Supporting Information

Photoinduced copper-catalyzed asymmetric cyanoalkylalkynyl-ation of alkenes, terminal alkynes, and oximes

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Content

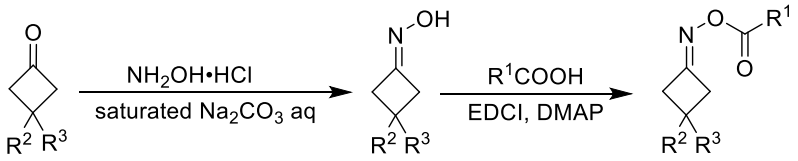
1 General information

NMR characterization data were collected on Bruker ASCENDTM operating at 400 MHz or bruker ASCENDTM 600 M. for ^{1}H NMR, 101 MHz for $^{13}C\{1H\}$ NMR (with complete proton decoupling), and 376 MHz for $^{19}F\{1H\}$ NMR (with complete proton decoupling). ^{1}H NMR and $^{13}C\{1H\}$ NMR: chemical shifts δ were recorded in ppm relative to tetramethylsilane and internally referenced to the residual solvent signal (for ^{1}H NMR: $CDCl_3$ = 7.26 ppm; for ^{13}C NMR: $CDCl_3$ = 77.16 ppm). $^{19}F\{1H\}$ NMR Chemical shifts are reported in ppm with relative to $CFCl_3$ (external reference, δ $^{19}F(CFCl_3)$ = 0. Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet), coupling constants (Hz), integration. High performance liquid chromatography (HPLC) was performed using Daicel Chiralcel columns at 23 °C with UV detector at 254 nm or 210 nm and enantiomeric excesses were determined in comparison with the authentic racemates. UPC^2 analysis used the corresponding commercial chiral column as stated in the experimental procedures at 35 ºC. High resolution mass spectra (HRMS) were performed on Thermo Q-Exactive Focus (ESI) and data were reported as (m/z). Infrared spectra (IR) were recorded on Bruker Tensor II spectrometer with Plantium ATR accessory and the peaks are reported as absorption maxima (ν, cm^{-1}). Optical rotations were measured on Rudolph Research Analytic Automatic Polarimeter, and reported as follows: $[\alpha]_D^T$ (c: g/100 mL, in CH_2Cl_2), which were measured at the light of 405 nm. UV-vis absorbance spectra were recorded on Hitachi U-3900H UV-vis spectrophotometer in a 10.0 mm quartz cuvette. Emission spectra were measured on FlouroMax$^+$ fluorescence spectrophotometer in a 10.0 mm quartz cuvette. Cyclic voltammograms were obtained on a CHI 605E potentiostat. The working electrode was glassy carbon electrode (φ 3 mm * 15 mm), the auxiliary electrode was platinum wire (φ 0.5 mm * 37 mm) and the reference electrode was Ag/AgCl electrode. Unless otherwise indicated, reagents obtained from commercial sources were used without further purification. Solvents were dried and distilled prior to use according to the standard methods. Metal salts obtained from commercial sources were used without further purification.

2 Synthesis of the Substrates

2.1 General procedure for the preparation of the cyclobutanone oxime esters.

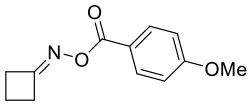
The Cyclobutanone Oxime Esters were prepared according to reported methods.[1]



The procedure for the synthesis of cyclobutanone oxime: The ketone (5.0 mmol, 1.0 equiv) and hydroxylamine hydrochloride (5.5 mmol, 1.1 equiv) were placed in a 100 mL flask equipped with stirrer, and methanol (10 mL) was added. The pH of the solution was held at 7–8 by adding saturated aq. sodium carbonate (10 mL). The resulting solution was stirred at 40 ℃ for 3h. After extraction with ethyl acetate, the solution was dried over Na_2SO_4 and evaporated to provide crude products which were used in the next step without further purification.

The procedure for the synthesis of cyclobutanone oxime esters: To a solution of cyclobutanone oxime (1.0 equiv.) in DCM (0.1 M) was added the carboxylic acid (1.1 equiv.), followed by EDCI (1.1 equiv.) and DMAP (0.1 equiv.). The mixture was stirred at room temperature for 12h. The mixture was extracted with DCM. The combined organic phase was dried over Na_2SO_4. The crude product was purified by silicon chromatography (petroleum ether/ ethyl acetate, 2:1, v/v) to give pure product.

cyclobutanone O-(4-methoxybenzoyl) oxime (A1)



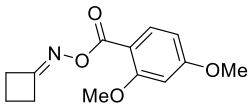
A1

white solid, 78% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ (ppm) 8.00 (d, J = 8.8 Hz, 2H), 6.93 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H), 3.13 (t, J = 8.0 Hz, 4H), 2.13 – 2.03 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 168.7, 163.7, 163.4, 131.5, 121.1, 113.6, 55.4, 31.8, 31.7, 14.2.

cyclobutanone O-(2,4-dimethoxybenzoyl) oxime (A2)



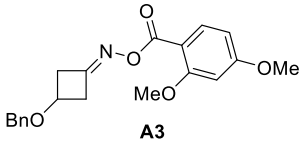
A2

white solid, 75% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 8.6 Hz, 1H), 6.51 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.48 (d, *J* = 2.4 Hz, 1H), 3.87 (s, 3H), 3.86 (s, 3H), 3.15 – 3.04 (m, 4H), 2.08 (p, *J* = 8.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.81, 164.55, 163.93, 161.29, 134.01, 111.47, 104.81, 99.15, 56.08, 55.65, 32.25, 31.98, 14.38.

3-(benzyloxy)cyclobutan-1-one O-(2,4-dimethoxybenzoyl) oxime (A3)



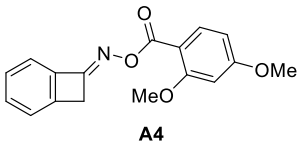
A3

colourless oil, 78% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.6 Hz, 1H), 7.32 – 7.16 (m, 5H), 6.45 – 6.36 (m, 2H), 4.47 – 4.35 (m, 2H), 4.24 – 4.12 (m, 1H), 3.76 (d, *J* = 3.6 Hz, 6H), 3.33 – 3.18 (m, 2H), 3.07 – 2.89 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.57, 163.69, 162.45, 161.23, 137.29, 133.98, 128.60, 128.07, 127.96, 111.06, 104.82, 99.02, 71.15, 66.77, 55.97, 55.57, 53.53, 40.63, 40.27.

bicyclo[4.2.0]octa-1(6),2,4-trien-7-one O-(2,4-dimethoxybenzoyl) oxime (A4)



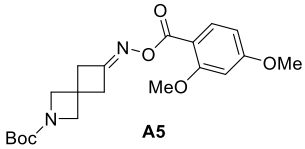
A4

white solid, 58% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.6 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.43 – 7.29 (m, 2H), 6.57 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.53 (d, *J* = 2.4 Hz, 1H), 4.03 (s, 2H), 3.92 (s, 3H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.64, 163.95, 161.23, 157.62, 146.05, 138.76, 134.19, 133.40, 128.54, 123.38, 111.01, 104.94, 99.09, 55.92, 55.58, 39.96.

tert-butyl 6-(((2,4-dimethoxybenzoyl)oxy)imino)-2-azaspiro[3.3]heptane-2-carboxylate (A5)



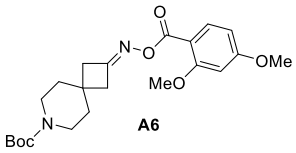
A5

white solid, 80% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 8.7 Hz, 1H), 6.52 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.48 (d, *J* = 2.3 Hz, 1H), 4.05 (q, *J* = 9.2 Hz, 4H), 3.87 (d, *J* = 6.4 Hz, 6H), 3.32 – 3.25 (m, 4H), 1.44 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.52, 163.40, 162.84, 161.12, 155.87, 133.84, 110.57, 104.77, 98.80, 79.64, 55.82, 55.43, 42.93, 42.58, 31.53, 28.22.

tert-butyl 2-(((2,4-dimethoxybenzoyl)oxy)imino)-7-azaspiro[3.5]nonane-7-carboxylate (A6)



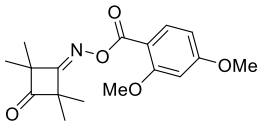
A6

white solid, 85% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 8.7 Hz, 1H), 6.54 – 6.50 (m, 1H), 6.48 (d, *J* = 2.4 Hz, 1H), 4.05 (q, *J* = 9.2 Hz, 4H), 3.87 (d, *J* = 6.4 Hz, 6H), 3.32 – 3.25 (m, 4H), 1.44 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.37, 164.22, 163.42, 161.03, 154.60, 133.70, 110.78, 104.68, 98.75, 79.41, 55.80, 55.36, 41.87, 41.59, 36.11, 32.99, 28.25.

3-(((2,4-dimethoxybenzoyl)oxy)imino)-2,2,4,4-tetramethylcyclobutan-1-one (A7)



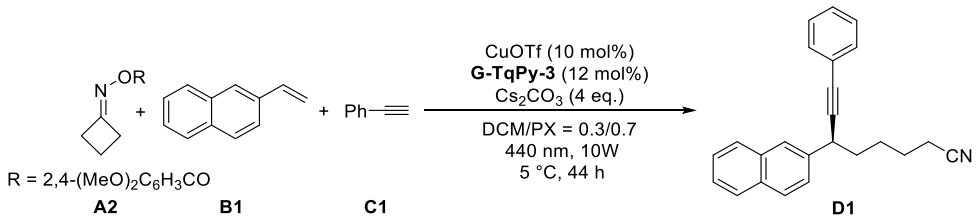
A7

white solid, 53% yield.

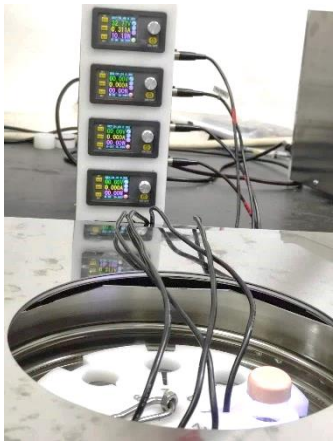
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.8 Hz, 1H), 6.55 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.49 (d, *J* = 2.4 Hz, 1H), 3.88 (s, 3H), 3.87 (s, 3H), 1.52 (s, 6H), 1.49 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 215.01, 173.26, 164.85, 164.07, 161.01, 134.65, 110.91, 105.06, 99.07, 65.60, 63.09, 55.83, 55.71, 21.55, 19.77.

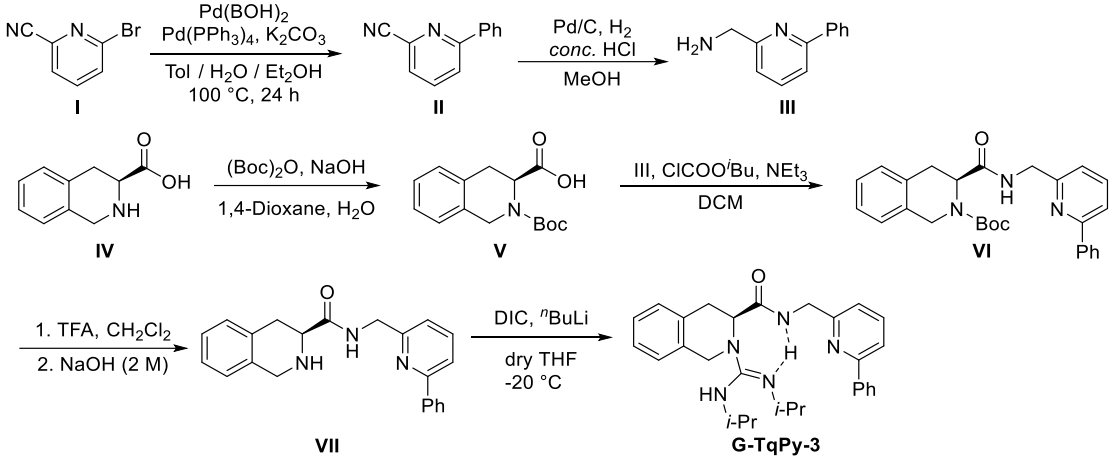
3 General procedure for the catalytic asymmetric reaction



In a glove box, a dry reaction tube was charged with CuOTf (10 mol%), **G-TqPy-3** (12 mol%) and Cs_2CO_3 (0.4 mmol), then **A2** (0.3 mmol), PX (0.7 mL) and dichloromethane (0.3 mL) were added. Subsequently **B1** (0.1 mmol) and **C1** (0.3 mmol) were added into the above solution with a microinjector. The mixture was stirred under 10 W LED (440 nm) irradiation at 5 ℃. After 44 h, the mixture was subjected to column chromatography on silica gel (eluent: petroleum ether/ acetone = 20/1, v/v) to afford the desired product.



4 Typical procedure for the synthesis of the ligand



The procedure for the synthesis of II: 6-Chloro-2-pyridinecarbonitrile (5.55 g, 30 mmol), phenylboric acid (4.40 g, 36 mmol), potassium carbonate (12.00 g, 90 mmol) and tetrakis(triphenylphosphine)palladium (0) (1.04 g, 0.9 mmol) were placed in a 250 mL flask. The mixture was deairated under reduced pressure for 3 times, then Tol (100 mL), Et_2OH (30 mL) and H_2O (30 mL) was added under nitrogen atmosphere. The reaction mixture was refluxed for 24 h. After that, the mixture was washed with with ethyl acetate and water. The organic layer was washed with saturated brine and dried over anhydrous sodium sulfate. The solvent was evaporated, and the residue was subjected to a silica gel column chromatography. The crude product was purified by silicon chromatography (petroleum ether/ ethyl acetate, 8:1, v/v) to give pure product. (4.8 g, 89 %).

The procedure for the synthesis of III: A Parr bottle was charged with II (4.8 g, 26.70 mmol) and methanol (150 mL). Stir vigorously to dissolve it. After adding 10% Pd-C (w/w, 1g) and concentrated hydrochloric acid (15 mL), place the Parr bottle on a Parr Hydrogenation Apparatus under 50 psig hydrogen at ambient temperature for 24 h. Filter the mixture through a pad of Celite. The filtrate concentrated under reduced pressure to remove methanol. Then the mixture was washed with with ethyl acetate and water. The water phase was collected and adjusted to alkaline with saturated sodium hydroxide solution. The water phase was extracted with ethyl acetate, then the combined organic layers were washed with saturated brine, dried over anhydrous Na_2SO_4, concentrated in vacuo, Use crude product in next step without further purification.

The procedure for the synthesis of V: To a 250 mL round-bottom flask was added IV (6.75 g, 50 mmol), NaOH (2.2 g, 55 mmol), H_2O (40 mL) and 1,4-Dixoane (60 mL). After fully dissolved, $(Boc)_2O$ (13,10 g, 60 mmol) was added in ice bath. The reaction mixture was stirred overnight at room temperature. After the 1,4-Dioxanet was removed under reduced pressure, the mixture was adjusted with 1 M $KHSO_4$ solution to acidity and extracted with DCM, the combined organics were washed with saturated brine, dried over anhydrous Na_2SO_4, vaporated to provide crude products which were used in the next step without further purification. (13.80 g, 99% yield)

The procedure for the synthesis of VI: To the solution of V (2.80 g, 10.0 mmol, 1.0 equiv.) in CH_2Cl_2 (20 mL) was added Et_3N (1.12 g, 12 mmol, 1.2 equiv.), isobutyl carbonochloridate (1.64 g, 12.0 mmol, 1.2 equiv.)at 0 °C under stirring. After 30 min, III (2.20 g, 12.0 mmol, 1.2 equiv.) was added. The reaction mixture was stirred at room temperature and detected by TLC. Overnight, the mixture was washed with 1 M $KHSO_4$ solution, saturated $NaHCO_3$ solution, brine, dried over

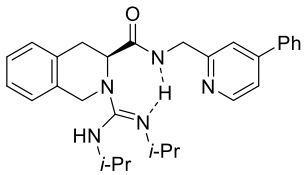
anhydrous Na_2SO_4, filtered, concentrated in vacuo, the crude product was purified by silicon chromatography (ethyl acetate) to give pure product. (3.50 g, 80 %).

The procedure for the synthesis of VII: TFA (10 mL) was added to the solution of amide VI in CH_2Cl_2 (15 mL) at 0 °C. The mixture was warmed to room temperature and stirred for 1h. Then, CH_2Cl_2 (20 mL) was added. The pH value of the mixture was brought into the range of 10–12 by the addition of 2 M NaOH solution. The aqueous phase was extracted with CH_2Cl_2. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated, the residue was subjected to flash column chromatography on silica gel and eluted with EtOAc (1/1, v/v) to give the white solid VII (2.41 g, 86% yield).

The procedure for the synthesis of G-TqPy-3: In an over-dried RB flask, amide VII (1.00 mmol, 1.0 equiv.) was dissolved in THF (20 mL) and cooled to -20 °C under nitrogen atmosphere. n-BuLi (2.4 M in hexane, 2.2 mmol, 2.2 equiv.) was added dropwise. After stirring at -20 °C for 30 mins, N,N'-diisopropylcarbodiimide (1.00 mmol, 1.0 equiv.) was added dropwise. The reaction mixture was slowly warmed up to rt and further stirred for 48 h. The reaction was quenched with ethanol and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel (eluent: DCM/MeOH/NEt_3 = 85:15:1). And the product was dissolved in ethyl acetate and washed by saturated sodium bicarbonate solution to afford the corresponding guanidine (0.34 g, 73% yield). [2] **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.63 (s, 1H), δ 8.03 – 7.97 (m, 2H), 7.78 – 7.62 (m, 2H), 7.48 – 7.31 (m, 4H), 7.15 – 7.10 (m, 3H), 7.02 – 6.97 (m, 1H), 6.12 (s, 1H), 4.28 – 3.61 (m, 6H), 3.71 – 3.28 (m, 1H), 2.95 – 2.79 (m, 1H), 1.23 – 1.05 (m, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.31, 156.54, 156.45, 138.50, 138.34, 135.93, 135.83, 134.12, 134.07, 129.46, 129.36, 129.29, 128.86, 126.86, 126.51, 126.48, 126.25, 125.82, 120.32, 119.69, 56.78, 56.61, 47.55, 47.35, 31.45, 31.20, 24.28, 22.72. **ESI-HRMS**: calcd for $C_{29}H_{36}N_5O^+$ ($[M + H]^+$) = 470.2914, found 470.2918.

The synthesis of the following guanidines followed the similar procedures.

Guanidine G-TqPy-4:



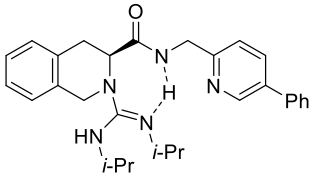
G-TqPy-4

white solid, 75% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.19 (s, 1H)δ 8.55 (t, *J* = 5.4 Hz, 1H), 7.89 – 7.56 (m, 3H), 7.49 – 7.39 (m, 4H), 7.15 – 7.07 (m, 3H), 7.03 – 6.97 (m, 1H), 6.12 (s, 1H), 4.32 – 3.56 (m, 6H), 3.21 – 3.13 (m, 1H), 2.84 – 2.97 (m, 1H), 1.26 – 0.97 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.13, 149.89, 149.79, 137.82, 136.02, 135.85, 134.22, 134.13, 129.66, 129.52, 129.47, 127.37, 127.34, 126.62, 126.41, 126.37, 125.99, 121.57, 120.21, 56.90, 47.72, 47.63, 31.52, 22.90, 14.36.

Guanidine G-TqPy-5:



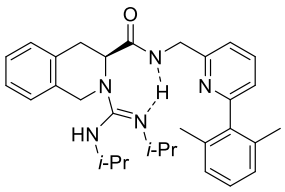
G-TqPy-5

white solid, 68% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.76 – 8.72 (m, 1H), 7.88 – 7.81 (m, 1H), 7.61 – 7.36 (m, 6H), 7.14 – 7.07 (m, 3H), 7.03 – 6.98 (m, 1H), 6.06 (s, 1H), 4.21 – 3.60 (m, 6H), 3.16 (dd, *J* = 16.4, 4.8 Hz, 1H), 2.97 – 2.84 (m, 1H), 1.10 – 1.21 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.45, 156.68, 138.64, 138.48, 136.07, 135.97, 134.26, 134.21, 129.60, 129.50, 129.43, 129.00, 127.01, 126.65, 126.62, 126.39, 125.96, 120.46, 119.83, 56.92, 56.75, 47.69, 47.49, 31.59, 31.34, 24.42, 22.86.

Guanidine G-TqPy-6:



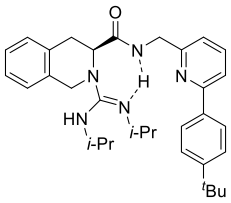
G-TqPy-6

white solid, 73% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.10 (s, 1H), δ 7.77 (q, *J* = 8.2 Hz, 1H), 7.56 – 7.38 (m, 1H), 7.22 – 7.15 (m, 2H), 7.16 – 7.08 (m, 5H), 7.07 – 6.95 (m, 1H), 6.15 (s, 1H), 4.25 – 3.58 (m, 6H), 3.15 (dt, *J* = 16.4, 4.4 Hz, 1H), 2.95 – 2.82 (m, 1H), 2.02 (d, *J* = 4.5 Hz, 6H), 1.07 – 1.19 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.32, 159.69, 140.27, 137.98, 136.03, 135.97, 135.93, 134.23, 134.18, 129.47, 129.41, 128.25, 127.80, 126.61, 126.57, 126.35, 125.96, 125.93, 124.39, 120.19, 56.92, 56.68, 47.69, 47.39, 31.81, 31.63, 29.92, 22.88, 20.55, 14.35, 11.66.

Guanidine G-TqPy-7：



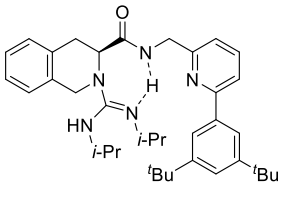
G-TqPy-7

white solid, 65% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) 8.00 – 7.97 (m, 2H), 7.74 – 7.66 (m, 2H), 7.52 – 7.49 (m, 2H), 7.23 – 7.14 (m, 4H), 7.07 – 7.03 (m, 1H), 5.98 (s, 1H), 4.29 – 3.55 (m, 6H), 3.24 – 3.17 (m, 1H), 2.96 – 2.89 (m, 1H), 1.38 (m, 9H), 1.18 – 0.96 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.66, 156.49, 138.14, 136.23, 129.55, 126.75, 126.44, 126.41, 125.99, 125.96, 119.26, 56.92, 47.80, 35.00, 31.57, 31.47, 29.97, 21.43.

Guanidine G-TqPy-8：



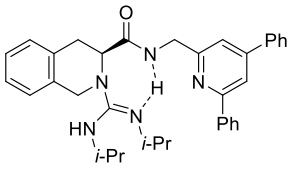
G-TqPy-8

white solid, 68% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.99 (s, 1H)δ 9.38 – 8.63 (m, 1H), 7.93 – 7.87 (m, 2H), 7.76 – 7.66 (m, 2H), 7.55 – 7.50 (m, 1H), 7.32 – 7.23 (m, 1H), 7.19 – 7.11 (m, 3H), 7.08 – 6.99 (m, 1H), 5.98 (s, 1H), 4.41 – 3.54 (m, 6H), 3.27 – 3.18 (m, 1H), 2.95 – 2.86 (m, 1H), 1.41 (d, *J* = 7.6 Hz, 18H), 1.18 – 0.95 (m, 12H).

13C NMR (101 MHz, CDCl3) δ 172.64, 157.61, 151.42, 138.03, 136.20, 136.02, 134.52, 134.42, 129.59, 126.69, 126.42, 126.38, 125.96, 125.92, 123.61, 121.57, 121.54, 119.80, 57.14, 57.00, 48.09, 48.00, 35.28, 31.78, 31.45, 24.22.

Guanidine G-TqPy-9：



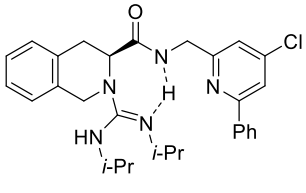
G-TqPy-9

white solid, 77% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.25 (s, 1H), δ 8.09 (d, *J* = 7.4 Hz, 2H), 7.87 (d, *J* = 6.0 Hz, 1H), 7.72 – 7.59 (m, 3H), 7.50 – 7.42 (m, 6H), 7.12 – 7.09 (m, 3H), 7.00 – 6.97 (m, 1H), 6.19 (s, 1H), 4.37 – 3.58 (m, 6H), 3.19 (dd, *J* = 16.4, 5.0 Hz, 1H), 2.98 – 2.88 (m, 1H), 1.24 – 1.10 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.22, 157.14, 157.06, 150.85, 138.78, 138.23, 135.97, 135.83, 134.17, 134.10, 129.52, 129.47, 129.37, 129.33, 128.91, 127.32, 127.29, 127.06, 126.52, 126.28, 126.25, 125.86, 118.49, 118.33, 117.98, 117.92, 56.81, 56.70, 47.53, 47.44, 31.45, 31.27, 23.29.

Guanidine G-TqPy-10：



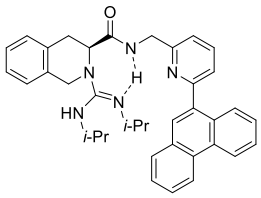
G-TqPy-10

white solid, 58% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 – 8.00 (m, 2H), 7.79 – 7.63 (m, 2H), 7.49 – 7.38 (m, 3H), 7.16 – 7.10 (m, 3H), 7.04 – 6.99 (m, 1H), 6.06 (s, 1H), 4.44 – 3.54 (m, 6H), 3.23 – 3.14 (m, 1H), 2.97– 2.86 (m, 1H), 1.23 – 1.00 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.20, 156.60, 138.81, 138.38, 136.09, 136.04, 134.32, 129.54, 129.50, 129.45, 129.00, 127.03, 126.68, 126.40, 125.96, 120.43, 120.26, 119.66, 56.91, 56.79, 47.70, 47.60, 31.83, 31.52, 22.89, 14.36, 11.67.

Guanidine G-TqPy-11：



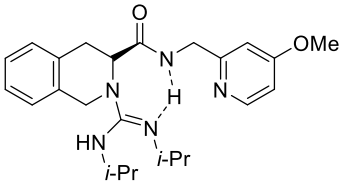
G-TqPy-11

white solid, 36% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.81 – 8.70 (m, 2H), 8.05 – 7.76 (m, 4H), 7.75 – 7.48 (m, 6H), 7.14 – 7.08 (dt, *J* = 6.8, 3.8 Hz, 3H),7.01 – 6.94 (dd, *J* = 9.0, 5.0 Hz, 1H), 6.20 (s, 1H), 4.43 – 3.46 (m, 6H), 3.21 – 3.14 (m, 1H), 2.98 – 2.87 (m, 1H), 1.24 – 0.99 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.80, 159.07, 138.40, 135.90, 134.11, 131.43, 130.99, 130.72, 130.38, 129.49, 129.43, 129.23, 128.85, 127.56, 127.27, 127.00, 126.92, 126.75, 126.58, 126.36, 125.98, 125.87, 124.94, 123.26, 122.86, 120.64, 56.88, 56.72, 47.90, 47.60, 47.39, 31.84, 31.63, 29.95, 22.91, 14.39.

Guanidine G-TqPy-12：



G-TqPy-12

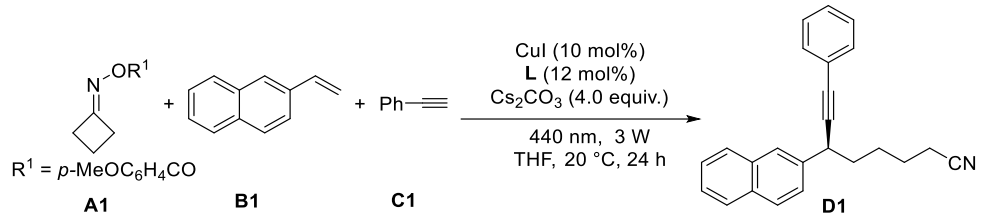
white solid, 62% yield. Synthesized from 4-methoxypicolinonitrile.

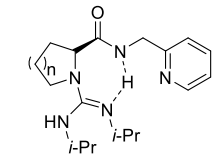
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (t, *J* = 5.6 Hz, 1H), 7.05 – 6.88 (m, 5H), 6.67 (td, *J* = 5.8, 2.4 Hz, 1H), 5.89 (s, 1H), 3.98 (s, 2H), 4.01 – 3.87 (m, 4H), δ 3.76 (d, *J* = 8.6 Hz, 1H), 3.63 – 3.57 (m, 1H), 3.14 – 3.04 (m, 1H), 2.81 (td, *J* = 16.2, 10.4 Hz, 1H), 1.15 – 1.00 (m, 12H).

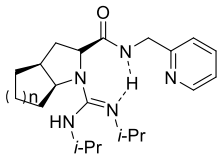
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.97, 166.76, 166.70, 150.33, 135.85, 135.69, 134.08, 133.98, 129.31, 129.28, 126.42, 126.19, 125.77, 110.01, 109.90, 107.89, 107.71, 56.72, 55.53, 55.46, 47.56, 47.51, 31.29, 31.23, 29.73, 23.13, 14.16.

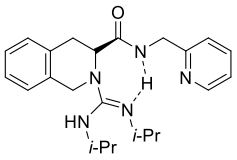
5 Optimization of the reaction conditions

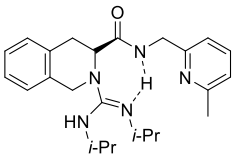
Table S1. Screening chiral ligands.

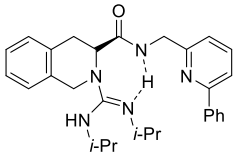


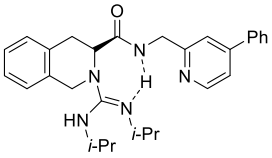

G-PrPy, n = 1
G-PiPy, n = 2

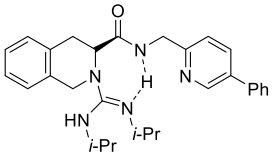

G-RaPy, n = 1
G-PePy, n = 2

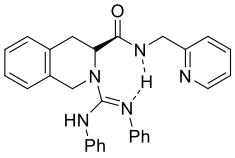

G-TqPy-1

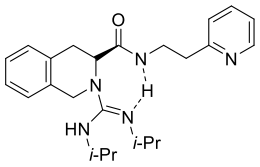

G-TqPy-2

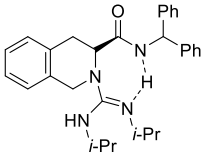

G-TqPy-3

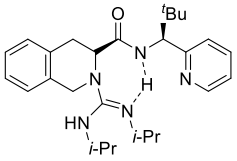

G-TqPy-4


G-TqPy-5


G²-TqPy


G³-TqPy


G⁴

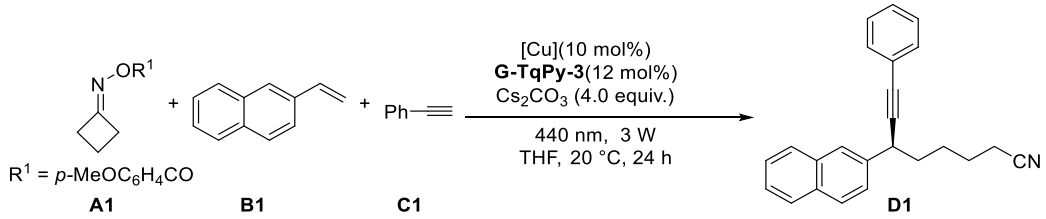

G-TqPy$^{(S)\text{-}t\text{Bu}}$

entry[a]	L	yield (%)[b]	ee (%)[c]
1	**G-RaPy**	15	40
2	**G-PrPy**	29	9
3	**G-PiPy**	12	34
4	**G-PePy**	15	42
5	**G-TqPy-1**	22	45
8	**G-TqPy-2**	24	43
9	**G-TqPy-3**	38	74
10	**G-TqPy-4**	18	45
11	**G-TqPy-5**	20	45
12	**G²-TqPy**	ND	-
13	**G³-TqPy**	ND	-
14	**G⁴**	ND	

15	**G-TqPy$^{(S)\text{-}t\text{Bu}}$**	ND	

[a] Unless otherwise noted, all reactions were performed with CuI/**Ligand** (1:1.2, 10 mol %), **A1** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), Cs_2CO_3 (0.4 mmol) in THF (1.0 mL) under 3 W LED (440 nm) irradiation at 20 ℃ for 24 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

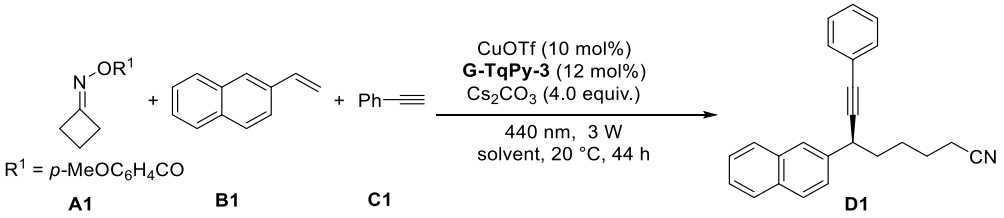
Table S2. Screening the copper salt.



entry[a]	[Cu]	yield (%)[b]	ee (%)[c]
1	$Cu(acac)_2$	36	71
2	$Cu(OTf)_2$	32	78
3	CuOTf	38	81
4	CuOTf•1/2C_6H_6	30	80
5	$Cu(ClO_4)_2$•$6H_2O$	30	73
6	CuTc	30	78
7	CuI	38	74
8[d]	CuOTf	46	85
9[d]	CuOAc	36	87
10[d]	CuC_2O_4	trace	83
11[d]	CuNTf	30	50

[a] Unless otherwise noted, all reactions were performed with [Cu]/**G-TqPy-3** (1:1.2, 10 mol %), **A1** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), Cs_2CO_3 (0.4 mmol) in THF (1.0 mL) under 3 W LED (440 nm) irradiation at 20 ℃ for 24 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2]. [d] The reactions were conducted in Tol (0.1 M) for 44 h.

Table S3. Screening the solvents.

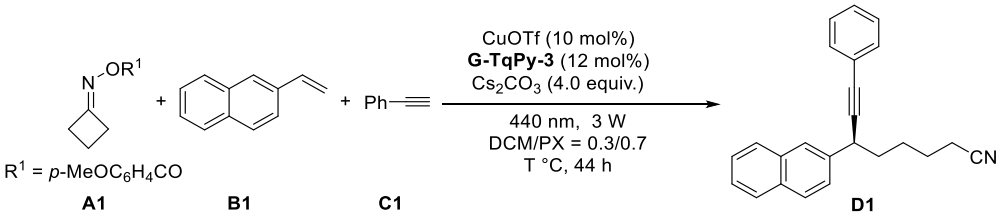


entry[a]	solvent	yield (%)[b]	ee (%)[c]

1	THF	36	85
2	DMF	ND	-
3	1,4-Dioxane	42	81
4	Cyclohexane	trace	72
5	EA	36	84
6	1,3,5-Trimethylbenzene	46	87
7	Tol	46	85
8	1,2-Xylene	44	87
9	p-Xylene (PX)	48	87
10	m-Xylene	46	86
11[d]	DCM	46	89
12 [d]	DCM / PX = 2/8	28	89
13[d]	DCM / PX = 3/7	34	91
14[d]	DCM / PX = 5/5	38	87
15[d]	DCM / PX = 7/3	37	88
16[d]	DCM / PX = 8/2	44	88

[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3** (1:1.2, 10 mol %), **A1** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol) , Cs_2CO_3 (0.4 mmol) in solvent (1.0 mL) under 3W LED (440 nm) irradiation at 20 ℃ for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2]. [d] The reactions were conducted under 3 W LED (440 nm) irradiation at 0 ℃ for 44 h.

Table S4. Screening reaction temperature.

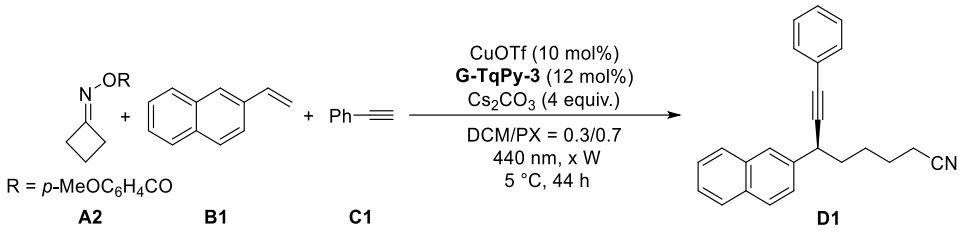


entry [a]	T (℃)	yield (%)[b]	ee (%)[c]
1	0	34	91
2	5	42	91
3	10	41	91
4	15	46	87

[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3** (1:1.2, 10 mol %), **A1** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol) , Cs_2CO_3 (0.4 mmol) in PX (0.7 mL) and DCM (0.3 mL) under 3W LED (440 nm)

irradiation for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

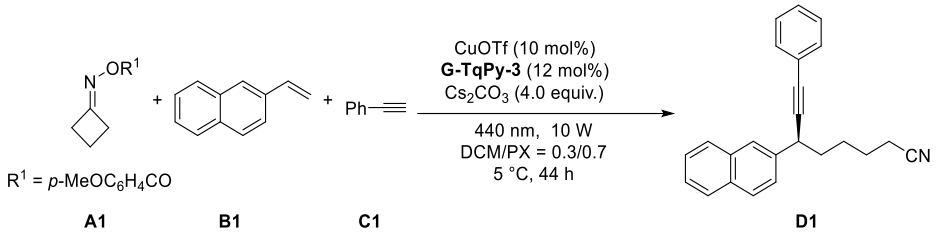
Table S5. Screening light sources.



entry [a]	x	yield (%)[b]	ee (%)[c]
1	3	42	91
2	5	47	86
3	10	51	87
4	15	47	84
5	20	48	85

[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3** (1:1.2, 10 mol %), **A1** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), Cs_2CO_3 (0.4 mmol) in PX (0.7 mL) and DCM (0.3 mL) under LED (440 nm) irradiation at 5 ℃ for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

Table S6. Screening the ratio of substrates.

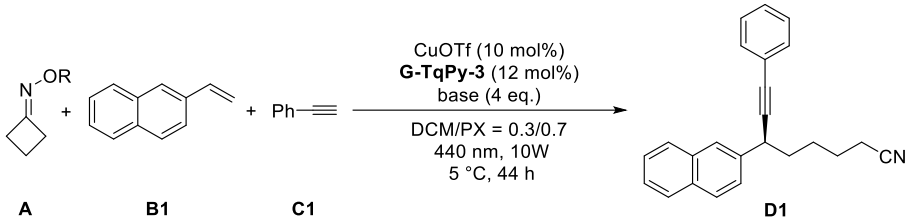


entry	ratio (**A1:B1:C1**)	yield of **D1** (%)[b]	ee (%)[c]
1	3:1:1	32	90
2	3:1:2	42	86
3	3:1:3	51	87
4	2:1:3	35	89
5	1:1:3	20	91
6	2:1:2	48	89
7	1:1:1	32	89
8	4:1:4	45	87
9	5:1:5	44	85
10	1:2:1	41	85

11	2:2:1	40	85
12	1:3:1	40	85

[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3** (1:1.2, 10 mol %), **A1** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), Cs_2CO_3 (0.4 mmol) in PX (0.7 mL) and DCM (0.3 mL) under 10 W LED (440 nm) irradiation at 5 °C for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

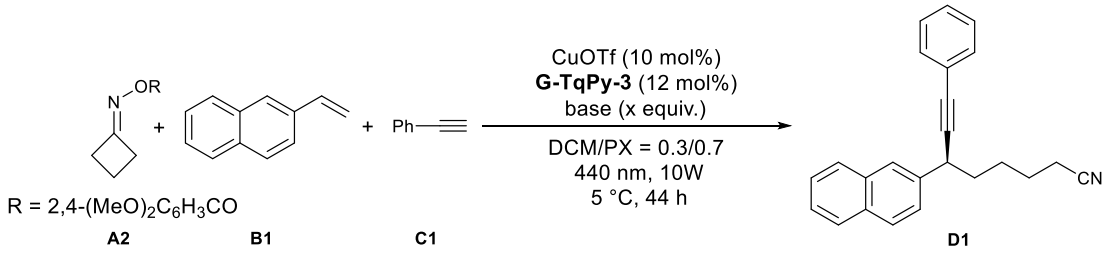
Table S7. Screening the N-protecting group of oximes.



entry	R	p*K*a of ROH in DMSO/AN (XGBoost)	yield (%)[b]	ee (%)[c]
1	R = C_6F_5CO	5.9/16.3	45	22
2	R = 3,5-$(CF_3)_2C_6H_3CO$	9.8/17.21	40	43
3	R = 4-$CF_3C_6H_4CO$	10.1/19.2	42	65
4	R = C_6H_5CO	10.2/20.9	48	87
5	R = 4-$MeOC_6H_4CO$	11.1/21.5	51	87
6	R = 2,4-$(MeO)_2C_6H_3CO$	11.7/20.7	52	91

[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3** (1:1.2, 10 mol %), **A** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), Cs_2CO_3 (0.4 mmol) in PX (0.7 mL) and DCM (0.3 mL) under 10W LED (440 nm) irradiation at 5 °C for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

Table S8. Screening basic additives.

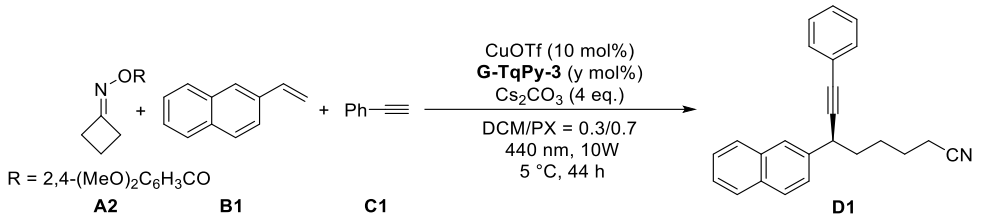


entry	base	yield (%)[b]	ee (%)[c]
1	K_3PO_4 (4.0 equiv.)	41	77
2	K_2CO_3 (4.0 equiv.)	28	60
3	Ba_2CO_3 (4.0 equiv.)	ND	
4	^{t}BuOK (4.0 equiv.)	ND	

5	NEt_3 (4.0 equiv.)	ND	
6	CH_3COOCs (4.0 equiv.)	ND	
7	Cs_2CO_3 (1.0 equiv.)	13	90
8	Cs_2CO_3 (2.0 equiv.)	42	90
9	Cs_2CO_3 (3.0 equiv.)	42	91
10	Cs_2CO_3 (4.0 equiv.)	52	91

[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3** (1:1.2, 10 mol %), **A2** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), base in PX (0.7 mL) and DCM (0.3 mL) under 10W LED (400 nm) irradiation at 5 ℃ for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

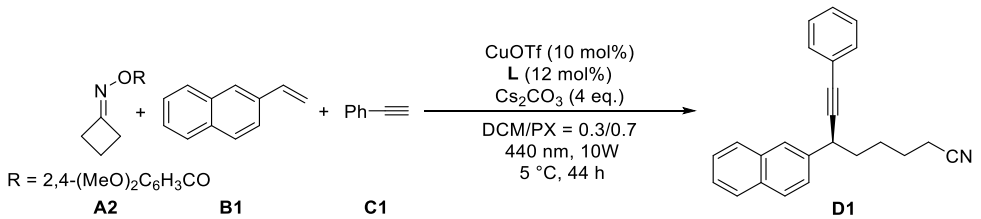
Table S9. Screening ligand loading.

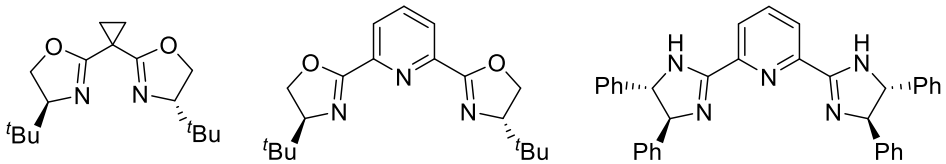


entry	y	yield (%)[b]	ee (%)[c]
1	5	37	76
2	10	50	90
3	12	52	91
4	15	50	90

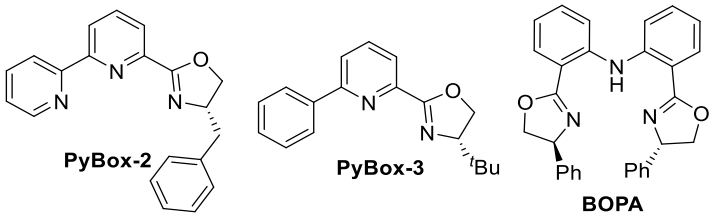
[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3**, **A2** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), Cs_2CO_3 (0.4 mmol) in PX (0.7 mL) and DCM (0.3 mL) under 10W LED (400 nm) irradiation at 5 ℃ for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

Table S10. Screening other chiral ligands





Box **PyBox-1** **PyImz**

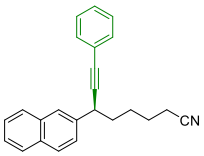


entry	L	yield (%)[b]	ee (%)[c]
1	**G-TqPy-1**	24	60
2	**G-TqPy-3**	52	91
3	**G-TqPy-4**	29	60
4	**G-TqPy-5**	29	65
5	**G-TqPy-6**	32	85
6	**G-TqPy-7**	48	86
7	**G-TqPy-8**	32	85
8	**G-TqPy-9**	52	88
9	**G-TqPy-10**	50	81
10	**G-TqPy-11**	46	81
11	**G-TqPy-12**	26	57
12	**Box**	ND	
13	**PyBox-1**	ND	
14	**PyImz**	ND	
15	**PyBox-2**	ND	
16	**PyBox-3**	ND	
17	**BOPA**	23	35

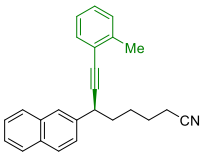
[a] Unless otherwise noted, all reactions were performed with CuOTf/ **L** (1:1.2, 10 mol %), **A2** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol), Cs_2CO_3 (0.4 mmol) in PX (0.7 mL) and DCM (0.3 mL) under 10W LED (440 nm) irradiation at 5 ℃ for 44 h. [b] NMR yield using dibromaethan as an internal standard. [c] The ee values were determined by UPC[2].

6 The list of substrates scope

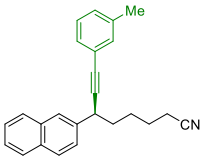
Table S11. Substrate scope of alkynes.



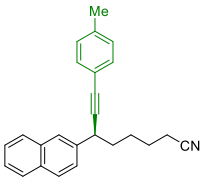
D1, 52% yield, 91% ee



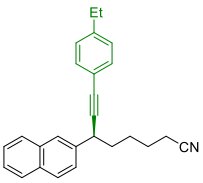
D2, 51% yield, 91% ee



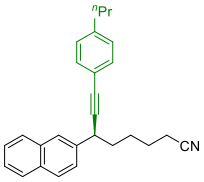
D3, 51% yield, 90% ee



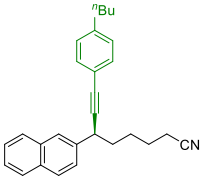
D4, 55% yield, 90% ee



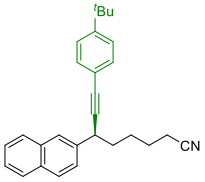
D5, 48% yield, 90% ee



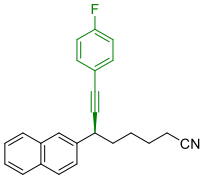
D6, 50% yield, 90% ee



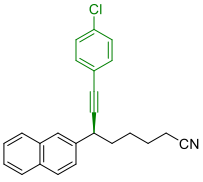
D7, 50% yield, 90 % ee



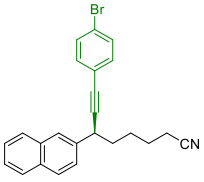
D8, 53% yield, 88% ee



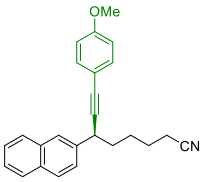
D9, 58% yield, 90% ee



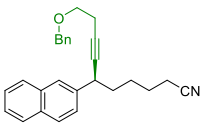
D10, 50% yield, 87% ee



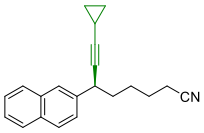
D11, 50% yield, 85% ee



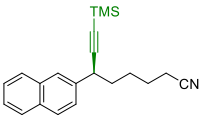
D12, 48% yield, 90% ee



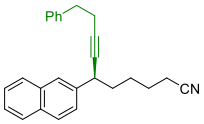
D13, 55% yield, 85% ee



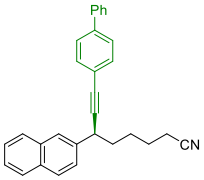
D14, 58% yield, 84% ee



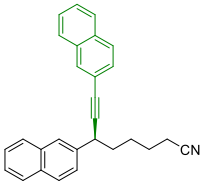
D15, 58% yield, 79% ee



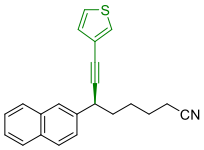
D16, 60% yield, 82% ee



D17, 58% yield, 89% ee

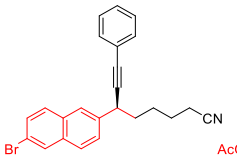


D18, 57% yield, 90% ee

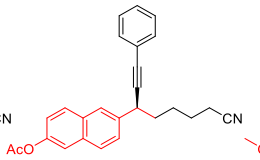


D19, 43% yield, 88% ee

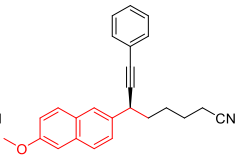
Table S12. Substrate scope of alkenes.



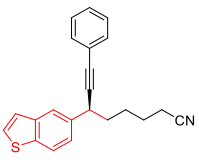
D20, 43% yield, 90% ee



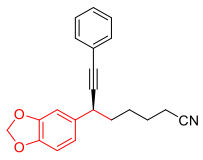
D21, 47% yield, 86% ee



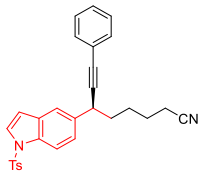
D22, 50% yield, 90% ee



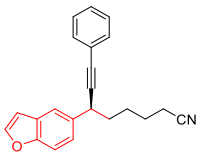
D23, 55% ee, 85% ee



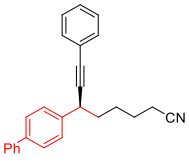
D24, 53% yield, 85% ee



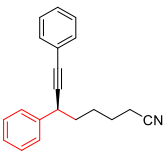
D25, 45% yield, 82% ee



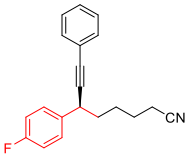
D26, 45% yield, 85% ee



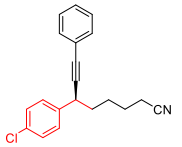
D27, 53% yield, 88% ee



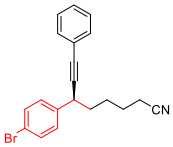
D28,64% yield, 90% ee



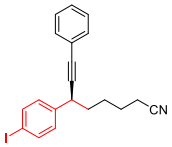
D29, 47% yield, 90% ee



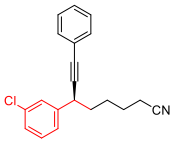
D30, 60% yield, 85% ee



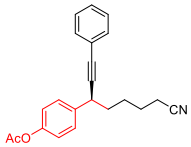
D31, 50% yield, 87% ee



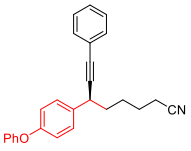
D32, 48% yield, 85% ee



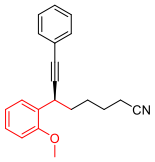
D33, 58% yield, 87% ee



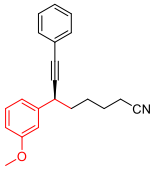
D34, 47% yield, 87% ee



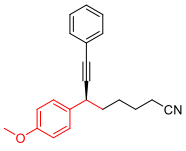
D35, 48% yield, 88% ee



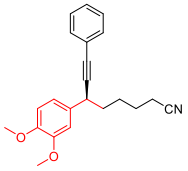
D36, 60% yield, 83% ee



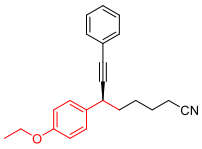
D37, 51% yield, 91% yield



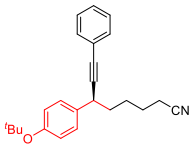
D38, 62% yield, 87% yield



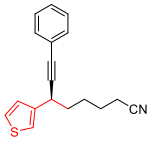
D39, 55% yield, 90% yield



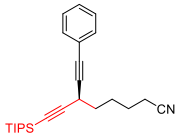
D40, 57% yield, 86% ee



D41, 30% yield, 90% ee

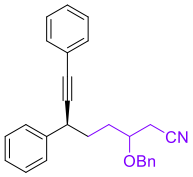


D42, 58% yield, 87% ee

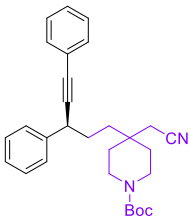


D43, 63% yield, 92% ee

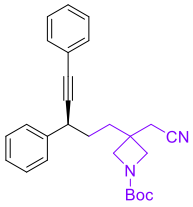
Table S13. Substrate scope of cycloketone oxime esters.



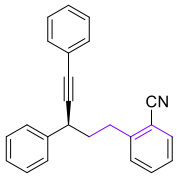
D44, 43% yield
1:1 dr, 80%/80% ee



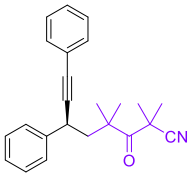
D45, 27% yield, 81% ee



D46, 50% yield, 85% ee



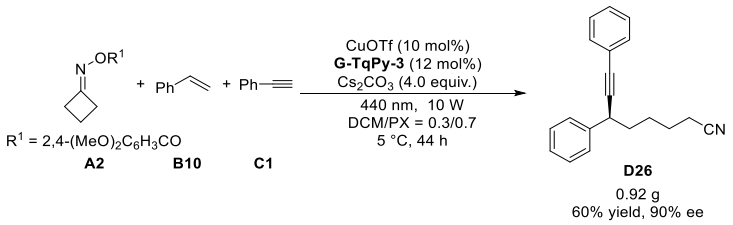
D47, 21% yield, 65% ee



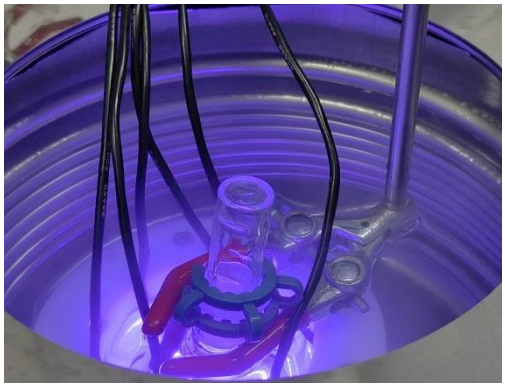
D48, 44% yield, 35% ee

7 The scale-up synthesis and Transformations

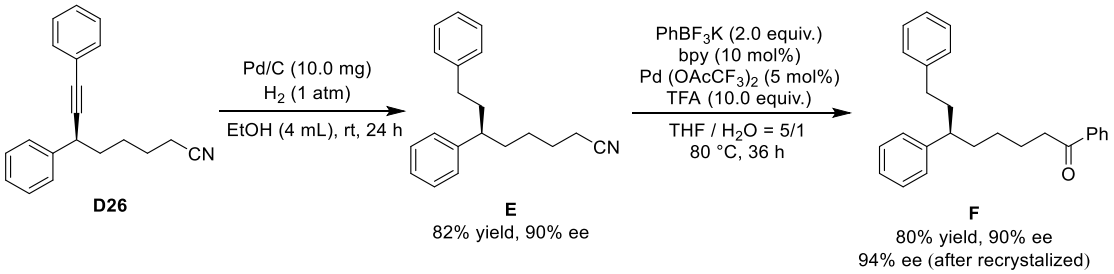
7.1 The scale-up synthesis of product D26



In a glove box, a dry reaction tube was charged with CuOTf (126 mg, 10 mol%), **G-TqPy-3** (342 mg, 12 mol%) and Cs_2CO_3 (7.8 g, 24.0 mmol) and **A2** (4.5 g, 18.0 mmol), then PX (42.0 mL) and Dichloromethane (18.0 mL) were added. Subsequently **B10** (625 mg, 6.0 mmol) and **C1** (1.8 g, 18.0 mmol) were added into the above solution. The mixture was stirred under 10 W LED (440 nm) irradiation at 5 ℃. After 44 h, the mixture was subjected to column chromatography on silica gel (eluent: petroleum ether/ acetone = 40/1, v/v) to afford the desired product.



7.2 Transformations of product D26



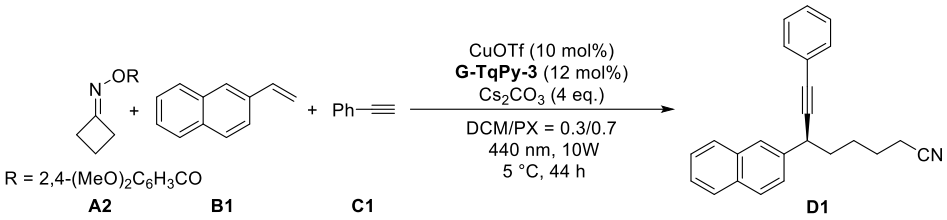
The procedure for the synthesis of E: The reaction was conducted with **D26** (546.3 mg, 2.0 mmol), Pd/C (50 mg) in EtOH (20.0 mL). Then, the reaction mixture was stirred at room temperature under a H_2 balloon until the reaction was completed as monitored by TLC analysis. The crude product was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate 20:1) directly to give the corresponding product in 82% yield as a colorless oil. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.31 (t, *J* = 8.2, 2H), 7.27 – 7.20 (m, 3H), 7.18 – 7.11 (m, 3H), 7.12 – 6.91 (m, 2H), 2.51 (tt, *J* = 10.0, 5.4 Hz, 1H), 2.46 – 2.40 (m, 2H), 2.20 (td, *J* = 7.2, 2.8 Hz, 2H), 2.02 – 1.77 (m, 2H), 1.73 – 1.40 (m, 4H), 1.39

– 1.13 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.93, 142.43, 128.61, 128.45, 128.39, 128.36, 127.77, 126.38, 125.80, 119.82, 45.38, 38.60, 36.28, 33.82, 26.81, 25.53, 17.09. HRMS (EI): m/z $[M + Na]^+$ calcd for $C_{20}H_{23}NNa^+$: 300.1727, found: 300.1718.

The procedure for the synthesis of F: To a flame-dried round Schlenk tube (50 mL) were added I (415.8 mg, 1.5 mmol), $PhBF_3K$ (552.0 mg, 3.0 mmol), bpy (23.4 mg, 0.15 mmol) and $Pd(OAcCF_3)_2$ (24.9 mg, 0.075 mmol). Subsequently, TFA (1.7 g, 15mmol), THF and water were added. After stirred under argon atmosphere at 80 ℃ for 36 h, the mixture was extracted with ethyl acetate and H_2O. And the organic phase was collected and dried over anhydrous Na_2SO_4, filtered, concentrated in vacuo. The crude product was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate 20:1) directly to give the corresponding product in 80% yield as a white solid. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 7.8 Hz, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.13 (m, 10H), 2.79 (t, *J* = 7.6 Hz, 2H), 2.51 – 2.42 (m, 1H), 2.36 (t, *J* = 8.2 Hz, 2H), 1.90 – 1.82 (m, 2H), 1.65 – 1.50 (m, 4H), 1.25 – 1.02 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.54, 145.53, 142.70, 137.15, 133.00, 128.67, 128.51, 128.39, 128.16, 127.90, 126.19, 125.76, 45.61, 38.74, 38.66, 37.04, 33.95, 27.46, 24.47. HRMS (EI): m/z $[M + H]^+$ calcd for $C_{26}H_{28}O^+$: 357.2212, found: 357.2210.

8 Mechanism Investigation

8.1 Control experiments.

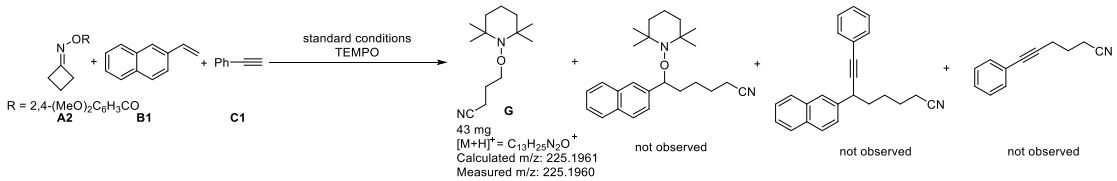


Entry	*hv*	CuOTf	**G-TqPy-3**	Cs_2CO_3	yield (%)[b]	ee (%)[c]
1[d]	×	√	√	√	30	88
2[e]	√	×	√	√	trace	
3[f]	√	√	×	√	trace	
4[g]	√	√	√	×	trace	
5	√	√	√	√	52	91

[a] Unless otherwise noted, all reactions were performed with CuOTf/**G-TqPy-3** (1:1.2, 10 mol %), **A2** (0.3 mmol), **B1** (0.1 mmol), **C1** (0.3 mmol) in PX (0.7 mL) and DCM (0.3 mL) under 10W LED (440 nm) irradiation for 44 h. [b] Determined by NMR analysis using tetrabromoethane as an internal standard. [c] The *ee* values were determined by UPC[2]. [d] No *hv*. [e] Without CuOTf. [f] Without **G-TqPy-3**. [g] Without Cs_2CO_3.

8.2 Radical Trapping Experiment.

In a glove box, a dry reaction tube was charged with CuOTf (10 mmol%), **G-TqPy-3** (12 mmol%) and Cs_2CO_3 (0.4 mmol), **A2** (0.3 mmol) and 2,2,6,6-tetramethyl-1-piperidinyloxyl (TEMPO, 0.3 mmol), then PX (0.7 mL) and dichloromethane (0.3 mL) were added. Subsequently **B1** (0.1 mmol) and **C1** (0.3 mmol) were added into the above solution with a microinjector. The mixture was stirred under 10 W LED (440 nm) irradiation at 5 ℃. After 44 h, the mixture was filtered through a short pad of silica and concentrated in vacuo. The reaction mixture was analyzed by nanospray ESI mass spectrometry (**Figure S3**) and yield was isolated yield.[3]



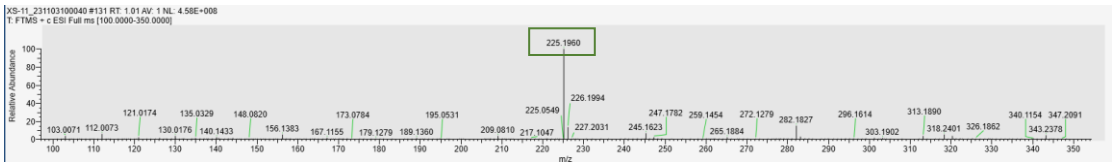
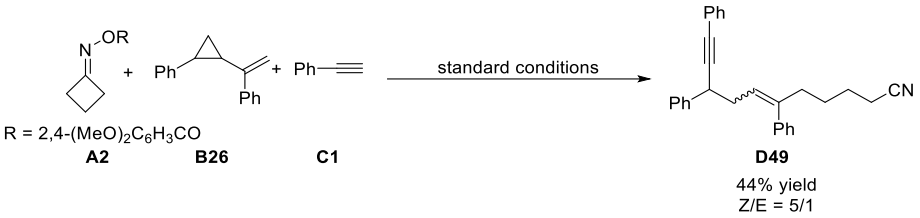


Figure S1. HRMS analysis

8.3 Radical Clock Experiment.



In a glove box, a dry reaction tube was charged with CuOTf (10 mol%), **G-TqPy-3** (12 mol%) and Cs_2CO_3 (0.4 mmol) and **A2** (0.3 mmol), then PX (0.7 mL) and dichloromethane (0.3 mL) were added. Subsequently **B26** (0.1 mmol) and **C1** (0.3 mmol) were added into the above solution with a microinjector. The mixture was stirred under 10 W LED (440 nm) irradiation at 5 °C. After 44 h, the mixture was subjected to column chromatography on silica gel (eluent: petroleum ether/ acetone = 20/1, v/v) to afford the desired product **D49**.

8.4 Electron paramagnetic resonance (EPR) analysis

EPR measurements: EPR spectra were recorded at room temperature on a Bruker EMXplus X-band spectrometer EPR: FrequencyMon = 9.86 GHz; Modulation Amplitude = 1.00 G; Center Field = 3510.00 G; Sweep Width 100.000 G; Conversion Time =150.00 ms; Sweep Time = 15.00 s; Power = 2.00 mW.

CuOTf + G-TqPy-3 + Cs_2CO_3 + A2+ DMPO: In a glove box, a dry reaction tube was charged with CuOTf (2.1 mg, 10 mol%), **G-TqPy-3** (5.7 mg, 12 mol%), Cs_2CO_3 (133 mg, 0.4 mmol), then PX (0.7 mL) and dichloromethane (0.3 mL) were added. After the mixture was stirred for 1 h, **A2** (74.7 mg, 0.3 mmol) and DMPO (33.9 mg, 0.3 mmol) were added. After 10 mins, a small aliquot of reaction solution was taken with pilet, and successfully transferred to an EPR capillary under a nitrogen atmosphere for X-band EPR measurement.

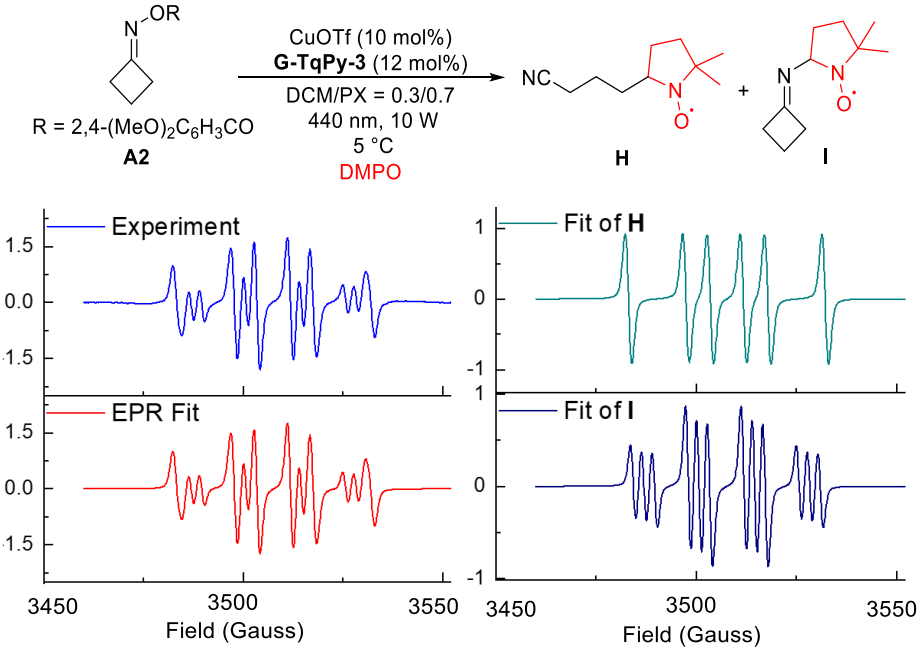


Figure S2. EPR analysis

8.5 UV-VIS Absorption Spectra

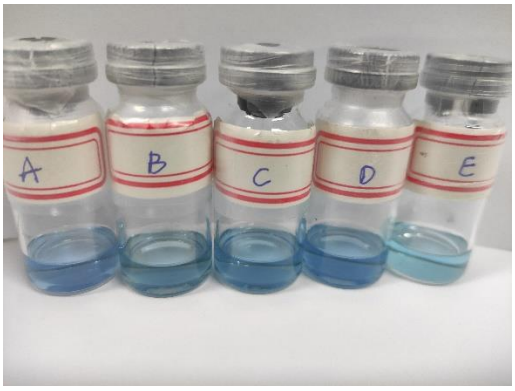


Figure S3. A: Solution of CuOTf/**G-TqPy-3** (1:1) in CH_2Cl_3 (0.01 M), B: Solution of CuOTf/**G-TqPy-3**/Cs_2CO_3 (1:1:1) in CH_2Cl_2 (0.01 M), C: Solution of CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1** (1:1:2:1) in CH_2Cl_2 (0.01 M), D: Solution of CuOTf/**G-TqPy-3**/Cs_2CO_3/**A2** (1:1:1:1) in CH_2Cl_2 (0.01 M), E: Solution of CuOTf/**G-TqPy-1**/Cs_2CO_3 (1:1:1) in CH_2Cl_2 (0.01 M).

UV-Vis absorption for CuOTf/**G-TqPy-1**/Cs_2CO_3 (1:1:1), CuOTf/**G-TqPy-3**/Cs_2CO_3 (1:1:1), G-**TqPy-3**, CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1** (1:1:2:1), CuOTf/**G-TqPy-1**/Cs_2CO_3/**C1** (1:1:2:1) at concentration (2.0 mM in DCM), all solutions were prepared in a glove box.

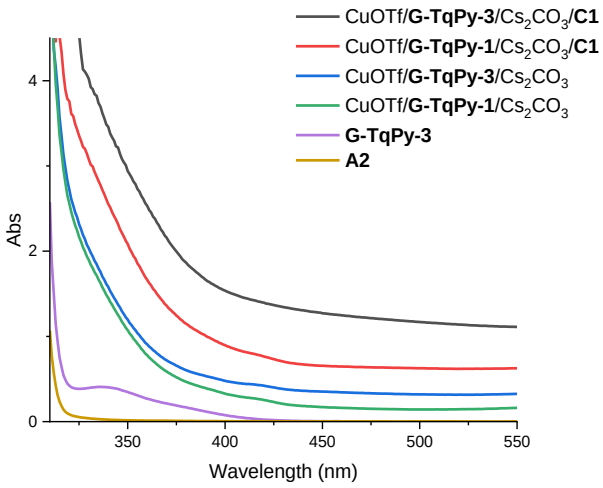
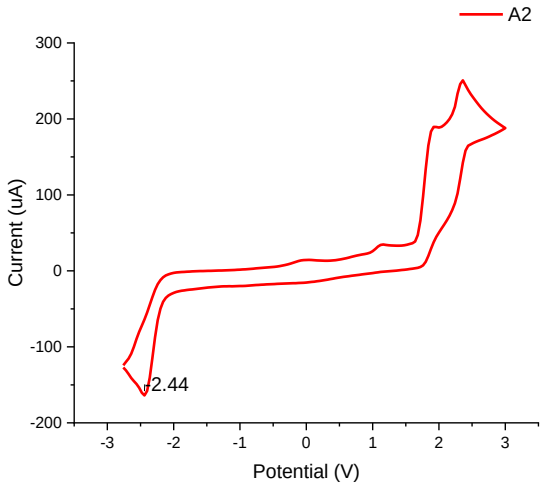


Figure S4. UV-VIS absorption spectra of the related mixtures (2.0 mM in DCM).

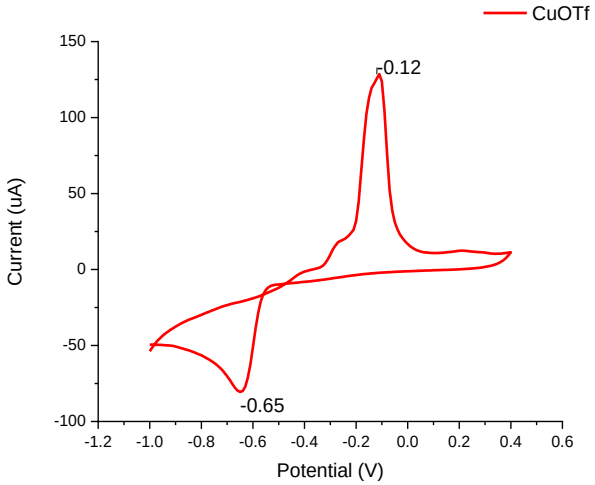
8.6 Cyclic voltammetry measurements

Cyclic voltammetry (CV) was performed in a three-electrode cell connected to a Schlenk line at room temperature. The working electrode was a platinum disk electrode. The counter electrode was a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from reaction by a salt bridge. 20 mL CH_3CN containing 0.1 M $TBAPF_6$ were poured into the electrochemical cell in all experiments. The scan rate is 0.1 V/s, 2 sweep segments. Ferrocene (Cp_2Fe) was used as a reference.

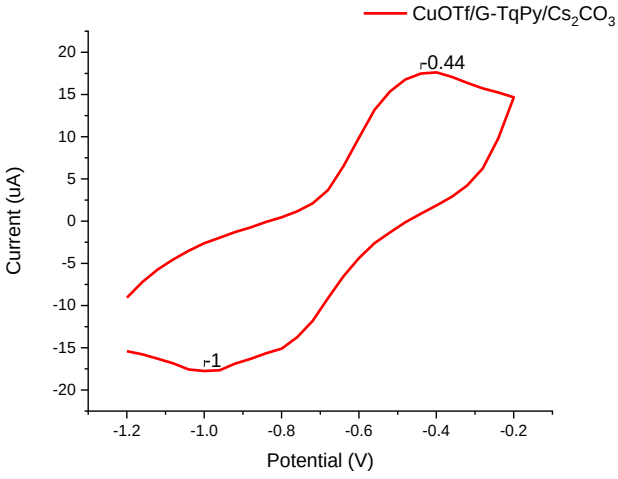
Cyclic voltammograms of **A2:**



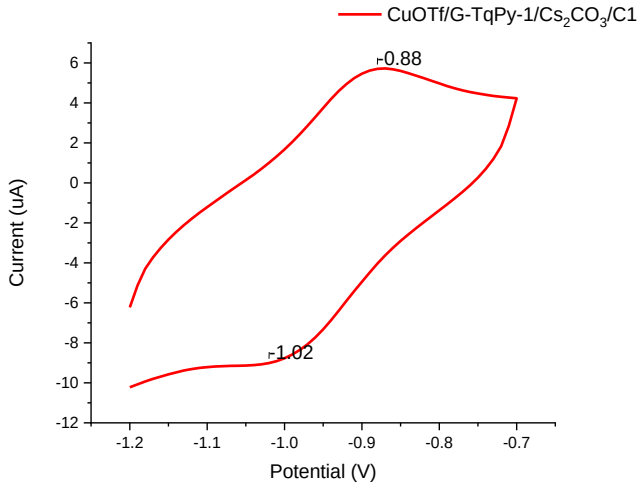
Cyclic voltammograms of CuOTf**:**



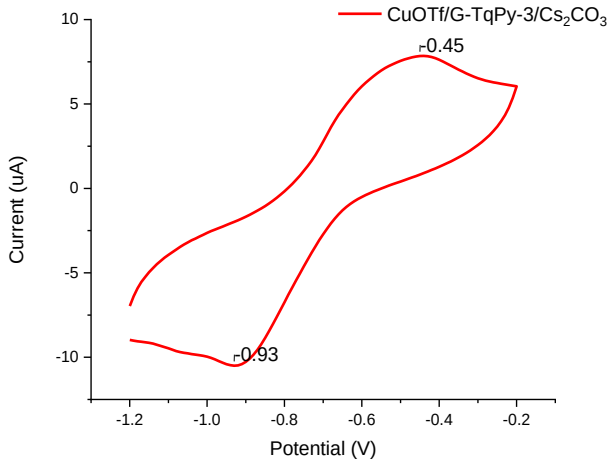
Cyclic voltammograms of CuOTf/**G-TqPy-1**/Cs_2CO_3 (-1.2 – 0.2 V):



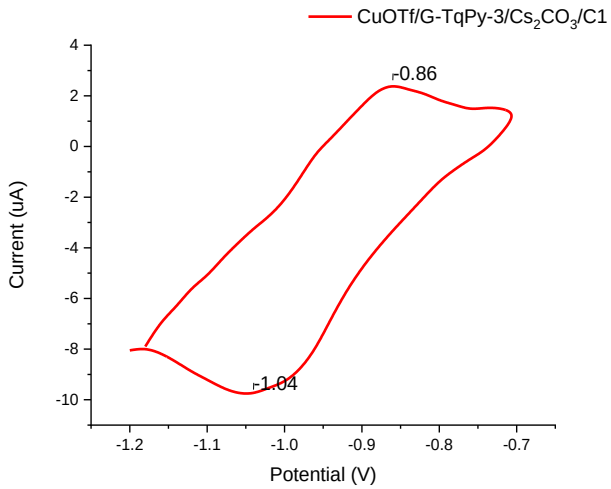
Cyclic voltammograms of CuOTf/**G-TqPy-1**/Cs_2CO_3/**C1** (-1.2 – -0.7 V):



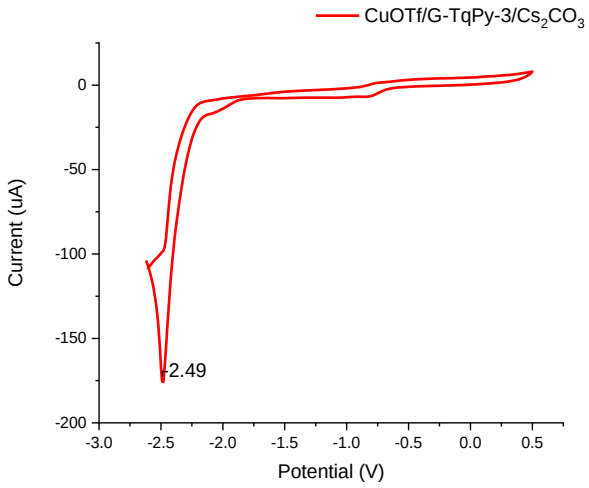
Cyclic voltammograms of CuOTf/**G-TqPy-3**/Cs_2CO_3 (-1.2 – 0.2 V):



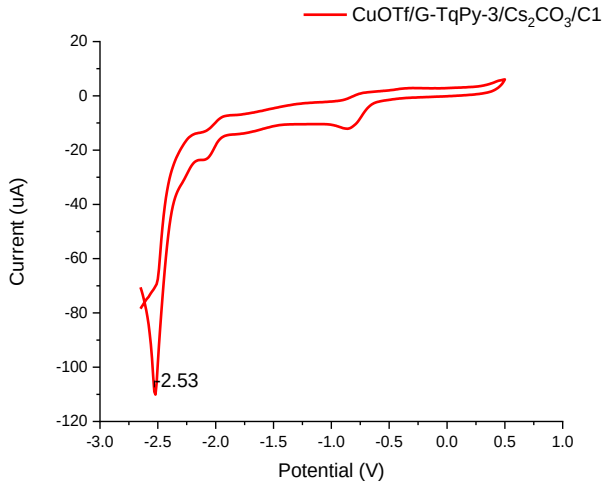
Cyclic voltammograms of CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1** (-1.2 – -0.7 V):



Cyclic voltammograms of CuOTf/**G-TqPy-3**/Cs_2CO_3 (-2.75 – 0.5 V):



Cyclic voltammograms of CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1** (-2.75 – 1.0 V):



Cyclic voltammograms of **G-TqPy-3**:

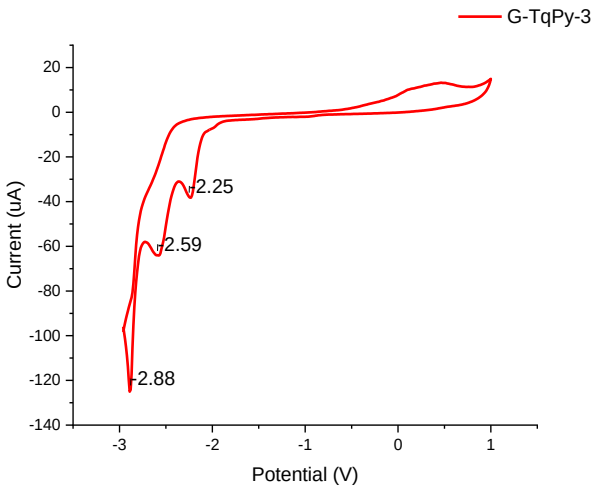


Figure S5. Cyclic voltammograms

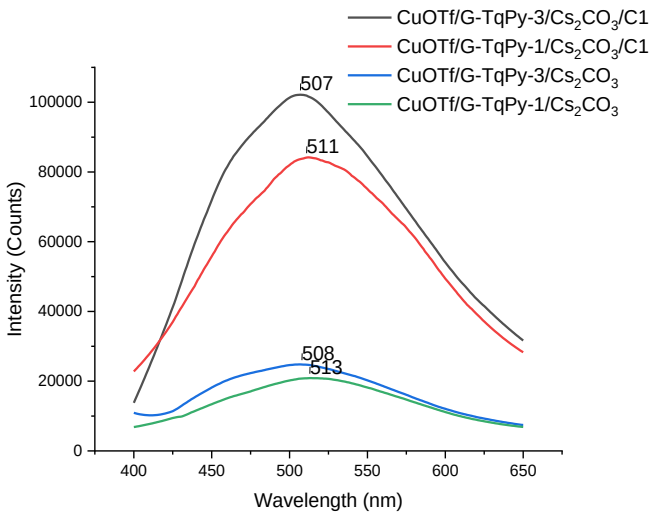


Figure S6. Phosphorescent emission spectrum of CuOTf/**G-TqPy-1**/Cs_2CO_3, CuOTf/**G-TqPy-1**/Cs_2CO_3/**C1**, CuOTf/**G-TqPy-3**/Cs_2CO_3, CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1**.

The excited state potential (E_{ox}*) was calculated using the following equation:

$E_{ox}^* = E_{ox} - E_{0,0}$; $E_{red}^* = E_{red} + E_{0,0}$

$E_{0,0} = \frac{hc}{\lambda}$ (λ: maximum emission wavel ength)

E_{ox}^*[CuOTf/**G-TqPy-1**/Cs_2CO_3] = -0.44 − 2.42 = -2.86 V vs. SCE

E_{ox}^*[CuOTf/**G-TqPy-1**/Cs_2CO_3/**C1**] = -0.88 − 2.43 = -3.31 V vs. SCE

E_{ox}^*[CuOTf/**G-TqPy-3**/Cs_2CO_3] = -0.45 − 2.44 = -2.89 V vs. SCE

E_{ox}^*[CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1**] = -0.86 − 2.44 = -3.30 V vs. SCE

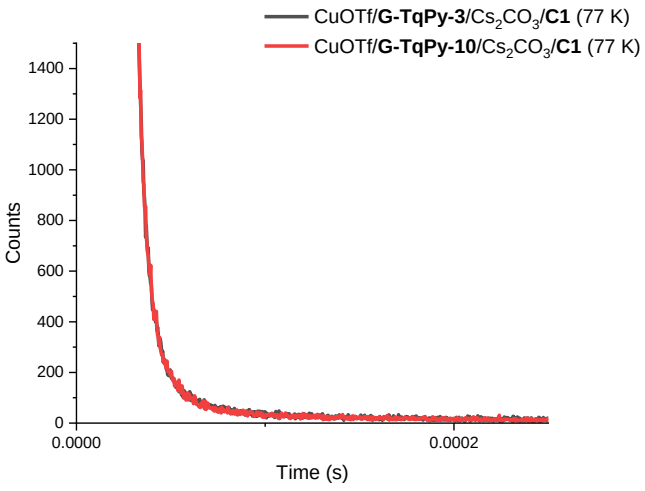
E_{red}^*[CuOTf/**G-TqPy-1**/Cs_2CO_3] = -1 +2.42 = 1.42 V vs. SCE

E_{red}^*[CuOTf/**G-TqPy-1**/Cs_2CO_3/**C1**] = -1.02 + 2.43 = 1.41 V vs. SCE

E_{red}^*[CuOTf/**G-TqPy-3**/Cs_2CO_3] = -0.93 + 2.44 = 1.51 V vs. SCE

E_{red}^*[CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1**] = -1.04 + 2.44 = 1.40 V vs. SCE

8.7 Lifetime measurements



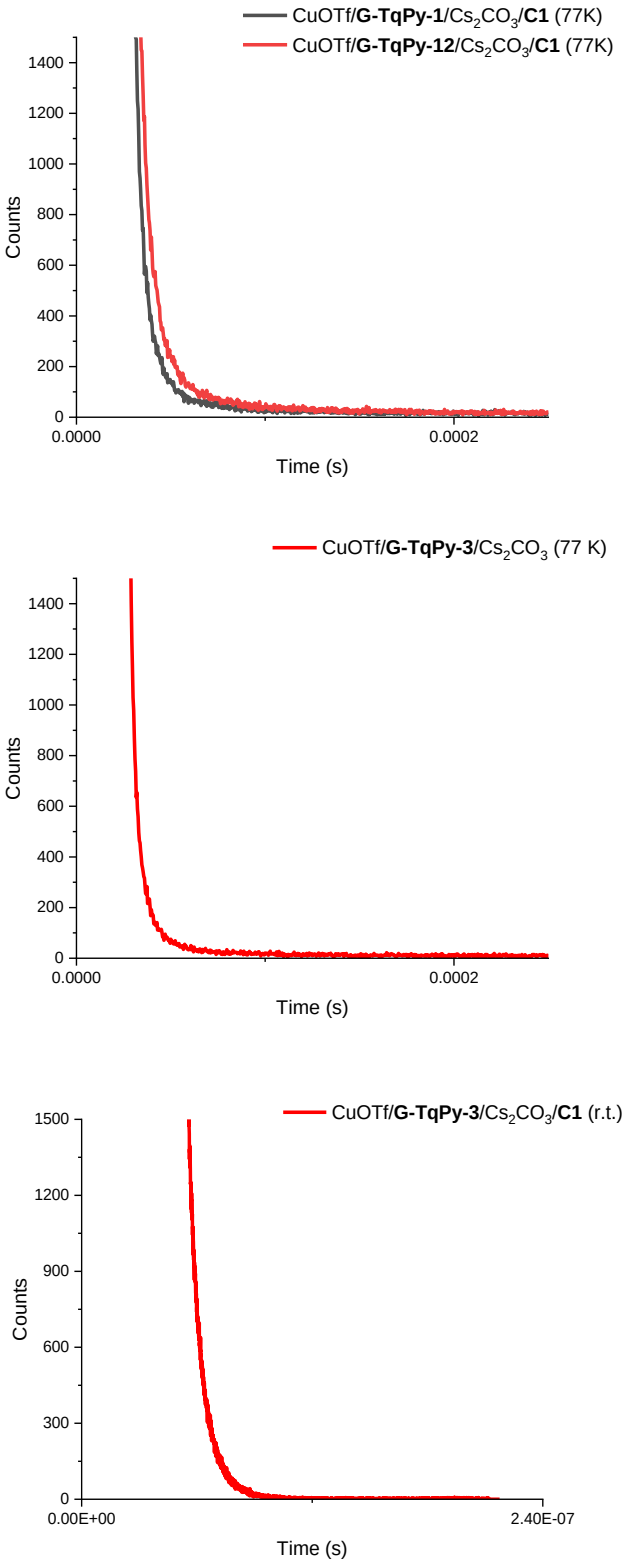


Figure S7. Phosphorescence lifetime of CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1**, CuOTf/**G-TqPy-10**/Cs_2CO_3/**C1**, CuOTf/**G-TqPy-1**/Cs_2CO_3/**C1**, CuOTf/**G-TqPy-12**/Cs_2CO_3/**C1**, CuOTf/**G-TqPy-3**/Cs_2CO_3.

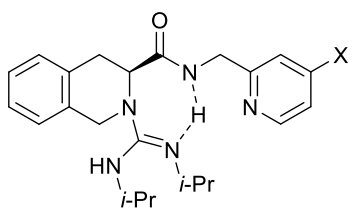
All measurements were carried out at a concentration of 2.0 mM in CH_2Cl_2.

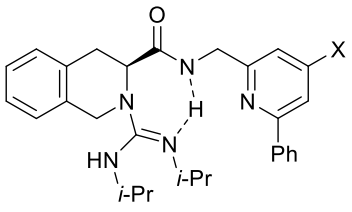
CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1** (average lifetime = 5.25 μs, 77 K);

CuOTf/**G-TqPy-10**/Cs_2CO_3/**C1** (average lifetime = 5.18 μs, 77 K);

CuOTf/**G-TqPy-1**/Cs_2CO_3/**C1** (average lifetime = 5.17 μs, 77 K);
CuOTf/**G-TqPy-12**/Cs_2CO_3/**C1** (average lifetime = 5.10 μs, 77 K);
CuOTf/**G-TqPy-3**/Cs_2CO_3 (average lifetime = 5.03 μs, 77 K);
CuOTf/**G-TqPy-3**/Cs_2CO_3/**C1** (average lifetime = 3.05 ns, room temperature);

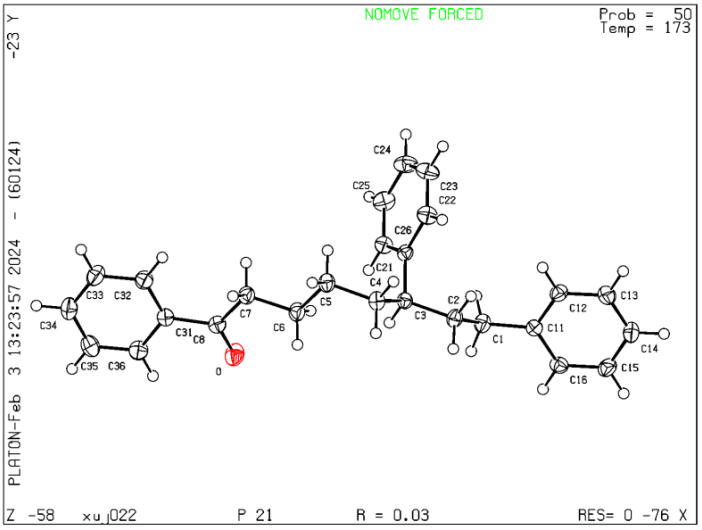
Phosphorescence data of the system containing CuOTf/**G**/Cs2CO3/**C1** (77 K)





	G-TqPy-1: X = H	**G-TqPy-12**: X = OMe	**G-TqPy-3**: X = H	**G-TqPy-10**: X = Cl
eV	2.42	2.42	2.45	2.45
τ (μs)	5.17	5.10	5.25	5.18

9 X-ray crystal structure



X-ray crystal structure of product **J**

The crystal of product **J** was obtained in the solvents of dichloromethane and petroleum ether. CCDC: 2331715 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via https://www.ccdc.cam.ac.uk/structures/.

Crystallographic Data for $C_{26}H_{28}O$.

Formula	C26H28O
Formula mass (amu)	356.48
Space group	P 21
a (Å)	13. 2149(3)
b (Å)	5.5084(1)
c (Å)	13.7281(4)

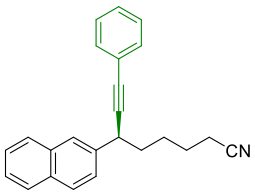
α (deg)	90
β (deg)	96.519(1)
γ (deg)	90
V (Å^3)	992.85(4)
Z	2
λ (Å)	1.54178
T (K)	173 K
ρ_{calcd} (g cm^{-3})	1.192
μ (mm^{-1})	0.536
Transmission factors	0.702–1.000
θ_{max} (deg)	68.252
No. of unique data, including $F_o^2 < 0$	3545
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	3421
No. of variables	245
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0304
$R_w(F_o^2)$ [b]	0.0793
Goodness of fit	1.066

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

10 The analytical and spectral characterization data for the products

(R)-6-(naphthalen-2-yl)-8-phenyloct-7-ynenitrile (D1)



D1

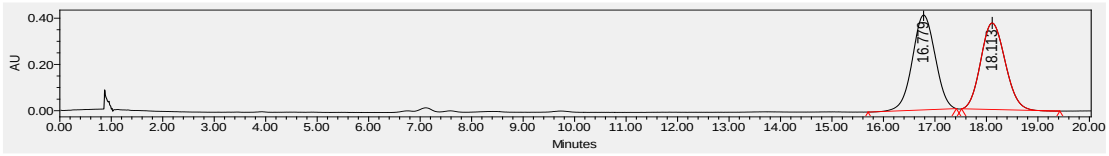
colourless oil, 52% yield, 91% ee. $[\alpha]^{20}_D$ = 47.2 (*c* = 0.36, in CH_2Cl_2). **UPC²** (Chiralcel OX column), CO_2/EtOH = 96/4, flow rate = 1.5 mL/min, λ = 254 nm, retention time: t_1 = 16.78 min, t_2 = 18.12 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 – 7.81 (m, 4H), 7.54 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.48 (m, 4H), 7.32 (m, 3H), 4.04 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.6 Hz, 2H), 1.96 (m, 2H), 1.63-1.78 (m, 4H).

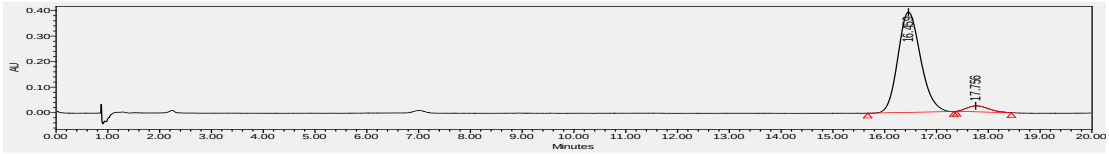
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.09, 133.59, 132.67, 131.85, 128.56, 128.44, 128.13, 127.93, 127.80, 126.35, 126.10, 125.90, 125.84, 123.62, 119.77, 90.87, 84.10, 38.43, 37.60, 26.72, 25.38, 17.27.

ESI-HRMS: calcd for $C_{24}H_{22}N^+$ ([M + H]$^+$) = 324.1746, found 324.1748.

IR (neat): 3054, 2924, 2856, 2246, 1718, 1603, 1508, 1459, 1269, 1120, 949, cm^{-1} .

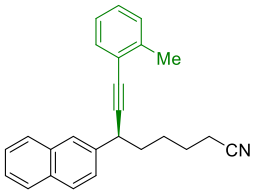


	Retention Time	Area	% Area
1	16.781	32642439	50.19
2	18.122	32398580	49.81



	Retention Time	Area	% Area
1	16.459	11947354	95.33
2	17.756	585920	4.67

(S)-6-(naphthalen-2-yl)-8-(o-tolyl)oct-7-ynenitrile (D2)



D2

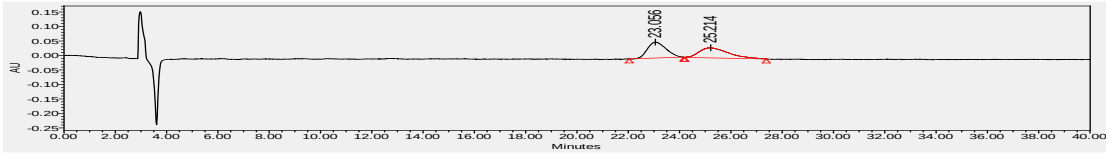
colourless liquid, 51% yield, 91% ee; $[\alpha]^{20}_D$ = 22.9 (*c* = 0.34, in CH_2Cl_2). **HPLC** (Chiralcel OD-H column), n-hexane/i-PrOH = 95/5, flow rate = 1.0mL/min, λ = 254 nm, retention time: t_1 = 23.06 min, t_2 = 25.21min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.86 – 7.81 (m, 3H), 7.55 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.50 – 7.42 (m, 3H), 7.22 (d, *J* = 4.3 Hz, 2H), 7.15 (m, 1H), 4.09 (t, *J* = 7.2 Hz, 1H), 2.48 (s, 3H), 2.35 (t, *J* = 6.6 Hz, 2H), 2.00 – 1.93 (m, 2H), 1.78 – 1.66 (m, 4H).

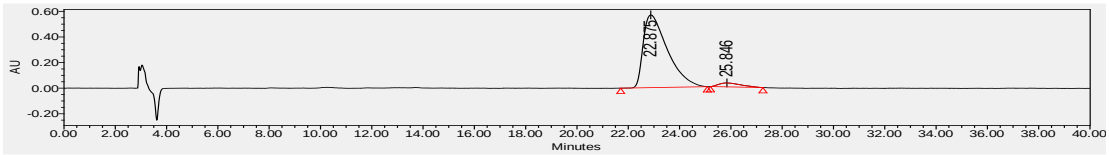
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.21, 139.23, 133.60, 132.66, 132.14, 129.57, 128.52, 128.11, 127.91, 127.80, 126.35, 126.10, 125.88, 125.85, 125.68, 123.41, 119.72, 94.84, 83.04, 38.64, 37.77, 26.74, 25.40, 21.08, 17.27.

ESI-HRMS: calcd for $C_{25}H_{24}N^+$ ([M + H]$^+$) = 338.1903, found 338.1902.

IR (neat): 3056, 2924, 2856, 2246, 1683, 1506,1371, 1268, 819, 755 cm^{-1}.

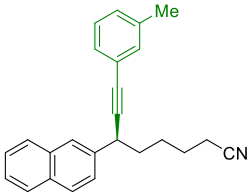


	Retention Time	Area	% Area
1	23.056	2763788	50.14
2	25.214	2748358	49.86



	Retention Time	Area	% Area
1	22.875	37265997	95.25
2	25.846	1857252	4.75

(S)-6-(naphthalen-2-yl)-8-(m-tolyl)oct-7-ynenitrile (D3)



D3

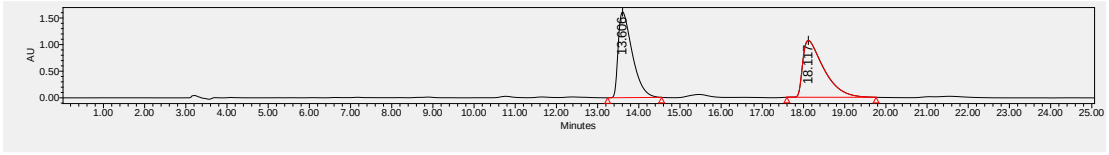
colourless liquid, 51% yield, 90% ee; $[\alpha]^{20}_D$ = 41.3 (*c* = 0.24, in CH_2Cl_2). **HPLC** (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 13.59 min, t_2 = 18.12min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 – 7.82 (m, 4H), 7.54 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.52 – 7.44 (m, 2H), 7.33 – 7.26 (m, 2H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 4.03 (t, *J* = 7.2 Hz, 1H), 2.34 (m, 5H), 1.97 – 1.92 (m, 2H), 1.76 – 1.66 (m, 4H).

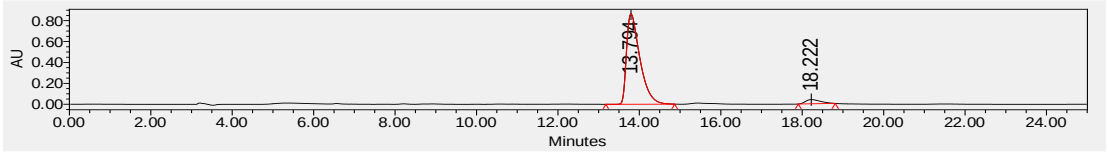
^{13}C NMR (151 MHz, $CDCl_3$) δ 139.15, 138.12, 133.58, 132.65, 132.44, 129.01, 128.88, 128.53, 128.34, 127.92, 127.79, 126.33, 126.09, 125.86, 123.39, 119.80, 90.46, 84.23, 38.42, 37.63, 26.72, 25.38, 21.36, 17.27.

ESI-HRMS: calcd for $C_{25}H_{24}N^+$ ($[M + H]^+$) = 338.1903, found 338.1900.

IR (neat): 3053, 2924, 2856, 2245, 1685, 1600, 1459, 1369, 1090, 819, 786 cm^{-1}.

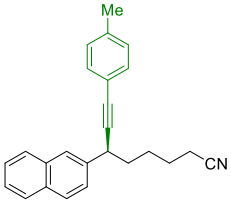


	Retention Time	Area	% Area
1	13.594	69705234	49.16
2	18.123	72076614	50.84



	Retention Time	Area	% Area
1	13.794	19658141	95.00
2	18.222	1034180	5.00

(S)-6-(naphthalen-2-yl)-8-(p-tolyl)oct-7-ynenitrile (D4)



D4

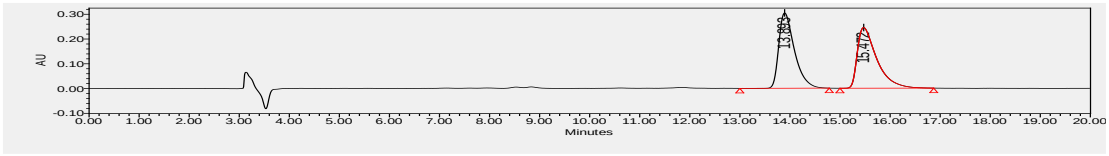
colourless liquid, 55% yield, 90% ee; $[\alpha]^{20}_D$ = 50.3 (*c* = 0.36, in CH_2Cl_2). **HPLC** (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 13.89 min, t_2 = 15.47 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.80 (m, 4H), 7.54 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.47 (m, 2H), 7.40 – 7.34 (m, 2H), 7.13 (d, *J* = 7.8 Hz, 2H), 4.03 (t, *J* = 7.2 Hz, 1H), 2.35 (m, 5H), 1.98 – 1.91 (m, 2H), 1.80 – 1.61 (m, 4H).

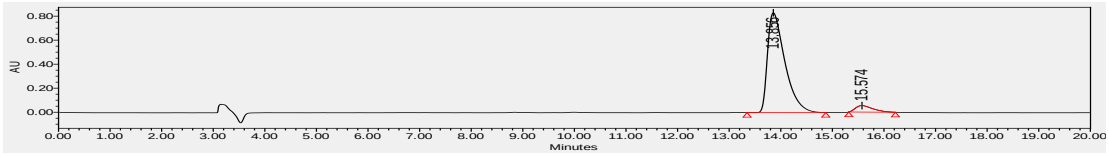
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.23, 138.16, 133.60, 132.66, 131.71, 129.18, 128.51, 127.92, 127.79, 126.32, 126.09, 125.86, 120.54, 119.76, 90.08, 84.17, 38.43, 37.62, 26.71, 25.38, 21.58, 17.25.

ESI-HRMS: calcd for $C_{25}H_{24}N^+$ ($[M + H]^+$) = 338.1903, found 338.1902.

IR (neat): 3053, 2924, 2857, 2246, 1685, 1508, 1459,1370, 1120, 818cm^{-1}.

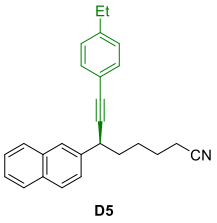


	Retention Time	Area	% Area
1	13.893	6609248	50.02
2	15.472	6602694	49.98



	Retention Time	Area	% Area
1	13.856	19296643	94.82
2	15.574	1054335	5.18

(S)-8-(4-ethylphenyl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D5)



D5

colourless liquid, 48% yield, 90% ee; $[\alpha]^{20}_D$ = 6.3 (*c* = 0.30, in CH_2Cl_2).

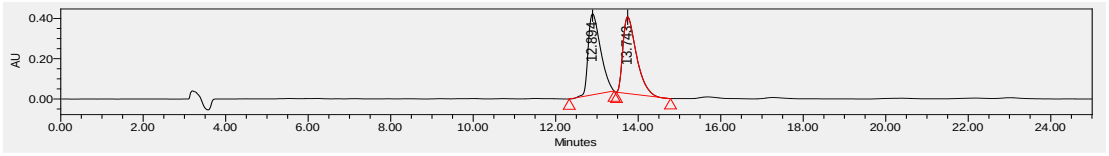
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 12.89 min, t_2 = 13.74 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.85 (s, 1H), 7.83 (d, *J* = 8.1 Hz, 3H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.47 (m, 2H), 7.40 (d, *J* = 7.8 Hz, 2H), 7.15 (d, *J* = 7.8 Hz, 2H), 4.02 (t, *J* = 7.2 Hz, 1H), 2.64 (q, *J* = 7.6 Hz, 2H), 2.33 (t, *J* = 6.6 Hz, 2H), 1.96 – 1.91 (m, 2H), 1.75 – 1.61 (m, 4H), 1.22 (t, *J* = 7.6 Hz, 3H).

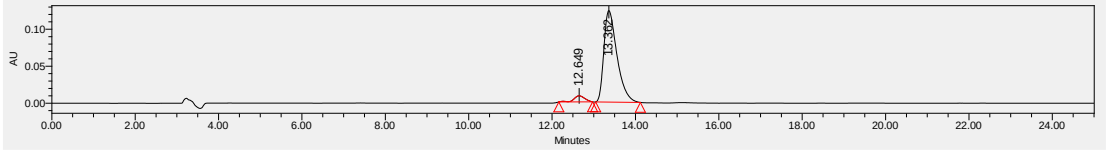
^{13}C NMR (151 MHz, $CDCl_3$) δ 144.41, 139.13, 133.47, 132.53, 131.69, 128.39, 127.90, 127.81, 127.68, 126.21, 125.97, 125.77, 125.74, 120.66, 119.70, 89.96, 84.09, 38.31, 37.54, 28.82, 26.60, 25.26, 17.15, 15.49.

ESI-HRMS: calcd for $C_{26}H_{26}N^+$ ($[M + H]^+$) = 352.059, found 352.2058.

IR (neat): 3053, 2931, 2866, 2246, 1684, 1604, 1508, 1420, 1289, 894, 831 cm^{-1}.



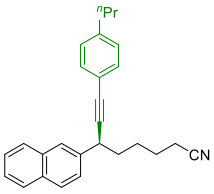
	Retention Time	Area	% Area
1	12.894	5292068	49.92
2	13.743	5308394	50.08



	Retention Time	Area	% Area
1	12.649	148025	5.19

2	13.362	2702302	94.81

(S)-6-(naphthalen-2-yl)-8-(4-propylphenyl)oct-7-ynenitrile (D6)



D6

colourless liquid, 50% yield, 90% ee; $[\alpha]^{20}_D$ = -12.5 (*c* = 0.32, in CH_2Cl_2).

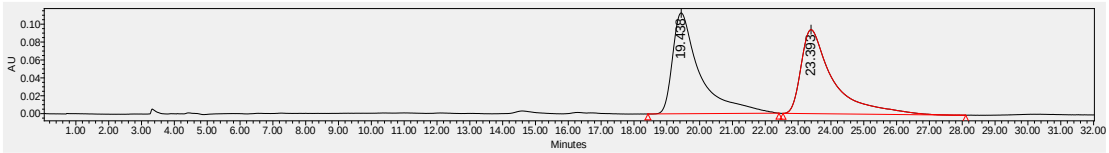
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 19.44 min, t_2 = 23.39 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 – 7.81 (m, 4H), 7.53 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.39 (d, *J* = 7.9 Hz, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 4.02 (t, *J* = 7.2 Hz, 1H), 2.58 (t, *J* = 7.6 Hz, 2H), 2.34 (t, *J* = 6.8 Hz, 2H), 1.94 (q, *J* = 7.4 Hz, 2H), 1.77 – 1.55 (m, 6H), 0.93 (t, *J* = 7.4 Hz, 3H).

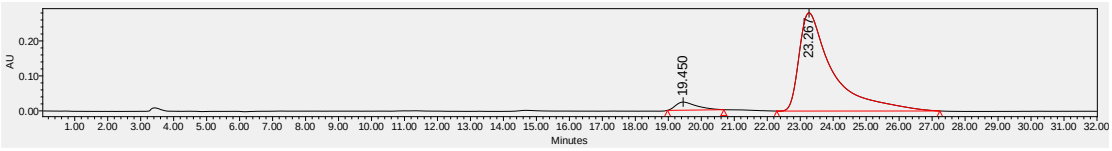
^{13}C NMR (151 MHz, $CDCl_3$) δ 142.96, 139.24, 133.58, 132.64, 131.70, 128.61, 128.50, 127.92, 127.79, 126.31, 126.08, 125.88, 125.84, 120.77, 119.80, 90.08, 84.21, 38.42, 38.05, 37.65, 26.71, 25.37, 24.55, 17.26, 13.89.

ESI-HRMS: calcd for $C_{27}H_{28}N^+$ ($[M + H]^+$) = 366.2216, found 366.2215.

IR (neat): 3053, 2929, 2865, 2246, 1685, 1603, 1508, 1460, 1371, 1178, 819 cm^{-1}.

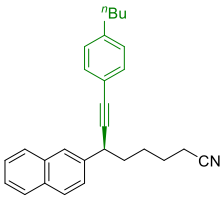


	Retention Time	Area	% Area
1	19.438	5612682	50.12
2	23.393	5585471	49.88



	Retention Time	Area	% Area
1	19.450	1504862	5.05
2	23.267	28271200	94.95

(S)-8-(4-butylphenyl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D7)



D7

colourless liquid, 50% yield, 90% ee; $[\alpha]^{20}_D$ = 58.3 (*c* = 0.15, in CH_2Cl_2).

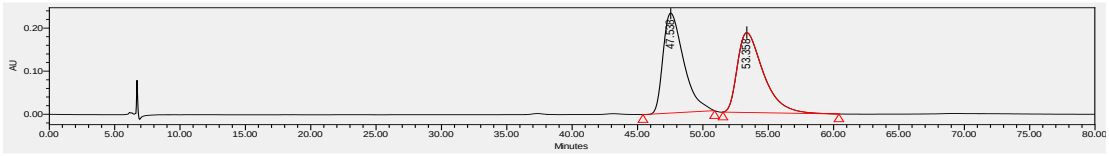
HPLC (Chiralcel IH column), n-hexane/i-PrOH = 99/1, flow rate = 0.5 mL/min, λ = 254 nm, retention time: t_1 = 47.54 min, t_2 = 53.36 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (s, 1H), 7.84 (dd, *J* = 7.6, 2.0 Hz, 3H), 7.54 – 7.52 (m, 1H), 7.48 (td, *J* = 8.0, 1.8 Hz, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H). 4.03 (t, *J* = 7.2 Hz, 1H), 2.61 (t, *J* = 7.6 Hz, 2H), 2.34 (t, *J* = 6.6 Hz, 2H), 1.95 (m, 2H), 1.75 – 1.67 (m, 4H), 1.63 – 1.53 (m, 4H), 1.97 – 1.92 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H).

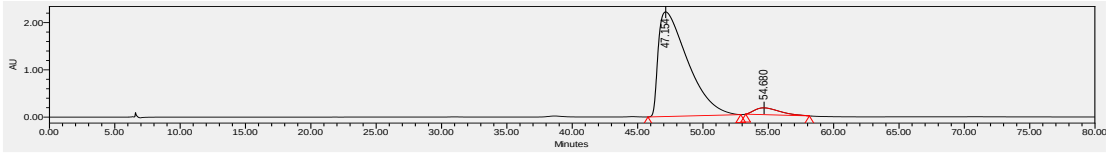
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.06, 139.12, 133.47, 132.53, 131.58, 128.42, 128.36, 127.79, 127.66, 126.18, 125.95, 125.75, 125.71, 120.61, 119.63, 89.94, 84.11, 38.30, 37.52, 35.55, 33.45, 26.58, 25.26, 22.28, 17.13, 13.93.

ESI-HRMS: calcd for $C_{28}H_{30}N^+$ ($[M + H]^+$) = 380.2372, found 380.2374.

IR (neat): 3053, 2927, 2858, 2246, 1685, 1508, 1460, 1371, 1178, 820, 750 cm^{-1}.

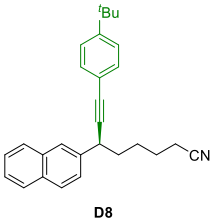


	Retention Time	Area	% Area
1	47.538	25472554	49.92
2	53.358	25552765	50.08



	Retention Time	Area	% Area
1	47.154	345713400	94.73
2	54.680	19229152	5.27

(S)-8-(4-(tert-butyl)phenyl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D8)



D8

colourless liquid, 53% yield, 88% ee; $[\alpha]^{20}_D = 44.6$ ($c = 0.32$, in CH_2Cl_2).

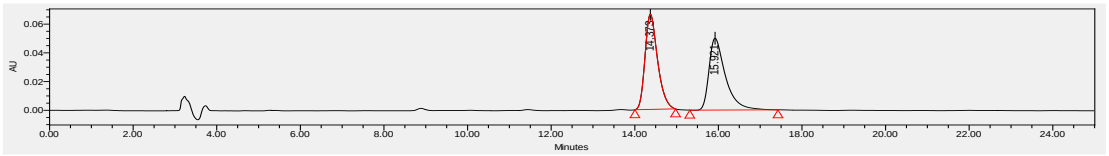
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: $t_1 = 14.37$ min, $t_2 = 15.92$ min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 (s, 1H), 7.84 (dd, *J* = 7.6, 2.0 Hz, 3H), 7.54 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.48 (td, *J* = 7.9, 1.8 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 4.04 (t, *J* = 7.1 Hz, 1H), 2.34 (t, *J* = 6.8 Hz, 2H), 1.94 (m, 2H), 1.80 – 1.65 (m, 4H), 1.32 (s, 9H).

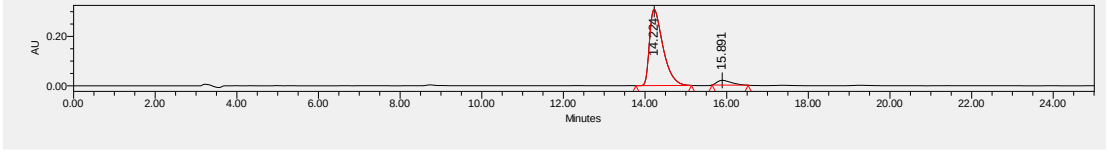
^{13}C NMR (151 MHz, $CDCl_3$) δ 151.35, 139.23, 133.58, 132.63, 131.54, 128.49, 127.92, 127.79, 126.31, 126.08, 125.89, 125.84, 125.44, 120.59, 119.80, 90.09, 84.17, 38.42, 37.67, 34.88, 31.32, 26.70, 25.37, 17.26.

ESI-HRMS: calcd for $C_{28}H_{30}N^+$ ($[M + H]^+$) = 380.2372, found 380.2369.

IR (neat): 3054, 2956, 2866, 2246, 1685, 1601, 1506, 1461, 1364, 1268, 855 cm^{-1}.

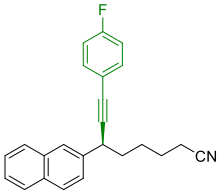


	Retention Time	Area	% Area
1	14.373	1379183	50.32
2	15.921	1361638	49.68



	Retention Time	Area	% Area
1	14.224	7057586	93.77
2	15.891	468862	6.23

(S)-8-(4-fluorophenyl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D9)



D9

colourless liquid, 58% yield, 90% ee; $[\alpha]^{20}_D$ = 50.0 (*c* = 0.08, in CH_2Cl_2).

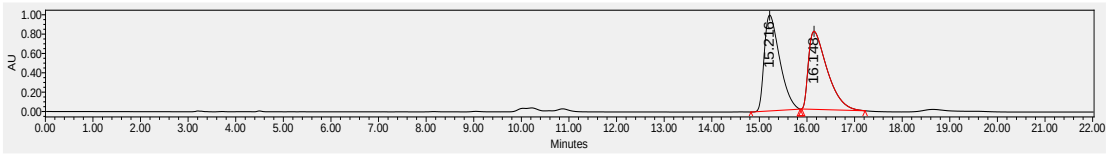
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 15.22 min, t_2 = 16.15 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (m, *J* = 5.6, 5.1, 3.0 Hz, 4H), 7.55 – 7.31 (m, 5H), 7.00 (t, *J* = 8.7 Hz, 2H), 4.01 (t, *J* = 7.2 Hz, 1H), 2.34 (t, *J* = 6.6 Hz, 2H), 1.98 – 1.90 (m, 2H), 1.76 – 1.63 (m, 4H).

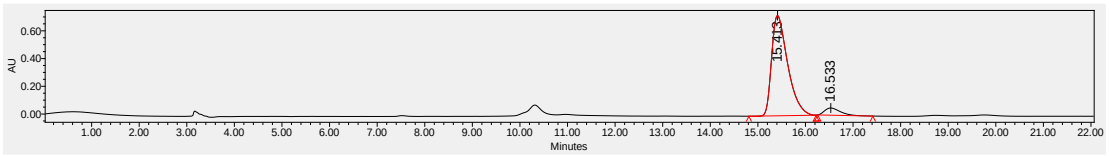
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.57, 161.10, 138.84, 133.58, 133.49, 133.46, 132.56, 128.46, 127.78, 127.68, 126.25, 125.95, 125.80, 125.64, 119.59, 119.56, 119.53, 115.64, 115.42, 90.42, 82.88, 38.26, 37.38, 26.55, 25.19, 17.12.

^{19}F NMR (376 MHz, $CDCl_3$) δ -111.57.

ESI-HRMS: calcd for $C_{24}H_{21}FN^+$ ($[M + H]^+$) = 342.1652, found 342,1641. **IR** (neat): 3054, 2921, 2853, 2244, 1600, 1506, 1265, 1227, 837, 734 cm^{-1}.

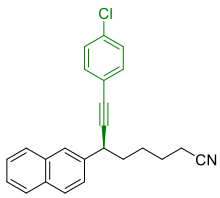


	Retention Time	Area	% Area
1	15.216	40741680	50.38
2	16.148	40132925	49.62



	Retention Time	Area	% Area
1	15.413	20232783	94.99
2	16.533	1066588	5.01

(S)-8-(4-chlorophenyl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D10)



D10

colourless liquid, 50% yield, 87% ee; $[\alpha]^{20}_D$ = 48.8 (*c* = 0.24, in CH_2Cl_2).

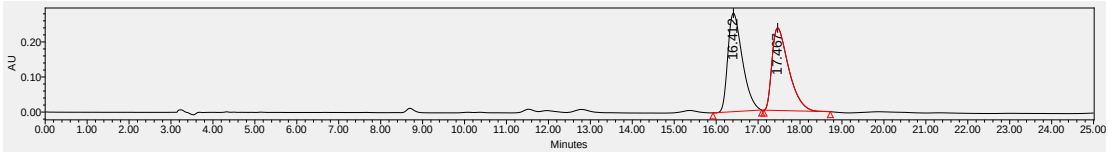
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 16.41 min, t_2 = 17.47 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (m, 4H), 7.55 – 7.44 (m, 3H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.32 – 7.25 (m, 2H), 4.02 (t, *J* = 7.2 Hz, 1H), 2.34 (t, *J* = 6.6 Hz, 2H), 2.01 – 1.90 (m, 2H), 1.77 – 1.62 (m, 4H).

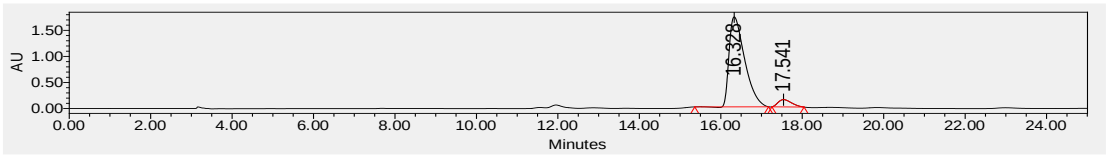
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.82, 134.09, 133.58, 133.08, 132.69, 128.75, 128.63, 127.91, 127.82, 126.42, 126.10, 125.97, 125.74, 122.10, 119.72, 91.96, 82.98, 38.45, 37.46, 26.69, 25.32, 17.27.

ESI-HRMS: calcd for $C_{24}H_{21}ClN^+$ ($[M + H]^+$) = 342.1652, found 342,1641.

IR (neat): 3055, 2940, 2864, 2245, 1681, 1595, 1488, 1398, 1091, 1013, 826 cm^{-1}.

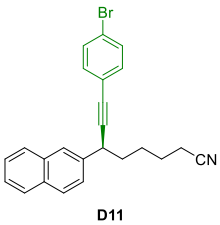


	Retention Time	Area	% Area
1	16.412	15946364	50.80
2	17.467	15442029	49.20



	Retention Time	Area	% Area
1	16.328	46390216	93.22
2	17.541	3373684	6.78

(S)-8-(4-bromophenyl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D11)



D11

colourless liquid, 50% yield, 85% ee; $[\alpha]^{20}_D$ = 39.3 (*c* = 0.3, in CH_2Cl_2).

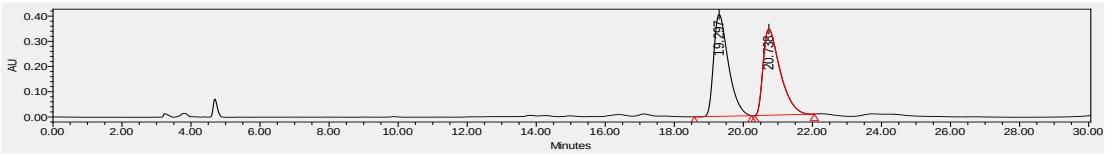
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 19.30 min, t_2 = 20.74 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.77 (m, 4H), 7.55 – 7.41 (m, 5H), 7.33 (d, *J* = 8.4 Hz, 2H), 4.02 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.4 Hz, 2H), 2.01 – 1.90 (m, 2H), 1.79 – 1.59 (m, 4H).

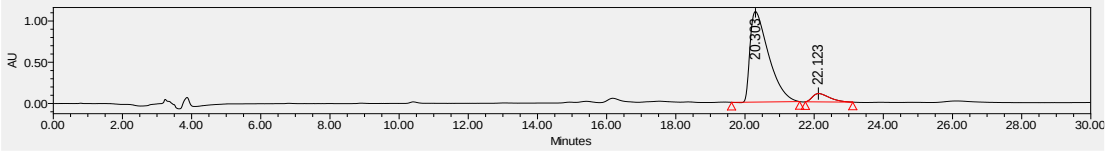
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.63, 133.44, 133.17, 132.55, 131.53, 128.50, 127.77, 127.68, 126.28, 125.96, 125.83, 125.60, 122.43, 122.14, 119.58, 92.04, 82.90, 38.33, 37.29, 26.54, 25.18, 17.13.

ESI-HRMS: calcd for $C_{24}H_{21}BrN^+$ ($[M + H]^+$) = 404.0831, found 404.0834.

IR (neat): 3957, 2928, 2859, 2246, 1596, 1485, 1444, 1181, 1071, 915, 760cm-1.

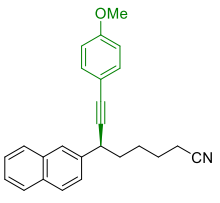


	Retention Time	Area	% Area
1	19.297	3788876	50.71
2	20.738	3682269	49.29



	Retention Time	Area	% Area
1	20.303	58751066	92.31
2	22.123	4894331	7.69

(S)-8-(4-methoxyphenyl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D12)



D12

colourless liquid, 48% yield, 90% ee; $[\alpha]^{20}_D$ = 64.3 (*c* = 0.18, in CH_2Cl_2).

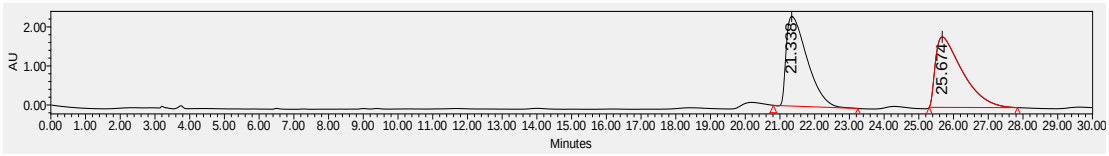
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 21.34 min, t_2 = 25.67 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.80 (m, 4H), 7.53 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.47 (m, 2H), 7.43 – 7.39 (m, 2H), 6.88 – 6.81 (m, 2H), 4.01 (t, *J* = 7.2 Hz, 1H), 3.81 (s, 3H), 2.34 (t, *J* = 6.6 Hz, 2H), 1.97 – 1.90 (m, 2H), 1.76 – 1.65 (m, 4H).

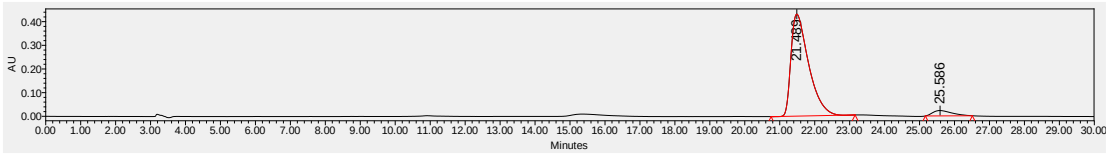
^{13}C NMR (151 MHz, $CDCl_3$) δ 159.47, 139.32, 133.58, 133.19, 132.63, 128.50, 127.91, 127.78, 126.30, 126.06, 125.88, 125.84, 119.80, 115.73, 114.02, 89.30, 83.85, 55.43, 38.43, 37.64, 26.70, 25.35, 17.25.

ESI-HRMS: calcd for $C_{25}H_{24}NO^+$ ($[M + H]^+$) = 354.1852, found 354.1849.

IR (neat): 3053, 2938, 2863, 2244, 1604, 1509, 1289, 1247, 1173, 1030, 831 cm^{-1}.

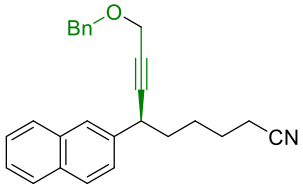


	Retention Time	Area	% Area
1	21.338	96605188	49.84
2	25.674	97206038	50.16



	Retention Time	Area	% Area
1	21.489	11371718	94.83
2	25.586	620223	5.17

(S)-10-(benzyloxy)-6-(naphthalen-2-yl)dec-7-ynenitrile (D13)



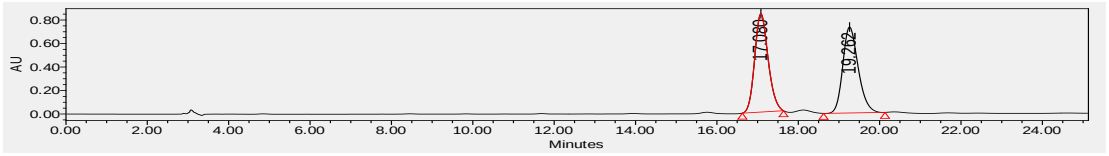
D13

colourless oil, 55% yield, 85% ee; $[\alpha]^{20}_D$ = 8.3 (*c* = 0.3, in CH_2Cl_2). **HPLC** (Chiralcel IF column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 17.08 min, t_2 = 19.26 min. **^{1}H NMR** (600 MHz, Chloroform-*d*) δ 7.86 – 7.80 (m, 4H), 7.52 – 7.41 (m, 3H), 7.40 – 7.36 (m, 5H), 4.64 (s, 2H), 4.29 (d, *J* = 2.0 Hz, 2H), 3.88 (t, *J* = 7.2 Hz, 1H), 2.31 (t, *J* = 6.8 Hz, 2H), 1.94 – 1.83 (m, 2H), 1.71 – 1.54 (m, 4H).

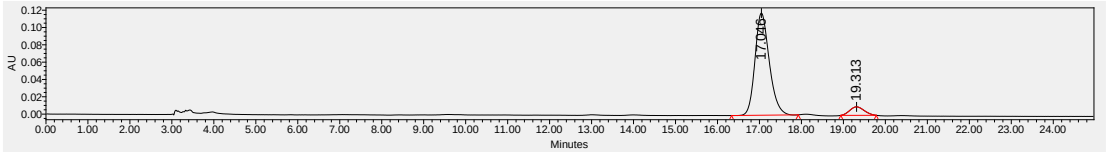
^{13}C NMR (151 MHz, $CDCl_3$) δ 138.82, 137.68, 133.53, 132.64, 128.59, 128.54, 128.22, 127.99, 127.88, 127.78, 126.37, 126.04, 125.91, 125.73, 119.74, 88.00, 79.56, 71.63, 57.86, 37.91, 37.37, 26.63, 25.31, 17.21.

ESI-HRMS: calcd for $C_{26}H_{26}NO^+$ ($[M + H]^+$) = 368.2008, found 368.2004.

IR (neat): 3056, 2938, 2860, 2244, 1600, 1503, 1454, 1355, 1070, 820, 739cm^{-1}.



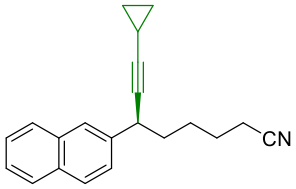
	Retention Time	Area	% Area
1	17.080	19153857	49.94
2	19.262	19196828	50.06



	Retention Time	Area	% Area
1	17.046	7275614	92.25

2	19.313	610850	7.75

(S)-8-cyclopropyl-6-(naphthalen-2-yl)oct-7-ynenitrile (D14)



D14

colourless oil, 58% yield, 84% ee; $[\alpha]^{20}_D$ = -12.5 (*c* = 0.32, in CH_2Cl_2).

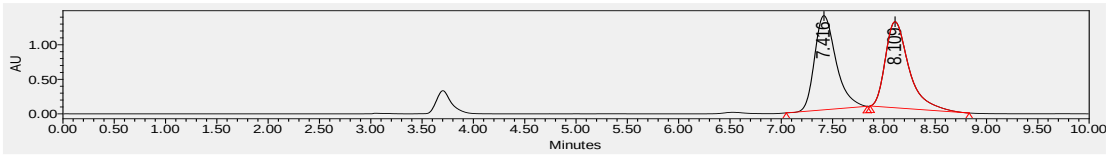
HPLC (Chiralcel IA column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 7.42 min, t_2 = 8.11 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.81 (t, *J* = 7.5 Hz, 3H), 7.76 (s, 1H), 7.54 – 7.43 (m, 3H), 3.75 (t, *J* = 7.2 Hz, 1H), 2.32 (t, *J* = 7.0 Hz, 2H), 1.83 – 1.77(m, 2H), 1.74 – 1.50 (m, 4H), 1.35 – 1.28 (m, 1H), 0.80 – 0.74 (m, 2H), 0.71– 0.65(m,, 2H).

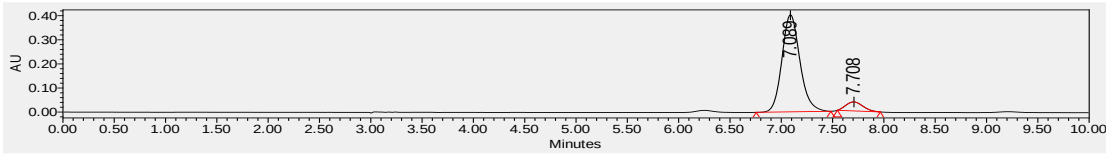
^{13}C NMR (151 MHz, $CDCl_3$) δ 139.77, 133.54, 132.56, 128.36, 127.87, 127.75, 126.22, 125.91, 125.85, 125.73, 119.82, 87.15, 76.43, 37.83, 37.75, 26.62, 25.32, 17.23, 8.44, 8.38, -0.20.

ESI-HRMS: calcd for $C_{21}H_{22}N^+$ ($[M + H]^+$) = 288.1746, found 288.1743.

IR (neat): 3026, 2926, 2858, 2245, 1600, 1500, 1454, 1339, 1023, 858, 820 cm^{-1}.

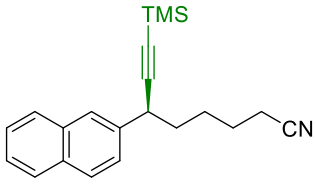


	Retention Time	Area	% Area
1	7.416	19800700	49.83
2	8.109	19934701	50.17



	Retention Time	Area	% Area
1	7.089	4907448	91.95
2	7.708	429437	8.05

(S)-6-(naphthalen-2-yl)-8-(trimethylsilyl)oct-7-ynenitrile (D15)



D15

colourless oil, 58% yield, 79% ee; $[\alpha]^{20}_D$ = -11.0 (*c* = 0.26, in CH_2Cl_2).

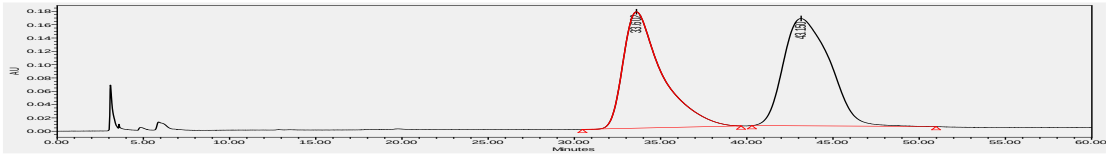
HPLC (Chiralcel OJ-H column), n-hexane/i-PrOH = 99/1, flow rate = 1.0 mL/min, λ = 211 nm, retention time: t_1 = 33.60 min, t_2 = 43.15 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 8.3 Hz, 3H), 7.79 (s, 1H), 7.51 – 7.40 (m, 3H), 3.83 (t, *J* = 7.2 Hz, 1H), 2.33 (t, *J* = 7.0 Hz, 2H), 1.87 – 1.82 (m, 2H), 1.76 – 1.54 (m, 4H), 0.21 (s, 9H).

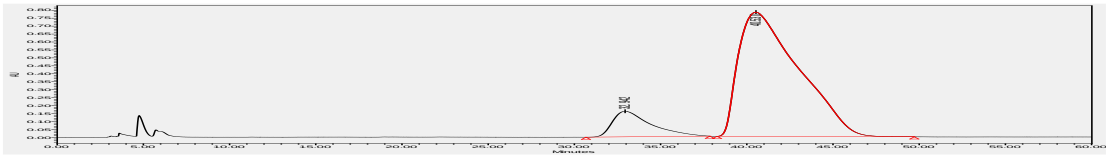
^{13}C NMR (151 MHz, $CDCl_3$) δ 138.79, 133.53, 132.62, 128.45, 127.90, 127.77, 126.30, 126.12, 125.86, 125.78, 119.75, 107.69, 88.28, 38.73, 37.47, 26.53, 25.30, 17.23, 0.28.

ESI-HRMS: calcd for $C_{21}H_{26}NSi^+$ ($[M + H]^+$) = 320.1829, found 320.1828.

IR (neat): 3055, 2953, 2862, 2169, 1600, 1507, 1248, 1085, 843 cm^{-1}.

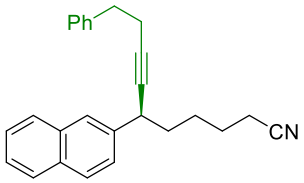


	Retention Time	Area	% Area
1	33.602	27345909	49.79
2	43.150	27575532	50.21



	Retention Time	Area	% Area
1	32.942	22798655	10.61
2	40.530	192080286	89.39

(S)-6-(naphthalen-2-yl)-10-phenyldec-7-ynenitrile (D16)



D16

colourless liquid, 60% yield, 82% ee; $[\alpha]^{20}_{D}$ = 23.8 (*c* = 0.29, in CH_2Cl_2).

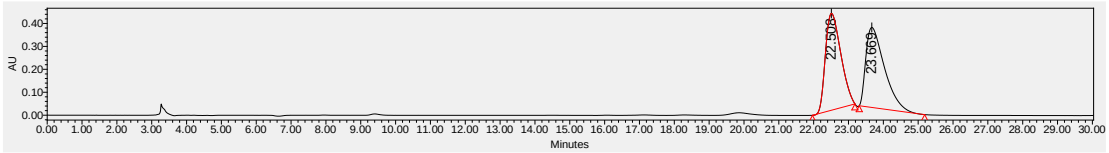
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 98/2, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 22.51 min, t_2 = 23.67 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.72 (s, 1H), 7.51 – 7.42 (m, 2H), 7.39 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.31 – 7.27 (m, 2H), 7.26 – 7.20 (m, 3H), 3.77 – 3.72 (t, *J* = 6.4, 1H), 2.87 (t, *J* = 7.4 Hz, 2H), 2.58 (t, *J* = 7.4, 2H), 2.27 (t, *J* = 7.2, 2H), 1.81 – 1.71 (m, 2H), 1.67 – 1.58 (m, 2H), 1.58 – 1.44 (m, 2H).

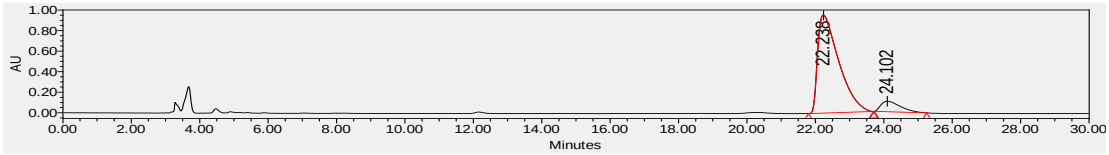
^{13}C NMR (151 MHz, $CDCl_3$) δ 140.97, 139.65, 133.53, 132.55, 128.73, 128.46, 128.33, 127.89, 127.74, 126.35, 126.20, 125.89, 125.73, 119.85, 83.27, 82.04, 37.82, 37.69, 35.43, 26.57, 25.32, 21.06, 17.20.

ESI-HRMS: calcd for $C_{26}H_{26}N^+$ ($[M + H]^+$) = 352.2059, found 352.2056.

IR (neat): 3026, 2926, 2858, 2245, 1600, 1500, 1454, 1367, 1339, 1023, 895, 858, 820cm^{-1}.

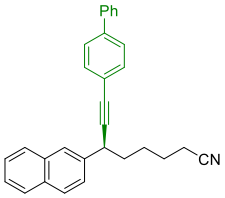


	Retention Time	Area	% Area
1	22.508	4762830	50.30
2	23.669	4705435	49.70



	Retention Time	Area	% Area
1	22.238	40868435	90.93
2	24.102	4076489	9.07

(S)-8-([1,1'-biphenyl]-4-yl)-6-(naphthalen-2-yl)oct-7-ynenitrile (D17)



D17

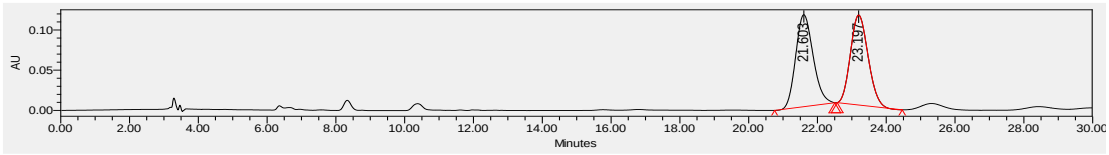
colourless oil, 58% yield, 89% ee. $[\alpha]^{20}_D$ = 38.9 (*c* = 0.54, in CH_2Cl_2). **HPLC** (Chiralcel IE column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 21.60 min, t_2 = 23.20 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.82 (m, 4H), 7.63 – 7.57 (m, 2H), 7.56 (m, 5H), 7.53 – 7.41 (m, 4H), 7.39 – 7.32 (m, 1H), 4.07 (t, *J* = 7.2 Hz, 1H), 2.40 – 2.32 (t, *J* = 6.6 Hz, 2H), 1.98 (m, 2H), 1.79 – 1.66 (m, 4H).

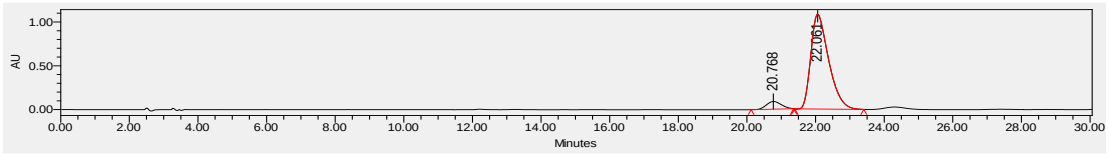
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.89, 140.59, 139.10, 133.62, 132.70, 132.28, 129.02, 128.60, 127.96, 127.83, 127.74, 127.18, 127.15, 126.39, 126.14, 125.93, 125.87, 122.56, 119.80, 91.60, 83.98, 38.54, 37.63, 26.75, 25.40, 17.30.

ESI-HRMS: calcd for $C_{30}H_{26}N^+$ ($[M + H]^+$) = 400.2059, found 400.2055.

IR (neat): 3055, 3031, 2919, 2852, 2246, 1683, 1601, 1485, 842, 821, 766, 697 cm^{-1} .

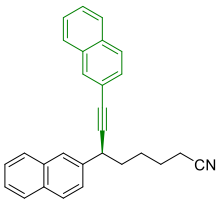


	Retention Time	Area	% Area
1	21.603	4446756	49.85
2	23.197	4473432	50.15



	Retention Time	Area	% Area
1	20.768	3840923	5.59
2	22.061	64927746	94.41

(S)-6,8-di(naphthalen-2-yl)oct-7-ynenitrile (D18)



D18

colourless oil, 57% yield, 90% ee. $[\alpha]^{20}_D$ = 90.6 (*c* = 0.07, in CH_2Cl_2).

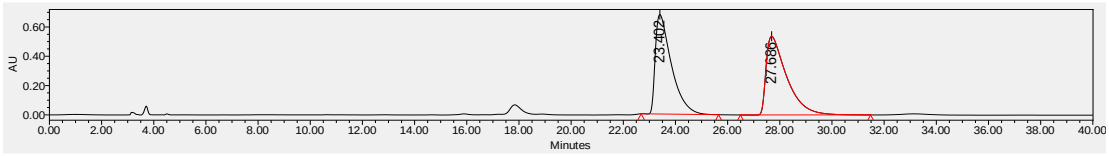
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 23.40 min, t_2 = 27.69 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 1.5 Hz, 1H), 7.89 (d, *J* = 1.8 Hz, 1H), 7.88 – 7.73 (m, 6H), 7.57 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.54 – 7.43 (m, 5H), 4.08 (t, *J* = 7.2 Hz, 1H), 2.39 – 2.28 (t, *J* = 6.6 Hz, 2H), 1.99 (m, 2H), 1.77 – 1.70 (m, 4H).

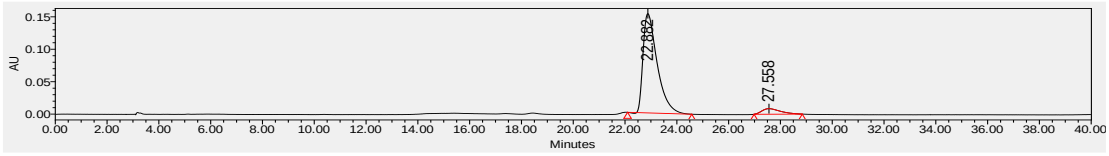
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.96, 133.50, 133.04, 132.69, 132.58, 131.37, 128.67, 128.47, 127.94, 127.81, 127.75, 127.68, 126.51, 126.24, 126.01, 125.79, 125.73, 120.79, 119.64, 91.15, 84.31, 38.42, 37.48, 26.63, 25.27, 17.15.

ESI-HRMS: calcd for $C_{28}H_{24}N^+$ ($[M + H]^+$) = 374.1903, found 374.1907.

IR (neat): 3055, 2924, 2855, 2244, 1683, 1597, 1503, 1461, 1369, 1126, 859 cm^{-1} .

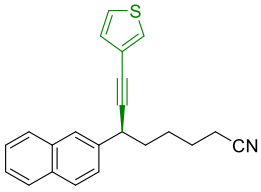


	Retention Time	Area	% Area
1	23.402	29074946	49.79
2	27.686	29315542	50.21



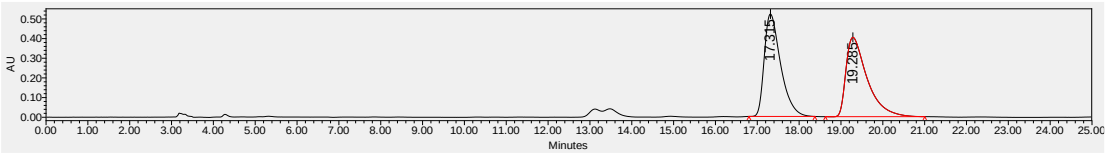
	Retention Time	Area	% Area
1	22.882	7122160	95.01
2	27.558	373994	4.99

(S)-6-(naphthalen-2-yl)-8-(thiophen-3-yl)oct-7-ynenitrile (D19)

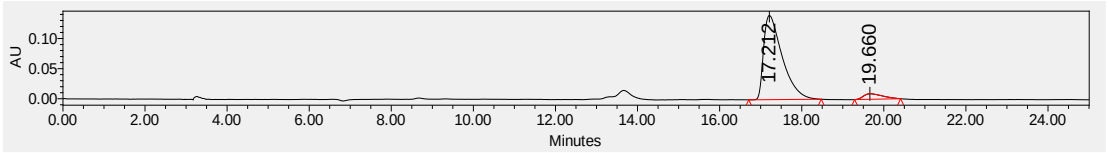


D19

colourless oil, 43% yield, 88% ee; $[\alpha]^{20}_D$ = 38.8 (*c* = 0.24, in CH_2Cl_2).
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 17.32 min, t_2 = 19.29 min.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.80 (m, 4H), 7.55 – 7.42 (m, 4H), 7.30 – 7.23 (m, 1H), 7.14 (dd, *J* = 5.0, 1.2 Hz, 1H), 4.01 (t, *J* = 7.2 Hz, 1H), 2.34 (t, *J* = 6.6 Hz, 2H), 1.94 (m, 2H), 1.74 – 1.56 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 138.89, 133.46, 132.55, 130.06, 128.43, 128.25, 127.78, 127.66, 126.22, 125.96, 125.76, 125.69, 125.21, 122.44, 119.61, 90.26, 78.98, 38.32, 37.37, 26.56, 25.21, 17.12.
ESI-HRMS: calcd for $C_{22}H_{20}NS^+$ ($[M + H]^+$) =330.1311, found 330.1309.
IR (neat): 3054, 2926, 2862, 2244, 1684, 1600, 1458, 1368, 1186, 820, 786 cm^{-1}.

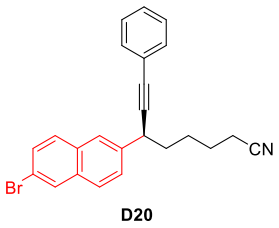


	Retention Time	Area	% Area
1	17.315	14172363	50.10
2	19.285	14116616	49.90



	Retention Time	Area	% Area
1	17.212	4415799	93.74
2	19.660	294990	6.26

(S)-6-(6-bromonaphthalen-2-yl)-8-phenyloct-7-ynenitrile (D20)



D20

colourless liquid, 43% yield, 90% ee; $[\alpha]^{20}_D$ = 7.9 (*c* = 0.30, in CH_2Cl_2).

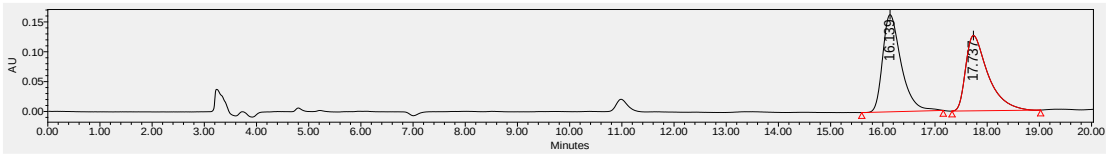
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 16.14 min, t_2 = 17.74 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 2.0 Hz, 1H), 7.83 (d, *J* = 1.8 Hz, 1H), 7.72 (dd, *J* = 16.8, 8.6 Hz, 2H), 7.58 – 7.52 (m, 2H), 7.51 – 7.44 (m, 2H), 7.34 – 7.29 (m, 3H), 4.02 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.6 Hz, 2H), 1.98 – 1.89 (m, 2H), 1.71 (m, 4H).

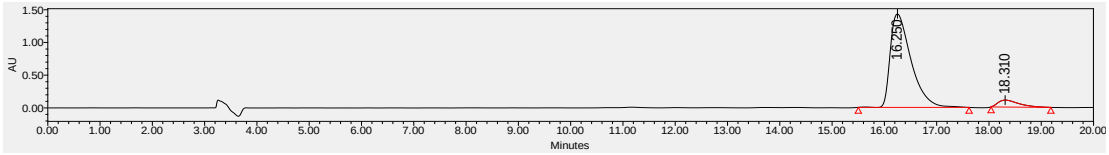
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.56, 133.60, 131.88, 131.72, 129.72, 129.61, 129.49, 128.35, 128.11, 127.54, 126.81, 125.94, 123.35, 119.69, 119.61, 90.33, 84.21, 38.28, 37.39, 26.57, 25.20, 17.15.

ESI-HRMS: calcd for $C_{24}H_{21}NBr^+$ ($[M + H]^+$) = 380.2372, found 380.2369.

IR (neat): 3030, 2938, 2846, 2246, 1684, 1601, 1487, 1229, 841, 762 cm^{-1}.

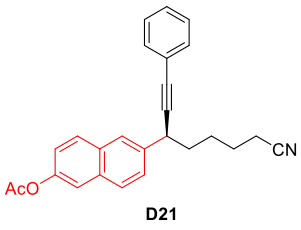


	Retention Time	Area	% Area
1	16.139	3779007	50.23
2	17.737	3744571	49.77



	Retention Time	Area	% Area
1	16.250	12946279	95.14
2	18.310	661439	4.86

(S)-6-(7-cyano-1-phenylhept-1-yn-3-yl)naphthalen-2-yl acetate (D21)



D21

colourless liquid, 47% yield, 86% ee; $[\alpha]^{20}_D$ = 27.3 (*c* = 0.31, in CH_2Cl_2).

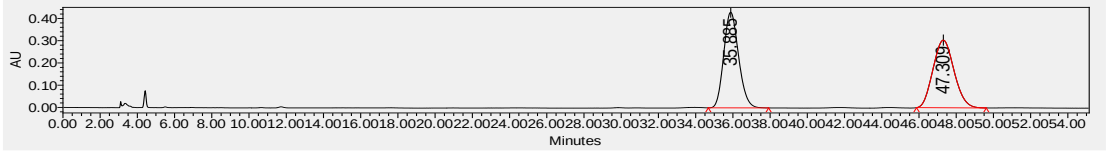
HPLC (Chiralcel IE column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 35.89 min, t_2 = 47.31 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.82 (d, 2H), 7.79 (d, *J* = 8.5 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.51 – 7.43 (m, 2H), 7.32 (m, 3H), 7.27 – 7.20 (m, 1H), 4.03 (t, *J* = 7.2 Hz, 1H), 2.35 (m, 5H), 1.98 – 1.89 (m, 2H), 1.80 – 1.56 (m, 4H).

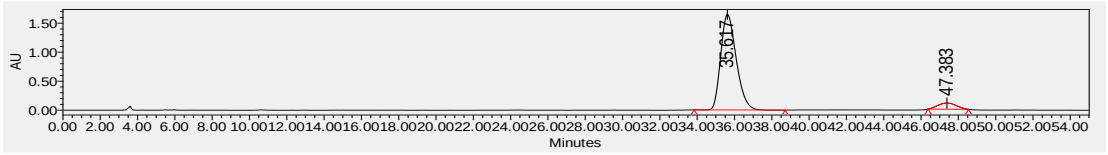
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.68, 148.32, 138.94, 132.83, 131.71, 131.50, 129.29, 128.31, 128.17, 128.02, 126.48, 125.86, 123.43, 121.50, 119.61, 118.39, 90.56, 84.07, 38.21, 37.43, 26.54, 25.22, 21.21, 17.13.

ESI-HRMS: calcd for $C_{26}H_{24}NO_2^+$ ($[M + H]^+$) = 382.1801, found 382.1798.

IR (neat): 2925, 2855, 2245, 1761, 1604, 1489, 1368, 1199, 1143, 908, 759 cm^{-1}.

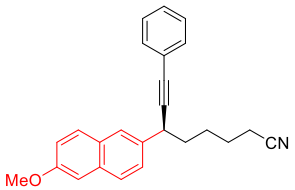


	Retention Time	Area	% Area
1	35.885	23916142	50.06
2	47.309	23855069	49.94



	Retention Time	Area	% Area
1	35.617	95248492	92.82
2	47.383	7363257	7.18

(S)-6-(6-methoxynaphthalen-2-yl)-8-phenyloct-7-ynenitrile (D22)



D22

colourless liquid, 50% yield, 90% ee; $[\alpha]^{20}_D$ = 65.0 (*c* = 0.14, in CH_2Cl_2).

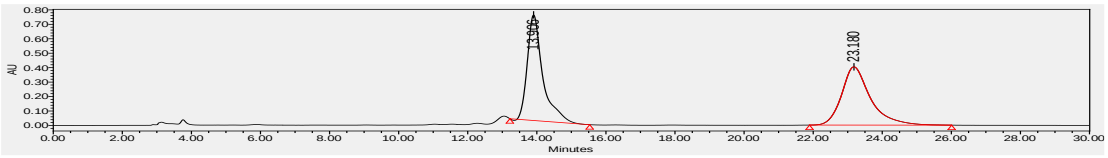
HPLC (Chiralcel IA column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 =13.91 min, t_2 = 23.18 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ7.79 (d, *J* = 1.8 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.51 (d, *J* = 1.8 Hz, 1H), 7.50 – 7.46 (m, 2H), 7.34 – 7.29 (m, 3H), 7.20 – 7.11 (m, 2H), 4.00 (t, *J* = 7.2 Hz, 1H), 3.93 (s, 3H), 2.34 (t, *J* = 6.6 Hz, 2H), 1.97 – 1.91 (m, 2H), 1.72 – 1.64 (m, 4H).

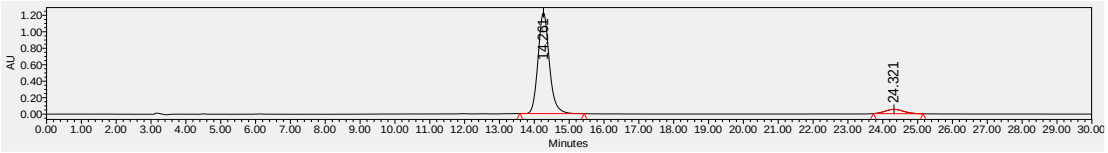
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.76, 136.78, 133.76, 131.83, 129.39, 129.05, 128.42, 128.07, 127.37, 126.34, 125.92, 123.69, 119.77, 119.14, 105.80, 91.09, 83.96, 55.45, 38.23, 37.66, 26.70, 25.37, 17.25.

ESI-HRMS: calcd for $C_{21}H_{20}NO_2^+$ ($[M + H]^+$) = 318.1488, found 318.1490.

IR (neat): 3056, 2938, 2862, 2245, 1605, 1485, 1266, 1214, 1168, 1030, 855 cm^{-1}.

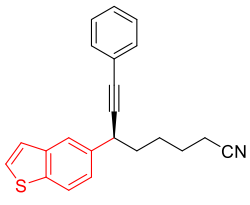


	Retention Time	Area	% Area
1	13.906	22840162	49.47
2	23.180	23327305	50.53



	Retention Time	Area	% Area
1	14.261	27678414	95.15
2	24.321	1410618	4.85

(S)-6-(benzo[b]thiophen-5-yl)-8-phenyloct-7-ynenitrile (D23)



D23

colourless liquid, 55% yield, 85% ee; $[\alpha]^{20}_D$ = 5.4 (*c* = 0.24, in CH_2Cl_2).

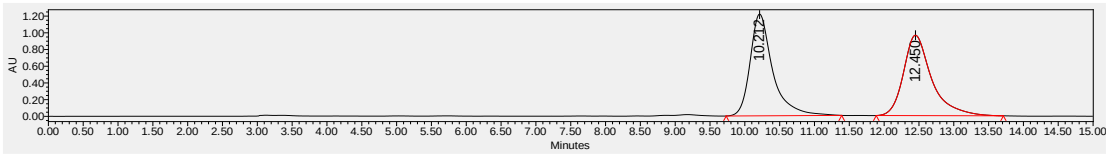
HPLC (Chiralcel IA column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 10.21 min, t_2 = 12.45 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ7.65 (d, *J* = 2.0 Hz, 1H), 7.63 (d, *J* = 2.0 Hz, 1H), 7.51 – 7.41 (m, 3H), 7.36 – 7.29 (m, 4H), 6.76 (d, *J* = 2.0 Hz, 1H), 3.99 (t, *J* = 7.2 Hz, 1H), 2.34 (t, *J* = 6.6 Hz, 2H), 1.93 – 1.88 (m, 2H), 1.62 – 1.76 (m, 4H).

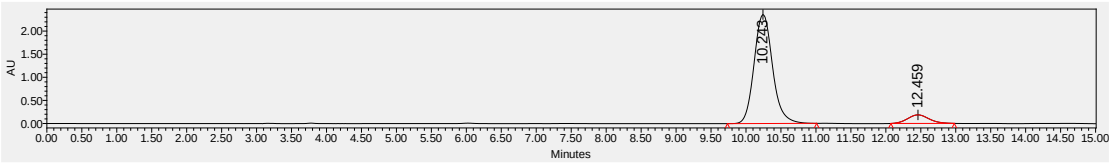
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.94, 138.37, 137.88, 131.69, 128.29, 127.97, 127.01, 124.01, 123.80, 123.49, 122.64, 122.25, 119.63, 90.95, 83.82, 38.13, 37.93, 26.57, 25.23, 17.13.

ESI-HRMS: calcd for $C_{22}H_{20}NS^+$ ([M + H]$^+$) = 330.1311, found 330.1313.

IR (neat): 3075, 2926, 2858, 2245, 1681, 1598, 1489, 1439, 1050,815, 758 cm^{-1}.

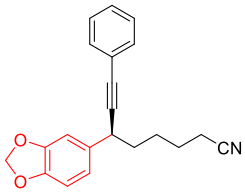


	Retention Time	Area	% Area
1	10.212	27412387	50.41
2	12.450	26968154	49.59



	Retention Time	Area	% Area
1	10.243	43346965	92.21
2	12.459	3662421	7.79

(S)-6-(benzo[d][1,3]dioxol-5-yl)-8-phenyloct-7-ynenitrile (D24)



D24

colourless liquid, 53% yield, 85% ee; $[\alpha]^{20}_D$ = -13.0 (*c* = 0.31, in CH_2Cl_2).

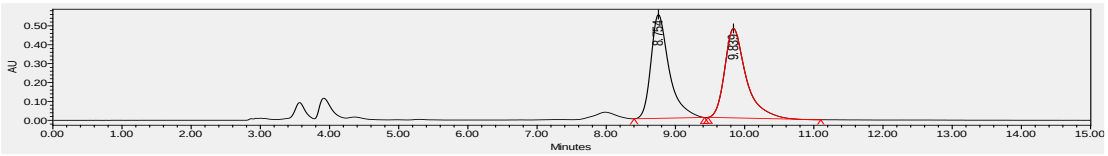
HPLC (Chiralcel IA column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 8.75 min, t_2 = 9.84 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.30 (dd, *J* = 5.0, 2.0 Hz, 3H), 6.93 (d, *J* = 1.8 Hz, 1H), 6.85 (m, *J* = 8.0, 1.8 Hz, 1H), 6.78 (d, *J* = 8.0 Hz, 1H), 5.96 (s, 2H), 3.79 (t, *J* = 7.2 Hz, 1H), 2.37 (t, *J* = 6.8 Hz, 2H), 1.86 – 1.78 (m, 2H), 1.77 – 1.55 (m, 4H).

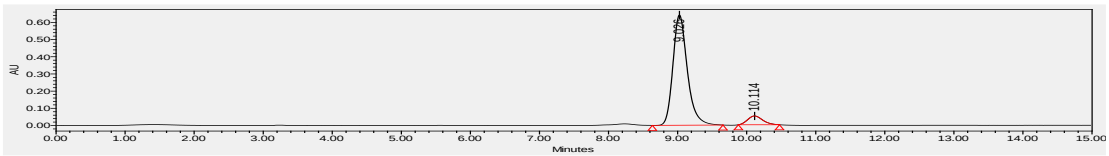
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.96, 146.59, 135.64, 131.78, 128.40, 128.09, 123.53, 120.61, 119.77, 108.35, 108.00, 101.18, 90.95, 83.81, 37.97, 37.94, 26.60, 25.33, 17.26.

ESI-HRMS: calcd for $C_{21}H_{20}NO_2^+$ ([M + H]$^+$) = 318.1488, found 318.1490.

IR (neat): 2930, 2855, 2246, 1676, 1486, 1441, 1246, 1038, 934, 759 cm^{-1}.

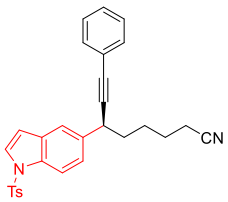


	Retention Time	Area	% Area
1	8.754	19134655	50.04
2	9.839	19106578	49.96



	Retention Time	Area	% Area
1	9.026	9287169	92.29
2	10.114	776339	7.71

(S)-8-phenyl-6-(1-tosyl-1H-indol-5-yl)oct-7-ynenitrile (D25)



D25

colourless liquid, 45% yield, 82% ee; $[\alpha]^{20}_D$ = 75.4 (*c* = 0.46, in CH_2Cl_2).

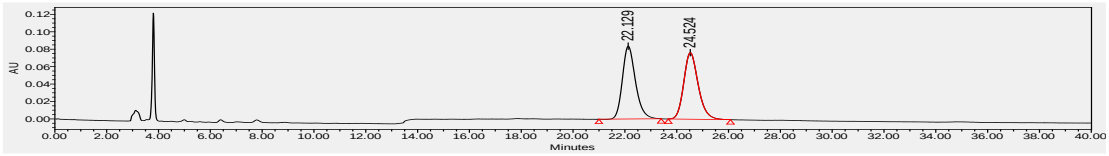
HPLC (Chiralcel IF column), n-hexane/i-PrOH = 85/15, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 22.13 min, t_2 = 24.52 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.6 Hz, 1H), 7.81 – 7.74 (m, 2H), 7.57 (m, 2H), 7.48 – 7.41 (m, 2H), 7.38 – 7.31 (m, 1H), 7.32 – 7.27 (m, 3H), 7.23 (d, *J* = 8.2 Hz, 2H), 6.64 (d, *J* = 3.6 Hz, 1H), 3.92 (t, *J* = 7.2 Hz, 1H), 2.34 (d, m, 5H), 1.90 – 1.82 (m, 2H), 1.76 – 1.55 (m, 4H).

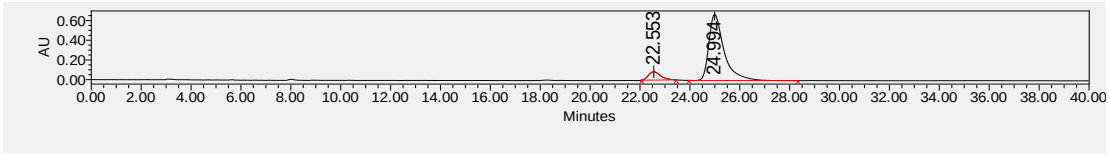
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.12, 136.93, 135.41, 133.94, 131.78, 131.15, 130.05, 128.41, 128.10, 126.98, 126.91, 124.32, 123.54, 120.12, 119.76, 113.71, 109.08, 91.06, 83.91, 38.15, 26.70, 25.30, 21.70, 17.23.

ESI-HRMS: calcd for $C_{29}H_{27}N_2O_2S^+$ ($[M + H]^+$) = 467.1787, found 467.1791.

IR (neat): 3055, 2927, 2859, 2245, 1596, 1458, 1370, 1172, 1091, 814, 760 cm^{-1}.

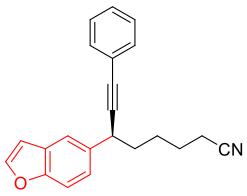


	Retention Time	Area	% Area
1	22.129	2937363	49.78
2	24.524	2963318	50.22



	Retention Time	Area	% Area
1	22.553	2848009	9.11
2	24.994	28404115	90.89

(S)-6-(benzofuran-5-yl)-8-phenyloct-7-ynenitrile (D26)



D26

colourless liquid, 45% yield, 85% ee; $[\alpha]^{20}_D$ = 4.2 (*c* = 0.26, in CH_2Cl_2).

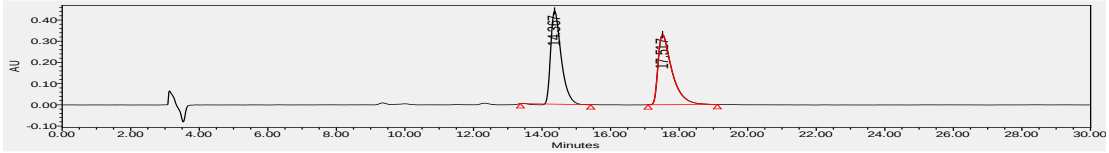
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 10.37 min, t_2 = 11.52 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 2.0 Hz, 1H), 7.63 (d, *J* = 2.2 Hz, 1H), 7.51 – 7.41 (m, 3H), 7.36 – 7.29 (m, 4H), 6.76 (d, *J* = 2.2 Hz, 1H), 3.97 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 7.0 Hz, 2H), 1.93 – 1.88 (m, 2H), 1.75 – 1.62 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 154.19, 145.65, 136.38, 131.82, 128.42, 128.07, 127.80, 123.95, 123.66, 119.96, 119.79, 111.53, 106.74, 91.35, 83.84, 38.31, 38.22, 26.71, 25.36, 17.28.

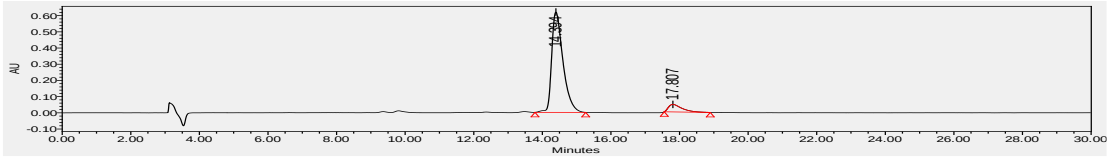
ESI-HRMS: calcd for $C_{22}H_{20}NO^+$ ($[M + H]^+$) = 314.1539, found 314.1541.

IR (neat): 3058, 2940, 2852, 2245, 1721, 1697, 1598, 1465, 1125, 1029, 892 cm^{-1}.



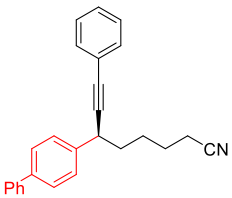
	Retention Time	Area	% Area
1	14.367	8609160	49.45

2	17.517	8800966	50.55



	Retention Time	Area	% Area
1	14.394	14198946	92.46
2	17.807	1158101	7.54

(S)-6-([1,1'-biphenyl]-4-yl)-8-phenyloct-7-ynenitrile (D27)



D27

colourless liquid, 53% yield, 88% ee; $[\alpha]^{20}_D$ = 16.7 (*c* = 0.24, in CH_2Cl_2).

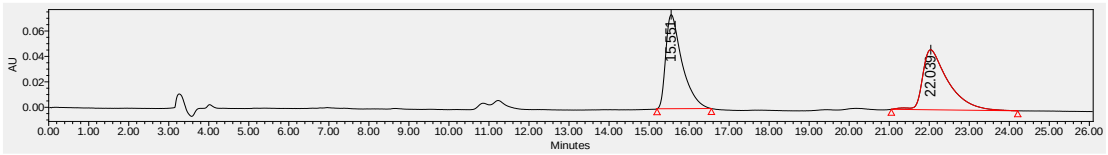
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 15.55 min, t_2 = 22.04 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.56 (m, 4H), 7.56 – 7.41 (m, 6H), 7.39 – 7.28 (m, 4H), 3.92 (t, *J* = 7.2 Hz, 1H), 2.45 – 2.33 (t, *J* = 6.6 Hz, 2H), 1.94 – 1.86 (m, 2H), 1.74 (m, 4H).

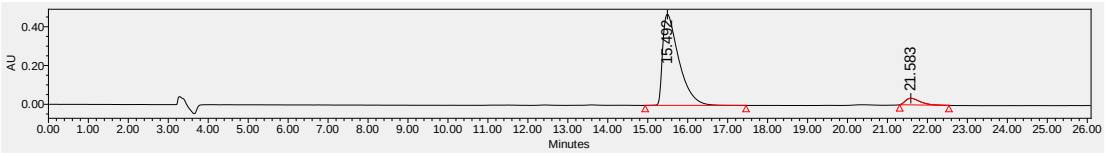
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.94, 140.83, 140.06, 131.82, 128.92, 128.42, 128.10, 127.98, 127.51, 127.40, 127.22, 123.59, 119.78, 90.80, 83.96, 37.98, 37.80, 26.72, 25.35, 17.27.

ESI-HRMS: calcd for $C_{26}H_{24}N^+$ ($[M + H]^+$) = 350.1903, found 350.1911.

IR (neat): 3030, 2940, 2865, 2246, 1684, 1601, 1487, 1406, 1228, 841, 735 cm^{-1}.

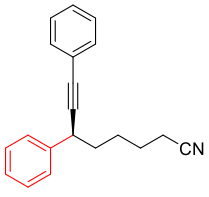


	Retention Time	Area	% Area
1	15.551	2094471	50.09
2	22.039	2087012	49.91



	Retention Time	Area	% Area
1	15.492	13289069	93.86
2	21.583	869005	6.14

(S)-6,8-diphenyloct-7-ynenitrile (D28)



D28

colourless liquid, 64% yield, 90% ee; $[\alpha]^{20}_D$ = 8.6 (*c* = 0.34, in CH_2Cl_2).

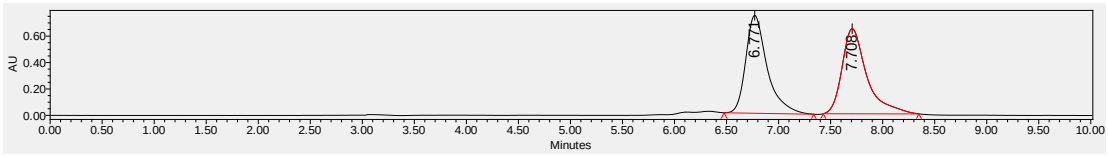
HPLC (Chiralcel IA column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 6.77 min, t_2 = 7.71 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.37 (m, 4H), 7.41 – 7.18 (m, 6H), 3.87 (t, *J* = 7.2 Hz, 1H), 2.34 (t, *J* = 6.8 Hz, 2H), 1.90 – 1.81 (m, 2H), 1.76 – 1.57 (m, 4H).

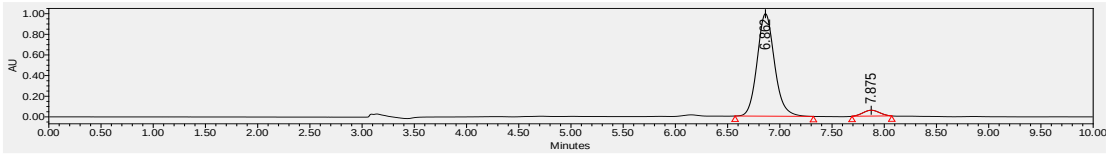
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.76, 131.80, 128.76, 128.40, 128.06, 127.55, 127.07, 123.65, 119.75, 90.90, 83.89, 38.30, 37.83, 26.69, 25.34, 17.25.

ESI-HRMS: calcd for $C_{20}H_{20}N^+$ ($[M + H]^+$) = 274.1590, found 374.1593.

IR (neat): 3029, 2927, 2859, 2346, 1598, 1490, 1449, 1347, 782 cm^{-1}.

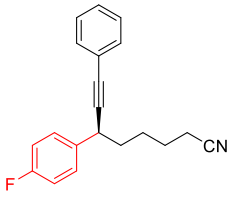


	Retention Time	Area	% Area
1	6.771	10601177	49.98
2	7.708	10611689	50.02



	Retention Time	Area	% Area
1	6.862	8968516	95.11
2	7.875	460844	4.89

(S)-6-(4-fluorophenyl)-8-phenyloct-7-ynenitrile (D29)



D29

colourless liquid, 47% yield, 90% ee; $[\alpha]^{20}_D$ = 6.7 (*c* = 0.18, in CH_2Cl_2).

HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 10.25 min, t_2 = 13.04 min.

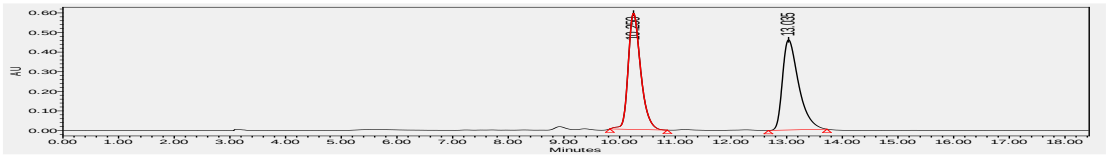
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.43 (m, 2H), 7.38 (dd, *J* = 8.8, 5.4 Hz, 2H), 7.34 – 7.24 (m, 3H), 7.04 (t, *J* = 8.8 Hz, 2H), 3.86 (t, *J* = 7.2 Hz, 1H). 2.36 (t, *J* = 6.8 Hz, 2H), 1.87 – 1.80 (m, 2H), 1.76 – 1.54 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.16, 160.72, 137.48, 137.44, 131.79, 129.06, 128.98, 128.44, 128.18, 123.45, 119.70, 115.66, 115.44, 90.60, 84.10, 37.90, 37.60, 26.62, 25.30, 17.27.

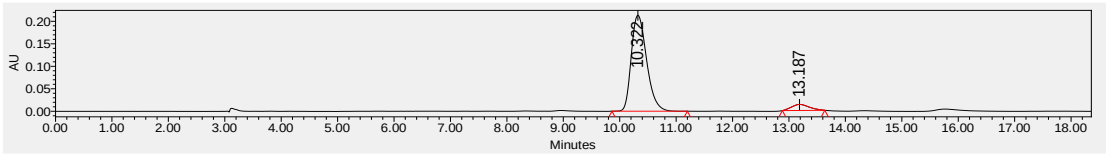
^{19}F NMR (376 MHz, $CDCl_3$) δ -116.06.

ESI-HRMS: calcd for $C_{20}H_{19}NF^+$ ($[M + H]^+$) = 292.1496, found 292.1495.

IR (neat): 3064, 2931, 2863, 2247, 1687, 1599, 1507, 1448, 1416, 1225cm^{-1}.

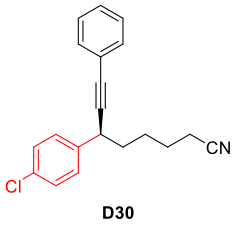


	Retention Time	Area	% Area
1	10.250	9230137	49.86
2	13.035	9283792	50.14



	Retention Time	Area	% Area
1	10.322	4035946	95.33
2	13.187	197561	4.67

(S)-6-(4-chlorophenyl)-8-phenyloct-7-ynenitrile (D30)



D30

colourless liquid, 60% yield, 85% ee; $[\alpha]^{20}_D$ = 6.7 (*c* = 0.18, in CH_2Cl_2).

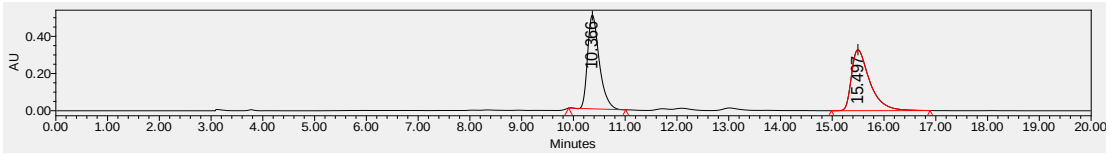
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 =10.37 min, t_2 = 15.50 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.40 (m, 2H), 7.37 – 7.17 (m, 7H), 3.85 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.8 Hz, 2H), 1.87 – 1.80 (m, 2H), 1.60 – 1.76 (m, 4H).

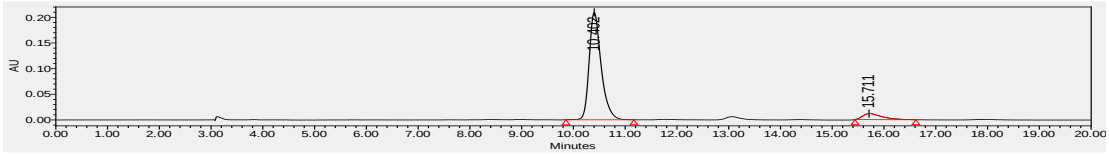
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.26, 132.83, 131.79, 128.92, 128.89, 128.45, 128.23, 123.38, 119.68, 90.25, 84.24, 37.74, 37.72, 26.60, 25.29, 17.27.

ESI-HRMS: calcd for $C_{20}H_{19}ClN^+$ ($[M + H]^+$) = 308.1200, found 308.1201.

IR (neat): 3059, 2935, 2864, 2246, 1688, 1594, 1489, 1289, 1091, 1014, 831 cm^{-1}.

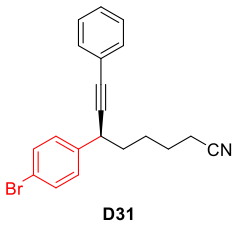


	Retention Time	Area	% Area
1	10.366	7952059	49.75
2	15.497	8031913	50.25



	Retention Time	Area	% Area
1	10.402	3375307	92.24
2	15.711	283852	7.76

(S)-6-(4-bromophenyl)-8-phenyloct-7-ynenitrile (D31)



D31

colourless liquid, 50% yield, 87% ee; $[\alpha]^{20}_D$ = 2.0 (*c* = 0.31, in CH_2Cl_2).

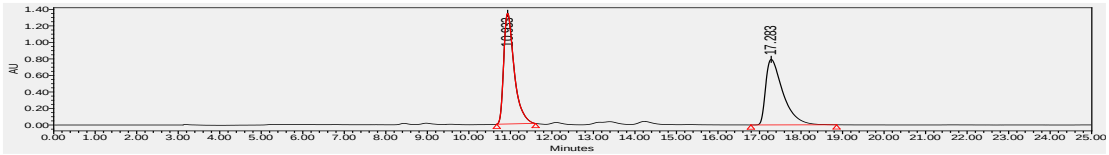
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 =10.93 min, t_2 = 17.28 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.37 (m, 4H), 7.40 – 7.23 (m, 5H), 3.83 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.8 Hz, 2H), 1.87 – 1.79 (m, 2H), 1.60 – 1.75(m, 4H).

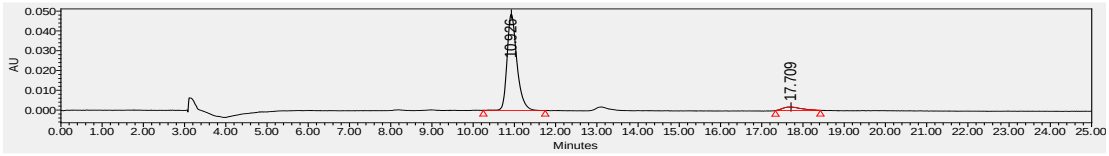
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.66, 131.71, 131.66, 129.18, 128.32, 128.10, 123.23, 120.74, 119.54, 90.02, 84.12, 37.69, 37.52, 26.46, 25.16, 17.13.

ESI-HRMS: calcd for $C_{20}H_{19}BrN^+$ ($[M + H]^+$) = 352.0695, found 352.0693.

IR (neat): 3056, 2926, 2858, 2246, 1596, 1486, 1404, 1071, 1010, 827, 758, 693 cm^{-1}.

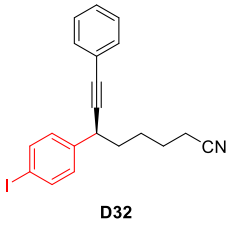


	Retention Time	Area	% Area
1	10.933	23435533	50.59
2	17.283	22891299	49.41



	Retention Time	Area	% Area
1	10.926	807070	93.54
2	17.709	55714	6.46

(S)-6-(4-iodophenyl)-8-phenyloct-7-ynenitrile (D32)



D32

colourless liquid, 48% yield, 85% ee; $[\alpha]^{20}_D$ = 38.9 (*c* = 0.20, in CH_2Cl_2).

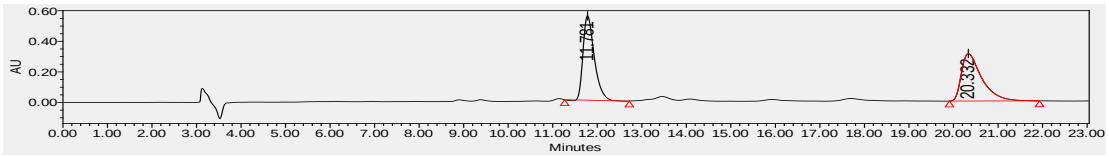
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 =11.78 min, t_2 = 20.33 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.59 (m, 2H), 7.47 – 7.33 (m, 2H), 7.36 – 7.28 (m, 3H), 7.20 – 7.14 (m, 2H), 3.82 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.8 Hz, 2H), 1.86 – 1.78 (m, 2H), 1.69 (m, 4H).

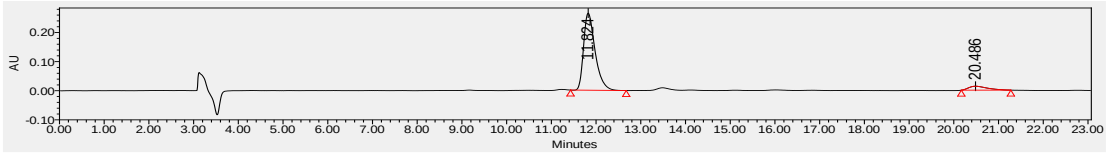
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.50, 137.82, 131.79, 129.63, 128.46, 128.24, 123.34, 119.70, 92.33, 90.10, 84.23, 37.92, 37.64, 26.61, 25.29, 17.28.

ESI-HRMS: calcd for $C_{20}H_{19}BrN^+$ ($[M + H]^+$) = 352.0695, found 352.0693.

IR (neat): 3059, 2940, 2867, 2244, 1687, 1580, 1484, 1395, 1224, 1004, 822 cm^{-1}.

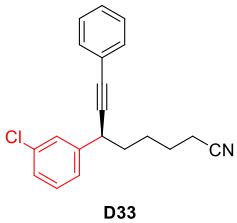


	Retention Time	Area	% Area
1	11.781	9776078	49.91
2	20.332	9810237	50.09



	Retention Time	Area	% Area
1	11.824	4755246	92.31
2	20.486	396025	7.69

(S)-6-(3-chlorophenyl)-8-phenyloct-7-ynenitrile (D33)



D33

colourless liquid, 58% yield, 87% ee; $[\alpha]^{20}_D$ = -6.2 (*c* = 0.29, in CH_2Cl_2).

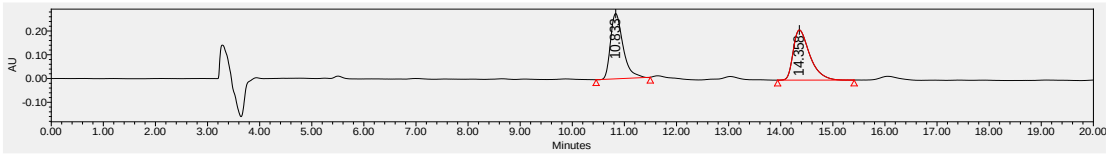
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 10.83 min, t_2 = 14.36 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.37 (m, 3H), 7.34 – 7.20 (m, 6H), 3.85 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.8 Hz, 2H), 1.89 – 1.81 (m, 2H), 1.76 – 1.57 (m, 4H).

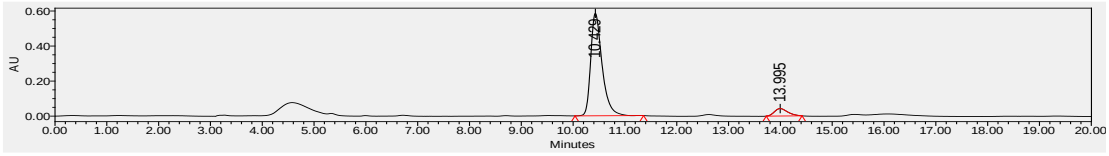
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.66, 134.44, 131.69, 129.88, 128.32, 128.13, 127.60, 127.17, 125.66, 123.20, 119.54, 89.79, 84.25, 37.90, 37.51, 26.49, 25.16, 17.12.

ESI-HRMS: calcd for $C_{20}H_{19}ClN^+$ ($[M + H]^+$) = 308.1200, found 308.1201.

IR (neat): 3061, 2938, 2865, 2246, 1690, 1595, 1424, 1221, 1075, 787 cm^{-1}.

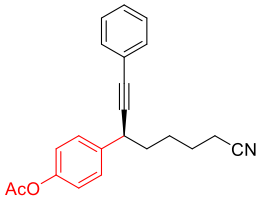


	Retention Time	Area	% Area
1	10.833	4593241	49.62
2	14.358	4663561	50.38



	Retention Time	Area	% Area
1	10.420	16363622	93.68
2	13.995	1104775	6.32

(S)-4-(7-cyano-1-phenylhept-1-yn-3-yl)phenyl acetate (D34)



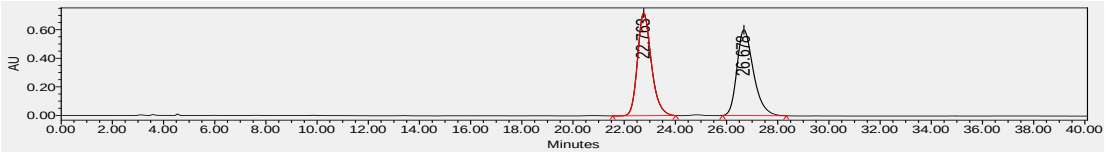
D34

colourless liquid, 47% yield, 87% ee; $[\alpha]^{20}_D$ = 7.2 (*c* = 0.32, in CH_2Cl_2). **HPLC** (Chiralcel IG column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 22.76 min, t_2 = 26.68 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.43 (m, 4H), 7.30 (m, 3H), 7.10 – 7.02 (m, 2H), 3.87 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 6.8 Hz, 2H), 2.30 (s, 3H), 1.88 – 1.81 (m, 2H), 1.75 – 1.61 (m, 4H).

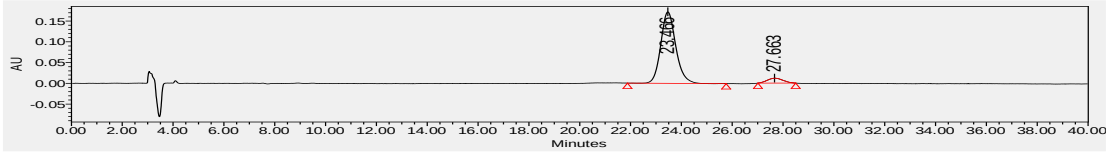
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.69, 149.65, 139.30, 131.79, 128.56, 128.42, 128.14, 123.49, 121.78, 119.72, 90.56, 84.08, 37.81, 37.78, 26.66, 25.31, 21.28, 17.25.

ESI-HRMS: calcd for $C_{22}H_{22}NO_2^+$ ($[M + H]^+$) = 332.1645, found 332.1642.

IR (neat): 3063, 2930, 2863, 2246, 1758, 1687, 1599, 1504, 1369, 1197, 1014, 913, 851 cm^{-1}.

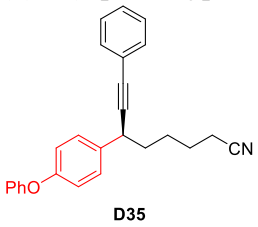


	Retention Time	Area	% Area
1	22.763	26963960	50.10
2	26.678	26854786	49.90



	Retention Time	Area	% Area
1	23.466	7065680	93.31
2	27.663	506440	6.69

(S)-6-(4-phenoxyphenyl)-8-(o-tolyl)oct-7-ynenitrile (D35)



D35

colourless liquid, 48% yield, 88% ee; $[\alpha]^{20}_D$ = 29.6 (*c* = 0.35, in CH_2Cl_2).

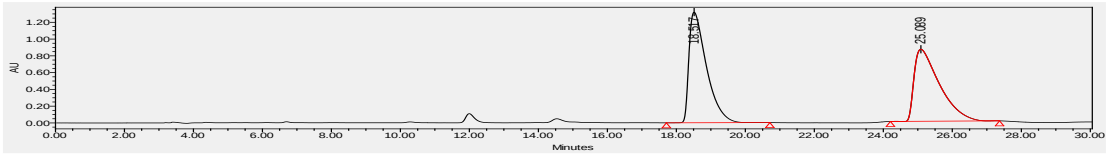
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 18.52 min, t_2 = 25.09 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.40 (m, 2H), 7.39 – 7.27 (m, 7H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.00 (m, 4H), 3.86 (t, *J* = 7.2 Hz, 1H), 2.36 (t, *J* = 6.8 Hz, 2H), 1.89 – 1.81 (m, 2H), 1.79 – 1.61 (m, 4H).

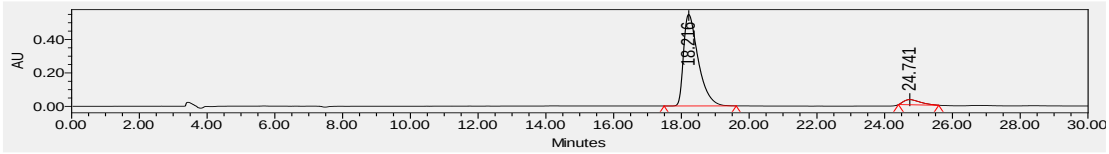
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.26, 156.14, 136.44, 131.66, 129.76, 128.69, 128.28, 127.97, 123.44, 123.26, 119.61, 118.97, 118.86, 90.77, 83.81, 37.76, 37.51, 26.55, 25.21, 17.15.

ESI-HRMS: calcd for $C_{26}H_{24}NO^+$ ($[M + H]^+$) = 366.1852, found 366.1856.

IR (neat): 3037, 2926, 2858, 2246, 1683, 1587, 1487, 1235, 1166, 843, 755 cm^{-1}.

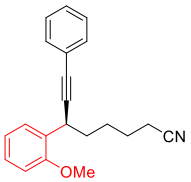


	Retention Time	Area	% Area
1	18.517	47923336	50.19
2	25.089	47555686	49.81



	Retention Time	Area	% Area
1	18.216	16446507	94.02
2	24.741	1045746	5.98

(R)-6-(2-methoxyphenyl)-8-phenyloct-7-ynenitrile (D36)



D36

colourless liquid, 60% yield, 83% ee; $[\alpha]^{20}_D$ = 17.2 (*c* = 0.35, in CH_2Cl_2).

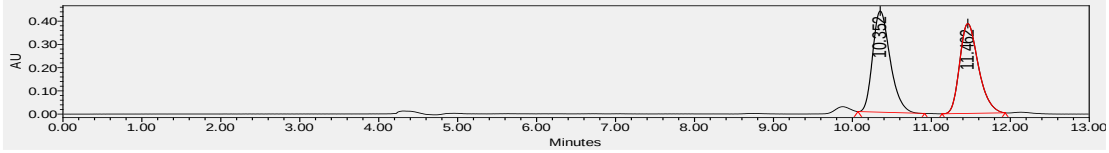
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 10.35 min, t_2 = 11.46 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.33 – 7.19 (m, 4H), 6.98 (t, *J* = 7.8 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 1H), 4.36 – 4.29 (t, *J* = 6.8 Hz, 1H), 3.86 (s, 2H), 2.35 (t, *J* = 7.0 Hz, 1H), 1.85 – 1.55 (m, 6H).

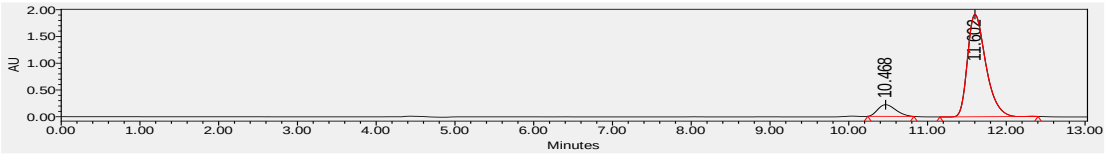
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.19, 131.81, 130.05, 128.64, 128.37, 128.11, 127.91, 123.89, 120.87, 119.90, 110.54, 91.46, 83.14, 55.55, 35.80, 31.35, 26.67, 25.22, 17.17.

ESI-HRMS: calcd for $C_{21}H_{22}NO^+$ ($[M + H]^+$) = 304.1695, found 304.1682.

IR (neat): 2938, 2863, 2837, 2245, 1596, 1491, 1460, 1440, 1243, 1028, 756 cm^{-1}.

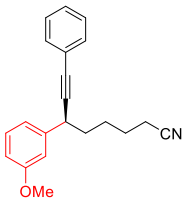


	Retention Time	Area	% Area
1	10.352	6446009	50.25
2	11.462	6382512	49.75



	Retention Time	Area	% Area
1	10.468	3249546	8.56
2	11.602	34713043	91.44

(S)-6-(3-methoxyphenyl)-8-phenyloct-7-ynenitrile (D37)



D37

colourless liquid, 51% yield, 91% ee; $[\alpha]^{20}_D$ = -7.2 (*c* = 0.21, in CH_2Cl_2).

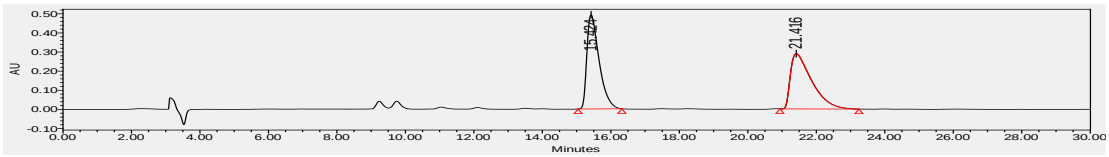
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 15.42 min, t_2 = 21.42 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (m, 2H), 7.32 – 7.18 (m, 4H), 7.02 – 6.95 (m, 2H), 6.80 (m, 1H), 3.82 (m, 4H), 2.34 (t, *J* = 6.8 Hz, 2H), 1.90 – 1.80 (m, 2H), 1.69 (m, 4H).

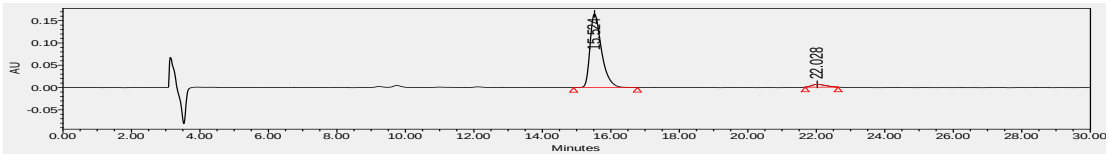
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.93, 143.37, 131.79, 129.73, 128.40, 128.07, 123.60, 119.94, 119.78, 113.52, 112.16, 90.76, 83.90, 55.37, 38.30, 37.71, 26.68, 25.34, 17.26.

ESI-HRMS: calcd for $C_{21}H_{22}NO^+$ ($[M + H]^+$) = 304.1695, found 304.1695.

IR (neat): 3054, 2937, 2862, 2244, 1601, 1488, 1437, 1257, 1149, 1045, 784 cm^{-1}.

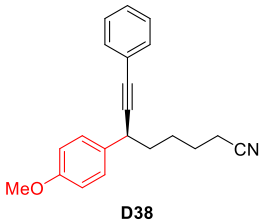


	Retention Time	Area	% Area
1	15.424	12234473	49.55
2	21.416	12456243	50.45



	Retention Time	Area	% Area
1	15.524	3861871	95.60
2	22.028	177637	4.40

(S)-6-(4-methoxyphenyl)-8-phenyloct-7-ynenitrile (D38)



D38

colourless liquid, 62% yield, 87% ee; $[\alpha]^{20}_D$ = 9.0 (*c* = 0.20, in CH_2Cl_2).

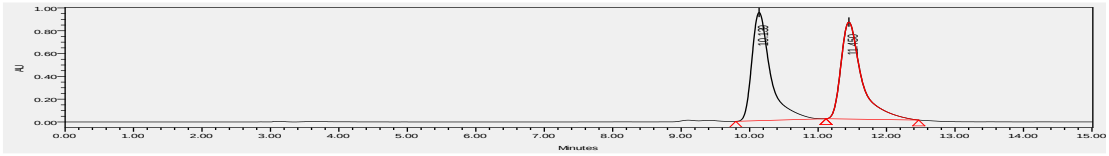
HPLC (Chiralcel IA column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 10.14 min, t_2 = 11.45 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.36 (m, 2H), 7.39 – 7.16 (m, 5H), 6.93 – 6.80 (m, 2H), 3.81 (m, 5H), 2.35 (t, *J* = 6.8 Hz, 2H), 1.92 – 1.78 (m, 2H), 1.72 – 1.57 (m, 4H).

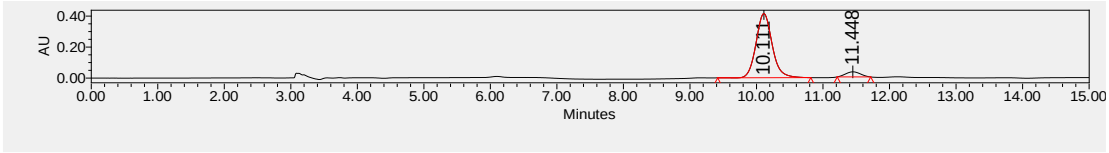
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.65, 133.83, 131.78, 128.52, 128.39, 128.02, 123.68, 119.80, 114.10, 91.25, 83.66, 55.45, 37.92, 37.45, 26.65, 25.35, 17.27.

ESI-HRMS: calcd for $C_{21}H_{22}NO^+$ ($[M + H]^+$) = 304.1695, found 304.1695.

IR (neat): 2937, 2865, 2245, 1676, 1602, 1510, 1298, 1248, 1175, 1032, 834 cm^{-1}.

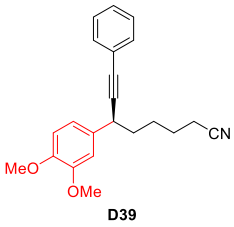


	Retention Time	Area	% Area
1	10.139	17972760	49.84
2	11.450	18088919	50.16



	Retention Time	Area	% Area
1	10.111	6966998	93.22
2	11.448	506521	6.78

(S)-6-(3,4-dimethoxyphenyl)-8-phenyloct-7-ynenitrile (D39)



D39

colourless liquid, 55% yield, 90% ee; $[\alpha]^{20}_D$ = -19.1 (*c* = 0.30, in CH_2Cl_2).

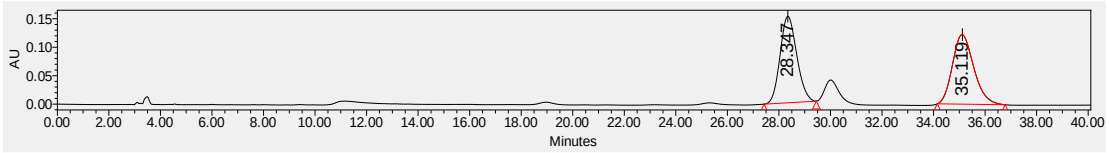
HPLC (Chiralcel IG column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 28.35 min, t_2 = 35.12 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.40 (m, 2H), 7.36 – 7.26 (m, 3H), 6.95 (dd, *J* = 6.4, 2.2 Hz, 2H), 6.85 (d, *J* = 8.8 Hz, 1H), 3.91 (s, 3H), 3.88 (s, 3H), 3.82 (t, *J* = 7.2 Hz, 1H), 2.36 (t, *J* = 6.8 Hz, 2H), 1.89 – 1.81 (m, 2H), 1.76 – 1.62 (m, 4H).

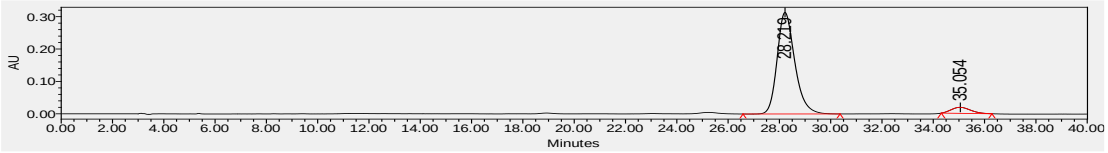
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.18, 148.12, 134.37, 131.77, 128.43, 128.07, 123.66, 119.77, 119.54, 111.36, 110.78, 91.15, 83.83, 56.11, 56.07, 37.93, 37.90, 26.73, 25.35, 17.29.

ESI-HRMS: calcd for $C_{22}H_{24}NO_2^+$ ($[M + H]^+$) = 334.1801, found 334.1802.

IR (neat): 2938, 2856, 2245, 1674, 1593, 1460, 1481, 1262, 1143, 1026, 761cm^{-1}.

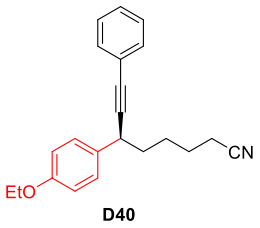


	Retention Time	Area	% Area
1	28.347	6833599	49.33
2	35.119	7018330	50.67



	Retention Time	Area	% Area
1	28.219	14962123	94.93
2	35.054	799867	5.07

(S)-6-(4-ethoxyphenyl)-8-phenyloct-7-ynenitrile (D40)



D40

colourless liquid, 57% yield, 86% ee; $[\alpha]^{20}_D$ = 9.8 (*c* = 0.33, in CH_2Cl_2).

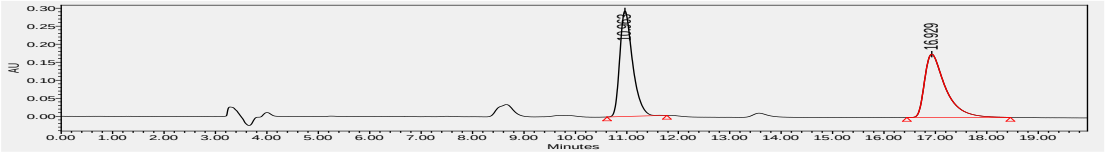
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 10.96 min, t_2 = 16.93 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.41 (m, 2H), 7.41 – 7.26 (m, 5H), 6.90 – 6.79 (m, 2H), 4.02 (q, *J* = 7.0 Hz, 2H), 3.81 (t, *J* = 7.2 Hz, 1H), 2.33 (t, *J* = 7.0 Hz, 2H), 1.83 (q, *J* = 7.0, 2.4 Hz, 2H), 1.77 – 1.55 (m, 4H), 1.41 (t, *J* = 7.0 Hz, 3H).

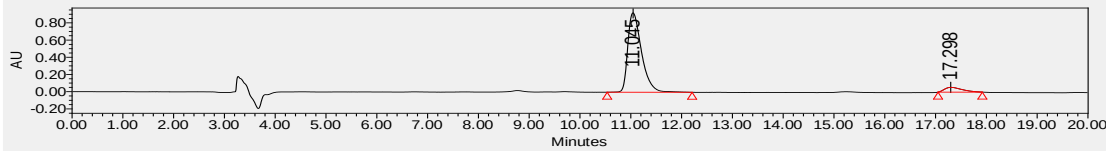
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.90, 133.53, 131.65, 128.36, 128.25, 127.86, 123.59, 119.65, 114.55, 91.18, 83.52, 63.47, 37.77, 37.31, 26.51, 25.22, 17.12, 14.87.

ESI-HRMS: calcd for $C_{22}H_{24}NO_2^+$ ($[M + H]^+$) = 318.1852, found 318.1852.

IR (neat): 2979, 2937, 2869, 2246, 1676, 1601, 1509, 1245, 1174, 1045, 835 cm^{-1}.

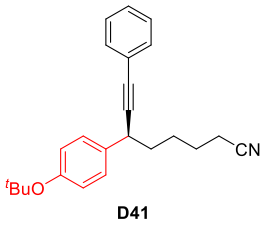


	Retention Time	Area	% Area
1	10.963	4987776	50.28
2	16.929	4932203	49.72



	Retention Time	Area	% Area
1	11.045	17372760	92.80
2	17.298	1347190	7.20

(S)-6-(4-(tert-butoxy)phenyl)-8-phenyloct-7-ynenitrile (D41)



D41

colourless liquid, 30% yield, 90% ee; $[\alpha]^{20}_D$ = 11.3 (*c* = 0.16, in CH_2Cl_2).

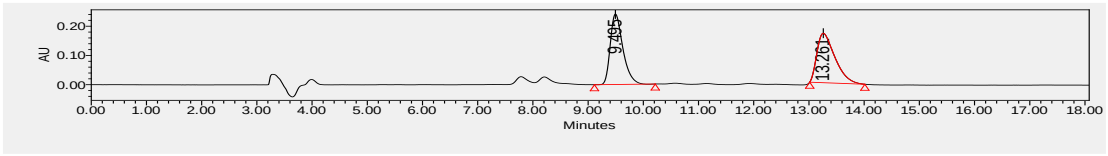
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 9.50 min, t_2 = 13.26 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.41 (m, 2H), 7.41 – 7.26 (m, 5H), 7.02 – 6.92 (m, 2H), 3.83 (t, *J* = 7.2 Hz, 1H), 2.35 (t, *J* = 7.0 Hz, 2H), 1.87 – 1.80 (m, 2H), 1.75 – 1.62 (m, 4H), 1.34 (s, 9H).

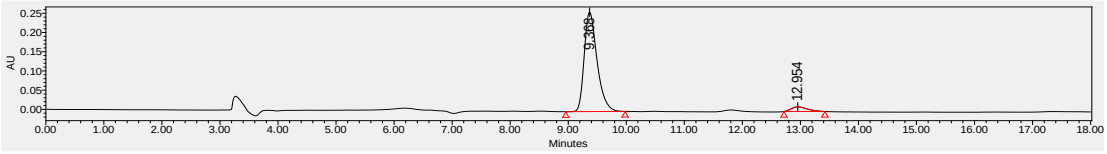
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.37, 136.49, 131.80, 128.41, 128.04, 127.90, 124.36, 123.70, 119.77, 91.15, 83.83, 78.56, 37.91, 37.66, 28.99, 26.71, 25.35, 17.28.

ESI-HRMS: calcd for $C_{24}H_{28}NO^+$ ($[M + H]^+$) = 346.2165, found 346.2164.

IR (neat): 2976, 2929, 2866, 2246, 1680, 1598, 1503, 1367, 1238, 1160, 896 cm^{-1}.

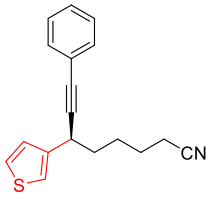


	Retention Time	Area	% Area
1	9.495	3830034	50.07
2	13.261	3819692	49.93



	Retention Time	Area	% Area
1	9.368	3975296	94.86
2	12.954	215285	5.14

(R)-8-phenyl-6-(thiophen-3-yl)oct-7-ynenitrile (D42)



D42

colourless liquid, 58% yield, 87% ee; $[\alpha]^{20}_D$ = -6.2 (*c* = 0.29, in CH_2Cl_2).

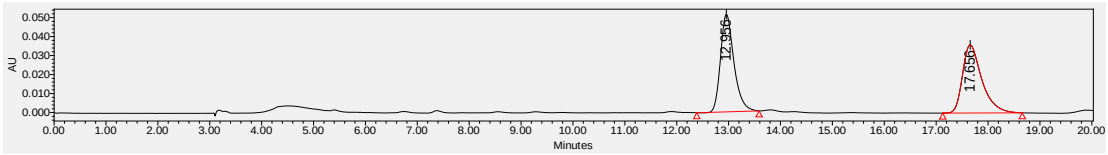
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 12.96 min, t_2 = 17.66 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.44 (m, 2H), 7.30 (m, 4H), 7.27 – 7.21 (m, 1H), 7.10 (dd, *J* = 5.0, 1.4 Hz, 1H), 3.98 (t, *J* = 8.2 Hz, 1H), 2.36 (t, *J* = 6.8 Hz, 2H), 1.97 – 1.89 (m, 2H), 1.82 – 1.61 (m, 4H).

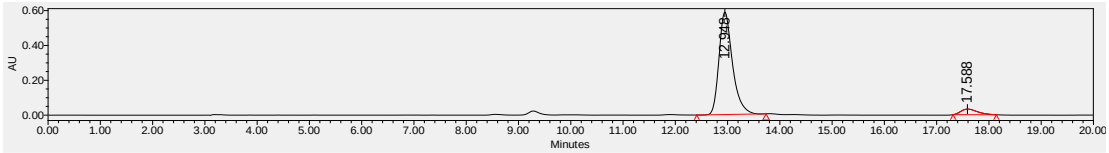
^{13}C NMR (151 MHz, $CDCl_3$) δ 142.11, 131.79, 128.42, 128.11, 126.96, 126.20, 123.53, 121.23, 119.76, 90.64, 83.29, 36.57, 33.55, 26.49, 25.33, 17.28.

ESI-HRMS: calcd for $C_{18}H_{18}NS^+$ ($[M + H]^+$) = 280.1154, found 280.1155.

IR (neat): 3102, 2939, 2865, 2246, 1677, 1598, 1511, 1447, 1417, 1232, 787 cm^{-1}.

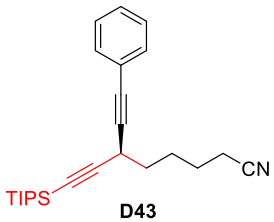


	Retention Time	Area	% Area
1	12.956	13359645	49.95
2	17.656	13385350	50.05



	Retention Time	Area	% Area
1	12.948	10517608	93.62
2	17.588	716585	6.38

(R)-8-phenyl-6-((triisopropylsilyl)ethynyl)oct-7-ynenitrile (D43)



D43

colourless liquid, 63% yield, 92% ee; $[\alpha]^{20}_D$ = -12.8 (*c* = 0.18, in CH_2Cl_2).

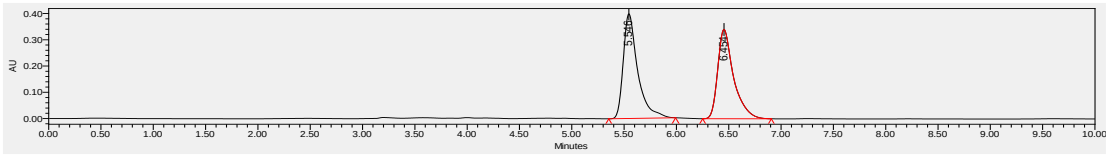
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 5.55 min, t_2 = 6.45 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.36 (m, 2H), 7.39 – 7.26 (m, 3H), 3.65 (t, *J* = 6.3 Hz, 1H), 2.41 – 2.29 (m, 2H), 1.88 – 1.74 (m, 6H), 1.08 (d, 21H).

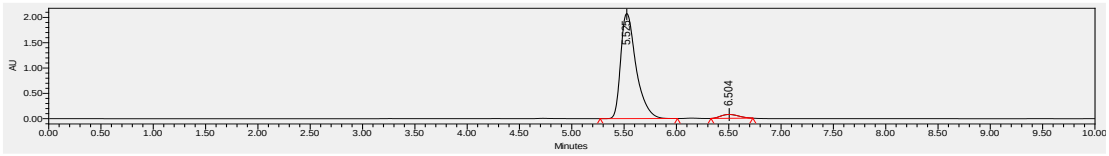
^{13}C NMR (101 MHz, $CDCl_3$) δ 131.79, 128.36, 128.19, 123.26, 119.59, 105.65, 87.52, 82.30, 81.52, 35.08, 26.14, 25.15, 24.87, 18.73, 17.26, 11.34.

ESI-HRMS: calcd for $C_{25}H_{35}NSiNa^+$ ($[M + Na]^+$) = 400.2431, found 400.2428.

IR (neat): 3639, 3547, 3256, 3029, 2943, 2865, 2246, 2174, 2346, 1598, 1490, 1449, 1347, 787 cm^{-1}.

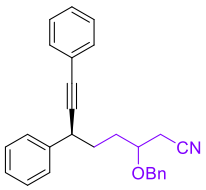


	Retention Time	Area	% Area
1	5.546	3613998	50.30
2	6.454	3571360	49.70



	Retention Time	Area	% Area
1	5.525	21217391	95.93
2	6.504	899972	4.07

(S)-3-(benzyloxy)-6,8-diphenyloct-7-ynenitrile (D44)



D44

colourless liquid, 43% yield, 80% ee; $[\alpha]^{20}_{D} = 8.0$ (*c* = 0.2, in CH_2Cl_2).

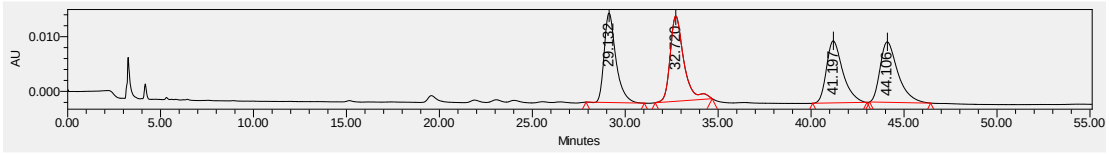
HPLC (Chiralcel IB column), n-hexane/i-PrOH = 98/2, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 29.13 min, t_2 = 32.72 min, t_2 = 41.20 min, t_2 = 44.11 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.23 (m, 15H), 4.66 – 4.48 (m, 2H), 3.92 – 3.82 (m, 1H), 3.79 – 3.68 (m, 1H), 2.54 (d, *J* = 5.8 Hz, 2H), 1.90 (m, 4H).

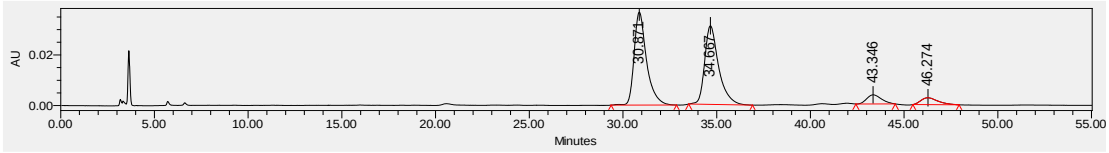
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.20, 137.23, 131.50, 128.47, 128.38, 128.10, 127.86, 127.80, 127.72, 127.28, 127.26, 126.82, 123.26, 117.31, 90.37, 83.84, 74.08, 73.87, 71.67, 37.96, 37.76, 33.53, 33.34, 31.74, 31.56, 22.86, 22.82.

ESI-HRMS: calcd for $C_{27}H_{25}NONa^+$ ($[M + Na]^+$) = 402.1824, found 402.1826.

IR (neat): 3060, 3029, 2924, 2865, 2250, 1599, 1491, 1451, 1348, 1093, 1028, 75c6, 696 m^{-1}.

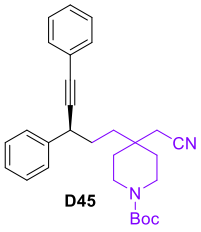


	Retention Time	Area	% Area
1	29.132	731007	25.04
2	32.720	740786	25.37
3	41.197	724704	24.82
4	44.106	722886	24.76



	Retention Time	Area	% Area
1	30.871	3342659	45.20
2	34.667	3317108	44.86
3	43.346	371870	5.03
4	46.274	363193	4.91

(S)-tert-butyl4-(cyanomethyl)-4-(3-phenyl-5-phenylpent-4-yn-1-yl)piperidine-1-carboxylate(D45)



D45

colourless liquid, 27% yield, 81% ee; $[\alpha]^{20}_D$ = -2.2 (*c* = 0.32, in CH_2Cl_2).

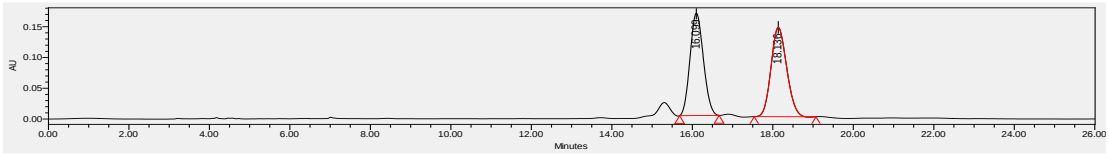
HPLC (Chiralcel IE column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 16.10 min, t_2 = 18.14 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.40 (m, 4H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.33 – 7.28 (m, 3H), 7.27 (d, *J* = 5.4 Hz, 1H), 3.86 (t, *J* = 6.6 Hz, 1H), 3.51 – 2.98 (m, 4H), 2.33 (s, 2H), 1.91 – 1.62 (m, 4H), 1.54 – 1.46 (m, 4H), 1.44 (s, 9H).

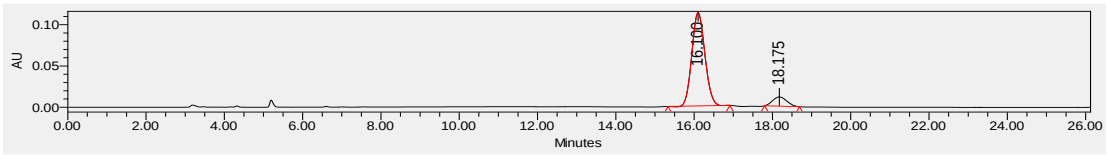
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.71, 141.32, 131.68, 128.71, 128.30, 128.01, 127.38, 127.11, 123.34, 117.36, 90.47, 84.08, 79.79, 38.55, 34.03, 33.83, 32.25, 28.40, 26.31.

ESI-HRMS: calcd for $C_{29}H_{35}N_2O_2^+$ ($[M + H]^+$) = 443.2693, found 443.2697.

IR (neat): 2974, 2924, 2854, 2242, 1687, 1423, 1366, 1247, 1154, 1020, 759 cm^{-1}.

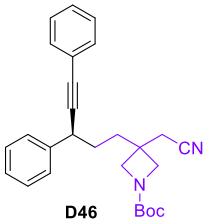


	Retention Time	Area	% Area
1	16.099	4501717	49.68
2	18.136	4559711	50.32



	Retention Time	Area	% Area
1	16.100	2619300	90.31
2	18.175	281175	9.69

(S)-tert-butyl 3-(cyanomethyl)-3-(3,5-diphenylpent-4-yn-1-yl)azetidine-1-carboxylate (D46)



D46

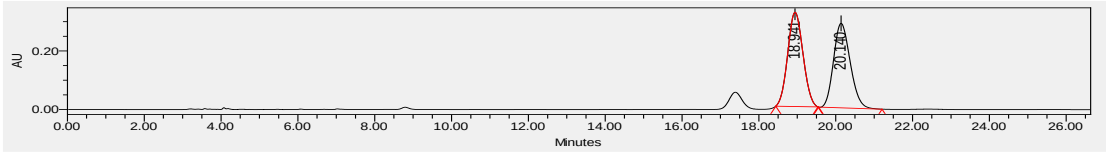
colourless liquid, 50% yield, 85% ee; $[\alpha]^{20}_D$ = 8.5 (*c* = 0.34, in CH_2Cl_2).

HPLC (Chiralcel IE column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 18.94 min, t_2 = 20.14 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.26 (m, 10H), 3.89 (t, *J* = 7.8Hz, 1H), 3.77 – 3.66 (m, 4H), 2.61 (s, 2H), 2.0 – 1.72 (m, 4H), 1.42 (s, 9H).

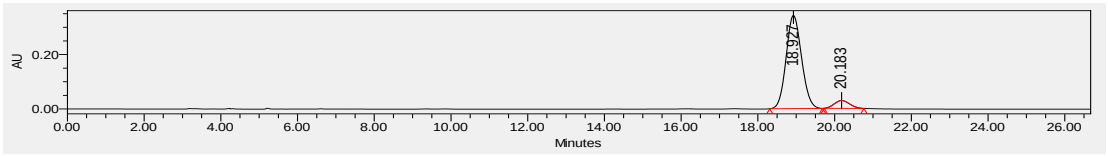
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.27, 141.14, 131.84, 128.91, 128.44, 128.23, 127.50, 127.33, 123.35, 117.01, 90.19, 84.44, 80.18, 38.42, 35.45, 34.30, 33.35, 28.45, 26.08.

ESI-HRMS: calcd for $C_{27}H_{31}N_2O_2^+$ ($[M + H]^+$) = 415.2380, found 443. 2383. **IR** (neat): 2972, 2928, 2880, 2245, 1698, 1398, 1150, 859, 759 cm^{-1}.



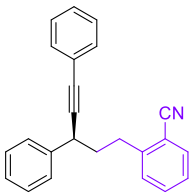
	Retention Time	Area	% Area
1	18.941	8878017	50.55

2	20.140	8686392	49.45



	Retention Time	Area	% Area
1	18.927	9547529	92.32
2	20.183	793899	7.68

(S)-2-(3,5-diphenylpent-4-yn-1-yl)benzonitrile (D47)



D47

colourless liquid, 21% yield, 65% ee; $[\alpha]^{20}_D$ = 28.3 (*c* = 0.36, in CH_2Cl_2).

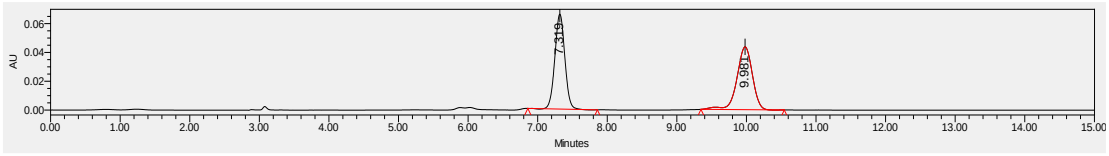
HPLC (Chiralcel AD-H column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 7.32 min, t_2 = 9.98 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.46 – 7.34 (m, 5H), 7.24 (m, 8H), 3.87 – 3.79 (t, *J* = 7.4 Hz, 1H), 3.12 – 2.91 (m, 2H), 2.19 – 2.05 (m, 2H).

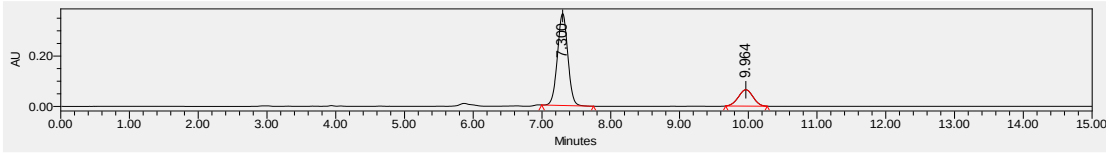
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.75, 141.40, 133.10, 132.90, 131.88, 129.81, 128.79, 128.40, 128.08, 127.59, 127.14, 126.78, 123.62, 118.08, 112.58, 90.48, 84.49, 39.43, 38.18, 32.71.

ESI-HRMS: calcd for $C_{24}H_{19}NNa^+$ ($[M + Na]^+$) = 379.2032, found 379.2030.

IR (neat): 3060, 3028, 2924, 2856, 2224, 1645, 1489, 1449, 1072, 758 cm^{-1}.

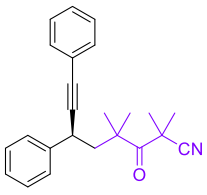


	Retention Time	Area	% Area
1	7.319	659691	49.54
2	9.981	671876	50.46



	Retention Time	Area	% Area
1	7.300	3900558	82.36
2	9.964	835398	17.64

(S)-2,2,4,4-tetramethyl-3-oxo-6,8-diphenyloct-7-ynenitrile (D48)



D48

colourless liquid, 44% yield, 35% ee; $[\alpha]^{20}_D$ = -12.4 (*c* = 0.23, in CH_2Cl_2).

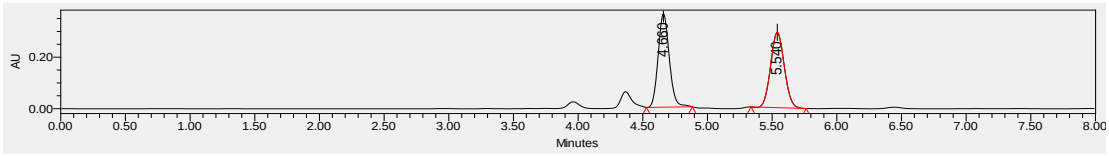
HPLC (Chiralcel AD-H column), n-hexane/i-PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm, retention time: t_1 = 4.66 min, t_2 = 5.54 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.31 (m, 4H), 7.31 – 7.05 (m, 6H), 3.82 (dd, *J* = 10.4, 4.2 Hz, 1H), 2.43 (dd, *J* = 14.3, 10.4 Hz, 1H), 2.08 (dd, *J* = 14.3, 4.0 Hz, 1H), 1.54 (s, 3H), 1.48 (d, *J* = 3.4 Hz, 6H), 1.41 (s, 3H).

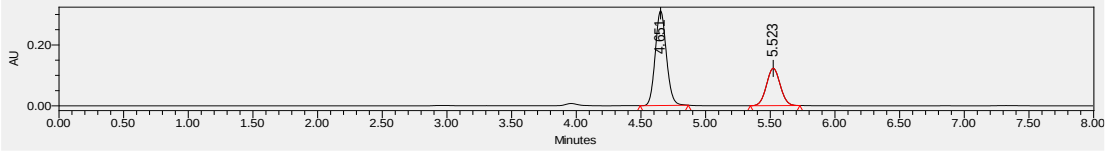
^{13}C NMR (101 MHz, $CDCl_3$) δ 207.47, 142.53, 131.55, 128.75, 128.25, 127.98, 127.48, 126.96, 123.47, 123.44, 91.48, 84.43, 49.85, 48.02, 40.27, 34.87, 26.86, 25.36, 25.06.

ESI-HRMS: calcd for $C_{24}H_{26}NO^+$ ($[M + H]^+$) = 344.2008, found 344.2010.

IR (neat): 3028, 2923, 2853, 2234, 1707, 1599, 1490, 1464, 1212, 1031, 999, 758 cm^{-1}.

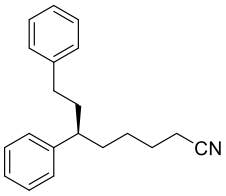


	Retention Time	Area	% Area
1	4.660	2176126	50.68
2	5.540	2117781	49.32



	Retention Time	Area	% Area
1	4.651	1934597	67.62
2	5.523	926228	32.38

(R)-6,8-diphenyloctanenitrile (E)



E

colourless liquid, 83% yield, 90% ee; $[\alpha]^{20}_D$ = 2.7 (*c* = 0.15, in CH_2Cl_2).

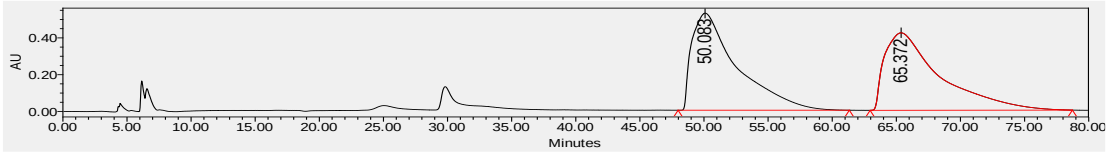
HPLC (Chiralcel OJ-H column), n-hexane/i-PrOH = 95/5, flow rate = 1.0 mL/min, λ = 211 nm, retention time: t_1 = 50.08 min, t_2 = 65.37 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 (t, *J* = 8.2, 2H), 7.24 (m, 3H), 7.18 – 7.11 (m, 3H), 7.12 – 6.91 (m, 2H), 2.51 (m, 1H), 2.46 – 2.39 (m, 2H), 2.20 (td, *J* = 7.2, 2.8 Hz, 2H), 2.02 – 1.77 (m, 2H), 1.77 – 1.40 (m, 4H), 1.39 – 1.13 (m, 2H).

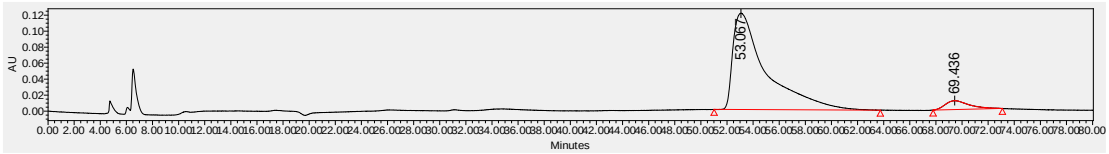
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.93, 142.43, 128.61, 128.45, 128.39, 128.36, 127.77, 126.38, 125.80, 119.82, 45.38, 38.60, 36.28, 33.82, 26.81, 25.53, 17.09.

ESI-HRMS: calcd for $C_{20}H_{23}NNa^+$ ($[M + Na]^+$) = 300.1727, found 300.1718.

IR (neat): 3060, 3026, 2924, 2854, 2246, 1645, 1601, 1494, 1453, 1261, 1028, 754 cm^{-1}.

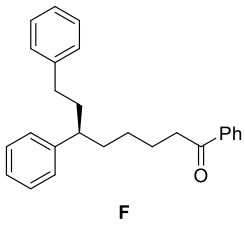


	Retention Time	Area	% Area
1	50.083	18974946	49.53
2	65.372	1119973	50.47



	Retention Time	Area	% Area
1	53.067	19056012	94.83
2	69.436	1038907	5.17

(R)-1,6,8-triphenyloctan-1-one (F)



F

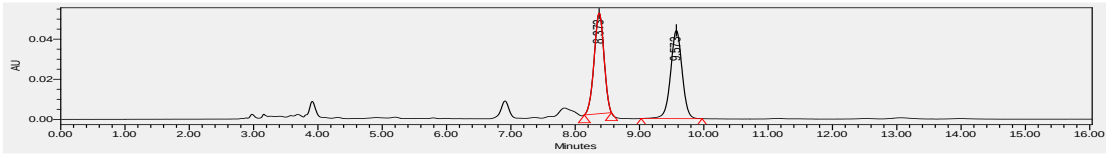
colourless liquid, 85% yield, 90% ee; $[\alpha]^{20}_{D}$ = 22.6 (*c* = 0.53, in CH_2Cl_2). **HPLC** (Chiralcel IA column), n-hexane/i-PrOH = 98/2, flow rate = 1.0 mL/min, λ = 245 nm, retention time: t_1 = 8.37 min, t_2 = 9.57 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 7.8 Hz, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.13 (m, 10H), 2.79 (t, *J* = 7.6 Hz, 2H), 2.47 (m, 1H), 2.36 (t, *J* = 8.2 Hz, 2H), 1.90 – 1.82 (m, 2H), 1.65 – 1.50 (m, 4H), 1.25 – 1.02 (m, 2H).

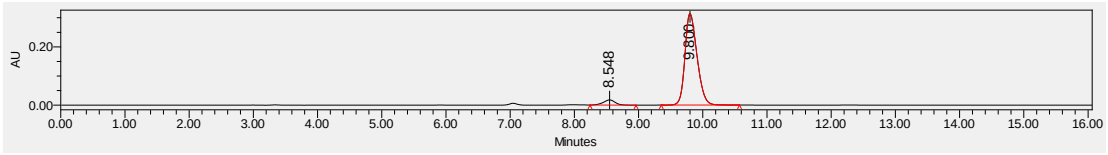
^{13}C NMR (101 MHz, $CDCl_3$) δ 200.54, 145.53, 142.70, 137.15, 133.00, 128.67, 128.51, 128.39, 128.16, 127.90, 126.19, 125.76, 45.61, 38.74, 38.66, 37.04, 33.95, 27.46, 24.47.

ESI-HRMS: calcd for $C_{26}H_{29}O^+$ ($[M + H]^+$) = 357.2213, found 357.2212.

IR (neat): 3060, 3026, 2927, 2855, 1684, 1599, 1493, 1450, 1408, 1218, 1028, 750 cm^{-1}.



	Retention Time	Area	% Area
1	8.373	535132	49.44
2	9.573	547171	50.56



	Retention Time	Area	% Area
1	8.548	541202	4.80
2	9.800	10722518	95.20

11 References

[1]. P. Wang; B. Zhao; Y. Yuan; Z. Shi. Radical-induced ring-opening and reconstruction of cyclobutanone oxime esters. *Chem. Commun*. **2019,** *55,* 1971.

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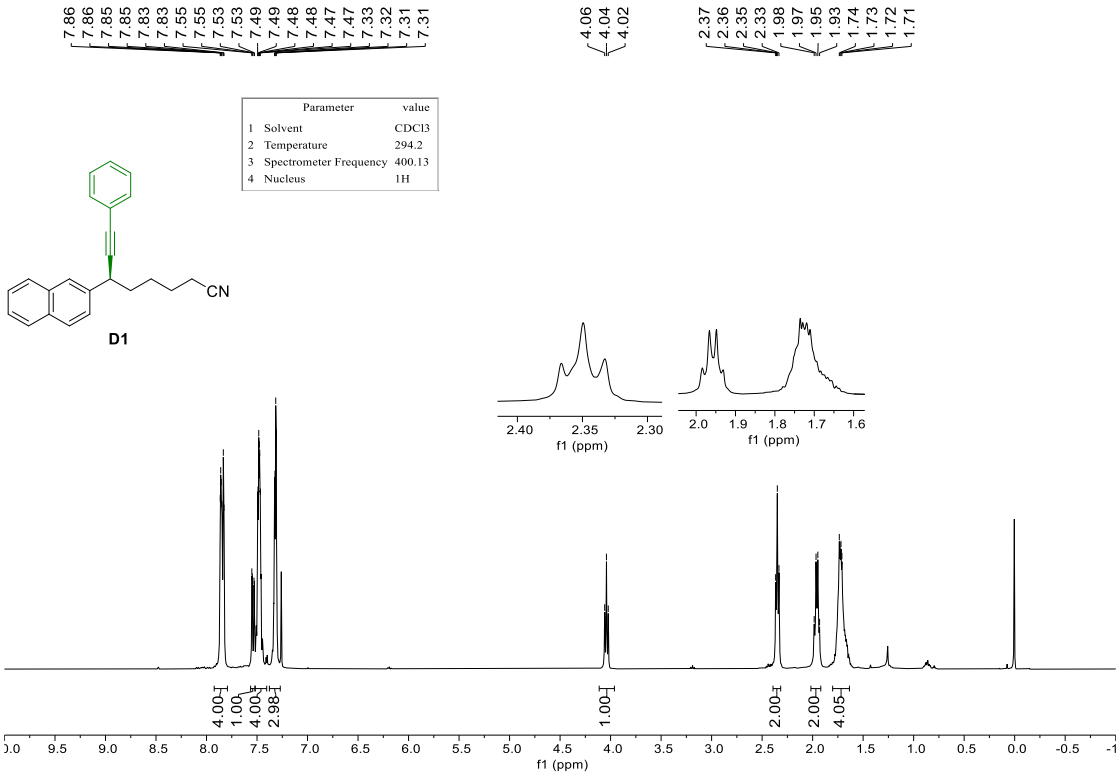
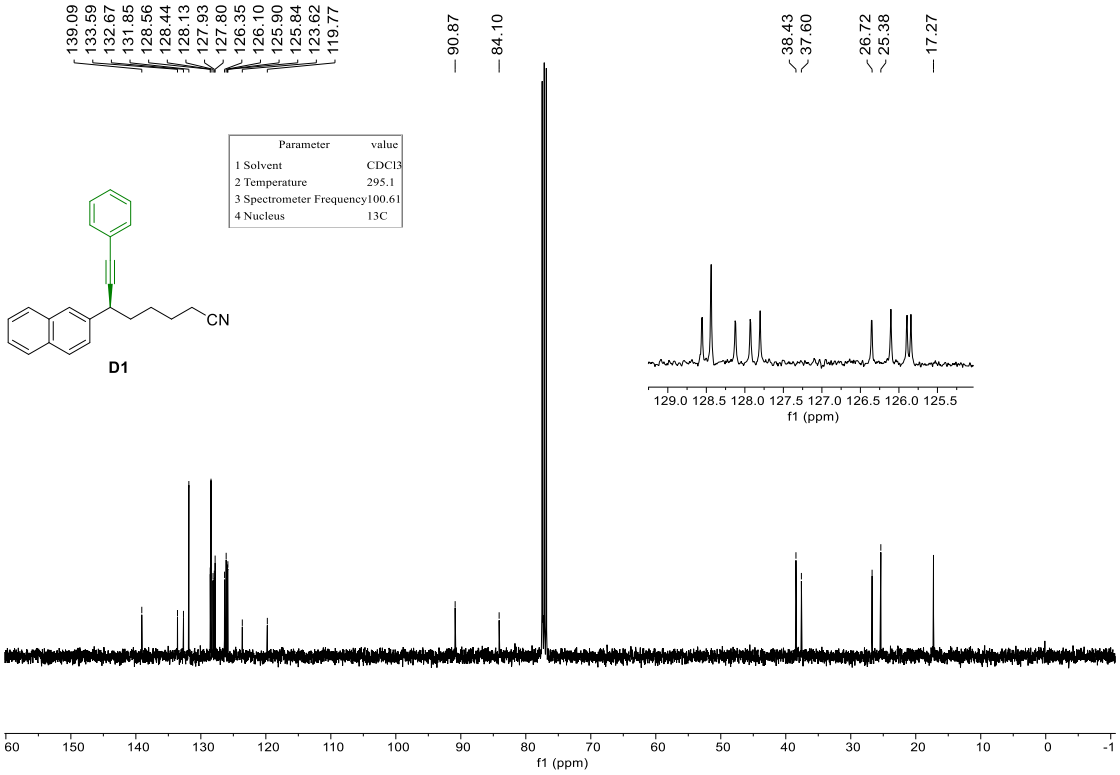
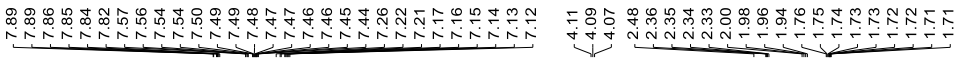
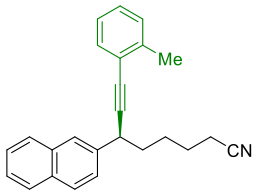
12 Copies of the NMR spectra for new compounds.



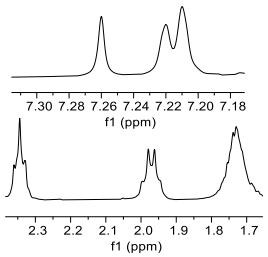


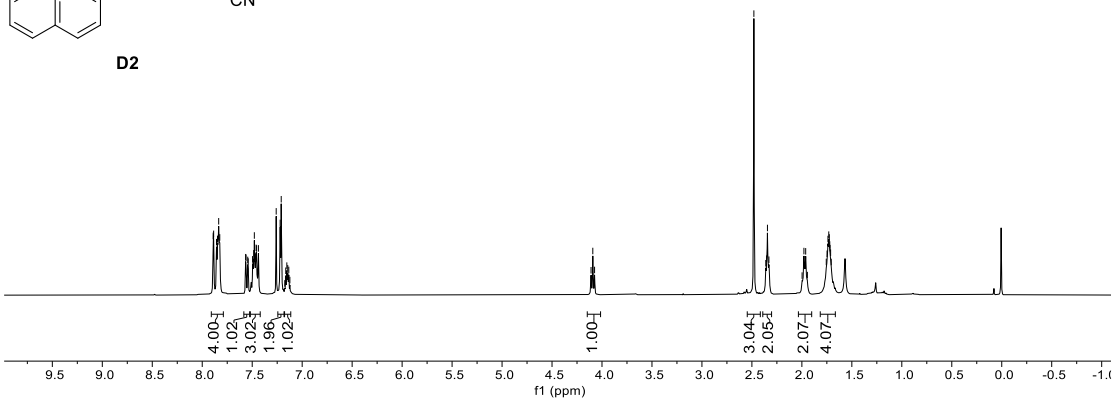


Parameter	value
1 Solvent	CDCl3
2 Temperature	296.4
3 Spectrometer Frequency	400.13
4 Nucleus	1H

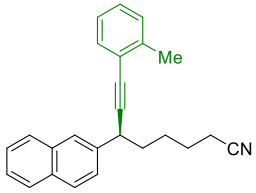


D2

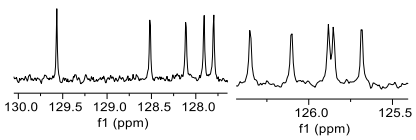


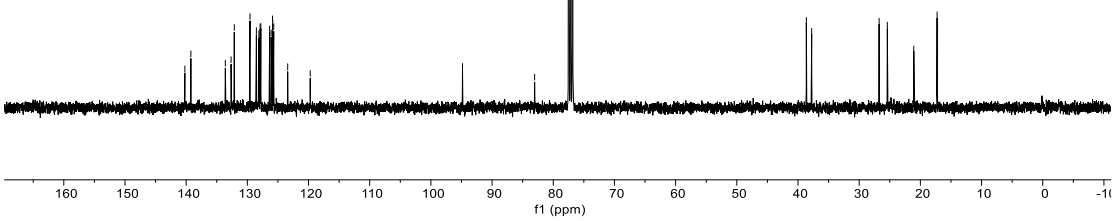


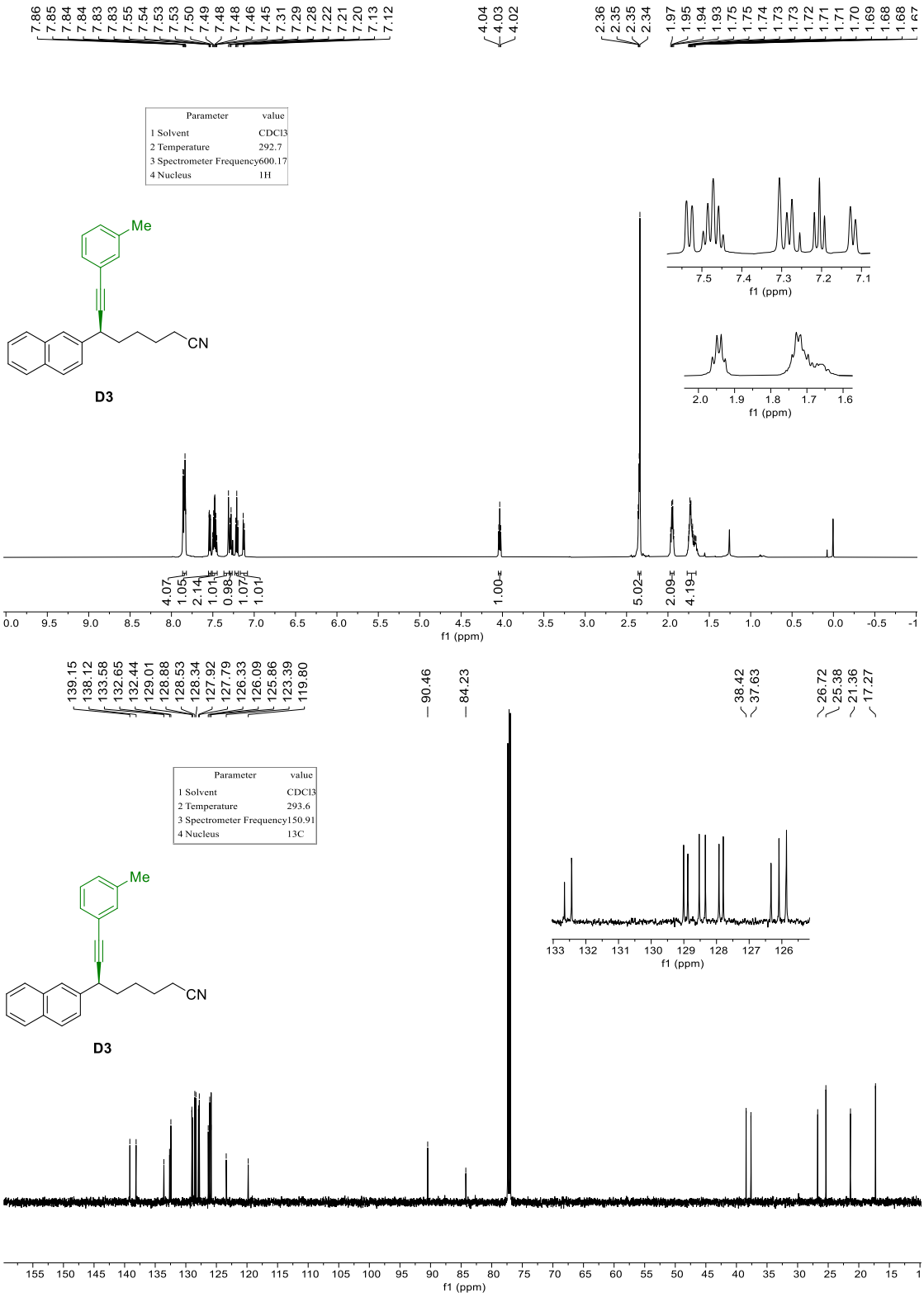
Parameter	value
1 Solvent	CDCl3
2 Temperature	297.2
3 Spectrometer Frequency	100.61
4 Nucleus	13C

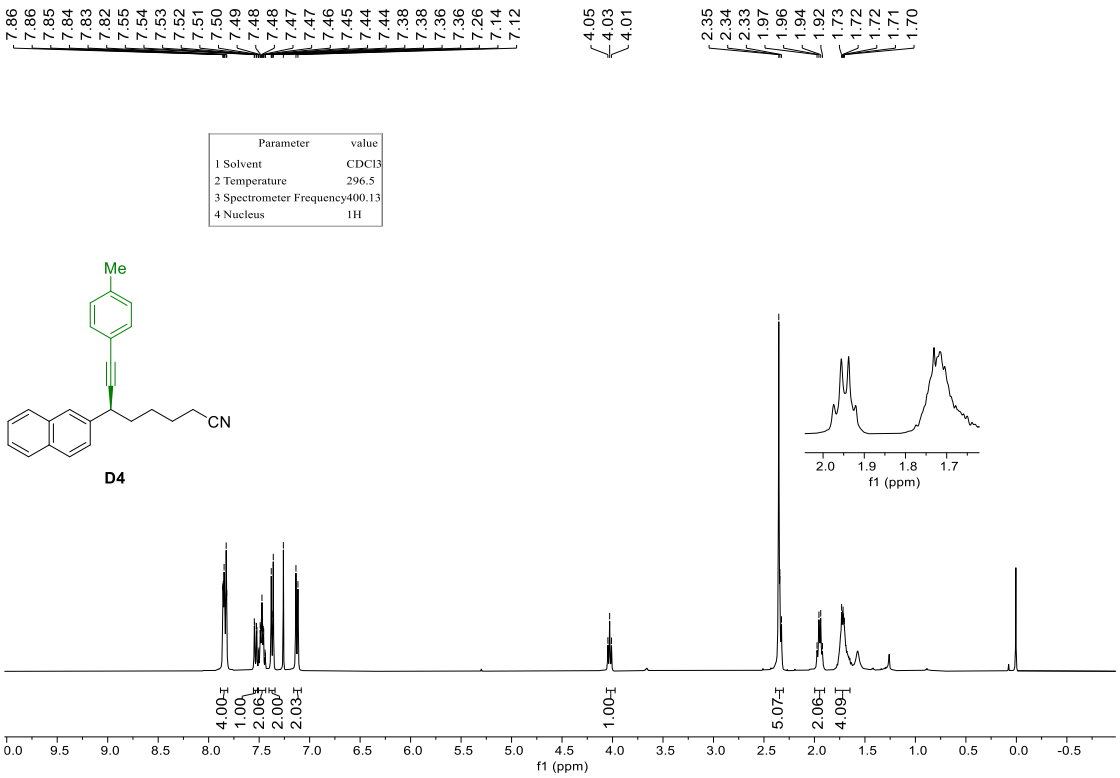


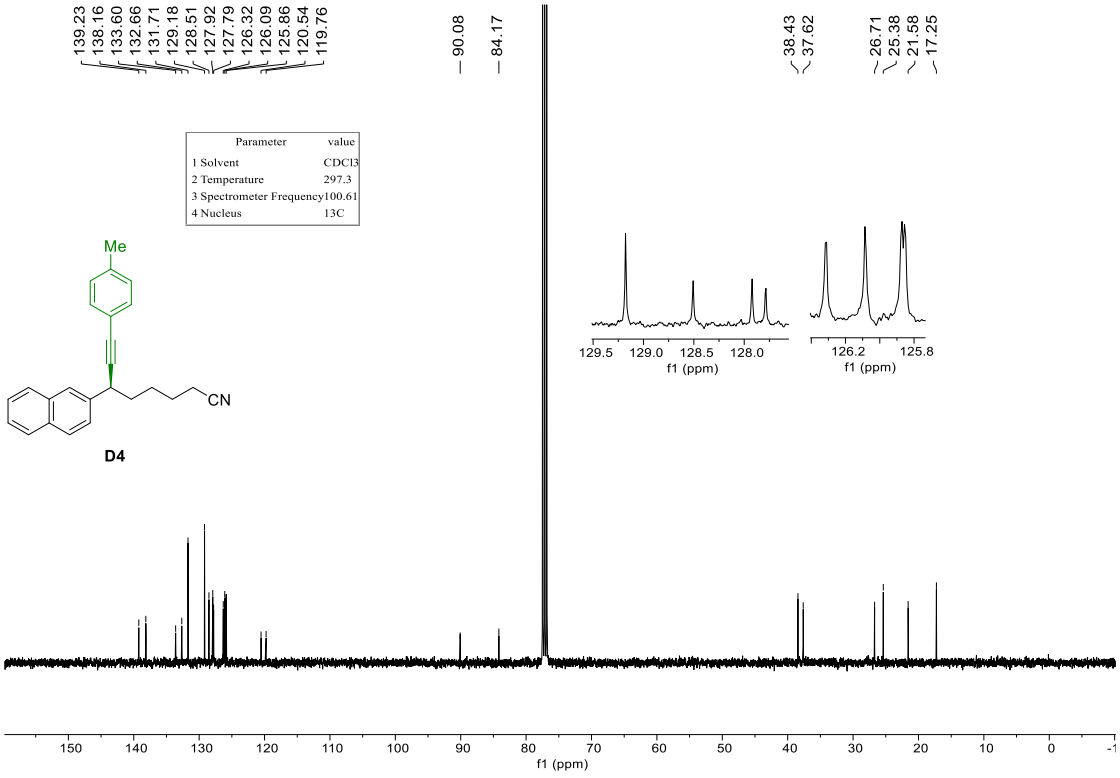
D2

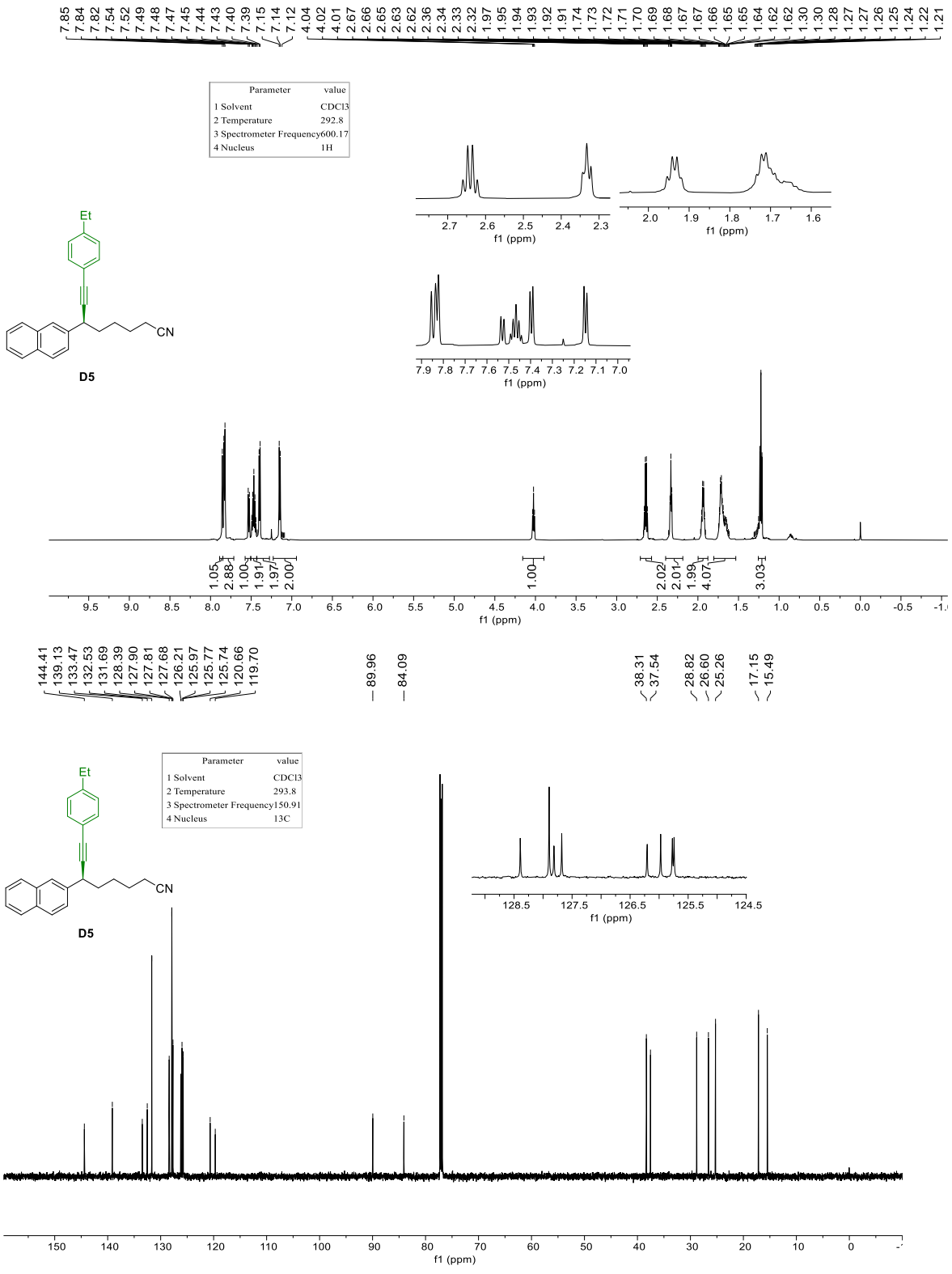


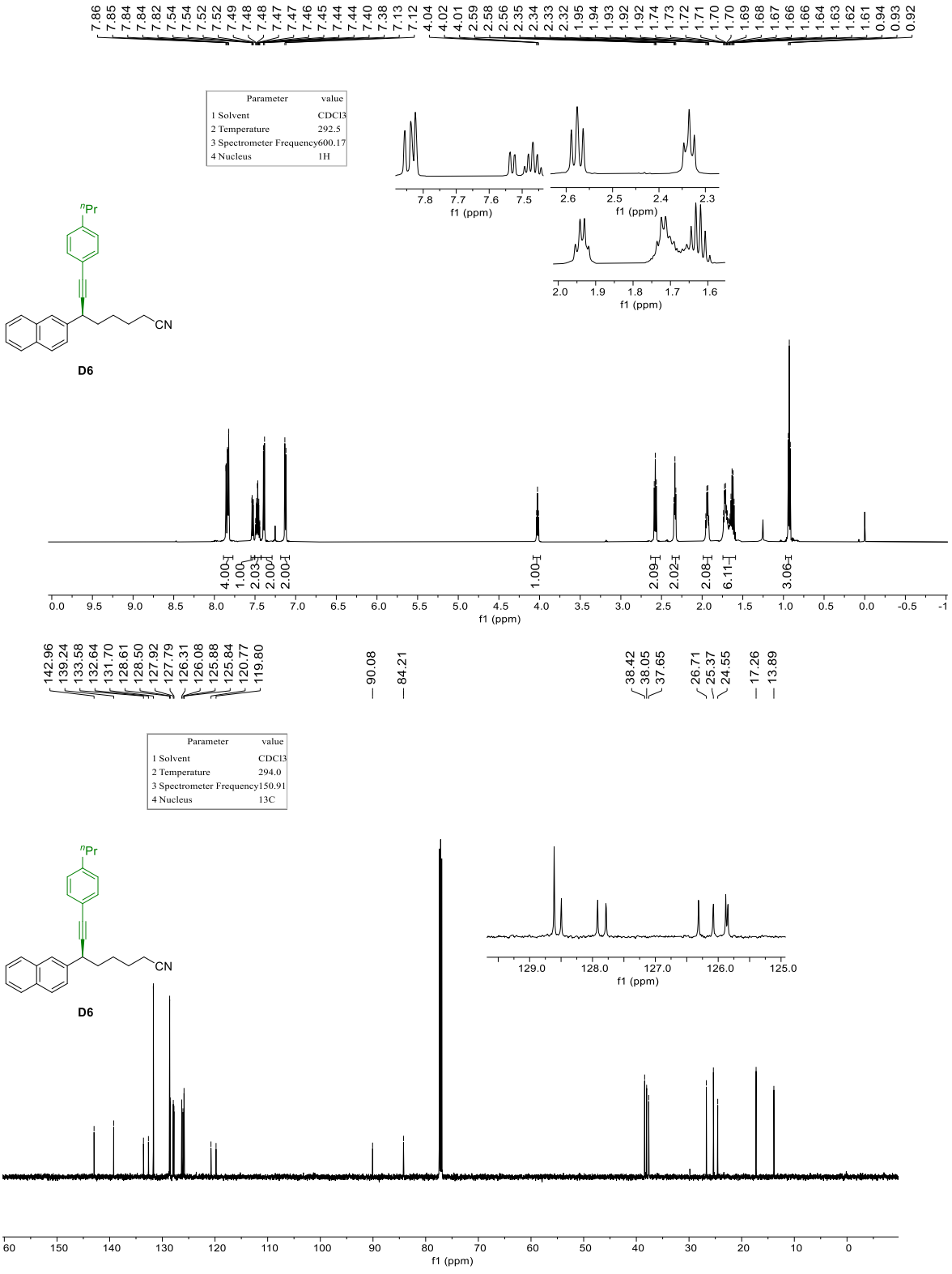


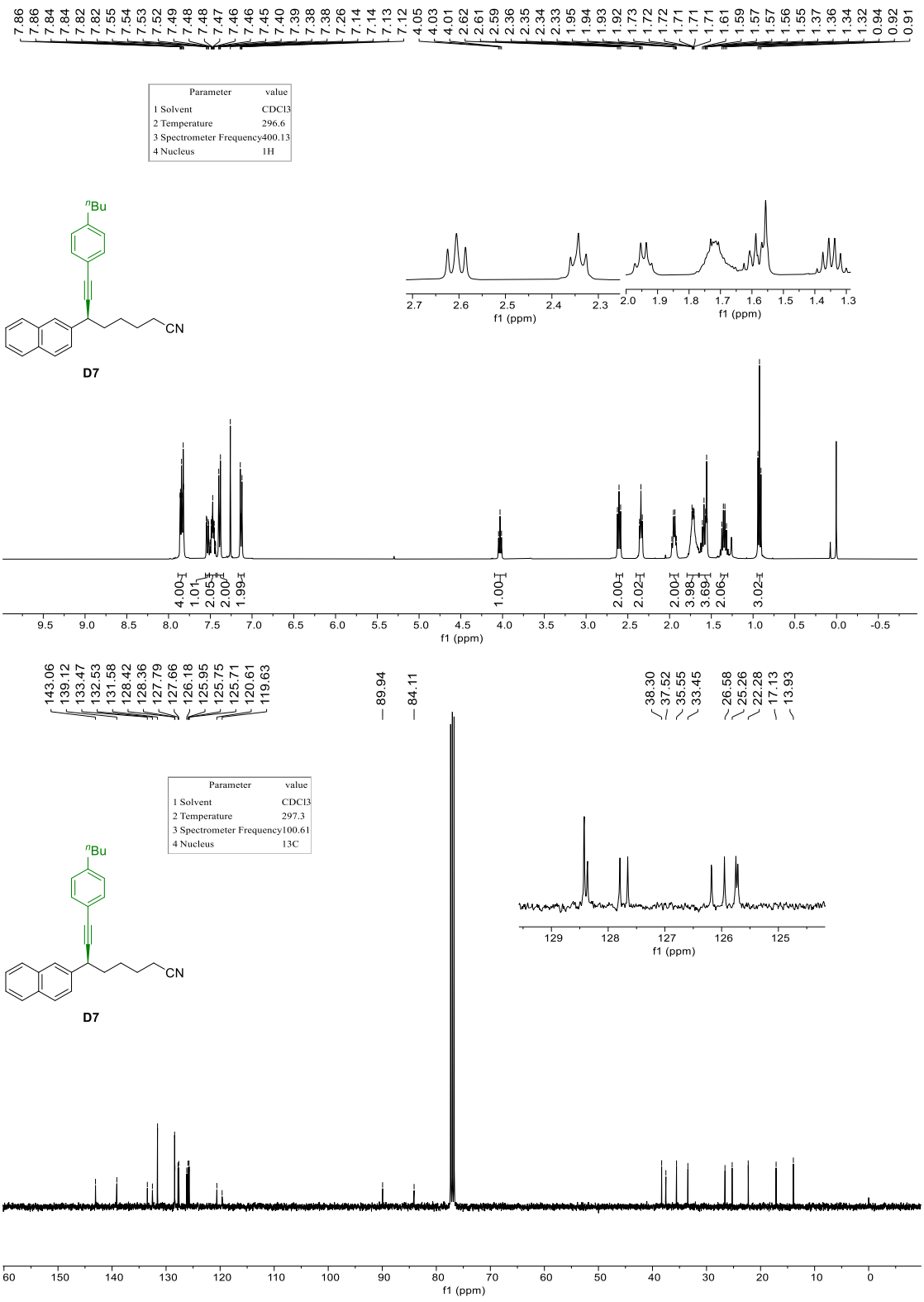

7.86 7.85 7.84 7.84 7.83 7.83 7.55 7.54 7.53 7.53 7.50 7.49 7.48 7.48 7.46 7.45 7.31 7.29 7.28 7.22 7.21 7.20 7.13 7.12
4.04 4.03 4.02
2.36 2.35 2.35 2.34
1.97 1.95 1.94 1.93 1.75 1.75 1.74 1.73 1.73 1.72 1.71 1.71 1.70 1.69 1.68 1.68
Parameter value
1 Solvent CDCl3
2 Temperature 292.7
3 Spectrometer Frequency 600.17
4 Nucleus 1H
Me
CN
D3
7.5 7.4 7.3 7.2 7.1
f1 (ppm)
2.0 1.9 1.8 1.7 1.6
f1 (ppm)
4.07 1.05 2.14 1.01 0.98 1.07 1.01
1.00
5.02
2.09 4.19
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)
139.15 138.12 133.58 132.65 132.44 129.01 128.88 128.53 128.34 127.92 127.79 126.33 126.09 125.86 123.39 119.80
90.46
84.23
38.42 37.63
26.72 25.38 21.36 17.27
Parameter value
1 Solvent CDCl3
2 Temperature 293.6
3 Spectrometer Frequency 150.91
4 Nucleus 13C
Me
CN
D3
133 132 131 130 129 128 127 126
f1 (ppm)
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 1
f1 (ppm)

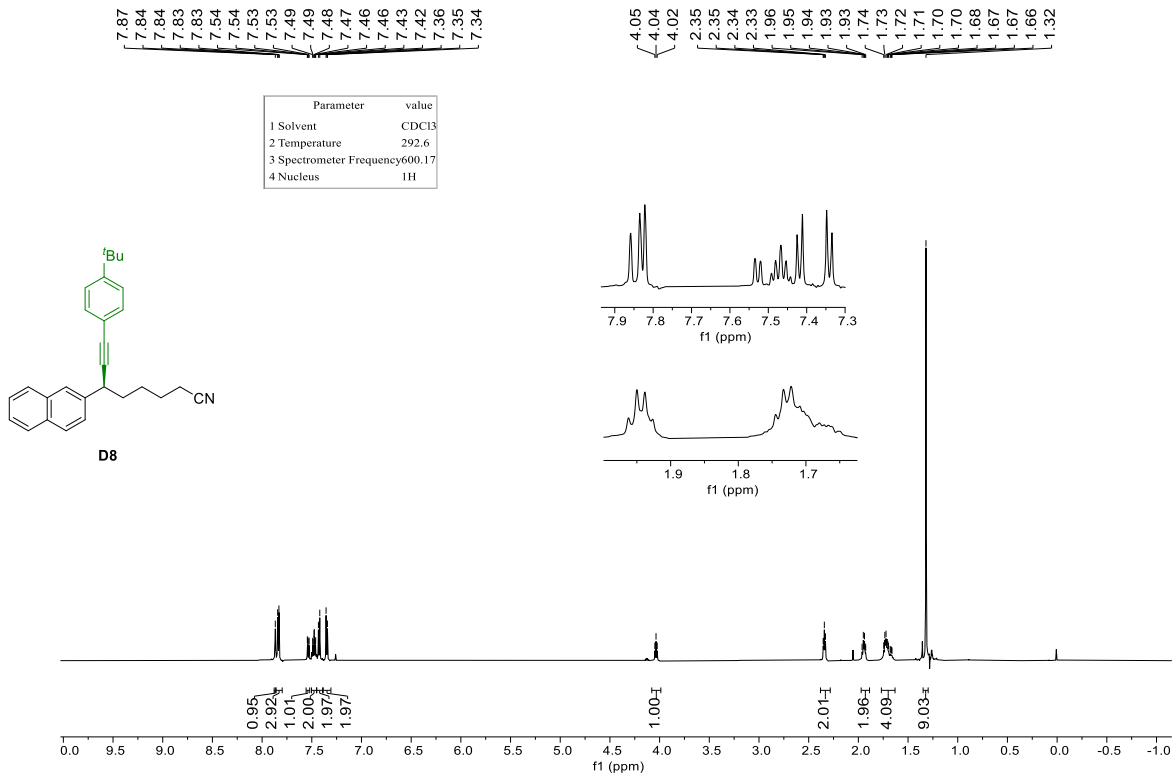

7.86 7.86 7.85 7.84 7.83 7.82 7.55 7.54 7.53 7.52 7.51 7.50 7.49 7.48 7.48 7.47 7.47 7.46 7.45 7.44 7.44 7.38 7.38 7.36 7.36 7.26 7.14 7.12
4.05 4.03 4.01
2.35 2.34 2.33 1.97 1.96 1.94 1.92 1.73 1.72 1.72 1.71 1.70
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
Me
CN
D4
2.0 1.9 1.8 1.7
f1 (ppm)
4.00 1.00 2.06 2.00 2.03 1.00 5.07 2.06 4.09
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


139.23 138.16 133.60 132.66 131.71 129.18 128.51 127.92 127.79 126.32 126.09 125.86 120.54 119.76
90.08 84.17
38.43 37.62
26.71 25.38 21.58 17.25
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
Me
CN
D4
129.5 129.0 128.5 128.0
f1 (ppm)
126.2 125.8
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


7.85 7.84 7.82 7.54 7.52 7.49 7.48 7.47 7.45 7.44 7.43 7.40 7.39 7.15 7.14 7.12
4.04 4.02 4.01 2.67 2.66 2.65 2.63 2.62 2.36 2.34 2.33 2.32 1.97 1.95 1.94 1.93 1.92 1.91 1.74 1.73 1.72 1.71 1.70 1.69 1.68 1.67 1.67 1.66 1.65 1.65 1.64 1.62 1.62 1.30 1.30 1.28 1.27 1.27 1.26 1.25 1.24 1.22 1.21
Parameter value
1 Solvent CDCl3
2 Temperature 292.8
3 Spectrometer Frequency 600.17
4 Nucleus 1H
Et
CN
D5
f1 (ppm)
1.05 2.88 1.00 1.91 1.97 2.00 1.00 2.02 2.01 1.99 4.07 3.03
144.41 139.13 133.47 132.53 131.69 128.39 127.90 127.81 127.68 126.21 125.97 125.77 125.74 120.66 119.70
89.96 84.09
38.31 37.54 28.82 26.60 25.26 17.15 15.49
Parameter value
1 Solvent CDCl3
2 Temperature 293.8
3 Spectrometer Frequency 150.91
4 Nucleus 13C
Et
CN
D5
f1 (ppm)


7.86 7.85 7.84 7.84 7.82 7.54 7.54 7.52 7.52 7.49 7.48 7.48 7.47 7.47 7.46 7.45 7.44 7.44 7.40 7.38 7.13 7.12
4.04 4.02 4.01 2.59 2.58 2.56 2.35 2.34 2.33 2.32 1.95 1.94 1.93 1.92 1.92 1.74 1.73 1.72 1.71 1.70 1.70 1.69 1.68 1.67 1.66 1.66 1.64 1.63 1.62 1.61 0.94 0.93 0.92
Parameter value
1 Solvent CDCl3
2 Temperature 292.5
3 Spectrometer Frequency 600.17
4 Nucleus 1H
nPr
CN
D6
f1 (ppm)
4.00 1.00 2.03 2.00 2.00 1.00 2.09 2.02 2.08 6.11 3.06
142.96 139.24 133.58 132.64 131.70 128.61 128.50 127.92 127.79 126.31 126.08 125.88 125.84 120.77 119.80
90.08 84.21
38.42 38.05 37.65 26.71 25.37 24.55 17.26 13.89
Parameter value
1 Solvent CDCl3
2 Temperature 294.0
3 Spectrometer Frequency 150.91
4 Nucleus 13C


7.86 7.86 7.84 7.84 7.82 7.82 7.55 7.54 7.53 7.52 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.40 7.39 7.38 7.38 7.26 7.14 7.14 7.13 7.12
4.05 4.03 4.01 2.62 2.61 2.59 2.36 2.35 2.34 2.33 1.95 1.94 1.93 1.92 1.73 1.72 1.72 1.71 1.71 1.71 1.61 1.59 1.57 1.57 1.56 1.55 1.37 1.36 1.34 1.32 0.94 0.92 0.91
Parameter value
1 Solvent CDCl3
2 Temperature 296.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
nBu
CN
D7
f1 (ppm)
4.00 1.01 2.05 2.00 1.99 1.00 2.00 2.02 2.00 3.98 3.69 2.06 3.02
143.06 139.12 133.47 132.53 131.58 128.42 128.36 127.79 127.66 126.18 125.95 125.75 125.71 120.61 119.63
89.94 84.11
38.30 37.52 35.55 33.45 26.58 25.26 22.28 17.13 13.93
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
nBu
CN
D7
f1 (ppm)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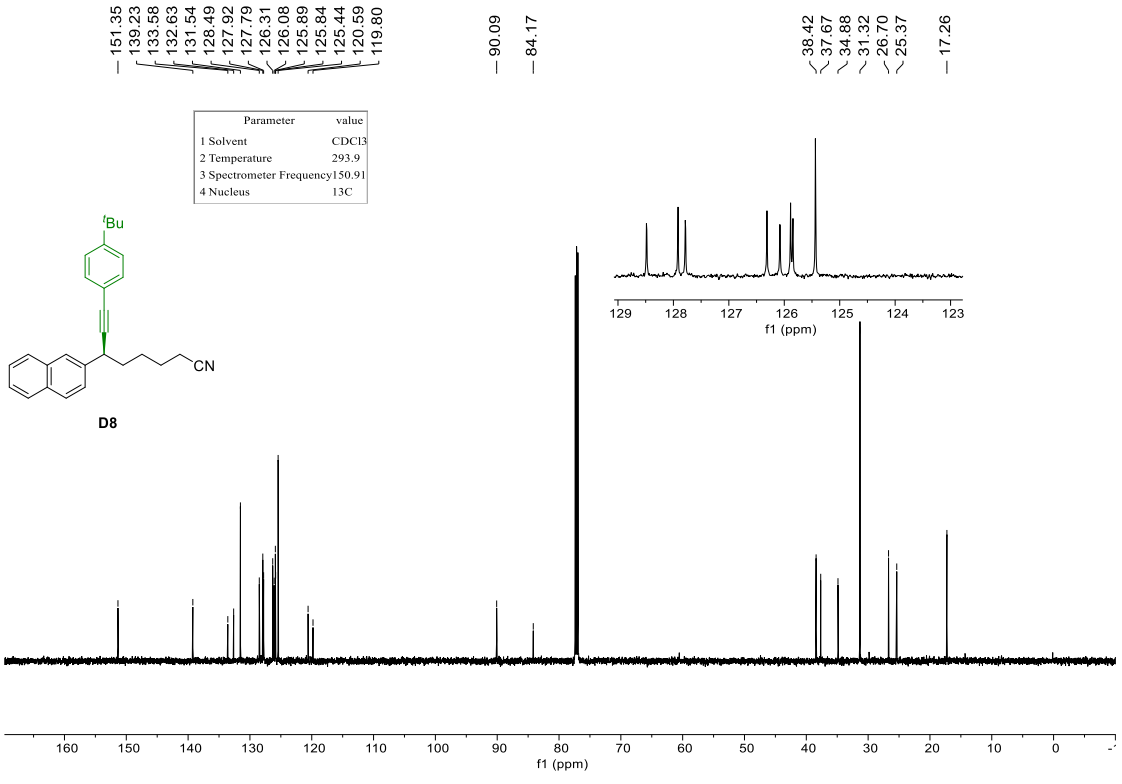
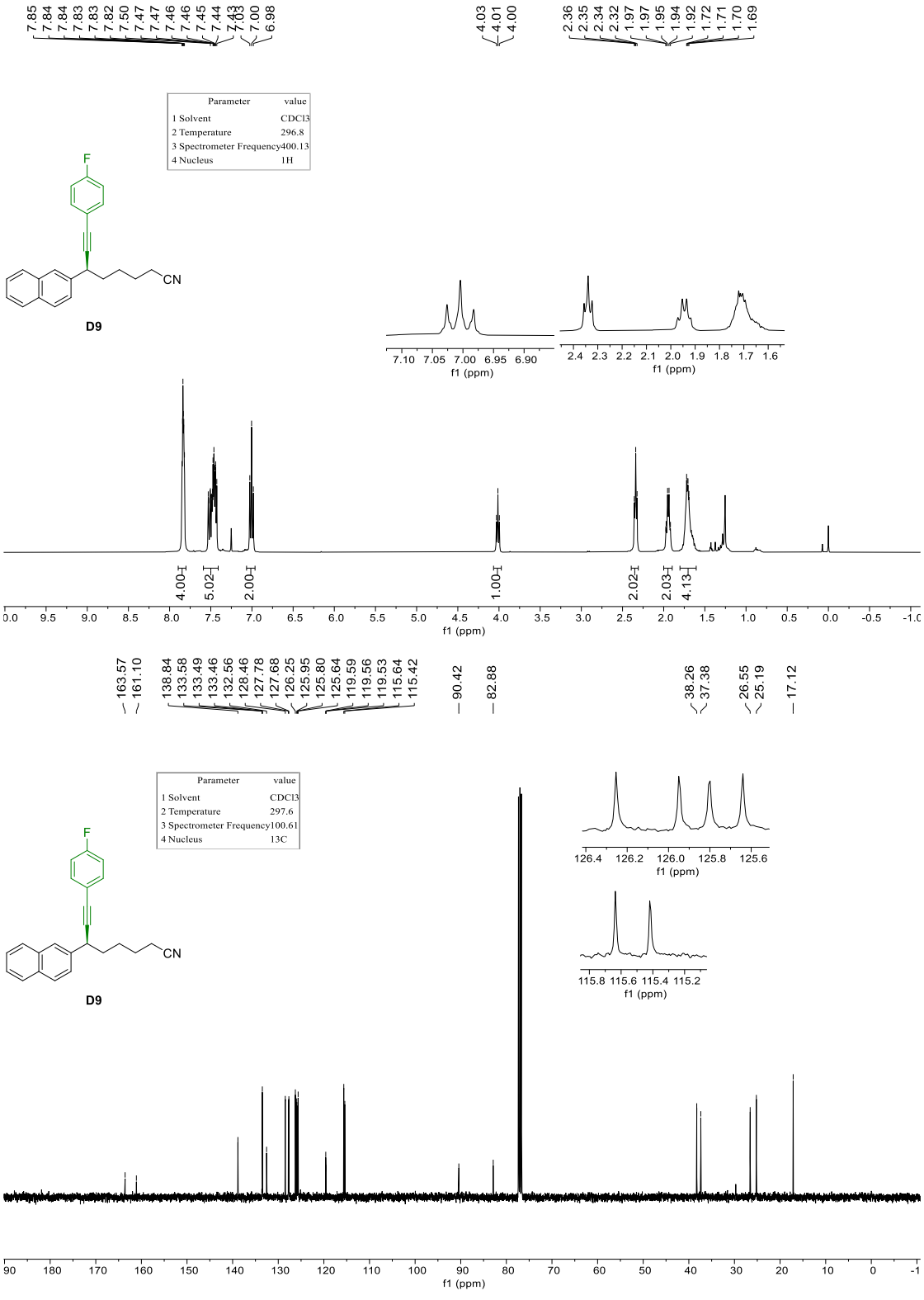
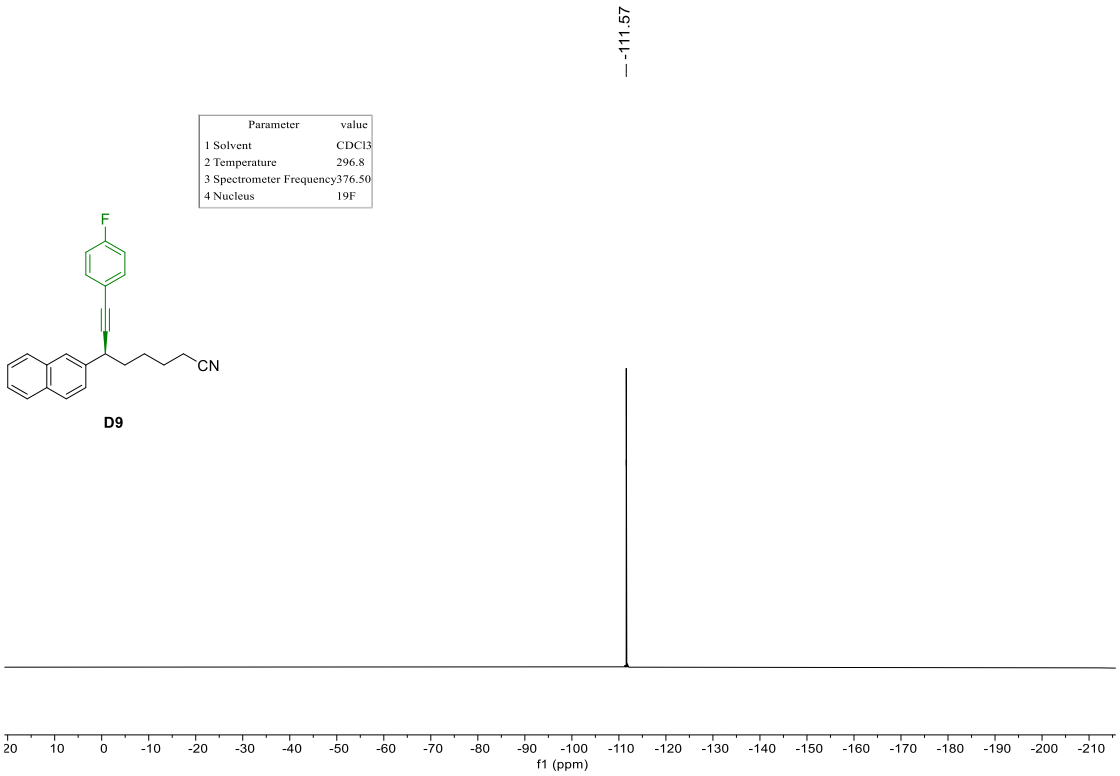
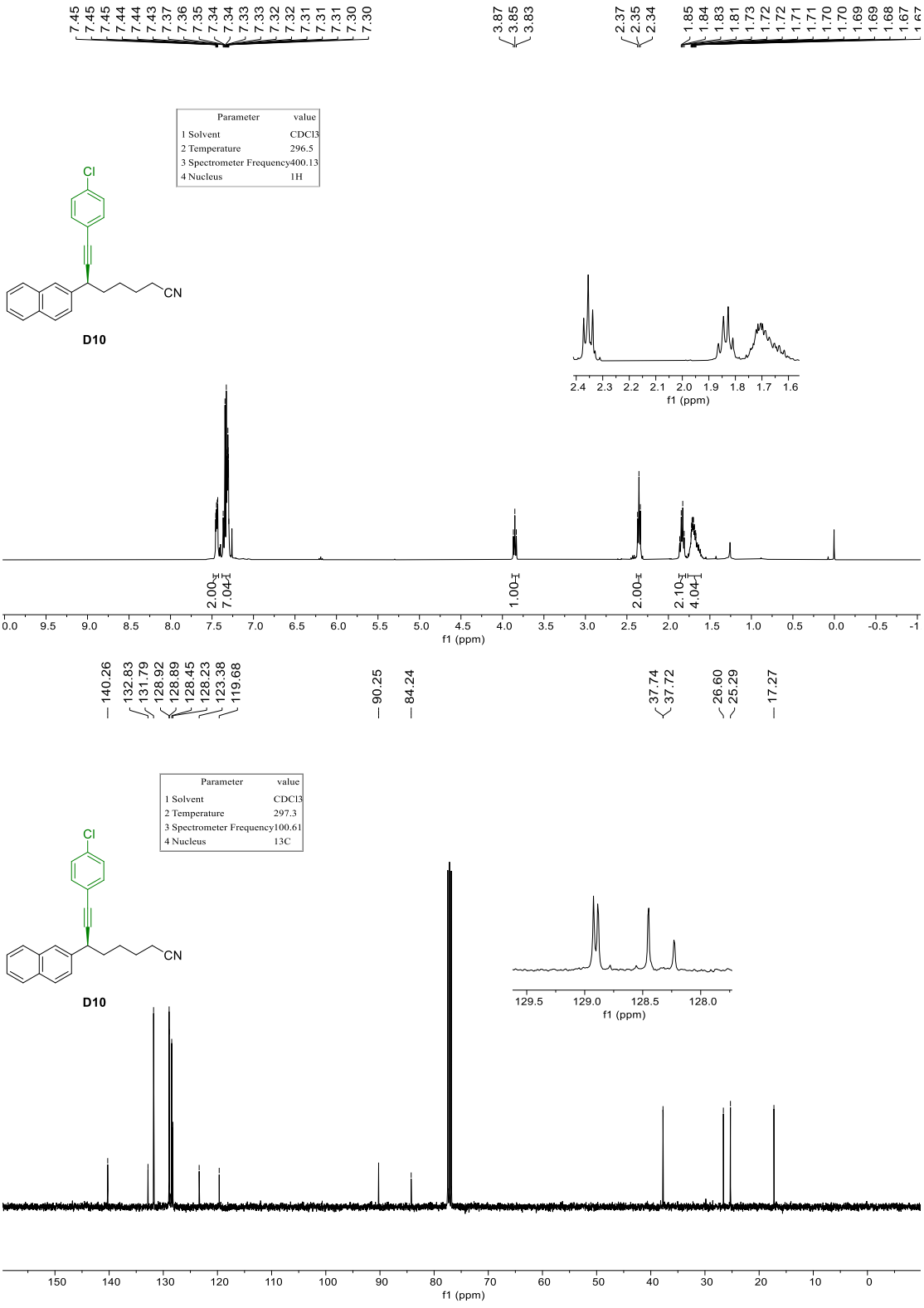
4.05 4.04 4.02 2.35 2.35 2.34 2.33 1.96 1.95 1.94 1.93 1.93 1.74 1.73 1.72 1.71 1.70 1.70 1.68 1.67 1.67 1.66 1.32
Parameter value
1 Solvent CDCl3
2 Temperature 292.6
3 Spectrometer Frequency 600.17
4 Nucleus 1H
tBu
CN
D8
7.9 7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
1.9 1.8 1.7
f1 (ppm)
0.95 2.92 1.01 2.00 1.97 1.97 1.00 2.01 1.96 4.09 9.03
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


151.35 139.23 133.58 132.63 131.54 128.49 127.92 127.79 126.31 126.08 125.89 125.84 125.44 120.59 119.80
90.09 84.17
38.42 37.67 34.88 31.32 26.70 25.37 17.26
Parameter value
1 Solvent CDCl3
2 Temperature 293.9
3 Spectrometer Frequency 150.91
4 Nucleus 13C
tBu
CN
D8
129 128 127 126 125 124 123
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.85 7.84 7.84 7.83 7.83 7.82 7.50 7.47 7.47 7.46 7.46 7.45 7.44 7.43 7.03 7.00 6.98
4.03 4.01 4.00
2.36 2.35 2.34 2.32 1.97 1.97 1.95 1.94 1.92 1.72 1.71 1.70 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 296.8
3 Spectrometer Frequency 400.13
4 Nucleus 1H
F
CN
D9
7.10 7.05 7.00 6.95 6.90
f1 (ppm)
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
4.00 5.02 2.00 1.00 2.02 2.03 4.13
f1 (ppm)
163.57 161.10 138.84 133.58 133.49 133.46 132.56 128.46 127.78 127.68 126.25 125.95 125.80 125.64 119.59 119.56 119.53 115.64 115.42 90.42 82.88 38.26 37.38 26.55 25.19 17.12
Parameter value
1 Solvent CDCl3
2 Temperature 297.6
3 Spectrometer Frequency 100.61
4 Nucleus 13C
F
CN
D9
126.4 126.2 126.0 125.8 125.6
f1 (ppm)
115.8 115.6 115.4 115.2
f1 (ppm)
f1 (ppm)


-111.57
Parameter value
1 Solvent CDCl3
2 Temperature 296.8
3 Spectrometer Frequency376.50
4 Nucleus 19F
F
CN
D9
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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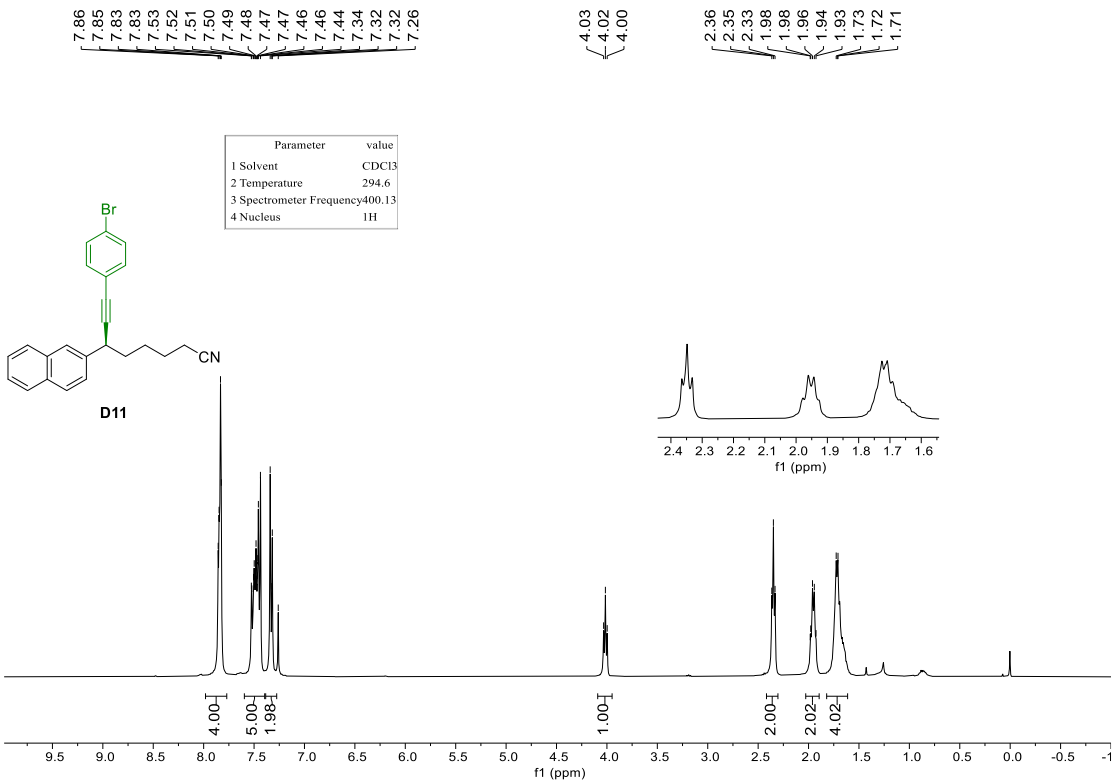
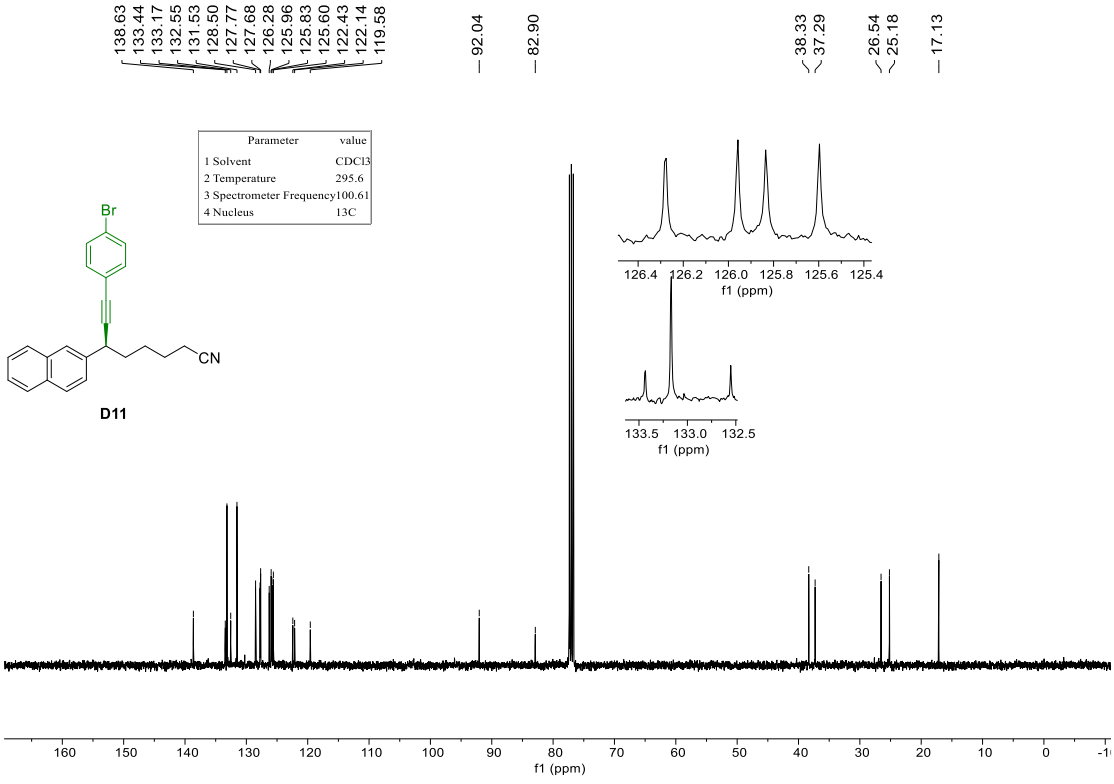
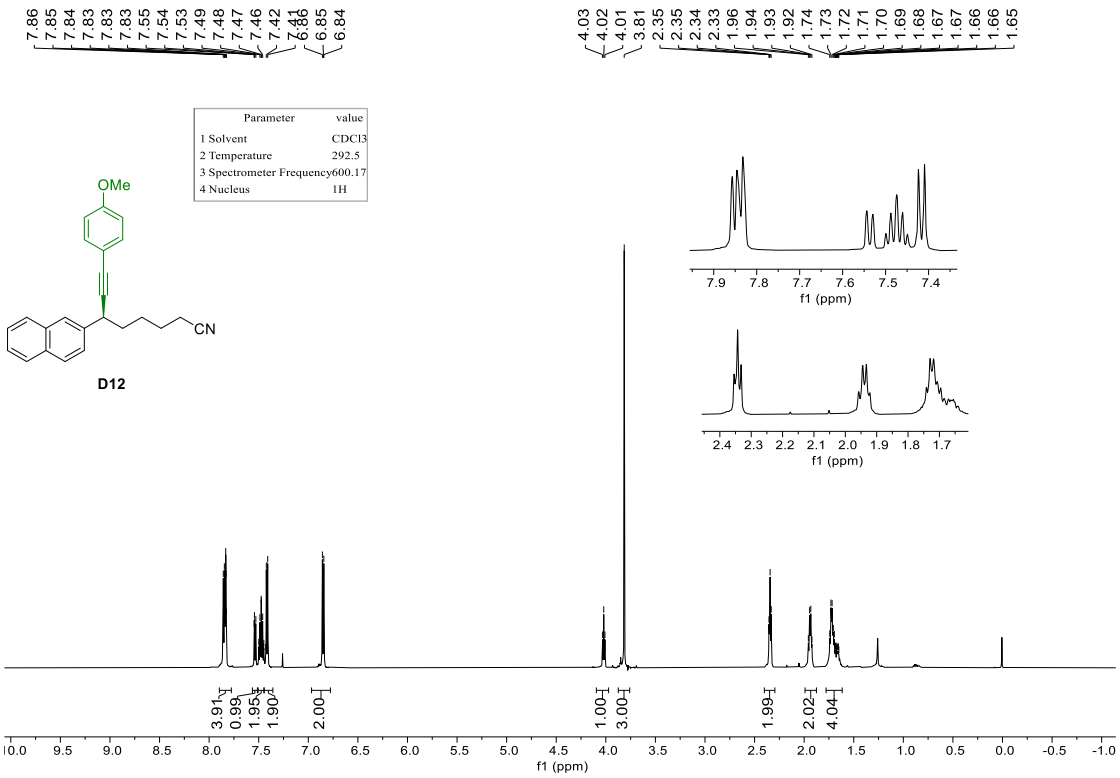
3.87 3.85 3.83
2.37 2.35 2.34
1.85 1.84 1.83 1.81 1.73 1.72 1.72 1.71 1.71 1.70 1.70 1.69 1.69 1.68 1.67
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
Cl
CN
D10
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
2.00 7.04 1.00 2.00 2.10 4.04
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)
140.26 132.83 131.79 128.92 128.89 128.45 128.23 123.38 119.68
90.25 84.24
37.74 37.72 26.60 25.29 17.27
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
Cl
CN
D10
129.5 129.0 128.5 128.0
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.86 7.85 7.83 7.83 7.53 7.52 7.51 7.50 7.49 7.48 7.47 7.47 7.46 7.46 7.44 7.34 7.32 7.32 7.26
4.03 4.02 4.00
2.36 2.35 2.33 1.98 1.98 1.96 1.94 1.93 1.73 1.72 1.71
Parameter value
1 Solvent CDCl3
2 Temperature 294.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
Br
CN
D11
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
4.00 5.00 1.98 1.00 2.00 2.02 4.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


138.63 133.44 133.17 132.55 131.53 128.50 127.77 127.68 126.28 125.96 125.83 125.60 122.43 122.14 119.58
92.04
82.90
38.33 37.29
26.54 25.18
17.13
Parameter value
1 Solvent CDCl3
2 Temperature 295.6
3 Spectrometer Frequency 100.61
4 Nucleus 13C
Br
CN
D11
126.4 126.2 126.0 125.8 125.6 125.4
f1 (ppm)
133.5 133.0 132.5
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.86 7.85 7.84 7.83 7.83 7.83 7.55 7.54 7.53 7.49 7.48 7.47 7.46 7.42 7.41 6.86 6.85 6.84
4.03 4.02 4.01 3.81 2.35 2.34 2.33 1.96 1.94 1.93 1.92 1.74 1.73 1.72 1.71 1.70 1.69 1.68 1.67 1.67 1.66 1.66 1.65
Parameter value
1 Solvent CDCl3
2 Temperature 292.5
3 Spectrometer Frequency 600.17
4 Nucleus 1H
OMe
CN
D12
7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7
f1 (ppm)
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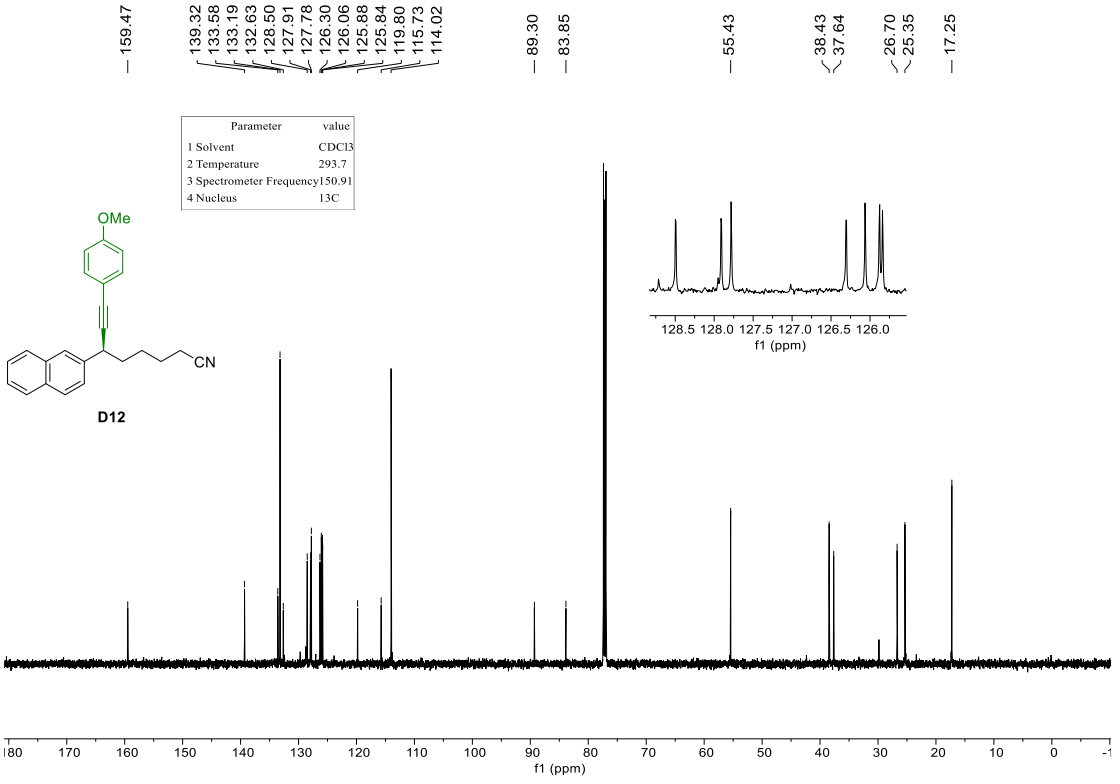
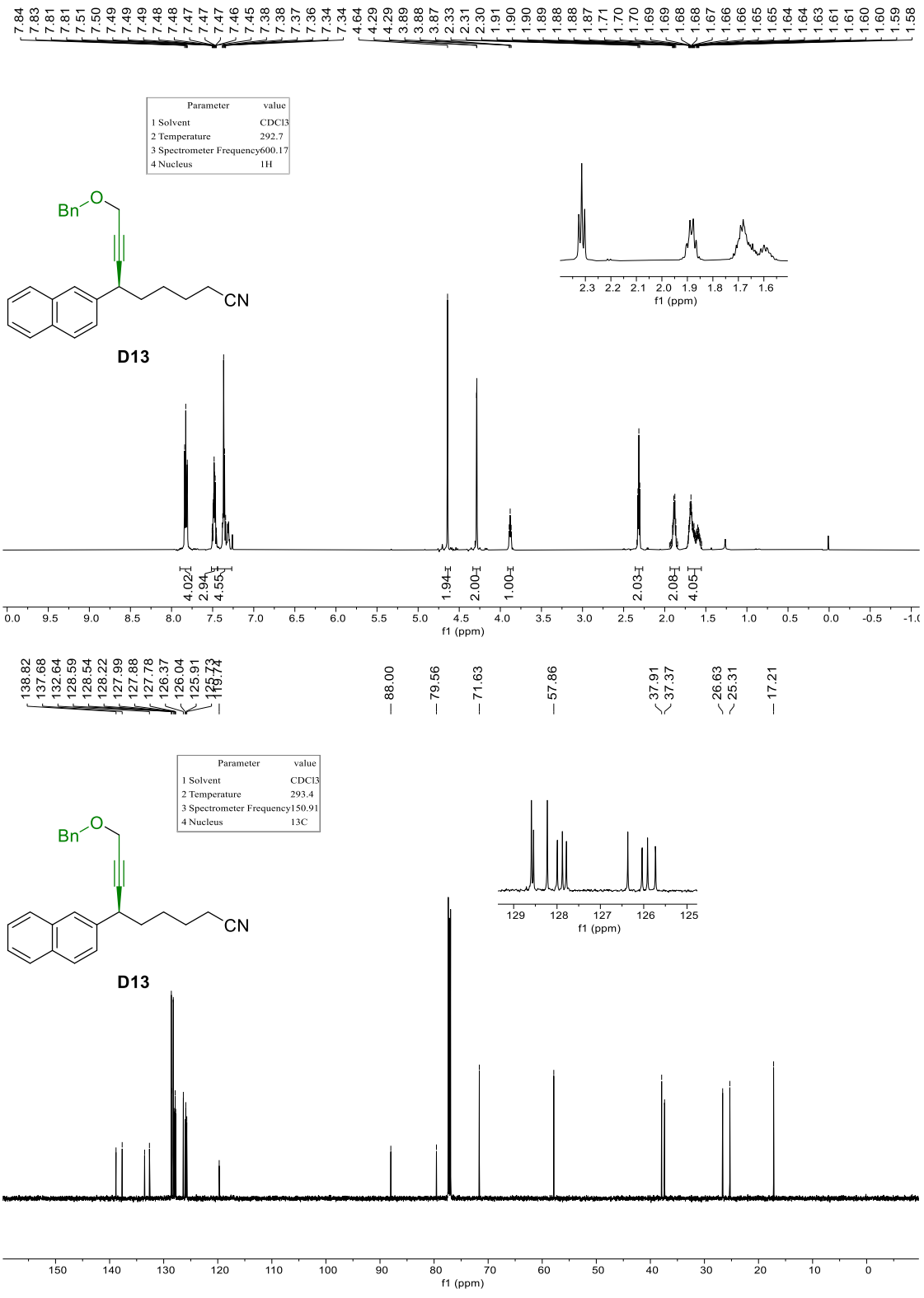
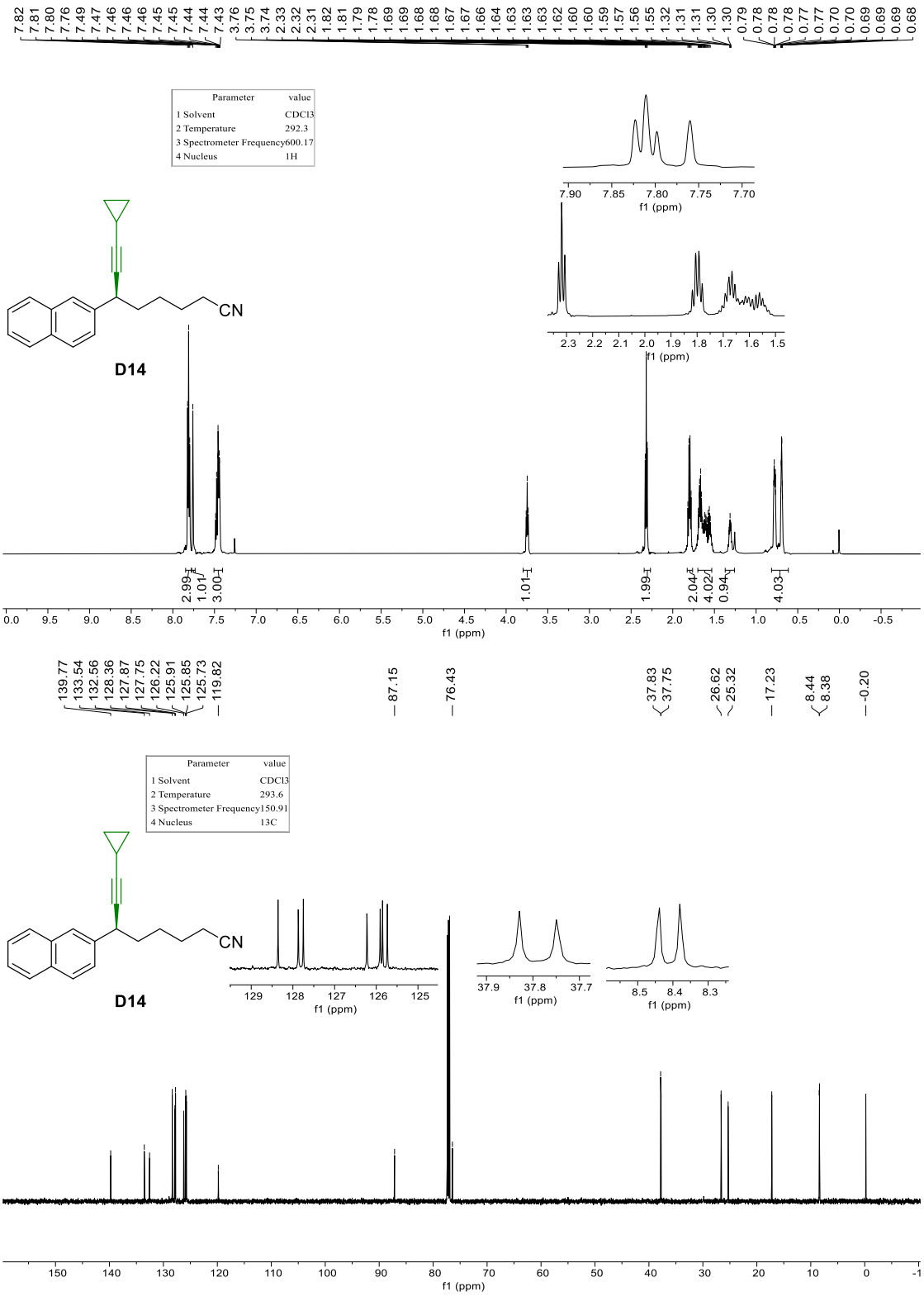
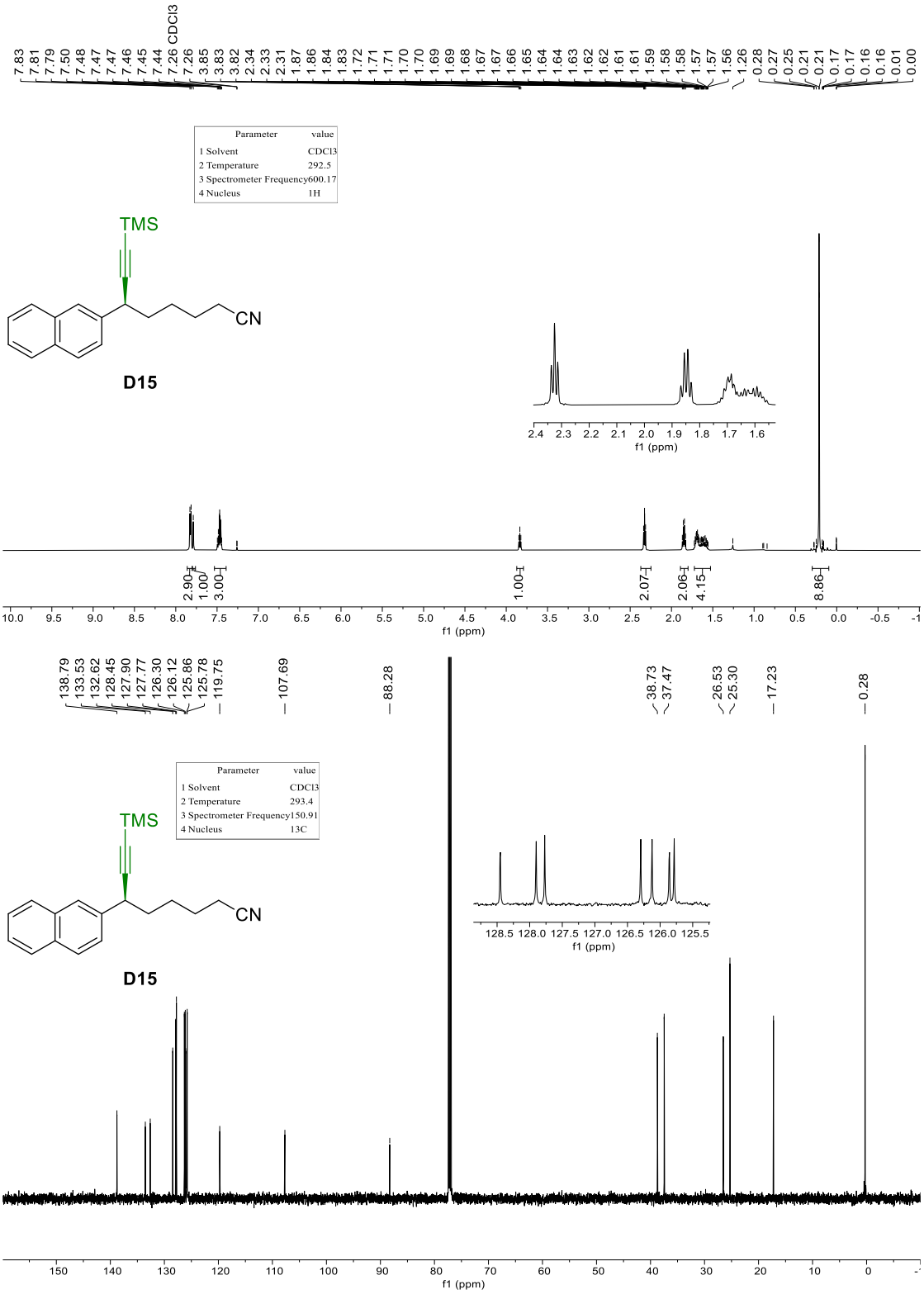
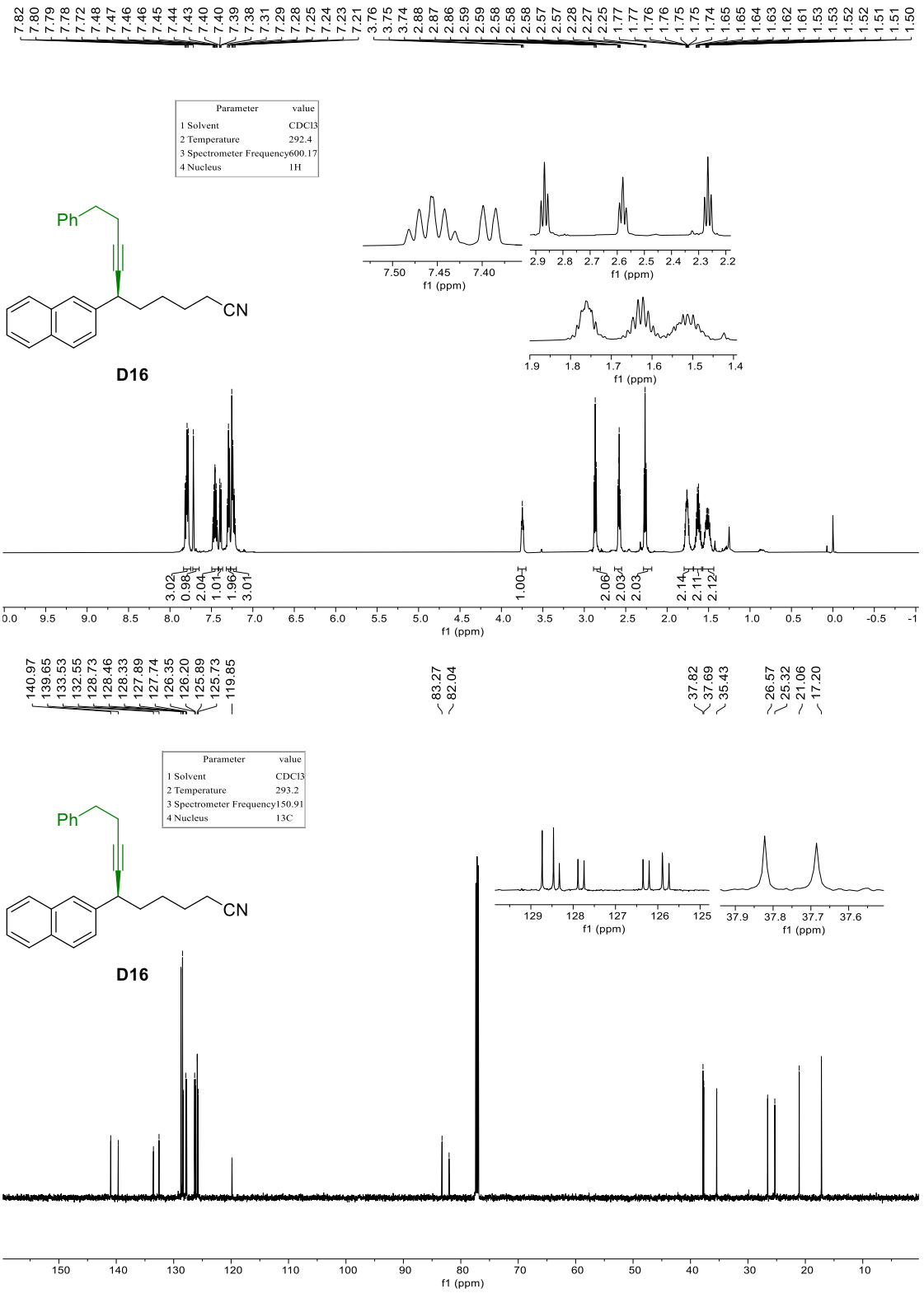
f1 (ppm)

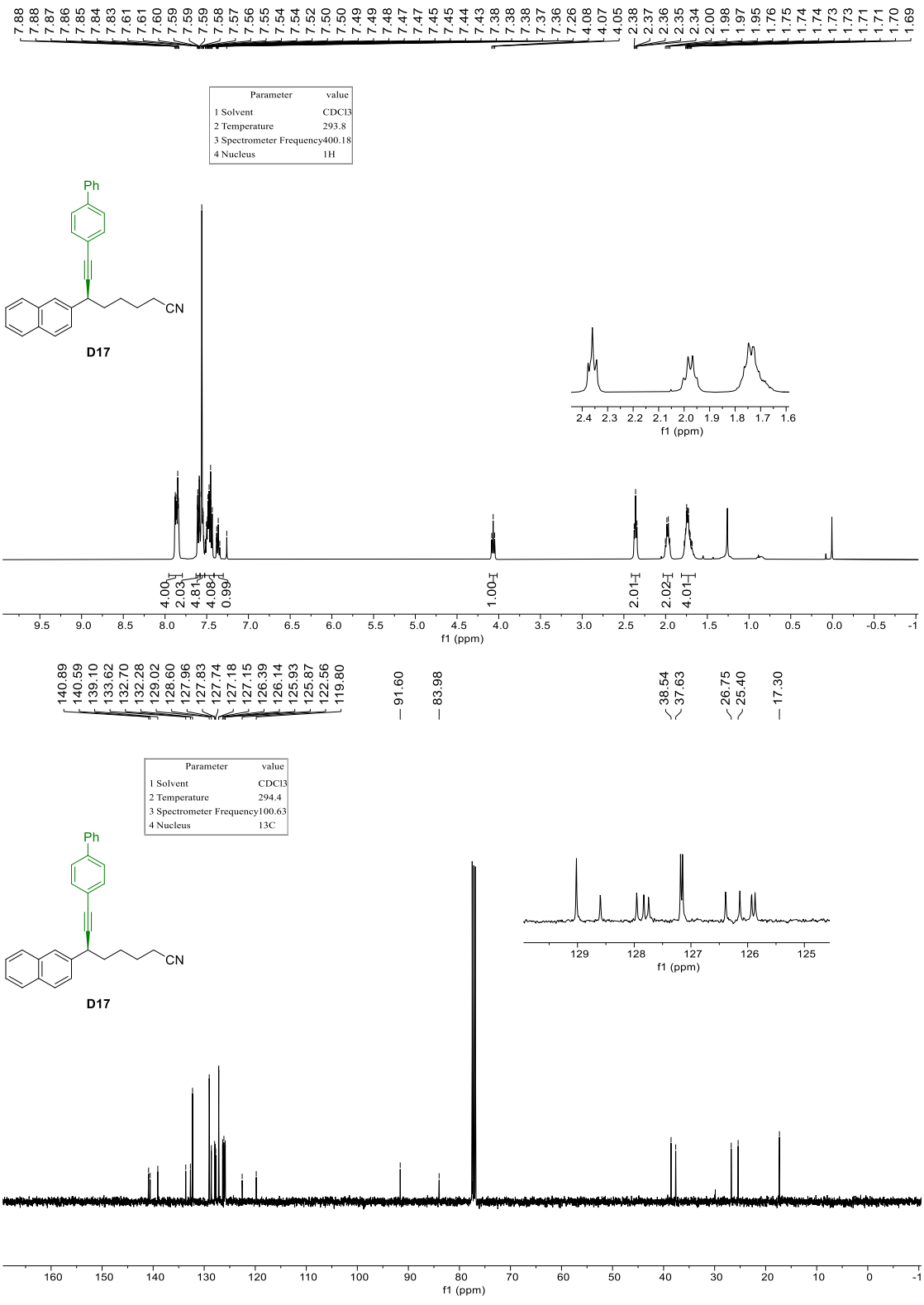

159.47
139.32 133.58 133.19 132.63 128.50 127.91 127.78 126.30 126.06 125.88 125.84 119.80 115.73 114.02
89.30 83.85
55.43
38.43 37.64
26.70 25.35
17.25
Parameter value
1 Solvent CDCl3
2 Temperature 293.7
3 Spectrometer Frequency 150.91
4 Nucleus 13C
OMe
CN
D12
128.5 128.0 127.5 127.0 126.5 126.0
f1 (ppm)
f1 (ppm)

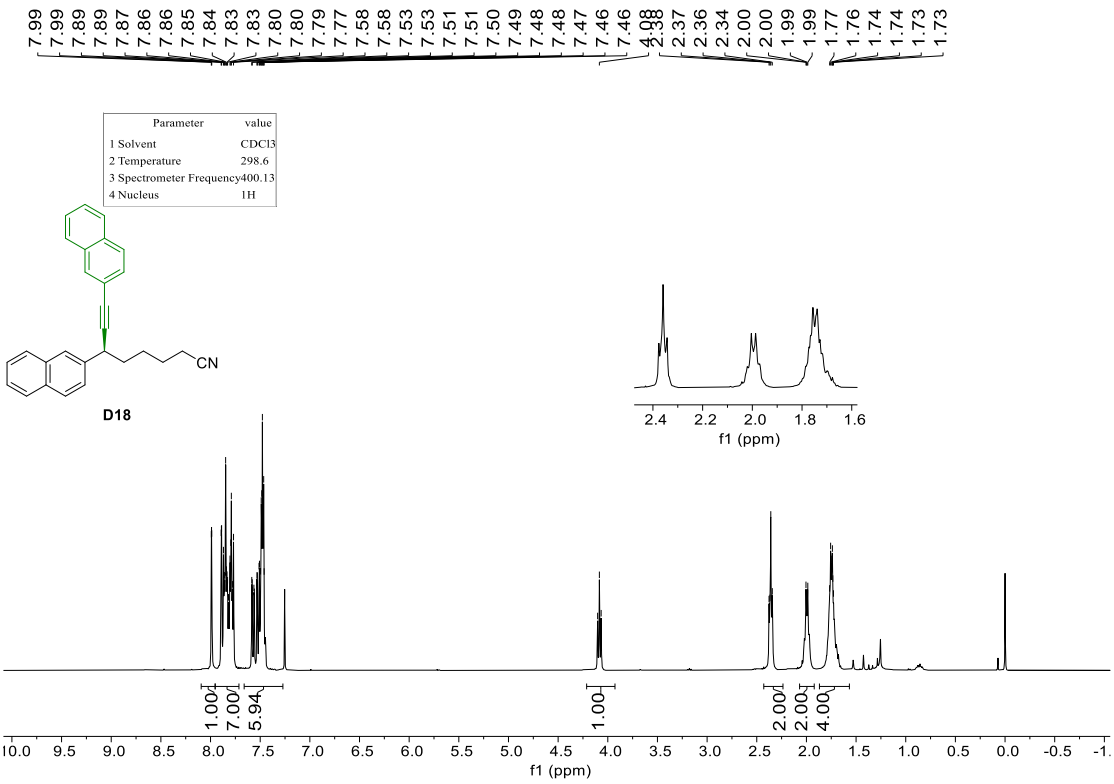

7.84 7.83 7.81 7.81 7.51 7.50 7.49 7.49 7.49 7.48 7.48 7.47 7.47 7.47 7.46 7.45 7.38 7.38 7.37 7.36 7.34 7.34
4.64 4.29 4.29 3.89 3.88 3.87 2.33 2.31 2.30 1.91 1.90 1.90 1.89 1.88 1.88 1.87 1.71 1.70 1.70 1.69 1.69 1.68 1.68 1.67 1.66 1.66 1.65 1.65 1.64 1.64 1.63 1.61 1.61 1.60 1.60 1.59 1.58
Parameter value
1 Solvent CDCl3
2 Temperature 292.7
3 Spectrometer Frequency 600.17
4 Nucleus 1H
Bn
O
CN
D13
2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
4.02 2.94 4.55 1.94 2.00 1.00 2.03 2.08 4.05
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
138.82 137.68 132.64 128.59 128.54 128.22 127.99 127.88 127.78 126.37 126.04 125.91
88.00 79.56 71.63 57.86 37.91 37.37 26.63 25.31 17.21
Parameter value
1 Solvent CDCl3
2 Temperature 293.4
3 Spectrometer Frequency 150.91
4 Nucleus 13C
Bn
O
CN
D13
129 128 127 126 125
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

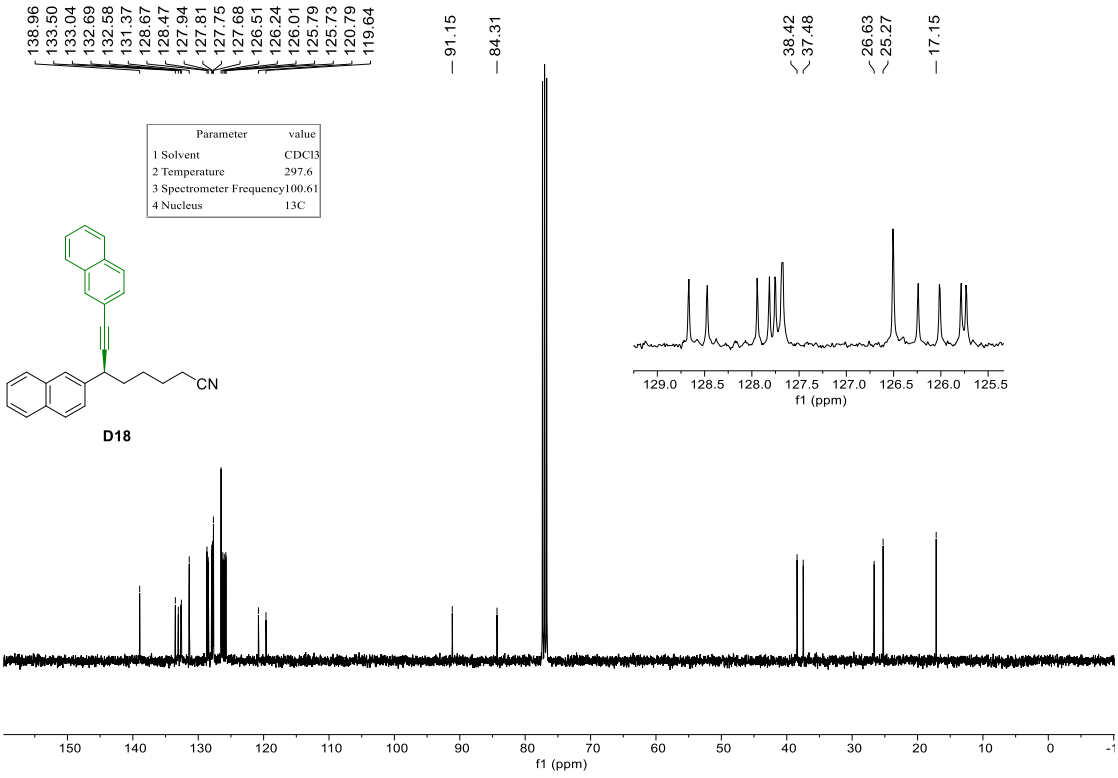

7.82 7.81 7.80 7.76 7.49 7.47 7.46 7.46 7.46 7.45 7.45 7.44 7.44 7.43
3.76 3.75 3.74 2.33 2.32 2.31 1.82 1.81 1.79 1.78 1.69 1.69 1.68 1.68 1.67 1.67 1.66 1.64 1.63 1.63 1.63 1.62 1.60 1.60 1.59 1.57 1.56 1.55 1.32 1.31 1.31 1.30 1.30 0.79 0.78 0.78 0.78 0.77 0.77 0.70 0.70 0.69 0.69 0.69 0.68
Parameter value
1 Solvent CDCl3
2 Temperature 292.3
3 Spectrometer Frequency 600.17
4 Nucleus 1H
CN
D14
7.90 7.85 7.80 7.75 7.70
f1 (ppm)
2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5
f1 (ppm)
2.99 1.01 3.00 1.01 1.99 2.04 4.02 0.94 4.03
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
139.77 133.54 132.56 128.36 127.87 127.75 126.22 125.91 125.85 125.73 119.82
87.15
76.43
37.83 37.75
26.62 25.32
17.23
8.44 8.38
-0.20
Parameter value
1 Solvent CDCl3
2 Temperature 293.6
3 Spectrometer Frequency 150.91
4 Nucleus 13C
CN
D14
129 128 127 126 125
f1 (ppm)
37.9 37.8 37.7
f1 (ppm)
8.5 8.4 8.3
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

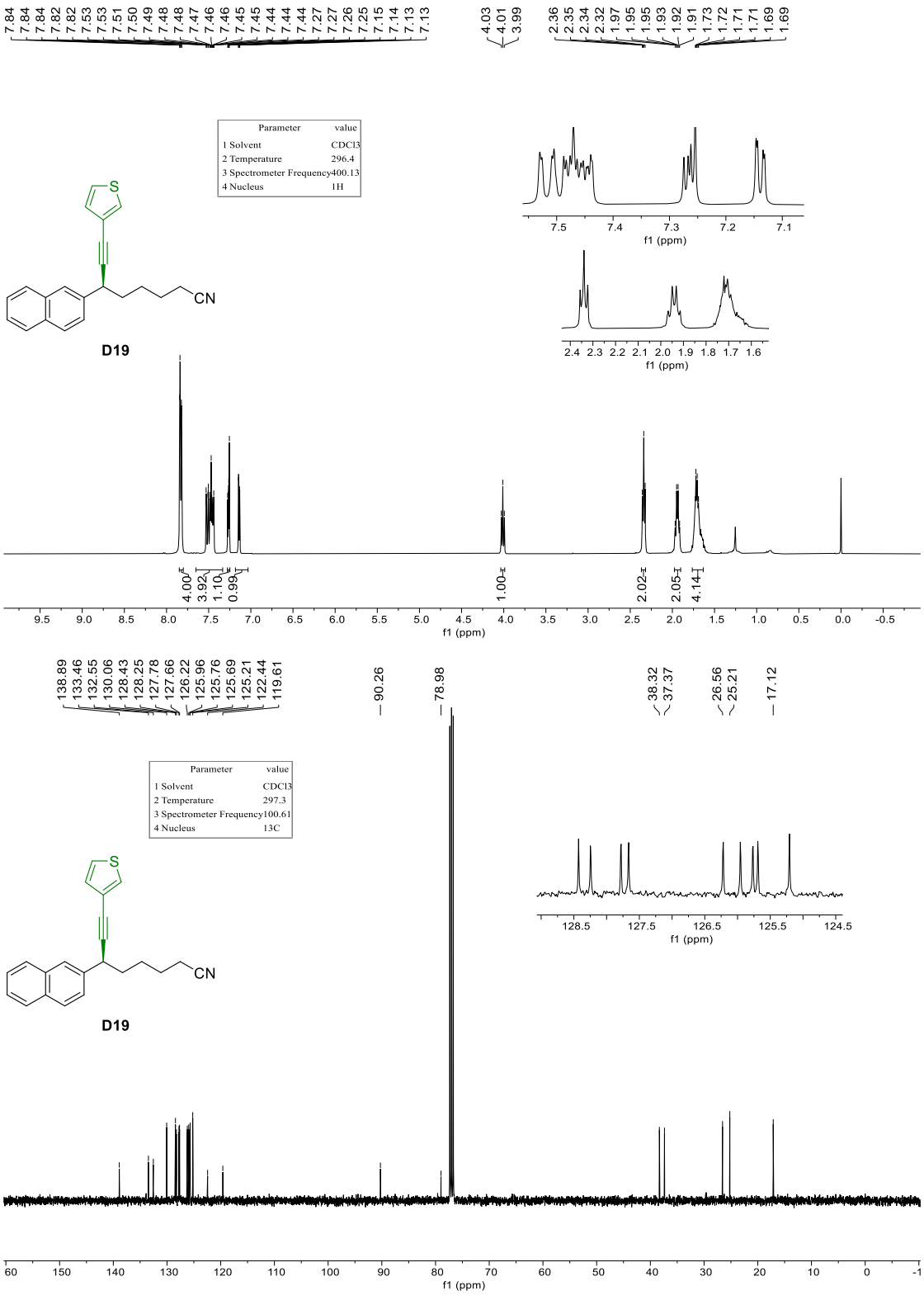

7.83 7.81 7.79 7.50 7.48 7.47 7.47 7.46 7.45 7.44 7.26 CDCl3 7.26 3.85 3.83 3.82 2.34 2.33 2.31 1.87 1.86 1.84 1.83 1.72 1.71 1.71 1.70 1.70 1.69 1.69 1.68 1.67 1.67 1.66 1.65 1.64 1.64 1.63 1.62 1.62 1.61 1.61 1.59 1.58 1.58 1.57 1.57 1.56 1.26 0.28 0.27 0.25 0.21 0.21 0.17 0.17 0.16 0.16 0.01 0.00
Parameter value
1 Solvent CDCl3
2 Temperature 292.5
3 Spectrometer Frequency 600.17
4 Nucleus 1H
TMS
CN
D15
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
2.90 1.00 3.00 1.00 2.07 2.06 4.15 8.86
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)
138.79 133.53 132.62 128.45 127.90 127.77 126.30 126.12 125.86 125.78 119.75 107.69 88.28 38.73 37.47 26.53 25.30 17.23 0.28
Parameter value
1 Solvent CDCl3
2 Temperature 293.4
3 Spectrometer Frequency 150.91
4 Nucleus 13C
TMS
CN
D15
128.5 128.0 127.5 127.0 126.5 126.0 125.5
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

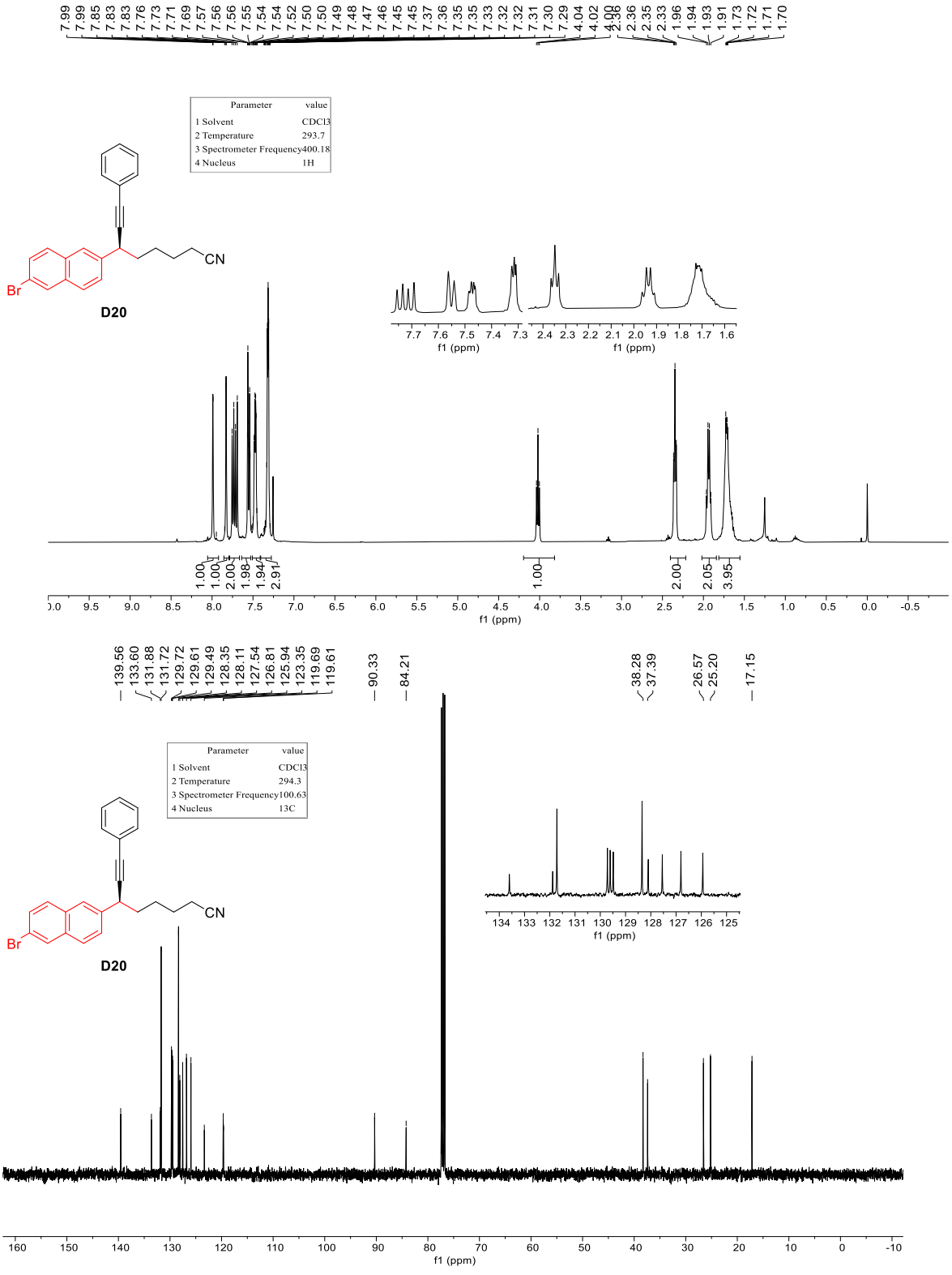

7.82 7.80 7.79 7.78 7.72 7.48 7.47 7.46 7.46 7.45 7.44 7.43 7.40 7.40 7.39 7.38 7.31 7.29 7.28 7.25 7.24 7.23 7.21
3.76 3.75 3.74 2.88 2.87 2.86 2.59 2.59 2.58 2.58 2.58 2.57 2.57 2.28 2.27 2.25 1.77 1.77 1.76 1.76 1.75 1.75 1.74 1.65 1.65 1.64 1.63 1.62 1.61 1.53 1.53 1.52 1.52 1.51 1.51 1.50
Parameter value
1 Solvent CDCl3
2 Temperature 292.4
3 Spectrometer Frequency 600.17
4 Nucleus 1H
Ph
CN
D16
f1 (ppm)
3.02 0.98 2.04 1.01 1.96 3.01 1.00 2.06 2.03 2.03 2.14 2.11 2.12
140.97 139.65 133.53 132.55 128.73 128.46 128.33 127.89 127.74 126.35 126.20 125.89 125.73 119.85
83.27 82.04
37.82 37.69 35.43
26.57 25.32 21.06 17.20
Parameter value
1 Solvent CDCl3
2 Temperature 293.2
3 Spectrometer Frequency 150.91
4 Nucleus 13C
Ph
CN
D16
f1 (ppm)

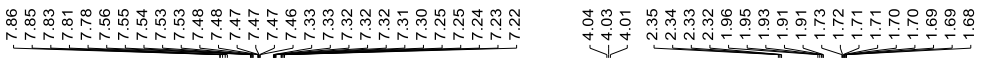

7.88 7.88 7.87 7.86 7.85 7.84 7.83 7.61 7.61 7.60 7.59 7.59 7.59 7.58 7.57 7.56 7.55 7.54 7.54 7.52 7.50 7.50 7.49 7.49 7.48 7.47 7.47 7.45 7.45 7.44 7.43 7.38 7.38 7.38 7.37 7.36 7.26 4.08 4.07 4.05
2.38 2.37 2.36 2.35 2.34 2.00 1.98 1.97 1.95 1.76 1.75 1.74 1.74 1.73 1.73 1.71 1.71 1.70 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 293.8
3 Spectrometer Frequency 400.18
4 Nucleus 1H
Ph
CN
D17
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
4.00 2.03 4.81 4.08 0.99 1.00 2.01 2.02 4.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)
140.89 140.59 139.10 133.62 132.70 132.28 129.02 128.60 127.96 127.83 127.74 127.18 127.15 126.39 126.14 125.93 125.87 122.56 119.80
91.60
83.98
38.54 37.63
26.75 25.40
17.30
Parameter value
1 Solvent CDCl3
2 Temperature 294.4
3 Spectrometer Frequency 100.63
4 Nucleus 13C
Ph
CN
D17
129 128 127 126 125
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


7.99 7.99 7.89 7.89 7.87 7.86 7.86 7.85 7.84 7.83 7.83 7.80 7.80 7.79 7.77 7.58 7.58 7.53 7.53 7.51 7.51 7.50 7.49 7.48 7.48 7.47 7.46 7.46 4.08 2.38 2.37 2.36 2.34 2.00 2.00 1.99 1.99 1.77 1.76 1.74 1.74 1.73 1.73
Parameter value
1 Solvent CDCl3
2 Temperature 298.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
D18
f1 (ppm)
1.00 7.00 5.94 1.00 2.00 2.00 4.00
f1 (ppm)


138.96 133.50 133.04 132.69 132.58 131.37 128.67 128.47 127.94 127.81 127.75 127.68 126.51 126.24 126.01 125.79 125.73 120.79 119.64
91.15 84.31
38.42 37.48 26.63 25.27 17.15
Parameter value
1 Solvent CDCl3
2 Temperature 297.6
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
D18
f1 (ppm)
f1 (ppm)


7.84 7.84 7.84 7.82 7.82 7.53 7.53 7.51 7.50 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.45 7.44 7.44 7.44 7.27 7.27 7.26 7.25 7.15 7.14 7.13 7.13
4.03 4.01 3.99
2.36 2.35 2.34 2.32 1.97 1.95 1.95 1.93 1.92 1.91 1.73 1.72 1.71 1.71 1.69 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 296.4
3 Spectrometer Frequency 400.13
4 Nucleus 1H
S
CN
D19
f1 (ppm)
4.00 3.92 1.10 0.99 1.00 2.02 2.05 4.14
138.89 133.46 132.55 130.06 128.43 128.25 127.78 127.66 126.22 125.96 125.76 125.69 125.21 122.44 119.61
90.26 78.98
38.32 37.37 26.56 25.21 17.12
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
S
CN
D19
f1 (ppm)


7.99 7.99 7.85 7.83 7.83 7.76 7.73 7.71 7.69 7.57 7.56 7.56 7.55 7.54 7.54 7.52 7.50 7.50 7.49 7.48 7.47 7.46 7.45 7.45 7.37 7.36 7.35 7.35 7.33 7.32 7.32 7.31 7.30 7.29 4.04 4.02 4.00 2.36 2.36 2.35 2.33 1.96 1.94 1.93 1.91 1.73 1.72 1.71 1.70
Parameter value
1 Solvent CDCl3
2 Temperature 293.7
3 Spectrometer Frequency 400.18
4 Nucleus 1H
CN
Br
D20
f1 (ppm)
1.00 1.00 2.00 1.98 1.94 2.91 1.00 2.00 2.05 3.95
f1 (ppm)
139.56 133.60 131.88 131.72 129.72 129.61 129.49 128.35 128.11 127.54 126.81 125.94 123.35 119.69 119.61 90.33 84.21 38.28 37.39 26.57 25.20 17.15
Parameter value
1 Solvent CDCl3
2 Temperature 294.3
3 Spectrometer Frequency 100.63
4 Nucleus 13C
CN
Br
D20
f1 (ppm)
f1 (ppm)


7.86
7.85
7.83
7.81
7.78
7.56
7.55
7.54
7.53
7.53
7.48
7.48
7.47
7.47
7.47
7.46
7.33
7.33
7.32
7.32
7.32
7.31
7.30
7.25
7.25
7.24
7.23
7.22
4.04
4.03
4.01
2.35
2.34
2.33
2.32
1.96
1.95
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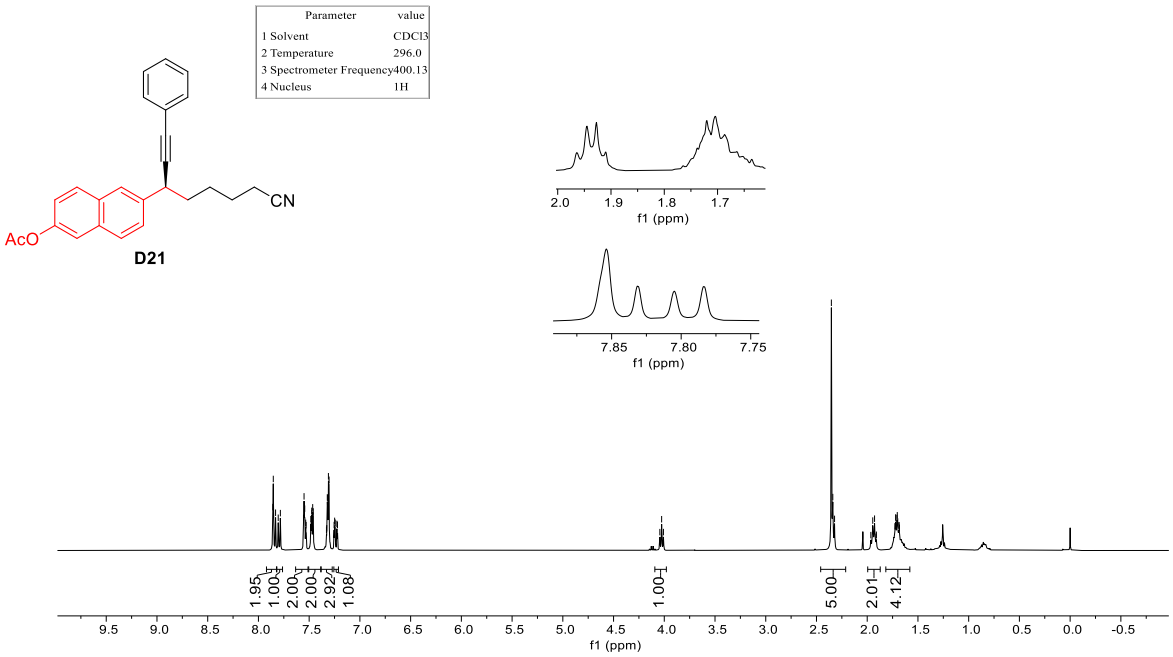
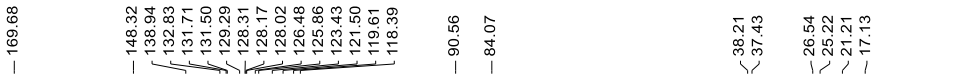
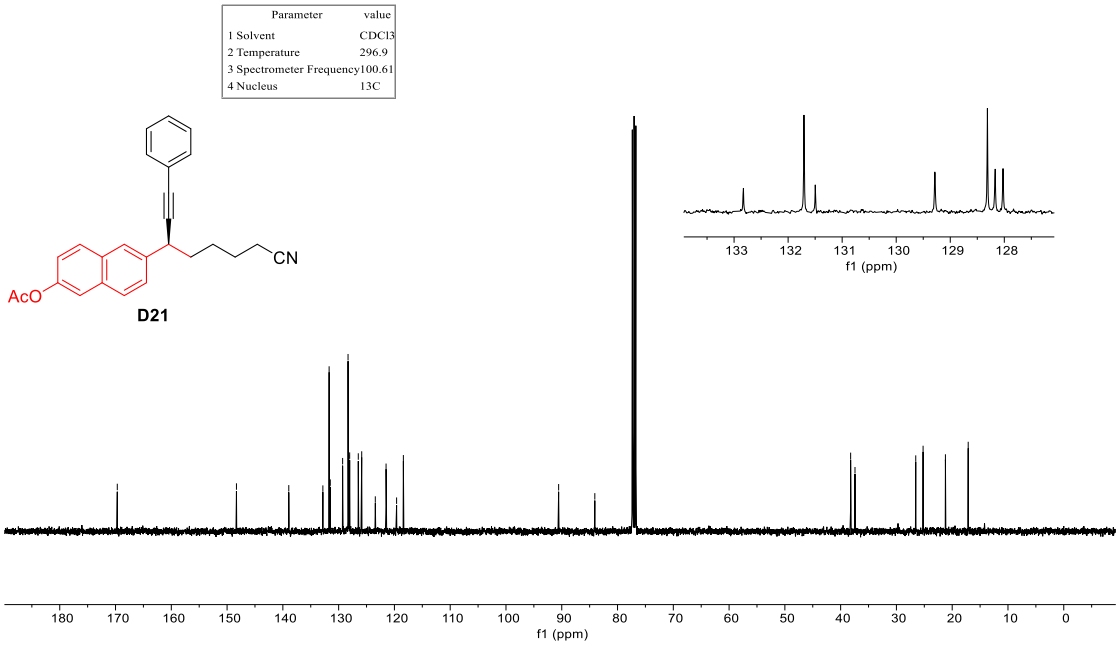
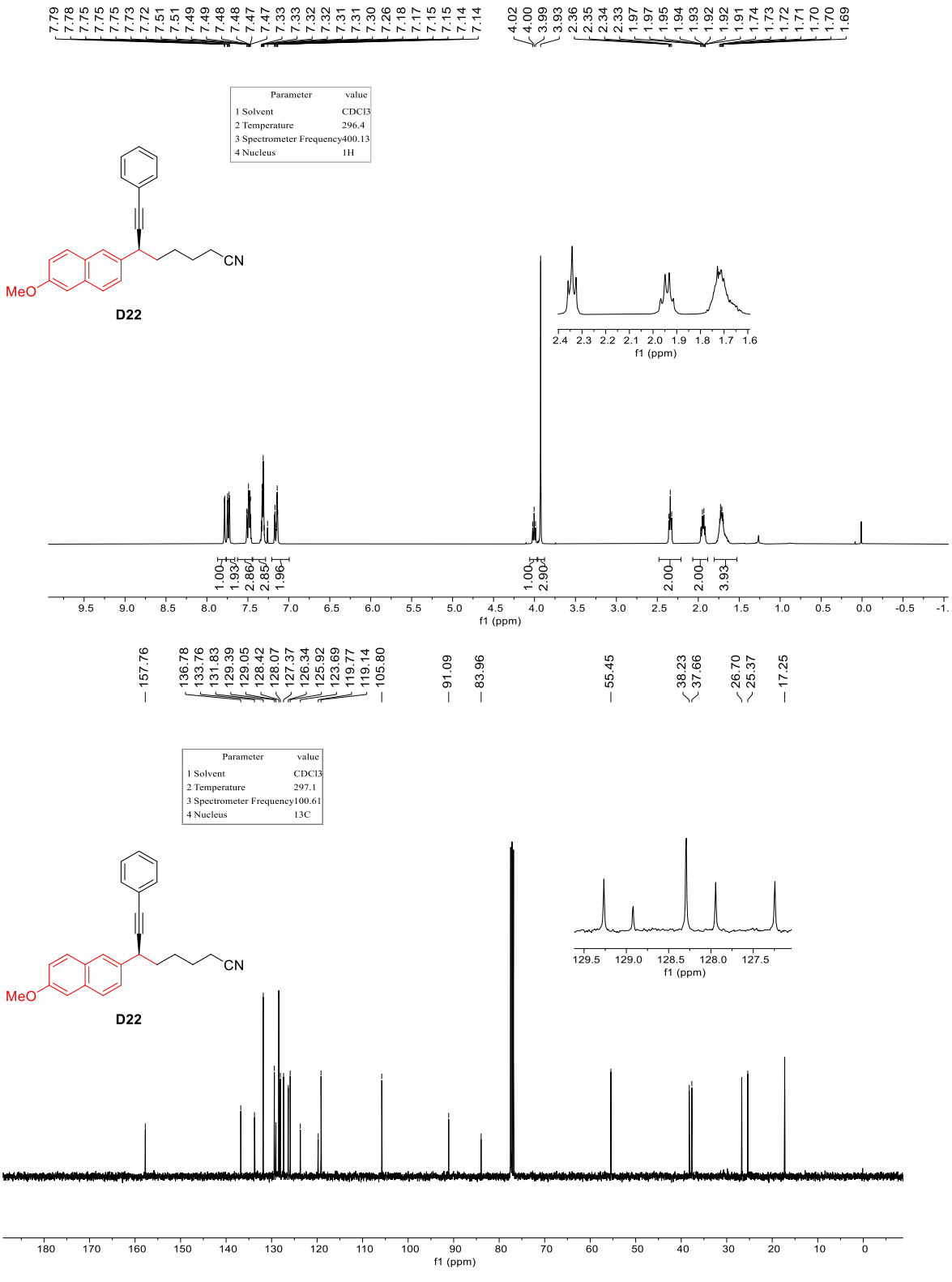
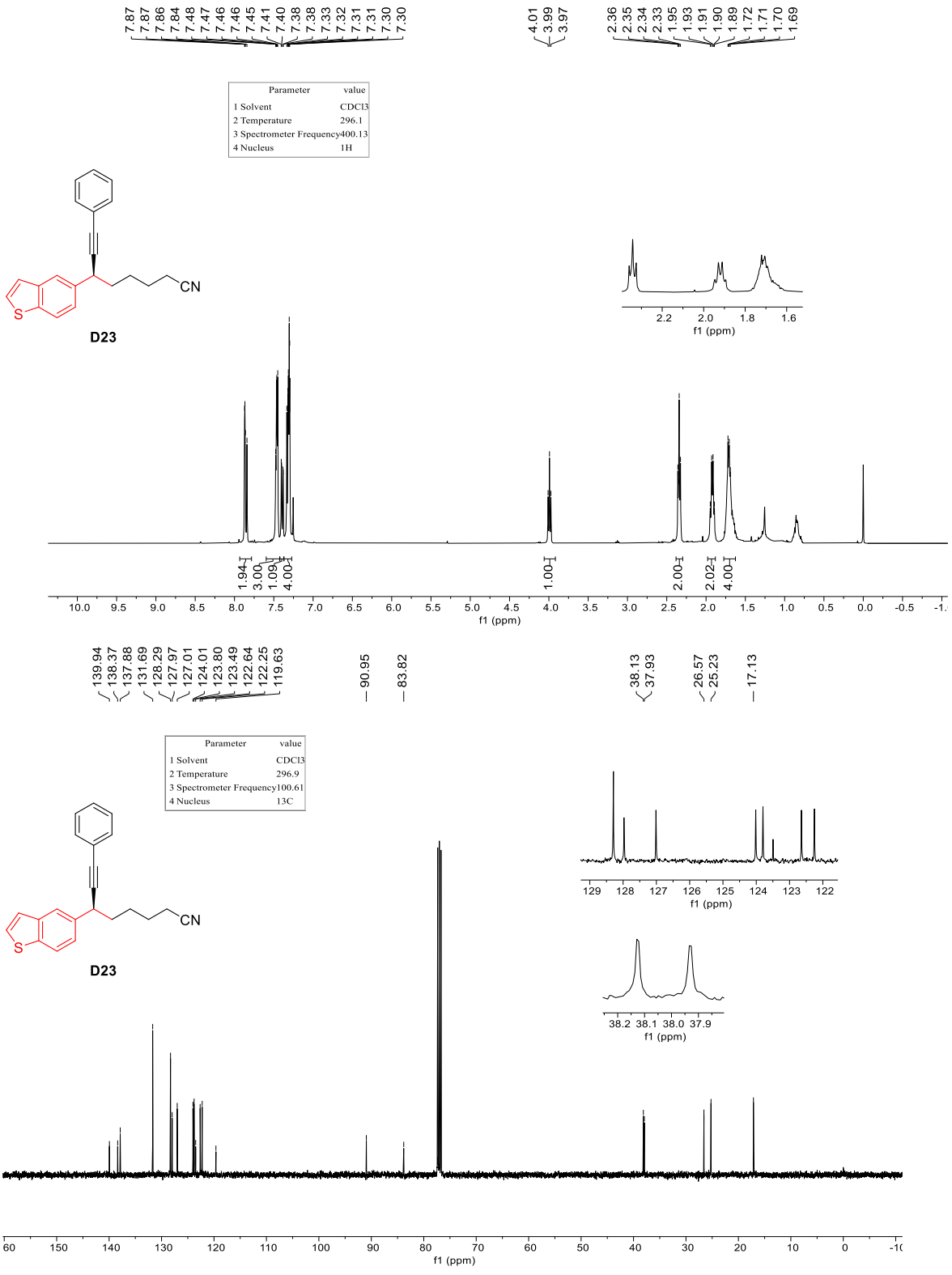
1.71
1.70
1.70
1.69
1.69
1.68

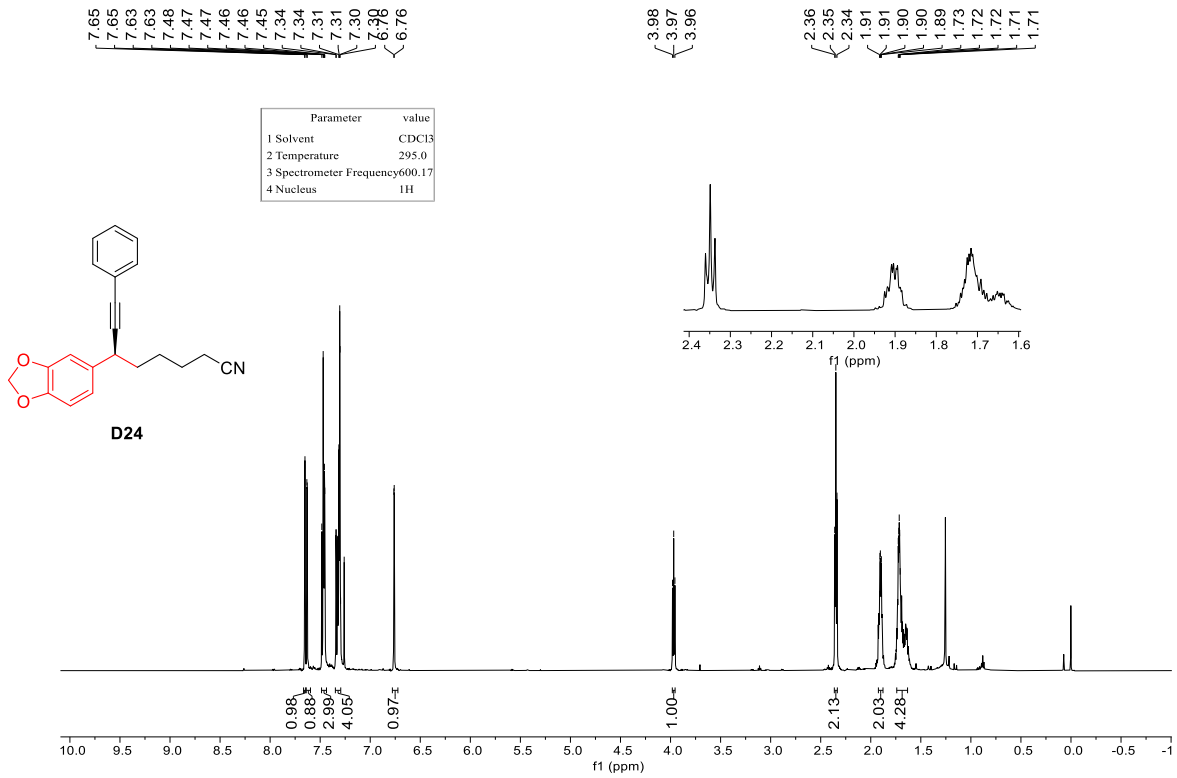

Parameter value
1 Solvent CDCl3
2 Temperature 296.0
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
AcO
D21
2.0 1.9 1.8 1.7
f1 (ppm)
7.85 7.80 7.75
f1 (ppm)
1.95 1.00 2.00 2.00 2.92 1.08
1.00
5.00
2.01 4.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

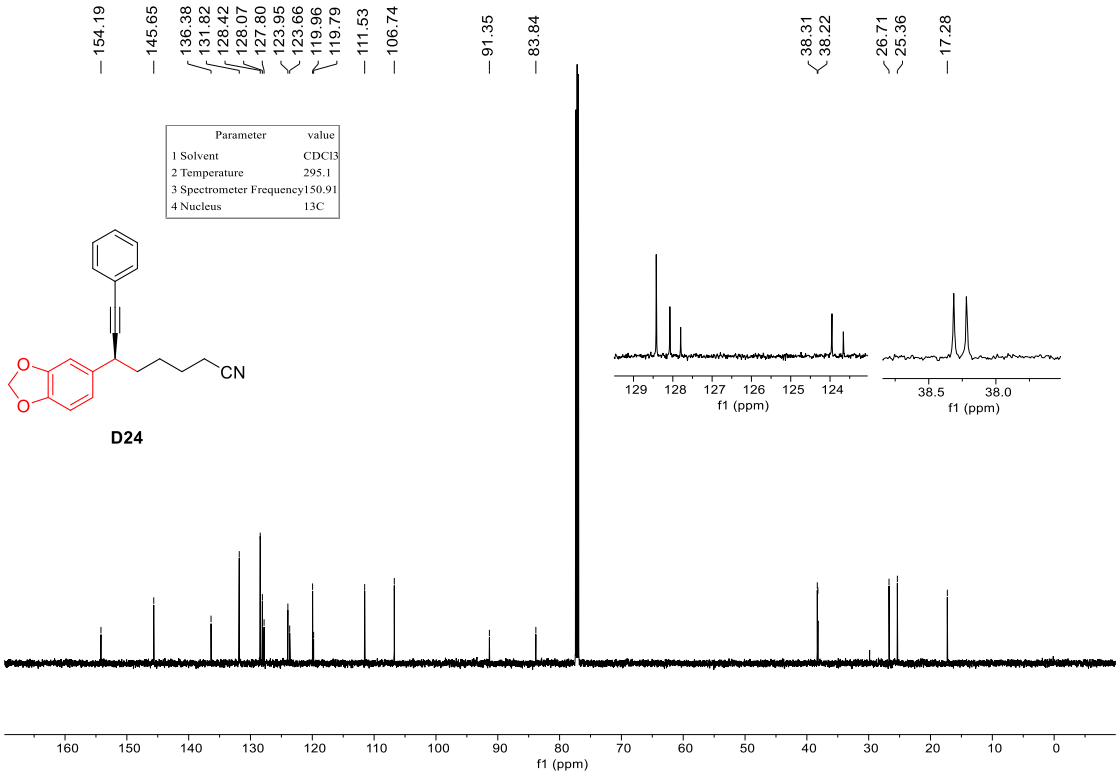

169.68
148.32
138.94
132.83
131.71
131.50
129.29
128.31
128.17
128.02
126.48
125.86
123.43
121.50
119.61
118.39
90.56
84.07
38.21
37.43
26.54
25.22
21.21
17.13

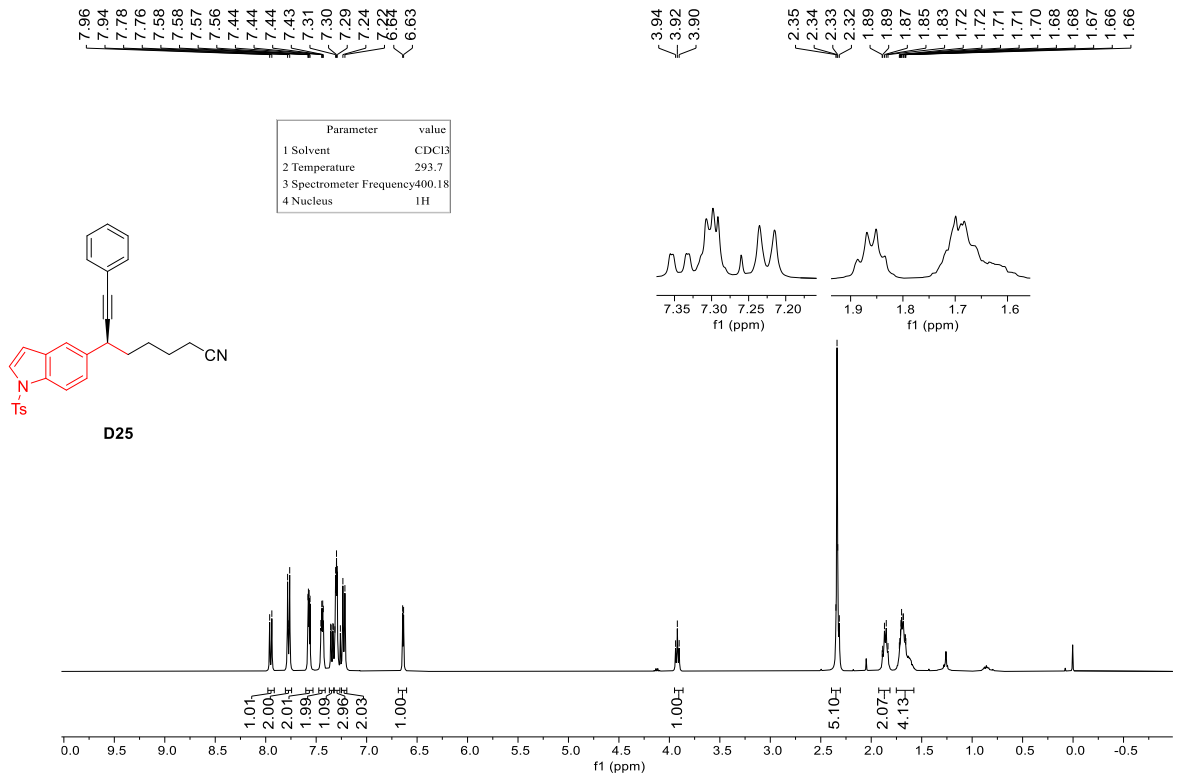

Parameter value
1 Solvent CDCl3
2 Temperature 296.9
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
AcO
D21
133 132 131 130 129 128
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

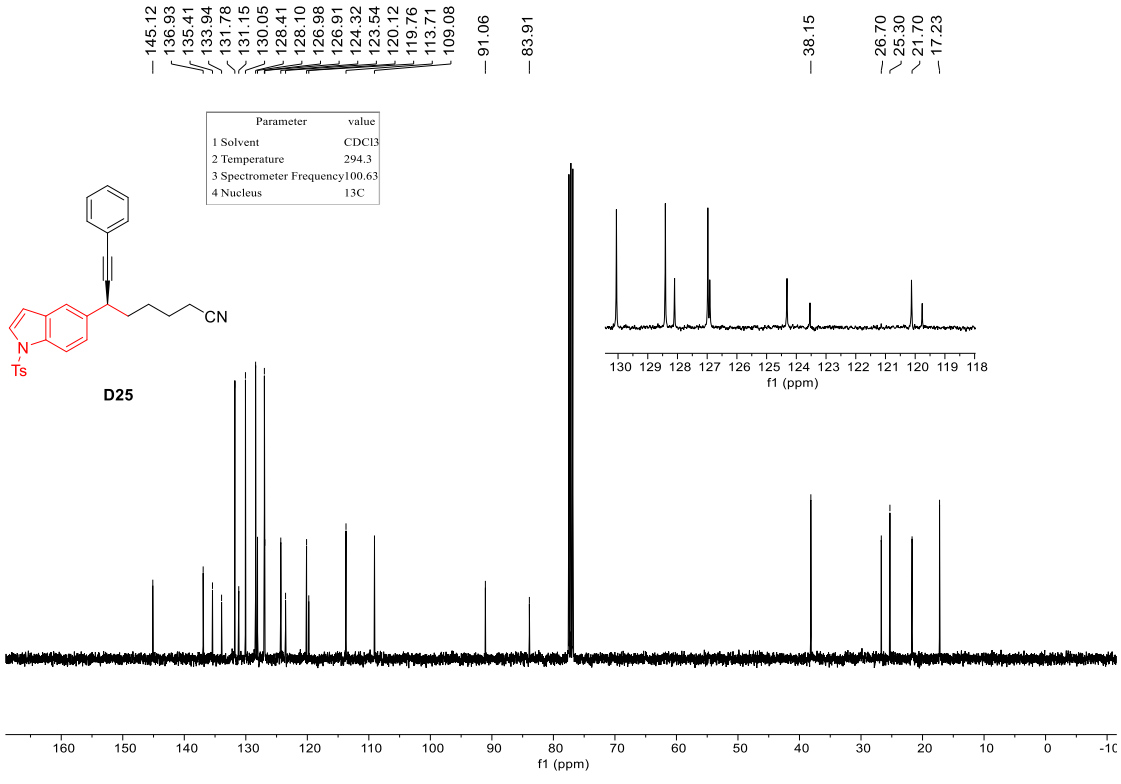

7.79 7.78 7.75 7.75 7.75 7.73 7.72 7.51 7.51 7.49 7.49 7.48 7.48 7.47 7.47 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.26 7.18 7.17 7.15 7.15 7.14 7.14
4.02 4.00 3.99 3.93 2.36 2.35 2.34 2.33 1.97 1.97 1.95 1.94 1.93 1.92 1.92 1.91 1.74 1.73 1.72 1.71 1.70 1.70 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 296.4
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
MeO
D22
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
1.00 1.93 2.86 2.85 1.96 1.00 2.90 2.00 2.00 3.93
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
157.76 136.78 133.76 131.83 129.39 129.05 128.42 128.07 127.37 126.34 125.92 123.69 119.77 119.14 105.80 91.09 83.96 55.45 38.23 37.66 26.70 25.37 17.25
Parameter value
1 Solvent CDCl3
2 Temperature 297.1
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
MeO
D22
129.5 129.0 128.5 128.0 127.5
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

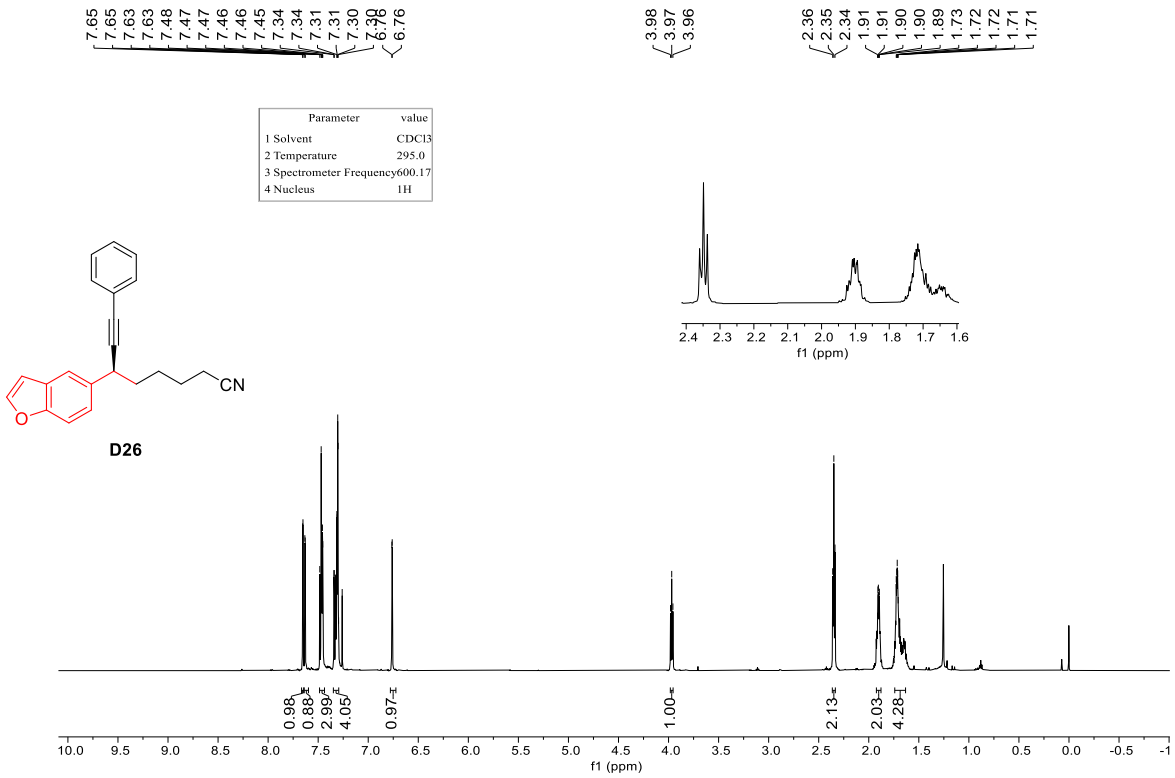

7.87 7.87 7.86 7.84 7.48 7.47 7.46 7.46 7.45 7.41 7.40 7.38 7.38 7.33 7.32 7.31 7.31 7.30 7.30
4.01 3.99 3.97
2.36 2.35 2.34 2.33 1.95 1.93 1.91 1.90 1.89 1.72 1.71 1.70 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 296.1
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
S
D23
f1 (ppm)
1.94 3.00 1.09 4.00 1.00 2.00 2.02 4.00
139.94 138.37 137.88 131.69 128.29 127.97 127.01 124.01 123.80 123.49 122.64 122.25 119.63
90.95
83.82
38.13 37.93
26.57 25.23
17.13
Parameter value
1 Solvent CDCl3
2 Temperature 296.9
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
S
D23
f1 (ppm)

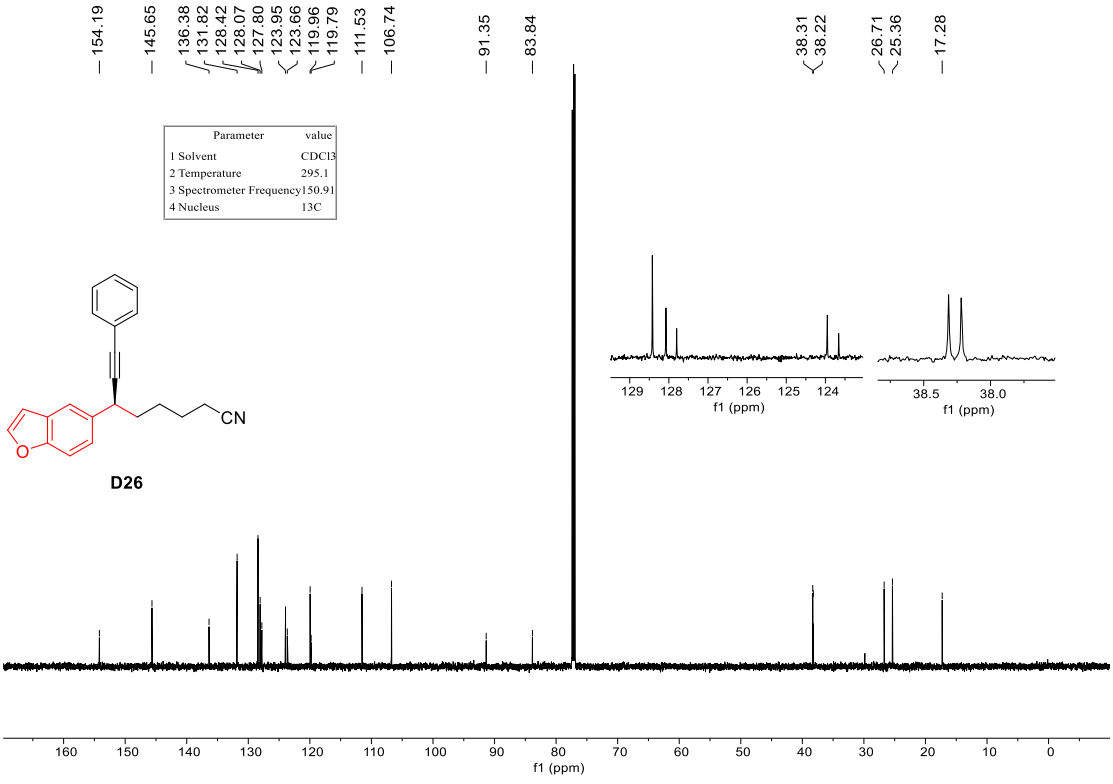

7.65 7.65 7.63 7.63 7.48 7.47 7.47 7.46 7.46 7.45 7.34 7.34 7.31 7.31 7.30 7.30 6.76 6.76
3.98 3.97 3.96
2.36 2.35 2.34 1.91 1.91 1.90 1.90 1.89 1.73 1.72 1.72 1.71 1.71
Parameter value
1 Solvent CDCl3
2 Temperature 295.0
3 Spectrometer Frequency 600.17
4 Nucleus 1H
CN
D24
0.98 0.88 2.99 4.05 0.97 1.00 2.13 2.03 4.28
f1 (ppm)

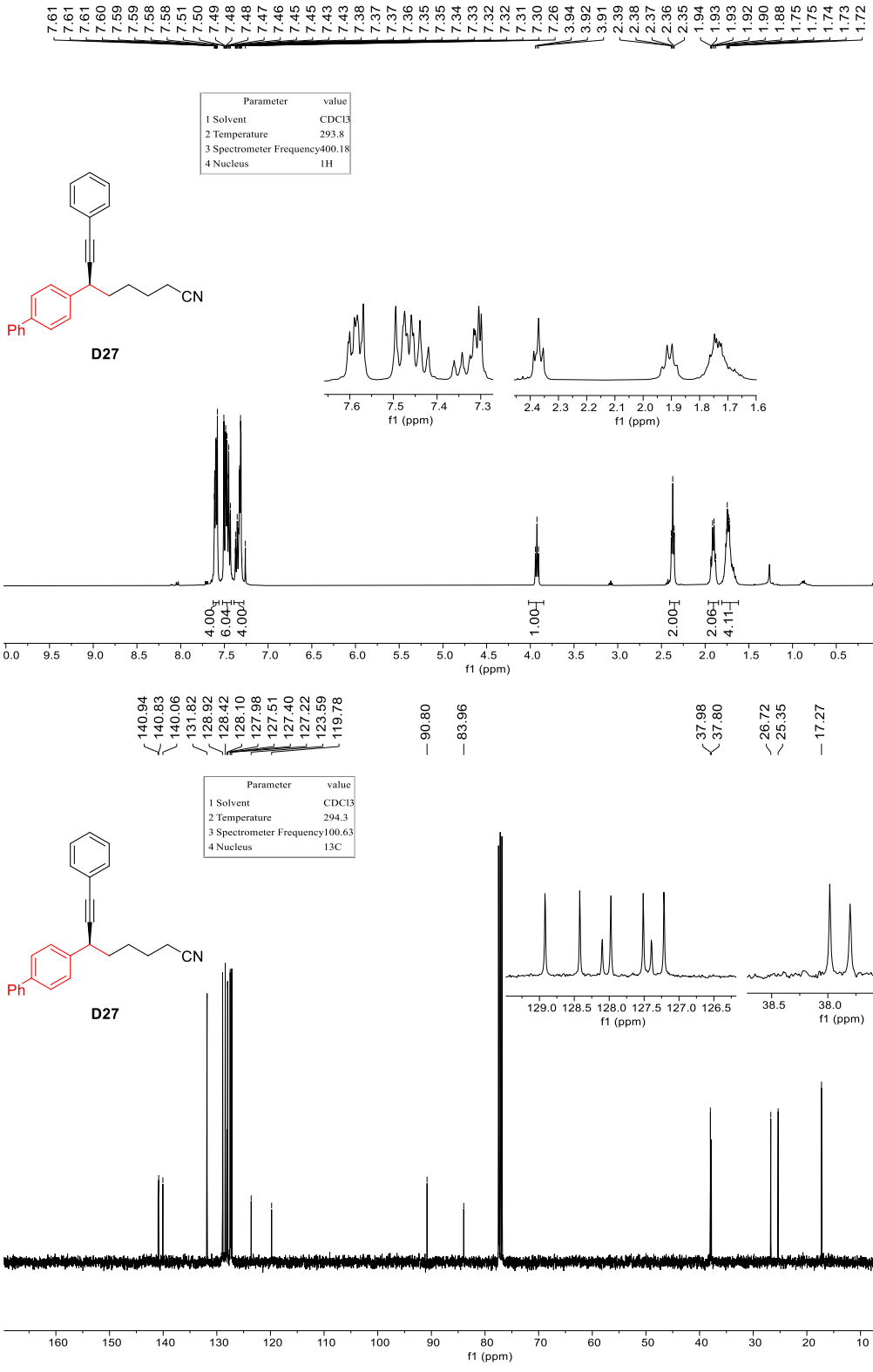

154.19 145.65 136.38 131.82 128.42 128.07 127.80 123.95 123.66 119.96 119.79 111.53 106.74 91.35 83.84 38.31 38.22 26.71 25.36 17.28
Parameter value
1 Solvent CDCl3
2 Temperature 295.1
3 Spectrometer Frequency 150.91
4 Nucleus 13C
CN
D24
f1 (ppm)

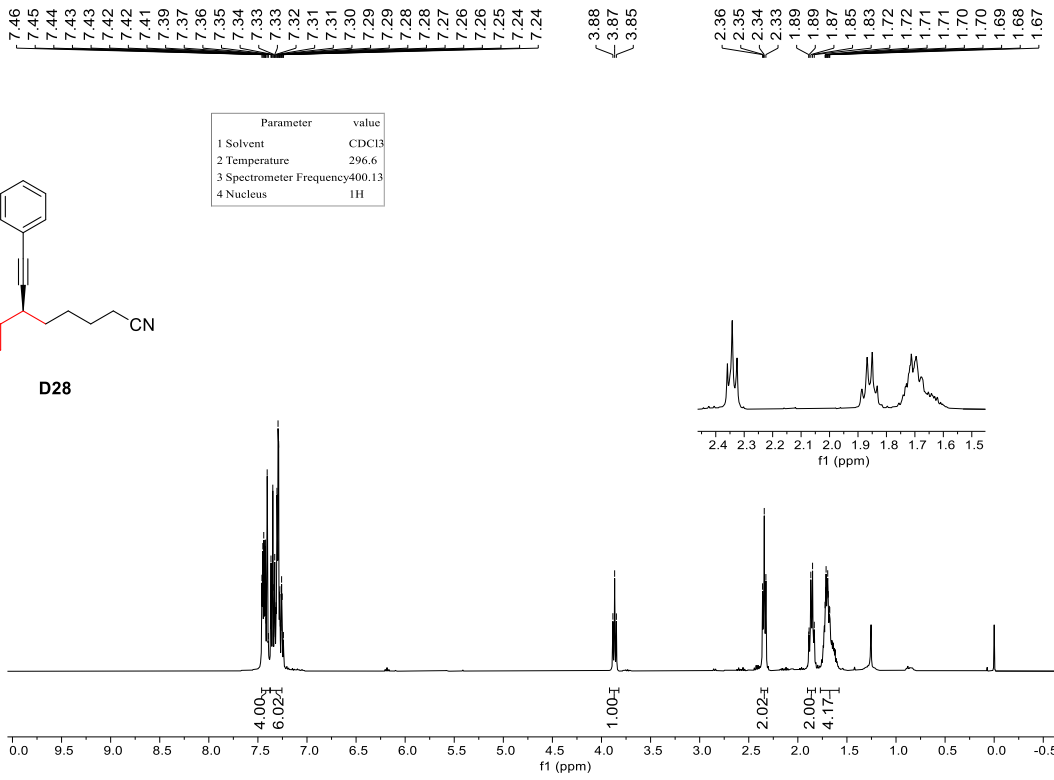

7.96 7.94 7.78 7.76 7.58 7.58 7.57 7.56 7.44 7.44 7.44 7.43 7.31 7.30 7.29 7.24 6.64 6.63
3.94 3.92 3.90
2.35 2.34 2.33 2.32 1.89 1.89 1.87 1.85 1.83 1.72 1.72 1.71 1.71 1.70 1.68 1.68 1.67 1.66 1.66
Parameter value
1 Solvent CDCl3
2 Temperature 293.7
3 Spectrometer Frequency 400.18
4 Nucleus 1H
CN
N
Ts
D25
7.35 7.30 7.25 7.20
f1 (ppm)
1.9 1.8 1.7 1.6
f1 (ppm)
1.01 2.00 2.01 1.99 1.09 2.96 2.03 1.00 1.00 5.10 2.07 4.13
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

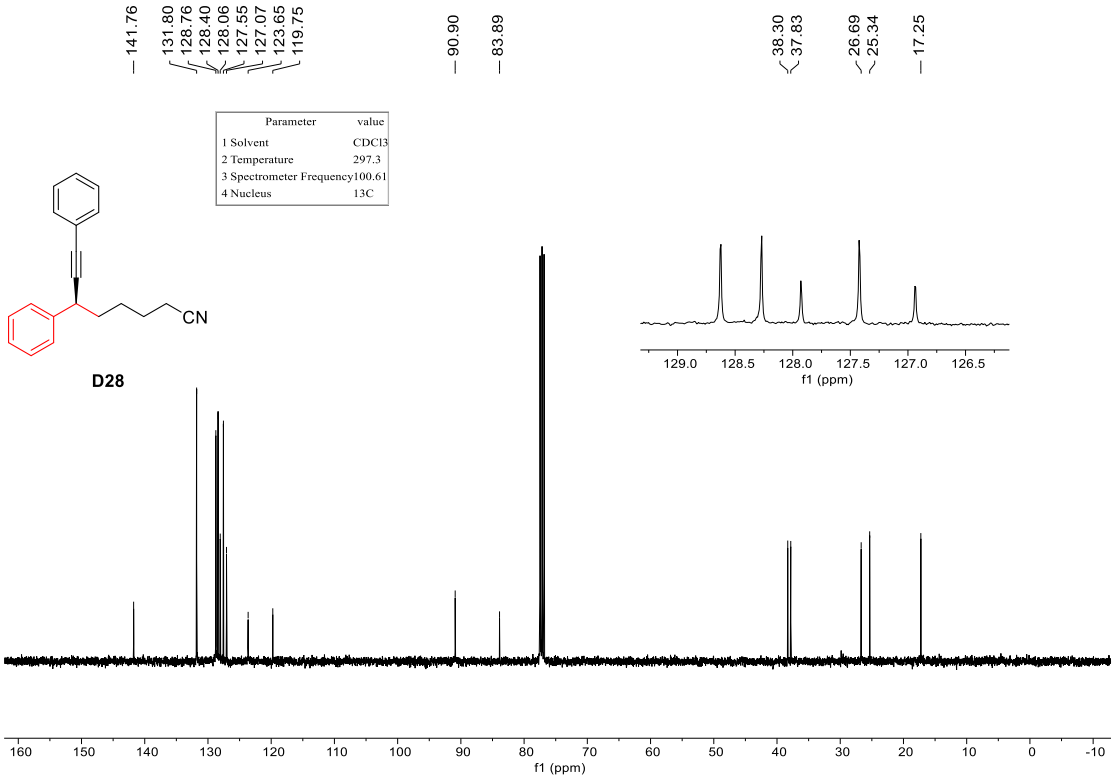

145.12 136.93 135.41 133.94 131.78 131.15 130.05 128.41 128.10 126.98 126.91 124.32 123.54 120.12 119.76 113.71 109.08
91.06
83.91
38.15
26.70 25.30 21.70 17.23
Parameter value
1 Solvent CDCl3
2 Temperature 294.3
3 Spectrometer Frequency 100.63
4 Nucleus 13C
CN
N
Ts
D25
130 129 128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

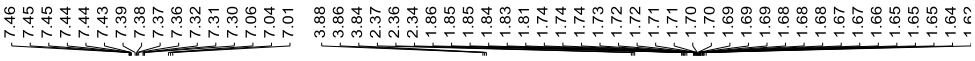

7.65 7.65 7.63 7.63 7.48 7.47 7.47 7.46 7.46 7.45 7.34 7.34 7.31 7.31 7.30 7.30 6.76 6.76
3.98 3.97 3.96
2.36 2.35 2.34 1.91 1.91 1.90 1.90 1.89 1.73 1.72 1.72 1.71 1.71
Parameter value
1 Solvent CDCl3
2 Temperature 295.0
3 Spectrometer Frequency 600.17
4 Nucleus 1H
CN
O
D26
f1 (ppm)
0.98 0.88 2.99 4.05 0.97 1.00 2.13 2.03 4.28
f1 (ppm)

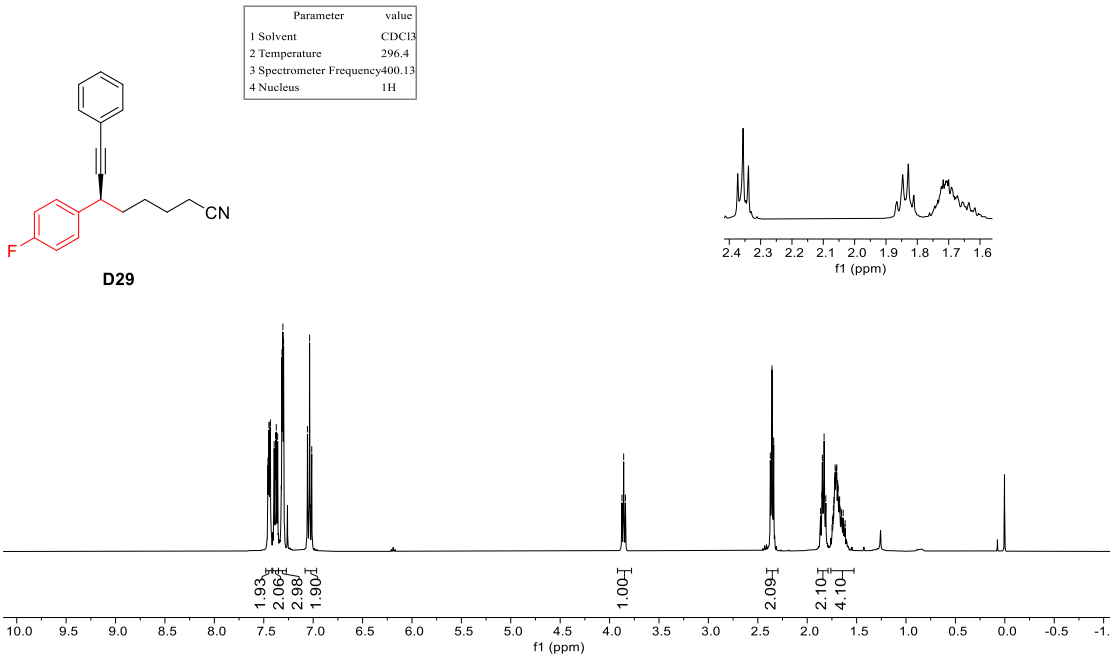

154.19 145.65 136.38 131.82 128.42 128.07 127.80 123.95 123.66 119.96 119.79 111.53 106.74 91.35 83.84 38.31 38.22 26.71 25.36 17.28
Parameter value
1 Solvent CDCl3
2 Temperature 295.1
3 Spectrometer Frequency 150.91
4 Nucleus 13C
CN
O
D26
f1 (ppm)
f1 (ppm)

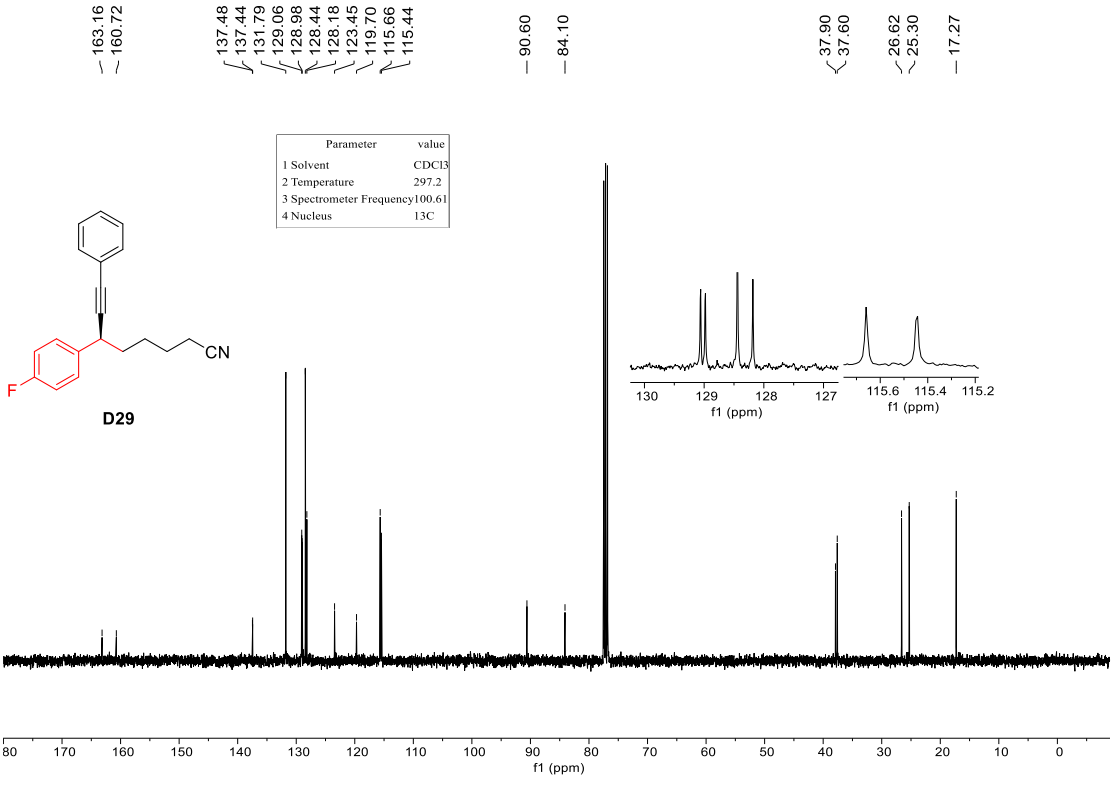

7.61 7.61 7.61 7.60 7.59 7.59 7.58 7.58 7.51 7.50 7.49 7.48 7.48 7.47 7.46 7.45 7.45 7.43 7.43 7.38 7.37 7.37 7.36 7.35 7.35 7.34 7.33 7.32 7.32 7.31 7.30 7.26 3.94 3.92 3.91 2.39 2.38 2.37 2.36 2.35 1.94 1.93 1.93 1.92 1.90 1.88 1.75 1.75 1.74 1.73 1.72
Parameter value
1 Solvent CDCl3
2 Temperature 293.8
3 Spectrometer Frequency 400.18
4 Nucleus 1H
CN
Ph
D27
f1 (ppm)
4.00 6.04 4.00 1.00 2.00 2.06 4.11
140.94 140.83 140.06 131.82 128.92 128.42 128.10 127.98 127.51 127.40 127.22 123.59 119.78 90.80 83.96 37.98 37.80 26.72 25.35 17.27
Parameter value
1 Solvent CDCl3
2 Temperature 294.3
3 Spectrometer Frequency 100.63
4 Nucleus 13C
CN
Ph
D27
f1 (ppm)


7.46 7.45 7.44 7.43 7.43 7.42 7.42 7.41 7.39 7.37 7.36 7.35 7.34 7.33 7.33 7.32 7.31 7.31 7.30 7.29 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.24 7.24
3.88 3.87 3.85
2.36 2.35 2.34 2.33 1.89 1.89 1.87 1.85 1.83 1.72 1.72 1.71 1.71 1.70 1.69 1.68 1.67
Parameter value
1 Solvent CDCl3
2 Temperature 296.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
D28
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5
f1 (ppm)
4.00 6.02 1.00 2.02 2.00 4.17
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

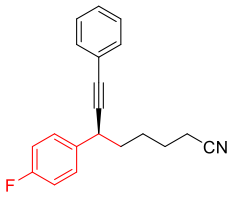

141.76 131.80 128.76 128.40 128.06 127.55 127.07 123.65 119.75
90.90 83.89
38.30 37.83 26.69 25.34 17.25
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
D28
129.0 128.5 128.0 127.5 127.0 126.5
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.46 7.45 7.45 7.44 7.44 7.43 7.39 7.38 7.37 7.36 7.32 7.31 7.30 7.06 7.04 7.01
3.88 3.86 3.84 2.37 2.36 2.34 1.86 1.85 1.85 1.84 1.83 1.81 1.74 1.74 1.74 1.73 1.72 1.72 1.71 1.71 1.70 1.70 1.69 1.69 1.68 1.68 1.67 1.67 1.66 1.65 1.65 1.64

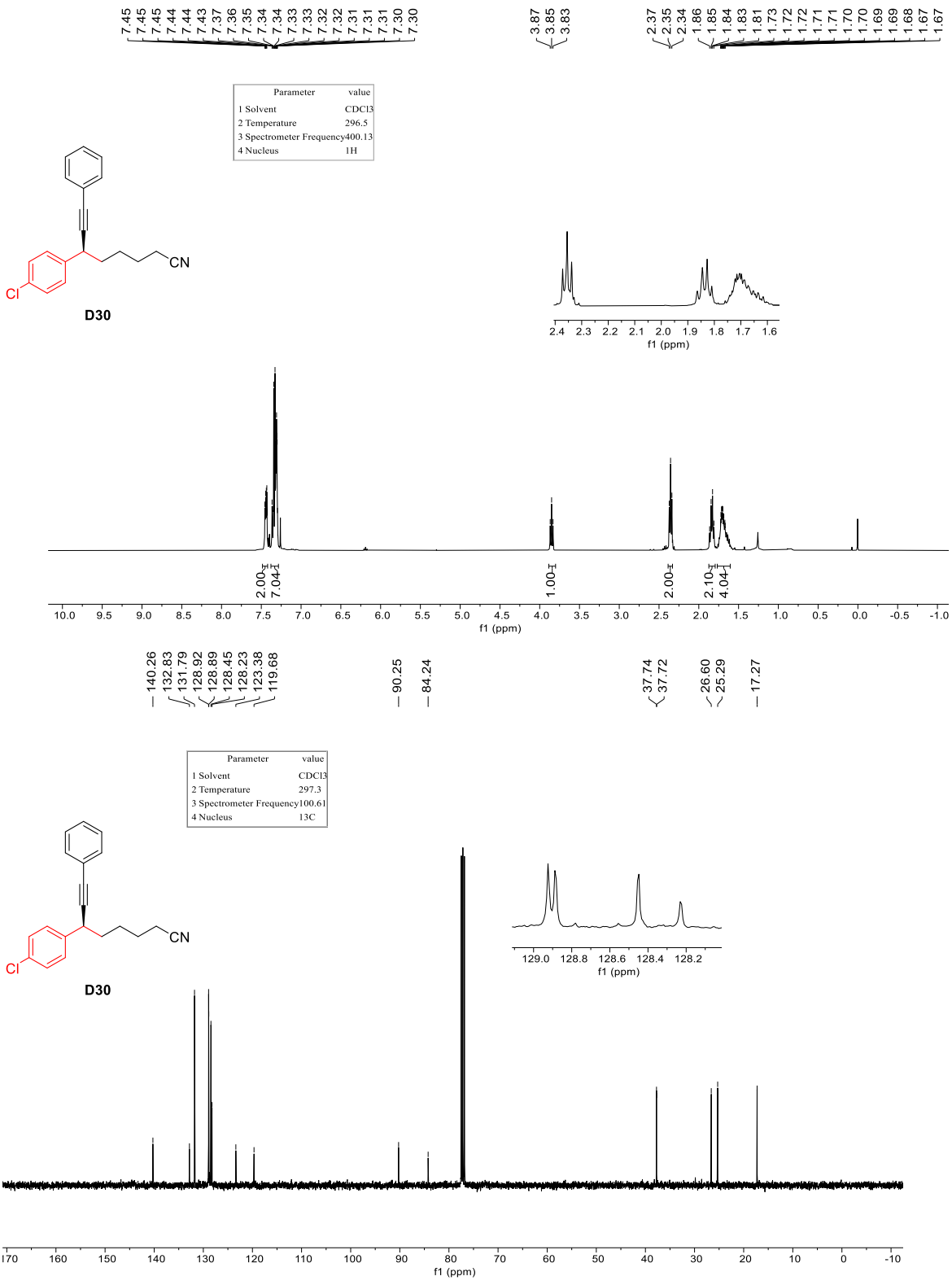

Parameter value
1 Solvent CDCl3
2 Temperature 296.4
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
F
D29
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
1.93 2.06 2.98 1.90 1.00 2.09 2.10 4.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

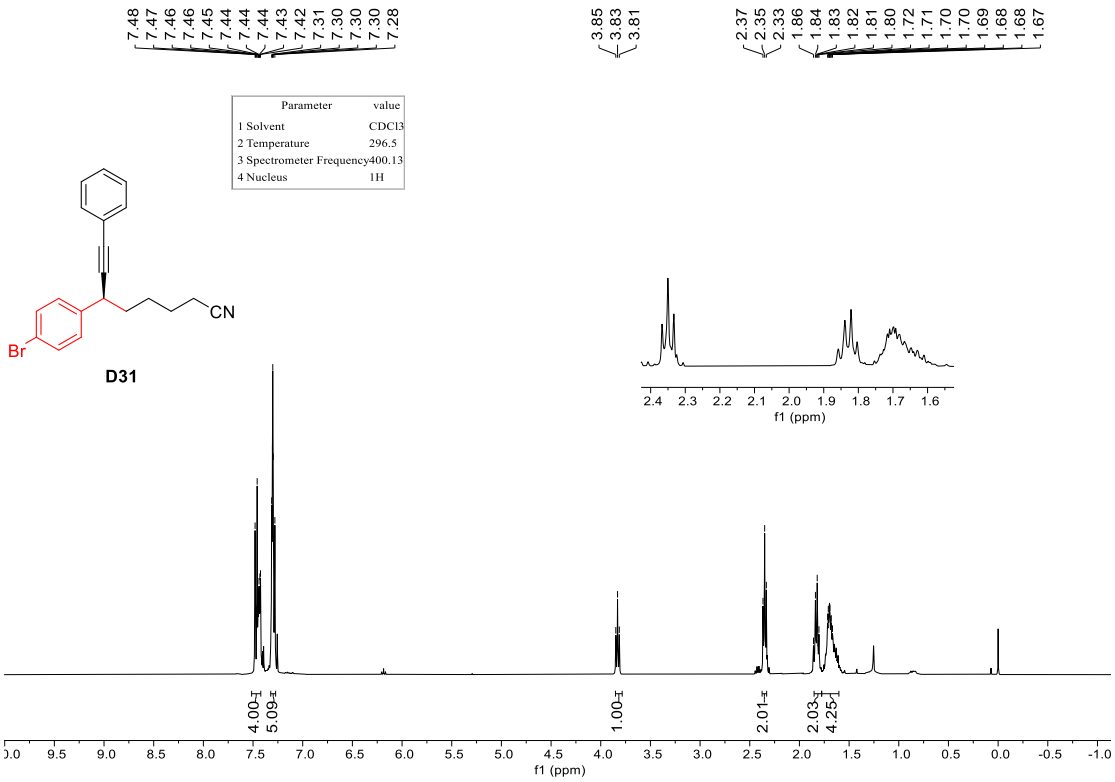

163.16 160.72 137.48 137.44 131.79 129.06 128.98 128.44 128.18 123.45 119.70 115.66 115.44 90.60 84.10 37.90 37.60 26.62 25.30 17.27
Parameter value
1 Solvent CDCl3
2 Temperature 297.2
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
F
D29
130 129 128 127
f1 (ppm)
115.6 115.4 115.2
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

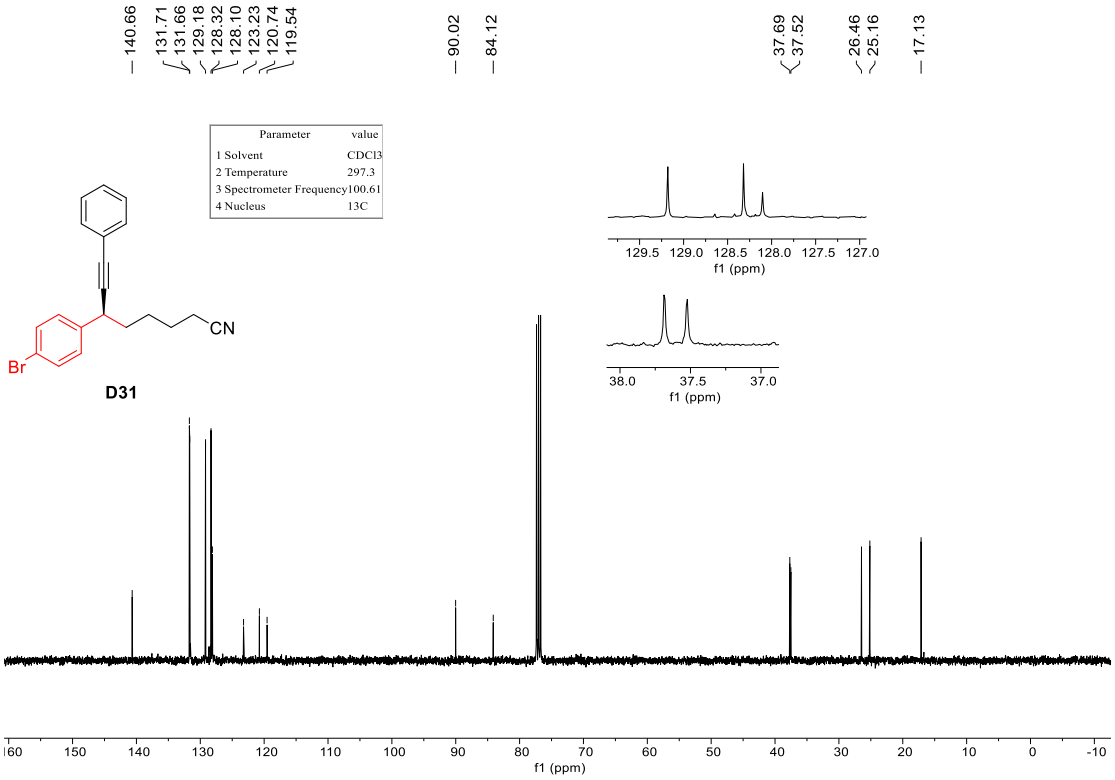
Parameter	value
1 Solvent	CDCl3
2 Temperature	296.8
3 Spectrometer Frequency	376.50
4 Nucleus	19F

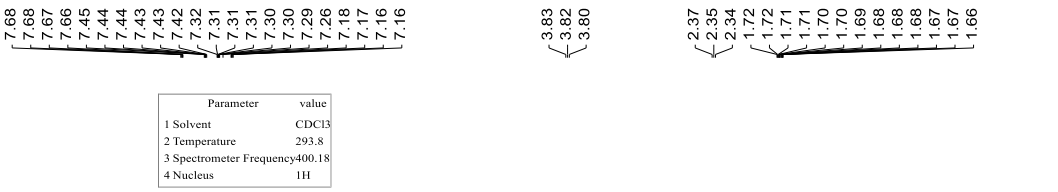


D29

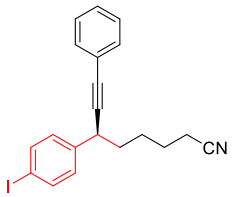

7.45 7.45 7.45 7.44 7.44 7.43 7.37 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.31 7.30 7.30
3.87 3.85 3.83
2.37 2.35 2.34 1.86 1.85 1.84 1.83 1.81 1.73 1.72 1.72 1.71 1.71 1.70 1.70 1.69 1.69 1.68 1.67 1.67
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
Cl
D30
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
2.00 7.04 1.00 2.00 2.10 4.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
140.26 132.83 131.79 128.92 128.89 128.45 128.23 123.38 119.68
90.25 84.24
37.74 37.72 26.60 25.29 17.27
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
Cl
D30
129.0 128.8 128.6 128.4 128.2
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.48 7.47 7.46 7.46 7.45 7.44 7.44 7.44 7.43 7.42 7.31 7.30 7.30 7.30 7.28
3.85 3.83 3.81
2.37 2.35 2.33 1.86 1.84 1.83 1.82 1.81 1.80 1.72 1.71 1.70 1.70 1.69 1.68 1.68 1.67
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
Br
D31
f1 (ppm)
4.00 5.09 1.00 2.01 2.03 4.25

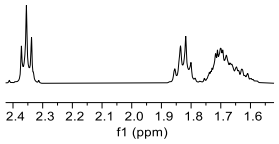

140.66 131.71 131.66 129.18 128.32 128.10 123.23 120.74 119.54
90.02 84.12
37.69 37.52 26.46 25.16 17.13
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
Br
D31
f1 (ppm)

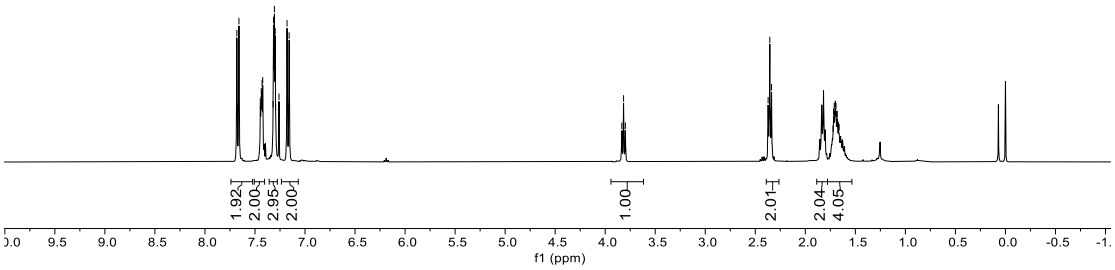


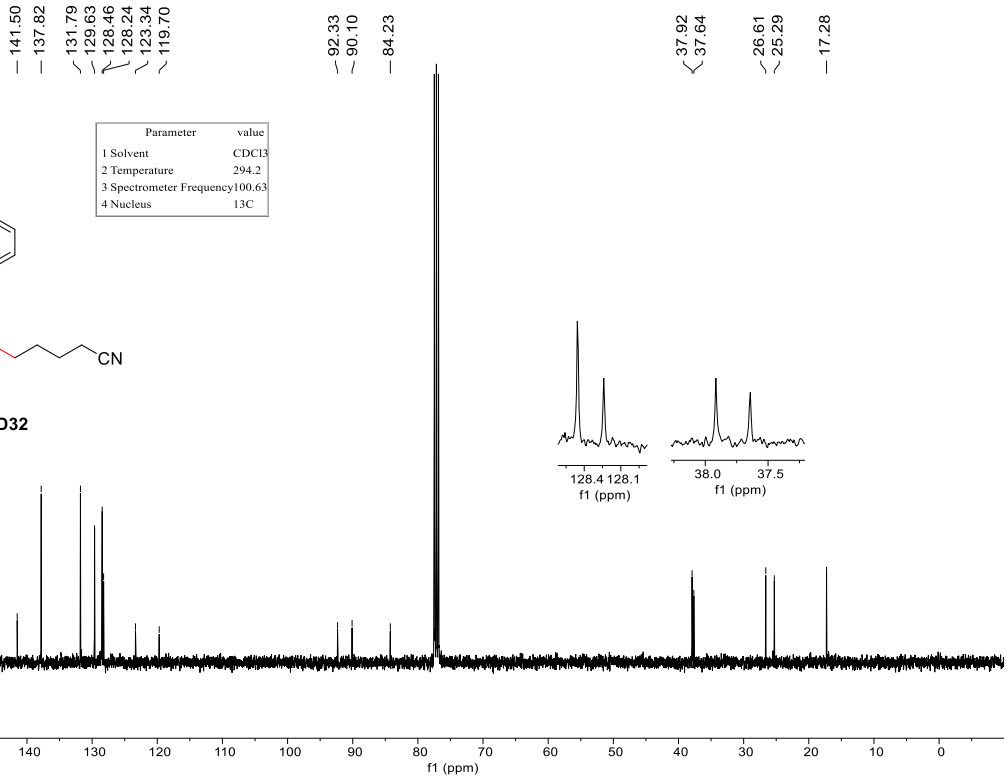
Parameter	value
1 Solvent	CDCl3
2 Temperature	293.8
3 Spectrometer Frequency	400.18
4 Nucleus	1H



D32

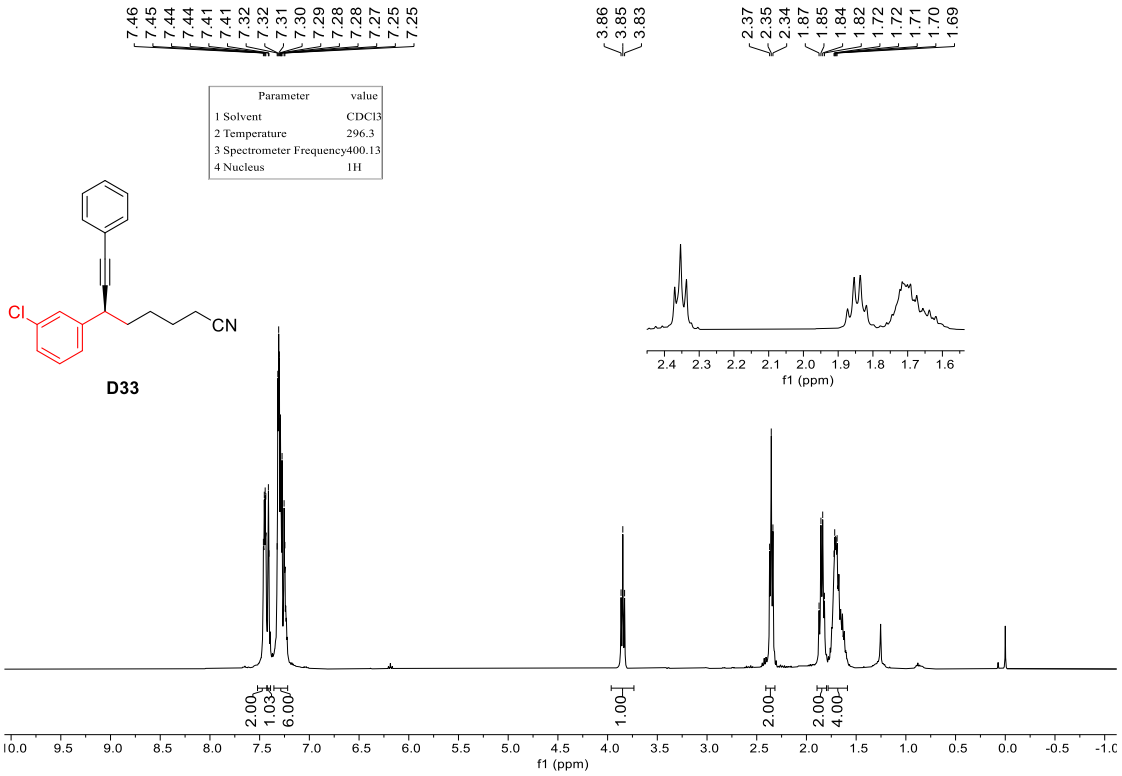


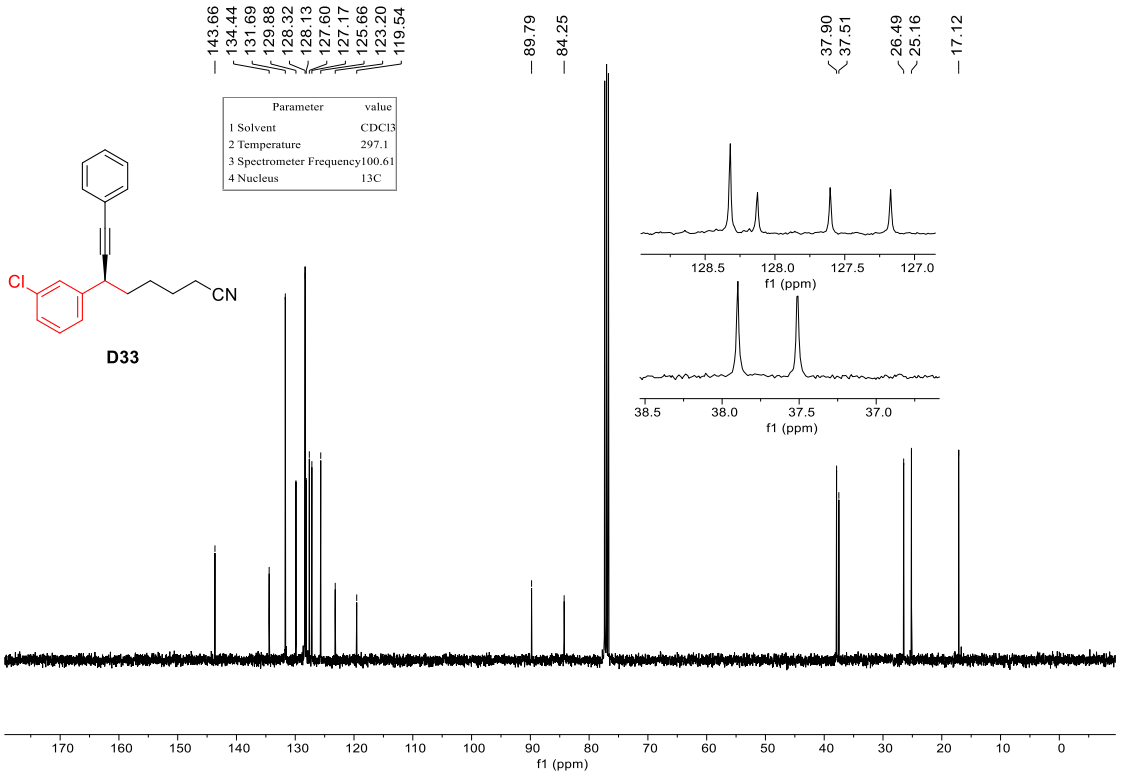


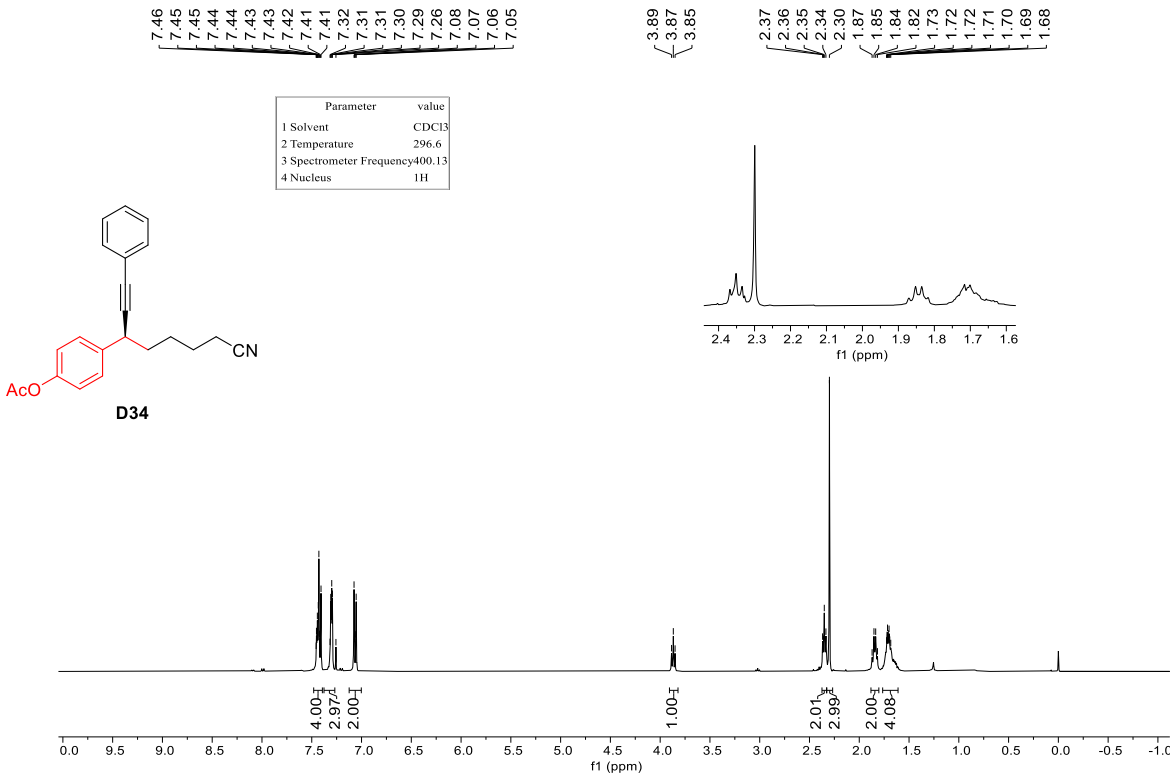


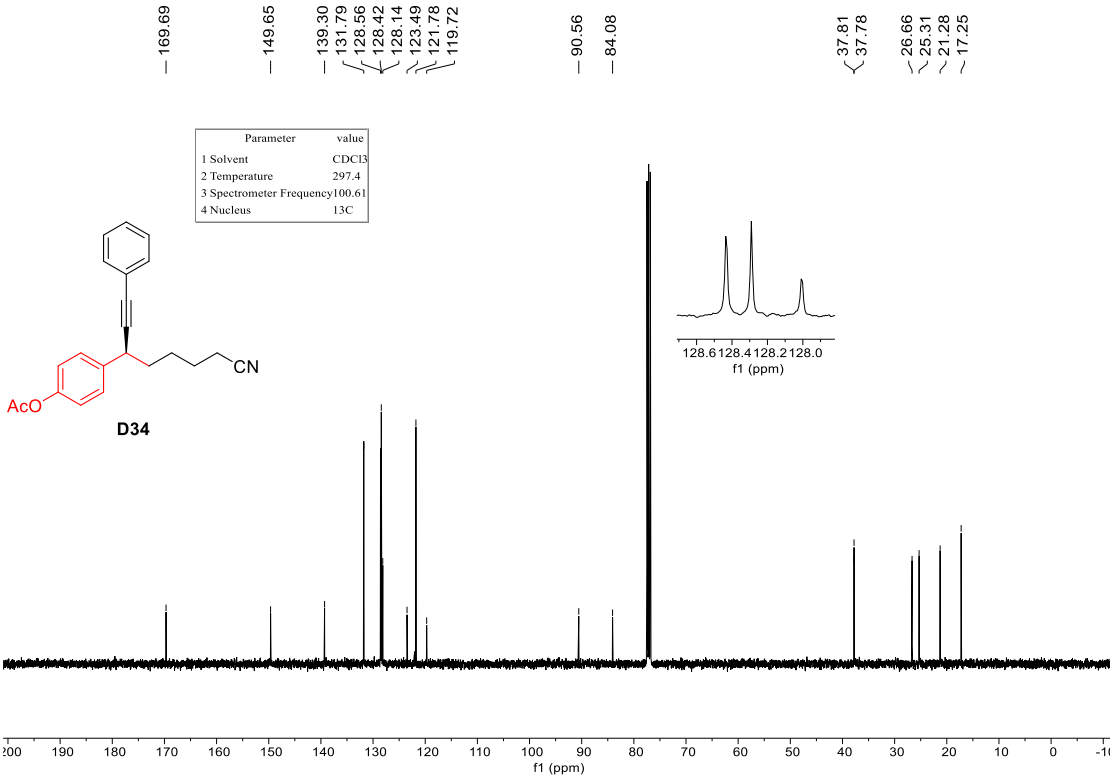
Parameter	value
1 Solvent	CDCl3
2 Temperature	294.2
3 Spectrometer Frequency	100.63
4 Nucleus	13C

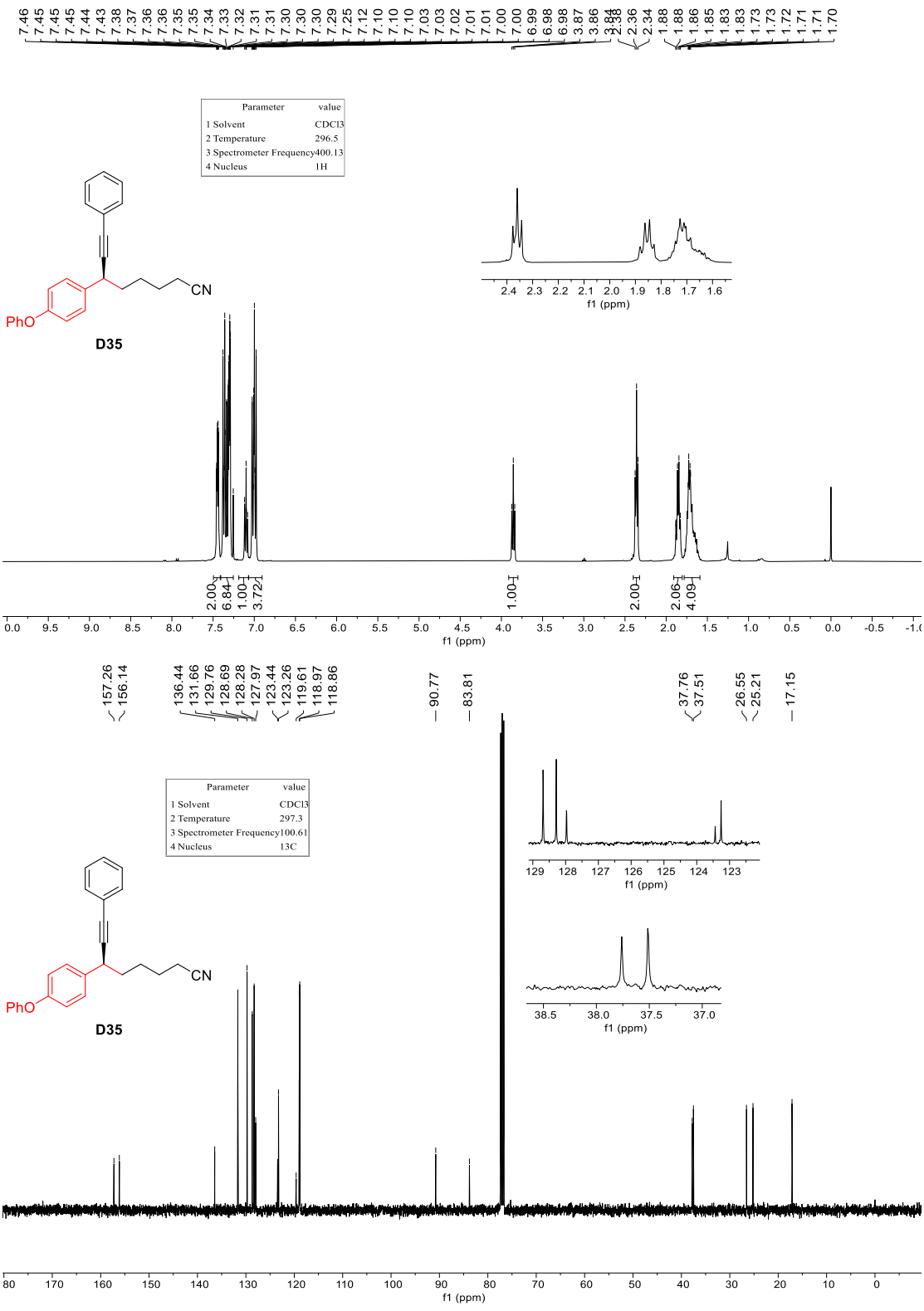
D32

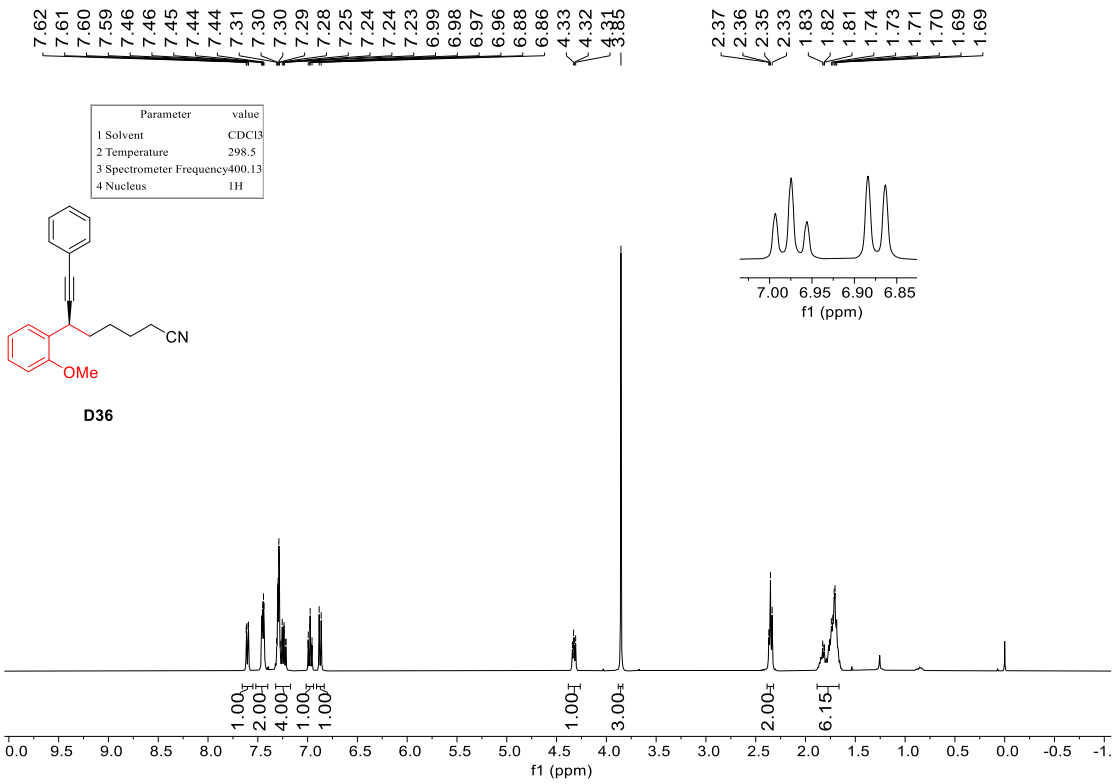

7.46 7.45 7.44 7.44 7.41 7.41 7.32 7.32 7.31 7.30 7.29 7.28 7.28 7.27 7.25 7.25
3.86 3.85 3.83
2.37 2.35 2.34 1.87 1.85 1.84 1.82 1.72 1.72 1.71 1.70 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 296.3
3 Spectrometer Frequency 400.13
4 Nucleus 1H
Cl
CN
D33
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
2.00 1.03 6.00 1.00 2.00 2.00 4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

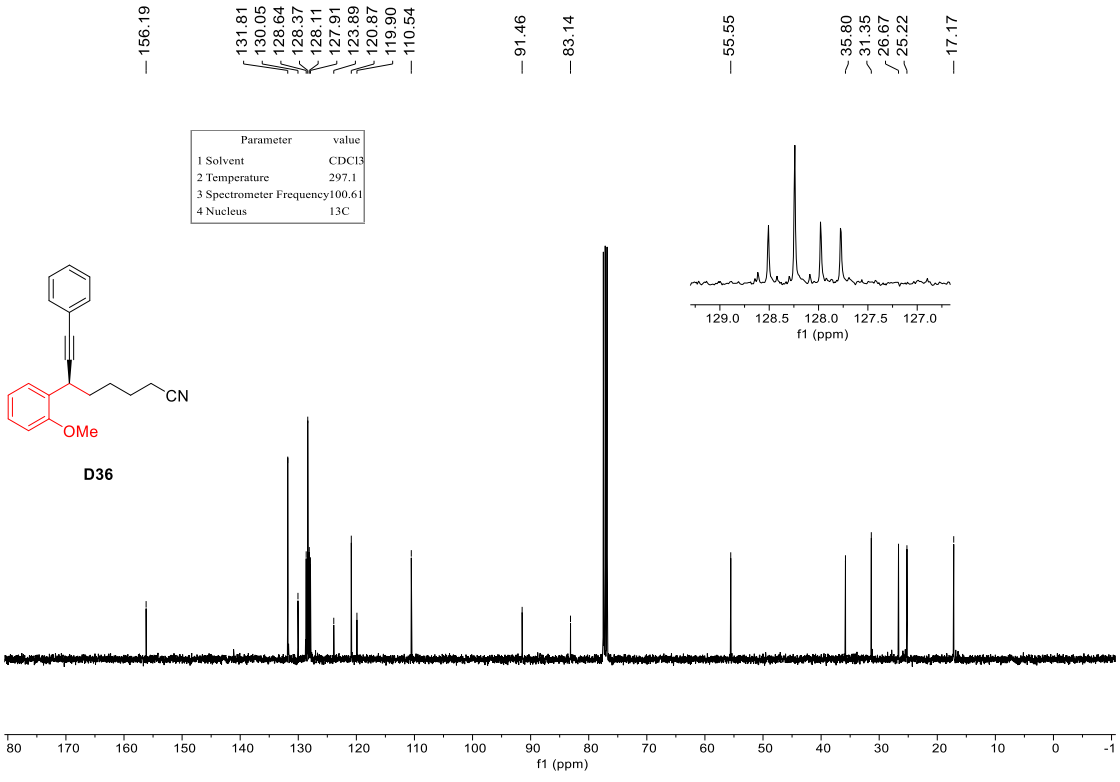

143.66 134.44 131.69 129.88 128.32 128.13 127.60 127.17 125.66 123.20 119.54
89.79 84.25
37.90 37.51 26.49 25.16 17.12
Parameter value
1 Solvent CDCl3
2 Temperature 297.1
3 Spectrometer Frequency 100.61
4 Nucleus 13C
Cl
CN
D33
128.5 128.0 127.5 127.0
f1 (ppm)
38.5 38.0 37.5 37.0
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.46 7.45 7.45 7.44 7.44 7.43 7.43 7.42 7.41 7.41 7.32 7.31 7.31 7.30 7.29 7.26 7.08 7.07 7.06 7.05
3.89 3.87 3.85
2.37 2.36 2.35 2.34 2.30 1.87 1.85 1.84 1.82 1.73 1.72 1.72 1.71 1.70 1.69 1.68
Parameter value
1 Solvent CDCl3
2 Temperature 296.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
AcO
D34
f1 (ppm)
4.00 2.97 2.00 1.00 2.01 2.99 2.00 4.08

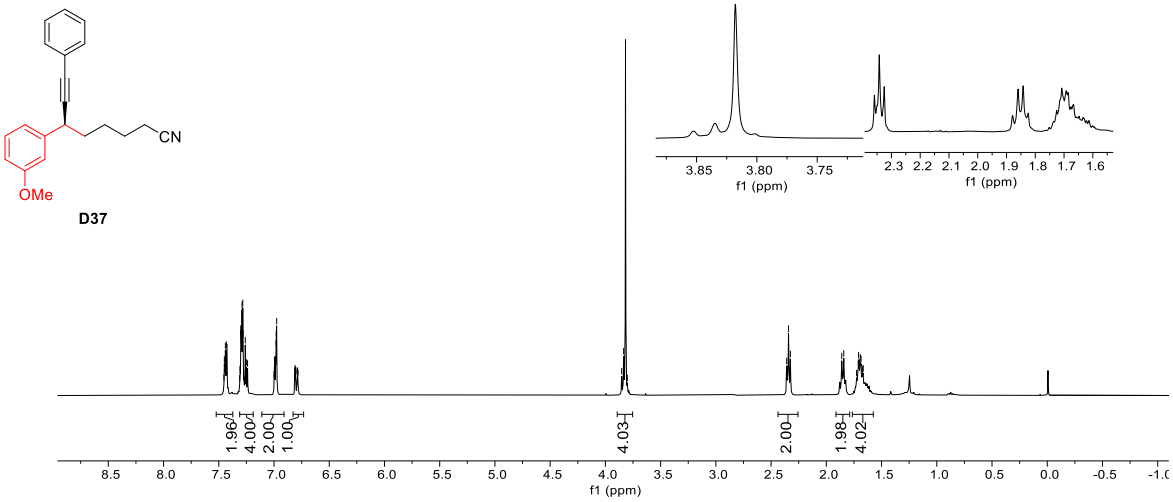

169.69 149.65 139.30 131.79 128.56 128.42 128.14 123.49 121.78 119.72 90.56 84.08 37.81 37.78 26.66 25.31 21.28 17.25
Parameter value
1 Solvent CDCl3
2 Temperature 297.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
AcO
D34
f1 (ppm)

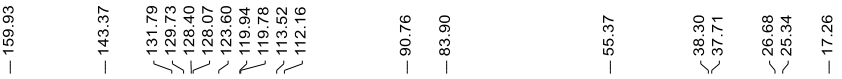

7.46 7.45 7.45 7.45 7.44 7.43 7.38 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.25 7.12 7.10 7.10 7.10 7.03 7.03 7.02 7.01 7.01 7.00 7.00 6.99 6.98 6.98 3.87 3.86 2.38 2.36 2.34 1.88 1.88 1.86 1.85 1.83 1.83 1.73 1.73 1.72 1.71 1.71 1.70
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
PhO
D35
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
2.00 6.84 1.00 3.72 1.00 2.00 2.06 4.09
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
157.26 156.14 136.44 131.66 129.76 128.69 128.28 127.97 123.44 123.26 119.61 118.97 118.86 90.77 83.81 37.76 37.51 26.55 25.21 17.15
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
PhO
D35
129 128 127 126 125 124 123
f1 (ppm)
38.5 38.0 37.5 37.0
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.62 7.61 7.60 7.59 7.46 7.46 7.45 7.44 7.44 7.31 7.30 7.30 7.29 7.28 7.25 7.24 7.24 7.23 6.99 6.98 6.97 6.96 6.88 6.86 4.33 4.32 4.31 3.85
2.37 2.36 2.35 2.33 1.83 1.82 1.81 1.74 1.73 1.71 1.70 1.69 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 298.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
OMe
D36
7.00 6.95 6.90 6.85
f1 (ppm)
1.00 2.00 4.00 1.00 1.00 3.00 2.00 6.15
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

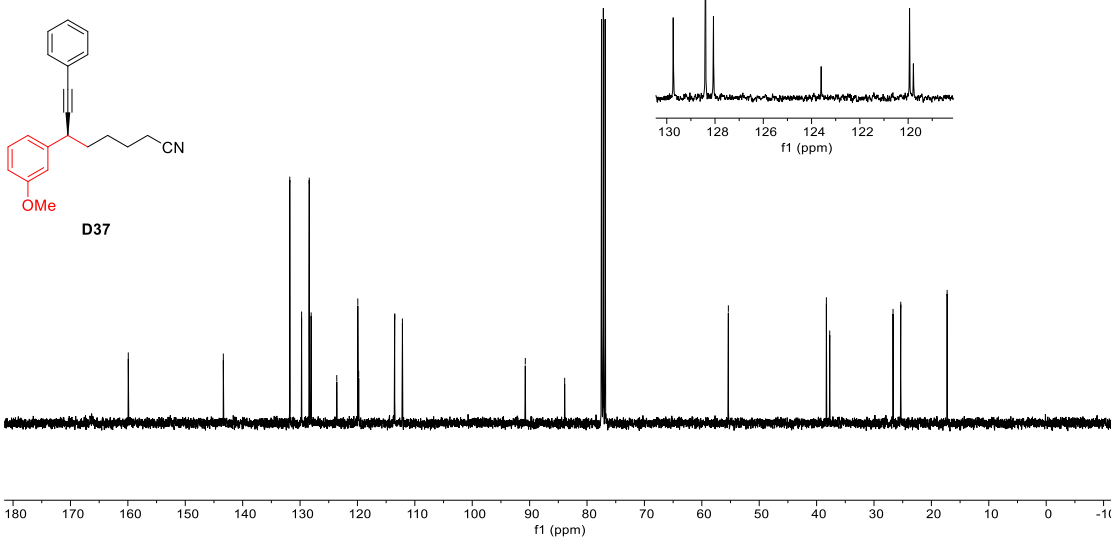

156.19
131.81 130.05 128.64 128.37 128.11 127.91 123.89 120.87 119.90 110.54
91.46
83.14
55.55
35.80 31.35 26.67 25.22
17.17
Parameter value
1 Solvent CDCl3
2 Temperature 297.1
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
OMe
D36
129.0 128.5 128.0 127.5 127.0
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

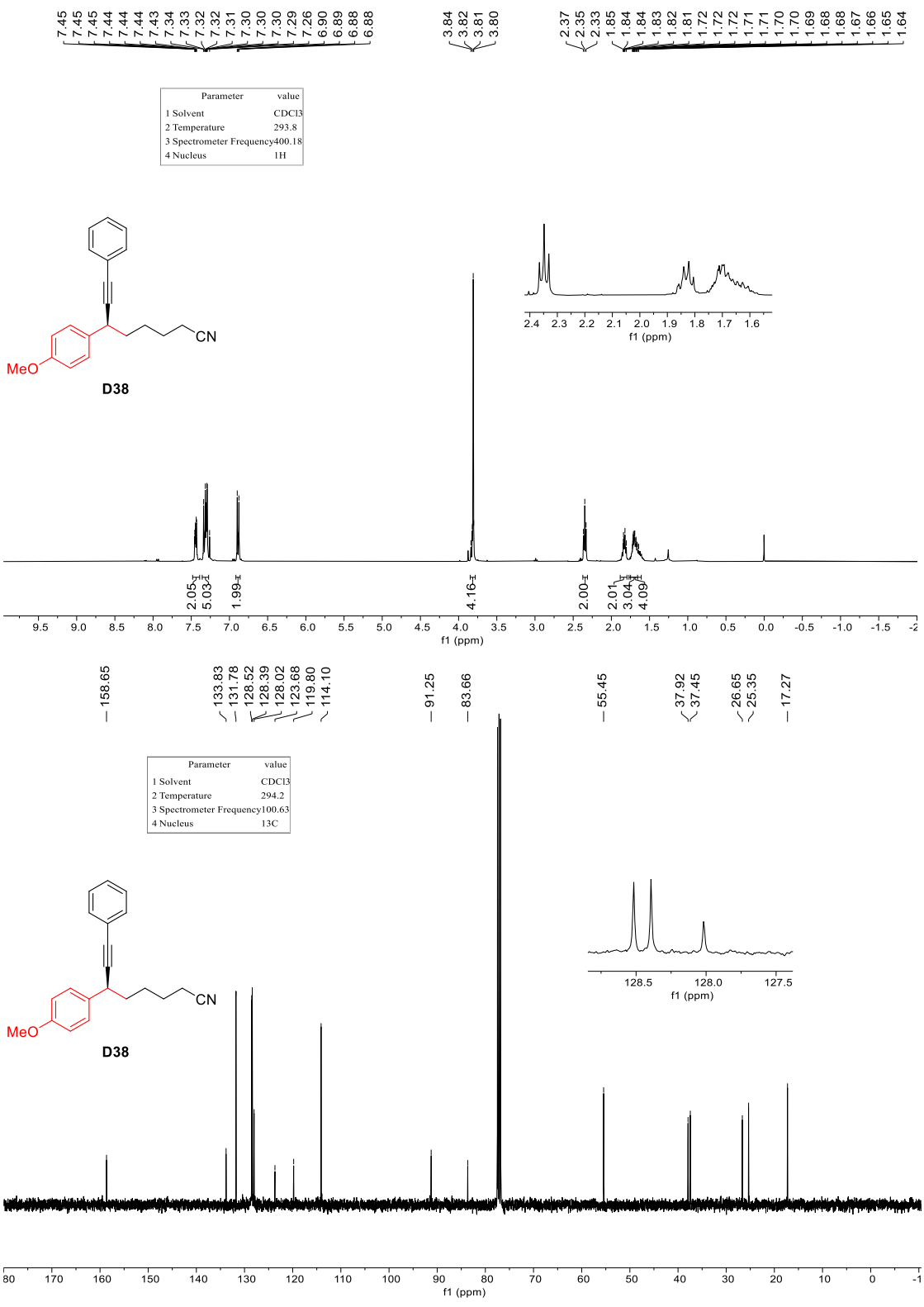
Parameter	value
1 Solvent	CDCl3
2 Temperature	293.8
3 Spectrometer Frequency	400.18
4 Nucleus	1H

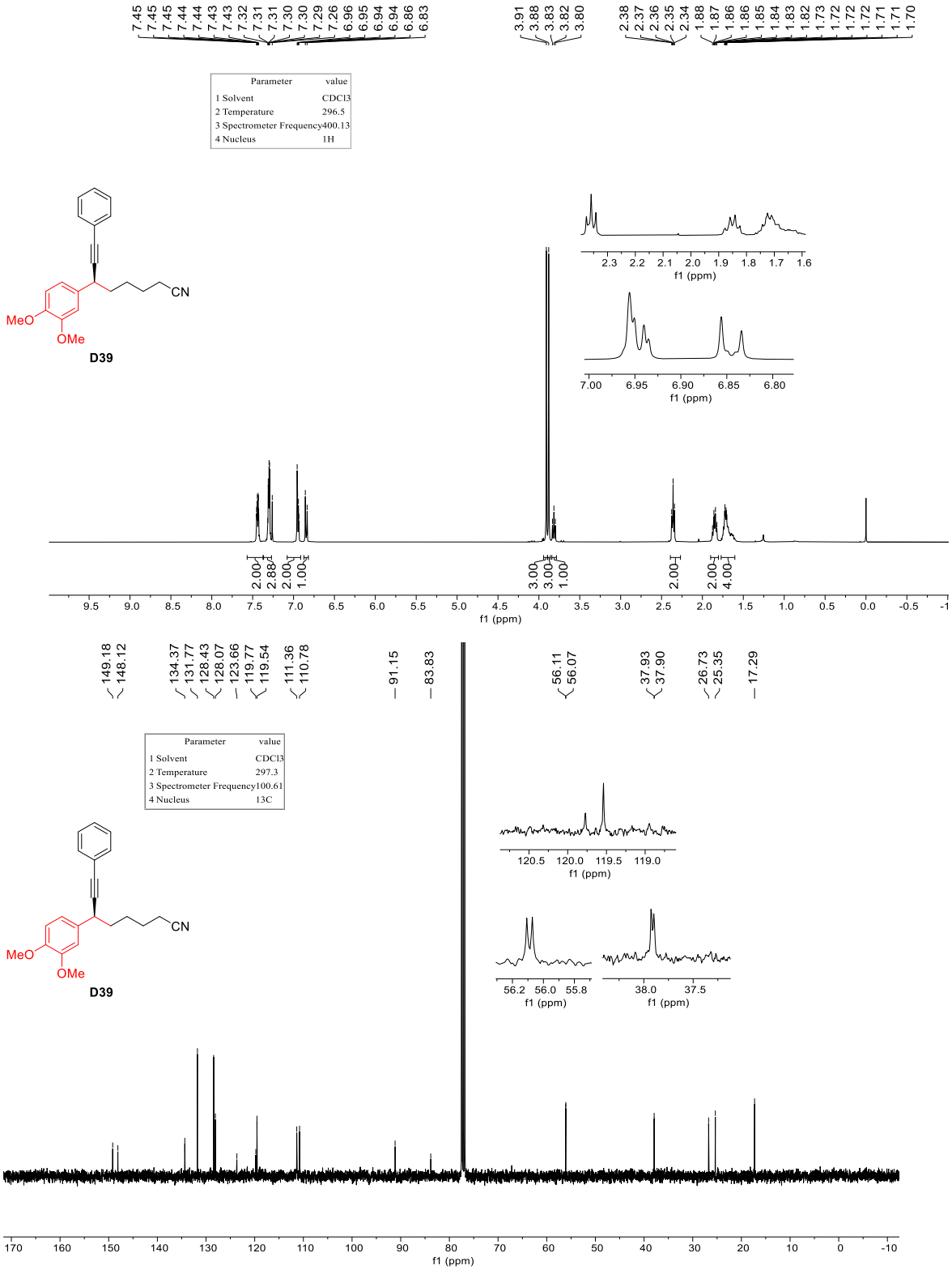


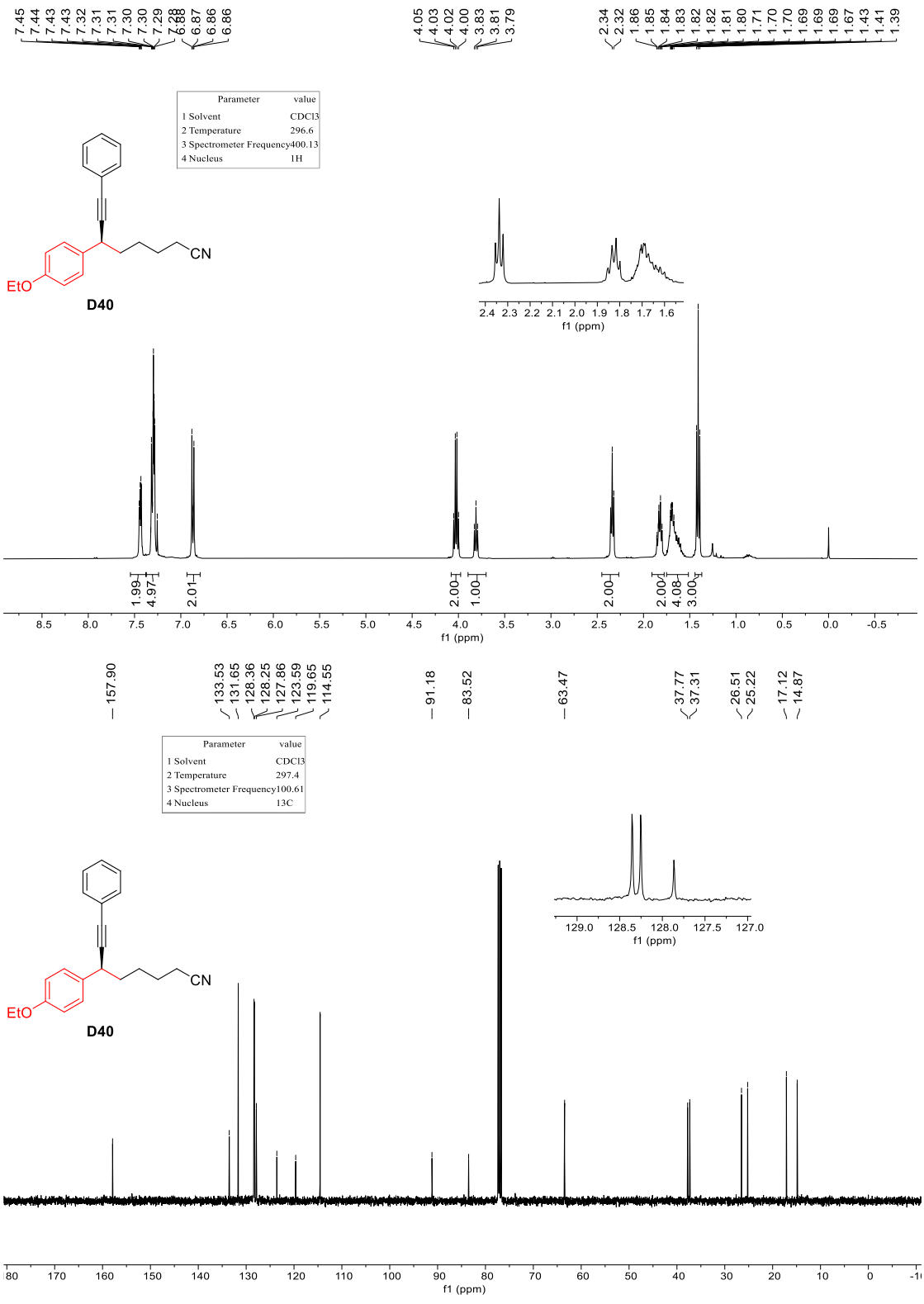


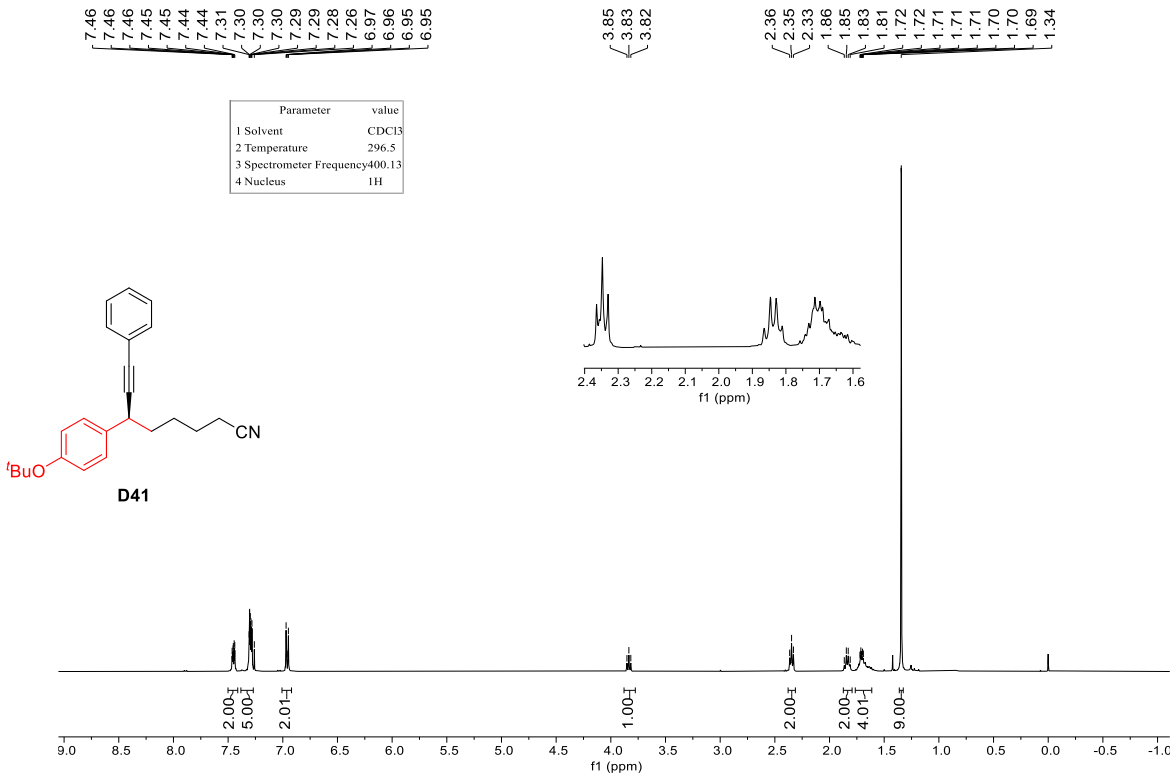
Parameter	value
1 Solvent	CDCl3
2 Temperature	294.2
3 Spectrometer Frequency	100.63
4 Nucleus	13C

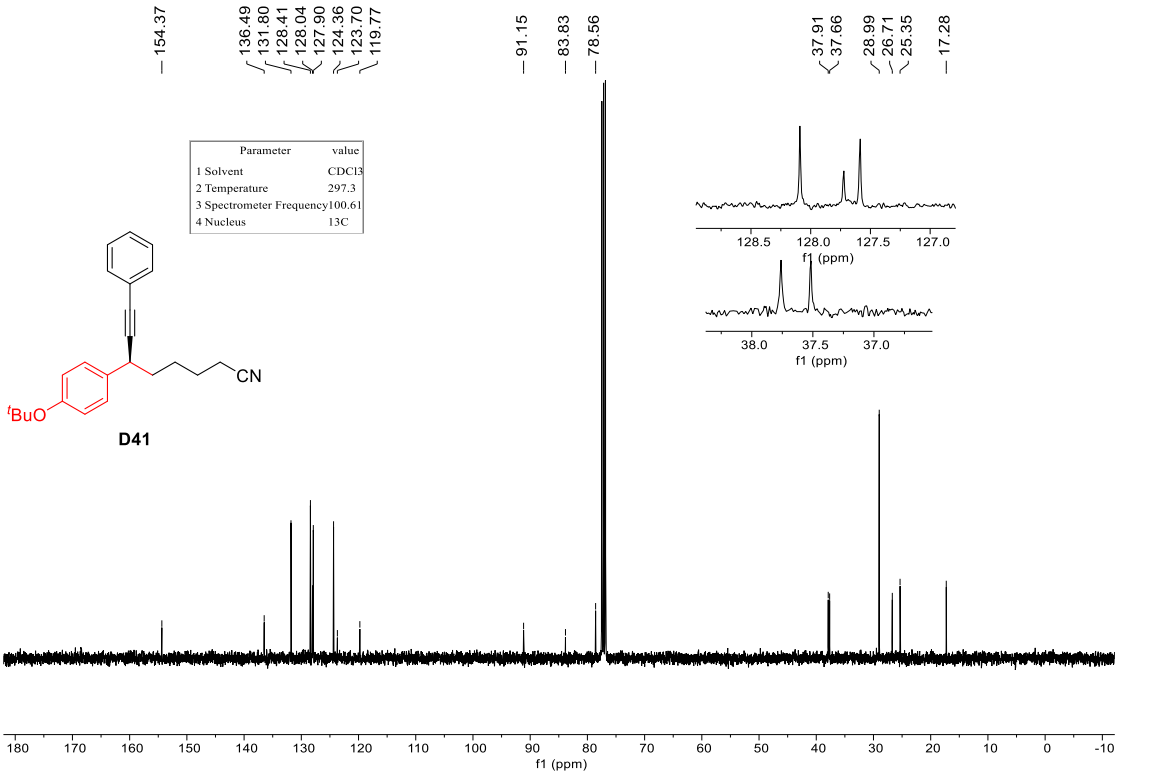


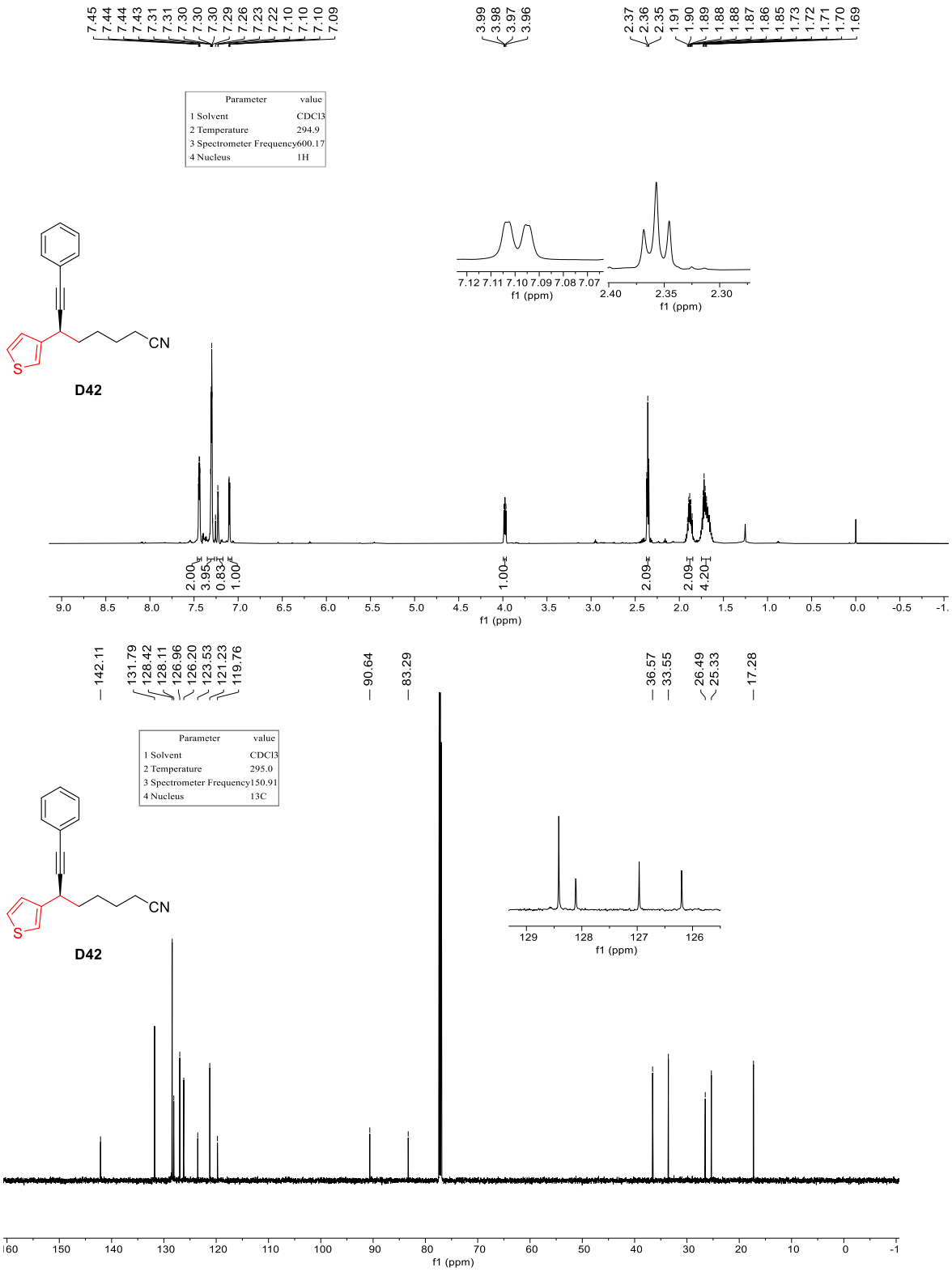

7.45 7.45 7.45 7.44 7.44 7.44 7.43 7.34 7.33 7.32 7.32 7.31 7.30 7.30 7.30 7.29 7.26 6.90 6.89 6.88 6.88
3.84 3.82 3.81 3.80
2.37 2.35 2.33 1.85 1.84 1.84 1.83 1.82 1.81 1.72 1.72 1.71 1.71 1.70 1.70 1.69 1.68 1.68 1.67 1.66 1.65 1.64
Parameter value
1 Solvent CDCl3
2 Temperature 293.8
3 Spectrometer Frequency 400.18
4 Nucleus 1H
CN
MeO
D38
f1 (ppm)
2.05 5.03 1.99 4.16 2.00 2.01 3.04 4.09
158.65 133.83 131.78 128.52 128.39 128.02 123.68 119.80 114.10 91.25 83.66 55.45 37.92 37.45 26.65 25.35 17.27
Parameter value
1 Solvent CDCl3
2 Temperature 294.2
3 Spectrometer Frequency 100.63
4 Nucleus 13C
CN
MeO
D38
f1 (ppm)

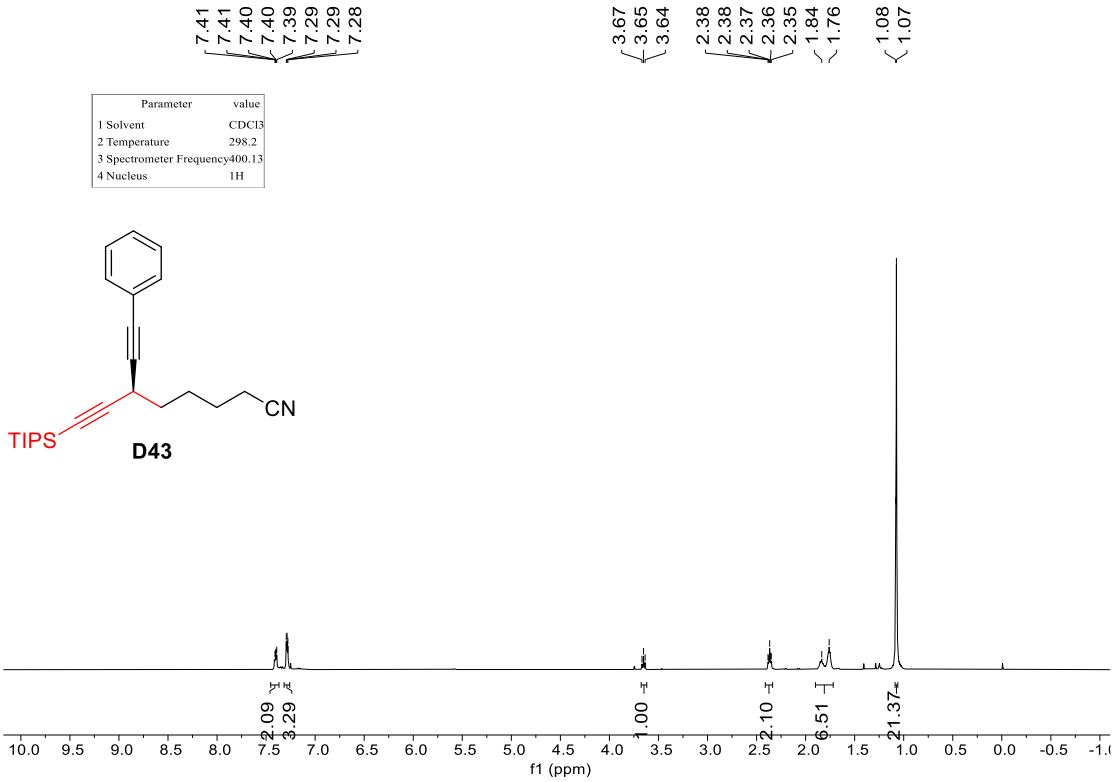

7.45 7.45 7.45 7.44 7.44 7.43 7.43 7.32 7.31 7.31 7.30 7.30 7.29 7.26 6.96 6.95 6.94 6.94 6.86 6.83
3.91 3.88 3.83 3.82 3.80
2.38 2.37 2.36 2.35 2.34 1.88 1.87 1.86 1.86 1.85 1.84 1.83 1.82 1.73 1.72 1.72 1.72 1.71 1.71 1.70
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
MeO
OMe
D39
f1 (ppm)
2.00 2.88 2.00 1.00 3.00 3.00 1.00 2.00 2.00 4.00
149.18 148.12 134.37 131.77 128.43 128.07 123.66 119.77 119.54 111.36 110.78 91.15 83.83 56.11 56.07 37.93 37.90 26.73 25.35 17.29
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
MeO
OMe
D39
f1 (ppm)

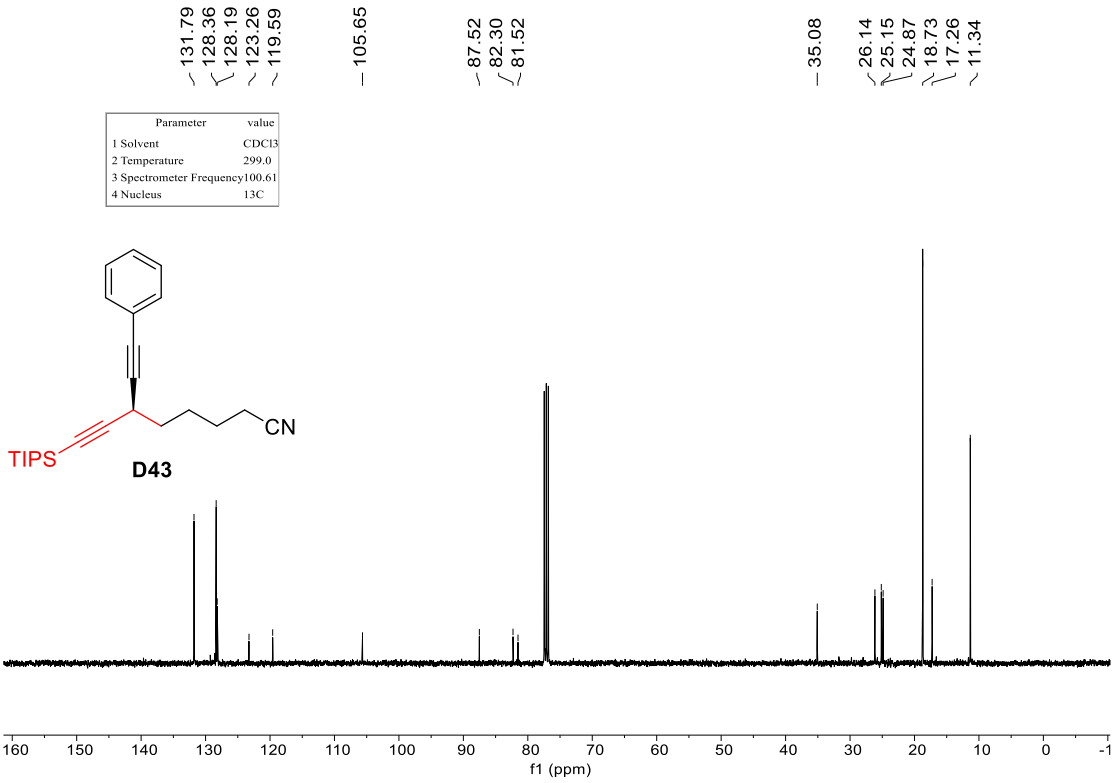

7.45 7.44 7.43 7.43 7.32 7.31 7.31 7.30 7.30 7.29 7.28 6.88 6.87 6.86 6.86
4.05 4.03 4.02 4.00 3.83 3.81 3.79
2.34 2.32 1.86 1.85 1.84 1.83 1.82 1.82 1.81 1.80 1.71 1.70 1.70 1.69 1.69 1.69 1.67 1.43 1.41 1.39
Parameter value
1 Solvent CDCl3
2 Temperature 296.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
EtO
D40
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (ppm)
1.99 4.97 2.01 2.00 1.00 2.00 2.00 4.08 3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
157.90
133.53 131.65 128.36 128.25 127.86 123.59 119.65 114.55
91.18
83.52
63.47
37.77 37.31
26.51 25.22
17.12 14.87
Parameter value
1 Solvent CDCl3
2 Temperature 297.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
EtO
D40
129.0 128.5 128.0 127.5 127.0
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

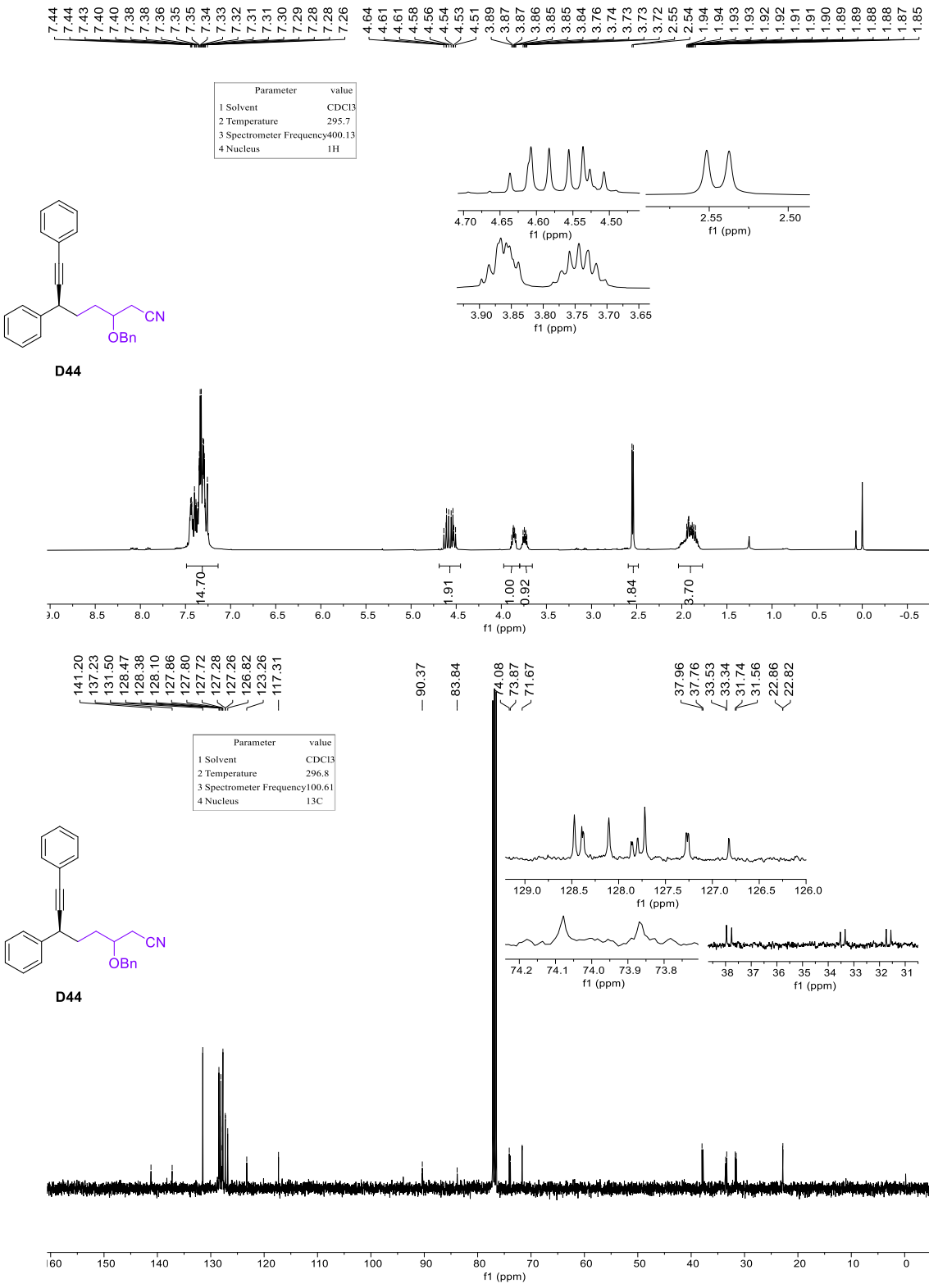

7.46 7.46 7.46 7.45 7.45 7.44 7.44 7.31 7.30 7.30 7.30 7.29 7.29 7.28 7.26 6.97 6.96 6.95 6.95
3.85 3.83 3.82
2.36 2.35 2.33 1.86 1.85 1.83 1.81 1.72 1.72 1.71 1.71 1.71 1.70 1.70 1.69 1.34
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
tBuO
D41
f1 (ppm)
2.00 5.00 2.01 1.00 2.00 2.00 4.01 9.00

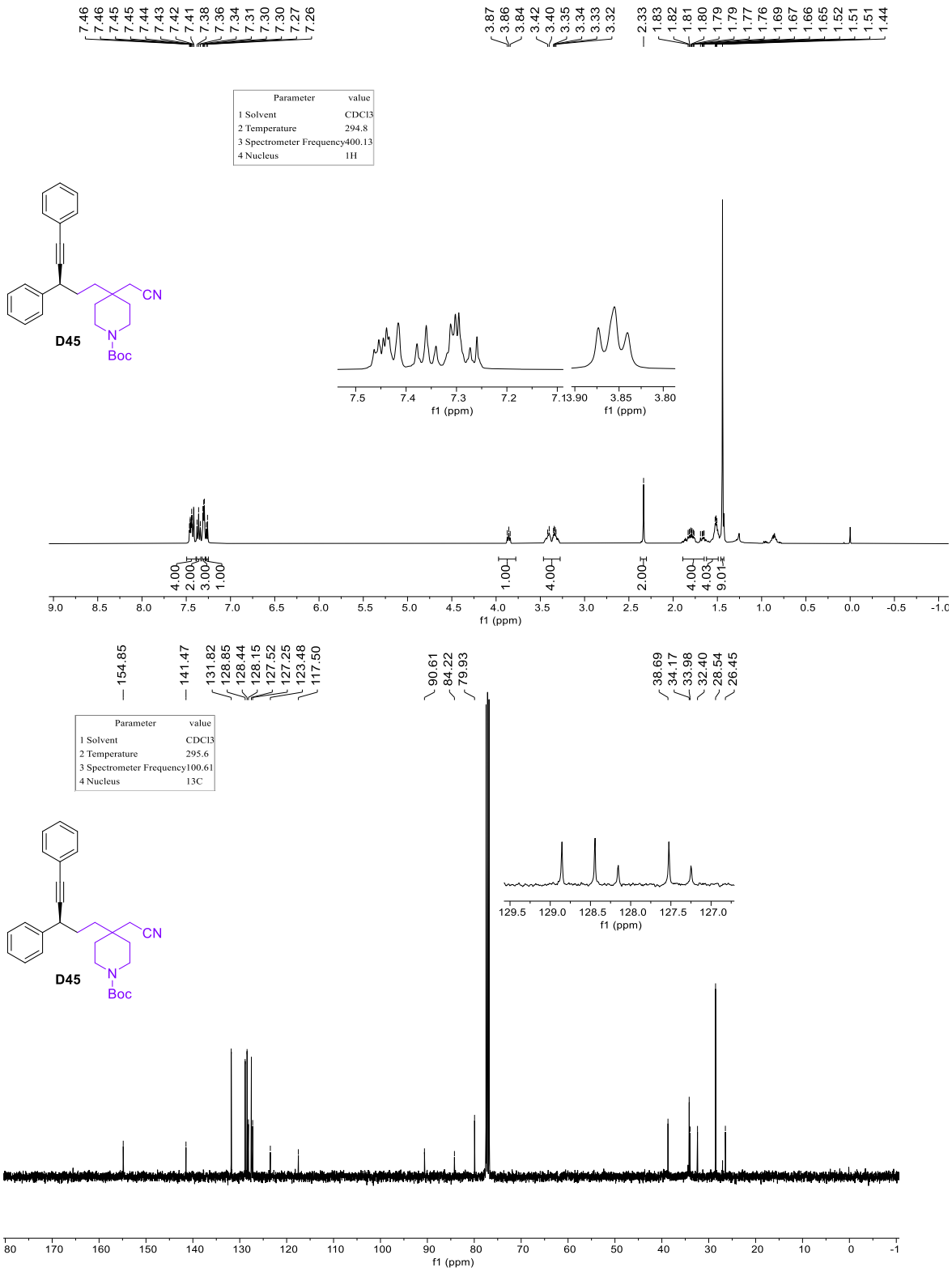

154.37
136.49 131.80 128.41 128.04 127.90 124.36 123.70 119.77
91.15 83.83 78.56
37.91 37.66 28.99 26.71 25.35 17.28
Parameter value
1 Solvent CDCl3
2 Temperature 297.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
tBuO
D41
f1 (ppm)

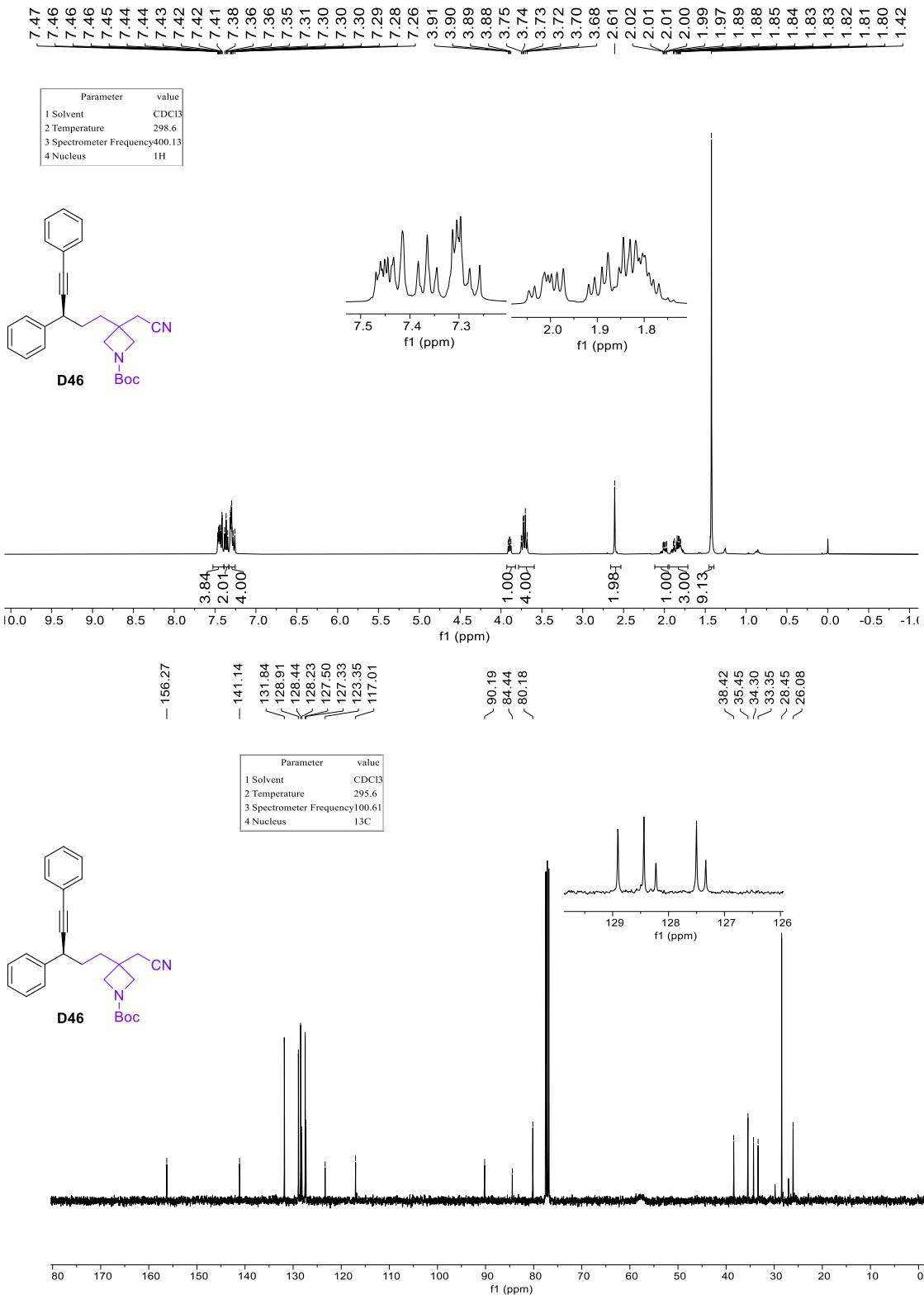

7.45 7.44 7.44 7.43 7.31 7.31 7.30 7.30 7.30 7.29 7.26 7.23 7.22 7.10 7.10 7.10 7.09
3.99 3.98 3.97 3.96
2.37 2.36 2.35 1.91 1.90 1.89 1.88 1.88 1.87 1.86 1.85 1.73 1.72 1.71 1.70 1.69
Parameter value
1 Solvent CDCl3
2 Temperature 294.9
3 Spectrometer Frequency 600.17
4 Nucleus 1H
CN
S
D42
7.12 7.11 7.10 7.09 7.08 7.07
f1 (ppm)
2.40 2.35 2.30
f1 (ppm)
2.00 3.95 0.83 1.00 1.00 2.09 2.09 4.20
f1 (ppm)
142.11 131.79 128.42 128.11 126.96 126.20 123.53 121.23 119.76
90.64 83.29
36.57 33.55 26.49 25.33 17.28
Parameter value
1 Solvent CDCl3
2 Temperature 295.0
3 Spectrometer Frequency 150.91
4 Nucleus 13C
CN
S
D42
129 128 127 126
f1 (ppm)
f1 (ppm)

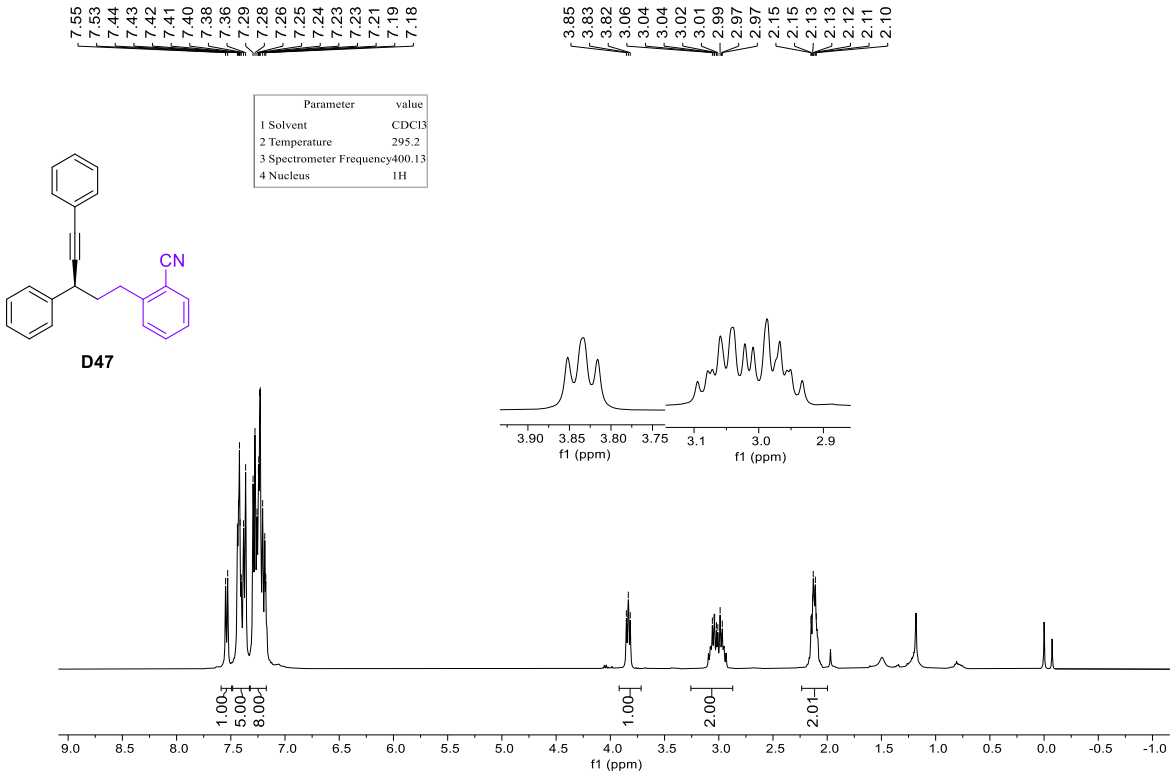

7.41
7.41
7.40
7.40
7.39
7.29
7.29
7.28
3.67
3.65
3.64
2.38
2.38
2.37
2.36
2.35
1.84
1.76
1.08
1.07
Parameter value
1 Solvent CDCl3
2 Temperature 298.2
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
TIPS
D43
2.09
3.29
1.00
2.10
6.51
21.37
f1 (ppm)

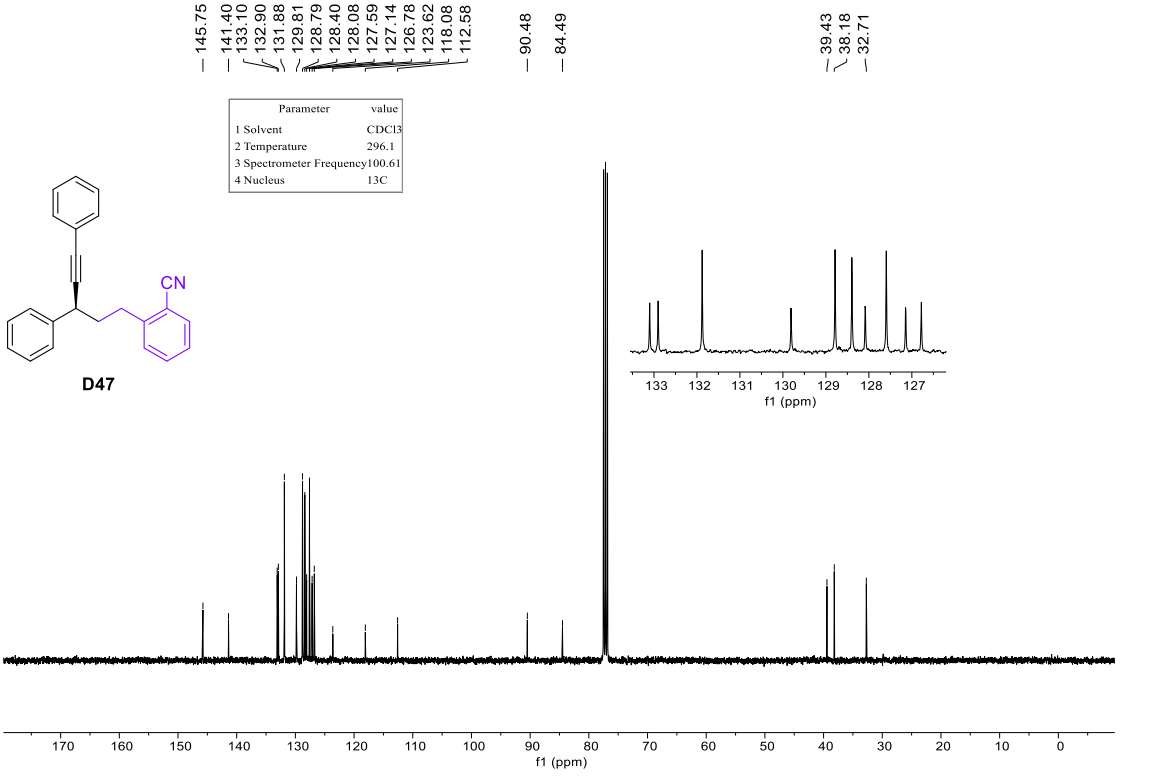

131.79
128.36
128.19
123.26
119.59
105.65
87.52
82.30
81.52
35.08
26.14
25.15
24.87
18.73
17.26
11.34
Parameter value
1 Solvent CDCl3
2 Temperature 299.0
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
TIPS
D43
f1 (ppm)

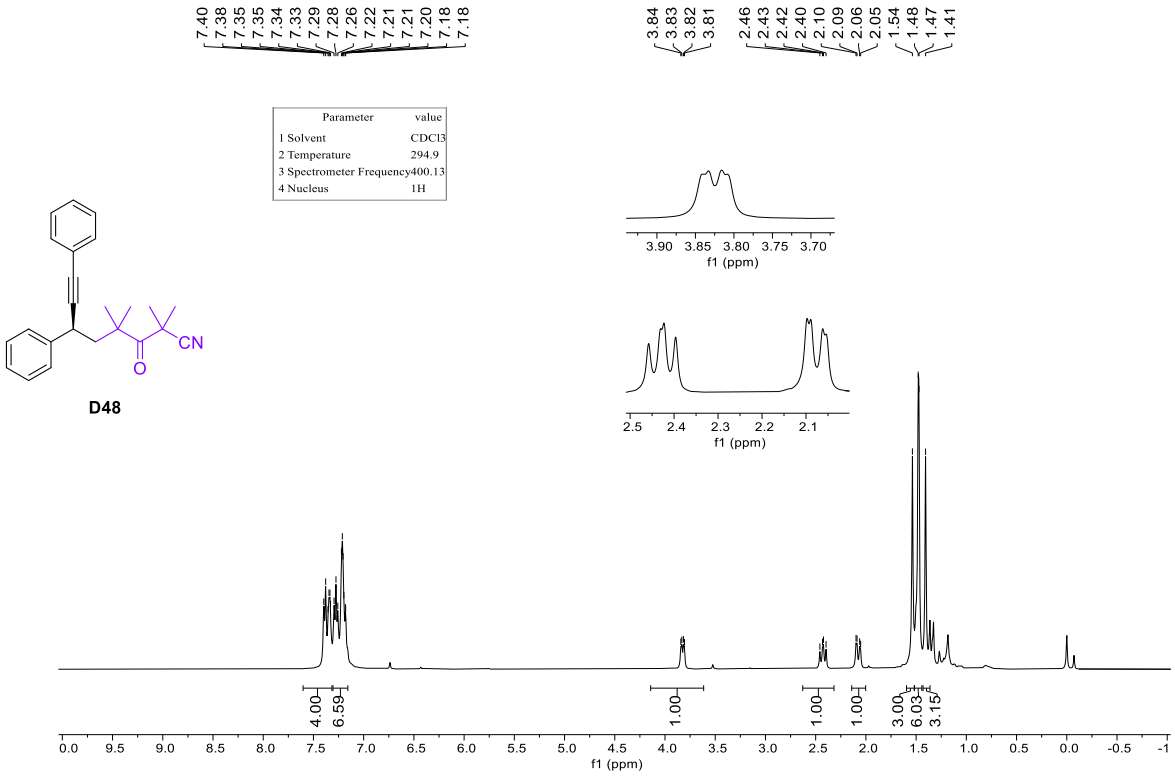

7.44 7.44 7.43 7.40 7.40 7.38 7.38 7.36 7.35 7.35 7.34 7.33 7.32 7.31 7.31 7.30 7.29 7.28 7.28 7.26
4.64 4.61 4.61 4.58 4.56 4.54 4.53 4.51
3.89 3.87 3.87 3.86 3.85 3.85 3.84 3.76 3.74 3.73 3.73 3.72
2.55 2.54 1.94 1.94 1.93 1.93 1.92 1.92 1.91 1.91 1.90 1.89 1.89 1.88 1.88 1.87 1.85
Parameter value
1 Solvent CDCl3
2 Temperature 295.7
3 Spectrometer Frequency 400.13
4 Nucleus 1H
4.70 4.65 4.60 4.55 4.50
f1 (ppm)
2.55 2.50
f1 (ppm)
3.90 3.85 3.80 3.75 3.70 3.65
f1 (ppm)
CN
OBn
D44
14.70
1.91
1.00
0.92
1.84
3.70
f1 (ppm)
141.20 137.23 131.50 128.47 128.38 128.10 127.86 127.80 127.72 127.28 127.26 126.82 123.26 117.31
90.37 83.84 74.08 73.87 71.67
37.96 37.76 33.53 33.34 31.74 31.56 22.86 22.82
Parameter value
1 Solvent CDCl3
2 Temperature 296.8
3 Spectrometer Frequency 100.61
4 Nucleus 13C
129.0 128.5 128.0 127.5 127.0 126.5 126.0
f1 (ppm)
74.2 74.1 74.0 73.9 73.8
f1 (ppm)
38 37 36 35 34 33 32 31
f1 (ppm)
CN
OBn
D44
f1 (ppm)

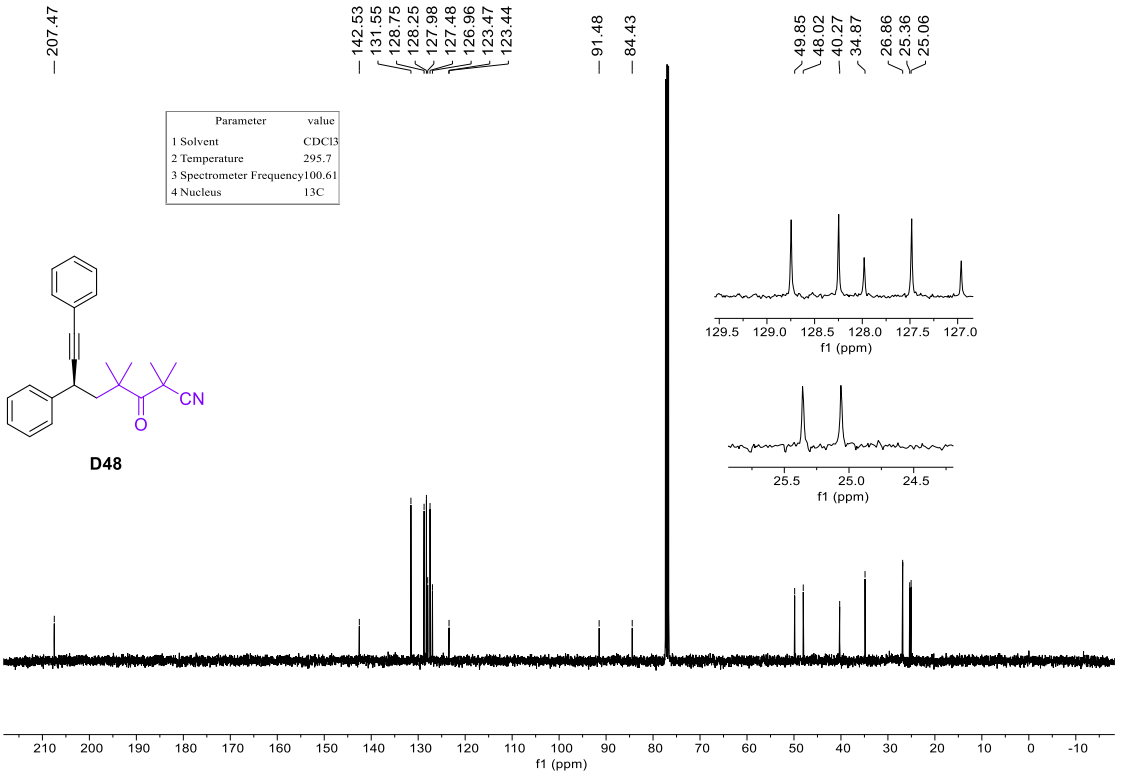

7.46 7.46 7.45 7.45 7.44 7.43 7.42 7.41 7.38 7.36 7.34 7.31 7.30 7.30 7.27 7.26
3.87 3.86 3.84 3.42 3.40 3.35 3.34 3.33 3.32
2.33 1.83 1.82 1.81 1.80 1.79 1.79 1.77 1.76 1.69 1.67 1.66 1.65 1.52 1.51 1.51 1.44
Parameter value
1 Solvent CDCl3
2 Temperature 294.8
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
N
Boc
D45
f1 (ppm)
4.00 2.00 3.00 1.00 1.00 4.00 2.00 4.00 4.03 9.01
154.85 141.47 131.82 128.85 128.44 128.15 127.52 127.25 123.48 117.50
90.61 84.22 79.93
38.69 34.17 33.98 32.40 28.54 26.45
Parameter value
1 Solvent CDCl3
2 Temperature 295.6
3 Spectrometer Frequency 100.61
4 Nucleus 13C

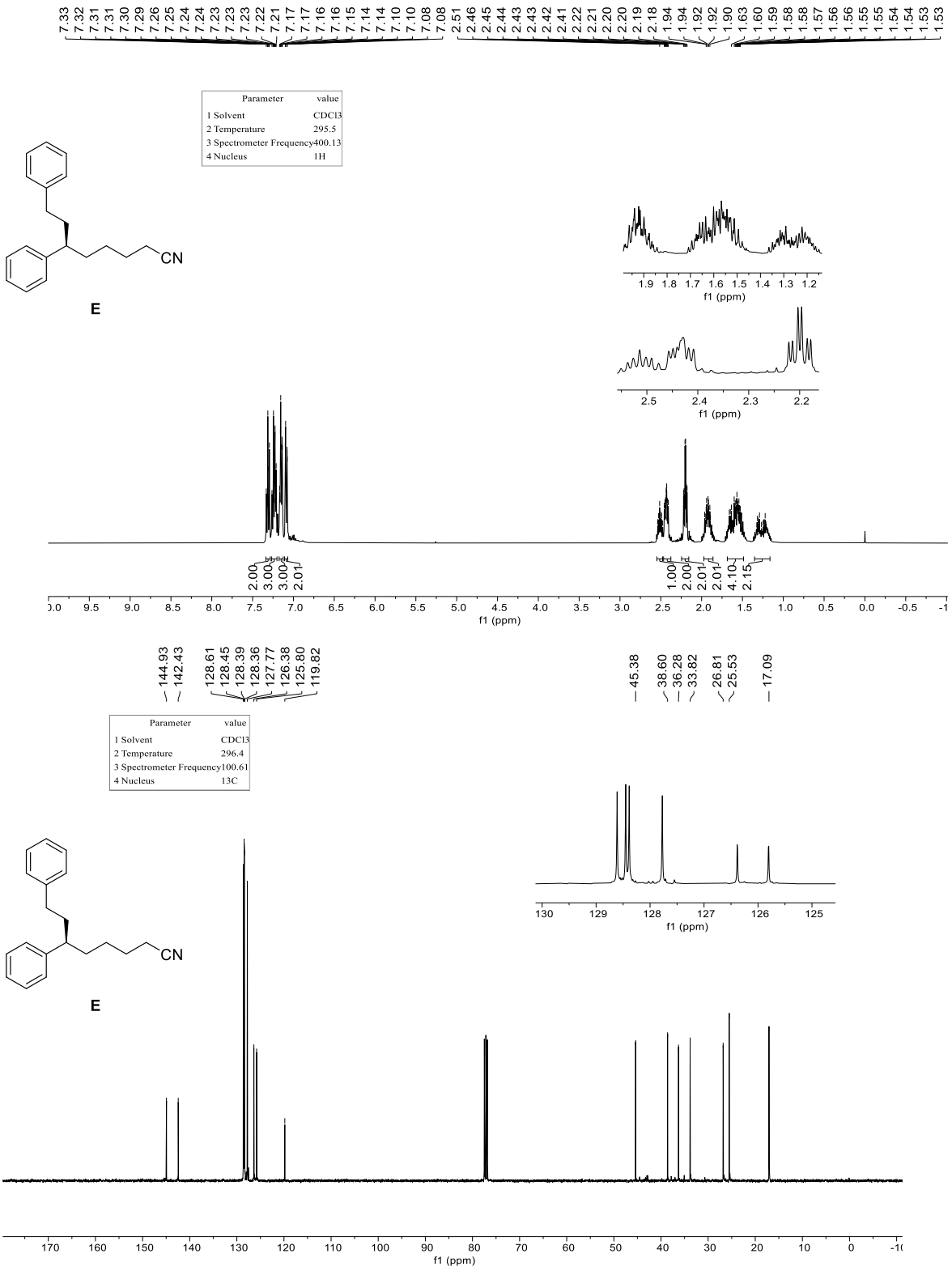

7.47 7.46 7.46 7.46 7.45 7.44 7.44 7.43 7.42 7.42 7.41 7.38 7.36 7.36 7.35 7.31 7.30 7.30 7.30 7.29 7.28 7.26
3.91 3.90 3.89 3.88 3.75 3.74 3.73 3.72 3.70 3.68
2.61
2.02 2.01 2.01 2.00 1.99 1.97 1.89 1.88 1.85 1.84 1.83 1.83 1.82 1.81 1.80 1.42
Parameter value
1 Solvent CDCl3
2 Temperature 298.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
N
Boc
D46
7.5 7.4 7.3
f1 (ppm)
2.0 1.9 1.8
f1 (ppm)
3.84 2.01 4.00 1.00 4.00 1.98 1.00 3.00 9.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
156.27 141.14 131.84 128.91 128.44 128.23 127.50 127.33 123.35 117.01
90.19 84.44 80.18
38.42 35.45 34.30 33.35 28.45 26.08
Parameter value
1 Solvent CDCl3
2 Temperature 295.6
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
N
Boc
D46
129 128 127 126
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

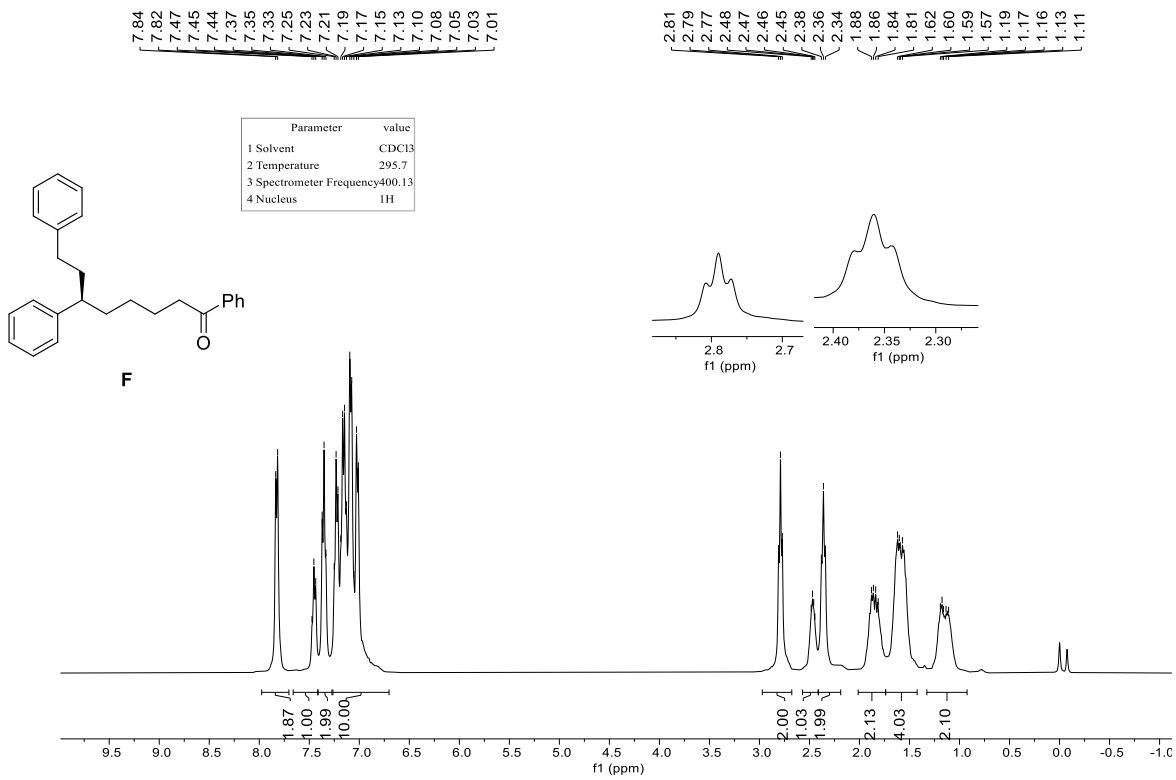

7.55 7.53 7.44 7.43 7.42 7.41 7.40 7.38 7.36 7.29 7.28 7.26 7.25 7.24 7.23 7.23 7.21 7.19 7.18
3.85 3.83 3.82 3.06 3.04 3.04 3.02 3.01 2.99 2.97 2.97 2.15 2.15 2.13 2.13 2.12 2.11 2.10
Parameter value
1 Solvent CDCl3
2 Temperature 295.2
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
D47
f1 (ppm)
1.00 5.00 8.00 1.00 2.00 2.01

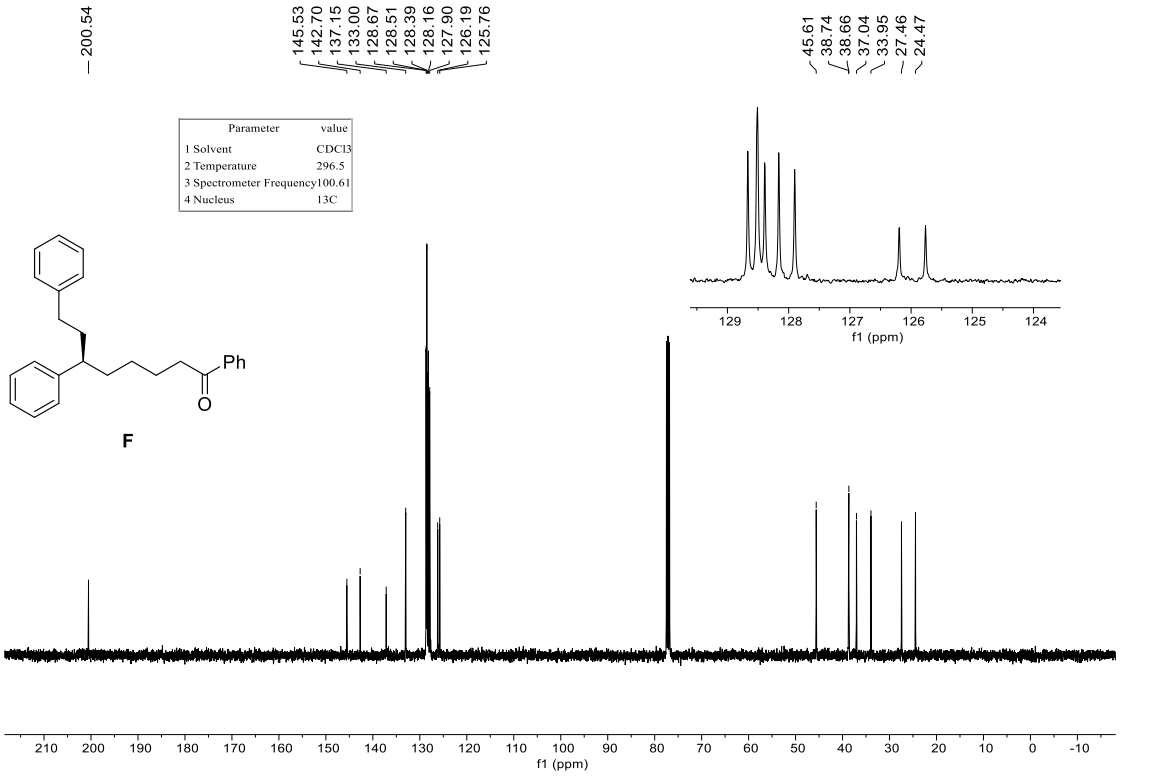

145.75 141.40 133.10 132.90 131.88 129.81 128.79 128.40 128.08 127.59 127.14 126.78 123.62 118.08 112.58
90.48 84.49
39.43 38.18 32.71
Parameter value
1 Solvent CDCl3
2 Temperature 296.1
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
D47
f1 (ppm)

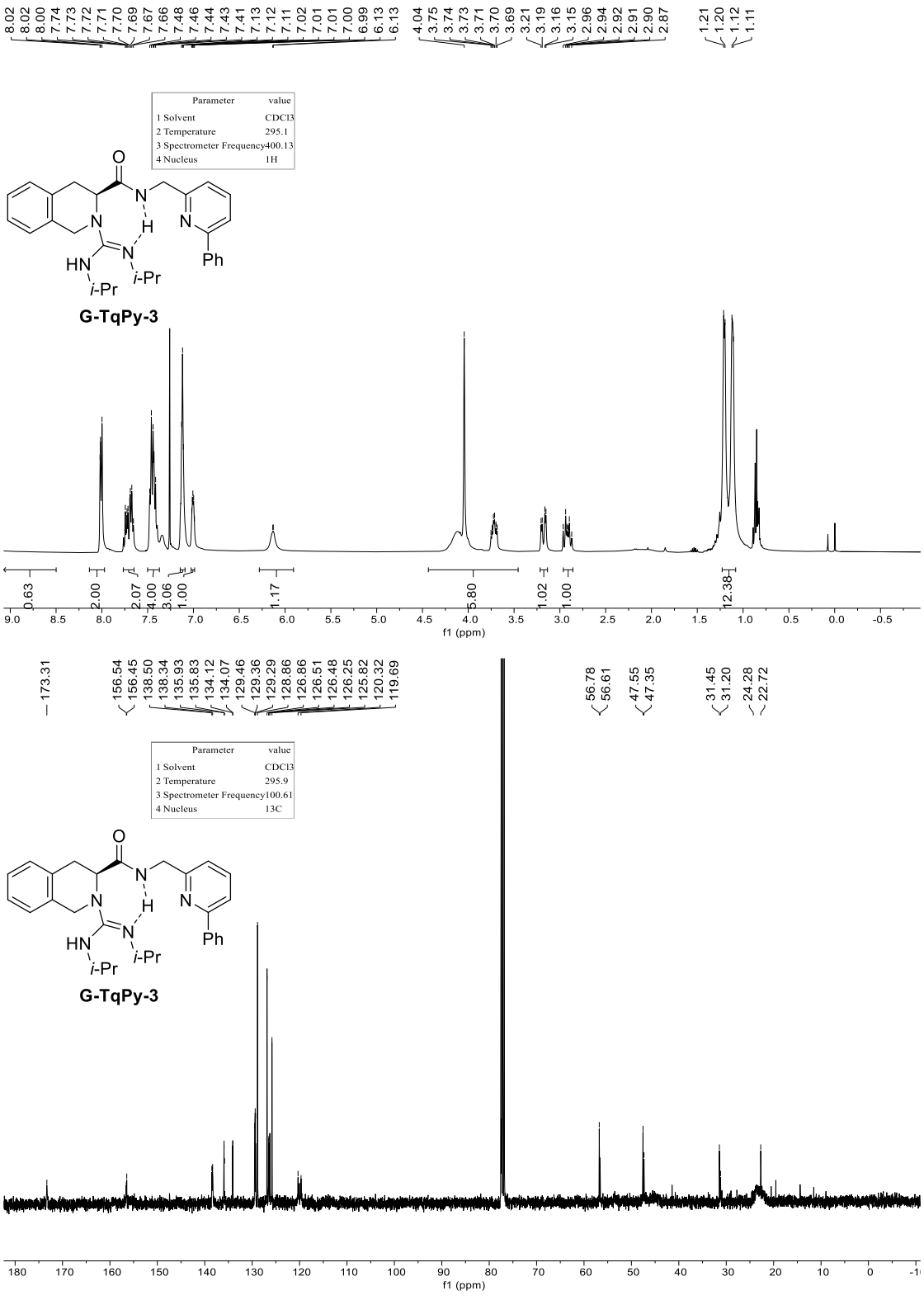

7.40
7.38
7.35
7.35
7.34
7.33
7.29
7.28
7.26
7.22
7.21
7.21
7.20
7.18
7.18
3.84
3.83
3.82
3.81
2.46
2.43
2.42
2.40
2.10
2.09
2.06
2.05
1.54
1.48
1.47
1.41
Parameter value
1 Solvent CDCl3
2 Temperature 294.9
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
O
D48
3.90 3.85 3.80 3.75 3.70
f1 (ppm)
2.5 2.4 2.3 2.2 2.1
f1 (ppm)
4.00
6.59
1.00
1.00
1.00
3.00
6.03
3.15
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

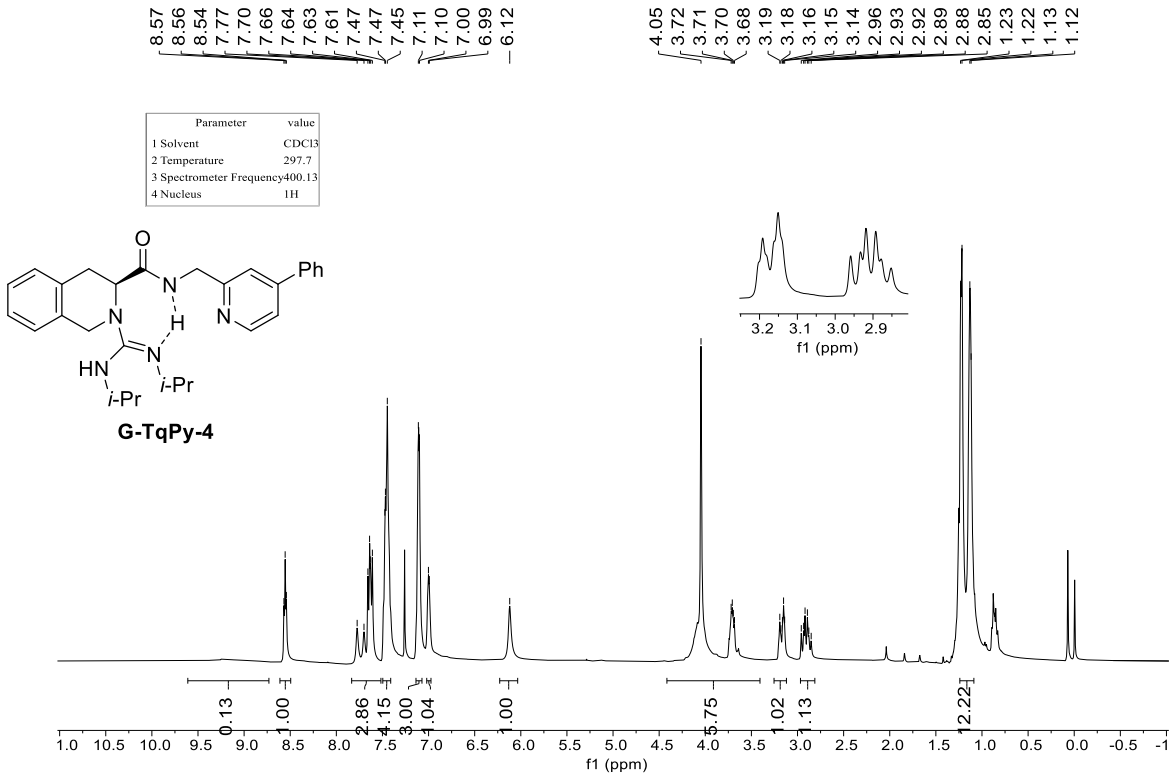

207.47
142.53
131.55
128.75
128.25
127.98
127.48
126.96
123.47
123.44
91.48
84.43
49.85
48.02
40.27
34.87
26.86
25.36
25.06
Parameter value
1 Solvent CDCl3
2 Temperature 295.7
3 Spectrometer Frequency 100.61
4 Nucleus 13C
CN
O
D48
129.5 129.0 128.5 128.0 127.5 127.0
f1 (ppm)
25.5 25.0 24.5
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

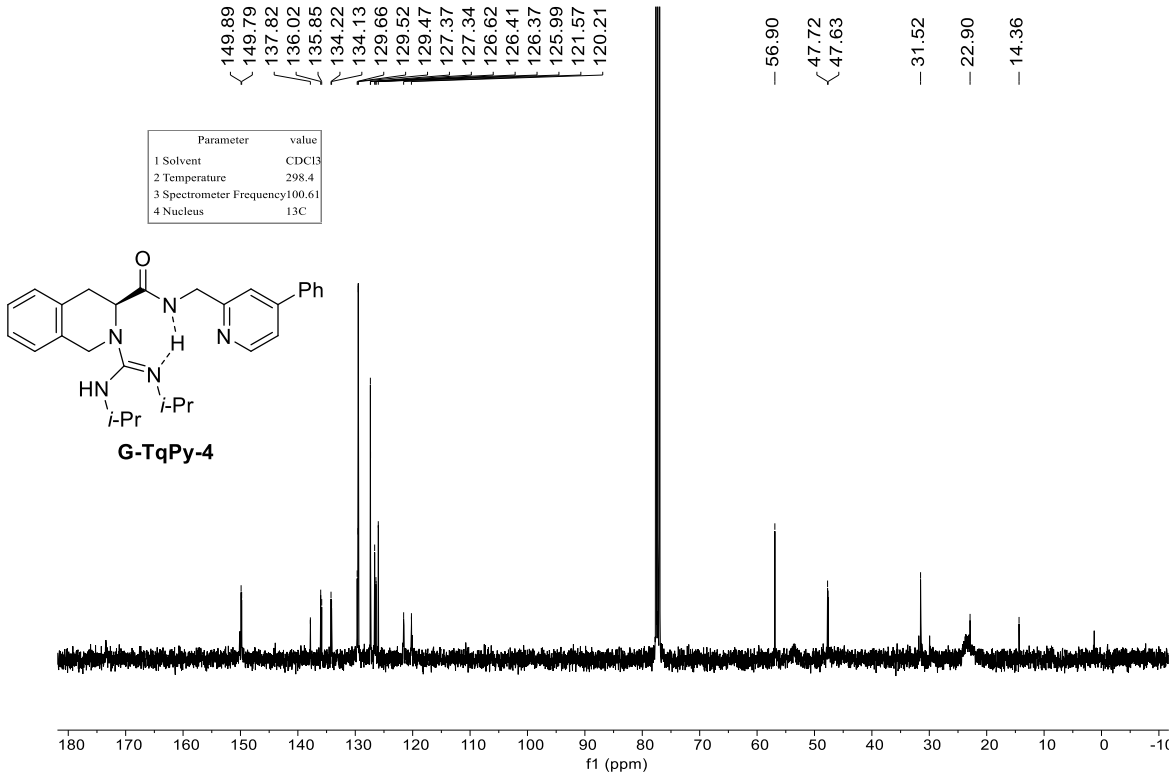

7.33 7.32 7.31 7.31 7.30 7.29 7.26 7.25 7.24 7.24 7.23 7.23 7.22 7.21 7.17 7.17 7.16 7.16 7.15 7.14 7.14 7.10 7.10 7.08 7.08
2.51 2.46 2.45 2.44 2.43 2.43 2.42 2.41 2.22 2.21 2.20 2.20 2.19 2.18 1.94 1.94 1.92 1.92 1.90 1.63 1.60 1.59 1.58 1.58 1.57 1.56 1.56 1.55 1.55 1.54 1.54 1.53 1.53
Parameter value
1 Solvent CDCl3
2 Temperature 295.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
CN
E
f1 (ppm)
2.00 3.00 3.00 2.01 1.00 2.00 2.01 2.01 4.10 2.15
144.93 142.43 128.61 128.45 128.39 128.36 127.77 126.38 125.80 119.82
45.38 38.60 36.28 33.82 26.81 25.53 17.09
Parameter value
1 Solvent CDCl3
2 Temperature 296.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C

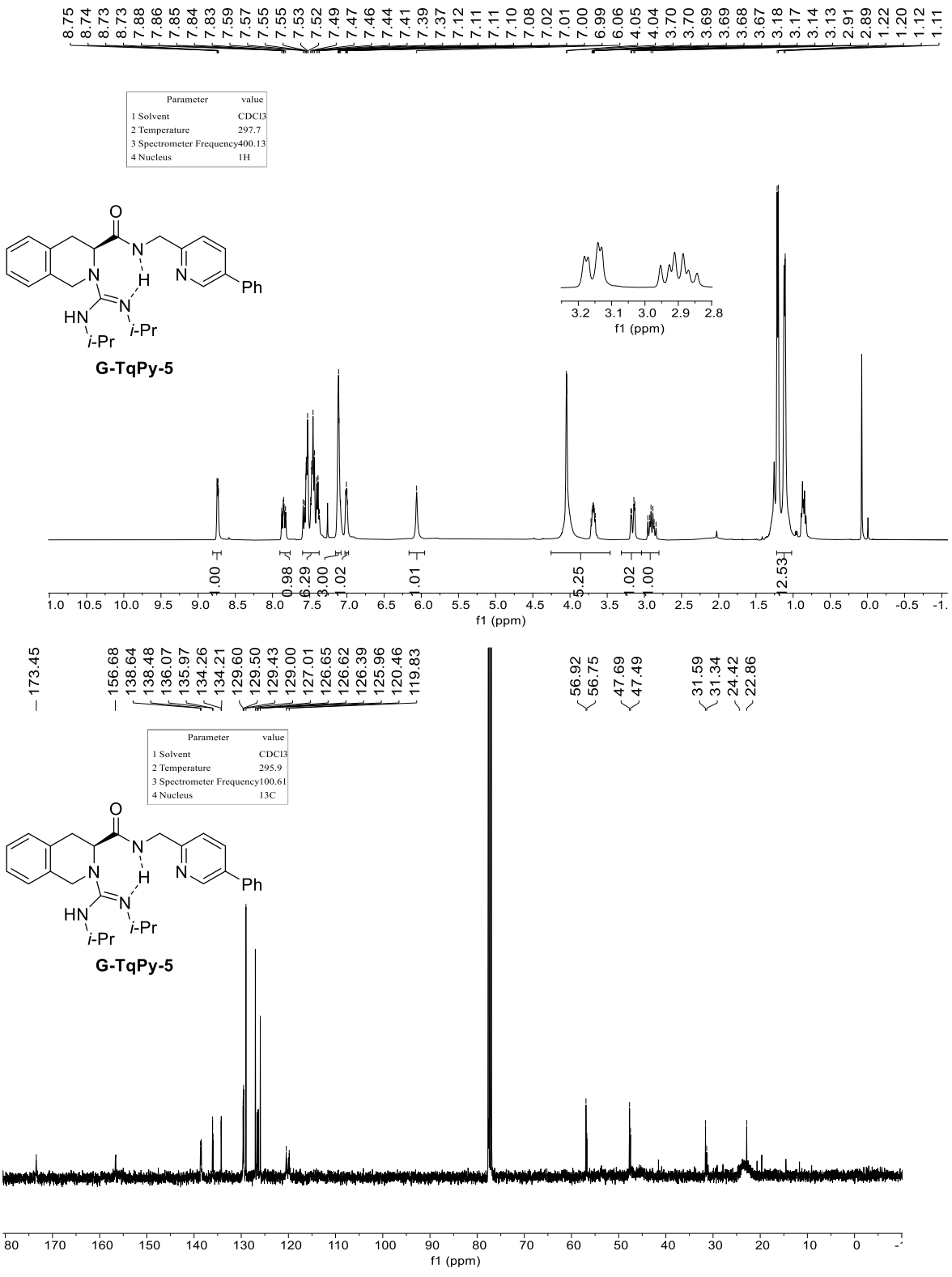

7.84
7.82
7.47
7.45
7.44
7.37
7.35
7.33
7.25
7.23
7.21
7.19
7.17
7.15
7.13
7.10
7.08
7.05
7.03
7.01
2.81
2.79
2.77
2.48
2.47
2.46
2.45
2.38
2.36
2.34
1.88
1.86
1.84
1.81
1.62
1.60
1.59
1.57
1.19
1.17
1.16
1.13
1.11
Parameter value
1 Solvent CDCl3
2 Temperature 295.7
3 Spectrometer Frequency 400.13
4 Nucleus 1H
Ph
O
F
2.8
2.7
2.40
2.35
2.30
f1 (ppm)
1.87
1.00
1.99
10.00
2.00
1.03
1.99
2.13
4.03
2.10
f1 (ppm)

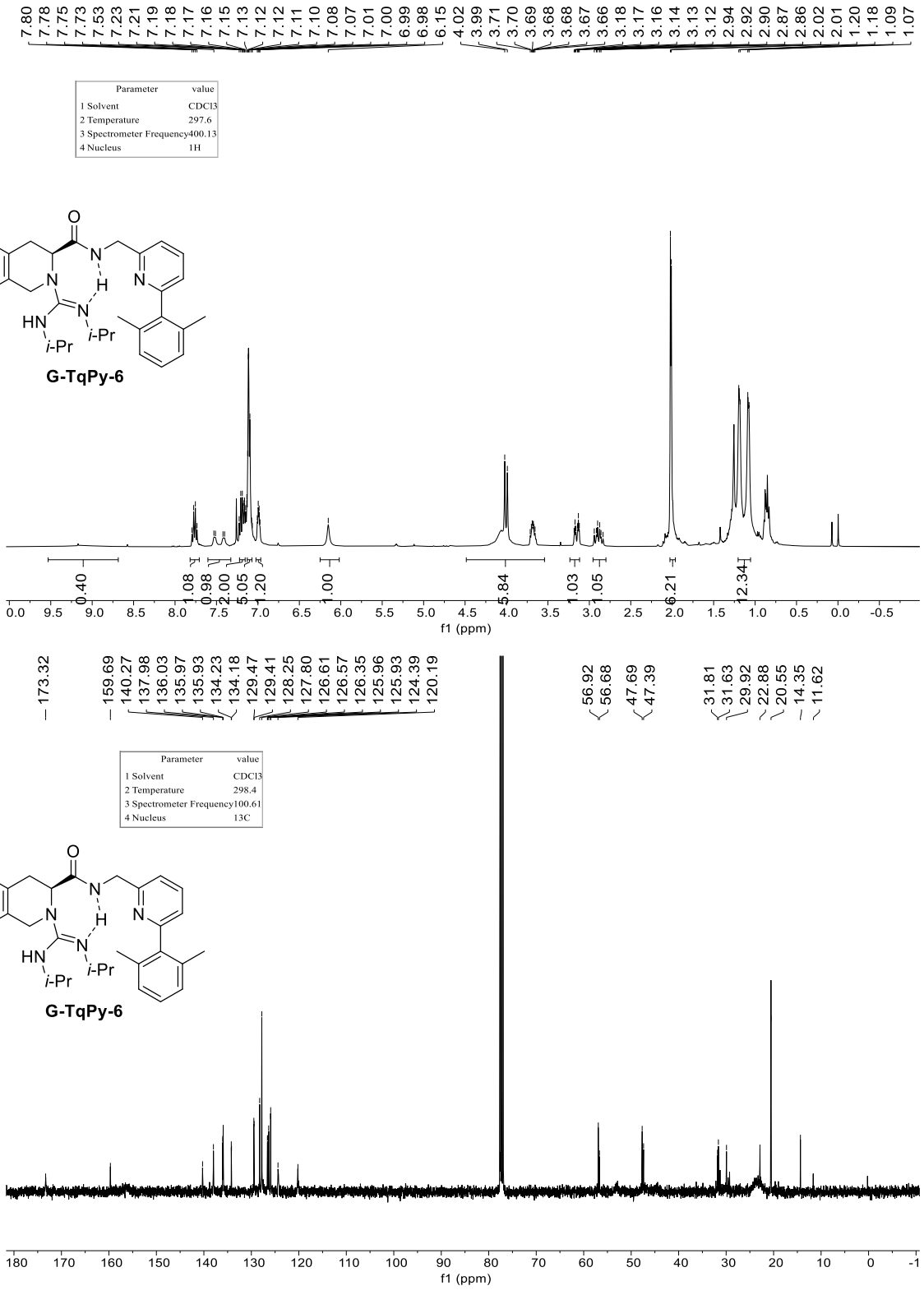

200.54
145.53
142.70
137.15
133.00
128.67
128.51
128.39
128.16
127.90
126.19
125.76
45.61
38.74
38.66
37.04
33.95
27.46
24.47
Parameter value
1 Solvent CDCl3
2 Temperature 296.5
3 Spectrometer Frequency 100.61
4 Nucleus 13C
Ph
O
F
129
128
127
126
125
124
f1 (ppm)
f1 (ppm)

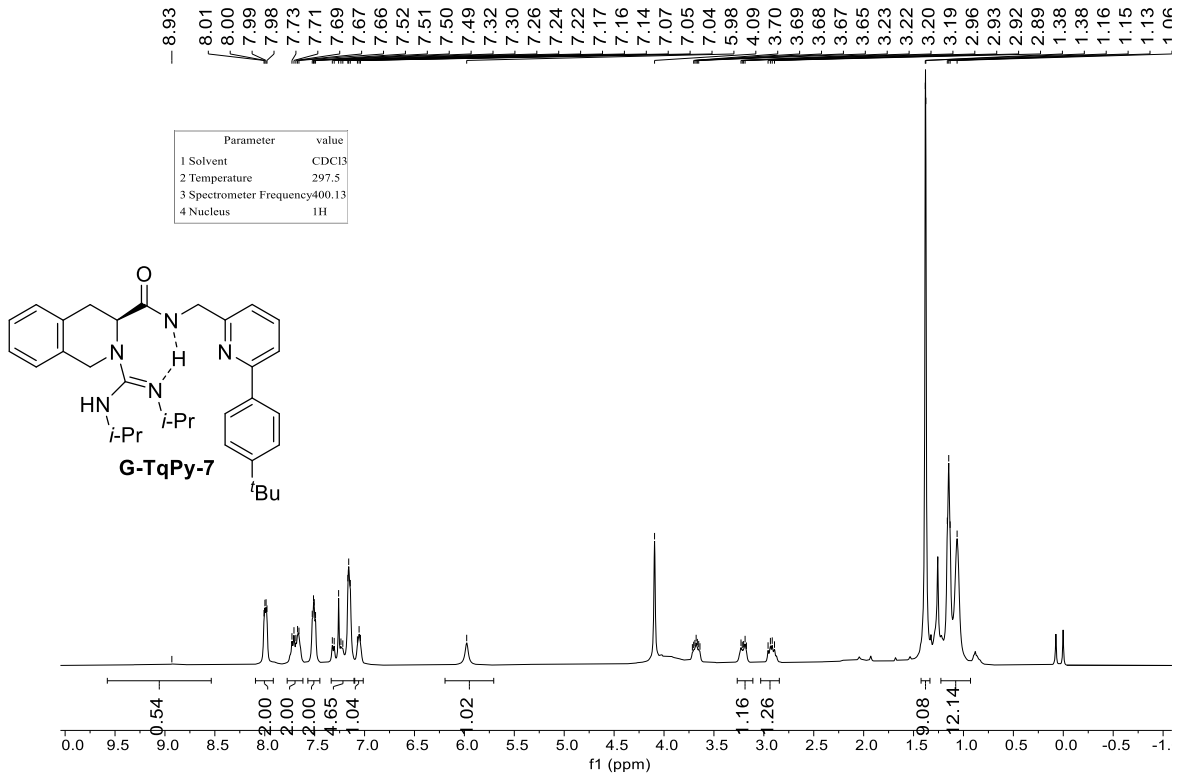

8.02 8.02 8.00 7.74 7.73 7.72 7.71 7.70 7.69 7.67 7.66 7.48 7.46 7.44 7.43 7.41 7.13 7.12 7.11 7.02 7.01 7.01 7.00 6.99 6.13 6.13
4.04 3.75 3.74 3.73 3.71 3.70 3.69 3.21 3.19 3.16 3.15 2.96 2.94 2.92 2.91 2.90 2.87
1.21 1.20 1.12 1.11
Parameter value
1 Solvent CDCl3
2 Temperature 295.1
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-3
0.63 2.00 2.07 4.00 3.06 1.00 1.17 5.80 1.02 1.00 12.38
f1 (ppm)
173.31
156.54 156.45 138.50 138.34 135.93 135.83 134.12 134.07 129.46 129.36 129.29 128.86 126.86 126.51 126.48 126.25 125.82 120.32 119.69
56.78 56.61 47.55 47.35 31.45 31.20 24.28 22.72
Parameter value
1 Solvent CDCl3
2 Temperature 295.9
3 Spectrometer Frequency 100.61
4 Nucleus 13C
G-TqPy-3
f1 (ppm)

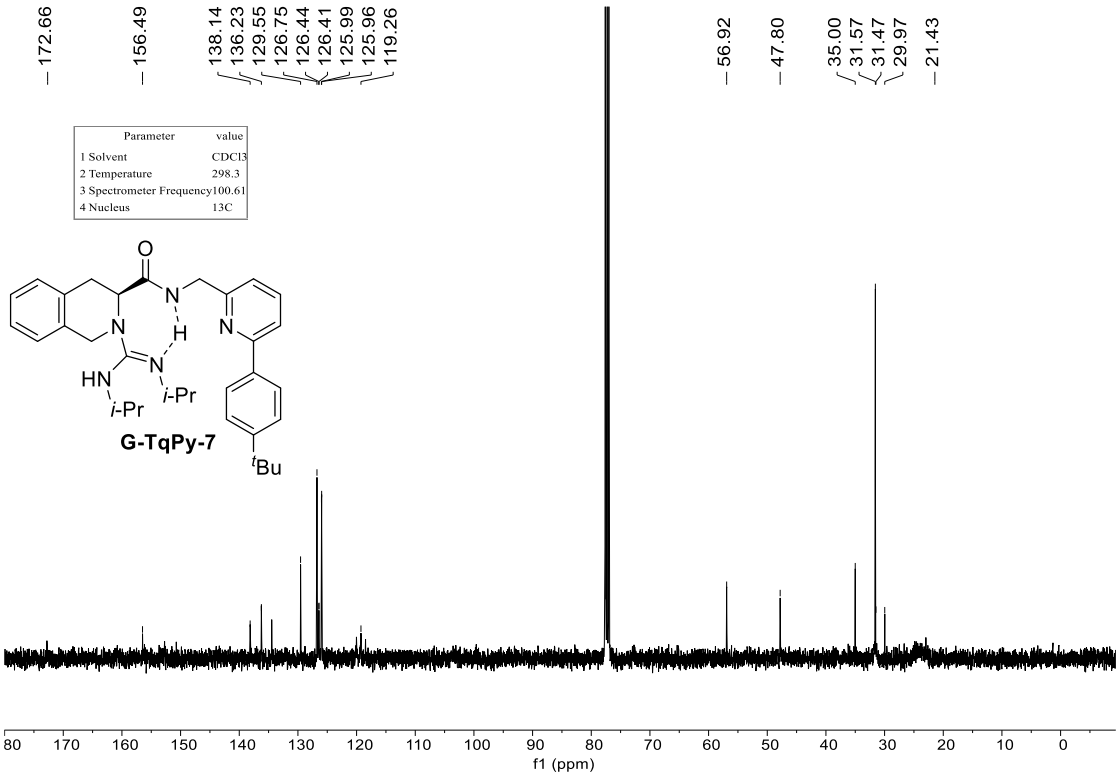

8.57 8.56 8.54 7.77 7.70 7.66 7.64 7.63 7.61 7.47 7.47 7.45 7.11 7.10 7.00 6.99 6.12
4.05 3.72 3.71 3.70 3.68 3.19 3.18 3.16 3.15 3.14 2.96 2.93 2.92 2.89 2.88 2.85 1.23 1.22 1.13 1.12
Parameter value
1 Solvent CDCl3
2 Temperature 297.7
3 Spectrometer Frequency 400.13
4 Nucleus 1H
Ph
HN
i-Pr
i-Pr
G-TqPy-4
3.2 3.1 3.0 2.9
f1 (ppm)
0.13 1.00 2.86 4.15 3.00 1.04 1.00 5.75 1.02 1.13 12.22
f1 (ppm)

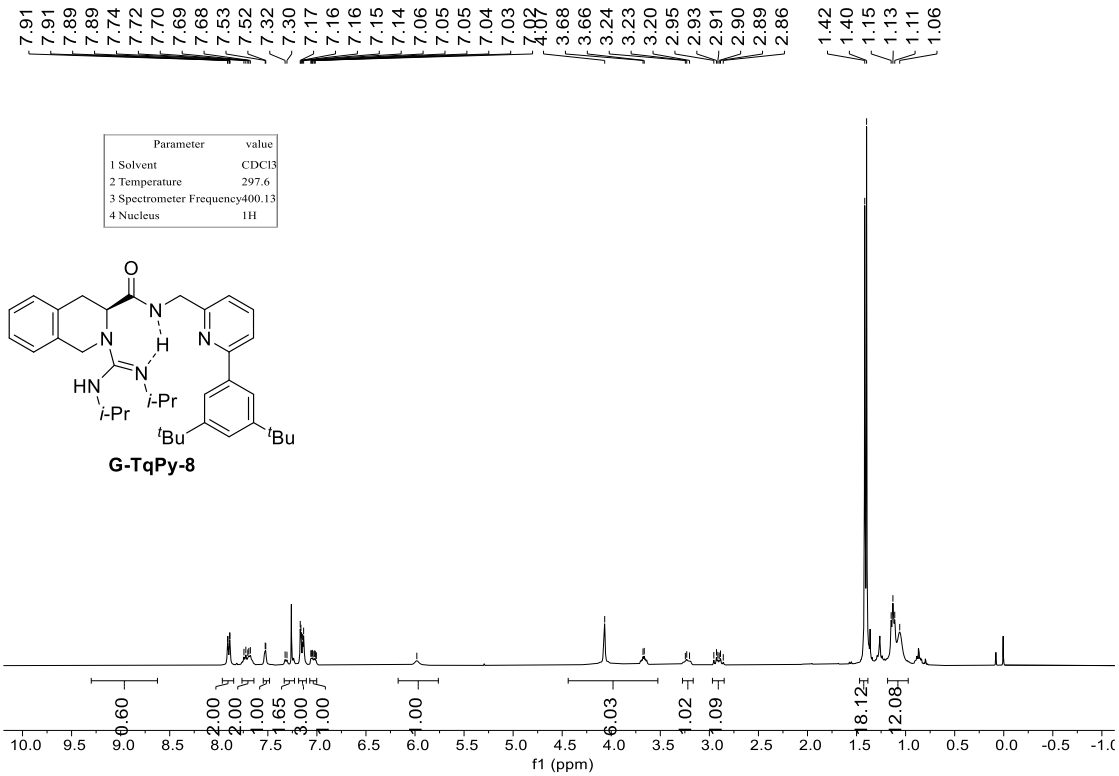

149.89 149.79 137.82 136.02 135.85 134.22 134.13 129.66 129.52 129.47 127.37 127.34 126.62 126.41 126.37 125.99 121.57 120.21
56.90 47.72 47.63 31.52 22.90 14.36
Parameter value
1 Solvent CDCl3
2 Temperature 298.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C
Ph
HN
i-Pr
i-Pr
G-TqPy-4
f1 (ppm)

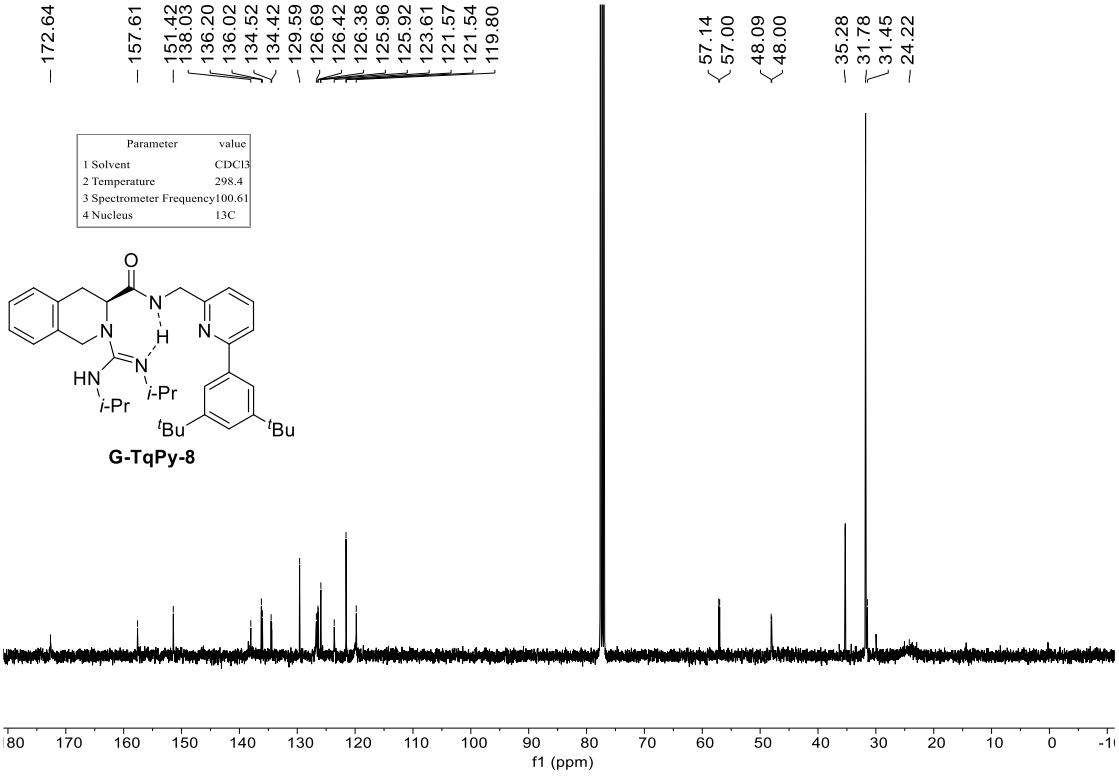

8.75 8.74 8.73 8.73 7.88 7.86 7.85 7.84 7.83 7.59 7.57 7.55 7.55 7.53 7.52 7.49 7.47 7.46 7.44 7.41 7.39 7.37 7.12 7.11 7.11 7.10 7.08 7.02 7.01 7.00 6.99 6.06 4.05 4.04 3.70 3.70 3.69 3.69 3.68 3.67 3.18 3.17 3.14 3.13 2.91 2.89 1.22 1.20 1.12 1.11
Parameter value
1 Solvent CDCl3
2 Temperature 297.7
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-5
f1 (ppm)
1.00 0.98 6.29 3.00 1.02 1.01 5.25 1.02 1.00 12.53
f1 (ppm)
173.45 156.68 138.64 138.48 136.07 135.97 134.26 134.21 129.60 129.50 129.43 129.00 127.01 126.65 126.62 126.39 125.96 120.46 119.83
56.92 56.75 47.69 47.49 31.59 31.34 24.42 22.86
Parameter value
1 Solvent CDCl3
2 Temperature 295.9
3 Spectrometer Frequency 100.61
4 Nucleus 13C
G-TqPy-5
f1 (ppm)

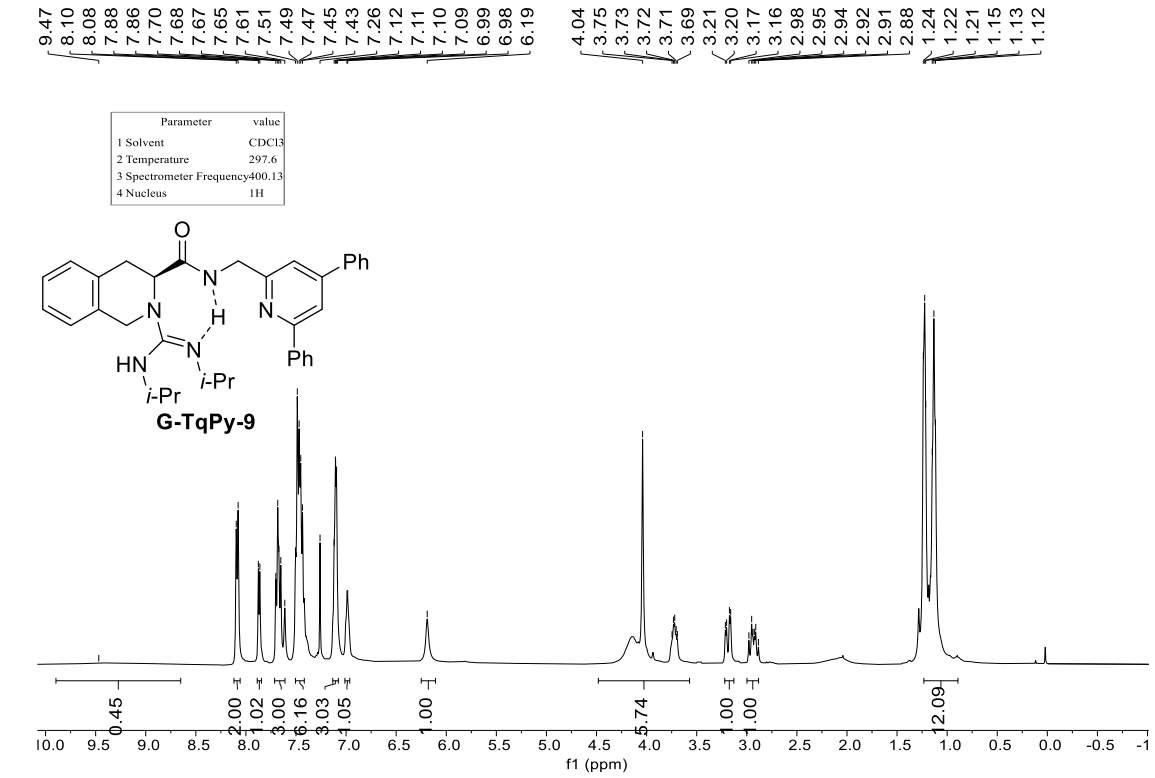

7.80 7.78 7.75 7.73 7.53 7.23 7.21 7.19 7.18 7.17 7.16 7.15 7.13 7.12 7.12 7.11 7.10 7.08 7.07 7.01 7.00 6.99 6.98 6.15 4.02 3.99 3.71 3.70 3.69 3.68 3.68 3.67 3.66 3.18 3.17 3.16 3.14 3.13 3.12 2.94 2.92 2.90 2.87 2.86 2.02 2.01 1.20 1.18 1.09 1.07
Parameter value
1 Solvent CDCl3
2 Temperature 297.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-6
0.40 1.08 0.98 2.00 5.05 1.20 1.00 5.84 1.03 1.05 6.21 12.34
f1 (ppm)
173.32 159.69 140.27 137.98 136.03 135.97 135.93 134.23 134.18 129.47 129.41 128.25 127.80 126.61 126.57 126.35 125.96 125.93 124.39 120.19 56.92 56.68 47.69 47.39 31.81 31.63 29.92 22.88 20.55 14.35 11.62
Parameter value
1 Solvent CDCl3
2 Temperature 298.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C
G-TqPy-6
f1 (ppm)

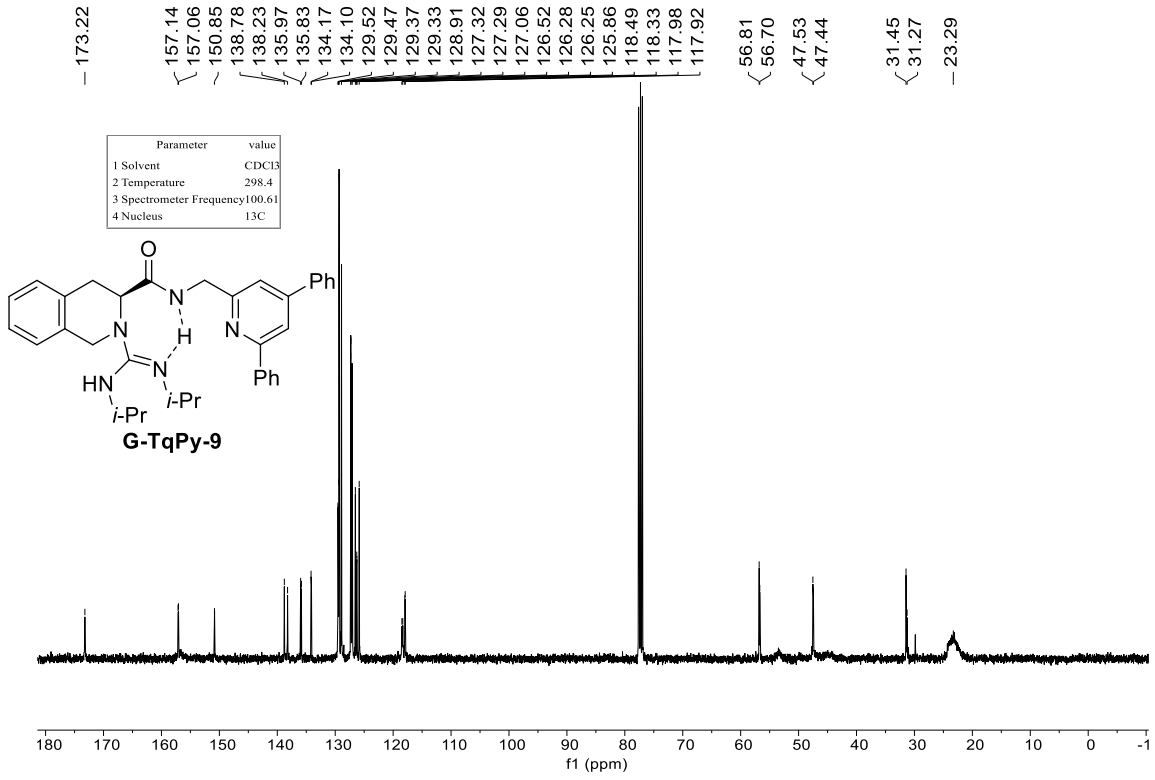

8.93
8.01
8.00
7.99
7.98
7.73
7.71
7.69
7.67
7.66
7.52
7.51
7.50
7.49
7.32
7.30
7.26
7.24
7.22
7.17
7.16
7.14
7.07
7.05
7.04
5.98
4.09
3.70
3.69
3.68
3.67
3.65
3.23
3.22
3.20
3.19
2.96
2.93
2.92
2.89
1.38
1.16
1.15
1.13
Parameter value
1 Solvent CDCl3
2 Temperature 297.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-7
0.54
2.00
2.00
2.00
4.65
1.04
1.02
1.16
1.26
9.08
12.14
f1 (ppm)

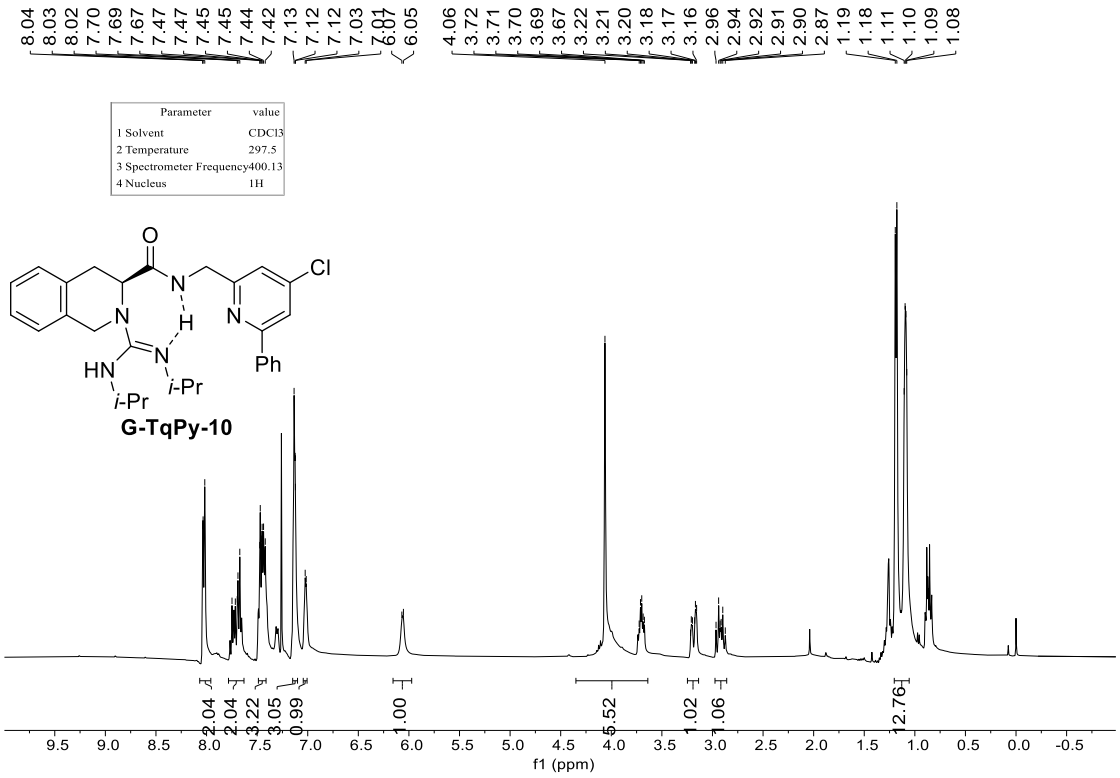

172.66
156.49
138.14
136.23
129.55
126.75
126.44
126.41
125.99
125.96
119.26
56.92
47.80
35.00
31.57
31.47
29.97
21.43
Parameter value
1 Solvent CDCl3
2 Temperature 298.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
G-TqPy-7
f1 (ppm)

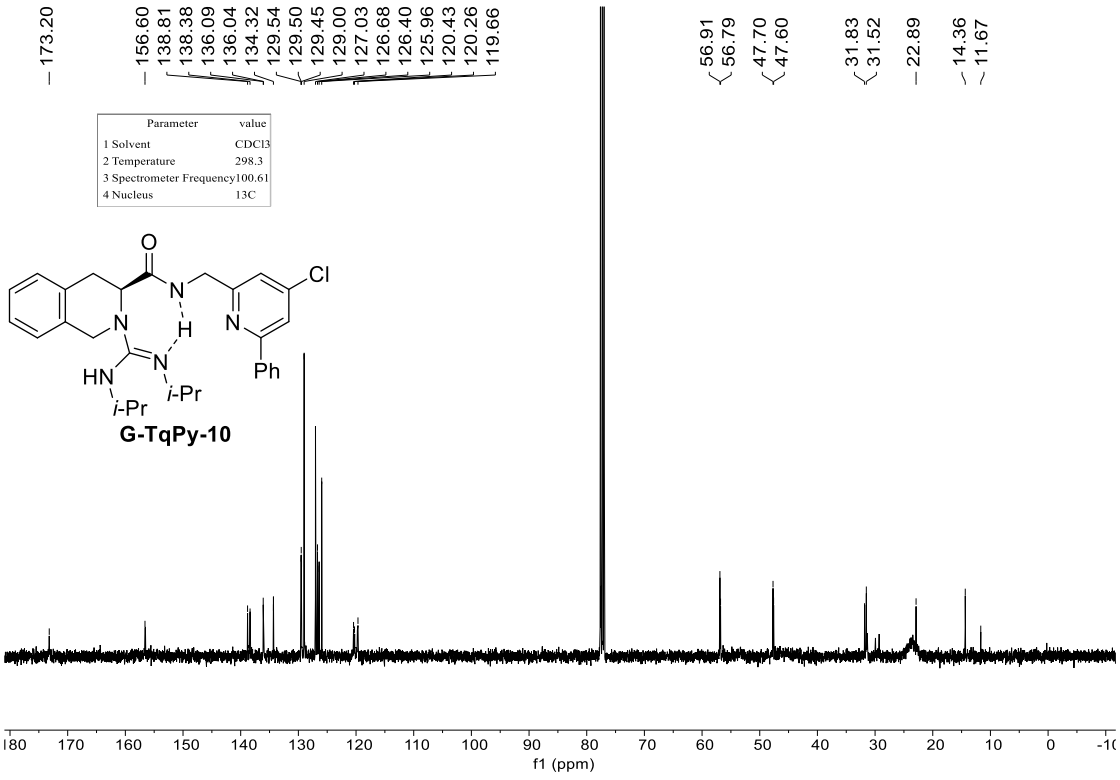

7.91 7.91 7.89 7.89 7.74 7.72 7.70 7.69 7.68 7.53 7.52 7.32 7.30 7.17 7.16 7.16 7.15 7.14 7.06 7.05 7.05 7.04 7.03 7.02 4.07 3.68 3.66 3.24 3.23 3.20 2.95 2.93 2.91 2.90 2.89 2.86 1.42 1.40 1.15 1.13 1.11 1.06
Parameter value
1 Solvent CDCl3
2 Temperature 297.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-8
0.60 2.00 2.00 1.00 1.65 3.00 1.00 4.00 6.03 1.02 1.09 18.12 12.08
f1 (ppm)

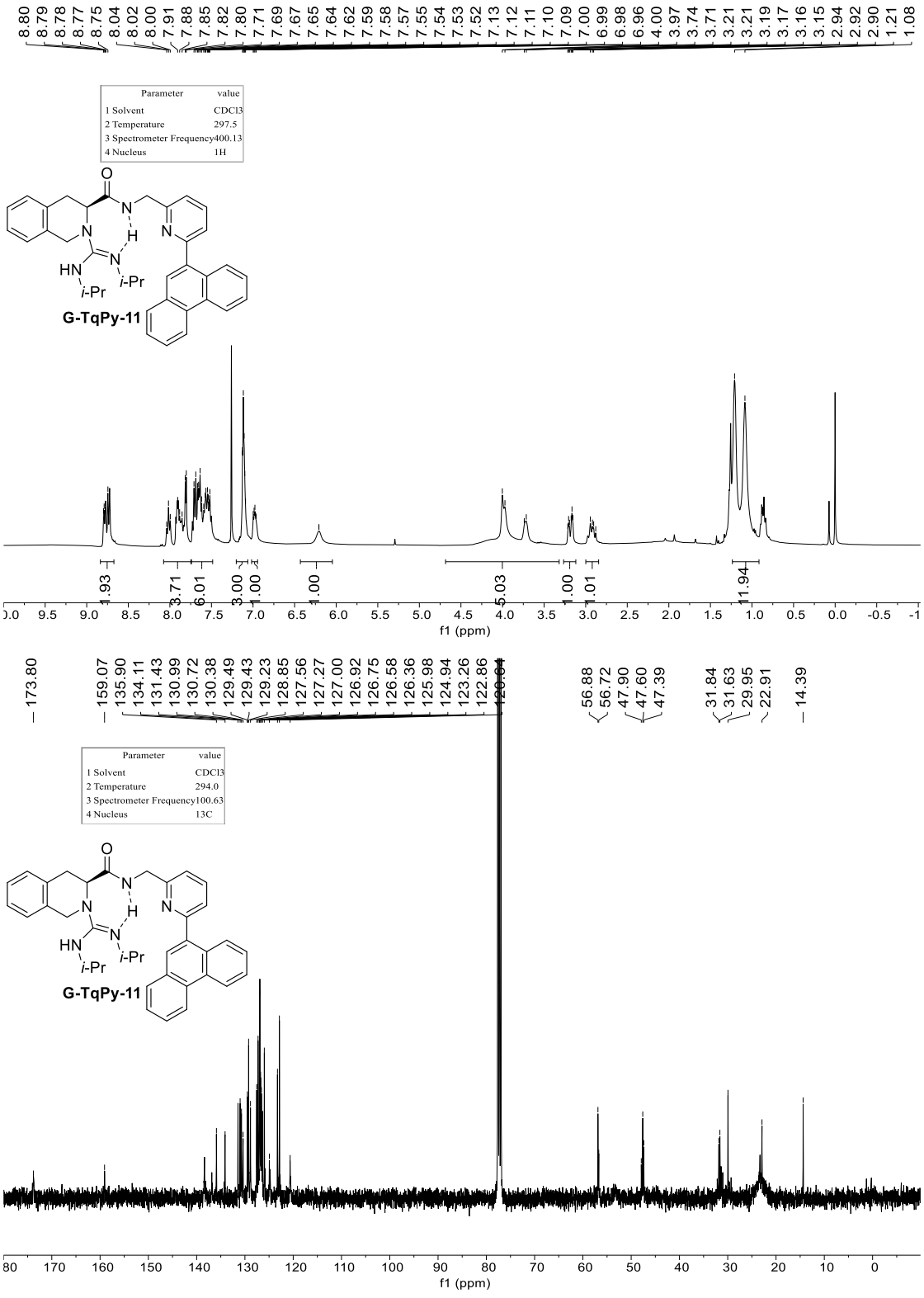

172.64 157.61 151.42 138.03 136.20 136.02 134.52 134.42 129.59 126.69 126.42 126.38 125.96 125.92 123.61 121.57 121.54 119.80 57.14 57.00 48.09 48.00 35.28 31.78 31.45 24.22
Parameter value
1 Solvent CDCl3
2 Temperature 298.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C
G-TqPy-8
f1 (ppm)

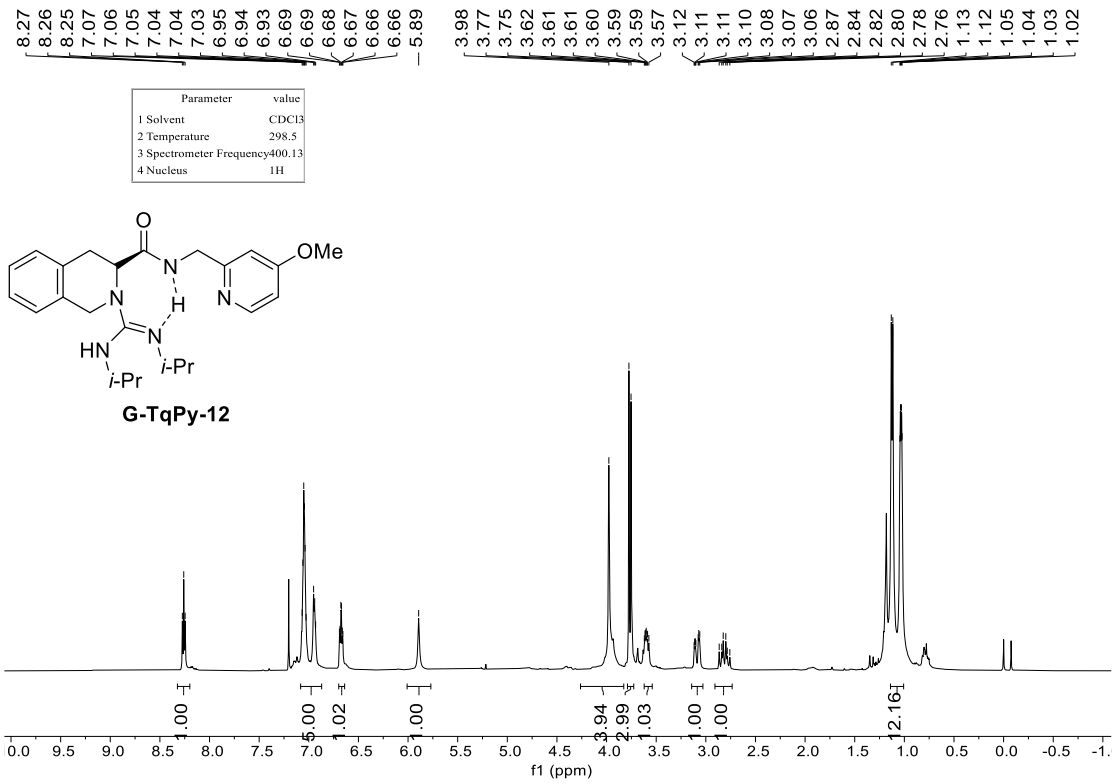

9.47
8.10
8.08
7.88
7.86
7.70
7.68
7.67
7.65
7.61
7.51
7.49
7.47
7.45
7.43
7.26
7.12
7.11
7.10
7.09
6.99
6.98
6.19
4.04
3.75
3.73
3.72
3.71
3.69
3.21
3.20
3.17
3.16
2.98
2.95
2.94
2.92
2.91
2.88
1.24
1.22
1.21
1.15
1.13
1.12
Parameter value
1 Solvent CDCl3
2 Temperature 297.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-9
0.45
2.00
1.02
3.00
6.16
3.03
1.05
1.00
5.74
1.00
1.00
12.09
f1 (ppm)

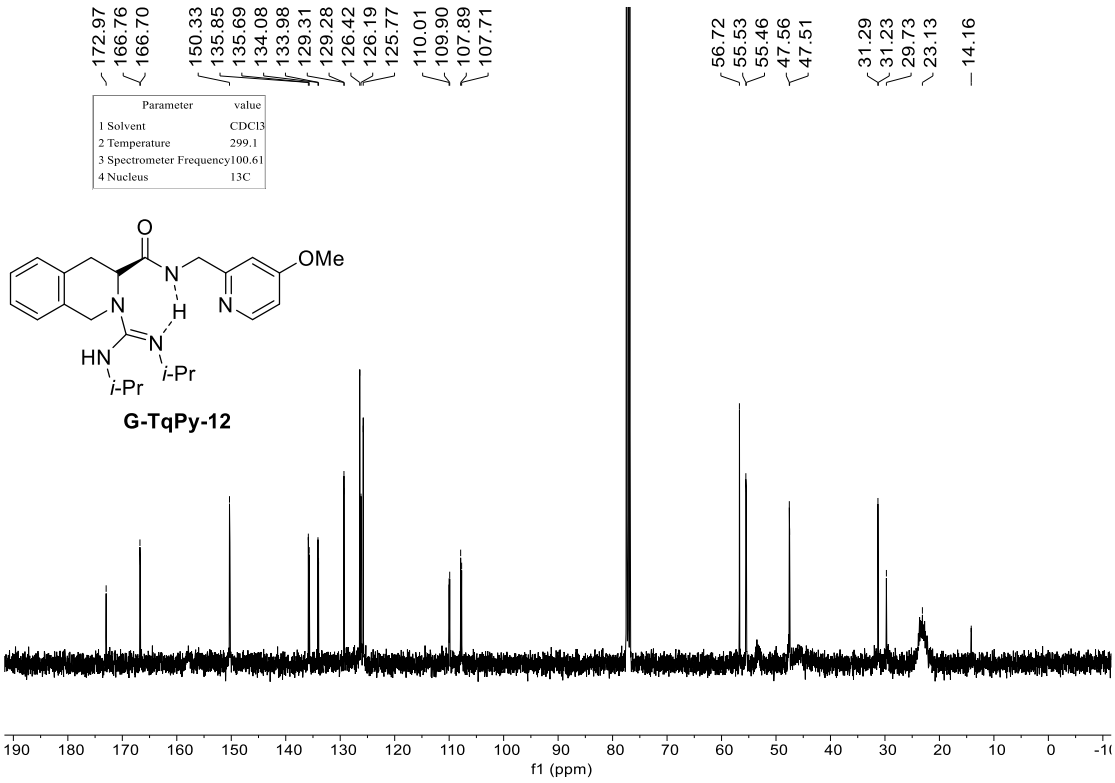

173.22
157.14
157.06
150.85
138.78
138.23
135.97
135.83
134.17
134.10
129.52
129.47
129.37
129.33
128.91
127.32
127.29
127.06
126.52
126.28
126.25
125.86
118.49
118.33
117.98
117.92
56.81
56.70
47.53
47.44
31.45
31.27
23.29
Parameter value
1 Solvent CDCl3
2 Temperature 298.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C
G-TqPy-9
f1 (ppm)


8.04 8.03 8.02 7.70 7.69 7.67 7.47 7.47 7.45 7.45 7.44 7.42 7.13 7.12 7.12 7.03 7.01 6.05
4.06 3.72 3.71 3.70 3.69 3.67 3.22 3.21 3.20 3.18 3.17 3.16 2.96 2.94 2.92 2.91 2.90 2.87 1.19 1.18 1.11 1.10 1.09 1.08
Parameter value
1 Solvent CDCl3
2 Temperature 297.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-10
2.04 2.04 3.22 3.05 0.99 1.00 5.52 1.02 1.06 12.76
f1 (ppm)


173.20
156.60 138.81 138.38 136.09 136.04 134.32 129.54 129.50 129.45 129.00 127.03 126.68 126.40 125.96 120.43 120.26 119.66
56.91 56.79 47.70 47.60 31.83 31.52 22.89 14.36 11.67
Parameter value
1 Solvent CDCl3
2 Temperature 298.3
3 Spectrometer Frequency 100.61
4 Nucleus 13C
G-TqPy-10
f1 (ppm)


8.80 8.79 8.78 8.77 8.75 8.04 8.02 8.00 7.91 7.88 7.85 7.82 7.80 7.71 7.69 7.67 7.65 7.64 7.62 7.59 7.58 7.57 7.55 7.54 7.53 7.52 7.13 7.12 7.11 7.10 7.09 7.00 6.99 6.98 6.96 4.00 3.97 3.74 3.71 3.21 3.21 3.19 3.17 3.16 3.15 2.94 2.92 2.90 1.21 1.08
Parameter value
1 Solvent CDCl3
2 Temperature 297.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
G-TqPy-11
1.93 3.71 6.01 3.00 1.00 1.00 5.03 1.00 1.01 11.94
f1 (ppm)
173.80 159.07 135.90 134.11 131.43 130.99 130.72 130.38 129.49 129.43 129.23 128.85 127.56 127.27 127.00 126.92 126.75 126.58 126.36 125.98 124.94 123.26 122.86 120.04 56.88 56.72 47.90 47.60 47.39 31.84 31.63 29.95 22.91 14.39
Parameter value
1 Solvent CDCl3
2 Temperature 294.0
3 Spectrometer Frequency 100.63
4 Nucleus 13C
G-TqPy-11
f1 (ppm)


8.27 8.26 8.25 7.07 7.06 7.05 7.04 7.04 7.03 6.95 6.94 6.93 6.69 6.69 6.68 6.67 6.66 6.66 5.89
3.98 3.77 3.75 3.62 3.61 3.61 3.60 3.59 3.59 3.57 3.12 3.11 3.11 3.10 3.08 3.07 3.06 2.87 2.84 2.82 2.80 2.78 2.76 1.13 1.12 1.05 1.04 1.03 1.02
Parameter value
1 Solvent CDCl3
2 Temperature 298.5
3 Spectrometer Frequency 400.13
4 Nucleus 1H
O
N
H
N
HN
N
i-Pr
i-Pr
OMe
G-TqPy-12
1.00 5.00 1.02 1.00 3.94 2.99 1.03 1.00 1.00 12.16
f1 (ppm)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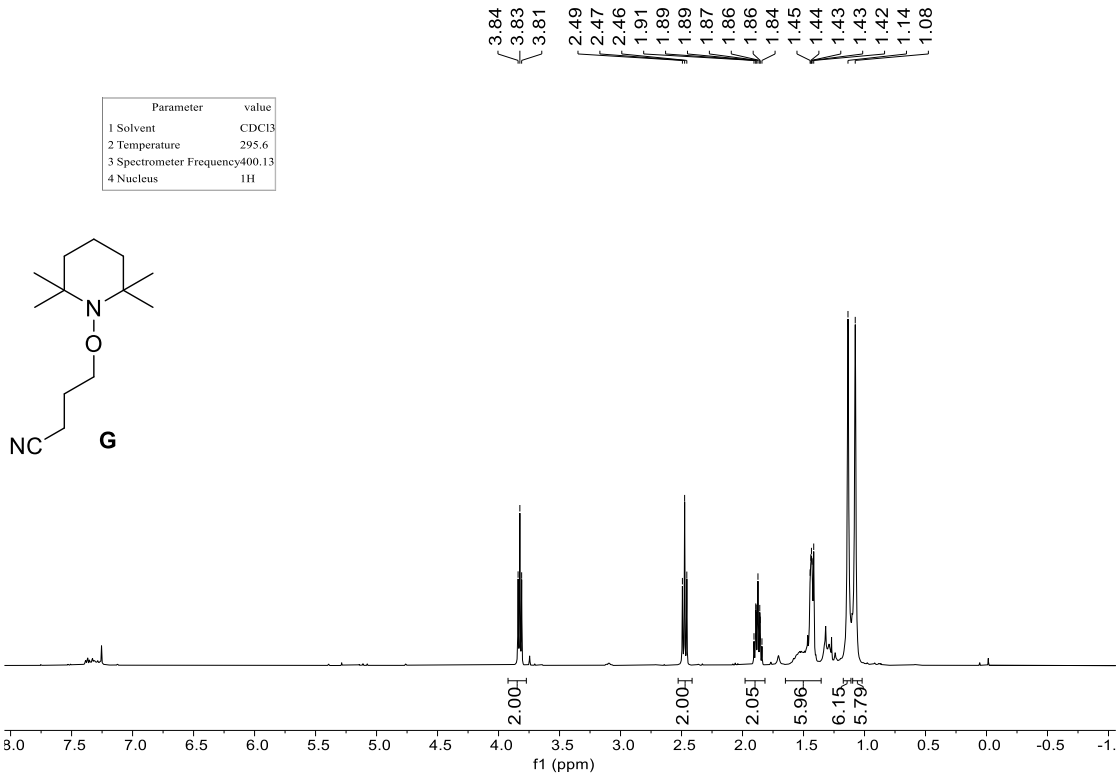
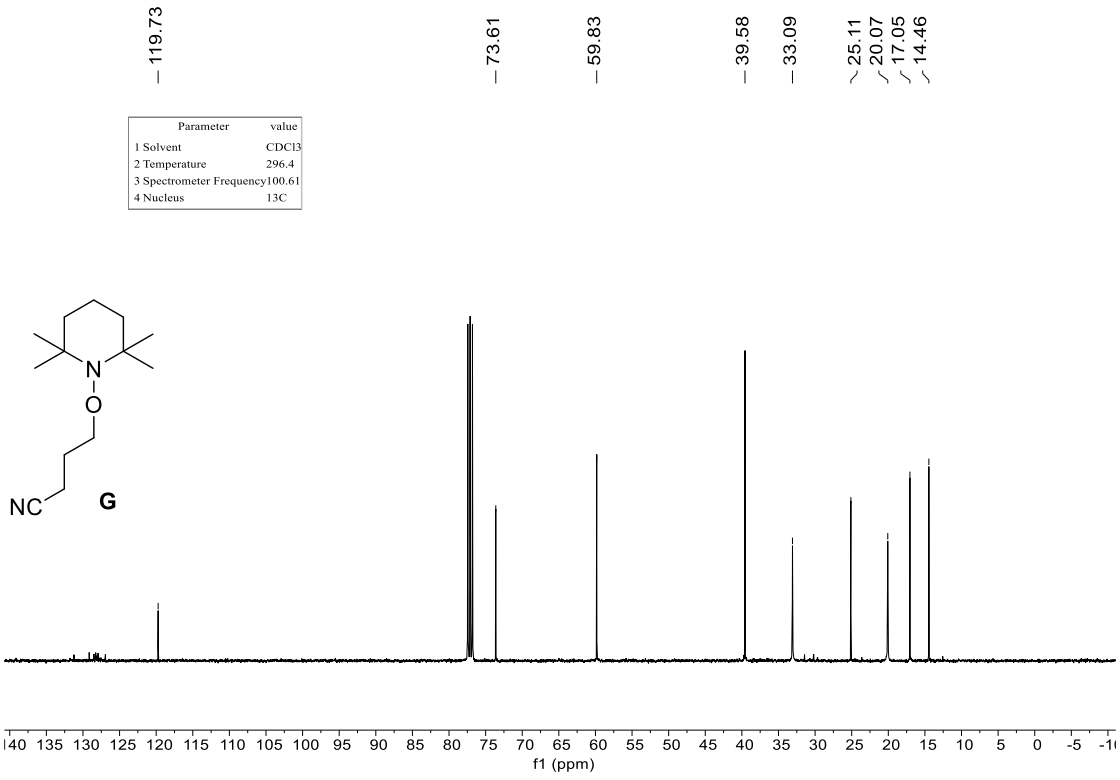
56.72 55.53 55.46 47.56 47.51 31.29 31.23 29.73 23.13 14.16
Parameter value
1 Solvent CDCl3
2 Temperature 299.1
3 Spectrometer Frequency 100.61
4 Nucleus 13C
O
N
H
N
HN
N
i-Pr
i-Pr
OMe
G-TqPy-12
f1 (ppm)


3.84
3.83
3.81
2.49
2.47
2.46
1.91
1.89
1.89
1.87
1.86
1.86
1.84
1.45
1.44
1.43
1.43
1.42
1.14
1.08
Parameter value
1 Solvent CDCl3
2 Temperature 295.6
3 Spectrometer Frequency 400.13
4 Nucleus 1H
N
O
NC
G
2.00
2.00
2.05
5.96
6.15
5.79
f1 (ppm)


119.73
73.61
59.83
39.58
33.09
25.11
20.07
17.05
14.46
Parameter value
1 Solvent CDCl3
2 Temperature 296.4
3 Spectrometer Frequency 100.61
4 Nucleus 13C
N
O
NC
G
f1 (ppm)