Supporting Information

Direct Synthesis of Pentasubstituted Pyrroles and Hexasubstituted Pyrrolines from Propargyl Sulfonylamides and Allenamides

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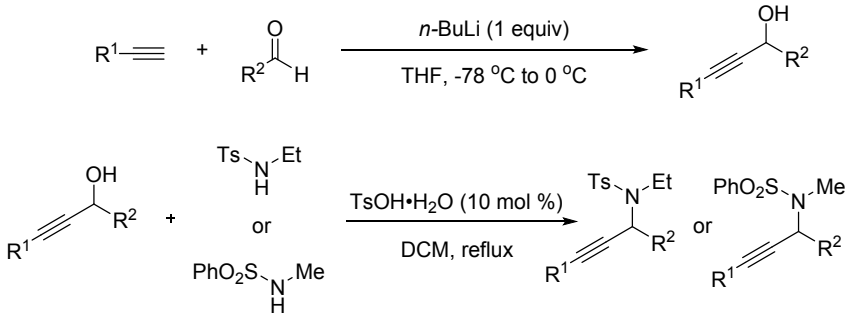
Materials and methods

All reactions were carried out under an atmosphere of nitrogen in a flame-dried glassware with magnetic stirring unless otherwise indicated. Commercially obtained reagents were used as received. Solvents were dried by Innovative Technology Solvent Purification System. Liquids and solutions were transferred via syringe. All reactions were monitored by thin-layer chromatography. GC-MS data were recorded on Thermo ISQ QD. ^{1}H, ^{19}F, and ^{13}C NMR spectra were recorded on Bruker-BioSpin AVANCE III HD and JEOL ECZ600S. Data for ^{1}H NMR spectra are reported relative to TMS as an internal standard and are reported as follows: chemical shift (ppm), multiplicity, coupling constant (Hz), and integration. Data for ^{13}C NMR spectra are reported relative to chloroform as an internal standard and are reported in terms of chemical shift (ppm). HRMS data were recorded on Thermo Fisher Scientific LTQ FTICR-MS, Waters Micromass GCT Premier or Thermo Finnigan DECAX-30000 LCQ Deca XP. Optical rotations were measured using a 1 mL cell with a 5 dm path length on an INESA SGW-1 polarimeter. All melting points were determined on a Beijing Science Instrument Dianguang Instrument Factory XT4B melting point apparatus without correction. IR data were recorded on Bruker Vertex 70.

Synthesis of propargyl sulfonylamides

All alkynes, aldehyde, sulfamide and primary amine were purchased from Adamas-beta, Energy Chemical and Bidepharmatech.

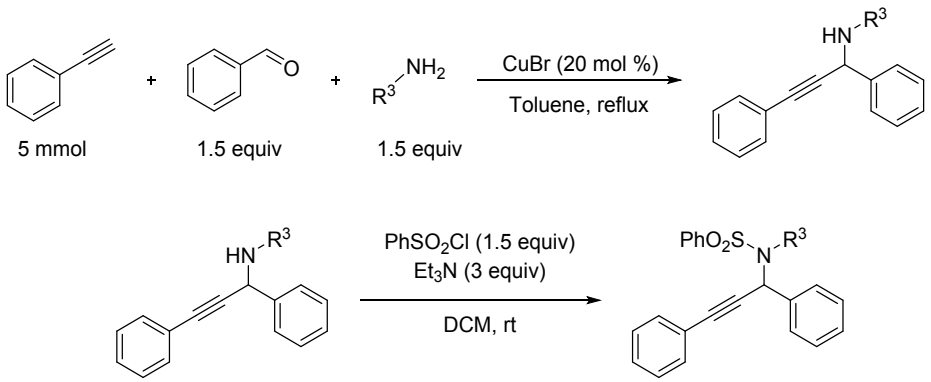
General procedure for synthesis of propargyl sulfonylamides **1a-1p**, **8**.



To a 50 mL round bottomed flask was charged with terminal alkyne (5 mmol, 1 equiv) and 10 mL of THF. The solution was cooled to -78 °C and *n*-BuLi (2.5 M in THF, 2 mL, 5 mmol, 1 equiv) was added. The resulting solution was stirred for 20 minutes at room temperature and then cooled to -78 °C again. Aldehyde (5 mmol, 1 equiv) in THF solution was added dropwise. The reaction mixture was then allowed to warm to room temperature and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous NH_4Cl (40 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (30 mL), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure to afford the crude propargyl alcohol.

A solution of the resulting crude propargyl alcohol and sulfonamide (1.2 equiv) in DCM was taken in a round bottom flask under nitrogen atmosphere and then $TsOH \cdot H_2O$ was added at room temperature. The reaction mixture was heated to reflux overnight and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the corresponding propargyl sulfonylamide.

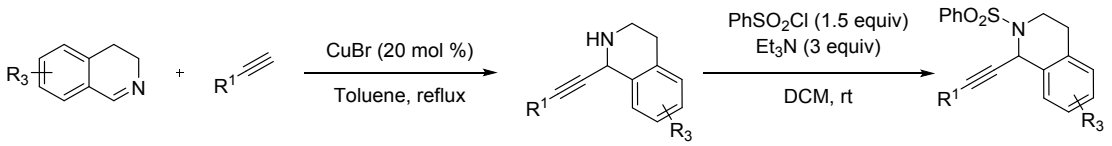
General procedure for synthesis of propargyl sulfonylamides **1q-1s**.



To a 50 mL round bottomed flask was charged with CuBr (1 mmol, 20 mol %), phenylacetylene (5 mmol, 1 equiv), benzaldehyde (7.5 mmol, 1.5 equiv), primary amine (7.5 mmol, 1.5 equiv) and 10 mL of toluene. The solution was heated to reflux and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure to afford the crude propargylamides.

The resulting crude propargylamine and Et_3N (3 equiv) were dissolved in dry DCM, and the mixture was cooled to 0 °C with a cooling bath. To this solution benzenesulfonyl chloride (1.5 equiv) was slowly added in drops, and the mixture was allowed to warm up to room temperature and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the desired product.

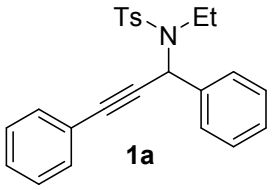
General procedure for synthesis of propargyl sulfonylamides **1t-1v**.



To a 50 mL round bottomed flask was charged with CuBr (1 mmol, 20 mol %), dihydroisoquinoline (5 mmol, 1 equiv), terminal alkyne (7.5 mmol, 1.5 equiv) and 10 mL of toluene. The solution was heated to reflux and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure to afford the crude material.

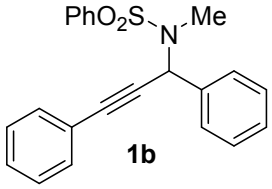
The resulting crude material and Et_3N (3 equiv) were dissolved in dry DCM, and the mixture was cooled to 0 °C with a cooling bath. To this solution benzenesulfonyl chloride (1.5 equiv) was slowly added in drops, and the mixture was allowed to warm up to room temperature and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the desired product.

Characterization data for propargyl sulfonylamides



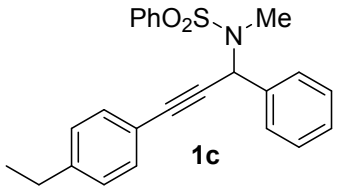
1a

Compound **1a** was obtained as yellow solid (m.p. = 67-68 °C, Rf = 0.64 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.70 (d, *J* = 7.5 Hz, 2H), 7.42 – 7.26 (m, 8H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.27 (s, 1H), 3.36 – 3.21 (m, 1H), 3.20 – 3.05 (m, 1H), 2.36 (s, 3H), 0.84 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.35, 137.03, 136.25, 131.55, 129.50, 128.63, 128.48, 128.35, 128.23, 128.10, 127.84, 122.12, 88.11, 83.68, 54.15, 40.72, 21.47, 16.04. HRMS (ESI) calcd for $[C_{24}H_{23}NNaO_2S]$ ($[M+Na]^+$): 412.1342, found: 412.1346. IR (thin film) *v* 1598.55, 2873.51, 2932.83, 2976.15 cm^{-1}.



1b

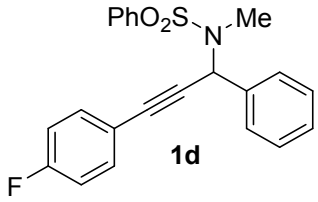
Compound **1b** was obtained as white solid (m.p. = 90-91 °C, Rf = 0.54 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.90 (m, 2H), 7.71 – 7.62 (m, 2H), 7.55 – 7.44 (m, 3H), 7.40 – 7.36 (m, 2H), 7.34 – 7.20 (m, 4H), 7.12 – 7.09 (m, 2H), 6.27 (s, 1H), 2.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.80, 136.04, 132.84, 131.64, 129.00, 128.81, 128.67, 128.52, 128.31, 128.02, 127.93, 121.84, 88.90, 82.20, 54.18, 29.97. HRMS (ESI) calcd for $[C_{22}H_{19}NNaO_2S]$ ($[M+Na]^+$): 384.1029, found: 384.1031. IR (thin film) *v* 1490.72, 1636.48, 2933.26 cm^{-1}.



1c

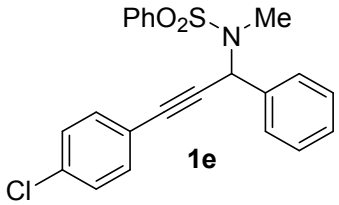
Compound **1c** was obtained as white solid (m.p. = 71-72 °C, Rf = 0.59 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.90 (m, 2H), 7.71 – 7.63 (m, 2H), 7.58 – 7.45 (m, 3H), 7.42 – 7.29 (m, 3H), 7.11 – 6.99 (m, 4H), 6.27 (s, 1H), 2.64 (s, 3H), 2.60 (q, *J* = 7.6 Hz, 2H), 1.20 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.25, 137.92, 136.21, 132.77, 131.64, 128.97, 128.61, 128.44, 128.01, 127.93, 127.84, 119.04, 89.08, 81.51, 54.21, 29.92, 28.86, 15.42. HRMS (ESI) calcd

for $[C_{24}H_{23}NNaO_2S]$ ($[M+Na]^+$): 412.1342, found: 412.1342. IR (thin film) *v* 1447.31, 1492.92, 1511.14, 2931.97, 2965.49 cm^{-1}.



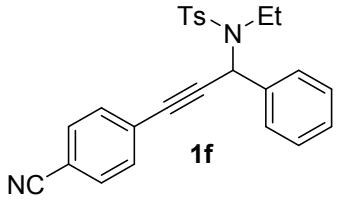
1d

Compound **1d** was obtained as white solid (m.p. = 134-135 °C, Rf = 0.57 (petroleum ether/ ethyl acetate = 5:1)). ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.92 (m, 2H), 7.68 – 7.62 (m, 2H), 7.60 – 7.47 (m, 3H), 7.44 – 7.31 (m, 3H), 7.13 – 7.05 (m, 2H), 6.95 (t, *J* = 8.6 Hz, 2H), 6.26 (s, 1H), 2.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.66 (d, *J* = 250.2 Hz), 137.88, 135.85, 133.52 (d, *J* = 8.4 Hz), 132.71, 128.90, 128.62, 128.49, 128.00, 127.84, 117.93 (d, *J* = 3.6 Hz), 115.55 (d, *J* = 22.1 Hz), 87.67, 82.02, 82.00, 54.06, 29.91. HRMS (ESI) calcd for $[C_{22}H_{18}FNNaO_2S]$ ($[M+Na]^+$): 402.0934, found: 402.0934. IR (thin film) *v* 1507.19, 1600.47, 2931.24 cm^{-1}.



1e

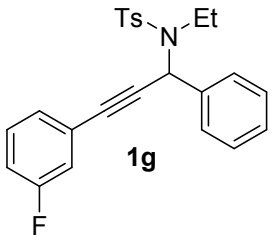
Compound **1e** was obtained as white solid (m.p. = 116-117 °C, Rf = 0.59 (petroleum ether/ ethyl acetate = 5:1)). ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.89 (m, 2H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.58 – 7.46 (m, 3H), 7.45 – 7.30 (m, 3H), 7.27 – 7.18 (m, 2H), 7.07 – 6.97 (m, 2H), 6.26 (s, 1H), 2.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.83, 135.72, 134.78, 132.82, 132.76, 128.93, 128.65, 128.59, 128.53, 128.00, 127.83, 120.30, 87.60, 83.31, 54.08, 29.94. HRMS (ESI) calcd for $[C_{24}H_{23}ClNNaO_2S]$ ($[M+Na]^+$): 418.0639, found: 418.0640. IR (thin film) *v* 1447.40, 1489.84, 2930.86 cm^{-1}.



1f

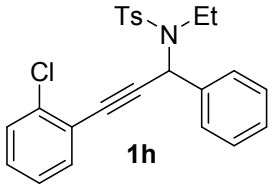
Compound **1f** was obtained as yellow liquid (Rf = 0.43 (petroleum ether/ ethyl acetate = 5:1)). ^1H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.1 Hz, 2H), 7.66 – 7.61 (m, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.41 – 7.34 (m, 3H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 8.2

Hz, 2H), 6.27 (s, 1H), 3.27 (dq, *J* = 14.4, 7.1 Hz, 1H), 3.08 (dq, *J* = 14.4, 7.1 Hz, 1H), 2.35 (s, 3H), 0.83 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.52, 136.32, 136.26, 132.15, 132.01, 129.59, 128.71, 128.04, 127.93, 126.96, 118.29, 112.15, 88.62, 86.34, 54.08, 40.88, 21.58, 16.09. HRMS (ESI) calcd for [$C_{25}H_{22}N_2NaO_2S$] ([M+Na]$^+$): 437.1294, found: 437.1294. IR (thin film) *v* 1602.44, 1640.70, 2228.90, 2978.34 cm^{-1}.



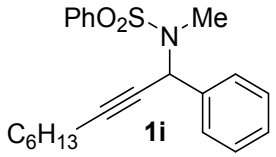
1g

Compound **1g** was obtained as white solid (m.p. = 80-81 ^{o}C, Rf = 0.61 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 – 7.81 (m, 2H), 7.67 (d, *J* = 5.4 Hz, 2H), 7.41 – 7.37 (m, 2H), 7.36 – 7.33 (m, 1H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.26 – 7.22 (m, 1H), 7.04 – 7.00 (m, 1H), 6.97 – 6.95 (m, 1H), 6.75 – 6.72 (m, 1H), 6.25 (s, 1H), 3.28 (dq, *J* = 13.8, 6.9 Hz, 1H), 3.09 (dq, *J* = 14.4, 7.2 Hz, 1H), 2.38 (s, 3H), 0.84 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.25 (d, *J* = 246.1 Hz), 143.60, 136.71, 136.23, 129.97 (d, *J* = 8.6 Hz), 129.63, 128.62, 128.54, 128.12, 127.94, 127.47, 127.46, 123.92 (d, *J* = 9.7 Hz), 118.50 (d, *J* = 23.0 Hz), 116.10 (d, *J* = 20.7 Hz), 86.90, 84.78, 54.15, 40.86, 21.48, 16.15. HRMS (ESI) calcd for [$C_{24}H_{22}FNNaO_2S$] ([M+Na]$^+$): 430.1247, found: 430.1249. IR (thin film) *v* 1581.02, 1644.09, 2935.68 cm^{-1}.



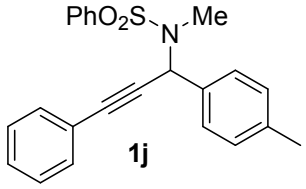
1h

Compound **1h** was obtained as white solid (m.p. = 122-123 ^{o}C, Rf = 0.57 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 – 7.81 (m, 2H), 7.76 (d, *J* = 7.7 Hz), 7.44 – 7.31 (m, 4H), 7.28 – 7.22 (m, 3H), 7.19 – 7.15 (m, 1H), 7.13 – 7.10 (m, 1H), 6.32 (s, 1H), 3.30 (dq, *J* = 14.4, 7.2 Hz, 1H), 3.18 (dq, *J* = 14.3, 7.0 Hz, 1H), 2.31 (s, 3H), 0.84 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.49, 136.98, 136.29, 136.02, 133.39, 129.81, 129.61, 129.33, 128.60, 128.47, 128.22, 127.85, 126.45, 122.18, 89.04, 85.02, 54.32, 40.95, 21.52, 16.17. HRMS (ESI) calcd for [$C_{24}H_{23}ClNNaO_2S$] ([M+Na]$^+$): 446.0952, found: 446.0952. IR (thin film) *v* 1599.48, 1644.58, 2934.90, 2977.97, cm^{-1}.



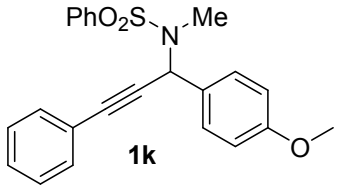
1i

Compound **1i** was obtained as colorless liquid (m.p. = 67-68 °C, Rf = 0.68 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.88 (m, 2H), 7.61 – 7.50 (m, 5H), 7.40 – 7.28 (m, 3H), 6.03 (s, 1H), 2.55 (s, 3H), 1.99 – 1.94 (m, 2H), 1.29 – 1.19 (m, 8H), 0.89 (t, *J* = 5.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.00, 136.58, 132.52, 128.69, 128.38, 128.16, 128.02, 127.86, 89.55, 72.90, 53.77, 31.25, 29.65, 28.49, 28.38, 22.53, 18.44, 14.07. HRMS (ESI) calcd for [$C_{22}H_{27}NNaO_2S$] ([M+Na]$^+$): 392.1655, found: 392.1655. IR (thin film) *v* 1448.00, 1493.44, 2858.23, 2931.09 cm^{-1}.



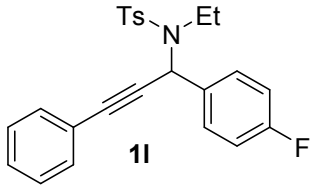
1j

Compound **1j** was obtained as white solid (m.p. = 86-87 °C, Rf = 0.68 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.88 (m, 2H), 7.59 – 7.44 (m, 5H), 7.34 – 7.15 (m, 5H), 7.10 (d, *J* = 6.8 Hz, 2H), 6.24 (s, 1H), 2.64 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.27, 137.91, 133.03, 132.70, 131.59, 129.28, 128.91, 128.67, 128.22, 127.99, 127.84, 121.94, 88.61, 82.48, 53.91, 29.83, 21.18. HRMS (ESI) calcd for [$C_{23}H_{21}NNaO_2S$] ([M+Na]$^+$): 398.1185, found: 398.1184. IR (thin film) *v* 1510.60, 2882.00, 2925.102970.0, 3026.20, 3057.96 cm^{-1}.



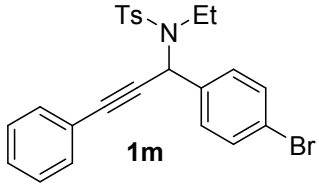
1k

Compound **1k** was obtained as white solid (m.p. = 89-90 °C, Rf = 0.58 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 – 7.91 (m, 2H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.52 – 7.48 (m, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.14 – 7.08 (m, 2H), 6.95 – 6.90 (m, 2H), 6.23 (s, 1H), 3.80 (s, 3H), 2.65 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.82, 137.92, 132.84, 131.69, 129.31, 129.04, 128.82, 128.35, 128.08, 121.98, 114.02, 88.74, 82.58, 55.45, 53.73, 29.81. HRMS (ESI) calcd for [$C_{23}H_{21}NnaO_3S$] ([M+Na]$^+$): 414.1134, found: 414.1134. IR (thin film) *v* 1510.33, 2838.59, 2929.89, 2957.89, 3036.67 cm^{-1}.



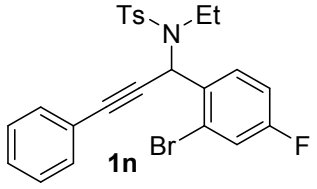
1l

Compound **1l** was obtained as white solid (m.p. = 111-112 °C, Rf = 0.68 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.0 Hz, 2H), 7.68 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.34 – 7.24 (m, 5H), 7.14 (d, *J* = 8.4 Hz, 2H), 7.06 (t, *J* = 8.5 Hz, 2H), 6.23 (s, 1H), 3.38 - 3.25 (m, 1H), 3.24 - 3.02 (m, 1H), 2.33 (s, 3H), 0.85 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.70 (d, *J* = 247.3 Hz), 143.52, 136.04, 133.02 (d, *J* = 3.2 Hz), 131.57, 129.86 (d, *J* = 8.2 Hz), 129.57, 128.81, 128.30, 127.80, 121.86, 115.37 (d, *J* = 21.7 Hz), 88.43, 83.28, 53.60, 40.69, 21.45, 16.15. HRMS (ESI) calcd for [$C_{24}H_{22}FNNaO_2S$] ([M+Na]$^+$): 430.1247, found: 430.1249. IR (thin film) *v* 1604.61, 1644.26, 2875.05, 2935.37, 2978.05 cm^{-1}.



1m

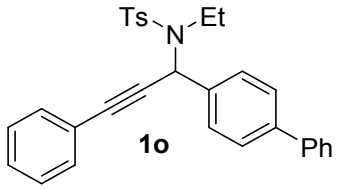
Compound **1m** was obtained as white solid (m.p. = 105-106 °C, Rf = 0.68 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 2H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.53 – 7.48 (m, 2H), 7.34 – 7.25 (m, 5H), 7.15 – 7.11 (m, 2H), 6.19 (s, 1H), 3.25 - 3.29 (m, 1H), 3.02 - 3.24 (m, 1H), 2.35 (s, 3H), 0.85 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.59, 136.41, 136.02, 131.68, 131.62, 129.84, 129.62, 128.88, 128.35, 127.87, 122.55, 121.88, 88.61, 83.00, 53.77, 40.88, 21.55, 16.19. HRMS (ESI) calcd for [$C_{24}H_{22}BrNNaO_2S$] ([M+Na]$^+$): 490.0447, found: 490.0444. IR (thin film) *v* 1597.80, 2874.07, 2933.91, 2976.31, 3062.60 cm^{-1}.



1n

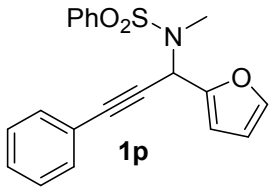
Compound **1n** was obtained as white solid (m.p. = 134-135 °C, Rf = 0.66 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.3 Hz, 2H), 7.80 (dd, *J* = 8.7, 5.9 Hz, 1H), 7.38 (dd, *J* = 8.1, 2.6 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.29 – 7.25 (m, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 7.15 – 7.08 (m, 2H), 7.05 (td, *J* = 8.2, 2.5 Hz, 1H), 6.46 (s, 1H), 3.23 – 3.12 (m, 1H), 3.07 – 2.95 (m, 1H), 2.30 (s, 3H), 0.72 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.52 (d, *J* = 252.9 Hz), 143.45, 136.01, 132.17 (d, *J* = 8.7 Hz), 131.61, 129.36, 128.89, 128.40, 128.33, 125.36 (d, *J* = 9.6 Hz),

121.87, 121.18 (d, J = 24.5 Hz), 114.49 (d, J = 20.9 Hz), 88.59, 84.20, 53.88, 40.25, 21.52, 15.70. HRMS (ESI) calcd for [$C_{24}H_{21}BrFNNaO_2S$] ([M+Na]$^+$): 508.0353, found: 508.0354. IR (thin film) v 1597.73, 2872.98, 2934.49, 2977.16, 3064.44 cm^{-1}.



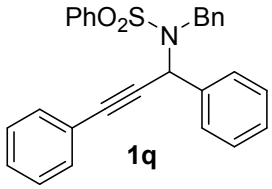
1o

Compound **1o** was obtained as white solid (m.p. = 93-94 ^{o}C, Rf = 0.68 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 8.0 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H), 7.65 – 7.59 (m, 4H), 7.45 (t, J = 7.6 Hz, 2H), 7.40 – 7.26 (m, 6H), 7.17 (d, J = 7.0 Hz, 2H), 6.31 (s, 1H), 3.75 -3.24 (m, 1H), 3.23 - 3.10 (m, 1H), 2.37 (s, 3H), 0.90 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.36, 141.20, 140.47, 136.25, 136.06, 131.56, 129.51, 128.84, 128.65, 128.51, 128.24, 127.83, 127.53, 127.15, 127.13, 122.10, 88.15, 83.69, 53.94, 40.79, 21.47, 16.12. HRMS (ESI) calcd for [$C_{30}H_{27}NNaO_2S$] ([M+Na]$^+$): 488.1655, found: 488.1656. IR (thin film) v 1639.29, 2854.78, 2874.72, 2932.84 cm^{-1}.



1p

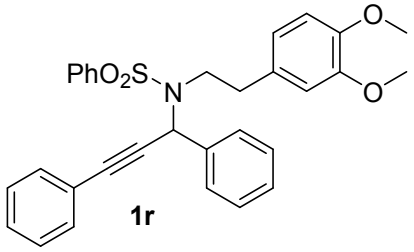
Compound **1p** was obtained as yellow liquid (Rf = 0.43 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 – 7.89 (m, 2H), 7.56 – 7.51 (m, 1H), 7.50 – 7.46 (m, 2H), 7.41 – 7.40 (m, 1H), 7.32 – 7.28 (m, 1H), 7.27 – 7.22 (m, 2H), 7.16 – 7.11 (m, 2H), 6.51 – 6.50 (m, 1H), 6.34 (dd, J = 3.2, 1.8 Hz, 1H), 6.27 (s, 1H), 2.73 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.05, 143.61, 138.00, 132.84, 131.73, 128.96, 128.94, 128.32, 128.00, 121.68, 110.44, 110.26, 86.93, 81.07, 48.88, 30.24. HRMS (ESI) calcd for [$C_{20}H_{17}NNaO_3S$] ([M+Na]$^+$): 374.0821, found: 374.0822. IR (thin film) v 1446.77, 1490.87, 2929.88, 2966.80, 3061.39 cm^{-1}.



1q

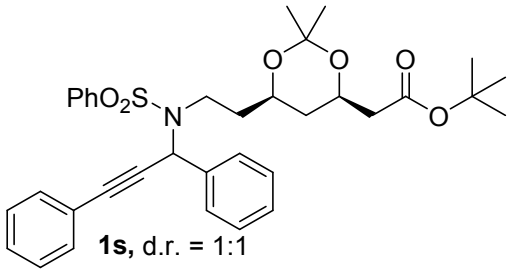
Compound **1q** was obtained as white solid (m.p. = 108-109 ^{o}C, Rf = 0.68 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 – 7.94 (m, 2H), 7.59 (t, J = 7.4 Hz, 1H), 7.55 – 7.50 (m, 4H), 7.38 – 7.34 (m, 1H), 7.34 – 7.30 (m, 2H), 7.25 –

7.22 (m, 2H), 7.21 – 7.15 (m, 3H), 7.07 – 7.01 (m, 5H), 6.42 (s, 1H), 4.58 (d, J = 10.4 Hz, 1H), 4.26 (d, J = 15.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.35, 136.53, 136.15, 132.87, 131.79, 129.11, 128.94, 128.72, 128.46, 128.44, 128.27, 128.22, 127.95, 127.86, 127.07, 122.05, 89.09, 83.41, 54.76, 49.37. HRMS (ESI) calcd for [$C_{28}H_{23}NNaO_2S$] ([M+Na]$^+$): 460.1342, found: 460.1341. IR (thin film) v 1446.37, 1492.01, 2922.60, 3031.68, 3062.26 cm^{-1}.



1r

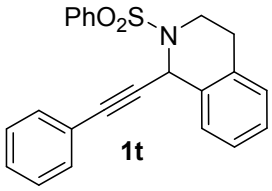
Compound **1r** was obtained as white solid (m.p. = 128-129 ^{o}C, Rf = 0.25 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 – 7.94 (m, 2H), 7.72 (d, J = 7.7 Hz, 2H), 7.57 – 7.52 (m, 1H), 7.51 – 7.47 (m, 2H), 7.42 (t, J = 7.4 Hz, 2H), 7.37 (t, J = 7.3 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.26 – 7.22 (m, 2H), 7.14 – 7.09 (m, 2H), 6.67 (d, J = 8.2 Hz, 1H), 6.43 (dd, J = 8.1, 1.9 Hz, 1H), 6.35 (d, J = 1.9 Hz, 1H), 6.29 (s, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 3.40 – 3.31 (m, 1H), 3.18 – 3.13 (m, 1H), 2.81 – 2.71 (m, 1H), 2.12 – 2.03 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.82, 147.56, 139.02, 136.81, 132.81, 131.65, 131.44, 129.05, 128.86, 128.69, 128.41, 128.34, 127.91, 121.89, 120.66, 111.99, 111.20, 88.46, 83.33, 55.95, 55.83, 54.44, 47.87, 36.91. HRMS (ESI) calcd for [$C_{31}H_{29}NNaO_4S$] ([M+Na]$^+$): 534.1710, found: 534.1708. IR (thin film) v 1590.69, 2833.82, 2870.09, 2935.17 cm^{-1}.



1s, d.r. = 1:1

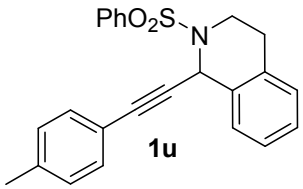
Compound **1h** was obtained as colorless liquid (Rf = 0.52 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.8 Hz, 2H), 7.69 (t, J = 7.6 Hz, 2H), 7.60 – 7.47 (m, 3H), 7.43 – 7.24 (m, 6H), 7.17 (t, J = 7.3 Hz, 2H), 6.30 (d, J = 7.6 Hz, 1H), 4.15 – 4.00 (m, 1H), 3.73 – 3.45 (m, 1H), 3.42 – 3.29 (m, 1H), 3.27 – 3.03 (m, 1H), 2.36 – 2.12 (m, 2H), 1.47 – 1.40 (m, 9H), 1.39 (m, 1.5H), 1.38 – 1.29 (m, 2H), 1.30 – 1.28 (m, 1.5H), 1.25 – 1.22 (m, 3H), 0.94 – 0.83 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.26, 170.22, 138.89, 138.86, 137.06, 136.82, 132.69, 132.66,

131.60, 128.94, 128.75, 128.60, 128.55, 128.49, 128.28, 128.16, 127.87, 127.84, 121.93, 98.69, 98.50, 88.85, 88.54, 83.23, 82.90, 80.55, 80.50, 66.69, 66.13, 66.03, 65.94, 54.33, 54.18, 42.72, 42.70, 42.07, 41.94, 36.37, 36.02, 35.91, 30.01, 29.96, 28.10, 19.69, 19.66. HRMS (ESI) calcd for [$C_{35}H_{41}NNaO_6S$] ([M+Na]$^+$): 626.2547, found: 626.2546. IR (thin film) *v* 1638.29, 1727.00, 2936.94, 2979.87 cm^{-1}. $^{[\alpha]}D^{26.6}$ -7.01 (*c* 0.38, $CHCl_3$).



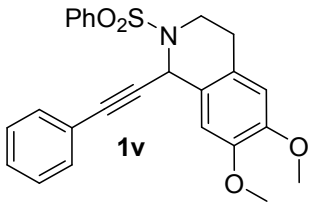
1t

Compound **1t** was obtained as white solid (m.p. = 124-125 ^{o}C, Rf = 0.52 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.5 Hz, 2H), 7.48 – 7.39 (m, 3H), 7.30 – 7.26 (m, 1H), 7.26 – 7.15 (m, 5H), 7.14 – 7.11 (m, 1H), 7.00 (d, *J* = 7.2 Hz, 2H), 6.01 (s, 1H), 4.06 (dd, *J* = 12.4, 6.5 Hz, 1H), 3.38 (td, *J* = 12.2, 4.0 Hz, 1H), 3.23 – 3.08 (m, 1H), 2.90 – 2.77 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.07, 133.98, 132.72, 132.63, 131.63, 129.39, 128.90, 128.52, 128.11, 127.93, 127.72, 127.36, 126.76, 122.15, 86.67, 85.77, 48.81, 40.12, 28.78. HRMS (ESI) calcd for [$C_{23}H_{19}NNaO_2S$] ([M+Na]$^+$): 396.1029, found: 369.1029. IR (thin film) *v* 1446.29, 1489.76, 2864.23, 2926.61, 3061.05 cm^{-1}.



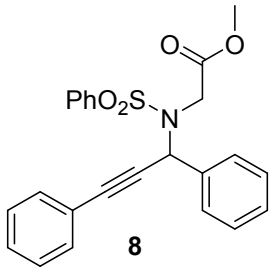
1u

Compound **1h** was obtained as colorless liquid (Rf = 0.52 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.42 (dt, *J* = 14.7, 7.0 Hz, 3H), 7.30 – 7.24 (m, 1H), 7.24 – 7.15 (m, 2H), 7.16 – 7.08 (m, 1H), 6.99 (d, *J* = 7.9 Hz, 2H), 6.90 (d, *J* = 7.9 Hz, 2H), 6.01 (s, 1H), 4.04 (dd, *J* = 12.5, 6.4 Hz, 1H), 3.38 (td, *J* = 12.2, 4.1 Hz, 1H), 3.14 (ddd, *J* = 18.0, 11.9, 6.5 Hz, 1H), 2.82 (dd, *J* = 16.5, 3.9 Hz, 1H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.07, 138.54, 134.09, 132.58, 132.53, 131.44, 129.26, 128.78, 128.76, 127.85, 127.57, 127.28, 126.63, 119.02, 86.72, 85.01, 48.78, 40.01, 28.71, 21.46. HRMS (ESI) calcd for [$C_{24}H_{21}NNaO_2S$] ([M+Na]$^+$): 410.1185, found: 410.1186. IR (thin film) *v* 1509.07, 1644.39, 2866.97, 2924.75, 3030.04 cm^{-1}.



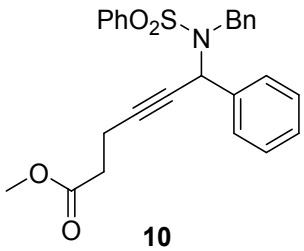
1v

Compound **1h** was obtained as yellow solid (m.p. = 63-64 °C, Rf = 0.16 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 – 7.89 (m, 2H), 7.44 (t, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.25 – 7.22 (m, 1H), 7.18 (t, *J* = 7.4 Hz, 2H), 7.06 – 6.95 (m, 2H), 6.73 (s, 1H), 6.57 (s, 1H), 5.91 (s, 1H), 4.04 (dd, *J* = 12.5, 6.5 Hz, 1H), 3.86 (s, 3H), 3.83 (s, 3H), 3.34 (td, *J* = 12.3, 4.1 Hz, 1H), 3.11 – 3.02 (m, 1H), 2.72 (dd, *J* = 16.2, 2.9 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.64, 147.98, 139.15, 132.66, 131.63, 128.87, 128.50, 128.11, 127.87, 125.78, 124.72, 122.19, 111.46, 109.72, 86.41, 85.90, 56.15, 55.99, 48.44, 40.12, 28.38. HRMS (ESI) calcd for [$C_{25}H_{23}NNaO_4S$] ([M+Na]$^+$): 456.1240, found: 456.1240. IR (thin film) *v* 1489.56, 1518.76, 2835.24, 2933.10 cm^{-1}.



8

Compound **8** was obtained as white solid (m.p. = 77-78 °C, Rf = 0.51 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 – 7.95 (m, 2H), 7.65 (d, *J* = 7.5 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.3 Hz, 2H), 7.34 – 7.30 (m, 2H), 7.27 (t, *J* = 7.4 Hz, 2H), 7.22 – 7.13 (m, 2H), 6.20 (s, 1H), 3.98 (d, *J* = 17.5 Hz, 1H), 3.88 (d, *J* = 17.5 Hz, 1H), 3.38 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.26, 139.00, 135.12, 133.16, 131.76, 129.12, 129.00, 128.88, 128.62, 128.55, 128.39, 128.10, 121.73, 88.55, 82.76, 54.46, 52.12, 45.97. HRMS (ESI) calcd for [$C_{24}H_{21}NNaO_4S$] ([M+Na]$^+$): 442.1083, found: 442.1085. IR (thin film) *v* 1739.41, 1760.98, 2951.37, 3033.04, 3063.36 cm^{-1}.



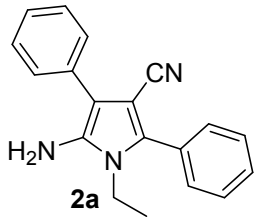
10

Compound **10** was obtained as white solid (m.p. = 82-83 ^{o}C, Rf = 0.46 (petroleum ether/ ethyl acetate = 5:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.9 Hz, 2H), 7.61 (t, *J* = 7.1 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.39 – 7.35 (m, 2H), 7.16 – 7.08 (m, 3H), 7.03 – 6.89 (m, 5H), 6.10 (s, 1H), 4.44 (d, *J* = 15.4 Hz, 1H), 4.11 (d, *J* = 15.4 Hz, 1H), 3.68 (s, 3H), 2.41 – 2.31 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.07, 139.37, 136.53, 136.14, 132.63, 128.83, 128.50, 128.26, 127.99, 127.94, 127.84, 127.66, 126.85, 87.54, 74.99, 54.17, 51.89, 48.95, 33.11, 14.55. HRMS (ESI) calcd for [$C_{26}H_{25}NNaO_4S$] ([M+Na]$^{+}$): 460.1342, found: 460.1341. IR (thin film) *v* 1644.39, 1737.03, 2849.83, 2922.26, 2952.68 cm^{-1}.

Synthesis of pentasubstituted pyrroles

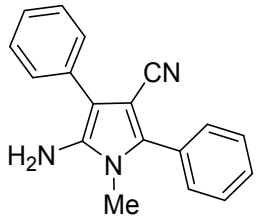
General procedure A: In a flame-dried Schlenk tube, propargyl sulfonylamide **1** (0.2 mmol, 1 equiv), TMSCN (0.6 mmol, 3 equiv) and Cs_2CO_3 (0.6 mmol, 3 equiv) were dissolved in DMF (2 mL) under a nitrogen atmosphere. The reaction mixture was stirred at 80 ^oC for 10 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with water (5 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by neutral alumina flash chromatography to yield the corresponding pentasubstituted pyrrole.

Characterization data for pentasubstituted pyrroles



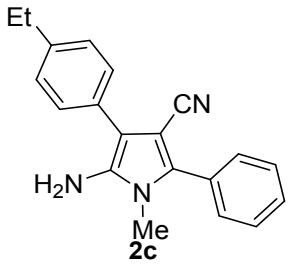
2a

Following the general procedure **A**, **2a** was obtained as a brown solid (37.3 mg, 65% yield, m.p. = 151-152 °C, Rf = 0.45 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.8 Hz, 2H), 7.49 – 7.35 (m, 7H), 7.27 (d, *J* = 7.4 Hz, 1H), 3.90 (q, *J* = 7.1 Hz, 2H), 3.49 (s, 2H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.50, 133.27, 133.11, 129.91, 129.58, 129.08, 128.89, 128.71, 128.05, 126.47, 117.66, 109.57, 90.45, 38.85, 15.76. HRMS (DART) calcd for $[C_{19}H_{18}N_3]^+$ ($[M+H]^+$): 288.1495, found: 288.1496. IR (thin film) *ν* 2211.10 cm^{-1}.



2b

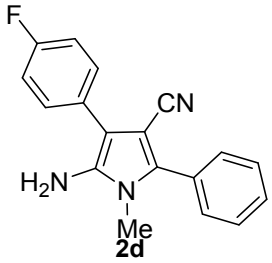
Following the general procedure **A**, **2b** was obtained as a brown liquid (36.0 mg, 66% yield, Rf = 0.34 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.37 (m, 9H), 7.31 – 7.25 (m, 1H), 3.49 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.61, 134.05, 133.08, 129.61, 129.33, 129.10, 128.87, 128.55, 128.00, 126.50, 117.69, 109.12, 90.05, 31.25. HRMS (ESI) calcd for $[C_{18}H_{15}N_3Na]$ ($[M+Na]^+$): 296.1158, found: 296.1160. IR (thin film) *ν* 2209.60 cm^{-1}.



2c

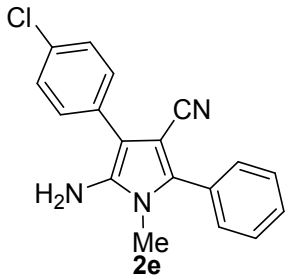
Following the general procedure **A**, **2c** was obtained as a brown liquid (47.0 mg, 78% yield, Rf = 0.41 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 – 7.43 (m, 4H), 7.42 – 7.36 (m, 3H), 7.29 – 7.25 (m, 2H), 3.50 (s, 2H), 3.46 (s,

3H), 2.67 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 142.59, 136.48, 134.12, 130.43, 129.78, 129.38, 128.93, 128.68, 128.54, 128.02, 118.02, 109.14, 90.05, 31.33, 28.69, 15.66. HRMS (ESI) calcd for [$C_{20}H_{19}N_3Na$] ([M+Na]$^+$): 324.1471, found: 324.1471. IR (thin film) v 2209.93 cm^{-1}.



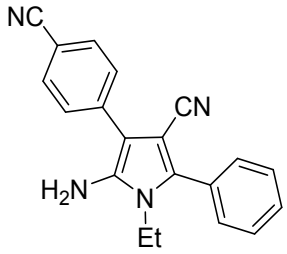
2d

Following the general procedure **A**, **2d** was obtained as a brown solid (37.2 mg, 64% yield, m.p. = 160-161 °C, Rf = 0.31 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 – 7.43 (m, 6H), 7.42 – 7.38 (m, 1H), 7.15 – 7.09 (m, 2H), 3.49 (s, 3H), 3.45 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.55 (d, J = 246.1 Hz), 136.58, 133.84, 129.71 (d, J = 8.0 Hz), 129.51, 129.30, 129.03, 128.90, 128.62, 117.54, 116.03 (d, J = 21.4 Hz), 108.44, 90.09, 31.27. HRMS (ESI) calcd for [$C_{18}H_{14}FN_3Na$] ([M+Na]$^+$): 314.1064, found: 314.1065. IR (thin film) v 2209.30 cm^{-1}.



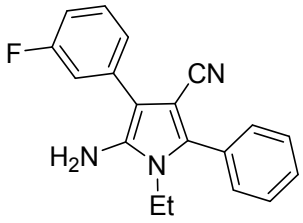
2e

Following the general procedure **A**, **2e** was obtained as a brown solid (39.3 mg, 64% yield, m.p. = 103-104 °C, Rf = 0.34 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 – 7.45 (m, 4H), 7.45 – 7.41 (m, 3H), 7.41 – 7.38 (m, 3H), 3.49 (s, 3H), 3.47 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 136.90, 134.16, 132.32, 131.63, 129.50, 129.38, 129.35, 129.30, 129.00, 128.77, 117.53, 108.07, 90.03, 31.34. HRMS (ESI) calcd for [$C_{18}H_{14}ClN_3Na$] ([M+Na]$^+$): 330.0768, found: 330.0767. IR (thin film) v 2211.78 cm^{-1}.



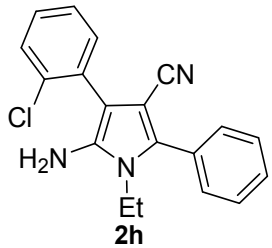
2f

Following the general procedure **A**, **2f** was obtained as a brown liquid (41.8 mg, 67% yield, Rf = 0.21 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 – 7.68 (m, 2H), 7.66 – 7.61 (m, 2H), 7.53 – 7.47 (m, 2H), 7.46 – 7.43 (m, 3H), 3.90 (q, *J* = 7.2 Hz, 2H), 3.61 (s, 2H), 1.30 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.36, 137.59, 134.64, 132.91, 129.62, 129.40, 129.20, 129.09, 128.08, 119.21, 117.24, 109.29, 106.98, 90.18, 38.98, 15.62. HRMS (ESI) calcd for $[C_{20}H_{16}N_4Na]$ ($[M+Na]^+$): 335.1267, found: 335.1267. IR (thin film) *v* 2213.94 cm^{-1}.



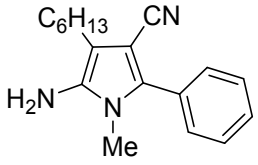
2g

Following the general procedure **A**, **2g** was obtained as a brown soild (48.8 mg, 80% yield, m.p. = 112-113 ^{o}C, Rf = 0.45 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 – 7.36 (m, 6H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 10.0 Hz, 1H), 6.95 (t, *J* = 7.5 Hz, 1H), 3.89 (q, *J* = 7.2 Hz, 2H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.29 (d, *J* = 246.7 Hz), 136.86, 135.38 (d, *J* = 9.7 Hz), 133.69, 130.68 (d, *J* = 8.6 Hz), 129.72, 129.64, 129.00, 128.93, 123.75, 117.46, 114.73 (d, *J* = 21.6 Hz), 113.33 (d, *J* = 21.6 Hz), 108.15, 90.38, 38.94, 15.75. HRMS (ESI) calcd for $[C_{19}H_{16}FN_3Na]$ ($[M+Na]^+$): 328.1220, found: 328.1222. IR (thin film) *v* 2211.63 cm^{-1}.



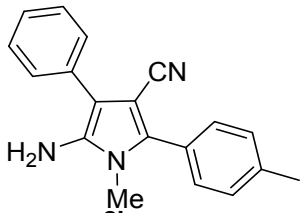
2h

Following the general procedure **A**, **2h** was obtained as a brown liquid (39.8 mg, 62% yield, Rf = 0.48 (petroleum ether/ ethyl acetate = 2:1)).[1]H NMR (600 MHz, $CDCl_3$) δ 7.51 – 7.43 (m, 6H), 7.43 – 7.39 (m, 1H), 7.33 (td, *J* = 7.6, 1.3 Hz, 1H), 7.27 (td, *J* = 7.7, 1.8 Hz, 1H), 3.93 (q, *J* = 7.2 Hz, 2H), 3.27 (s, 2H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 136.60, 133.72, 133.53, 132.69, 131.62, 130.09, 129.96, 129.62, 128.95, 128.89, 128.80, 127.26, 117.33, 108.70, 91.60, 39.00, 15.96. HRMS (ESI) calcd for [$C_{19}H_{16}ClN_3Na$] ([M+Na]$^+$): 344.0925, found: 344.0925. IR (thin film) *v* 2212.23 cm^{-1}.



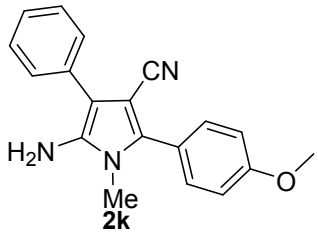
2i

Following the general procedure **A**, **2i** was obtained as a brown liquid (29.8 mg, 53% yield, Rf = 0.45 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 – 7.38 (m, 4H), 7.37 – 7.32 (m, 1H), 3.44 (s, 3H), 3.01 (s, 2H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.61 – 1.54 (m, 2H), 1.39 – 1.32 (m, 2H), 1.32 – 1.28 (m, 4H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 135.53, 132.67, 130.18, 129.18, 128.83, 128.24, 117.90, 111.53, 90.69, 31.81, 31.19, 30.60, 29.24, 24.69, 22.76, 14.22. HRMS (ESI) calcd for [$C_{18}H_{23}N_3Na$] ([M+Na]$^+$): 304.1784, found: 304.1784. IR (thin film) *v* 2202.50 cm^{-1}.



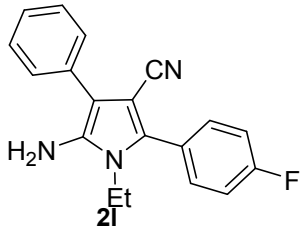
2j

Following the general procedure **A**, **2j** was obtained as a brown solid (46.5 mg, 81% yield, Rf = 0.36 (petroleum ether/ ethyl acetate = 2:1)).[1]H NMR (600 MHz, $CDCl_3$) δ 7.51 – 7.47 (m, 2H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.25 (m, 3H), 3.48 (s, 5H), 2.40 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.67, 136.95, 133.95, 133.25, 129.66, 129.30, 129.16, 128.04, 126.75, 126.50, 117.97, 108.96, 89.75, 31.27, 21.44. HRMS (ESI) calcd for [$C_{19}H_{17}N_3Na$] ([M+Na]$^+$): 310.1315, found: 310.1316. IR (thin film) *v* 2207.86 cm^{-1}.



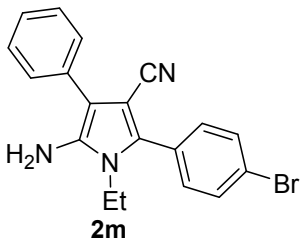
2k

Following the general procedure **A**, **2k** was obtained as a brown liquid (42.4 mg, 70% yield, Rf = 0.24 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.40 – 7.36 (m, 2H), 7.29 – 7.23 (m, 1H), 7.02 – 6.96 (m, 2H), 3.84 (s, 3H), 3.48 (s, 2H), 3.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.82, 136.74, 133.67, 133.22, 130.72, 129.06, 127.94, 126.38, 121.94, 117.97, 114.36, 108.75, 89.47, 55.38, 31.10. HRMS (ESI) calcd for [$C_{19}H_{17}N_3NaO$] ([M+Na]$^+$): 326.1264, found: 326.1263. IR (thin film) *v* 2207.57 cm^{-1}.



2l

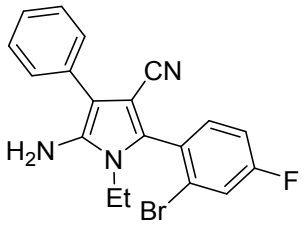
Following the general procedure **A**, **2l** was obtained as a brown solid (48.2 mg, 79% yield, m.p. = 179-180 ^{o}C, Rf = 0.39 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.2 Hz, 2H), 7.45 – 7.41 (m, 4H), 7.31 – 7.24 (m, 1H), 7.21 – 7.12 (m, 2H), 3.87 (q, *J* = 7.2 Hz, 2H), 3.48 (s, 2H), 1.26 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.92 (d, *J* = 249.2 Hz), 135.27, 133.28, 132.97, 131.50 (d, *J* = 8.4 Hz), 129.09, 128.00, 126.52, 125.97 (d, *J* = 3.4 Hz), 117.49, 116.06 (d, *J* = 21.8 Hz), 109.53, 90.69, 38.80, 15.73. HRMS (ESI) calcd for [$C_{19}H_{16}FN_3Na$] ([M+Na]$^+$): 328.1220, found: 328.1216. IR (thin film) *v* 2210.73 cm^{-1}.



2m

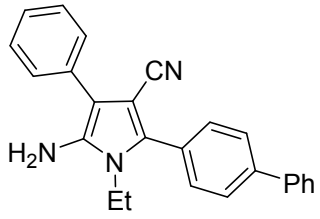
Following the general procedure **A**, **2m** was obtained as a brown solid (55.5 mg, 76% yield, m.p. = 143-144 ^{o}C, Rf = 0.45 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 – 7.57 (m, 2H), 7.50 – 7.47 (m, 2H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.35 – 7.32 (m, 2H), 7.29 – 7.25 (m, 1H), 3.88 (q, *J* = 7.2 Hz, 2H), 3.49 (s, 2H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 135.04, 133.71, 132.92, 132.26, 131.10, 129.19, 128.86, 128.09, 126.69, 123.12, 117.43, 109.87, 90.96, 38.98, 15.84.

HRMS (ESI) calcd for [$C_{19}H_{16}BrN_3Na$] ([M+Na]$^+$): 388.0420, found: 388.0421. IR (thin film) v 2210.48 cm^{-1}.



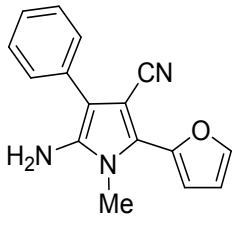
2n

Following the general procedure **A**, **2n** was obtained as a brown liquid (55.2 mg, 72% yield, Rf = 0.45 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 2H), 7.49 – 7.39 (m, 4H), 7.32 – 7.25 (m, 1H), 7.16 (td, J = 8.2, 2.6 Hz, 1H), 3.92 - 3.75 (m, 1H), 3.74 - 3.61 (m, 1H), 3.48 (s, 2H), 1.17 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.03 (d, J = 254.3 Hz), 134.26 (d, J = 8.8 Hz), 133.24, 133.01, 132.82, 129.15, 128.02, 127.49 (d, J = 4.0 Hz), 126.59, 126.33 (d, J = 9.9 Hz), 120.71 (d, J = 24.6 Hz), 116.81, 115.17 (d, J = 21.6 Hz), 109.60, 91.81, 39.05, 15.54. HRMS (ESI) calcd for [$C_{19}H_{15}BrFN_3Na$] ([M+Na]$^+$): 406.0326, found: 406.0327. IR (thin film) v 2214.18 cm^{-1}.



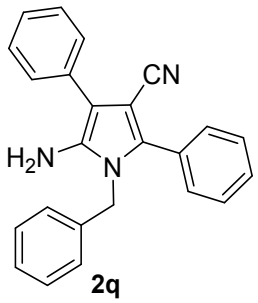
2o

Following the general procedure **A**, **2o** was obtained as a yellow solid (56.6 mg, 78% yield, m.p. = 183-184 ^{o}C, Rf = 0.45 (petroleum ether/ ethyl acetate = 2:1)). NMR (600 MHz, $CDCl_3$) δ 7.69 (d, J = 8.2 Hz, 2H), 7.63 (d, J = 7.8 Hz, 2H), 7.54 – 7.51 (m, 4H), 7.48 – 7.43 (m, 4H), 7.38 (t, J = 7.4 Hz, 1H), 7.28 (t, J = 7.7 Hz, 1H), 3.94 (q, J = 7.2 Hz, 2H), 3.51 (s, 2H), 1.31 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.37, 140.30, 136.14, 133.63, 133.12, 129.87, 129.10, 128.93, 128.76, 128.04, 127.70, 127.57, 127.11, 126.48, 117.83, 109.51, 90.49, 38.97, 15.80. HRMS (ESI) calcd for [$C_{25}H_{21}N_3Na$] ([M+Na]$^+$): 386.1628, found: 386.1627. IR (thin film) v 2210.51 cm^{-1}.



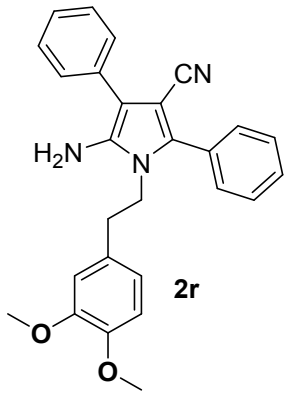
2p

Following the general procedure **A**, **2p** was obtained as a brown liquid (32.0 mg, 61% yield, Rf = 0.21 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 (d, *J* = 1.9 Hz, 1H), 7.47 – 7.41 (m, 5H), 7.28 (t, *J* = 7.2 Hz, 1H), 6.80 (d, *J* = 3.4 Hz, 1H), 6.52 (dd, *J* = 3.4, 1.9 Hz, 1H), 3.67 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.34, 142.43, 134.49, 132.81, 129.20, 128.12, 126.78, 126.29, 117.31, 111.70, 109.95, 109.76, 89.78, 31.69. HRMS (ESI) calcd for $[C_{16}H_{13}N_3NaO]$ ($[M+Na]^+$): 286.0951, found: 286.0951. IR (thin film) *ν* 2209.37 cm^{-1}.



2q

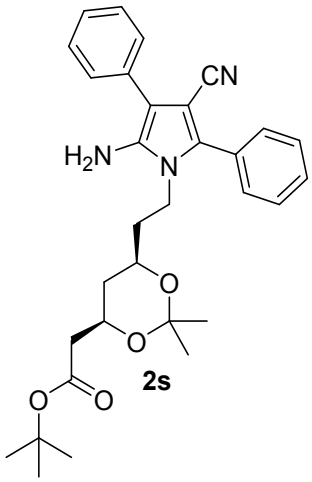
Following the general procedure **A**, **2q** was obtained as a yellow solid (37.7 mg, 54% yield, m.p. = 193-194 ^{o}C, Rf = 0.6 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.4 Hz, 2H), 7.48 – 7.36 (m, 9H), 7.34 – 7.26 (m, 2H), 7.09 (d, *J* = 7.4 Hz, 2H), 5.14 (s, 2H), 3.36 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.04, 136.57, 134.11, 132.95, 129.46, 129.37, 129.29, 129.12, 128.97, 128.78, 128.02, 127.99, 126.55, 125.70, 117.57, 109.17, 90.78, 47.54. HRMS (DART) calcd for $[C_{24}H_{20}N_3]^+$ ($[M+H]^+$): 350.1652, found: 350.1652. IR (thin film) *ν* 2211.83 cm^{-1}.



2r

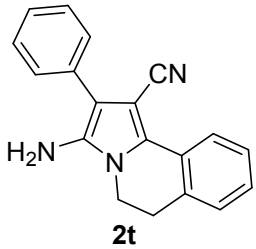
Following the general procedure **A**, **2r** was obtained as a brown liquid (39.8 mg, 47% yield, Rf = 0.45 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 – 7.38 (m, 7H), 7.35 – 7.31 (m, 2H), 7.29 – 7.21 (m, 1H), 6.70 (d, *J* = 8.1 Hz, 1H), 6.45 (dd, *J* = 8.1, 1.9 Hz, 1H), 6.27 (d, *J* = 1.9 Hz, 1H), 4.12 (t, *J* = 7.0 Hz, 2H), 3.83 (s, 3H), 3.69 (s, 3H), 3.06 (s, 2H), 2.71 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.04, 148.10, 136.84, 133.84, 133.13, 130.06, 129.93, 129.78, 129.18, 128.88, 128.82, 128.12, 126.61, 120.87, 117.64, 111.74, 111.39, 109.73, 90.68, 56.04, 55.76,

45.24, 35.98. HRMS (DART) calcd for $[C_{27}H_{26}O_2N_3]^+$ ($[M+H]^+$): 424.2020, found: 424.2020. IR (thin film) *v* 2210.37, cm^{-1}.



2s

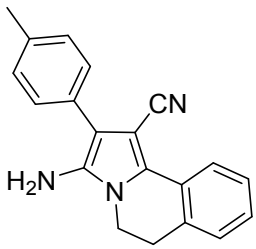
Following the general procedure **A**, **2s** was obtained as a brown liquid (69.0 mg, 67% yield, Rf = 0.21 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 – 7.48 (m, 2H), 7.47 – 7.37 (m, 7H), 7.27 – 7.24 (m, 1H), 4.20 – 4.15 (m, 1H), 4.01 (td, *J* = 13.6, 12.3, 6.2 Hz, 2H), 3.85 (s, 2H), 3.77 – 3.60 (m, 1H), 2.36 (dd, *J* = 15.3, 7.1 Hz, 1H), 2.23 (dd, *J* = 15.3, 6.0 Hz, 1H), 1.82 – 1.60 (m, 4H), 1.47 – 1.43 (m, 1H), 1.41 (s, 9H), 1.40 – 1.38 (m, 1H), 1.35 (s, 3H), 1.32 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.16, 136.03, 134.36, 133.29, 129.99, 129.57, 129.18, 129.01, 128.77, 127.97, 126.40, 117.74, 107.79, 99.07, 90.78, 80.89, 77.35, 77.14, 76.93, 66.03, 65.99, 42.49, 39.13, 36.72, 36.08, 30.08, 28.17, 19.79. HRMS (DART) calcd for $[C_{31}H_{38}O_4N_3]^+$ ($[M+H]^+$): 516.2857, found: 516.2856. IR (thin film) *v* 2212.20, 1726.00 cm^{-1}. $[\alpha]D^{26.6}$ 23.69 (*c* 0.38, $CHCl_3$).



2t

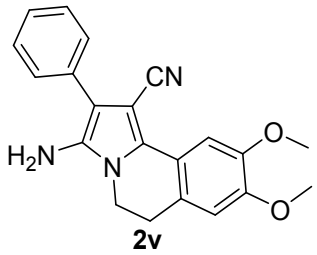
Following the general procedure **A**, **2t** was obtained as a brown liquid (43.9 mg, 77% yield, Rf = 0.26 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 7.8 Hz, 1H), 7.59 – 7.35 (m, 4H), 7.35 – 7.20 (m, 4H), 3.97 (t, *J* = 6.6 Hz, 2H), 3.50 (s, 2H), 3.09 (t, *J* = 6.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.80, 132.46, 130.80, 130.32, 129.12, 128.13, 128.00, 127.83, 127.50, 127.14, 126.67,

123.51, 118.23, 110.72, 86.17, 39.22, 28.72. HRMS (DART) calcd for $[C_{19}H_{16}N_3]^+$ ($[M+H]^+$): 286.1339, found: 286.1340. IR (thin film) *v* 2205.09 cm^{-1}.



2u

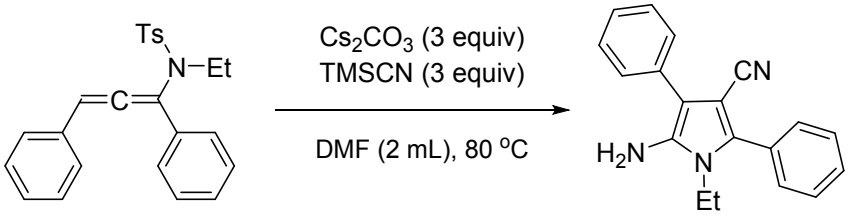
Following the general procedure **A**, **2u** was obtained as a brown liquid (44.3 mg, 74% yield, Rf = 0.30 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (d, *J* = 7.5 Hz, 1H), 7.45 – 7.28 (m, 4H), 7.28 – 7.18 (m, 3H), 5.11 (s, 2H), 3.97 (t, *J* = 6.4 Hz, 2H), 3.04 (t, *J* = 6.1 Hz, 2H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 136.45, 135.24, 131.80, 130.72, 129.74, 128.89, 128.65, 127.99, 127.74, 127.42, 127.29, 122.18, 119.03, 105.91, 85.27, 28.40, 21.22. HRMS (ESI) calcd for $[C_{20}H_{18}N_3]$ ($[M+H]^+$): 300.1495, found: 300.1496. IR (thin film) *v* 2212.23 cm^{-1}.



2v

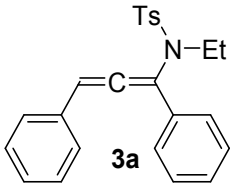
Following the general procedure **A**, **2v** was obtained as a brown liquid (30.4 mg, 44% yield, Rf = 0.1 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (600 MHz, DMSO-d_6) δ 7.52 (s, 1H), 7.43 (d, *J* = 7.0 Hz, 2H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.19 (t, *J* = 7.3 Hz, 1H), 6.93 (s, 1H), 5.07 (s, 2H), 3.89 (t, *J* = 6.7 Hz, 2H), 3.76 (s, 3H), 3.73 (s, 3H), 2.94 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 148.59, 148.30, 136.20, 133.99, 129.96, 129.22, 127.97, 125.94, 124.93, 119.86, 119.50, 112.57, 106.30, 104.99, 83.69, 56.13, 56.01, 27.92. HRMS (ESI) calcd for $[C_{21}H_{20}O_2N_3]$ ($[M+H]^+$): 346.1550, found: 346.1551. IR (thin film) *v* 2212.23 cm^{-1}.

Synthesis of substituted pyrrole 2a directly from allene 3a



3a **2a**, 82%

In a flame-dried Schlenk tube, allenamide **3a** (0.2 mmol, 1 equiv), TMSCN (0.6 mmol, 3 equiv) and Cs_2CO_3 (0.6 mmol, 3 equiv) were dissolved in DMF (2 mL) under a nitrogen atmosphere. The reaction mixture was stirred at 80 °C for 10 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with water (5 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by neutral alumina flash chromatography to yield the product **2a** in 82% yield.

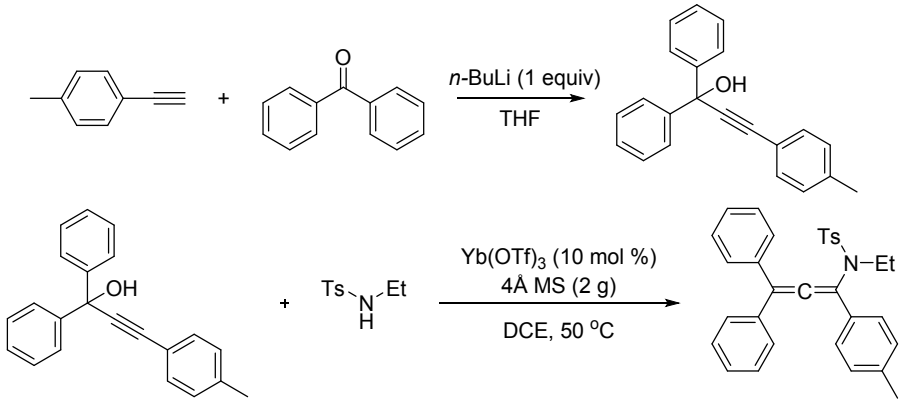


3a

Compound **3a** was obtained as colorless oil (Rf = 0.64 (petroleum ether/ ethyl acetate = 5:1)).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 7.4 Hz, 2H), 7.38 – 7.25 (m, 6H), 7.20 – 7.07 (m, 4H), 6.47 (s, 1H), 3.57 – 3.33 (m, 2H), 2.34 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.66, 143.39, 135.04, 134.91, 132.22, 129.34, 128.84, 128.51, 128.35, 128.21, 127.93, 127.64, 126.15, 115.34, 103.72, 46.05, 21.53, 13.74. HRMS (ESI) calcd for [$C_{24}H_{23}NNaO_2S$] ([M+Na]$^+$): 412.1342, found: 412.1342. IR (thin film) *v* 1910.63, 2827.17, 2924.17, 2976.03, 3027.14, 3057.01, 3081.99 cm^{-1}.

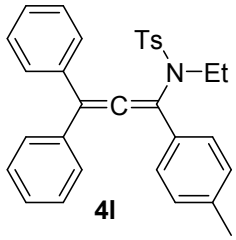
Synthesis of tetrasubstituted allenamides

Tetrasubstituted allenamides **4a-4k** were prepare according our previous work.[1] And **4l** was prepared as following procedure.



To a 50 mL round bottomed flask was charged with 1-ethynyl-4-methylbenzene (5 mmol, 1 equiv) and 10 mL of THF. The solution was cooled to -78 °C and *n*-BuLi (2.5 M in THF, 2 mL, 5 mmol, 1 equiv) was added. The resulting solution was stirred for 20 minutes at room temperature and then cooled to -78 °C again. benzophenone (5 mmol, 1 equiv) in THF solution was added dropwise. The reaction mixture was then allowed to warm to room temperature and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous NH_4Cl (40 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (30 mL), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the propargyl alcohol.

To a 50 mL round bottomed flask was charged with $Yb(OTf)_3$ (10 mol %), the resulting propargyl alcohol (1 equiv), *N*-ethyl-4-methylbenzenesulfonamide (1.5 equiv)， 4A MS (2 g) and DCE (0.2 M). The solution was heated to 50 °C and stirred for 12 h. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the mixture was concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the corresponding tetrasubstituted allenamide.[2]



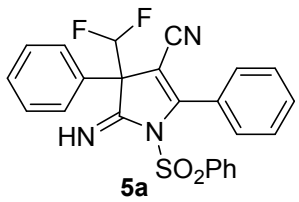
4l

Compound **4l** was obtained as white solid (m.p. = 147-148 °C, Rf = 0.73 (petroleum ether/ ethyl acetate = 3:1)).^{1}H NMR (600 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.2 Hz, 4H), 7.35 – 7.25 (m, 6H), 7.19 – 7.10 (m, 6H), 6.91 (d, *J* = 8.0 Hz, 2H), 3.53 (q, *J* = 7.1 Hz, 2H), 2.35 (s, 3H), 2.28 (s, 3H), 1.10 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 206.37, 143.07, 138.15, 135.60, 135.39, 132.45, 129.38, 129.30, 128.78, 128.52, 128.32, 127.83, 126.15, 119.05, 114.39, 46.14, 21.59, 21.33, 13.91. HRMS (ESI) calcd for [$C_{31}H_{29}NNaO_2S$] ([M+Na]$^+$): 502.1811, found: 502.1812. IR (thin film) *v* 1911.00, 2872.17, 2977.26, 3082.60 cm^{-1}.

Synthesis of hexasubstituted pyrrolines

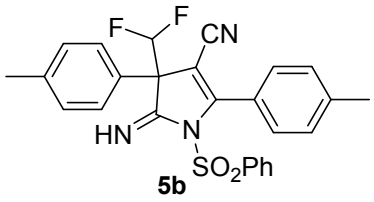
General procedure B: In a flame-dried Schlenk tube, tetrasubstituted allenamide **4** (0.1 mmol, 1 equiv), TMSCN (0.3 mmol, 3 equiv) and K_2CO_3 (0.3 mmol, 3 equiv) were dissolved in DMF (1 mL) under a nitrogen atmosphere. The reaction mixture was stirred at 80 ^oC for 10 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with water (5 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by silica gel flash chromatography to yield the corresponding hexasubstituted pyrroline.

Characterization data for hexasubstituted pyrrolines



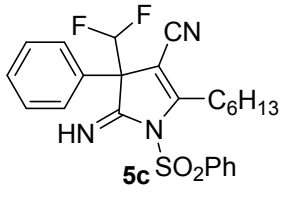
5a

Following the general procedure **B**, **5a** was obtained as a white solid (32.8 mg, 73% yield, m.p. = 128-129 °C, Rf = 0.53 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.10 (s, 1H), 7.57 – 7.47 (m, 3H), 7.46 – 7.37 (m, 3H), 7.32 – 7.26 (m, 2H), 7.22 (d, *J* = 7.6 Hz, 3H), 7.20 – 7.09 (m, 4H), 6.36 (t, *J* = 54.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.35 (d, *J* = 8.2 Hz), 158.32, 136.16, 134.99, 133.79, 132.06, 129.73, 129.41, 129.31, 129.09, 128.43, 127.57, 127.41, 126.49, 116.61 (dd, *J* = 251.4, 247.0 Hz), 114.28, 94.07, 61.08 (t, *J* = 21.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -122.87 – -125.82(m, 2F). HRMS (ESI) calcd for [$C_{24}H_{17}F_2N_3NaO_2S$] ([M+Na]$^+$): 472.0902, found: 472.0899. IR (thin film) *v* 1690.80, 2223.19 cm^{-1}.



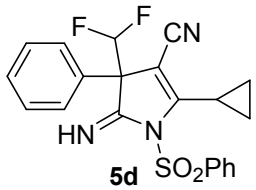
5b

Following the general procedure **B**, **5b** was obtained as a white solid (36.3 mg, 76% yield, m.p. = 137-138 °C, Rf = 0.35 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.12 (s, 1H), 7.52 – 7.48 (m, 1H), 7.48 – 7.44 (m, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.25 – 7.22 (m, 4H), 7.21 – 7.18 (m, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 6.38 (t, *J* = 54.7 Hz, 1H), 2.45 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.61 (d, *J* = 7.4 Hz), 158.30, 142.65, 138.98, 136.25, 134.72, 130.88, 130.03, 129.67, 129.21, 129.09, 127.48, 126.35, 124.68, 116.55 (dd, *J* = 246.5, 246.5 Hz), 114.50, 93.77, 60.78 (t, *J* = 20.9 Hz), 21.83, 21.15. ^{19}F NMR (376 MHz, $CDCl_3$) δ -122.94 – -125.98 (m, 2F). HRMS (ESI) calcd for [$C_{26}H_{21}F_2N_3NaO_2S$] ([M+Na]$^+$): 500.1215, found: 500.1210. IR (thin film) *v* 1687.51, 2219.73 cm^{-1}.



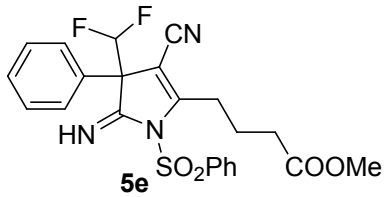
5c

Following the general procedure **B**, **5c** was obtained as a white soild (33.8 mg, 74% yield, m.p. = 73-74 °C, Rf = 0.44 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.01 (s, 1H), 7.57 – 7.53 (m, 3H), 7.37 – 7.33 (m, 2H), 7.29 – 7.26 (m, 1H), 7.26 – 7.21 (m, 4H), 6.36 (t, *J* = 54.8 Hz, 1H), 3.04 – 2.99 (m, 1H), 2.96 – 2.90 (m, 1H), 1.82 – 1.75 (m, 2H), 1.47 – 1.40 (m, 2H), 1.36 – 1.31 (m, 4H), 0.90 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$)) δ 161.50, 159.13 (d, *J* = 8.3 Hz), 136.78, 135.02, 133.82 (d, *J* = 4.2 Hz), 129.72, 129.28, 128.99, 126.82, 126.44, 118.07, 116.42 (dd, *J* = 250.7, 246.4 Hz), 93.02, 60.45 (t, *J* = 21.7 Hz), 31.35, 29.99, 28.69, 22.56, 14.08. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.35 – -125.93(m, 2F). HRMS (ESI) calcd for [$C_{24}H_{25}F_2N_3NaO_2S$] ([M+Na]$^+$): 480.1528, found: 480.1529. IR (thin film) *v* 1688.44, 2221.13 cm^{-1}.



5d

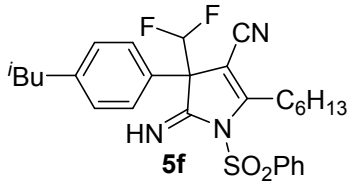
Following the general procedure **B**, **5d** was obtained as a colorless liquid (31.8 mg, 77% yield, Rf = 0.29 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.72 – 7.62 (m, 3H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.42 – 7.28 (m, 5H), 6.43 (t, *J* = 54.6 Hz, 1H), 2.16 – 2.07 (m, 1H), 1.32 – 1.23 (m, 1H), 1.24 – 1.15 (m, 1H), 1.14 – 0.99 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.36, 158.67 (d, *J* = 7.8 Hz), 137.87, 134.98, 133.94, 129.65, 129.35, 129.11, 126.91, 126.61, 116.56 (dd, *J* = 251.1, 245.9 Hz), 114.02, 89.98, 60.89 (t, *J* = 23.8 Hz), 11.08, 9.72, 9.63. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.95 – -125.87 (m, 2F). HRMS (ESI) calcd for [$C_{21}H_{17}F_2N_3NaO_2S$] ([M+Na]$^+$): 436.0902, found: 436.0902. IR (thin film) *v* 1670.92, 2219.26 cm^{-1}.



5e

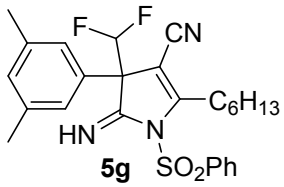
Following the general procedure **B**, **5e** was obtained as a colorless liquid (35.5 mg, 75% yield, Rf = 0.18 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 7.62 – 7.53 (m, 3H), 7.41 – 7.34 (m, 2H), 7.33 – 7.18 (m, 5H), 6.36 (t, *J* = 54.7 Hz, 1H), 3.72 (s, 3H), 3.16 – 2.98 (m, 2H), 2.48 (t, *J* = 7.4 Hz, 2H), 2.25 – 2.10 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.77, 160.03, 158.84 (d, *J* = 7.4 Hz), 136.54,

135.00, 133.48, 129.66, 129.25, 128.99, 126.77, 126.33, 116.25 (dd, J = 251.4, 246.6 Hz), 113.63, 93.87, 60.44 (t, J = 21.8 Hz), 51.87, 32.77, 28.97, 23.70. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.20 – -125.85 (m, 2F). HRMS (ESI) calcd for [$C_{23}H_{21}F_2NaO_4S$] ([M+Na]$^+$): 496.1113, found: 496.1113. IR (thin film) v 1687.26, 1734.93, 2221.07 cm^{-1}.



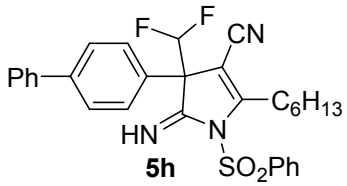
5f

Following the general procedure **B**, **5f** was obtained as a colorless liquid (35.4 mg, 69% yield, Rf = 0.52 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.00 (s, 1H), 7.61 – 7.54 (m, 3H), 7.37 (t, J = 7.8 Hz, 2H), 7.13 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 8.0 Hz, 2H), 6.35 (t, J = 54.8 Hz, 1H), 3.06 – 2.97 (m, 1H), 2.97 – 2.89 (m, 1H), 2.42 (d, J = 7.2 Hz, 2H), 1.86 – 1.76 (m, 3H), 1.49 – 1.40 (m, 2H), 1.38 – 1.31 (m, 4H), 0.93 – 0.87 (m, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.26, 159.26 (d, J = 8.5 Hz), 142.71, 136.92, 134.92, 131.02, 129.95, 129.69, 126.88, 126.13, 116.44 (dd, J = 251.2, 246.6 Hz), 114.19, 93.20, 60.27 (t, J = 21.7 Hz), 44.95, 31.35, 30.17, 29.98, 28.71, 22.57, 22.44, 22.44, 14.07. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.34 – -125.98(m, 2F). HRMS (DART) calcd for [$C_{28}H_{34}O_2N_3F_2S$]$^+$ ([M+H]$^+$): 514.2334, found: 514.2325. IR (thin film) v 1689.73, 2222.35 cm^{-1}.



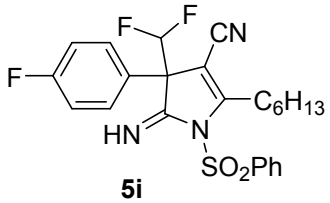
5g

Following the general procedure **B**, **5g** was obtained as a colorless liquid (32.5 mg, 67% yield, Rf = 0.32 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 7.61 – 7.54 (m, 3H), 7.37 (t, J = 7.9 Hz, 2H), 6.92 (s, 1H), 6.77 (s, 2H), 6.37 (t, J = 54.8 Hz, 1H), 3.07 – 2.88 (m, 2H), 2.22 (s, 6H), 1.87 – 1.74 (m, 2H), 1.51 – 1.40 (m, 2H), 1.39 – 1.32 (m, 4H), 0.91 (t, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.05, 159.31 (d, J = 8.0 Hz), 138.74, 136.70, 134.81, 133.64, 130.69, 129.48, 126.81, 123.99, 116.31 (dd, J = 250.4, 246.4 Hz), 114.05, 93.40, 60.36 (t, J = 21.6 Hz), 31.31, 29.95, 28.60, 28.58, 22.53, 21.48, 14.03. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.66, – -125.76 (m, 2F). HRMS (ESI) calcd for [$C_{26}H_{29}F_2N_3NaO_2S$] ([M+Na]$^+$): 508.1841, found: 508.1843. IR (thin film) v 1623.75, 1687.50, 2212.23 cm^{-1}.



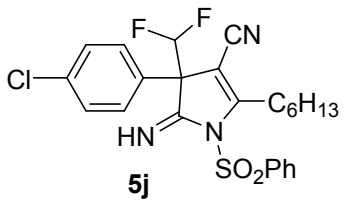
5h

Following the general procedure **B**, **5h** was obtained as a white soild (38.9 mg, 73% yield, m.p. = 95-96 °C, Rf = 0.32 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.05 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 7.6 Hz, 3H), 7.50 – 7.42 (m, 4H), 7.41 – 7.26 (m, 5H), 6.40 (t, *J* = 54.7 Hz, 1H), 3.09 – 2.93 (m, 2H), 1.87 – 1.77 (m, 2H), 1.51 – 1.40 (m, 2H), 1.41 – 1.30 (m, 4H), 0.91 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.52, 159.14 (d, *J* = 7.9 Hz), 141.83, 139.90, 136.70, 134.87, 132.59, 129.65, 128.99, 127.91, 127.85, 127.06, 126.82, 116.29 (dd, *J* = 247.9, 248.3 Hz), 113.84, 92.99, 60.23 (t, *J* = 21.8 Hz), 31.30, 30.00, 28.65, 22.53, 14.05. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.19 – -125.83(m, 2F). HRMS (ESI) calcd for [$C_{30}H_{29}F_2N_3NaO_2S$] ([M+Na]$^+$): 556.1841, found: 556.1832. IR (thin film) *v* 1621.19, 1688.47, 2220.92 cm^{-1}.



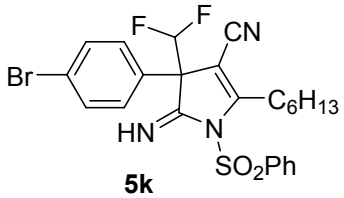
5i

Following the general procedure **B**, **5i** was obtained as a colorless liquid (39.4 mg, 83% yield, m.p. = 60-61 °C, Rf = 0.42 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.57 (d, *J* = 8.3 Hz, 3H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.28 – 7.21 (m, 2H), 6.94 (t, *J* = 8.5 Hz, 2H), 6.31 (t, *J* = 54.7 Hz, 1H), 3.08 – 2.99 (m, 1H), 2.98 – 2.89 (m 1H), 1.84 – 1.74 (m, 2H), 1.49 – 1.39 (m, 2H), 1.38 – 1.30 (m, 4H), 0.90 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.77 (d, *J* = 249.6 Hz), 161.70, 158.90 (d, *J* = 8.2 Hz), 136.58, 134.99, 129.67, 129.53, 128.39 (d, *J* = 8.4 Hz), 126.74, 116.15 (d, *J* = 21.7 Hz), 116.19 (t, *J* = 249.0 Hz), 113.96, 92.66, 59.75 (t, *J* = 21.9 Hz), 31.25, 29.94, 28.60, 28.58, 22.48, 14.00. ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.18 (s, 1F), -121.45 – -126.16 (m, 2F). HRMS (ESI) calcd for [$C_{24}H_{24}F_3N_3NaO_2S$] ([M+Na]$^+$): 498.1434, found: 498.1434. IR (thin film) *v* 1621.49, 1688.86, 2221.47 cm^{-1}.



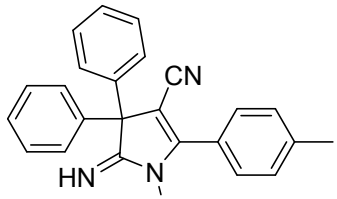
5j

Following the general procedure **B**, **5j** was obtained as a colorless liquid (30.4 mg, 62% yield, m.p. = 63-64 °C, Rf = 0.45 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.21 – 7.09 (m, 4H), 6.22 (t, *J* = 54.7 Hz, 1H), 3.00 – 2.91 (m, 1H), 2.90 – 2.81 (m, 1H), 1.77 – 1.66 (m, 2H), 1.40 – 1.32 (m, 2H), 1.32 – 1.25 (m, 4H), 0.84 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.80, 158.78 (d, *J* = 8.2 Hz), 136.61, 135.23, 134.99, 132.20, 129.69, 129.34, 127.83, 126.76, 116.04 (dd, *J* = 250.7, 247.4 Hz), 113.85, 92.52, 59.84 (t, *J* = 22.0 Hz), 31.26, 29.98, 28.62, 28.60, 22.49, 14.01. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.03 – -125.93 (m, 2F). HRMS (ESI) calcd for [$C_{24}H_{24}ClF_2N_3NaO_2S$] ([M+Na]$^+$): 514.1138, found: 514.1139. IR (thin film) *v* 1652.87, 1685.26, 2221.18 cm^{-1}.



5k

Following the general procedure **B**, **5k** was obtained as a colorless liquid (34.2 mg, 64% yield, m.p. = 85-86 °C, Rf = 0.53 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.59 – 7.53 (m, 2H), 7.43 – 7.36 (m, 4H), 7.15 – 7.09 (m, 2H), 6.29 (t, *J* = 54.7 Hz, 1H), 3.07 – 2.98 (m, 1H), 2.97 – 2.89 (m, 1H), 1.84 – 1.74 (m, 2H), 1.51 – 1.39 (m, 2H), 1.39 – 1.30 (m, 4H), 0.91 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.83, 158.72 (d, *J* = 8.1 Hz), 136.59, 135.00, 132.73 (d, *J* = 4.3 Hz), 132.30, 129.69, 128.10, 126.75, 123.46, 115.97 (dd, *J* = 251.0, 247.5 Hz), 113.83, 92.46, 59.91 (t, *J* = 22.9 Hz), 31.25, 29.98, 28.60, 22.49, 14.01. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.02 – -125.92 (m, 2F). HRMS (ESI) calcd for [$C_{24}H_{24}BrF_2N_3NaO_2S$] ([M+Na]$^+$): 558.0633, found: 558.0624. IR (thin film) *v* 1620.44, 1688.56, 2221.17 cm^{-1}.



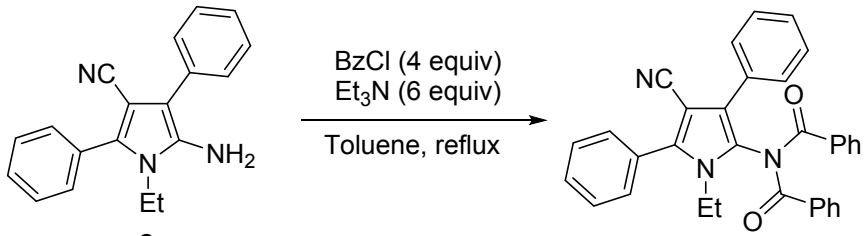
5l

Following the general procedure **B**, **5l** was obtained as a white solid (30.9 mg, 82% yield, m.p. = 155-156 °C, Rf = 0.2 (petroleum ether/ ethyl acetate = 3:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.37 (m, 6H), 7.37 – 7.26 (m, 8H), 3.70 (q, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 1.11 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.08, 159.36,

141.34, 140.67, 129.82, 129.16, 128.37, 127.91, 127.88, 125.23, 117.06, 92.38, 64.24, 37.67, 21.55, 13.57. HRMS (DART) calcd for $[C_{26}H_{24}N_3]^+$ ($[M+H]^+$): 378.1965, found: 378.1963. IR (thin film) *v* 1598.08, 1617.54, 1650.46, 2198.45, 2212.23 cm^{-1}.

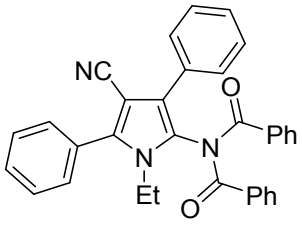
Synthetic applications

1) Protection of the amine group

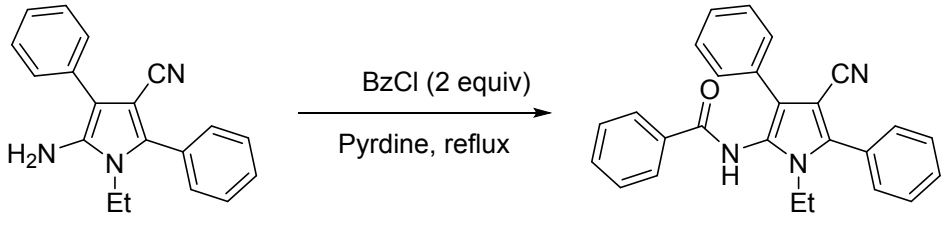


2a **6**, yield:76%

In a flame-dried Schlenk tube was charged with pentasubstituted pyrrole (**2a**, 0.2 mmol), Et_3N (1.2 mmol), toluene (1 mL) and BzCl (0.8 mmol). The resulting suspension was stirred under reflux for 10 h. Upon completion of the reaction as monitored by TLC, the solvent was concentrated under vacuum. The crude residue was purified by flash column chromatography on silica gel to give product **6** as a white soild in 76% yield.

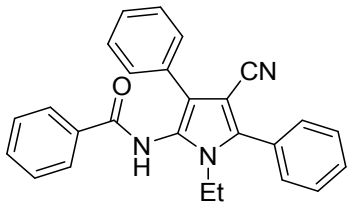


Compound **6** was obtained as white solid (m.p. = 79-80 °C, Rf = 0.48 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 9H), 7.42 (t, J = 7.5 Hz, 2H), 7.35 – 7.29 (m, 5H), 7.27 (t, J = 7.8 Hz, 4H), 4.00 (q, J = 7.2 Hz, 2H), 1.14 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.28, 140.64, 133.85, 132.93, 130.92, 129.75, 129.72, 129.25, 129.16, 129.02, 128.89, 128.85, 128.53, 128.28, 125.27, 124.41, 116.12, 93.03, 39.94, 15.66. HRMS (DART) calcd for $[C_{33}H_{25}O_2N_3]^+$ ($[M+H]^+$): 495.1941, found: 495.1938. IR (thin film) ν 1698.71, 2220.56.23 cm^{-1}.



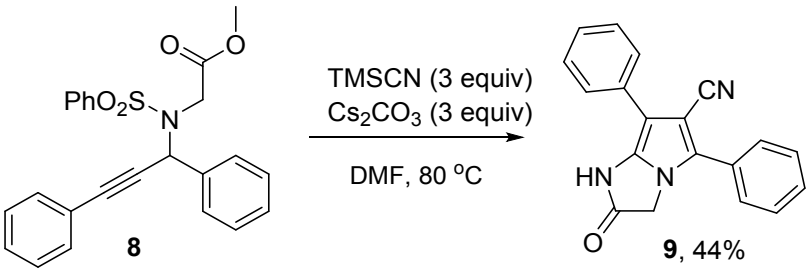
2a **7**, yield:97%

In a flame-dried Schlenk tube was charged with pentasubstituted pyrrole (**2a**, 0.2 mmol), pyridine (1 mL) and BzCl (0.4 mmol). The resulting suspension was stirred under reflux for 1 h. Upon completion of the reaction as monitored by TLC, the solvent was concentrated under vacuum. The crude residue was purified by flash column chromatography on silica gel to give product **7** as a white solid in 97% yield.

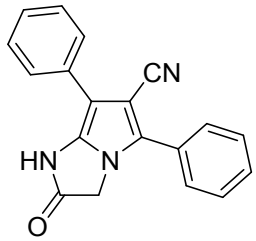


Compound **7** was obtained as white solid (m.p. = 186-187 ^{o}C, Rf = 0.32 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 2H), 7.79 (s, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.52 – 7.40 (m, 9H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.26 (t, *J* = 7.4 Hz, 1H), 3.89 (q, *J* = 7.2 Hz, 2H), 1.15 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.79, 140.07, 132.82, 131.68, 129.77, 129.49, 129.44, 129.08, 129.05, 128.92, 128.34, 127.62, 127.59, 122.92, 122.13, 116.88, 91.65, 39.91, 16.26. HRMS (DART) calcd for $[C_{26}H_{22}ON_3]^+$ ($[M+H]^+$): 392.1757, found: 392.1757. IR (thin film) *v* 1657.70, 2218.22 cm^{-1}.

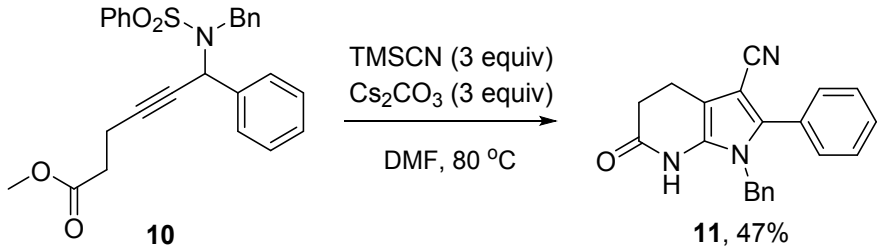
2) Synthesis of lactams



In a flame-dried Schlenk tube, propargyl sulfonylamide **8** (0.2 mmol, 1 equiv), TMSCN (0.6 mmol, 3 equiv) and Cs_2CO_3 (0.6 mmol, 3 equiv) were dissolved in DMF (2 mL) under a nitrogen atmosphere. The reaction mixture was stirred at 80 °C for 10 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with water (5 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by silica gel flash chromatography to yield the product **9** as a white solid in 44% yield.

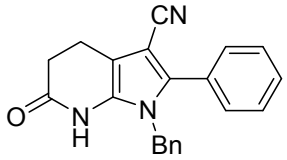


Compound **9** was obtained as white solid (m.p. = 100-101 °C, Rf = 0.79 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (400 MHz, DMSO-d_6) δ 11.66 (s, 1H), 7.67 (d, J = 7.8 Hz, 2H), 7.47 (t, J = 7.4 Hz, 4H), 7.37 (t, J = 7.6 Hz, 3H), 7.21 (t, J = 7.3 Hz, 1H), 4.80 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.07, 135.17, 134.74, 131.64, 129.68, 129.30, 129.24, 129.10, 127.28, 127.02, 126.89, 118.24, 102.67, 89.00, 50.10. HRMS (ESI) calcd for [$C_{19}H_{13}N_3NaO$] ([M+Na]$^+$): 322.0951, found: 322.0951. IR (thin film) v 1673.73, 2218.03 cm^{-1}.



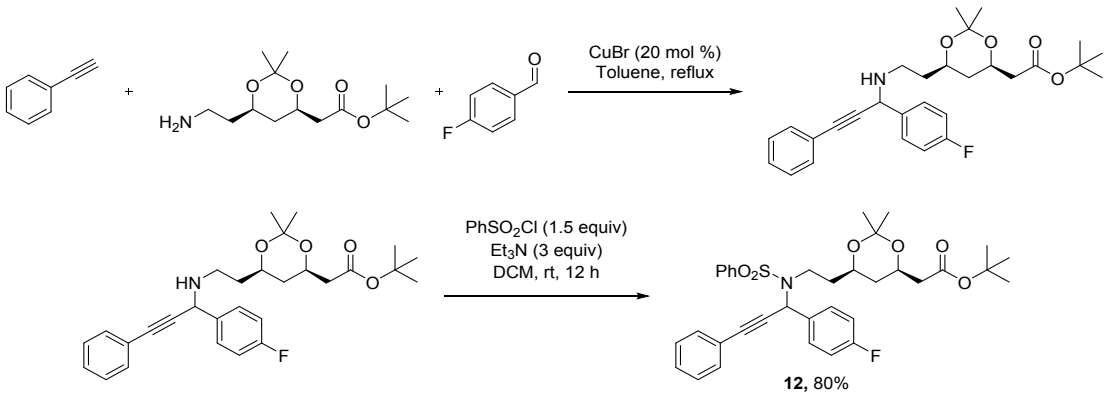
In a flame-dried Schlenk tube, propargyl sulfonylamide **10** (0.2 mmol, 1 equiv),

TMSCN (0.6 mmol, 3 equiv) and Cs_2CO_3 (0.6 mmol, 3 equiv) were dissolved in DMF (2 mL) under a nitrogen atmosphere. The reaction mixture was stirred at 80 °C for 10 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with water (5 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by silica gel flash chromatography to yield the product **11** in 47% yield.



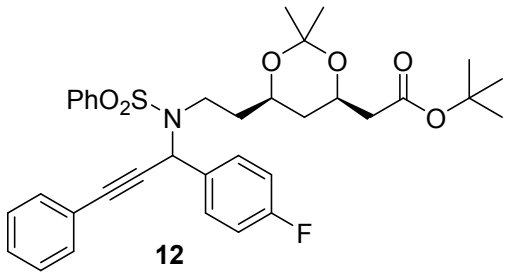
Compound **11** was obtained as white solid (m.p. = 189-190 °C, Rf = 0.23 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (600 MHz, $CDCl_3$) δ 9.19 (s, 1H), 7.42 – 7.36 (m, 3H), 7.36 – 7.33 (m, 2H), 7.32 – 7.25 (m, 3H), 6.92 (d, J = 6.6 Hz, 2H), 5.10 (s, 2H), 2.84 (t, J = 7.7 Hz, 2H), 2.61 (t, J = 7.7 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.91, 137.17, 135.82, 130.03, 129.38, 129.22, 129.17, 128.86, 128.19, 125.85, 116.40, 102.99, 90.65, 47.33, 31.76, 17.80. HRMS (DART) calcd for $[C_{21}H_{18}ON_3]^+$ ($[M+H]^+$): 328.1444, found: 328.1444. IR (thin film) ν 1673.43, 2218.09 cm^{-1}.

3) Synthesis of atorvastatin analogues



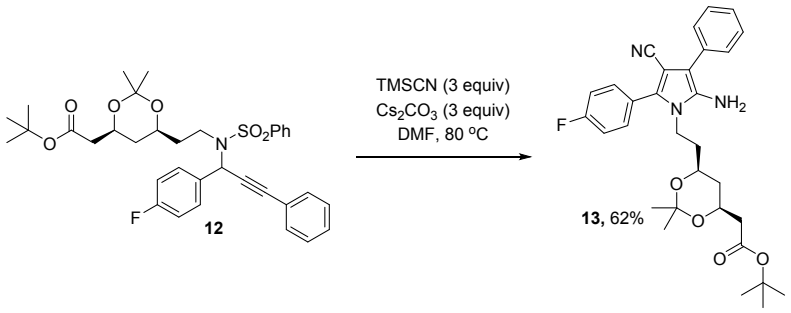
To a 50 mL round bottomed flask was charged with CuBr (1 mmol, 20 mol %), phenylacetylene (5 mmol, 1 equiv), benzaldehyde (7.5 mmol, 1.5 equiv), primary amine (7.5 mmol, 1.5 equiv) and 10 mL of toluene. The solution was heated to reflux and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure to afford the crude propargylamide.

The resulting crude propargylamide and Et_3N (3 equiv) were dissolved in dry DCM, and the mixture was cooled to 0 °C with a cooling bath. To this solution benzenesulfonyl chloride (1.5 equiv) was slowly added in drops, and the mixture was allowed to warm to room temperature and was monitored by TLC for completion. On completion the reaction was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the desired product **12** in 80% yield.

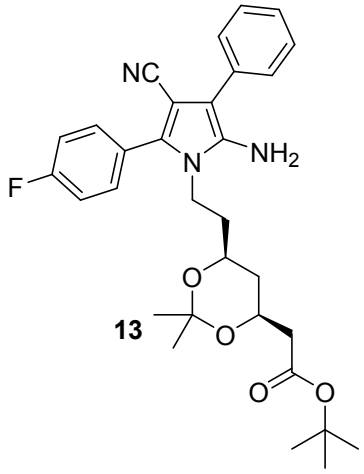


Compound **12** was obtained as colorless liquid (Rf = 0.75 (petroleum ether/ ethyl acetate = 2:1)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.5 Hz, 2H), 7.74 – 7.63 (m, 2H), 7.59 – 7.48 (m, 3H), 7.35 – 7.25 (m, 3H), 7.17 (t, J = 7.2 Hz, 2H), 7.08 (t, J = 8.4 Hz, 2H), 6.27 (s, 1H), 4.21 – 4.02 (m, 1H), 3.78 – 3.47 (m, 1H), 3.42 – 3.29 (m, 1H),

3.29 – 3.02 (m, 1H), 2.41 – 2.14 (m, 2H), 1.82 – 1.57 (m, 1H), 1.50 – 1.35 (m, 12H), 1.29 – 1.26 (m, 3H), 1.22 – 0.90 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.22, 170.17, 162.73 (d, *J* = 247.9 Hz), 138.80, 138.73, 132.92 (d, *J* = 3.1 Hz), 132.77 (d, *J* = 3.9 Hz), 131.59, 129.92 (d, *J* = 8.3 Hz), 128.98, 128.88, 128.32, 128.31, 127.81, 127.78, 121.72, 115.48 (d, *J* = 21.8 Hz), 115.46 (d, *J* = 21.6 Hz), 98.69, 98.52, 88.96, 88.80, 82.89, 82.73, 80.58, 80.55, 66.60, 66.10, 66.08, 66.03, 53.70, 53.63, 42.68, 42.66, 41.94, 36.33, 36.31, 36.00, 35.86, 30.01, 29.96, 28.08, 19.67, 19.63. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.36 (s, 1F), -113.53 (s, 1F). HRMS (DART) calcd for $[C_{35}H_{41}O_6NFS]^+$ ($[M+H]^+$): 622.2633, found: 622.2632. $^{[\alpha]}D^{26.6}$ 28.65 (*c* 0.44, $CHCl_3$).

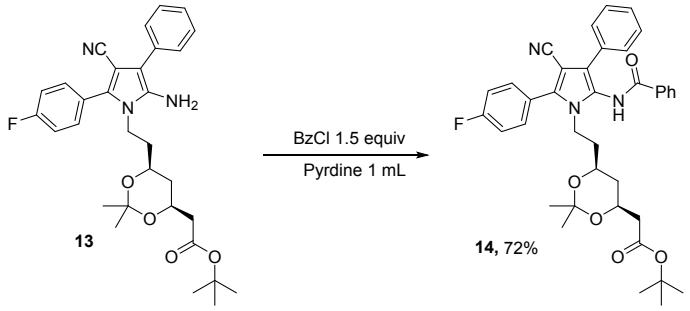


In a flame-dried Schlenk tube, propargyl sulfonylamide **12** (0.2 mmol, 1 equiv), TMSCN (0.6 mmol, 3 equiv) and Cs_2CO_3 (0.6 mmol, 3 equiv) were dissolved in DMF (2 mL) under a nitrogen atmosphere. The reaction mixture was stirred at 80 °C for 10 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with water (5 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by neutral alumina flash chromatography to yield the product **13** as a brown liquid in 62% yield.

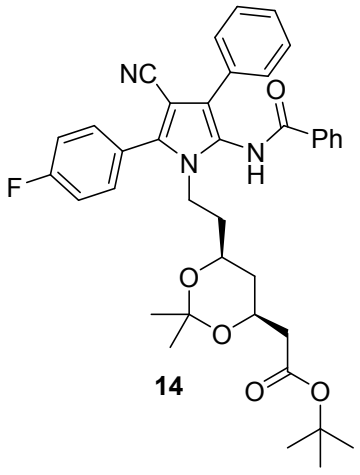


Compound **13** was obtained as brown liquid (Rf = 0.43 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.39 (m, 6H), 7.27 (t, *J* = 7.2 Hz, 1H), 7.17 (t, *J* = 8.5 Hz, 2H), 4.27 – 4.12 (m, 1H), 3.98 (t, *J* = 6.6 Hz, 2H), 3.84 (s, 2H), 3.73

(t, *J* = 10.1 Hz, 1H), 2.39 (dd, *J* = 15.3, 7.0 Hz, 1H), 2.25 (dd, *J* = 15.3, 6.1 Hz, 1H), 1.71 – 1.62 (m, 2H), 1.43 (s, 9H), 1.37 (s, 3H), 1.34 (s, 3H), 1.23 – 1.05 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.04, 162.89 (d, *J* = 249.4 Hz), 134.74, 134.26, 133.09, 131.45 (d, *J* = 8.2 Hz), 129.10, 127.86, 126.39, 125.99 (d, *J* = 3.5 Hz), 117.46, 116.09 (d, *J* = 21.8 Hz), 107.76, 99.00, 90.98, 80.81, 65.95, 65.90, 42.41, 39.07, 36.67, 36.03, 30.01, 28.09, 19.72. ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.08 (s, 1F). HRMS (DART) calcd for $[C_{31}H_{37}O_4N_3F]^+$ ($[M+H]^+$): 534.2763, found: 534.2760. IR (thin film) *v* 1686.42, 1731.14, 2214.02 cm^{-1}. $[\alpha]D^{26.6}$ -8.02 (*c* 0.69, $CHCl_3$).

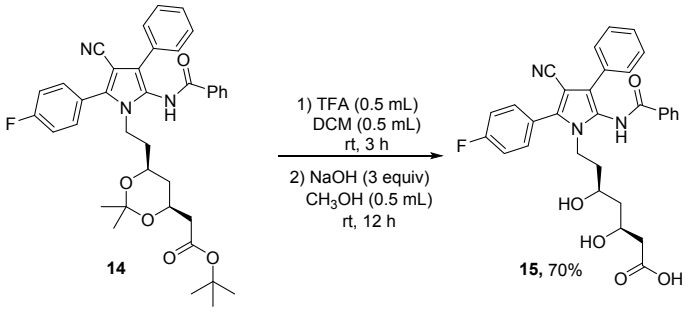


In a flame-dried Schlenk tube was charged with pentasubstituted pyrrole (**13**, 0.2 mmol), pyridine (1 mL) and BzCl (0.3 mmol). The resulting suspension was stirred under reflux for 1 h. Upon completion of the reaction as monitored by TLC, the solvent was concentrated under vacuum. The crude residue was purified by flash column chromatography on silica gel to give the product **14** as a yellow solid in 72% yield.



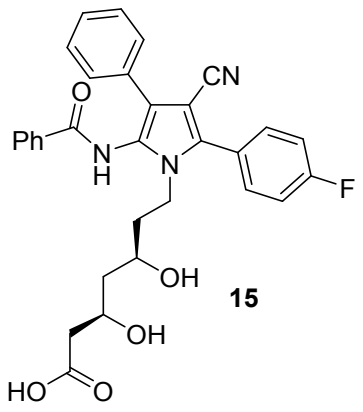
Compound **7** was obtained as yellow solid (m.p. = 68-69 °C, Rf = 0.43 (petroleum ether/ ethyl acetate = 2:1)).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.5 Hz, 2H), 7.70 (s, 1H), 7.62 – 7.44 (m, 7H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 7.3 Hz, 1H), 7.22 (t, *J* = 8.6 Hz, 2H), 4.16 – 4.07 (m, 2H), 3.99 – 3.89 (m, 1H), 3.63 – 3.56 (m, 1H), 2.31 (dd, *J* = 15.4, 7.0 Hz, 1H), 2.18 (dd, *J* = 15.3, 6.1 Hz, 1H), 1.68 – 1.65 (m, 2H), 1.41 (s, 9H), 1.36 – 1.29 (m, 2H), 1.25 (s, 3H), 1.12 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.10, 168.65, 163.29 (d, *J* = 250.4 Hz), 138.87, 132.97, 132.70, 131.65 (d, *J* = 8.5 Hz),

131.45, 128.97, 128.86, 128.21, 127.62, 127.51, 125.39 (d, J = 3.2 Hz), 122.88, 122.55, 116.31 (d, J = 21.8 Hz), 98.78, 92.10, 80.81, 66.11, 65.86, 42.31, 40.84, 36.76, 35.89, 29.83, 28.07, 19.58. ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.89 (s, 1F). HRMS (DART) calcd for $[C_{38}H_{41}O_5N_3F]^+$ ($[M+H]^+$): 638.3025, found: 638.3017. IR (thin film) v 1662.18, 1726.90, 2218.74 cm^{-1}. $[\alpha]D^{26.6}$ 17.71 (c 0.41, $CHCl_3$).



In a flame-dried Schlenk tube was charged with **14** (0.1 mmol), DCM (0.5 mL) and TFA (0.5 mL). The resulting suspension was stirred at room temperature for 3 h. Upon completion of the reaction as monitored by TLC, the solvent was concentrated under vacuum. The crude residue was extracted with ethyl acetate and saturated aqueous $NaHCO_3$. And the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure to afford the crude material.

The resulting crude material and NaOH (3 equiv) were dissolved in MeOH (0.5 mL). The resulting suspension was stirred at room temperature for 12 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with 2 M HCl. The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine, dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by flash chromatography to yield the desired product **15** as a white solid in 70% yield.

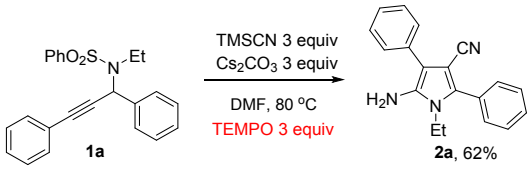


15

Compound **15** was obtained as white solid (m.p. = 145-146 °C, Rf = 0.38 (DCM/MeOH = 10:1)).^{1}H NMR (400 MHz, DMSO-d_6) δ 10.43 (s, 1H), 7.97 (d, J = 7.3 Hz, 2H), 7.72 – 7.58 (m, 3H), 7.53 (q, J = 7.3 Hz, 4H), 7.43 (q, J = 8.5, 8.0 Hz, 4H), 7.30 (t, J = 7.4 Hz, 1H), 4.00 (dd, J = 17.3, 7.3 Hz, 1H), 3.86 – 3.74 (m, 2H), 2.12 (d, J = 4.2 Hz, 1H), 1.99 (dd, J = 15.2, 8.1 Hz, 1H), 1.78 – 1.68 (m, 1H), 1.65 – 1.55 (m, 1H), 1.37 (dd, J = 15.0, 7.6 Hz, 1H), 1.24 (t, J = 8.1 Hz, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 170.92 168.69, 163.15 (d, J = 247.8 Hz), 138.50, 133.71, 132.74, 132.60 (d, J = 8.3 Hz), 132.33, 129.21, 129.17, 128.33, 128.23, 127.79, 125.98, 124.73, 121.82, 117.20, 116.70 (d, J = 21.6 Hz), 90.64, 66.40, 44.31, 43.73, 42.08, 38.09. ^{19}F NMR (376 MHz, DMSO-d_6) δ -111.47 (s, 1F). HRMS (ESI) calcd for [$C_{31}H_{28}N_3FNaO_5$] ([M+Na]$^+$): 564.1905, found: 564.1906. IR (thin film) v 1655.41, 2221.13 cm^{-1}. $^{[\alpha]}D^{26.6}$ -168.4 (*c* 0.29, MeOH).

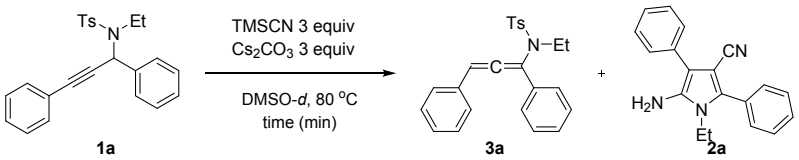
Preliminary mechanism study

a) Radical trapping reaction

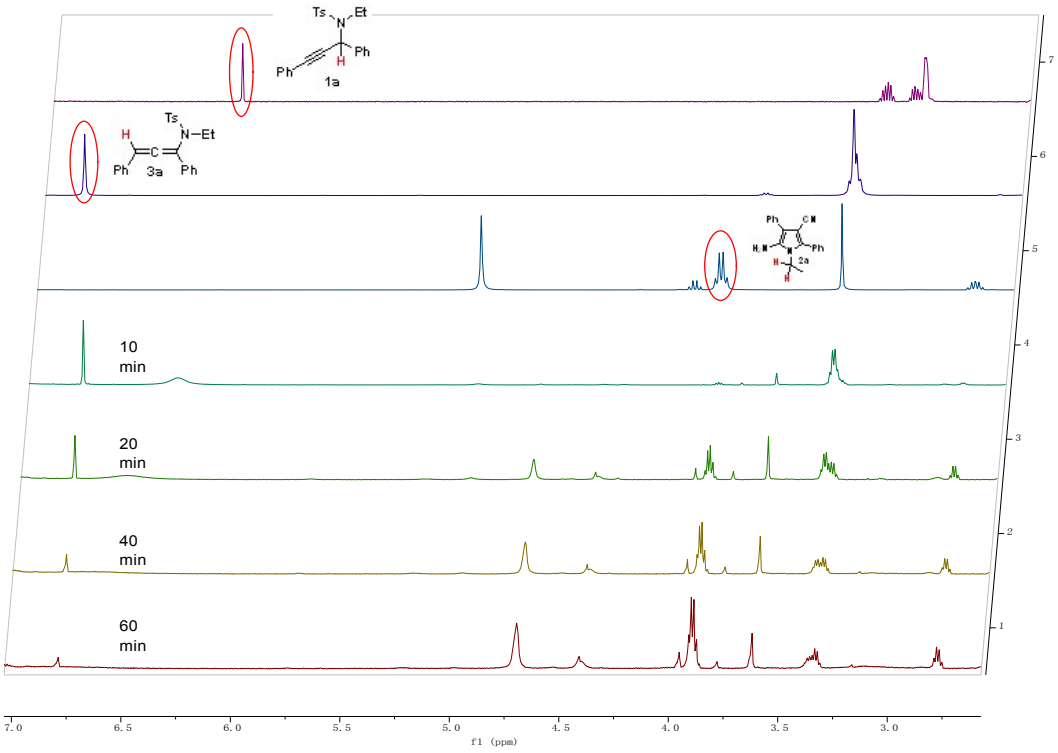


In a flame-dried Schlenk tube, propargyl sulfonylamide **1a** (0.2 mmol, 1 equiv), TMSCN (0.6 mmol, 3 equiv) Cs_2CO_3 (0.6 mmol, 3 equiv) and TEMPO (0.6 mmol, 3 equiv) were dissolved in DMF (2 mL) under a nitrogen atmosphere. The reaction mixture was stirred at 80 °C for 10 h. Upon completion of the reaction as monitored by TLC, the reaction was quenched with water (5 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers were washed with brine (10 mL*3), water (10 mL*3), dried over $MgSO_4$ and filtered. Then the solution was concentrated under reduced pressure. The crude material was purified by silica gel flash chromatography to yield the product **2a** in 62% yield.

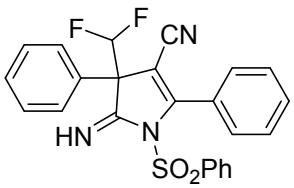
b) ^{1}H NMR of crude reaction solution



In a flame-dried NMR tube, propargyl sulfonylamide **1a** (0.1 mmol, 1 equiv), TMSCN (0.3 mmol, 3 equiv) Cs_2CO_3 (0.3 mmol, 3 equiv) and were dissolved in DMSO-*d* (0.5 mL) under a nitrogen atmosphere. And the reaction was carried out in NMR machine at 80 °C and was monitored in situ after 10, 20, 40 and 60 minutes.



Single crystal data of 5a



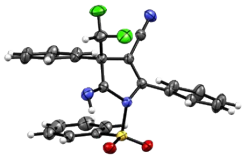
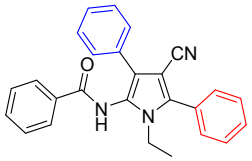


Table S1 Crystal data and structure refinement for 5a.

Identification code	**5a**
Empirical formula	$C_{24}H_{17}F_2N_3O_2S$
Formula weight	449.46
Temperature/K	292.90(11)
Crystal system	monoclinic
Space group	C2/c
a/Å	27.864(4)
b/Å	9.0235(19)
c/Å	17.39(2)
α/°	90
β/°	94.11(4)
γ/°	90
Volume/Å^3	4362(6)
Z	8
ρ_{calc}g/cm^3	1.369
μ/mm^{-1}	1.699
F(000)	1856.0
Crystal size/mm^3	0.3 × 0.2 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.198 to 130.88
Index ranges	-27 ≤ h ≤ 32, -10 ≤ k ≤ 6, -20 ≤ l ≤ 19
Reflections collected	8983
Independent reflections	3649 [R_{int} = 0.0214, R_{sigma} = 0.0249]
Data/restraints/parameters	3649/0/297
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0406, wR_2 = 0.1061
Final R indexes [all data]	R_1 = 0.0499, wR_2 = 0.1155
Largest diff. peak/hole / e Å^{-3}	0.14/-0.30

Single crystal data of 7



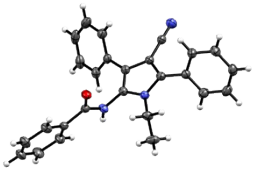


Table S2 Crystal data and structure refinement for 7.

Identification code	**7**
Empirical formula	$C_{26}H_{21}N_3O$
Formula weight	391.46
Temperature/K	110.43(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	24.8324(4)
b/Å	9.05410(10)
c/Å	21.9042(4)
α/°	90
β/°	109.819(2)
γ/°	90
Volume/Å^3	4633.12(14)
Z	8
ρ_{calc}g/cm^3	1.122
μ/mm^{-1}	0.351
F(000)	1648.0
Crystal size/mm^3	0.9 × 0.7 × 0.5
Radiation	GaKα (λ = 1.3405)
2Θ range for data collection/°	9.108 to 120.92
Index ranges	-31 ≤ h ≤ 31, -8 ≤ k ≤ 11, -28 ≤ l ≤ 27
Reflections collected	28636
Independent reflections	5187 [R_{int} = 0.0193, R_{sigma} = 0.0123]
Data/restraints/parameters	5187/0/272
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2 = 0.0944
Final R indexes [all data]	R_1 = 0.0376, wR_2 = 0.0953
Largest diff. peak/hole / e Å^{-3}	0.28/-0.20

Computational methods and details

All of structures were optimized at B3LYP[3]-D3[4]/Def2-SVP[5] level of theory in gas-phase to analyze the frequencies and thermal energies at 353K. Single point energies based upon the optimized structures were then calculated at the B3LYP-D3/Def2-TZVP level of theory with SMD solvation model[6] calculation in N,N-dimethylformamide (DMF) solution. The presented Gibbs free energies are obtained by adding the solution-phase electronic energy with the gas-phase Gibbs free energy correction. In addition, natural bond orbital (NBO) charge analysis[7] was calculated at the same level in solution-phase. The intrinsic reaction coordinate (IRC) path calculations have also been conducted to confirm the connections of cyanation from TSs to intermediates. The integration grid option were required at ultrafine for all of calculations. All calculations were carried out by the Gaussian 09 package.[8]

For the cynao nucleophilic addition, we calculated two conformations of **3b** with different C-N(Me)(SO_2Ph) orientations. Figure S1 depicts the other pathways of cyanation in which the cyanide anion adds onto the internal and terminal carbons of $\mathbf{3b_{rot}}$. The tendency of cyanide addition onto $\mathbf{3b_{rot}}$ is similar to addition onto **3b** where the preference site is still the internal carbon. Similarly, the NBO charges on the carbons of the allene moieties in $\mathbf{3b_{rot}}$ are 0.13 and -0.27 for internal and terminal carbons, respectively. It is worth noting that the relative free energy of $\mathbf{3b_{rot}}$ is -3.7 kcal/mol lower than that of **3b**, but the barrier of $\mathbf{TS1_{rot}}$ is 2.9 kcal/mol higher than that of **TS1**. This means that the path of cynao nucleophilic addition possibly should be $\mathbf{3b_{rot}}$-**3b**-**TS1**-**int1**-$\mathbf{int1_{rot}}$.

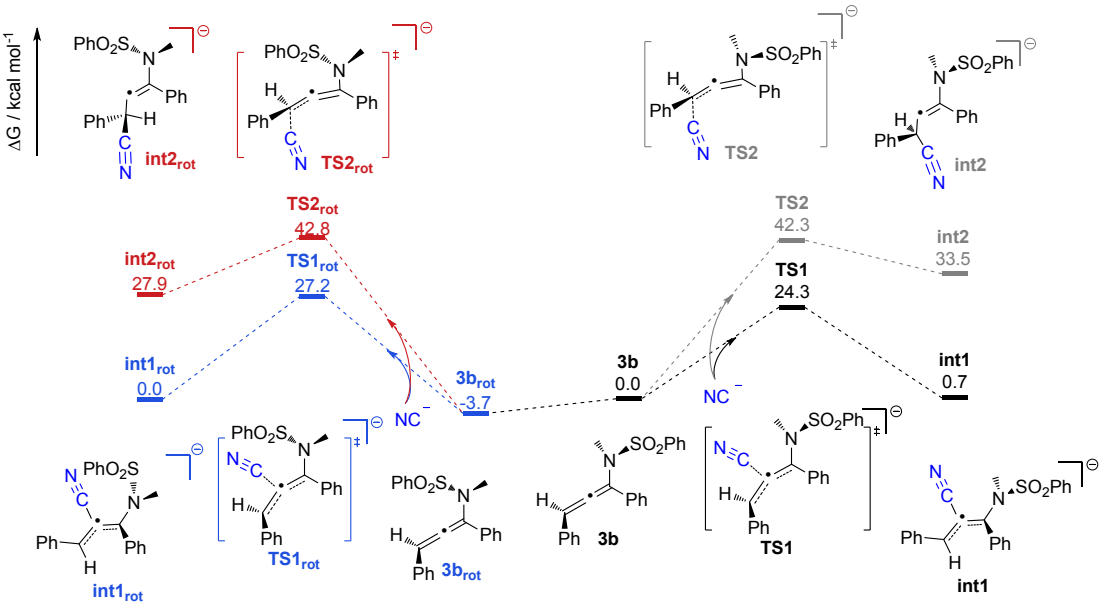


Figure S1. Energy profile of cyano nucleophilic addition on **3b**$_{rot}$.

Table S3. Electronic potential energies and correction to zero point energies, thermal energies, enthalpies, free energies (in Hartree) and imaginary frequencies (cm^{-1}) of optimized structures calculated at the B3LYP-D3/Def2-TZVP/(SMD-DMF)//B3LYP-D3/Def2-SVP.

Entry	Structure	$E_{el,sol}$	$E_{el,gas}$	$cZPE_{gas}$	$cU_{298,gas}$	$cH_{298,gas}$	$cG_{298,gas}$	Imaginary Frequency
1	**3b**	-1453.593562	-1452.225456	0.355749	0.386686	0.387804	0.286481	
2	**4a**	-2432.034066	-2429.801818	0.432580	0.476165	0.477284	0.346261	
3	CN^-	-92.998838	-92.763823	0.004942	0.007740	0.008858	-0.018278	
4	**TS1**	-1546.569519	-1545.002565	0.360230	0.394883	0.396002	0.284072	-165.0093
5	**int1**	-1546.614548	-1545.082624	0.363713	0.397410	0.398529	0.291358	
6	**TS2**	-1546.542124	-1544.994107	0.360575	0.394836	0.395954	0.285244	-339.5953
7	**int2**	-1546.561623	-1545.015106	0.362757	0.396463	0.397582	0.290727	
8	**$3b_{rot}$**	-1453.597893	-1452.224831	0.355781	0.386753	0.387872	0.284880	
9	**$TS1_{rot}$**	-1546.567503	-1545.018789	0.360806	0.395198	0.396317	0.286664	-216.2856
10	**$int1_{rot}$**	-1546.613913	-1545.086779	0.363731	0.397460	0.398579	0.289711	
11	**$TS2_{rot}$**	-1546.540377	-1544.995730	0.360667	0.394886	0.396004	0.284300	-376.3601
12	**$int2_{rot}$**	-1546.568726	-1545.025977	0.363309	0.396936	0.398054	0.289010	

Coordinate of optimized structures

Structure S1. $3b_{rot}$

E(B3LYP)sol = -1453.59789306

E(B3LYP)gas = -1452.22483148

7	-1.118341	-0.173967	1.273376
16	-1.944718	-1.594932	0.792919
6	-0.734051	-2.499756	-0.175708
6	-0.676908	-2.288308	-1.557142
6	0.178508	-3.332109	0.479589
6	0.331578	-2.915055	-2.292699
1	-1.418449	-1.645120	-2.033240
6	1.183405	-3.951589	-0.268222
1	0.085751	-3.496346	1.554483
6	1.263060	-3.738787	-1.648978
1	0.387756	-2.763232	-3.373435
1	1.902738	-4.607363	0.228104
1	2.050733	-4.226027	-2.229187
8	-3.012898	-1.170847	-0.109088
8	-2.208883	-2.344725	2.021437
6	5.289563	2.058872	0.768680
6	4.052336	2.465881	1.285579
6	2.869197	1.926181	0.784898
6	2.899006	0.964303	-0.243807
6	4.145780	0.566828	-0.757737
6	5.331581	1.108362	-0.254967
1	4.012377	3.212536	2.082893
1	1.904756	2.250601	1.184287
1	4.182661	-0.177997	-1.557750
1	6.292208	0.786684	-0.665370
6	1.664997	0.361500	-0.786394
6	0.442157	0.567388	-0.350021
6	-0.757016	0.715186	0.191617
1	6.215895	2.484659	1.162260
6	-1.742050	1.749513	-0.212141
6	-2.955634	1.892745	0.479585
6	-1.467360	2.616173	-1.286684
6	-3.868583	2.882252	0.107888
1	-3.182629	1.213381	1.300088
6	-2.379976	3.603029	-1.654727
1	-0.528081	2.509922	-1.835607
6	-3.586652	3.741417	-0.957467
1	-4.810551	2.977381	0.654002
1	-2.150887	4.267505	-2.491909
1	-4.303825	4.513501	-1.247604
1	1.793863	-0.336768	-1.625938
6	-0.148404	-0.332322	2.358783
1	0.785790	-0.825119	2.031432
1	0.100028	0.668790	2.738880
1	-0.609211	-0.915945	3.164933

Structure S2. 4a

E(B3LYP)sol = -2432.03406623

E(B3LYP)gas = -2429.80181839

9	4.232993	0.225018	1.485734
7	-0.698204	0.561060	0.068069
16	-0.676042	2.075023	0.910070
6	0.855984	2.826638	0.394316
6	2.000128	2.595960	1.162110
6	0.880260	3.582820	-0.781940
6	3.214336	3.129125	0.724475
1	1.936745	2.002438	2.072949
6	2.101203	4.116922	-1.196660
1	-0.032928	3.724632	-1.359182
6	3.263369	3.887234	-0.449552
1	4.121398	2.935088	1.299712
1	2.146252	4.710158	-2.112942
1	4.216270	4.301106	-0.788973
8	-0.582998	1.713647	2.322692
8	-1.799644	2.850771	0.392412
16	-1.343108	0.400438	-1.538499
8	-1.091283	1.655993	-2.237258

8	-0.804146	-0.870883	-2.024461
6	-3.101145	0.198146	-1.293877
6	-3.609603	-1.096226	-1.151085
6	-3.915473	1.332621	-1.236514
6	-4.979658	-1.253691	-0.934994
1	-2.940258	-1.955635	-1.200246
6	-5.283356	1.155193	-1.019569
1	-3.476257	2.324063	-1.341236
6	-5.812810	-0.131720	-0.867679
1	-5.393928	-2.257007	-0.813952
1	-5.938246	2.028037	-0.967852
1	-6.884399	-0.260587	-0.695550
6	4.322467	-3.128055	-2.636084
6	2.967347	-2.780152	-2.699272
6	2.359709	-2.109220	-1.640173
6	3.098689	-1.774914	-0.486259
6	4.464195	-2.112111	-0.439583
6	5.067046	-2.786470	-1.505374
1	2.377797	-3.026318	-3.585928
1	1.308631	-1.820987	-1.715233
1	5.079840	-1.833870	0.416583
1	6.128926	-3.039109	-1.449803
6	3.267641	-0.674110	1.846114
1	3.775667	-1.548045	2.291826
6	2.431016	-1.075588	0.644776
6	1.138023	-0.828008	0.665780
6	-0.163050	-0.628213	0.676412
1	4.796354	-3.653142	-3.469218
6	-1.147232	-1.602632	1.215535
6	-2.279249	-1.146524	1.910543
6	-0.978547	-2.979467	0.997003
6	-3.224467	-2.057943	2.382689
1	-2.406821	-0.077162	2.083514
6	-1.929256	-3.887661	1.467380
1	-0.110578	-3.327700	0.432131
6	-3.055248	-3.428963	2.160523
1	-4.101330	-1.693801	2.923551
1	-1.796187	-4.956730	1.283093
1	-3.801701	-4.139812	2.524145
9	2.511366	-0.094417	2.810894

Structure S3. CN^-

E(B3LYP)sol = -92.9988381353

E(B3LYP)gas = -92.7638229989

7	0.000000	0.000000	0.544137
6	0.000000	0.000000	-0.634826

Structure S4. $\mathbf{TS1_{rot}}$

E(B3LYP)sol = -1546.56750275

E(B3LYP)gas = -1545.01878855

7	-1.748061	-0.579814	0.917673
6	5.284059	2.086674	0.172556
6	4.273036	2.355647	1.101923
6	2.960877	1.936963	0.872278
6	2.632277	1.221309	-0.298880
6	3.661893	0.961724	-1.228895
6	4.970287	1.386790	-0.999042
1	4.508003	2.901231	2.020582
1	2.176167	2.135554	1.600633
1	3.422736	0.402208	-2.138362
1	5.750892	1.168063	-1.734062
6	1.281851	0.746522	-0.591470
6	0.214362	0.610583	0.192744
6	-1.127105	0.553693	0.304512
1	6.308889	2.421943	0.357481
6	-1.998900	1.669328	-0.119084
6	-3.368866	1.448919	-0.376312
6	-1.501474	2.981191	-0.278193
6	-4.200348	2.496248	-0.778016
1	-3.761693	0.434876	-0.296790
6	-2.334567	4.022058	-0.685723
1	-0.446856	3.174035	-0.068884
6	-3.693465	3.790406	-0.936562
1	-5.256941	2.294144	-0.979017
1	-1.921379	5.029202	-0.798294
1	-4.347428	4.609194	-1.250058

1	1.123817	0.383996	-1.616815
6	-2.319061	-0.470976	2.259012
1	-3.159219	0.246399	2.263167
1	-2.688296	-1.455488	2.570989
1	-1.531732	-0.154073	2.956414
7	0.910260	-0.825080	3.180603
6	1.044494	0.008244	2.363052
16	-1.960796	-1.957214	-0.007904
6	-0.285528	-2.422365	-0.468263
6	0.062055	-2.459851	-1.820294
6	0.640669	-2.693905	0.541253
6	1.378030	-2.775288	-2.169735
1	-0.693244	-2.220348	-2.570187
6	1.954430	-2.994021	0.177764
1	0.371977	-2.588747	1.593159
6	2.323397	-3.036492	-1.171230
1	1.669018	-2.800936	-3.223633
1	2.697083	-3.156092	0.962062
1	3.358997	-3.255950	-1.445842
8	-2.659835	-1.626221	-1.262895
8	-2.522398	-2.993771	0.869847

Frequencies -- -216.2856
Red. masses -- 8.5020
Frc consts -- 0.2343
IR Inten -- 157.1470

Structure S5. int1$_{rot}$

E(B3LYP)sol = -1546.61391251
E(B3LYP)gas = -1545.08677918

7	1.836691	-0.679748	-1.000056
6	-5.569310	1.354528	-0.166293
6	-4.891890	0.680798	-1.191529
6	-3.500529	0.606346	-1.218488
6	-2.704731	1.202846	-0.199422
6	-3.419809	1.891056	0.824214
6	-4.809093	1.963259	0.842328
1	-5.461073	0.203470	-1.996042
1	-3.021931	0.078900	-2.041384
1	-2.847739	2.370421	1.624793
1	-5.308438	2.501710	1.654724
6	-1.264556	1.164792	-0.101962
6	-0.295835	0.445432	-0.802213
6	1.126293	0.499992	-0.606398
1	-6.661465	1.408272	-0.155798
6	1.888020	1.637613	-0.124666
6	3.252454	1.493929	0.261588
6	1.368394	2.964667	-0.084336
6	4.023268	2.585172	0.655271
1	3.692419	0.498019	0.281521
6	2.149698	4.048717	0.307757
1	0.339722	3.143923	-0.397955
6	3.487703	3.879319	0.689279
1	5.063904	2.417287	0.952337
1	1.704045	5.049290	0.310915
1	4.094207	4.731948	1.007404
1	-0.863446	1.758147	0.722333
6	2.622317	-0.712544	-2.228429
1	3.405828	0.065949	-2.219646
1	3.093627	-1.698140	-2.343900
1	1.953038	-0.544275	-3.087238
7	-0.964574	-1.248515	-2.670948
6	-0.685084	-0.505988	-1.819833
16	2.067072	-1.920984	0.127290
6	0.417590	-2.126394	0.812063
6	0.065095	-1.423520	1.966421
6	-0.491551	-2.949640	0.145990
6	-1.240886	-1.528862	2.446517
1	0.807848	-0.788081	2.450541
6	-1.793403	-3.053640	0.641780
1	-0.183830	-3.464379	-0.764685
6	-2.170036	-2.338619	1.782902
1	-1.541993	-0.959914	3.329641
1	-2.523379	-3.674719	0.116925
1	-3.198620	-2.397839	2.147904
8	2.926546	-1.503540	1.251162
8	2.435278	-3.139204	-0.617067

Structure S6. $TS2_{rot}$

E(B3LYP)sol = -1546.54037749

E(B3LYP)gas = -1544.99573027

7	-1.392566	0.501690	-1.318600
16	-2.091362	1.821314	-0.543772
6	-0.781323	2.565372	0.445996
6	-0.540977	2.074967	1.733527
6	0.026071	3.554088	-0.119675
6	0.540844	2.577756	2.458774
1	-1.195684	1.304779	2.142597
6	1.106601	4.051301	0.615466
1	-0.201598	3.921249	-1.121871
6	1.367431	3.559703	1.898523
1	0.745593	2.192802	3.461084
1	1.749007	4.823171	0.182934
1	2.219705	3.943164	2.466246
8	-3.092879	1.306281	0.393395
8	-2.464636	2.800765	-1.577989
6	5.155676	-1.205293	-1.642757
6	3.899829	-1.392063	-2.231430
6	2.734901	-1.227451	-1.476760
6	2.801678	-0.887130	-0.118394
6	4.065759	-0.717512	0.466615
6	5.232819	-0.865314	-0.287858
1	3.826011	-1.663505	-3.288876
1	1.752319	-1.354711	-1.936642
1	4.126727	-0.478780	1.532269
1	6.208372	-0.719918	0.186039
6	1.551001	-0.706850	0.710323
6	0.387472	-0.396511	0.019441
6	-0.864460	-0.546719	-0.396661
1	6.067541	-1.325916	-2.235045
6	-1.849097	-1.632127	-0.130564
6	-3.106412	-1.669008	-0.766281
6	-1.533798	-2.675768	0.762776
6	-4.004487	-2.712469	-0.529305
1	-3.377085	-0.857291	-1.440262
6	-2.433902	-3.715121	0.999388
1	-0.576828	-2.675526	1.282035
6	-3.676096	-3.745441	0.353929
1	-4.974657	-2.712221	-1.036498
1	-2.155468	-4.507523	1.700441
1	-4.381273	-4.560858	0.542123
1	1.715912	0.012807	1.525759
6	-0.549610	0.816093	-2.467702
1	0.456532	1.157889	-2.161532
1	-0.431152	-0.107105	-3.055339
1	-1.041273	1.575223	-3.089676
7	1.411075	-2.996869	2.674650
6	1.680020	-2.187646	1.874124

Frequencies -- -376.3601

Red. masses -- 11.6671

Frc consts -- 0.9737

IR Inten -- 514.4017

Structure S7. $int2_{rot}$

E(B3LYP)sol = -1546.56872606

E(B3LYP)gas = -1545.02597729

7	-1.176285	1.698985	-0.682732
16	-0.241324	2.543146	0.418694
6	1.495616	2.127530	0.177656
6	2.019227	0.985572	0.791829
6	2.284405	2.944526	-0.633830
6	3.363682	0.666793	0.595064
1	1.378054	0.369060	1.419295
6	3.627185	2.607180	-0.839235
1	1.844042	3.837156	-1.081147
6	4.164081	1.471281	-0.225370
1	3.774927	-0.228812	1.064316
1	4.255216	3.238906	-1.473948
1	5.214000	1.209243	-0.386378
8	-0.597661	2.061450	1.761726
8	-0.372754	3.974060	0.089575
6	3.491272	-3.129545	1.265674
6	3.443248	-2.822262	-0.101092
6	2.233190	-2.474480	-0.702041
6	1.044330	-2.454914	0.042807

6	1.099423	-2.758583	1.407768	6	-6.094594	0.521873	-0.433227
6	2.316082	-3.087367	2.020223	1	-4.059881	-0.714872	-2.876507
1	4.360270	-2.838127	-0.697370	1	-2.398551	-0.545781	-1.039403
1	2.194632	-2.192929	-1.756524	1	-5.468953	0.997436	1.580084
1	0.179873	-2.723559	1.999247	1	-7.133668	0.811516	-0.256048
1	2.341983	-3.312718	3.090435	6	-2.843449	0.392935	1.494381
6	-0.276838	-2.026066	-0.595933	6	-1.539803	0.284550	1.360188
6	-0.225989	-0.517642	-0.849876	6	-0.233580	0.168825	1.208699
6	-1.294139	0.233194	-0.508817	1	-6.433497	-0.038254	-2.495827
1	4.441834	-3.392087	1.739248	6	0.639965	1.325448	0.870937
6	-2.650242	-0.159256	-0.019779	6	1.951449	1.393484	1.370540
6	-3.289316	0.531279	1.033495	6	0.173919	2.355404	0.036587
6	-3.343561	-1.242015	-0.600826	6	2.778643	2.467434	1.041570
6	-4.545413	0.137833	1.496937	1	2.320280	0.582811	2.000592
1	-2.769732	1.372755	1.492179	6	1.003044	3.429952	-0.290446
6	-4.601493	-1.637537	-0.133726	1	-0.838291	2.293165	-0.370233
1	-2.901958	-1.762190	-1.453231	6	2.308987	3.488786	0.208682
6	-5.210711	-0.952523	0.921133	1	3.799246	2.503106	1.430618
1	-5.011521	0.688035	2.320841	1	0.631677	4.220237	-0.948004
1	-5.112802	-2.479734	-0.610534	1	2.960596	4.325591	-0.055553
1	-6.196069	-1.258035	1.286152	1	-3.259423	0.601574	2.490331
1	-1.095537	-2.373137	0.075950	6	-0.136271	-2.019489	2.375300
6	-1.099377	2.144854	-2.070162	1	-1.157871	-2.362579	2.135633
1	-0.228523	1.696159	-2.583010	1	0.518923	-2.892756	2.473696
1	-2.012987	1.805212	-2.582993	1	-0.162095	-1.473849	3.329001
1	-1.055965	3.241706	-2.114092	16	0.792517	-1.876831	-0.146560
7	-0.712663	-3.269767	-2.873927	6	2.315072	-1.075841	-0.642734
6	-0.503426	-2.733827	-1.865455	6	2.277617	-0.084430	-1.623884
6	3.505613	-1.460453	-0.020649				
6	3.467843	0.557325	-1.972962				
1	1.326345	0.184077	-2.083736				
6	4.687814	-0.811681	-0.380062				
1	3.496432	-2.255584	0.726907				
6	4.667104	0.198623	-1.349723				
1	3.454774	1.346285	-2.728047				
1	5.629467	-1.096465	0.095425				
1	5.594866	0.707628	-1.622698				
8	-0.231635	-1.536986	-1.142492				
8	1.091439	-3.272724	0.184247				

Structure S8. 3b

E(B3LYP)sol = -1453.59356227

E(B3LYP)gas = -1452.22545574

7	0.416980	-1.107495	1.365882
6	-5.702305	0.046691	-1.687791
6	-4.369463	-0.329257	-1.901658
6	-3.431351	-0.226598	-0.875438
6	-3.817078	0.261982	0.389718
6	-5.158832	0.625462	0.599223

Structure S9. TS1

E(B3LYP)sol = -1546.56951874

E(B3LYP)gas = -1545.00256512

7	-0.748269	-0.950090	-0.858090
6	6.291295	0.148675	1.196332
6	5.065734	-0.300739	1.703667
6	3.915892	-0.289764	0.913333
6	3.973890	0.171548	-0.421837
6	5.217280	0.609573	-0.924895
6	6.361282	0.603482	-0.126238
1	5.004252	-0.672114	2.730885
1	2.966649	-0.674020	1.291734
1	5.278486	0.958511	-1.960758
1	7.314124	0.950705	-0.537809
6	2.786721	0.209981	-1.271496
6	1.556268	-0.154774	-0.917027
6	0.250127	0.066670	-0.771717
1	7.186802	0.140469	1.824820
6	-0.245240	1.449928	-0.534562
6	-1.475248	1.869780	-1.074154
6	0.493512	2.372915	0.231377
6	-1.945293	3.169180	-0.868594
1	-2.067617	1.155807	-1.649135
6	0.022065	3.668804	0.438868
1	1.437771	2.049626	0.673995
6	-1.200851	4.077953	-0.110573
1	-2.905952	3.468617	-1.298041
1	0.608477	4.364512	1.046305
1	-1.571367	5.093085	0.058569
1	2.937090	0.525527	-2.313193
6	-0.734921	-1.926151	-1.954950
1	-0.022858	-2.743134	-1.763737
1	-1.750011	-2.327346	-2.102331
1	-0.441990	-1.381163	-2.864056
7	1.882788	-3.552349	-0.601733
6	1.805444	-2.523301	-0.039346
16	-1.452755	-1.450180	0.601855
6	-3.114143	-0.732022	0.500485
6	-3.359459	0.517246	1.075352
6	-4.127854	-1.439632	-0.152873
6	-4.635372	1.077135	0.969749
1	-2.549104	1.035275	1.589234
6	-5.399212	-0.868827	-0.259224
1	-3.912817	-2.432700	-0.551651
6	-5.652805	0.390124	0.298341
1	-4.831957	2.058161	1.410240
1	-6.197769	-1.413104	-0.770993
1	-6.649179	0.833338	0.215359
8	-0.789308	-0.760940	1.709564
8	-1.663850	-2.898661	0.560379

Frequencies --	-165.0093
Red. masses --	7.5313
Frc consts --	0.1208
IR Inten --	98.9277

Structure S10. int1

E(B3LYP)sol = -1546.61454754

E(B3LYP)gas = -1545.08262417

7	0.717893	-1.190469	0.967298
6	-6.749573	0.349383	-0.623492
6	-5.924293	-0.753754	-0.881421
6	-4.559351	-0.722734	-0.602933
6	-3.942318	0.427079	-0.032130
6	-4.803609	1.538303	0.207351
6	-6.165129	1.500697	-0.077433
1	-6.352350	-1.661703	-1.318957
1	-3.958632	-1.599768	-0.837562
1	-4.370937	2.448145	0.635536
1	-6.781630	2.381868	0.129940
6	-2.542030	0.577474	0.288929
6	-1.495441	-0.348466	0.362749
6	-0.114213	-0.076420	0.619386
1	-7.819316	0.315133	-0.848042
6	0.530740	1.226164	0.624774
6	1.753724	1.423732	1.331273
6	0.062236	2.348264	-0.117344

6	2.443344	2.630181	1.298561	6	-3.395012	0.613781	2.091064
1	2.176800	0.588591	1.890576	1	-1.357587	-0.149945	2.038324
6	0.763696	3.552742	-0.151137	6	-4.907267	-0.332931	0.446450
1	-0.840559	2.248841	-0.719330	1	-4.036917	-1.831813	-0.871762
6	1.959204	3.719032	0.559228	6	-4.663976	0.547040	1.507882
1	3.382552	2.720682	1.853696	1	-3.200505	1.311580	2.908599
1	0.370489	4.376782	-0.756056	1	-5.902000	-0.387013	-0.004349
1	2.502471	4.667586	0.532977	1	-5.467904	1.189045	1.878176
1	-2.264263	1.597328	0.558105	8	-0.241485	-2.120821	0.908620
6	0.688963	-1.788093	2.300224	8	-1.883057	-3.290303	-0.646444
1	-0.228439	-2.380901	2.456984	6	5.324333	-1.164215	1.811895
1	1.554269	-2.449564	2.441996	6	3.964492	-1.492377	1.814310
1	0.725057	-0.979460	3.047426	6	3.109400	-0.990976	0.827395
7	-2.068663	-2.892614	0.320394	6	3.602659	-0.137286	-0.173056
6	-1.808856	-1.759937	0.300365	6	4.967678	0.192473	-0.163989
16	1.570259	-1.959495	-0.264891	6	5.823622	-0.319209	0.813818
6	2.910759	-0.814832	-0.652191	1	3.560919	-2.153880	2.586721
6	2.689428	0.207507	-1.578007	1	2.054050	-1.276165	0.817313
6	4.125432	-0.932331	0.026869	1	5.348778	0.879626	-0.924458
6	3.697184	1.146560	-1.803973	1	6.884560	-0.050825	0.801906
1	1.727243	0.267809	-2.087040	6	2.694115	0.417370	-1.243543
6	5.131562	0.006602	-0.214513	6	1.442599	-0.173147	-1.343818
1	4.265813	-1.756165	0.729160	6	0.137141	-0.020830	-1.159738
6	4.914530	1.049747	-1.121789	1	5.991658	-1.563495	2.581835
1	3.522454	1.968053	-2.502737	6	-0.574119	1.193582	-0.673269
1	6.087305	-0.073393	0.311036	6	-1.830933	1.564727	-1.191805
1	5.697286	1.793279	-1.295381	6	-0.013970	1.993411	0.338673
8	0.752488	-2.029794	-1.479167	6	-2.501826	2.691114	-0.716898
8	2.189972	-3.167836	0.306919	1	-2.288269	0.933447	-1.956408
----------				6	-0.680661	3.126657	0.808264
				1	0.951689	1.714124	0.758689

Structure S11. TS2

E(B3LYP)sol = -1546.54212439

E(B3LYP)gas = -1544.99410699

----------				6	-1.929809	3.480304	0.288649
7	-0.776830	-1.137120	-1.483066	1	-3.482426	2.951553	-1.126945
16	-1.276110	-2.048335	-0.134784	1	-0.214394	3.738134	1.585566
6	-2.613463	-1.050390	0.542291	1	-2.455325	4.363518	0.663811
6	-2.360541	-0.194333	1.614101	1	3.207273	0.542498	-2.204706
6	-3.877761	-1.138330	-0.044120	6	-0.430171	-1.937721	-2.659631
				1	-0.371456	-1.245438	-3.511944
				1	0.551276	-2.431305	-2.557658
				1	-1.210624	-2.686734	-2.844943

7	2.762983	3.534427	-0.860890
6	2.871510	2.370334	-0.893417

Frequencies -- -339.5953
Red. masses -- 11.3836
Frc consts -- 0.7735
IR Inten -- 445.2308

Structure S12. int2

E(B3LYP)sol = -1546.56162271
E(B3LYP)gas = -1545.01510624

7	0.897824	-1.304830	1.373823
16	1.476928	-1.941817	-0.084244
6	2.705521	-0.722953	-0.600890
6	2.404286	0.172244	-1.626240
6	3.939080	-0.693441	0.054475
6	3.350589	1.135573	-1.985403
1	1.425767	0.123222	-2.103480
6	4.880150	0.269185	-0.314531
1	4.145670	-1.420528	0.842011
6	4.584452	1.186873	-1.330625
1	3.111611	1.860175	-2.767437
1	5.847645	0.307136	0.193974
1	5.318625	1.948542	-1.607842
8	0.448117	-1.952779	-1.138199
8	2.227133	-3.175737	0.217615
6	-4.918761	-0.739836	-2.219344
6	-3.636725	-1.267365	-2.042674
6	-2.920805	-1.027459	-0.862513
6	-3.486931	-0.250186	0.158856
6	-4.775940	0.274970	-0.025090
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1	-3.177661	-1.871451	-2.830727
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1	-5.218786	0.889514	0.764831
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6	0.212959	0.949236	0.704452
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6	-0.445014	1.597915	-0.356859
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6	-0.001621	2.832215	-0.838574
1	-1.304232	1.111766	-0.820276
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1	-0.534392	3.309872	-1.666467
1	1.468214	4.415891	-0.655840
1	-3.421282	-0.342539	2.268704
6	0.827172	-2.262028	2.480840
1	0.694542	-1.673049	3.399565
1	-0.040843	-2.934173	2.394003
1	1.759934	-2.838752	2.537331
7	-2.617705	2.586342	2.068081
6	-2.660686	1.470017	1.747265

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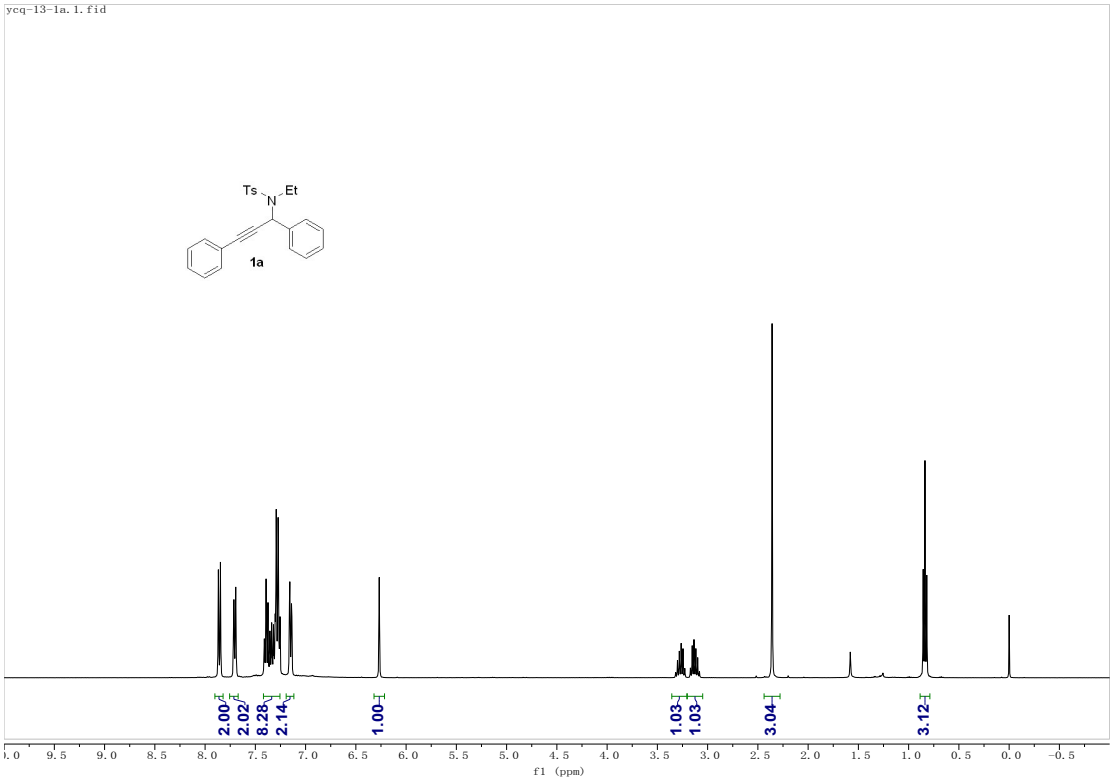
NMR spectra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1.03
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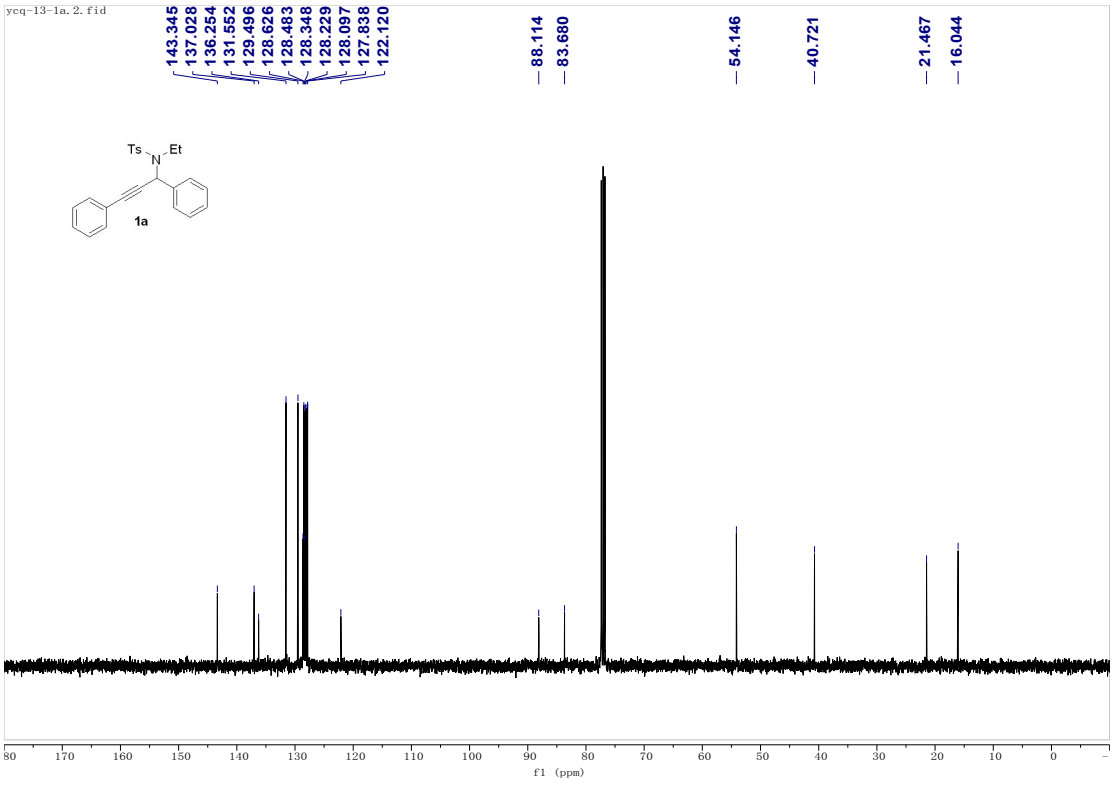
3.12
f1 (ppm)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Ts
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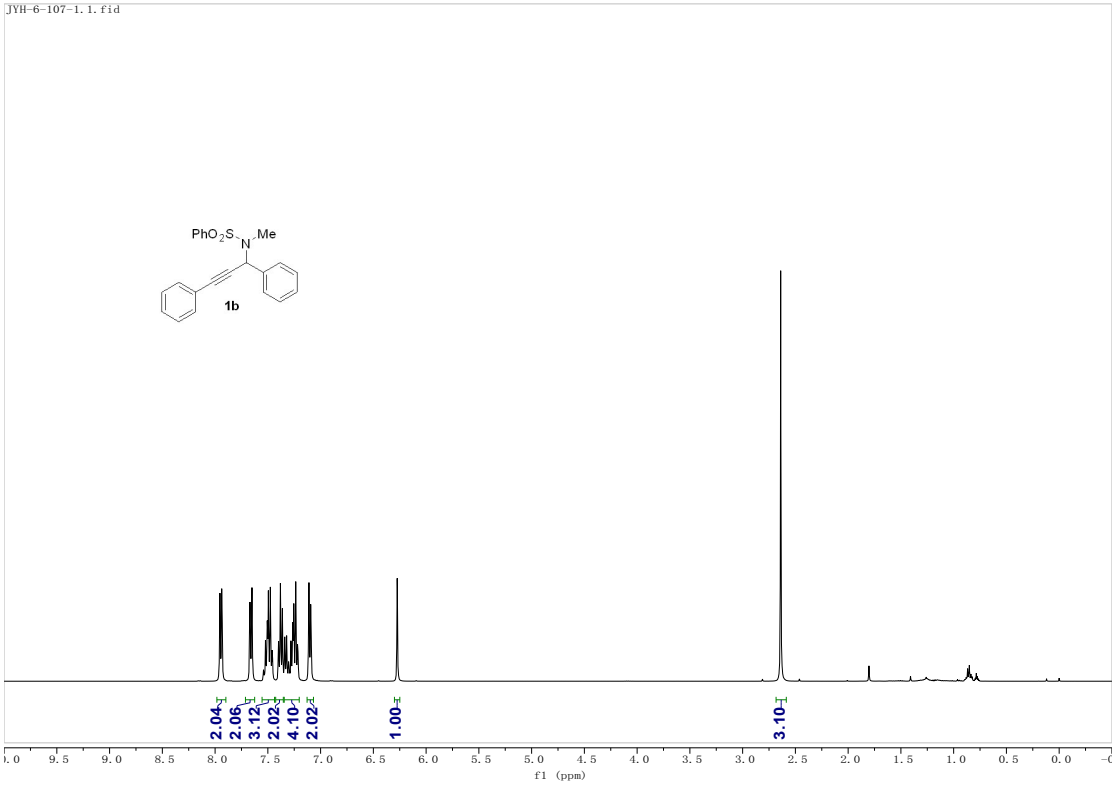
Et
1a
f1 (ppm)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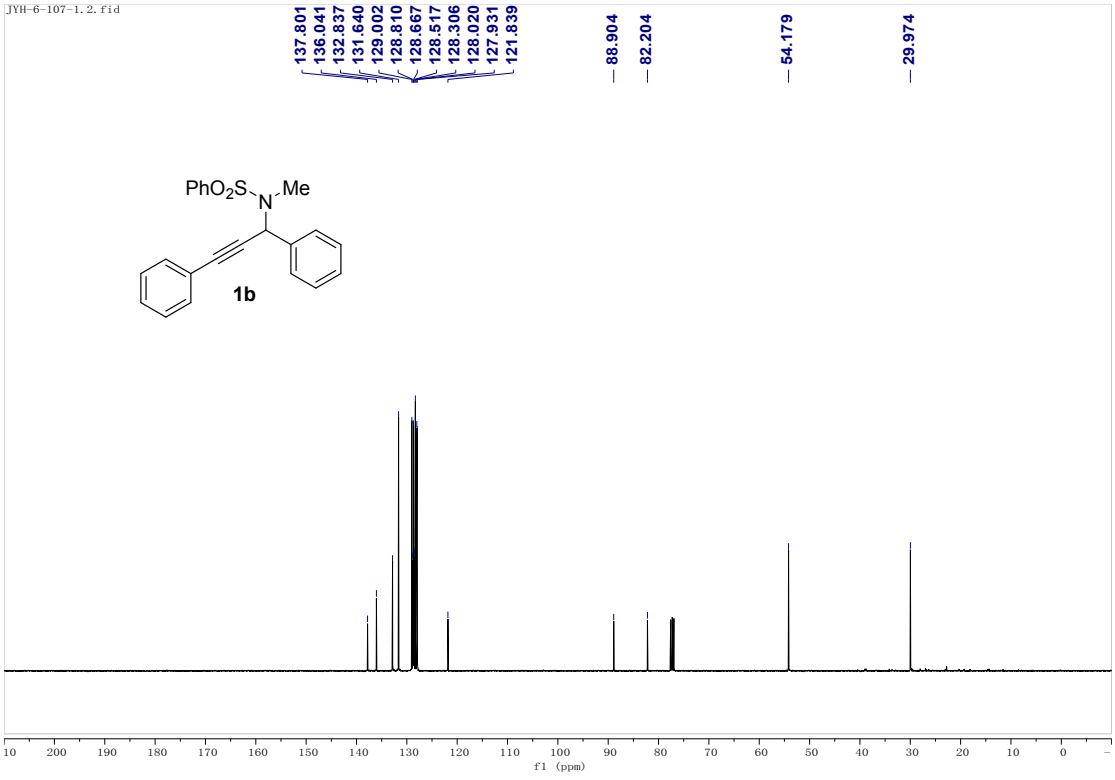
f1 (ppm)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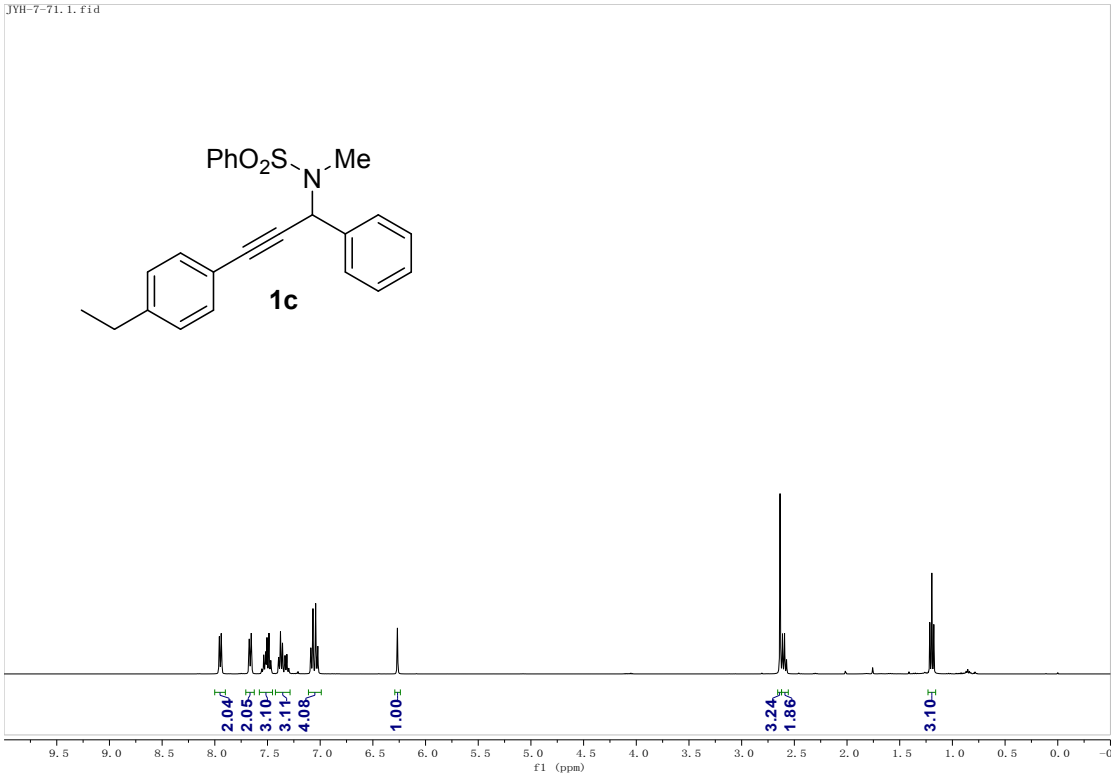
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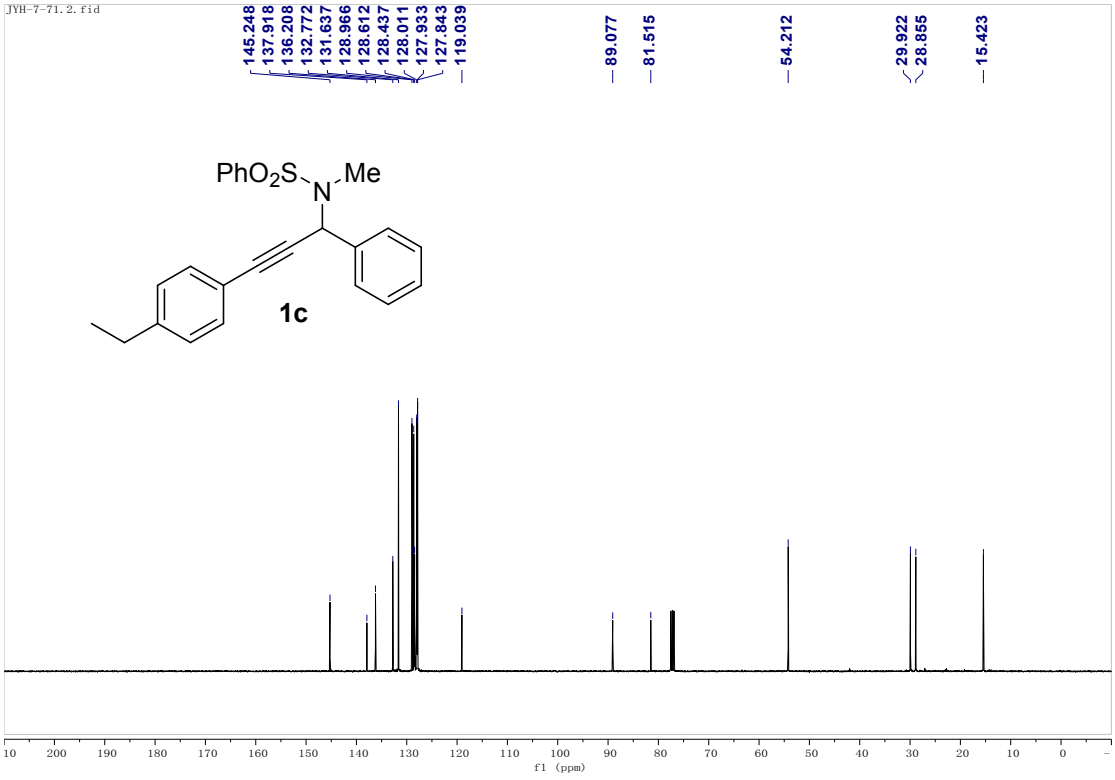
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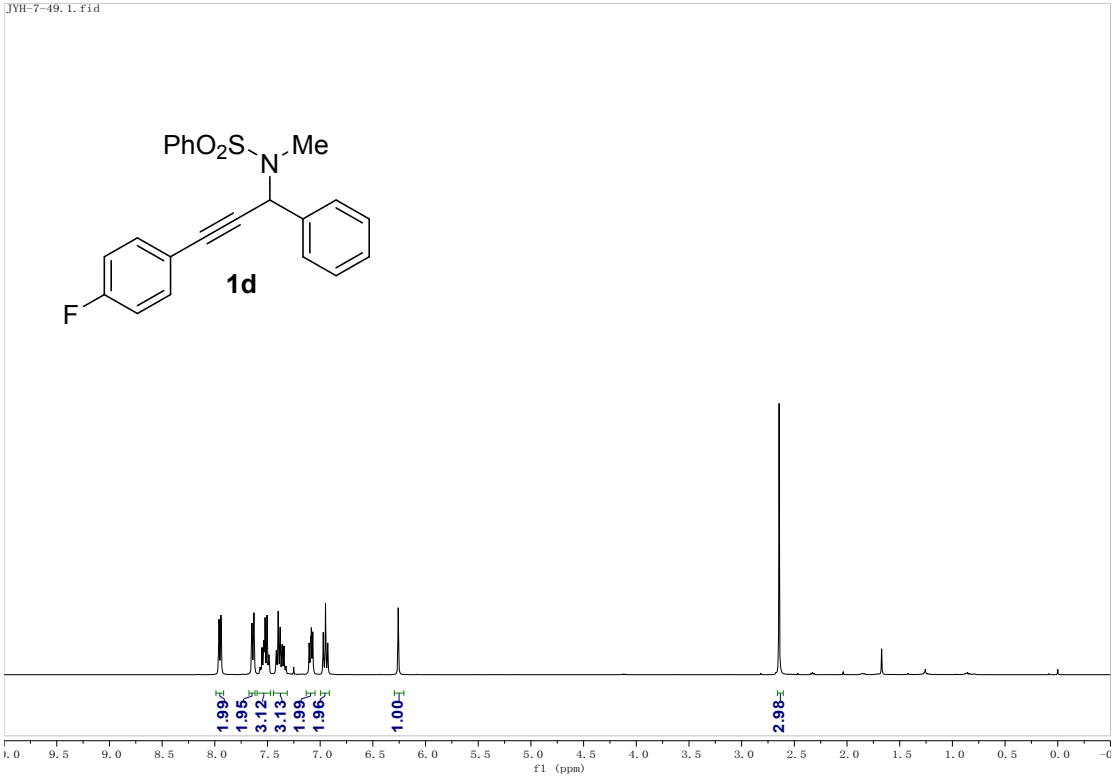
Me
1c
f1 (ppm)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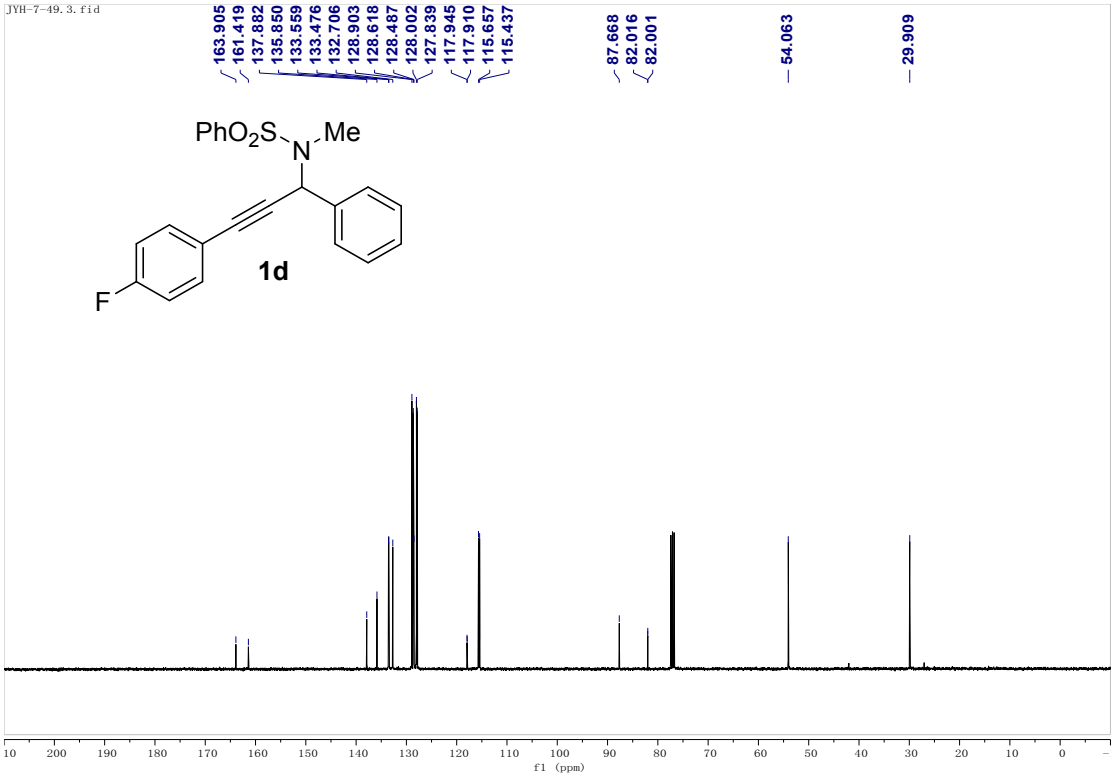
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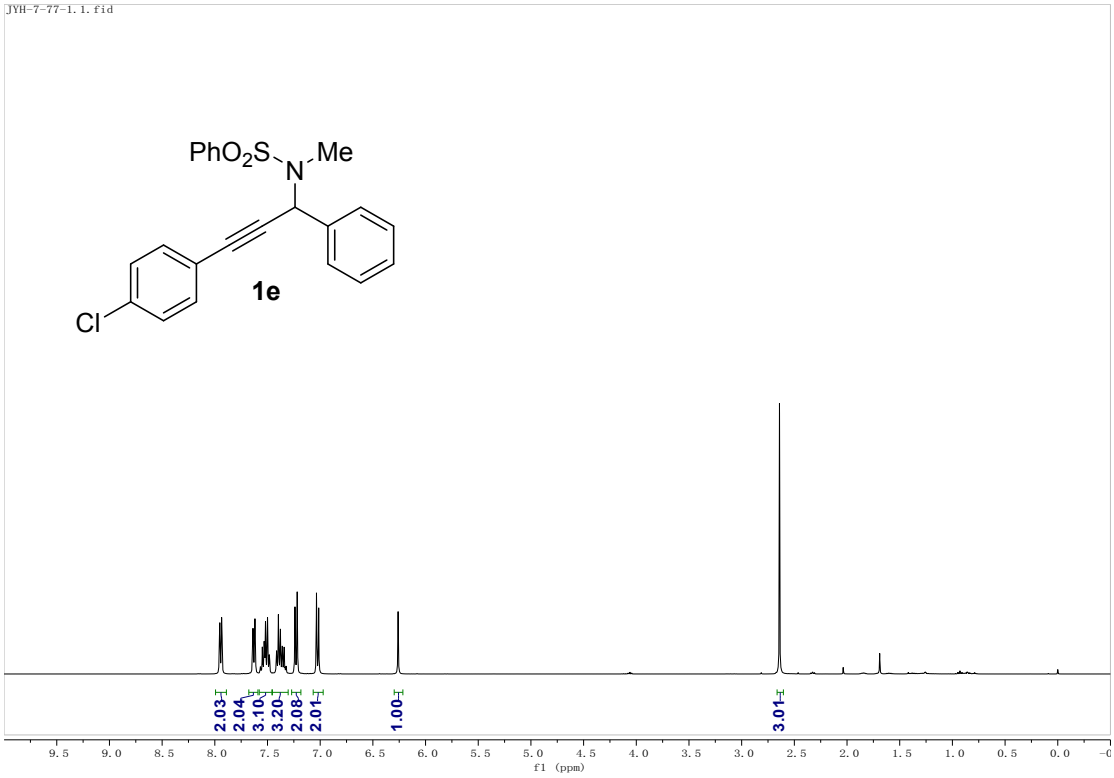
PhO2S
N
Me
1d
F
f1 (ppm)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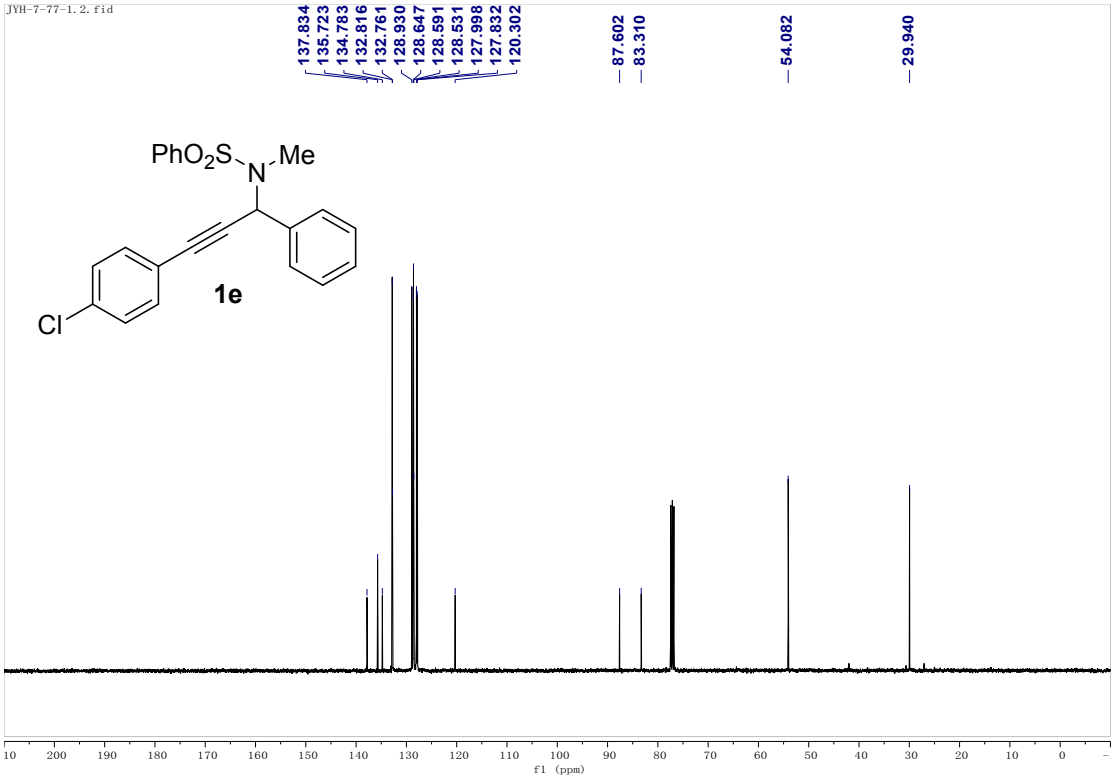
3.01
f1 (ppm)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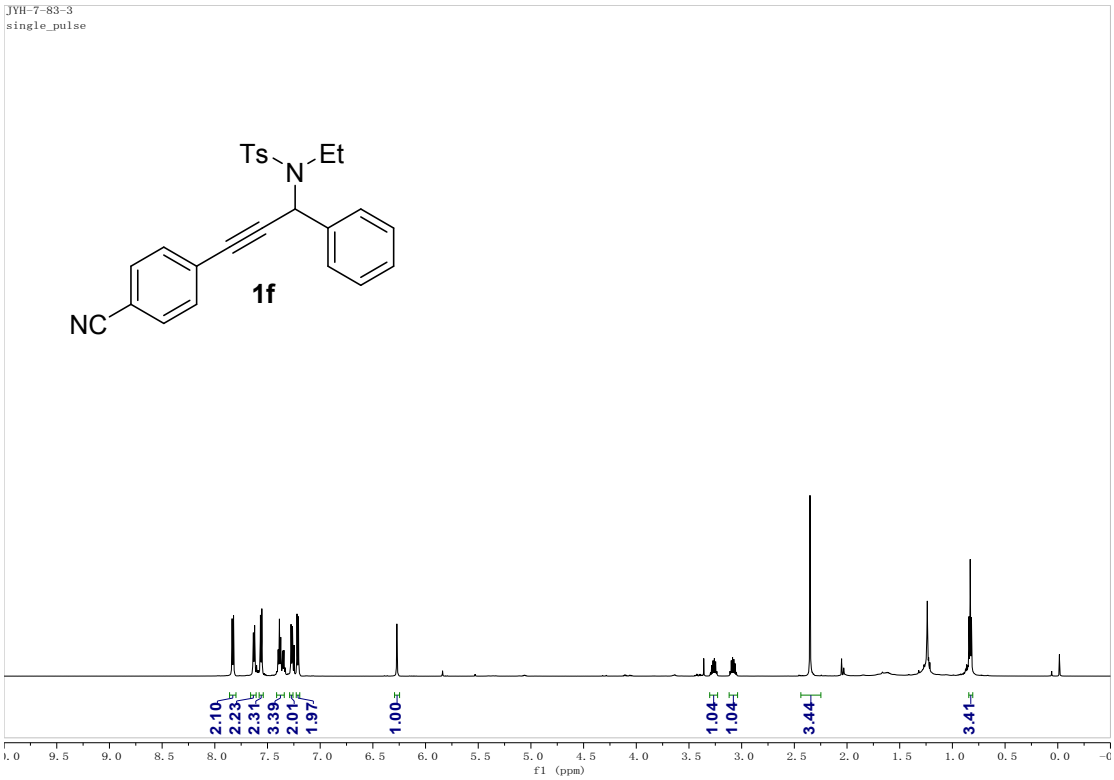
PhO2S
N
Me
1e
Cl
f1 (ppm)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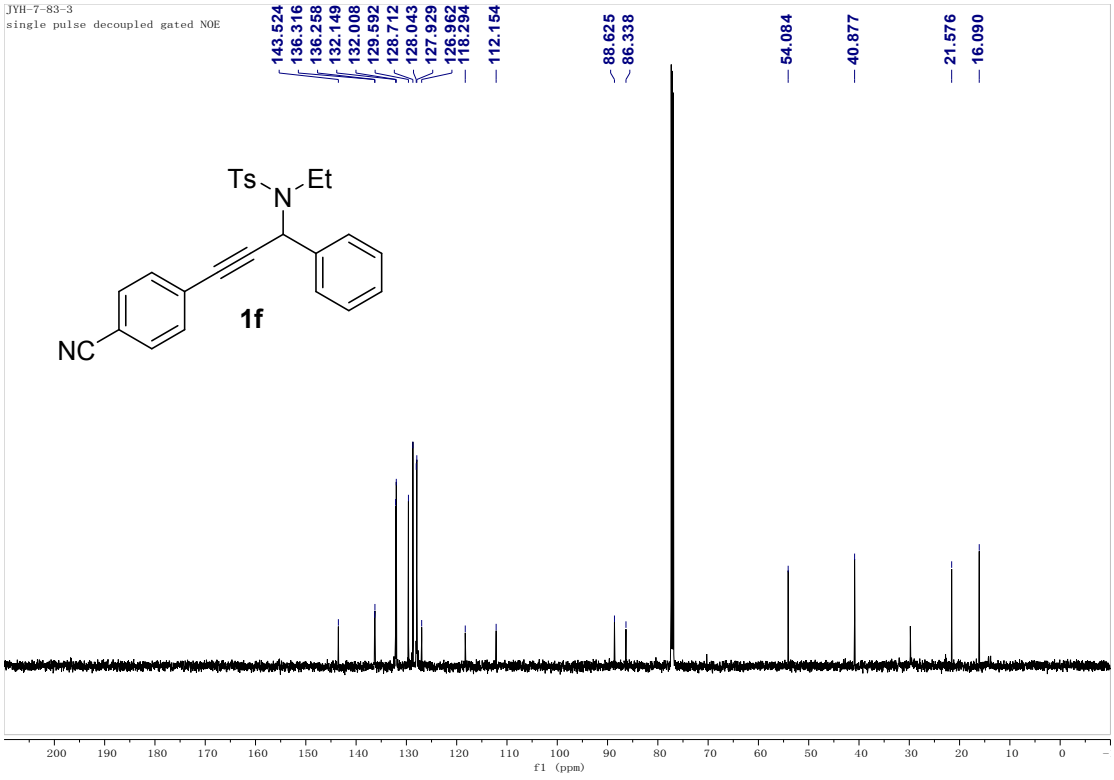
f1 (ppm)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Ts
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Et
1f
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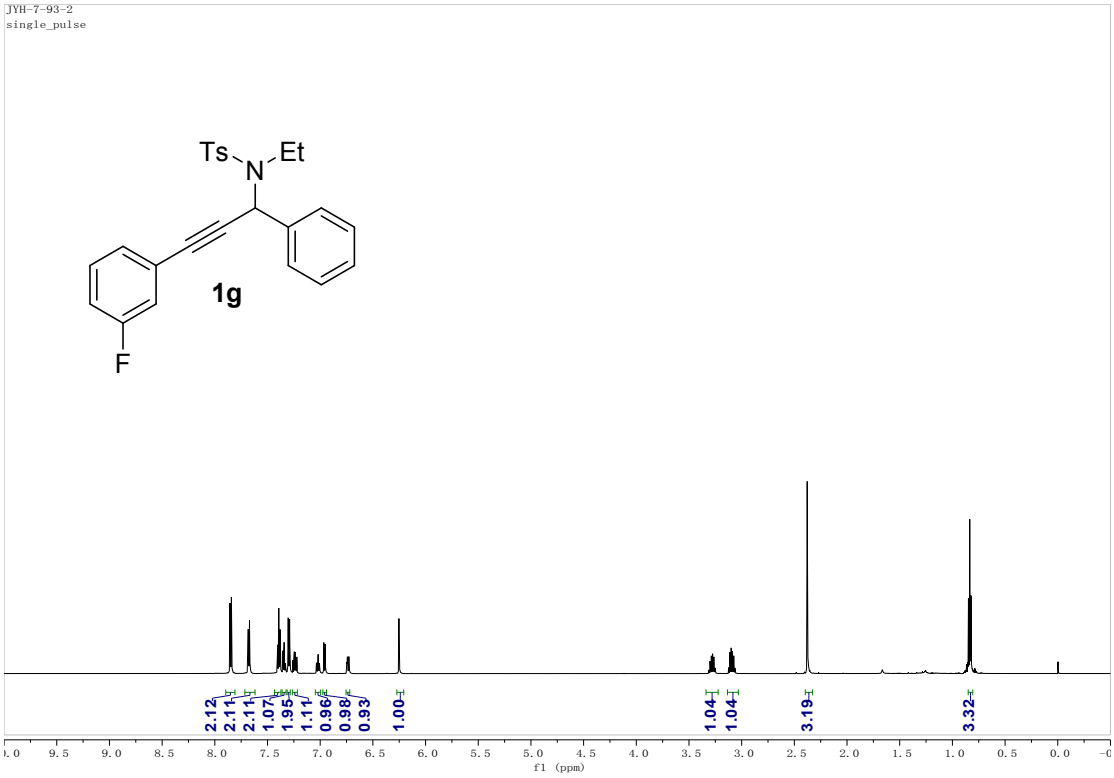
f1 (ppm)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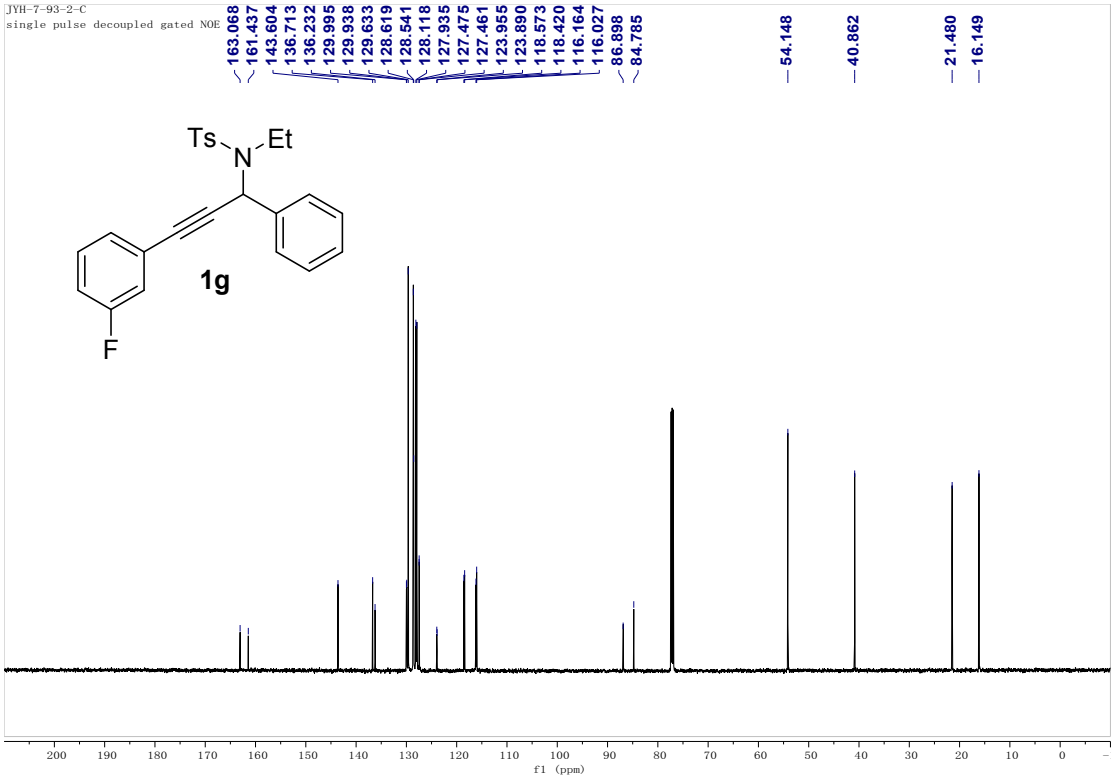
f1 (ppm)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Ts
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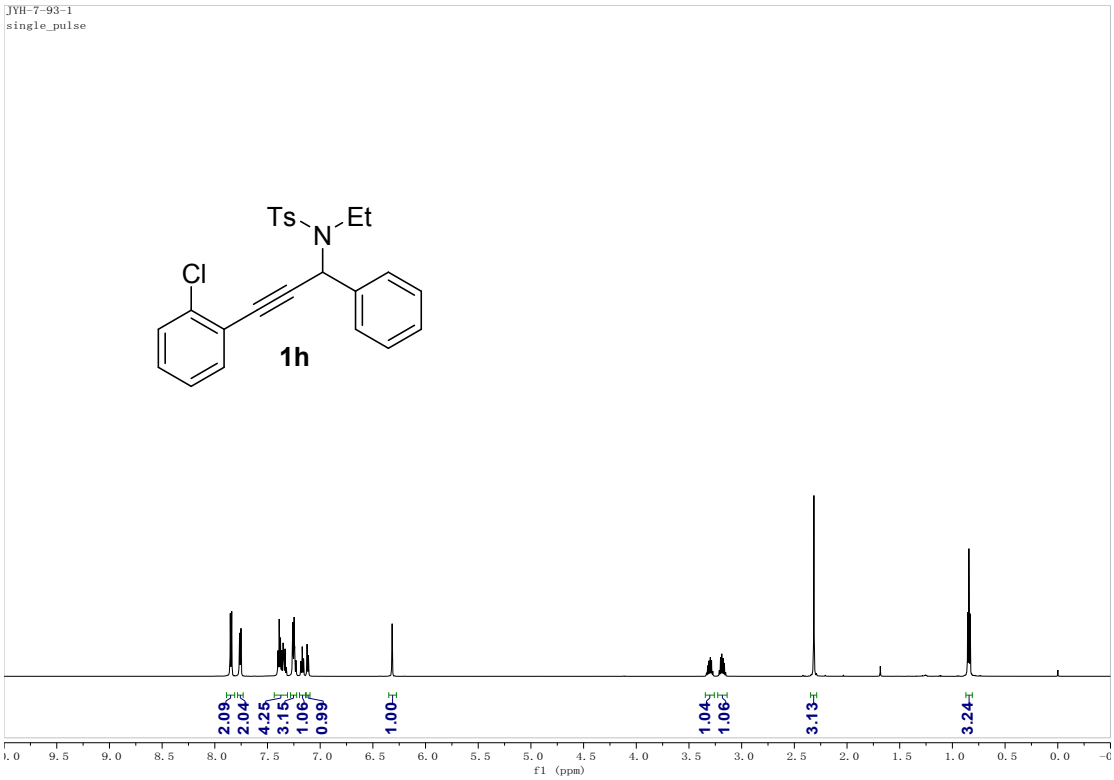
Et
1g
F
f1 (ppm)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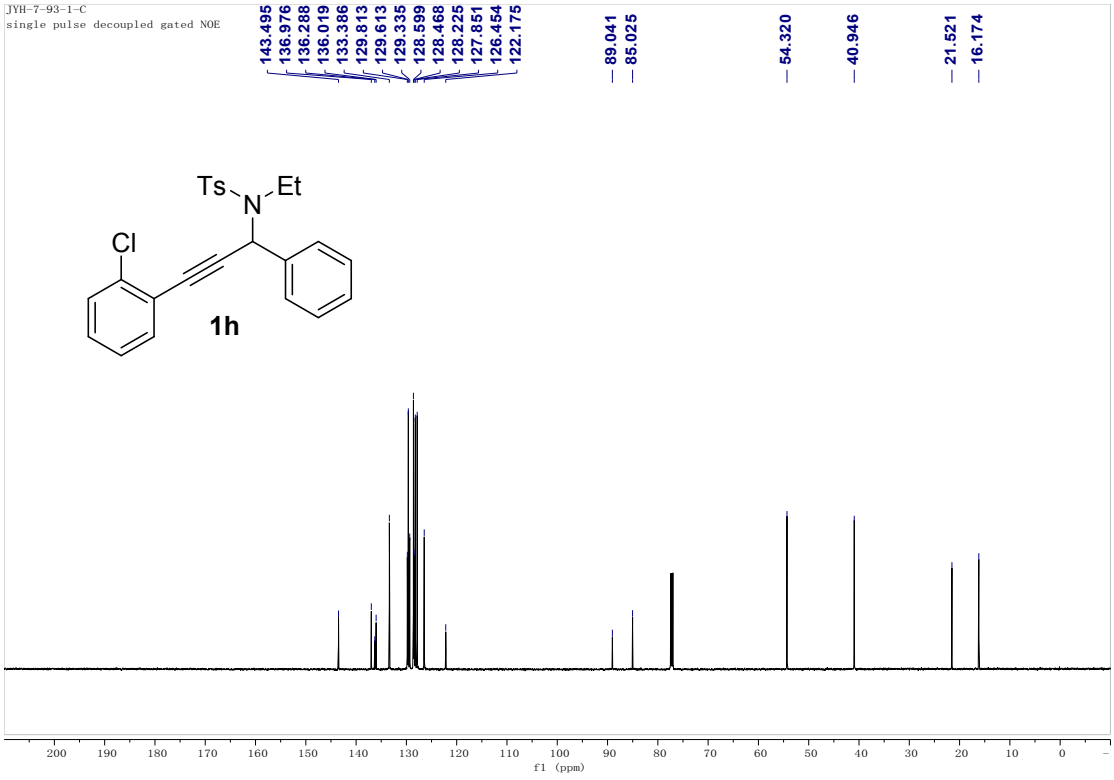
f1 (ppm)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Ts
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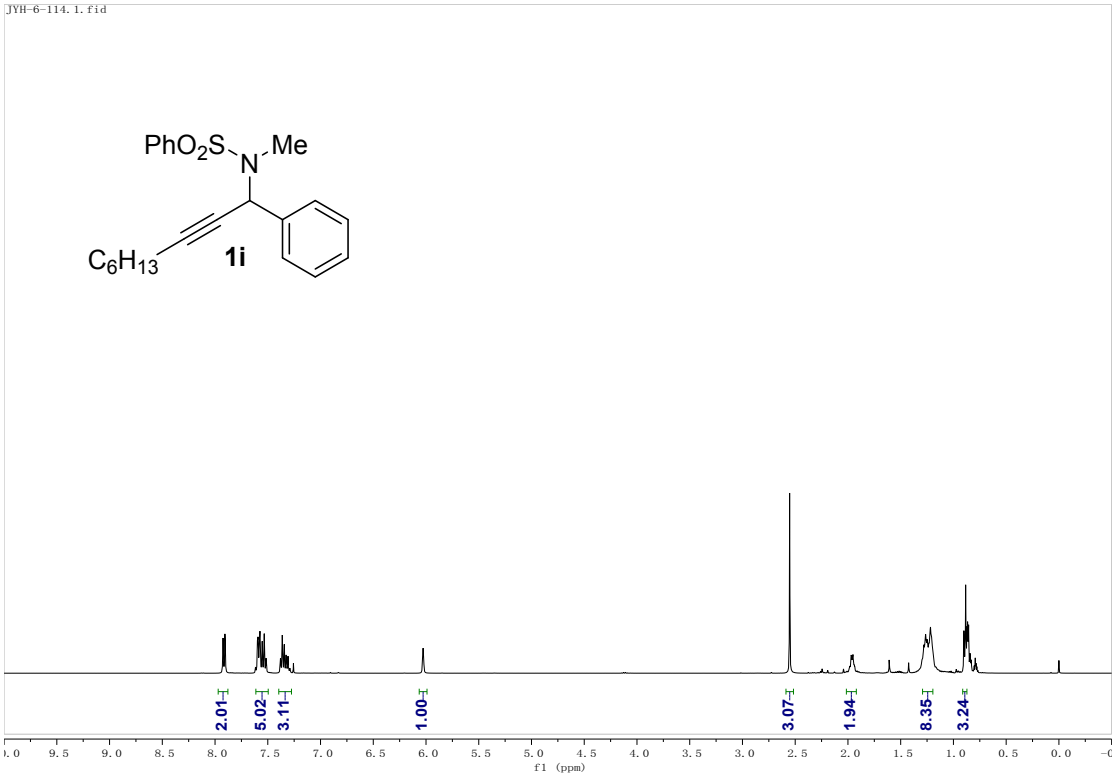
Et
Cl
1h
f1 (ppm)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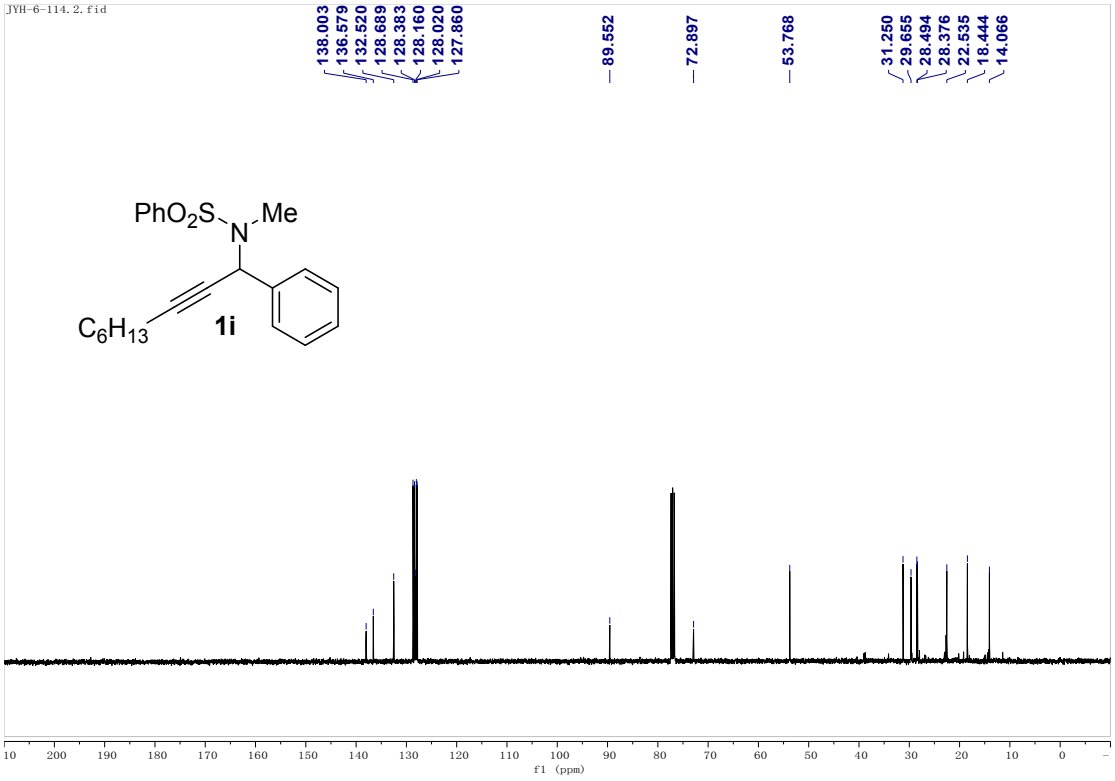
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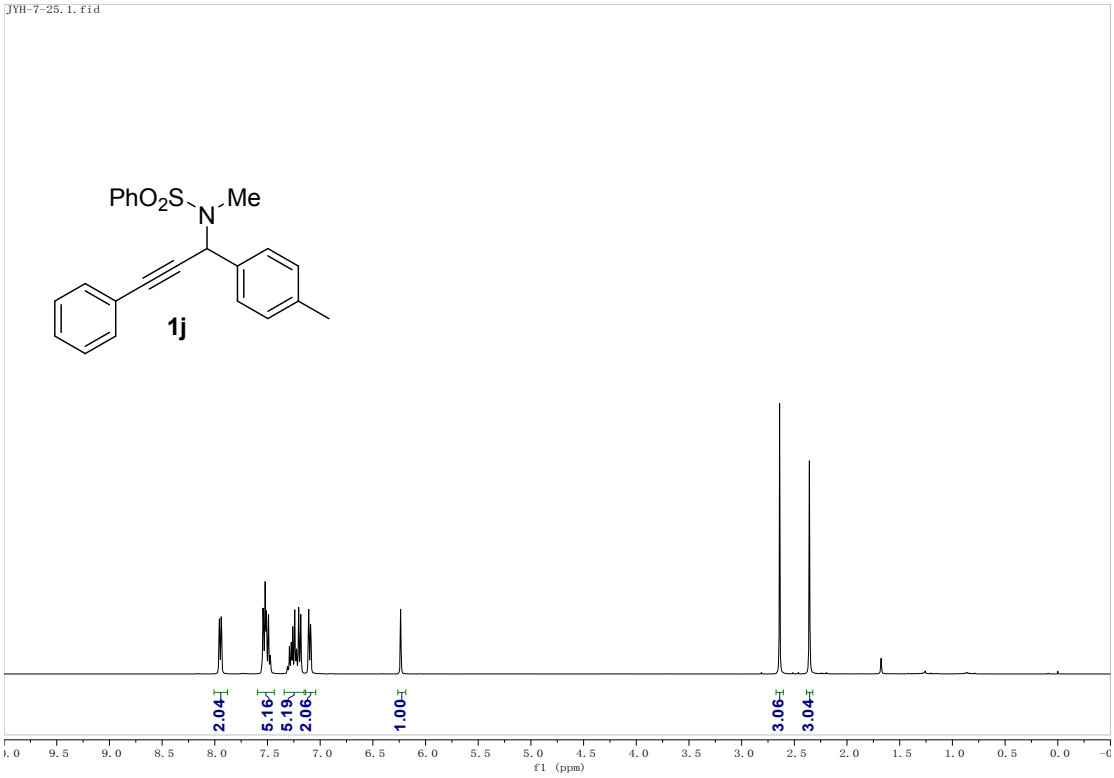
N
Me
C6H13
1i
f1 (ppm)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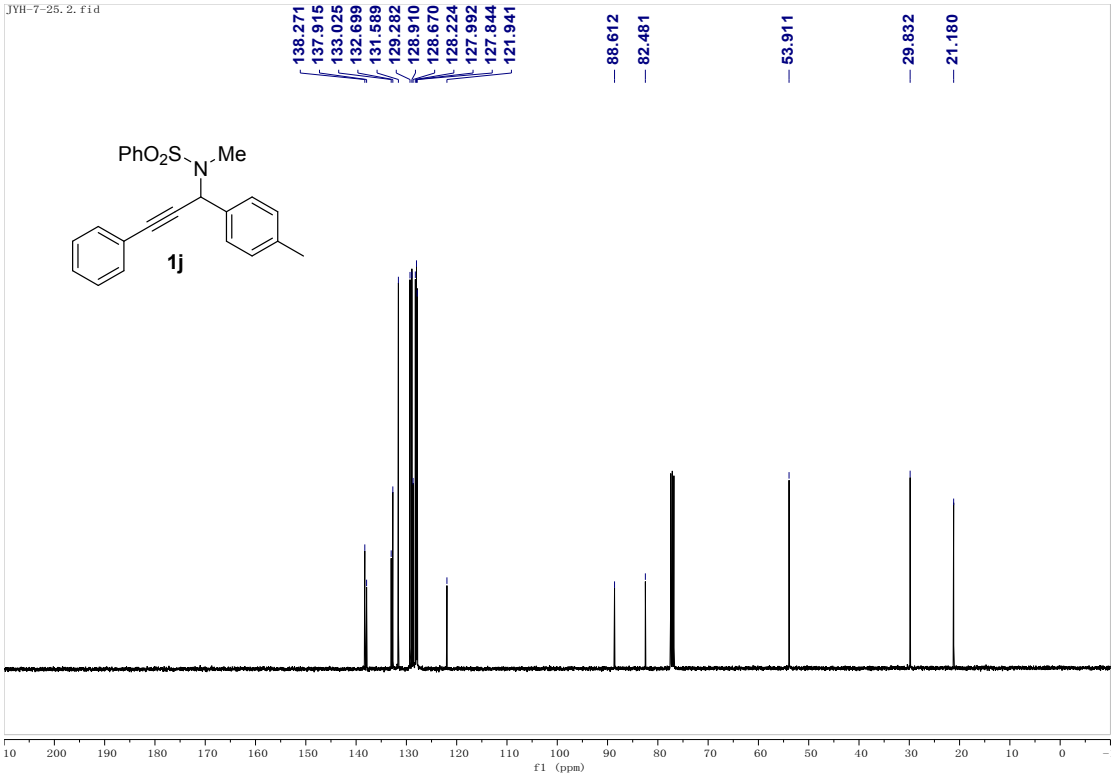
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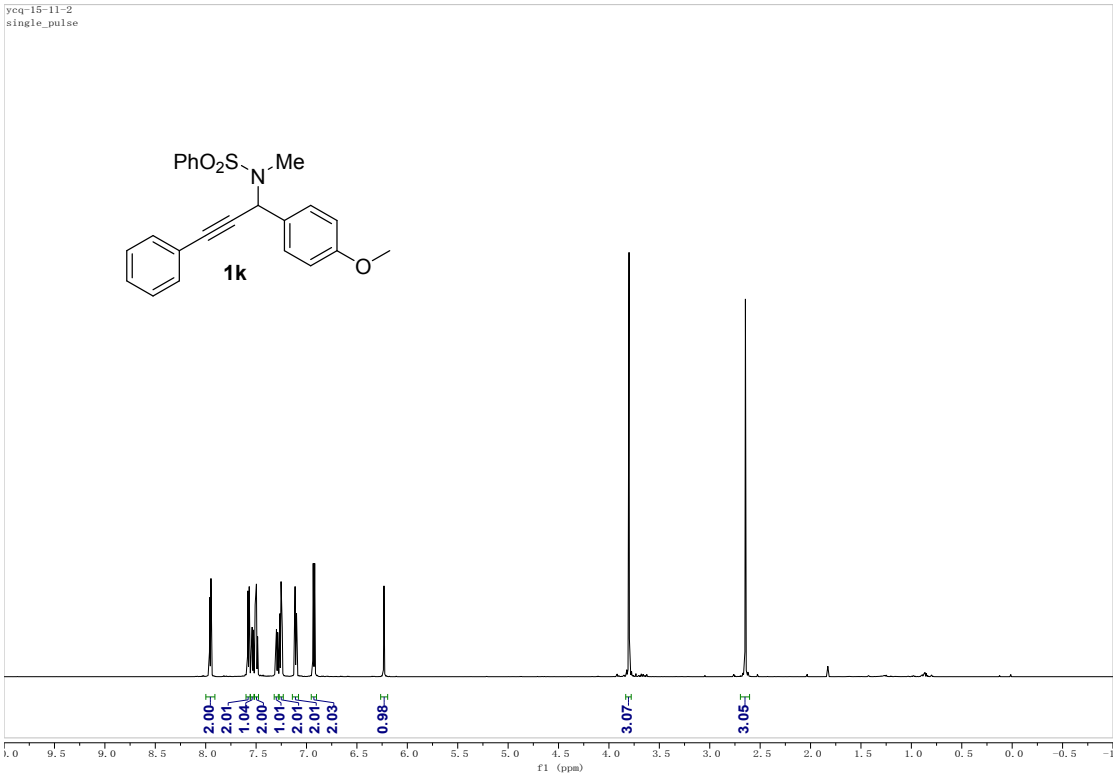
Me
1j
f1 (ppm)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O
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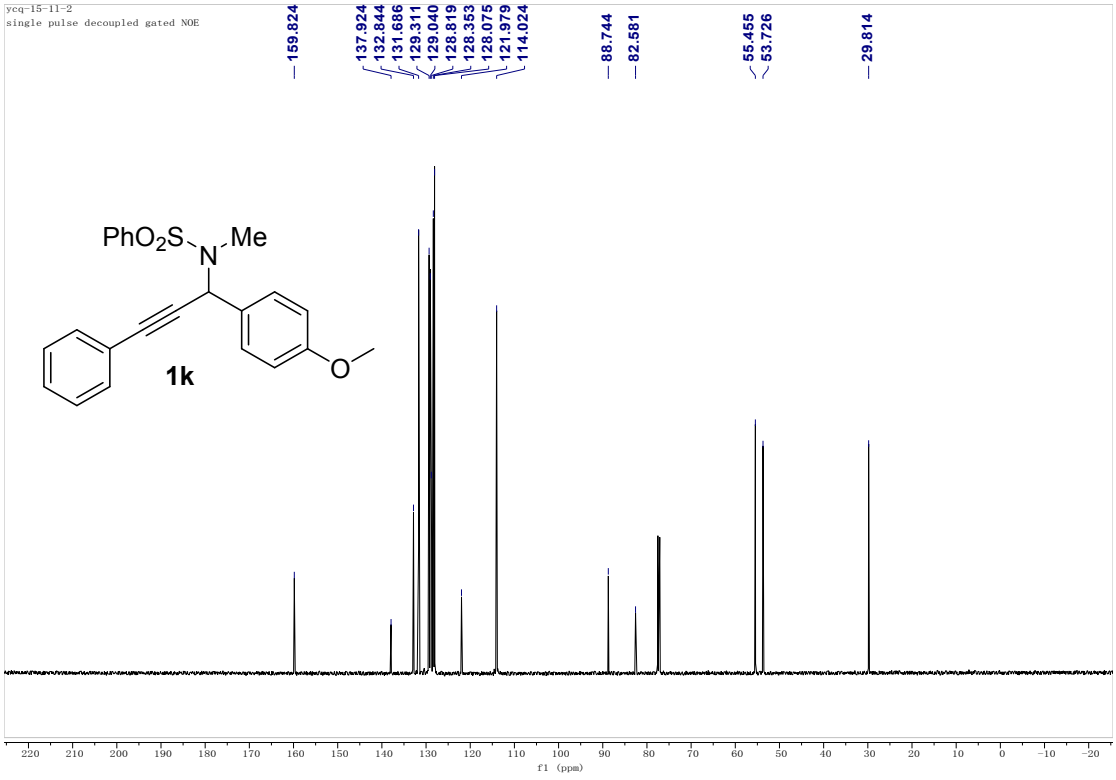
f1 (ppm)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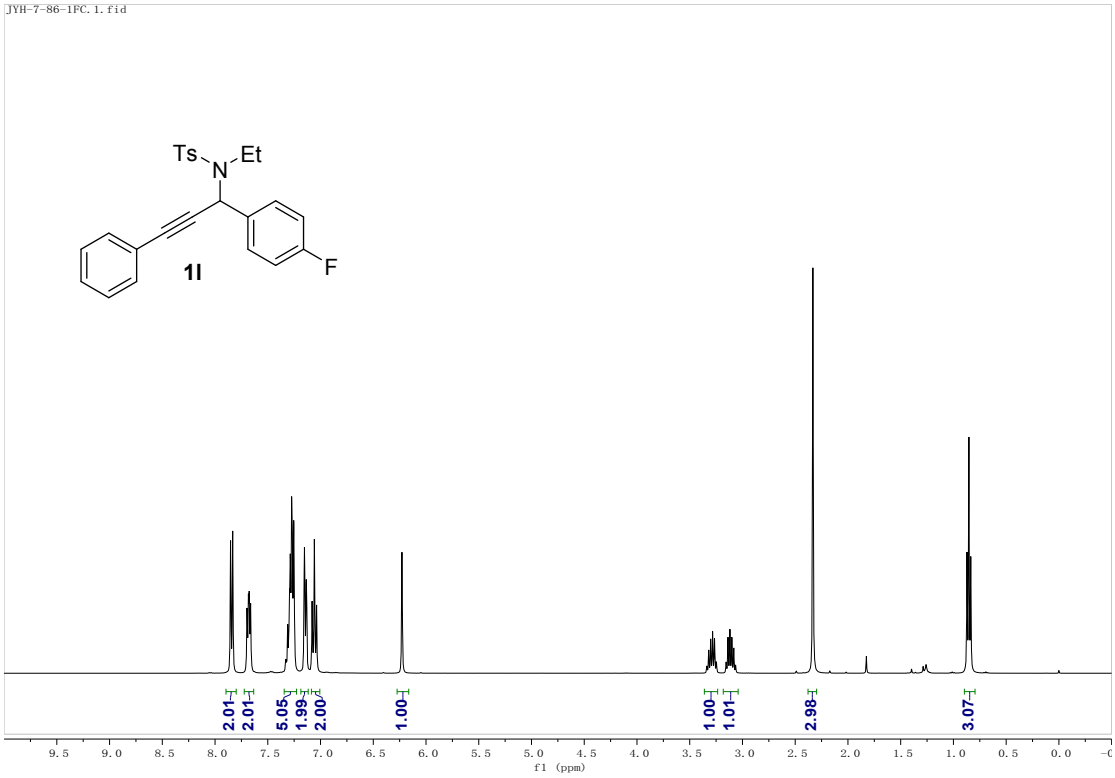
Me
O
1k
f1 (ppm)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Et
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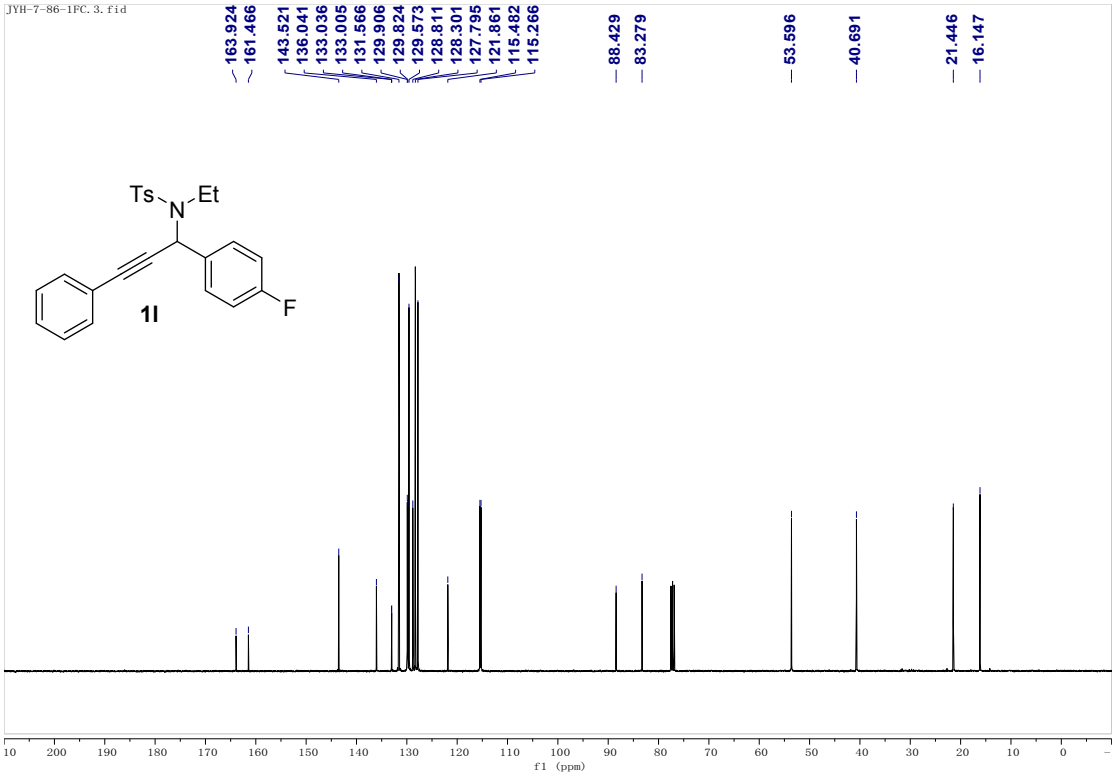
3.07
f1 (ppm)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Ts
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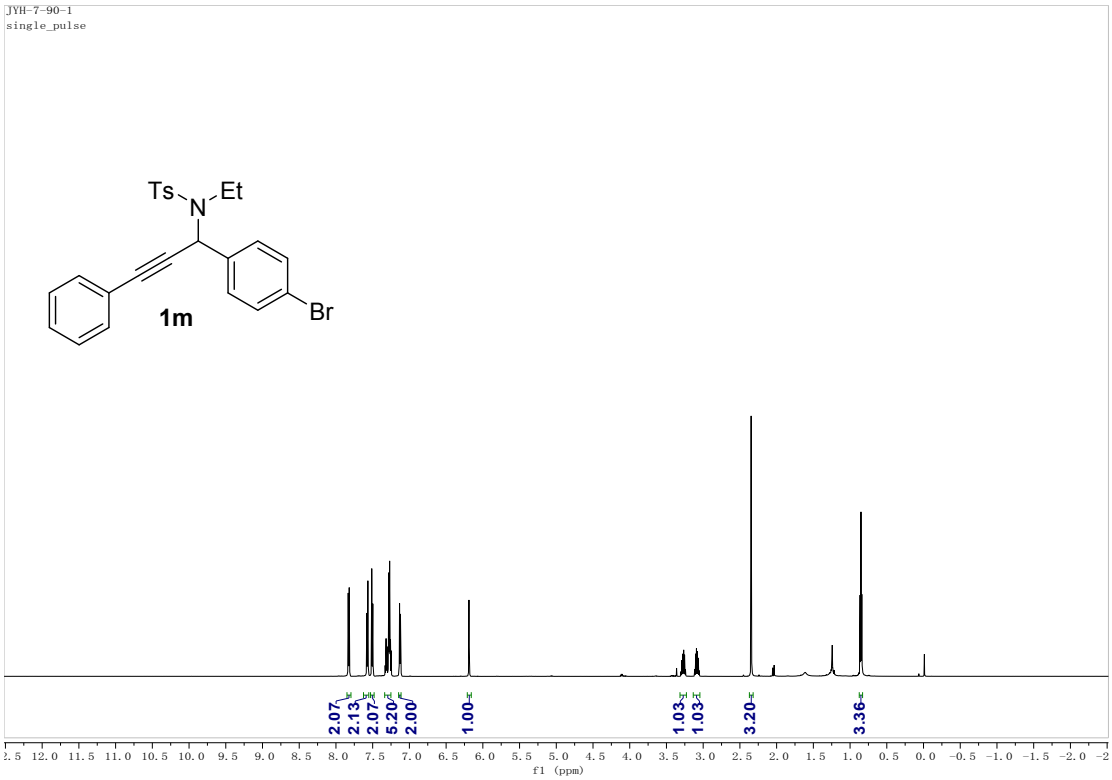
Et
F
1l
f1 (ppm)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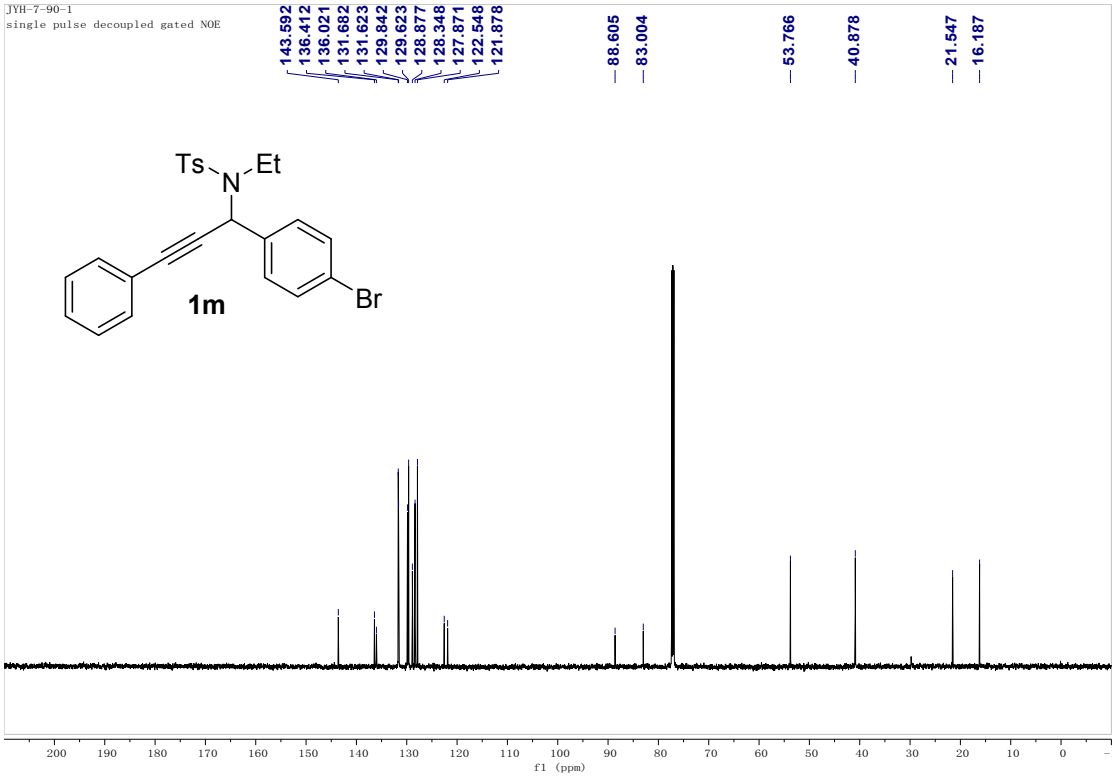
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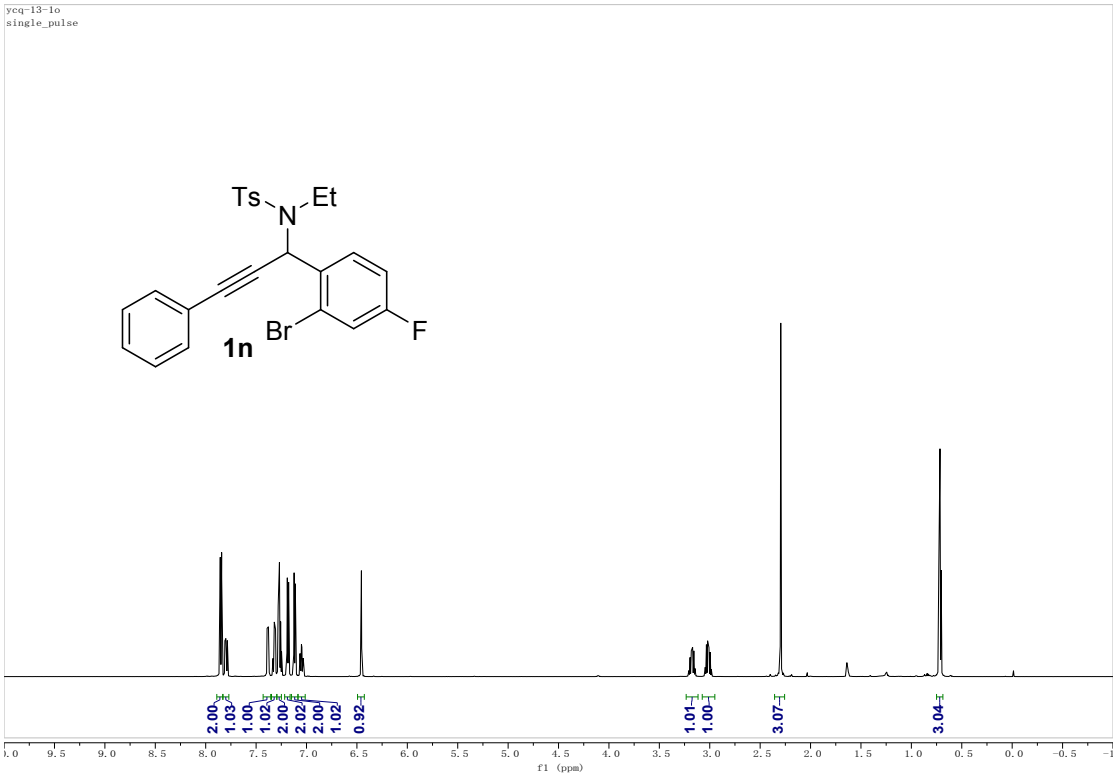
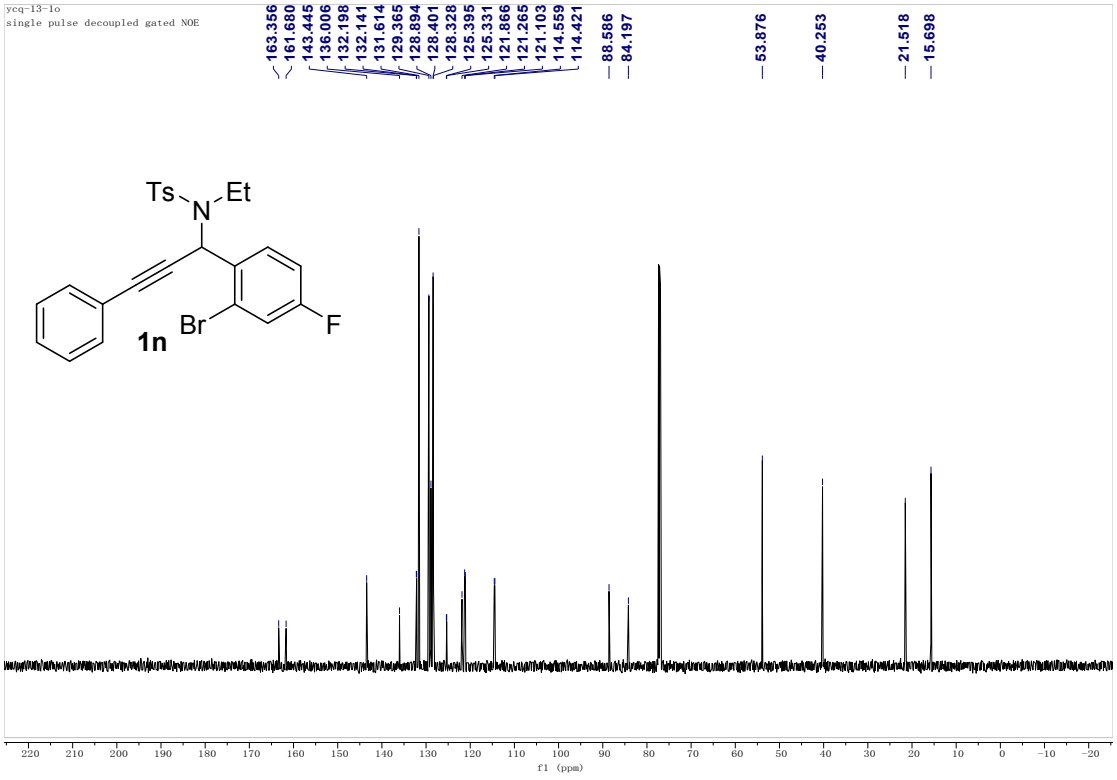
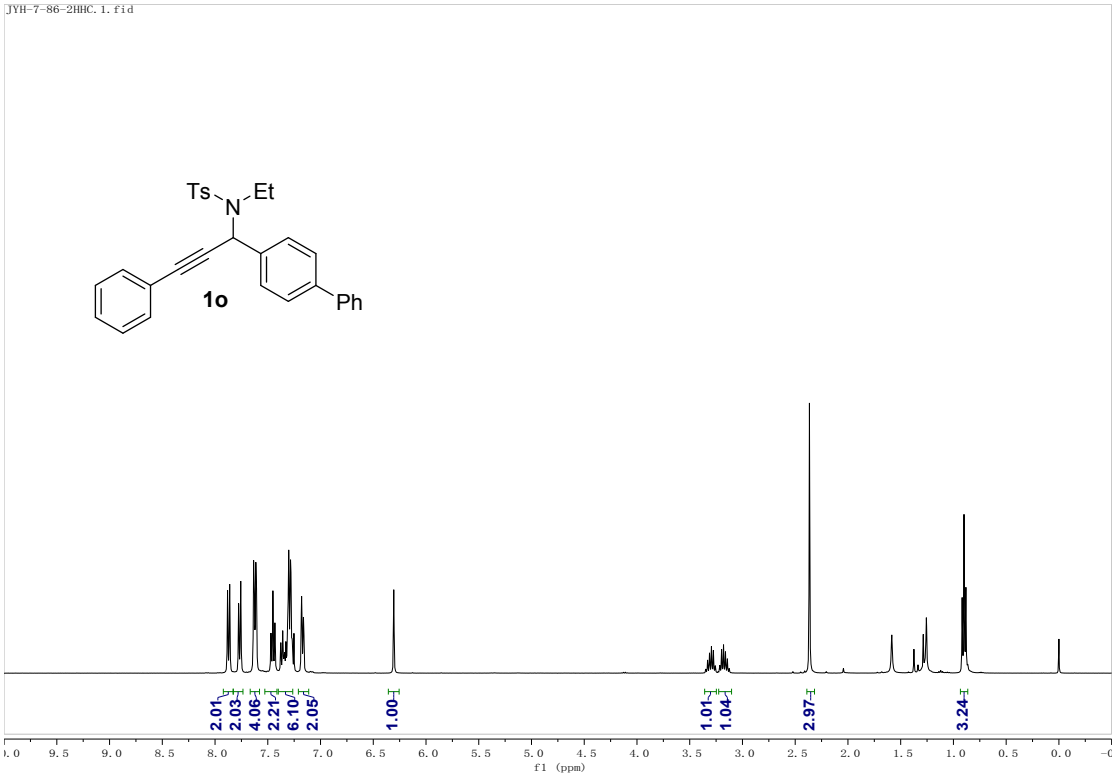
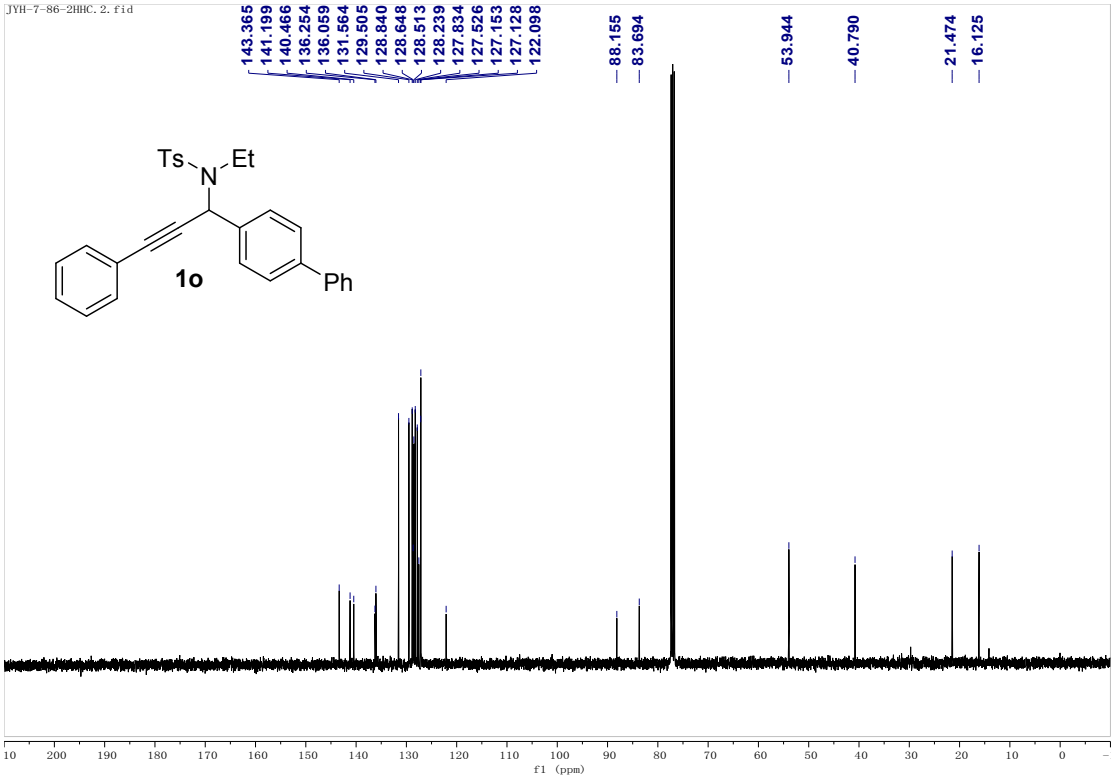
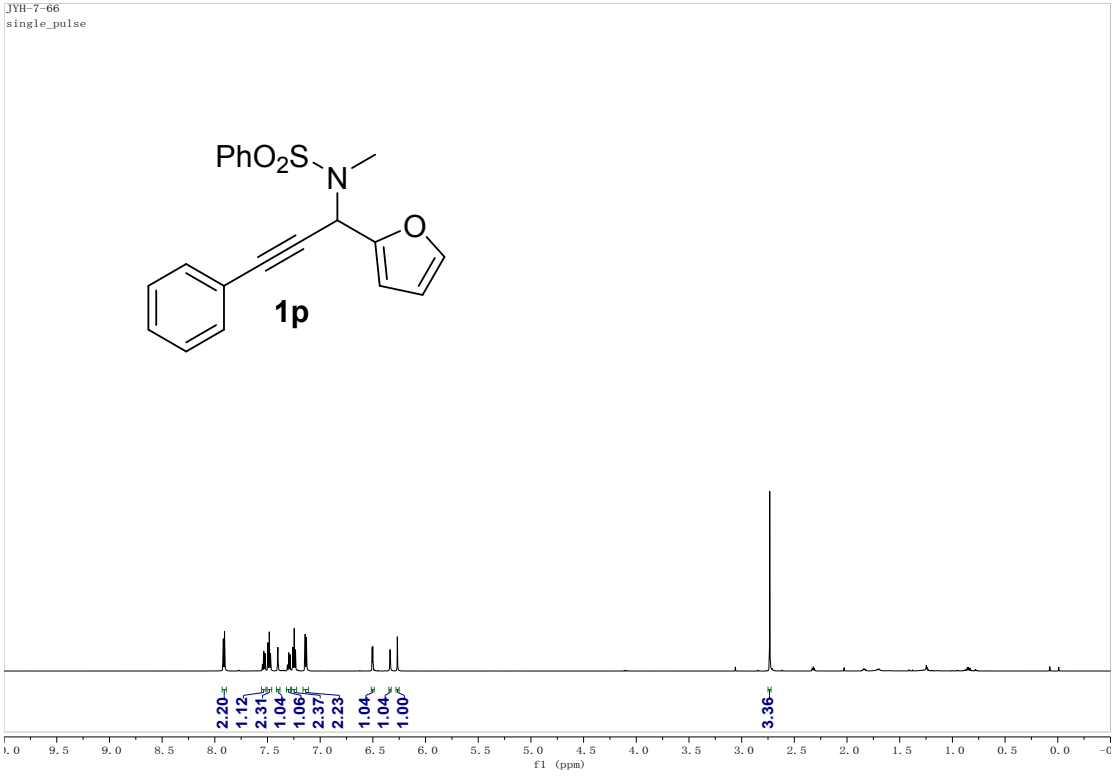
128.877
128.348
127.871
122.548
121.878
88.605
83.004
53.766
40.878
21.547
16.187
Ts
N
Et
Br
1m
f1 (ppm)

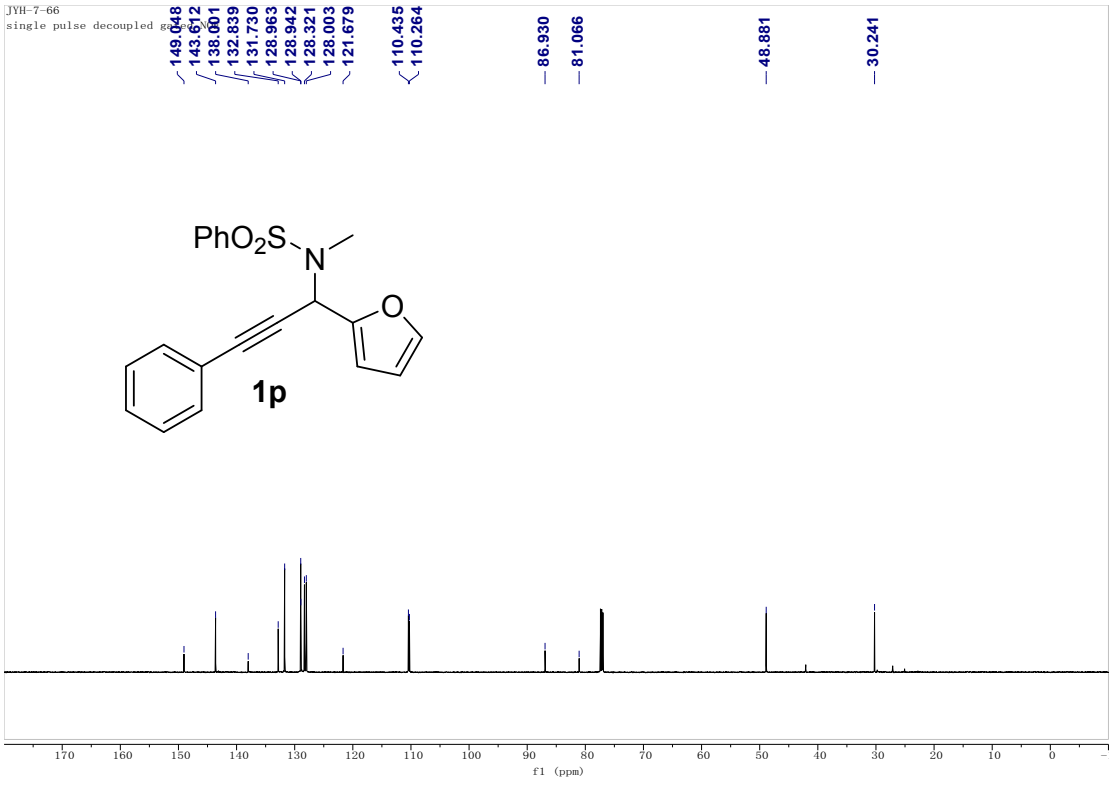

ycq-13-1o
single_pulse
Ts
N
Et
Br
F
1n
2.00
1.03
1.00
1.02
2.00
2.02
2.00
1.02
0.92
1.01
1.00
3.07
3.04
f1 (ppm)

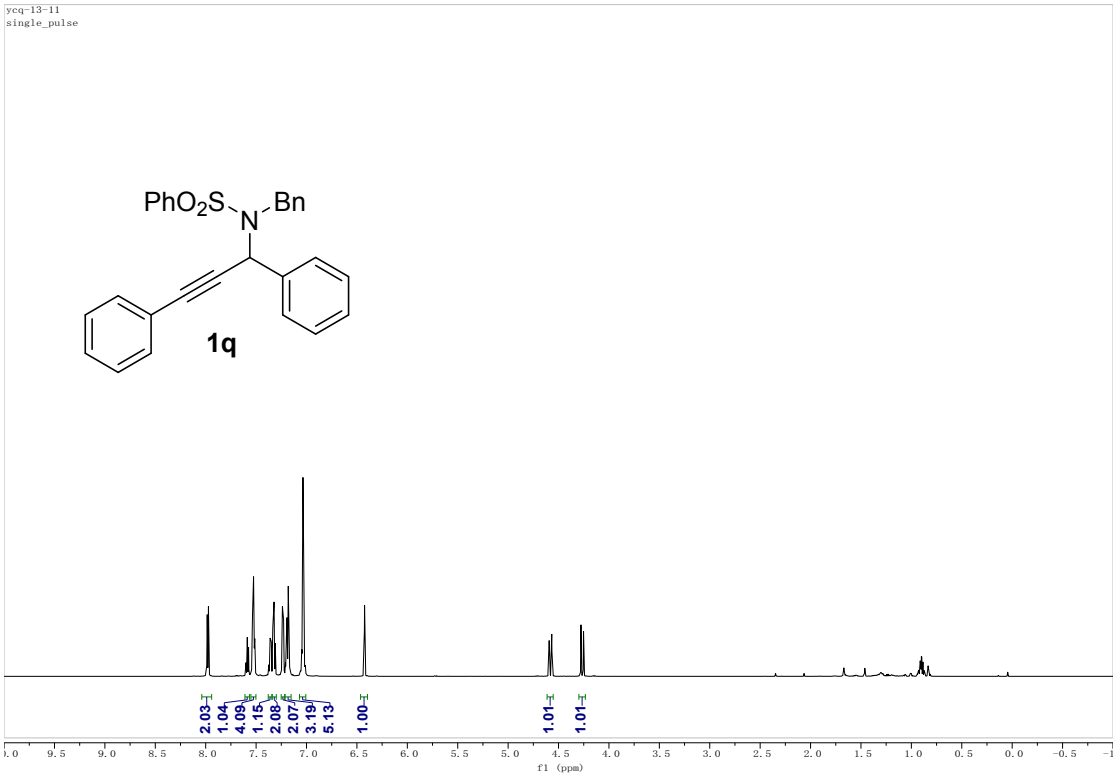

ycq-13-1o
single pulse decoupled gated NOE
163.356
161.680
143.445
136.006
132.198
132.141
131.614
129.365
128.894
128.401
128.328
125.395
125.331
121.866
121.265
121.103
114.559
114.421
88.586
84.197
53.876
40.253
21.518
15.698
Ts
N
Et
Br
F
1n
f1 (ppm)

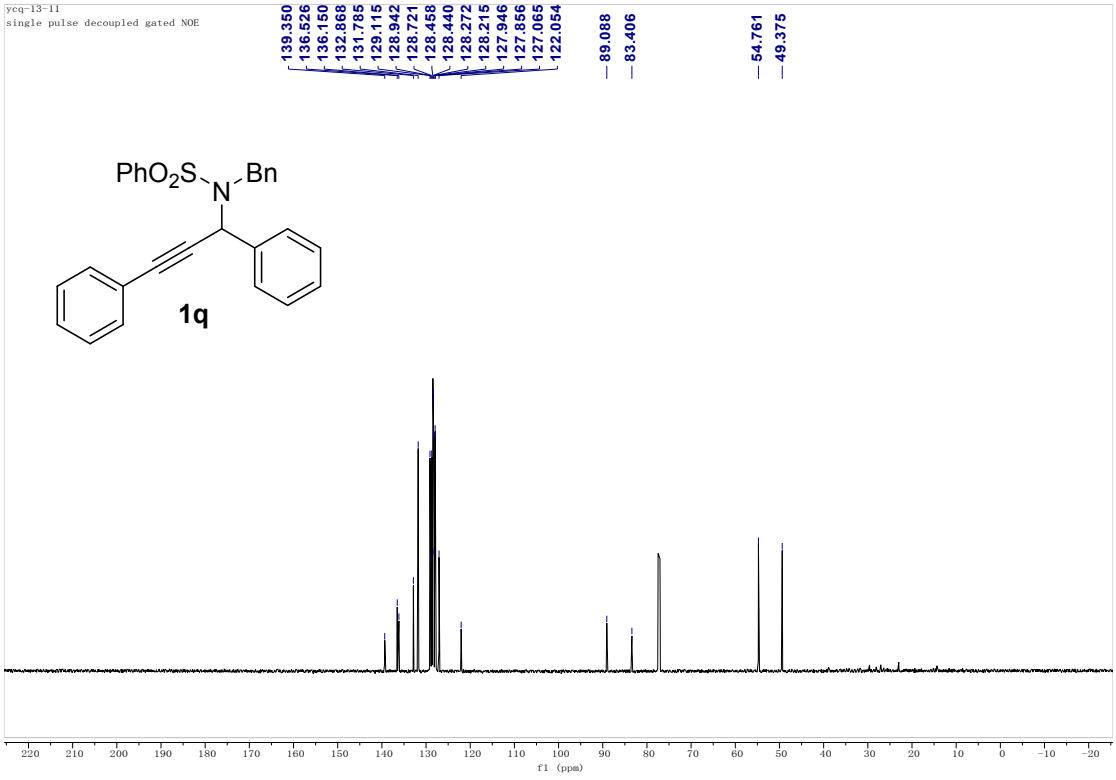

JYH-7-86-2HHC.1.fid
Ts
N
Et
1o
Ph
2.01
2.03
4.06
2.21
6.10
2.05
1.00
1.01
1.04
2.97
3.24
f1 (ppm)

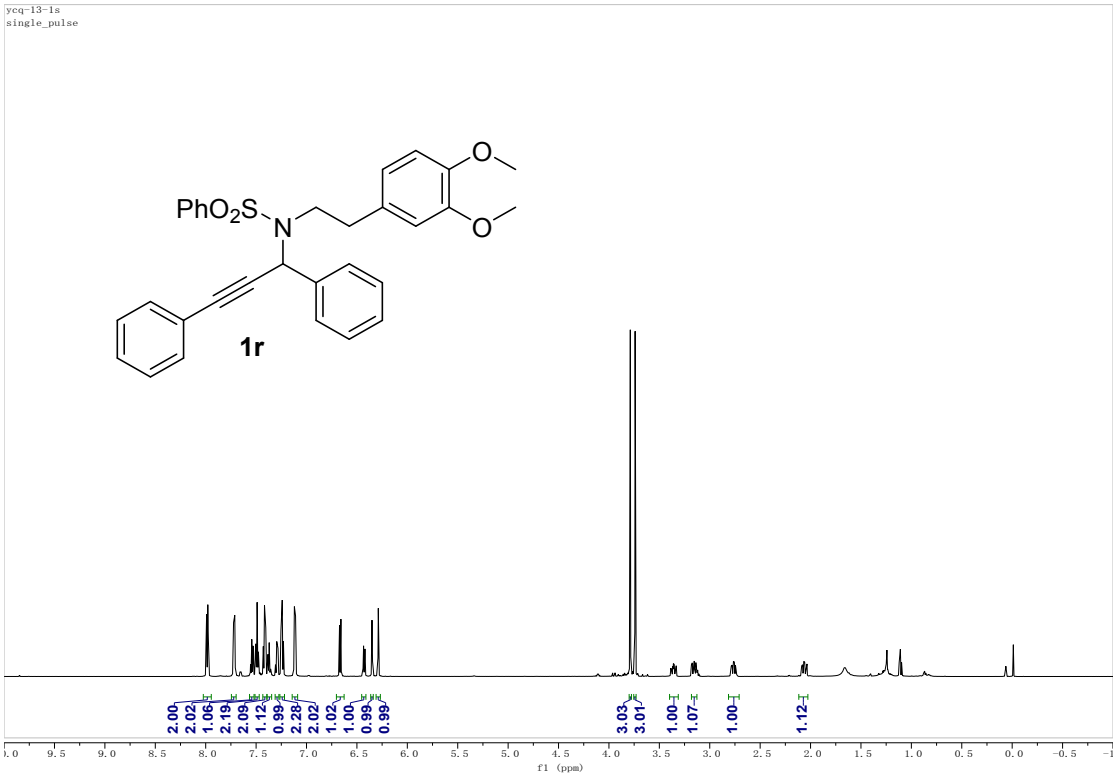

JYH-7-86-2HHC.2.fid
143.365
141.199
140.466
136.254
136.059
131.564
129.505
128.840
128.648
128.513
128.239
127.834
127.526
127.153
127.128
122.098
88.155
83.694
53.944
40.790
21.474
16.125
Ts
N
Et
1o
Ph
f1 (ppm)

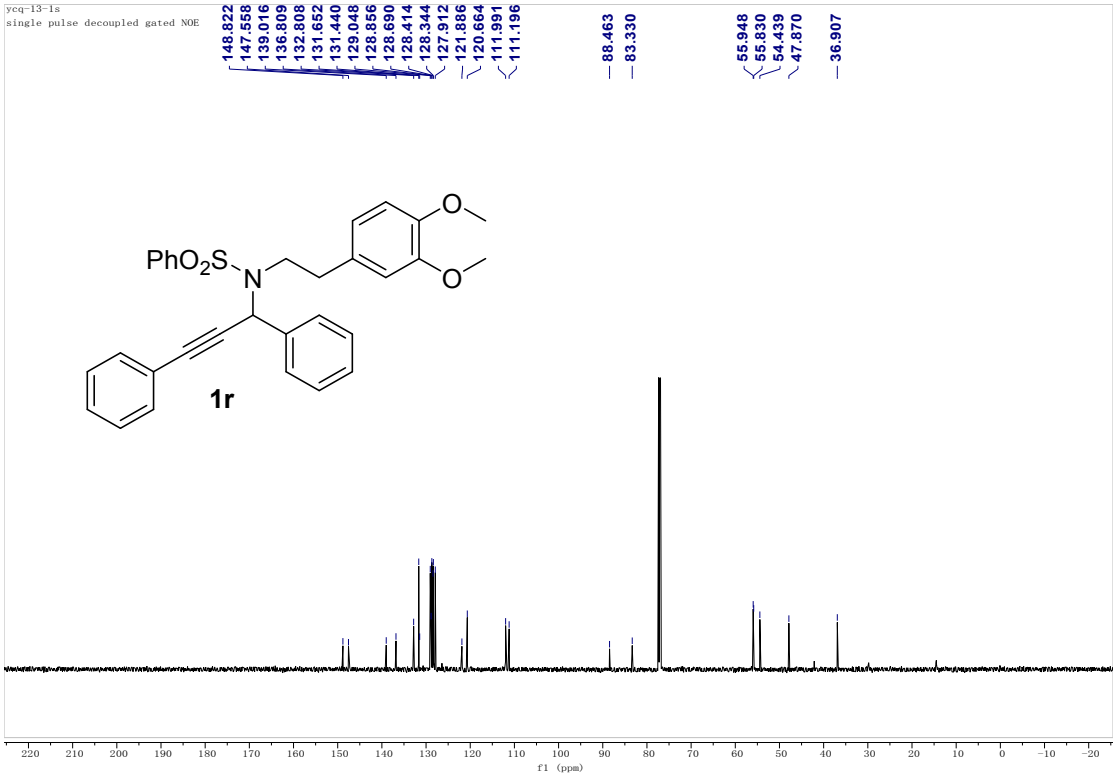

JYH-7-66
single_pulse
PhO2S
N
O
1p
2.20
1.12
2.31
1.04
1.06
2.37
2.23
1.04
1.04
1.00
3.36
f1 (ppm)

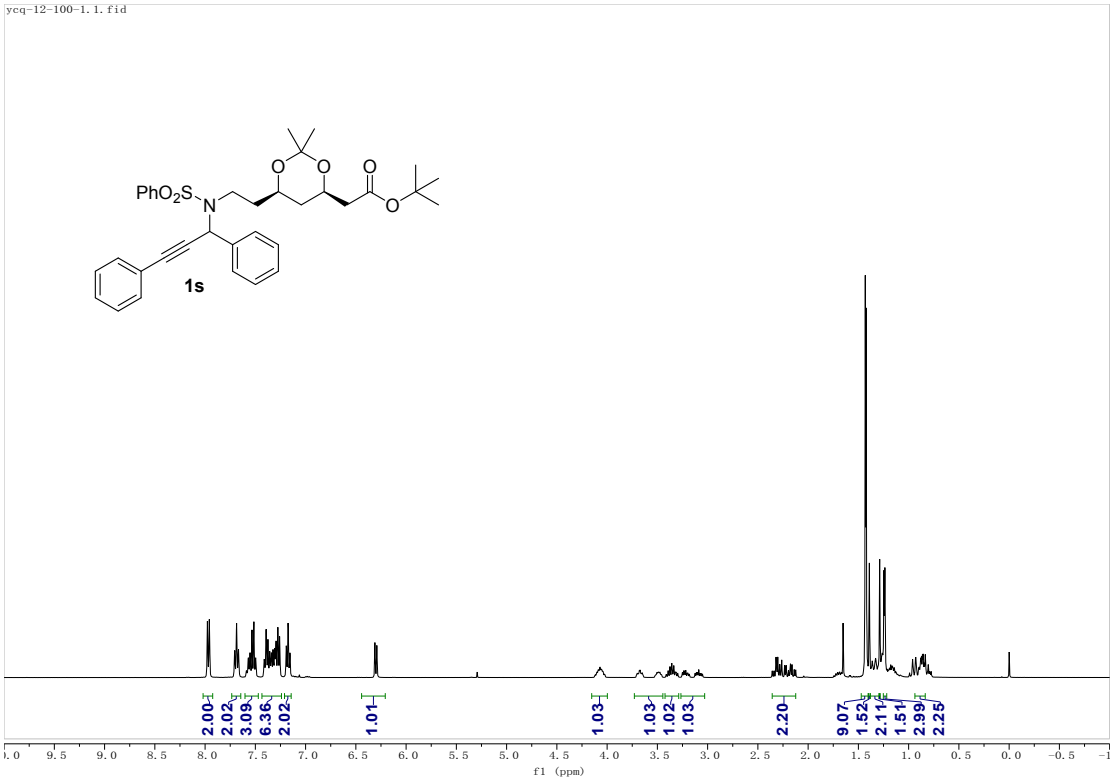

JYH-7-66
single pulse decoupled gated
149.048
143.512
138.001
132.839
131.730
128.963
128.942
128.321
128.003
121.679
110.435
110.264
86.930
81.066
48.881
30.241
PhO2S
N
O
1p
f1 (ppm)

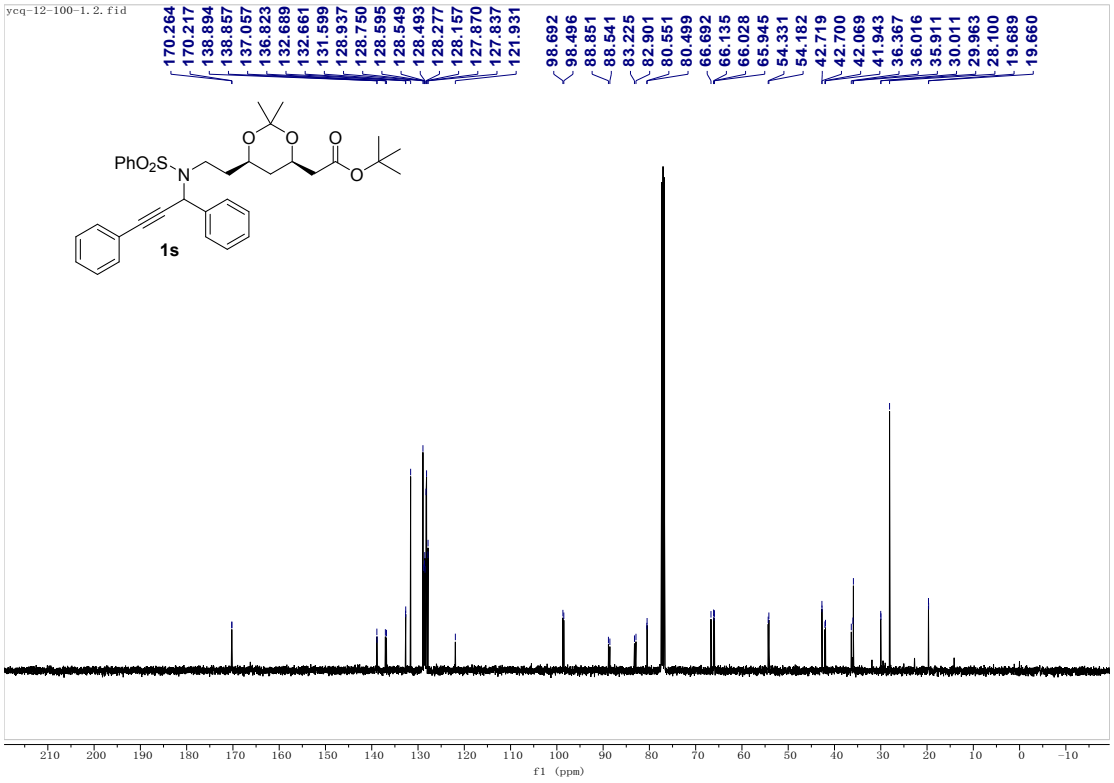

ycq-13-11
single_pulse
PhO2S
N
Bn
1q
2.03
1.04
4.09
1.15
2.08
2.07
3.19
5.13
1.00
1.01
1.01
f1 (ppm)

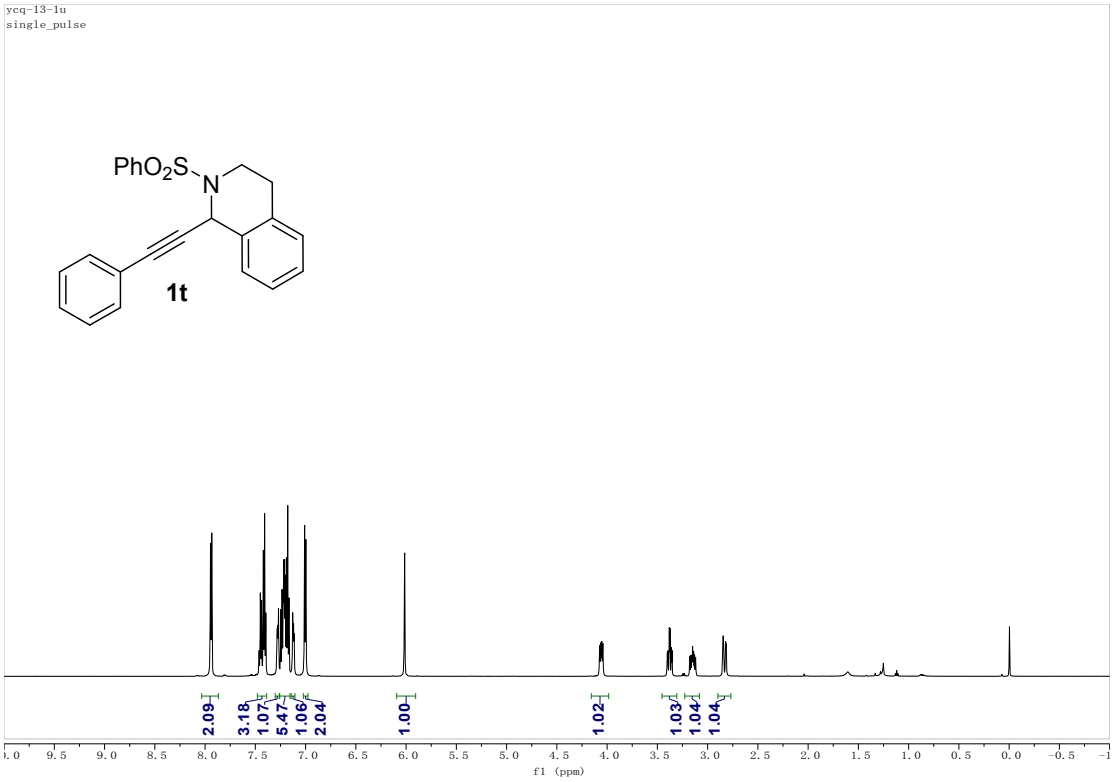

ycq-13-11
single pulse decoupled gated NOE
139.350
136.526
136.150
132.868
131.785
129.115
128.942
128.721
128.458
128.440
128.272
128.215
127.946
127.856
127.065
122.054
89.088
83.406
54.761
49.375
PhO2S
N
Bn
1q
f1 (ppm)

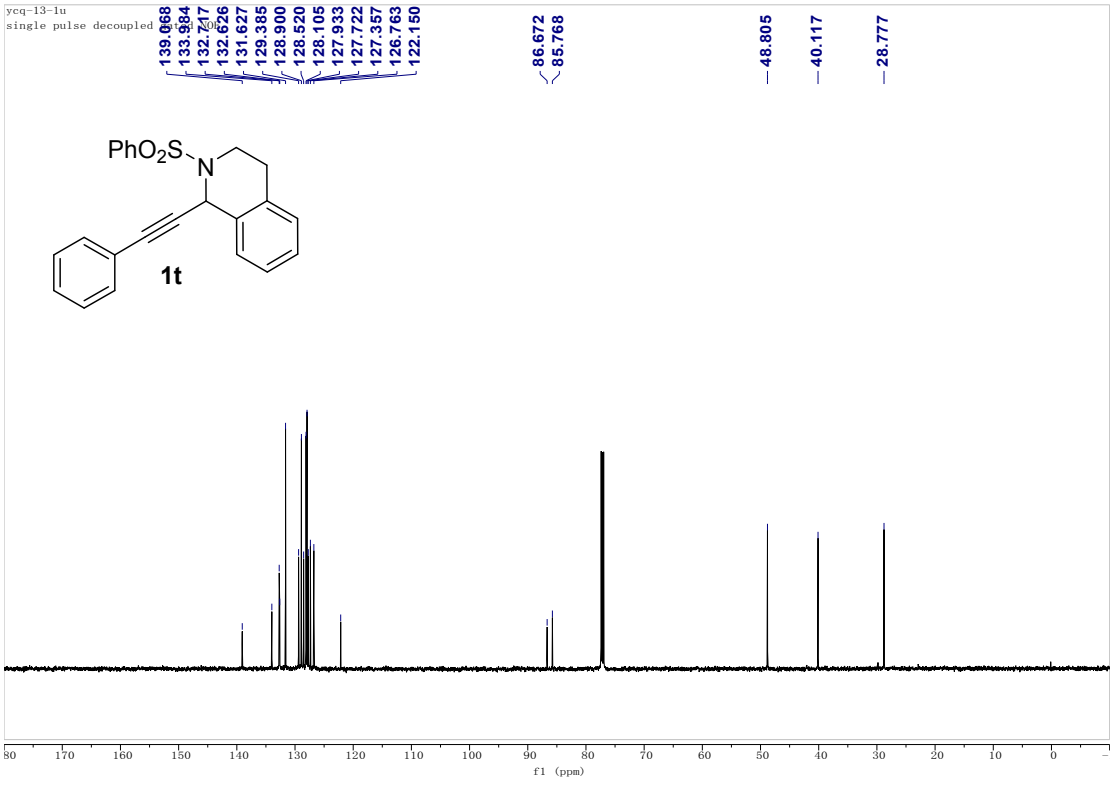

ycq-13-1s
single_pulse
PhO2S
N
O
O
1r
2.00
2.02
1.06
2.19
2.09
1.12
0.99
2.28
2.02
1.02
1.00
0.99
0.99
3.03
3.01
1.00
1.07
1.00
1.12
f1 (ppm)

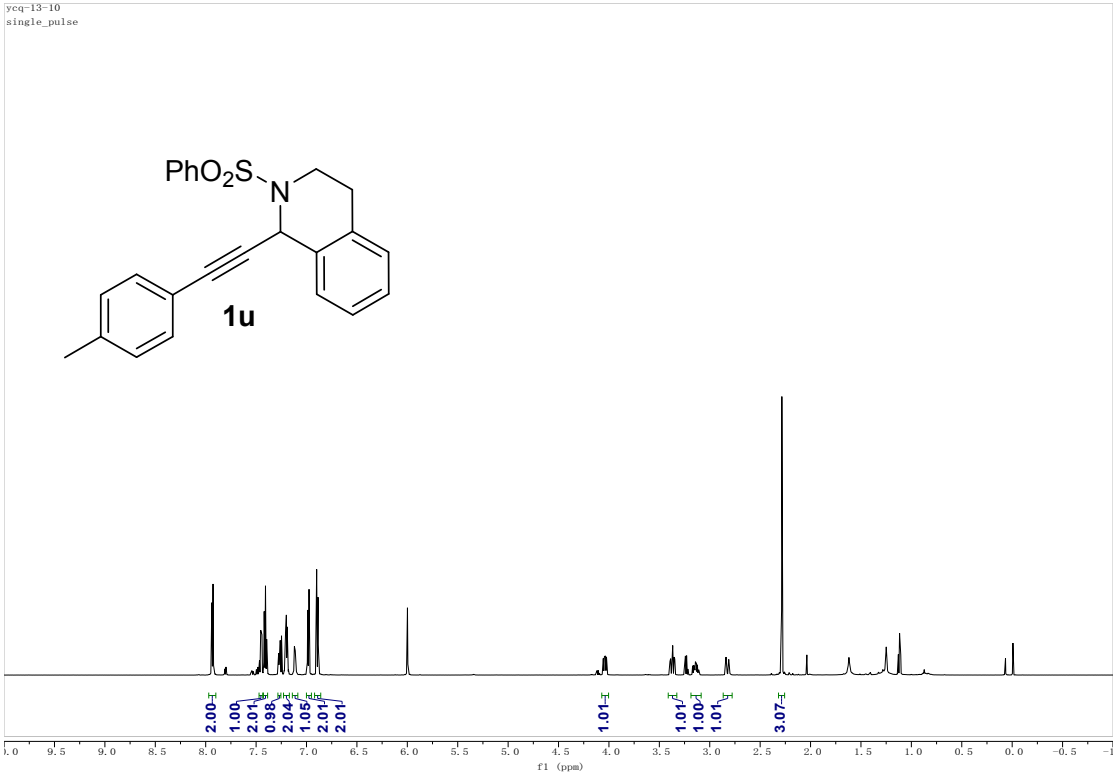

ycq-13-1s
single pulse decoupled gated NOE
148.822
147.558
139.016
136.809
132.808
131.652
131.440
129.048
128.856
128.690
128.414
128.344
127.912
121.886
120.664
111.991
111.196
88.463
83.330
55.948
55.830
54.439
47.870
36.907
PhO2S
N
O
O
1r
f1 (ppm)

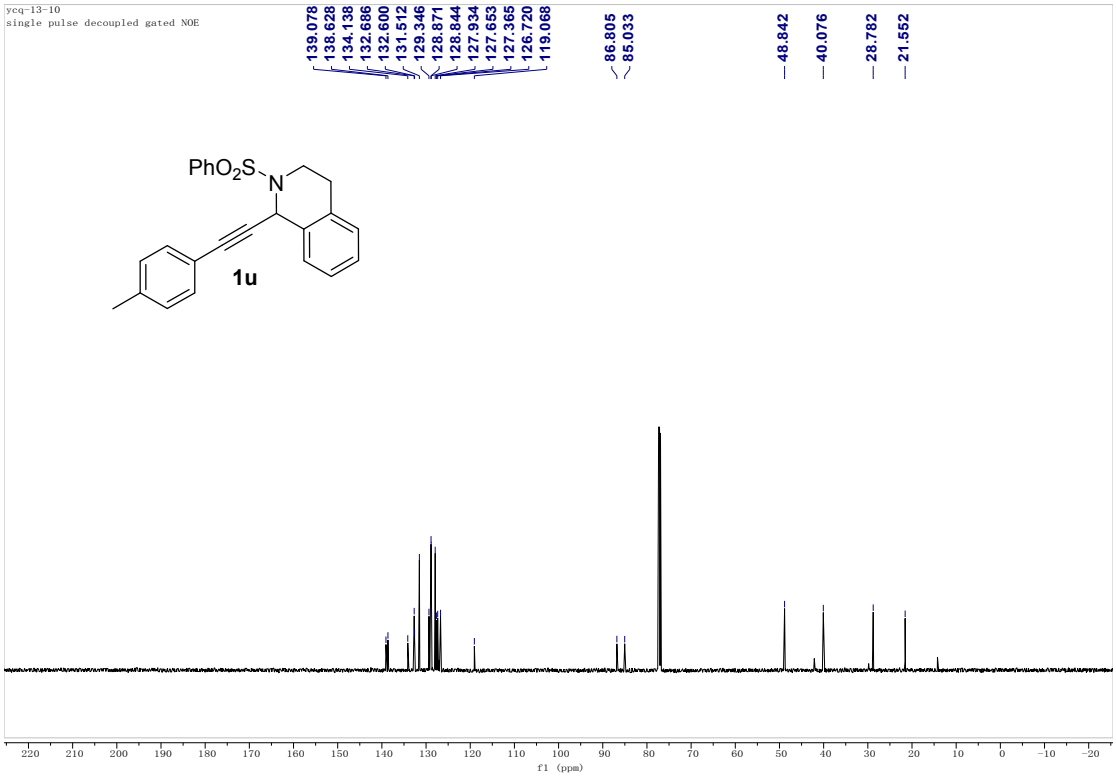

ycq-12-100-1.1.fid
PhO2S
N
O
O
O
O
1s
2.00
2.02
3.09
6.36
2.02
1.01
1.03
1.03
1.02
1.03
2.20
9.07
1.52
2.11
1.51
2.99
2.25
f1 (ppm)

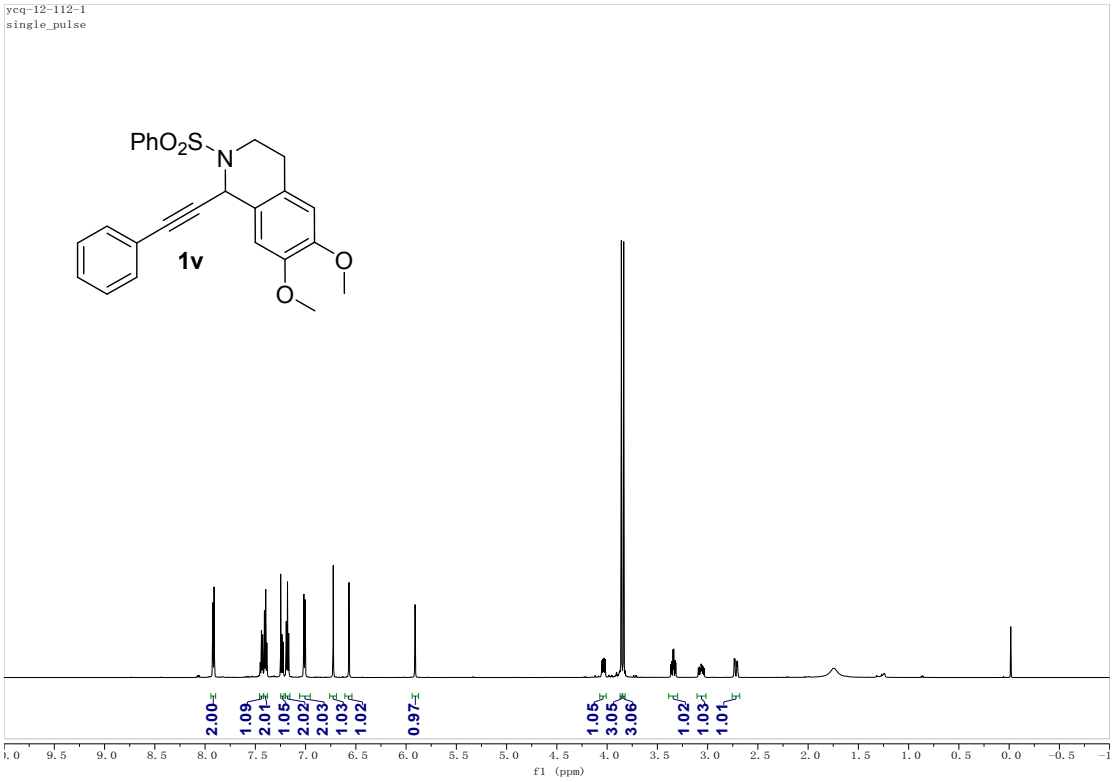

ycq-12-100-1.2.fid
170.264
170.217
138.894
138.857
137.057
136.823
132.689
132.661
131.599
128.937
128.750
128.595
128.549
128.493
128.277
128.157
127.870
127.837
121.931
98.692
98.496
88.851
88.541
83.225
82.901
80.551
80.499
66.692
66.135
66.028
65.945
54.331
54.182
42.719
42.700
42.069
41.943
36.367
36.016
35.911
30.011
29.963
28.100
19.689
19.660
PhO2S
N
O
O
O
O
1s
f1 (ppm)

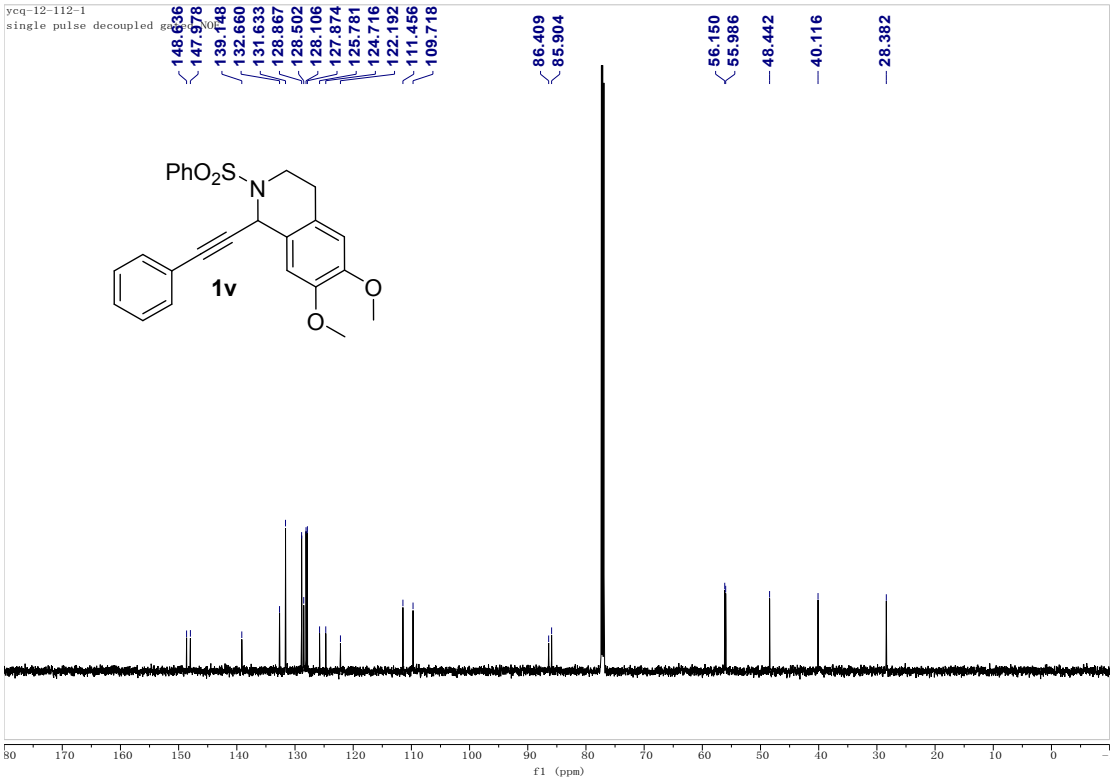

ycq-13-1u
single_pulse
PhO2S
N
1t
2.09
3.18
1.07
5.47
1.06
2.04
1.00
1.02
1.03
1.04
1.04
f1 (ppm)

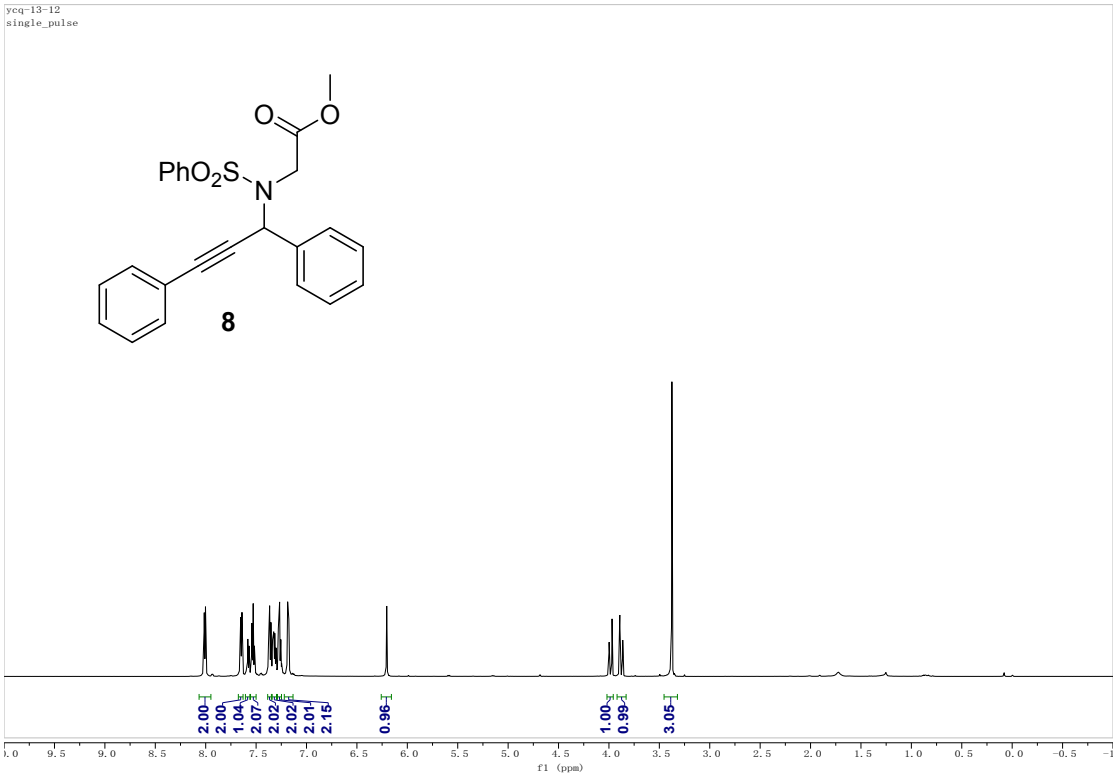

ycq-13-1u
single pulse decoupled
139.068
133.984
132.717
132.626
131.627
129.385
128.900
128.520
128.105
127.933
127.722
127.357
126.763
122.150
86.672
85.768
48.805
40.117
28.777
PhO2S
N
1t
f1 (ppm)

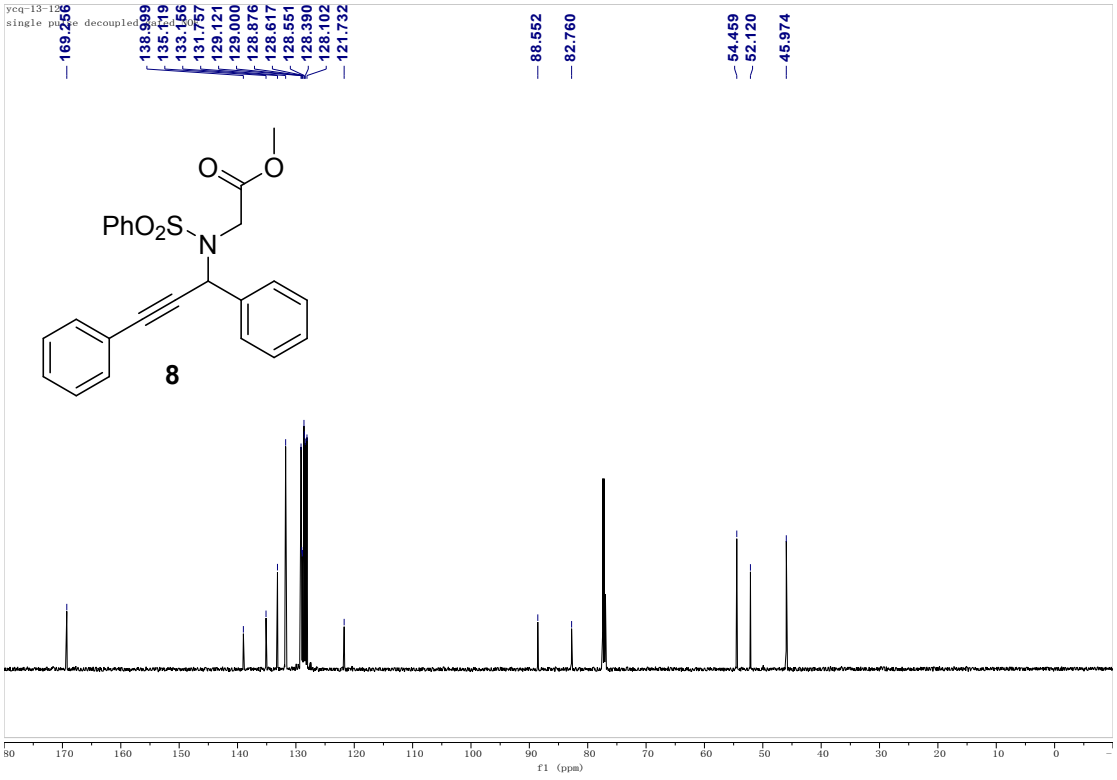

ycq-13-10
single_pulse
PhO2S
N
1u
2.00
1.00
2.01
0.98
2.04
1.05
2.01
2.01
1.01
1.01
1.00
1.01
3.07
f1 (ppm)

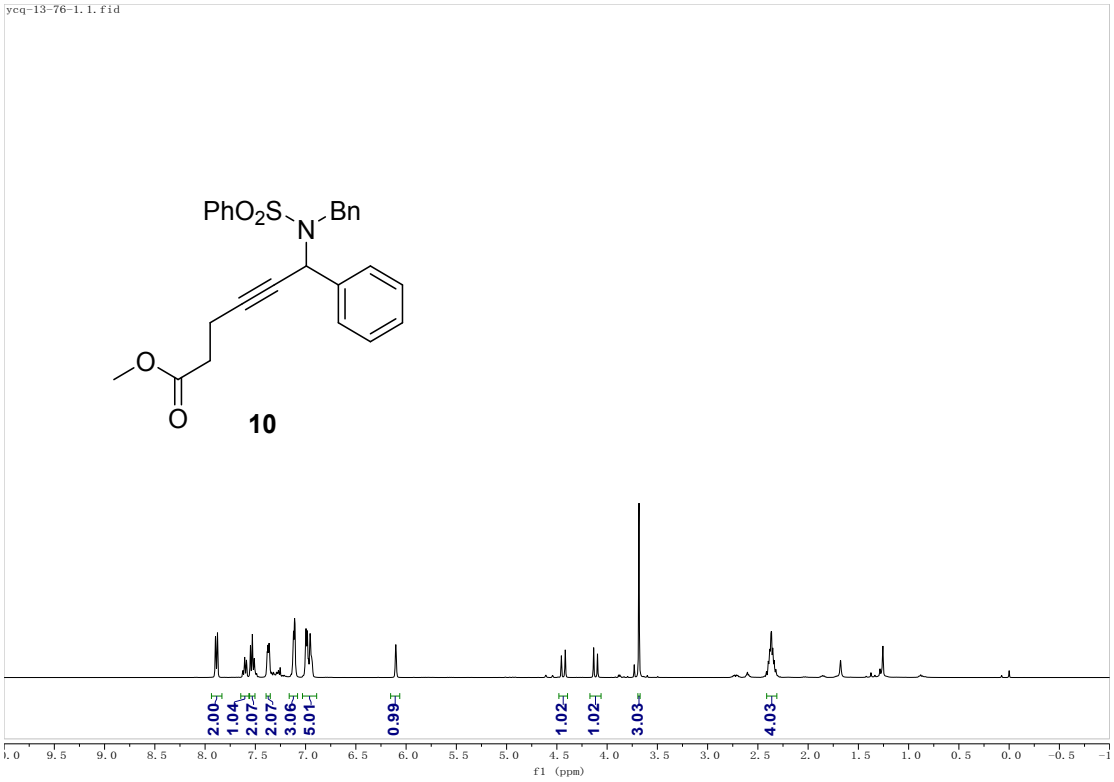

ycq-13-10
single pulse decoupled gated NOE
139.078
138.628
134.138
132.686
132.600
131.512
129.346
128.871
128.844
127.934
127.653
127.365
126.720
119.068
86.805
85.033
48.842
40.076
28.782
21.552
PhO2S
N
1u
f1 (ppm)

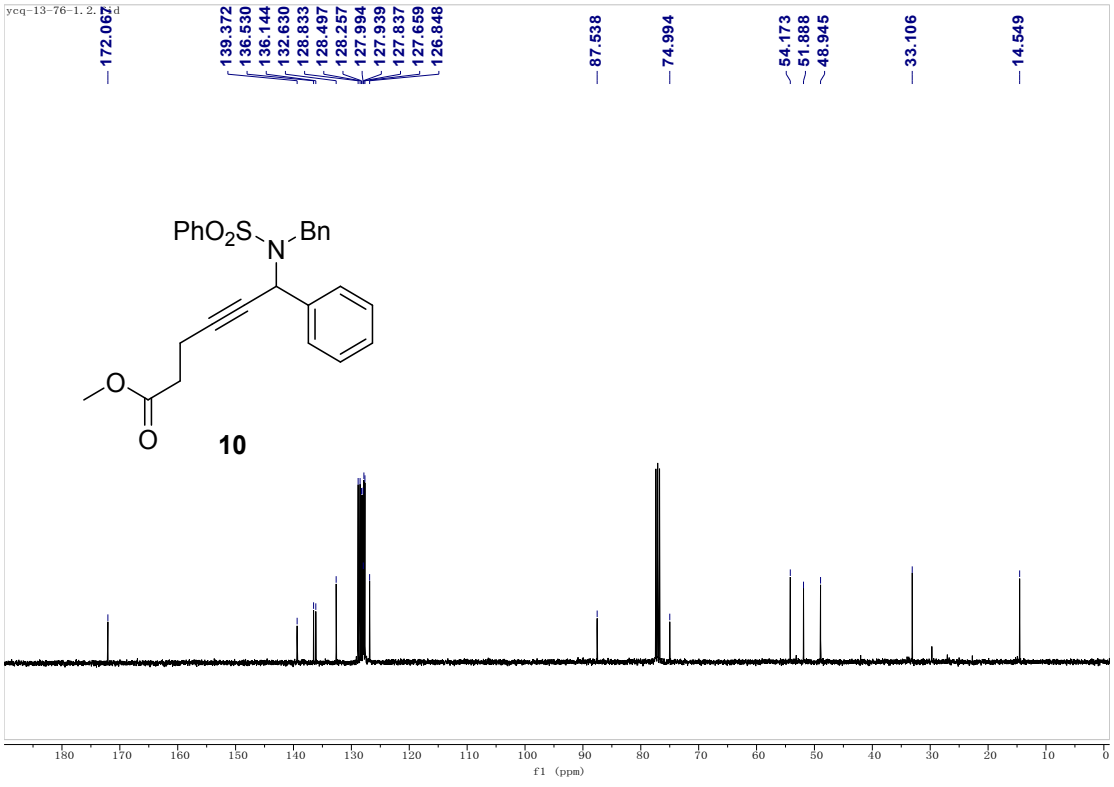

ycq-12-112-1
single_pulse
PhO2S
N
1v
O
O
2.00
1.09
2.01
1.05
2.02
2.03
1.03
1.02
0.97
1.05
3.05
3.06
1.02
1.03
1.01
f1 (ppm)

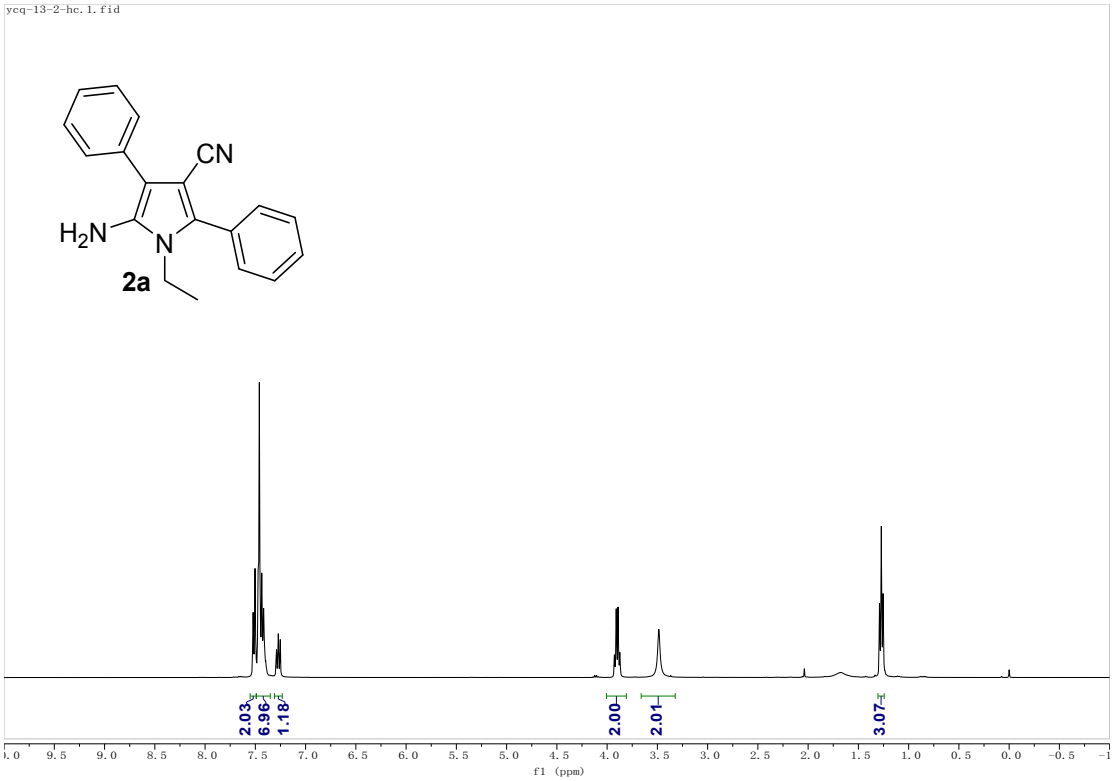

ycq-12-112-1
single pulse decoupled gated NOE
148.636
147.978
139.148
132.660
131.633
128.867
128.502
128.106
127.874
125.781
124.716
122.192
111.456
109.718
86.409
85.904
56.150
55.986
48.442
40.116
28.382
PhO2S
N
1v
O
O
f1 (ppm)

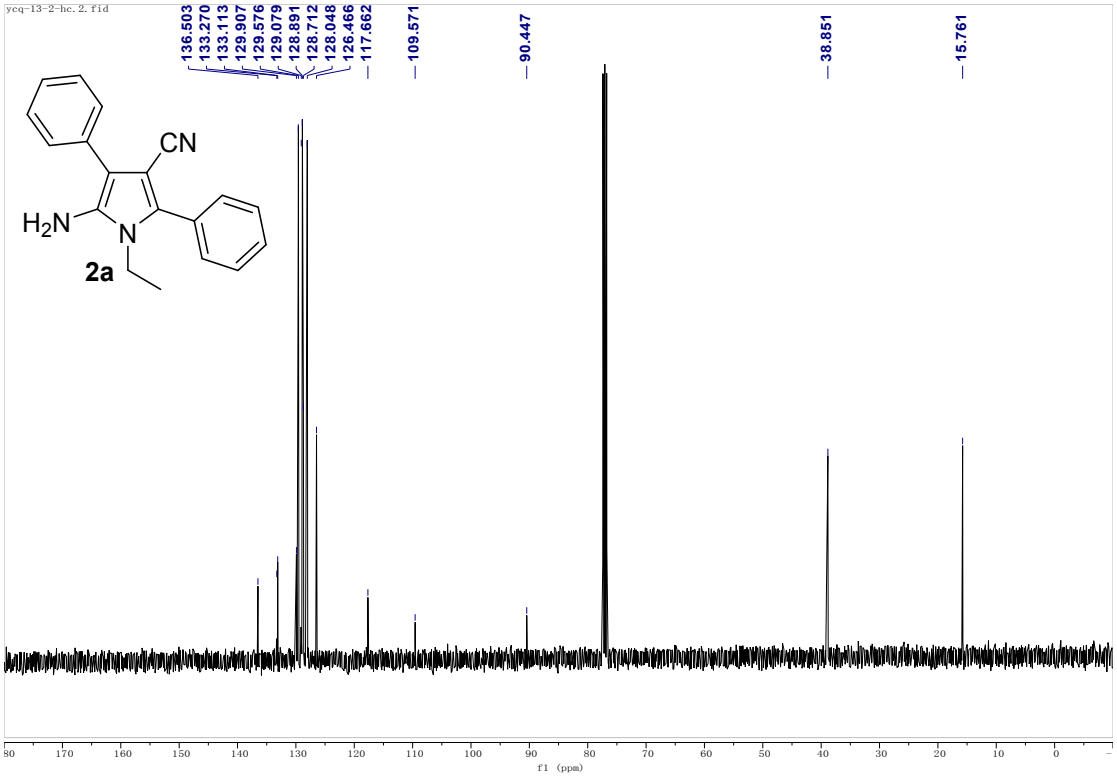

ycq-13-12
single_pulse
O
O
PhO2S
N
8
2.00
2.00
1.04
2.07
2.02
2.02
2.01
2.15
0.96
1.00
0.99
3.05
f1 (ppm)

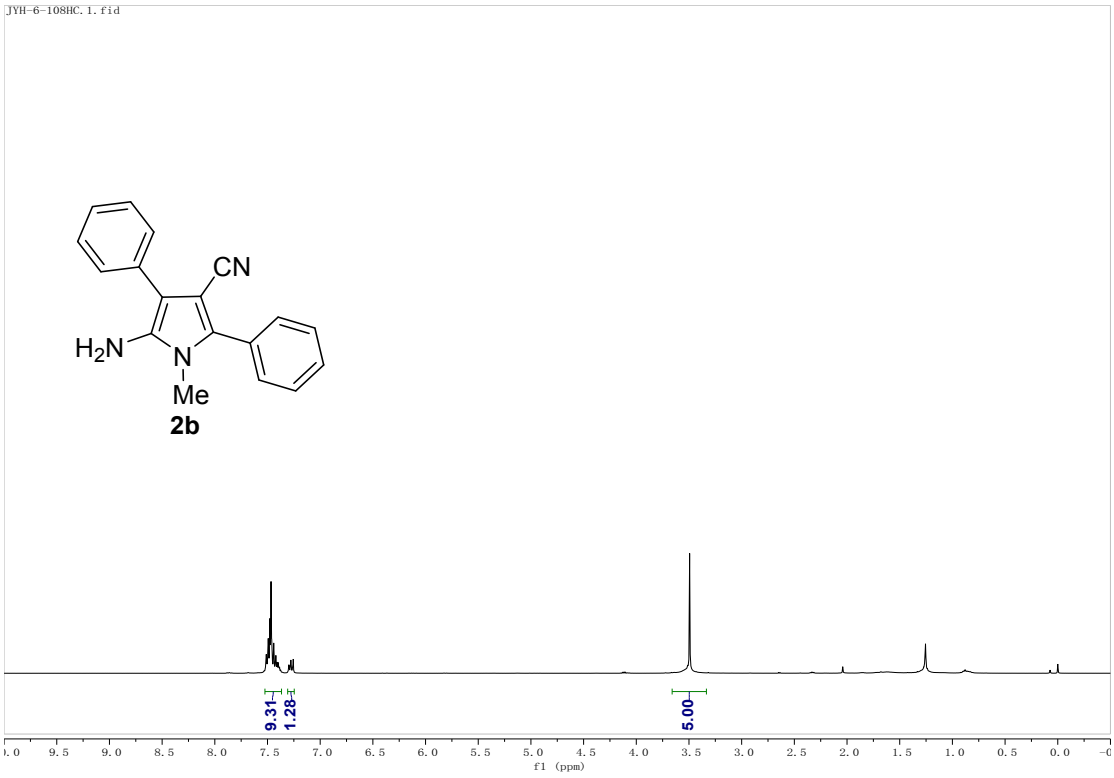

ycq-13-12
single pulse decoupled carbon
169.256
138.399
135.119
133.156
131.757
129.121
129.000
128.876
128.617
128.551
128.390
128.102
121.732
88.552
82.760
54.459
52.120
45.974
O
O
PhO2S
N
8
f1 (ppm)

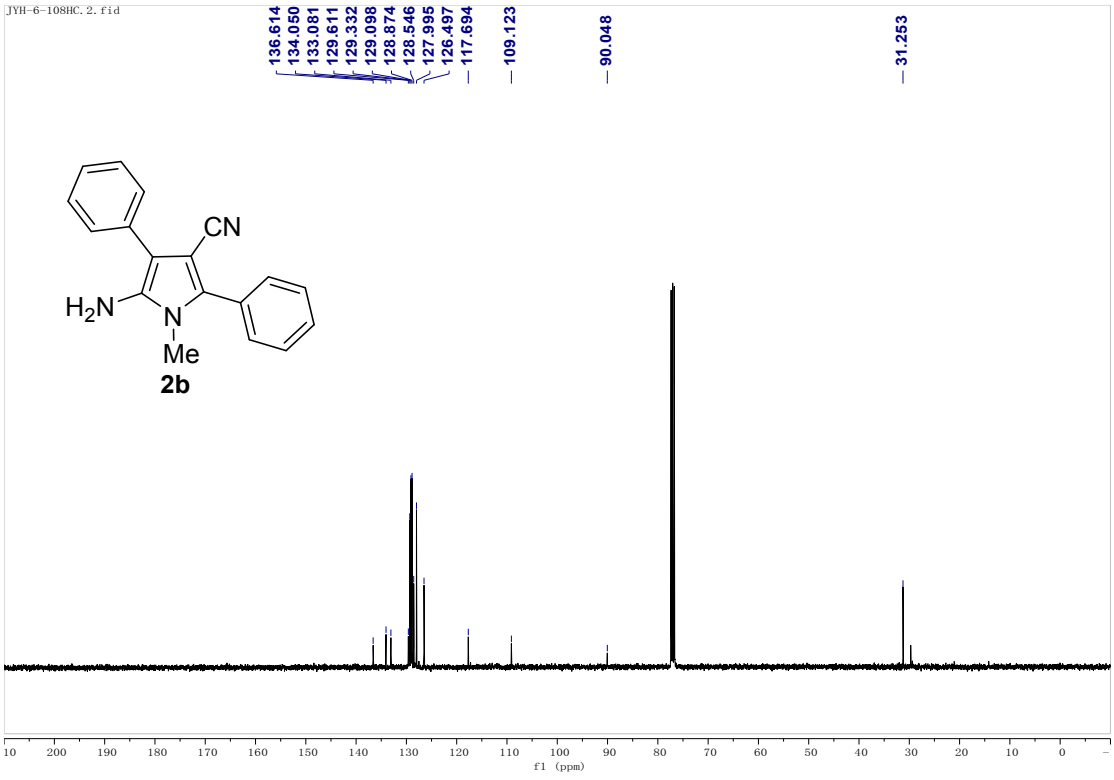

ycq-13-76-1.1.fid
PhO2S
N
Bn
O
O
10
2.00
1.04
2.07
2.07
3.06
5.01
0.99
1.02
1.02
3.03
4.03
f1 (ppm)

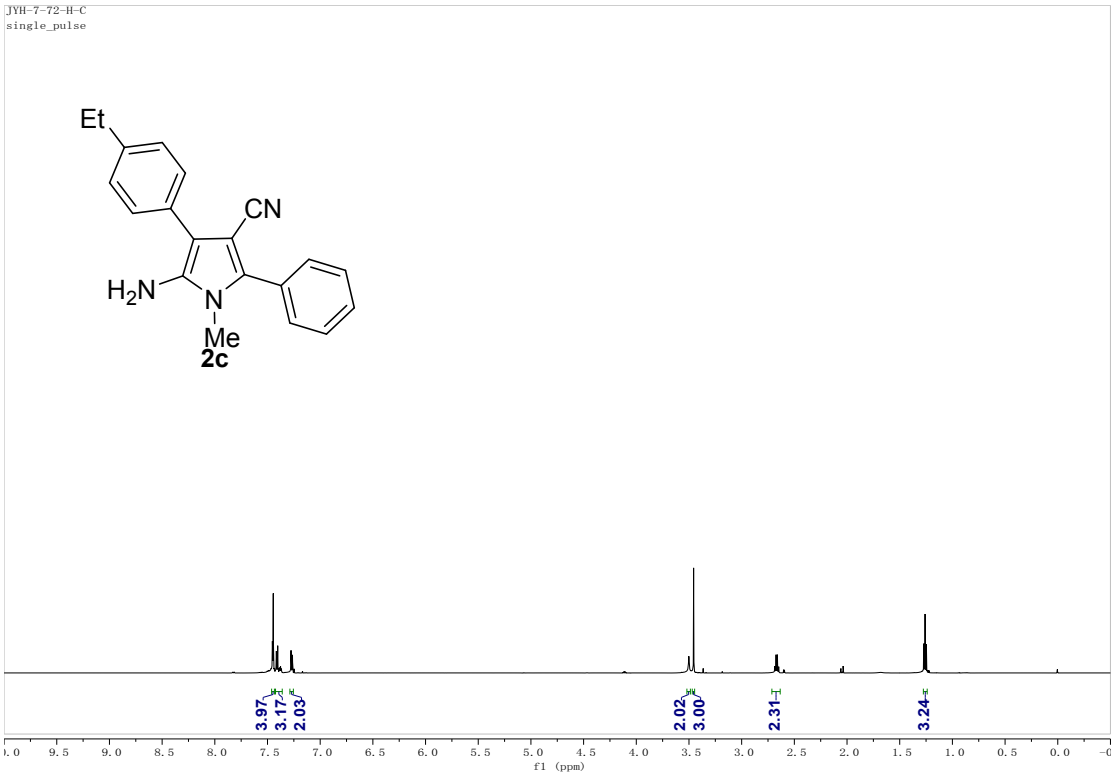

ycq-13-76-1.2.fid
172.067
139.372
136.530
136.144
132.630
128.833
128.497
128.257
127.994
127.939
127.837
127.659
126.848
87.538
74.994
54.173
51.888
48.945
33.106
14.549
PhO2S
N
Bn
O
O
10
f1 (ppm)

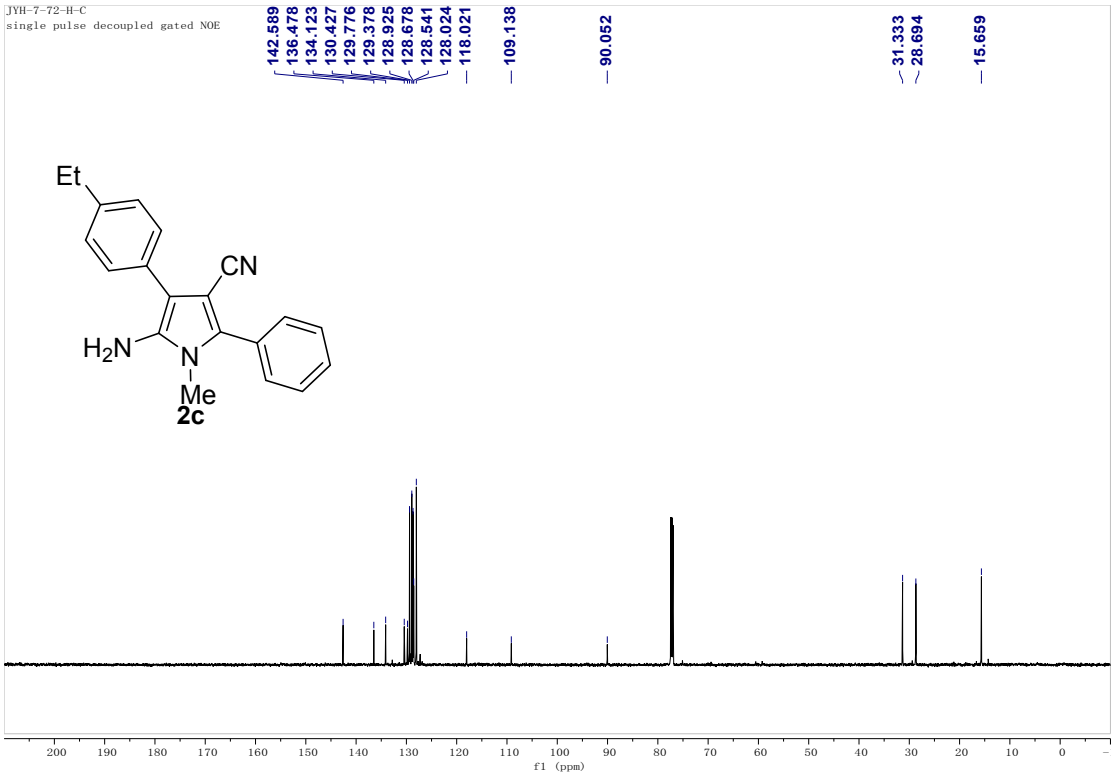

ycq-13-2-hc.1.fid
CN
H_2N
N
2a
2.03
6.96
1.18
2.00
2.01
3.07
f1 (ppm)

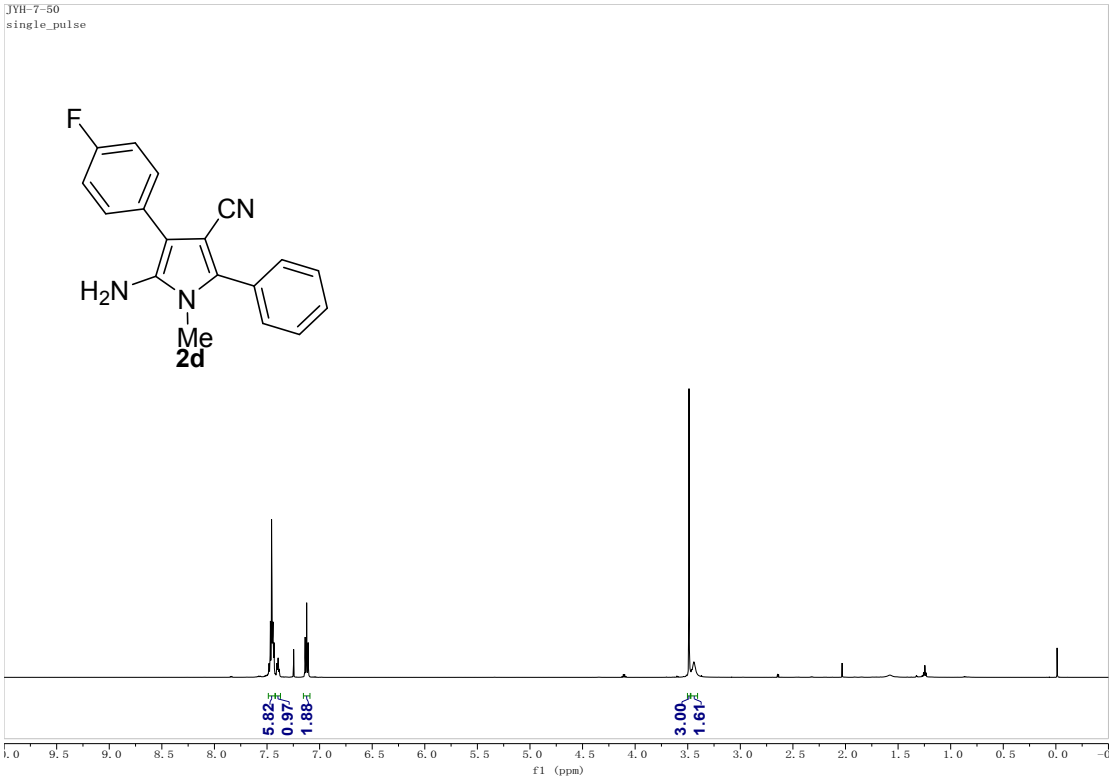

ycq-13-2-hc.2.fid
136.503
133.270
133.113
129.907
129.576
129.079
128.891
128.712
128.048
126.466
117.662
109.571
90.447
38.851
15.761
CN
H_2N
N
2a
f1 (ppm)

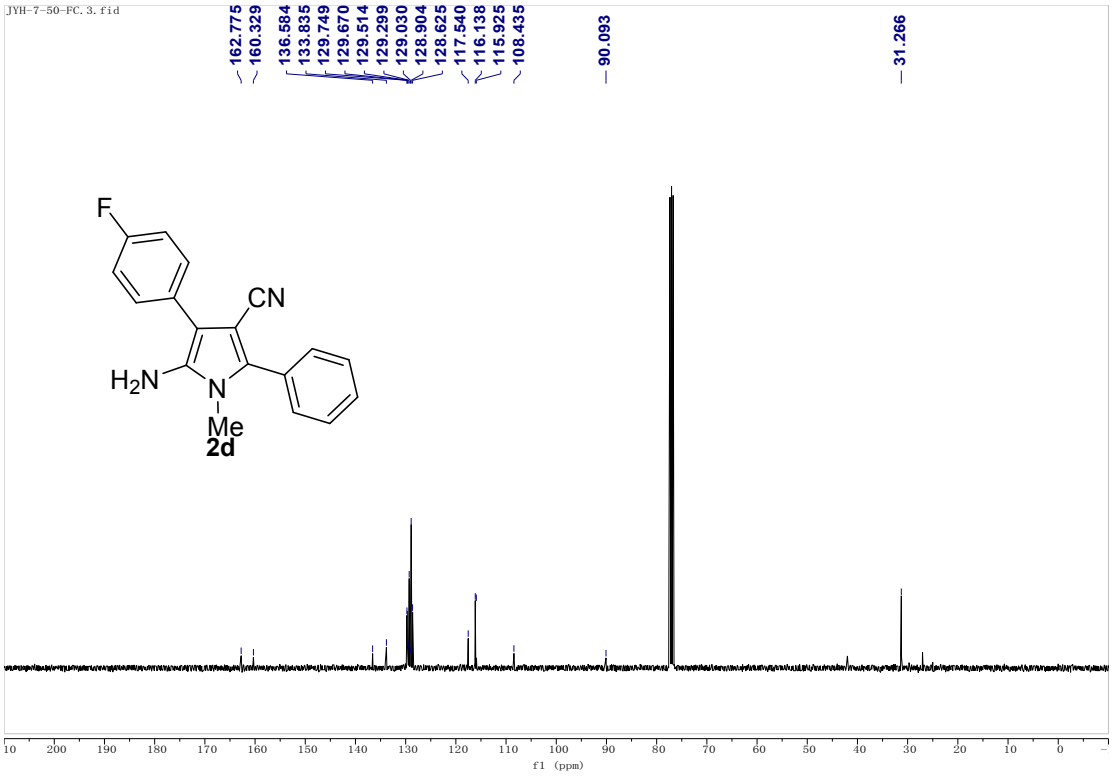

JYH-6-108HC.1.fid
CN
H2N
N
Me
2b
9.31
1.28
5.00
f1 (ppm)

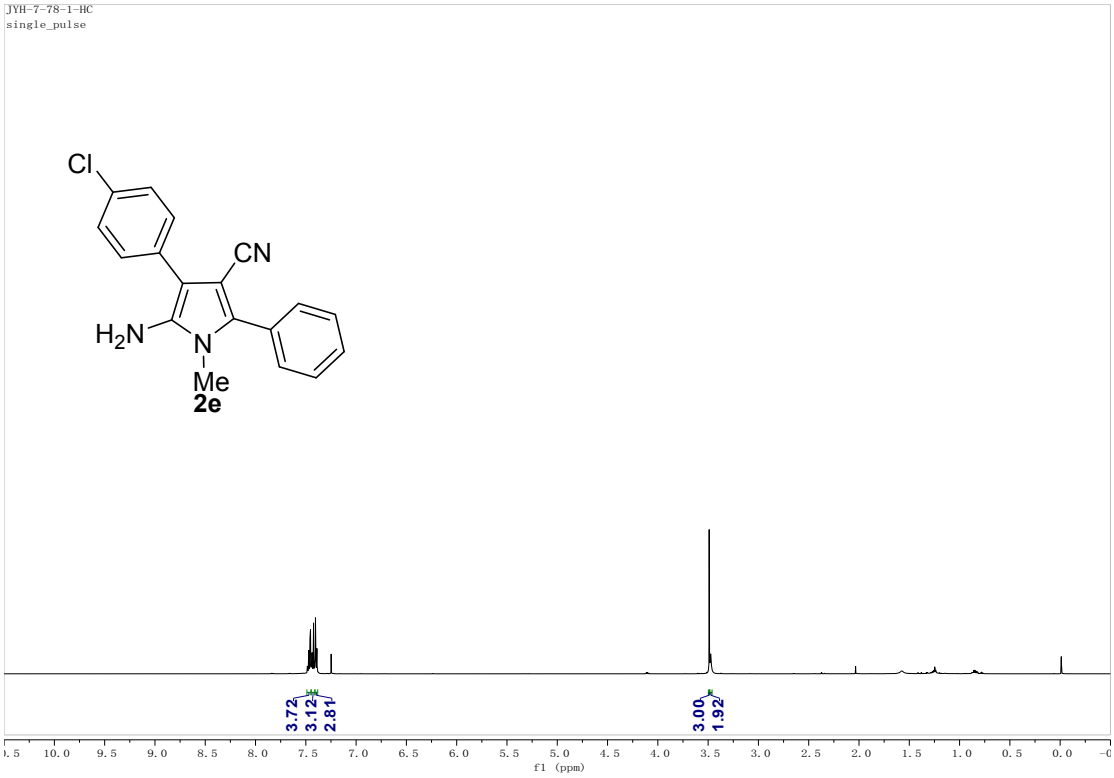

JYH-6-108HC.2.fid
136.614
134.050
133.081
129.611
129.332
129.098
128.874
128.546
127.995
126.497
117.694
109.123
90.048
31.253
CN
H2N
N
Me
2b
f1 (ppm)

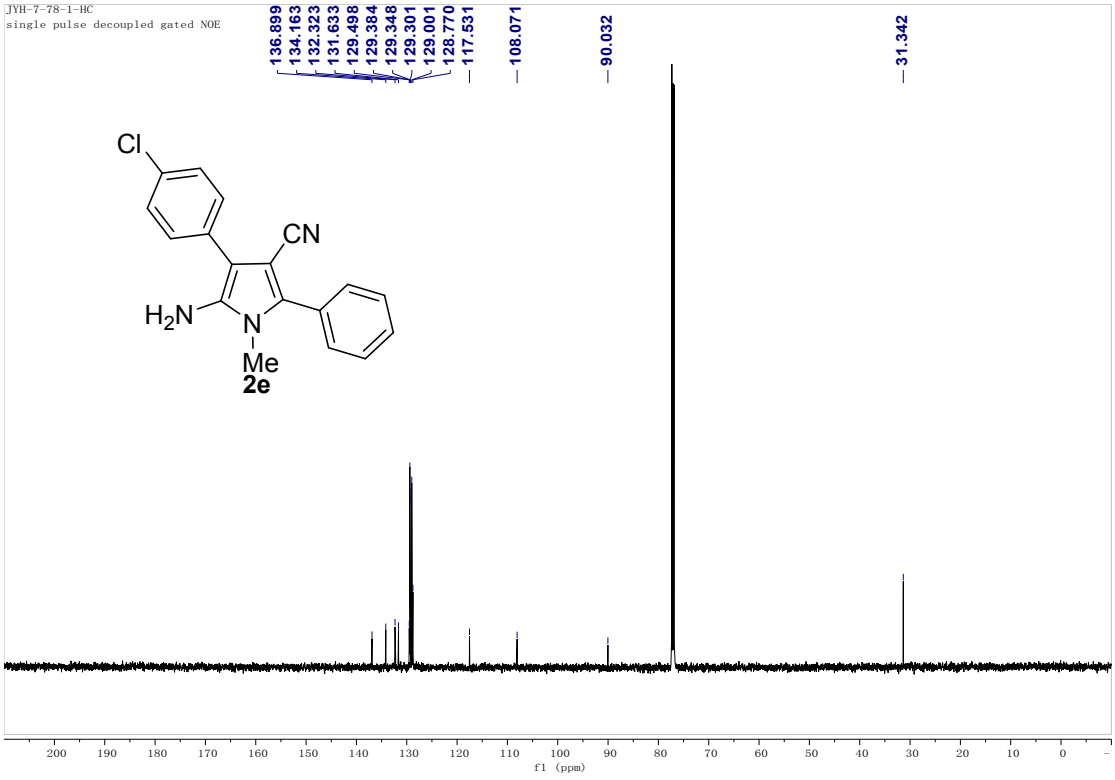

JYH-7-72-H-C
single_pulse
Et
CN
H2N
N
Me
2c
3.97
3.17
2.03
2.02
3.00
2.31
3.24
f1 (ppm)

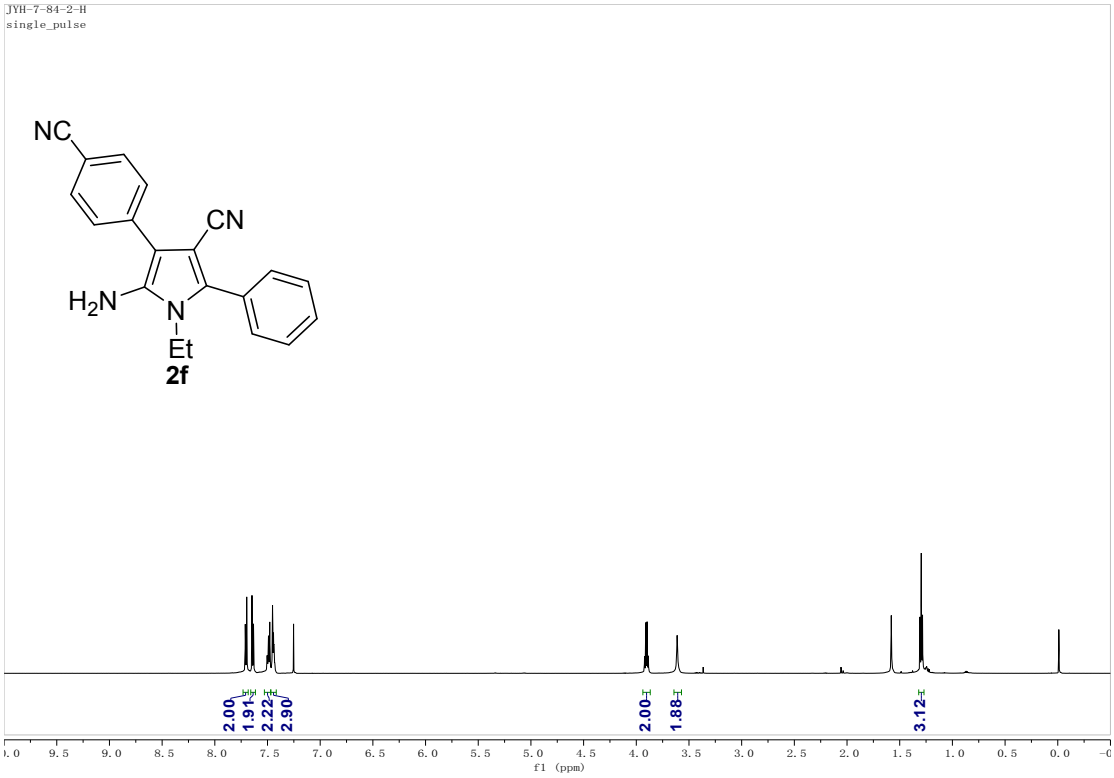

JYH-7-72-H-C
single pulse decoupled gated NOE
142.589
136.478
134.123
130.427
129.776
129.378
128.925
128.678
128.541
128.024
118.021
109.138
90.052
31.333
28.694
15.659
Et
CN
H2N
N
Me
2c
f1 (ppm)

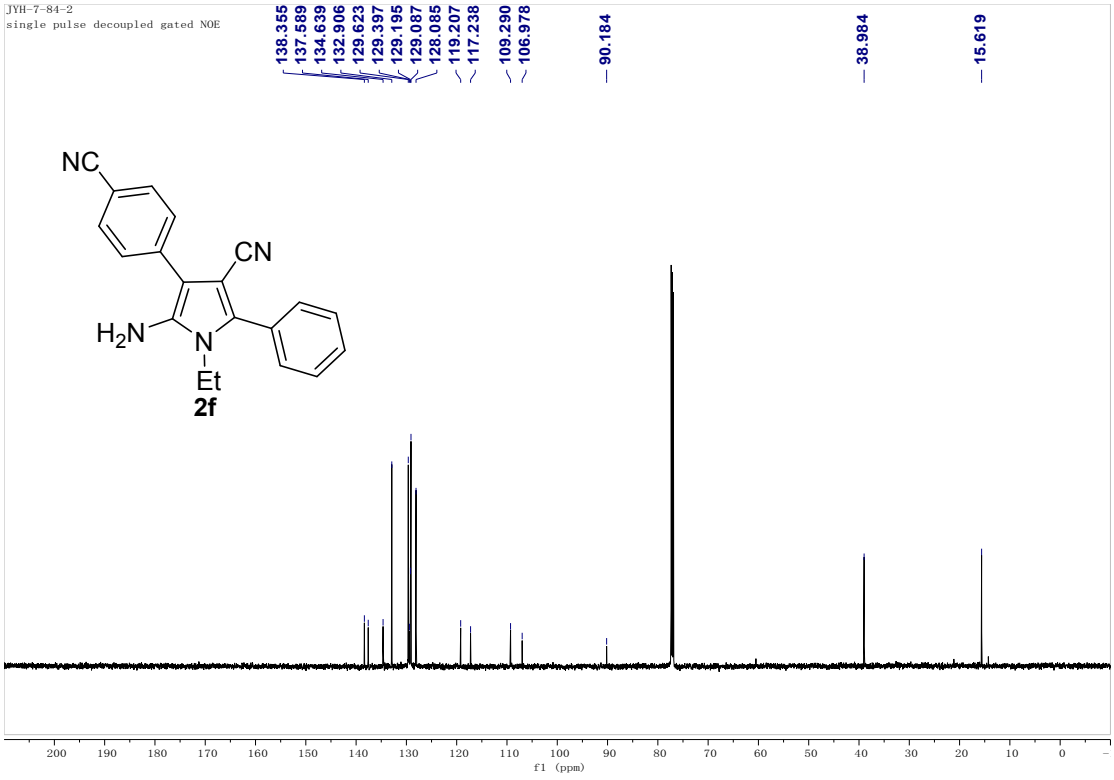

JYH-7-50
single_pulse
F
CN
H2N
N
Me
2d
5.82
0.97
1.88
3.00
1.61
f1 (ppm)

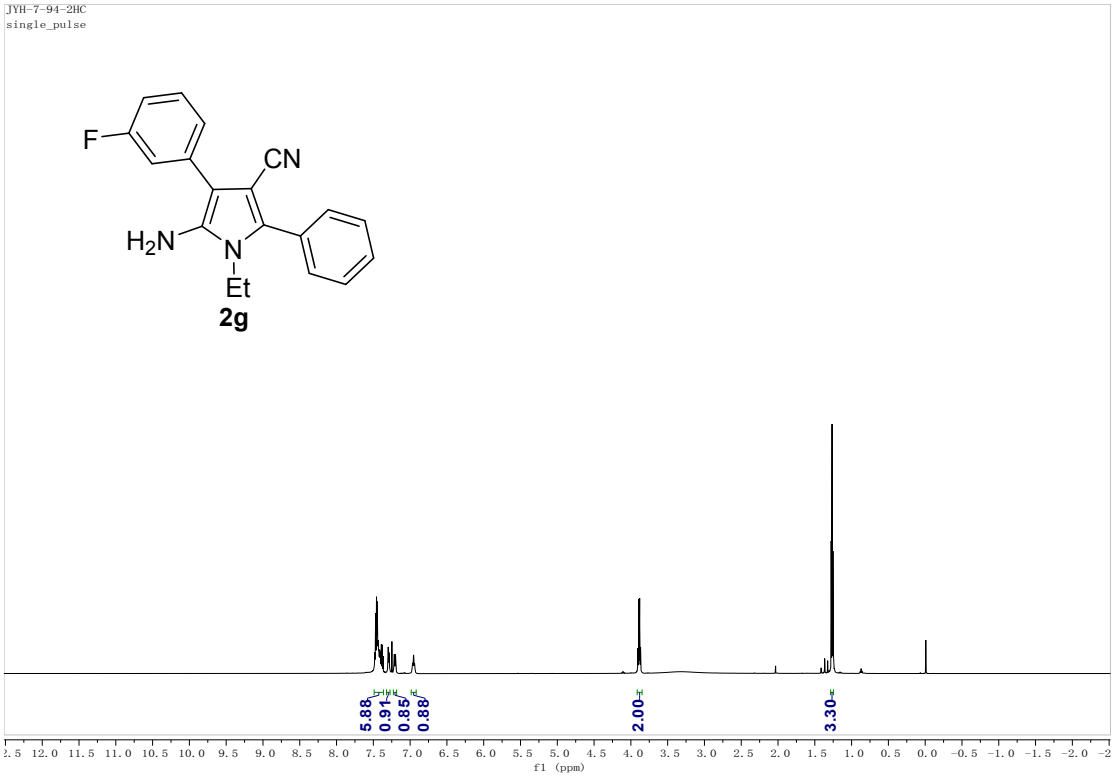

JYH-7-50-FC.3.fid
162.775
160.329
136.584
133.835
129.749
129.670
129.514
129.299
129.030
128.904
128.625
117.540
116.138
115.925
108.435
90.093
31.266
F
CN
H2N
N
Me
2d
f1 (ppm)

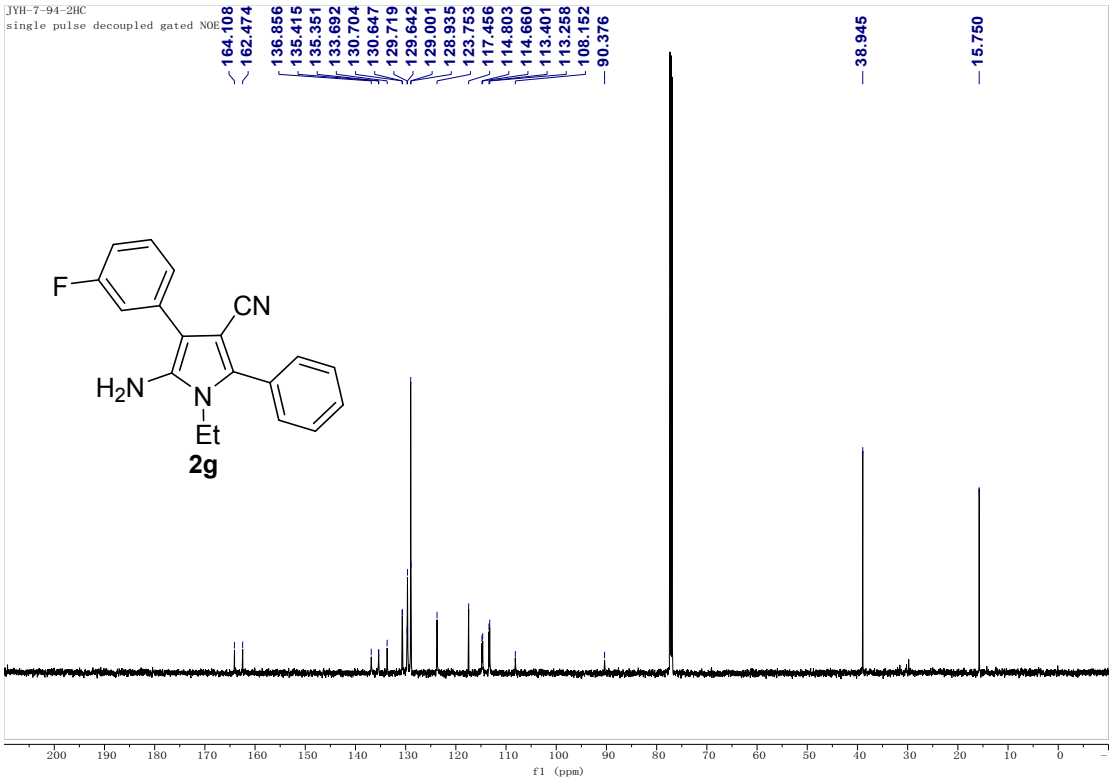

JYH-7-78-1-HC
single_pulse
Cl
CN
H_2N
N
Me
2e
3.72
3.12
2.81
3.00
1.92
f1 (ppm)

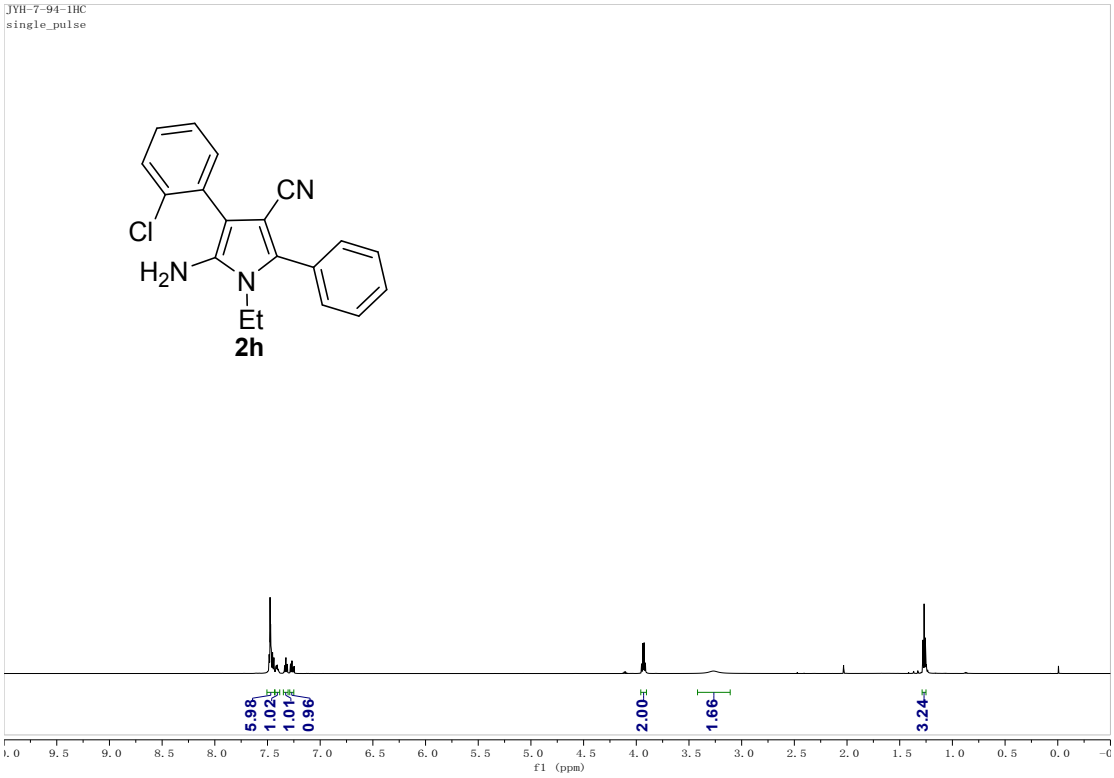

JYH-7-78-1-HC
single pulse decoupled gated NOE
136.899
134.163
132.323
131.633
129.498
129.384
129.348
129.301
129.001
128.770
117.531
108.071
90.032
31.342
Cl
CN
H_2N
N
Me
2e
f1 (ppm)

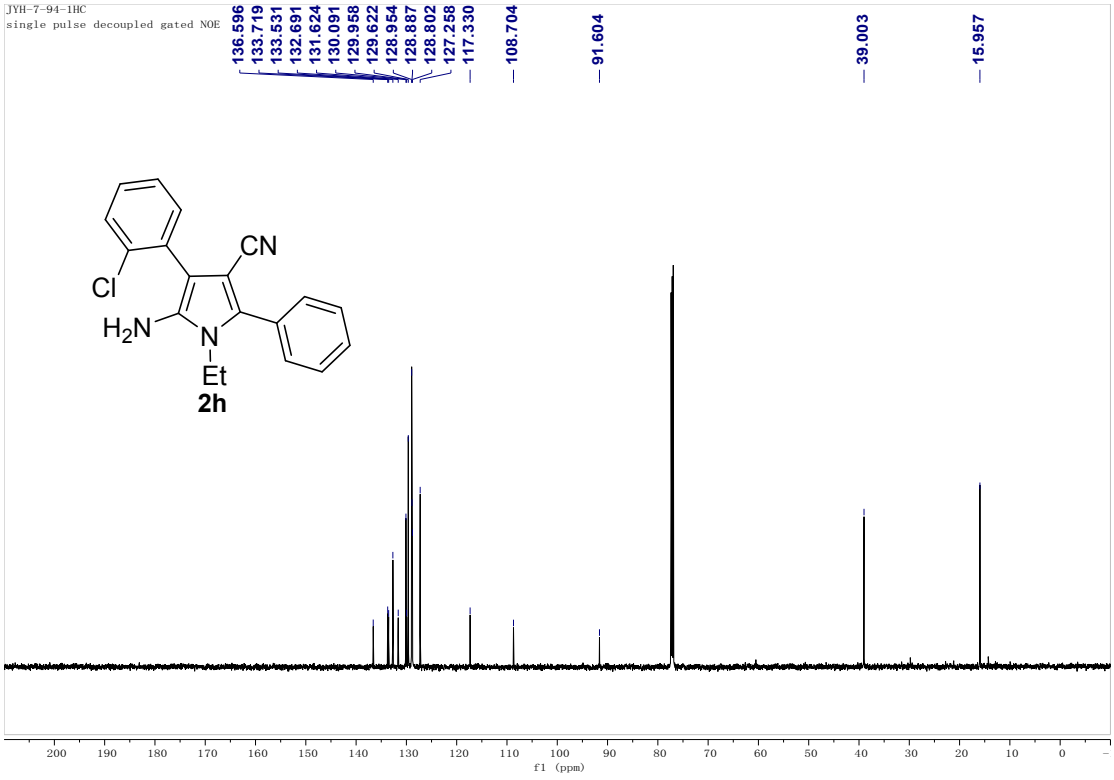

JYH-7-84-2-H
single_pulse
NC
CN
H_2N
N
Et
2f
2.00
1.91
2.22
2.90
2.00
1.88
3.12
f1 (ppm)

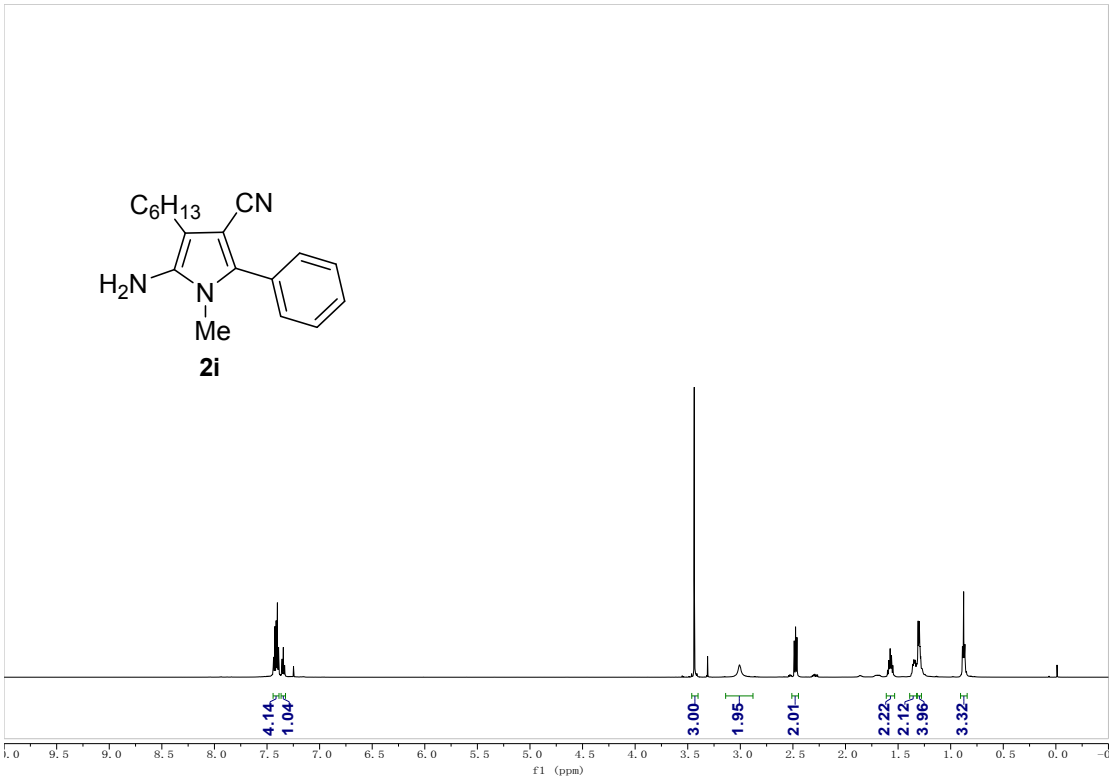

JYH-7-84-2
single pulse decoupled gated NOE
138.355
137.589
134.639
132.906
129.623
129.397
129.195
129.087
128.085
119.207
117.238
109.290
106.978
90.184
38.984
15.619
NC
CN
H_2N
N
Et
2f
f1 (ppm)

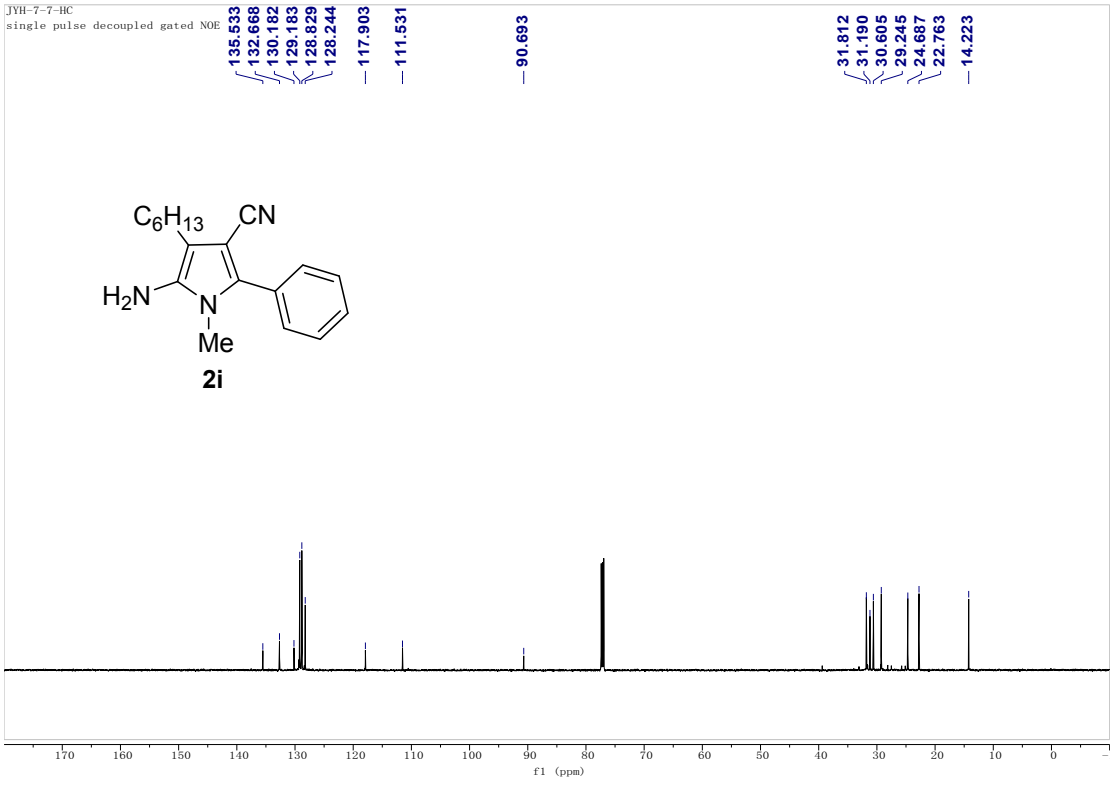

JYH-7-94-2HC
single_pulse
F
CN
H2N
N
Et
2g
5.88
0.91
0.85
0.88
2.00
3.30
f1 (ppm)

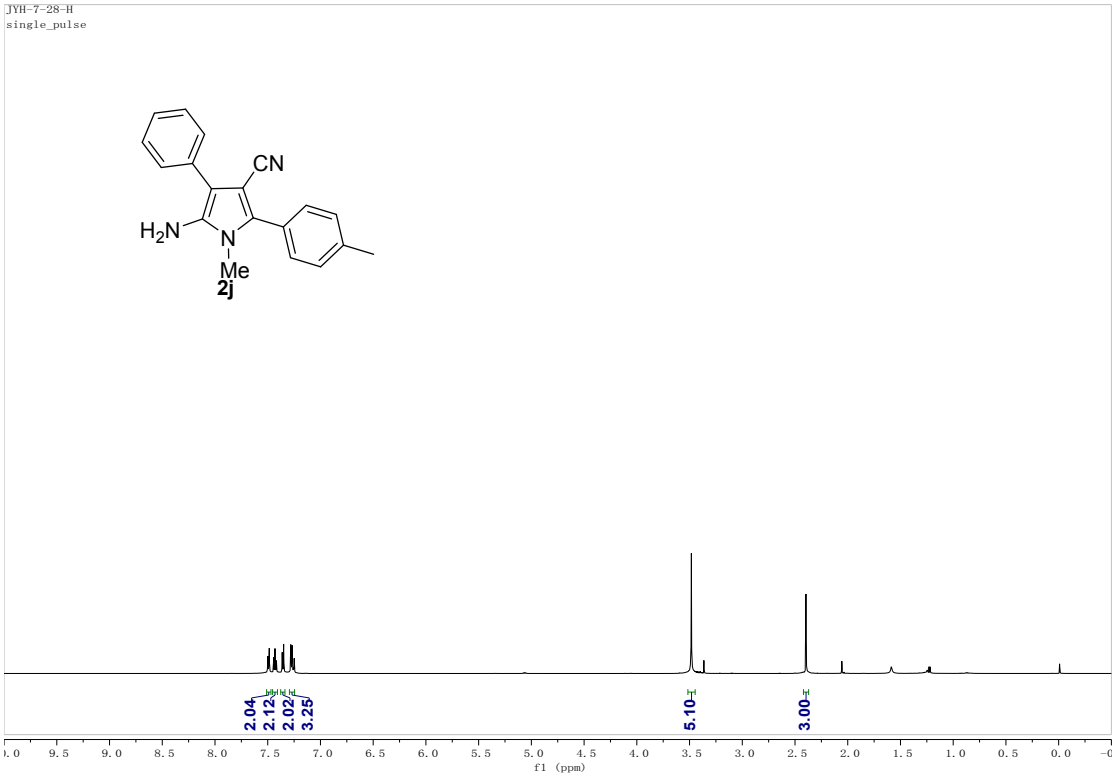

JYH-7-94-2HC
single pulse decoupled gated NOE
164.108
162.474
136.856
135.415
135.351
133.692
130.704
130.647
129.719
129.642
129.001
128.935
123.753
117.456
114.803
114.660
113.401
113.258
108.152
90.376
38.945
15.750
F
CN
H2N
N
Et
2g
f1 (ppm)

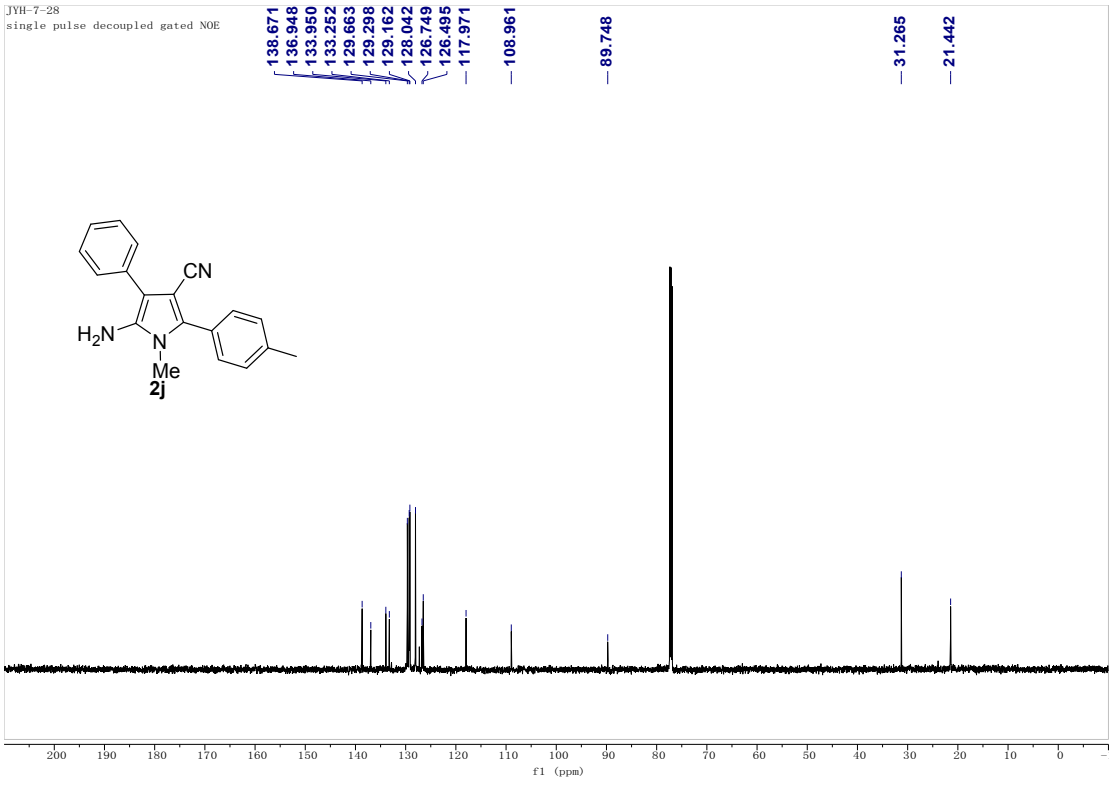

JYH-7-94-1HC
single_pulse
CN
Cl
H2N
N
Et
2h
5.98
1.02
1.01
0.96
2.00
1.66
3.24
f1 (ppm)

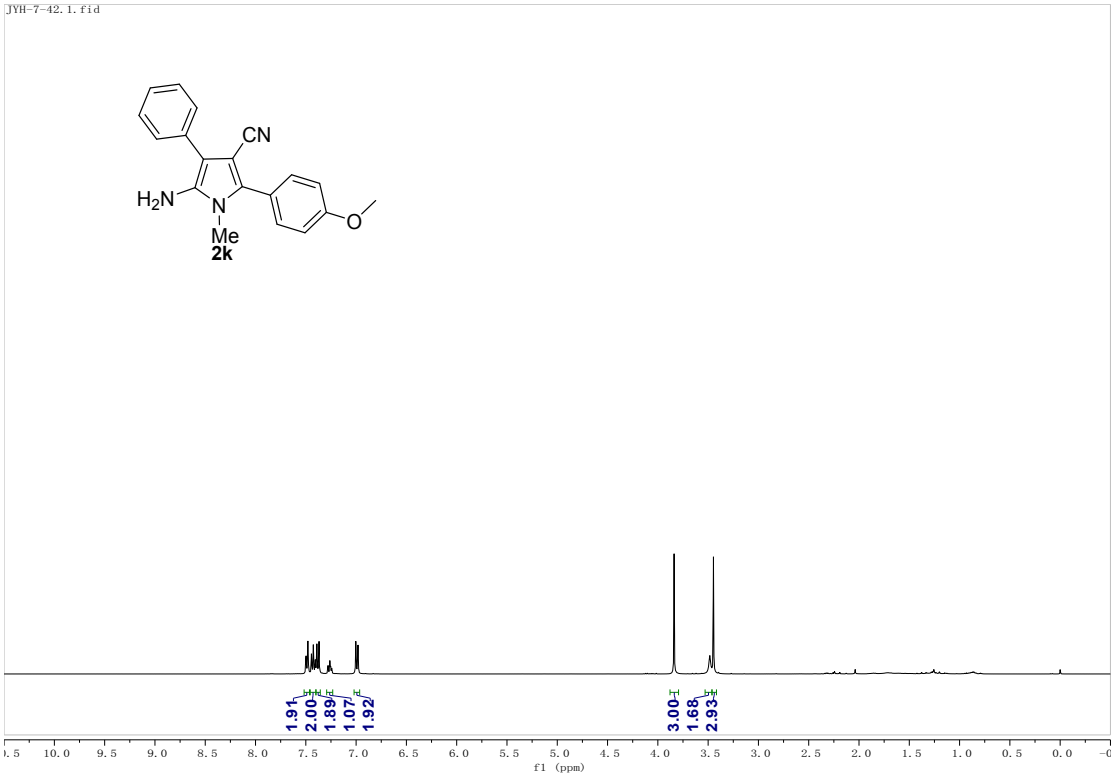

JYH-7-94-1HC
single pulse decoupled gated NOE
136.596
133.719
133.531
132.691
131.624
130.091
129.958
129.622
128.954
128.887
128.802
127.258
117.330
108.704
91.604
39.003
15.957
CN
Cl
H2N
N
Et
2h
f1 (ppm)

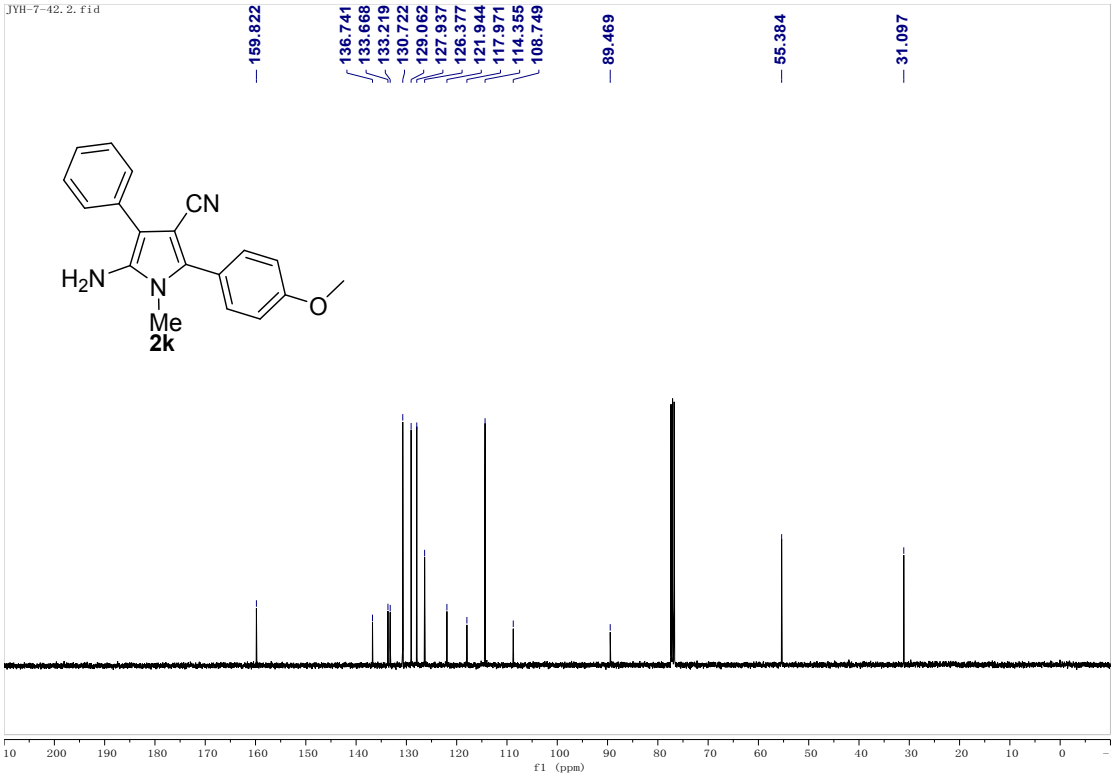

C6H13
CN
H2N
N
Me
2i
4.14
1.04
3.00
1.95
2.01
2.22
2.12
3.96
3.32
f1 (ppm)

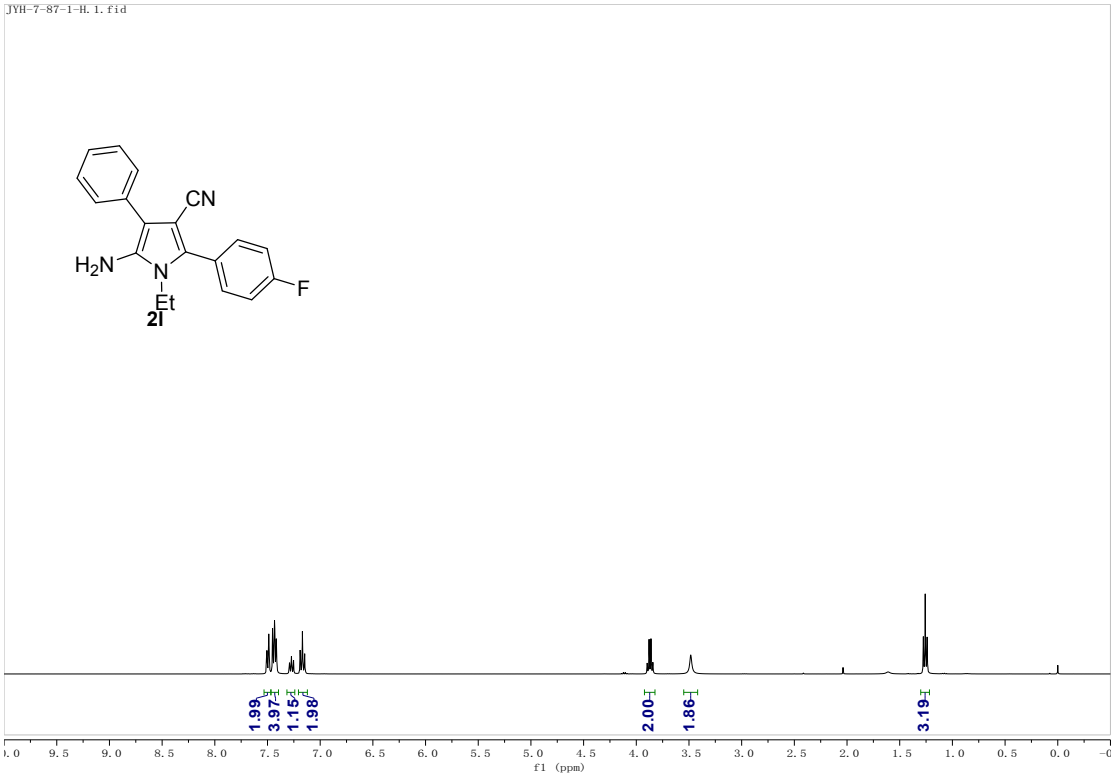

JYH-7-7-HC
single pulse decoupled gated NOE
135.533
132.668
130.182
129.183
128.829
128.244
117.903
111.531
90.693
31.812
31.190
30.605
29.245
24.687
22.763
14.223
C6H13
CN
H2N
N
Me
2i
f1 (ppm)

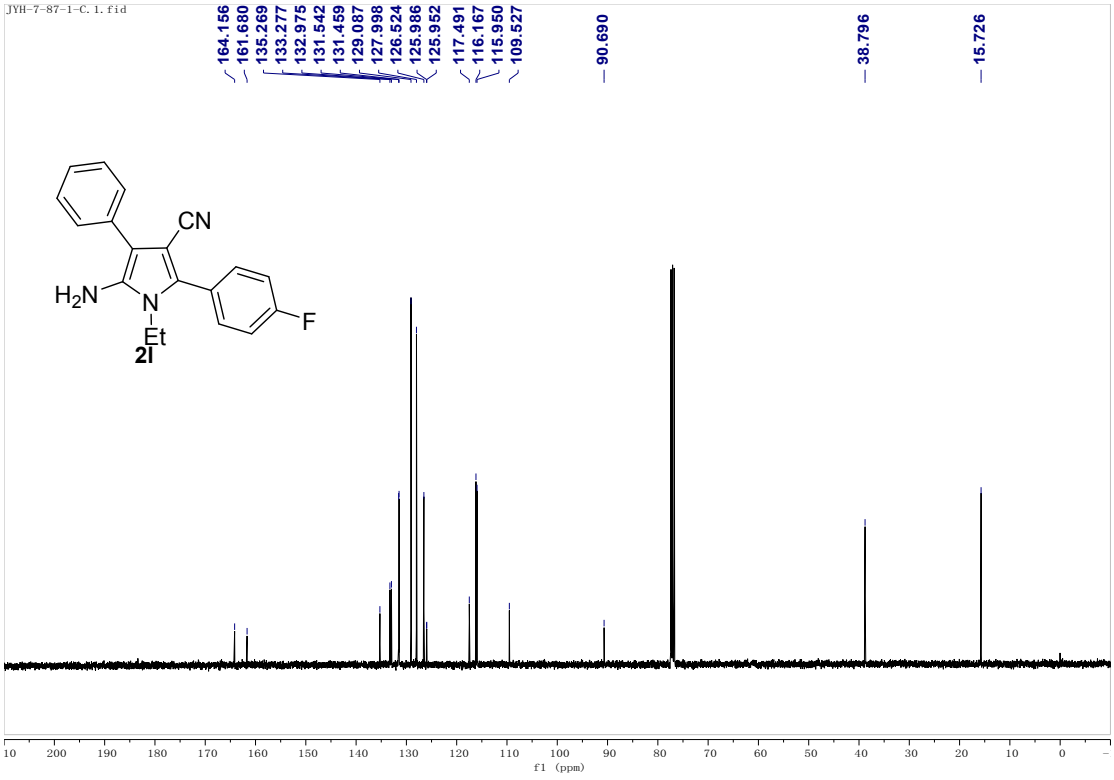

JYH-7-28-H
single_pulse
CN
H2N
N
Me
2j
2.04
2.12
2.02
3.25
5.10
3.00
f1 (ppm)

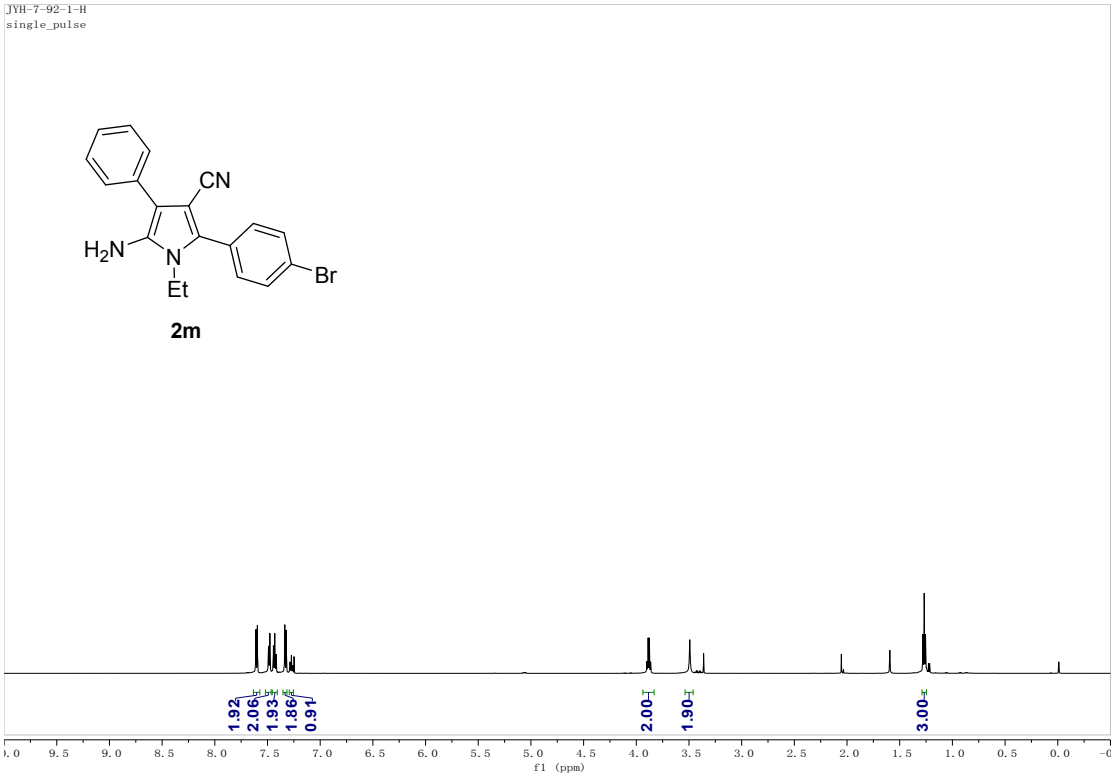

JYH-7-28
single pulse decoupled gated NOE
138.671
136.948
133.950
133.252
129.663
129.298
129.162
128.042
126.749
126.495
117.971
108.961
89.748
31.265
21.442
CN
H2N
N
Me
2j
f1 (ppm)

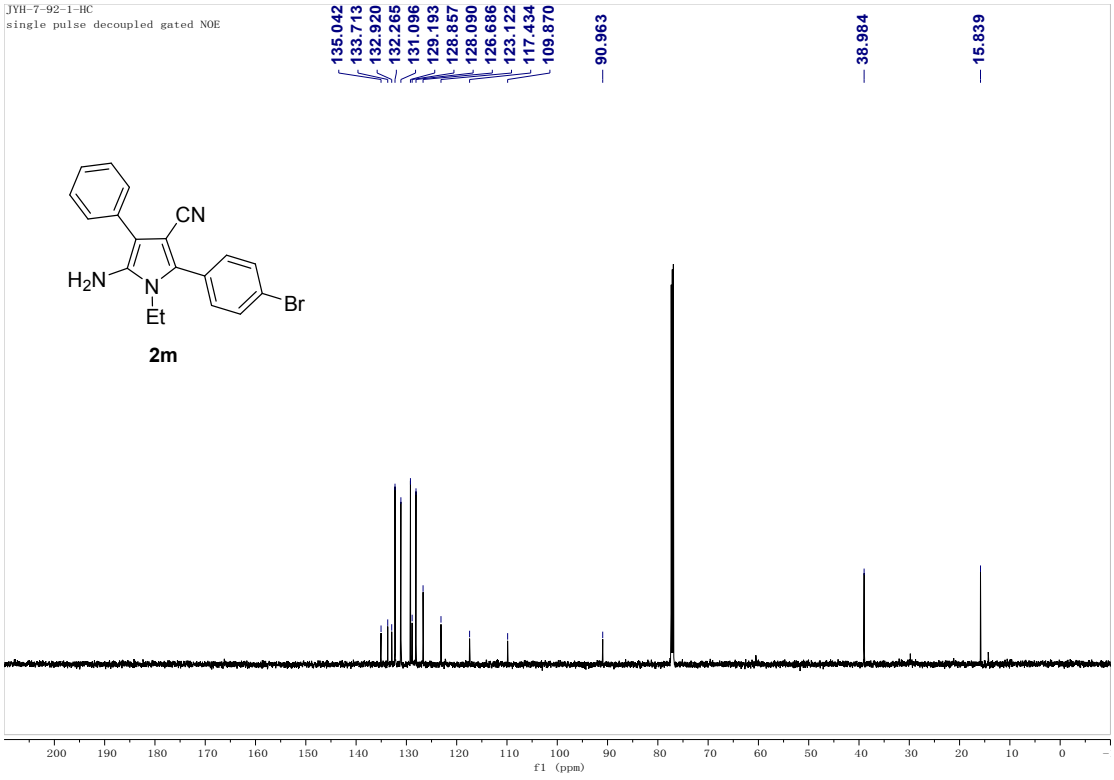

JYH-7-42.1.fid
CN
H2N
N
Me
O
2k
1.91
2.00
1.89
1.07
1.92
3.00
1.68
2.93
f1 (ppm)

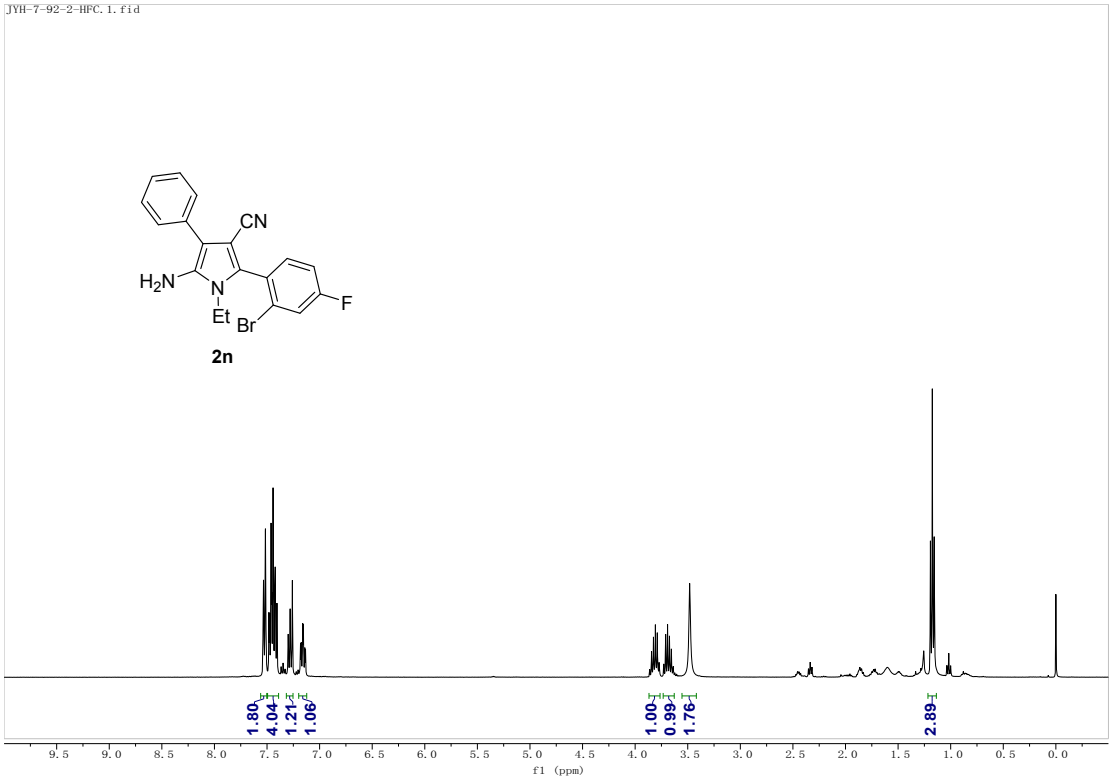

JYH-7-42.2.fid
159.822
136.741
133.668
133.219
130.722
129.062
127.937
126.377
121.944
117.971
114.355
108.749
89.469
55.384
31.097
CN
H2N
N
Me
O
2k
f1 (ppm)

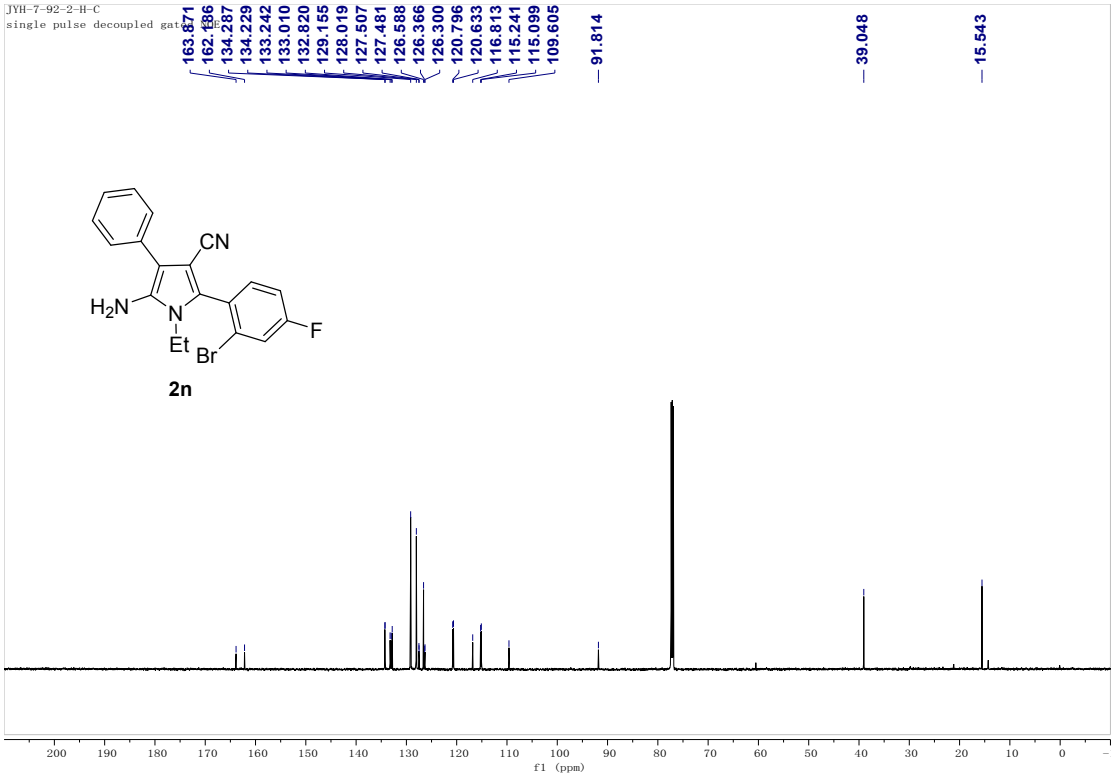

JYH-7-87-1-H.1.fid
CN
H2N
N
Et
F
2l
1.99
3.97
1.15
1.98
2.00
1.86
3.19
f1 (ppm)

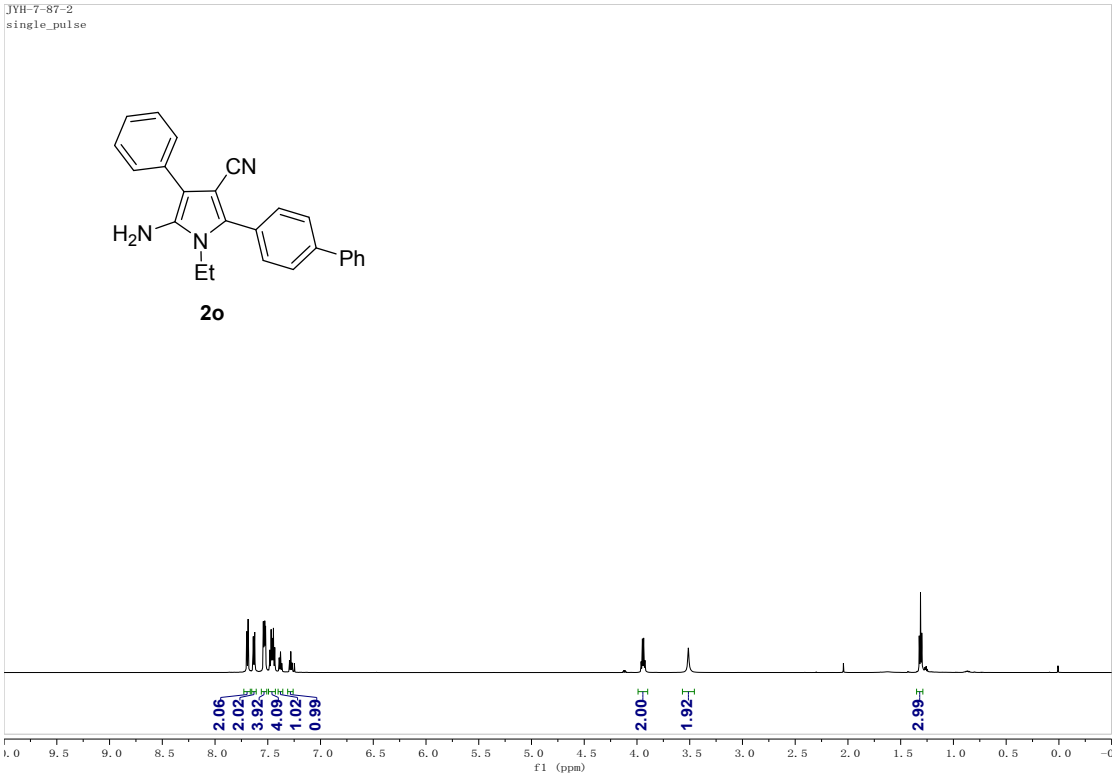

JYH-7-87-1-C.1.fid
164.156
161.680
135.269
133.277
132.975
131.542
131.459
129.087
127.998
126.524
125.986
125.952
117.491
116.167
115.950
109.527
90.690
38.796
15.726
CN
H2N
N
Et
F
2l
f1 (ppm)

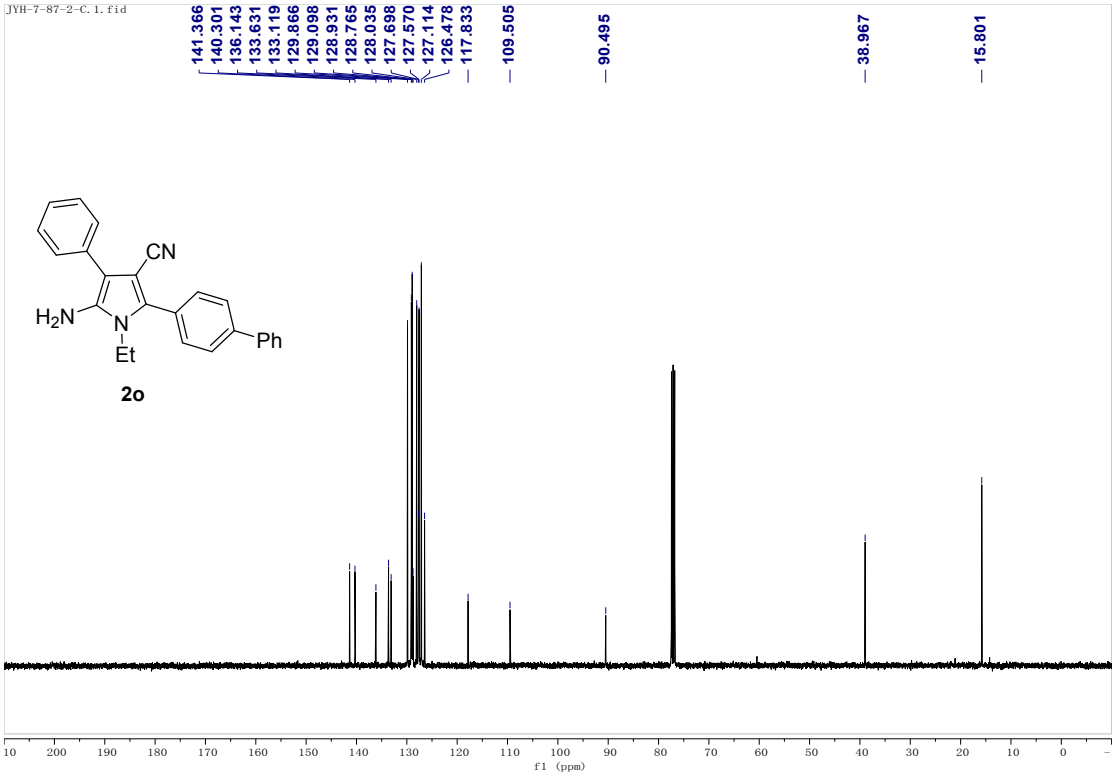

JYH-7-92-1-H
single_pulse
CN
H2N
N
Et
Br
2m
1.92
2.06
1.93
1.86
0.91
2.00
1.90
3.00
f1 (ppm)

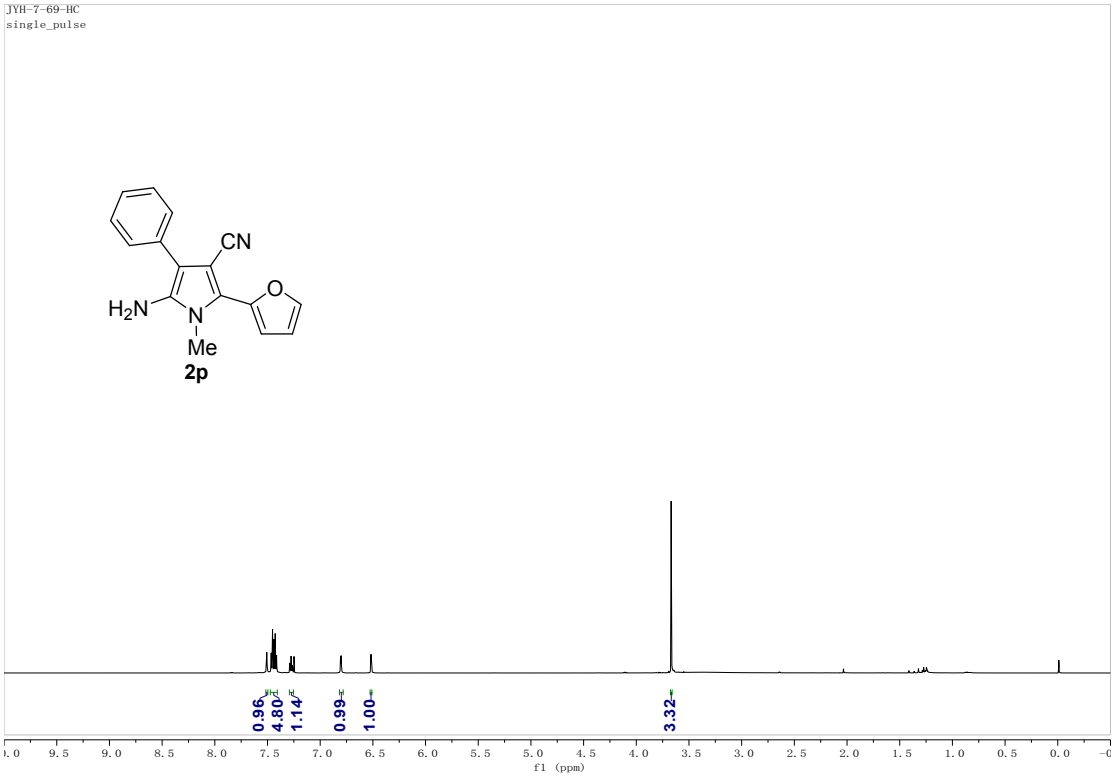

JYH-7-92-1-HC
single pulse decoupled gated NOE
135.042
133.713
132.920
132.265
131.096
129.193
128.857
128.090
126.686
123.122
117.434
109.870
90.963
38.984
15.839
CN
H2N
N
Et
Br
2m
f1 (ppm)

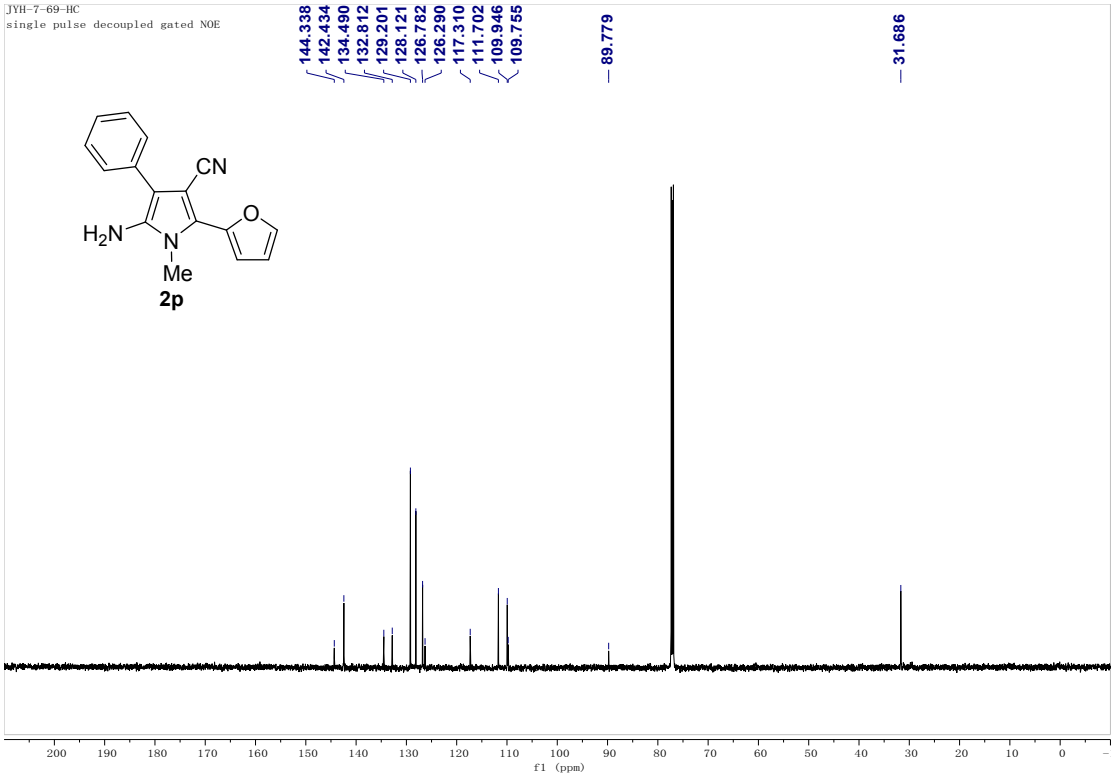

JYH-7-92-2-HFC.1.fid
CN
H2N
N
Et
Br
F
2n
1.80
4.04
1.21
1.06
1.00
0.99
1.76
2.89
f1 (ppm)

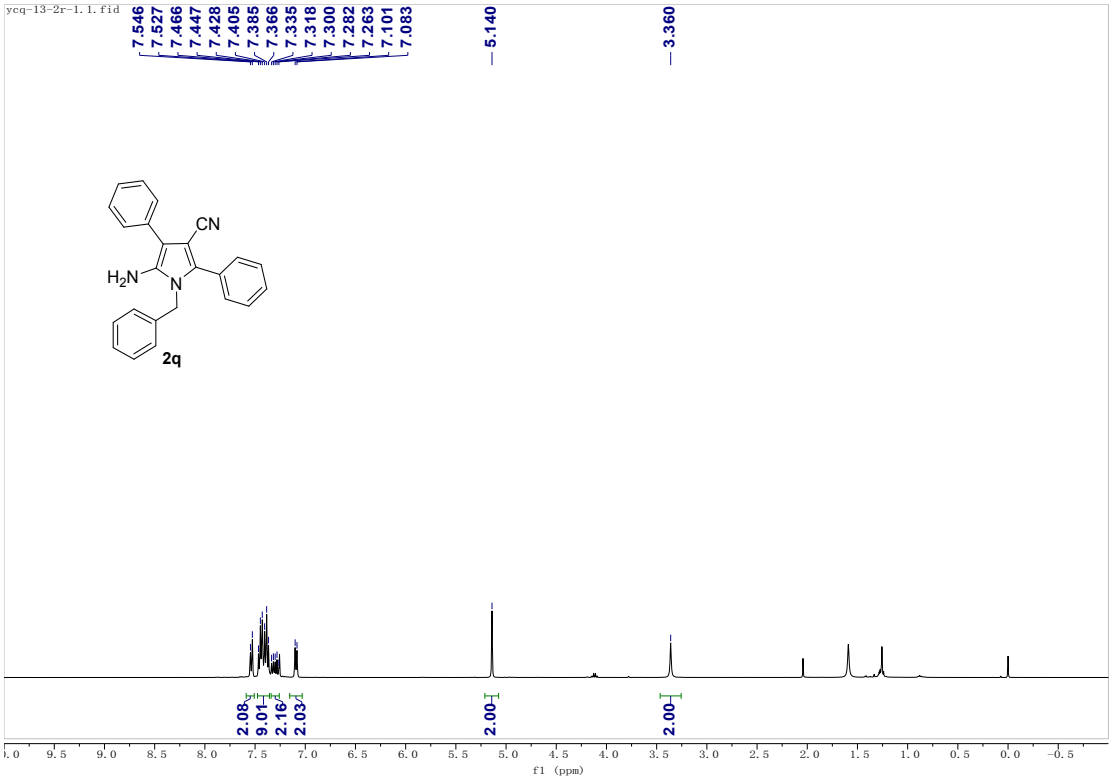

JYH-7-92-2-H-C
single pulse decoupled gated DE
163.871
162.186
134.287
134.229
133.242
133.010
132.820
129.155
128.019
127.507
127.481
126.588
126.366
126.300
120.796
120.633
116.813
115.241
115.099
109.605
91.814
39.048
15.543
CN
H2N
N
Et
Br
F
2n
f1 (ppm)

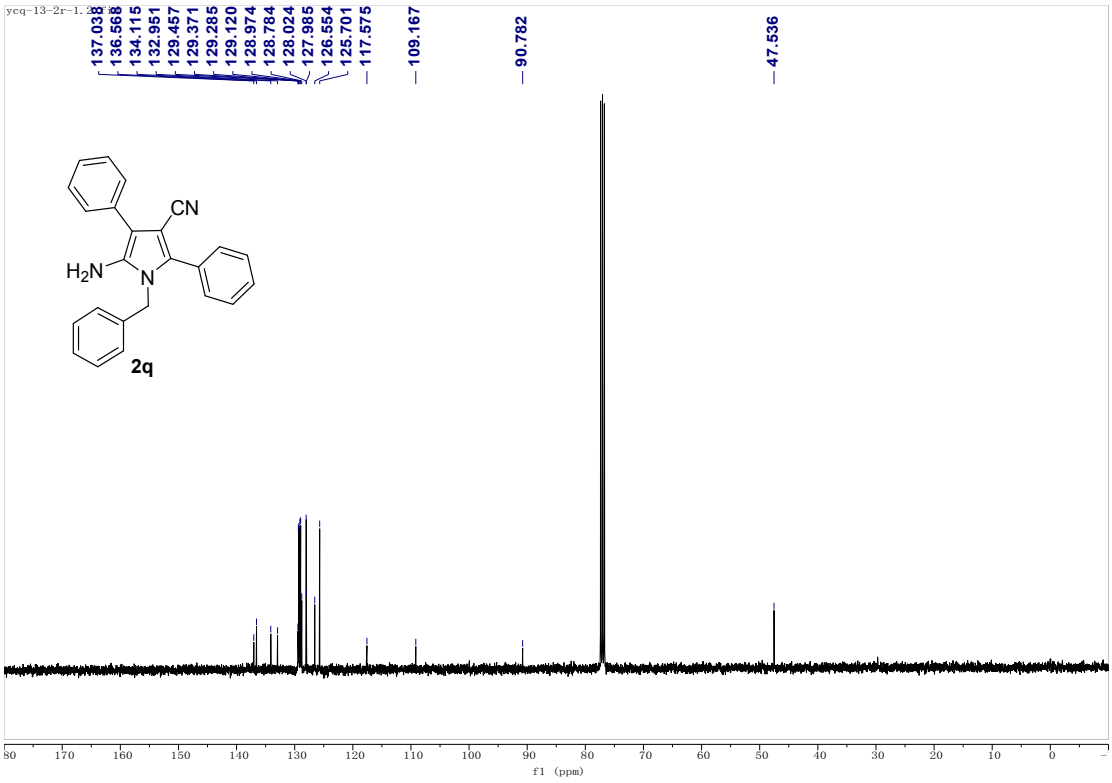

JYH-7-87-2
single_pulse
CN
H2N
N
Et
Ph
2o
2.06
2.02
3.92
4.09
1.02
0.99
2.00
1.92
2.99
f1 (ppm)

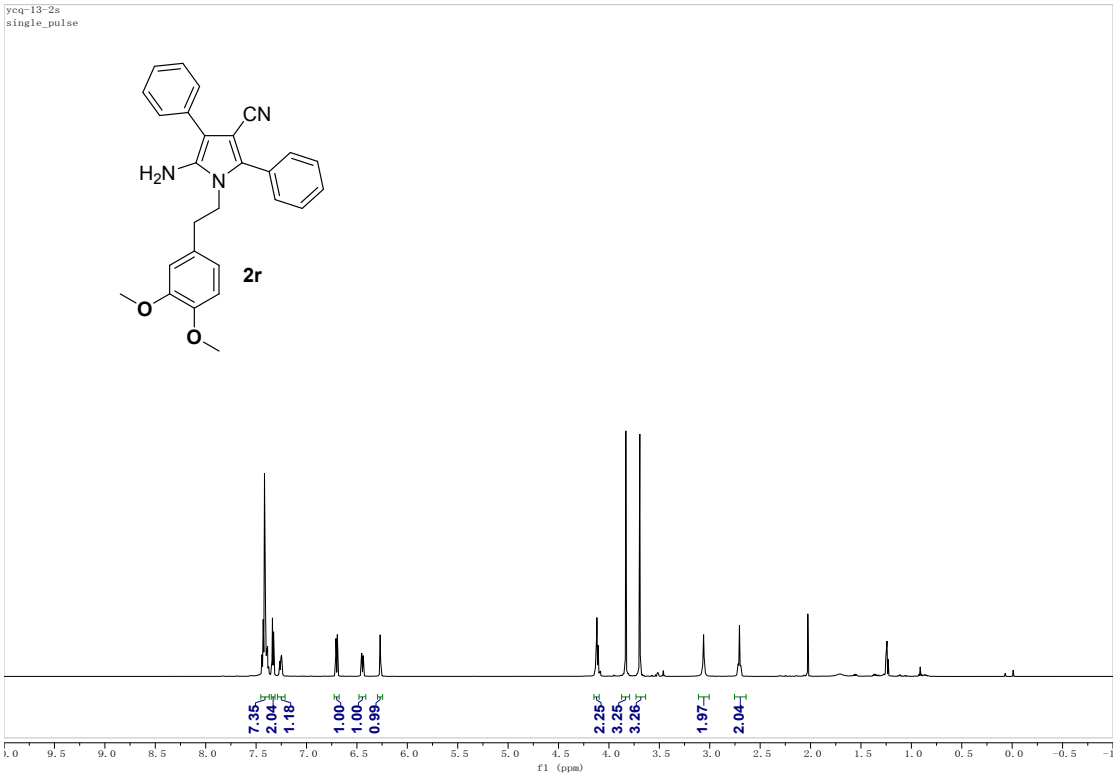

JYH-7-87-2-C.1.fid
141.366
140.301
136.143
133.631
133.119
129.866
129.098
128.931
128.765
128.035
127.698
127.570
127.114
126.478
117.833
109.505
90.495
38.967
15.801
CN
H2N
N
Et
Ph
2o
f1 (ppm)

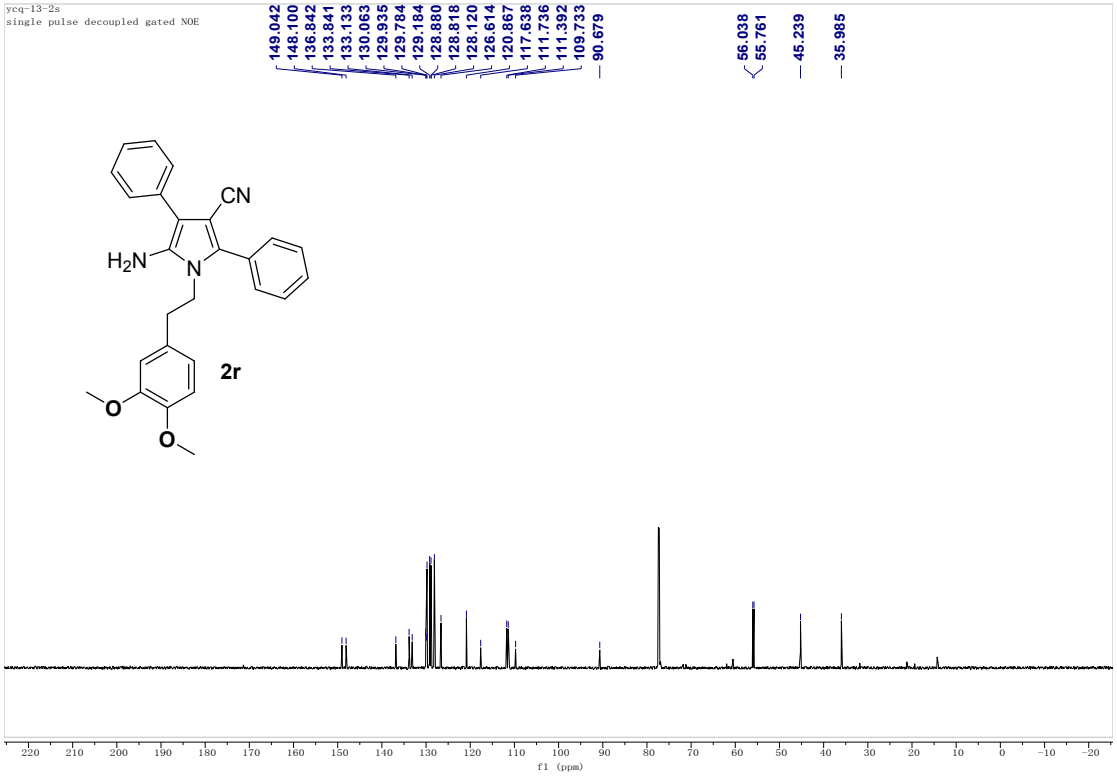

JYH-7-69-HC
single_pulse
CN
H_2N
N
Me
O
2p
0.96
4.80
1.14
0.99
1.00
3.32
f1 (ppm)

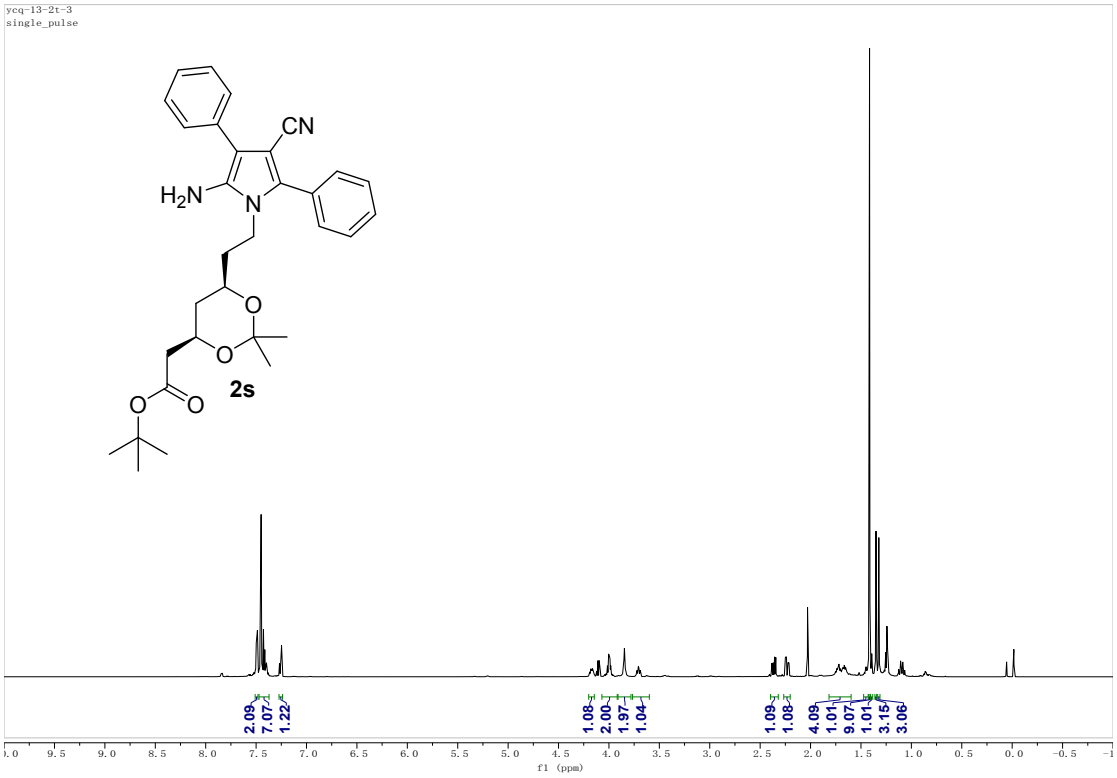

JYH-7-69-HC
single pulse decoupled gated NOE
144.338
142.434
134.490
132.812
129.201
128.121
126.782
126.290
117.310
111.702
109.946
109.755
89.779
31.686
CN
H_2N
N
Me
O
2p
f1 (ppm)

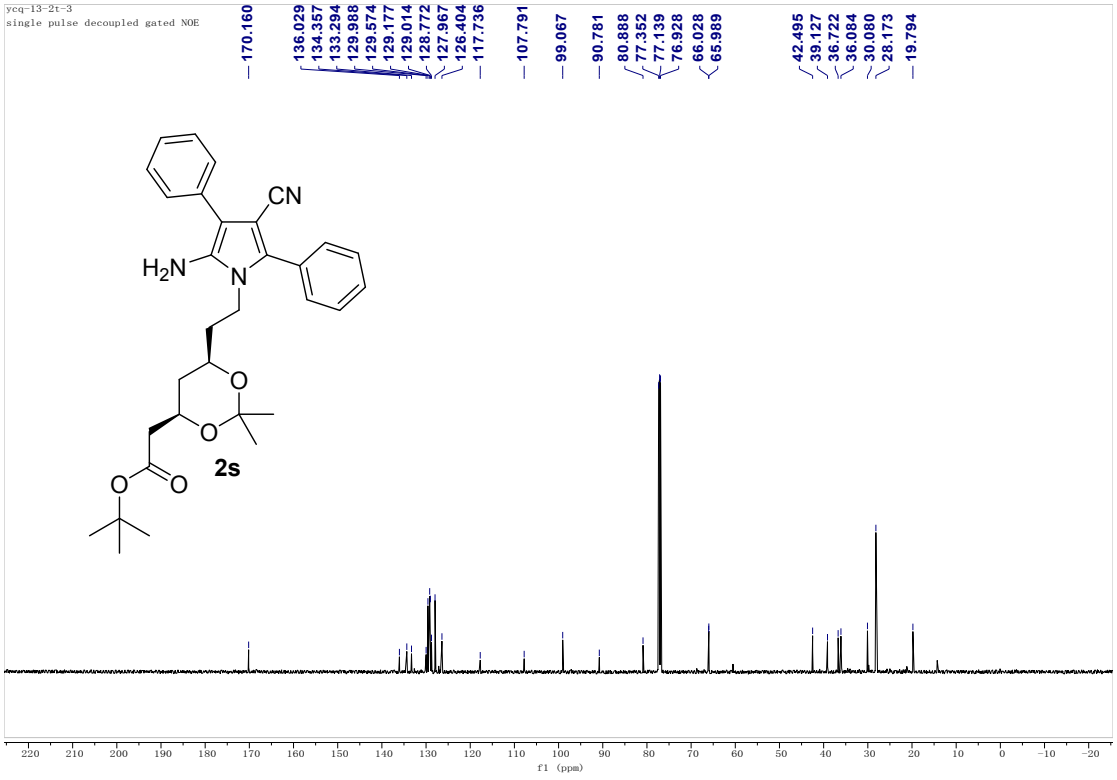

ycq-13-2r-1.1.fid
7.546
7.527
7.466
7.447
7.428
7.405
7.385
7.366
7.335
7.318
7.300
7.282
7.263
7.101
7.083
5.140
3.360
CN
H2N
N
2q
2.08
9.01
2.16
2.03
2.00
2.00
f1 (ppm)

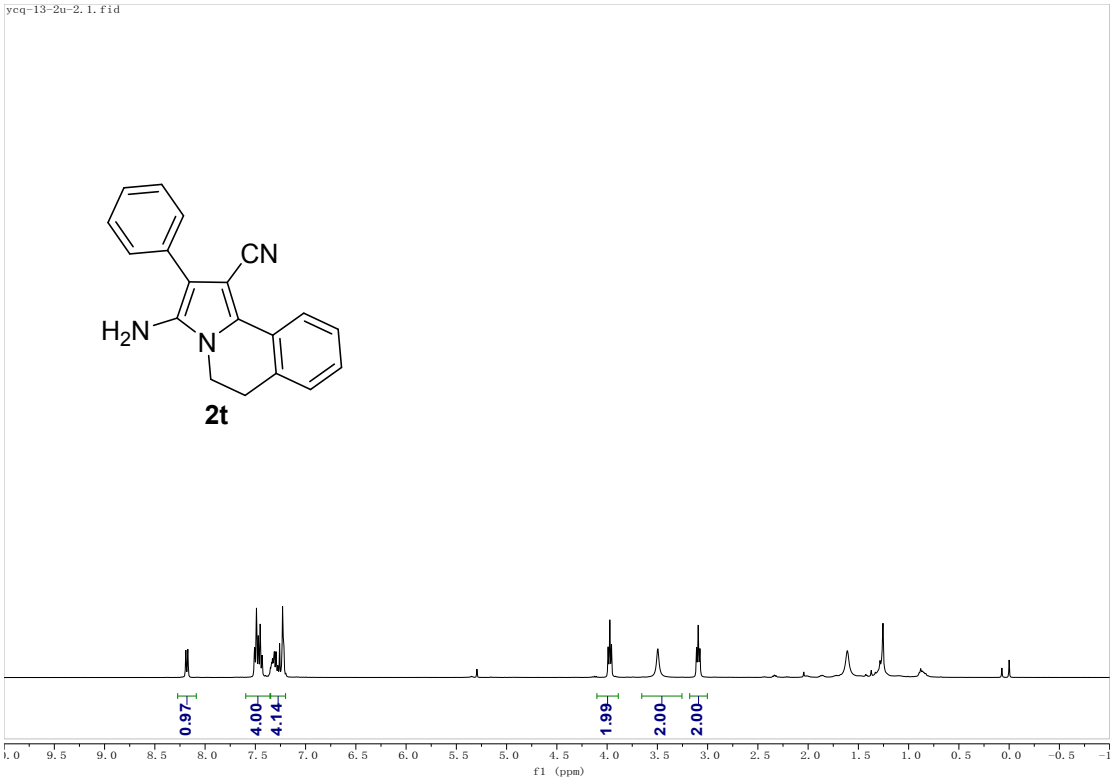

137.038
136.568
134.115
132.951
129.457
129.371
129.285
129.120
128.974
128.784
128.024
127.985
126.554
125.701
117.575
109.167
90.782
47.536
CN
H2N
N
2q
f1 (ppm)

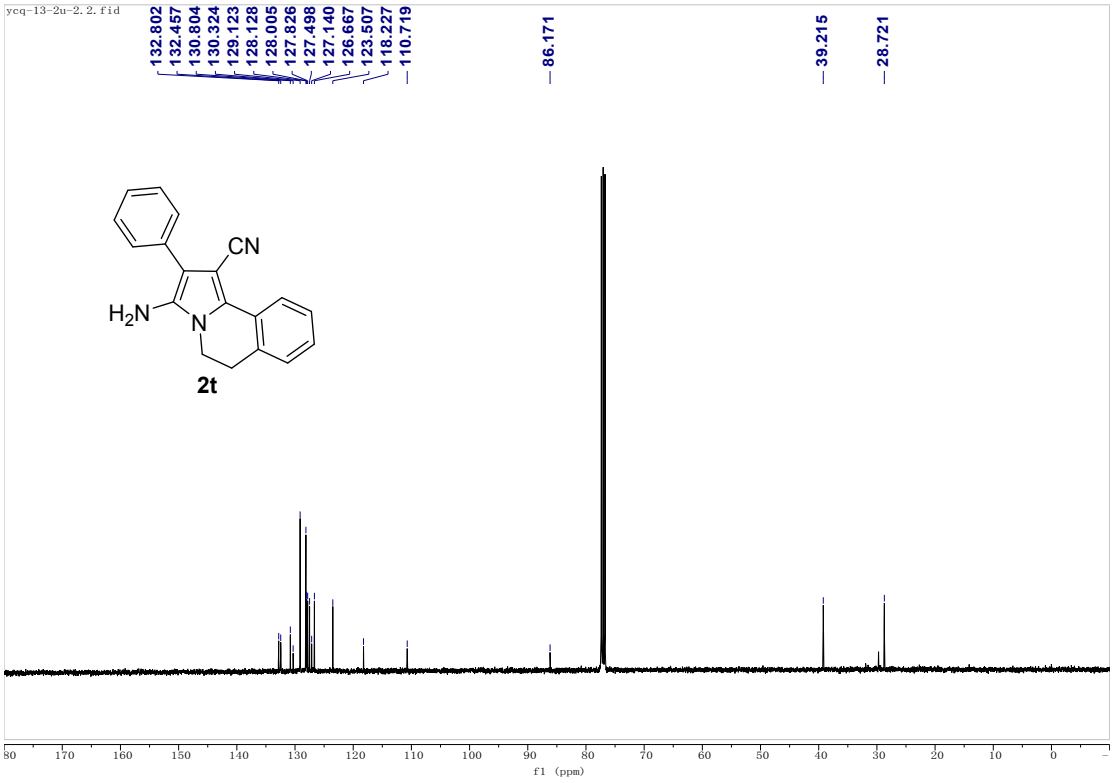

ycq-13-2s
single_pulse
CN
H2N
N
2r
O
O
7.35
2.04
1.18
1.00
1.00
0.99
2.25
3.25
3.26
1.97
2.04
f1 (ppm)

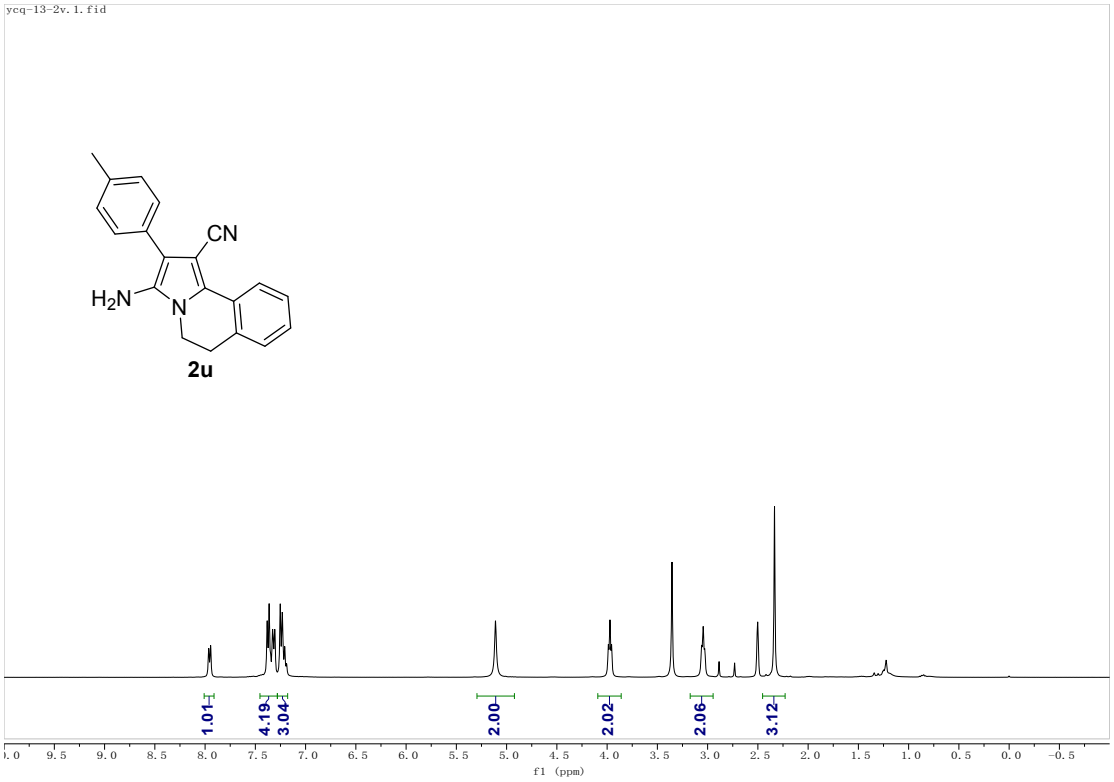

ycq-13-2s
single pulse decoupled gated NOE
149.042
148.100
136.842
133.841
133.133
130.063
129.935
129.784
129.184
128.880
128.818
128.120
126.614
120.867
117.638
111.736
111.392
109.733
90.679
56.038
55.761
45.239
35.985
CN
H2N
N
2r
O
O
f1 (ppm)

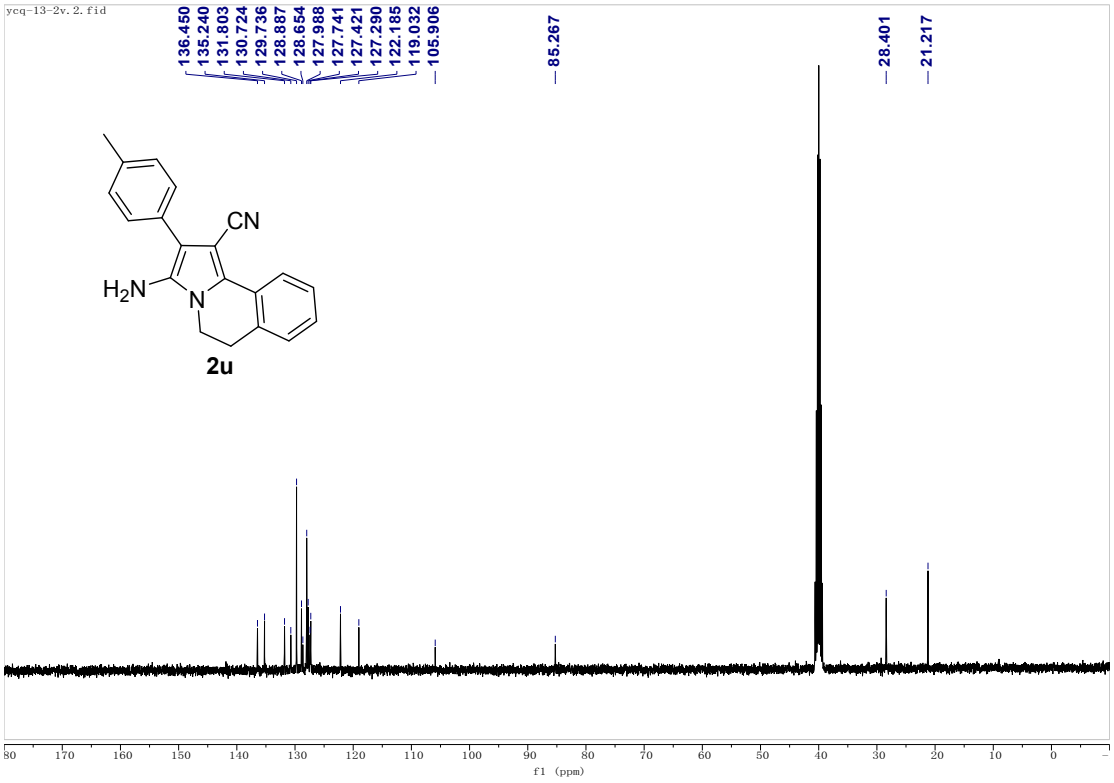

ycq-13-2t-3
single_pulse
CN
H2N
N
O
O
O
O
2s
2.09
7.07
1.22
1.08
2.00
1.97
1.04
1.09
1.08
4.09
1.01
9.07
1.01
3.15
3.06
f1 (ppm)

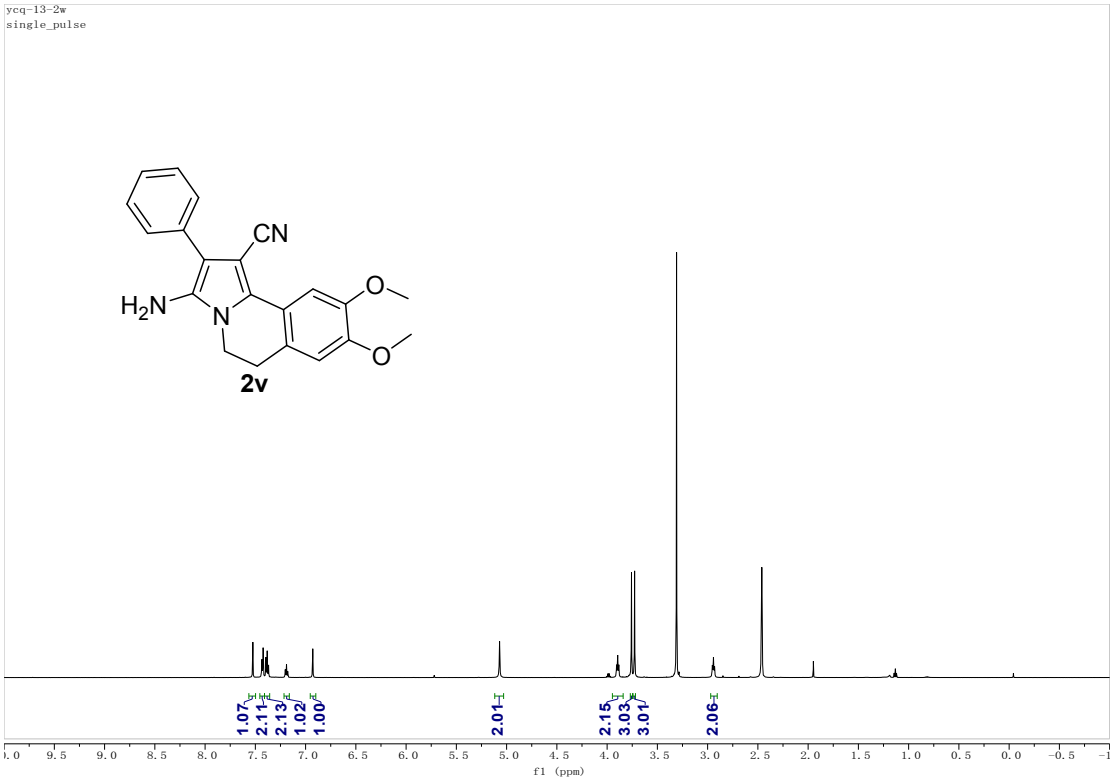

ycq-13-2t-3
single pulse decoupled gated NOE
170.160
136.029
134.357
133.294
129.988
129.574
129.177
129.014
128.772
127.967
126.404
117.736
107.791
99.067
90.781
80.888
77.352
77.139
76.928
66.028
65.989
42.495
39.127
36.722
36.084
30.080
28.173
19.794
CN
H2N
N
O
O
O
O
2s
f1 (ppm)

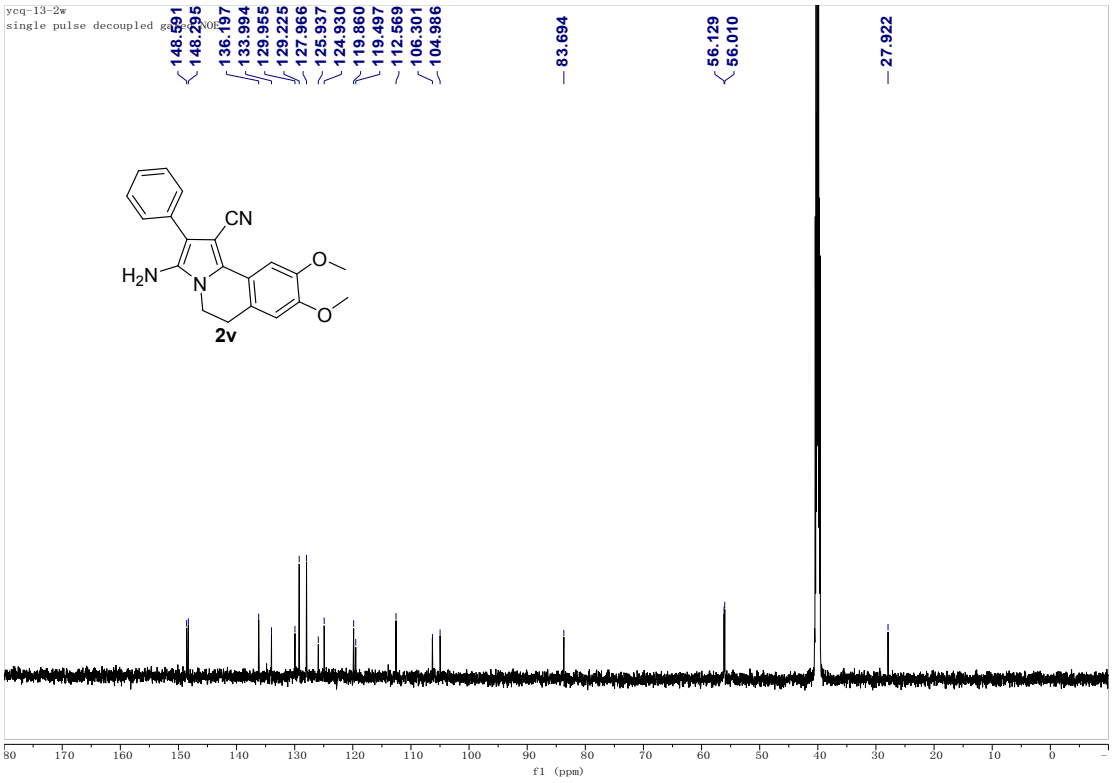

ycq-13-2u-2.1.fid
CN
H2N
N
2t
0.97
4.00
4.14
1.99
2.00
2.00
f1 (ppm)

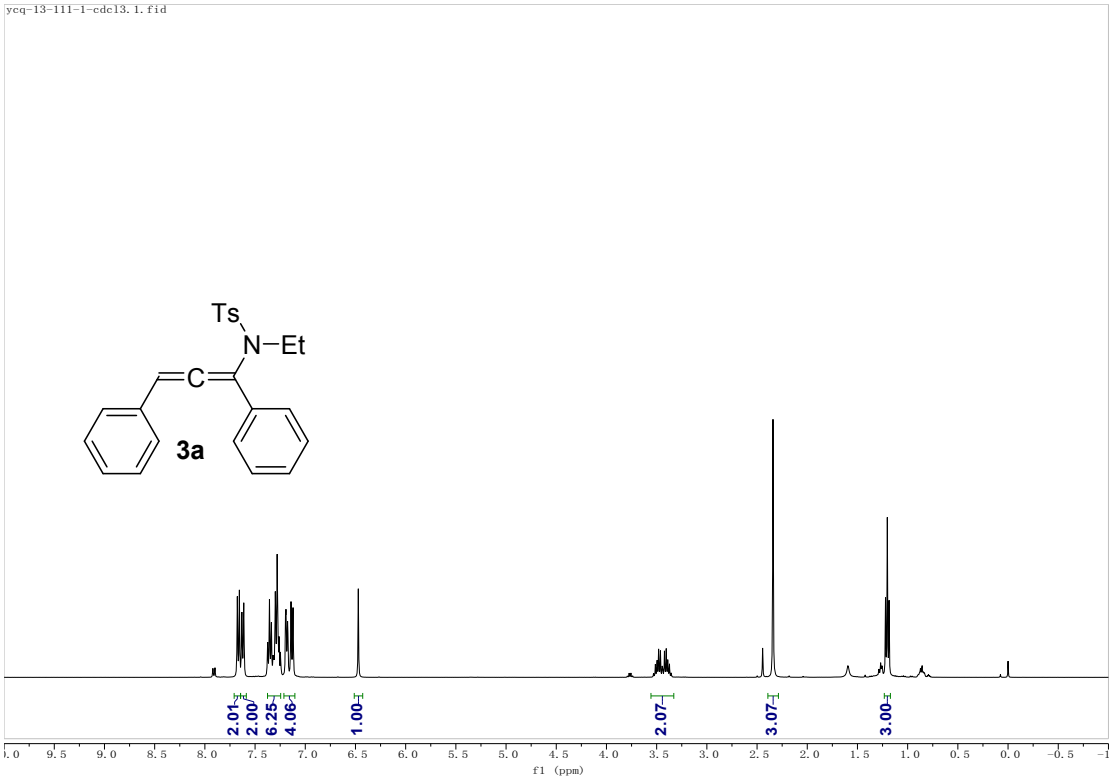

ycq-13-2u-2.2.fid
132.802
132.457
130.804
130.324
129.123
128.128
128.005
127.826
127.498
127.140
126.667
123.507
118.227
110.719
86.171
39.215
28.721
CN
H2N
N
2t
f1 (ppm)

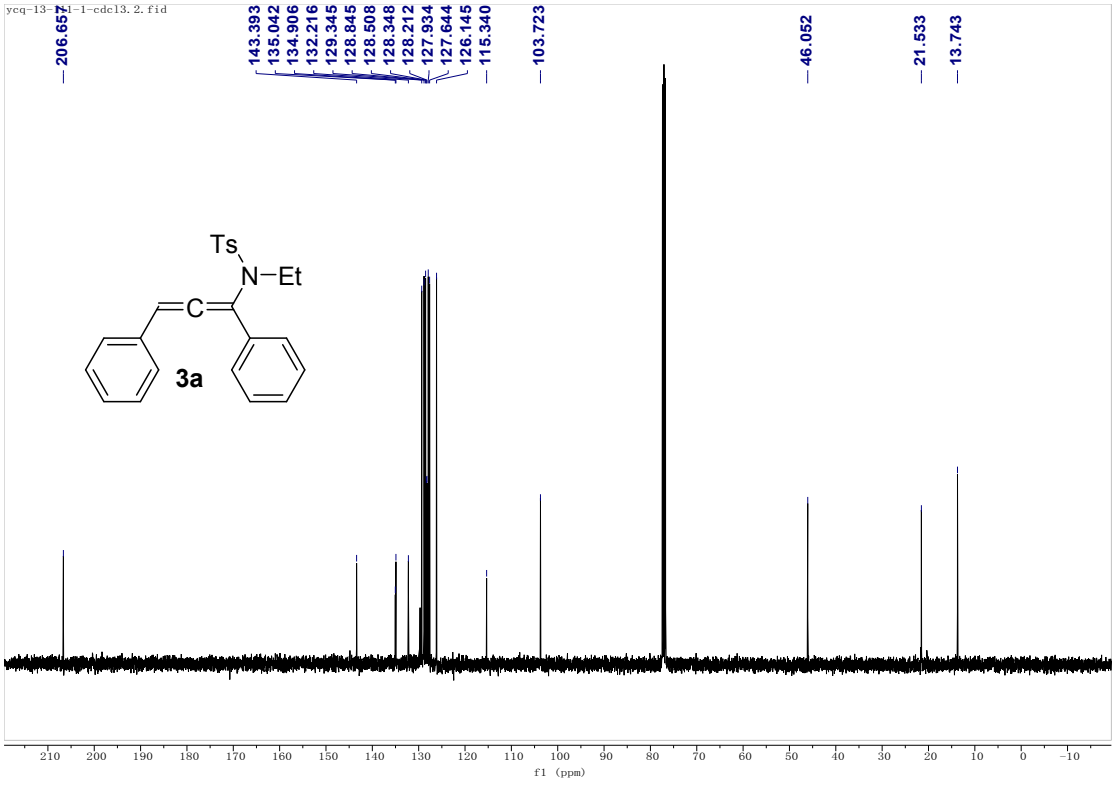

ycq-13-2v.1.fid
CN
H_2N
N
2u
1.01
4.19
3.04
2.00
2.02
2.06
3.12
f1 (ppm)

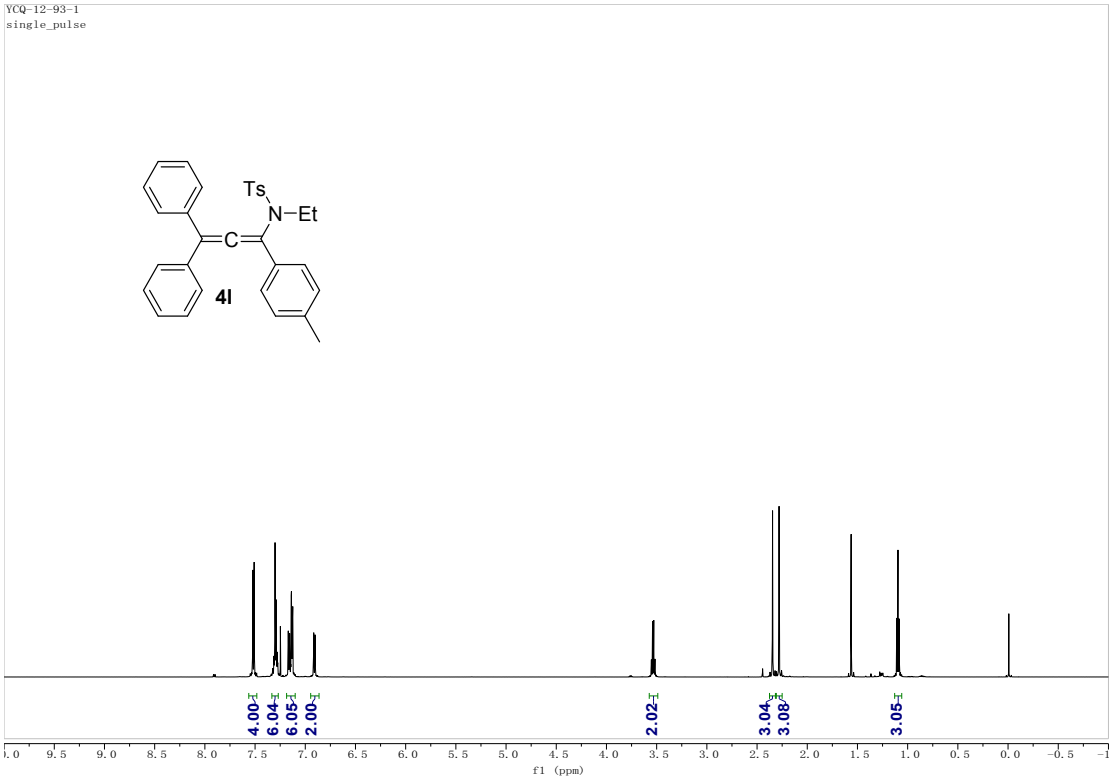

ycq-13-2v.2.fid
136.450
135.240
131.803
130.724
129.736
128.887
128.654
127.988
127.741
127.421
127.290
122.185
119.032
105.906
85.267
28.401
21.217
CN
H_2N
N
2u
f1 (ppm)

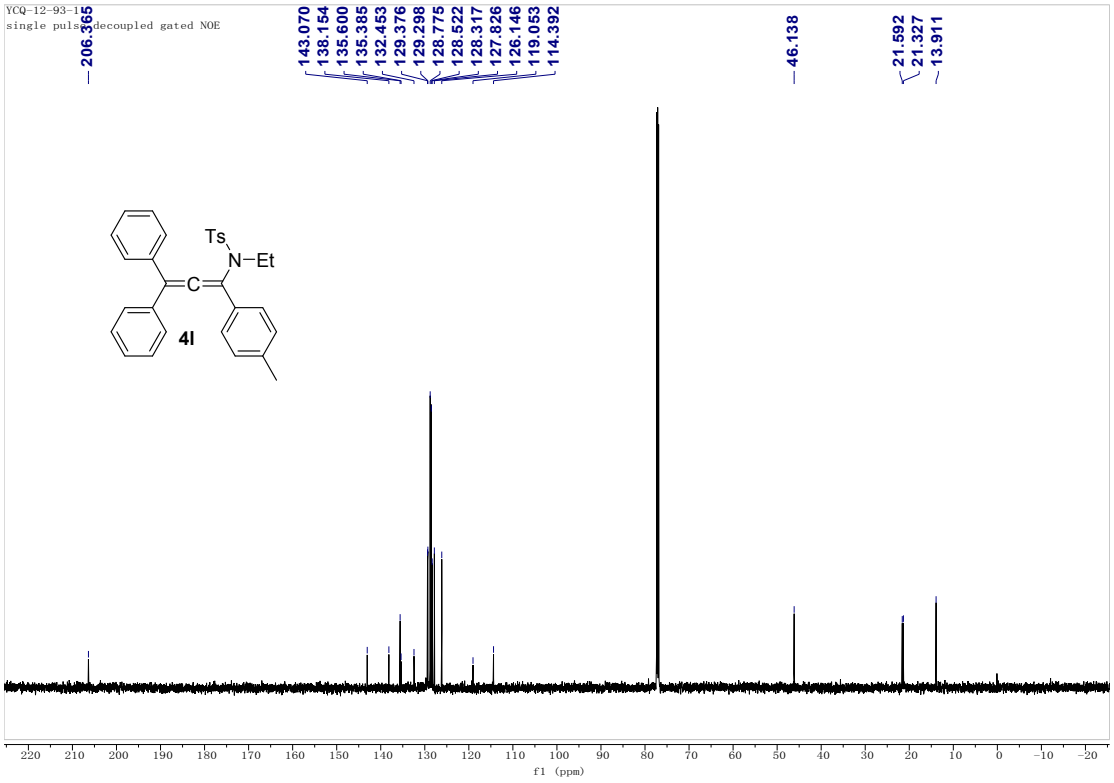

ycq-13-2w
single_pulse
CN
H_2N
N
O
O
2v
1.07
2.11
2.13
1.02
1.00
2.01
2.15
3.03
3.01
2.06
f1 (ppm)

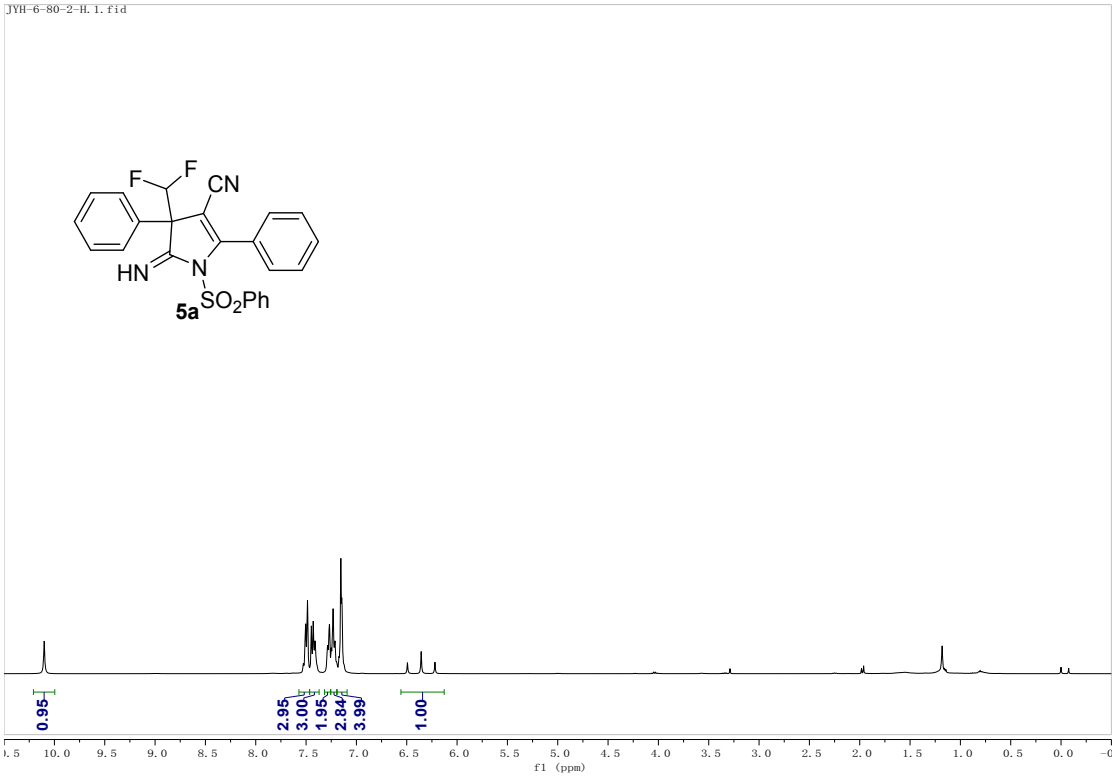

ycq-13-2w
single pulse decoupled gated NOE
148.591
148.295
136.197
133.994
129.955
129.225
127.966
125.937
124.930
119.860
119.497
112.569
106.301
104.986
83.694
56.129
56.010
27.922
CN
H_2N
N
O
O
2v
f1 (ppm)

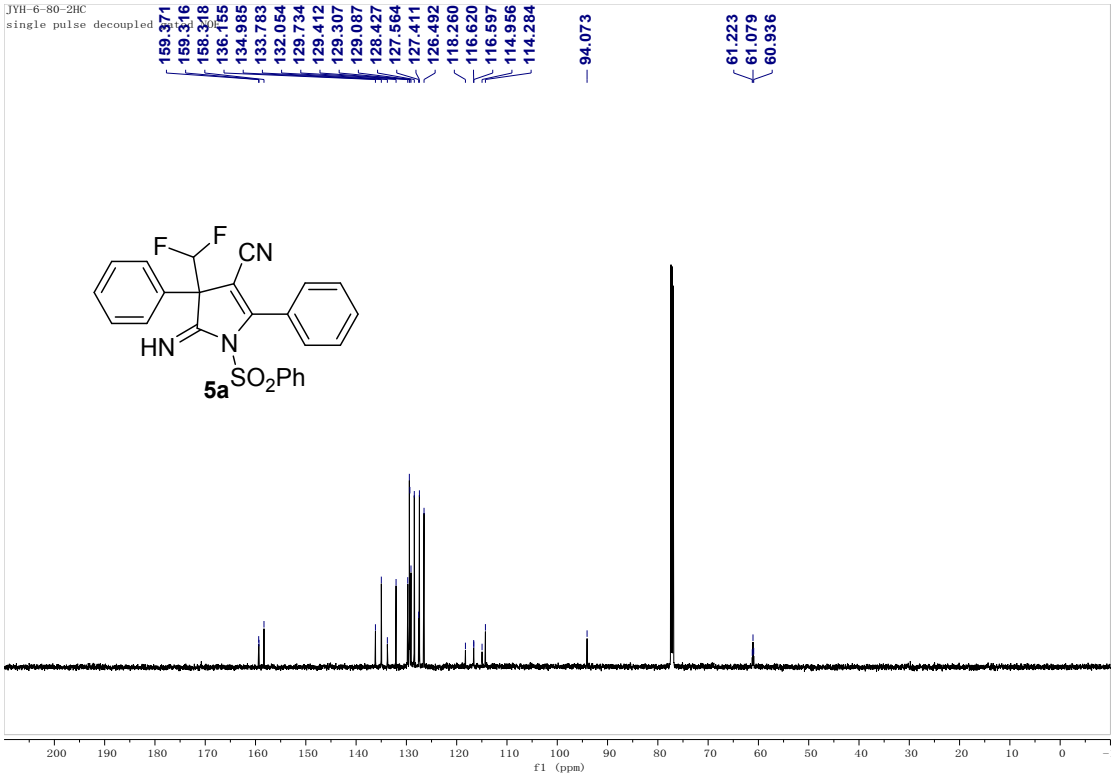

ycq-13-111-1-cdcl3.1.fid
Ts
N–Et
C
3a
2.01
2.00
6.25
4.06
1.00
2.07
3.07
3.00
f1 (ppm)

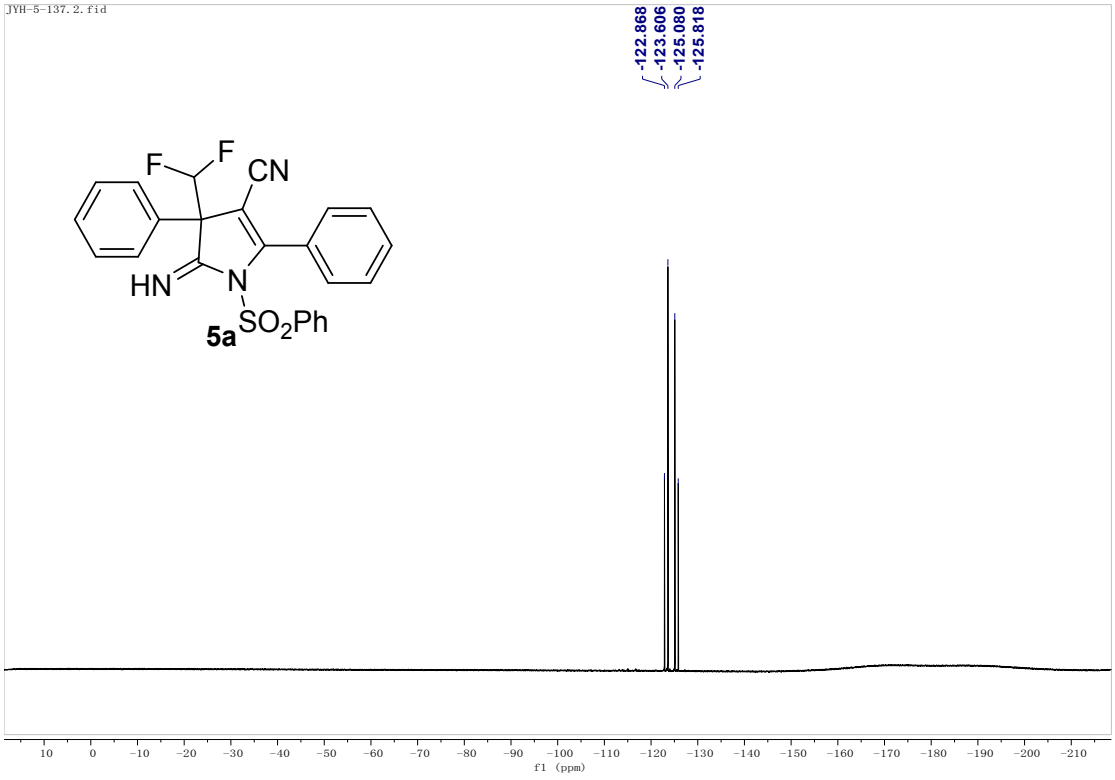

ycq-13-111-1-cdcl3.2.fid
206.657
143.393
135.042
134.906
132.216
129.345
128.845
128.508
128.348
128.212
127.934
127.644
126.145
115.340
103.723
46.052
21.533
13.743
Ts
N–Et
C
3a
f1 (ppm)

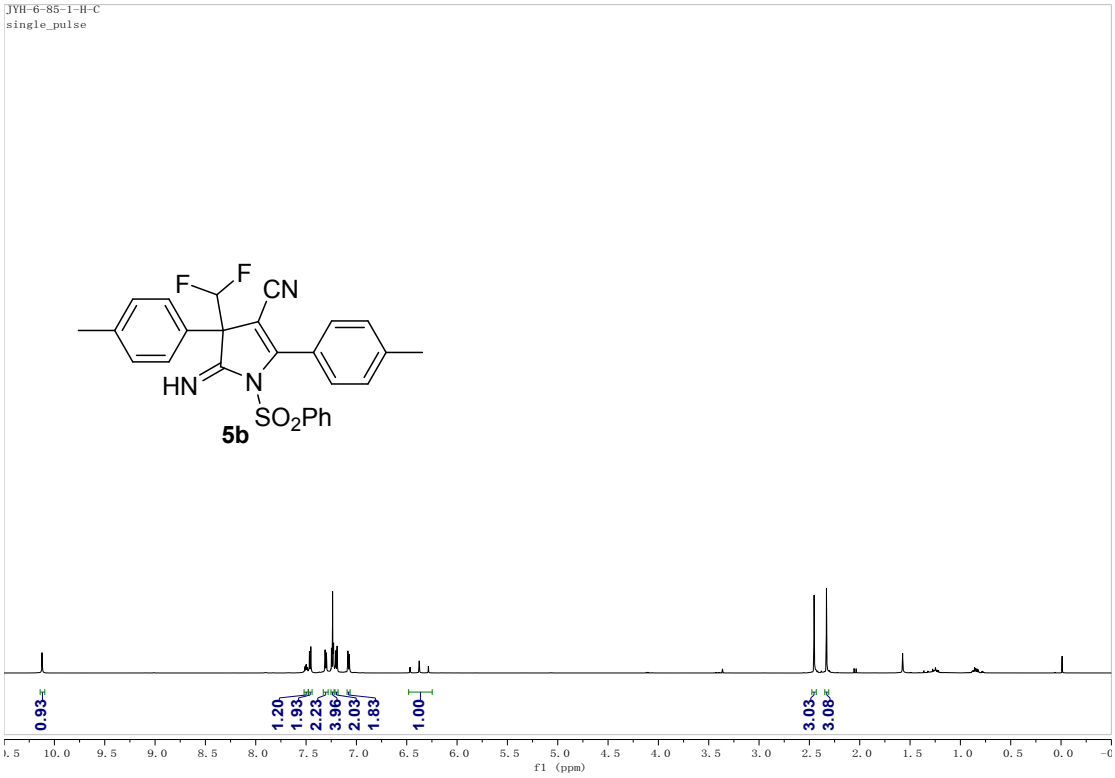

YCQ-12-93-1
single_pulse
Ts
N–Et
C
4l
4.00
6.04
6.05
2.00
2.02
3.04
3.08
3.05
f1 (ppm)

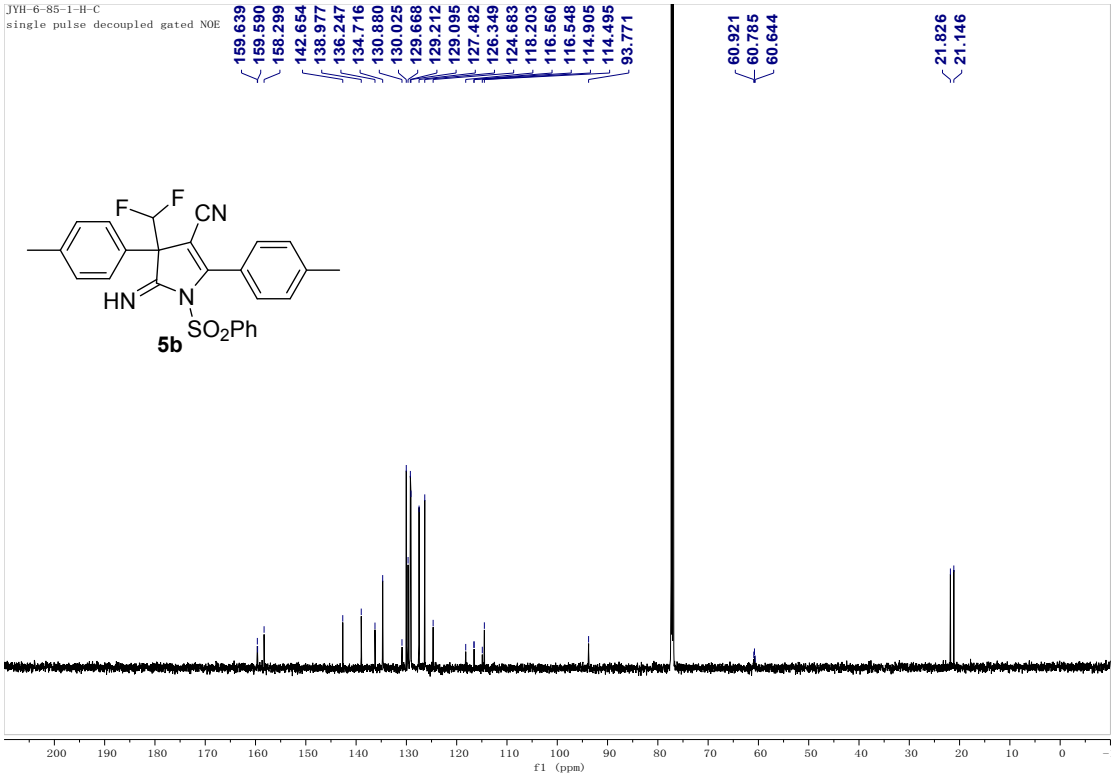

YCQ-12-93-1
single pulse decoupled gated NOE
206.365
143.070
138.154
135.600
135.385
132.453
129.376
129.298
128.775
128.522
128.317
127.826
126.146
119.053
114.392
46.138
21.592
21.327
13.911
Ts
N–Et
C
4l
f1 (ppm)

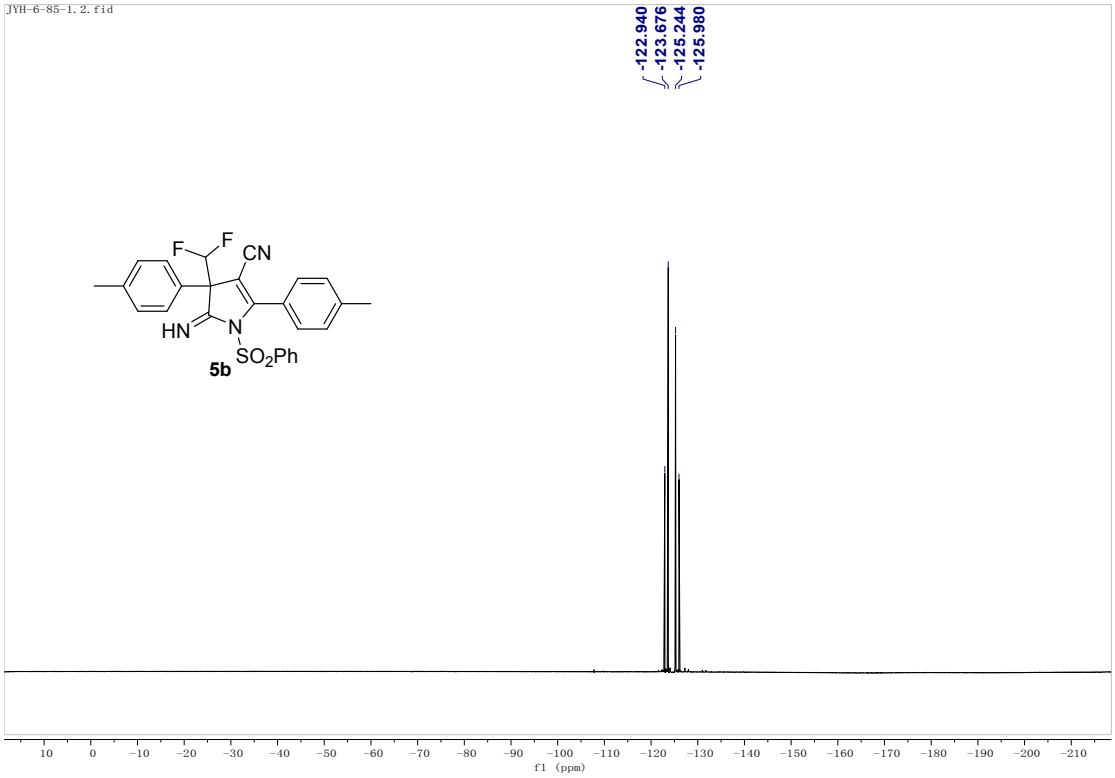

JYH-6-80-2-H.1.fid
F
F
CN
HN
N
SO2Ph
5a
0.95
2.95
3.00
1.95
2.84
3.99
1.00
f1 (ppm)

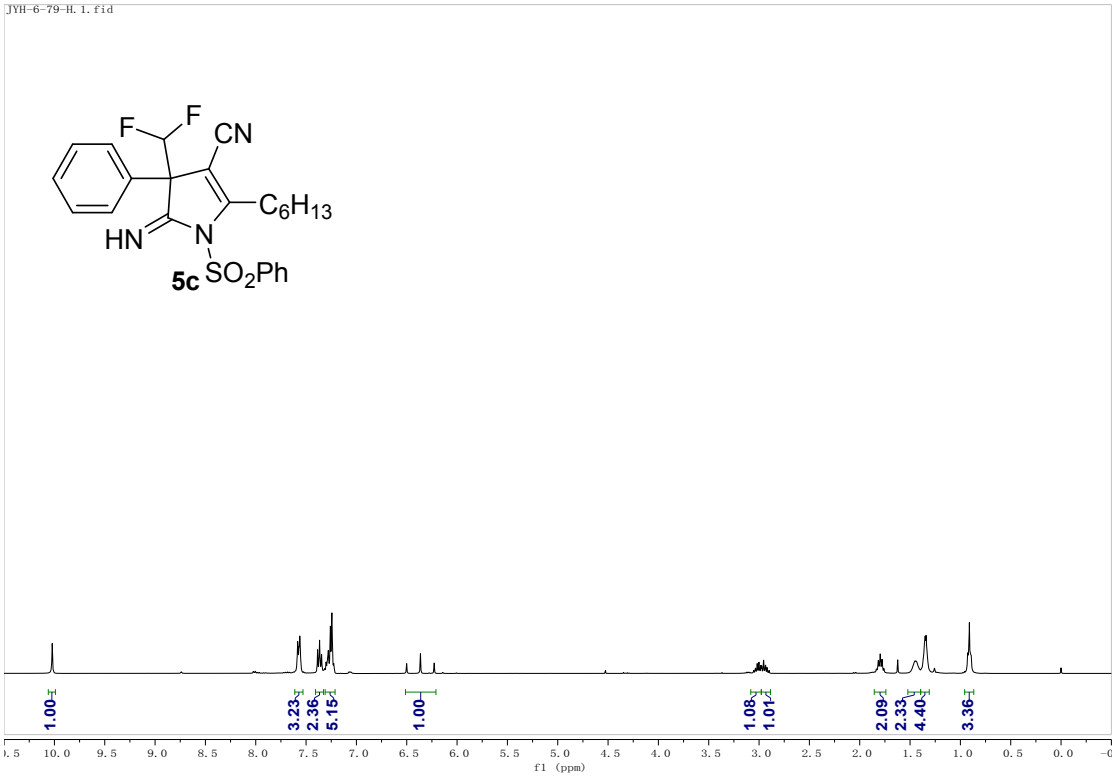

JYH-6-80-2HC
single pulse decoupled
159.371
159.316
158.318
136.155
134.985
133.783
132.054
129.734
129.412
129.307
129.087
128.427
127.564
127.411
126.492
118.260
116.620
116.597
114.956
114.284
94.073
61.223
61.079
60.936
F
F
CN
HN
N
SO2Ph
5a
f1 (ppm)

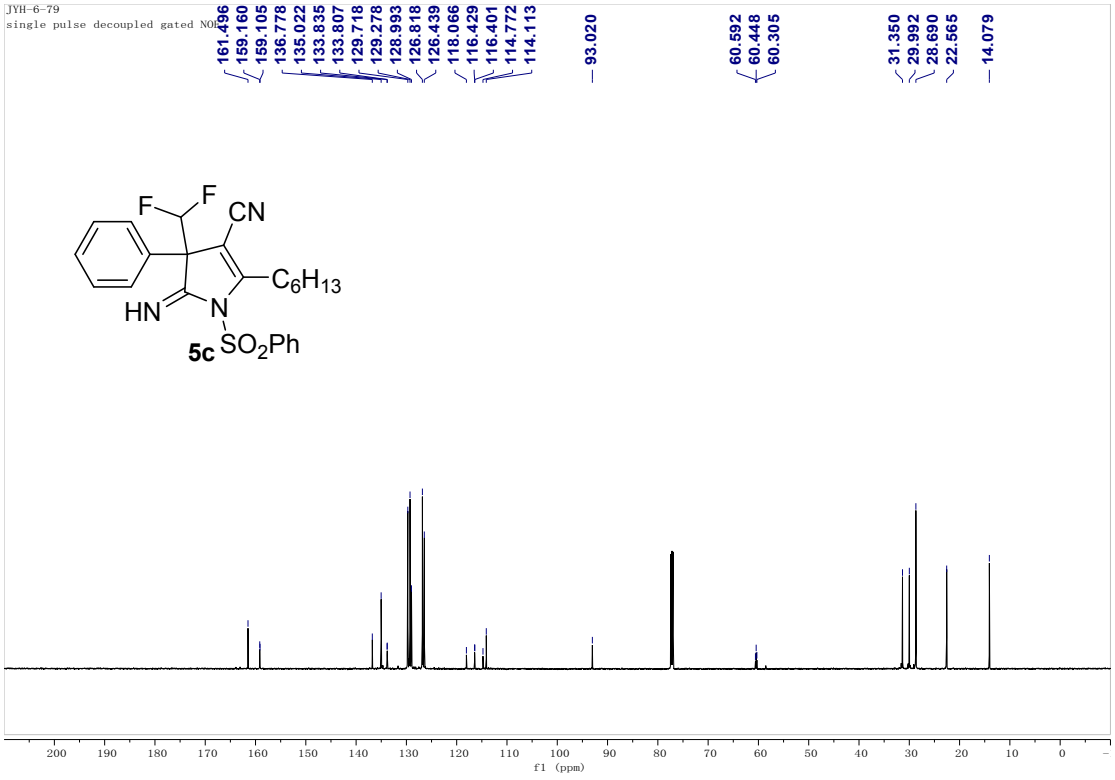

JYH-5-137.2.fid
-122.868
-123.606
-125.080
-125.818
F
F
CN
HN
N
SO2Ph
5a
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

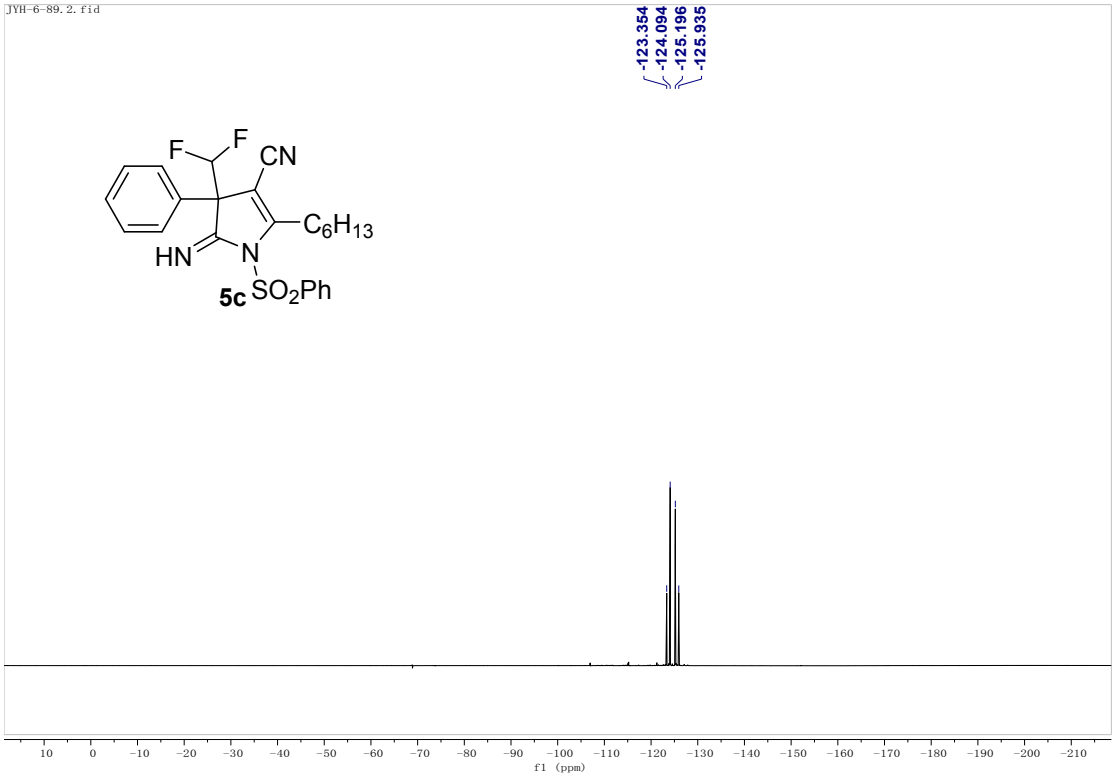

JYH-6-85-1-H-C
single_pulse
F
F
CN
HN
N
SO2Ph
5b
0.93
1.20
1.93
2.23
3.96
2.03
1.83
1.00
3.03
3.08
f1 (ppm)

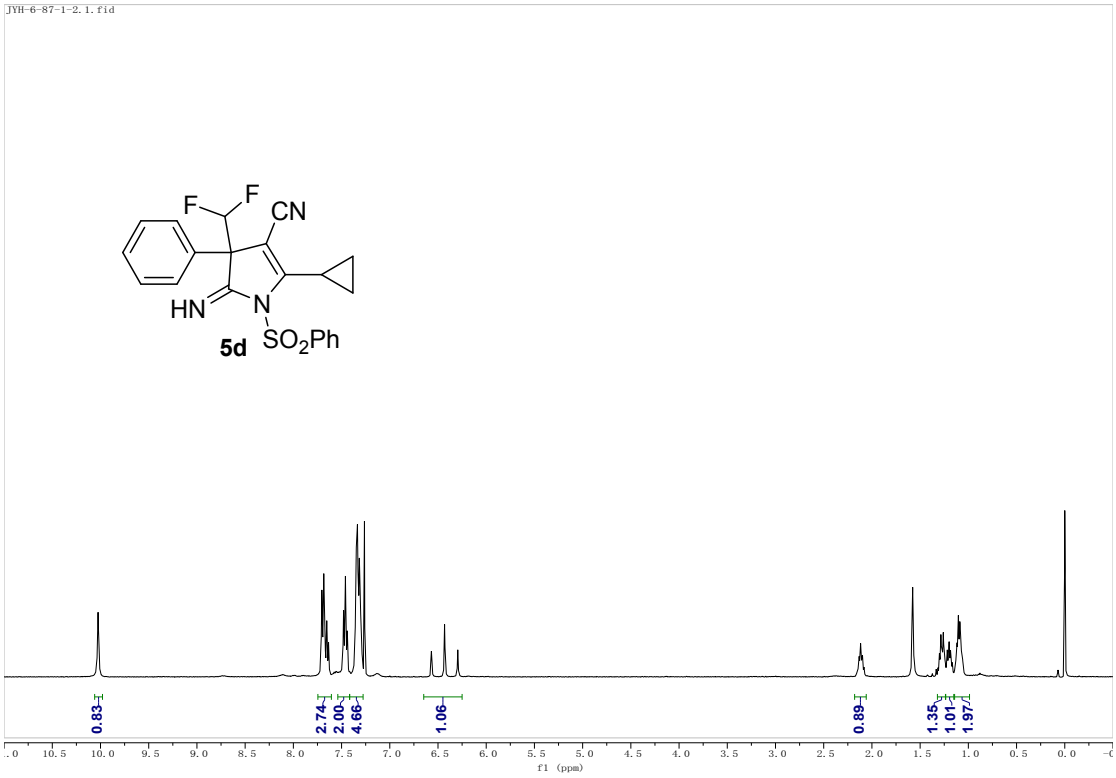

JYH-6-85-1-H-C
single pulse decoupled gated NOE
159.639
159.590
158.299
142.654
138.977
136.247
134.716
130.880
130.025
129.668
129.212
129.095
127.482
126.349
124.683
118.203
116.560
116.548
114.905
114.495
93.771
60.921
60.785
60.644
21.826
21.146
F
F
CN
HN
N
SO2Ph
5b
f1 (ppm)

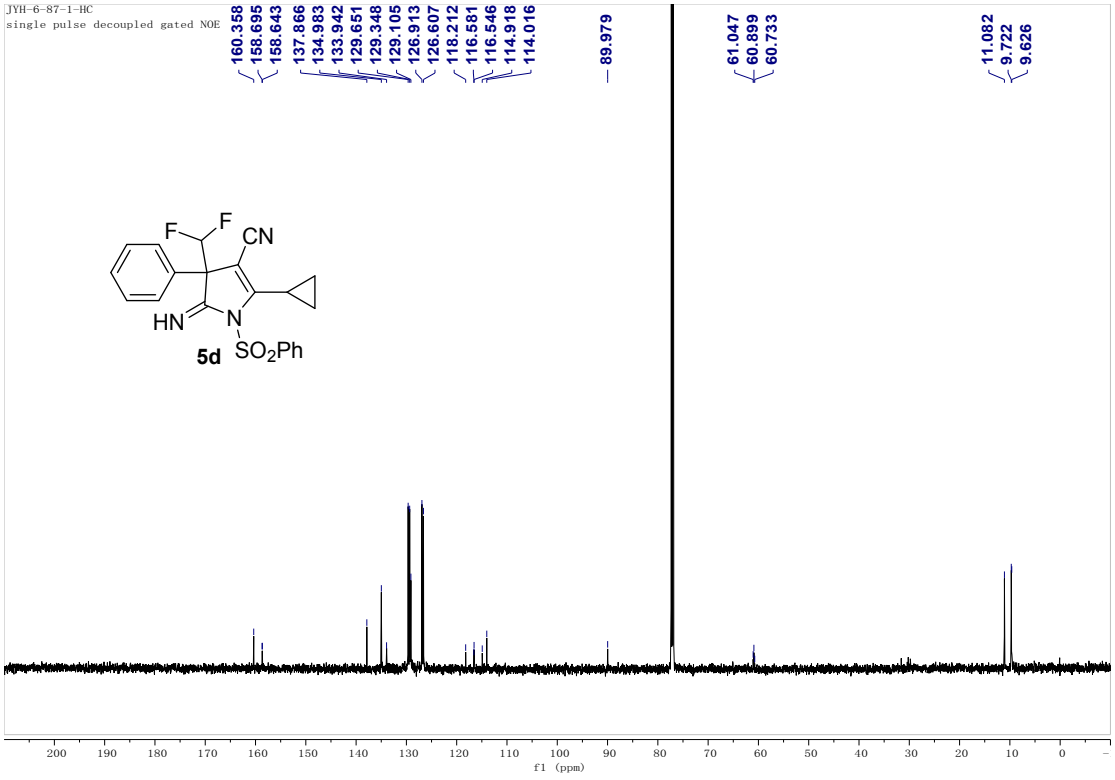

JYH-6-85-1.2.fid
-122.940
-123.676
-125.244
-125.980
F
F
CN
HN
N
SO2Ph
5b
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

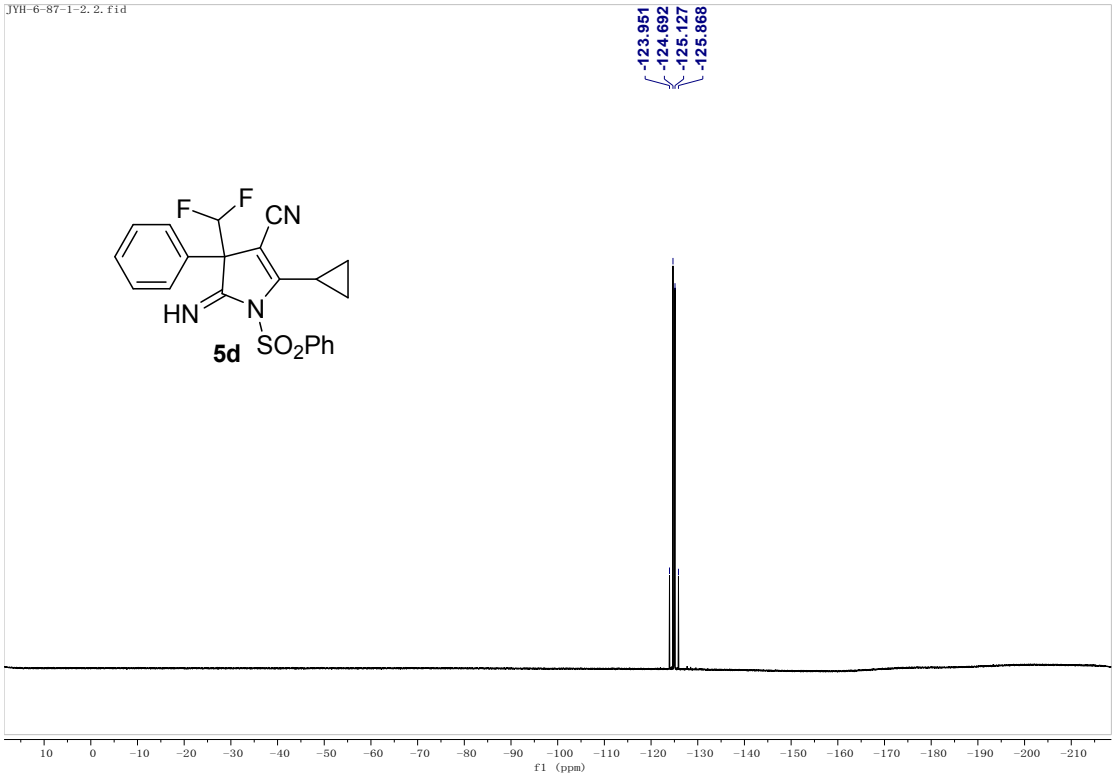

JYH-6-79-H.1.fid
F
F
CN
C6H13
HN
N
SO2Ph
5c
1.00
3.23
2.36
5.15
1.00
1.08
1.01
2.09
2.33
4.40
3.36
f1 (ppm)

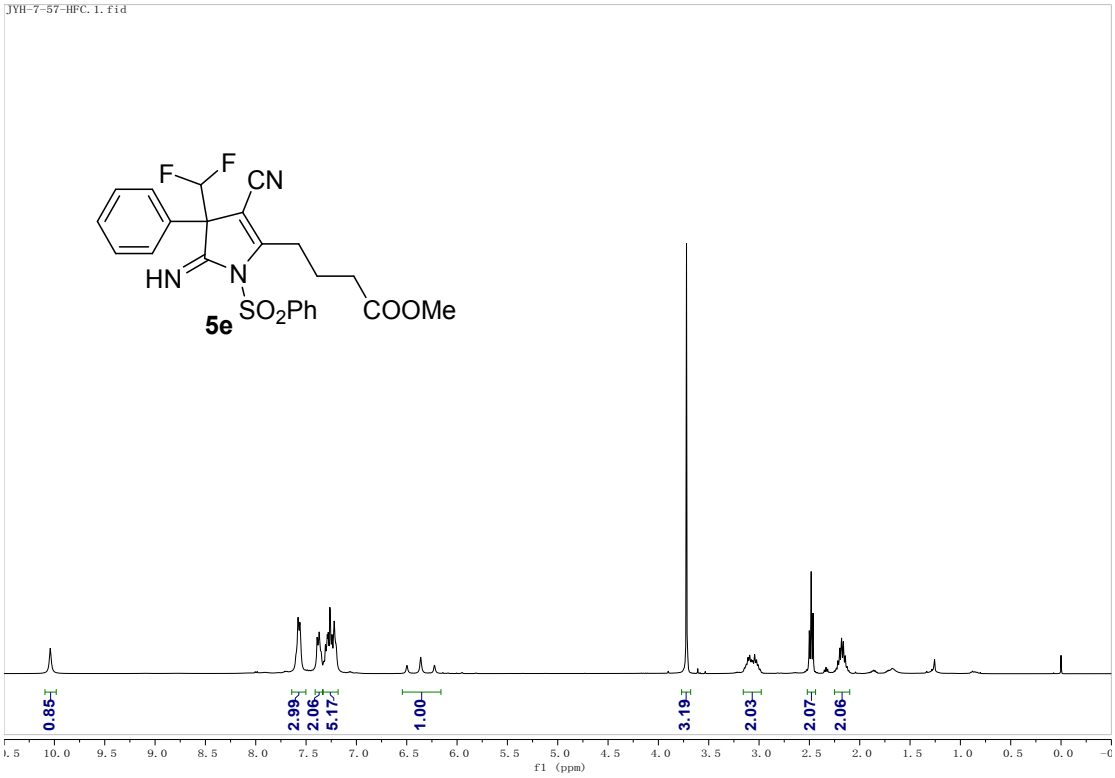

JYH-6-79
single pulse decoupled gated NOE
161.496
159.160
159.105
136.778
135.022
133.835
133.807
129.718
129.278
128.993
126.818
126.439
118.066
116.429
116.401
114.772
114.113
93.020
60.592
60.448
60.305
31.350
29.992
28.690
22.565
14.079
F
F
CN
C6H13
HN
N
SO2Ph
5c
f1 (ppm)

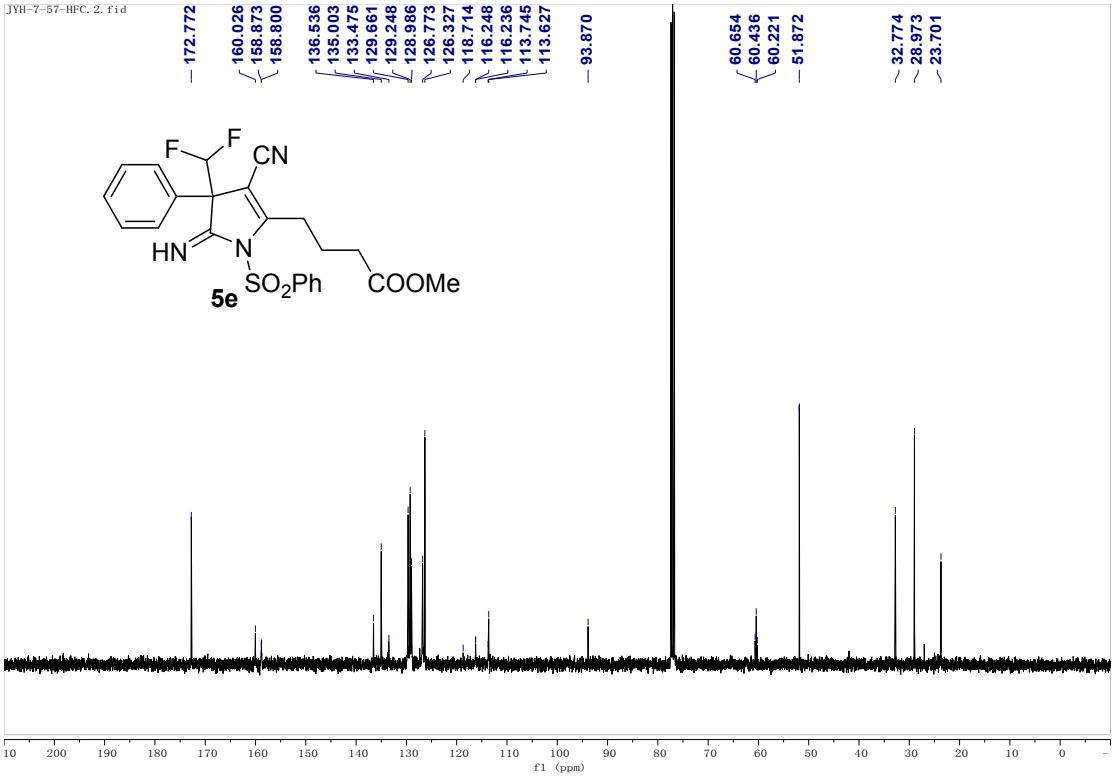

JYH-6-89.2.fid
-123.354
-124.094
-125.196
-125.935
F
F
CN
C6H13
HN
N
SO2Ph
5c
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

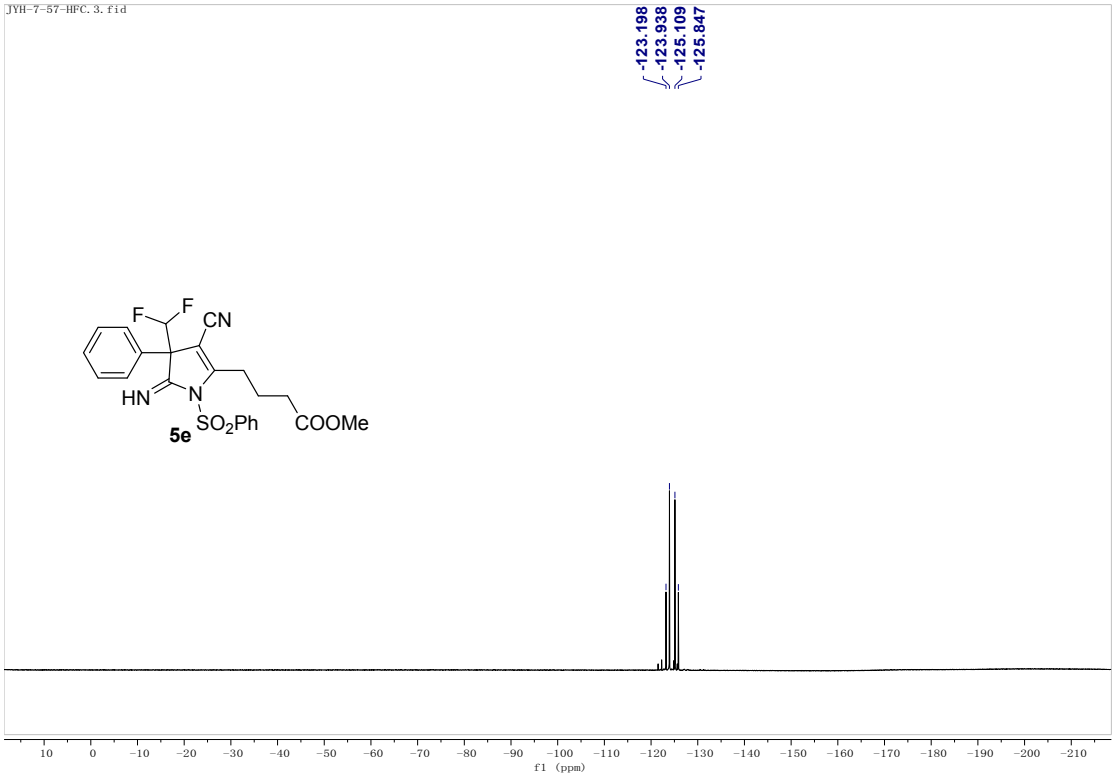

JYH-6-87-1-2.1.fid
F
F
CN
HN
N
SO2Ph
5d
0.83
2.74
2.00
4.66
1.06
0.89
1.35
1.01
1.97
f1 (ppm)

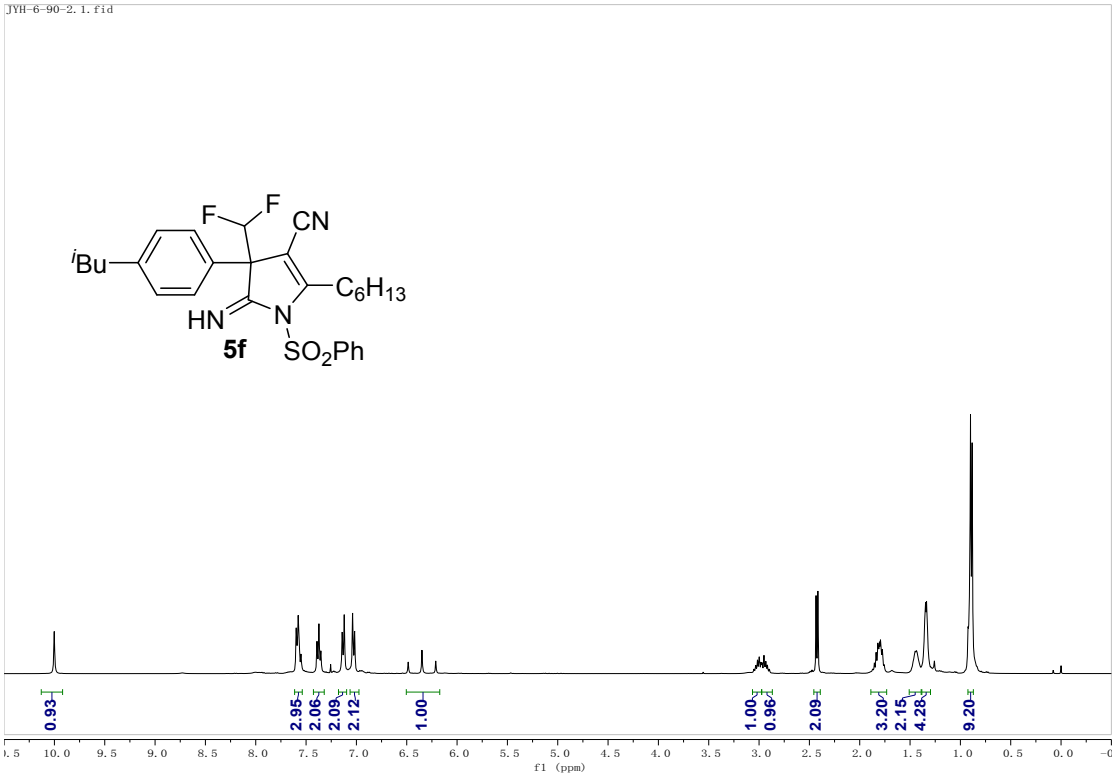

JYH-6-87-1-HC
single pulse decoupled gated NOE
160.358
158.695
158.643
137.866
134.983
133.942
129.651
129.348
129.105
126.913
126.607
118.212
116.581
116.546
114.918
114.016
89.979
61.047
60.899
60.733
11.082
9.722
9.626
F
F
CN
HN
N
SO2Ph
5d
f1 (ppm)

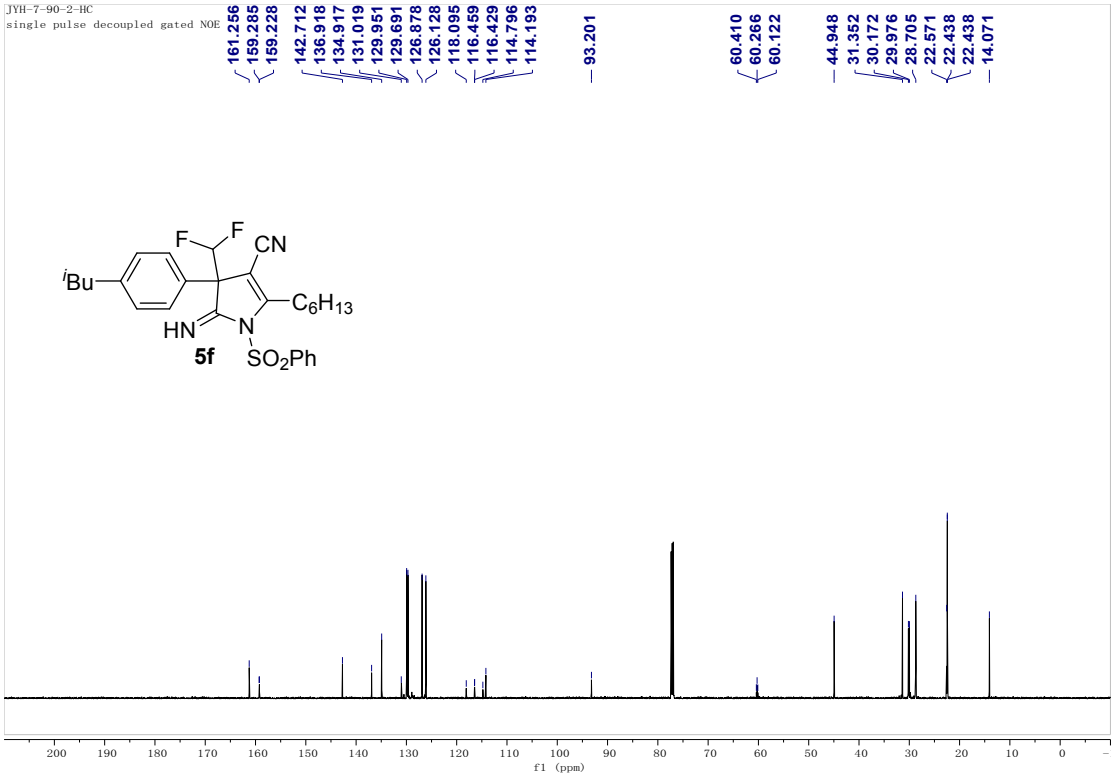

JYH-6-87-1-2.2.fid
-123.951
-124.692
-125.127
-125.868
F
F
CN
HN
N
SO2Ph
5d
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

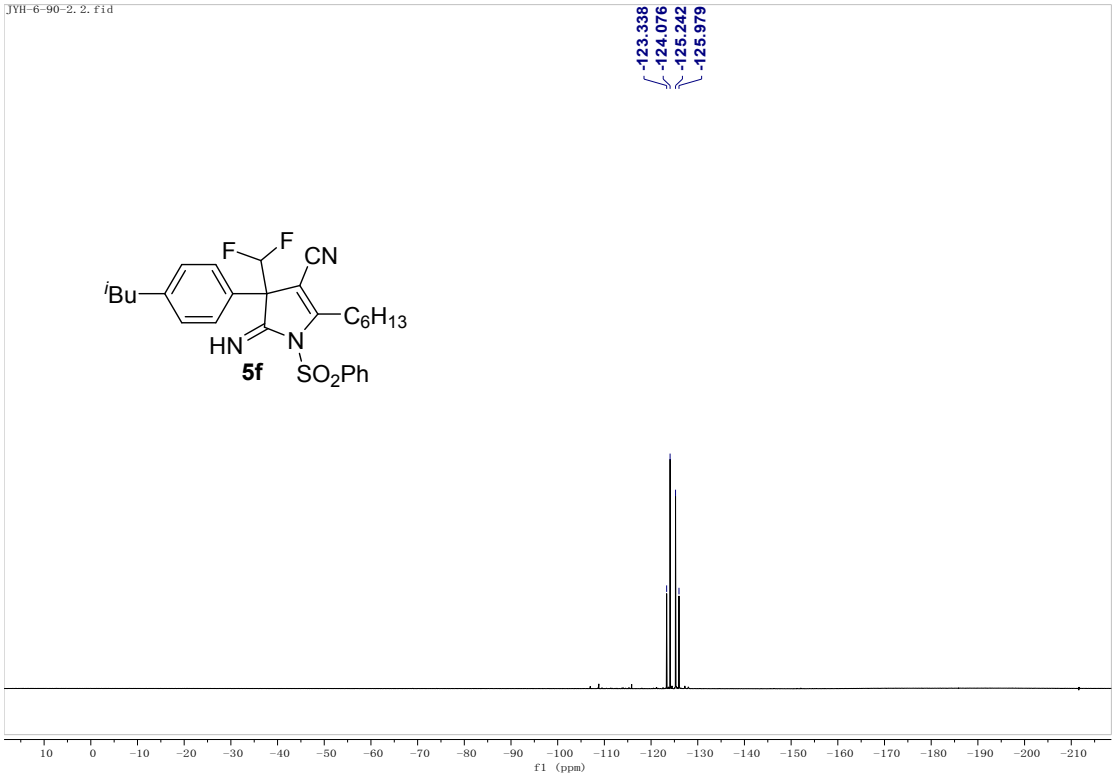

JYH-7-57-HFC.1.fid
F
F
CN
HN
N
SO2Ph
COOMe
5e
0.85
2.99
2.06
5.17
1.00
3.19
2.03
2.07
2.06
f1 (ppm)

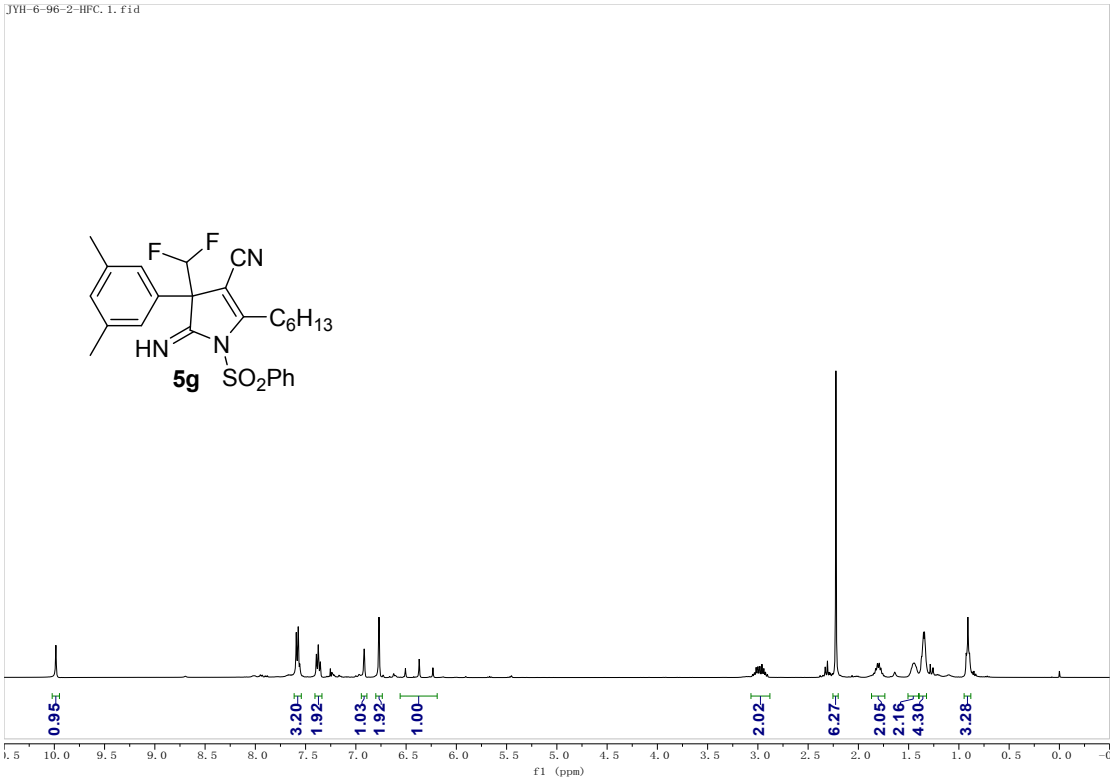

JYH-7-57-HFC.2.fid
172.772
160.026
158.873
158.800
136.536
135.003
133.475
129.661
129.248
128.986
126.773
126.327
118.714
116.248
116.236
113.745
113.627
93.870
60.654
60.436
60.221
51.872
32.774
28.973
23.701
F
F
CN
HN
N
SO2Ph
COOMe
5e
f1 (ppm)

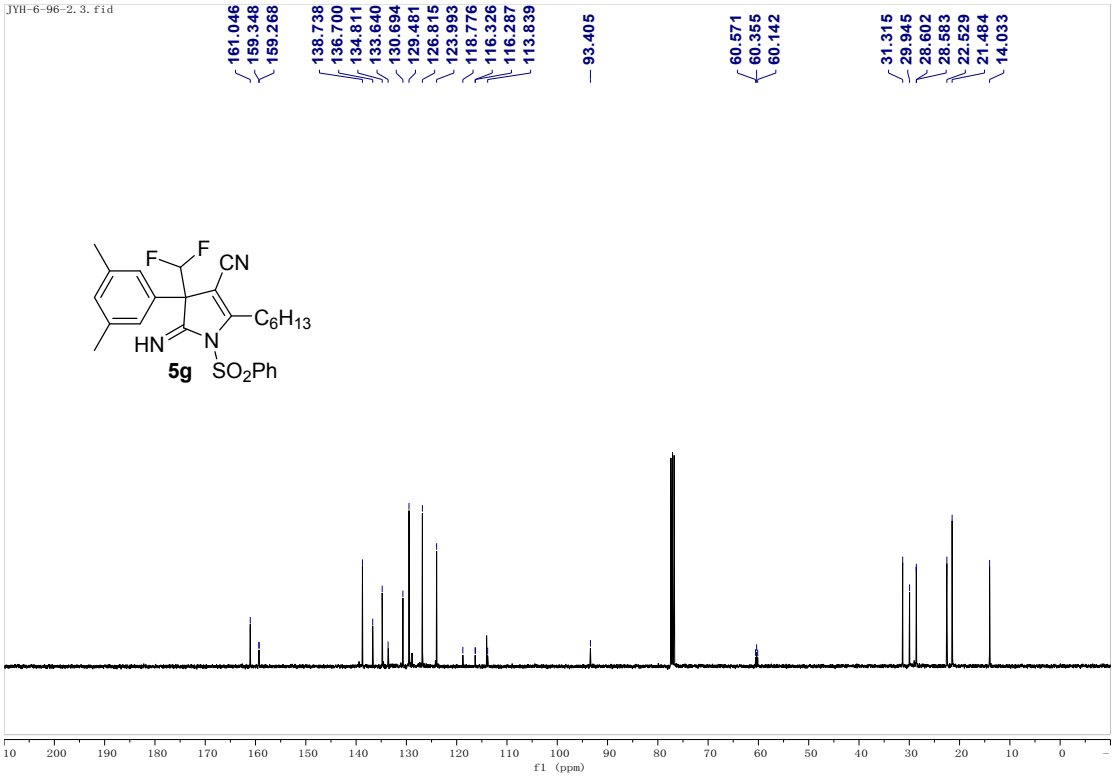

JYH-7-57-HFC.3.fid
-123.198
-123.938
-125.109
-125.847
F
F
CN
HN
N
SO2Ph
COOMe
5e
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

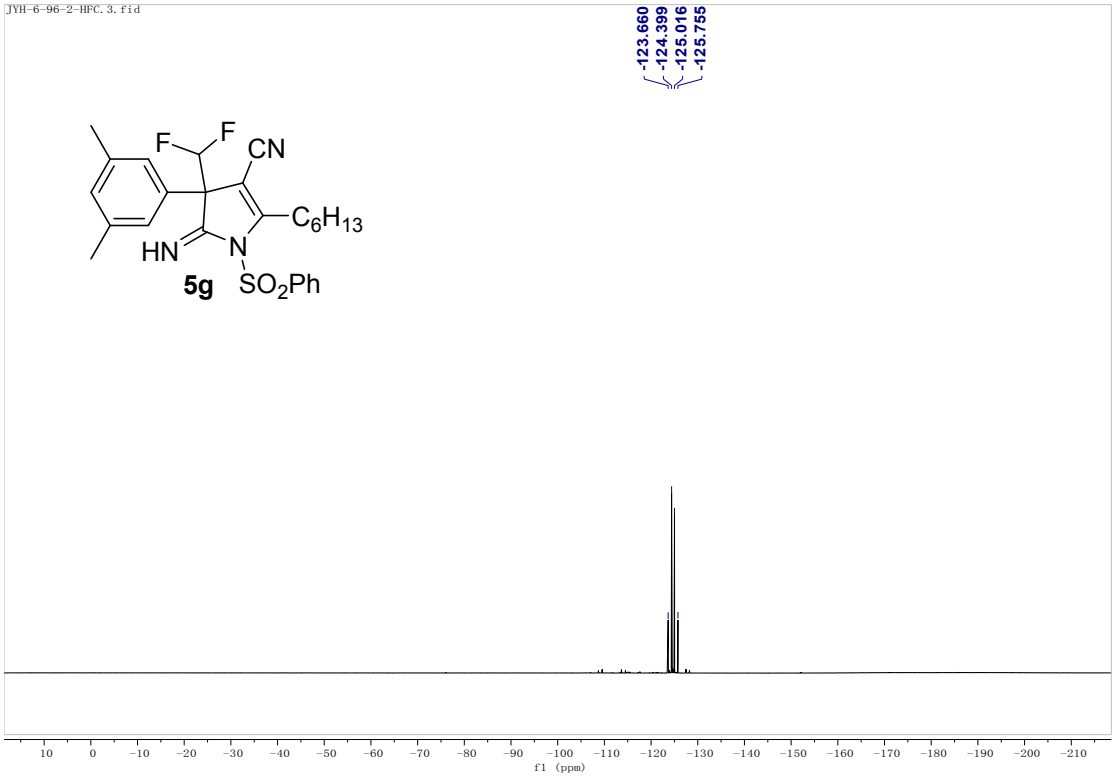

JYH-6-90-2.1.fid
F
F
CN
iBu
C6H13
HN
N
SO2Ph
5f
0.93
2.95
2.06
2.09
2.12
1.00
1.00
0.96
2.09
3.20
2.15
4.28
9.20
f1 (ppm)

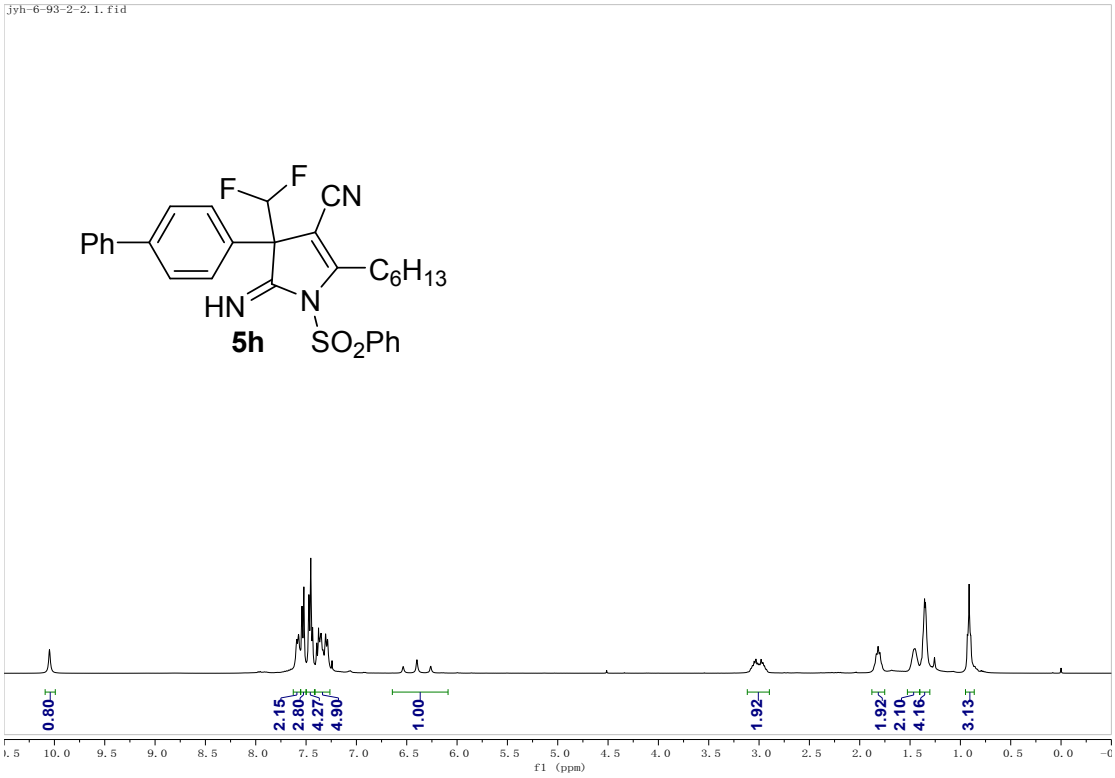

JYH-7-90-2-HC
single pulse decoupled gated NOE
161.256
159.285
159.228
142.712
136.918
134.917
131.019
129.951
129.691
126.878
126.128
118.095
116.459
116.429
114.796
114.193
93.201
60.410
60.266
60.122
44.948
31.352
30.172
29.976
28.705
22.571
22.438
22.438
14.071
F
F
CN
iBu
C6H13
HN
N
SO2Ph
5f
f1 (ppm)

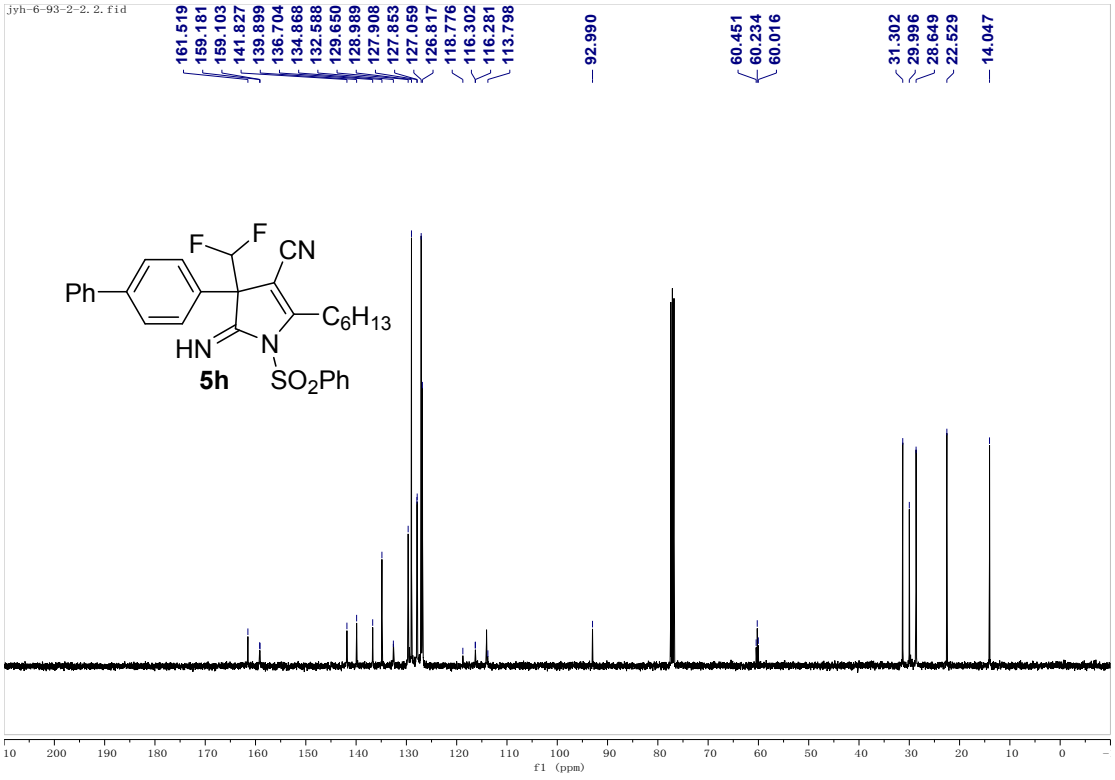

JYH-6-90-2.2.fid
-123.338
-124.076
-125.242
-125.979
F
F
CN
iBu
C6H13
HN
N
SO2Ph
5f
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

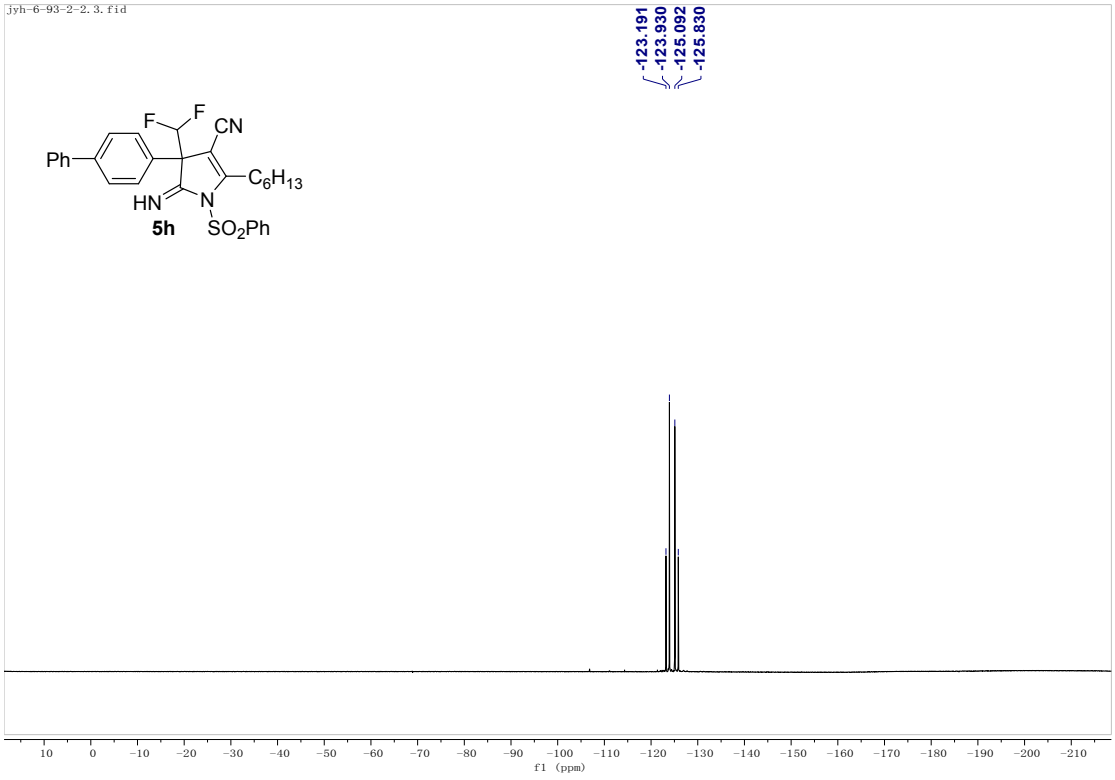

JYH-6-96-2-HFC.1.fid
F
F
CN
C6H13
HN
N
SO2Ph
5g
0.95
3.20
1.92
1.03
1.92
1.00
2.02
6.27
2.05
2.16
4.30
3.28
f1 (ppm)

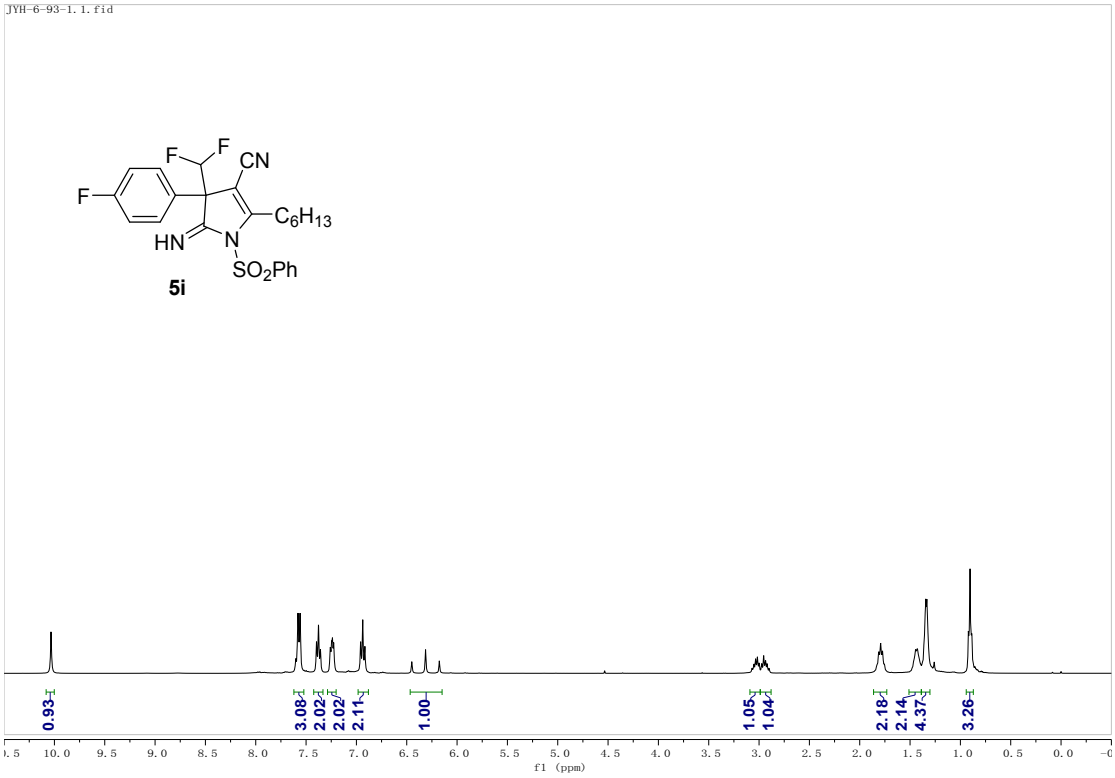

JYH-6-96-2.3.fid
161.046
159.348
159.268
138.738
136.700
134.811
133.640
130.694
129.481
126.815
123.993
118.776
116.326
116.287
113.839
93.405
60.571
60.355
60.142
31.315
29.945
28.602
28.583
22.529
21.484
14.033
F
F
CN
C6H13
HN
N
SO2Ph
5g
f1 (ppm)

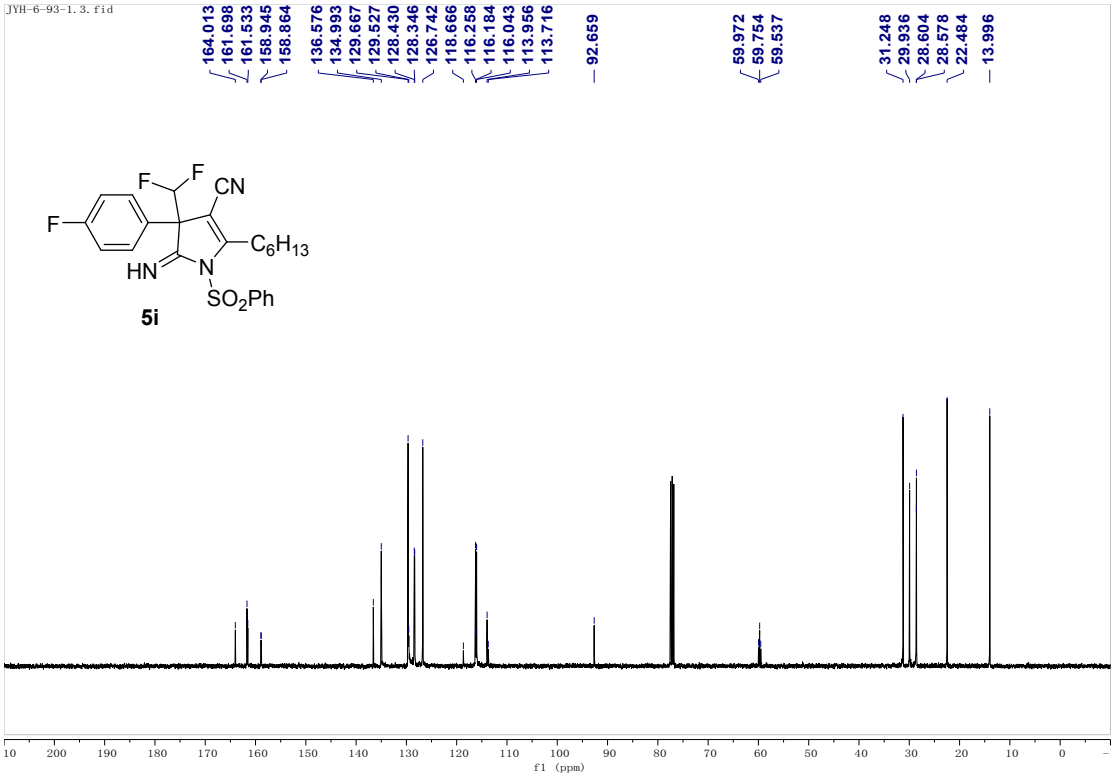

JYH-6-96-2-HFC.3.fid
-123.660
-124.399
-125.016
-125.755
F
F
CN
C6H13
HN
N
SO2Ph
5g
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

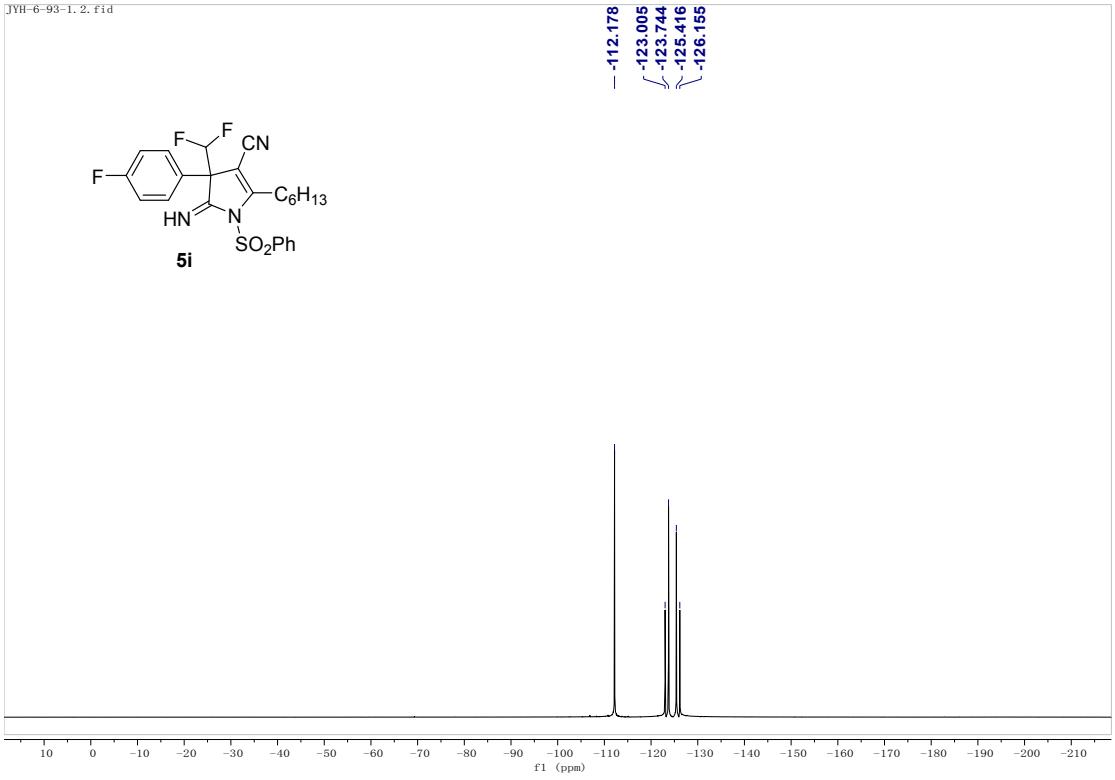

jyh-6-93-2-2.1.fid
F
F
CN
Ph
C6H13
HN
N
5h
SO2Ph
0.80
2.15
2.80
4.27
4.90
1.00
1.92
1.92
2.10
4.16
3.13
f1 (ppm)

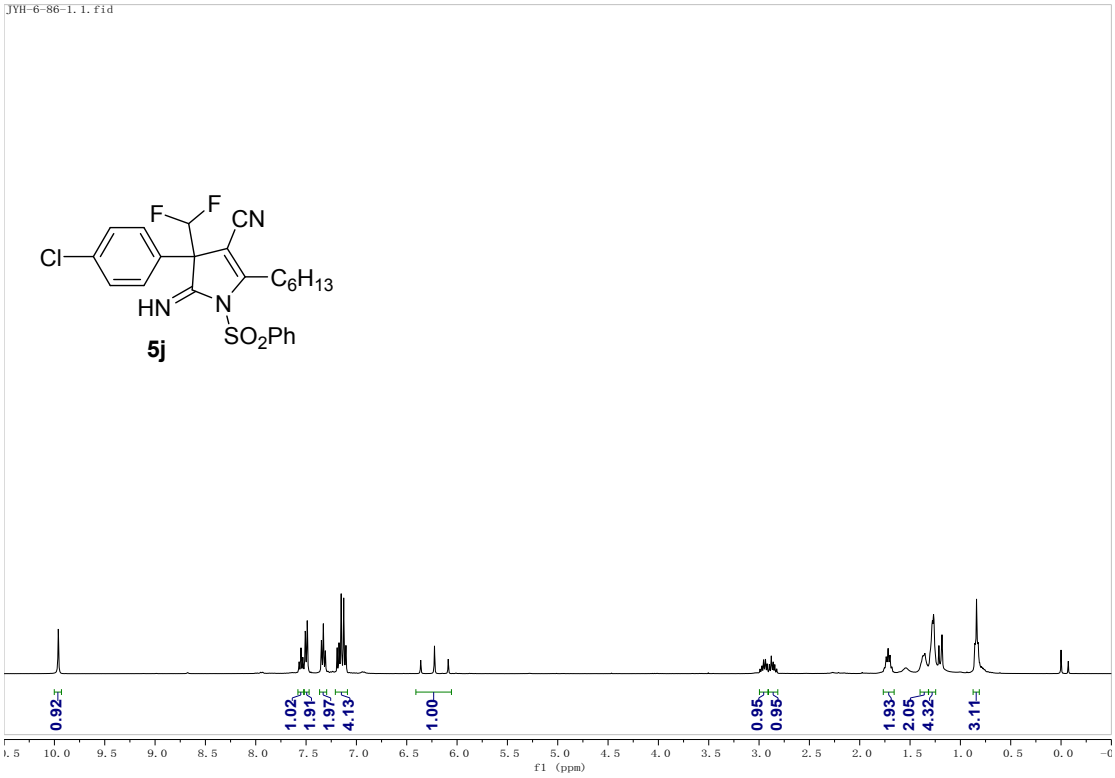

jyh-6-93-2-2.2.fid
161.519
159.181
159.103
141.827
139.899
136.704
134.868
132.588
129.650
128.989
127.908
127.853
127.059
126.817
118.776
116.302
116.281
113.798
92.990
60.451
60.234
60.016
31.302
29.996
28.649
22.529
14.047
F
F
CN
Ph
C6H13
HN
N
5h
SO2Ph
f1 (ppm)

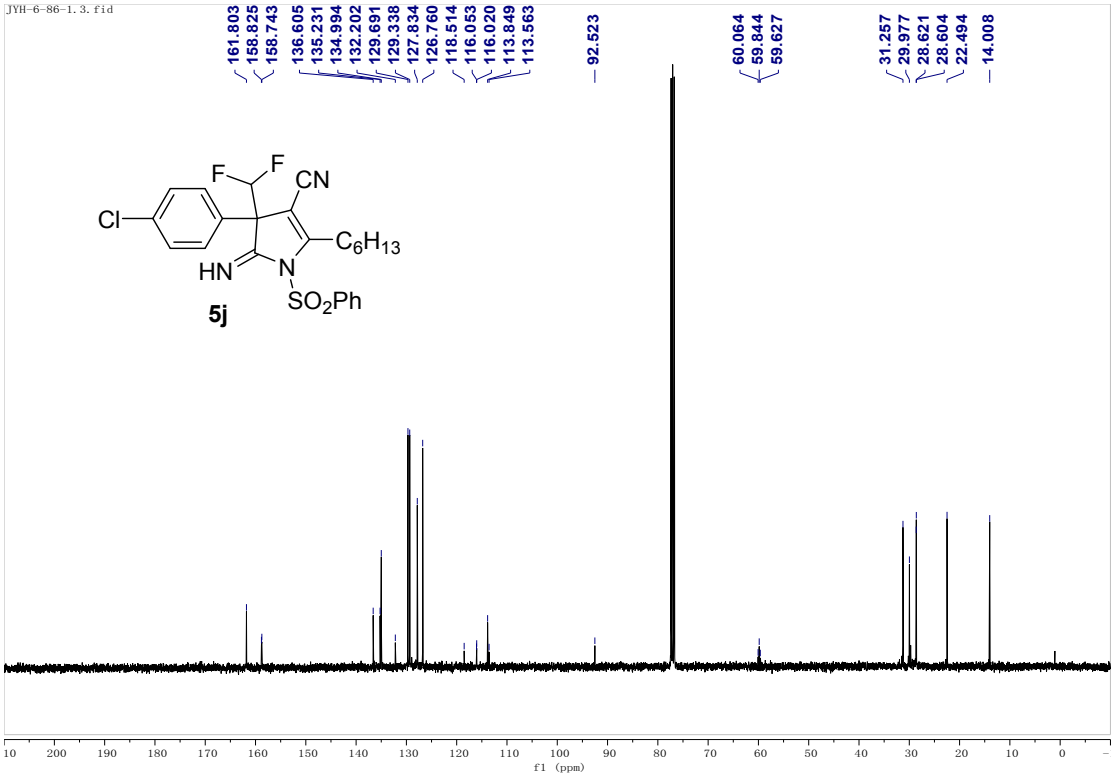

jyh-6-93-2-2.3.fid
-123.191
-123.930
-125.092
-125.830
F
F
CN
Ph
C6H13
HN
N
SO2Ph
5h
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

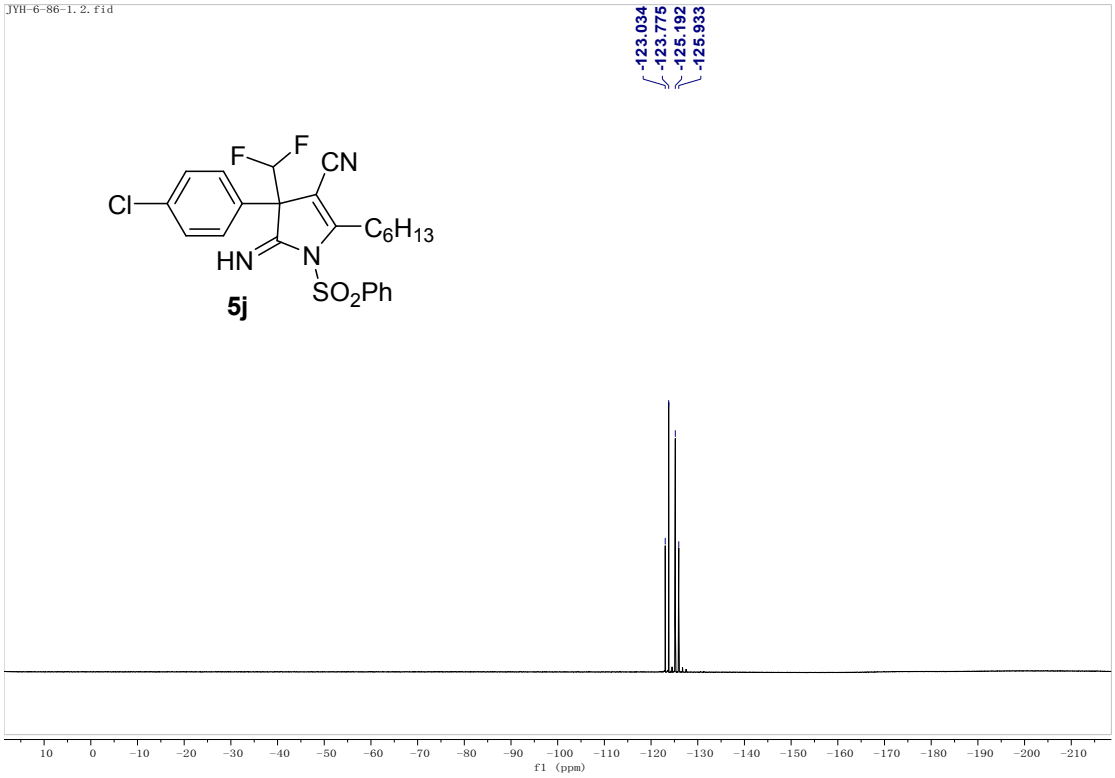

JYH-6-93-1.1.fid
F
F
CN
F
C6H13
HN
N
SO2Ph
5i
0.93
3.08
2.02
2.02
2.11
1.00
1.05
1.04
2.18
2.14
4.37
3.26
f1 (ppm)

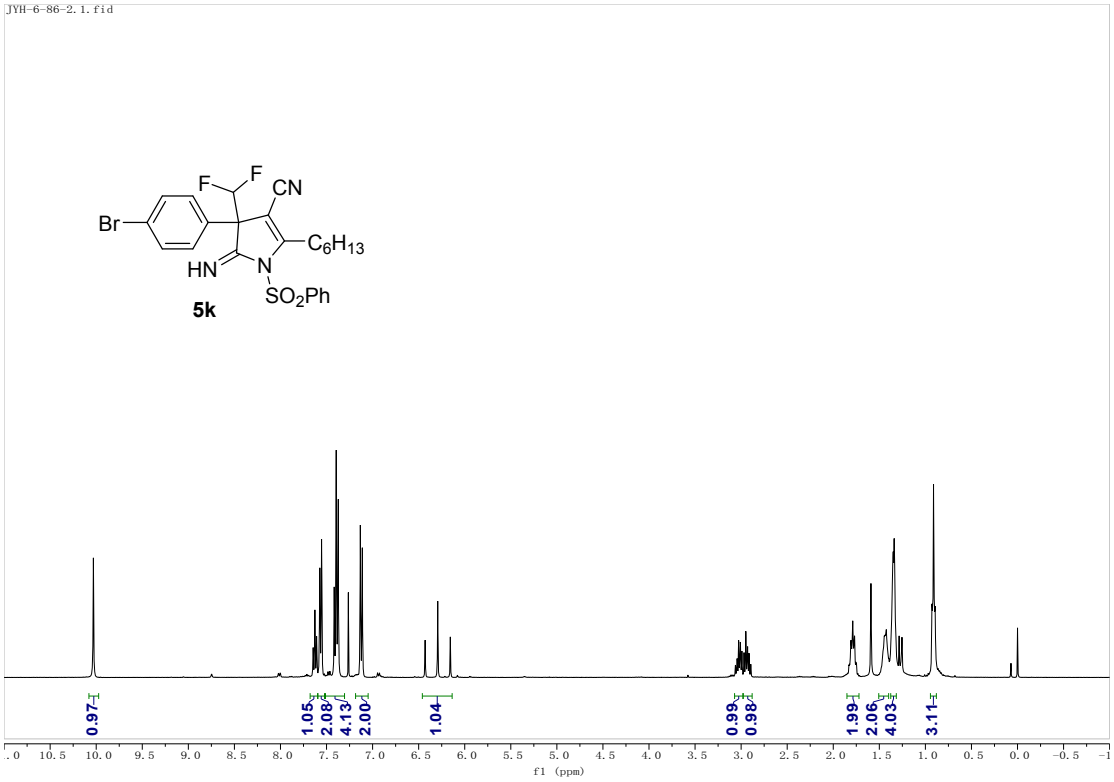

JYH-6-93-1.3.fid
164.013
161.698
161.533
158.945
158.864
136.576
134.993
129.667
129.527
128.430
128.346
126.742
118.666
116.258
116.184
116.043
113.956
113.716
92.659
59.972
59.754
59.537
31.248
29.936
28.604
28.578
22.484
13.996
F
F
CN
F
C6H13
HN
N
SO2Ph
5i
f1 (ppm)

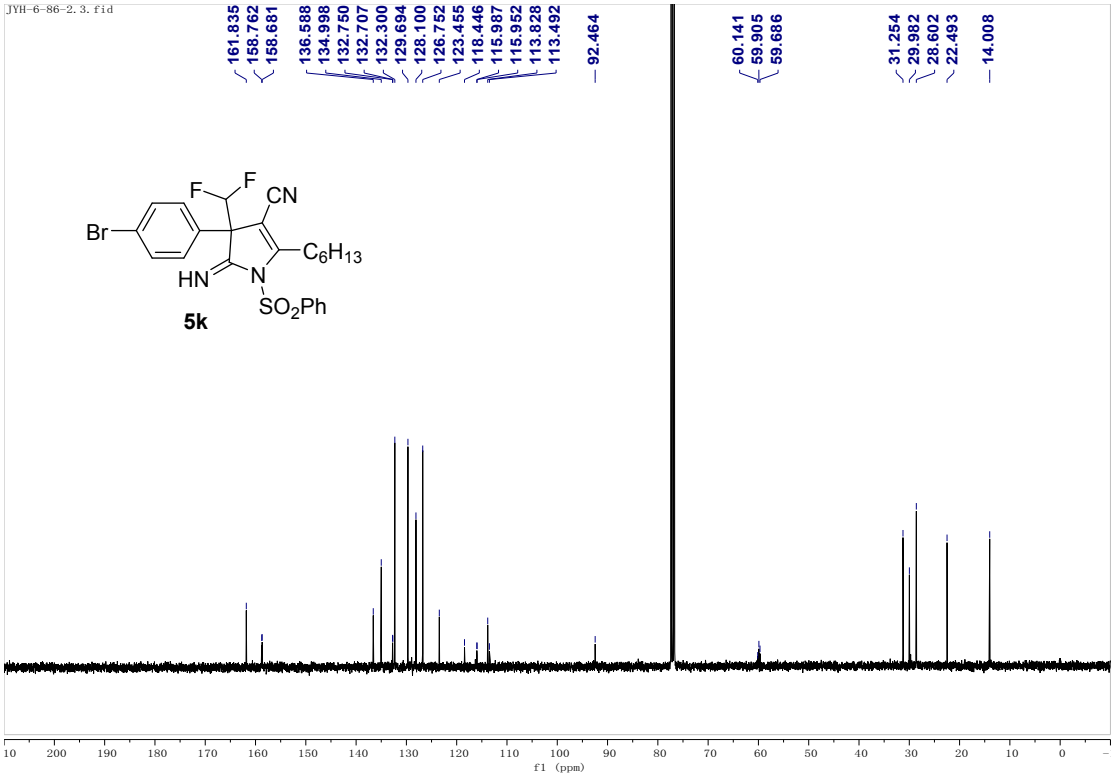

JYH-6-93-1.2.fid
-112.178
-123.005
-123.744
-125.416
-126.155
F
F
F
CN
C6H13
HN
N
SO2Ph
5i
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

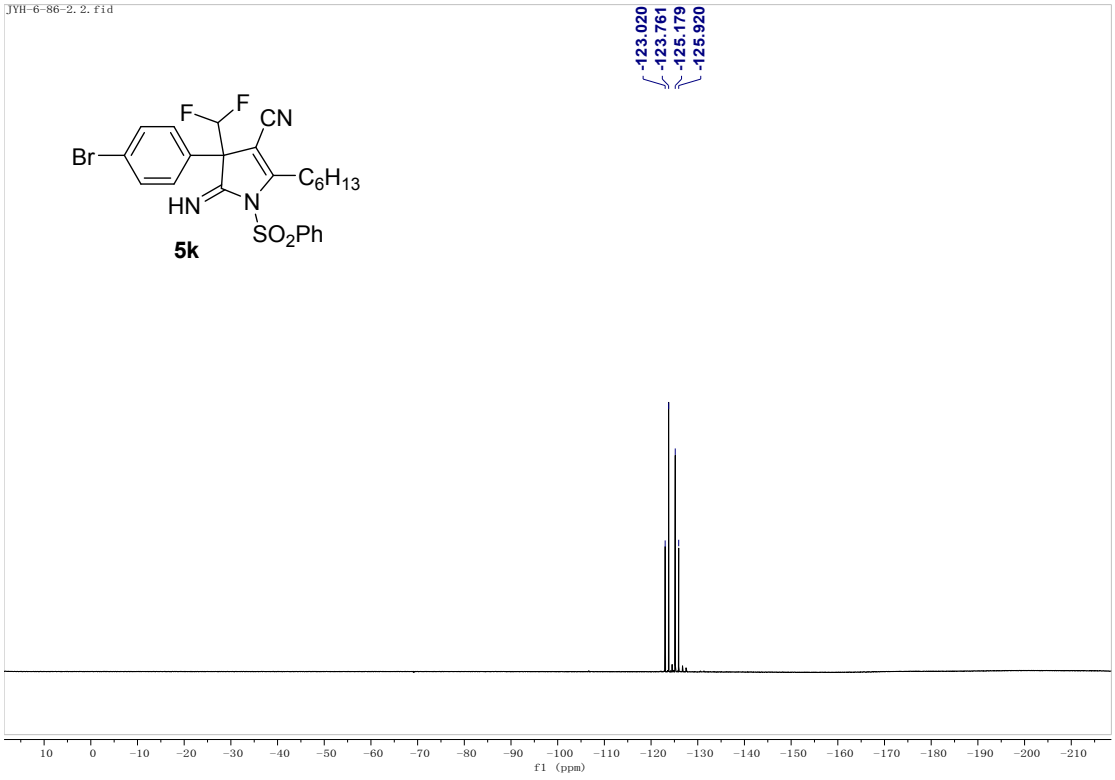

JYH-6-86-1.1.fid
F
F
CN
Cl
C6H13
HN
N
SO2Ph
5j
0.92
1.02
1.91
1.97
4.13
1.00
0.95
0.95
1.93
2.05
4.32
3.11
f1 (ppm)

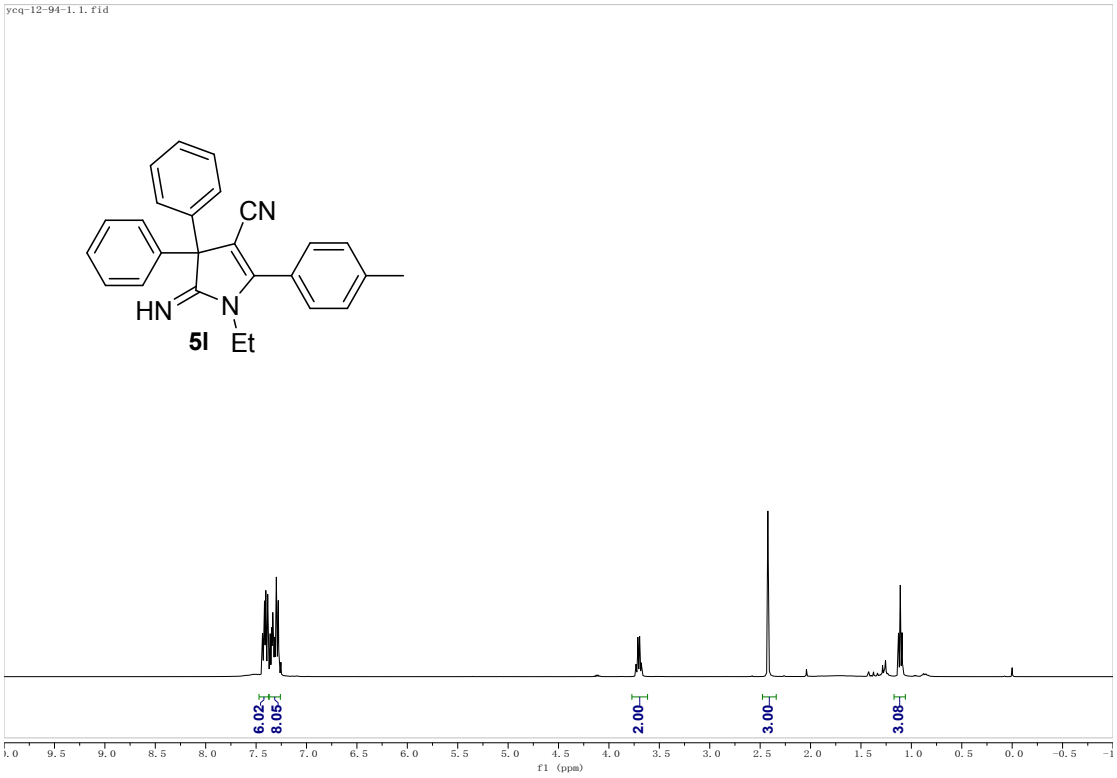

JYH-6-86-1.3.fid
161.803
158.825
158.743
136.605
135.231
134.994
132.202
129.691
129.338
127.834
126.760
118.514
116.053
116.020
113.849
113.563
92.523
60.064
59.844
59.627
31.257
29.977
28.621
28.604
22.494
14.008
F
F
CN
Cl
C6H13
HN
N
SO2Ph
5j
f1 (ppm)

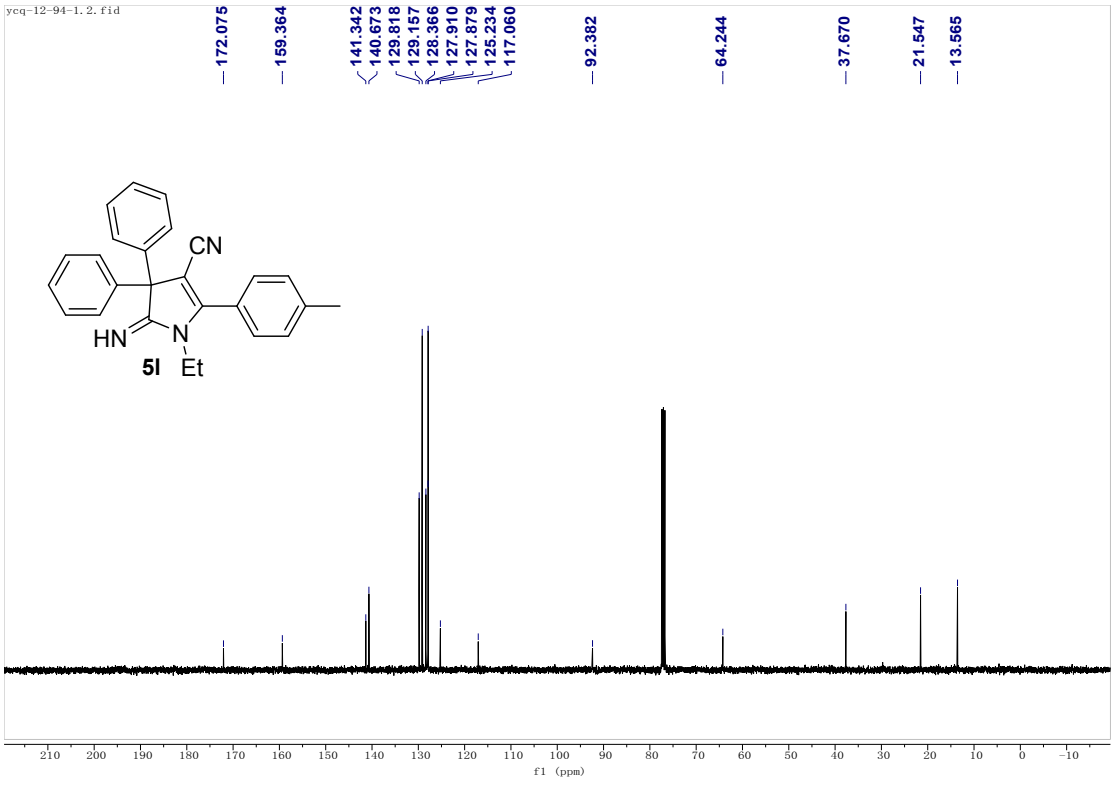

JYH-6-86-1.2.fid
-123.034
-123.775
-125.192
-125.933
F
F
CN
Cl
C6H13
HN
N
SO2Ph
5j
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

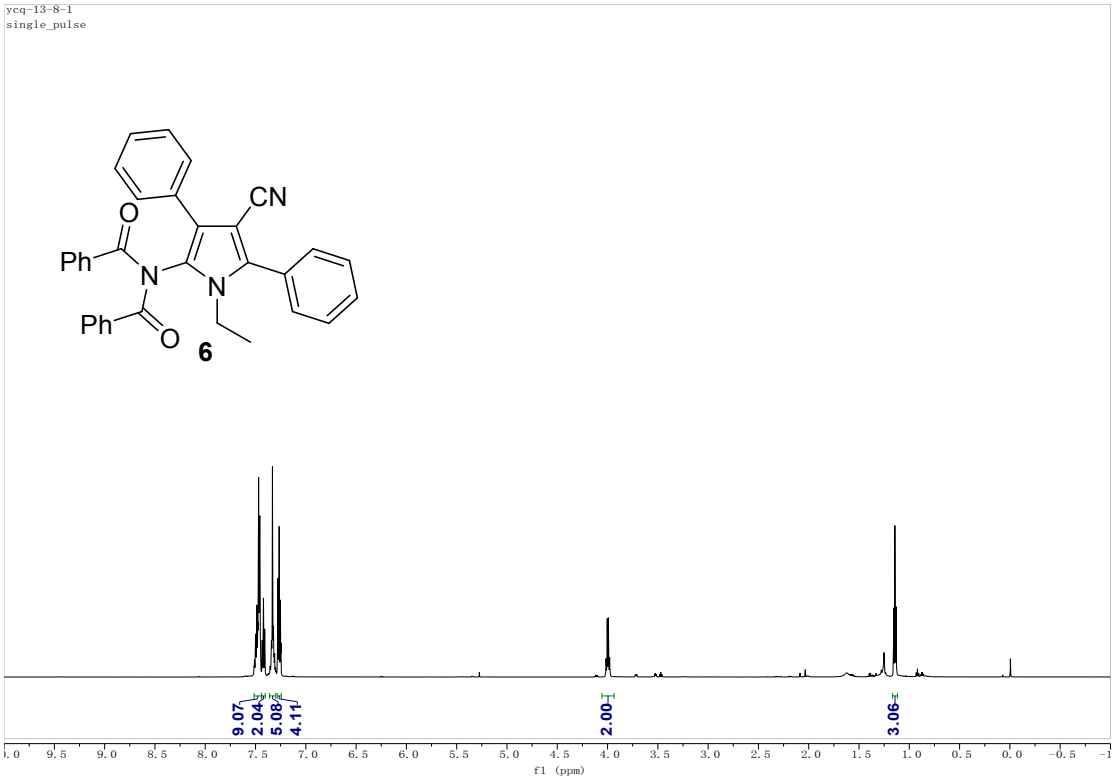

JYH-6-86-2.1.fid
F
F
CN
Br
C6H13
HN
N
SO2Ph
5k
0.97
1.05
2.08
4.13
2.00
1.04
0.99
0.98
1.99
2.06
4.03
3.11
f1 (ppm)

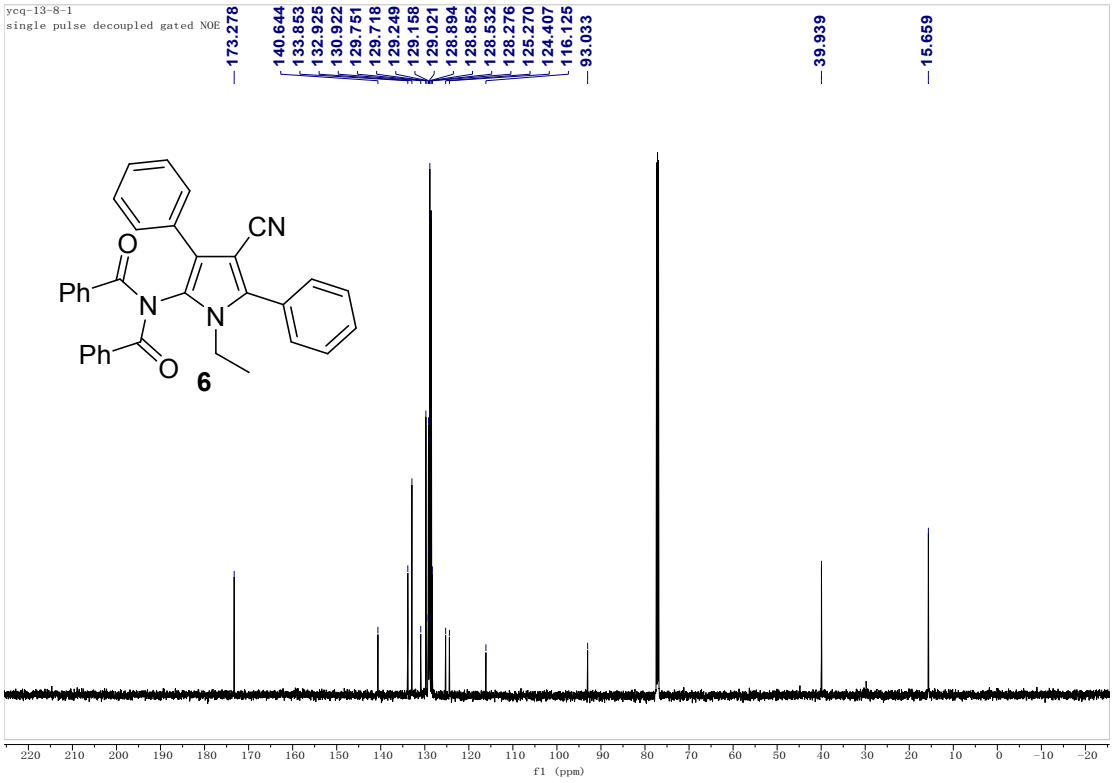

JYH-6-86-2.3.fid
161.835
158.762
158.681
136.588
134.998
132.750
132.707
132.300
129.694
128.100
126.752
123.455
118.446
115.987
115.952
113.828
113.492
92.464
60.141
59.905
59.686
31.254
29.982
28.602
22.493
14.008
F
F
CN
Br
C6H13
HN
N
SO2Ph
5k
f1 (ppm)

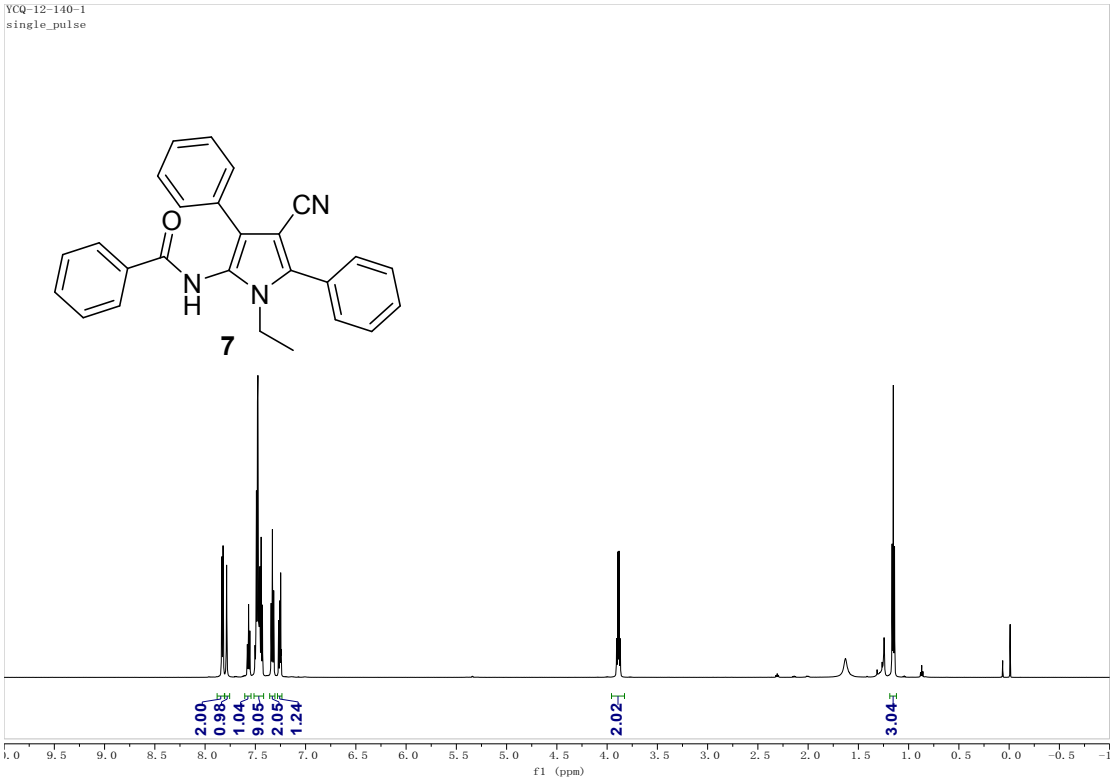

JYH-6-86-2.2.fid
-123.020
-123.761
-125.179
-125.920
F
F
CN
Br
C_6H_{13}
HN
N
SO_2Ph
5k
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

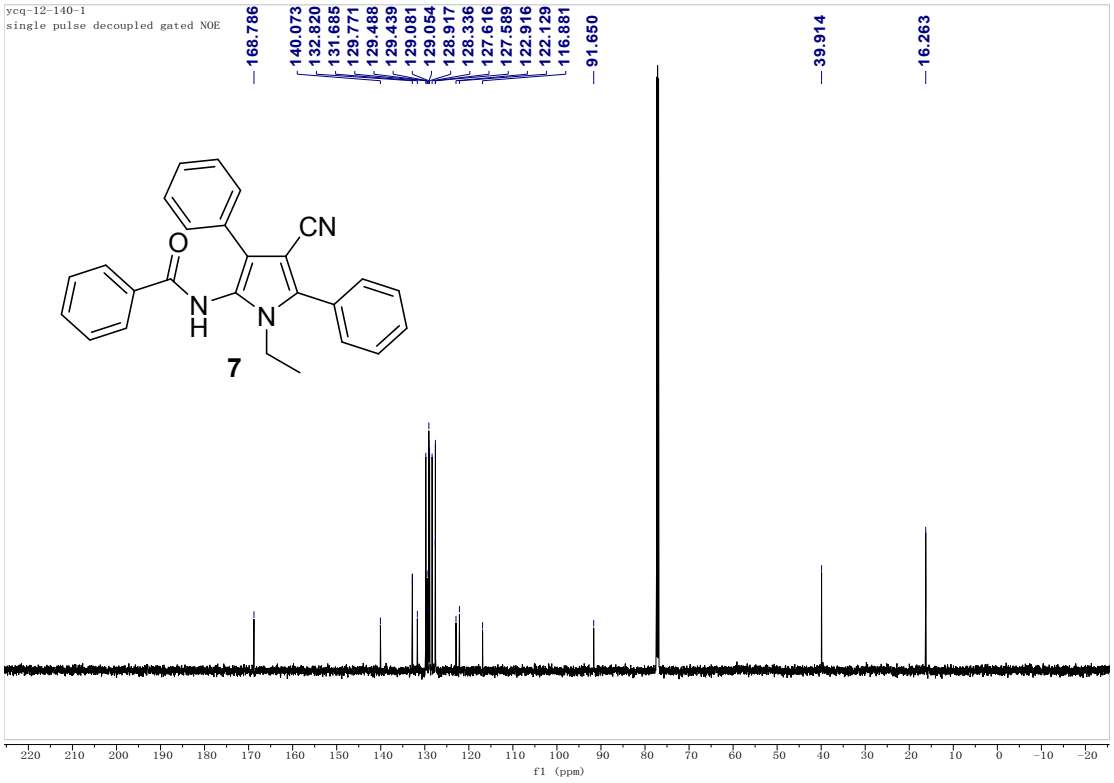

ycq-12-94-1.1.fid
CN
HN
N
Et
5l
6.02
8.05
2.00
3.00
3.08
f1 (ppm)

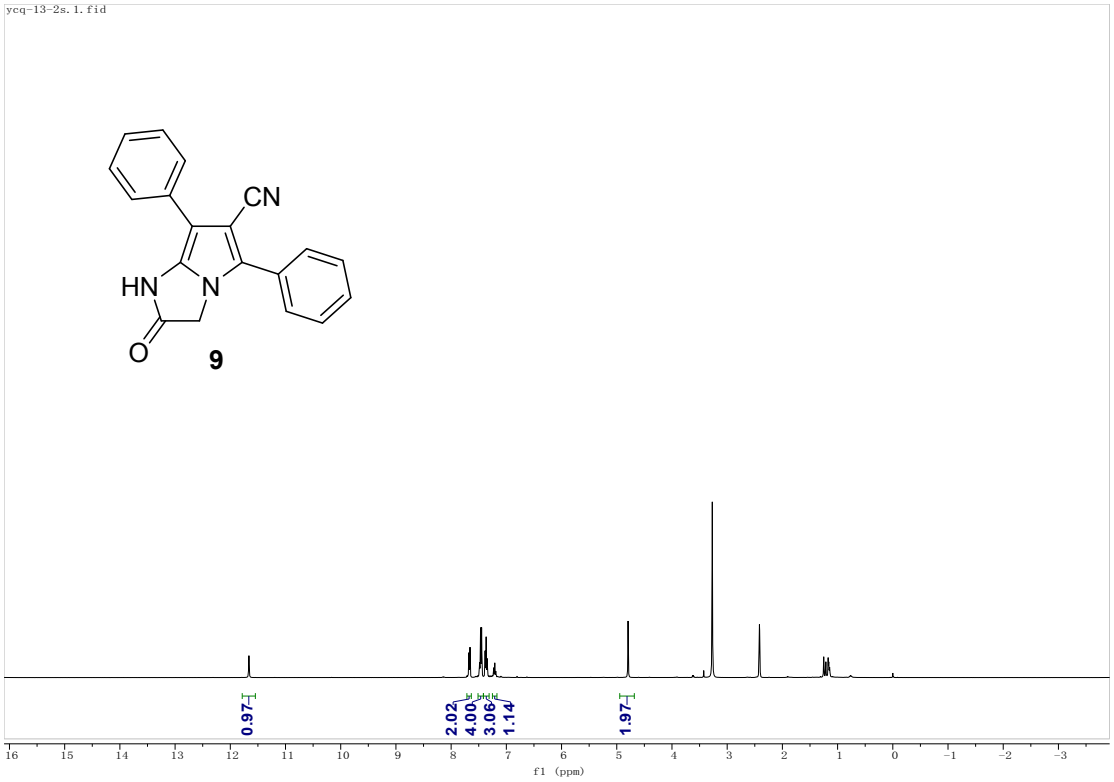

ycq-12-94-1.2.fid
172.075
159.364
141.342
140.673
129.818
129.157
128.366
127.910
127.879
125.234
117.060
92.382
64.244
37.670
21.547
13.565
CN
HN
N
Et
5l
f1 (ppm)

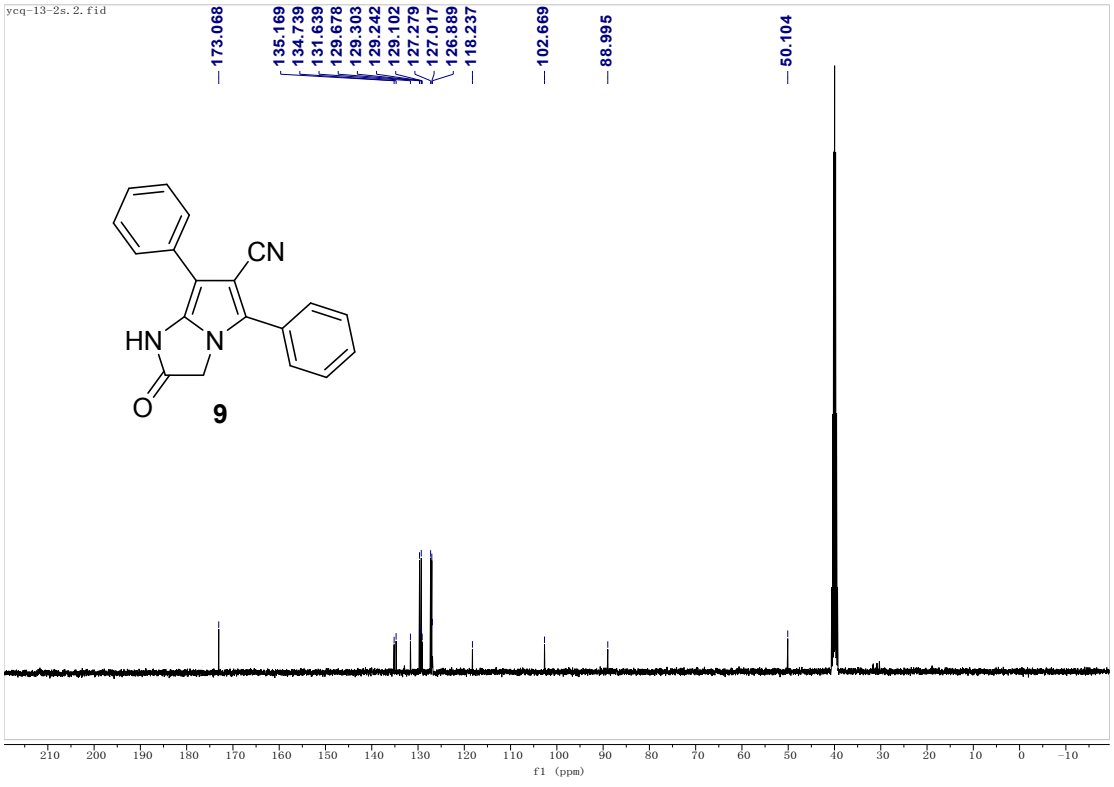

ycq-13-8-1
single_pulse
CN
O
Ph
N
N
Ph
O
6
9.07
2.04
5.08
4.11
2.00
3.06
f1 (ppm)

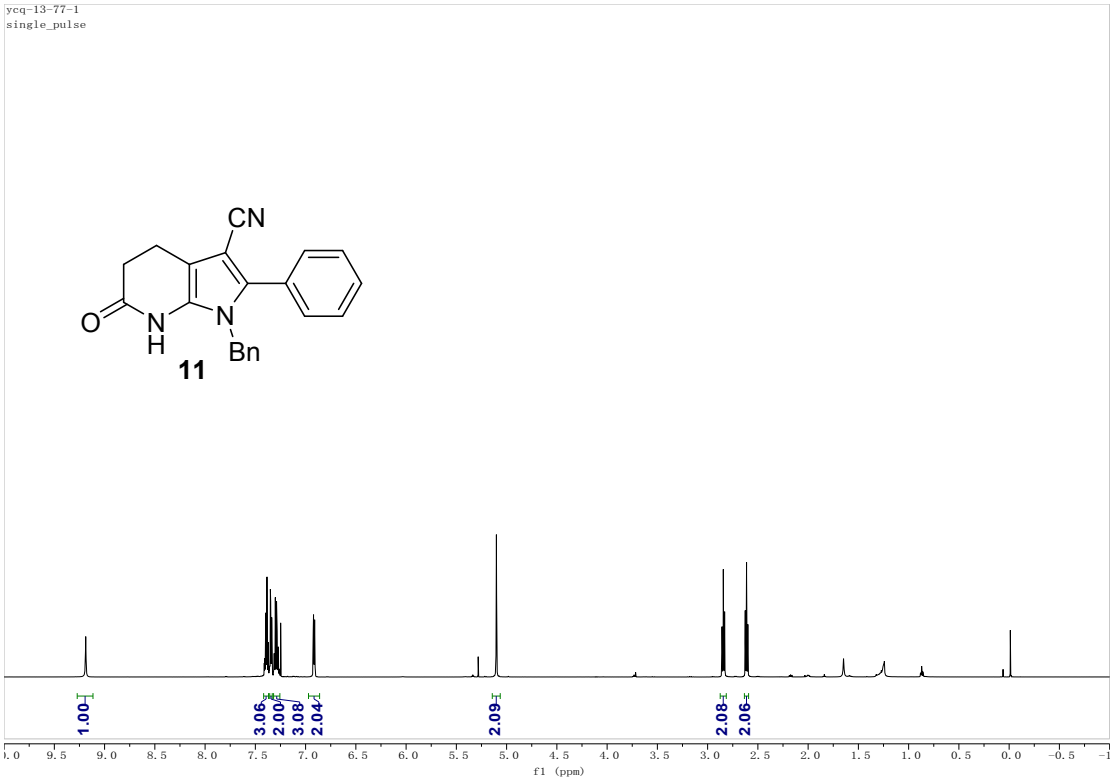

ycq-13-8-1
single pulse decoupled gated NOE
173.278
140.644
133.853
132.925
130.922
129.751
129.718
129.249
129.158
129.021
128.894
128.852
128.532
128.276
125.270
124.407
116.125
93.033
39.939
15.659
CN
O
Ph
N
N
Ph
O
6
f1 (ppm)

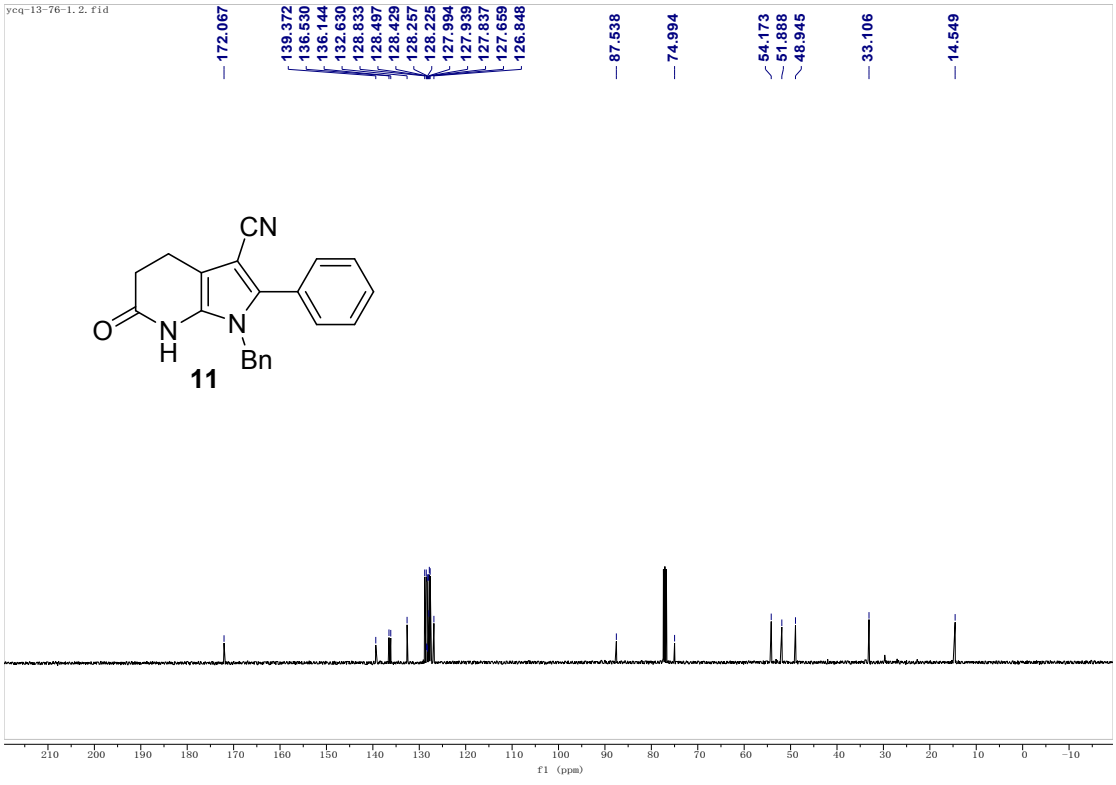

YCQ-12-140-1
single_pulse
CN
O
N
H
N
7
2.00
0.98
1.04
9.05
2.05
1.24
2.02
3.04
f1 (ppm)

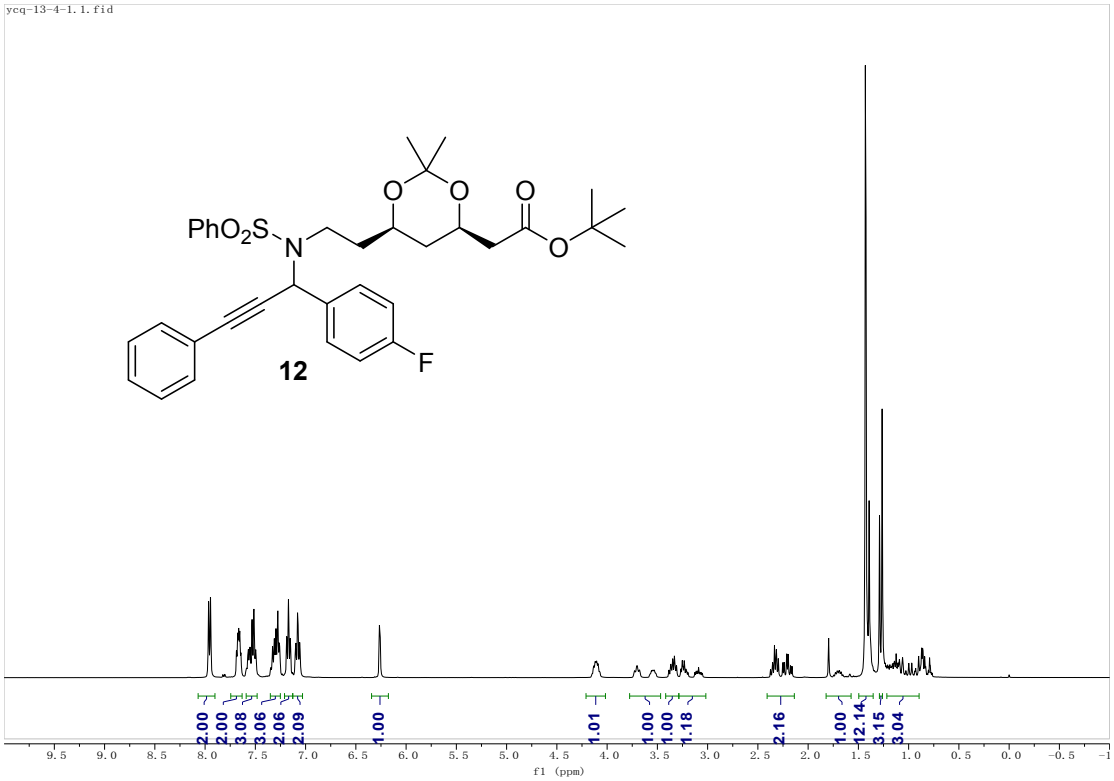

ycq-12-140-1
single pulse decoupled gated NOE
168.786
140.073
132.820
131.685
129.771
129.488
129.439
129.081
129.054
128.917
128.336
127.616
127.589
122.916
122.129
116.881
91.650
39.914
16.263
CN
O
N
H
N
7
f1 (ppm)

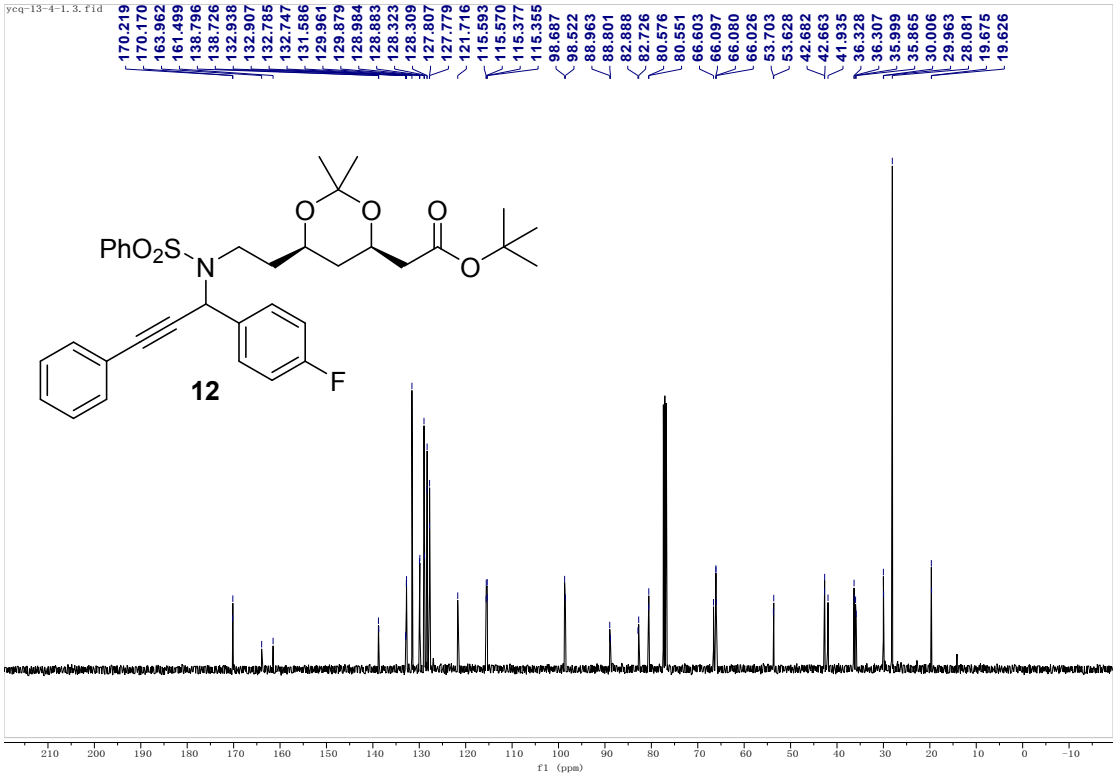

ycq-13-2s.1.fid
CN
HN
N
O
9
0.97
2.02
4.00
3.06
1.14
1.97
f1 (ppm)

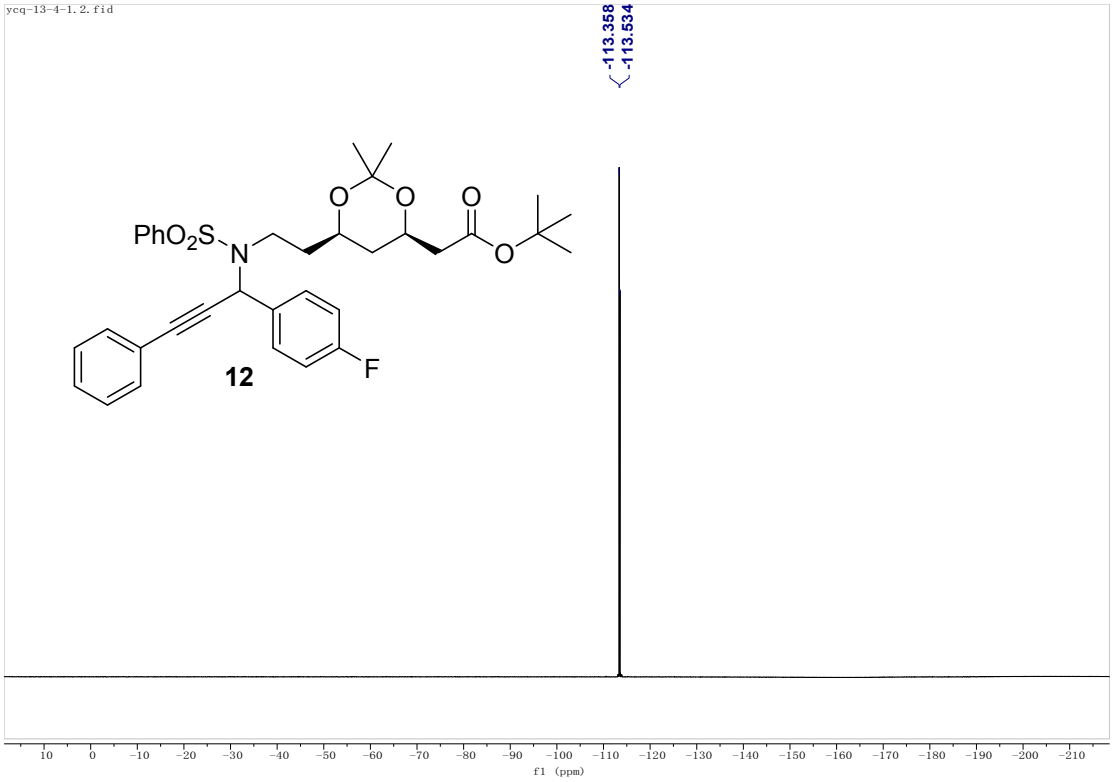

ycq-13-2s.2.fid
173.068
135.169
134.739
131.639
129.678
129.303
129.242
129.102
127.279
127.017
126.889
118.237
102.669
88.995
50.104
CN
HN
N
O
9
f1 (ppm)

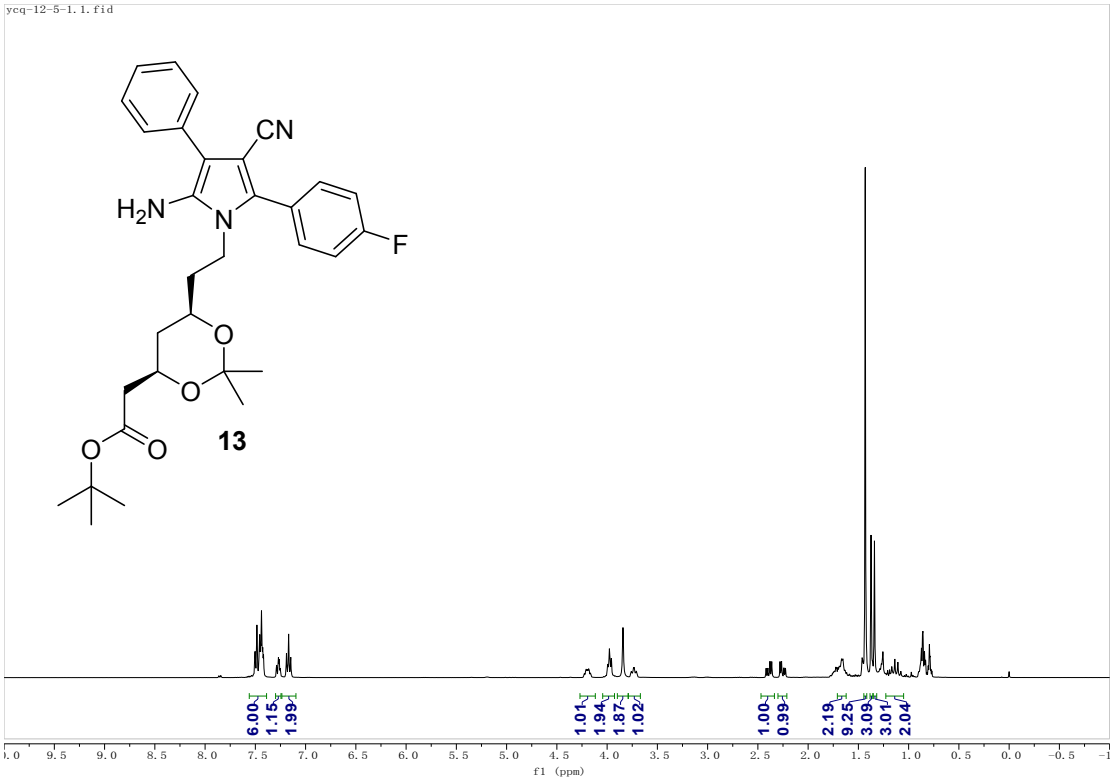

ycq-13-77-1
single_pulse
CN
O
N
H
N
Bn
11
1.00
3.06
2.00
3.08
2.04
2.09
2.08
2.06
f1 (ppm)

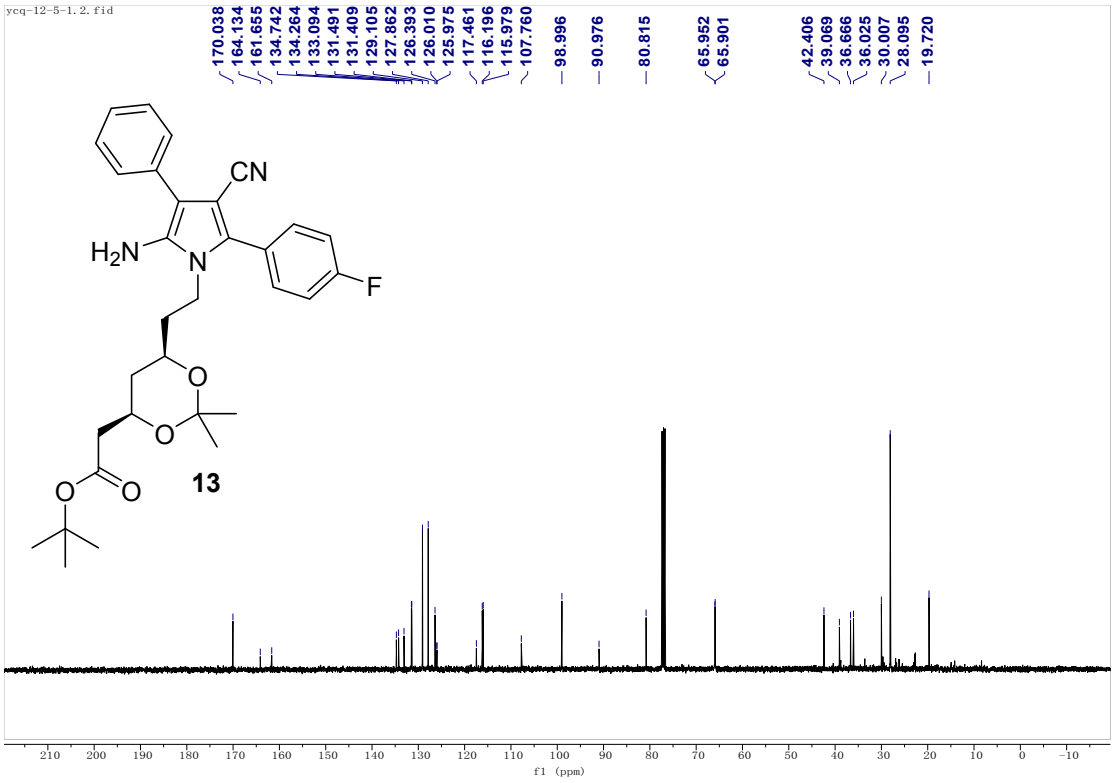

ycq-13-76-1.2.fid
172.067
139.372
136.530
136.144
132.630
128.833
128.497
128.429
128.257
128.225
127.994
127.939
127.837
127.659
126.848
87.538
74.994
54.173
51.888
48.945
33.106
14.549
CN
O
N
H
N
Bn
11
f1 (ppm)

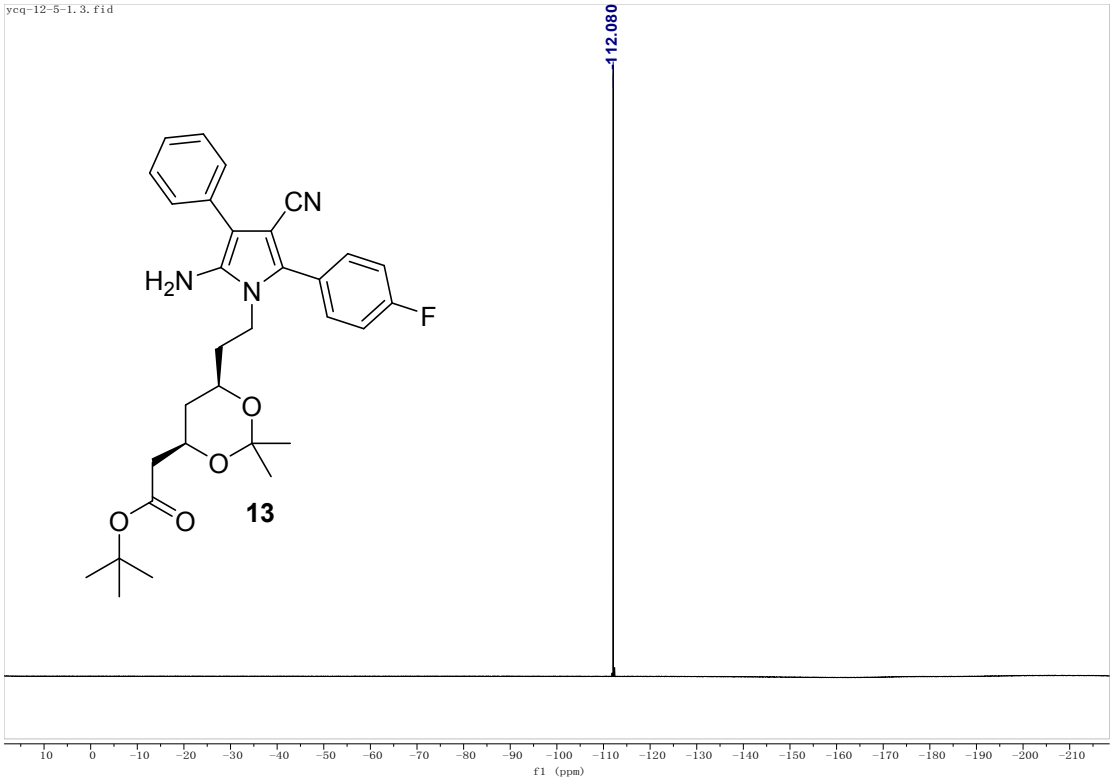

ycq-13-4-1.1.fid
PhO2S
N
O
O
O
O
F
12
2.00
2.00
3.08
3.06
2.06
2.09
1.00
1.01
1.00
1.00
1.18
2.16
1.00
12.14
3.15
3.04
f1 (ppm)

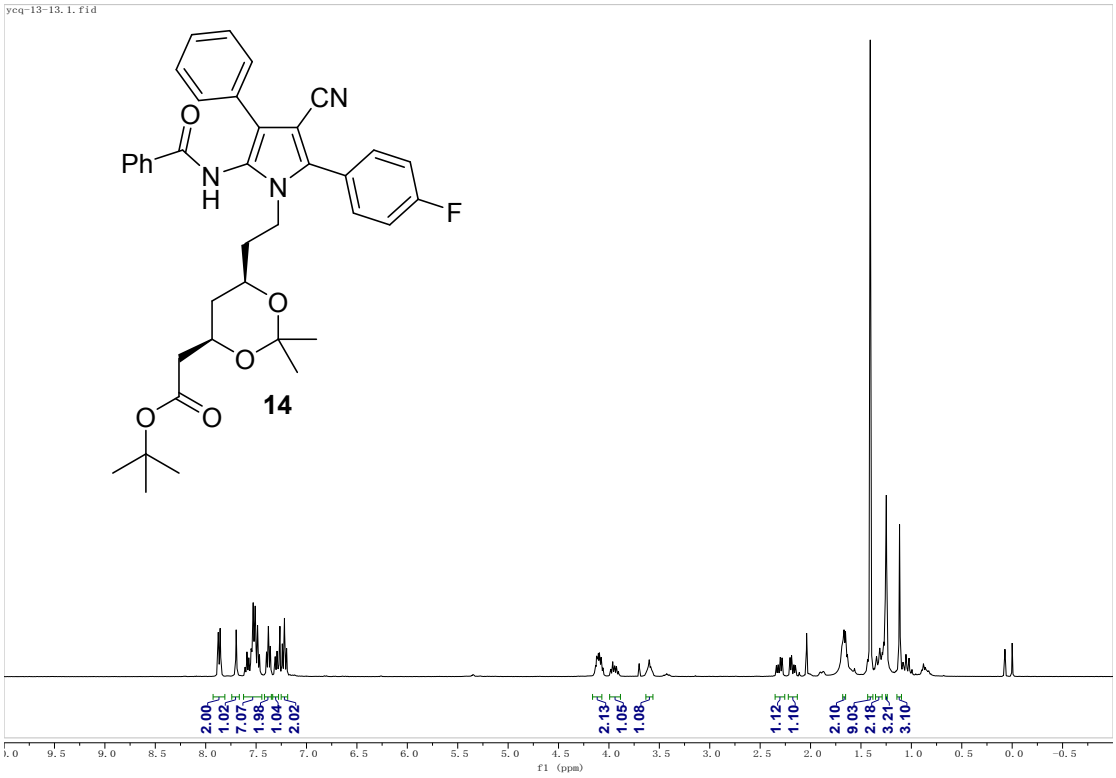

ycq-13-4-1.3.fid
170.219
170.170
163.962
161.499
138.796
138.726
132.938
132.907
132.785
132.747
131.586
129.961
129.879
128.984
128.883
128.323
128.309
127.807
127.779
121.716
115.593
115.570
115.377
115.355
98.687
98.522
88.963
88.801
82.888
82.726
80.576
80.551
66.603
66.097
66.080
66.026
53.703
53.628
42.682
42.663
41.935
36.328
36.307
35.999
35.865
30.006
29.963
28.081
19.675
19.626
PhO2S
N
O
O
O
O
F
12
f1 (ppm)

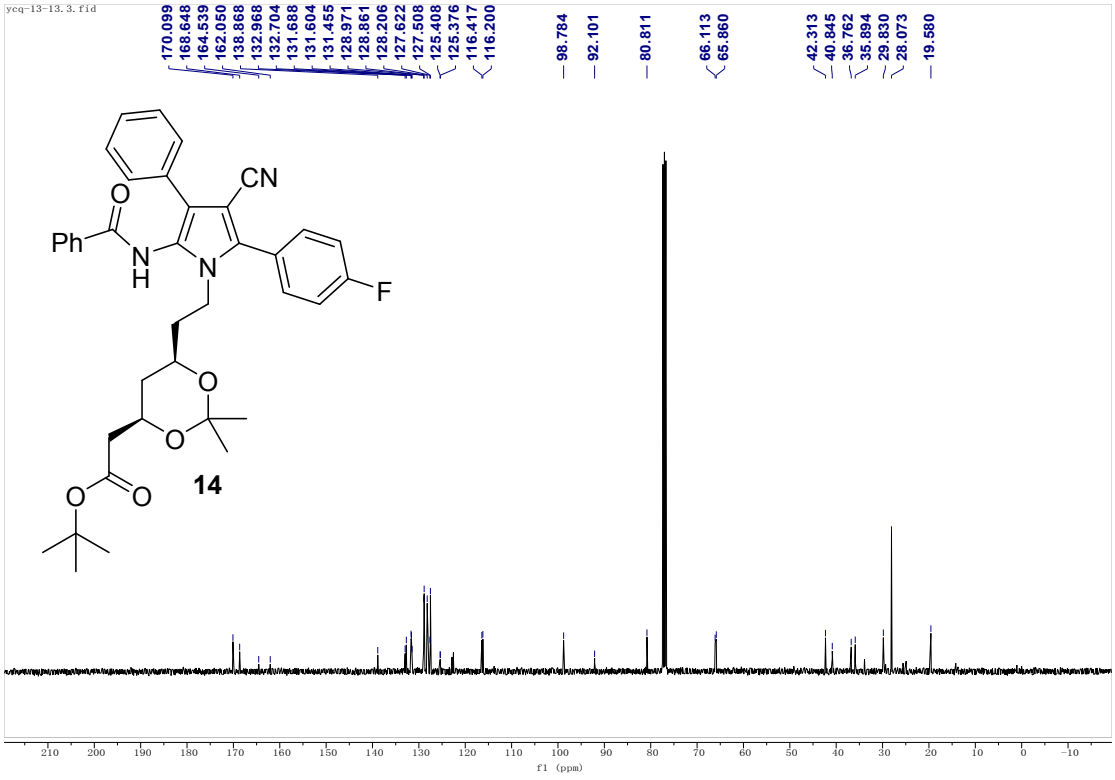

ycq-13-4-1.2.fid
-113.358
-113.534
PhO2S
N
O
O
O
O
F
12
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

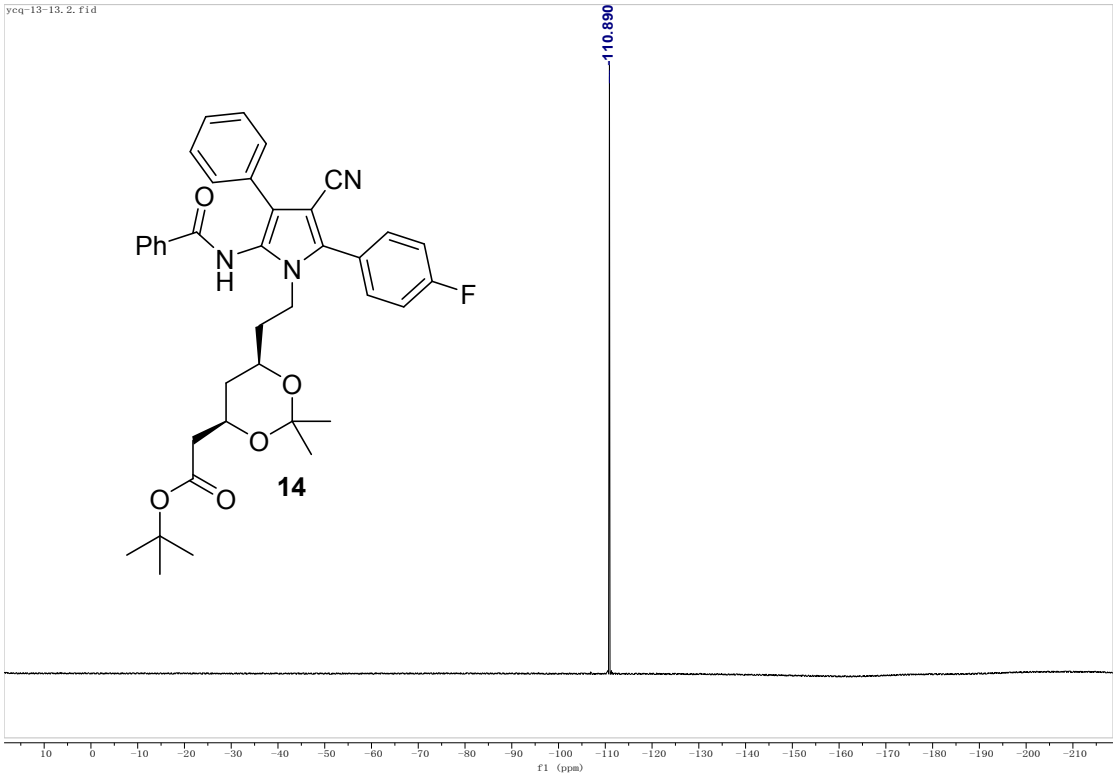

ycq-12-5-1.1.fid
CN
H_2N
N
F
O
O
O
O
13
6.00
1.15
1.99
1.01
1.94
1.87
1.02
1.00
0.99
2.19
9.25
3.09
3.01
2.04
f1 (ppm)

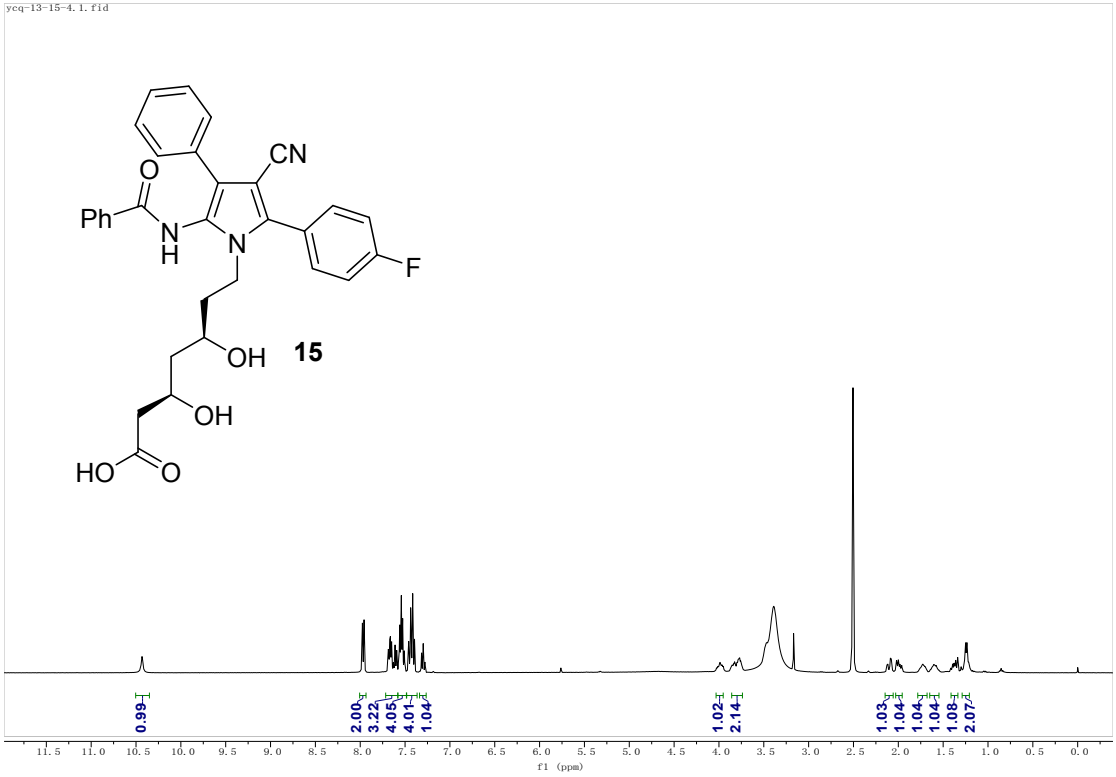

ycq-12-5-1.2.fid
170.038
164.134
161.655
134.742
134.264
133.094
131.491
131.409
129.105
127.862
126.393
126.010
125.975
117.461
116.196
115.979
107.760
98.996
90.976
80.815
65.952
65.901
42.406
39.069
36.666
36.025
30.007
28.095
19.720
CN
H_2N
N
F
O
O
O
O
13
f1 (ppm)

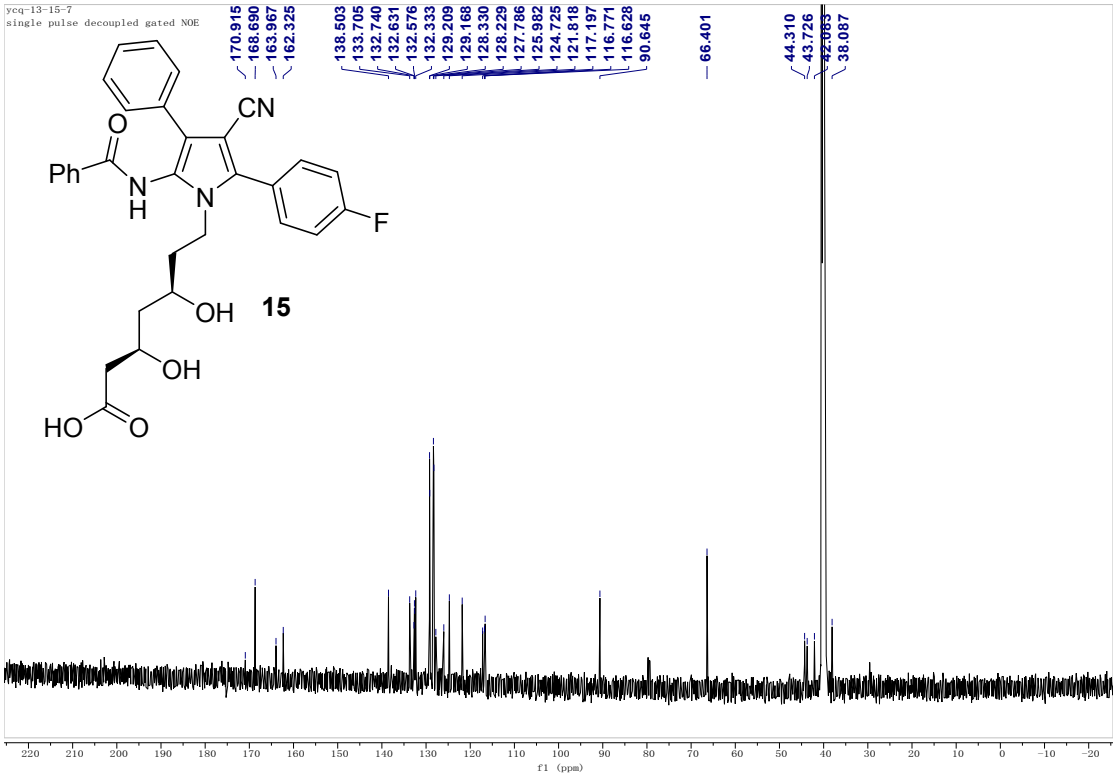

ycq-12-5-1.3.fid
112.080
CN
H2N
N
F
O
O
O
O
13
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

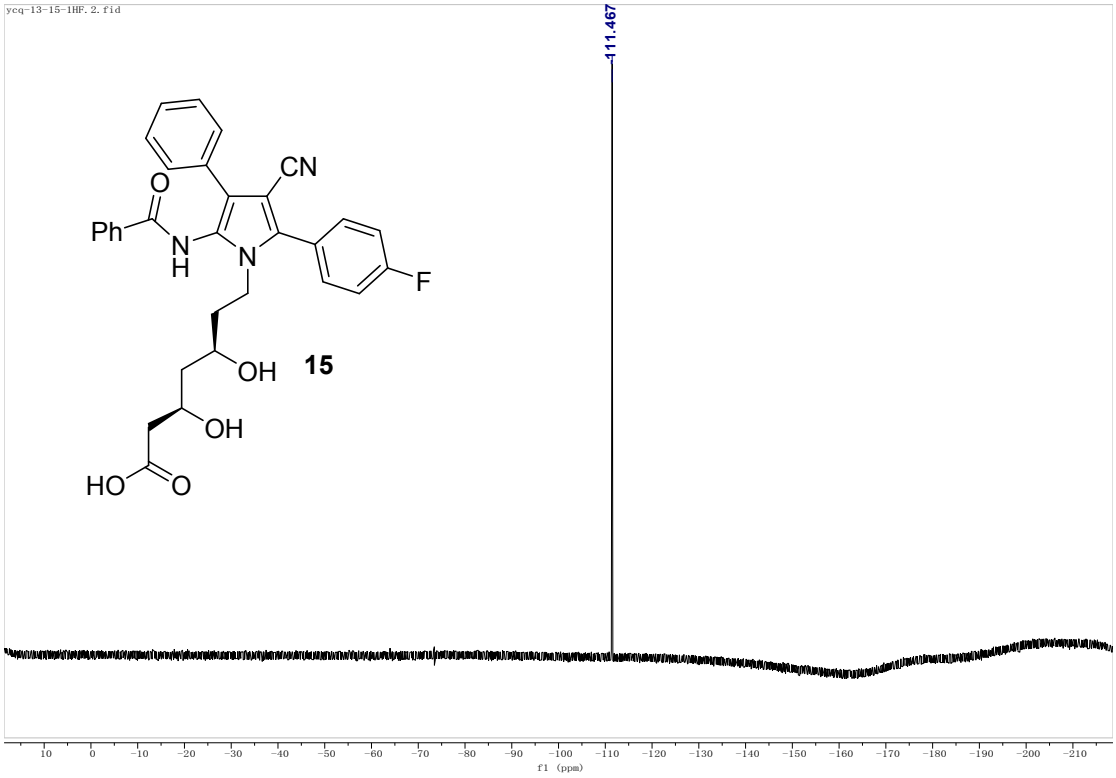

ycq-13-1.1.fid
CN
O
Ph
N
H
N
F
O
O
O
O
14
2.00
1.02
7.07
1.98
1.04
2.02
2.13
1.05
1.08
1.12
1.10
2.10
9.03
2.18
3.21
3.10
f1 (ppm)


ycq-13-3.1.fid
170.099
168.648
164.539
162.050
138.868
132.968
132.704
131.688
131.604
131.455
128.971
128.861
128.206
127.622
127.508
125.408
125.376
116.417
116.200
98.784
92.101
80.811
66.113
65.860
42.313
40.845
36.762
35.894
29.830
28.073
19.580
CN
O
Ph
N
H
N
F
O
O
O
O
14
f1 (ppm)


ycq-13-13.2.fid
110.890
CN
O
Ph
N
H
N
F
O
O
O
O
14
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)


ycq-13-15-4.1.fid
CN
O
Ph
N
H
N
F
OH
15
OH
HO
O
0.99
2.00
3.22
4.05
4.01
1.04
1.02
2.14
1.03
1.04
1.04
1.08
2.07
f1 (ppm)


ycq-13-15-7
single pulse decoupled gated NOE
170.915
168.690
163.967
162.325
138.503
133.705
132.740
132.631
132.576
132.333
129.209
129.168
128.330
128.229
127.786
125.982
124.725
121.818
117.197
116.771
116.628
90.645
66.401
44.310
43.726
42.063
38.087
CN
O
Ph
N
H
N
F
OH
15
OH
HO
O
f1 (ppm)


ycq-13-15-1HF.2.fid
111.467
CN
O
Ph
N
H
N
F
OH
OH
HO
O
15
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)