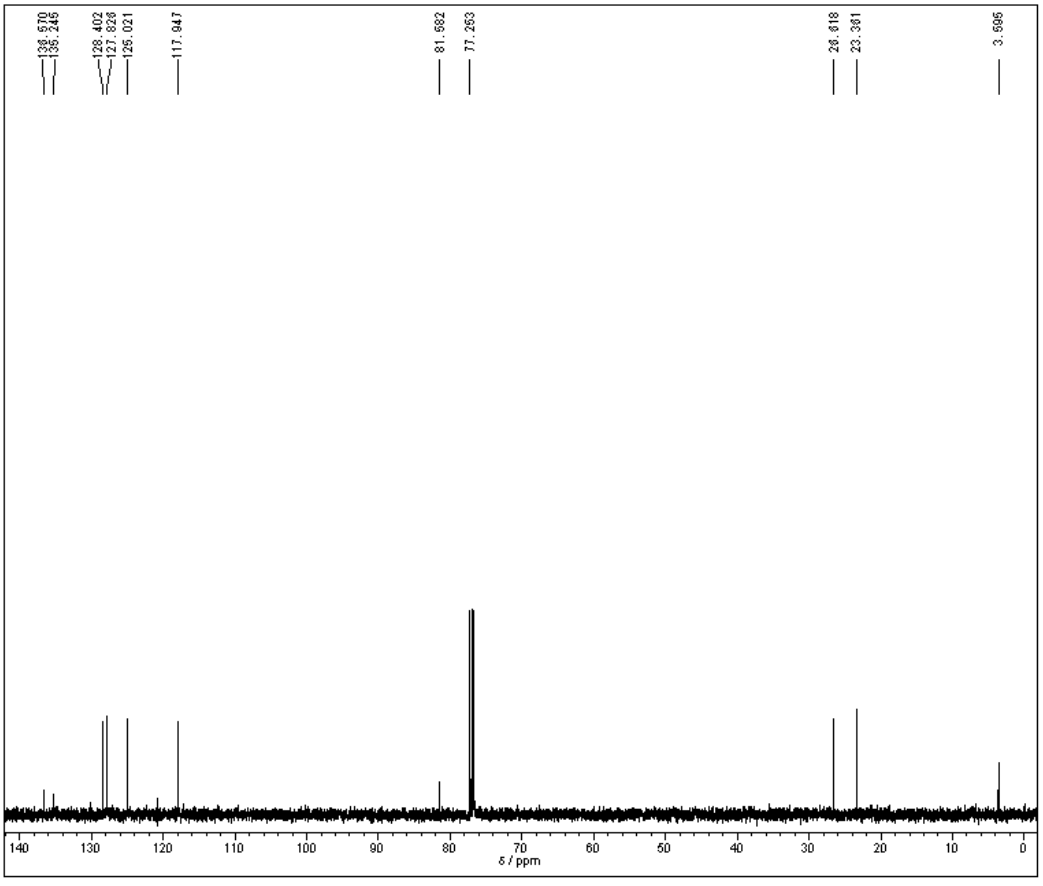
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCL_3$

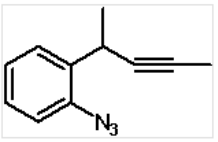
10a





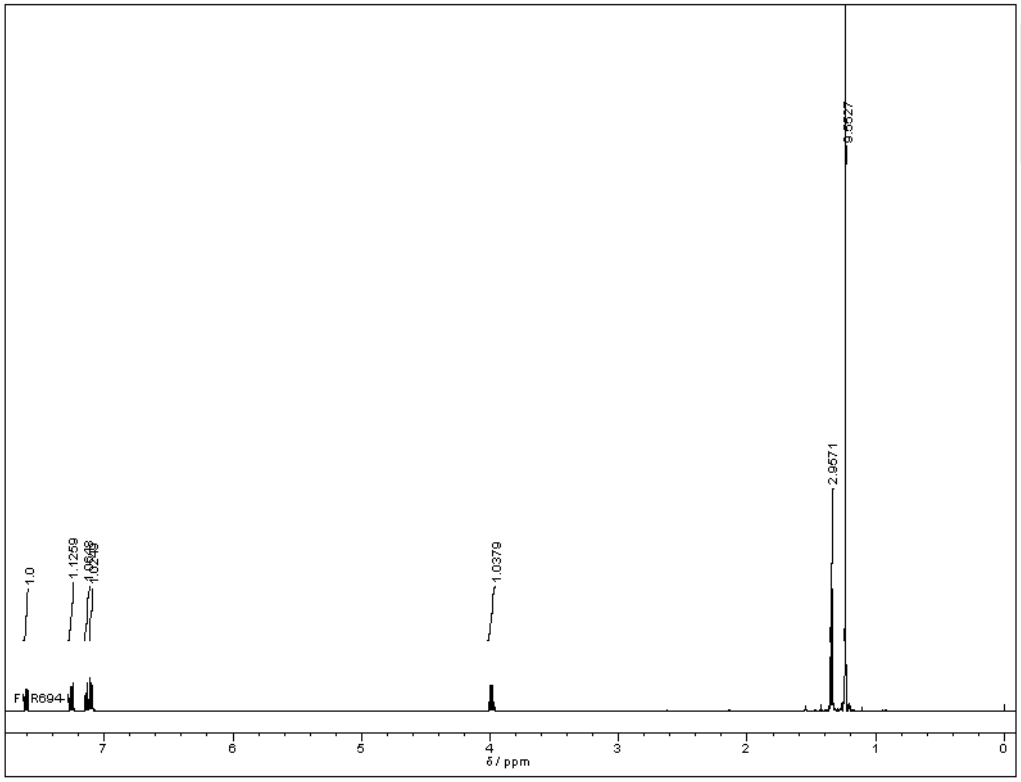
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

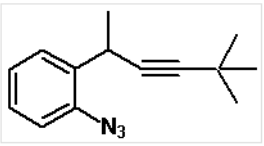




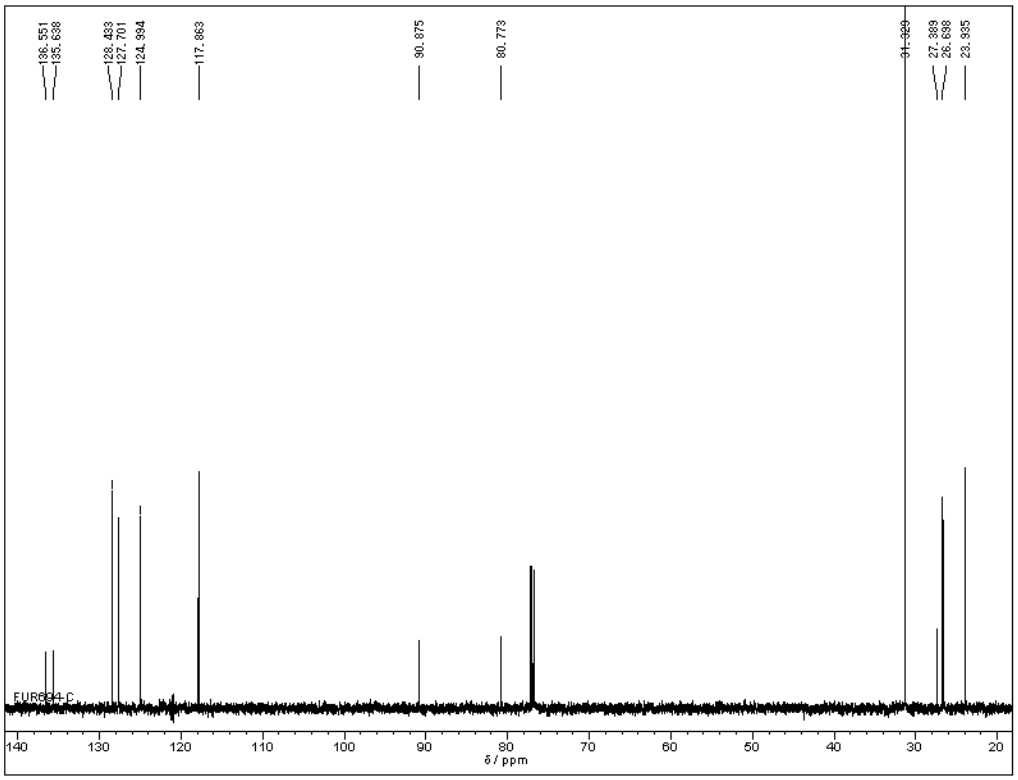
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

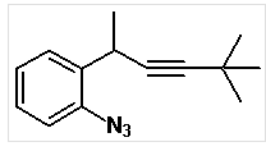
10b





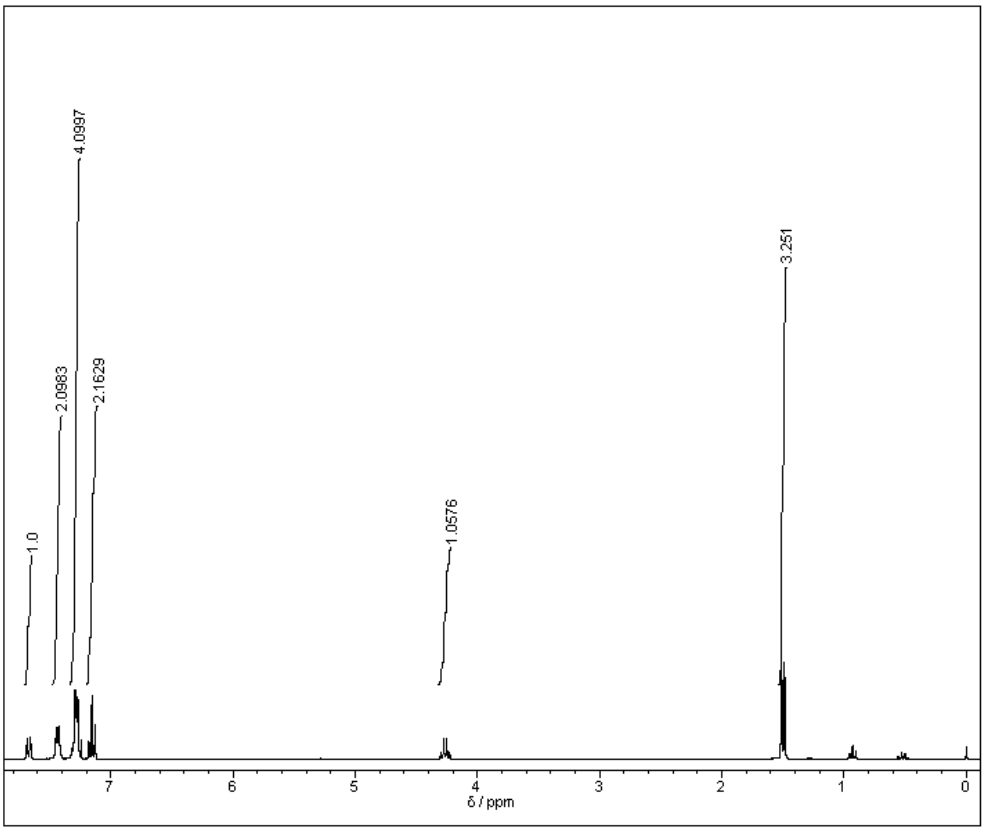
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	CDCL3

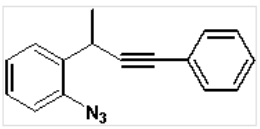




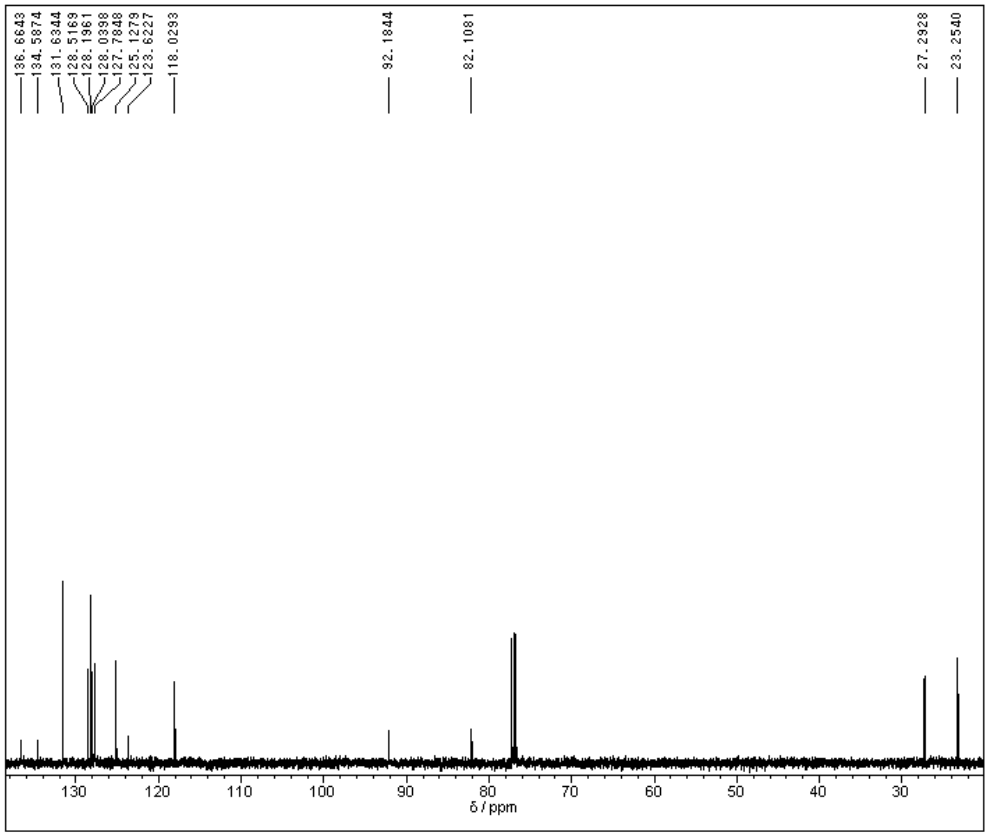
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	CDCL3

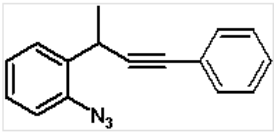
10c





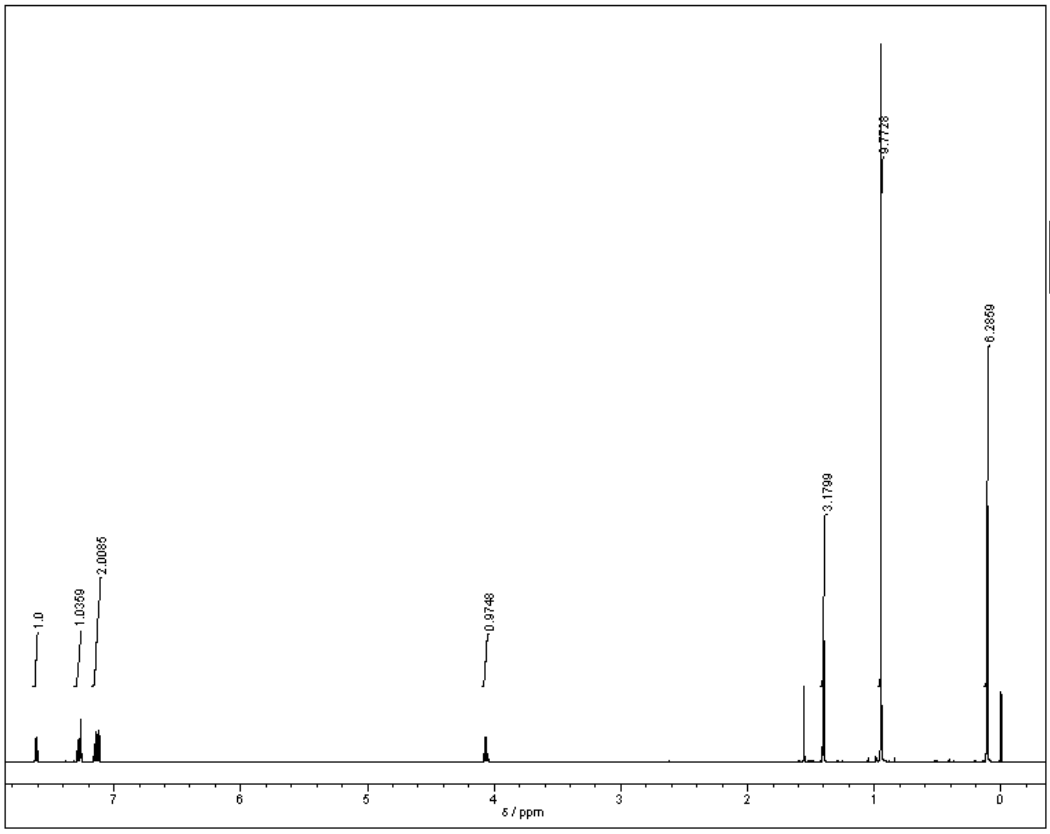
ObsNuc 1H
ObsFreq 300.01 MHz
Solvent $CDCl_3$

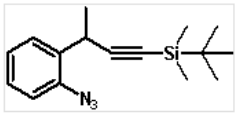




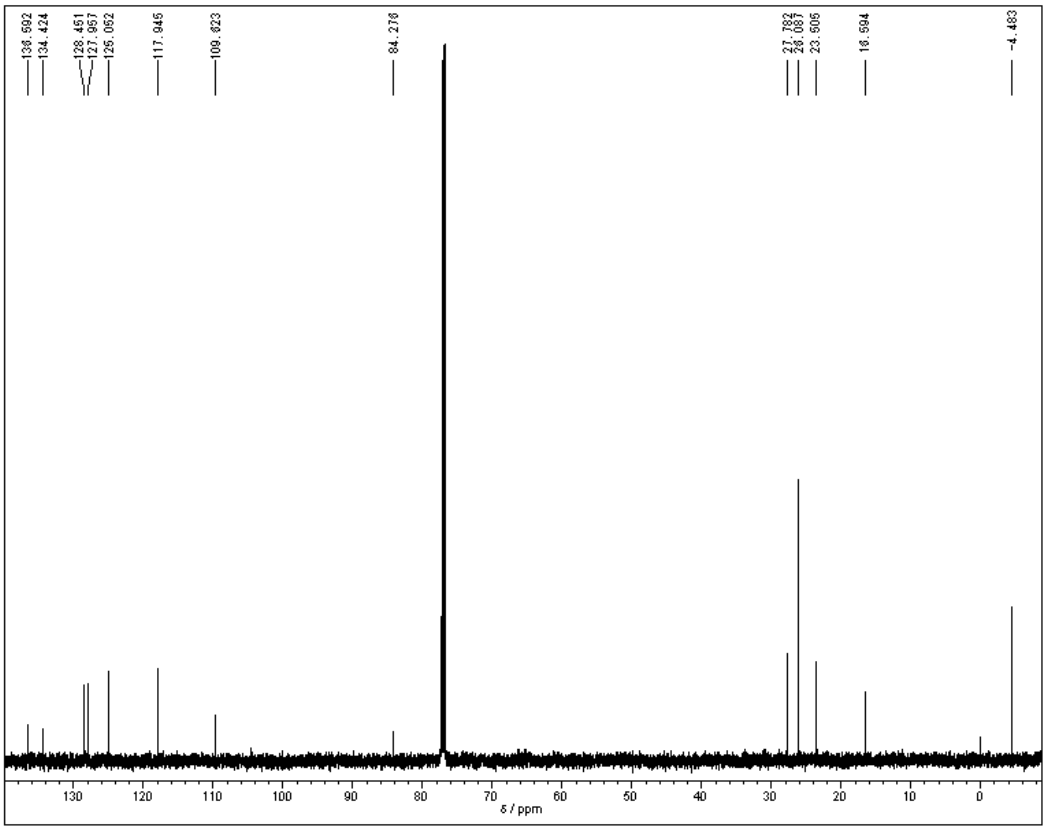
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

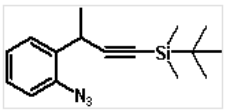
10d





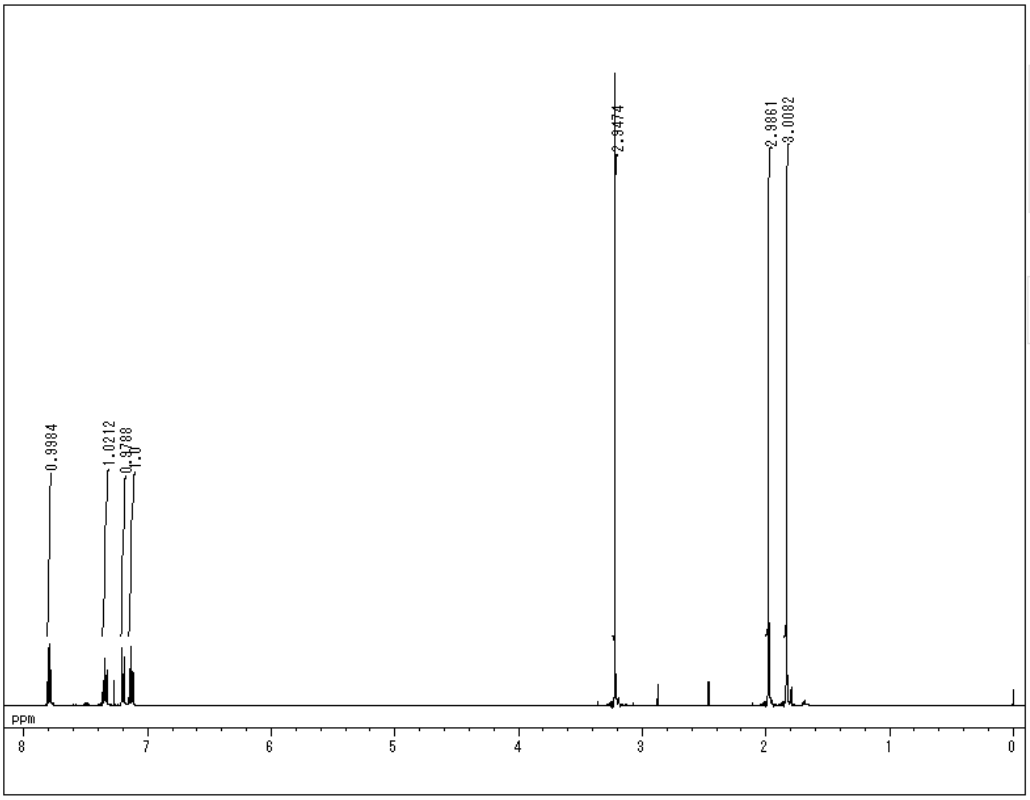
ObsNuc	^{1}H
ObsFreq	600.13 MHz
Solvent	CDCL^{3}

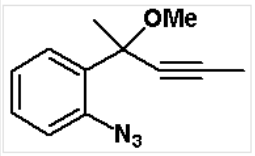




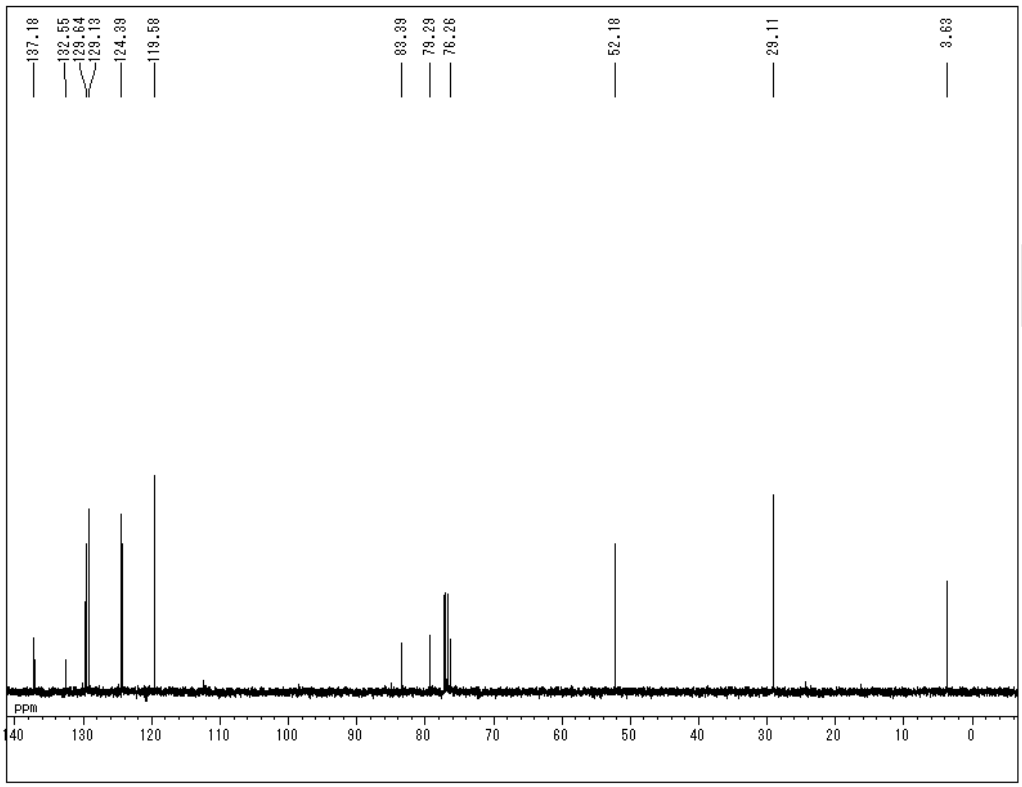
ObsNuc	^{13}C
ObsFreq	150.9 MHz
Solvent	CDCL^{3}

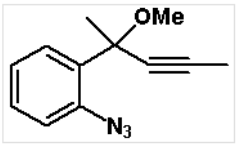
11a





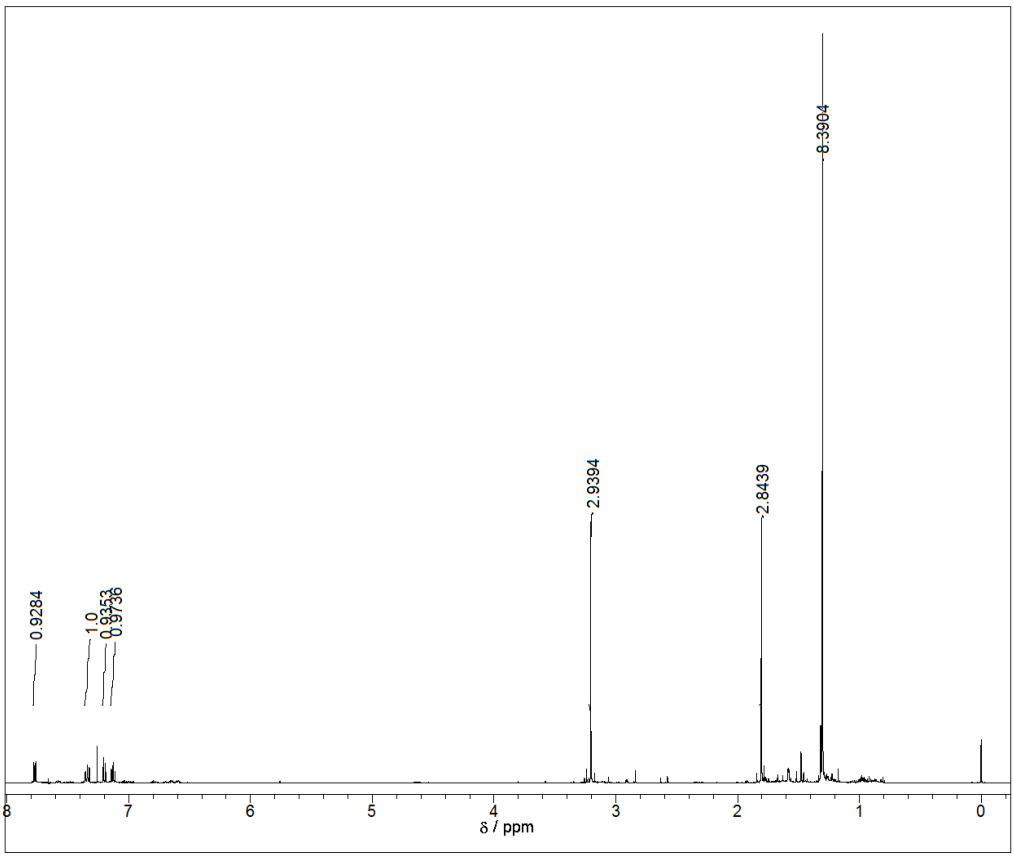
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

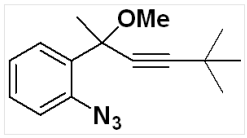




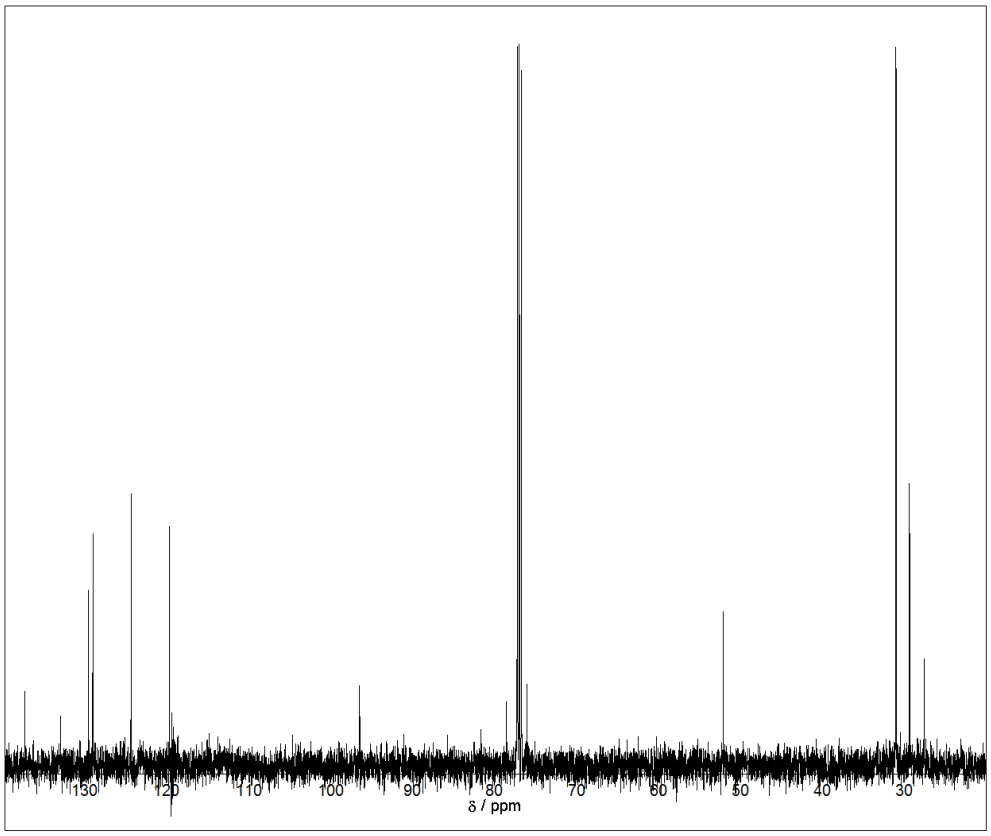
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

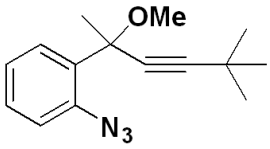
11b





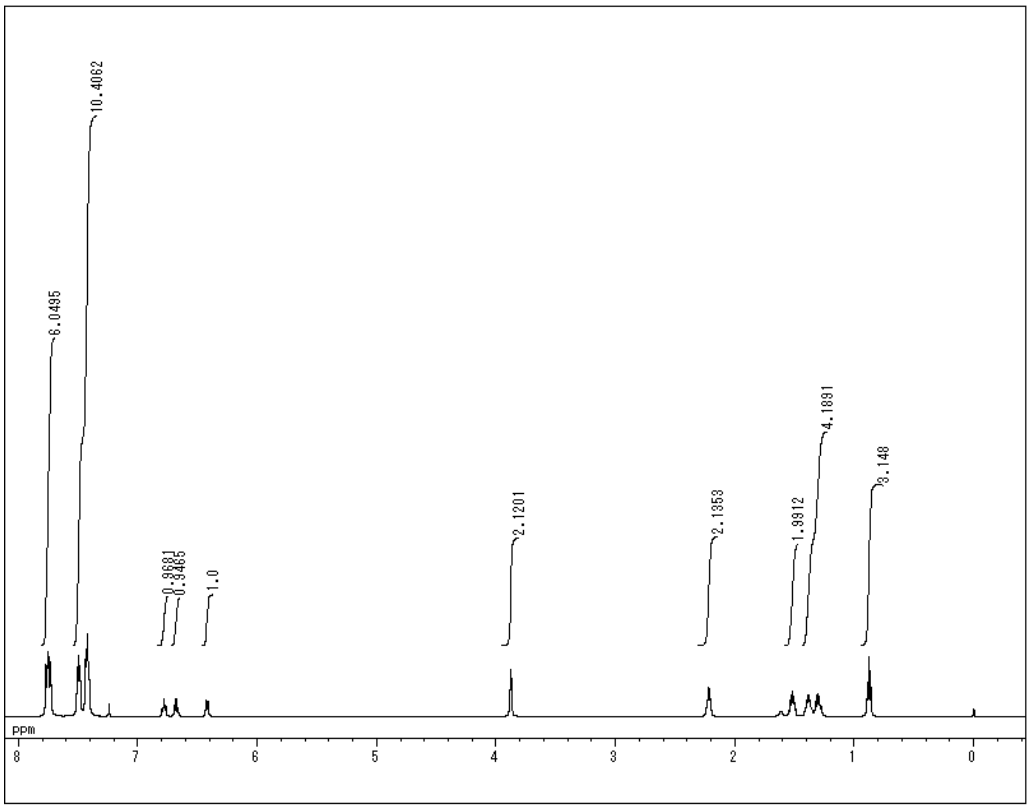
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

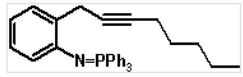




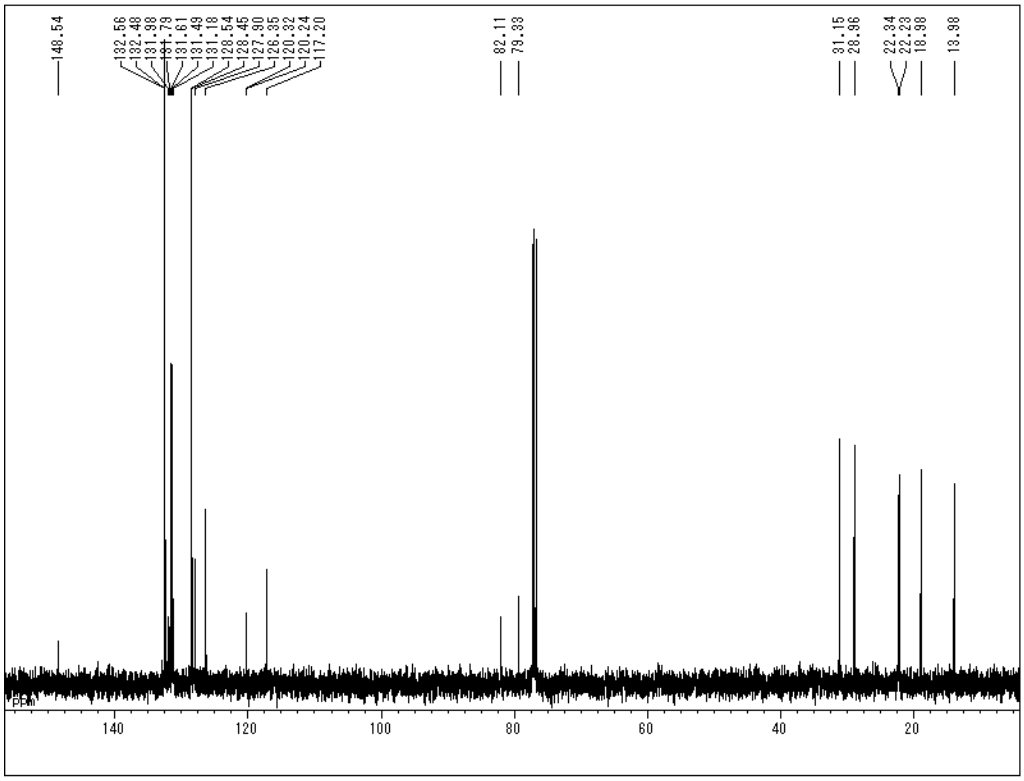
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

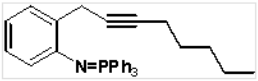
12a





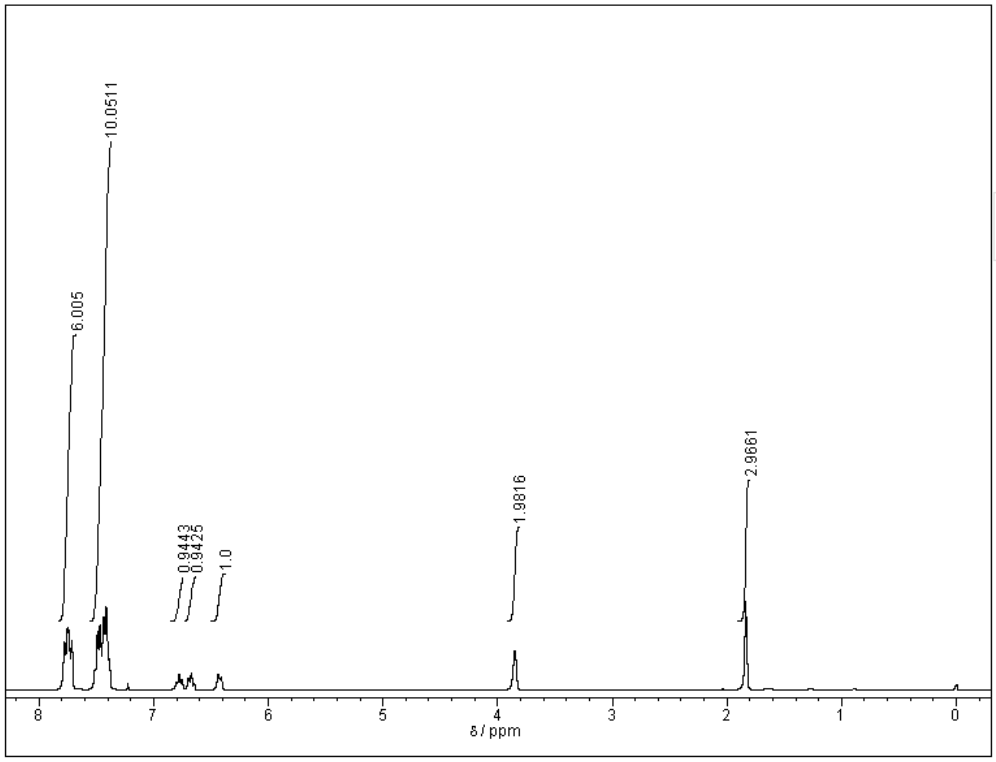
ObsNuc ¹H
ObsFreq 500.0 MHz
Solvent CDCL₃

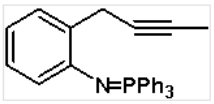




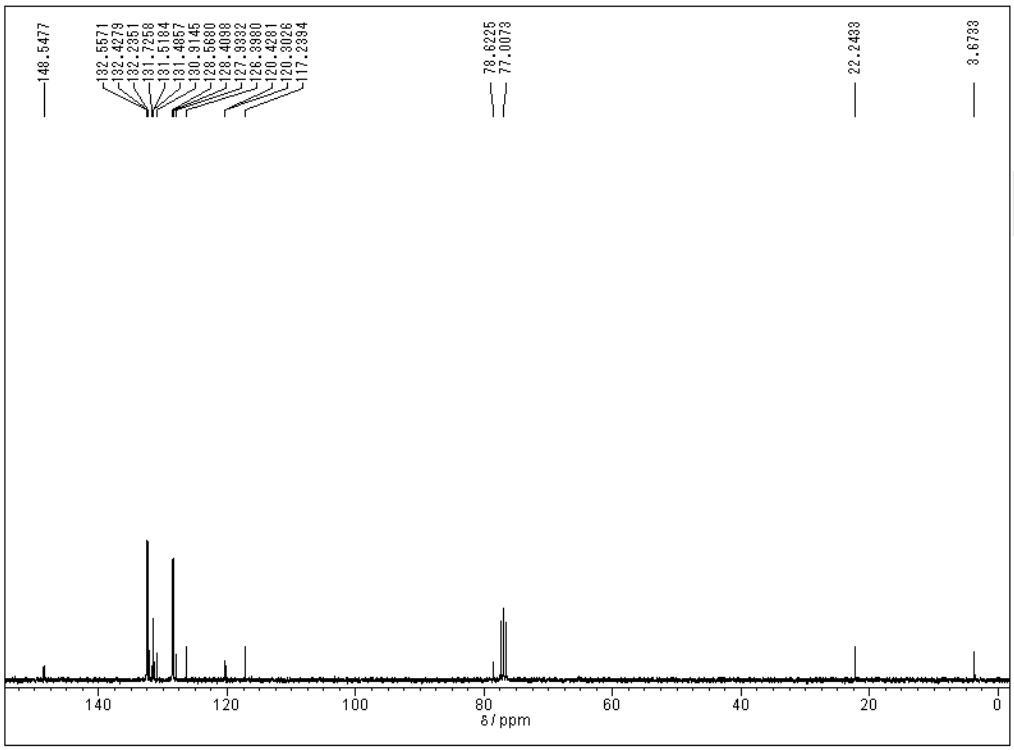
ObsNuc ¹³C
ObsFreq 125.65 MHz
Solvent CDCL₃

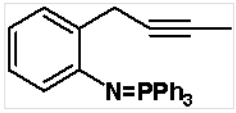
12b





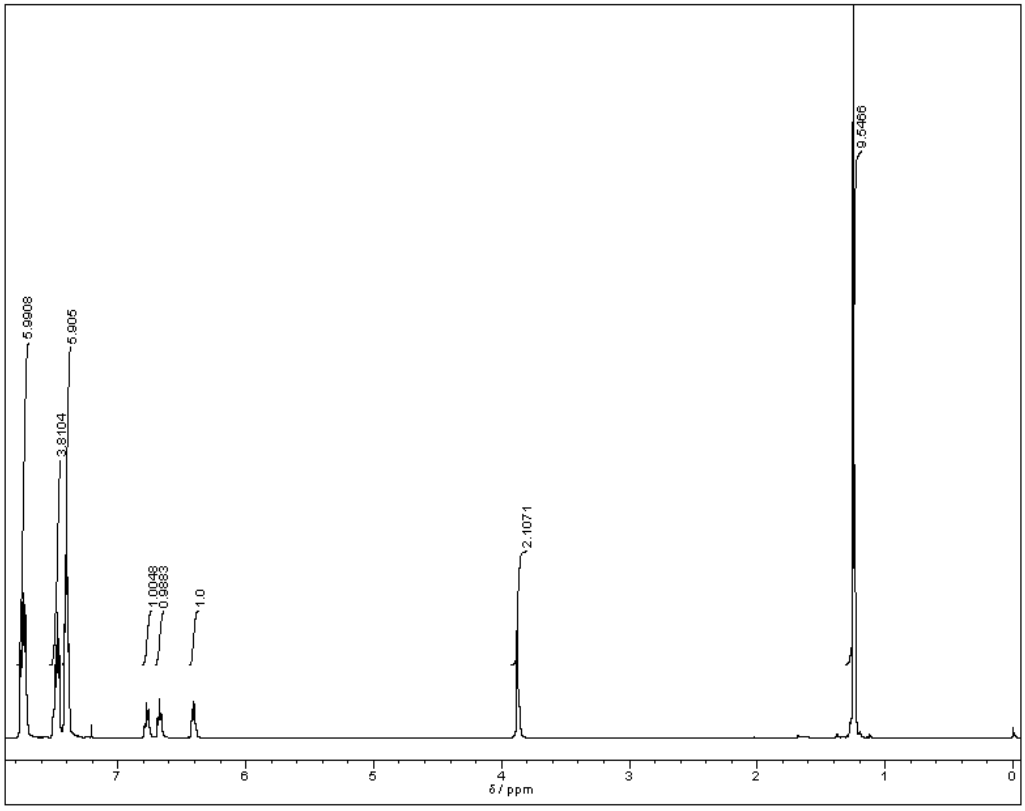
ObsNuc ¹H
ObsFreq 300.01 MHz
Solvent CDCL₃

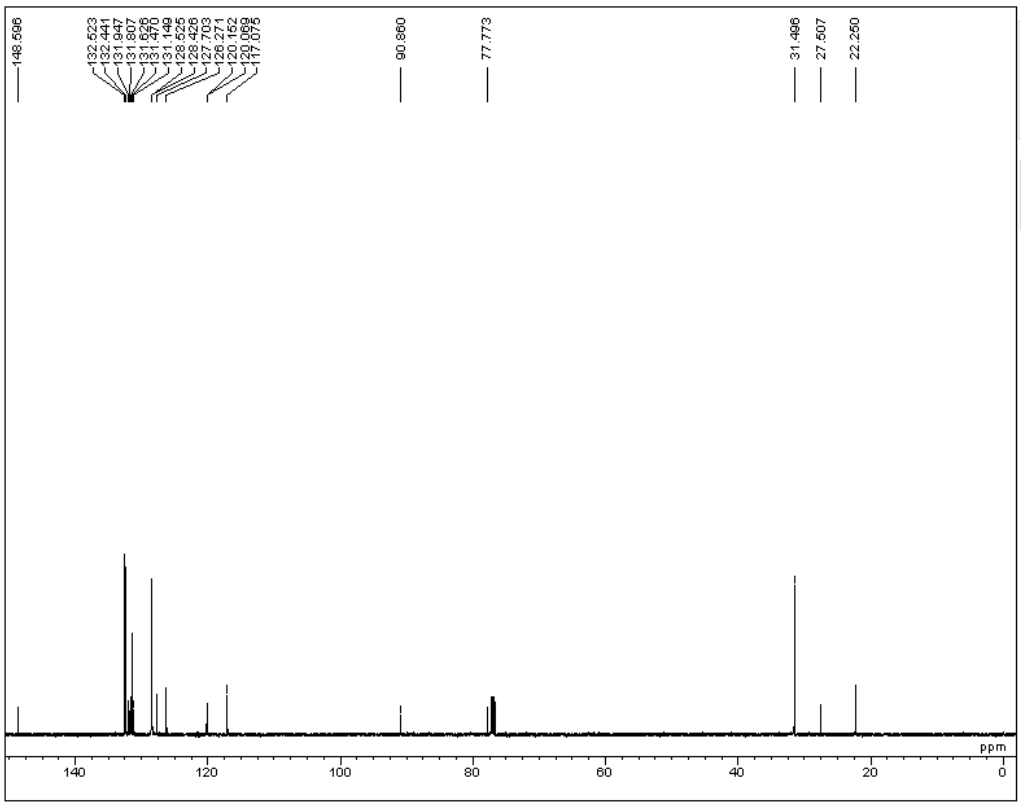




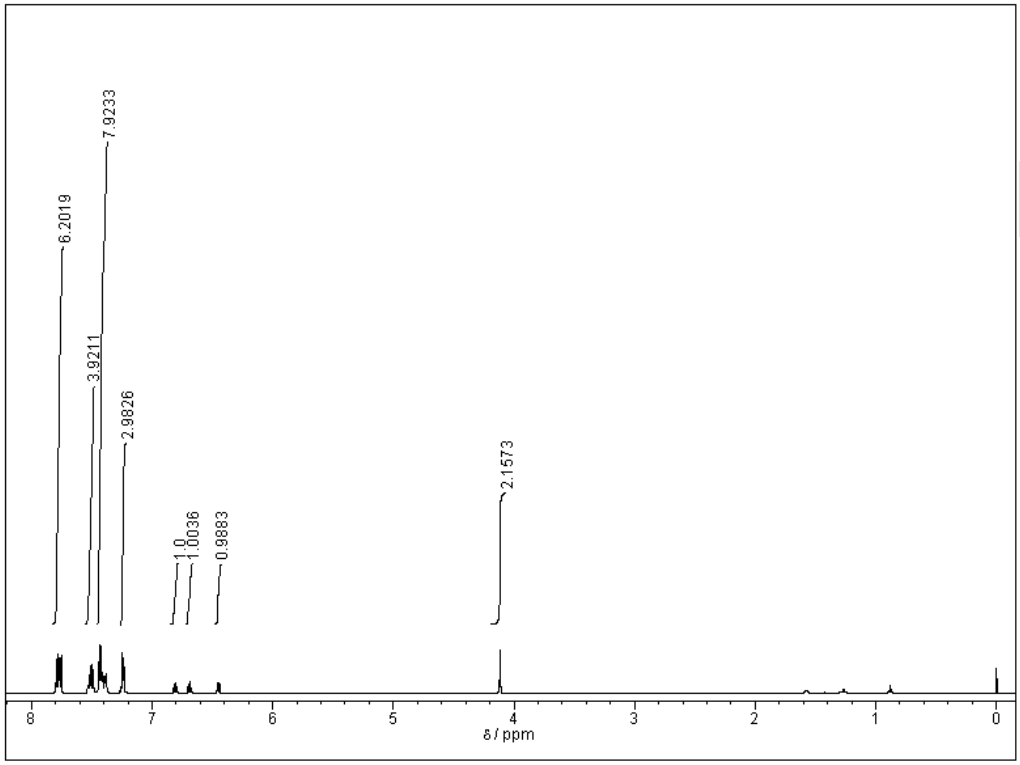
ObsNuc ¹³C
ObsFreq 75.44 MHz
Solvent CDCL₃

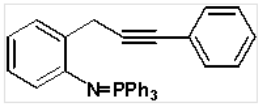
12c


5.9908
5.905
3.8104
1.0048
0.9883
1.0
2.1071
9.5466
δ / ppm
N=PPh3
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

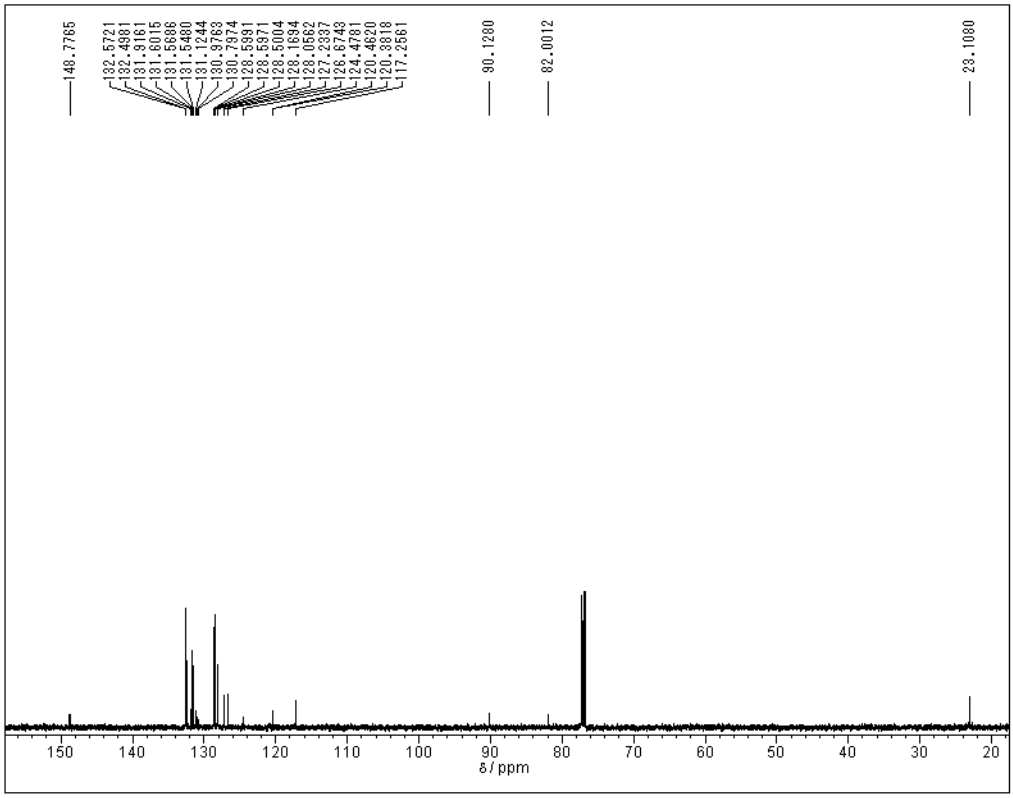

148.596
132.523
132.441
131.947
131.807
131.626
131.470
131.149
128.525
128.426
127.703
126.271
120.152
120.069
117.075
90.860
77.773
31.496
27.507
22.250
ppm
N=PPh3
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

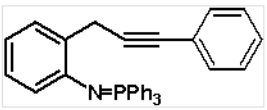
12d





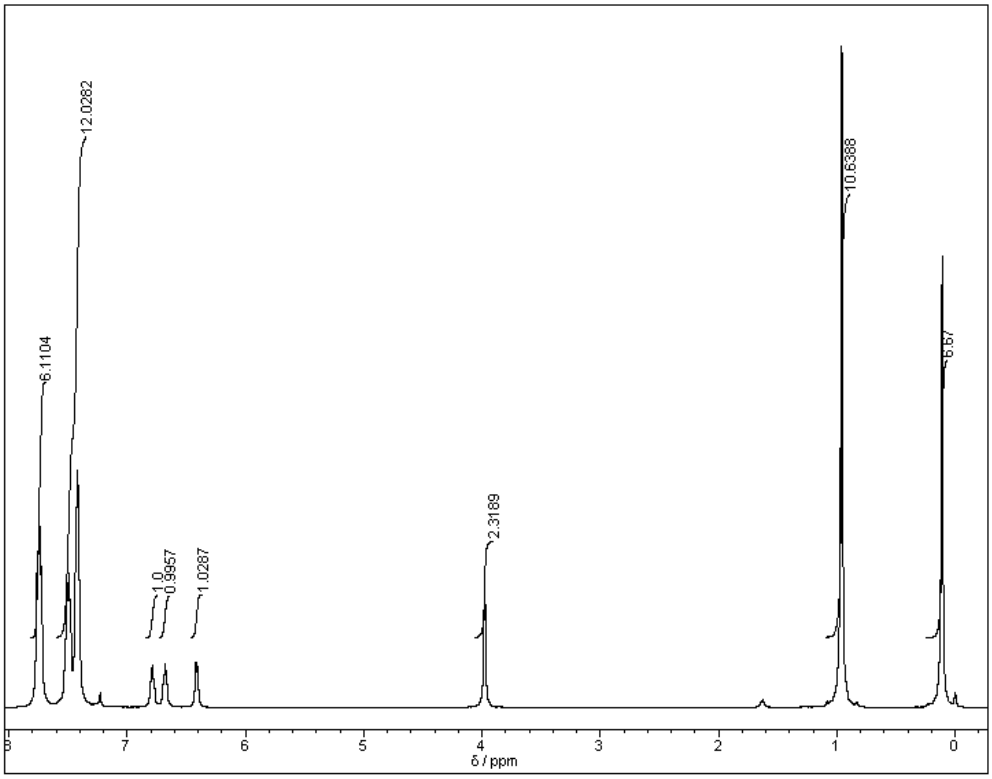
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

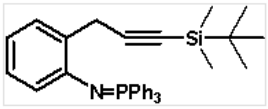




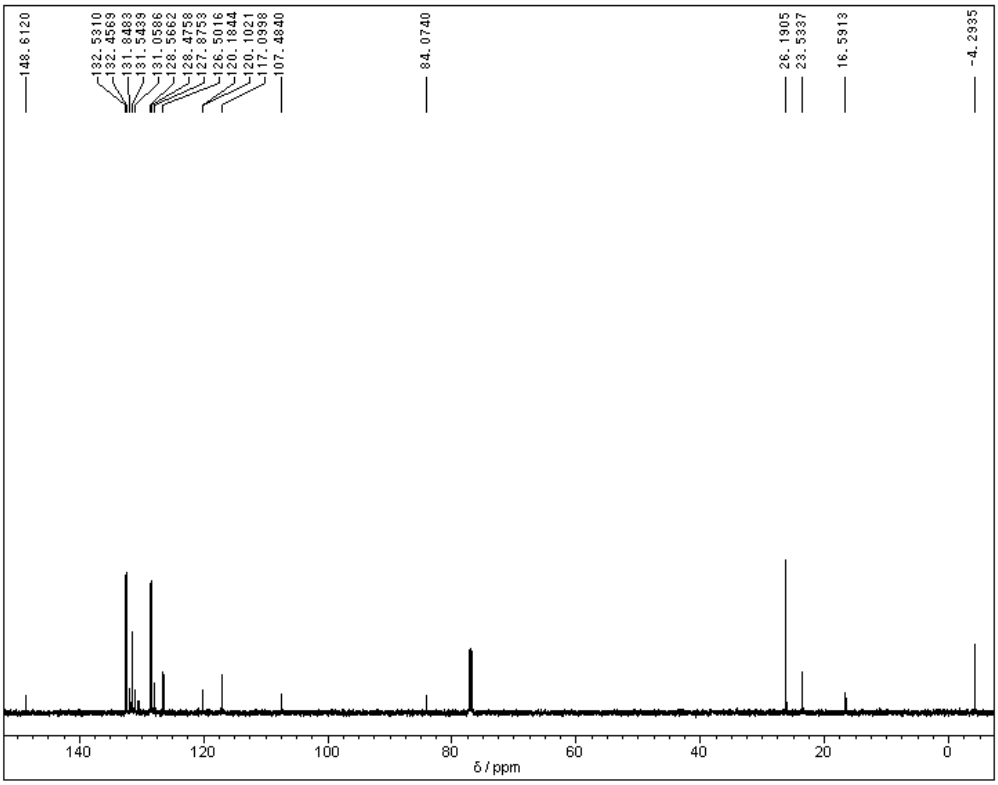
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

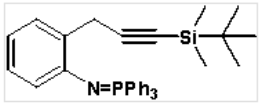
12e





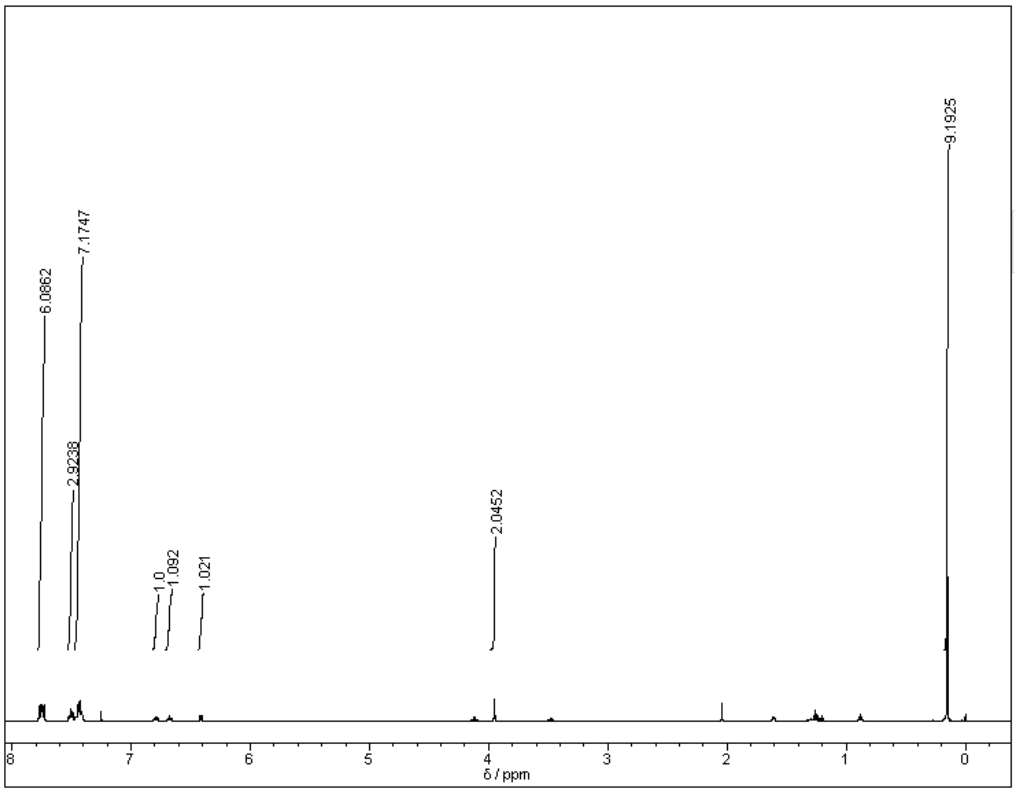
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCL_3$

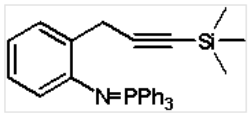




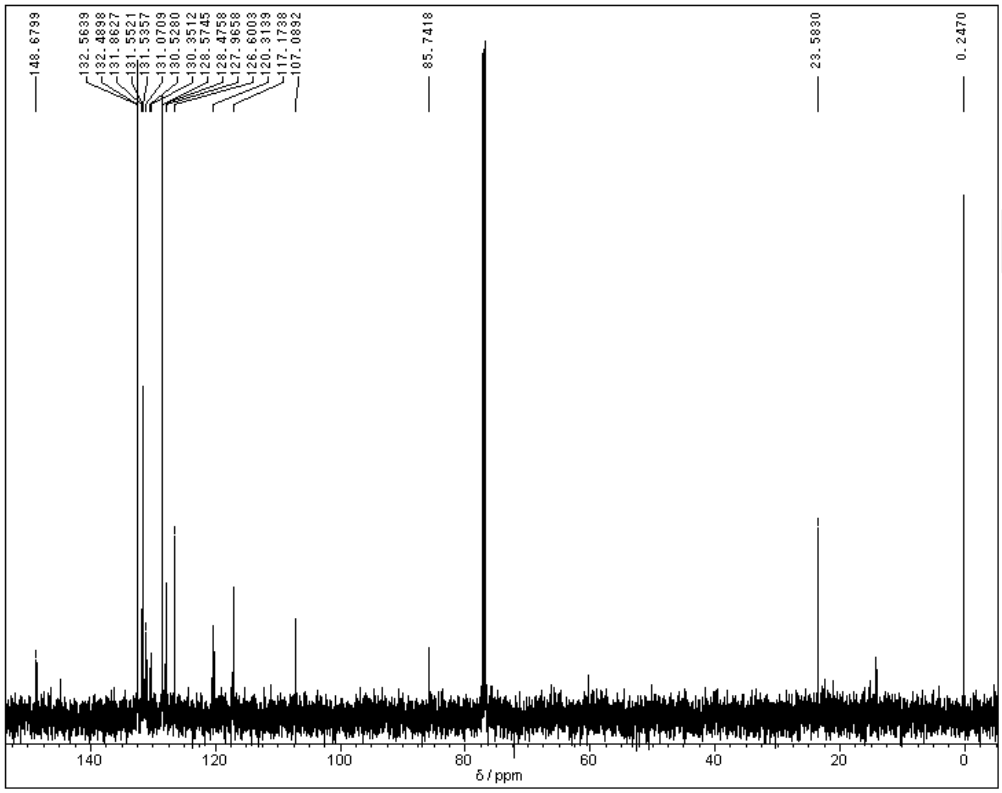
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCL_3$

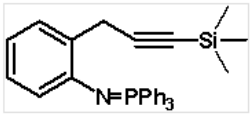
12f





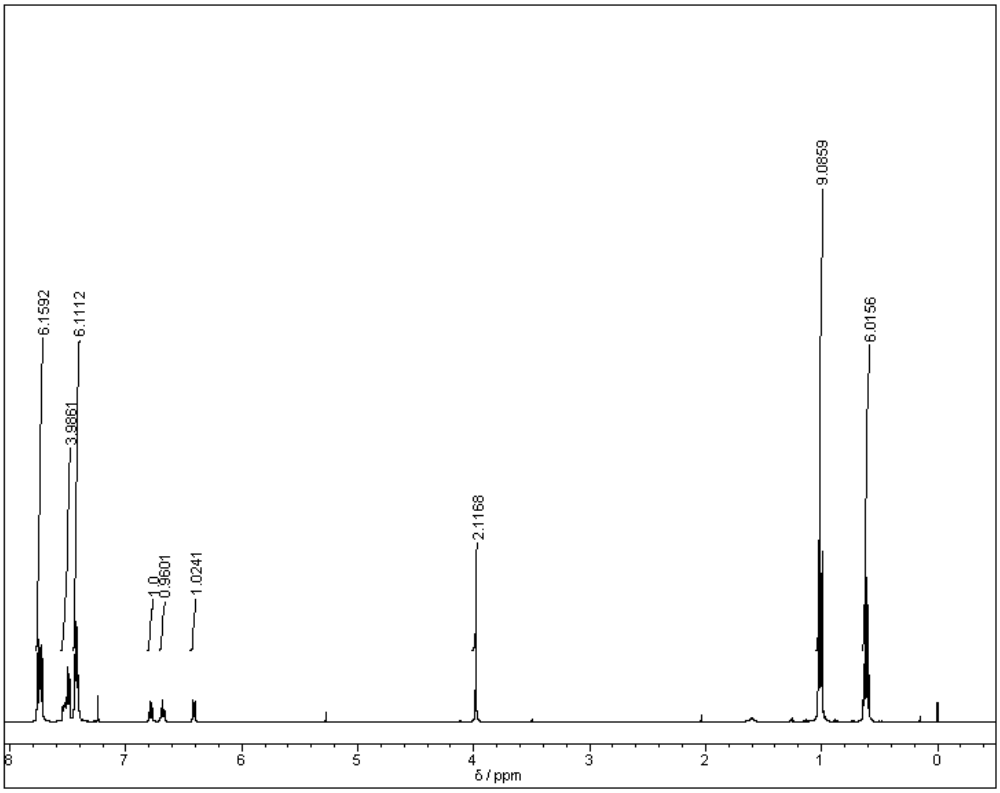
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

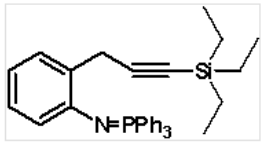




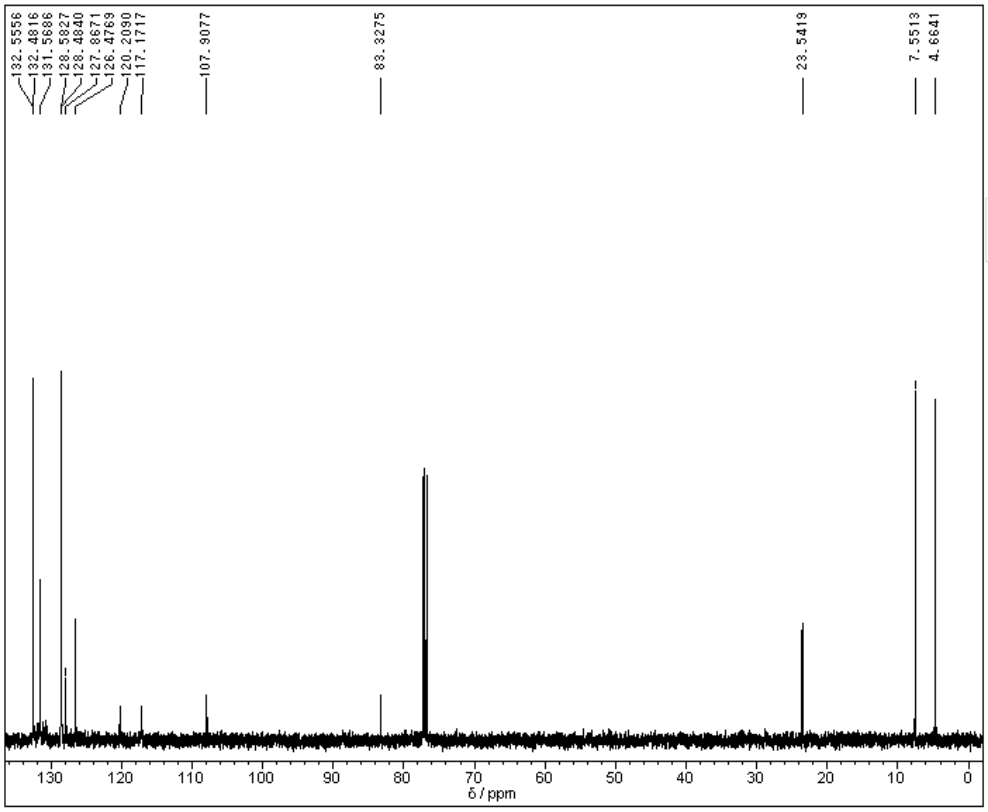
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

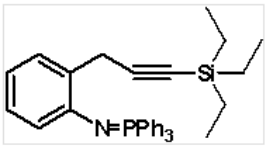
12g





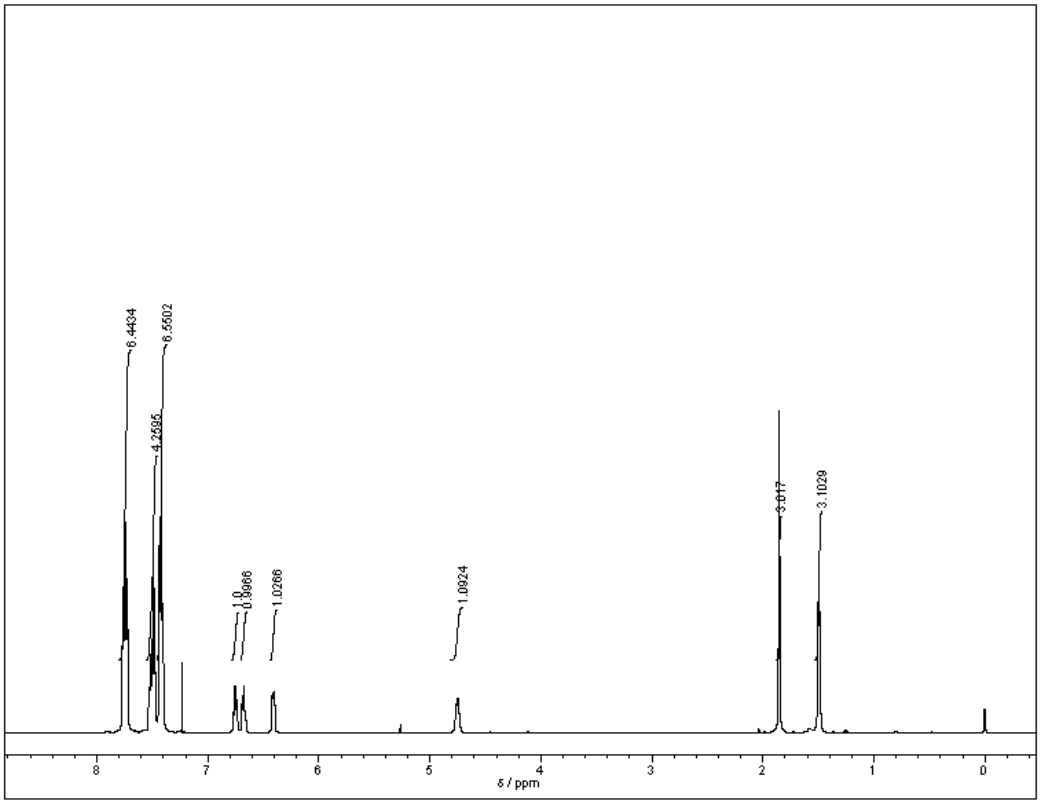
ObsNuc	1H
ObsFreq	500.0 MHz
Solvent	$CDCL_3$

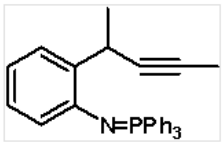




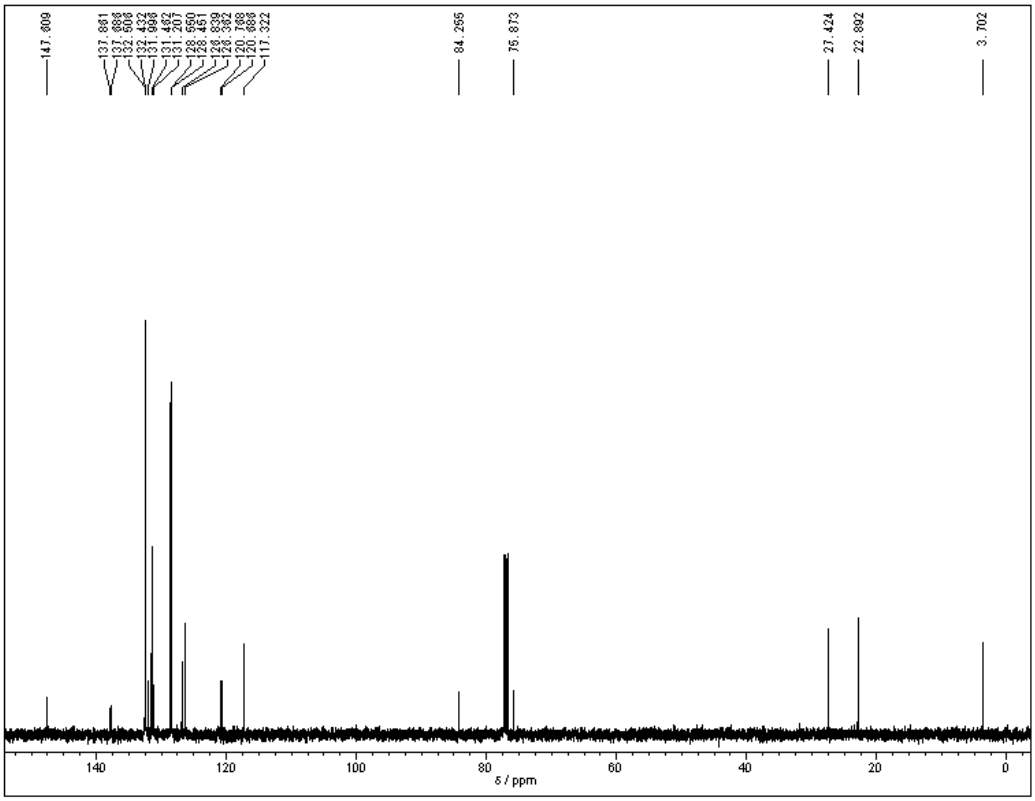
ObsNuc	13C
ObsFreq	125.65 MHz
Solvent	$CDCL_3$

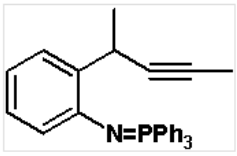
13a





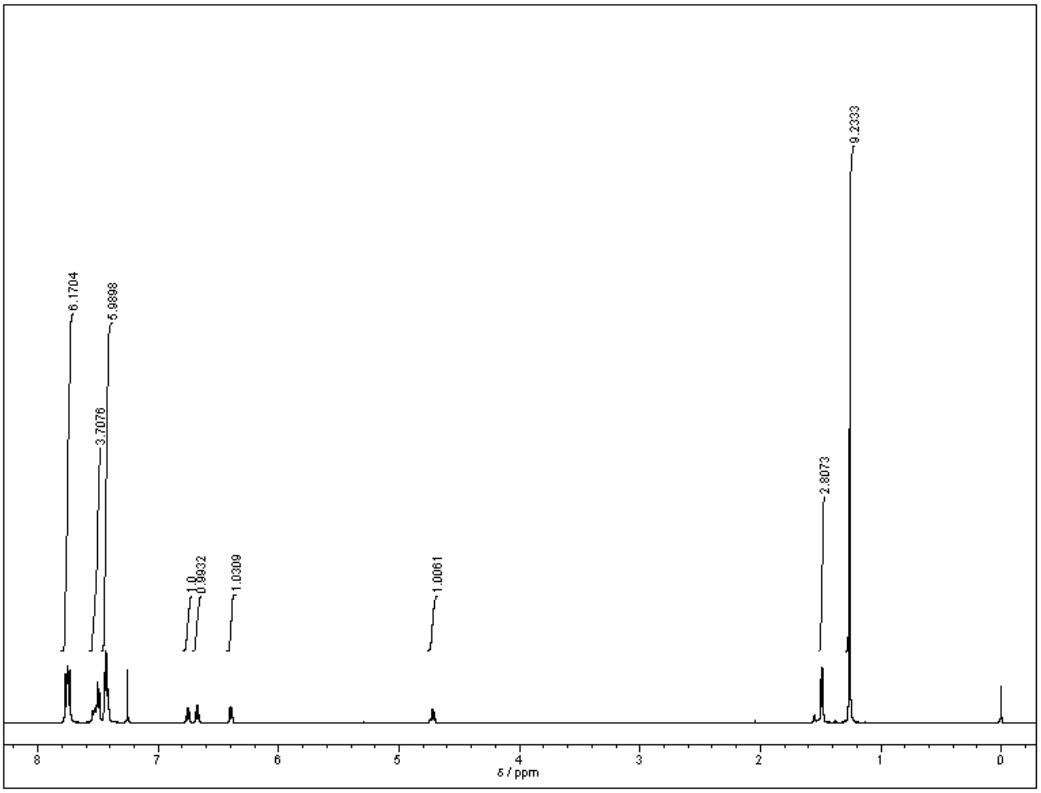
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

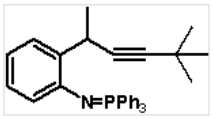




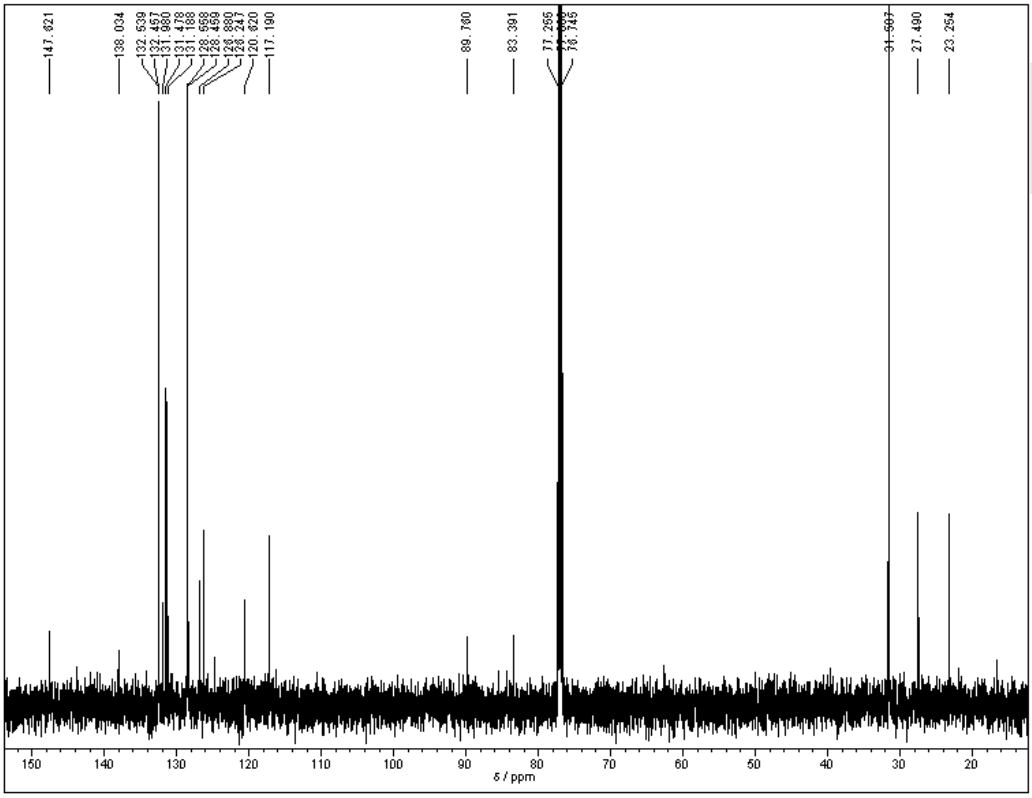
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

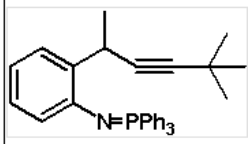
13b





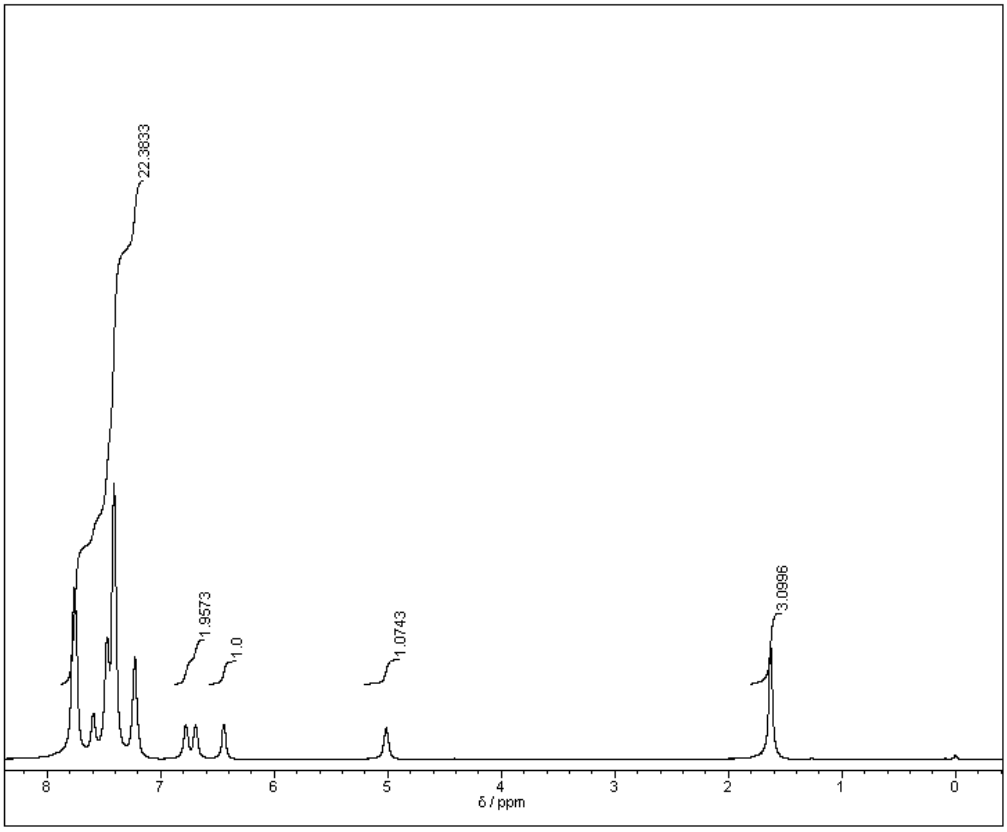
Obs Nuc ^{1}H
Obs Freq 500.0 MHz
Solvent $CDCl_3$

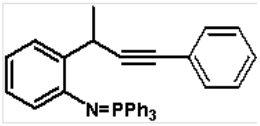




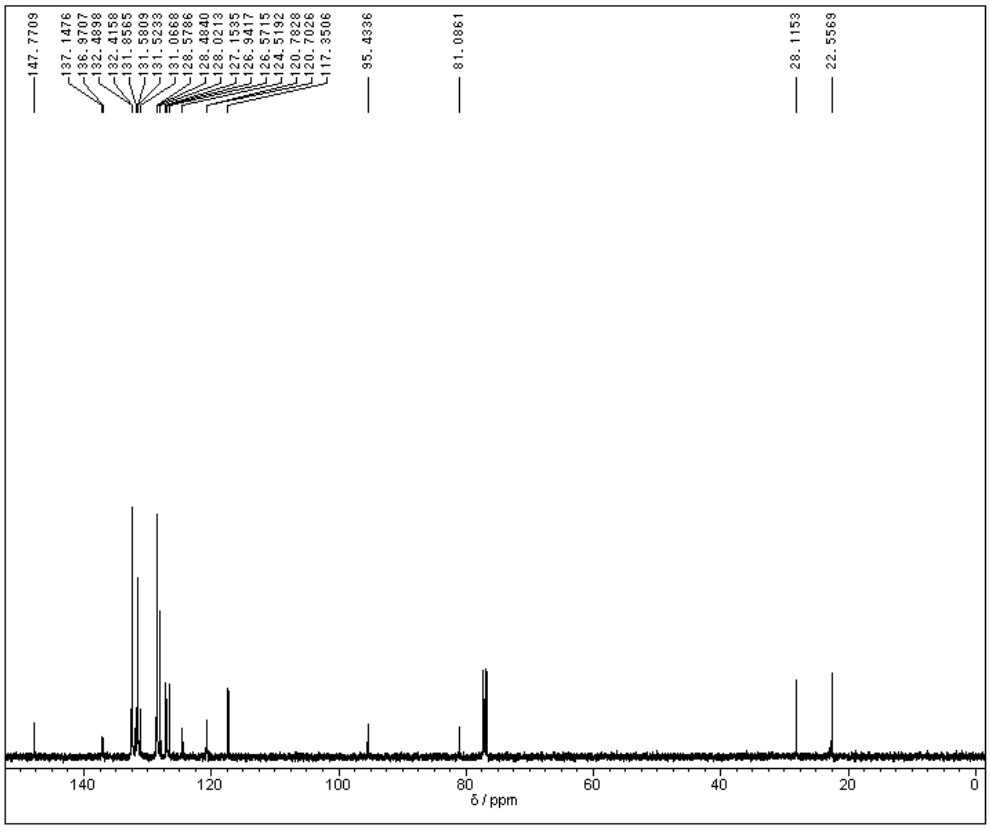
Obs Nuc ^{13}C
Obs Freq 125.65 MHz
Solvent $CDCl_3$

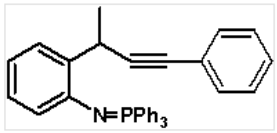
13c





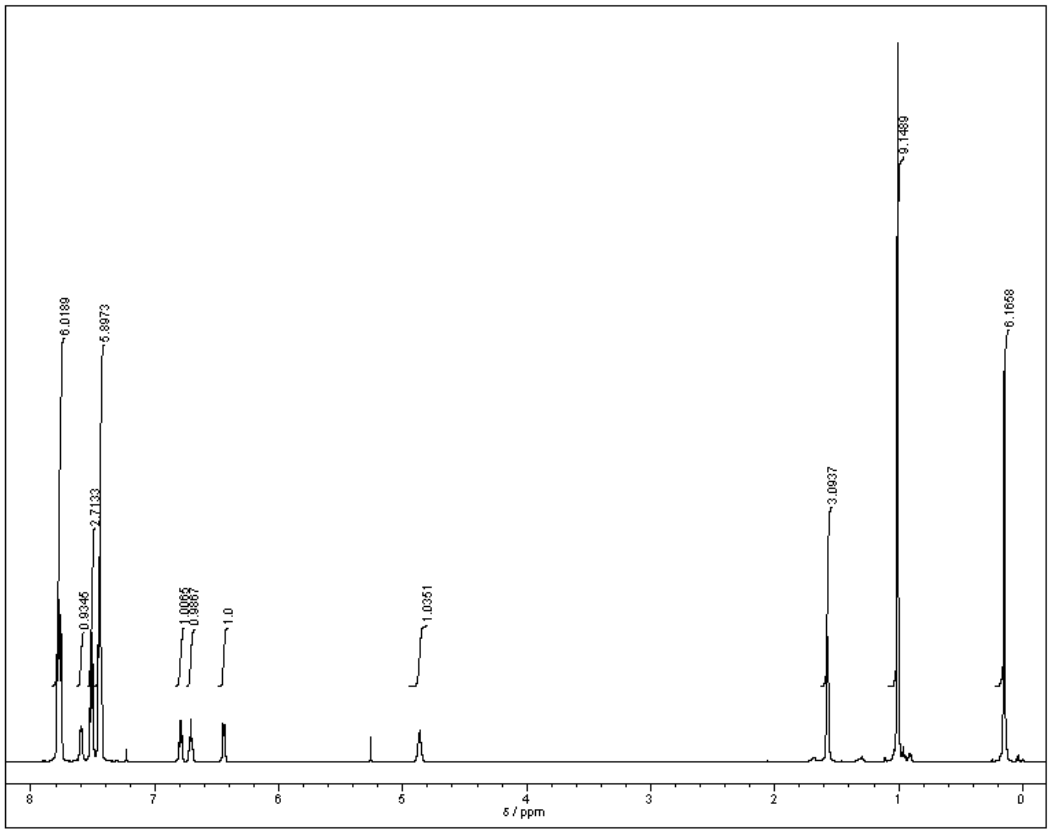
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

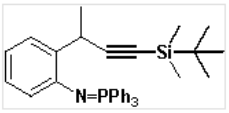




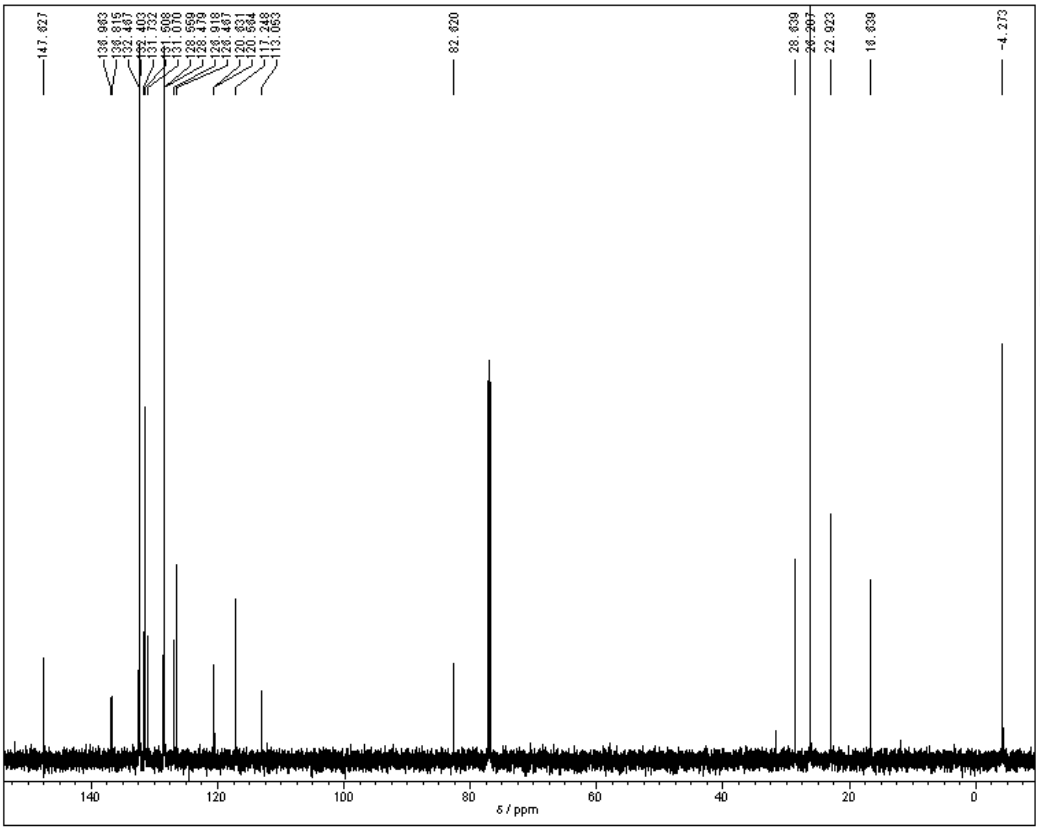
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

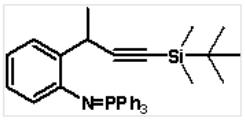
13d





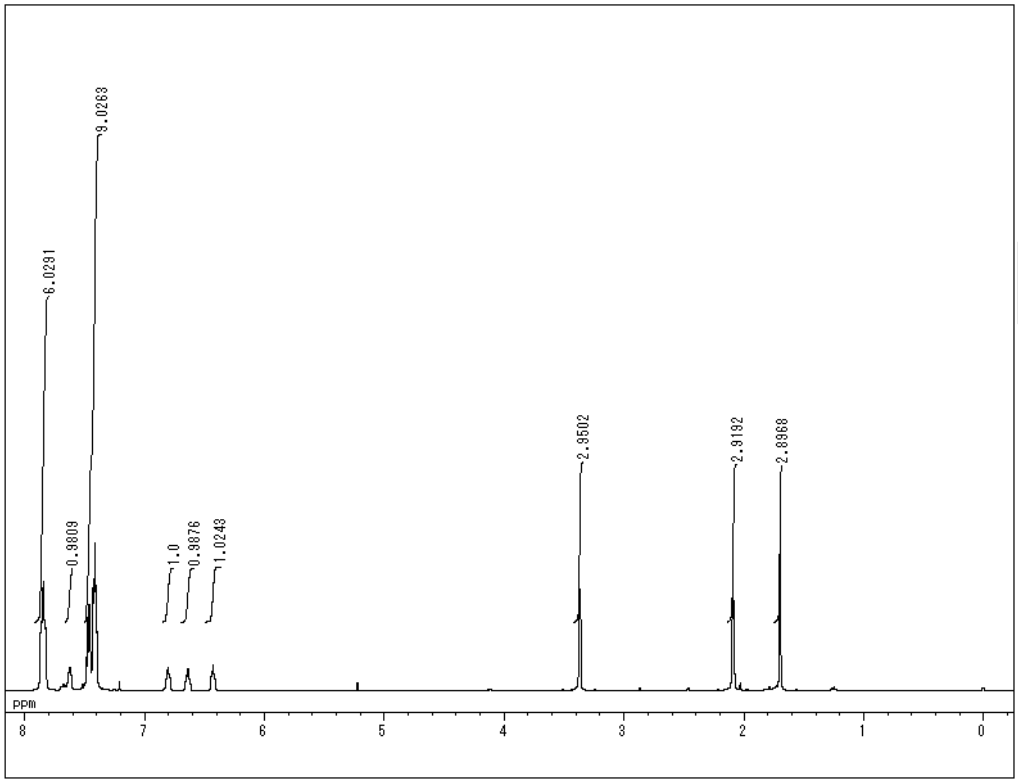
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCL^{3}$

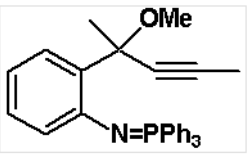




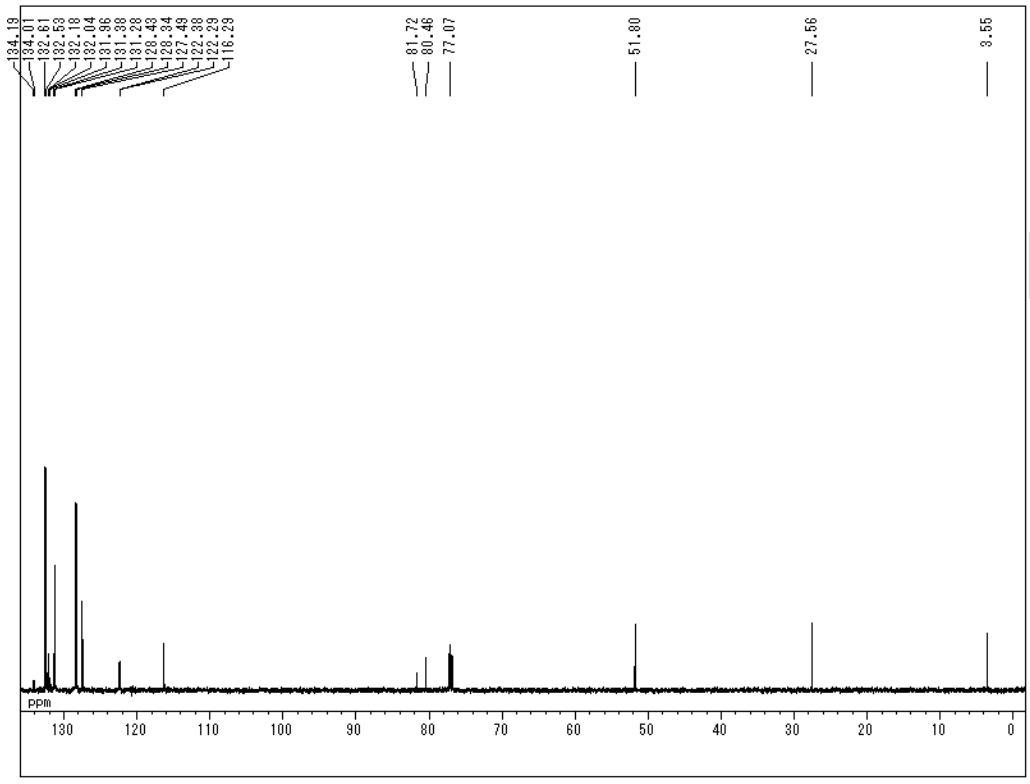
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCL^{3}$

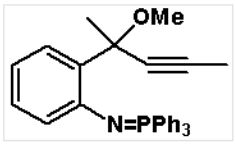
14a





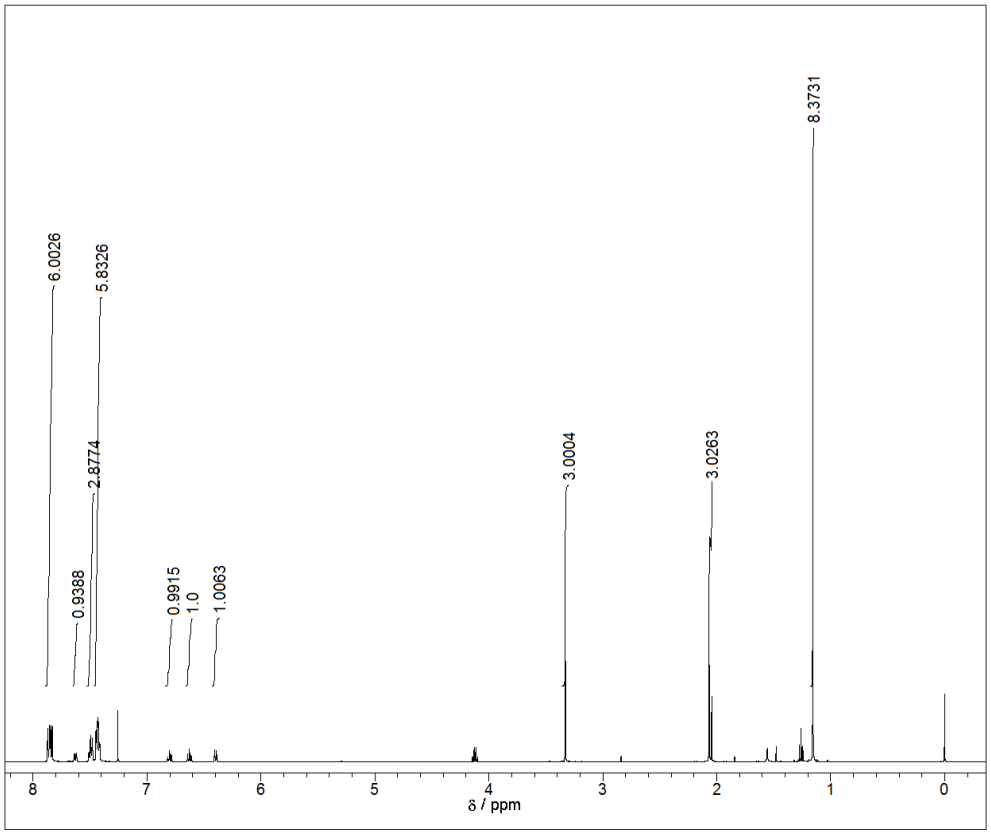
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCL_3$

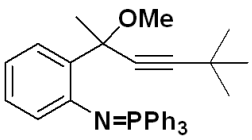




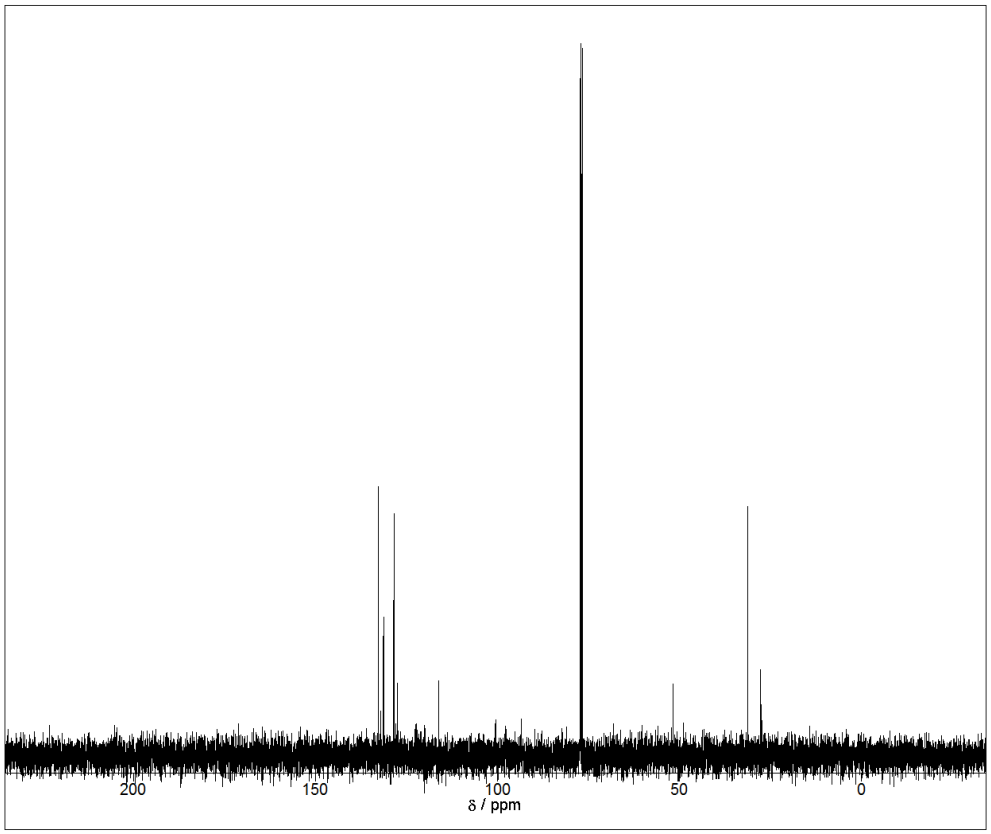
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCL_3$

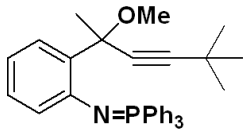
14b





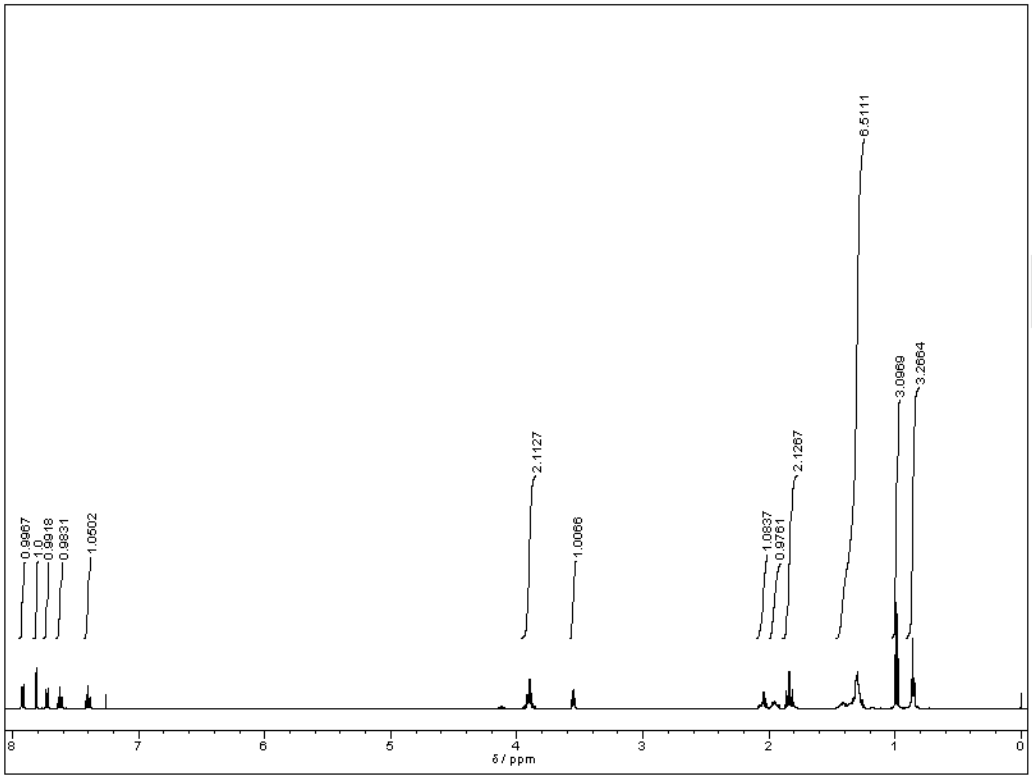
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCL_3$

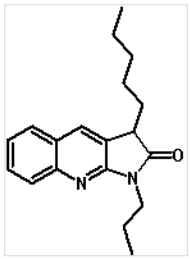




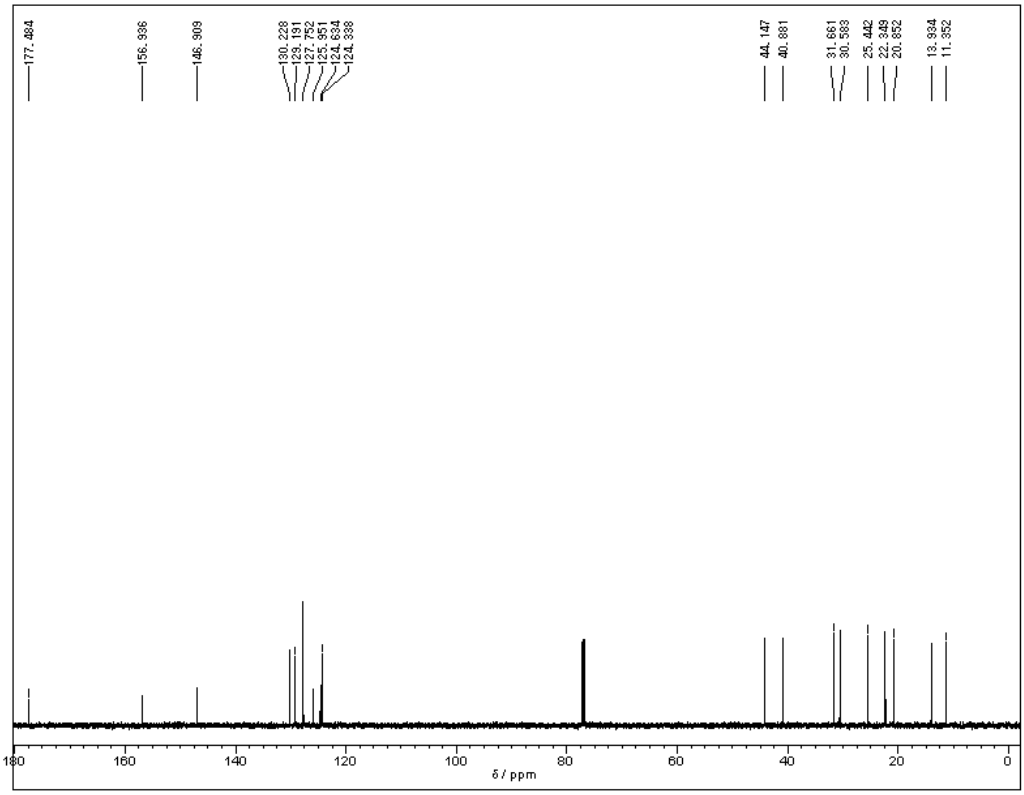
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCL_3$

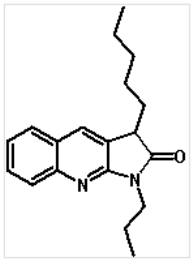
15a





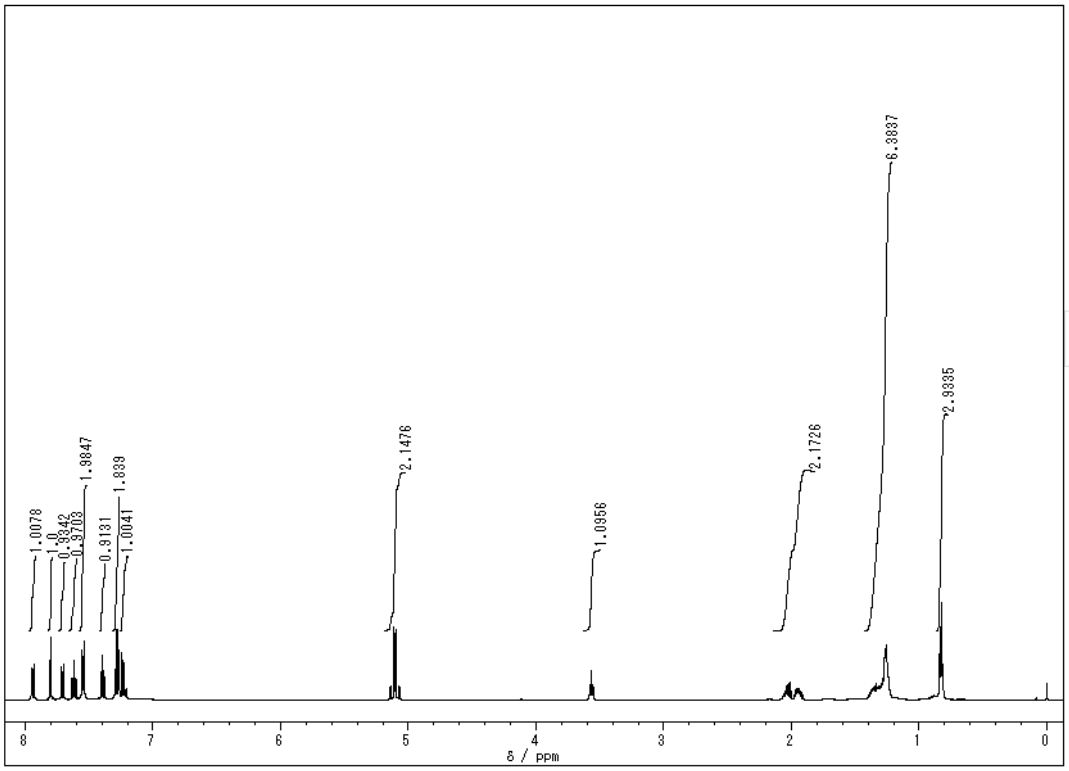
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

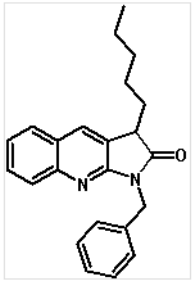




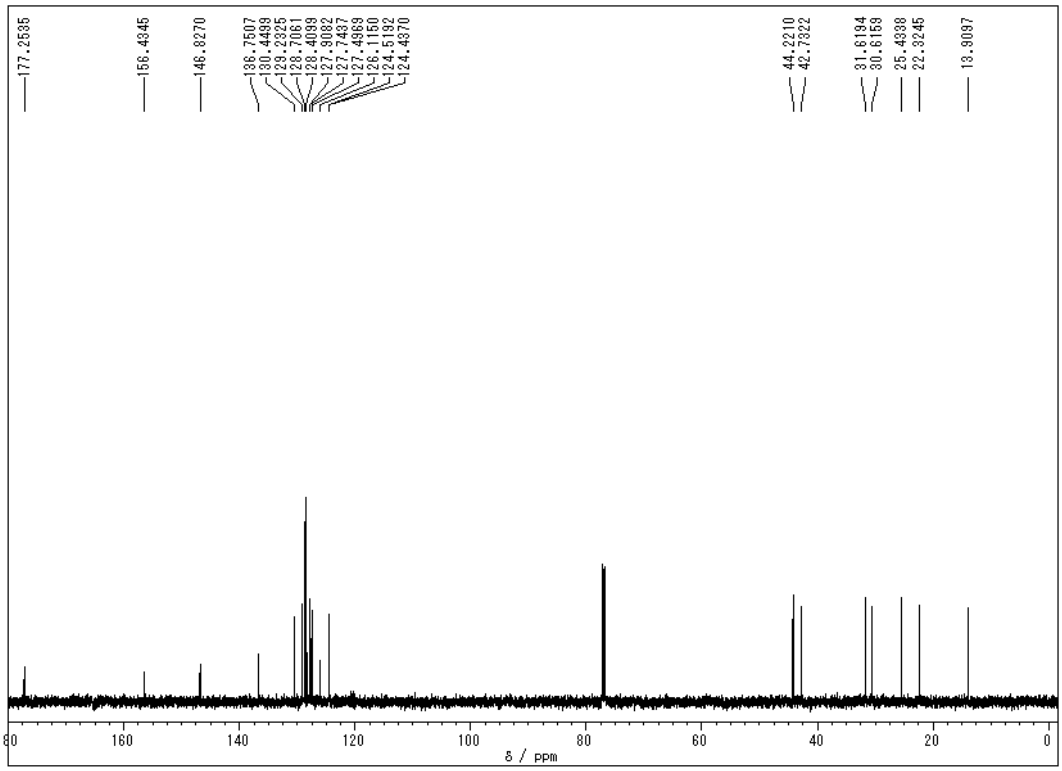
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

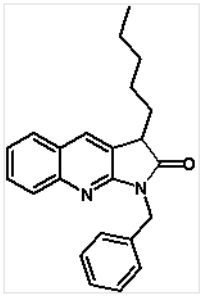
15b





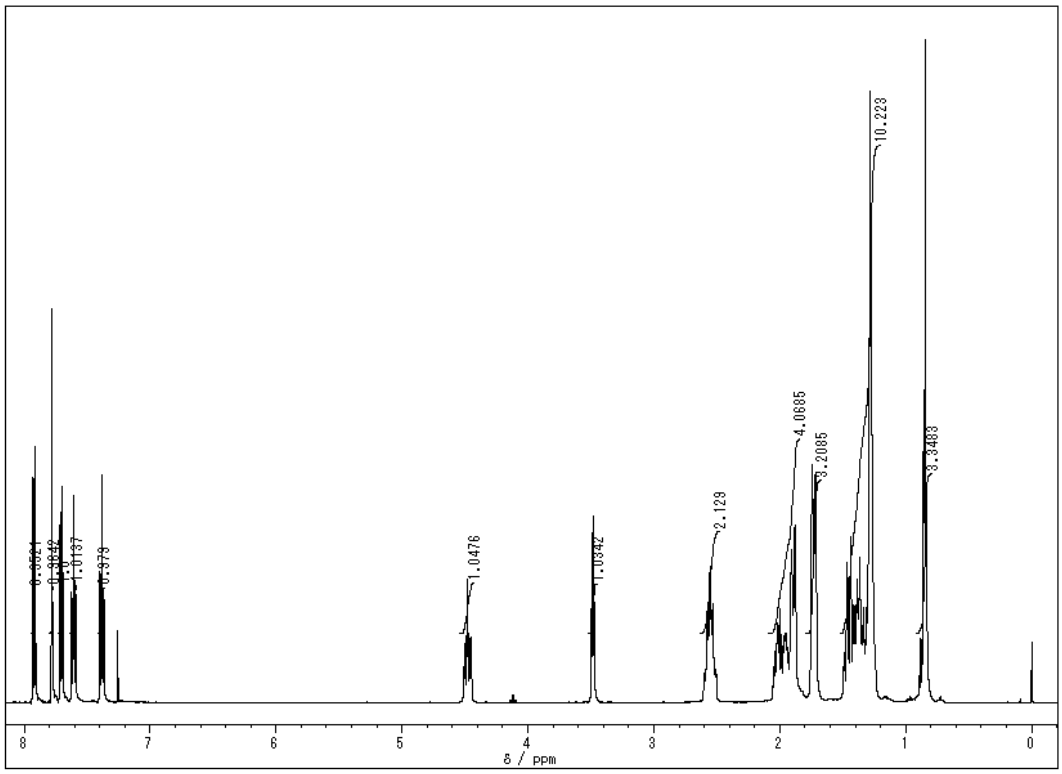
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

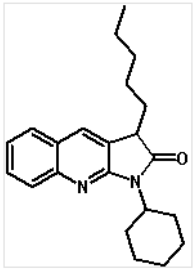




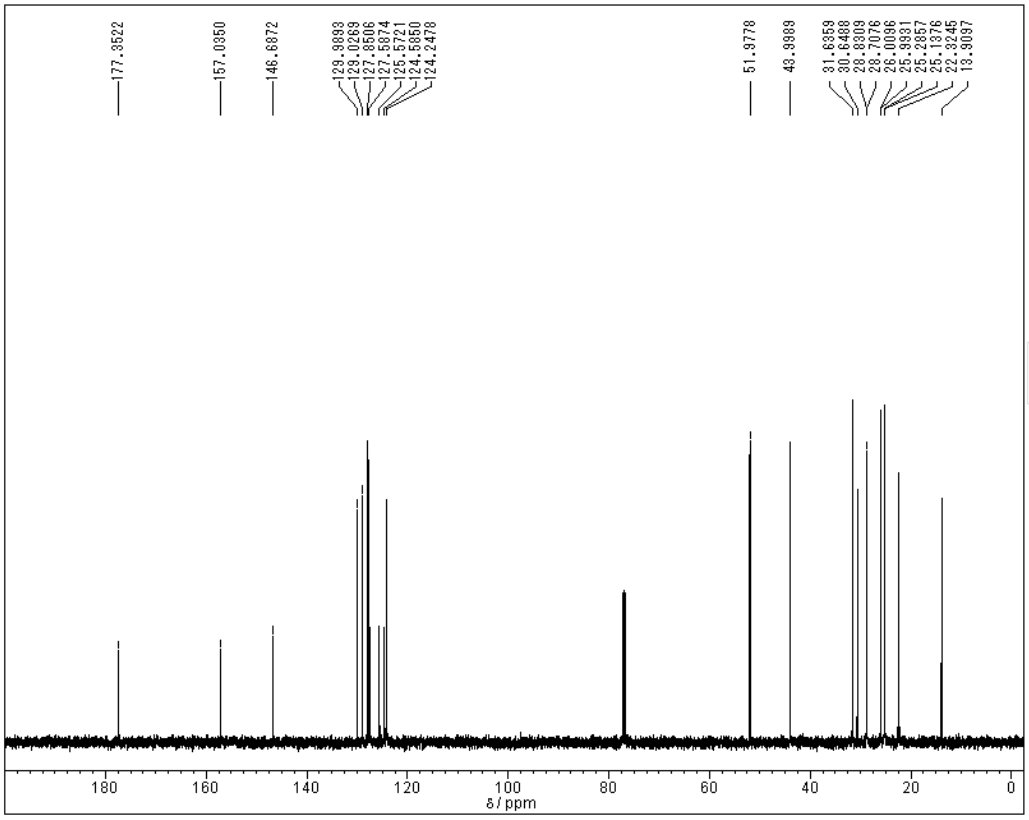
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

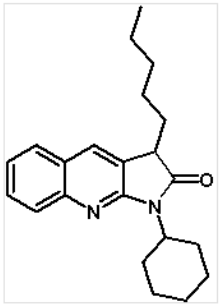
15c





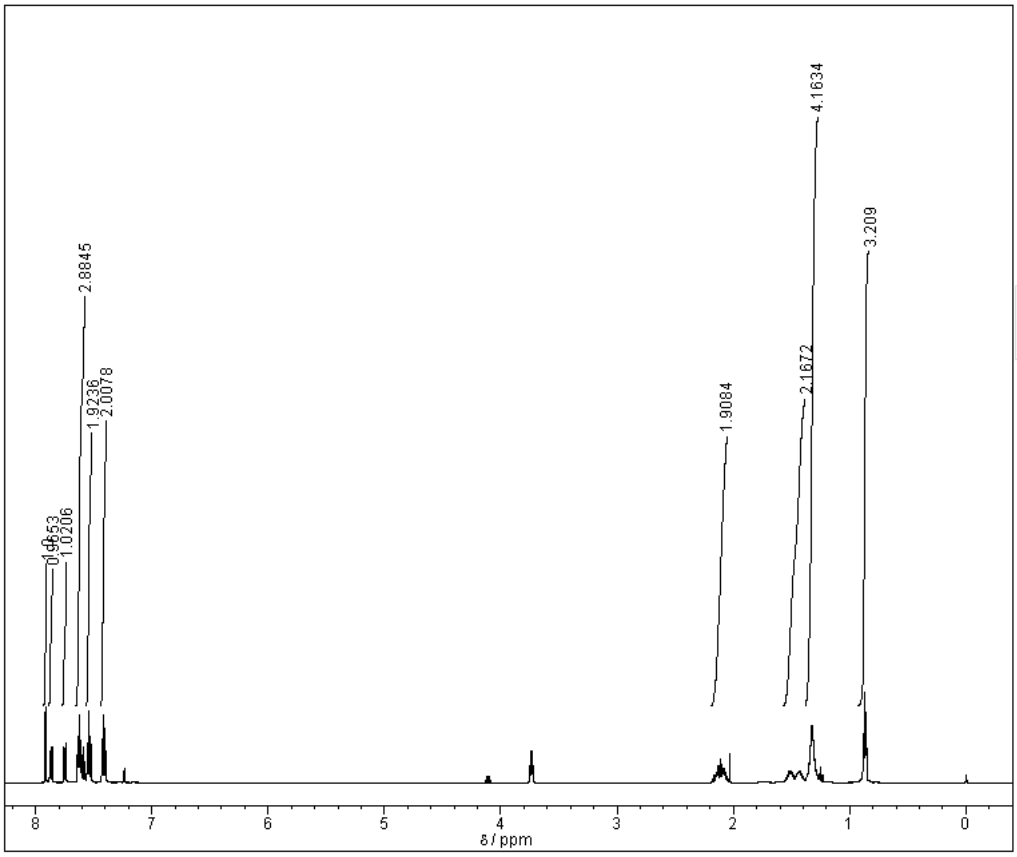
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

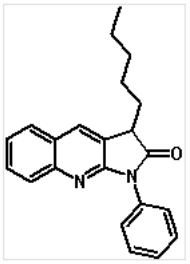




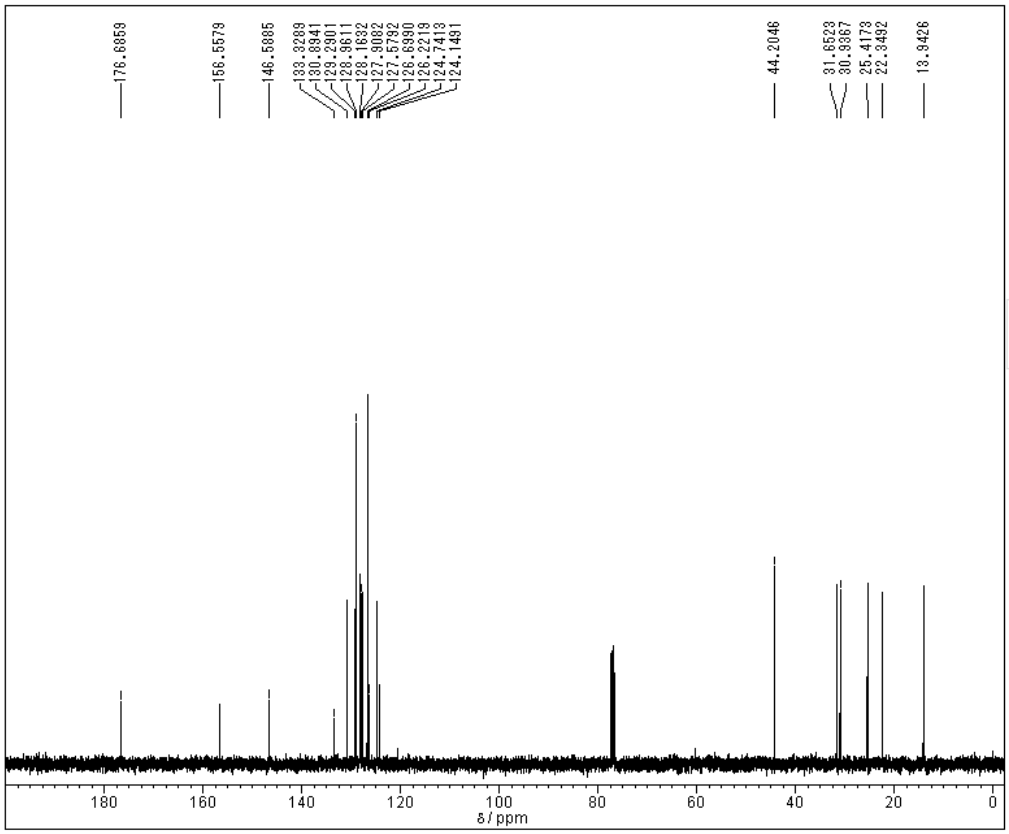
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

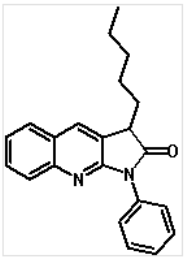
15d





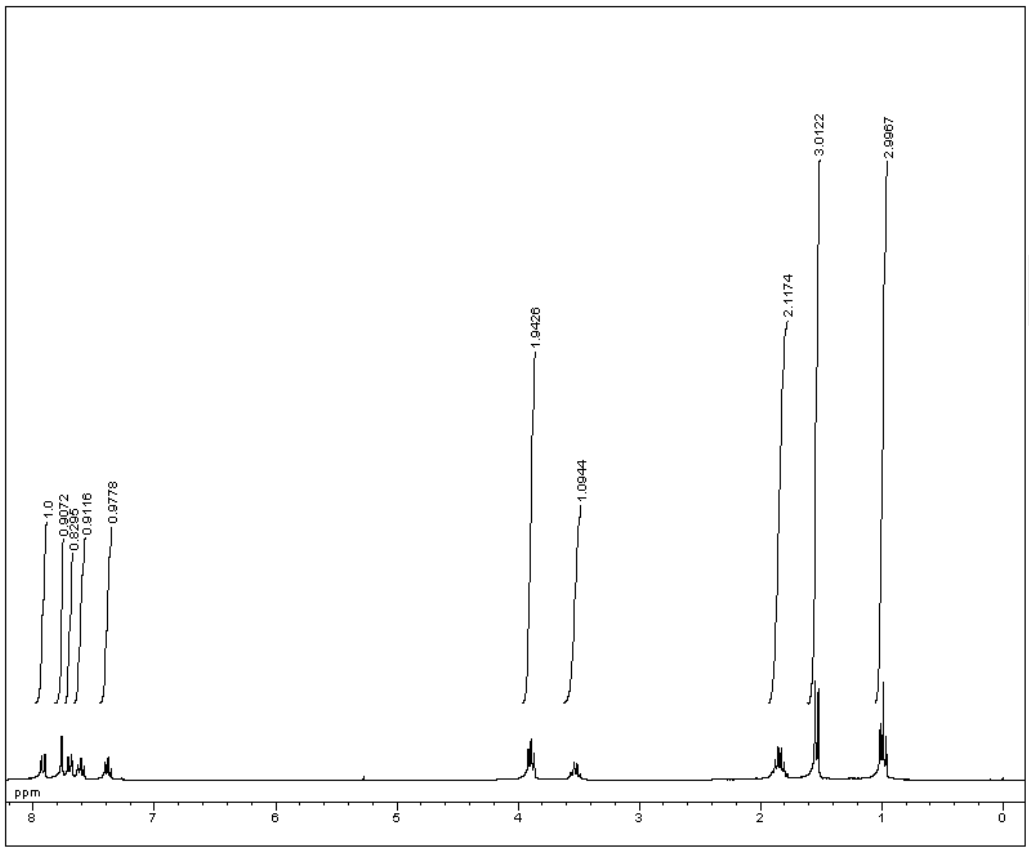
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

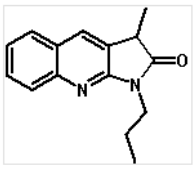




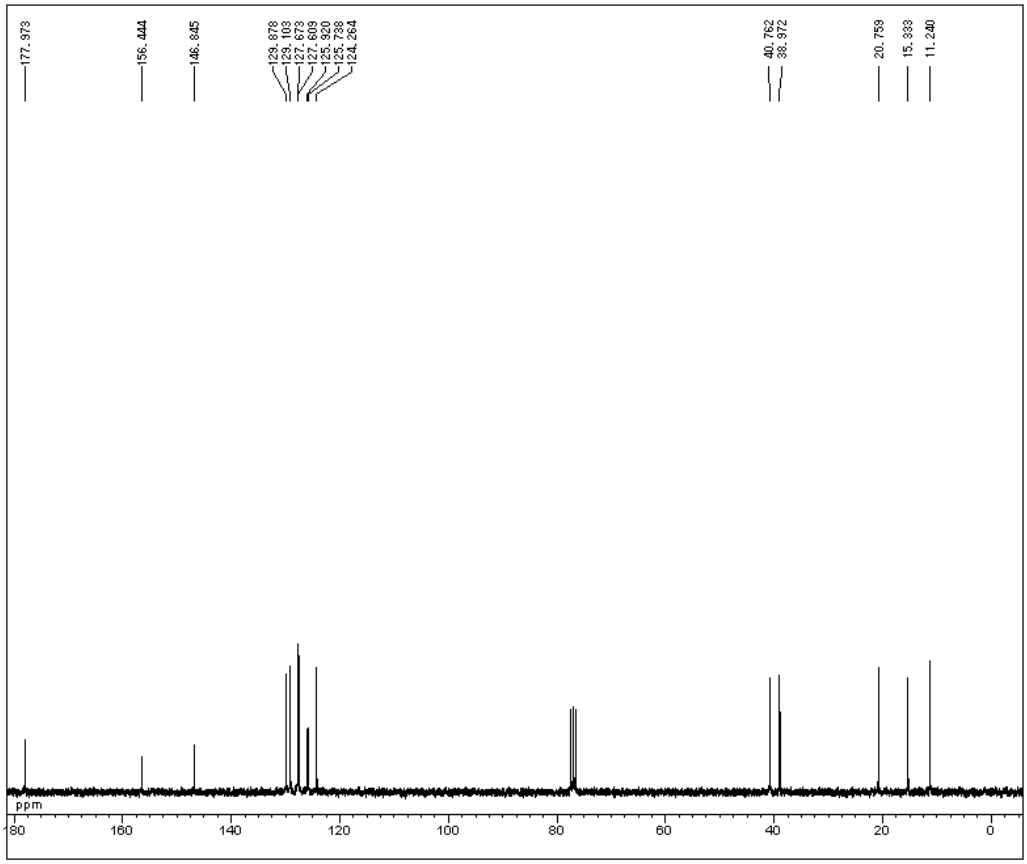
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

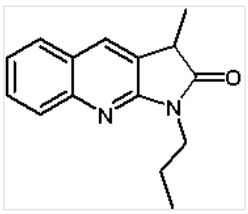
15e





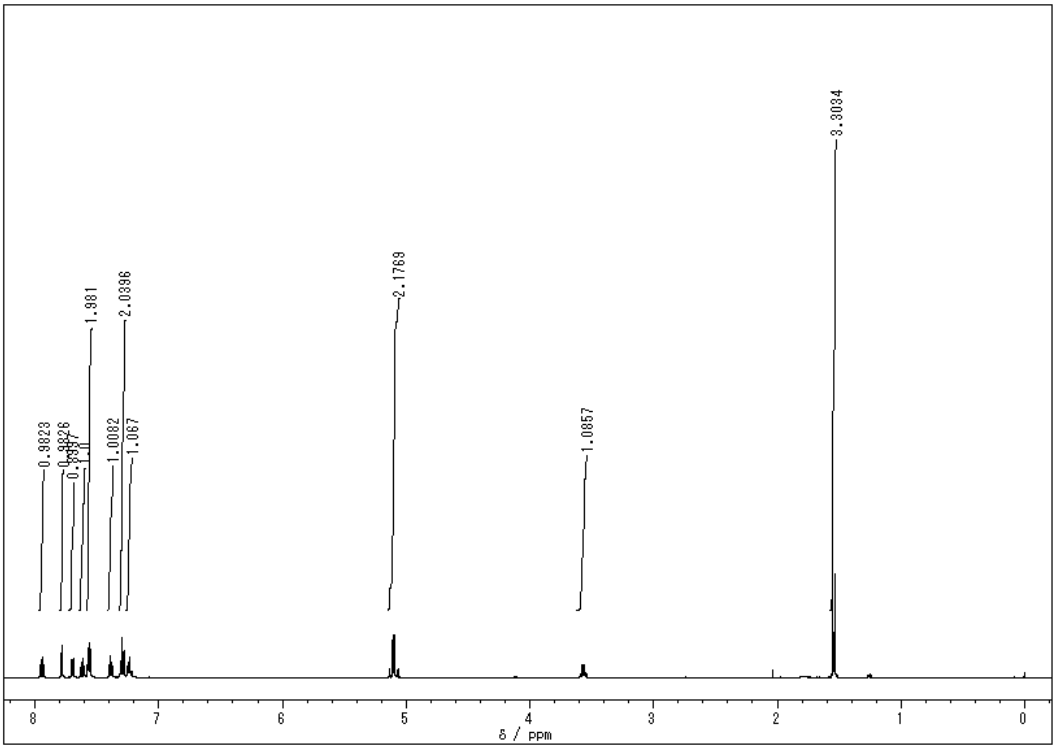
ObsNuc ^{1}H
ObsFreq 300.01 MHz
Solvent $CDCl_3$

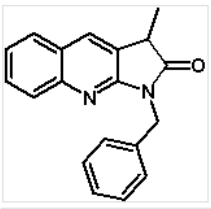




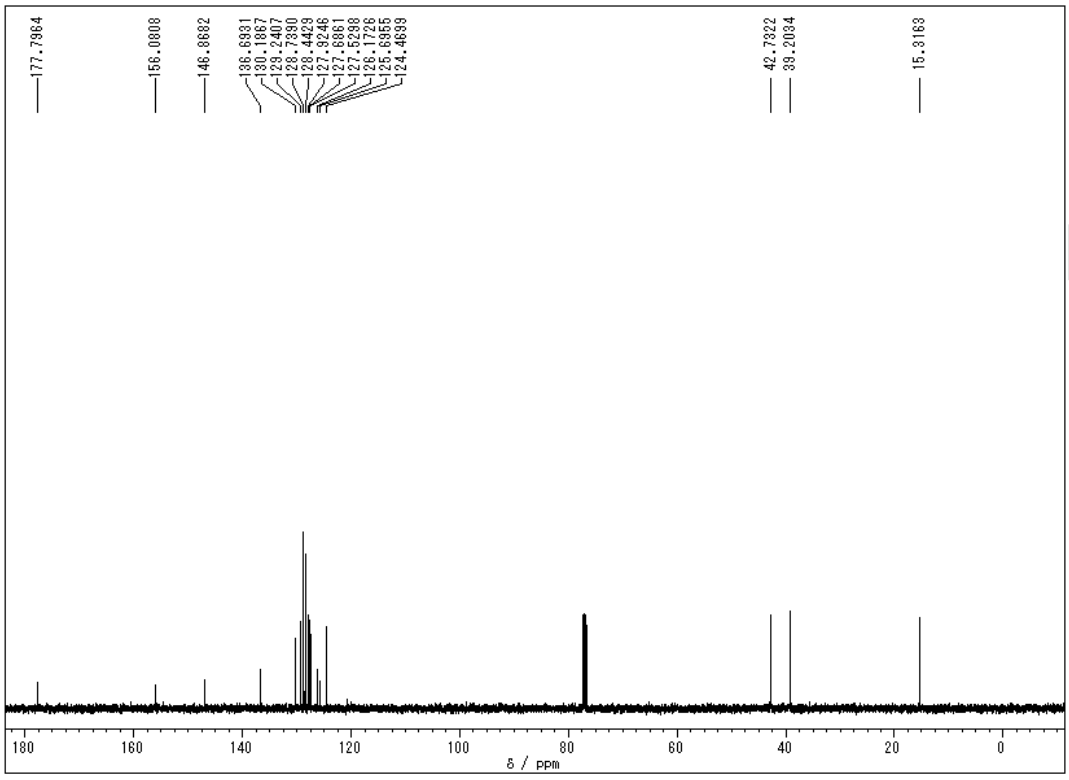
ObsNuc ^{13}C
ObsFreq 75.44 MHz
Solvent $CDCl_3$

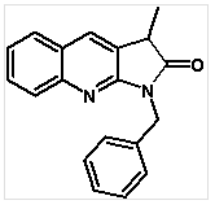
15f





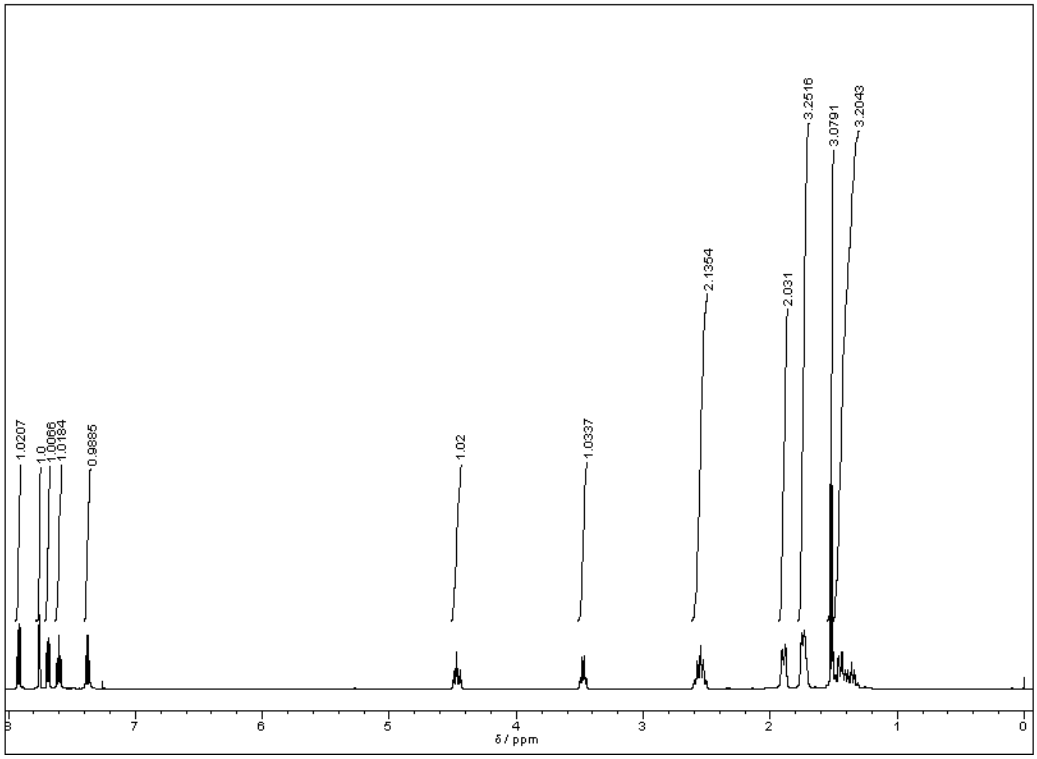
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

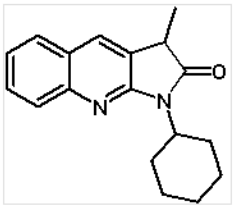




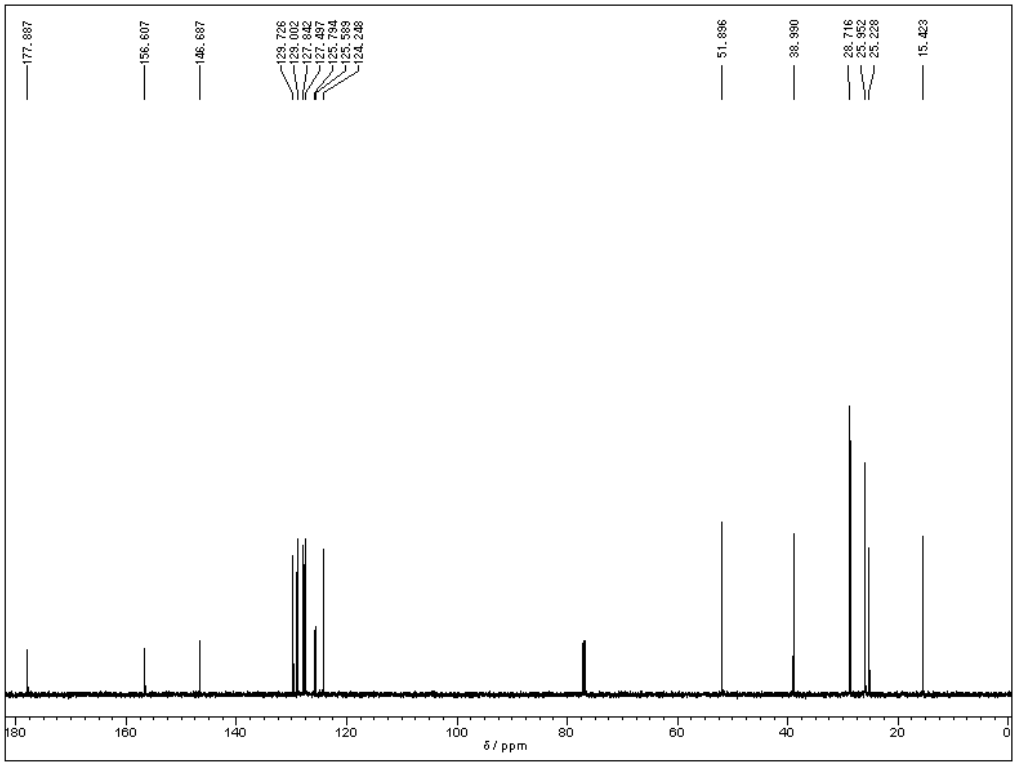
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

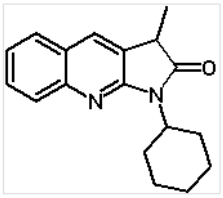
15g





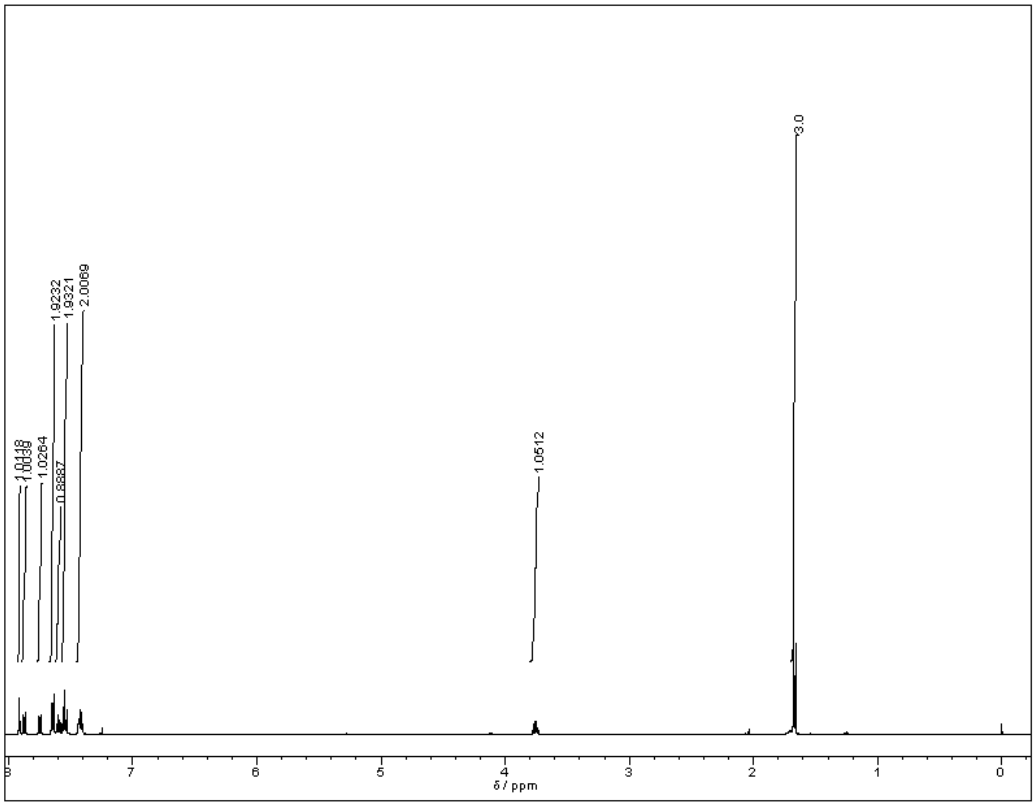
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

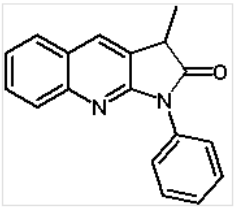




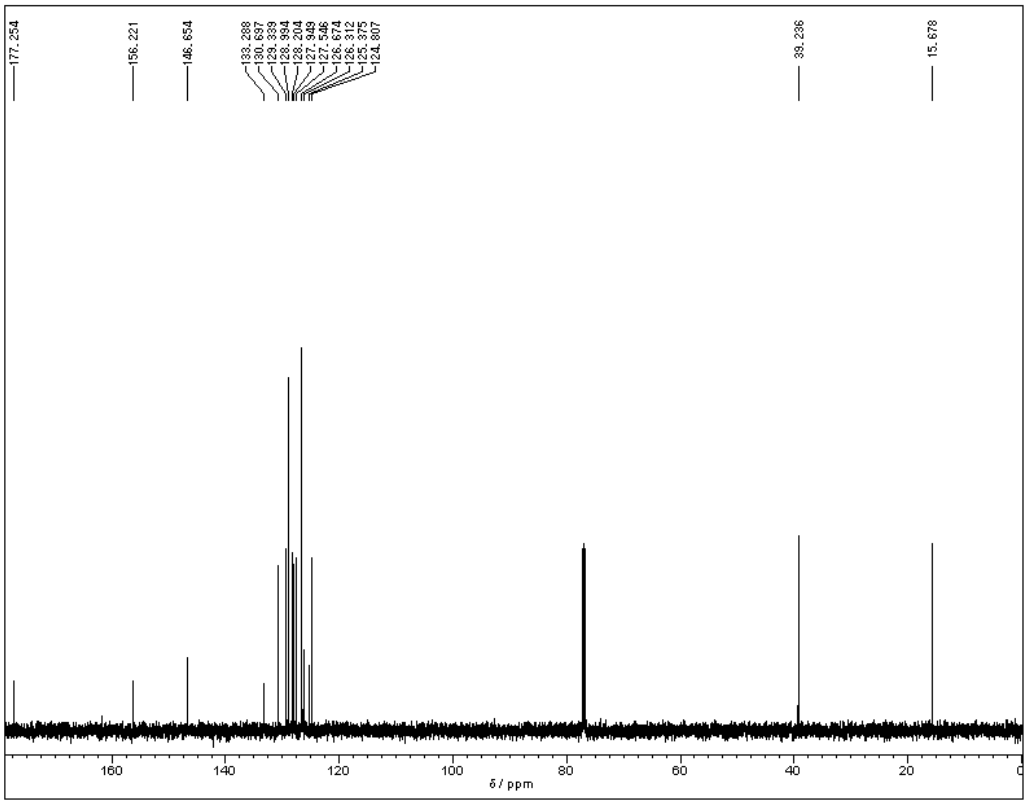
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

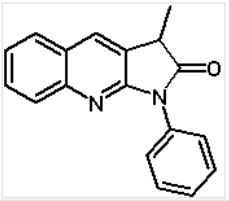
15h





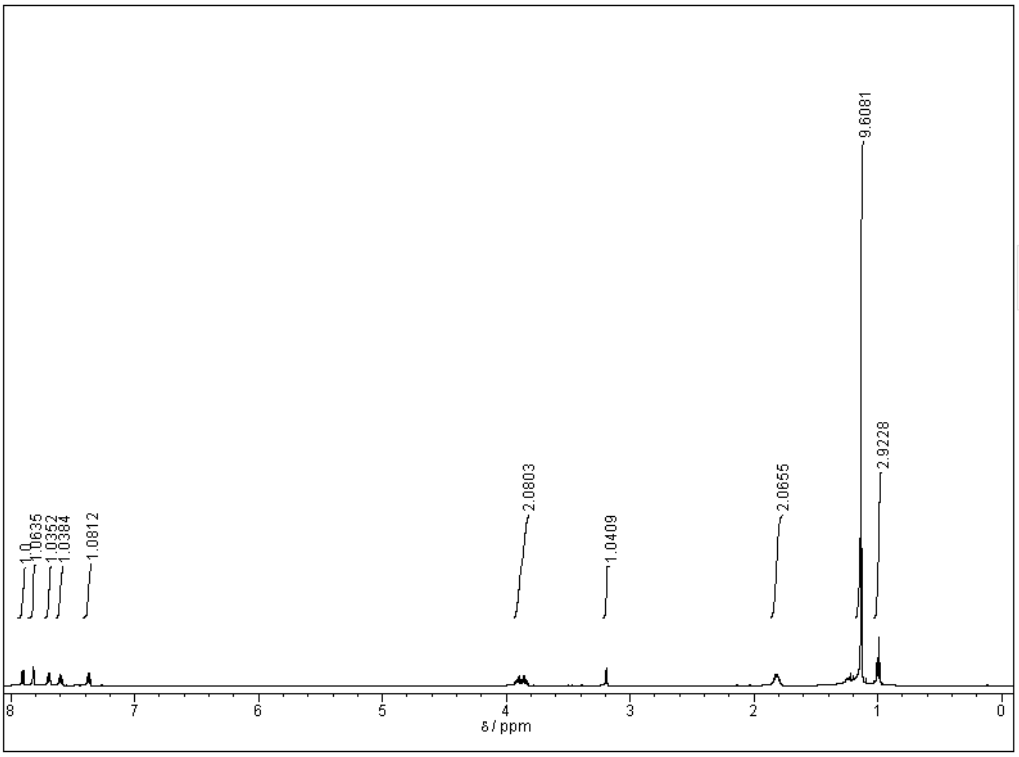
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

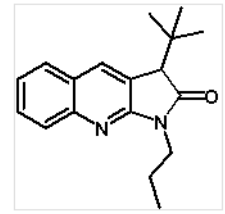




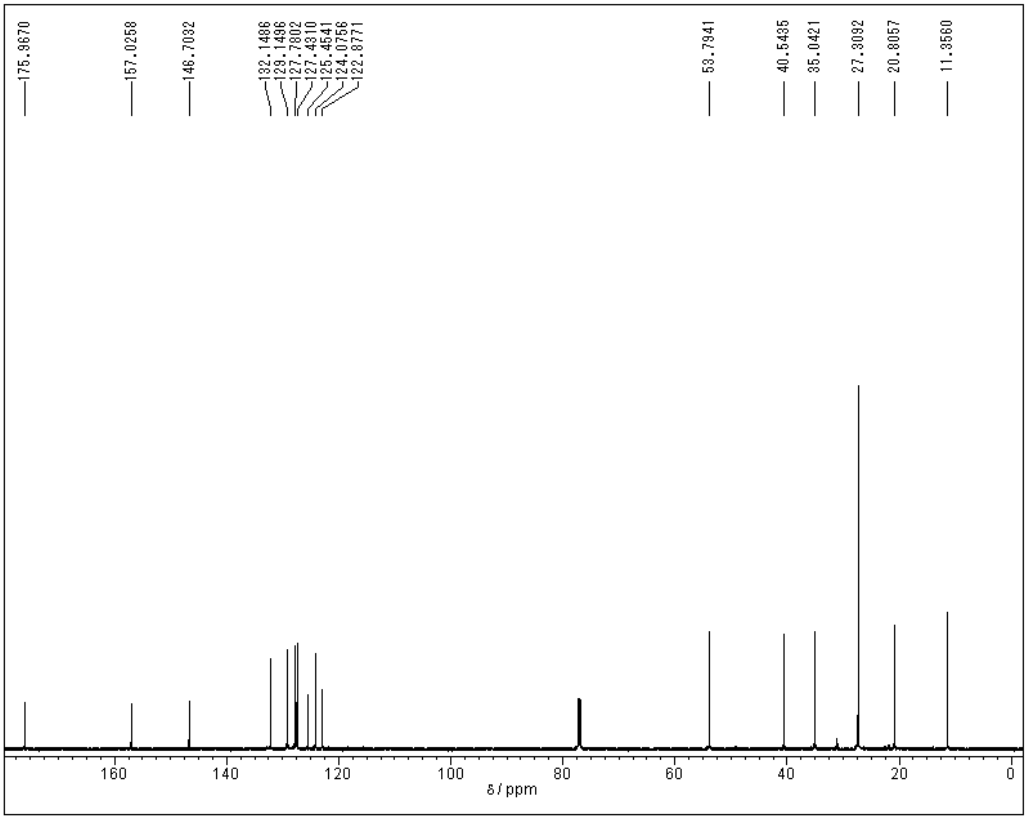
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

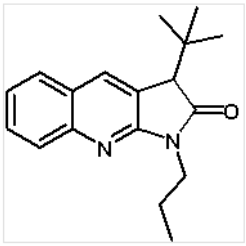
15i





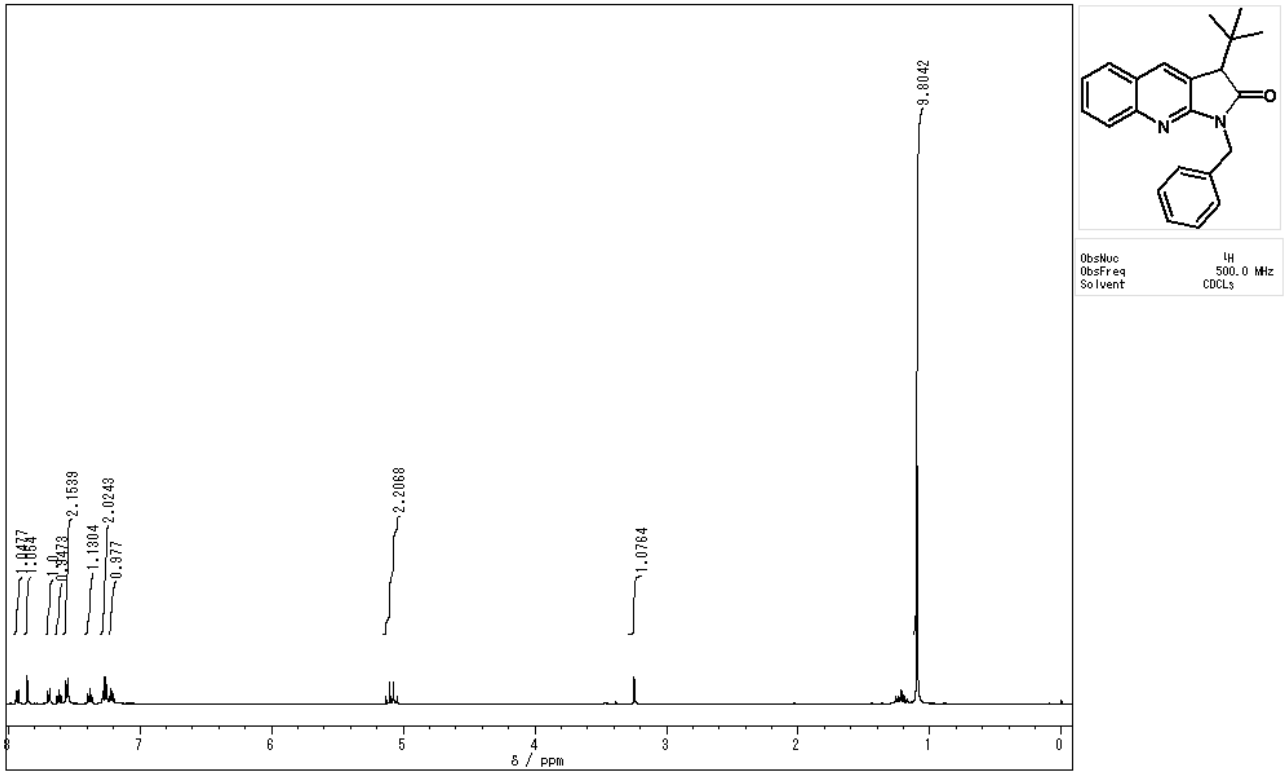
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

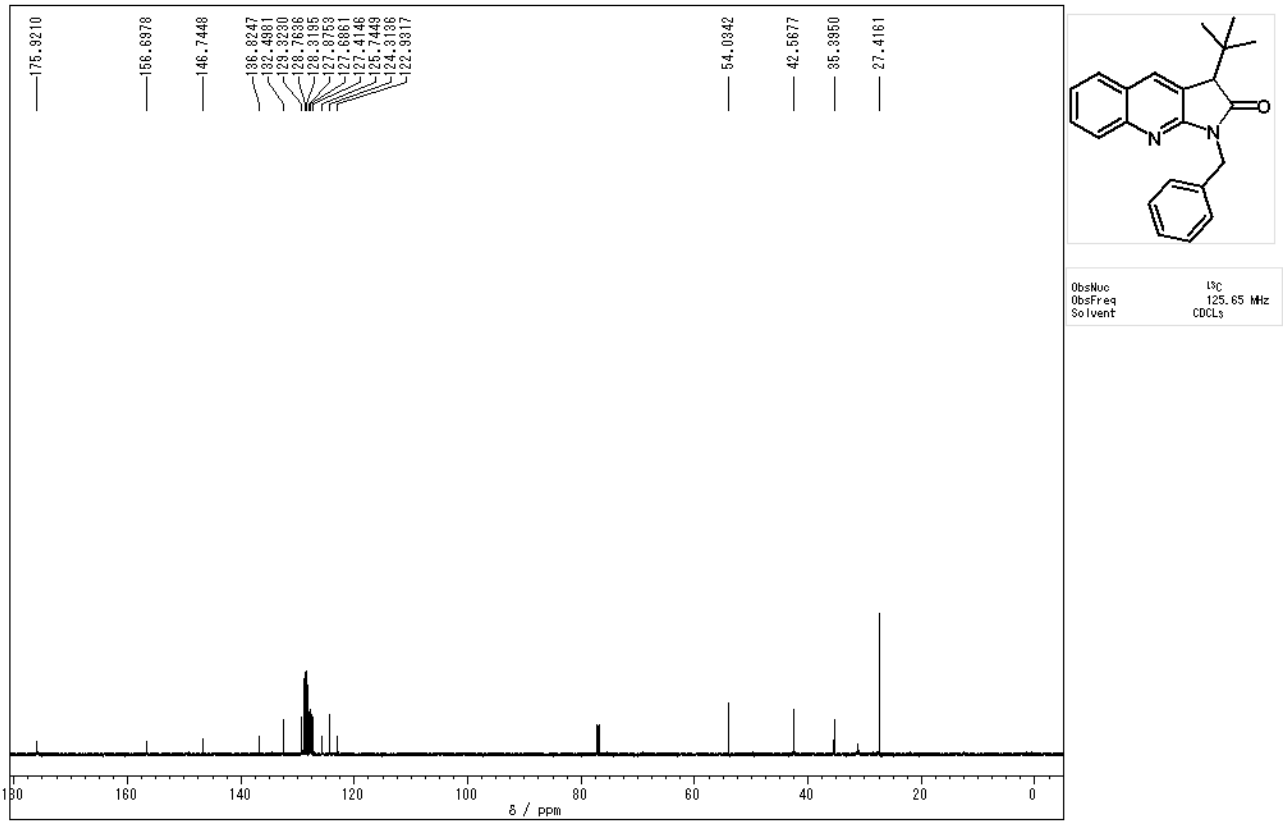




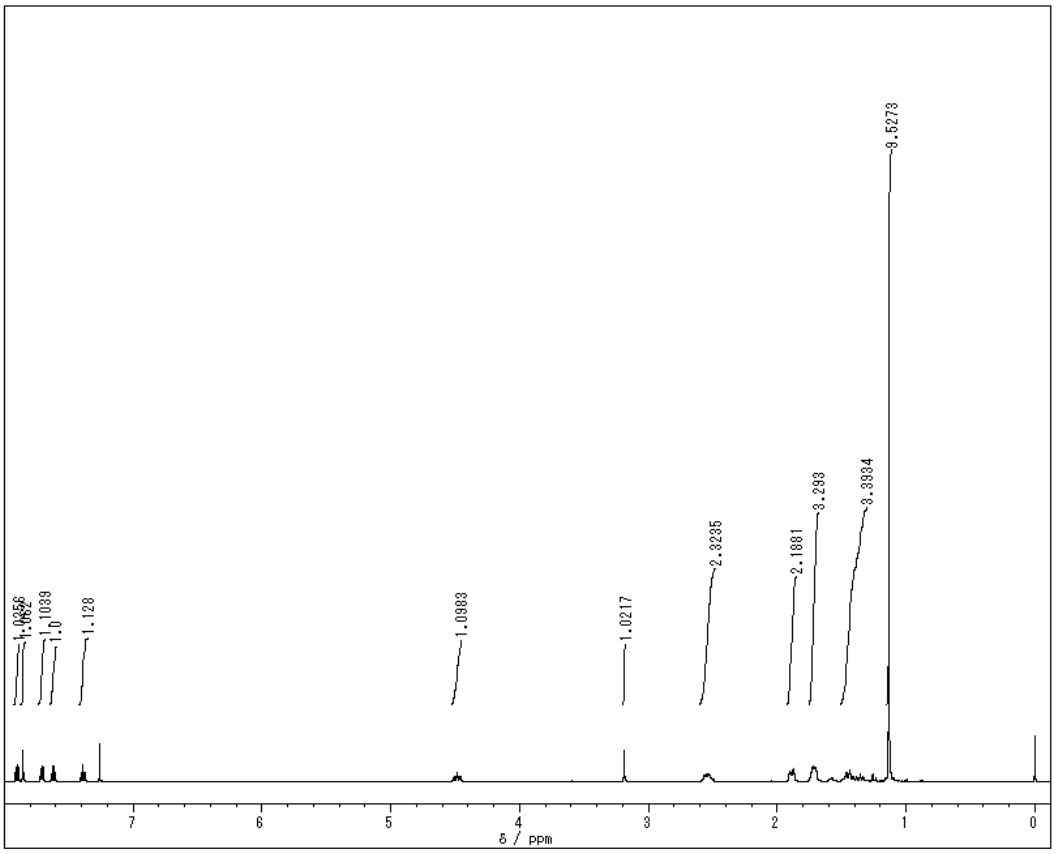
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

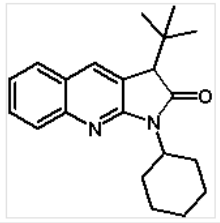
15j


9.8042
2.2068
2.1539
2.0243
1.1304
1.0764
0.977
δ / ppm
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3

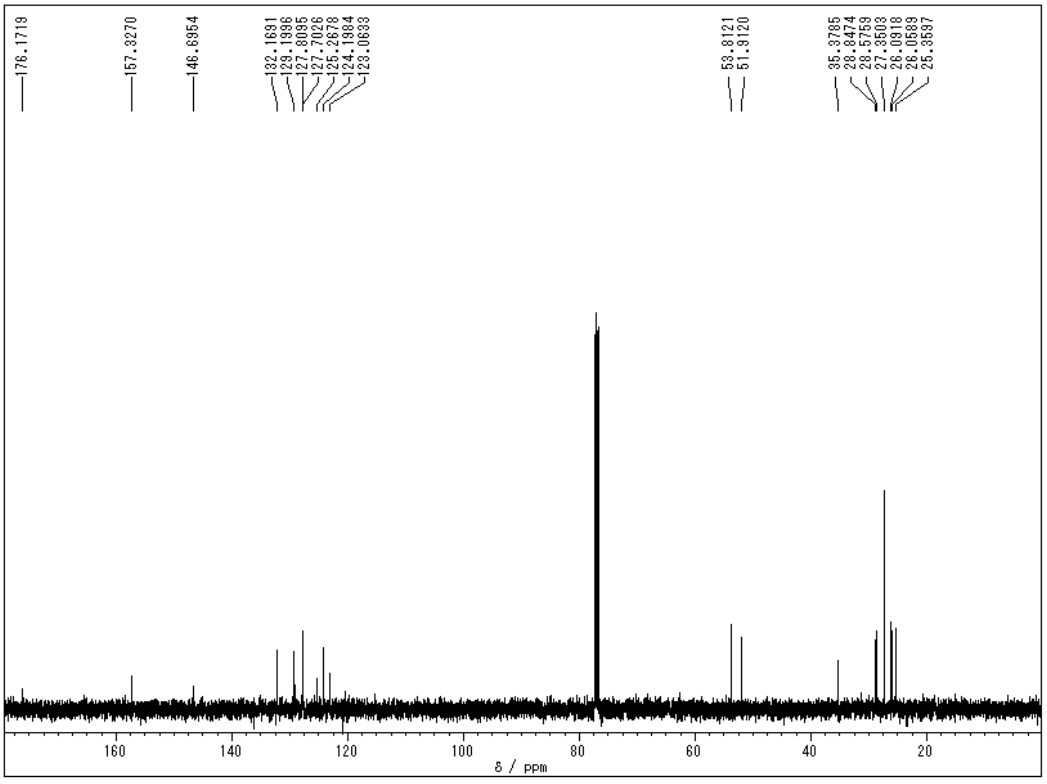

175.9210
156.6978
146.7448
136.8247
132.4881
129.3230
128.7636
128.3195
127.8753
127.6861
127.4146
125.7449
124.3136
122.8317
54.0342
42.5677
35.3950
27.4161
δ / ppm
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

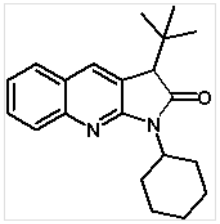
15k





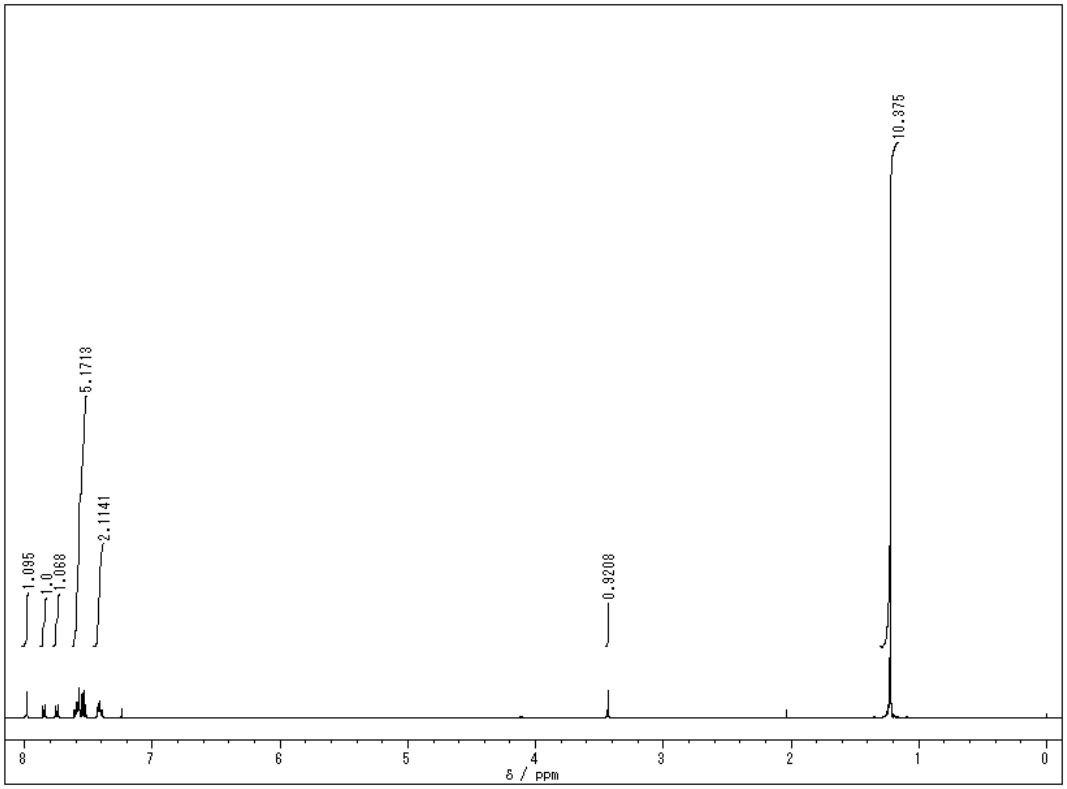
ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCl3

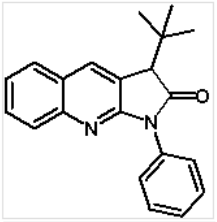




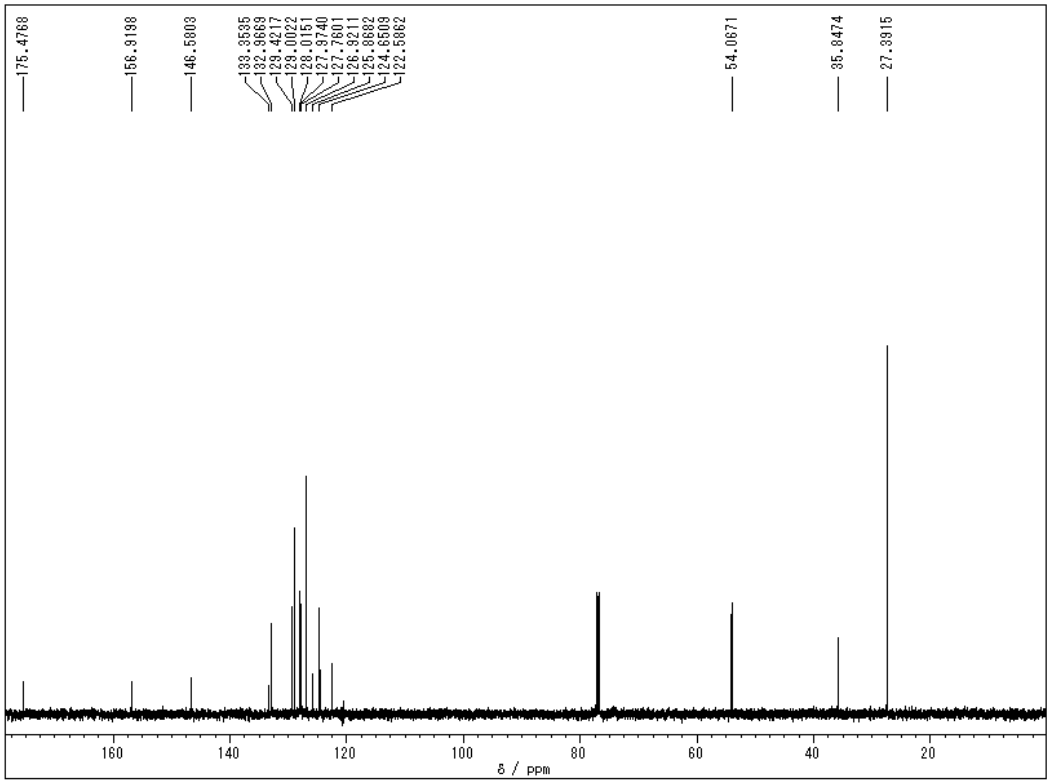
ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCl3

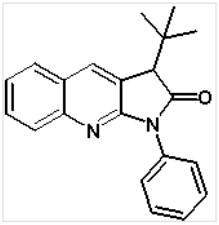
15l





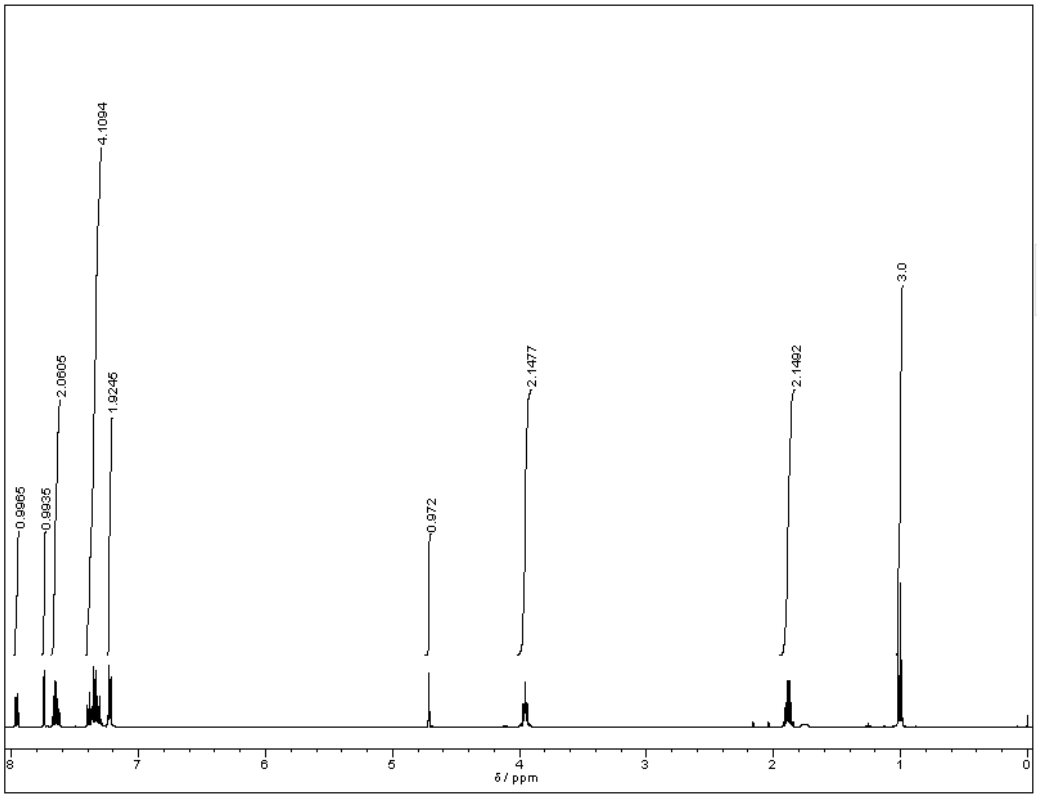
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	CDCl$_3$

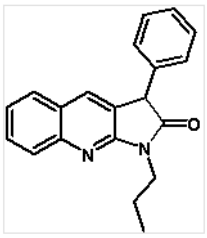




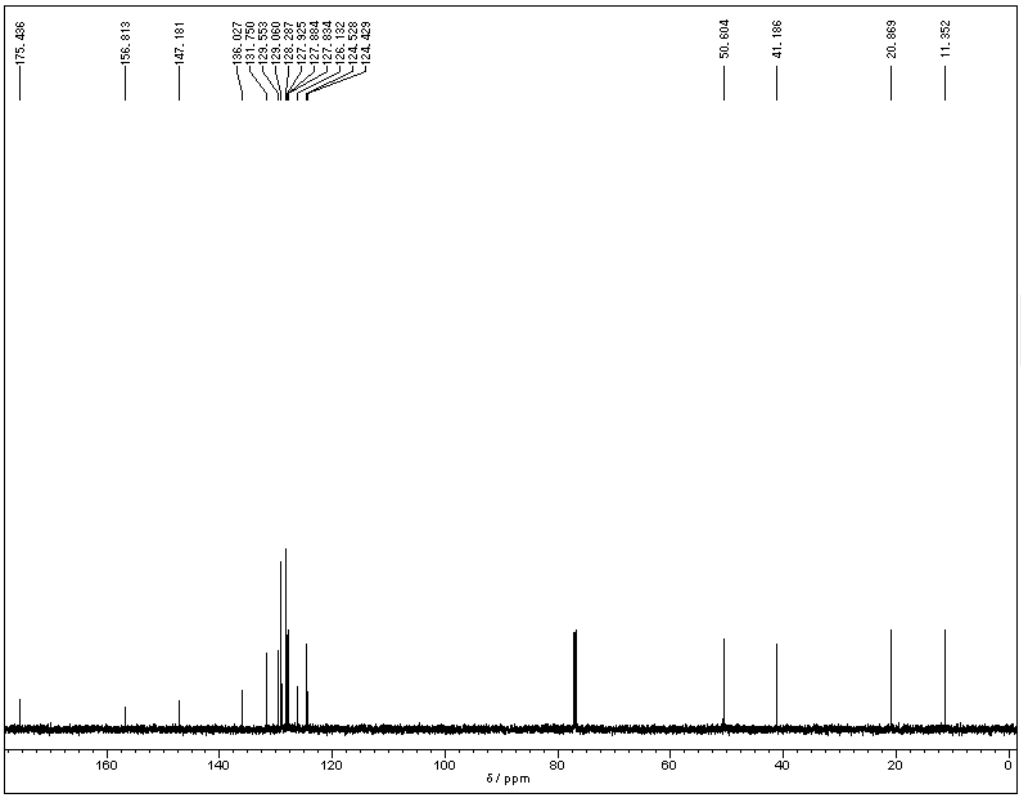
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	CDCl$_3$

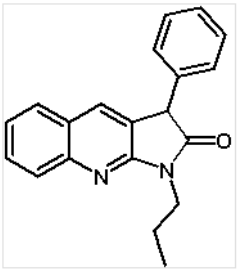
15m





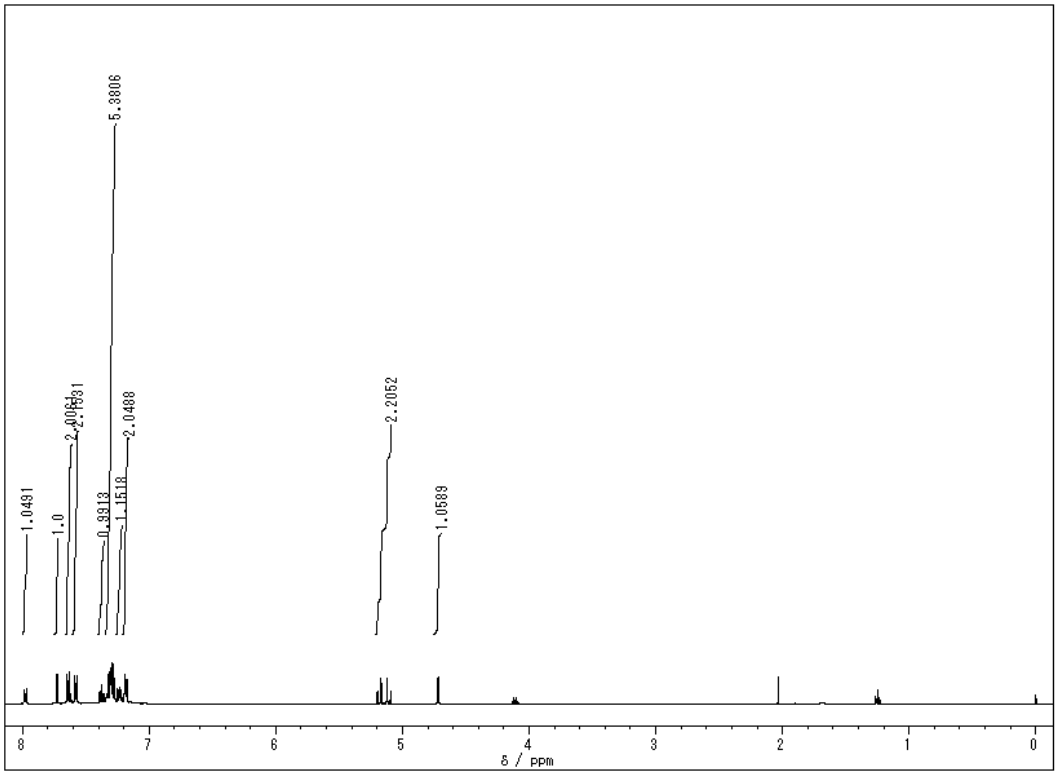
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

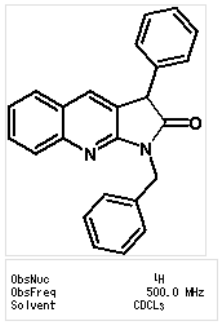


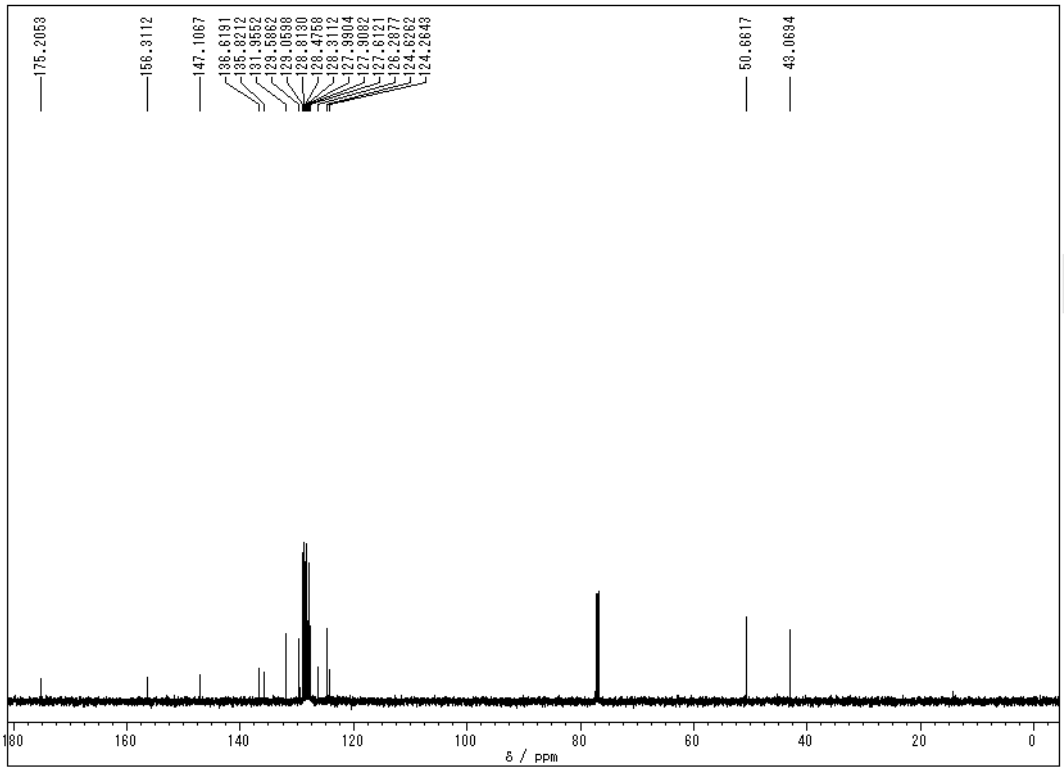


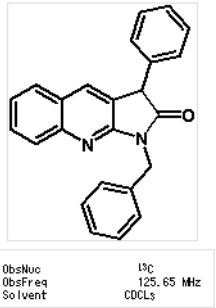
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

15n

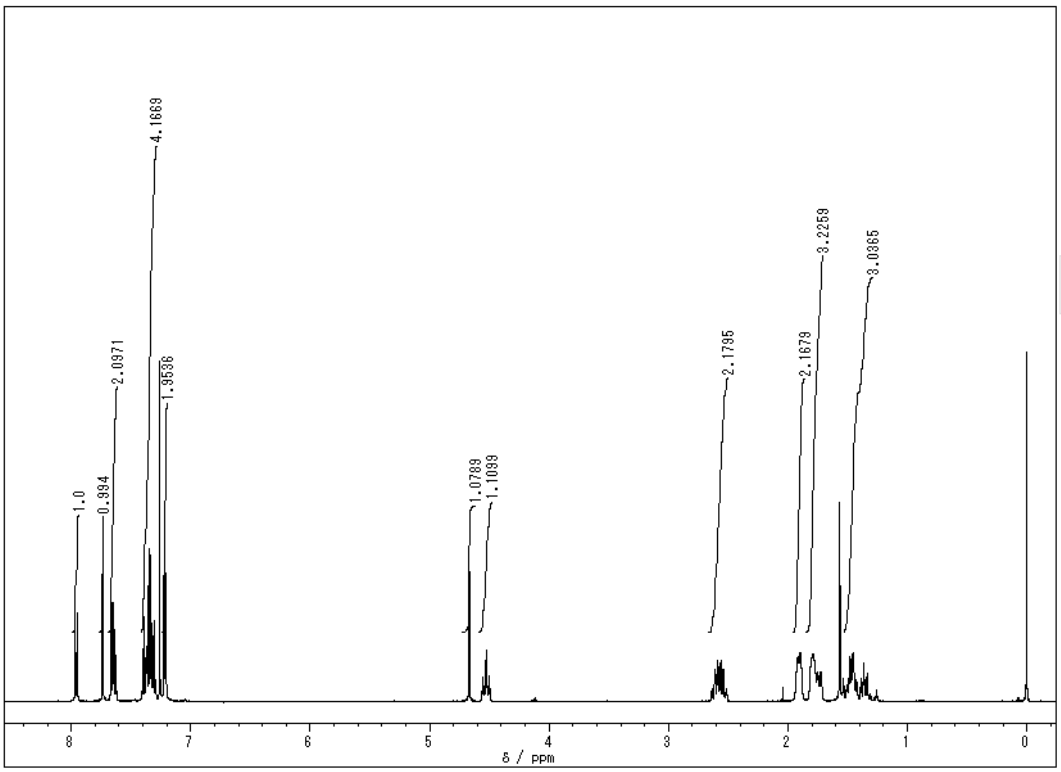

5.3806
2.0061
2.0931
2.0488
2.2052
1.0491
1.0
0.9813
1.1518
1.0589
8
7
6
5
4
3
2
1
0
δ / ppm

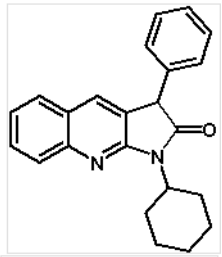

ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCl3

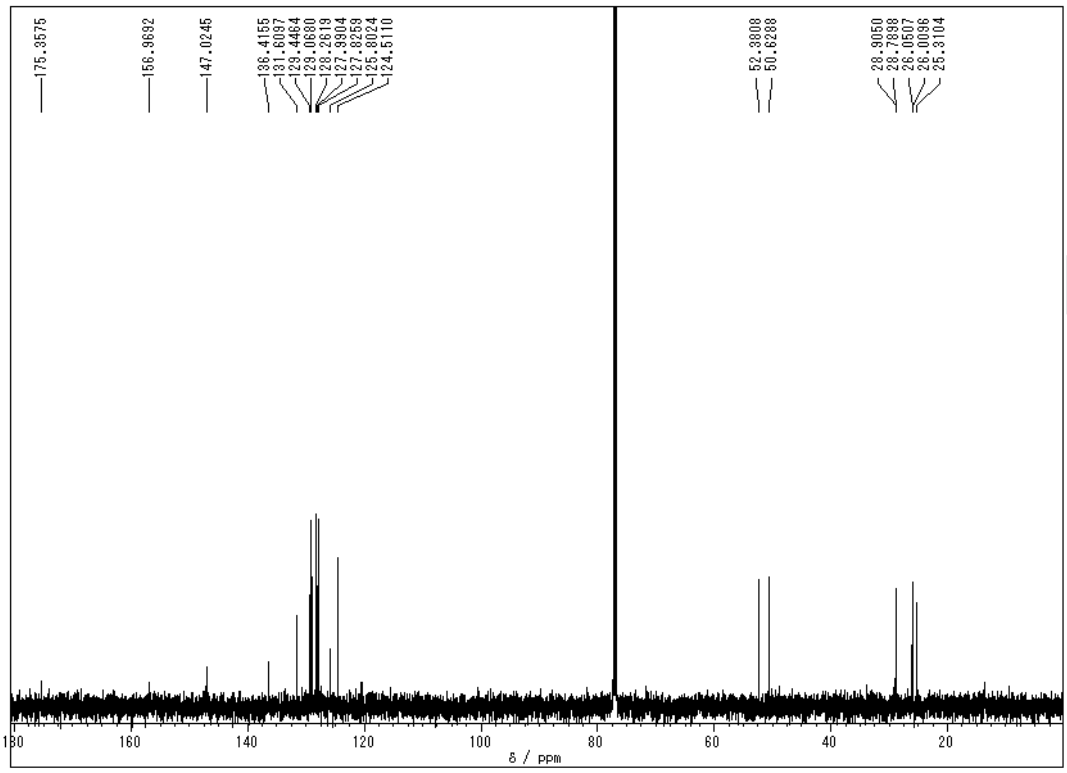

175.2053
156.3112
147.1067
138.6191
135.8212
131.9552
129.5862
129.0598
128.8130
128.4758
128.3112
127.9804
127.9082
127.6121
126.2877
124.6262
124.2643
50.6617
43.0694
180
160
140
120
100
80
60
40
20
0
δ / ppm


ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCl3

15o


1.0
0.994
2.0971
4.1668
1.9536
1.0789
1.1038
2.1795
2.1679
3.2259
3.0365
8
7
6
5
4
3
2
1
0
δ / ppm


ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCl3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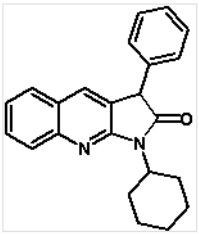
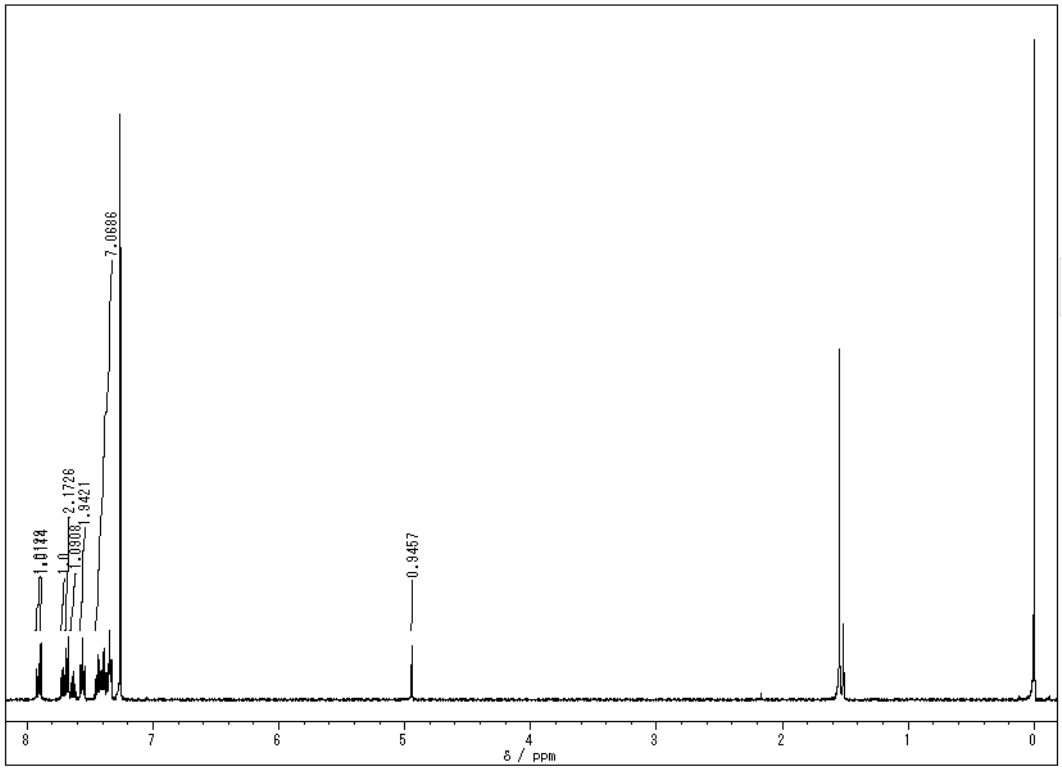
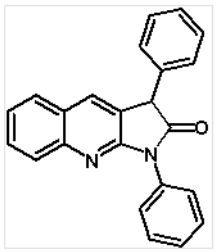
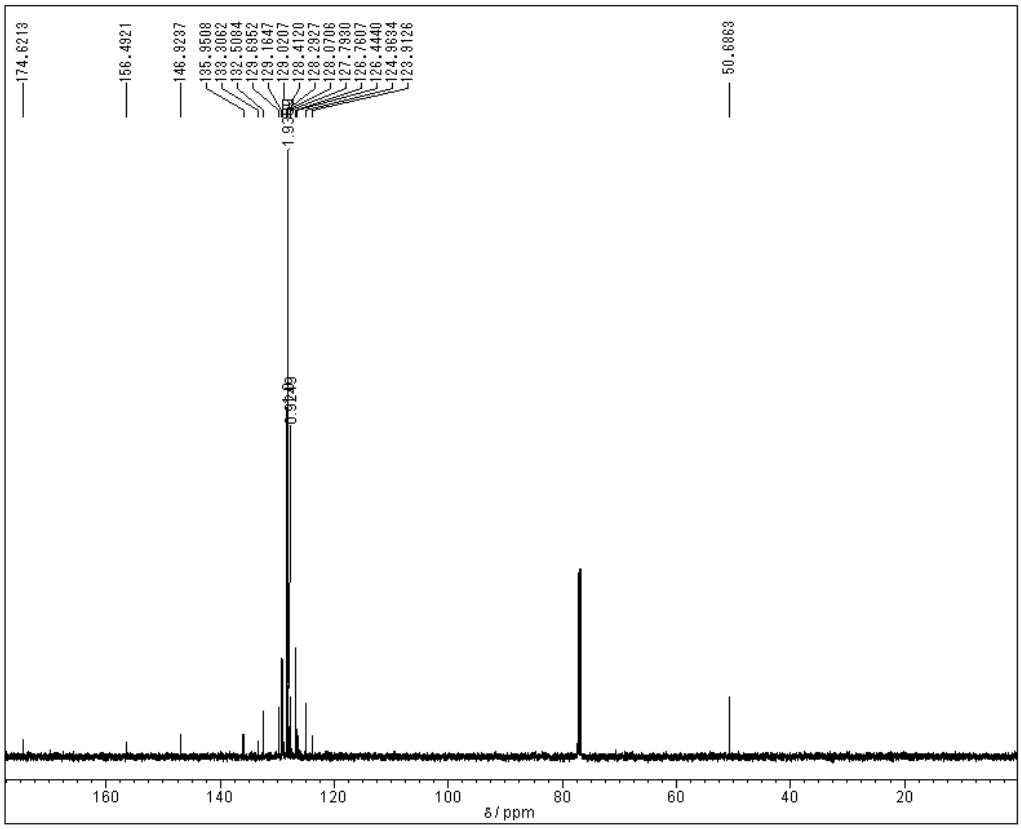
147.0245
136.4155
131.6097
129.4464
129.0680
128.2619
127.3804
127.8269
125.8024
124.5110
52.3808
50.6288
28.9050
28.7898
26.0507
26.0096
25.3104
180
160
140
120
100
80
60
40
20
δ / ppm


ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCl3

15p


1.0144
1.0
2.1728
1.0908
1.9421
7.0686
0.9457
8
7
6
5
4
3
2
1
0
δ / ppm


ObsNuc 1H
ObsFreq 500.0 MHz
Solvent CDCL3


174.6213
156.4921
146.9237
135.9508
133.3062
132.5084
129.6852
129.1647
128.0207
128.4120
128.2927
128.0706
127.7930
126.7607
126.4440
124.9634
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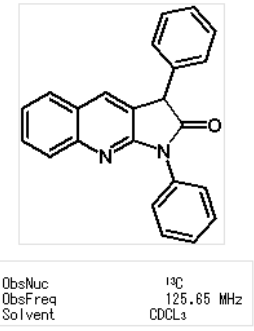
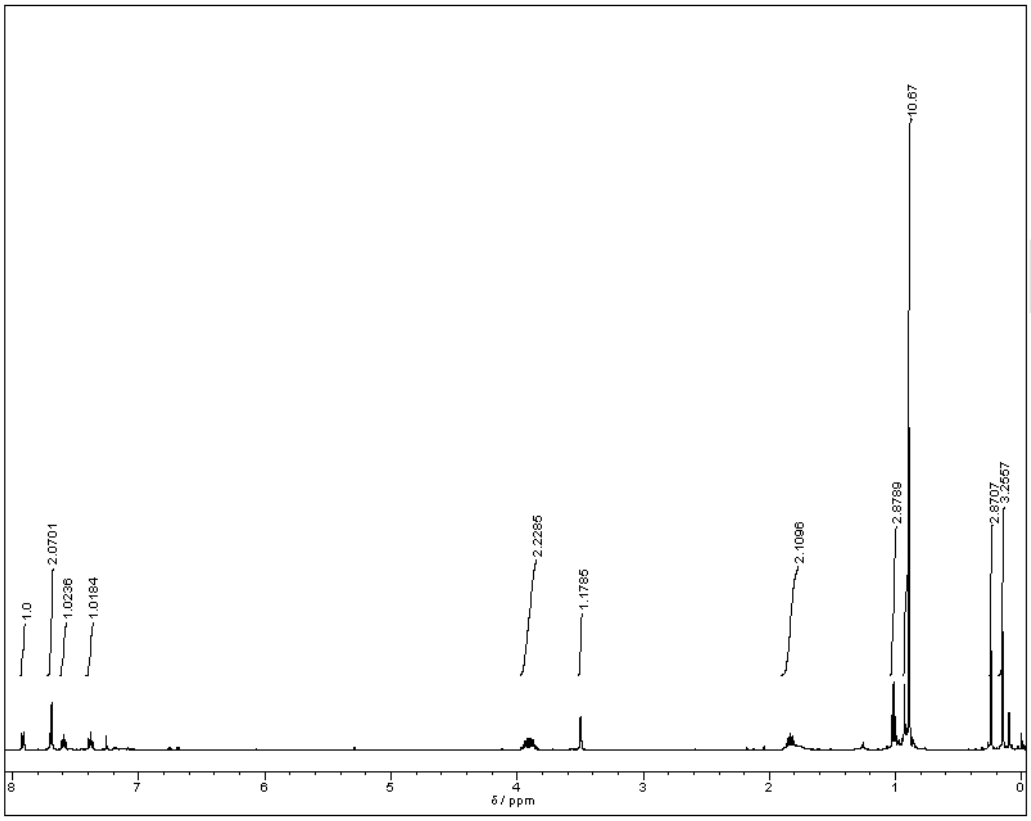
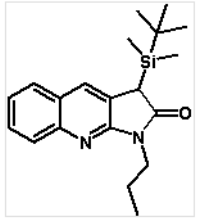
50.6883
1.9360
0.9240
160
140
120
100
80
60
40
20
δ/ppm

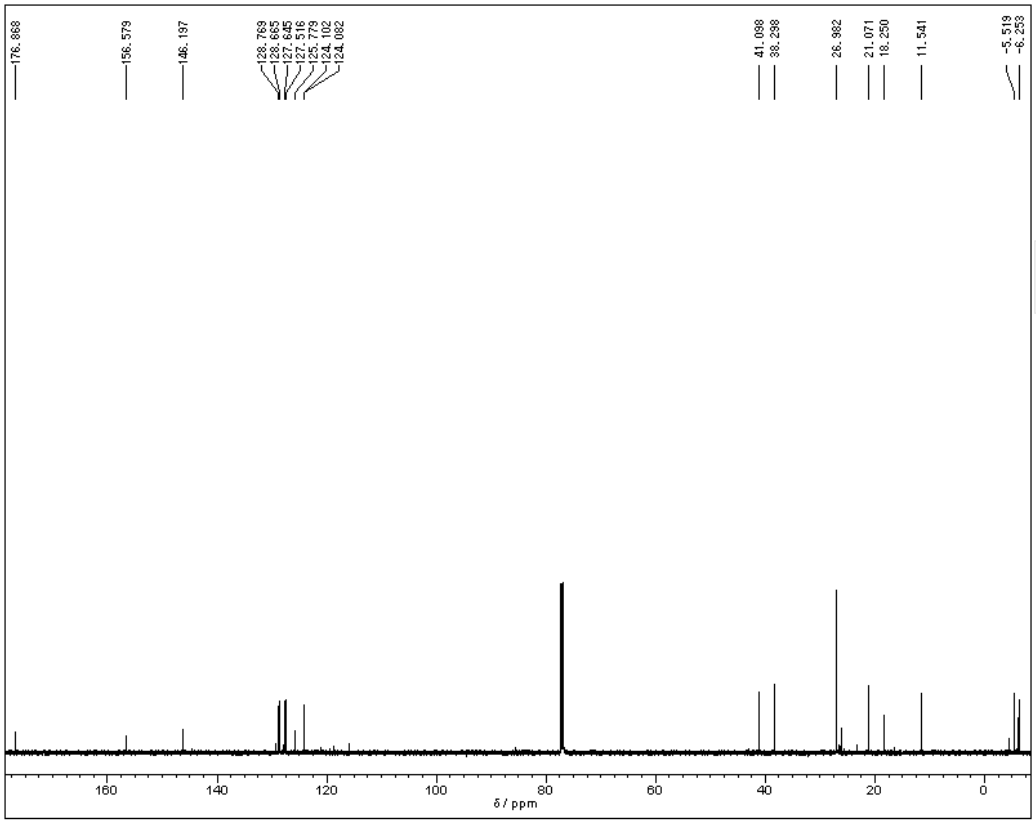

ObsNuc 13C
ObsFreq 125.65 MHz
Solvent CDCL3

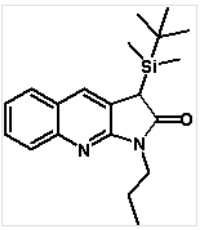
15q





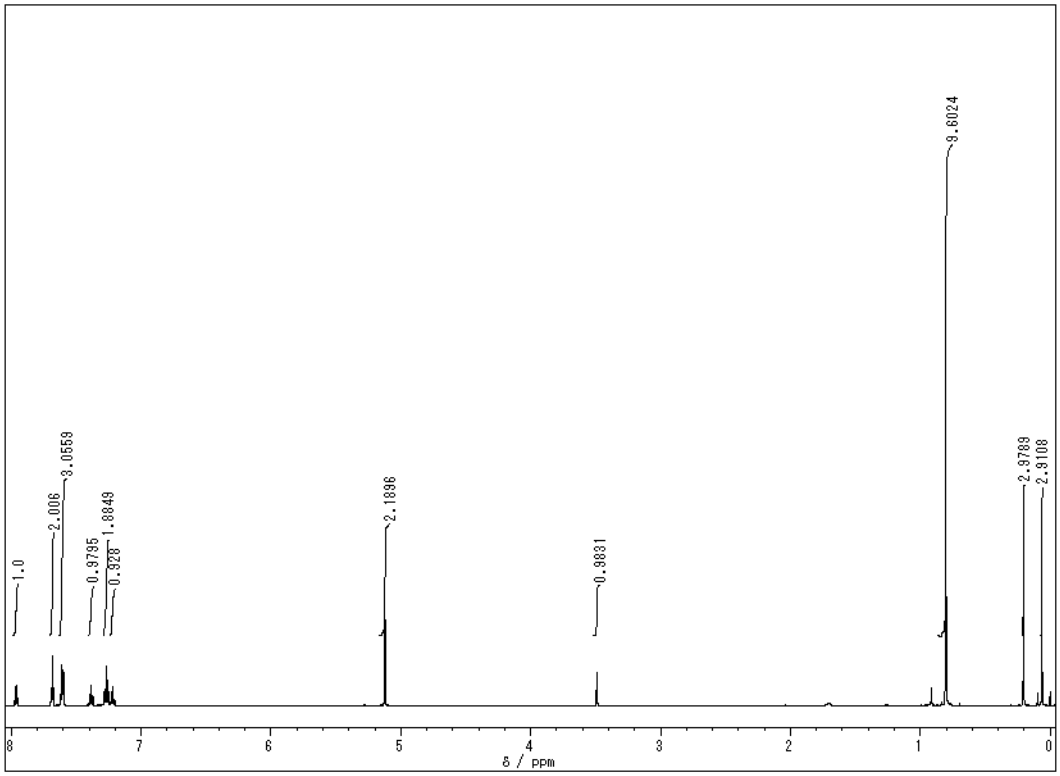
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

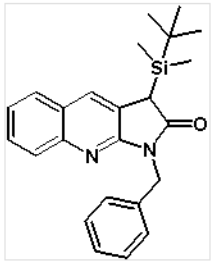




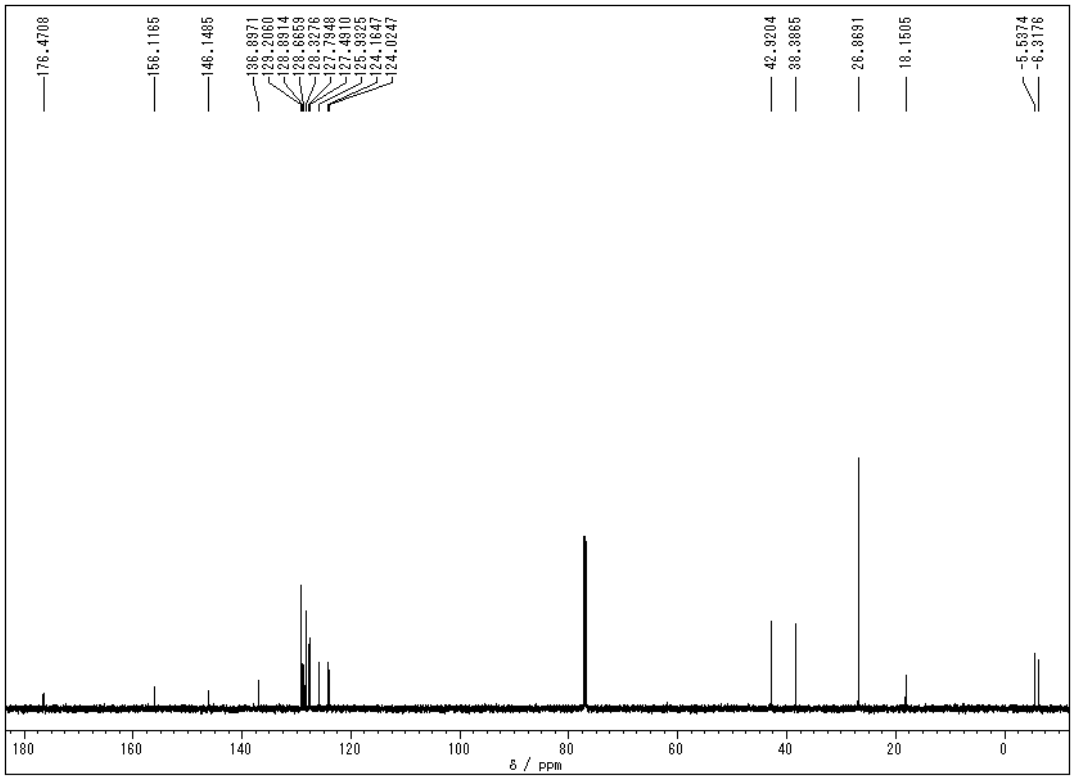
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

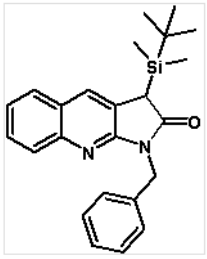
15r





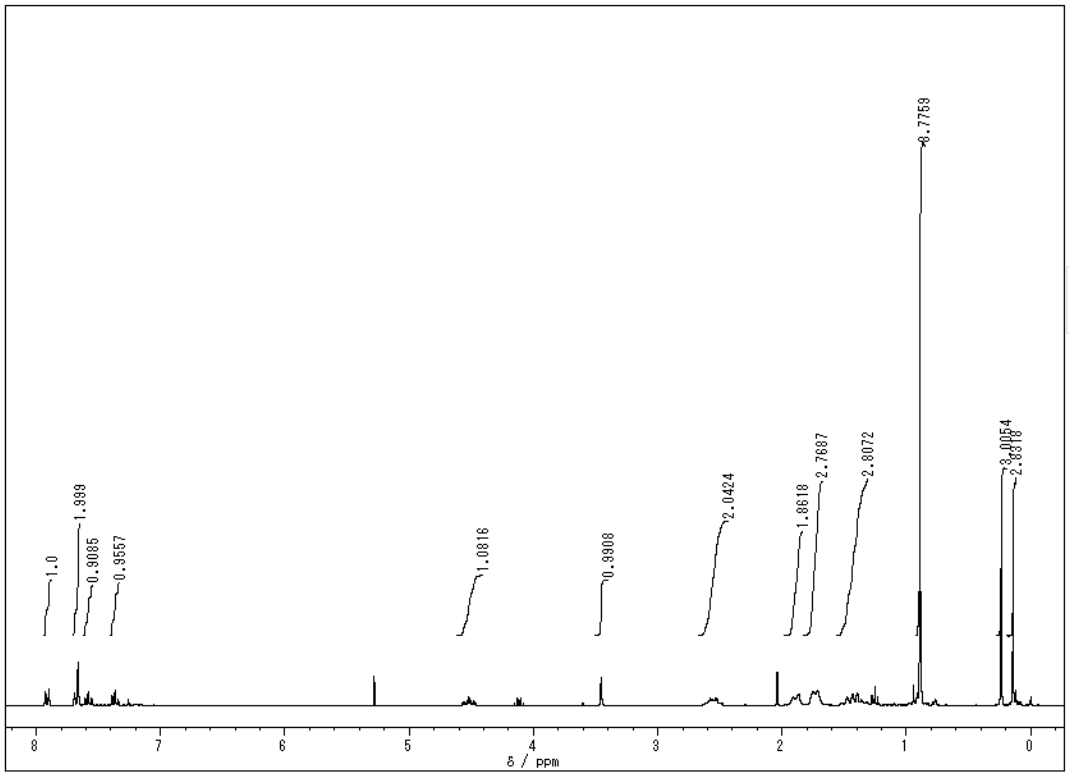
ObsNuc 1H
ObsFreq 600.13 MHz
Solvent CDgCLg

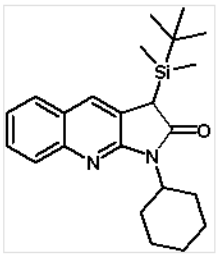




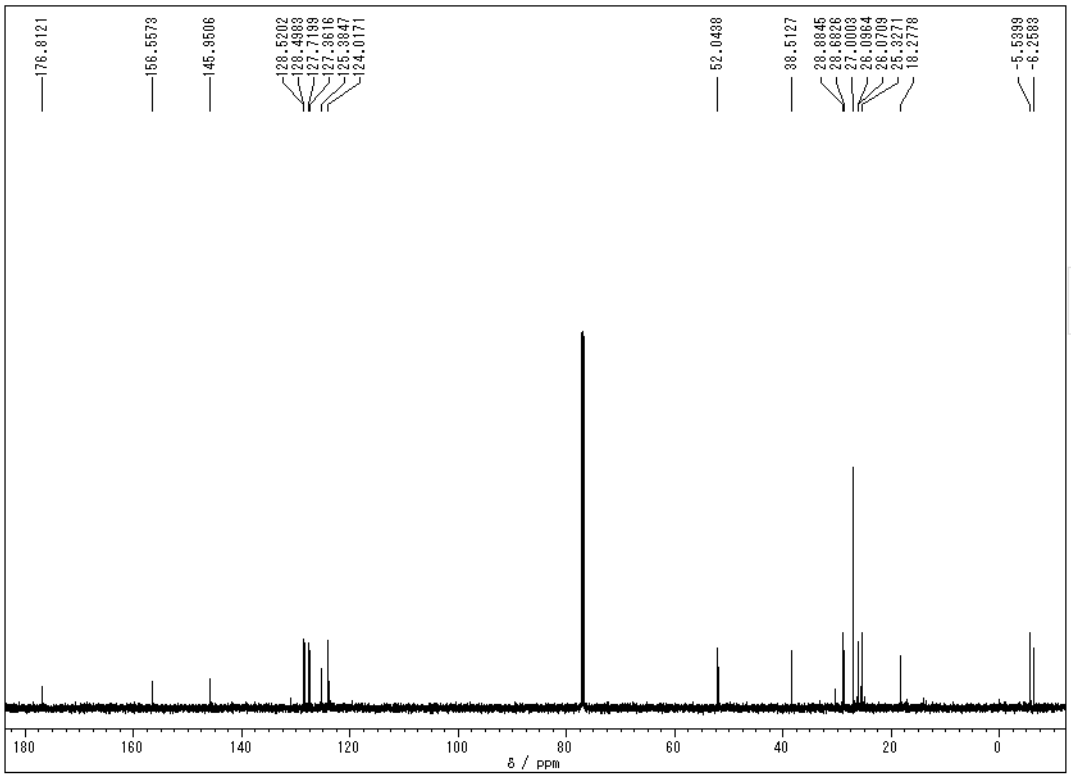
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent CDCLs

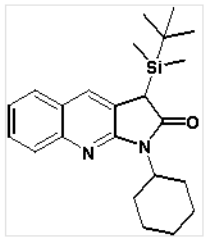
15s





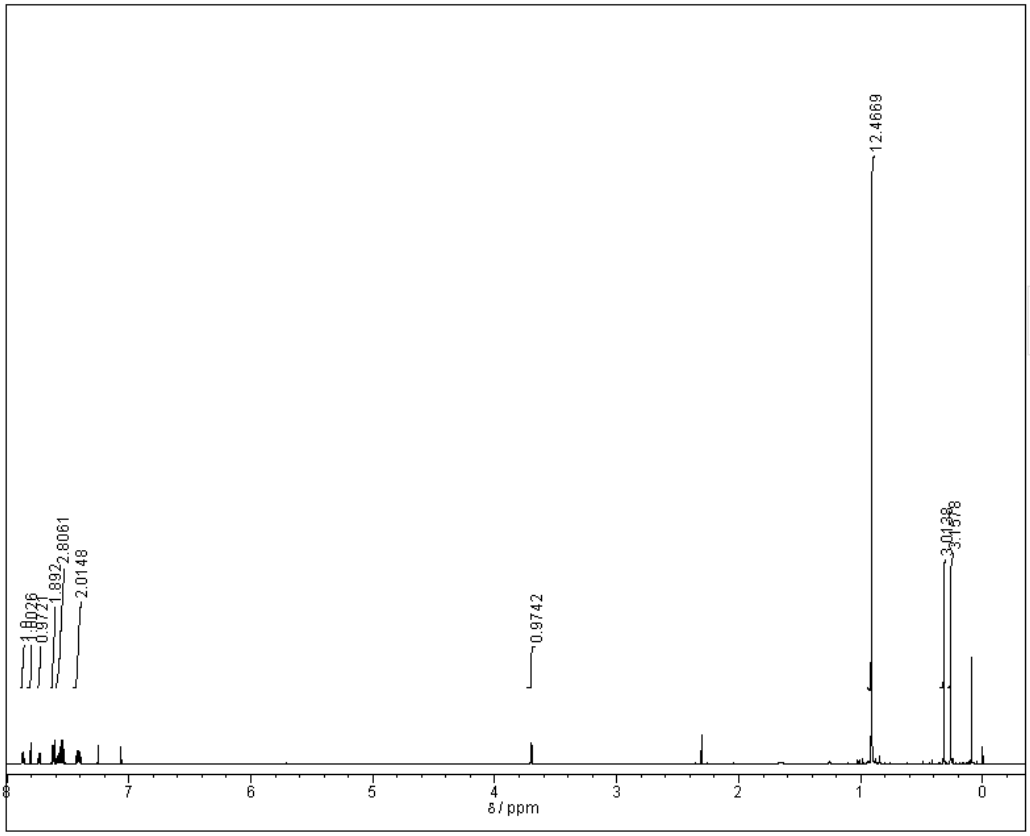
ObsNuc 1H
ObsFreq 300.01 MHz
Solvent CDCL3

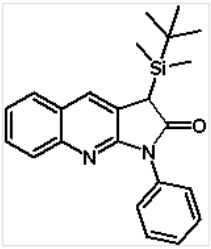




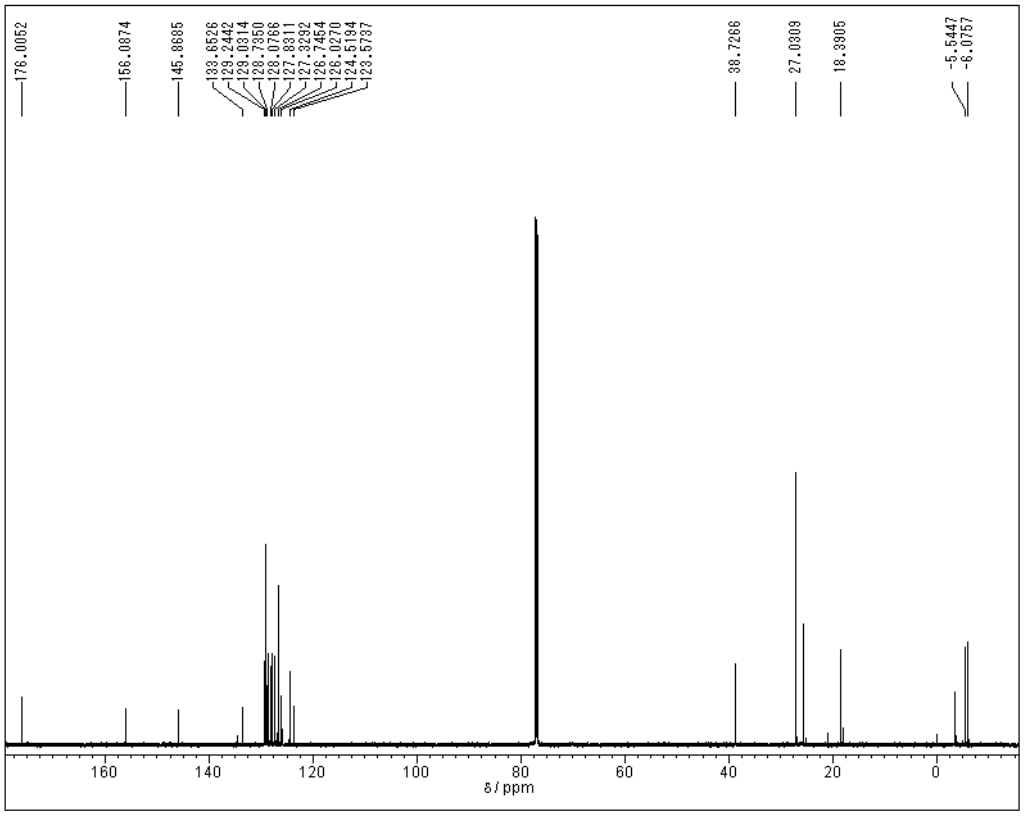
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent CDCL3

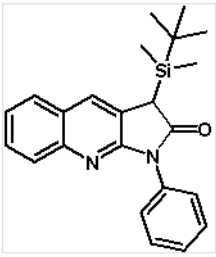
15t





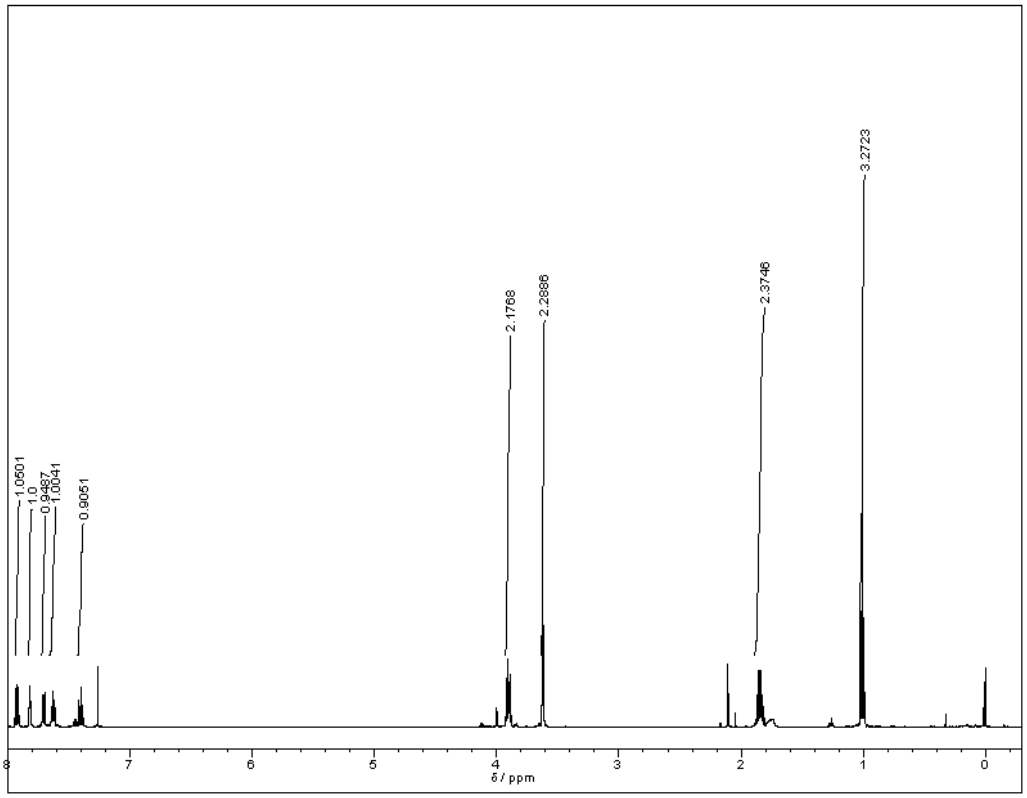
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent CDCL₃

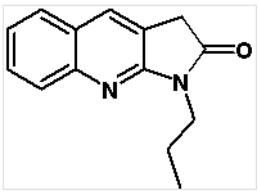




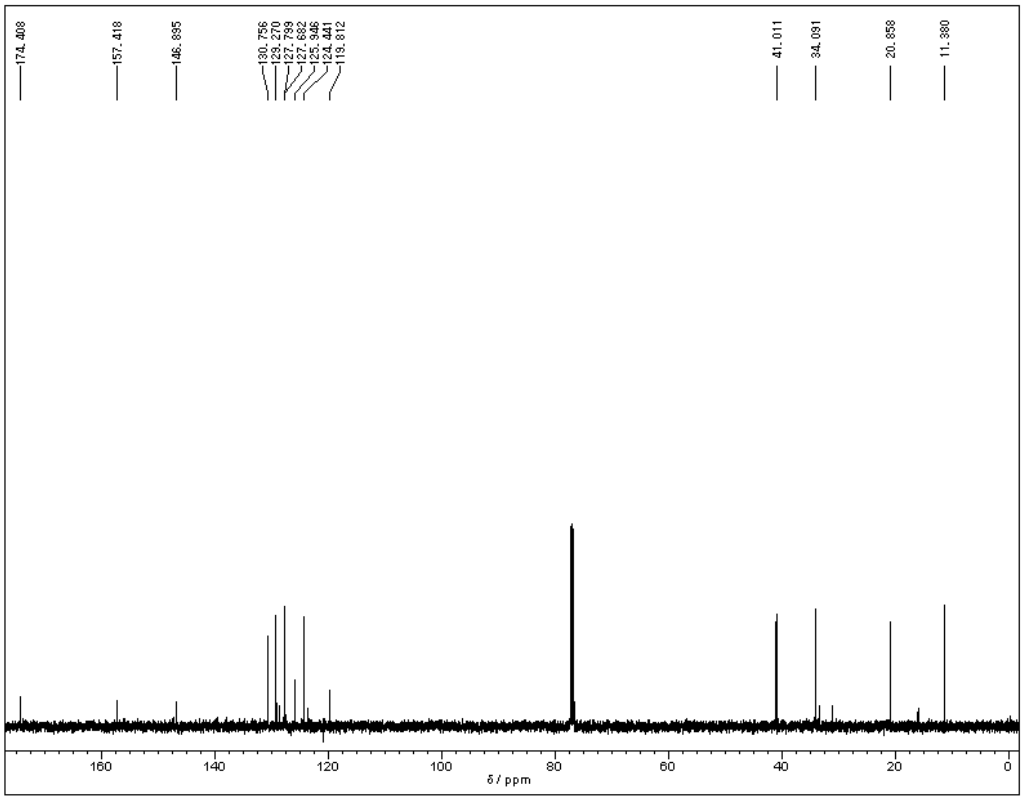
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent CDCL₃

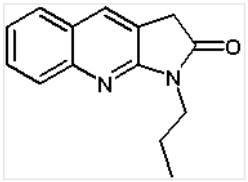
15u





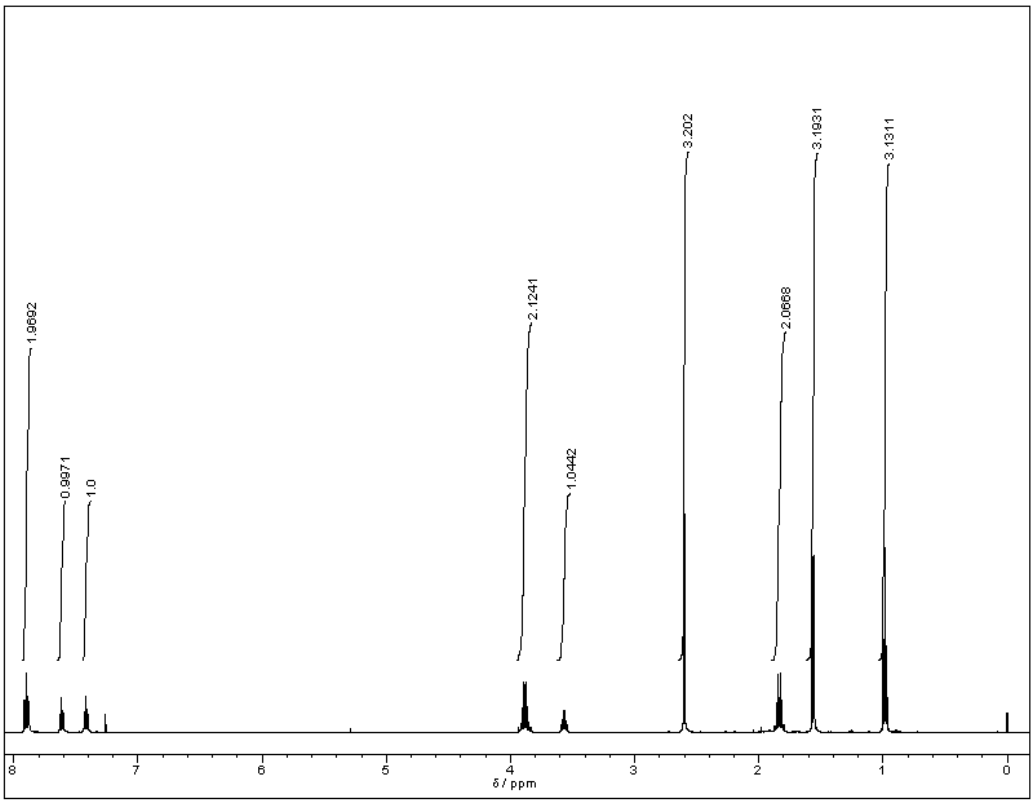
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent $CDCl_3$

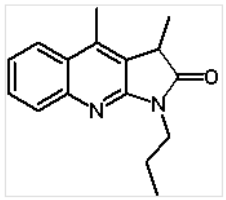




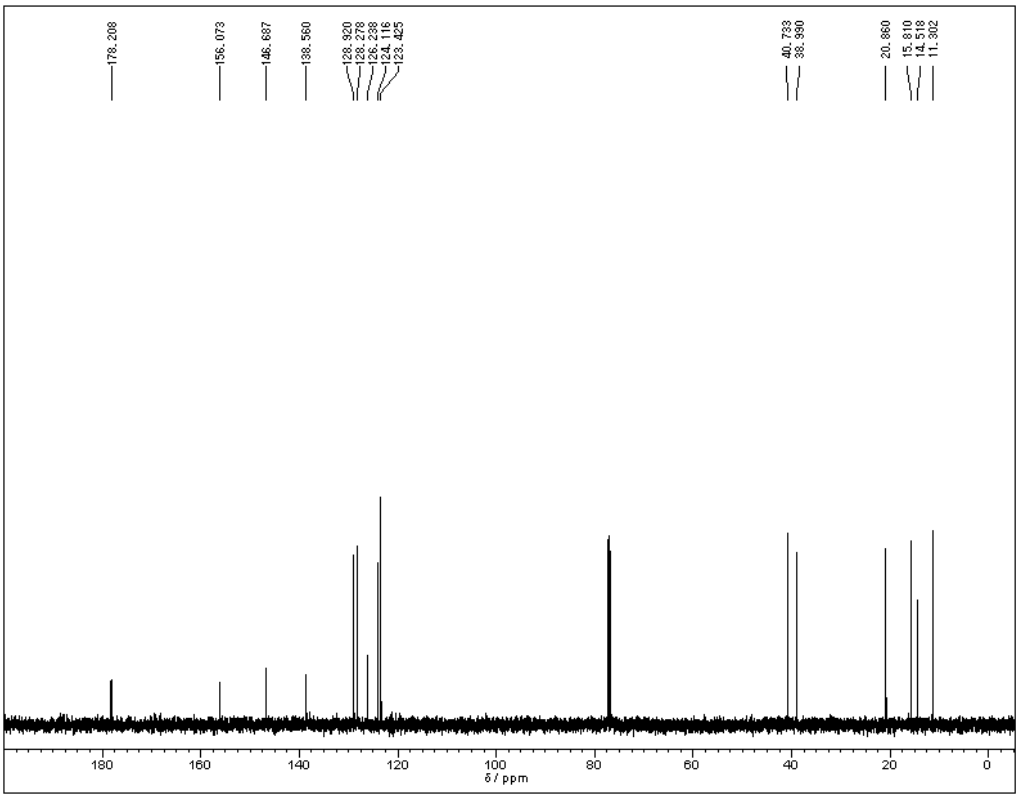
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent $CDCl_3$

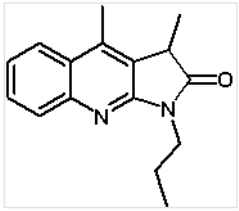
17a





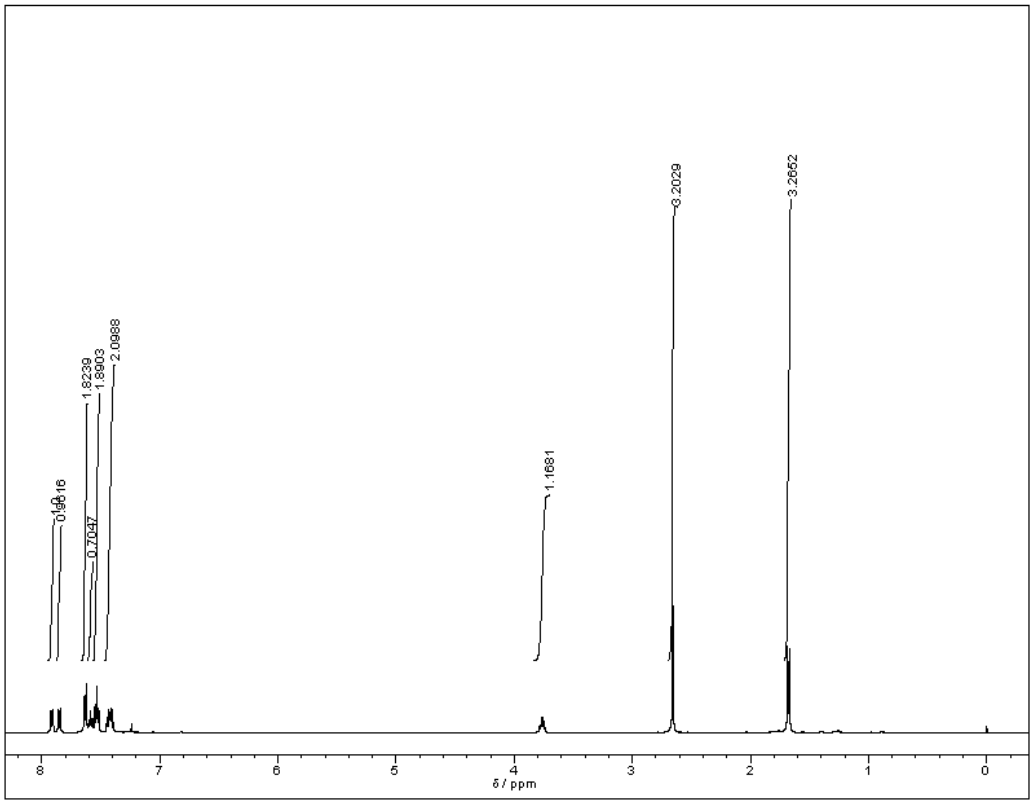
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent CDCL3

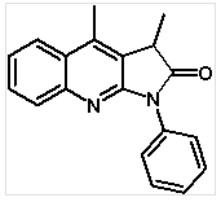




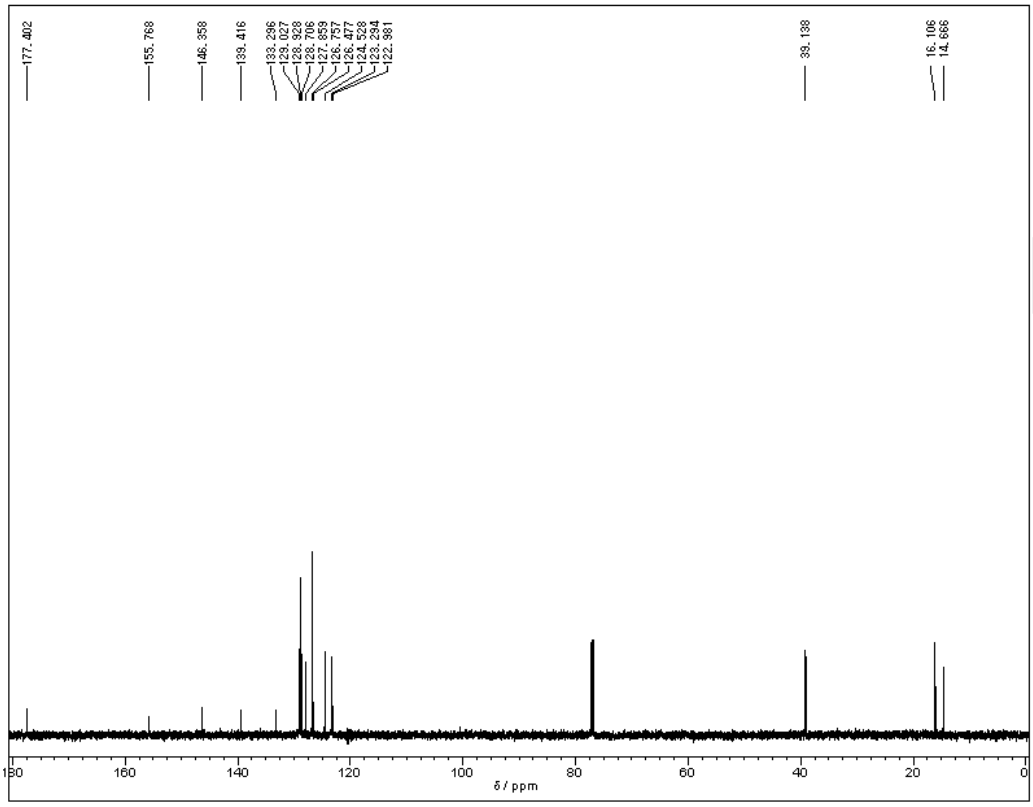
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent CDCL3

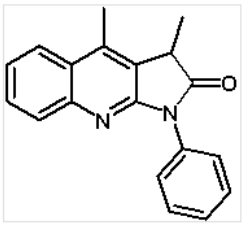
17b





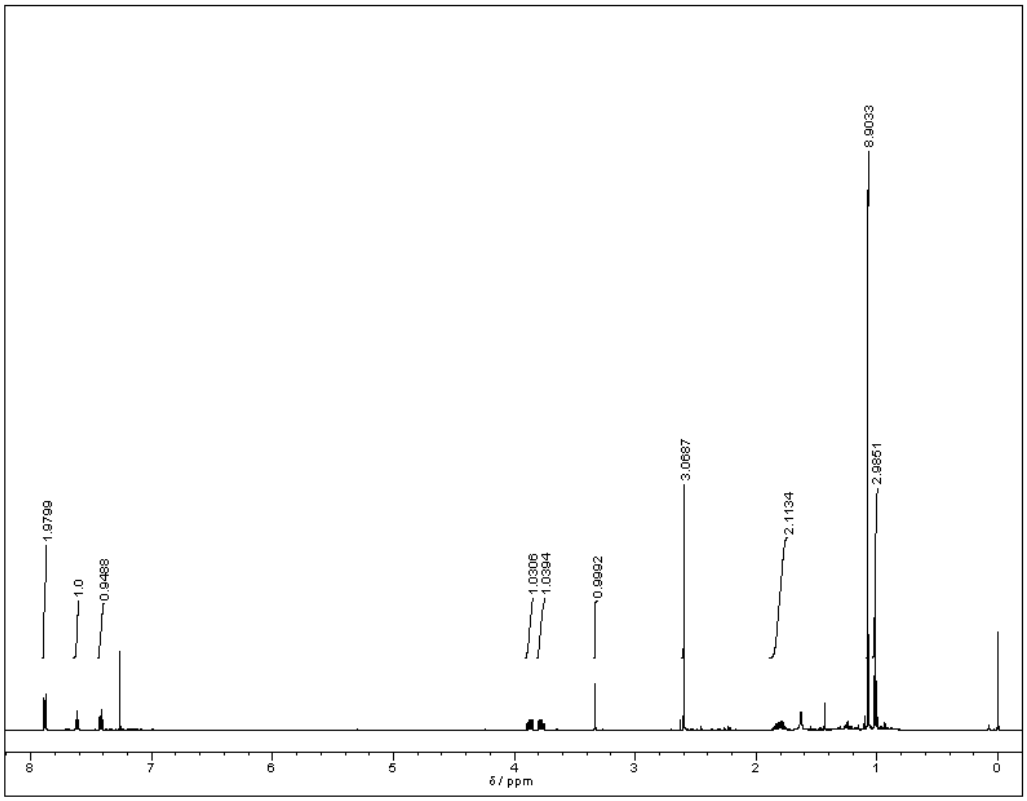
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	CDCL3

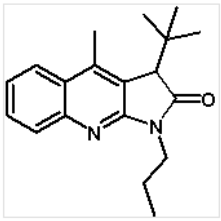




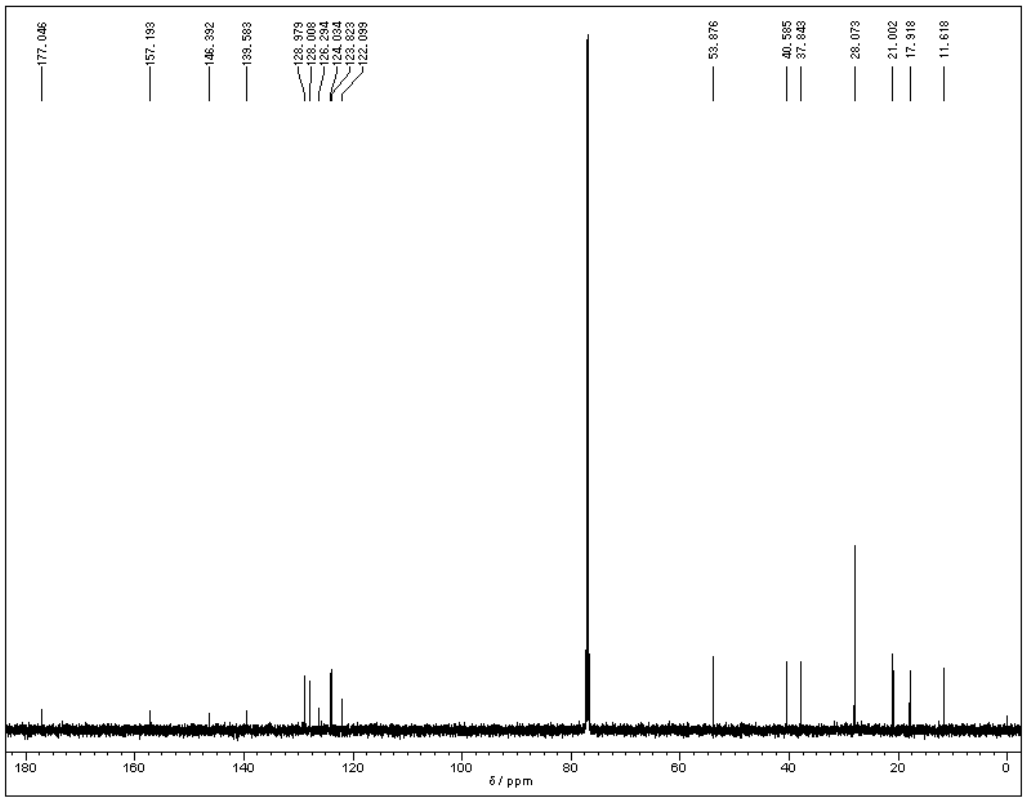
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	CDCL3

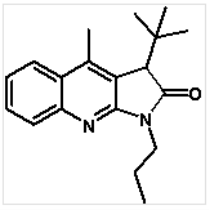
17c





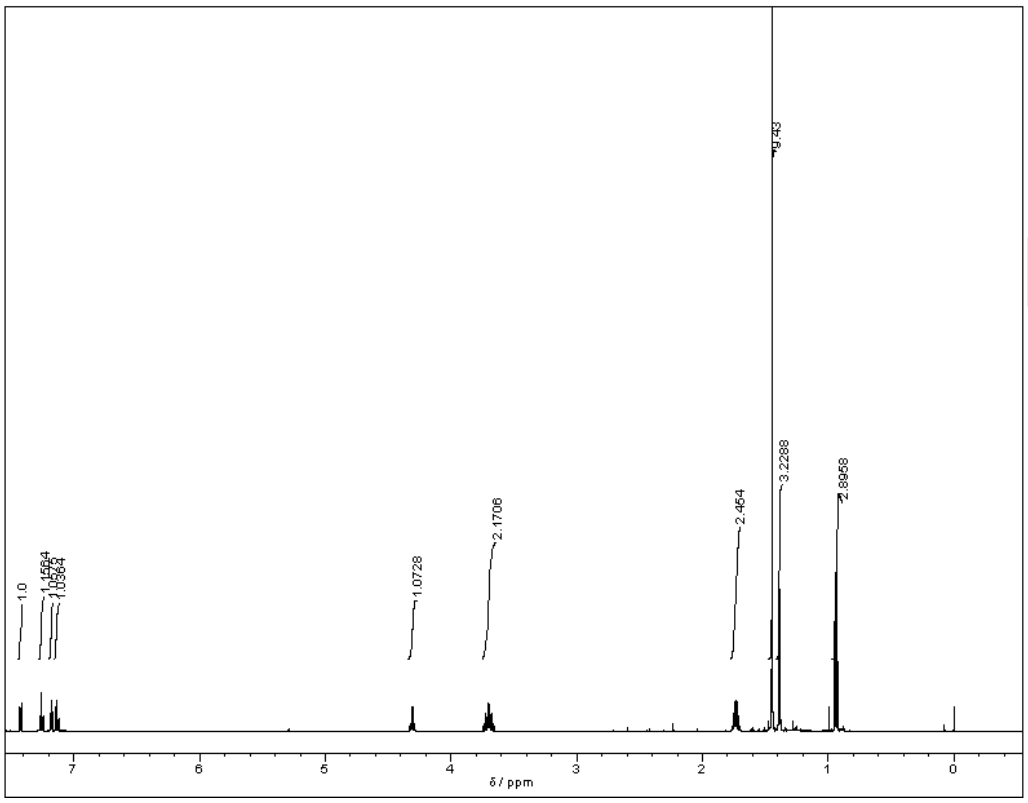
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

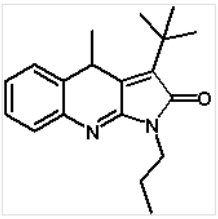




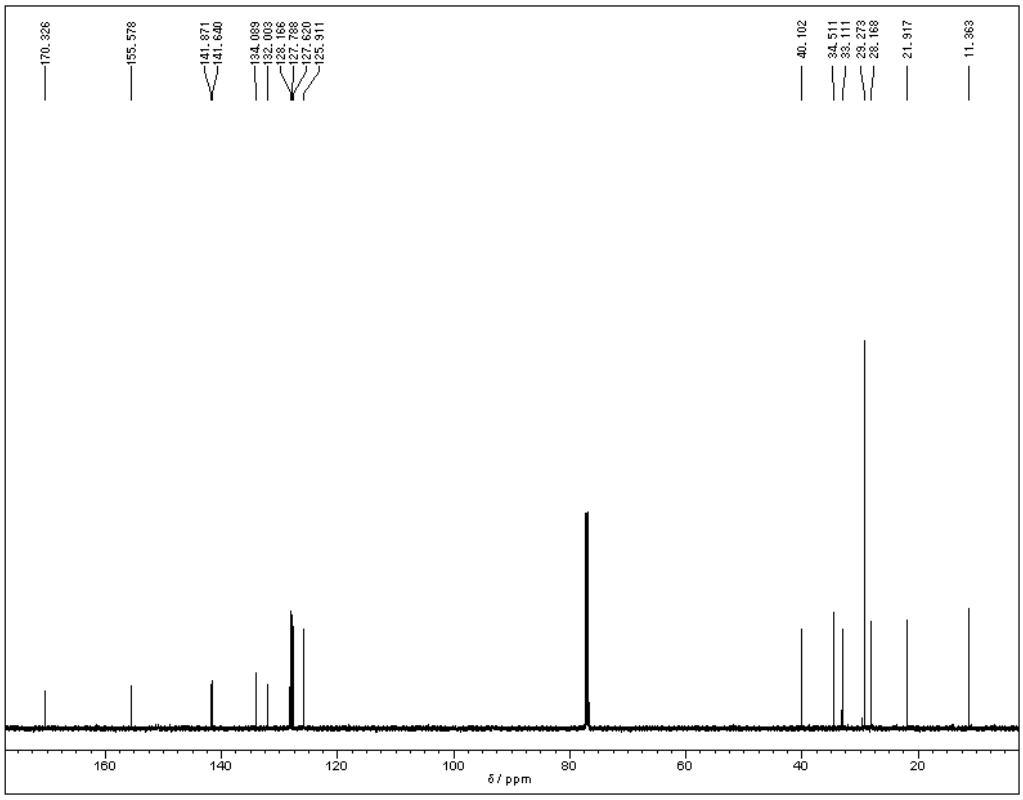
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

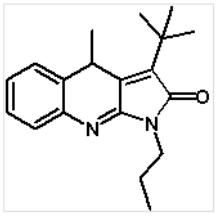
18a





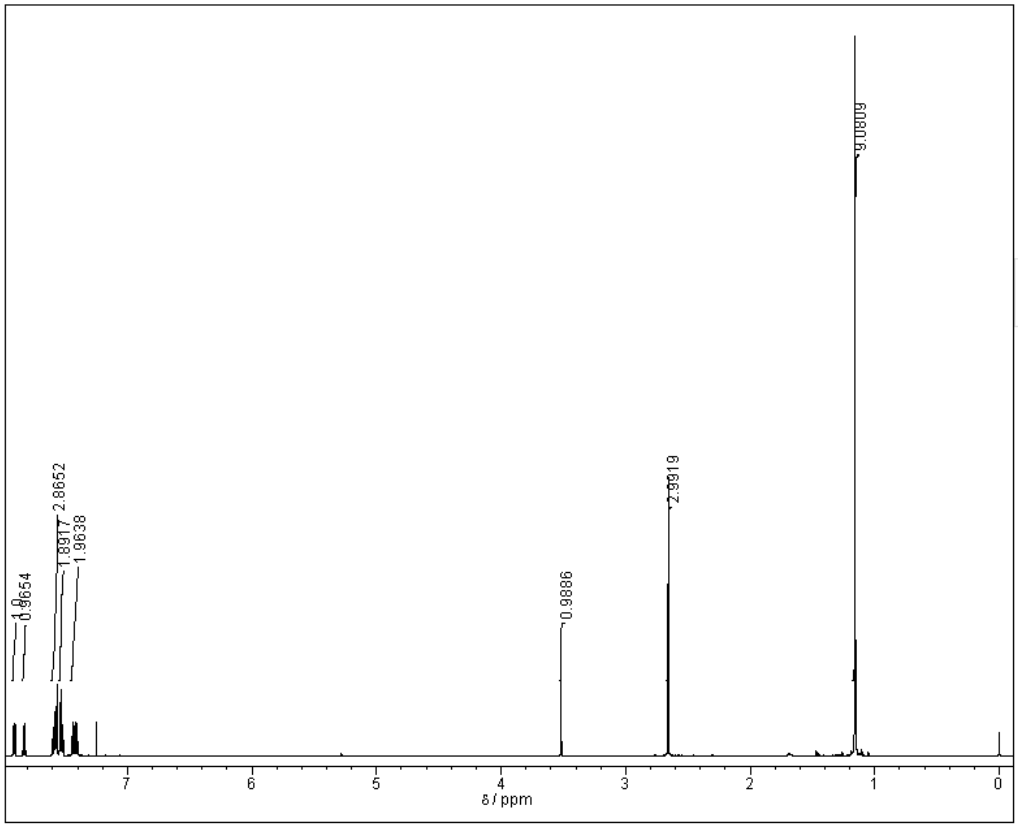
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent CDCL3

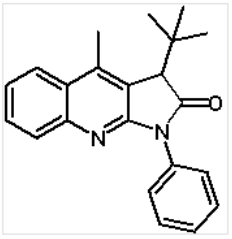




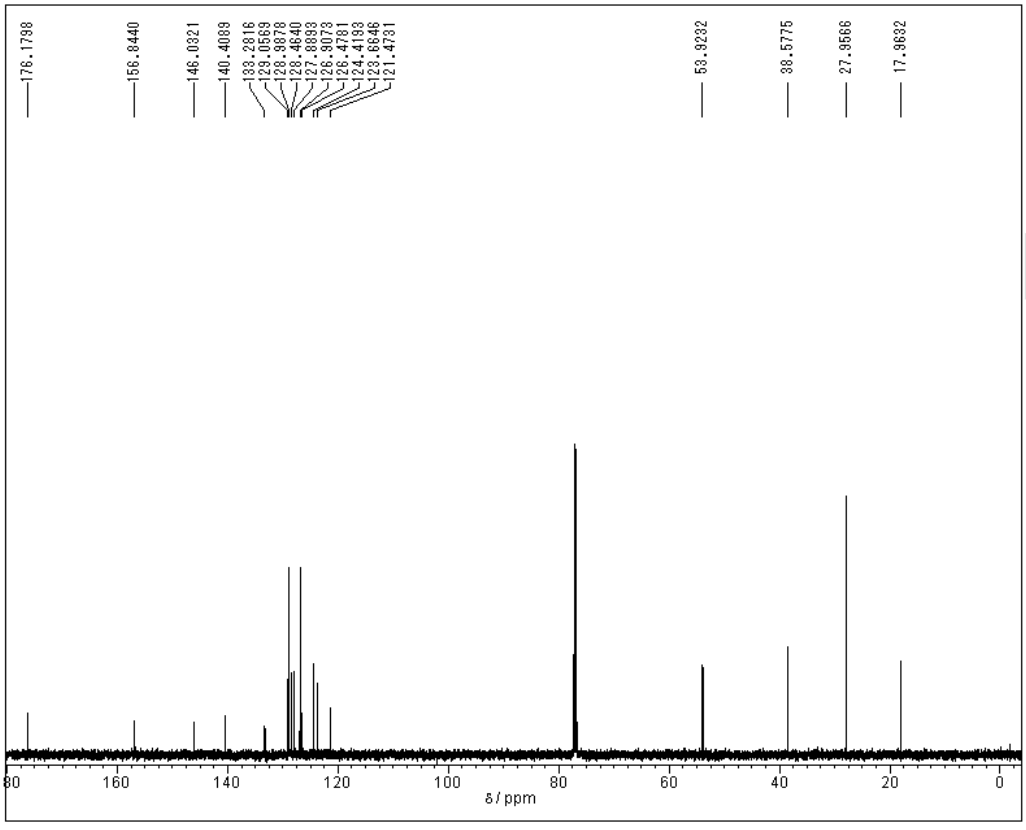
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent CDCL3

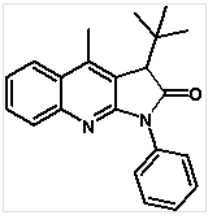
17d





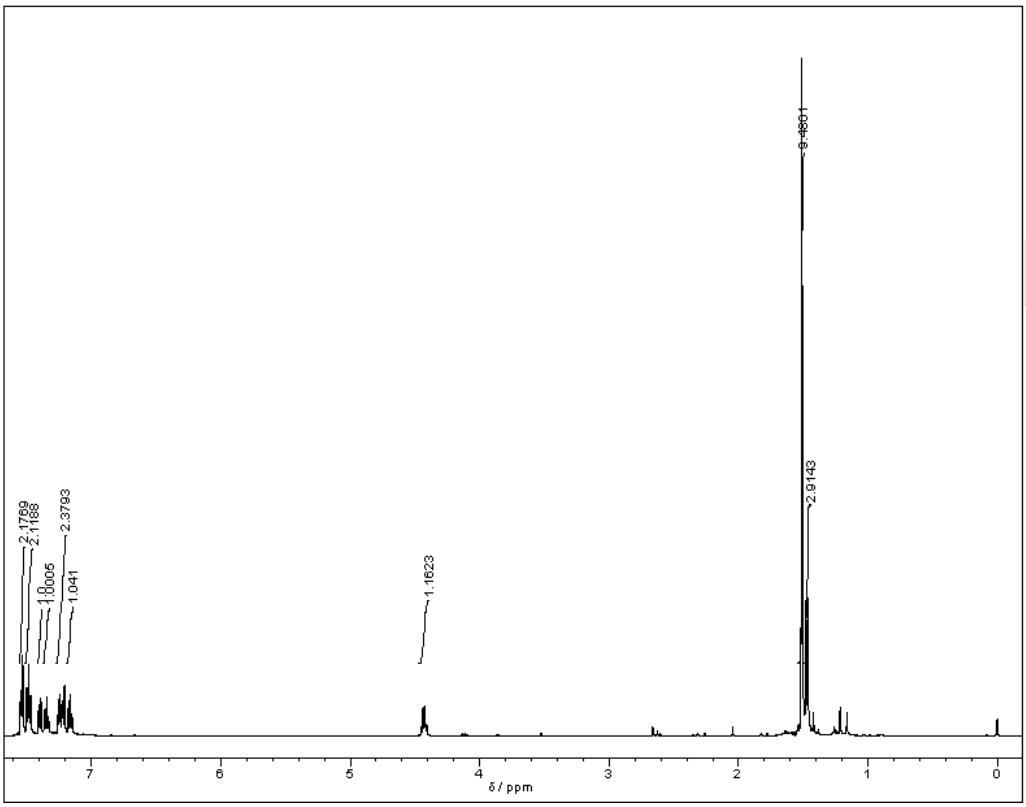
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent CDCL₃

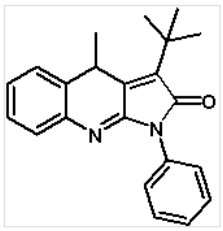




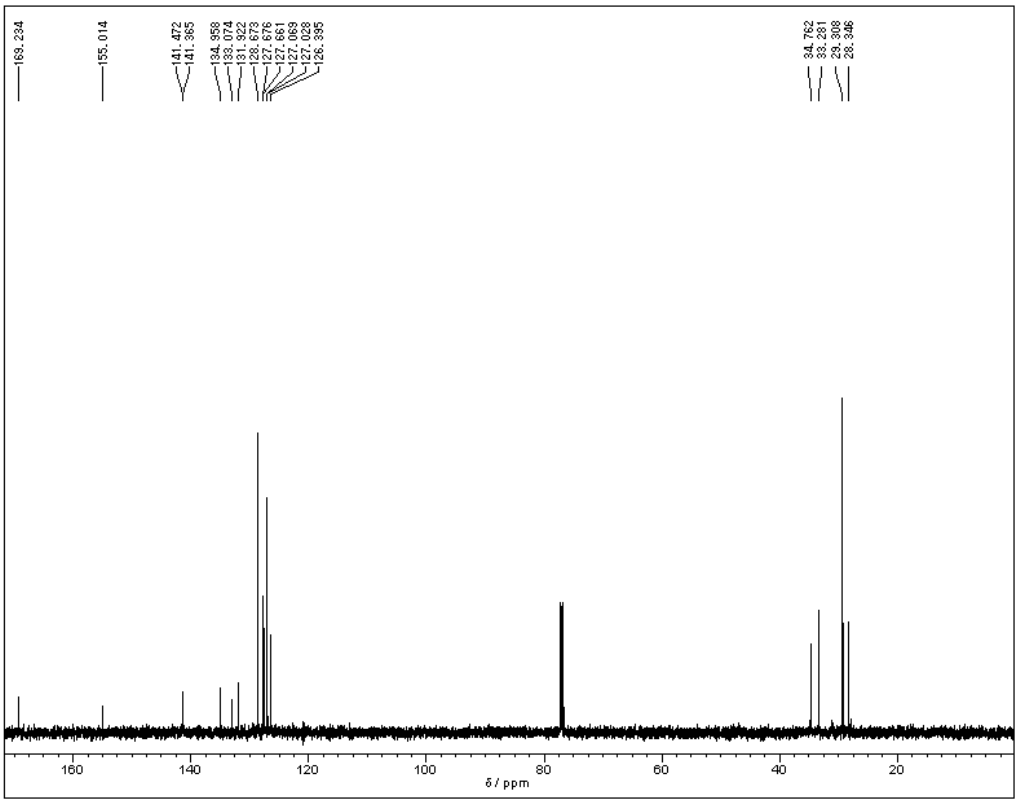
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent CDCL₃

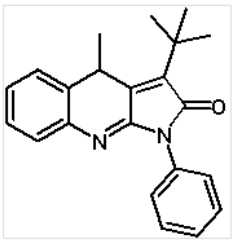
18b





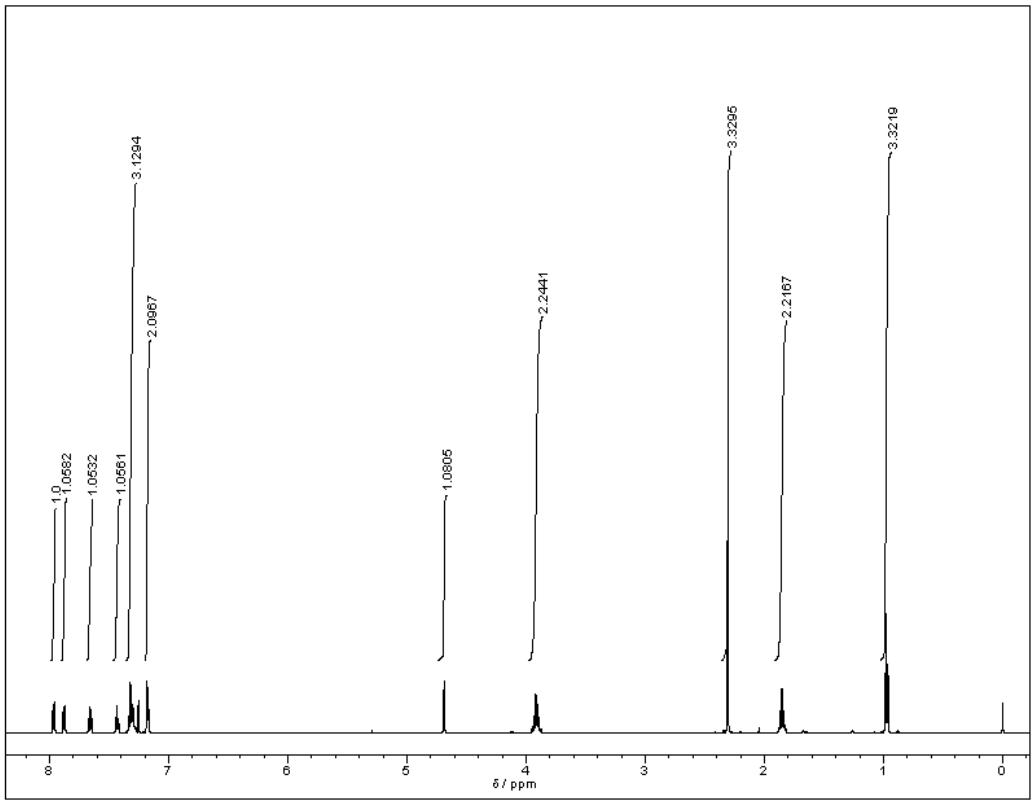
ObsNuc ^{1}H
ObsFreq 500.0 MHz
Solvent CDCL3

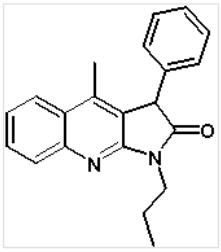




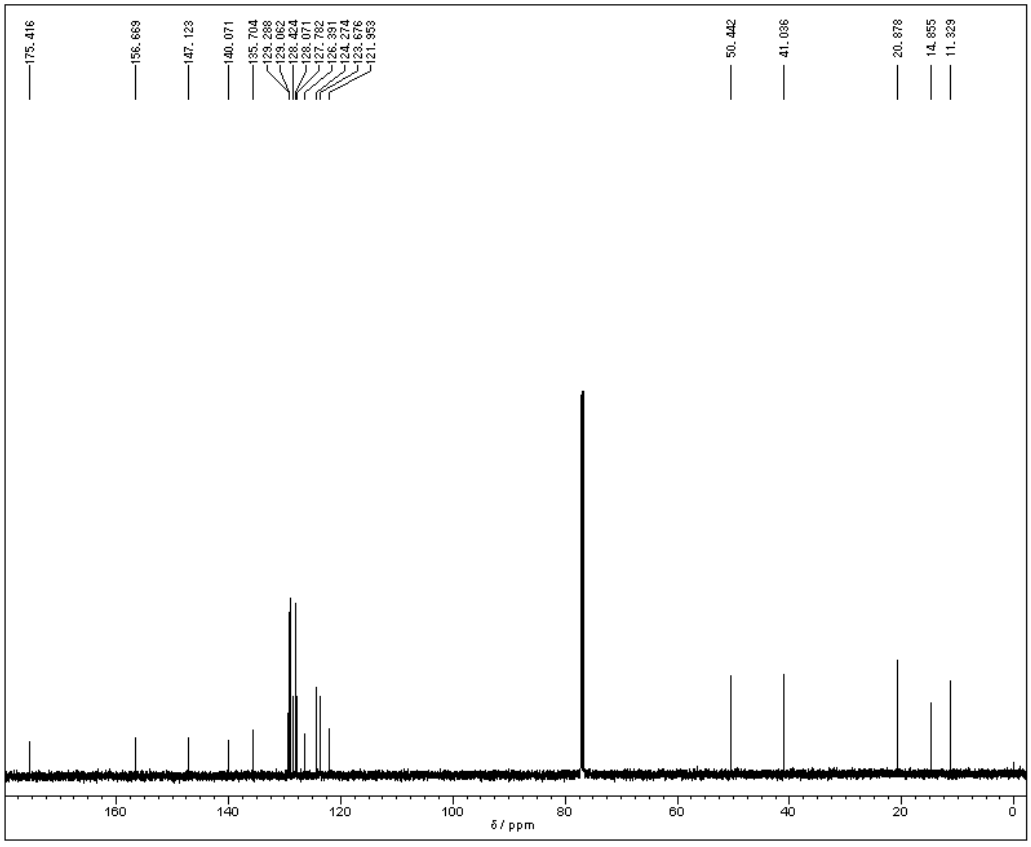
ObsNuc ^{13}C
ObsFreq 125.65 MHz
Solvent CDCL3

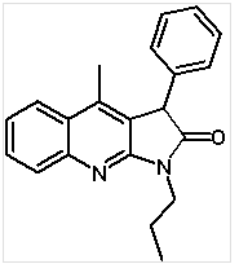
17e





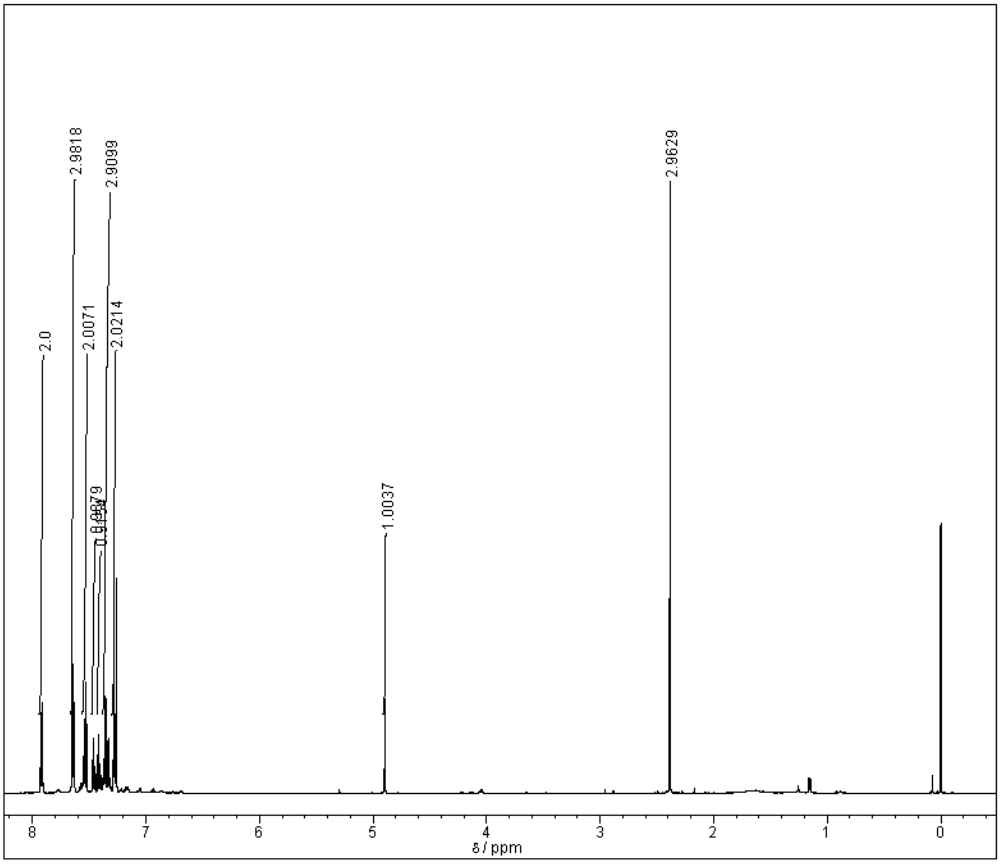
ObsNuc ^{1}H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

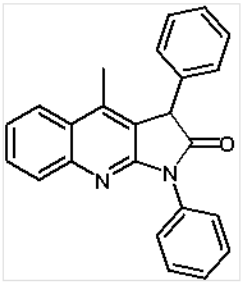




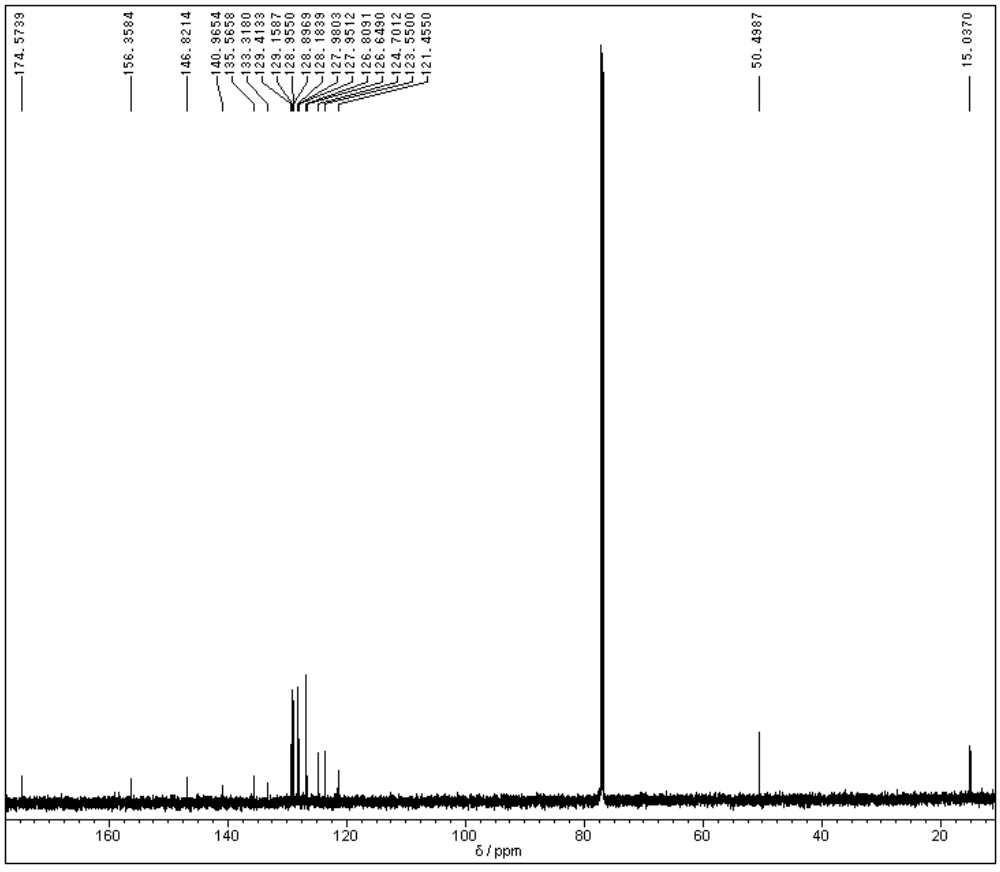
ObsNuc ^{13}C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

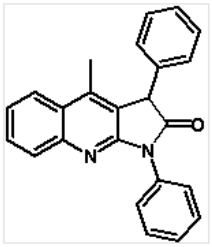
17f





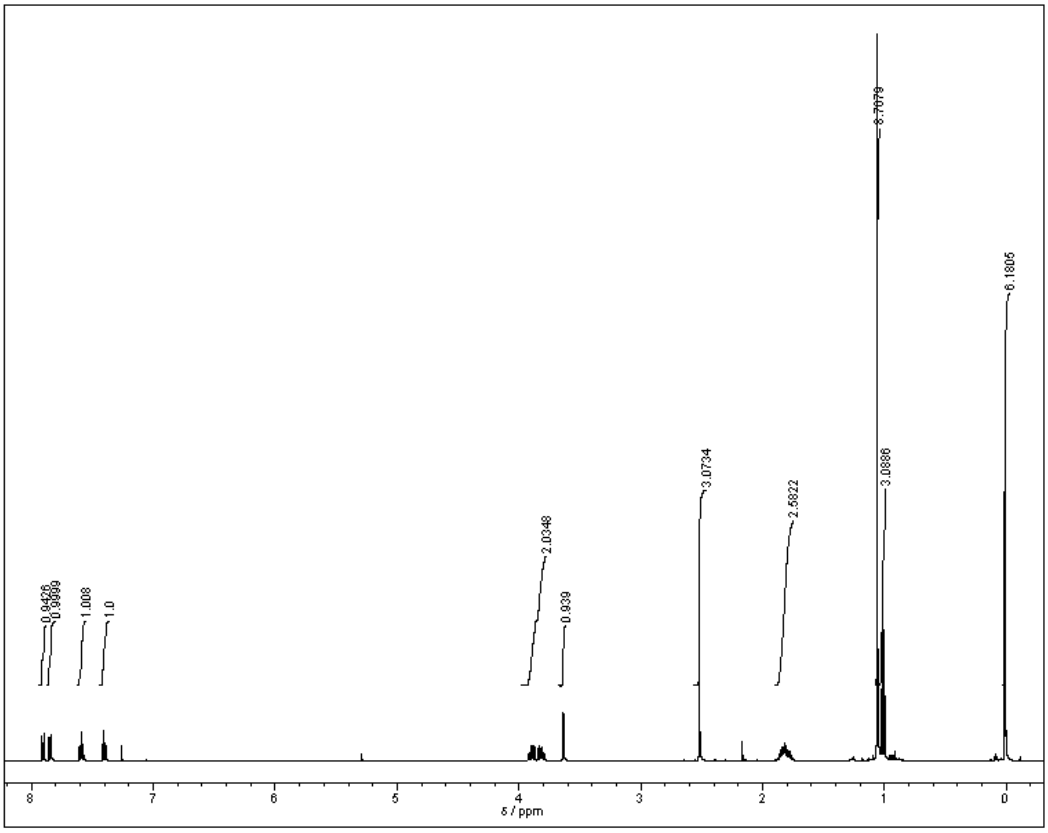
ObsNuc ¹H
ObsFreq 600.13 MHz
Solvent $CDCl_3$

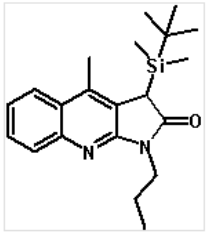




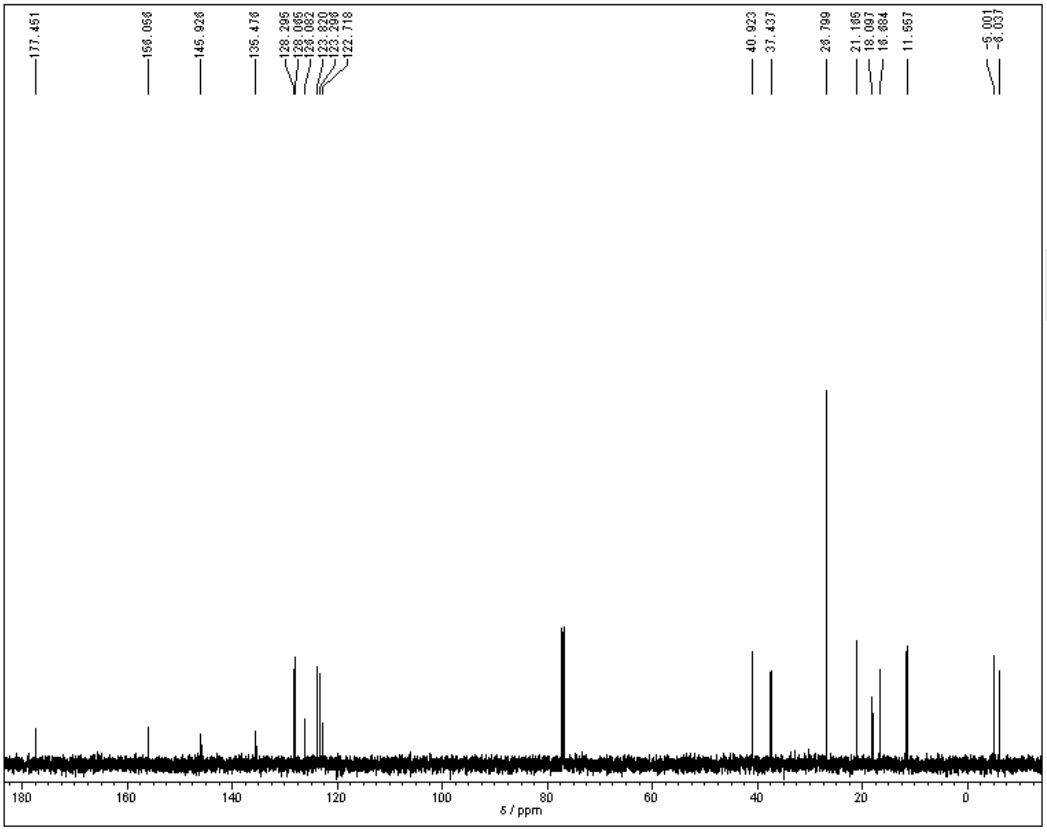
ObsNuc ¹³C
ObsFreq 150.9 MHz
Solvent $CDCl_3$

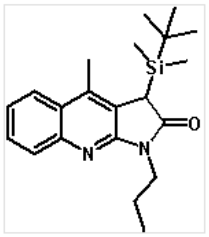
17g





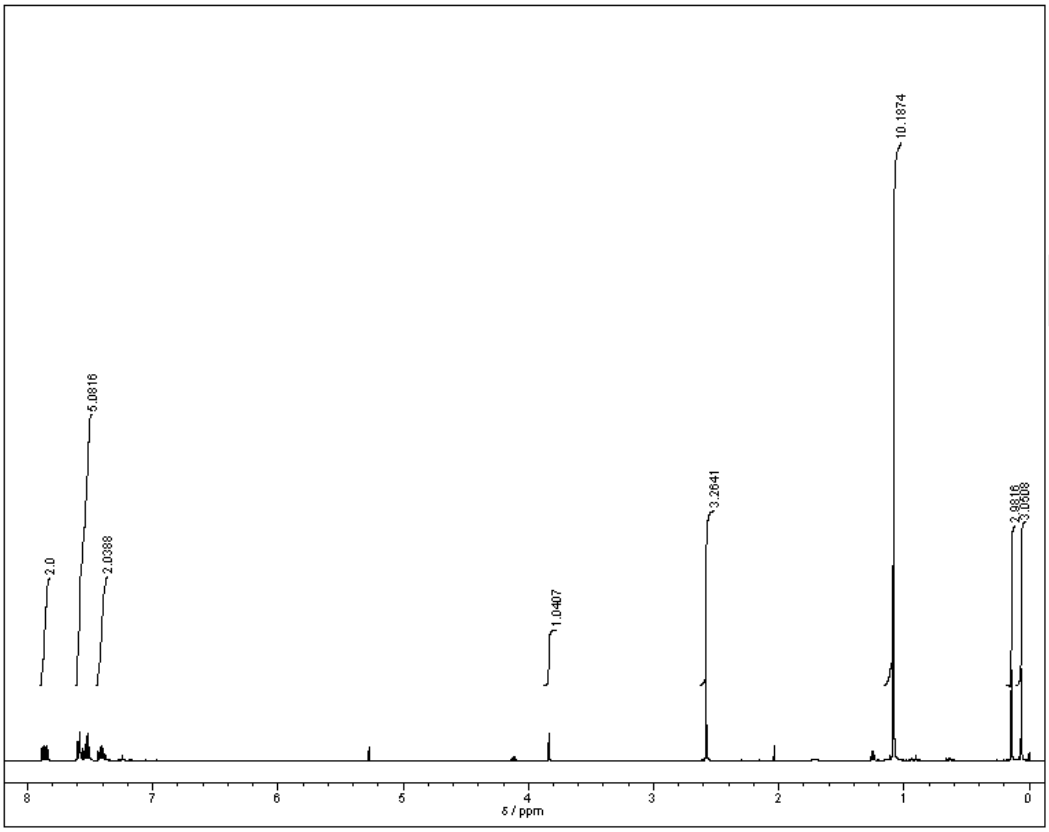
Obs Nuc	^{1}H
Obs Freq	500.0 MHz
Solvent	$CDCl_3$

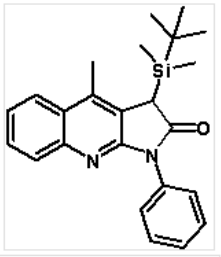




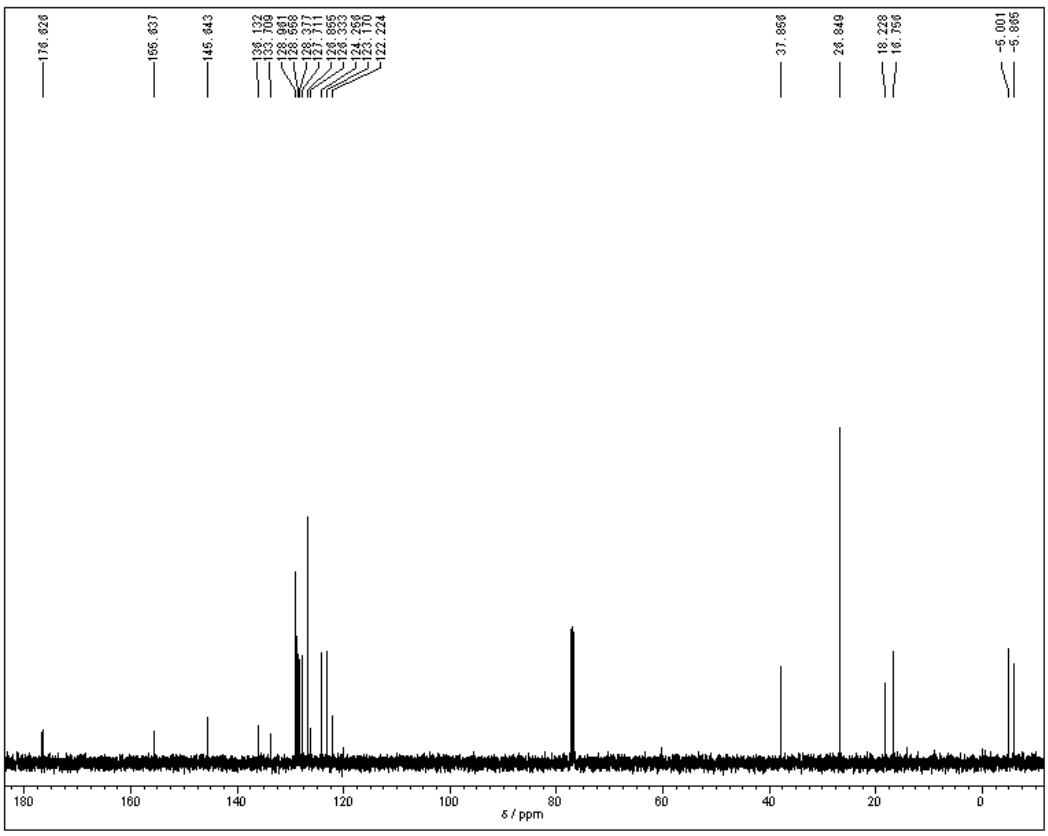
Obs Nuc	^{13}C
Obs Freq	125.65 MHz
Solvent	$CDCl_3$

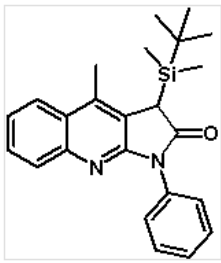
17h





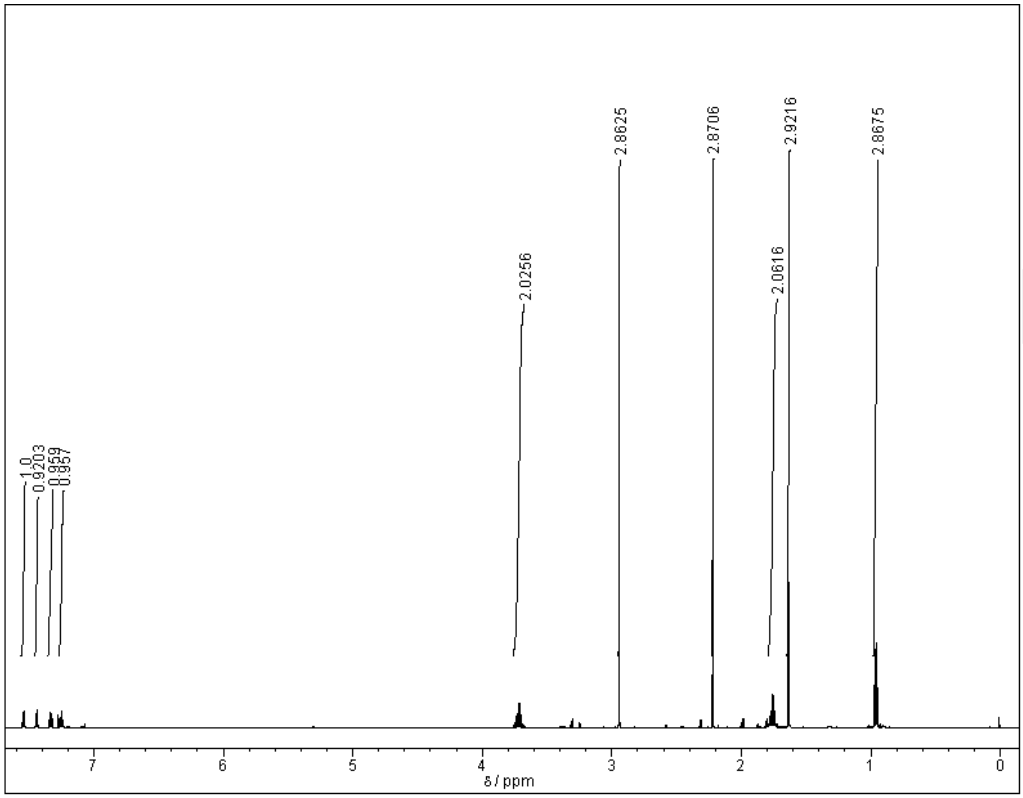
ObsNuc	^{1}H
ObsFreq	500.0 MHz
Solvent	$CDCl_3$

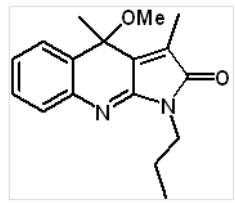




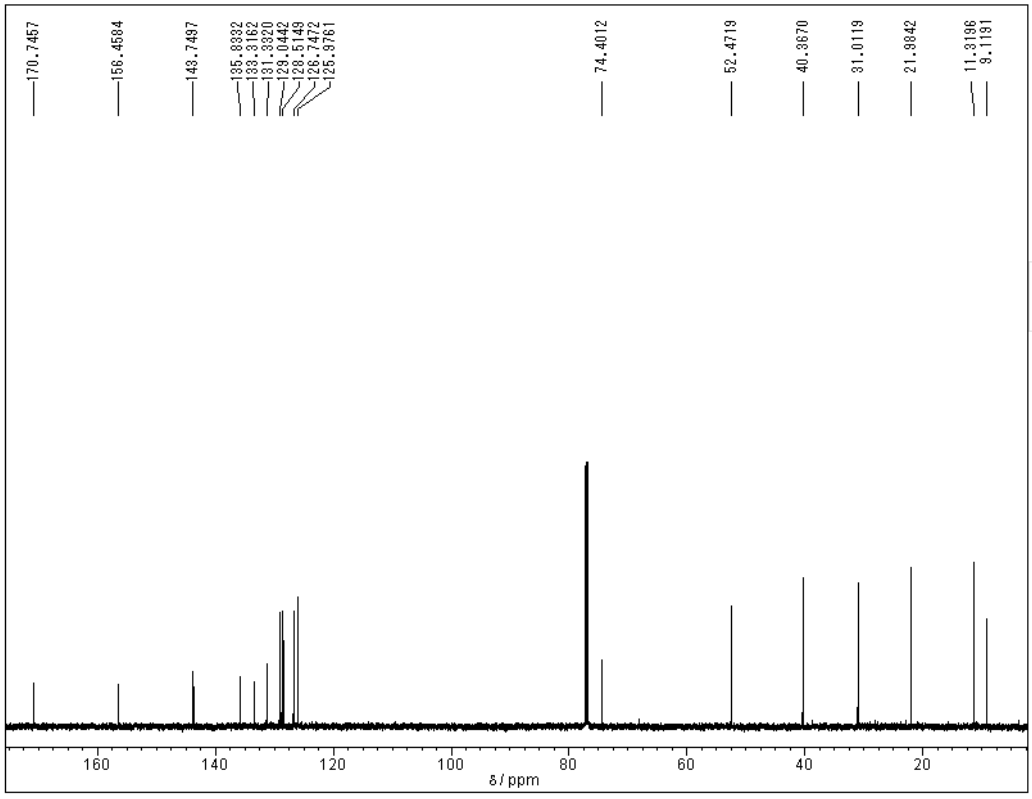
ObsNuc	^{13}C
ObsFreq	125.65 MHz
Solvent	$CDCl_3$

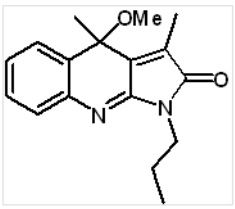
19a





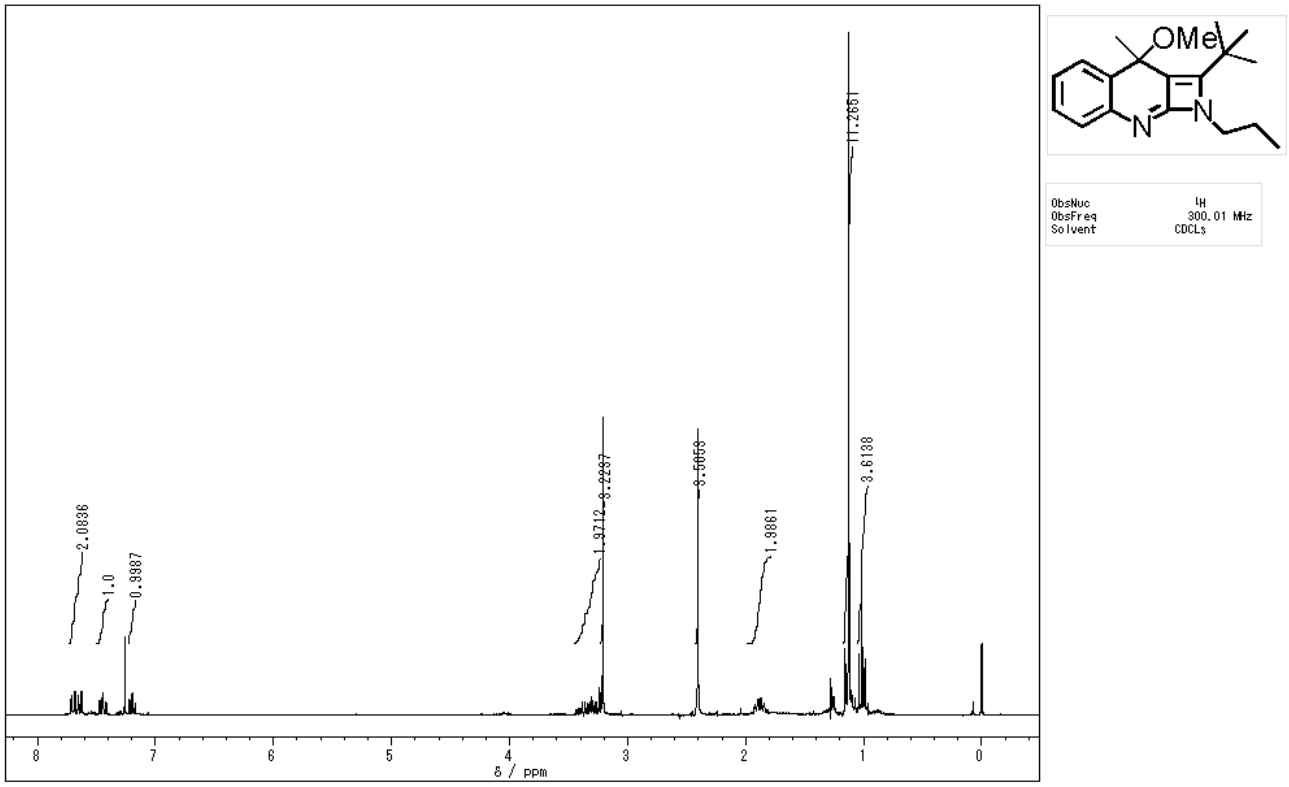
ObsFreq 600.13 MHz
ObsNuo ^{1}H
Solvent $CDCl_3$

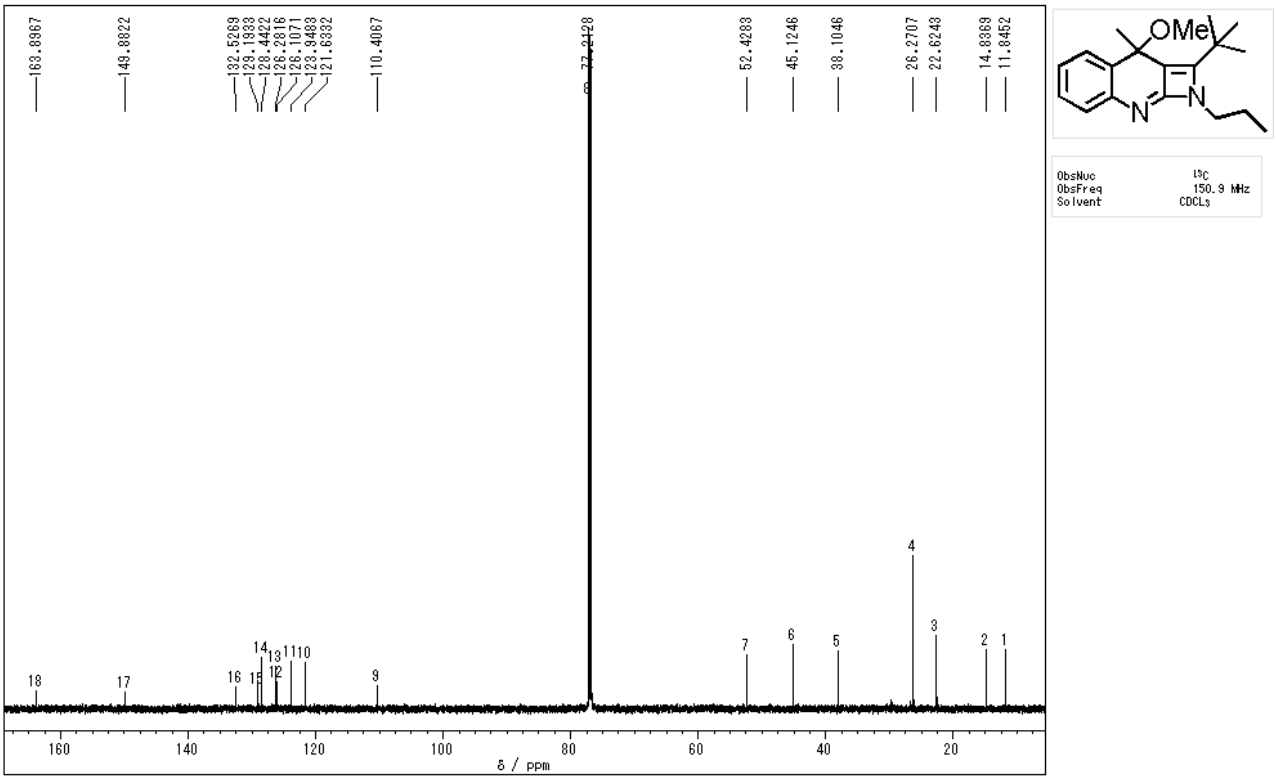




ObsFreq 150.9 MHz
ObsNuo ^{13}C
Solvent $CDCl_3$

20


2.0836
1.0
0.9887
1.9712
3.2837
3.5053
1.9861
11.2661
3.6138
8
7
6
5
4
3
2
1
0
δ / ppm
OMe
N
N
ObsNuc 1H
ObsFreq 300.01 MHz
Solvent CDCL3


168.8867
149.8822
132.5269
129.1933
128.4422
126.2816
126.1071
123.9483
121.6332
110.4067
77.2428
52.4283
45.1246
38.1046
28.2707
22.6243
14.8369
11.8452
18
17
16
15
14
13
12
11
10
9
7
6
5
4
3
2
1
160
140
120
100
80
60
40
20
δ / ppm
OMe
N
N
ObsNuc 13C
ObsFreq 150.9 MHz
Solvent CDCL3