Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Copper-Catalyzed Three-component Oxycyanation of Alkenes

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Materials and methods

All reactions were carried out under an atmosphere of nitrogen in glassware with magnetic stirring unless otherwise indicated. Commercially obtained reagents were used as received. Solvents were dried by Inert PureSolv MD5. Liquids and solutions were transferred via syringe. All reactions were monitored by thin-layer chromatography. ^{1}H and ^{13}C NMR spectra were recorded on Bruker-BioSpin AVANCE III HD. Data for ^{1}H NMR spectra are reported relative to chloroform as an internal standard (7.26 ppm) 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 (77.23 ppm) and are reported in terms of chemical shift (ppm). HRMS data were recorded on Bruker Impact II UHR-TOF, Waters Micromass GCT Premier or Thermo Fisher Scientific LTQ FT Ultra. IR data were obtained from Bruker VERTEX 70. GC-MS data were recorded on Thermo ISQ QD. High performance liquid chromatography (HPLC) analysis was performed on chiral columns. Optical rotations were measured in the solvent indicated.

Synthesis of diacyl peroxides

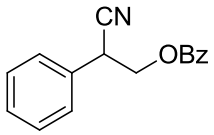
Caution: Diacyl peroxides and peresters have potentials to explode. Any diacyl peroxide involved reaction (as product or substrate) should be carried out with precautions!

Benzoyl peroxide (BPO) **2a** was purchased from Adamas. Other peroxides were prepared according to our previous work.[1]

General procedure

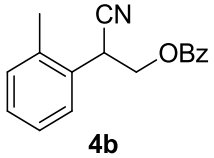
To a flame-dried Schlenk tube with a stirring bar were added $Cu(CH_3CN)_4PF_6$ (5 mol %), 1,10-Phen (7 mol %), BPO (0.75 mmol, 1.5 equiv), TFEA (0.5 mL), TMSCN (1.0 mmol, 2 equiv), and styrene (0.5 mmol, 1 equiv) sequentially under the nitrogen atmosphere. The reaction mixture was heated at 50 ^oC for 24 hours, and then was cooled to room temperature. The solvent was removed by rotary evaporation under vacuum and the residue was chromatographed on silica gel (petroleum ether/ethyl acetate = 10:1~3:1) to yield the desired product**.**

Characterization data for products



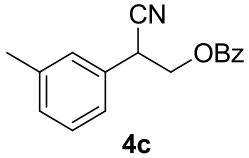
4a

Following the general procedure, product **4a** was obtained as a colorless liquid (102 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.03 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.41 (m, 6H), 7.41 – 7.37 (m, 1H), 4.67 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.52 (dd, *J* = 10.9, 8.5 Hz, 1H), 4.32 (dd, *J* = 8.5, 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.89, 133.59, 131.49, 129.82, 129.39, 129.08, 128.98, 128.57, 127.80, 118.51, 65.50, 37.58. IR (thin film): υ 2248, 1720 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{13}NNaO_2]^+$ ($[M+Na]^+$): 274.0844, found: 274.0839.



4b

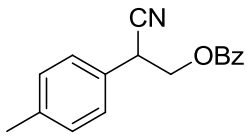
Following the general procedure, product **4b** was obtained as a yellow liquid (70 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 – 8.04 (m, 2H), 7.63 – 7.51 (m, 2H), 7.46 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.28 (dd, *J* = 5.7, 3.4 Hz, 2H), 7.251 – 7.218 (m, 1H), 4.64 (dd, *J* = 10.5, 4.8 Hz, 1H), 4.50 (dd, *J* = 9.1, 4.8 Hz, 1H), 4.42 (dd, *J* = 10.5, 9.1 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.05, 135.74, 133.62, 131.29, 129.85, 129.68, 129.12, 129.06, 128.59, 128.12, 127.11, 119.05, 64.36, 34.62, 19.16. IR (thin film): υ 2247, 1724 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0995.



4c

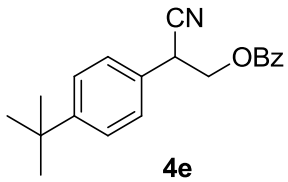
Following the general procedure, product **4c** was obtained as a yellow liquid (73 mg, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.6 Hz, 2H), 7.62 – 7.55 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.27 – 7.21 (m, 2H), 7.19 (d, *J* = 7.5 Hz, 1H), 4.64 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.49 (dd, *J* = 10.9, 8.7 Hz, 1H), 4.28 (dd, *J* = 8.7, 5.5 Hz, 1H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.90, 139.30, 133.58, 131.35, 129.83, 129.70, 129.24, 129.14, 128.56, 128.47, 124.85, 118.68,

65.57, 37.51, 21.36. IR (thin film): υ 2247, 1724 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0996.



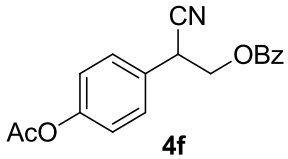
4d

Following the general procedure, product **4d** was obtained as a colorless liquid (57 mg, 43% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.66 – 7.55 (m, 1H), 7.45 (dd, *J* = 8.4, 7.2 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 4.63 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.49 (dd, *J* = 10.9, 8.5 Hz, 1H), 4.28 (dd, *J* = 8.5, 5.6 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.90, 138.91, 133.56, 130.03, 129.83, 129.15, 128.56, 128.46, 127.66, 118.72, 65.59, 37.22, 21.14. IR (thin film): υ 2247, 1724 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0995.



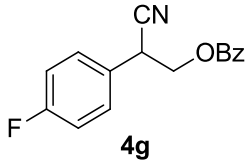
4e

Following the general procedure, product **4e** was obtained as a white solid (101 mg, 66% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 – 8.01 (m, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.51 – 7.42 (m, 4H), 7.42 – 7.37 (m, 2H), 4.67 (dd, *J* = 10.9, 5.5 Hz, 1H), 4.50 (dd, *J* = 10.9, 8.7 Hz, 1H), 4.32 (dd, *J* = 8.8, 5.5 Hz, 1H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.92, 152.12, 133.56, 129.84, 129.19, 128.57, 128.43, 127.53, 126.34, 118.75, 65.60, 37.14, 34.69, 31.26. IR (thin film): υ 2248, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{20}H_{21}NNaO_2]^+$ ($[M+Na]^+$): 330.1470, found: 330.1463.



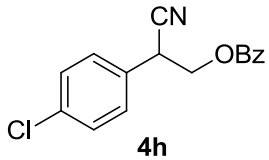
4f

Following the general procedure, product **4f** was obtained as a yellow liquid (102 mg, 66% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 7.96 (m, 2H), 7.71 – 7.54 (m, 1H), 7.484 – 7.435 (m, 4H), 7.16 (d, *J* = 8.6 Hz, 2H), 4.65 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.50 (dd, *J* = 11.0, 8.4 Hz, 1H), 4.33 (dd, *J* = 8.4, 5.6 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.19, 165.86, 151.06, 133.64, 129.82, 129.01, 128.99, 128.59, 122.65, 118.32, 65.37, 37.01, 21.10. IR (thin film): υ 2248, 1724 cm^{-1}. HRMS (ESI) calcd for $[C_{18}H_{15}NNaO_4]^+$ ($[M+Na]^+$): 332.0899, found: 332.0892.



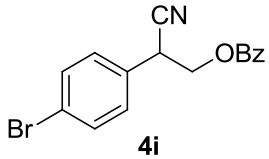
4g

Following the general procedure, product **4g** was obtained as a yellow liquid (90 mg, 67% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.52 – 7.39 (m, 4H), δ 7.12 (t, *J* = 8.5 Hz, 2H). 4.64 (dd, *J* = 11.0, 5.7 Hz, 1H), 4.51 (dd, *J* = 11.0, 8.2 Hz, 1H), 4.31 (dd, *J* = 8.2, 5.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.84, 162.91 (d, *J* = 248.9 Hz), 133.67, 129.80, 129.61 (d, *J* = 8.4 Hz), 128.95, 128.60, 127.36 (d, *J* = 3.5 Hz), 118.30, 116.47 (d, *J* = 22.0 Hz), 65.35 (d, *J* = 1.1 Hz), 36.86. IR (thin film): υ 2248, 1724 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}FNNaO_2]^+$ ($[M+Na]^+$): 292.0750, found: 292.0744.



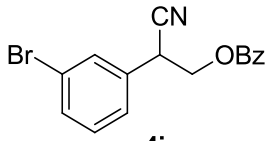
4h

Following the general procedure, product **4h** was obtained as a colorless liquid (88 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.45 (dd, *J* = 8.4, 7.2 Hz, 2H), 7.41-7.37 (m, 4H), 4.63 (dd, *J* = 10.9, 5.7 Hz, 1H), 4.51 (dd, *J* = 10.9, 8.0 Hz, 1H), 4.30 (dd, *J* = 8.0, 5.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.79, 135.09, 133.69, 130.11, 129.80, 129.60, 129.18, 128.93, 128.62, 118.12, 65.20, 36.97. IR (thin film): υ 2248, 1723 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}ClNNaO_2]^+$ ($[M+Na]^+$): 308.0454, found: 308.0451.



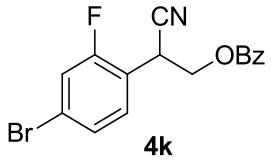
4i

Following the general procedure, product **4i** was obtained as a yellow liquid (87 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.93 (m, 2H), 7.57 – 7.45 (m, 3H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 4.56 (dd, *J* = 11.0, 5.7 Hz, 1H), 4.44 (dd, *J* = 10.9, 8.0 Hz, 1H), 4.21 (dd, *J* = 8.0, 5.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.81, 133.70, 132.58, 130.59, 129.81, 129.45, 128.90, 128.62, 123.22, 118.00, 65.12, 37.07. IR (thin film): υ 2248, 1723 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}BrNNaO_2]^+$ ($[M+Na]^+$): 351.9949, found: 351.9944.



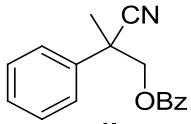
4j

Following the general procedure, product **4j** was obtained as a yellow liquid (105 mg, 64% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 8.01 (m, 2H), 7.68 – 7.57 (m, 2H), 7.551 – 7.524 (m, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.4415 – 7.388 (m, 1H), 7.31 (t, *J* = 7.9 Hz, 1H), 4.66 (dd, *J* = 10.9, 5.7 Hz, 1H), 4.52 (dd, *J* = 10.9, 8.2 Hz, 1H), 4.30 (dd, *J* = 8.2, 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.80, 133.70, 133.64, 132.25, 130.98, 130.89, 129.82, 128.89, 128.62, 126.43, 123.33, 117.85, 65.16, 37.11. IR (thin film): υ 2248, 1721 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}BrNNaO_2]^+$ ($[M+Na]^+$): 351.9949, found: 351.9945.



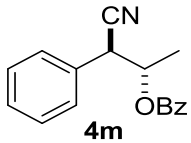
4k

Following the general procedure, product **4k** was obtained as a yellow liquid (97 mg, 56% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.63 – 7.55 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 3H), 7.38 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.32 (dd, *J* = 9.5, 1.9 Hz, 1H), 4.66 – 4.54 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.62, 159.73 (d, *J* = 253.4 Hz), 133.67, 130.67 (d, *J* = 3.5 Hz), 129.78, 128.86, 128.60, 128.47 (d, *J* = 3.7 Hz), 123.74 (d, *J* = 9.5 Hz), 119.83 (d, *J* = 24.4 Hz), 118.40 (d, *J* = 14.2 Hz), 117.15, 63.60 (d, *J* = 1.5 Hz), 31.35 (d, *J* = 2.9 Hz). IR (thin film): υ 2251, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}FBrNNaO_2]^+$ ($[M+Na]^+$): 369.9855, found: 369.9848.



4l

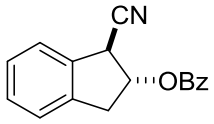
Following the general procedure, product **4l** was obtained as a yellow liquid (70 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.87 (m, 2H), 7.53 – 7.43 (m, 3H), 7.38 – 7.30 (m, 4H), 7.30 – 7.23 (m, 1H), 4.47 (d, *J* = 1.4 Hz, 2H), 1.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.71, 136.71, 133.51, 129.79, 129.20, 129.15, 128.68, 128.56, 125.94, 121.64, 69.58, 42.59, 23.63. IR (thin film): υ 2241, 1726 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0994.



4m

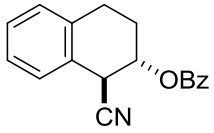
Following the general procedure, product **4m** was obtained as a yellow liquid (70 mg, 53% yield, dr = 1:1 as detected by GC-MS and one of the isomer was lost during separation). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 – 8.05 (m, 2H), 7.64 – 7.57 (m, 1H), 7.50 – 7.35 (m, 7H), 5.37 (qd, *J* = 6.4, 4.7 Hz, 1H), 4.44 (d, *J* = 4.7 Hz, 1H), 1.43 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (100

MHz, $CDCl_3$) δ 165.24, 133.39, 131.98, 129.73, 129.45, 129.10, 128.77, 128.50, 128.26, 118.08, 71.36, 43.67, 18.35. IR (thin film): υ 2318, 1721 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0994.



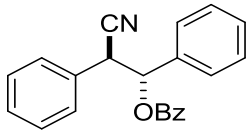
4n

Following the general procedure, product **4n** was obtained as a yellow liquid (67 mg, 51% yield, dr > 20:1 as detected by GC-MS). ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.91 (m, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.40 – 7.31 (m, 3H), 7.26 – 7.16 (m, 3H), 5.80 (dt, *J* = 7.3, 5.7 Hz, 1H), 4.30 (d, *J* = 5.7 Hz, 1H), 3.58 (dd, *J* = 16.6, 7.2 Hz, 1H), 3.05 (dd, *J* = 16.6, 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.77, 138.21, 133.28, 132.53, 128.74, 128.38, 128.08, 127.47, 127.04, 124.25, 123.57, 117.57, 76.82, 40.24, 37.07. IR (thin film): υ 2243, 1722 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{13}NNaO_2]^+$ ($[M+Na]^+$): 286.0844, found: 286.0837.



4o

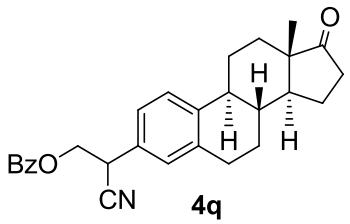
Following the general procedure, product **4o** was obtained as a yellow liquid (60 mg, 43% yield, dr = 5:1 as detected by ^1H NMR). ^1H NMR (400 MHz, $CDCl_3$, major and minor) δ 8.16 – 8.06 (m, 0.17H), 8.07 – 7.98 (m, 1.99H), 7.66 – 7.52 (m, 1.09H), 7.48 – 7.38 (m, 3.25H), 7.34 – 7.10 (m, 3.55H), 5.70 – 5.56 (m, 1H), 5.45 (ddd, *J* = 10.4, 5.3, 3.3 Hz, 0.08H), 4.30 (d, *J* = 7.0 Hz, 0.99H), 4.11 (q, *J* = 7.1 Hz, 0.06H), 3.21 – 2.97 (m, 2.23H), 2.464 – 2.391 (m, 1.08H), 2.14 – 1.97 (m, 1.12H). ^{13}C NMR (100 MHz, $CDCl_3$, major and minor) δ 165.53, 135.08, 133.51, 129.92, 129.78, 129.56, 129.49, 129.31, 129.02, 128.78, 128.53, 127.53, 127.10, 119.14, 70.63, 36.64, 26.63, 25.95. IR (thin film): υ 2251, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{18}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 300.1000, found: 300.0996.



4p

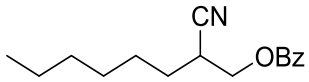
Following the general procedure, product **4p** was obtained as a yellow liquid (49 mg, 30% yield, dr = 2:1 as detected by GC-MS). ^1H NMR (400 MHz, $CDCl_3$) δ 8.11 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.64 – 7.55 (m, 1H), 7.47 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.36 – 7.32 (m, 5H), 7.31 – 7.28 (m, 3H), 7.32 – 7.22 (m, 2H), 6.24 (d, *J* = 5.7 Hz, 1H), 4.34 (d, *J* = 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.80, 136.33, 133.60, 131.69, 129.86, 129.23, 129.12, 128.99, 128.81, 128.71, 128.63, 128.47, 126.58, 117.92, 76.63, 45.15.

IR (thin film): υ 2318, 1724 cm^{-1}. HRMS (ESI) calcd for $[C_{22}H_{17}NNaO_2]^+$ ($[M+Na]^+$): 350.1157, found: 350.1151.



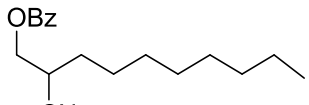
4q

Following the general procedure, 5 mol % of Hantzsch ester (diethyl 1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate) was added and product **4q** was obtained as a yellow liquid (98 mg, 46% yield, dr = 1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.02 (m, 2H), 7.64 – 7.55 (m, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.25 – 7.16 (m, 2H), 4.64 (dd, *J* = 10.7, 5.4 Hz, 1H), 4.48 (dd, *J* = 10.9, 8.7 Hz, 1H), 4.26 (dd, *J* = 8.7, 5.5 Hz, 1H), 2.97 – 2.89 (m, 2H), 2.51 (dd, *J* = 18.7, 8.7 Hz, 1H), 2.448 – 2.397 (m, 1H), 2.30 (td, *J* = 10.7, 4.3 Hz, 1H), 2.22 – 2.10 (m, 1H), 2.11 – 1.99 (m, 2H), 2.02 – 1.92 (m, 1H), 1.69 – 1.57 (m, 2H), 1.60 – 1.40 (m, 4H), 0.91 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.91, 140.73, 137.83, 133.58, 129.83, 129.14, 128.81, 128.56, 128.32, 126.40, 125.12, 118.72, 65.58, 50.47, 47.93, 44.28, 37.95, 37.16, 35.84, 31.55, 29.34, 26.30, 25.67, 21.59, 13.84. IR (thin film): υ 2246, 1727 cm^{-1}. HRMS (ESI) calcd for $[C_{28}H_{29}NNaO_3]^+$ ($[M+Na]^+$): 450.2054, found: 450.2039.



6a

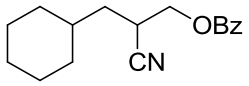
Following the general procedure, product **6a** was obtained as a colorless liquid (52 mg, 40% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.63 – 7.56 (m, 1H), 7.46 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.47 (dd, *J* = 11.0, 5.4 Hz, 1H), 4.38 (dd, *J* = 11.0, 7.5 Hz, 1H), 3.04 (ddt, *J* = 9.1, 7.5, 5.5 Hz, 1H), 1.81 – 1.45 (m, 4H), 1.41 – 1.25 (m, 6H), 0.92 – 0.85 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.97, 133.51, 129.79, 129.20, 128.54, 119.79, 63.60, 31.75, 31.45, 28.94, 28.68, 26.87, 22.49, 14.01. IR (thin film): υ 2244, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{21}NNaO_2]^+$ ($[M+Na]^+$): 282.1470, found: 282.1464.



6b

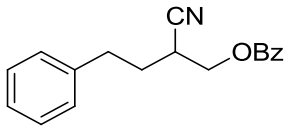
Following the general procedure, product **6b** was obtained as a colorless liquid (64.6 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.05 (m, 2H), 7.62 – 7.56 (m, 1H), 7.46 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.47 (dd, *J* = 11.0, 5.4 Hz, 1H), 4.38 (dd, *J* = 11.0, 7.5 Hz, 1H), 3.08 – 2.99 (m, 1H), 1.82 – 1.67 (m, 2H), 1.66 – 1.56 (m, 1H), 1.56 – 1.45 (m, 1H), 1.40 – 1.22 (m, 10H), 0.93 – 0.85 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.97, 133.51, 129.79, 129.20, 128.54, 119.79, 63.59, 31.79, 31.76, 29.24, 29.13,

29.03, 28.95, 26.91, 22.63, 14.09. IR (thin film): υ 2245, 1726 cm^{-1}. HRMS (ESI) calcd for $[C_{18}H_{25}NNaO_2]^+$ ($[M+Na]^+$): 310.1783, found: 310.1778.



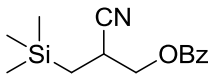
6c

Following the general procedure, product **6c** was obtained as a colorless liquid (46 mg, 34% yield). ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 – 7.98 (m, 2H), 7.73 – 7.55 (m, 1H), 7.47 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.47 (dd, *J* = 10.9, 5.3 Hz, 1H), 4.35 (dd, *J* = 11.0, 7.6 Hz, 1H), 3.17 – 3.08 (m, 1H), 1.89 – 1.65 (m, 6H), 1.53 – 1.44 (m, 1H), 1.36 – 1.23 (m, 3H), 1.22 – 1.08 (m, 1H), 1.06 – 0.80 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.99, 133.51, 129.80, 129.20, 128.54, 119.98, 63.96, 36.32, 35.18, 33.44, 32.30, 29.28, 26.26, 25.97, 25.85. IR (thin film): υ 2244, 1724 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{21}NNaO_2]^+$ ($[M+Na]^+$): 294.1470, found: 294.1466.



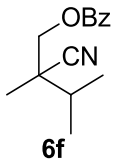
6d

Following the general procedure, product **6d** was obtained as a colorless liquid (46 mg, 33% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 7.91 (m, 2H), 7.66 – 7.54 (m, 1H), 7.45 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.32 (dd, *J* = 7.9, 6.6 Hz, 2H), 7.26 – 7.19 (m, 3H), 4.55 – 4.24 (m, 2H), 3.02 – 2.92 (m, 2H), 2.81 (dt, *J* = 14.0, 8.2 Hz, 1H), 2.19 – 2.06 (m, 1H), 2.06 – 1.94 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.91, 139.48, 133.56, 129.81, 129.12, 128.81, 128.57, 128.45, 126.70, 119.48, 63.43, 32.89, 31.06, 30.65. IR (thin film): υ 2244, 1722 cm^{-1}. HRMS (ESI) calcd for $[C_{18}H_{17}NNaO_2]^+$ ($[M+Na]^+$): 302.1157, found: 302.1151.



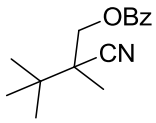
6e

Following the general procedure, product **6e** was obtained as a yellow liquid (39 mg, 30% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 8.05 (m, 2H), 7.62 – 7.56 (m, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 4.45 (dd, *J* = 10.9, 5.2 Hz, 1H), 4.30 (dd, *J* = 10.8, 8.4 Hz, 1H), 3.11 – 3.02 (m, 1H), 1.05 (dd, *J* = 14.7, 10.6 Hz, 1H), 0.89 (dd, *J* = 14.7, 5.2 Hz, 1H), 0.16 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.35, 134.85, 131.16, 129.89, 122.26, 67.36, 28.81, 17.86, 0.01. IR (thin film): υ 2243, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{14}H_{19}NNaO_2Si]^+$ ($[M+Na]^+$): 284.1083, found: 284.1078.



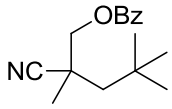
6f

Following the general procedure, product **6f** was obtained as a yellow liquid (45 mg, 39% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 – 8.04 (m, 2H), 7.64 – 7.55 (m, 1H), 7.47 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.42 (d, *J* = 11.1 Hz, 1H), 4.32 (d, *J* = 11.0 Hz, 1H), 2.03 (p, *J* = 6.8 Hz, 1H), 1.41 (s, 3H), 1.17 (d, *J* = 6.8 Hz, 3H), 1.09 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.91, 133.48, 129.76, 129.30, 128.56, 121.85, 67.12, 41.69, 32.74, 18.77, 18.37, 17.39. IR (thin film): υ 2237, 1726 cm^{-1}. HRMS (ESI) calcd for $[C_{14}H_{17}NNaO_2]^+$ ([M+Na]$^+$): 254.1157, found: 254.1150.



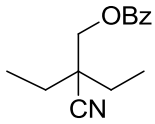
6g

Following the general procedure, product **6g** was obtained as a yellow liquid (63.7 mg, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 8.05 (m, 2H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.47 (dd, *J* = 8.3, 7.0 Hz, 2H), 4.50 (d, *J* = 10.9 Hz, 1H), 4.32 (d, *J* = 10.9 Hz, 1H), 1.45 (s, 3H), 1.16 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.15, 133.45, 129.78, 129.36, 128.56, 122.04, 66.14, 45.11, 35.27, 26.03, 17.98. IR (thin film): υ 2236, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{15}H_{19}NNaO_2]^+$ ([M+Na]$^+$): 268.1313, found: 268.1309.



6h

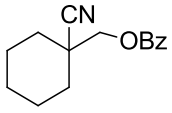
Following the general procedure, product **6h** was obtained as a yellow liquid (58 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.06 (m, 2H), 7.65 – 7.56 (m, 1H), 7.47 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.39 (d, *J* = 10.9 Hz, 1H), 4.23 (d, *J* = 10.9 Hz, 1H), 1.77 (d, *J* = 14.6 Hz, 1H), 1.54 (d, *J* = 14.7 Hz, 1H), 1.54 (s, 3H), 1.15 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.86, 133.49, 129.77, 129.29, 128.58, 122.90, 69.62, 48.72, 35.56, 31.58, 30.86, 24.26. IR (thin film): υ 2237, 1726 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{21}NNaO_2]^+$ ([M+Na]$^+$): 282.1470, found: 282.1464.



6i

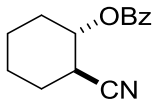
Following the general procedure, product **6i** was obtained as a yellow liquid (46 mg, 40% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 8.03 (m, 2H), 7.63 – 7.56 (m, 1H),

7.47 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.37 (s, 2H), 1.78 (d, *J* = 7.6 Hz, 4H), 1.11 (t, *J* = 7.5 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.87, 133.48, 129.74, 129.30, 128.56, 121.41, 65.55, 42.49, 26.92, 8.78. IR (thin film): υ 2238, 1726 cm^{-1}. HRMS (ESI) calcd for $[C_{14}H_{17}NNaO_2]^+$ ($[M+Na]^+$): 254.1157, found: 254.1152.



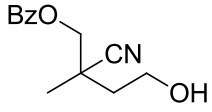
6j

Following the general procedure, product **6j** was obtained as a white liquid (74 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 – 8.01 (m, 2H), 7.63 – 7.54 (m, 1H), 7.46 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.31 (s, 2H), 2.10 (dd, *J* = 12.8, 2.1 Hz, 2H), 1.79 – 1.75 (m, 3H), 1.74 – 1.59 (m, 2H), 1.40 (td, *J* = 13.0, 3.5 Hz, 2H), 1.30 – 1.16 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.92, 133.45, 129.78, 129.31, 128.53, 121.64, 69.07, 39.60, 32.48, 25.23, 22.40. IR (thin film): υ 2237, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{15}H_{17}NNaO_2]^+$ ($[M+Na]^+$): 266.1157, found: 266.1152.



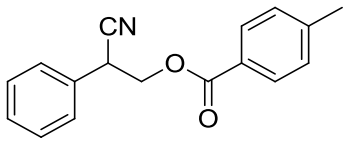
6k

Following the general procedure, product **6k** was obtained as a colorless liquid (73 mg, 64% yield, dr > 20:1 as detected by GC-MS). ^{1}H NMR (400 MHz, $CDCl_3$, major and minor) δ 8.10 – 8.02 (m, 2H), 7.62 – 7.52 (m, 1H), 7.49 – 7.40 (m, 2H), 5.17 – 5.00 (m, 1H), 3.27 (q, *J* = 4.1 Hz, 0.32H), 2.87 (td, *J* = 9.2, 4.0 Hz, 0.69H), 2.26 – 2.05 (m, 1.56H), 2.00 – 1.90 (m, 0.64H), 1.89 – 1.73 (m, 2.77H), 1.66 (tq, *J* = 7.7, 3.5 Hz, 0.72H), 1.58 – 1.32 (m, 2.49H), 0.93 – 0.79 (m, 0.36H). ^{13}C NMR (100 MHz, $CDCl_3$, major and minor) δ 165.50, 165.37, 133.39, 133.31, 129.80, 129.74, 129.72, 129.64, 119.88, 119.29, 71.86, 70.72, 33.60, 33.29, 30.16, 28.33, 27.70, 27.29, 23.48, 23.06, 22.65, 21.67. IR (thin film): υ 2243, 1721 cm^{-1}. HRMS (ESI) calcd for $[C_{14}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 252.1000, found: 252.0995.



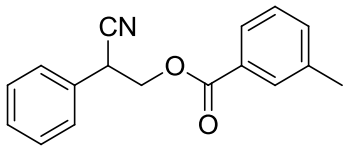
6l

Following the general procedure, product **6l** was obtained as a colorless liquid (55 mg, 47% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 8.05 (m, 2H), 7.62 – 7.55 (m, 1H), 7.46 (dd, *J* = 8.4, 7.1 Hz, 2H), 4.44 (d, *J* = 11.0 Hz, 1H), 4.33 (d, *J* = 11.0 Hz, 1H), 4.00 – 3.90 (m, 1H), 2.05 (dt, *J* = 14.3, 6.5 Hz, 2H), 1.89 (dt, *J* = 14.2, 6.3 Hz, 1H), 1.52 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.91, 133.58, 129.78, 129.17, 128.60, 122.07, 68.48, 58.93, 38.43, 36.10, 22.17. IR (thin film): υ 2240, 1724, 1274 cm^{-1}. HRMS (ESI) calcd for $[C_{13}H_{15}NNaO_3]^+$ ($[M+Na]^+$): 256.0950, found: 256.0945.



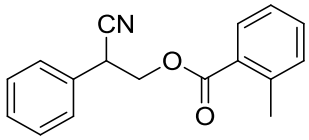
7a

Following the general procedure, product **7a** was obtained as a colorless liquid (89 mg, 67% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.92 (m, 2H), 7.50 – 7.34 (m, 5H), 7.32 – 7.21 (m, 2H), 4.64 (dd, *J* = 10.9, 5.7 Hz, 1H), 4.50 (dd, *J* = 10.9, 8.5 Hz, 1H), 4.31 (dd, *J* = 8.5, 5.6 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.94, 144.42, 131.58, 129.86, 129.36, 129.28, 128.93, 127.81, 126.33, 118.57, 65.36, 37.60, 21.75. IR (thin film): υ 2248, 1721 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0994.



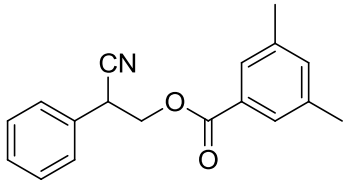
7b

Following the general procedure, product **7b** was obtained as a colorless liquid (86 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 6.8, 1.5 Hz, 2H), 7.49 – 7.36 (m, 6H), 7.38 – 7.29 (m, 1H), 4.64 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.51 (dd, *J* = 10.9, 8.6 Hz, 1H), 4.32 (dd, *J* = 8.6, 5.6 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.07, 138.40, 134.37, 131.54, 130.33, 129.38, 129.01, 128.96, 128.46, 127.81, 126.97, 118.57, 65.47, 37.58, 21.30. IR (thin film): υ 2248, 1721 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0996.



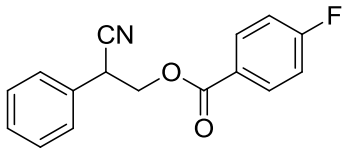
7c

Following the general procedure, product **7c** was obtained as a colorless liquid (58 mg, 44% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.47 – 7.35 (m, 6H), 7.29 – 7.22 (m, 2H), 4.63 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.50 (dd, *J* = 10.9, 8.5 Hz, 1H), 4.31 (dd, *J* = 8.5, 5.6 Hz, 1H), 2.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.64, 140.82, 132.66, 131.86, 131.56, 130.93, 129.38, 128.95, 128.28, 127.81, 125.93, 118.65, 65.39, 37.55, 21.86. IR (thin film): υ 2248, 1723 cm^{-1}. HRMS (ESI) calcd for $[C_{17}H_{15}NNaO_2]^+$ ($[M+Na]^+$): 288.1000, found: 288.0992.



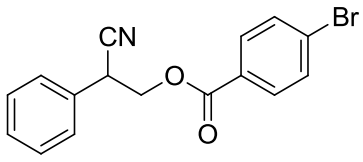
7d

Following the general procedure, product **7d** was obtained as a colorless liquid (85 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 1.6 Hz, 2H), 7.50 – 7.37 (m, 5H), 7.23 (s, 1H), 4.64 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.51 (dd, *J* = 10.9, 8.7 Hz, 1H), 4.32 (dd, *J* = 8.7, 5.6 Hz, 1H), 2.37 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.26, 138.24, 135.27, 131.56, 129.37, 128.95, 127.82, 127.53, 118.61, 65.45, 37.59, 21.19. IR (thin film): 2248, 1720 cm^{-1}. IR (thin film): υ 2248, 1723 cm^{-1}. HRMS (ESI) calcd for $[C_{18}H_{17}NNaO_2]^+$ ($[M+Na]^+$): 302.1157, found: 302.1152.



7e

Following the general procedure, product **7e** was obtained as a colorless liquid (102 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 – 8.03 (m, 2H), 7.50 – 7.35 (m, 5H), 7.13 (t, *J* = 8.6 Hz, 2H), 4.66 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.51 (dd, *J* = 10.9, 8.5 Hz, 1H), 4.32 (dd, *J* = 8.5, 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.12 (d, *J* = 255.1 Hz), 164.87, 132.43 (d, *J* = 9.5 Hz), 131.40, 129.41, 129.01, 127.78, 125.33 (d, *J* = 3.0 Hz), 118.48, 115.81 (d, *J* = 22.1 Hz), 65.56, 37.55. IR (thin film): υ 2248, 1723 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}FNNaO_2]^+$ ($[M+Na]^+$): 292.0750, found: 292.0744.

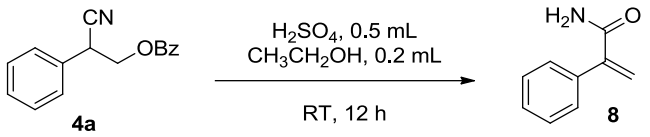


7f

Following the general procedure, product **7f** was obtained as a yellow liquid (76 mg, 46% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.87 (m, 2H), 7.63 – 7.56 (m, 2H), 7.48 – 7.36 (m, 5H), 4.65 (dd, *J* = 10.9, 5.6 Hz, 1H), 4.52 (dd, *J* = 10.9, 8.5 Hz, 1H), 4.31 (dd, *J* = 8.5, 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.16, 131.97, 131.32, 131.29, 129.43, 129.05, 128.87, 127.96, 127.77, 118.40, 65.63, 37.53. IR (thin film): υ 2249, 1722 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}BrNNaO_2]^+$ ($[M+Na]^+$): 351.9949, found: 351.9943.

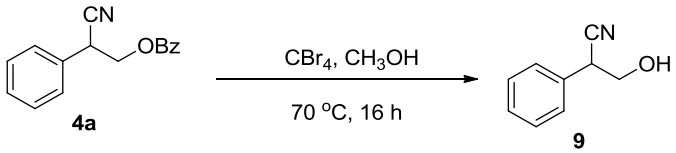
Transformations of the oxycyanation products

1. Synthesis of compound 8



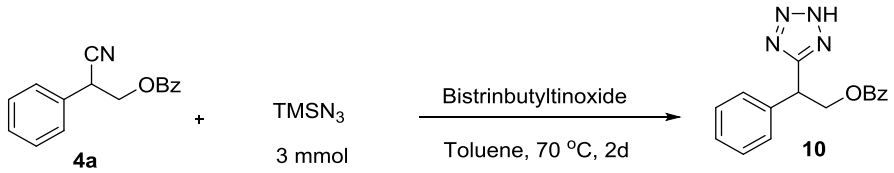
A solution of **4a** (0.1 mmol), EtOH (0.2 mL), and H_2SO_4 (1 mL) was stirred at rt for 12 h. On completion the reaction was quenched with ice-H_2O (3 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers was washed with brine (10 mL), dried over $MgSO_4$ and concentrated under vacuum. The residue was purified by column chromatography to yield **8** (12 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.35 (m, 5H), 6.21 – 6.17 (m, 2H), 5.68 – 5.65 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.35, 144.11, 137.07, 128.72, 128.59, 128.16, 123.25. These data matches with the reported value.[2]

2. Synthesis of compound 9



A solution of **4a** (0.2 mmol), CH_3OH (0.6 mL), and CBr_4 (0.04 mmol) was stirred at 70 °C for 16 h. On completion the reaction was quenched with H_2O (3 mL). The aqueous layer was extracted with diethyl ether and the combined organic layers was washed with brine (3 mL), dried over $MgSO_4$ and concentrated under vacuum. The residue was purified by column chromatography to yield **9** as a clear oil (18 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.33 (m, 5H), 4.04 – 3.88 (m, 3H), 2.25 (t, J = 6.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.16, 129.29, 128.69, 127.81, 119.35, 65.36, 40.98. These data matches with the reported value.[3]

3. Synthesis of compound 10

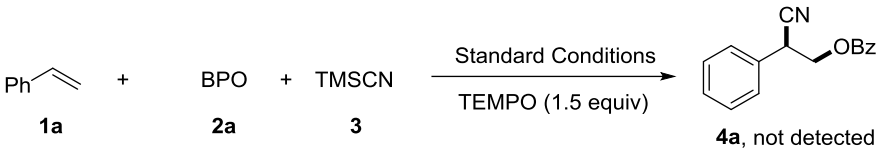


A solution of **4a** (0.18 mmol), $TMSN_3$ (3 mmol), and Bu_2SnO (0.6 equiv), toluene was stirred at 70 °C for 2 d. On completion the reaction was quenched with H_2O (3 mL). The aqueous layer was extracted with ethyl acetate and the combined organic layers was washed with brine (3 mL), dried over $MgSO_4$ and concentrated under vacuum. The residue was purified by column chromatography to yield **10** as a yellow oil (72 mg, 82% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.83 – 7.77 (m, 2H), 7.64 – 7.58 (m, 1H), 7.47 (t, J = 7.7 Hz, 2H), 7.41 – 7.37 (m, 2H), 7.29 (t, J = 7.5 Hz, 2H), 7.24 – 7.18 (m, 1H), 4.89 – 4.59 (m, 3H). ^{13}C NMR (400 MHz, DMSO-d_6) δ 165.91, 159.24, 140.04, 133.80, 130.02, 129.48, 129.16, 128.81, 128.79, 127.39, 67.60, 41.86. IR (thin film): υ 1714 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{14}N_4NaO_2]^+$ ($[M+Na]^+$): 317.1014, found: 317.1008.[4]

Mechanism studies

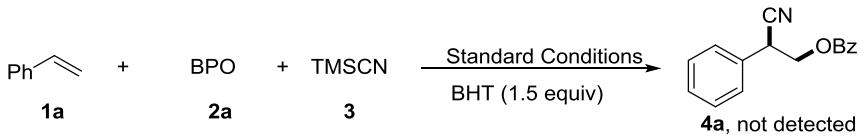
1. Radical trapping experiments

(a) With TEMPO



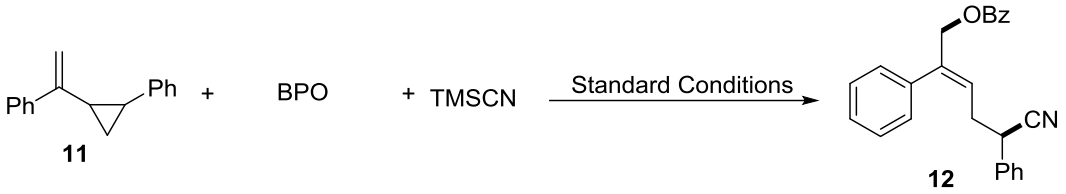
In a flame-dried Schlenk tube, $Cu(CH_3CN)_4PF_6$ (0.025 mmol, 5 mol %) and 1,10-phenanthroline (0.035 mmol, 7 mol %) were dissolved in TFEA (0.5 mL) under a nitrogen atmosphere, and the mixture was stirred at room temperature for 30 minutes. Then styrene **1a** (0.5 mmol, 1.0 equiv), BPO (0.75 mmol, 1.5 equiv), TEMPO (0.75 mmol, 1.5 equiv) and TMSCN (1 mmol, 2 equiv) were sequentially added. The reaction mixture was stirred at 50 ^oC for 24 hours. The reaction mixture was detected by GC-MS analysis and no trace of product **4a** was detected.

(b) With BHT

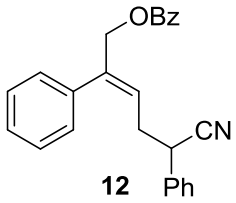


In a flame-dried Schlenk tube, $Cu(CH_3CN)_4PF_6$ (0.025 mmol, 5 mol %) and 1,10-phenanthroline (0.035 mmol, 7 mol %) were dissolved in TFEA (0.5 mL) under a nitrogen atmosphere, and the mixture was stirred at room temperature for 30 minutes. Then styrene **1a** (0.5 mmol, 1.0 equiv), BPO (0.75 mmol, 1.5 equiv), BHT (0.75 mmol, 1.5 equiv) and TMSCN (1 mmol, 2 equiv) were sequentially added. The reaction mixture was stirred at 50 ^oC for 24 hours. The reaction mixture was detected by GC-MS analysis and no trace of product **4a** was detected.

2. Ring-opening experiment



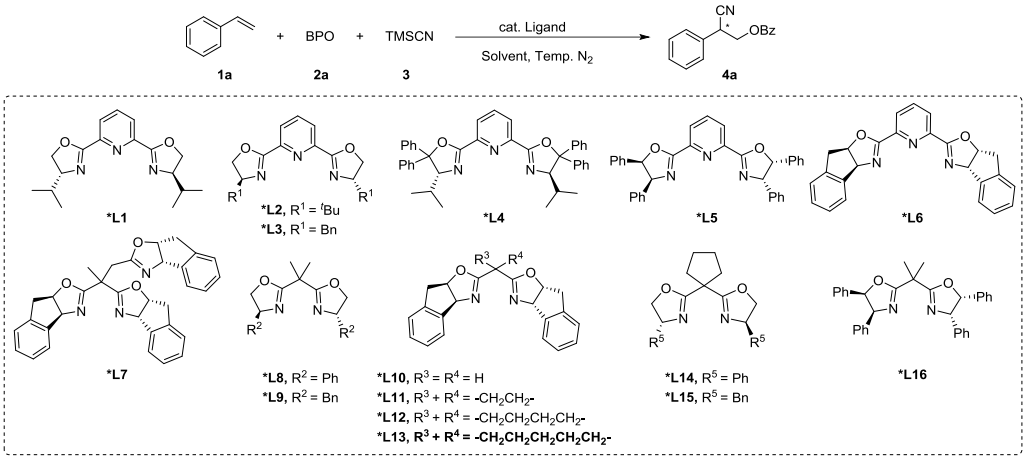
In a flame-dried Schlenk tube, $Cu(CH_3CN)_4PF_6$ (0.025 mmol, 5 mol %) and 1,10-phenanthroline (0.035 mmol, 7 mol %) were dissolved in TFEA (0.5 mL) under a nitrogen atmosphere, and the mixture was stirred at room temperature for 30 minutes. Then styrene **11** (0.5 mmol, 1.0 equiv), BPO (0.75 mmol, 1.5 equiv) and TMSCN (1 mmol, 2 equiv) were sequentially added. The reaction mixture was stirred at 50 ^oC for 24 hours. After the reaction completion, the solvent was evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the product **12**.



Product **12** was obtained as a yellow liquid (61 mg, 33% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.81 (m, 2H), 7.48 – 7.40 (m, 1H), 7.36 – 7.31 (m, 3H), 7.29 (t, *J* = 4.4 Hz, 6H), 7.27 – 7.19 (m, 3H), 5.98 (t, *J* = 7.8 Hz, 1H), 5.07 (d, *J* = 12.6 Hz, 1H), 4.97 (d, *J* = 12.6 Hz, 1H), 3.92 (dd, *J* = 7.6, 6.6 Hz, 1H), 3.01 – 2.85 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.33, 139.97, 138.68, 134.91, 133.09, 129.87, 129.64, 129.20, 128.52, 128.39, 128.36, 127.90, 127.82, 127.43, 126.40, 120.22, 61.33, 37.53, 34.73. IR (thin film): υ 2242, 1719 cm^{-1}. HRMS (ESI) calcd for $[C_{25}H_{21}NNaO_2]^+$ ($[M+Na]^+$): 390.1470, found: 390.1466.

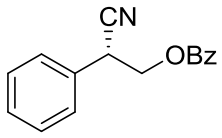
Asymmetric oxycyanation

Table S1. Optimization of reaction conditions



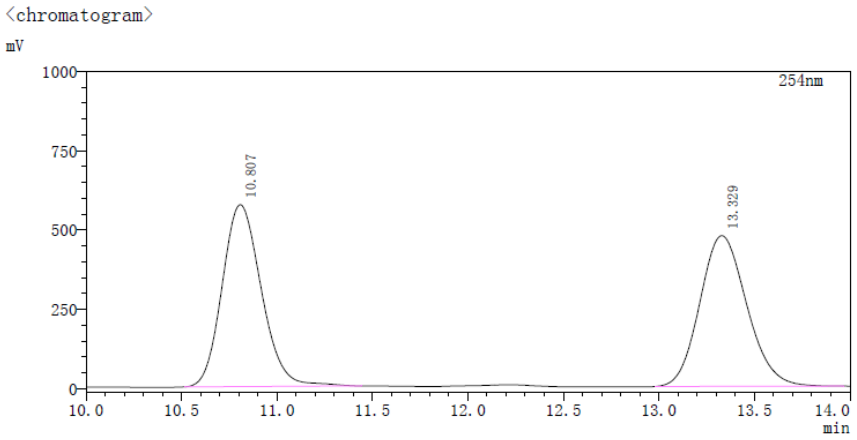
Entry	Cat.	Ligand	Solvent	Temp (^oC)	Yield (%)[b]	Er value
1	$Cu(CH_3CN)_4PF_6$	*L1	TFEA	50	54	33:67
2	$Cu(CH_3CN)_4PF_6$	*L2	TFEA	50	62	63.5:36.5
3	$Cu(CH_3CN)_4PF_6$	*L3	TFEA	50	75	81.5:18.5
4	$Cu(CH_3CN)_4PF_6$	*L4	TFEA	50	31	32.5:67.5
5	$Cu(CH_3CN)_4PF_6$	*L5	TFEA	50	35	65.5:34.5
6	$Cu(CH_3CN)_4PF_6$	*L6	TFEA	50	32	65.5:34.5
7	$Cu(CH_3CN)_4PF_6$	*L7	TFEA	50	70	82:18
8	$Cu(CH_3CN)_4PF_6$	*L8	TFEA	50	77	77.5:22.5
9	$Cu(CH_3CN)_4PF_6$	*L9	TFEA	50	66	83:17
10	$Cu(CH_3CN)_4PF_6$	*L10	TFEA	50	54	71:29
11	$Cu(CH_3CN)_4PF_6$	*L11	TFEA	50	69	77:23
12[c]	$Cu(CH_3CN)_4PF_6$	*L9	TFEA	50	80	87:13
13	$Cu(OAc)_2$	*L9	TFEA	50	82	89:11
14	CuTc	*L9	TFEA	50	86	85:15
15	$Cu(OAc)_2$	*L9	TFEA	RT	84	88:12
16	$Cu(OAc)_2$	*L12	TFEA	RT	89	85:15
17	$Cu(OAc)_2$	*L13	TFEA	RT	88	90:10
18	$Cu(OAc)_2$	*L14	TFEA	RT	84	23.5:76.5
19	$Cu(OAc)_2$	*L15	TFEA	RT	71	14:86
20	$Cu(OAc)_2$	*L16	TFEA	RT	80	70:30
21[c]	$Cu(OAc)_2$	*L13	TFEA	RT	83	91:9

[a] Reaction conditions: styrene **1a** (0.2 mmol), BPO **2a** (0.3 mmol), TMSCN **3** (0.4 mmol), cat. (5 mol %), ligand (7 mol %), solvent (0.5 mL), 24 h. [b] isolated yields. [c] 2.5 mol % of $Cu(OAc)_2$ and 3.5 mol % of ligand were used instead.

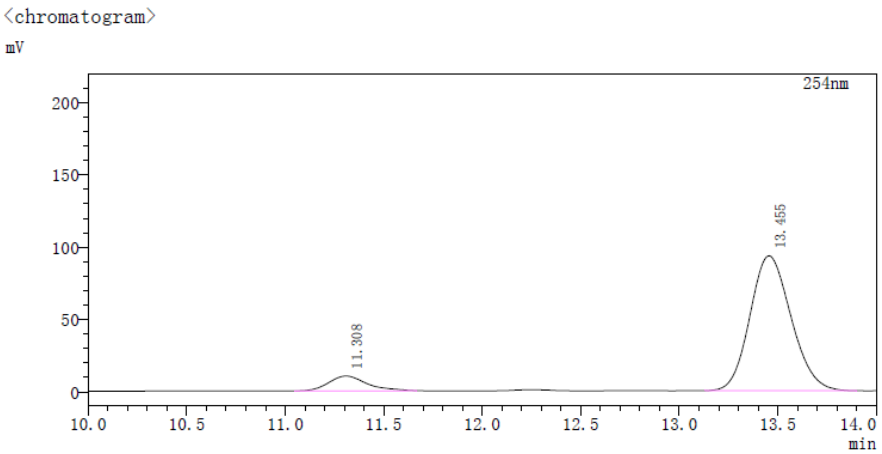


(*R*)-4a

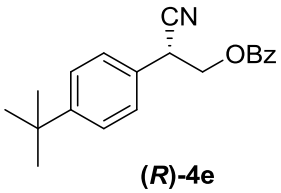
The reaction was conducted following the general procedure: the mixture of $Cu(OAc)_2$ (2.5 mol %), ***L13** (3.5 mol %), BPO (181.5 mg, 0.75 mmol, 1.5 equiv), TFEA (0.5 mL), TMSCN (0.75 mmol, 1.5 equiv), and styrene (0.5 mmol, 1 equiv) was stirred at rt for 24 hours, and **(*R*)-4a** was obtained (102 mg, 81% yield, 91:9 er). $[\alpha]^{24.5}_{D}$ = 44.596 (*c* 0.32, $CHCl_3$). HPLC (Chiralcel OD-H, hexane: *i*-PrOH = 91:9, flow rate: 1 mL/min, λ = 254 nm), t_{minor} = 11.308, t_{major} = 13.455.



Peak#	Ret. Time	Height	Height%	Area	Area%
1	10.807	573320	54.710	8173327	50.171
2	13.329	474608	45.290	8117557	49.829
Total		1047928	100.000	16290884	100.000

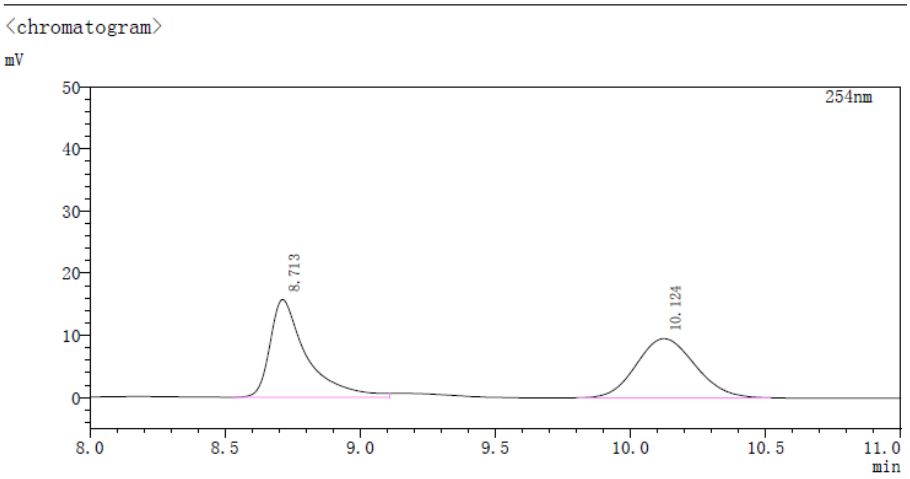


Peak#	Ret. Time	Height	Height%	Area	Area%
1	11.308	10286	9.937	138610	9.270
2	13.455	93225	90.063	1356614	90.730
Total		103511	100.000	1495223	100.000

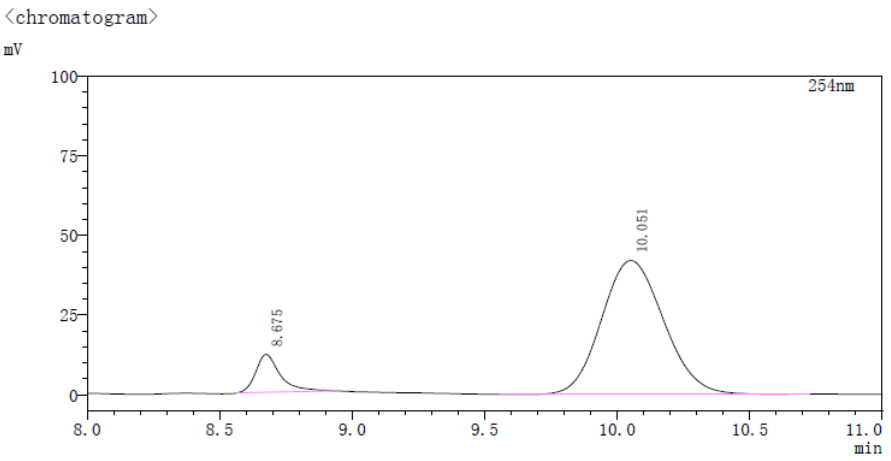


(*R*)-4e

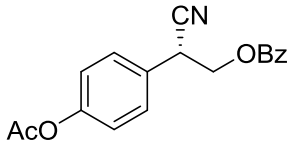
The reaction was conducted following the general procedure: the mixture of $Cu(OAc)_2$ (2.5 mol %), ***L13** (3.5 mol %), BPO (181.5 mg, 0.75 mmol, 1.5 equiv), TFEA (0.5 mL), TMSCN (0.75 mmol, 1.5 equiv), and 1-(tert-butyl)-4-vinylbenzene (0.5 mmol, 1 equiv) was stirred at rt for 24 hours, and **(*R*)-4e** was obtained (101 mg, 66% yield, 90:10 er). $[\alpha]^{24.6}_D$ = 10.964 (*c* 0.59, $CHCl_3$). HPLC (Chiralcel OD-H, hexane: *i*-PrOH = 95:5, flow rate: 1 mL/min, λ = 254 nm), t_{minor} = 8.675, t_{major} = 10.051.



Peak#	Ret. Time	Height	Height%	Area	Area%
1	8.713	15709	62.247	149350	50.896
2	10.124	9527	37.753	144089	49.104
Total		25236	100.000	293440	100.000

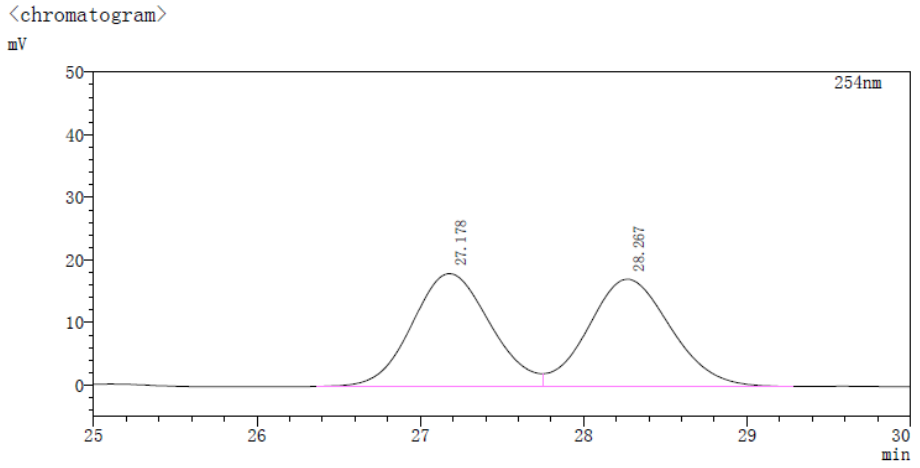


Peak#	Ret. Time	Height	Height%	Area	Area%
1	8.675	11962	22.190	77432	10.193
2	10.051	41943	77.810	682252	89.807
Total		53904	100.000	759684	100.000

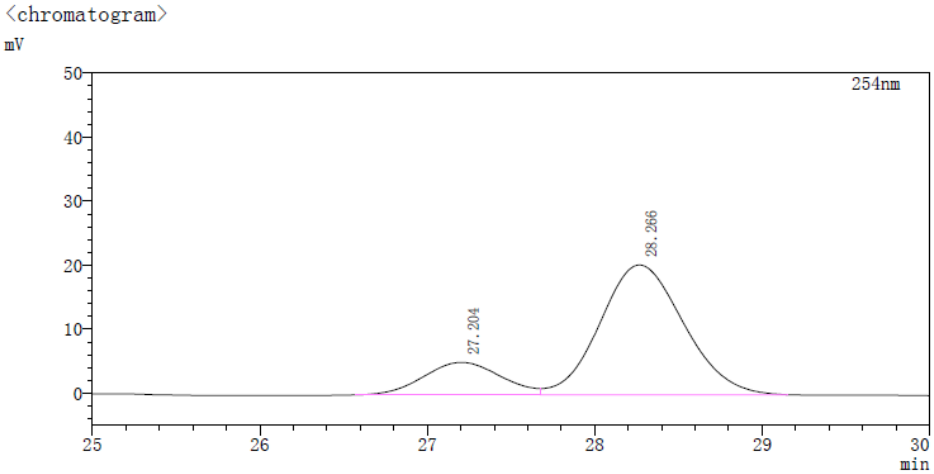


(*R*)-4f

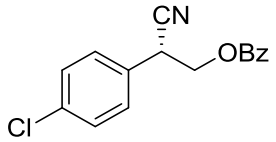
The reaction was conducted following the general procedure: the mixture of $Cu(OAc)_2$ (2.5 mol %), ***L13** (3.5 mol %), BPO (181.5 mg, 0.75 mmol, 1.5 equiv), TFEA (0.5 mL), TMSCN (0.75 mmol, 1.5 equiv), and 4-vinylphenyl acetate (0.5 mmol, 1 equiv) was stirred at rt for 24 hours, and **(*R*)-4f** was obtained (102 mg, 66% yield, 81:19 er). $[\alpha]^{24.7}_D$ = -31.627 (*c* 0.35, $CHCl_3$). HPLC (Chiralcel OD-H, hexane: *i*-PrOH = 90: 10, flow rate: 1 mL/min, λ = 254 nm), t_{minor} = 27.204, t_{major} = 28.266.



Peak#	Ret. Time	Height	Height%	Area	Area%
1	27.178	18013	51.266	599308	49.996
2	28.267	17123	48.734	599413	50.004
Total		35136	100.000	1198721	100.000

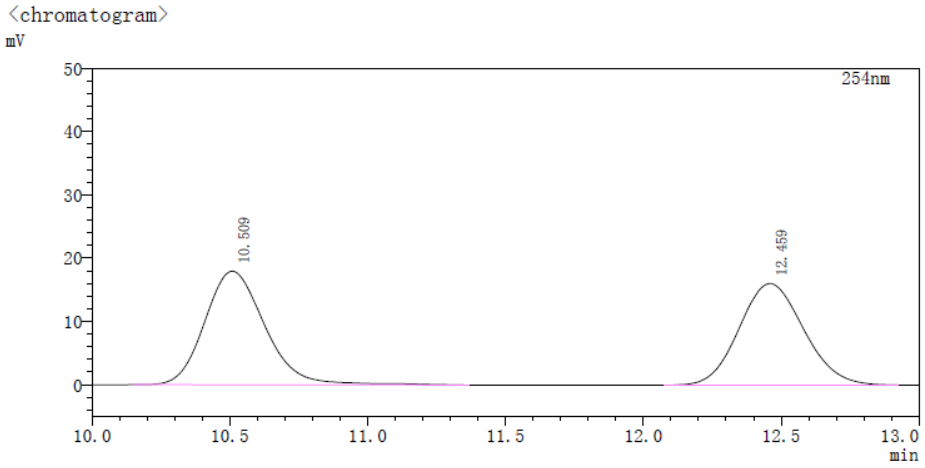


Peak#	Ret. Time	Height	Height%	Area	Area%
1	27.204	5085	20.048	162973	18.782
2	28.266	20278	79.952	704744	81.218
Total		25362	100.000	867716	100.000

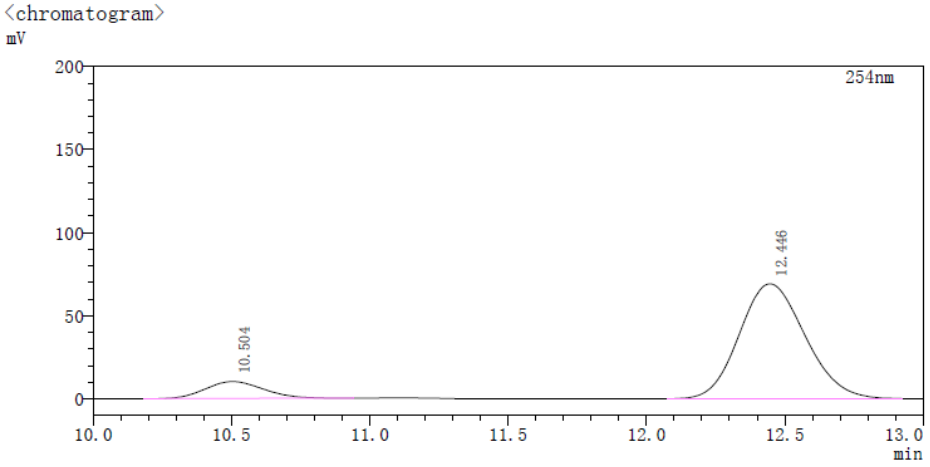


(*R*)-4h

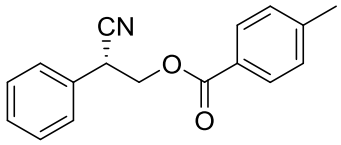
The reaction was conducted following the general procedure: the mixture of $Cu(OAc)_2$ (2.5 mol %), ***L13** (3.5 mol %), BPO (181.5 mg, 0.75 mmol, 1.5 equiv), TFEA (0.5 mL), TMSCN (0.75 mmol, 1.5 equiv), and 1-chloro-4-vinylbenzene (0.5 mmol, 1 equiv) was stirred at rt for 24 hours, and **(*R*)-4h** was obtained (88 mg, 62% yield, 88:12 er). $[\alpha]^{24.5}_D$ = -25.986 (*c* 0.97, $CHCl_3$). HPLC (Chiralcel OD-H, hexane: *i*-PrOH = 90: 10, flow rate: 1 mL/min, λ = 254 nm), t_{minor} = 10.504, t_{major} = 12.446.



Peak#	Ret. Time	Height	Height%	Area	Area%
1	10.509	17968	52.810	273467	51.134
2	12.459	16056	47.190	261333	48.866
Total		34024	100.000	534799	100.000

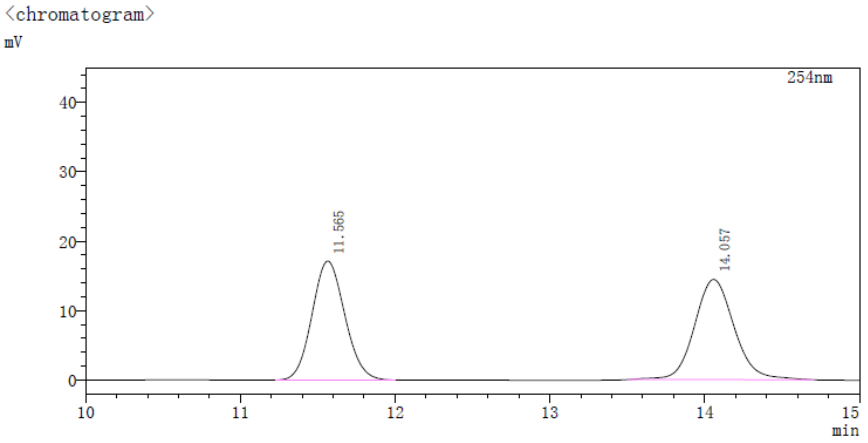


Peak#	Ret. Time	Height	Height%	Area	Area%
1	10.504	10184	12.839	148921	11.541
2	12.446	69141	87.161	1141408	88.459
Total		79326	100.000	1290328	100.000

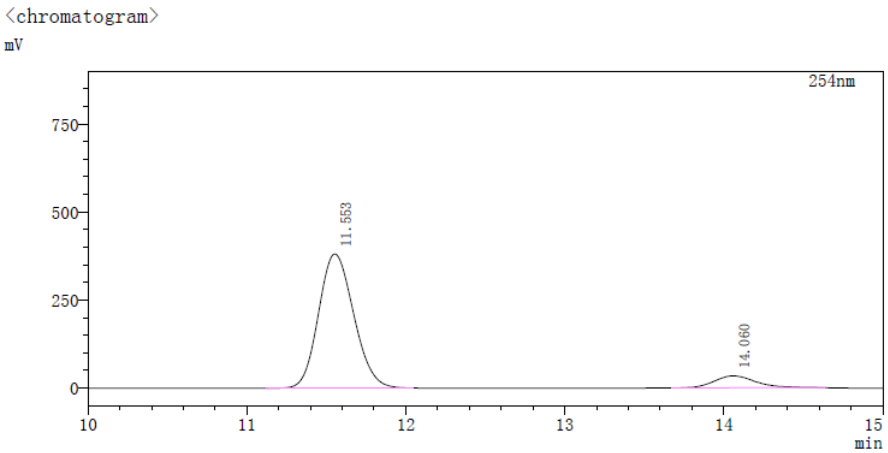


(*R*)-7a

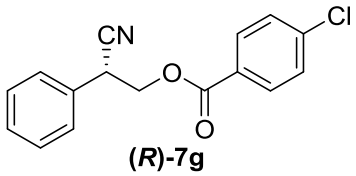
The reaction was conducted following the general procedure: the mixture of $Cu(OAc)_2$ (2.5 mol %), ***L13** (3.5 mol %), 4-methylbenzoic peroxyanhydride (0.75 mmol, 1.5 equiv), TFEA (0.5 mL), TMSCN (0.75 mmol, 1.5 equiv), and styrene (0.5 mmol, 1 equiv) was stirred at rt for 24 hours, and **(*R*)-7a** was obtained (89 mg, 67% yield, 90.5:9.5 er). $[\alpha]^{24.7}_D$ = 37.425 (*c* 1.65, $CHCl_3$). Chiralcel (Chiralcel OD-H, hexane: *i*-PrOH = 90: 10, flow rate: 1 mL/min, λ = 254 nm), t_{major} = 11.553, t_{minor} = 14.060.



Peak#	Ret. Time	Height	Height%	Area	Area%
1	11.565	17143	54.258	252649	49.624
2	14.057	14452	45.742	256482	50.376
Total		31595	100.000	509131	100.000

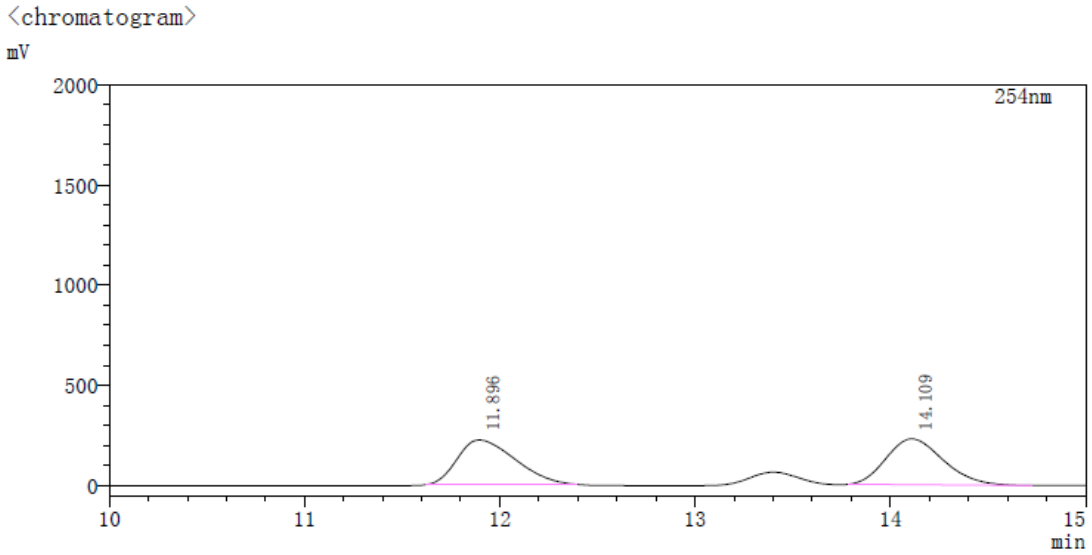


Peak#	Ret. Time	Height	Height%	Area	Area%
1	11.553	380991	91.860	5859226	90.470
2	14.060	33762	8.140	617223	9.530
Total		414753	100.000	6476449	100.000



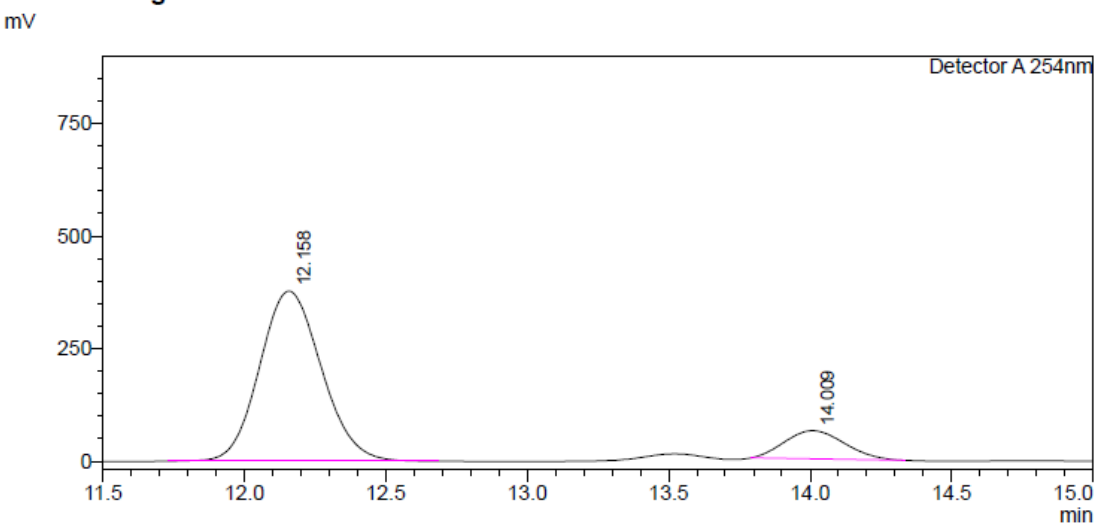
(*R*)-7g

The reaction was conducted following the general procedure: the mixture of $Cu(OAc)_2$ (2.5 mol %), ***L13** (3.5 mol %), 4-chlorobenzoic peroxyanhydride (0.75 mmol, 1.5 equiv), TFEA (0.5 mL), TMSCN (0.75 mmol, 1.5 equiv), and styrene (0.5 mmol, 1 equiv) was stirred at rt for 24 hours, and **(*R*)-7g** was obtained (71 mg, 46% yield, 86:14 er). $[\alpha]^{24.7}_D$ = 31.391 (*c* 0.41, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.6 Hz, 1H), 7.54 – 7.36 (m, 4H), 4.66 (dd, J = 10.9, 5.6 Hz, 1H), 4.51 (dd, J = 10.9, 8.5 Hz, 1H), 4.32 (dd, J = 8.5, 5.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.02, 140.16, 131.31, 131.20, 129.44, 129.06, 128.98, 127.78, 127.48, 118.46, 65.64, 37.53. IR (thin film): υ 2248, 1725 cm^{-1}. HRMS (ESI) calcd for $[C_{16}H_{12}ClNNaO_2]^+$ ($[M+Na]^+$): 308.0454, found: 308.0448. HPLC (Chiralcel IC, hexane/*i*-PrOH = 95:5, flow rate: 1 mL/min, λ = 254 nm), t_{major} = 12.158, t_{minor} = 14.009.



Peak#	Ret. Time	Height	Height%	Area	Area%
1	11.896	221822	49.257	4548611	49.451
2	14.109	228511	50.743	4649546	50.549
Total		450333	100.000	9198157	100.000

<Chromatogram>



Detector A 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	12.158	377570	85.810	5743052	86.192
2	14.009	62438	14.190	920032	13.808
Total		440008	100.000	6663084	100.000

Single crystal data of (*R*)-4e

CCDC 2040065 **(*R*)-4e** contains the supplementary crystallographic data (dimer). Crystal data and structure refinements of **(*R*)-4e** is listed in Table S2. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/

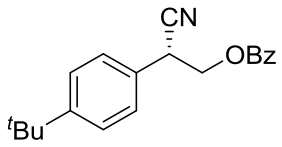


Table S2. Crystal data and structure refinement for **(*R*)-4e**.

Identification code	(*R*)-4e	
Empirical formula	$C_{20}H_{21}NO_2$	
Formula weight	307.38	
Temperature (K)	100(2)	
Wavelength (Å)	1.54178	
Crystal system	monoclinic	
Space group	$P2_1$	
Unit cell dimensions (Å, °)	*a* = 9.4303(5)	α = 90
	b = 19.9537(11)	β = 111.9060(10)
	c = 9.8206(5)	γ = 90
Volume (Å)	1714.51(16)	
Z	4	
Calculated density (g cm^{-3})	1.191	
Absorption coefficient (mm^{-1})	0.605	
F_{000}	656	
Crystal size (mm^3)	× ×	
θ range for data collection (°)	4.432 to 72.480	
Miller index ranges	$-11 \le h \le 10$, $-24 \le k \le 24$, $-12 \le l \le 12$	
Reflections collected	32674	
Independent reflections	6739 [R_{int} = 0.0377]	
Completeness to θ_{max} (%)	0.995	
Max. and min. transmission	and	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	6739 / 2 / 443
Goodness-of-fit on F^2	1.052
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0354, $wR2$ = 0.0864
R indices (all data)	$R1$ = 0.0356, $wR2$ = 0.0866
Extinction coefficient	0.0041(7)
Largest diff. peak and hole (e $Å^{-3}$)	0.321 and -0.221
Absolute structure parameter	.11(5)

References

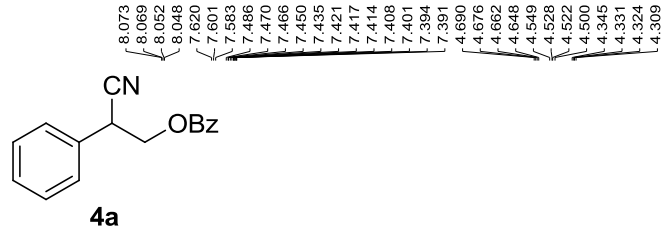
1 B. Qian, S. Chen, T. Wang, X. Zhang and H. Bao, Iron-Catalyzed Carboamination of Olefins: Synthesis of Amines and Disubstituted beta-Amino Acids, *J. Am. Chem. Soc.,* 2017, **139**, 13076.

2 X. Ji, B. Gao, X. Zhou, Z. Liu and H. Huang, Palladium-Catalyzed Regioselective Hydroaminocarbonylation of Alkynes to alpha,beta-Unsaturated Primary Amides with Ammonium Chloride, *J. Org. Chem.*, 2018, **83**, 10134.

3 E. Farber, J. Herget, J. A. Gascon and A. R. Howell, Unexpected cleavage of 2-azido-2-(hydroxymethyl)oxetanes: conformation determines reaction pathway?, *J. Org. Chem.*, 2010, **75**, 7565.

4 A. L. Fuentes de Arriba, E. Lenci, M. Sonawane, O. Formery and D. J. Dixon, Iridium-Catalyzed Reductive Strecker Reaction for Late-Stage Amide and Lactam Cyanation, *Angew. Chem. Int. Ed.*, 2017, **56**, 3655.

NMR spectra



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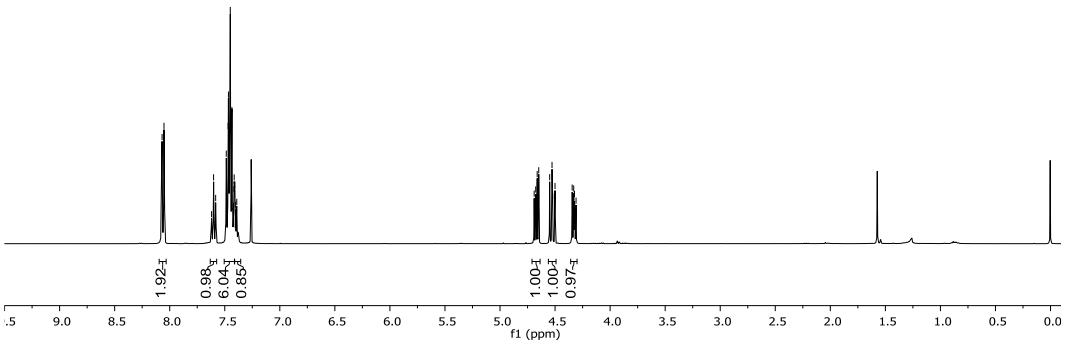

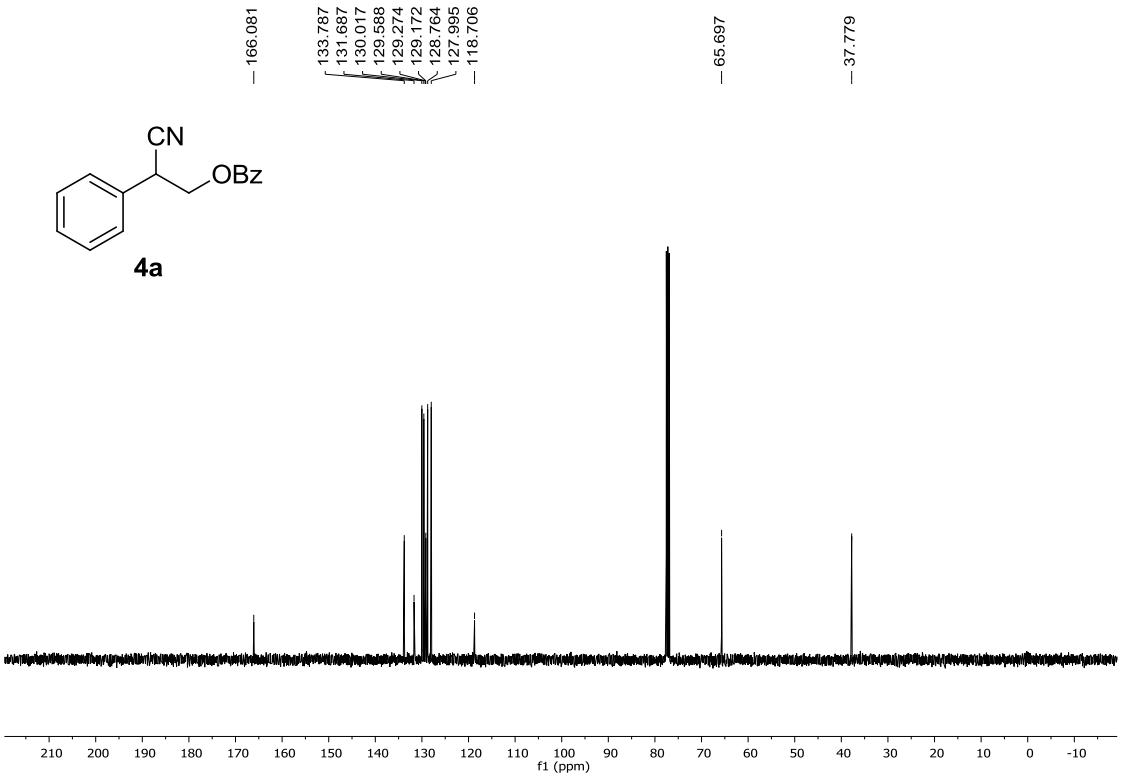

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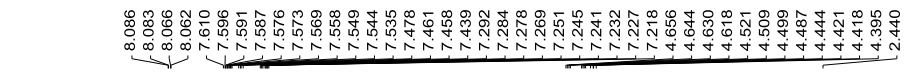
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7.535
7.478
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7.458
7.439
7.292
7.284
7.278
7.269
7.251
7.245
7.241
7.232
7.227
7.218
4.656
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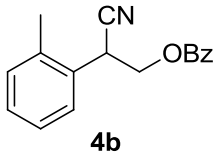
2.440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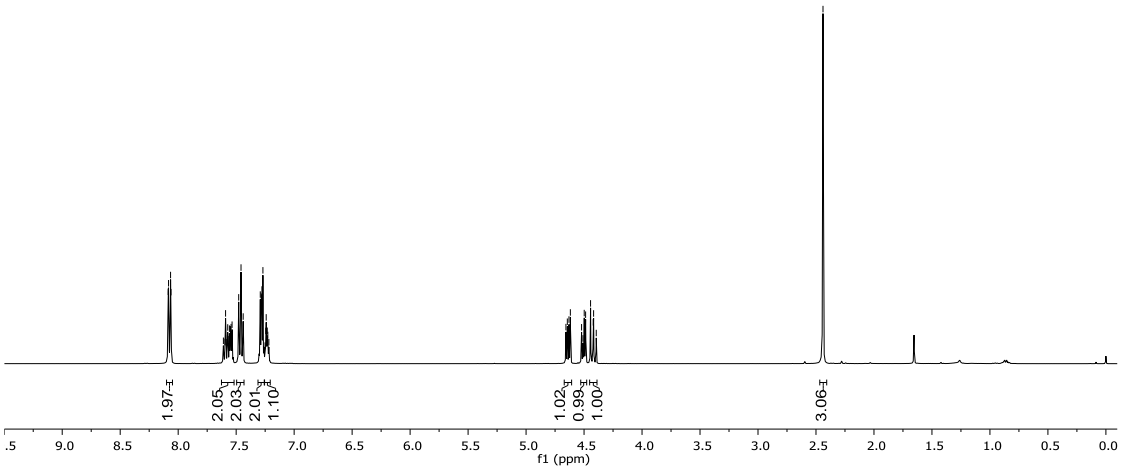
OBz

4b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1.10
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f1 (ppm)


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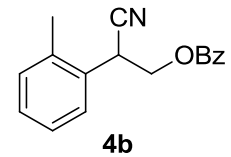
19.155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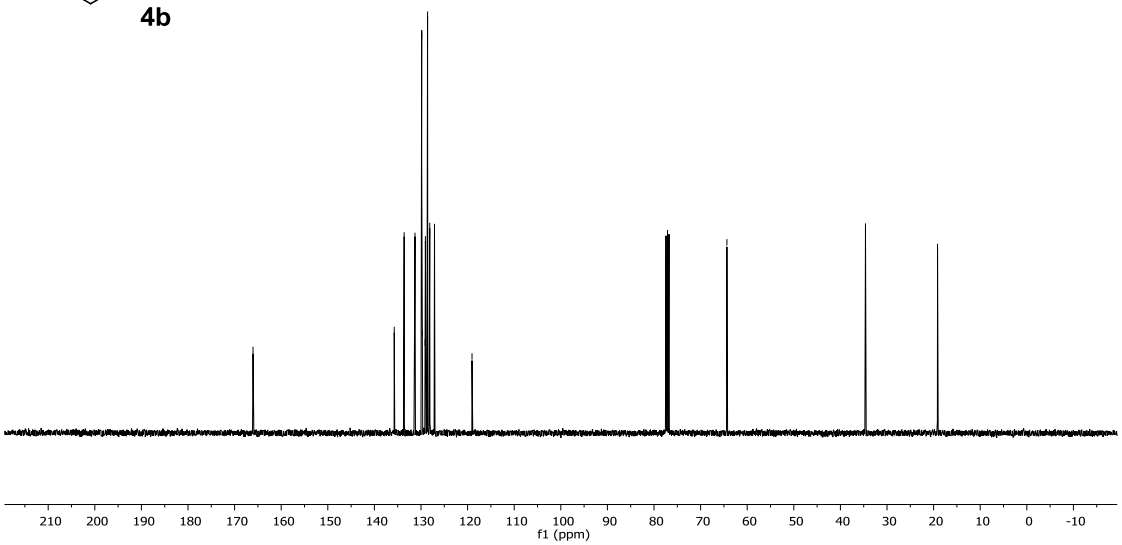
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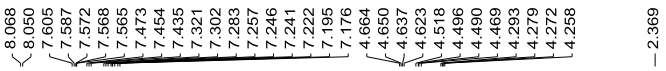
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7.195
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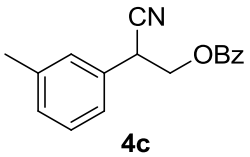
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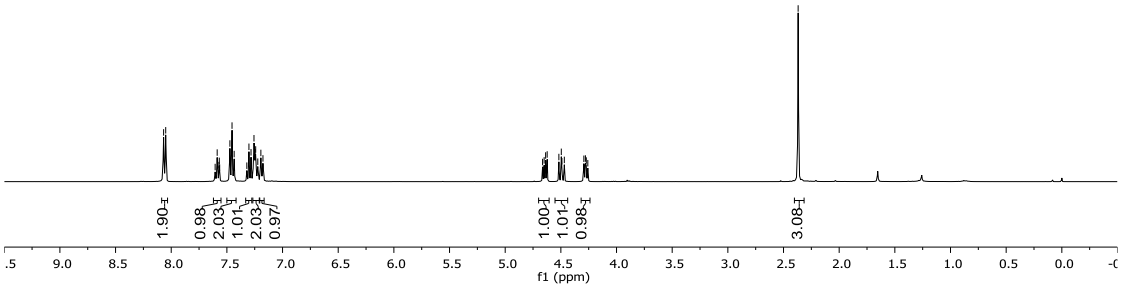
4c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2.03
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f1 (ppm)


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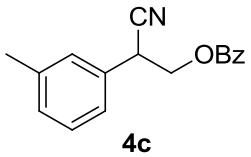
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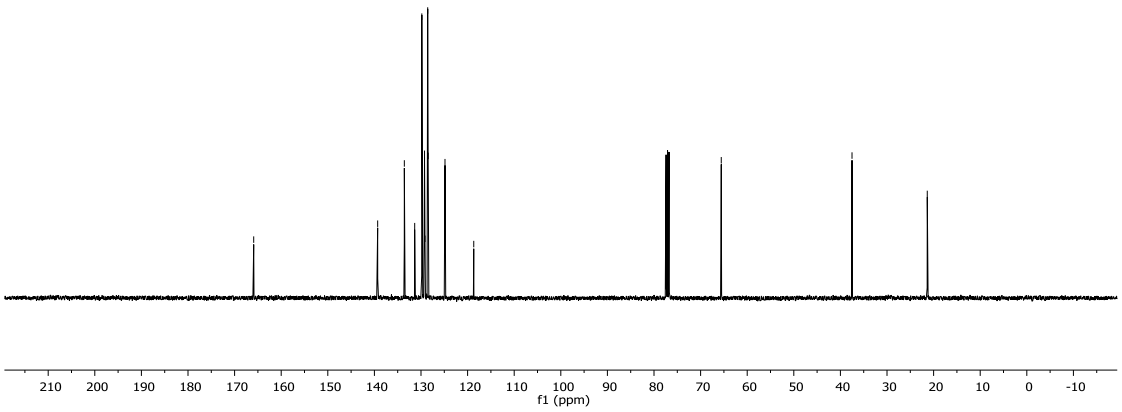
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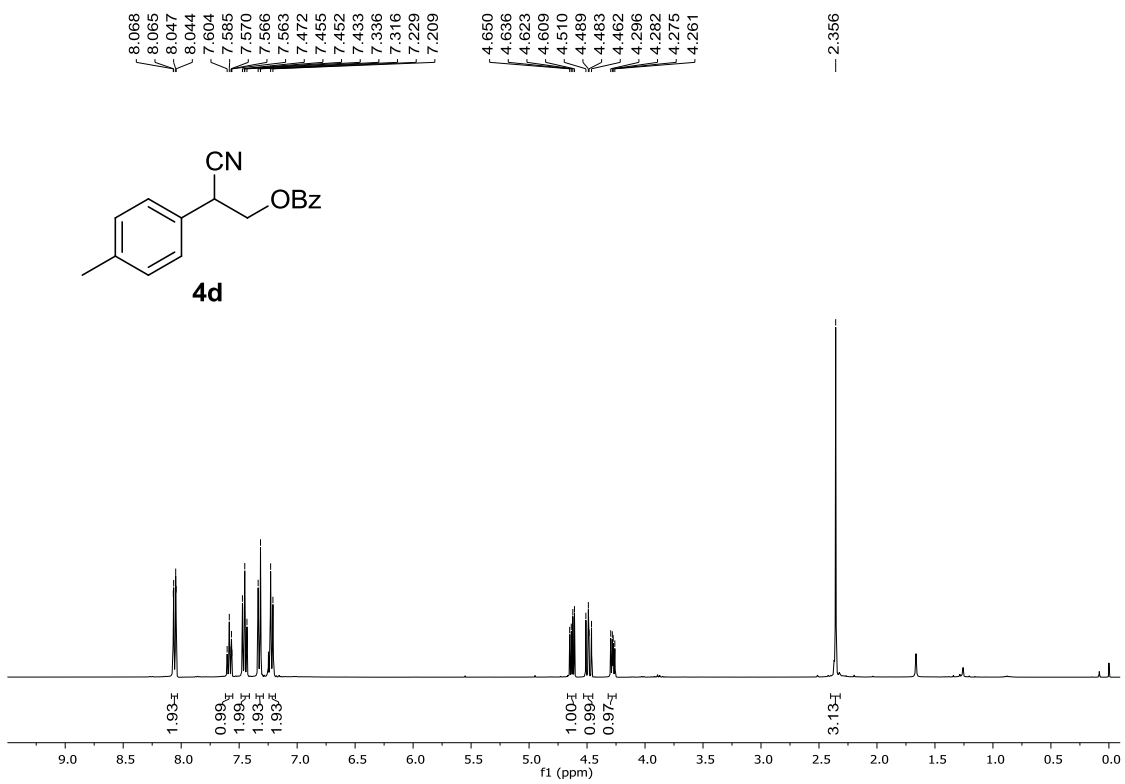
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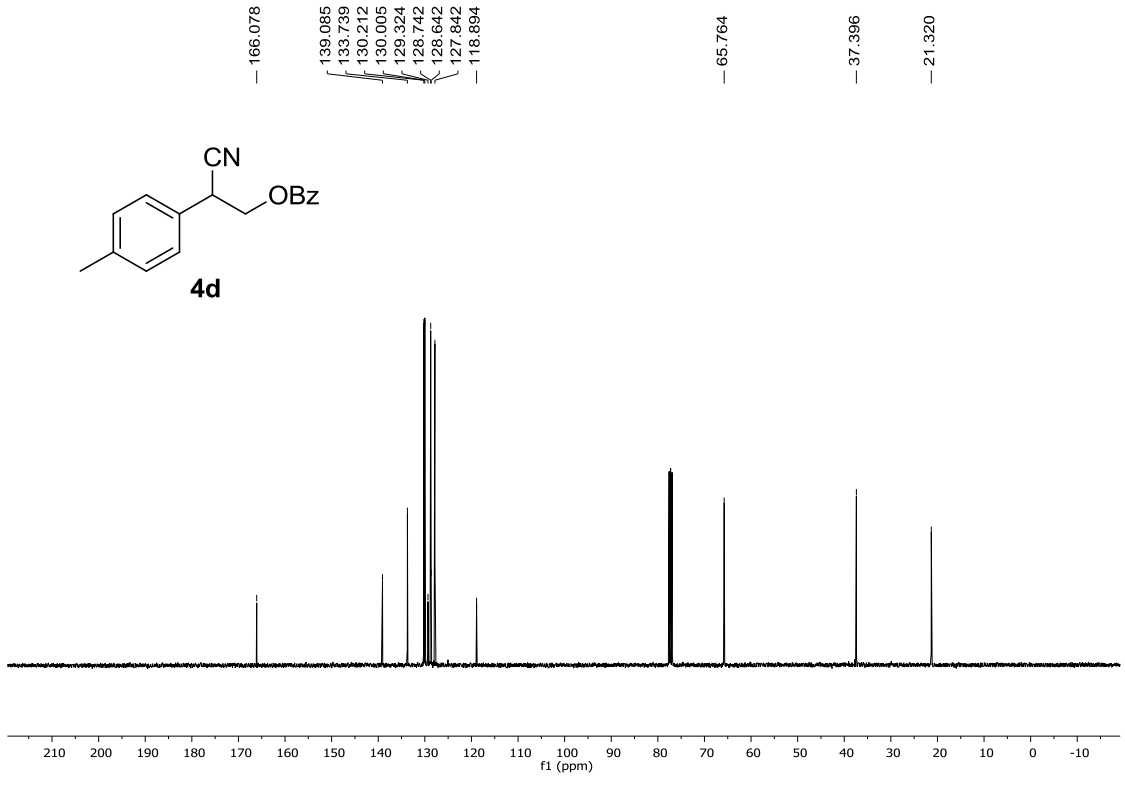
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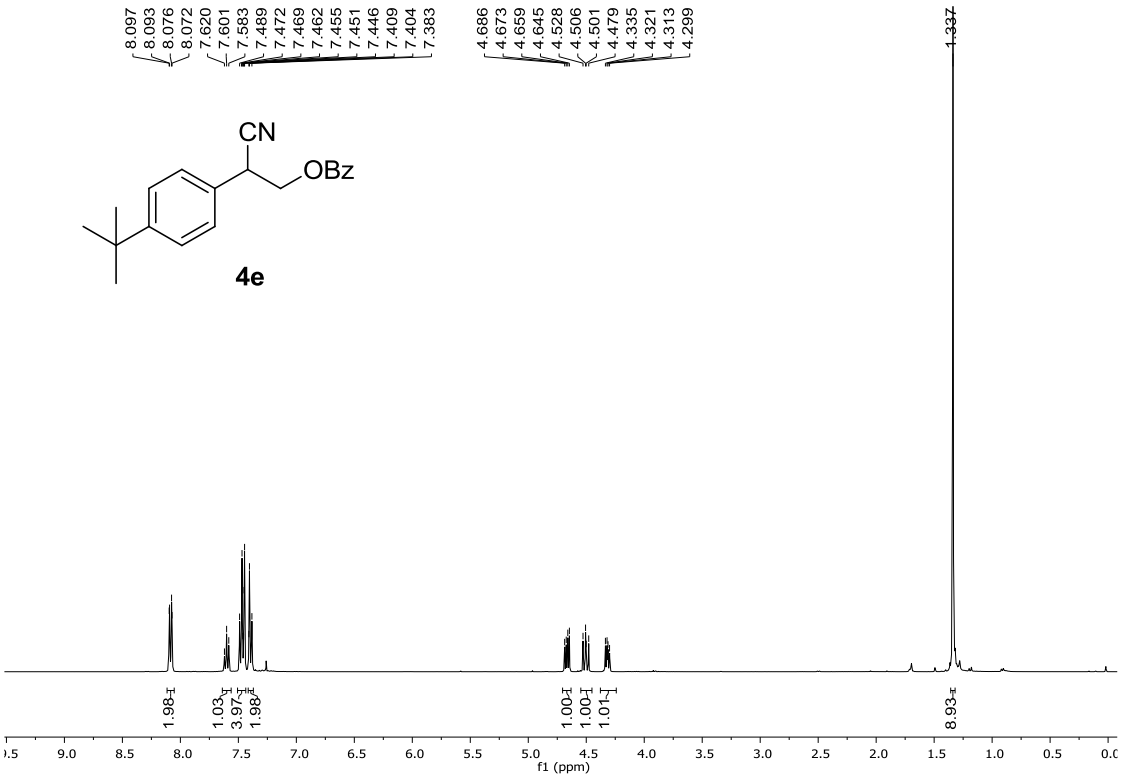
f1 (ppm)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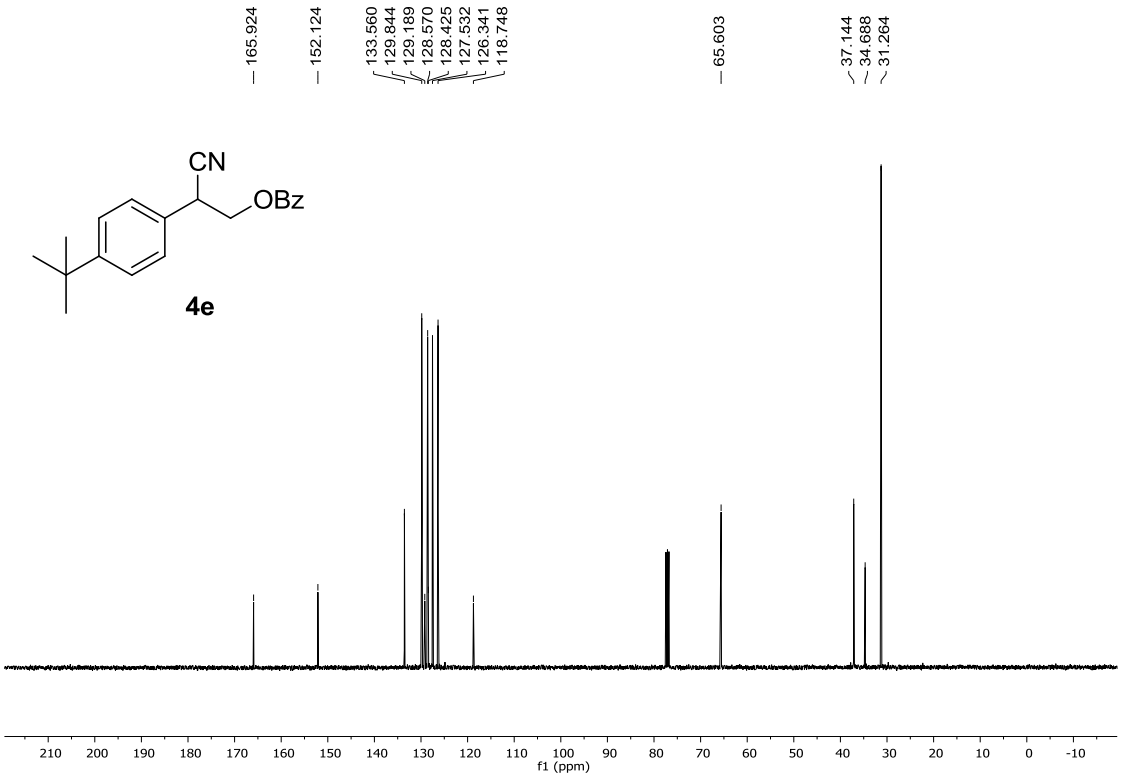
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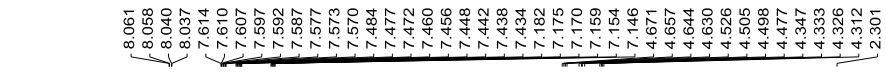
OBz
4e
f1 (ppm)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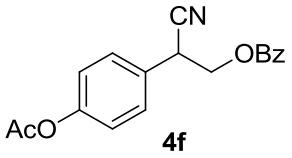
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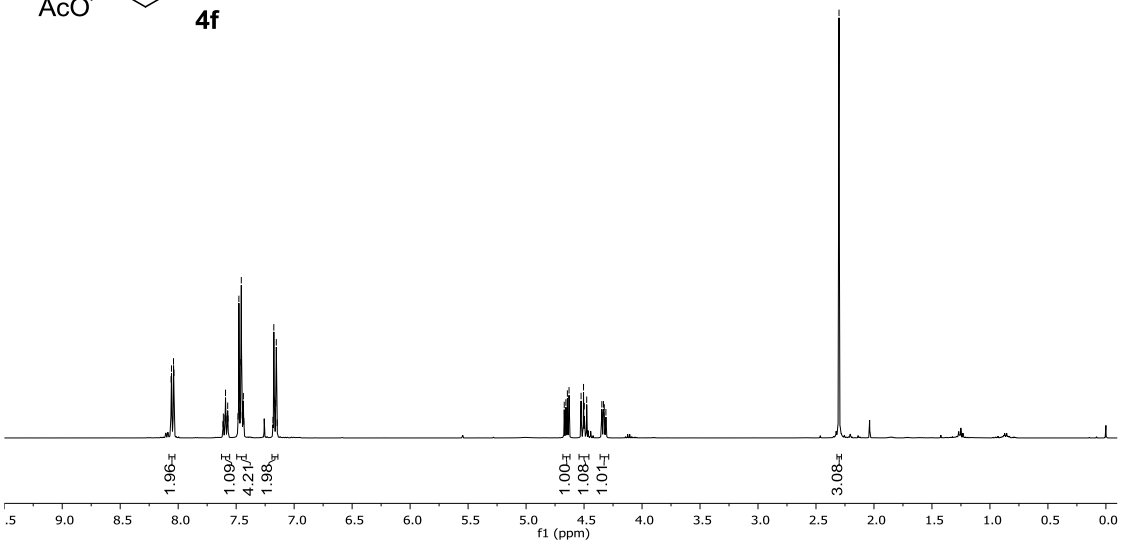
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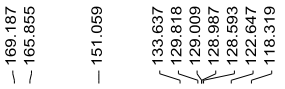
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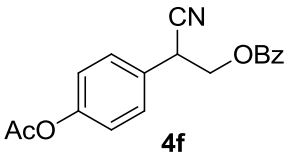
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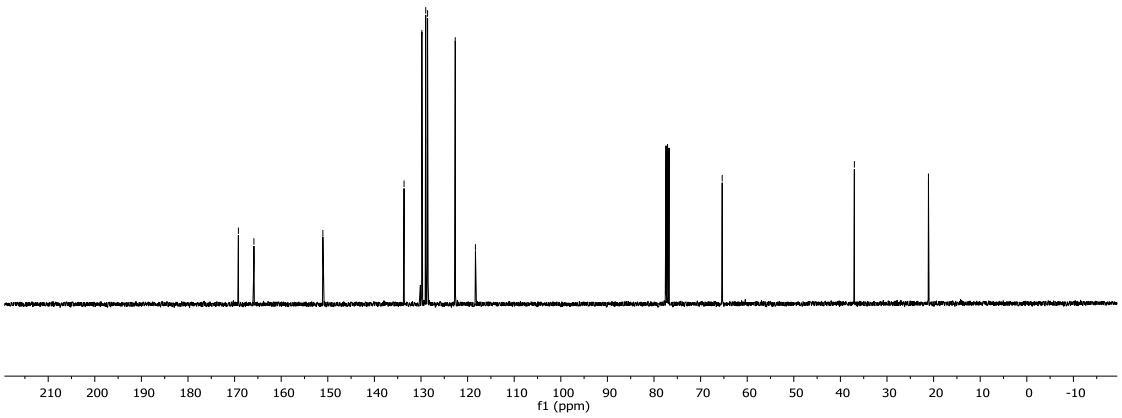
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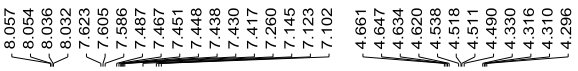
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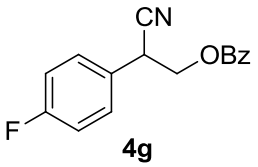
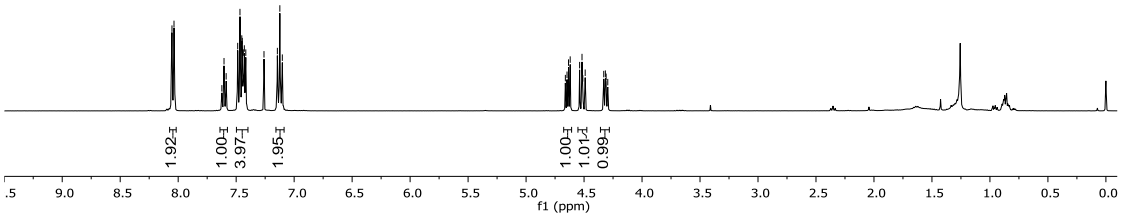

CN
OBz
F

4g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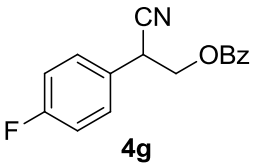
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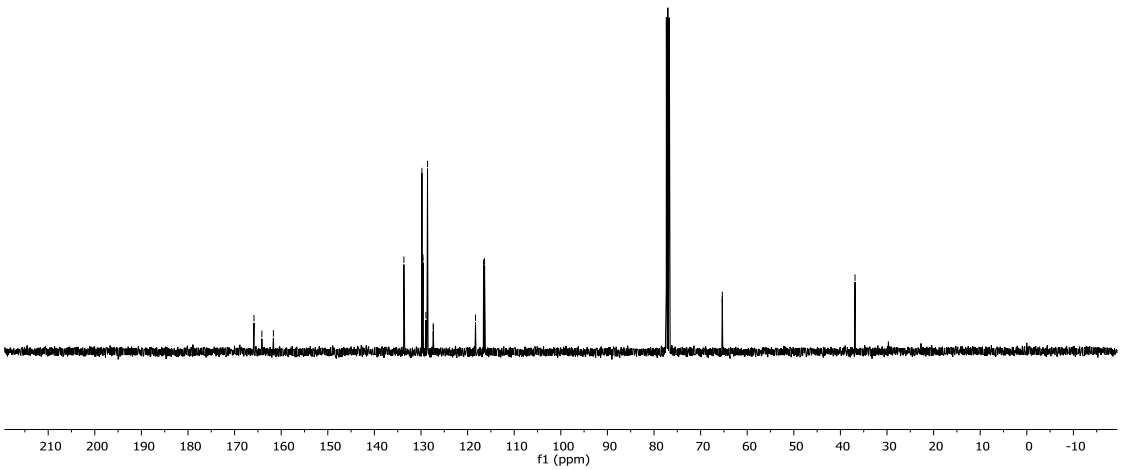
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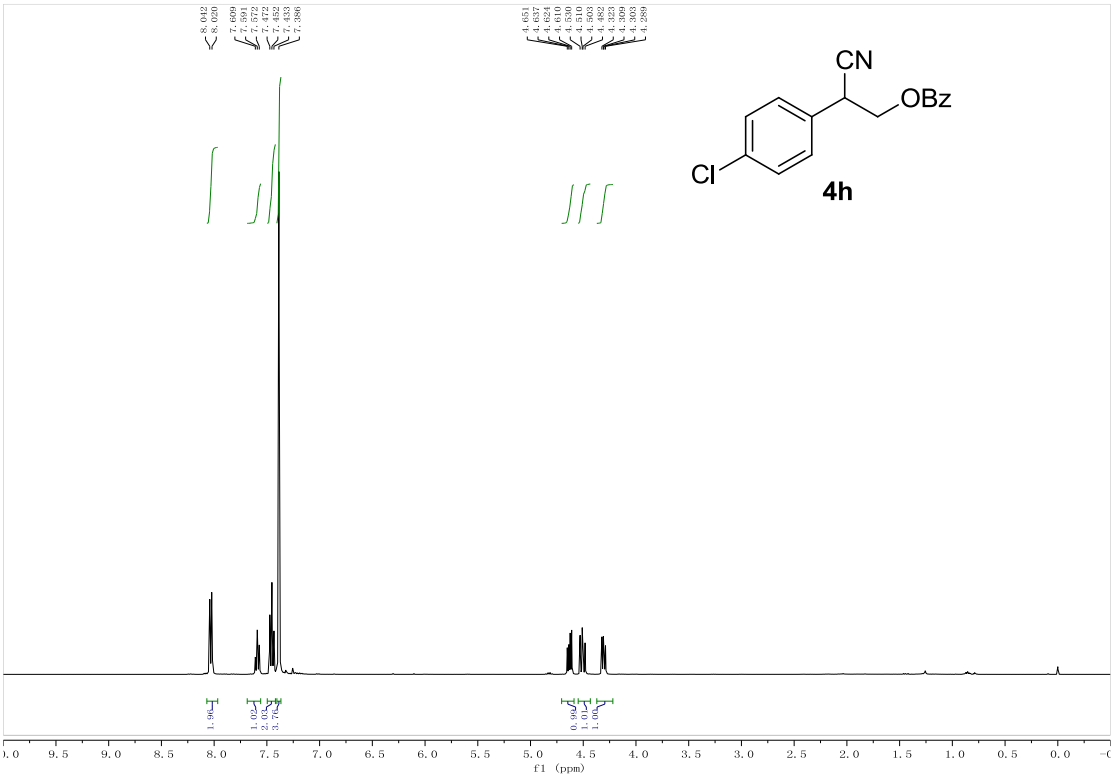
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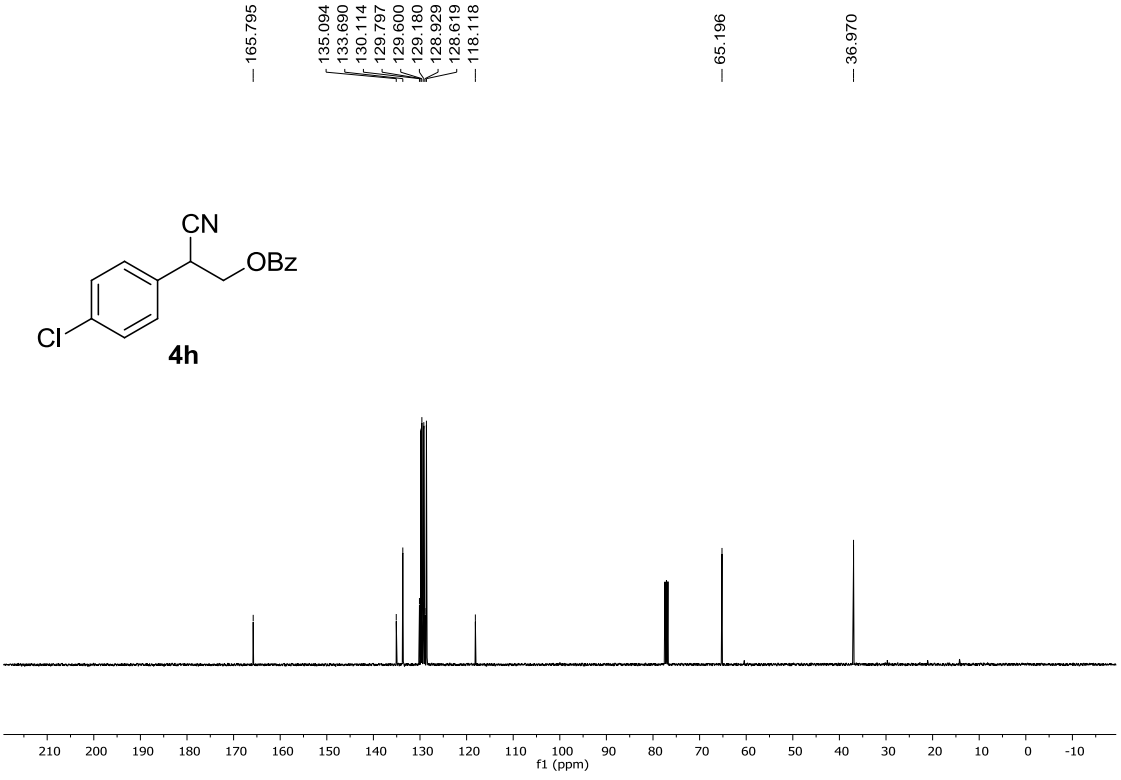
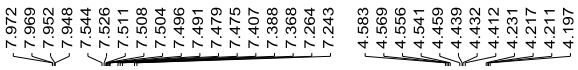
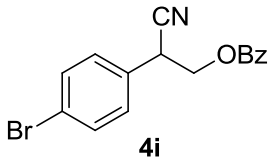
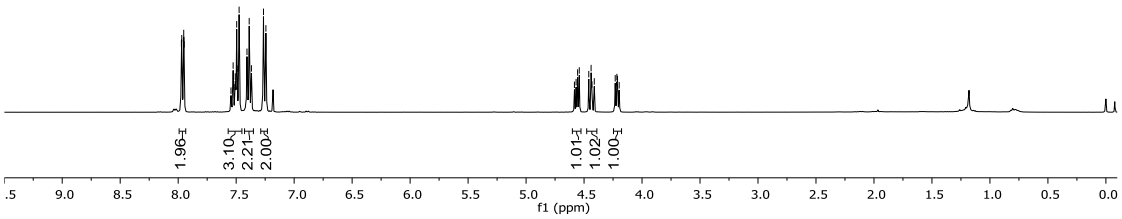
7.386
4.651
4.637
4.624
4.610
4.530
4.510
4.483
4.462
4.323
4.309
4.303
4.288
CN
OBz
Cl
4h
1.96
1.00
2.00
3.74
0.90
1.01
1.00
f1 (ppm)


165.795
135.094
133.690
130.114
129.797
129.600
129.180
128.929
128.619
118.118
65.196
36.970
CN
OBz
Cl
4h
f1 (ppm)

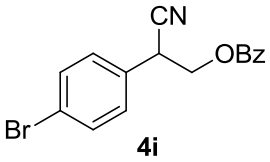

7.972
7.969
7.952
7.948
7.544
7.526
7.511
7.508
7.504
7.496
7.491
7.479
7.475
7.407
7.388
7.368
7.264
7.243
4.583
4.569
4.556
4.541
4.459
4.439
4.432
4.412
4.231
4.217
4.211
4.197


CN
OBz
Br

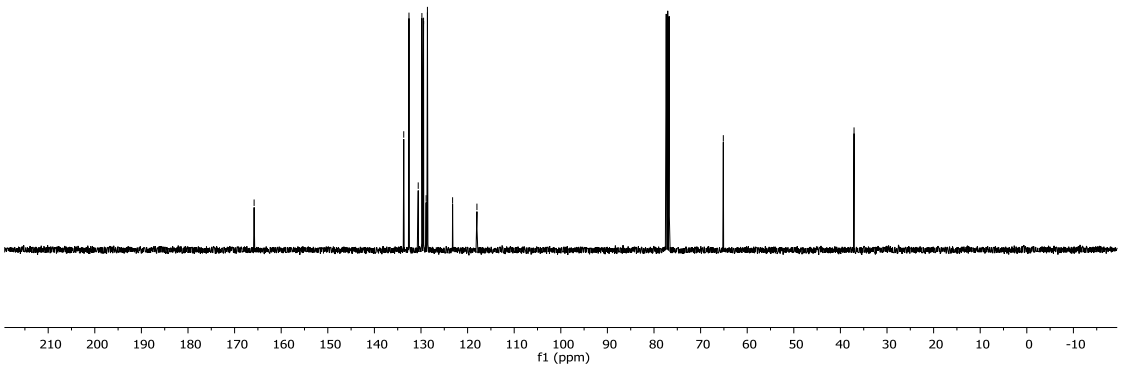
4i

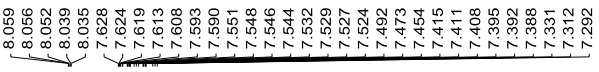

1.96
3.10
2.21
2.00
1.01
1.02
1.00
f1 (ppm)


165.812
133.704
132.581
130.595
129.807
129.451
128.900
128.619
123.222
117.997
65.125
37.072


CN
OBz
Br

4i


f1 (ppm)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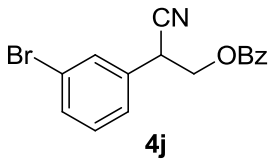
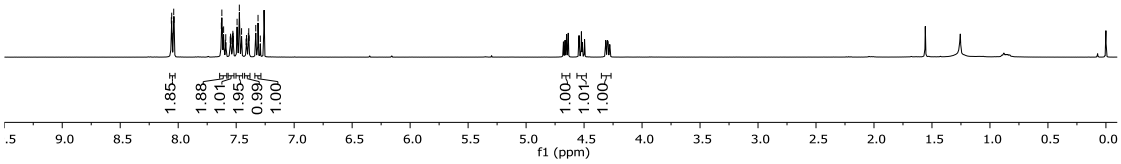
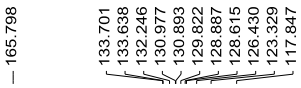
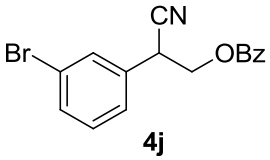
8.056
8.052
8.039
8.035
7.628
7.624
7.619
7.613
7.608
7.593
7.590
7.551
7.548
7.546
7.544
7.532
7.529
7.527
7.524
7.492
7.473
7.454
7.415
7.411
7.408
7.395
7.392
7.388
7.331
7.312
7.292


CN
Br
OBz

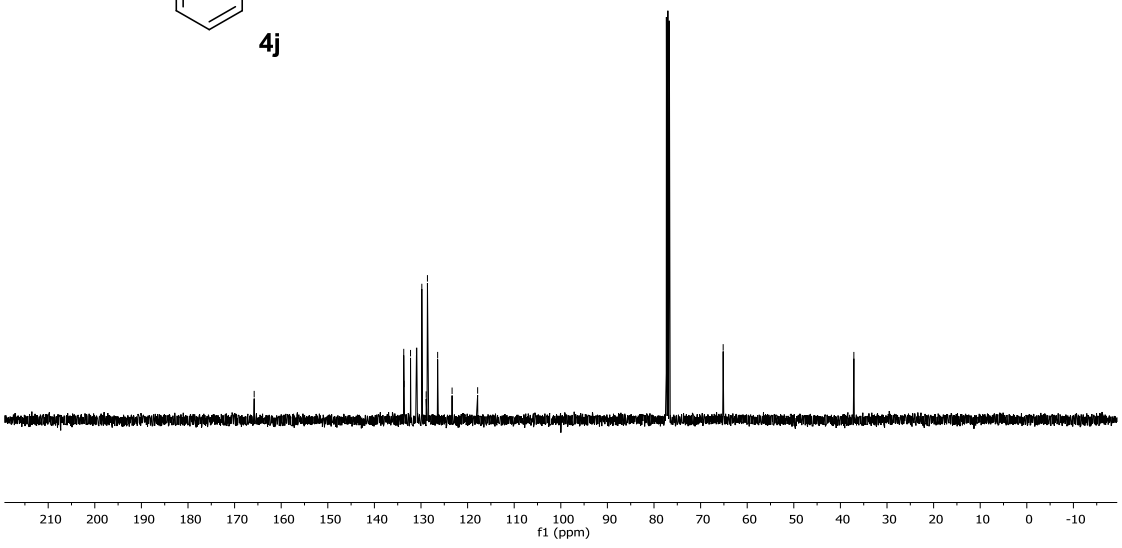
4j

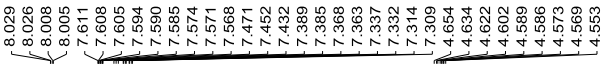

1.85
1.88
1.01
1.95
0.99
1.00
1.00
1.01
1.00
f1 (ppm)

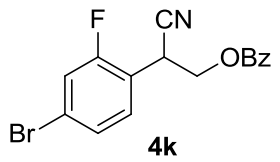

165.798
133.701
133.638
132.246
130.977
130.893
129.822
128.887
128.615
126.430
123.329
117.847
65.159
37.113


CN
Br
OBz

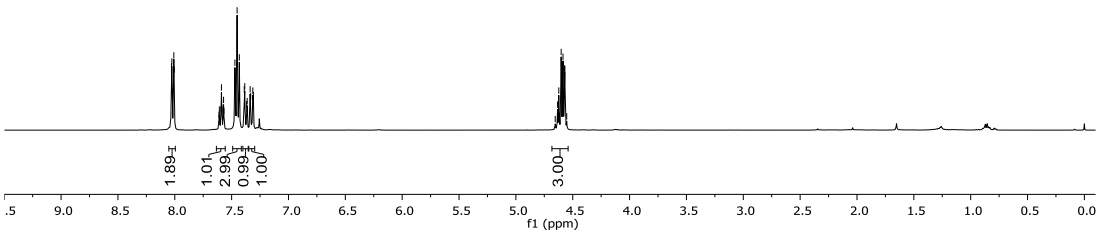
4j

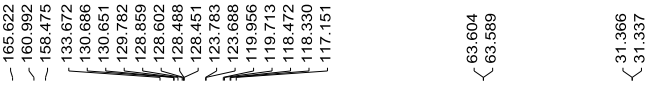

f1 (ppm)

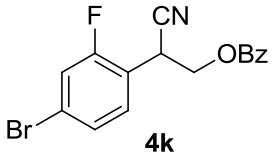

8.029
8.026
8.008
8.005
7.611
7.608
7.605
7.594
7.590
7.585
7.574
7.571
7.568
7.471
7.452
7.432
7.389
7.385
7.368
7.363
7.337
7.332
7.314
7.309
4.654
4.634
4.622
4.602
4.589
4.586
4.573
4.569
4.553


F
CN
OBz
Br

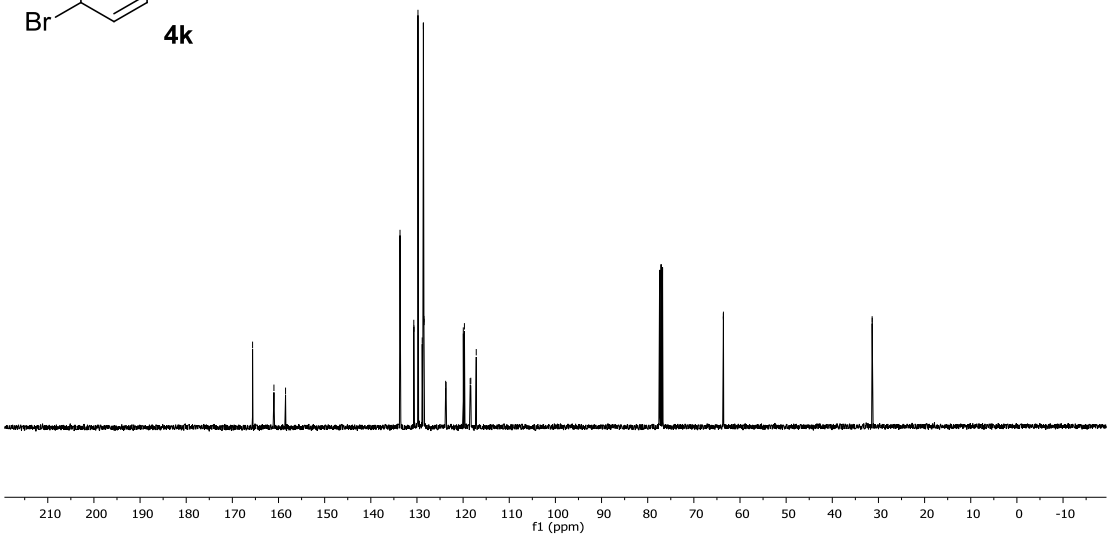
4k

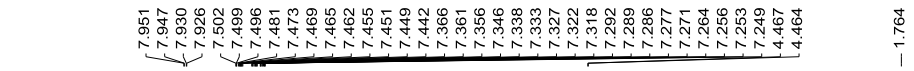

1.89
1.01
2.99
0.99
1.00
3.00
f1 (ppm)

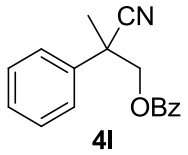

165.622
160.992
158.475
133.672
130.686
130.651
129.782
128.859
128.602
128.488
128.451
123.783
123.688
119.956
119.713
118.472
118.330
117.151
63.604
63.589
31.366
31.337


F
CN
OBz
Br

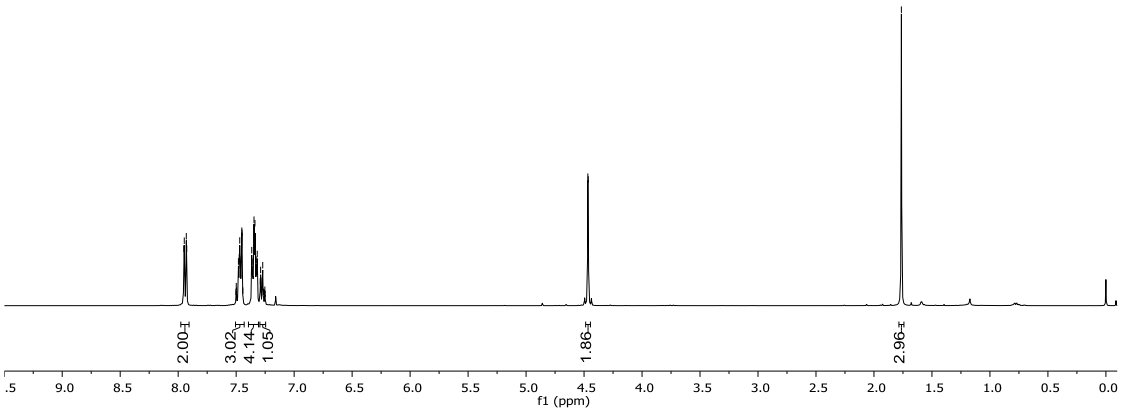
4k


f1 (ppm)

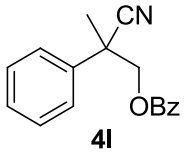

7.951
7.947
7.930
7.926
7.502
7.499
7.496
7.481
7.473
7.469
7.465
7.462
7.455
7.451
7.449
7.442
7.366
7.361
7.356
7.346
7.338
7.333
7.327
7.322
7.318
7.292
7.289
7.286
7.277
7.271
7.264
7.256
7.253
7.249
4.467
4.464
1.764


CN
OBz

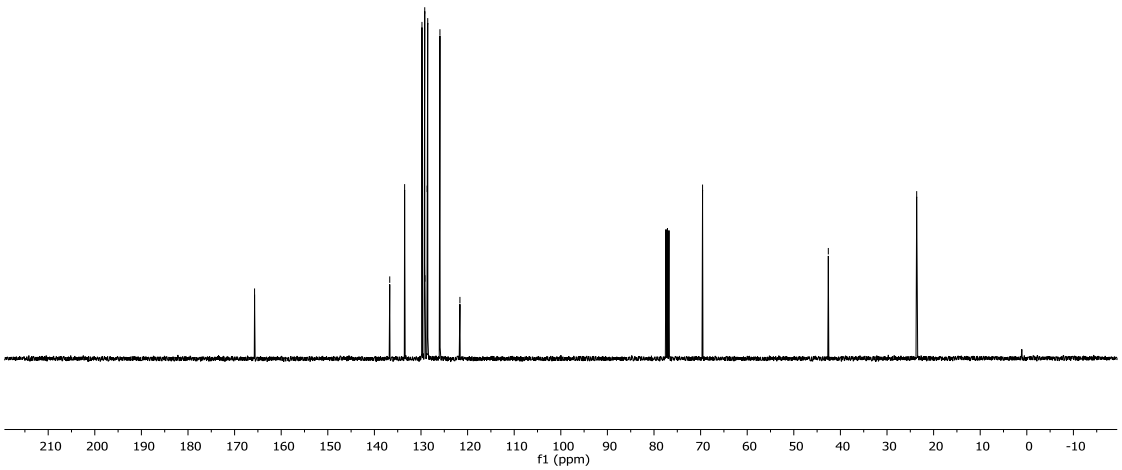
4l

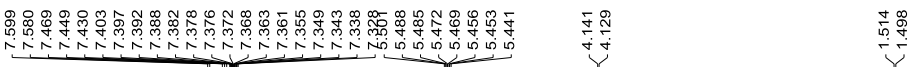

2.00
3.02
4.14
1.05
1.86
2.96
f1 (ppm)


165.714
136.708
133.515
129.792
129.198
129.151
128.681
128.556
125.935
121.645
69.580
42.594
23.633


CN
OBz

4l


f1 (ppm)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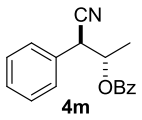
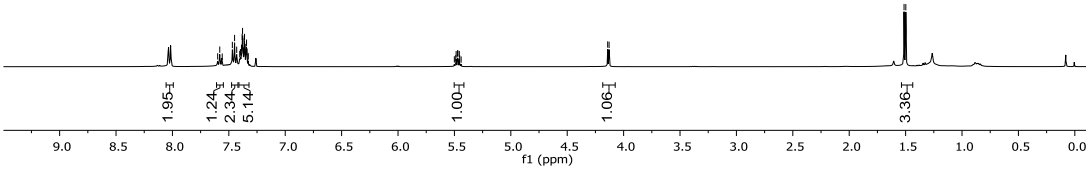
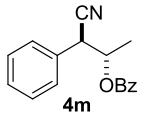
7.469
7.449
7.430
7.403
7.397
7.392
7.388
7.382
7.378
7.376
7.372
7.368
7.363
7.361
7.355
7.349
7.343
7.338
5.501
5.488
5.485
5.472
5.469
5.456
5.453
5.441
4.141
4.129
1.514
1.498


CN
OBz

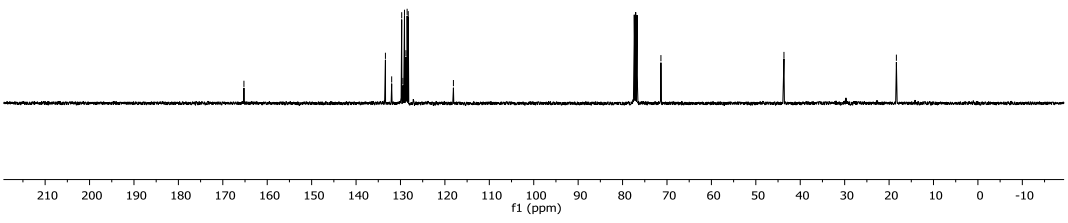
4m

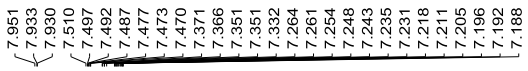

1.95
1.24
2.34
5.14
1.00
1.06
3.36
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


165.244
133.387
131.982
129.726
129.454
129.100
128.765
128.502
128.294
128.255
118.080
71.362
43.665
18.355


CN
OBz

4m


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.951
7.933
7.930
7.510
7.497
7.492
7.487
7.477
7.473
7.470
7.371
7.366
7.351
7.351
7.332
7.264
7.261
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7.248
7.243
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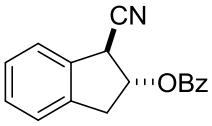
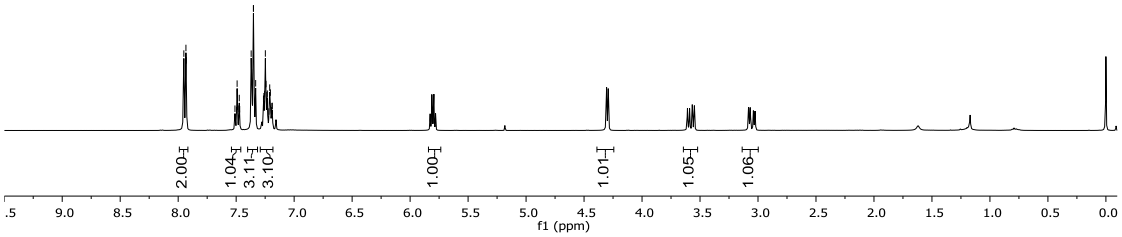
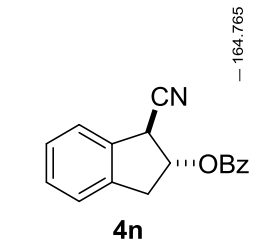
7.231
7.218
7.211
7.205
7.196
7.192
7.188


CN
OBz

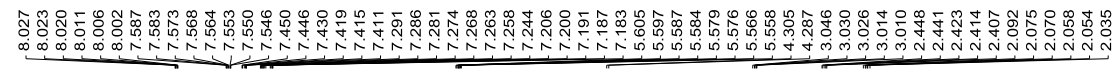
4n


2.00
1.04
3.11
3.10
1.00
1.01
1.05
1.06
f1 (ppm)


CN
OBz

4n

164.765
138.210
133.277
132.534
128.739
128.384
128.079
127.473
127.037
124.255
123.566
117.565
76.819
40.236
37.067
f1 (ppm)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8.020
8.011
8.006
8.002
7.587
7.583
7.573
7.568
7.564
7.553
7.550
7.546
7.450
7.446
7.430
7.419
7.415
7.411
7.291
7.286
7.281
7.274
7.268
7.263
7.258
7.244
7.206
7.200
7.191
7.187
7.183
5.605
5.597
5.587
5.584
5.579
5.576
5.566
5.558
4.305
4.287
3.046
3.030
3.026
3.014
3.010
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2.441
2.423
2.414
2.407
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2.075
2.070
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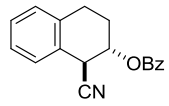
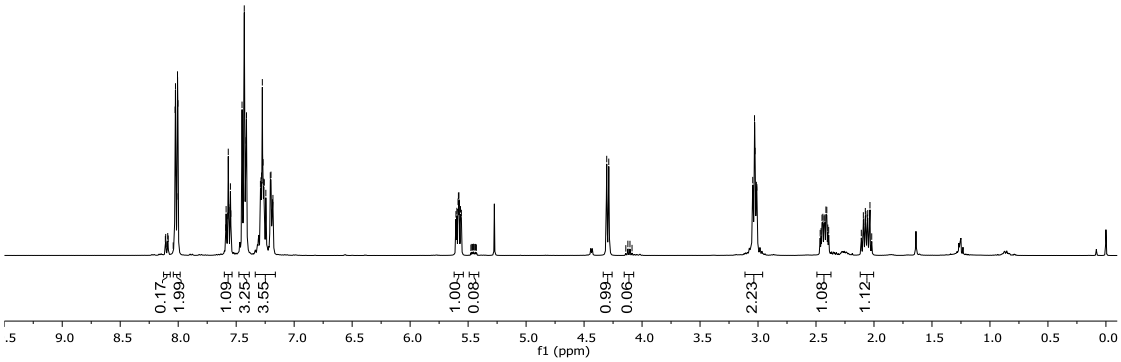
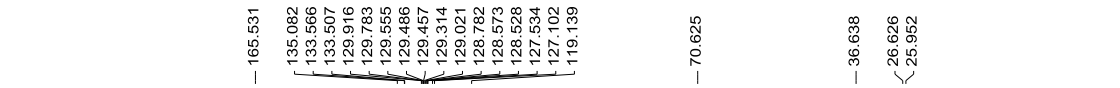
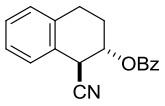
2.054
2.035


OBz
CN

4o

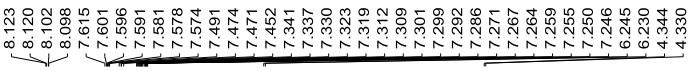

0.17
1.99
1.09
3.25
3.55
1.00
0.08
0.99
0.06
2.23
1.08
1.12
f1 (ppm)


165.531
135.082
133.566
133.507
129.916
129.783
129.555
129.486
129.457
129.314
129.021
128.782
128.573
128.528
127.534
127.102
119.139
70.625
36.638
26.626
25.952


OBz
CN

4o

f1 (ppm)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8.098
7.615
7.601
7.596
7.591
7.581
7.578
7.574
7.491
7.474
7.471
7.452
7.341
7.337
7.330
7.323
7.319
7.312
7.309
7.301
7.299
7.292
7.286
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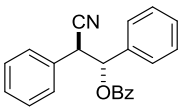
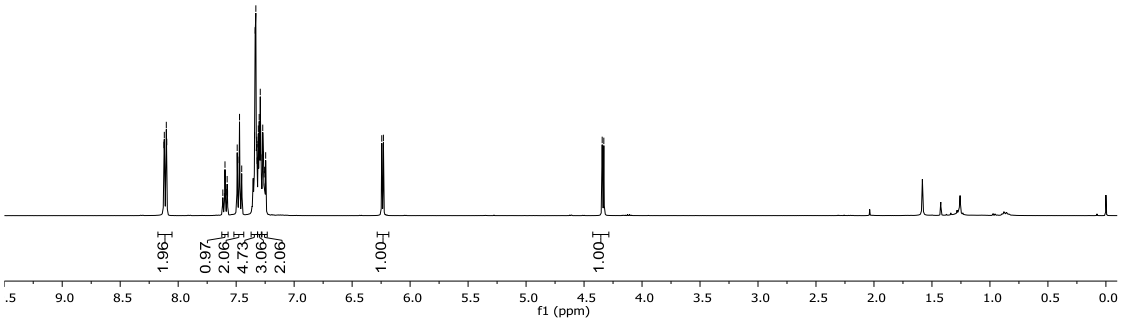
7.267
7.264
7.259
7.255
7.250
7.246
6.245
6.230
4.344
4.330


CN
OBz

4p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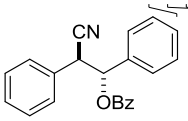
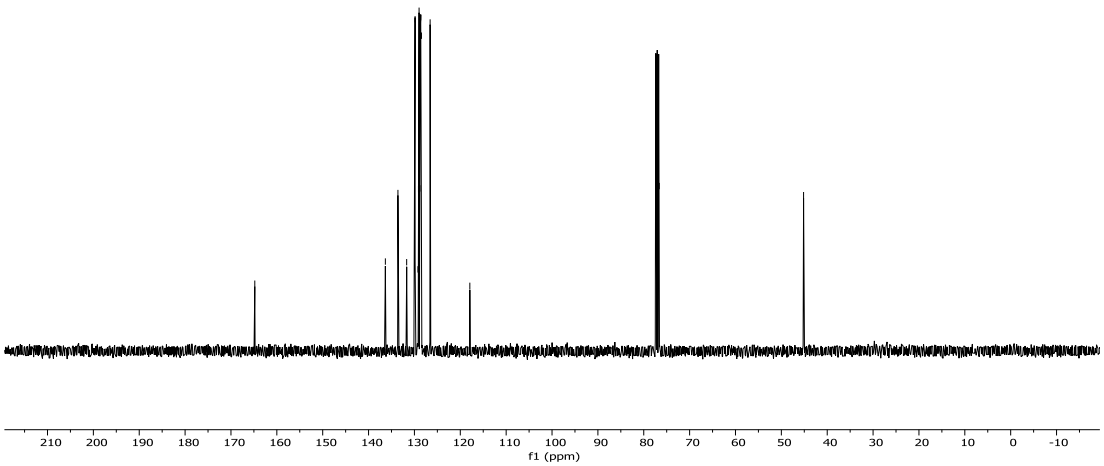
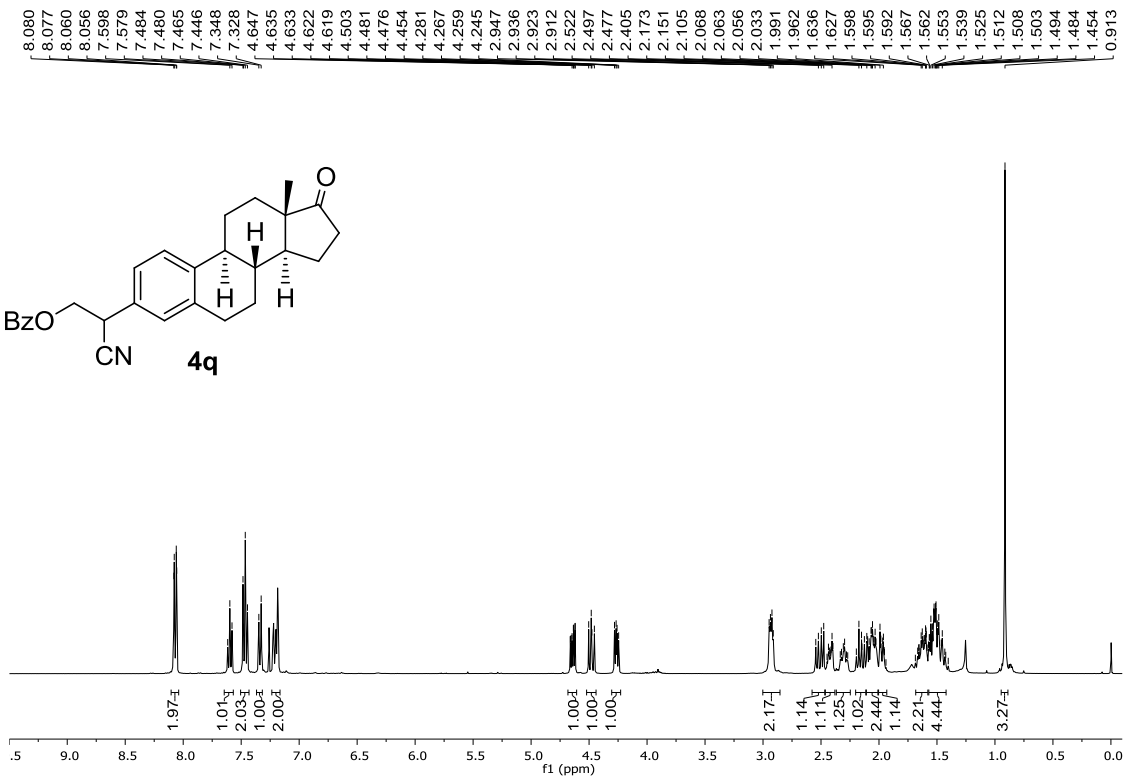
0.97
2.06
4.73
3.06
2.06
1.00
1.00
f1 (ppm)


164.805
136.335
133.597
131.690
129.859
129.230
129.118
128.987
128.805
128.706
128.627
128.468
126.578
117.919
76.629
45.154


CN
OBz

4p


f1 (ppm)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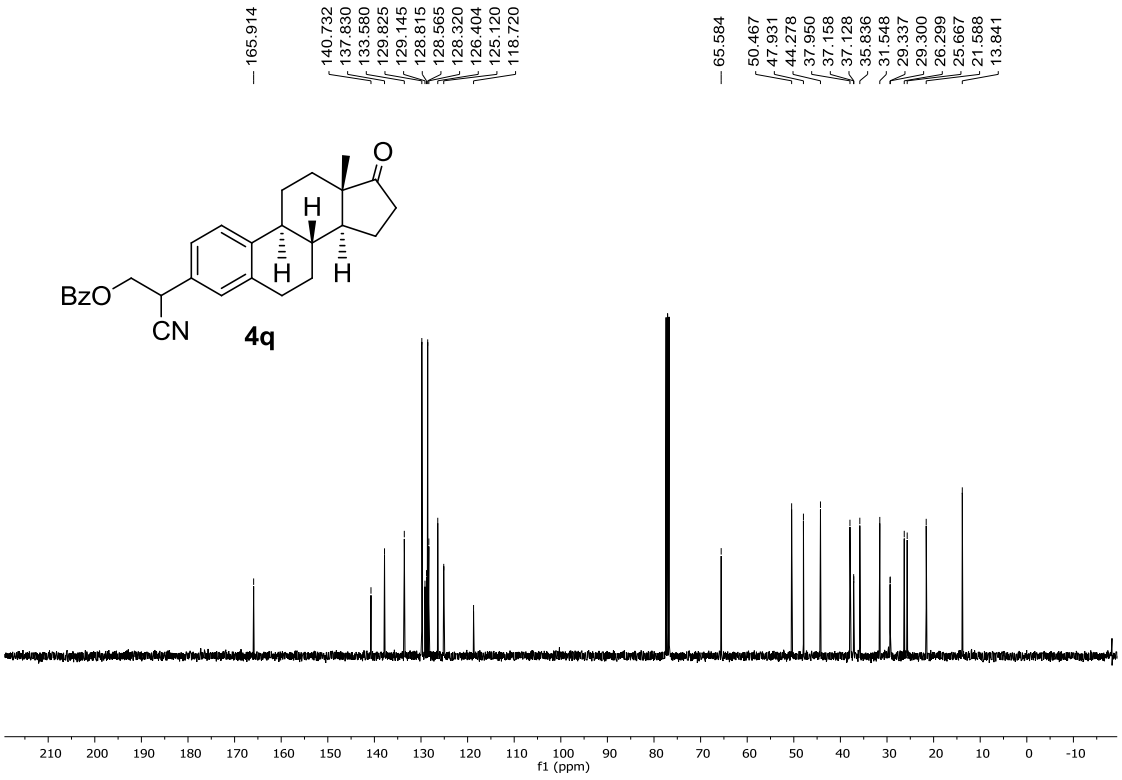
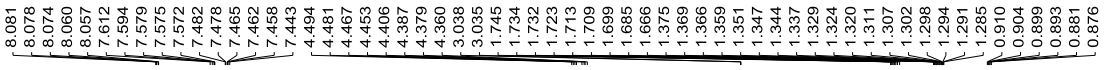
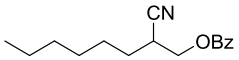
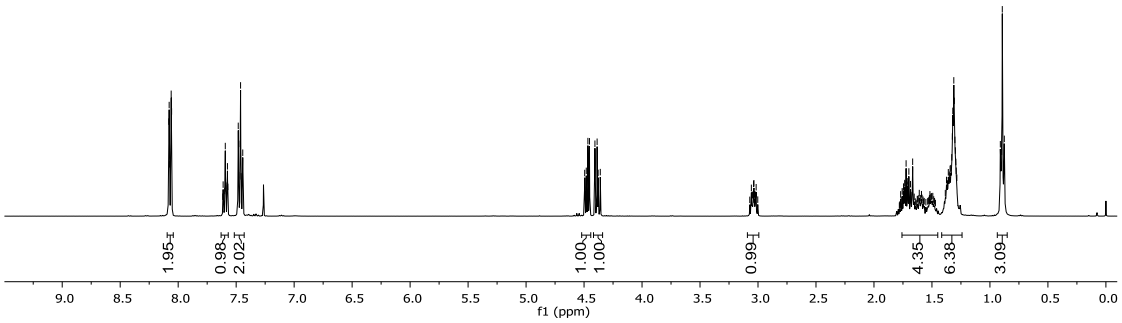
8.060
8.056
7.598
7.579
7.484
7.480
7.465
7.446
7.348
7.328
4.647
4.635
4.633
4.622
4.619
4.503
4.481
4.476
4.454
4.281
4.267
4.259
4.245
2.947
2.936
2.923
2.912
2.522
2.497
2.477
2.405
2.173
2.151
2.105
2.068
2.063
2.056
2.033
1.991
1.962
1.636
1.627
1.598
1.595
1.592
1.567
1.562
1.553
1.539
1.525
1.512
1.508
1.503
1.494
1.484
1.454
0.913
O
H
H
H
BzO
CN
4q
1.97
1.01
2.03
1.00
2.00
1.00
1.00
1.00
2.17
1.14
1.11
1.25
1.02
2.44
1.14
2.21
4.44
3.27
f1 (ppm)

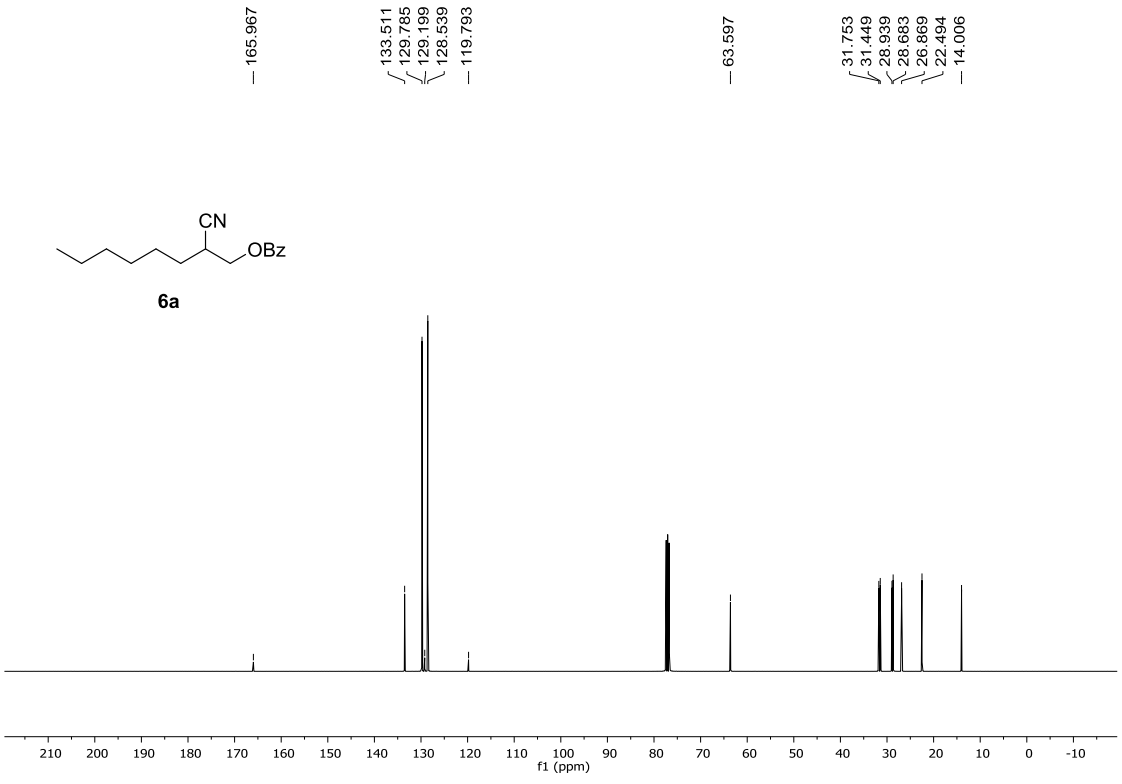

165.914
140.732
137.830
133.580
129.825
129.145
128.815
128.565
128.320
126.404
125.120
118.720
65.584
50.467
47.931
44.278
37.950
37.158
37.128
35.836
31.548
29.337
29.300
26.299
25.667
21.588
13.841
O
H
H
H
BzO
CN
4q
f1 (ppm)


8.081
8.078
8.074
8.060
8.057
7.612
7.594
7.579
7.575
7.572
7.482
7.478
7.465
7.462
7.458
7.443
4.494
4.481
4.467
4.453
4.406
4.387
4.379
4.360
3.038
3.035
1.745
1.734
1.732
1.723
1.713
1.709
1.699
1.685
1.666
1.375
1.369
1.366
1.359
1.351
1.347
1.344
1.337
1.329
1.324
1.320
1.311
1.307
1.302
1.298
1.294
1.291
1.285
0.910
0.904
0.899
0.893
0.881
0.876


CN
OBz

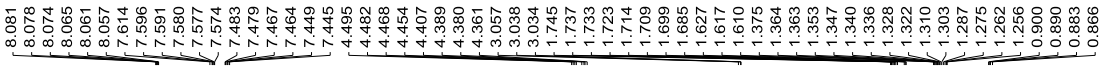
6a

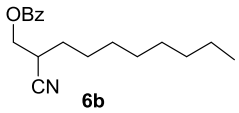

1.95
0.98
2.02
1.00
1.00
0.99
4.35
6.38
3.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


165.967
133.511
129.785
129.199
128.539
119.793
63.597
31.753
31.449
28.939
28.683
26.869
22.494
14.006
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

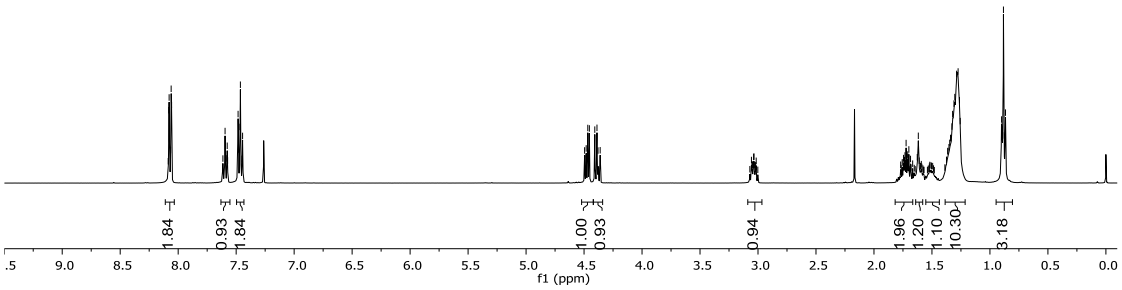
CN
OBz

6a

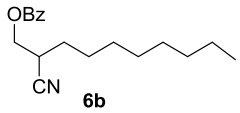

8.081
8.078
8.074
8.065
8.061
8.057
7.614
7.596
7.591
7.580
7.577
7.574
7.483
7.479
7.467
7.464
7.449
7.445
4.495
4.482
4.468
4.454
4.407
4.389
4.380
4.361
3.057
3.038
3.034
1.745
1.737
1.733
1.723
1.714
1.709
1.699
1.685
1.627
1.617
1.610
1.375
1.364
1.363
1.353
1.347
1.340
1.336
1.328
1.322
1.310
1.303
1.287
1.275
1.262
1.256
0.900
0.890
0.883
0.866


OBz
CN

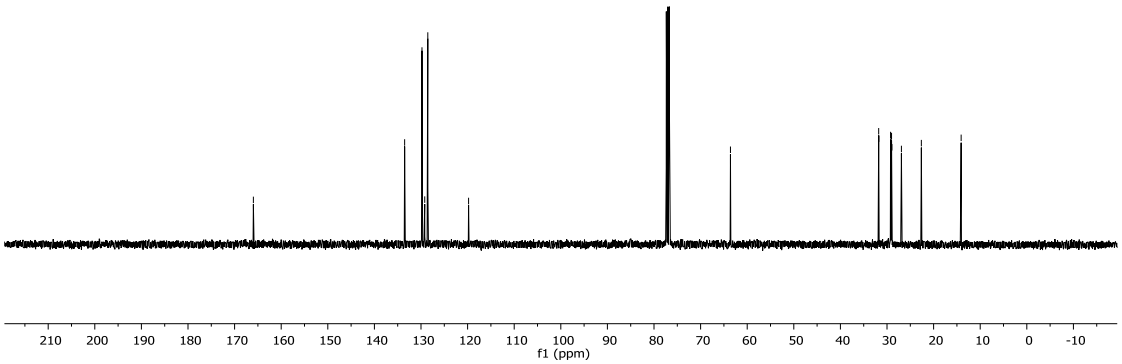
6b

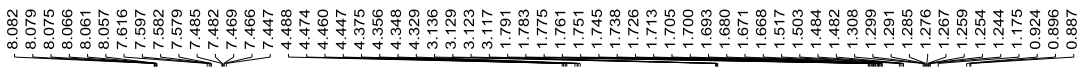

1.84
0.93
1.84
1.00
0.93
0.94
1.96
1.20
1.10
10.30
3.18
f1 (ppm)

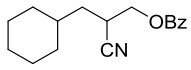

165.969
133.511
129.790
129.199
128.539
119.791
63.595
31.786
31.757
29.238
29.130
29.026
28.947
26.908
22.631
14.092


OBz
CN

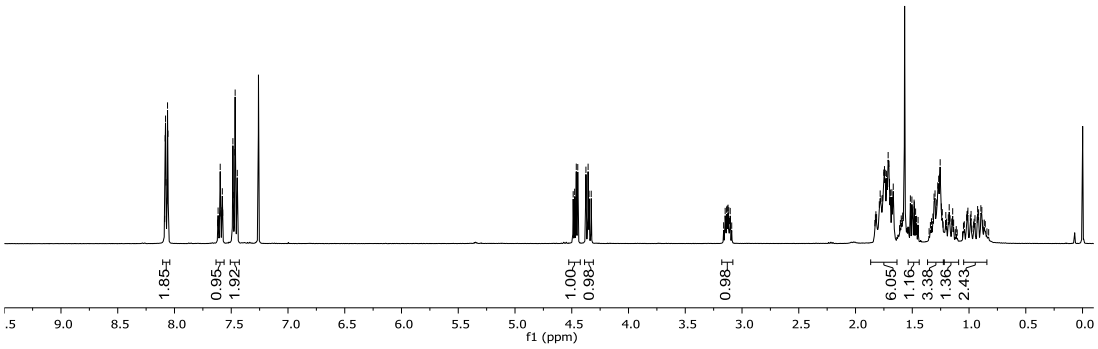
6b


f1 (ppm)

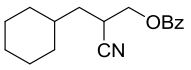

8.082
8.079
8.075
8.066
8.061
8.057
7.616
7.597
7.582
7.579
7.485
7.482
7.469
7.466
7.447
4.488
4.474
4.460
4.447
4.375
4.356
4.348
4.329
3.136
3.129
3.123
3.117
1.791
1.783
1.775
1.761
1.751
1.745
1.738
1.726
1.713
1.705
1.700
1.693
1.680
1.671
1.668
1.517
1.503
1.484
1.482
1.308
1.299
1.291
1.285
1.276
1.267
1.259
1.254
1.244
1.175
0.924
0.896
0.887


OBz
CN

6c

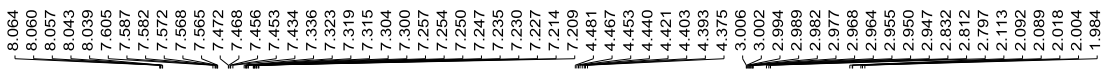

1.85
0.95
1.92
1.00
0.98
0.98
6.05
1.16
3.38
1.36
2.43
f1 (ppm)


165.993
133.512
129.796
129.202
128.543
119.979
63.958
36.319
35.185
33.444
32.296
29.282
26.255
25.975
25.850


OBz
CN

6c

f1 (ppm)


8.064
8.060
8.057
8.043
8.039
7.605
7.587
7.582
7.572
7.568
7.565
7.472
7.468
7.456
7.453
7.434
7.336
7.323
7.319
7.315
7.304
7.300
7.257
7.254
7.250
7.247
7.235
7.230
7.227
7.214
7.209
4.481
4.467
4.453
4.440
4.421
4.403
4.393
4.375
3.006
3.002
2.994
2.989
2.982
2.977
2.968
2.964
2.955
2.950
2.947
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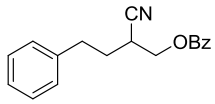
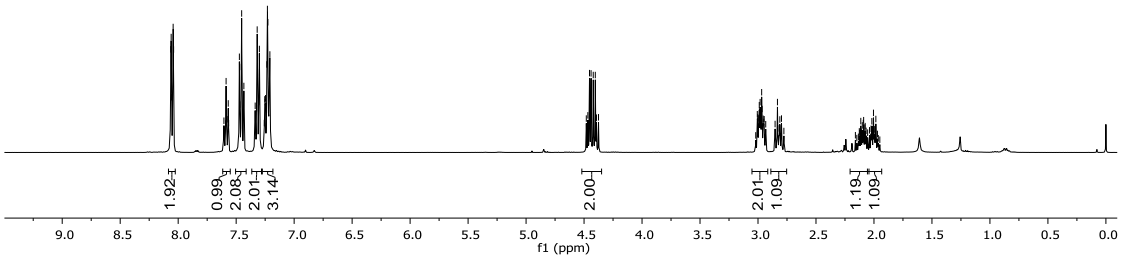
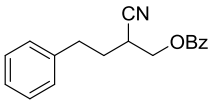
2.113
2.092
2.089
2.018
2.004
1.984


CN
OBz

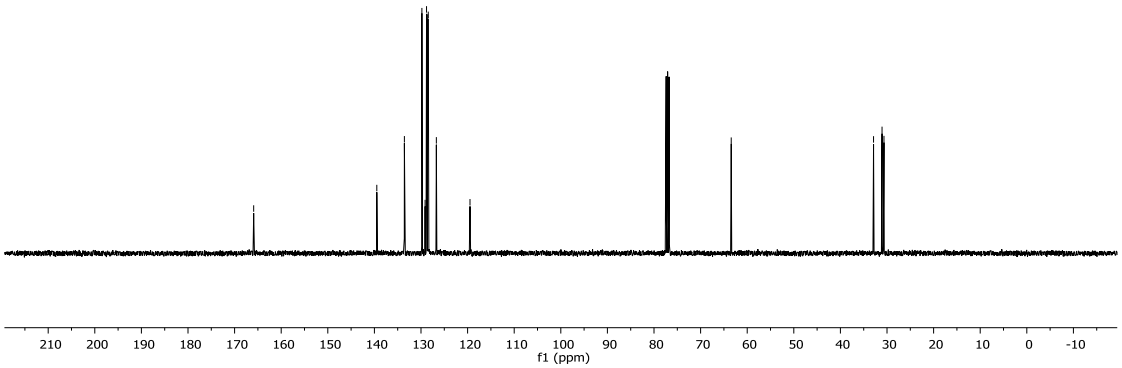
6d

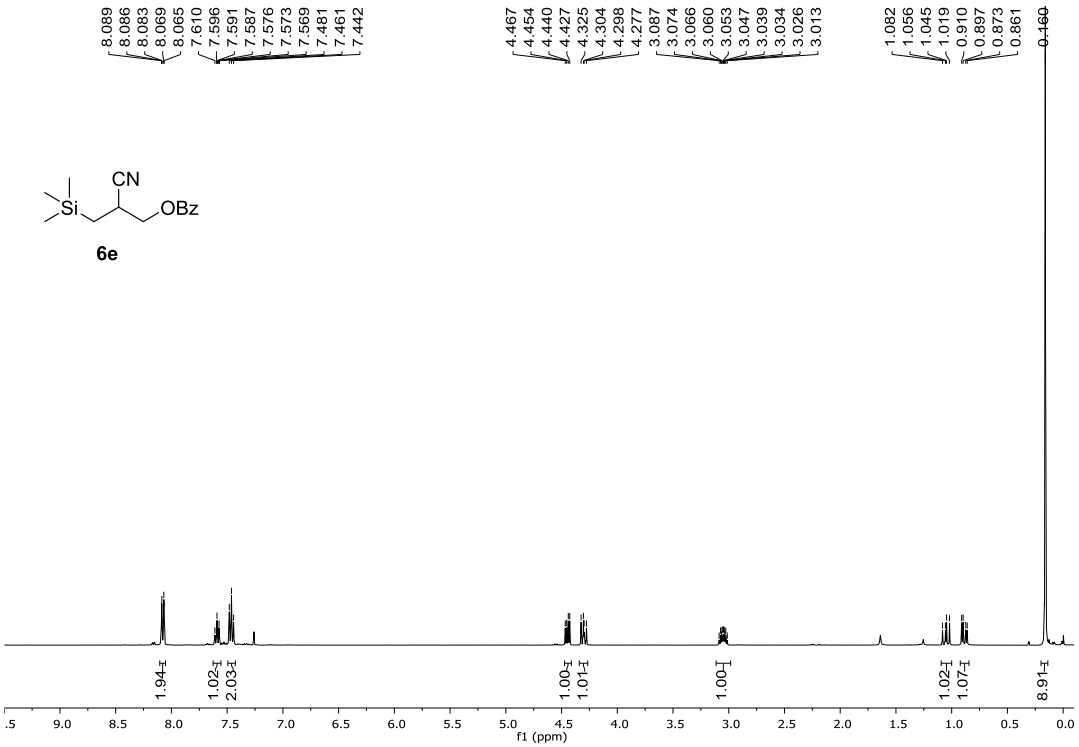

1.92
0.99
2.08
2.01
3.14
2.00
2.01
1.09
1.19
1.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


165.905
139.482
133.565
129.807
129.123
128.812
128.567
128.448
126.704
119.484
63.430
32.890
31.064
30.653

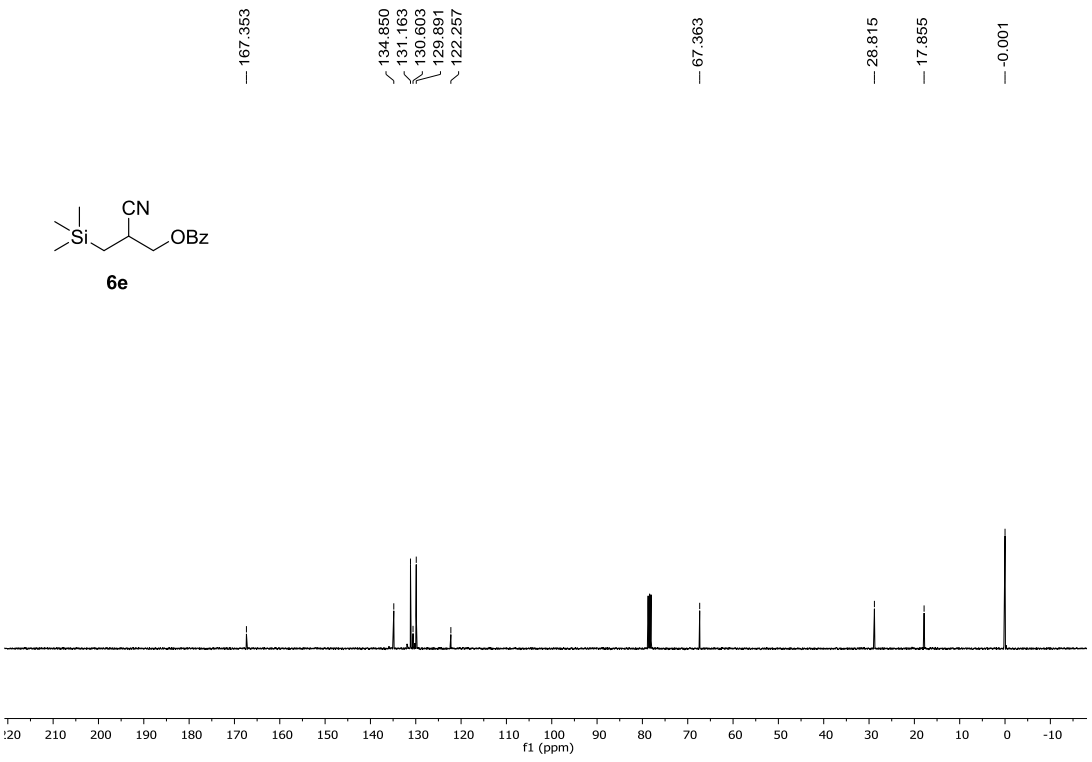

CN
OBz

6d

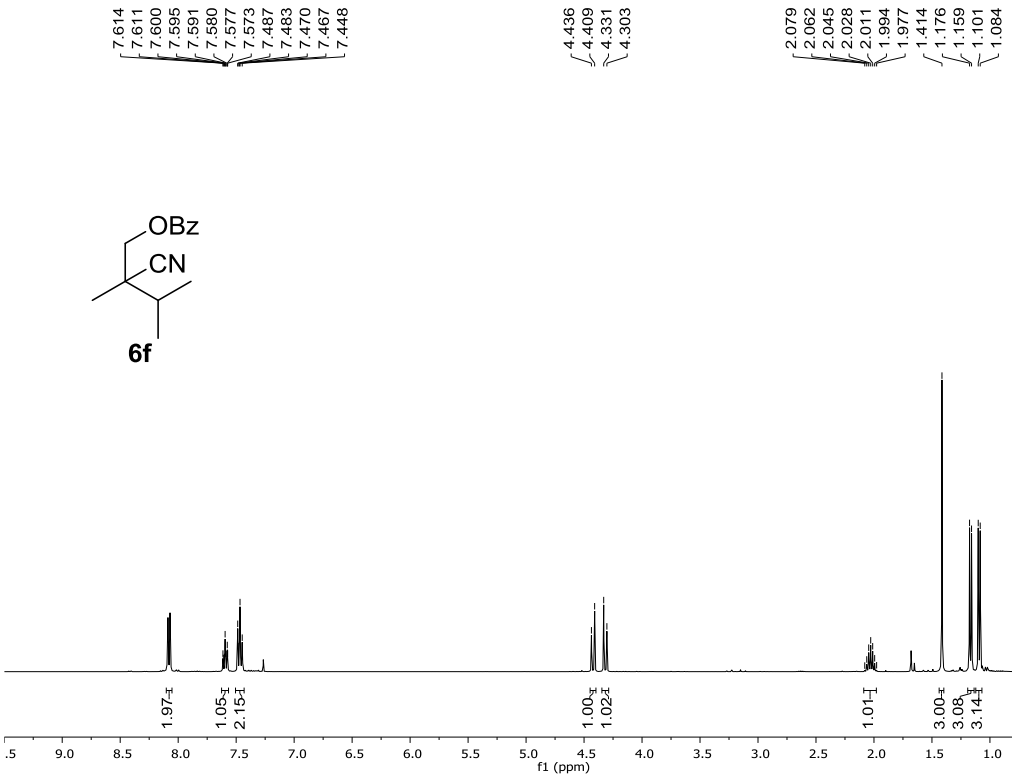

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

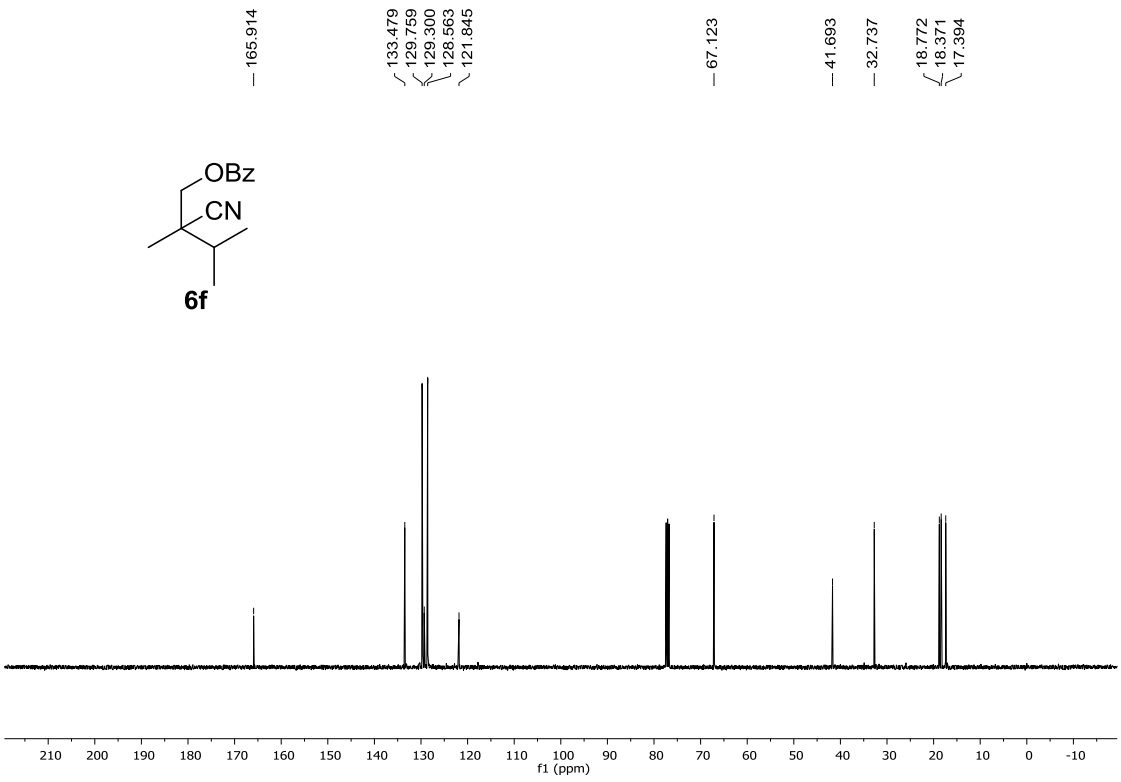

8.089
8.086
8.083
8.069
8.065
7.610
7.596
7.591
7.587
7.576
7.573
7.569
7.481
7.461
7.442
4.467
4.454
4.440
4.427
4.325
4.304
4.298
4.277
3.087
3.074
3.066
3.060
3.053
3.047
3.039
3.034
3.026
3.013
1.082
1.056
1.045
1.019
0.910
0.897
0.873
0.861
0.160
CN
Si
OBz
1.94
1.02
2.03
1.00
1.01
1.00
1.02
1.07
8.91
f1 (ppm)

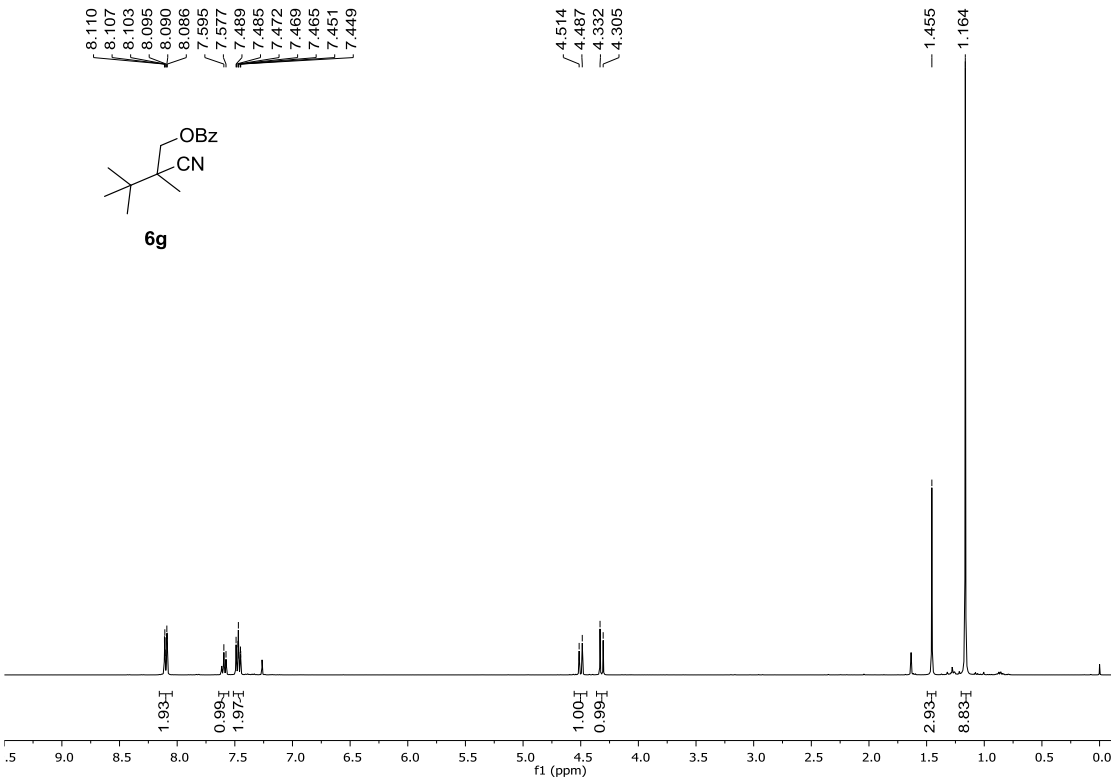
6e

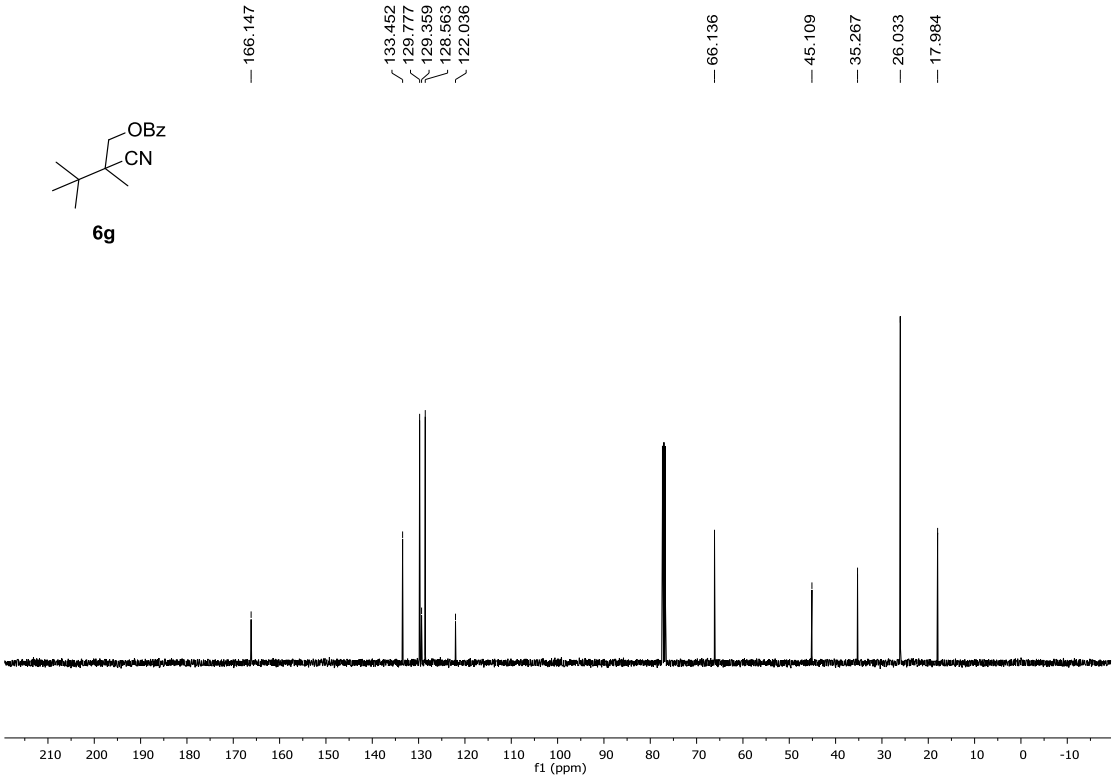

167.353
134.850
131.163
130.603
129.891
122.257
67.363
28.815
17.855
-0.001
CN
Si
OBz
f1 (ppm)

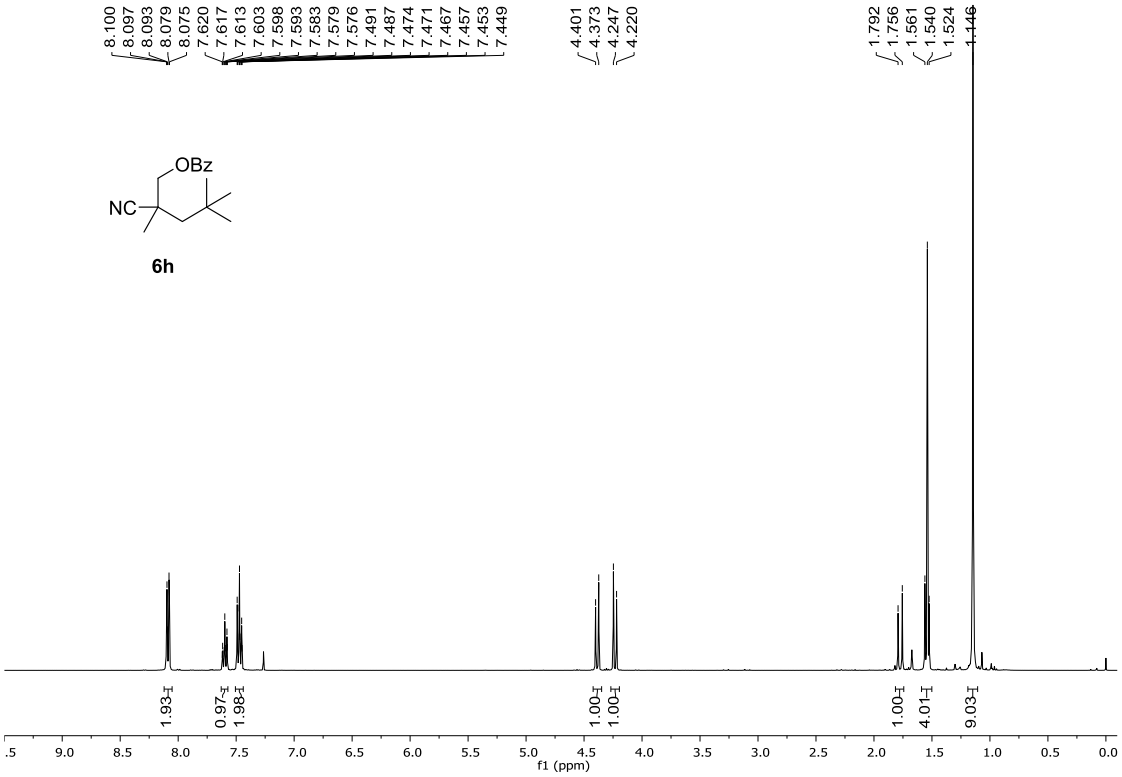
6e


7.614
7.611
7.600
7.595
7.591
7.580
7.577
7.573
7.487
7.483
7.470
7.467
7.448
4.436
4.409
4.331
4.303
2.079
2.062
2.045
2.028
2.011
1.994
1.977
1.414
1.176
1.159
1.101
1.084
OBz
CN
6f
1.97
1.05
2.15
1.00
1.02
1.01
3.00
3.08
3.14
f1 (ppm)

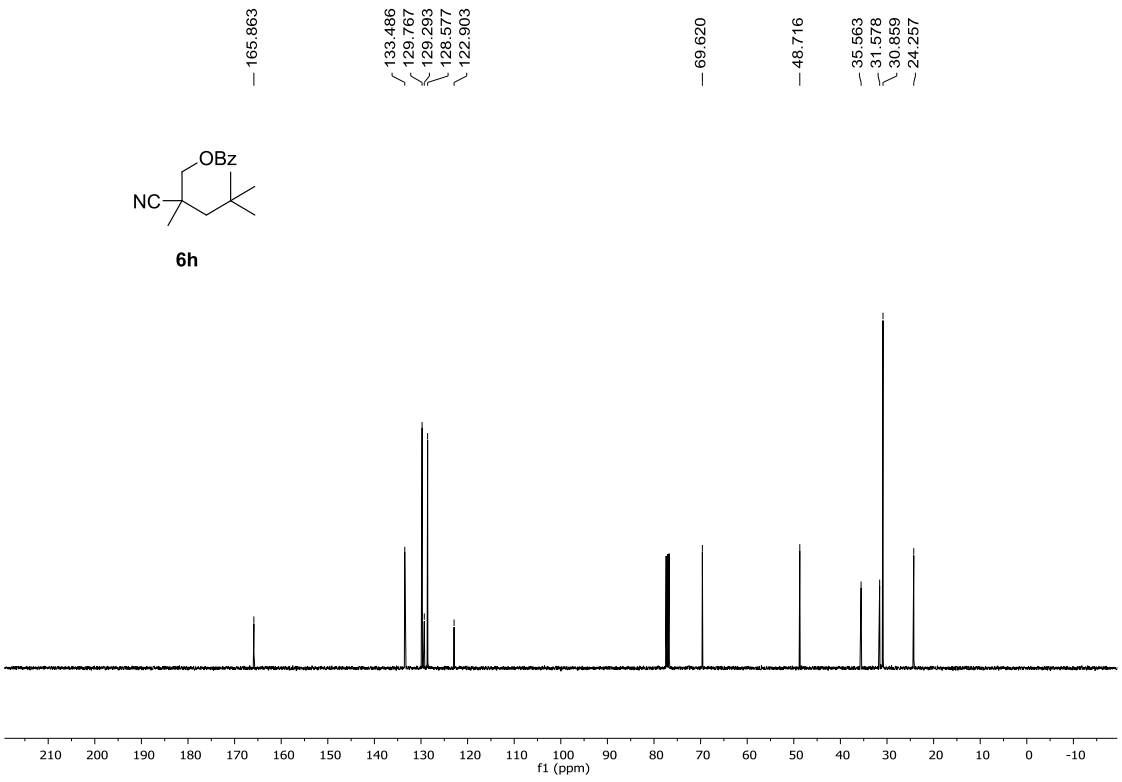

165.914
133.479
129.759
129.300
128.563
121.845
67.123
41.693
32.737
18.772
18.371
17.394
OBz
CN
6f
f1 (ppm)


8.110
8.107
8.103
8.095
8.090
8.086
7.595
7.577
7.489
7.485
7.472
7.469
7.465
7.451
7.449
4.514
4.487
4.332
4.305
1.455
1.164
OBz
CN
6g
1.93
0.99
1.97
1.00
0.99
2.93
8.83
f1 (ppm)


166.147
133.452
129.777
129.359
128.563
122.036
66.136
45.109
35.267
26.033
17.984
OBz
CN
6g
f1 (ppm)

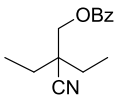

8.100
8.097
8.093
8.079
8.075
7.620
7.617
7.613
7.603
7.598
7.593
7.583
7.579
7.576
7.491
7.487
7.474
7.471
7.467
7.457
7.453
7.449
4.401
4.373
4.247
4.220
1.792
1.756
1.561
1.540
1.524
1.146
OBz
NC
1.93
0.97
1.98
1.00
1.00
1.00
4.01
9.03
f1 (ppm)

6h

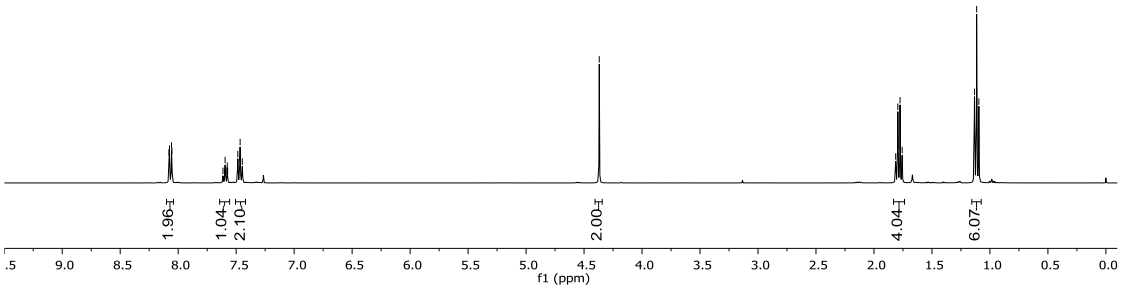

165.863
133.486
129.767
129.293
128.577
122.903
69.620
48.716
35.563
31.578
30.859
24.257
OBz
NC
f1 (ppm)

6h

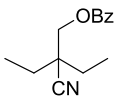

8.078
8.078
8.075
8.058
8.054
7.614
7.600
7.595
7.591
7.580
7.577
7.573
7.486
7.469
7.466
7.447
4.369
1.813
1.794
1.775
1.757
1.133
1.115
1.096


OBz
CN

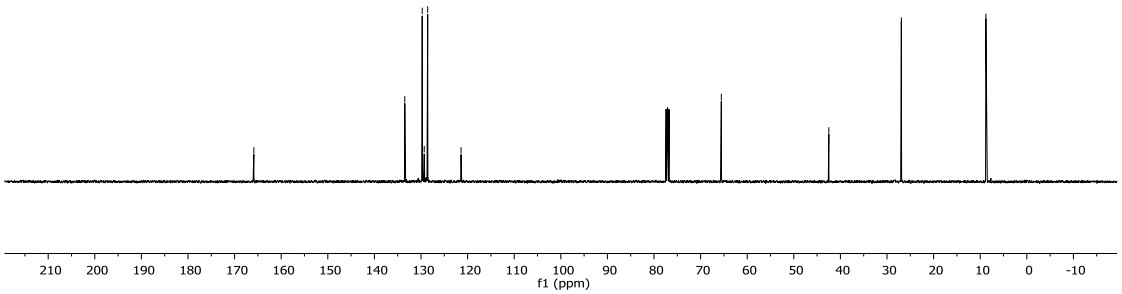
6i

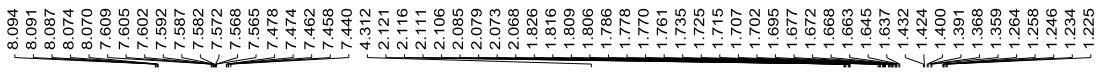

1.96
1.04
2.10
2.00
4.04
6.07
f1 (ppm)


165.868
133.478
129.742
129.300
128.564
121.406
65.552
42.486
26.922
8.781


OBz
CN

6i


f1 (ppm)


8.094
8.091
8.087
8.074
8.070
7.609
7.605
7.602
7.592
7.587
7.582
7.572
7.568
7.565
7.478
7.474
7.462
7.458
7.440
4.312
2.121
2.116
2.111
2.106
2.085
2.079
2.073
2.068
1.826
1.816
1.809
1.806
1.786
1.778
1.770
1.761
1.735
1.725
1.715
1.707
1.702
1.695
1.677
1.672
1.668
1.663
1.645
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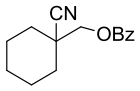
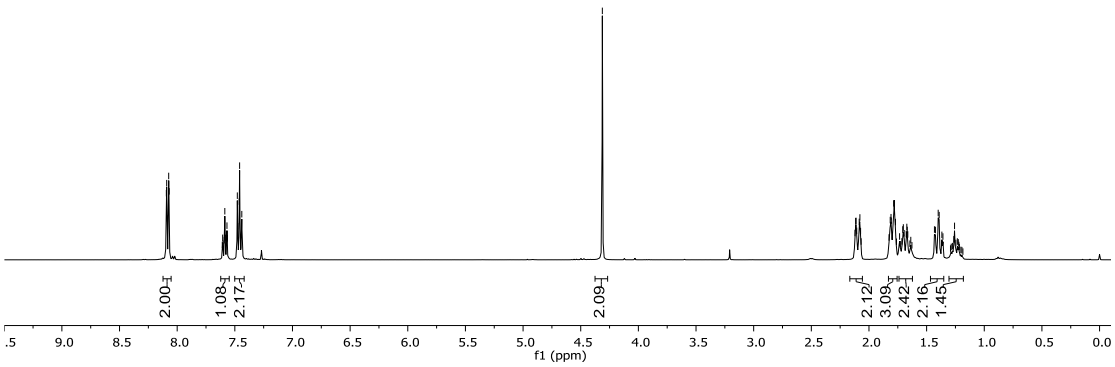
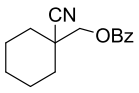
1.359
1.264
1.258
1.246
1.234
1.225


CN
OBz

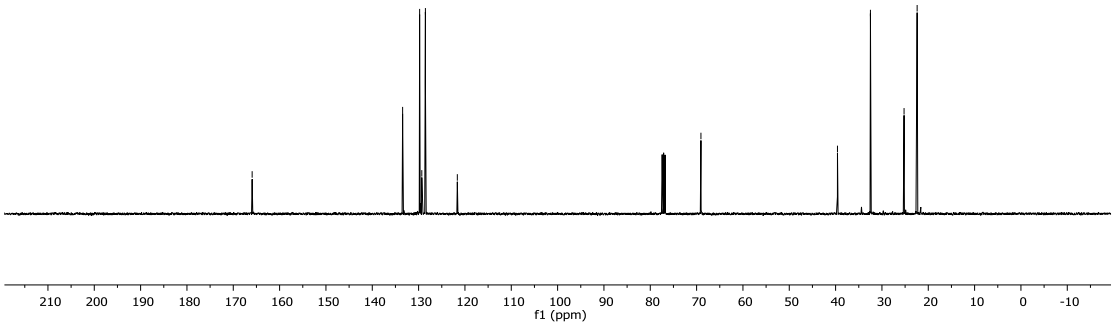
6j

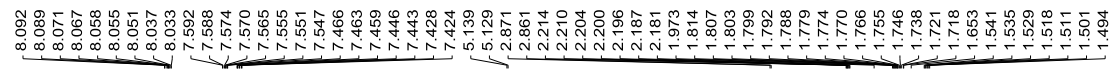

2.00
1.08
2.17
2.09
2.12
3.09
2.42
2.16
1.45
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

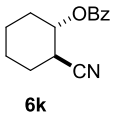

165.925
133.448
129.778
129.310
128.533
121.642
69.065
39.597
32.481
25.226
22.403


CN
OBz

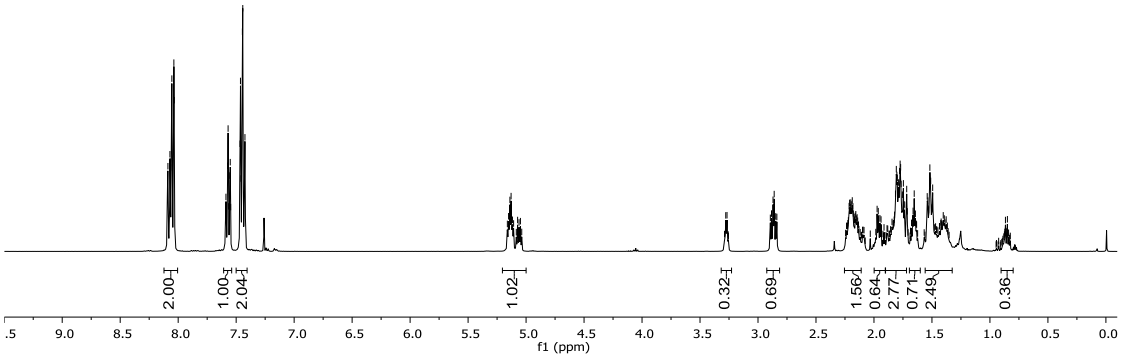
6j


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

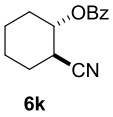

8.092
8.089
8.071
8.067
8.058
8.055
8.051
8.037
8.033
7.592
7.588
7.574
7.570
7.565
7.555
7.551
7.547
7.466
7.463
7.459
7.446
7.443
7.428
7.424
5.139
5.129
2.871
2.861
2.214
2.210
2.204
2.200
2.196
2.187
2.181
1.973
1.814
1.807
1.803
1.799
1.792
1.788
1.779
1.774
1.770
1.766
1.755
1.746
1.738
1.721
1.718
1.653
1.541
1.535
1.529
1.518
1.511
1.501
1.494


OBz
CN

6k

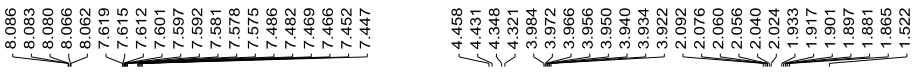

2.00
1.00
2.04
1.02
0.32
0.69
1.56
0.64
2.77
0.71
2.49
0.36
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


165.502
165.373
133.394
133.315
129.801
129.738
129.716
129.636
128.487
128.459
119.878
119.291
71.863
70.718
33.599
33.285
30.156
28.325
27.696
27.285
23.481
23.057
22.651
21.671


OBz
CN

6k

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.086
8.083
8.080
8.066
8.062
7.619
7.615
7.612
7.601
7.597
7.592
7.581
7.578
7.575
7.486
7.482
7.469
7.466
7.452
7.447
4.458
4.431
4.348
4.321
3.984
3.972
3.966
3.956
3.950
3.940
3.934
3.922
2.092
2.076
2.060
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2.040
2.024
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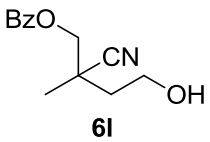
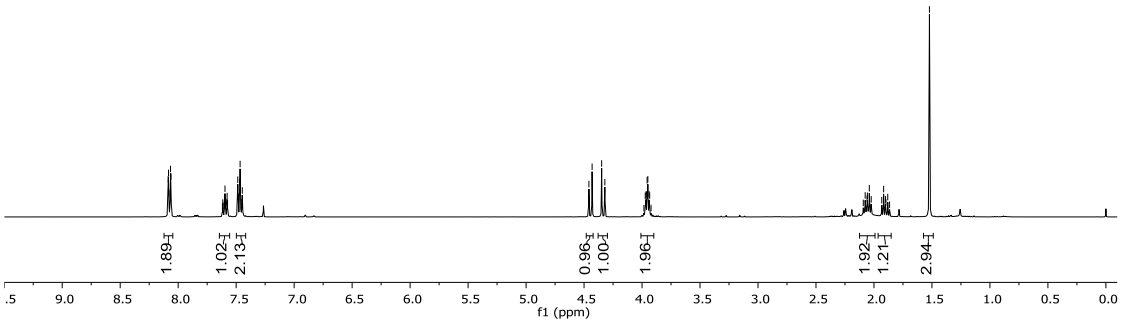
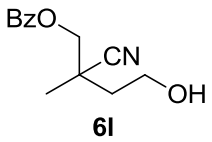
1.917
1.901
1.897
1.881
1.865
1.522


BzO
CN
OH

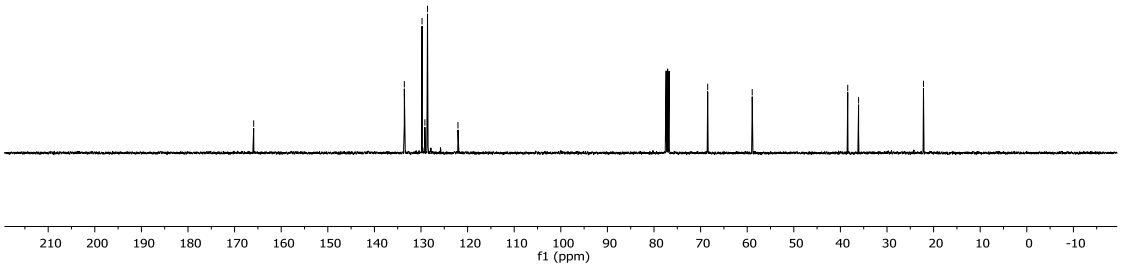
6l

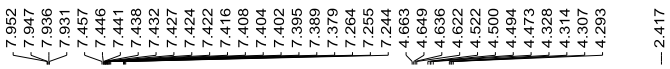

1.89
1.02
2.13
0.96
1.00
1.96
1.92
1.21
2.94
f1 (ppm)

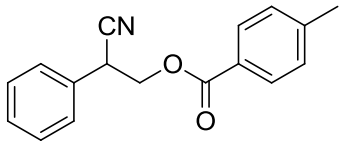

165.906
133.576
129.777
129.165
128.601
122.066
68.481
58.925
38.427
36.098
22.173


BzO
CN
OH

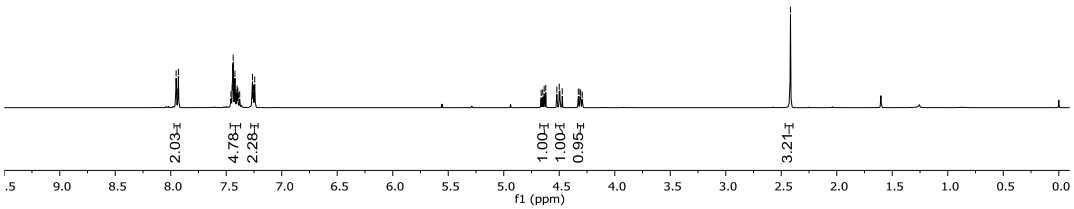
6l

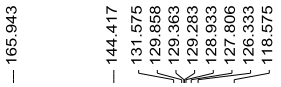

f1 (ppm)

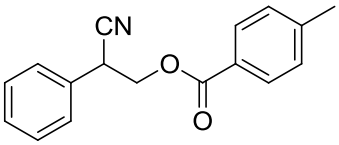

7.952
7.947
7.936
7.931
7.457
7.446
7.441
7.438
7.432
7.427
7.424
7.422
7.416
7.408
7.404
7.402
7.395
7.389
7.379
7.264
7.255
7.244
4.663
4.649
4.636
4.622
4.522
4.500
4.494
4.473
4.328
4.314
4.307
4.293
2.417


CN
O
O

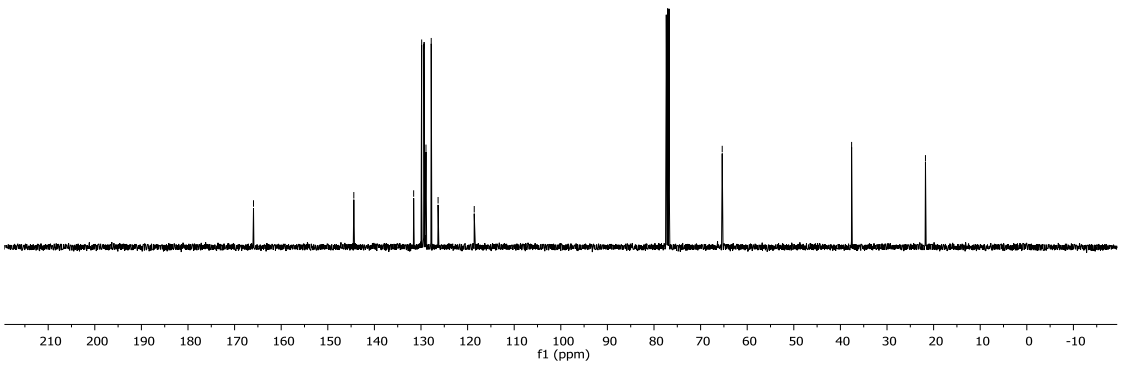
7a

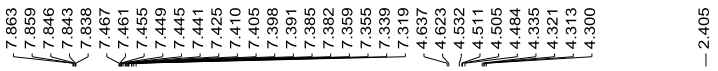

2.03
4.78
2.28
1.00
1.00
0.95
3.21
f1 (ppm)

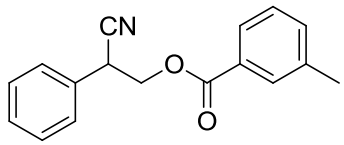

165.943
144.417
131.575
129.858
129.363
129.283
128.933
127.806
126.333
118.575
65.361
37.595
21.746


CN
O
O

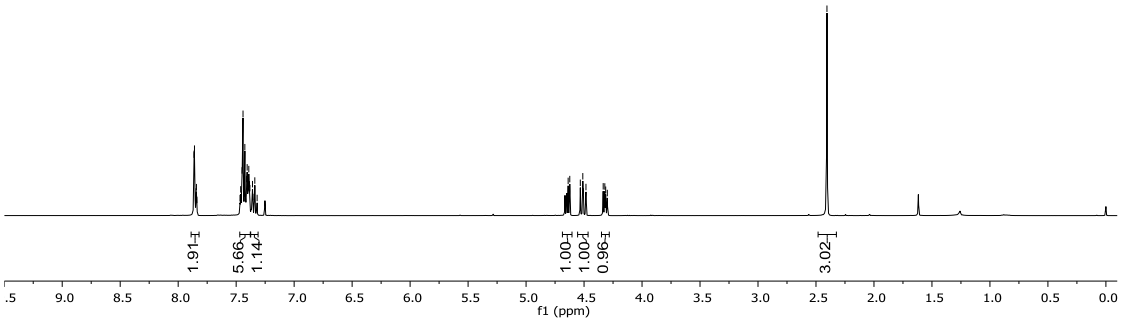
7a


f1 (ppm)

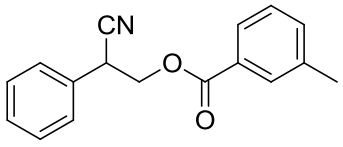

7.863
7.859
7.846
7.843
7.838
7.467
7.461
7.455
7.449
7.445
7.441
7.425
7.410
7.405
7.398
7.391
7.385
7.382
7.359
7.355
7.339
7.319
4.637
4.623
4.532
4.511
4.505
4.484
4.335
4.321
4.313
4.300
2.405


CN
O
O

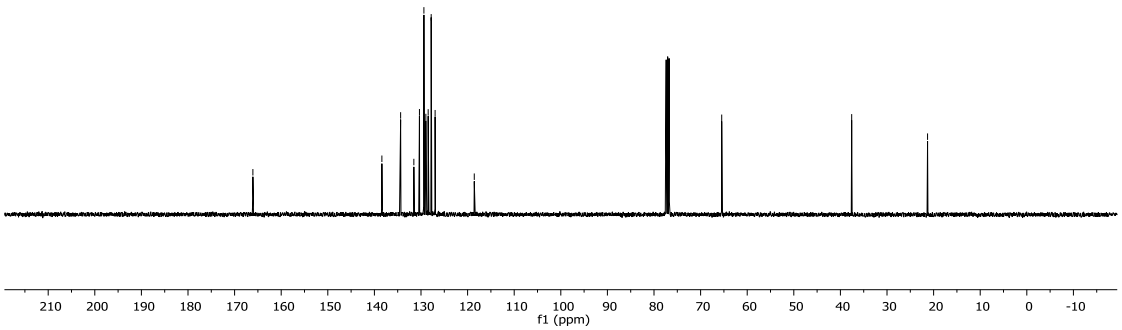
7b

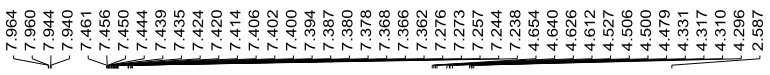

1.91
5.66
1.14
1.00
1.00
0.96
3.02
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

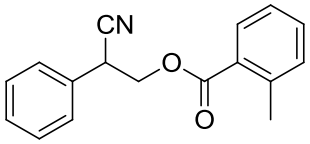

166.074
138.396
134.371
131.535
130.332
129.377
129.006
128.959
128.462
127.814
126.971
118.568
65.470
37.580
21.298


CN
O
O

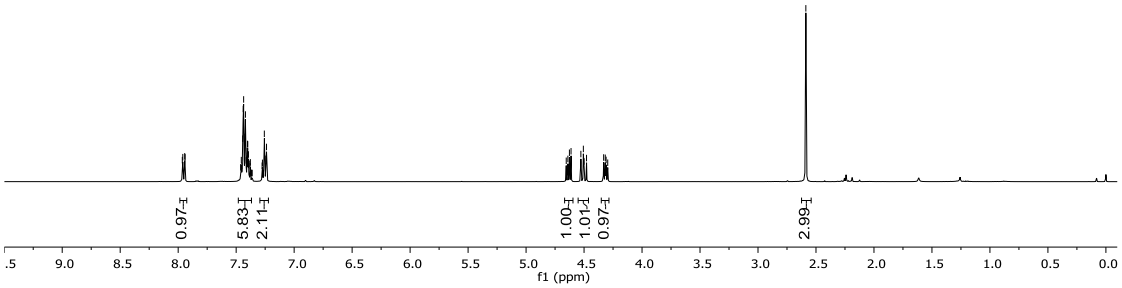
7b

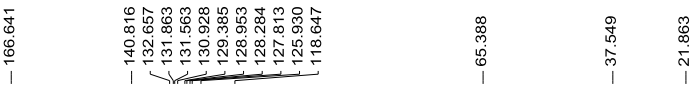

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

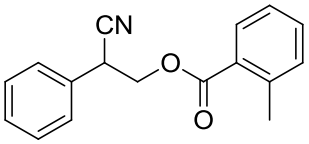

7.964
7.960
7.944
7.940
7.461
7.456
7.450
7.444
7.439
7.435
7.424
7.420
7.414
7.406
7.402
7.400
7.394
7.387
7.380
7.378
7.368
7.366
7.362
7.276
7.273
7.257
7.244
7.238
4.654
4.640
4.626
4.612
4.527
4.506
4.500
4.479
4.331
4.317
4.310
4.296
2.587


CN
O
O

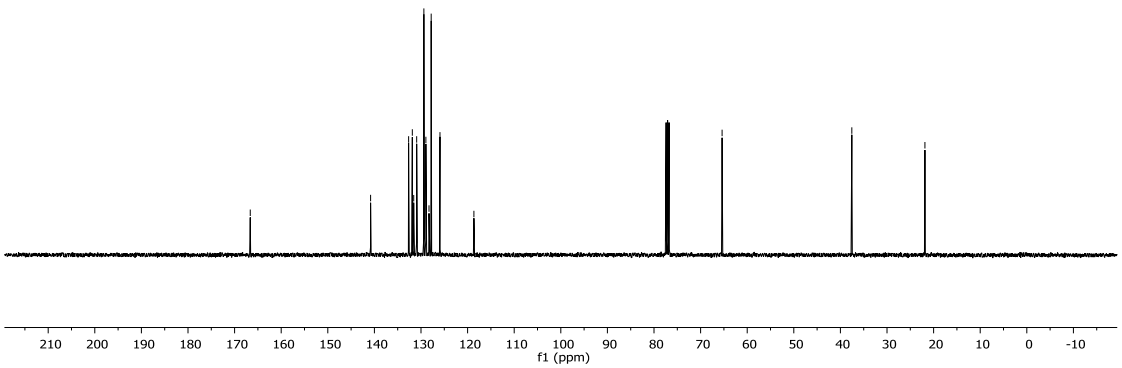
7c

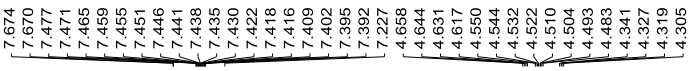

0.97
5.83
2.11
1.00
1.01
0.97
2.99
f1 (ppm)

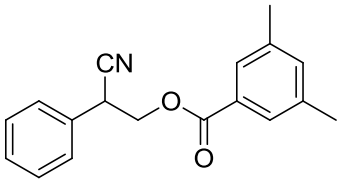

166.641
140.816
132.657
131.863
131.563
130.928
129.385
128.953
128.284
127.813
125.930
118.647
65.388
37.549
21.863


CN
O
O

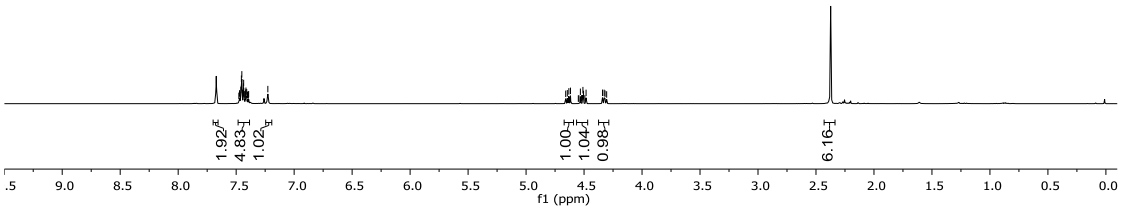
7c

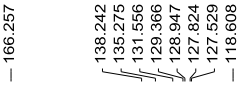

f1 (ppm)

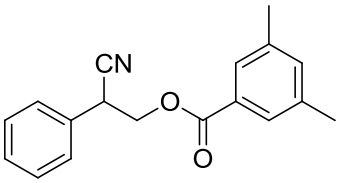

7.674
7.670
7.477
7.471
7.465
7.459
7.455
7.451
7.446
7.441
7.438
7.435
7.430
7.422
7.418
7.416
7.409
7.402
7.395
7.392
7.227
4.658
4.644
4.631
4.617
4.550
4.544
4.532
4.522
4.510
4.504
4.493
4.483
4.341
4.327
4.319
4.305


CN
O
O

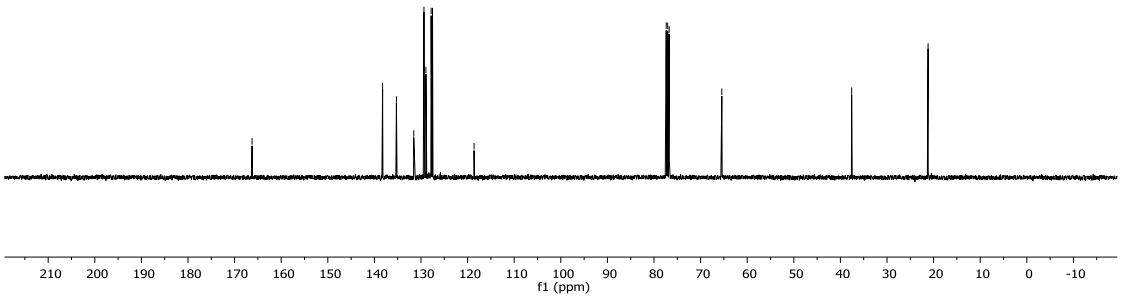
7d


1.92
4.83
1.02
1.00
1.04
0.98
6.16
f1 (ppm)

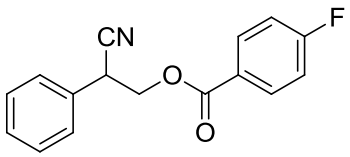

166.257
138.242
135.275
131.556
129.366
128.947
127.824
127.529
118.608
77.377
77.060
76.743
65.446
37.589
21.186


CN
O
O

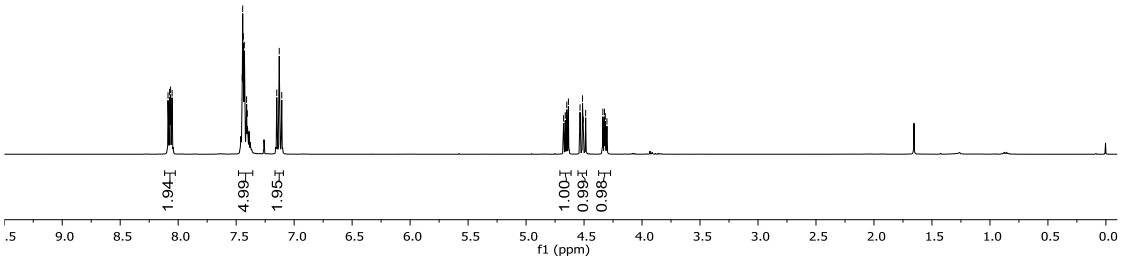
7d

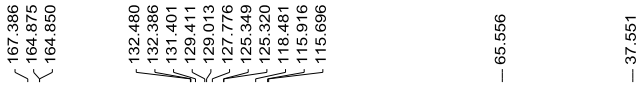

f1 (ppm)

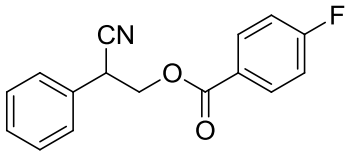

8.088
8.074
8.070
8.065
8.052
7.447
7.444
7.438
7.430
7.410
7.404
7.150
7.128
7.107
4.676
4.662
4.649
4.635
4.535
4.513
4.507
4.486
4.338
4.324
4.317
4.303


CN
O
O
F

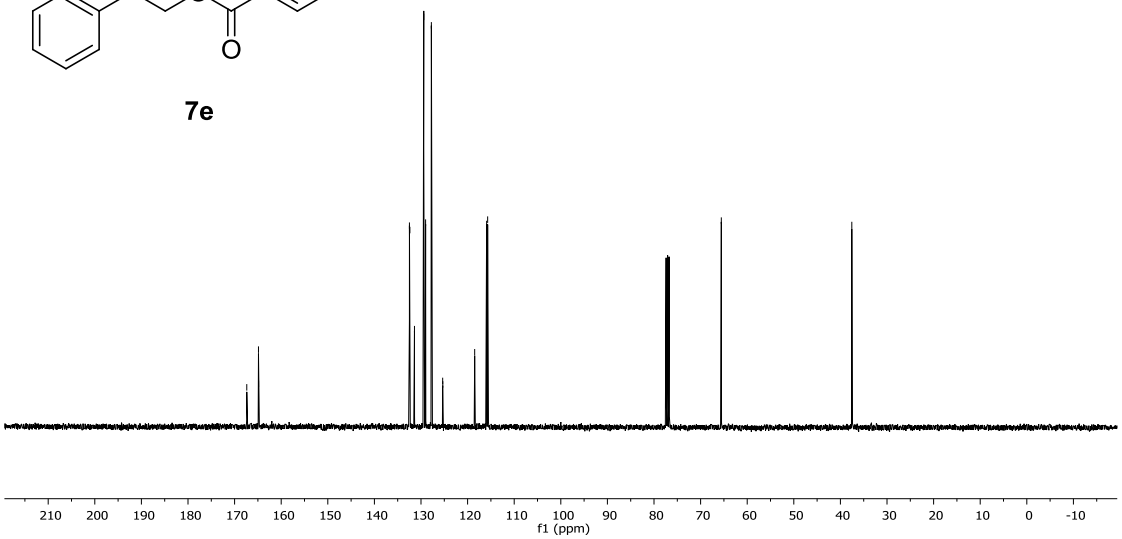
7e

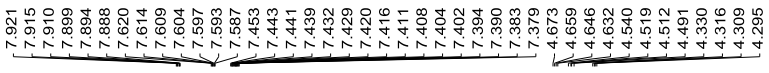

1.94
4.99
1.95
1.00
0.99
0.98
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

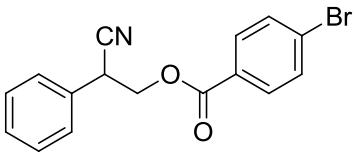

167.386
164.875
164.850
132.480
132.386
131.401
129.411
129.013
127.776
125.349
125.320
118.481
115.916
115.696
65.556
37.551


CN
O
O
F

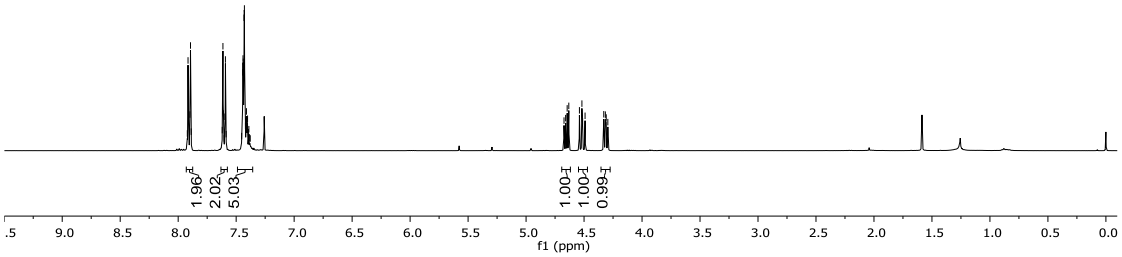
7e


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

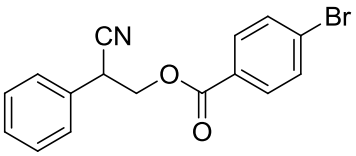

7.921
7.915
7.910
7.899
7.894
7.888
7.620
7.614
7.609
7.604
7.597
7.593
7.587
7.453
7.443
7.441
7.439
7.432
7.429
7.420
7.416
7.411
7.408
7.404
7.402
7.394
7.390
7.383
7.379
4.673
4.659
4.646
4.632
4.540
4.519
4.512
4.491
4.330
4.316
4.309
4.295


CN
O
O
Br

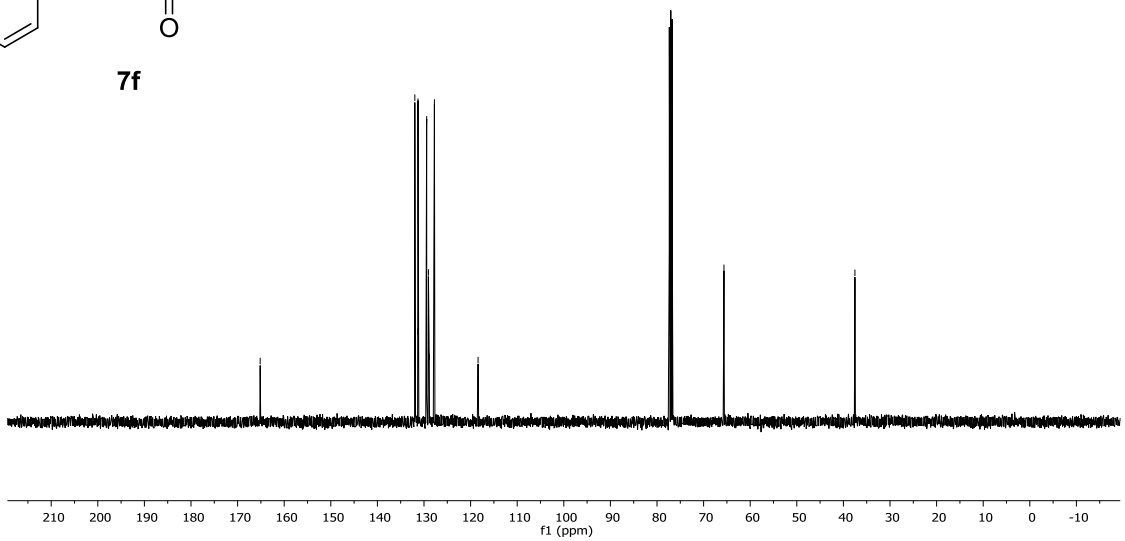
7f

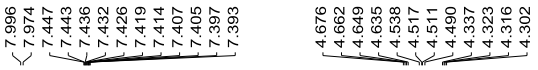

1.96
2.02
5.03
1.00
1.00
0.99
f1 (ppm)

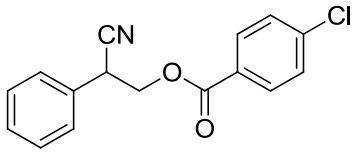

165.156
131.969
131.317
131.287
129.427
129.046
128.867
127.957
127.766
118.397
65.633
37.529


CN
O
O
Br

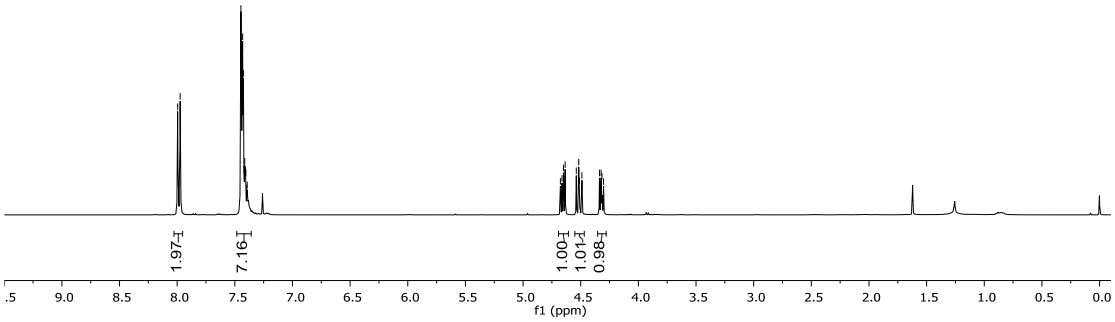
7f


f1 (ppm)

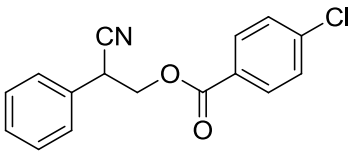

7.996
7.974
7.447
7.443
7.436
7.432
7.426
7.419
7.414
7.407
7.405
7.397
7.393
4.676
4.662
4.649
4.635
4.538
4.517
4.511
4.490
4.337
4.323
4.316
4.302


CN
O
O
Cl

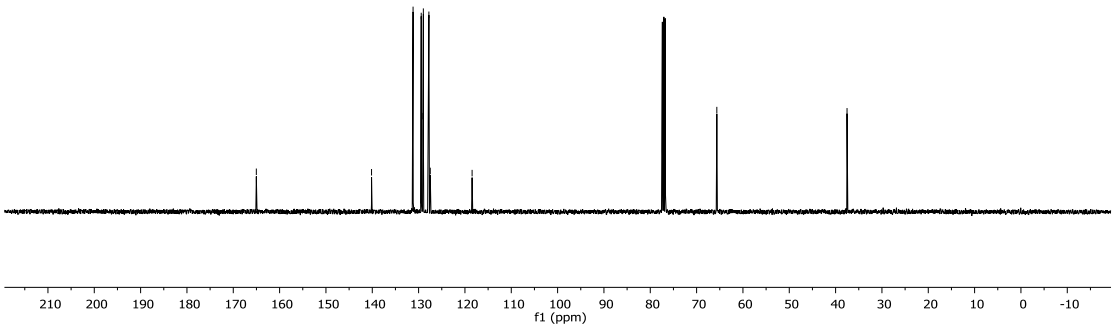
7g

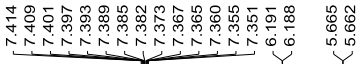

1.97
7.16
1.00
1.01
0.98
f1 (ppm)

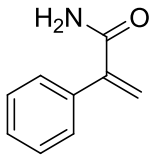

165.023
140.158
131.307
131.195
129.436
129.055
128.978
127.781
127.485
118.455
65.636
37.533


CN
O
O
Cl

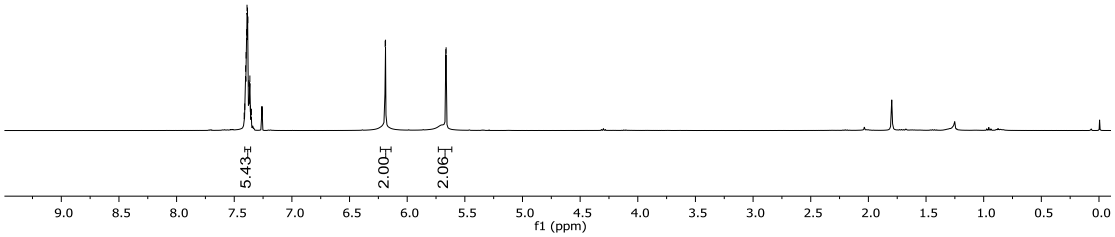
7g

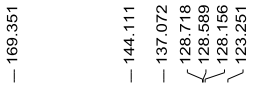

f1 (ppm)

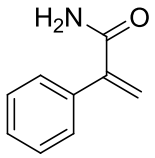

7.414
7.409
7.401
7.397
7.393
7.389
7.385
7.382
7.373
7.367
7.365
7.360
7.355
7.351
6.191
6.188
5.665
5.662


H2N
O

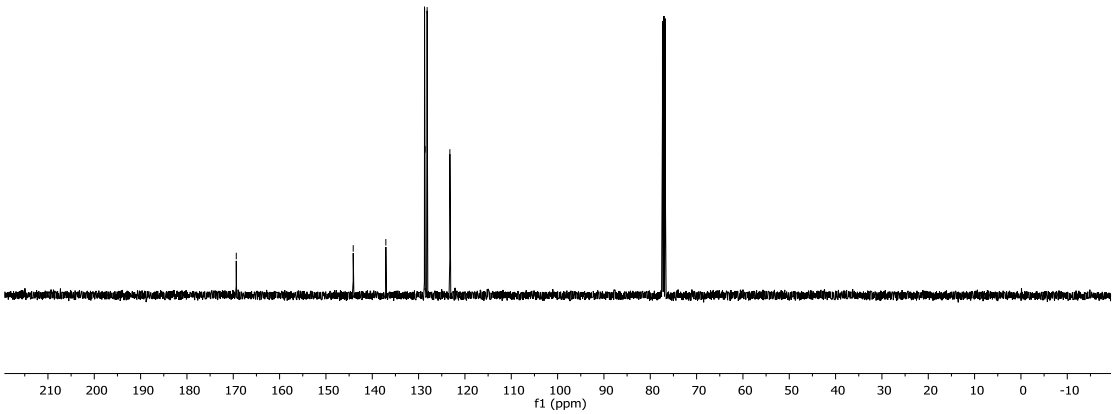
8

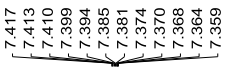

5.43
2.00
2.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

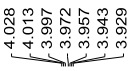

169.351
144.111
137.072
128.718
128.589
128.156
123.251


H2N
O

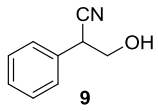
8


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

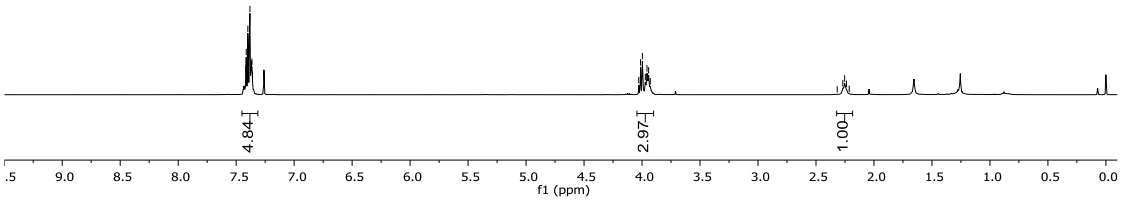

7.417
7.413
7.410
7.399
7.394
7.385
7.381
7.374
7.370
7.368
7.364
7.359


4.028
4.013
3.997
3.972
3.957
3.943
3.929

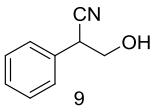

2.317
2.269
2.253
2.237
2.214


CN
OH

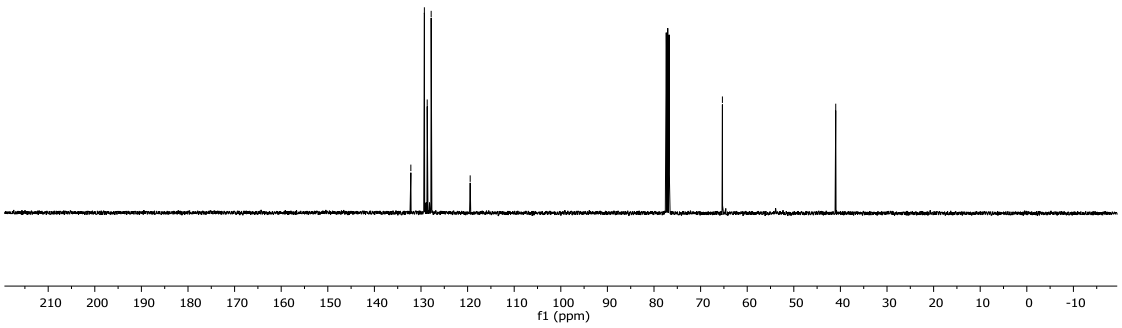
9

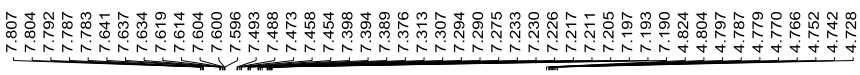

4.84
2.97
1.00
f1 (ppm)

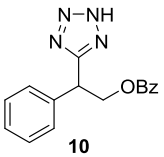

132.180
129.275
128.666
127.816
119.445
65.319
41.001


CN
OH

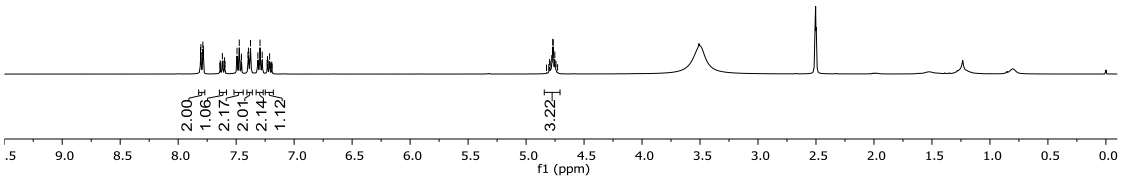
9

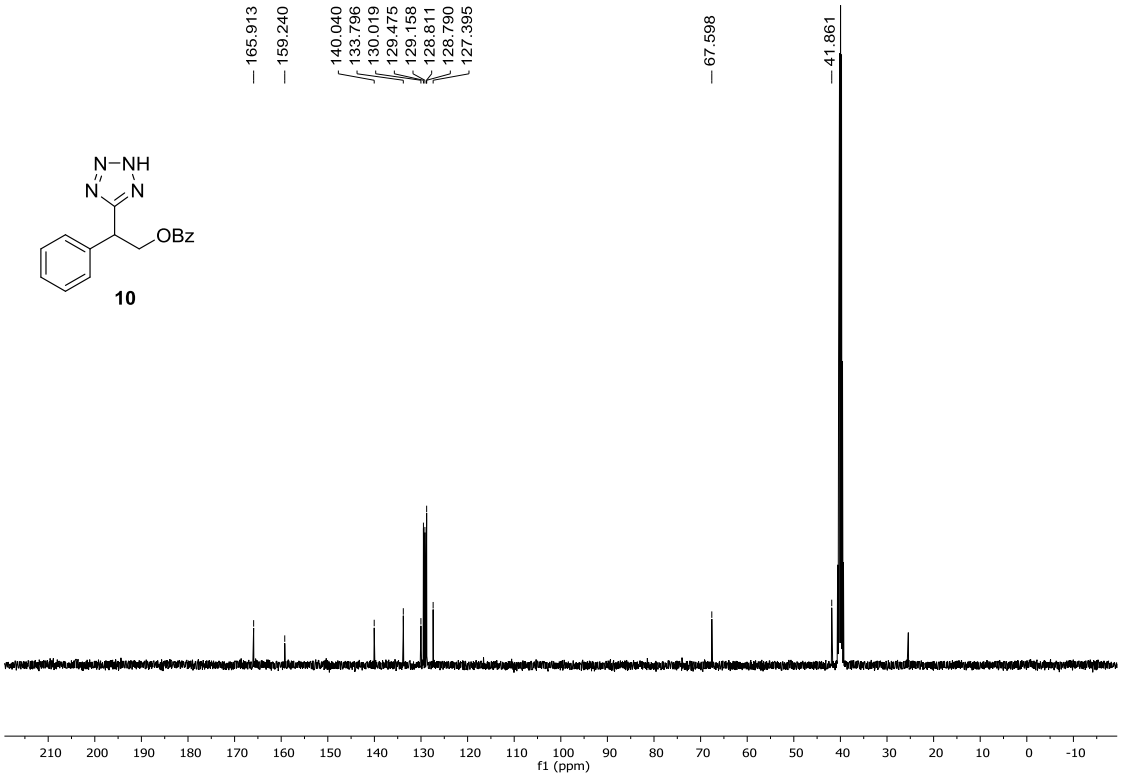

f1 (ppm)


7.807
7.804
7.792
7.787
7.783
7.641
7.637
7.634
7.619
7.614
7.604
7.600
7.596
7.493
7.488
7.473
7.458
7.454
7.398
7.394
7.389
7.376
7.313
7.307
7.294
7.290
7.275
7.233
7.230
7.226
7.217
7.211
7.205
7.197
7.193
7.190
4.824
4.804
4.797
4.787
4.779
4.770
4.766
4.752
4.742
4.728

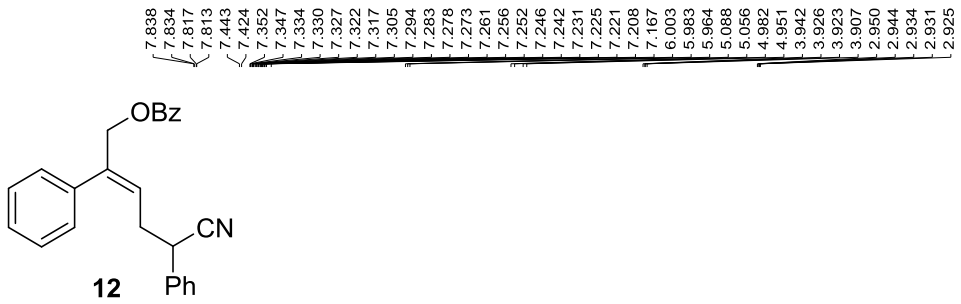

N–NH
N
N
OBz

10


2.00
1.06
2.17
2.01
2.14
1.12
3.22
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

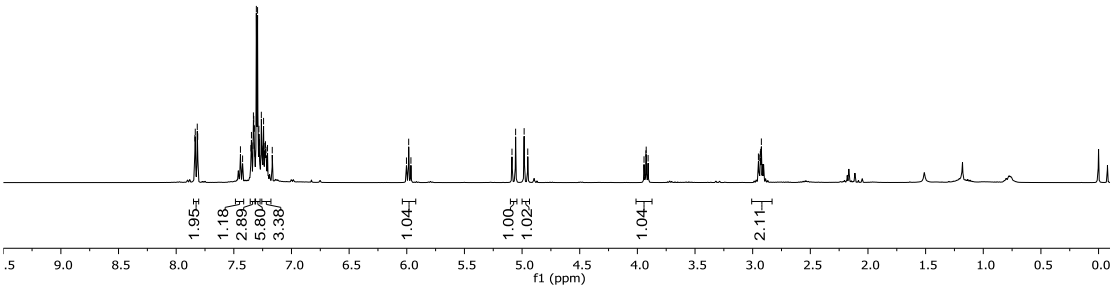

165.913
159.240
140.040
133.796
130.019
129.475
129.158
128.811
128.790
127.395
67.598
41.861
N–NH
N
N
OBz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

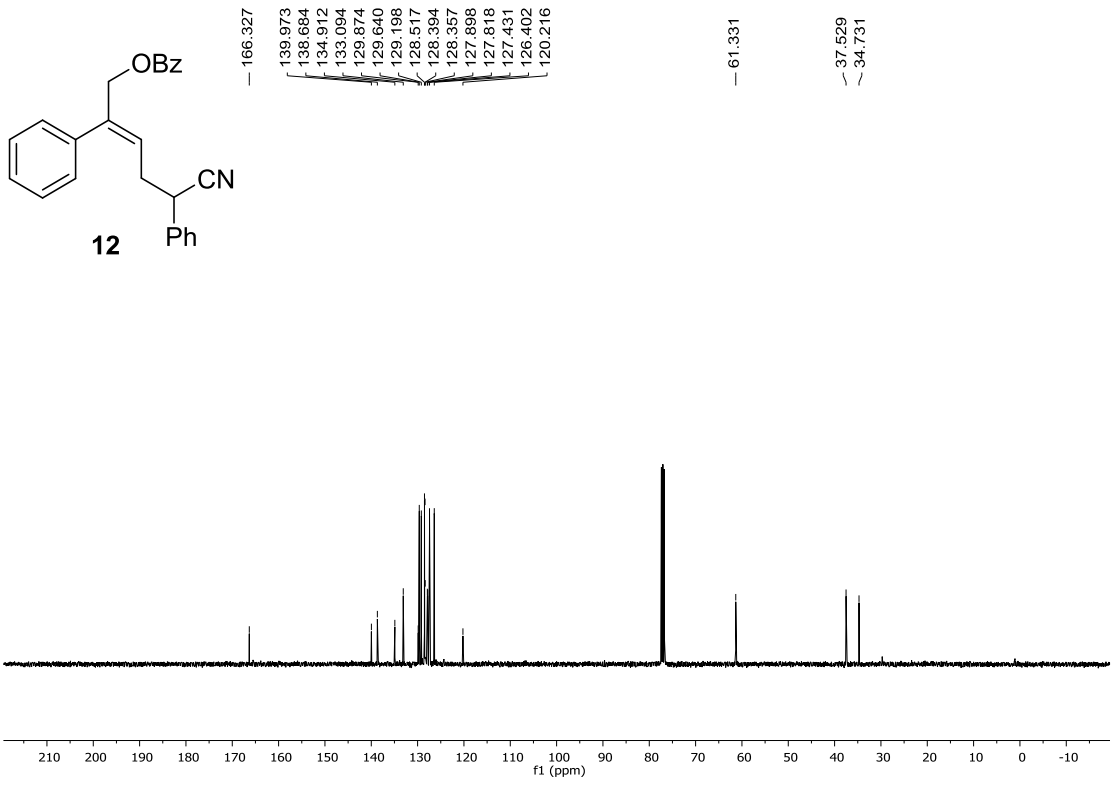
10


7.838
7.834
7.817
7.813
7.443
7.424
7.352
7.347
7.334
7.330
7.327
7.322
7.317
7.305
7.294
7.283
7.278
7.273
7.261
7.256
7.252
7.246
7.242
7.231
7.225
7.221
7.208
7.167
6.003
5.983
5.964
5.088
5.056
4.982
4.951
3.942
3.926
3.923
3.907
2.950
2.944
2.934
2.931
2.925

OBz
CN
Ph

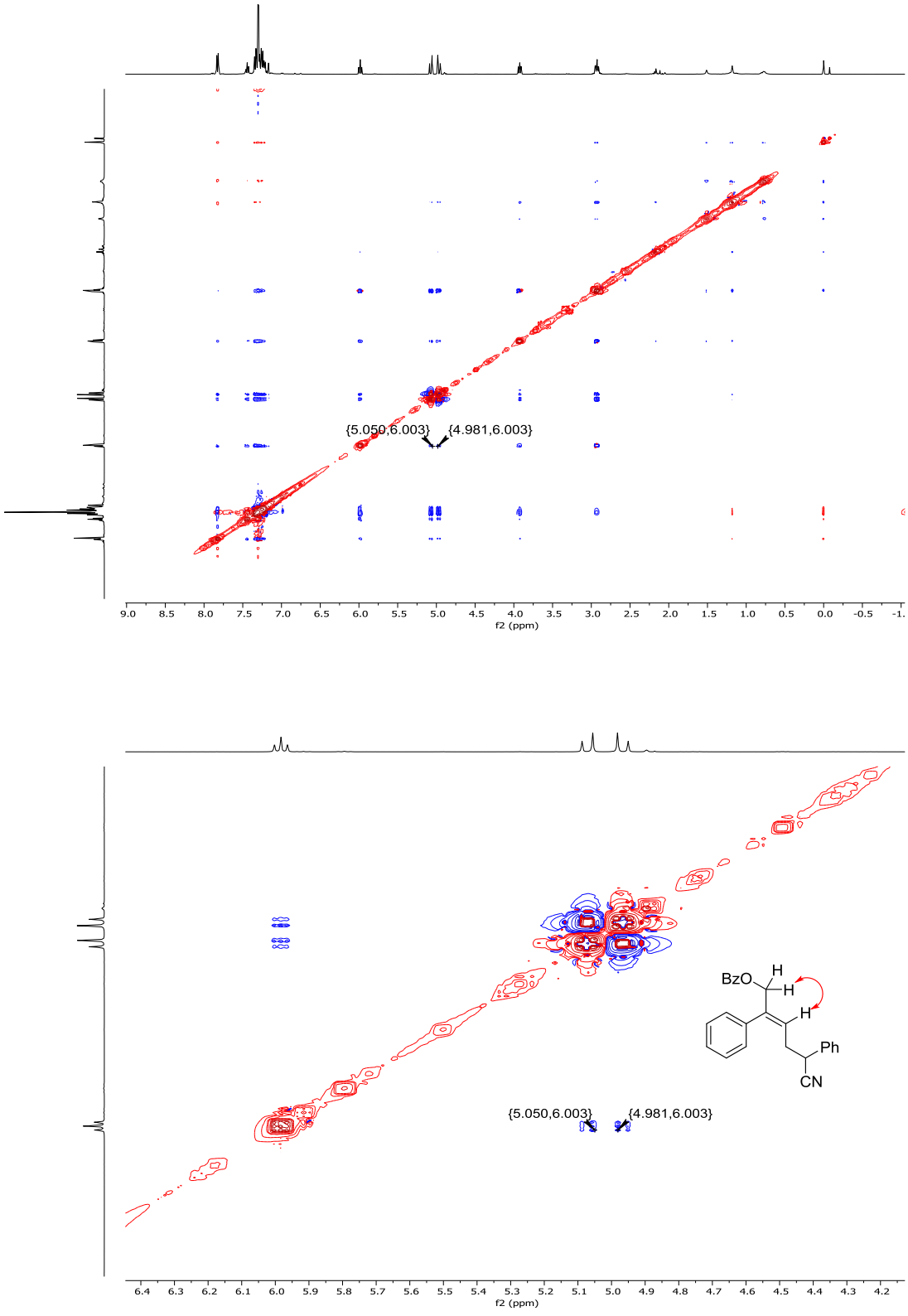
12


1.95
1.18
2.89
5.80
3.38
1.04
1.00
1.02
1.04
2.11
f1 (ppm)


166.327
139.973
138.684
134.912
133.094
129.874
129.640
129.198
128.517
128.394
128.357
127.898
127.818
127.431
126.402
120.216
61.331
37.529
34.731
f1 (ppm)

OBz
CN
Ph

12



2D-NOESY spectrum of compound **12**