Supporting Information

Fei-Phos Ligand-controlled Asymmetric Palladium -Catalyzed Allylic Substitutions with Structurally Diverse Nucleophiles: Scope and Limitation

Jian-Xing Xu[a], Fei Ye[a], Xing-Feng Bai[a,b], Jin Zhang[a], Zheng Xu[a], Zhan-Jiang Zheng[a], and Li-Wen Xu [a,b]*

[a] Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education, Hangzhou Normal University, Hangzhou 311121, P. R. China
Fax: (+) 86-571-28867756, E-mail: liwenxu@hznu.edu.cn

[b] State Key Laboratory for Oxo Synthesis and Selective Oxidation, Lanzhou Institute of Chemical Physics (CAS) and University of the Chinese Academy of Sciences, Lanzhou 730000, P. R. China

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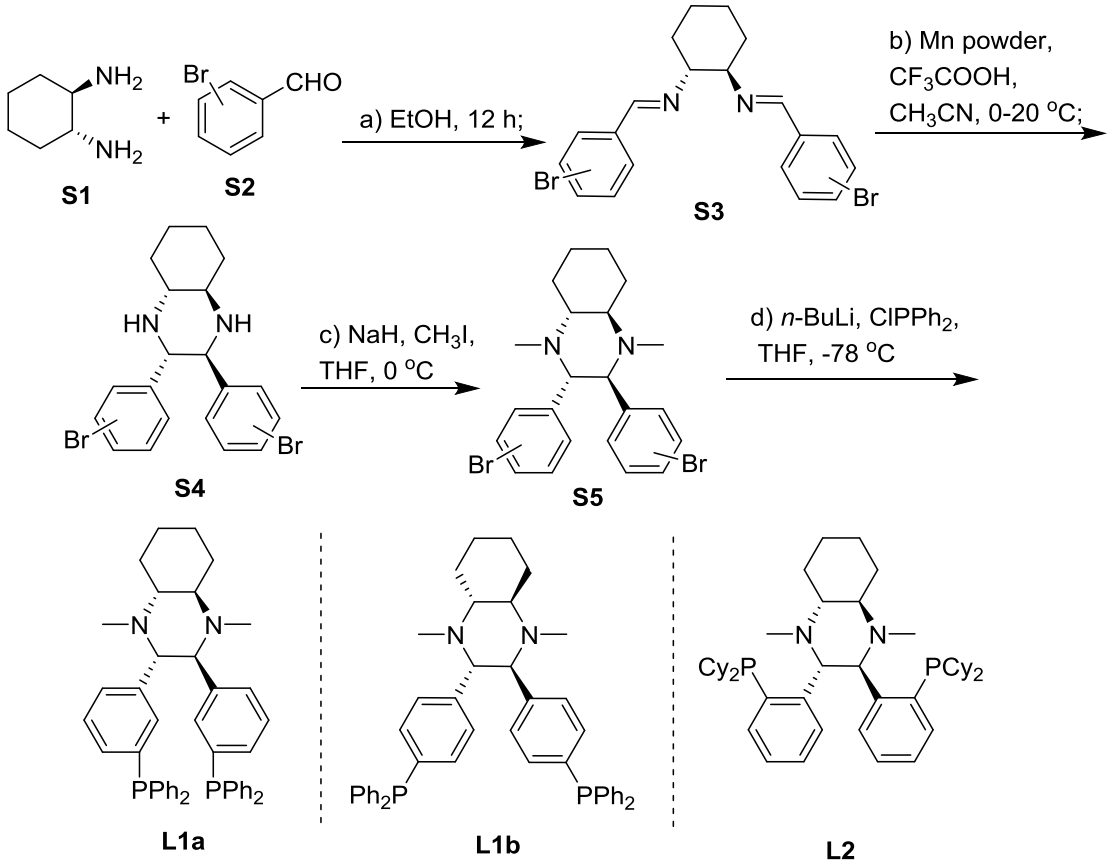
1. General Information

All the reactions dealing with air or moisture sensitive compounds were carried out in a dry reaction vessel under positive pressure of argon. Reagents were purchased from commercial sources and were used as received unless mentioned otherwise. Reactions were monitored by thin layer chromatography using silica gel. Air- and moisture-sensitive liquids and solutions were transferred via a syringe or a stainless steel cannula. ^{1}HNMR was recorded at 400 MHz or 500 MHz: chemical shifts are reported in ppm relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($CDCl_3$: δ = 7.26 ppm). ^{13}C NMR was recorded at 100 MHz or 125 MHz: chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard (CDCl3: δ = 77.20 ppm). High resolution mass spectra (HRMS) of the products were obtained on a Bruker Daltonics micro TOF-spectrometer. Infrared spectra were recorded on a Nexus 870 FTIR spectrometer. Toluene, N,N-Dimethylacetamide (DMAc), and $CHCl_3$ was dried and distilled over CaH_2. THF were distilled from sodium benzophenone ketyl. The preparation of allylic substrates, such as 1,3-diphenyl-2-propenyl acetate was carried out easily according to reported methods[1].

2. Synthesis of chiral ligands[2]

The product of similar chiral ligands in the previous report.[2]



A solution of Bromobenzylaldehyde **S2** (9.2 g, 50 mmol) in EtOH (25 mL) was added dropwise to the ethanol/H_2O (1.5/1) solution (50 mL) of trans-(*R*,*R*)-diaminocyclohexane **S1** (2.85 g, 25 mmol) at room temperature over 1 h. After stirring at reflux temperature for 12 h, H_2O (30 mL) was added to the mixture and cooled to 0 °C. After maintain it for 5 h at the same temperature, the precipitate was filtrated, the filter residue was washed with cooled ethanol and cooled H_2O.

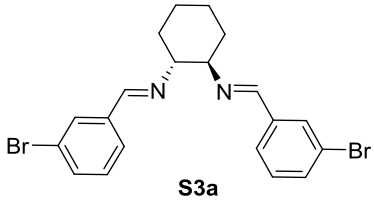
The **S3** was dissolved in a mixture of dry acetonitrile (200 mL) and toluene (20 mL). To the solution was added manganese powder (300 mesh; 2.2 g, 40 mmol), and the resulting mixture was cooled to 0 °C before trifluoroacetic acid (7.6 mL, 80 mmol) was added dropwise over a period of 30 min under an Ar atmosphere. The reaction mixture was stirred vigorously at 20 °C for 24 h followed by addition of two additional equivalents of trifluoroacetic acid at 0 °C. After standing at that temperature

for 2 h, the resulting mixture was filtered and the residue was washed with petroleum ether (bp 60-90 ^{o}C, 10 mL×2) to afford a white solid. The solid was dissolved in H_2O (10 mL) and neutralized with saturated $NaHCO_3$ solution to pH = 8. The aqueous solution was extracted with dichloromethane (20 mL×3). The combined organic layer was washed with H_2O (10 mL), dried over anhydrous Na_2SO_4, and concentrated. The resulting product can be applied directly to the next step reaction without further purification .

S4 (12 mmol) was dissolved in THF (20 mL), which was added dropwise to the solution of sodium hydride (80% purity, 0.86 g, 28.8 mmol) at 0 ^{o}C. After stirring at the same temperature for 3 h. Iodomethane (1.86 mL, 30 mmol) was added to the above mixture at the same temperature and the resulting mixture was stirred at room temperature for 12 h. A solution of 1M aqueous $NaHSO_3$ was added slowly to quench the reaction. The aqueous phase was extracted with dichloromethane (3×20 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum/acetate, 20/1 to 5/1) to give the targeted compound.

To a solution of **S5** (10 mmol) in 20 mL THF at -78 ^{o}C was dropwise added 10 mL (25 mmol) of 2.5 M solution of *n*-BuLi in hexanes. The resulting solution was stirred at -78 ^{o}C fot 1 h, and then a solution of 4.5 mL of chlorodiphenylphosphine (25 mmol) in 20 mL of THF was added dropwise during 15 mins. The reaction mixture was stirred for another 3 h at the same temperature, and then warmed at room temperature. After stirring for another 4 h, a solution of 1M aqueous NH_4Cl was added slowly until the reaction mixture became clear in both phases. The aqueous phase was extracted with dichloromethane (3×20 mL). Combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum/acetate, 20/1 to 5/1) to give the targeted compound.

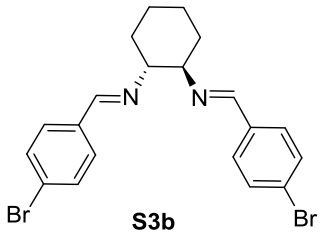
N,N'-((1R,2R)-cyclohexane-1,2-diyl)bis(1-(3-bromophenyl)methanimine) (S3a):



S3a

White solid, Yield: 89%. $[\alpha]_D^{25}$ = -194.1 (c = 2.32, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 2H), 7.79 (s, 2H), 7.44 (dd, *J* = 7.8, 1.3 Hz, 4H), 7.17 (t, *J* = 7.8 Hz, 2H), 3.44 – 3.33 (m, 2H), 1.93 – 1.73 (m, 6H), 1.48 (t, *J* = 9.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.40, 138.29, 133.23, 130.36, 129.99, 126.89, 122.82, 73.74, 32.82, 24.40. HRMS (ESI) calcd. for $C_{20}H_{20}Br_2N_2[M+H]^+$: 447.0066, Found: 447.0068.

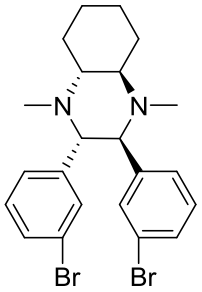
N,N'-((1R,2R)-cyclohexane-1,2-diyl)bis(1-(4-bromophenyl)methanimine) (S3b):



S3b

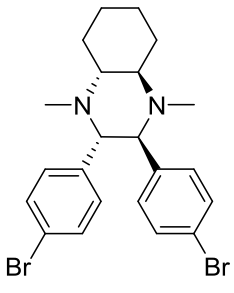
White solid, Yield: 83%. $[\alpha]_D^{25}$ = -253.7 (c = 2.37, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 2H), 7.49 – 7.38 (m, 8H), 3.44 – 3.28 (m, 2H), 1.93 – 1.73 (m, 6H), 1.48 (t, *J* = 9.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.73, 135.15, 131.68, 129.32, 124.69, 73.77, 32.81, 24.42. HRMS (ESI) calcd. for $C_{20}H_{20}Br_2N_2[M+H]^+$: 447.0066, Found: 447.0066.

(2S,3S,5R,6R)-2,3-bis(3-bromophenyl)-1,4-dimethyldecahydroquinoxaline (S5a):



S5a

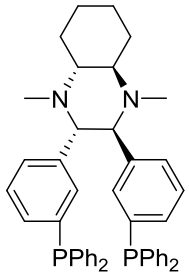
White solid, Yield: 78%. $[\alpha]_D^{25}$ = -104.1 (c = 2.32, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.63 – 6.39 (m, 8H), 3.05 (s, 2H), 2.21 (d, *J* = 13.0 Hz, 2H), 2.07 (d, *J* = 8.9 Hz, 2H), 1.97 (s, 6H), 1.80 (d, *J* = 8.0 Hz, 2H), 1.38 – 1.14 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.19, 131.35, 130.06, 129.24, 127.66, 122.07, 75.75, 67.31, 39.90, 29.50, 24.92. HRMS (ESI) calcd. for $C_{22}H_{26}Br_2N_2[M+H]^+$: 477.0536, Found: 447.0538.



S5b

(2S,3S,5R,6R)-2,3-bis(4-bromophenyl)-1,4-dimethyldecahydroquinoxaline (S5b): White solid, Yield: 70%. $[\alpha]_D^{25}$ = -139.0 (c

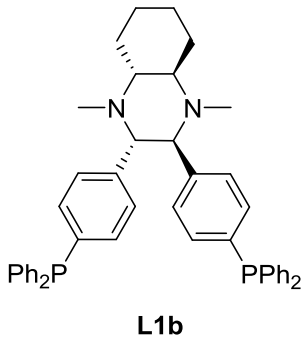
= 2.23, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 6.37 (m, 8H), 3.05 (s, 2H), 2.21 (d, *J* = 13.0 Hz, 2H), 2.07 (d, *J* = 8.9 Hz, 2H), 1.97 (s, 6H), 1.80 (d, *J* = 8.0 Hz, 2H), 1.39 – 1.14 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.19, 131.35, 130.06, 129.24, 127.66, 122.07, 75.75, 67.31, 39.90, 29.50, 24.92. HRMS (ESI) calcd. for $C_{22}H_{26}Br_2N_2[M+H]^+$: 477.0536, Found: 447.0537.



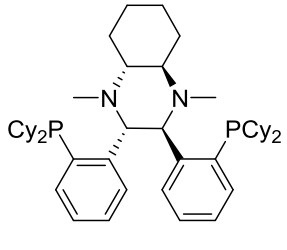
L1a

(2S,3S,5R,6R)-2,3-bis(3-(diphenylphosphanyl)phenyl)-1,4-dimethyldecahydroquinoxaline (L1a): White solid, Yield: 78%. $[\alpha]_D^{25}$ = -135.8 (c = 2.32, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 6.67 (m, 28H), 3.10 (s, 2H), 2.16 (d, *J* = 12.4 Hz, 2H), 2.03 (d, *J* = 10.0 Hz, 2H), 1.90 (s, 6H), 1.75 (d, *J* = 8.1 Hz, 2H), 1.33 – 1.12 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.04, 137.46, 137.35, 133.87, 133.66, 133.47, 128.58, 128.50, 128.44, 128.38, 75.85, 67.58, 39.66, 29.54, 24.98. HRMS (ESI) calcd. for $C_{46}H_{46}N_2P_2[M+H]^+$: 689.3209, Found: 689.3211.

(2S,3S,5R,6R)-2,3-bis(4-(diphenylphosphanyl)phenyl)-1,4-dimethyldecahydroquinoxaline (L1b): White solid, Yield: 68%. $[\alpha]_D^{25}$ = -288.5 (c = 2.32, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 6.73 (m, 28H), 3.14 (s, 2H), 2.21 (d, *J* = 11.6 Hz, 2H), 2.10 (s, 2H), 1.99 (s, 6H), 1.78 (d, *J* = 6.7 Hz, 2H), 1.40 – 1.28 (m, 3H), 1.24 – 1.19 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.40, 137.30, 137.11, 137.00, 133.83, 133.64, 133.44, 133.25, 128.66, 128.50, 128.43, 128.37, 76.06, 67.55, 39.95, 29.51, 24.96. HRMS (ESI) calcd. for $C_{46}H_{46}N_2P_2[M+H]^+$: 689.3209, Found: 689.3207.



L1b



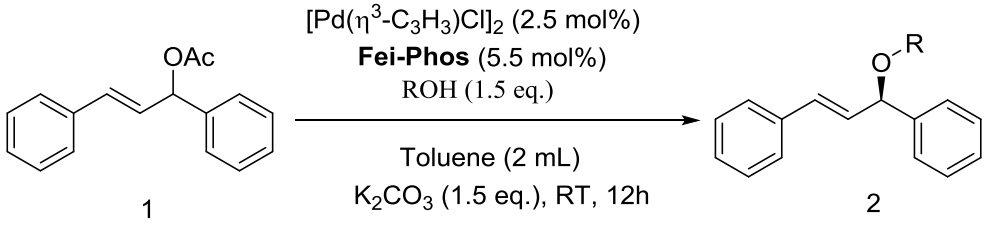
L2

(2S,3S,5R,6R)-2,3-bis(2-(dicyclohexylphosphanyl)phenyl)-1,4-dimethyldecahydroquinoxaline (L2): White solid, Yield: 79%. $[\alpha]_D^{25}$ = -11.2 (c = 2.32, $CHCl_3$). ^{1}H NMR (400

MHz, $CDCl_3$) δ 8.00 (d, *J* = 6.2 Hz, 2H), 7.38 – 7.08 (m, 6H), 4.90 – 4.74 (m, 2H), 2.26 (d, *J* = 9.1 Hz, 2H), 2.15 (d, *J* = 12.2 Hz, 2H), 1.80 (s, 6H), 1.77 – 1.28 (m, 22H), 1.22 – 0.93 (m, 17H), 0.81 (dd, *J* = 26.1, 13.7 Hz, 4H), 0.37 (t, *J* = 11.1 Hz, 2H), 0.09 (q, *J* = 12.4 Hz, 2H). HRMS (ESI) calcd. for $C_{46}H_{70}N_2P_2[M+H]^+$: 713.5087, Found: 713.5081.

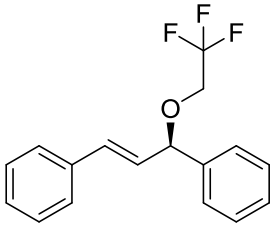
3. General procedures for Pd-catalyzed asymmetric allylation alkylation to the formation of products 2a-2f, 3a-3j, 5a-5g and 6a-6g.

3.1 General procedure for Pd-catalyzed asymmetric allylic etherification of alcohols in the presence of (2*S*,3*S*,5*R*,6*R*)-Fei-Phos.



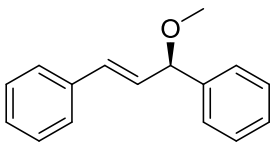
A flame-dried Schlenk tube was charged with $[Pd(\eta^3\text{-allyl})Cl]_2$ (4.5 mg, 0.0125 mmol, 2.5 mol%) and (2*S*,3*S*,5*R*,6*R*)-**Fei-Phos** (18.9 mg, 0.0275 mmol, 5.5 mol%) under N_2 atmosphere, and the mixture was dissolved in dry Toluene (2.0 mL). The solution was stirred at room temperature for 30 min and then adding (*E*)-1,3-diphenyl-2-propenyl acetate (0.5 mmol). The mixture solution was further stirred for 10 minutes at room temperature, and anhydrous K_2CO_3 (104 mg, 0.75 mmol) was added in to the vial followed by alcohol (0.75 mmol). The reaction mixture was stirred at room temperature for 12 h. The solution was quenched with EtOAc and saturated aqueous NH_4Cl solution. The mixture was then extracted twice with EtOAc (20×3 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude product was purified by flash column chromatography to afford the product.

The product of catalytic asymmetric allylic etherification in the previous report.[2]



2a

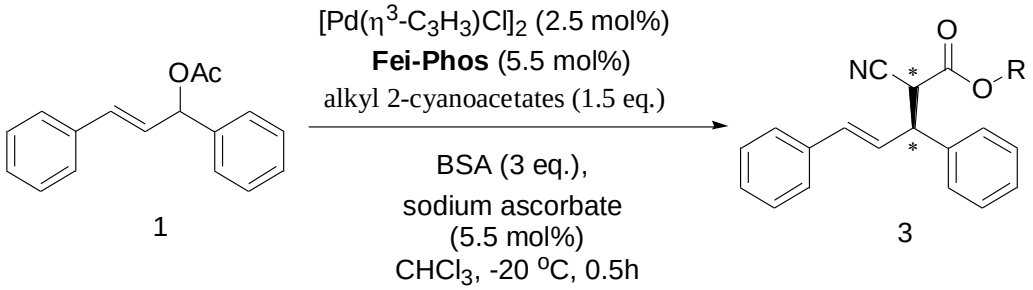
(*R*,*E*)-(3-(2,2,2-trifluoroethoxy)prop-1-ene-1,3-diyl)dibenzene (2a): Yellow oil, Yield: 98%. $[\alpha]_D^{25}$ = 6.5 (c = 4.35, $CHCl_3$), 31% *ee* [determined by HPLC analysis using a Chiralcel OJ-H column; *n*-Hex / *i*-PrOH = 98:2, 1 mL/min, 254 nm; t_R (minor) = 16.65 min; t_R (major) =20.20 min]. ^{1}H NMR (400 MHz, CDCl3) δ 7.41 – 7.19 (m, 11H), 6.64 (d, J = 15.9 Hz, 1H), 6.27 (dd, J = 15.9, 7.2 Hz, 1H), 5.07 (d, J = 7.2 Hz, 1H), 3.90 – 3.79 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.60, 136.12, 132.90, 128.78, 128.66, 128.53, 128.32, 128.19, 126.91, 126.78, 124.21 (q, J = 278.9 Hz), 83.82, 65.51 (q, J = 34.2 Hz). HRMS (ESI) calcd. for $C_{17}H_{14}F_3O[M+Na]^+$: 315.0967, Found: 315.0962.



2c

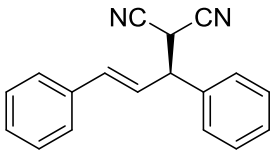
(*R*,*E*)-(3-methoxyprop-1-ene-1,3-diyl)dibenzene (2c): Colorless oil, Yield: 95% . $[\alpha]_D^{25}$ = 7.3 (c = 5.26, $CHCl_3$), 97% *ee* [determined by HPLC analysis using a Chiralcel OJ-H column; *n*-Hex / *i*-PrOH = 96:4, 1 mL/min, 254 nm; t_R (minor) = 10.43 min; t_R (major) = 11.00 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.08 (m, 10H), 6.54 (d, J = 15.9 Hz, 1H), 6.19 (dd, J = 15.9, 7.0 Hz, 1H), 4.70 (d, J = 7.0 Hz, 1H), 3.28 (d, J = 1.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.12, 136.68, 131.51, 130.25, 128.56, 127.75, 126.90, 126.64, 84.36, 56.47. HRMS (ESI) calcd. for $C_{16}H_{16}O[M+Na]^+$: 247.1093, Found: 247.0944.

3.2 General procedure for Pd-catalyzed asymmetric allylic alkylation of cyanoacetates in the presence of (2*S*,3*S*,5*R*,6*R*)-Fei-Phos.



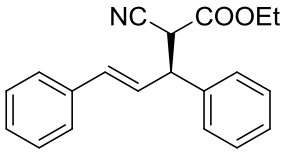
1 3

A flame-dried Schlenk tube was charged with $[Pd(\eta^3\text{-allyl})Cl]_2$ (4.5 mg, 0.0125 mmol, 2.5 mol%) and (2*S*,3*S*,5*R*,6*R*)-**Fei-Phos** (18.9 mg, 0.0275 mmol, 5.5 mol%) and sodium ascorbate (5.4 mg, 0.0275 mmol, 5.5mol%) under an N_2 atmosphere, and the mixture was dissolved in dry $CHCl_3$ (2.0 mL). The solution was stirred at -20 ^oC for 30 min and then (*E*)-1,3-diphenyl-2-propenyl acetate (0.5 mmol), cyanoacetate (0.75 mmol), BSA (1.5 mmol) was added to the above solution. The reaction mixture was stirred at -20 ^oC for 30 min. The solution was quenched with EtOAc and saturated aqueous NH_4Cl solution. The mixture was then extracted twice with EtOAc (20×3 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude product was purified by flash column chromatography to afford the alkylated product.



3a

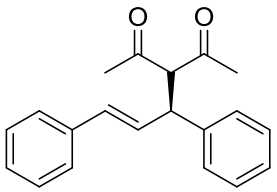
(*S*,*E*)-2-(1,3-diphenylallyl)malononitrile (3a): Light yellow oil, Yield: 72%. $[\alpha]_D^{25}$ = 24.2 (c = 3.33, $CHCl_3$), 92% *ee* [determined by HPLC analysis using a Chiralcel OJ-H column; *n*-Hex / *i*-PrOH = 70:30, 1 mL/min, 254 nm; t_R (minor) =17.85 min; t_R (major) =20.00 min]. ^1H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.25 (m, 10H), 6.71 (d, *J* = 15.7 Hz, 1H), 6.47 (dd, *J* = 15.7, 8.0 Hz, 1H), 4.15 – 3.99 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.09, 134.34, 134.01, 127.93, 127.45, 127.23, 127.12, 126.21, 125.29, 122.45, 110.19, 110.11, 48.30, 28.70. HRMS (ESI) calcd. for $C_{18}H_{14}N_2[M+Na]^+$: 281.1049, Found: 281.1039.



3b

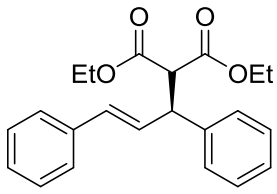
(*E*)-ethyl-2-cyano-3,5-diphenylpent-4-enoate (3b): Colorless oil, Yield: 92%. $[\alpha]_D^{25}$ = 19.2 (c = 7.22, $CHCl_3$), 90% *ee*, *dr*>99:1 [determined by HPLC analysis using a Chiralcel IB column; *n*-Hex / *i*-PrOH = 99:1, 0.5 mL/min, 254 nm; t_R (minor) = 29.93 min; t_R (major) = 34.36 min]. ^1H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.20 (m, 10H), 6.59 (dd, *J* = 15.7, 11.5 Hz, 1H), 6.48 (ddd, *J* = 31.0, 15.7, 8.3 Hz, 1H), 4.24 (dd, *J* = 8.2, 6.5 Hz, 1H), 4.18 – 4.10 (m, 2H), 3.90 (dd, *J* = 15.4, 7.0 Hz, 1H), 1.16 (td, *J* = 7.1, 3.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.95, 164.91, 138.80,

138.12, 136.23, 136.16, 134.35, 133.28, 129.09, 129.06, 128.68, 128.66, 128.19, 128.15, 128.03, 127.72, 127.10, 126.68, 126.58, 125.75, 115.49, 62.93, 62.88, 49.47, 49.22, 44.88, 44.55, 13.97.



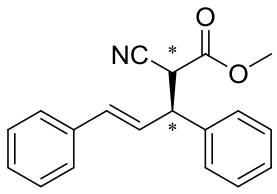
3c

(*S,E*)-3-(1,3-diphenylallyl)pentane-2,4-dione (3c): White solid, Yield: 92%. $[\alpha]_D^{25}$ = 4.7 (c = 7.06, $CHCl_3$), 94% *ee* [determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 95:5, 1 mL/min, 254 nm; t_R (minor) = 10.73 min; t_R (major) = 11.92 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.11 (m, 3H), 6.42 (d, *J* = 15.9 Hz, 1H), 6.19 (ddd, *J* = 15.8, 4.7, 3.1 Hz, 1H), 4.51 – 4.14 (m, 1H), 2.24 (s, 1H), 1.91 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.74, 202.58, 140.18, 136.63, 131.72, 129.36, 129.02, 128.53, 127.96, 127.71, 127.26, 126.38, 74.55, 49.16, 29.97, 29.71. HRMS (ESI) calcd. for $C_{20}H_{20}O_2$[M+Na]$^+$: 315.1356, Found: 315.1340.



3d

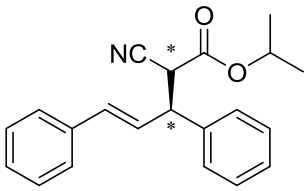
diethyl (*S,E*)-2-(1,3-diphenylallyl)malonate (3d): Yield: 90%. 94% *ee* [determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 90:10, 1 mL/min, 254 nm; t_R (minor) =9.67 min; t_R (major) =12.88 min].^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.11 (m, 10H), 6.47 (d, *J* = 15.8 Hz, 1H), 6.34 (dd, *J* = 15.7, 8.5 Hz, 1H), 4.26 (dd, *J* = 10.9, 8.5 Hz, 1H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.97 (qd, *J* = 7.1, 1.4 Hz, 2H), 3.92 (d, *J* = 10.9 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.00 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.85, 167.43, 140.36, 136.90, 131.71, 129.41, 128.65, 128.47, 128.02, 127.52, 127.09, 126.37, 61.57, 61.36, 57.82, 49.22, 14.14, 13.79.



3e

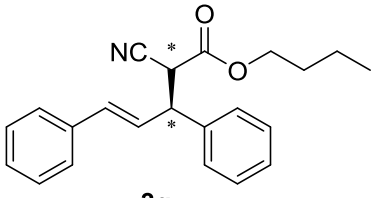
methyl (*E*)-2-cyano-3,5-diphenyl-pent-4-enoate (3e): Colorless oil, Yield: 86% . $[\alpha]_D^{25}$ = 26.5 (c = 5.23 $CHCl_3$), 91% *ee*, *dr*>99:1 [determined by HPLC analysis using a Chiralcel IB column; *n*-Hex / *i*-PrOH = 99:1, 0.5 mL/min, 254 nm; t_R

(minor) = 40.54 min; t_R (major) =46.56 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.21 (m, 10H), 6.59 (dd, *J* = 15.8, 10.0 Hz, 1H), 6.48 (ddd, *J* = 31.9, 15.7, 8.3 Hz, 1H), 4.27 – 4.17 (m, 1H), 3.93 (dd, *J* = 16.8, 6.8 Hz, 1H), 3.71 (d, *J* = 7.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.42, 165.39, 138.82, 138.08, 136.26, 136.19, 134.41, 133.33, 129.11, 129.07, 128.68, 128.65, 128.21, 128.16, 128.05, 127.98, 127.66, 127.05, 126.69, 126.60, 125.69, 115.33, 115.27, 53.49, 53.41, 49.37, 49.09, 44.75, 44.43.



3f

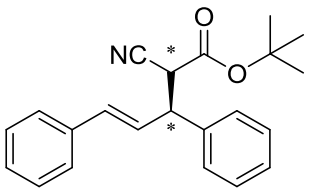
isopropyl (*E*)-2-cyano-3,5-diphenyl-pent-4-enoate (3f): Light yellow oil, Yield: 83%. $[\alpha]_D^{25}$ = 19.2 (c = 4.47 $CHCl_3$), 90%/92% *ee*, 54:46 *dr* [determined by HPLC analysis using a Chiralcel IC column; *n*-Hex / *i*-PrOH = 99:1, 0.5 mL/min, 254 nm; t_R = 51.30 min, t_R = 54.49 min, t_R = 59.28 min, t_R = 85.69 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.23 (m, 10H), 6.58 (dd, *J* = 15.7, 12.4 Hz, 1H), 6.54 – 6.39 (m, 1H), 4.97 (hept, *J* = 6.2 Hz, 1H), 4.25 – 4.13 (m, 1H), 3.87 (dd, *J* = 13.3, 7.2 Hz, 1H), 1.19 – 1.08 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.48, 164.44, 138.78, 138.19, 136.23, 136.16, 134.28, 133.25, 129.07, 129.05, 128.68, 128.66, 128.16, 128.13, 128.06, 128.01, 127.78, 127.18, 126.67, 126.58, 125.87, 115.59, 71.06, 49.55, 49.36, 45.00, 44.68, 21.55, 21.53, 21.48, 21.42.



3g

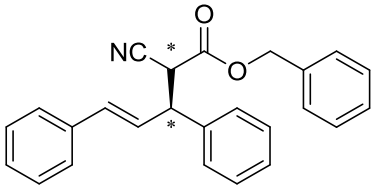
butyl (*E*)-2-cyano-3,5-diphenyl-pent-4-enoate (3g): Light yellow oil, Yield: 84%. $[\alpha]_D^{25}$ = 18.4 (c = 4.65 $CHCl_3$), 92%/88% *ee*, 54:46 *dr* [determined by HPLC analysis using a Chiralcel IC column; *n*-Hex / *i*-PrOH = 99:1, 0.5 mL/min, 254 nm; t_R = 50.27 min, t_R = 53.74 min, t_R = 64.58 min, t_R = 83.84 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.22 (m, 10H), 6.59 (dd, *J* = 15.8, 10.3 Hz, 1H), 6.48 (ddd, *J* = 31.7, 15.7, 8.2 Hz, 1H), 4.26 – 4.16 (m, 1H), 4.09 (dd, *J* = 6.0, 4.6 Hz, 1H), 3.91 (dd, *J* = 14.0, 6.9 Hz, 1H), 1.51 (dq, *J* = 13.7, 6.9 Hz, 2H), 1.35 – 1.19 (m, 2H), 0.83 (td, *J* = 7.3, 1.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.02, 164.98,

138.86, 138.17, 136.25, 136.19, 134.36, 133.29, 129.07, 129.03, 128.65, 128.62, 128.11, 128.02, 127.6, 127.14, 126.67, 126.58, 125.72, 115.41, 66.71, 66.66, 49.46, 49.22, 44.88, 44.56, 30.36, 29.71, 18.92, 13.52.



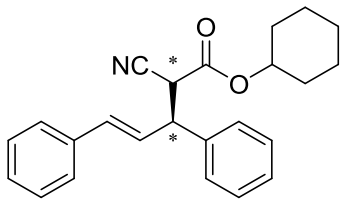
3h

tert-butyl (*E*)-2-cyano-3,5-diphenyl-pent-4-enoate (3h): Light yellow oil, Yield: 80%. $[\alpha]_D^{25}$ = 22.1 (c = 2.26 $CHCl_3$), 94%/94% *ee*, 54:46 *dr* [determined by HPLC analysis using a Chiralcel IC column; *n*-Hex / *i*-PrOH = 99:1, 0.5 mL/min, 254 nm; t_R = 34.00 min, t_R = 36.30 min, t_R = 43.35 min, t_R = 52.63 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.16 (m, 10H), 6.57 (t, *J* = 15.2 Hz, 1H), 6.46 (ddd, *J* = 28.4, 15.7, 8.3 Hz, 1H), 4.23 – 4.07 (m, 1H), 3.81 (dd, *J* = 12.1, 7.3 Hz, 1H), 1.34 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.84, 163.78, 138.88, 138.32, 136.28, 136.22, 134.13, 133.10, 129.02, 128.98, 128.67, 128.66, 128.14, 128.08, 127.94, 127.83, 127.44, 126.64, 126.56, 126.13, 115.88, 84.33, 49.51, 49.44, 45.61, 45.30, 27.72, 27.69.



3i

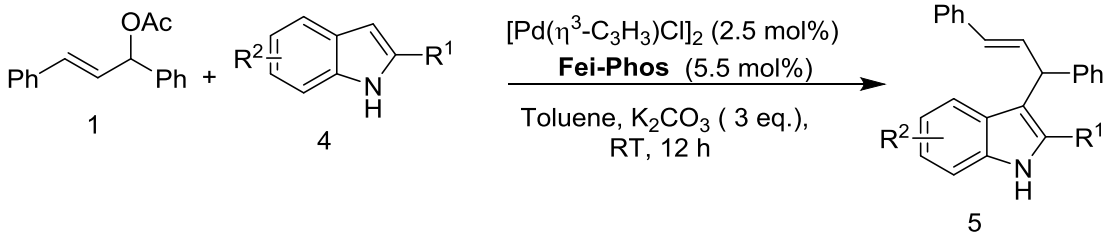
benzyl (*E*)-2-cyano-3,5-diphenyl-pent-4-enoate (3i): Light yellow oil, Yield: 89%. $[\alpha]_D^{25}$ = 16.9 (c = 6.67 $CHCl_3$), 90%/92% *ee*, 55:45 *dr* [determined by HPLC analysis using a Chiralcel IC column; *n*-Hex / *i*-PrOH = 99:1, 0.5 mL/min, 254 nm; t_R = 72.33 min, t_R = 87.46 min, t_R = 103.01 min, t_R = 113.32 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.15 (m, 15H), 6.55 – 6.50 (m, 1H), 6.50 – 6.35 (m, 1H), 5.15 – 5.07 (m, 2H), 4.20 (dt, *J* = 16.1, 7.2 Hz, 1H), 3.94 (dd, *J* = 12.7, 7.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.86, 164.83, 138.69, 137.99, 136.14, 136.08, 134.47, 134.36, 134.30, 133.35, 129.12, 129.11, 128.78, 128.73, 128.70, 128.68, 128.65, 128.62, 128.55, 128.20, 128.16, 128.15, 128.05, 127.96, 127.68, 126.91, 126.73, 126.63, 125.49, 115.28, 115.26, 68.48, 49.52, 49.19, 44.93, 44.57.



3j

cyclohexyl (*E*)-2-cyano-3,5-diphenyl-pent-4-enoate (3j): White solid, Yield: 88%. $[\alpha]_D^{25}$ = 27.9 (c = 6.93 $CHCl_3$), 94%/94% *ee*, 54:46 *dr* [determined by HPLC analysis using a Chiralcel IC column; *n*-Hex / *i*-PrOH = 99:1, 0.5 mL/min, 254 nm; t_R = 47.99 min, t_R = 51.77 min, t_R = 62.21 min, t_R = 79.37 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 9H), 7.26 – 7.21 (m, 1H), 6.60 (d, *J* = 15.8 Hz, 1H), 6.51 (dd, *J* = 16.2, 8.7 Hz, 1H), 4.84 – 4.69 (m, 1H), 4.23 (t, *J* = 7.3 Hz, 1H), 3.87 (d, *J* = 7.3 Hz, 1H), 1.74 – 1.26 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.36, 138.88, 136.28, 134.27, 129.03, 128.60, 128.06, 127.95, 127.74, 126.63, 125.93, 115.53, 75.56, 49.29, 45.01, 31.16, 31.07, 25.15, 23.31. HRMS (ESI) calcd. for $C_{24}H_{25}NO_2$[M+Na]: 382.1778, Found: 382.1785.

3.3 General procedure for Pd-catalyzed asymmetric allylic alkylation of indoles in the presence of (2*S*,3*S*,5*R*,6*R*)-Fei-Phos.



1 4 5

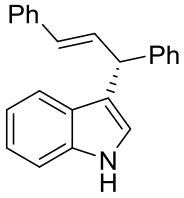
A flame-dried Schlenk tube was charged with $[Pd(\eta^3\text{-allyl})Cl]_2$ (4.5 mg, 0.0125 mmol, 2.5 mol%) and (2*S*,3*S*,5*R*,6*R*)-**Fei-Phos** (18.9 mg, 0.0275 mmol, 5.5 mol%) under an N_2 atmosphere, and the mixture was dissolved in dry toluene (2.0 mL). The solution was stirred at room temperature for 30 min and then adding (*E*)-1,3-diphenyl-2-propenyl acetate **1** (126 mg, 0.5 mmol). The mixture solution was further stirred for 10 minutes at room temperature, and anhydrous K_2CO_3 (207 mg, 1.5 mmol) was added in to the vial followed by indoles **4** (1.5 mmol). The reaction mixture was stirred at room temperature for 12 h. The solution was quenched with EtOAc and saturated aqueous NH_4Cl solution. The mixture was then extracted twice with EtOAc (20×3 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo.

The crude product was purified by flash column chromatography to afford the alkylated product **5**. And the product **5** was directly conversed to *N*-Boc-protected derivatives **6**.

3.4 The preparation of *N*-Boc-protected indoles 6

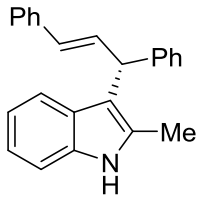
5 **6**

To a solution of **5** (0.1 mmol) and DMAP (0.6 mg, 0.005 mmol) in CH_2Cl_2 (2 mL) was added $(Boc)_2O$ (32.7 mg, 0.15 mmol), and the solution was stirred for 2 h at room temperature. The resulting mixture was evaporated under reduced pressure and purified by flash column chromatography to afford the *N*-Boc-protected alkylated indole **6**. Enantiomeric excess was determined on an aliquot before the addition of the acetic anhydride by HPLC with chiral stationary phase.



5a

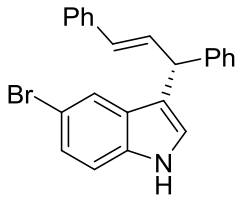
(*R,E*)-3-(1,3-diphenylallyl)-1H-indole (5a): White solid, 124-127 ^oC. 82% yield. $[\alpha]_D^{25}$ = -38.3 (*c* = 0.6, $CDCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 7.89 (bs, 1H), 7.48-7.33 (m, 9H), 7.32-7.20 (m, 3H), 7.15-7.07 (m, 1H), 6.82 (d, J = 3.75Hz, 1H), 6.85-6.75 (m, 1H), 6.56-6.48 (m, 1H), 5.23-5.15 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.5, 137.6, 136.7, 132.7, 130.6, 128.6, 127.3, 126.9, 126.5, 126.4, 122.7, 122.1, 119.9, 119.5, 118.7, 111.2, 46.3. IR (cm^{-1}, neat) 3384.5, 3022.1, 2852.2, 1597.7, 1489.4, 1449.4, 1419.2, 1335.1, 1220.5, 1007.5, 962.9, 742.3, 694.3. GC-MS (EI): calcd for $C_{23}H_{19}N$ [M]: 309.1; Found: 309.2, 254.1, 232.1, 206.1, 178.1, 152.1, 115.1.



5b

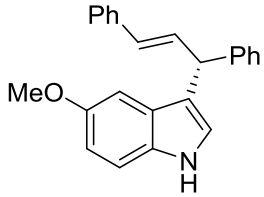
(*R,E*)-3-(1,3-diphenylallyl)-2-methyl-1H-indole (5b): Yellow solid,

mp: 39-40 °C. 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (bs, 1H), 7.49-7.44 (m, 6H), 7.39-7.34 (m, 5H), 7.33-7.30 (m, 1H), 7.19-7.15 (m, 1H), 7.10-7.05 (m, 1H), 6.94 (dd, J = 7.0 Hz, 32.0 Hz, 1H), 6.52 (d, J = 31.5 Hz, 1H), 5.24 (d, J = 7.5 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.6, 137.7, 135.5, 132.3, 130.7, 129.8, 129.1, 128.6, 128.4, 128.3, 128.0, 127.2, 126.4, 126.2, 120.9, 119.4, 119.3, 112.8, 110.5, 45.2, 12.4. IR (cm^{-1}, neat) 3338.43, 3058.2, 3027.6, 2924.7, 1685.1, 1616.4, 1491.1, 1450.0, 1264.4, 968.7, 734.1, 696.9.



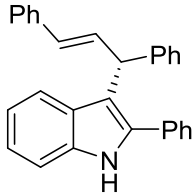
5c

(*R*,*E*)-5-bromo-3-(1,3-diphenylallyl)-1H-indole (5c): Colorless oil. 81% yield. $[\alpha]_D^{25}$ = -28.1 (*c* = 0.85, $CDCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (bs, 1H), 7.67-7.63 (m, 1H), 7.45-7.29 (m, 11H), 7.21-7.17 (m, 1H), 6.89 (s, 1H), 6.76 (dd, J = 7.5 Hz, 16.0 Hz, 1H), 6.50 (d, J = 16.0 Hz, 1H), 5.13 (d, J = 7.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.1, 137.4, 135.3, 132.2, 130.9, 128.6, 128.5, 127.5, 126.7, 126.5, 125.1, 124.0, 122.3, 118.3, 112.8, 46.0. IR (cm^{-1}, neat) 3420.4, 3024.5, 2921.4, 2851.0, 1693.0, 1492.4, 1449.1, 1213.5, 1094.7, 1028.4, 882.2, 794.9, 695.3.



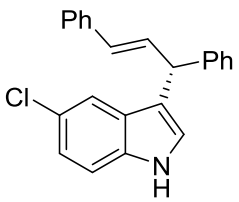
5d

(*R*,*E*)-3-(1,3-diphenylallyl)-5-methoxy-1H-indole (5d): Colorless oil. 88% yield. $[\alpha]_D^{25}$ = -30.2 (*c* = 0.9, $CDCl_3$). The product **5d** was directly conversed to *N*-Boc-protected derivatives **6d**.



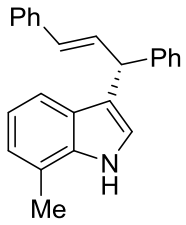
5e

(*R*,*E*)-3-(1,3-diphenylallyl)-2-phenyl-1H-indole (5e): Yellow oil. 85% yield. $[\alpha]_D^{25}$ = -36.4 (*c* = 0.7, $CDCl_3$). The product **5e** was directly conversed to *N*-Boc-protected derivatives **6e**.



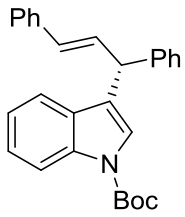
5f

(*R,E*)-5-chloro-3-(1,3-diphenylallyl)-1H-indole (5f): Yellow oil. 80% yield. $[\alpha]_D^{25}$ = -28.9 (*c* = 0.8, $CDCl_3$). The product **5f** was directly conversed to *N*-Boc-protected derivatives **6f**.



5g

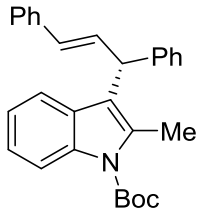
(*R,E*)-3-(1,3-diphenylallyl)-7-methyl-1H-indole (5g): Yellow oil. 80% yield. $[\alpha]_D^{25}$ = -14.1 (*c* = 0.5, $CDCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (bs, 1H), 7.52-7.47 (m, 4H), 7.47-7.31(m, 7H), 7.14-7.09 (m, 2H), 6.93 (d, J = 1.5 Hz, 1H), 6.88 (dd, J = 7.5 Hz, 16.0 Hz, 1H), 6.59 (d, J = 15.5 Hz, 1H), 5.26 (d, J = 7.5 Hz, 1H), 2.55 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.6, 137.7, 136.4, 132.8, 130.7, 128.7, 128.6, 127.4, 126.6, 126.5, 122.7, 122.6, 120.4, 119.8, 119.2, 117.8, 46.5, 16.7. IR (cm^{-1}, neat) 3427.3, 3026.1, 2964.1, 2964.2, 2921.2, 2853.4, 2245.7, 1598.5, 1493.3, 1449.4, 1340.5, 1029.1, 905.7, 786.8, 726.5, 695.6.



6a

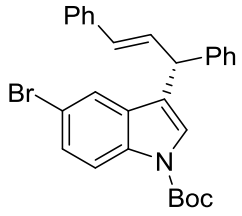
(*R,E*)-tert-butyl 3-(1,3-diphenylallyl)-1H-indole-1-carboxylate (6a):

White solid, 56-58 °C. 79% yield, 96% *ee*. $[\alpha]_D^{25}$ = -31.7 (*c* = 1.2, $CDCl_3$). HPLC conditions: chiralcel OD-H, n-hexane/2-propanol = 99/1, 0.7 mL/min, 254 nm. minor enantiomer: t_R = 7.53 min (S); major enantiomer: t_R = 8.51 min (R). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33-8.21 (m, 1H), 7.55-7.52 (m, 1H), 7.47-7.28 (m, 12H), 7.25-7.21(m, 1H), 6.82 (dd, J=7.5 Hz, 16.0 Hz, 1H), 6.56 (d, J = 15.5 Hz, 1H), 5.15 (d, J = 7.0 Hz, 1H), 1.77 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.0, 142.2, 137.3, 131.4, 131.3, 130.0, 129.1, 128.7, 128.6, 128.5, 127.5, 126.8, 126.5, 124.5, 123.9, 122.6, 120.3, 115.4, 83.8, 46.1, 28.3. IR (cm^{-1}, neat) 3057.4, 2976.4, 2930.4, 1727.7, 1599.7, 1450.5, 1368.2, 1308.0, 1254.4, 1150.4, 1074.1, 966.8, 852.4, 742.8. GC-MS (EI): calcd for $C_{28}H_{27}NO_2$ [M]: 409.2; Found: 309.2, 268.0, 232.1, 204.1, 165.0, 130.1, 91.0.



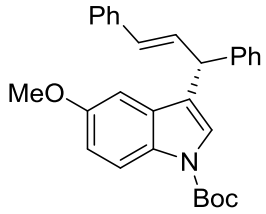
6b

(*R*,*E*)-tert-butyl 3-(1,3-diphenylallyl)-2-methyl-1H-indole-1-carboxylate (6b): White solid, mp: 130-132 ^{o}C. 75% yield, 99% *ee*. $[\alpha]_D^{25}$ = -8.5 (*c* = 0.6, $CDCl_3$). HPLC conditions: chiralcel OJ-H, n-hexane/2-propanol = 80/20, 0.3 mL/min, 254 nm. major enantiomer: t_R = 20.48 min (R); minor enantiomer: t_R = 26.93 min (S). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23-8.19 (m, 1H), 7.46-7.42 (m, 2H), 7.42-7.38 (m, 2H), 7.37-7.32 (m, 5H), 7.29-7.25 (m, 3H), 7.16-7.11(m, 1H), 6.87 (dd, J=7.5 Hz, 16.0 Hz, 1H), 6.53 (d, J = 16.0 Hz, 1H), 5.25 (d, J = 7.5 Hz, 1H), 2.68 (s, 3H), 1.75 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.8, 142.5, 137.3, 136.1, 134.1, 131.6, 130.7, 129.0, 128.6, 128.4, 128.1, 127.3, 126.4, 126.3, 123.2, 122.3, 119.6, 119.3, 115.5, 83.7, 44.6, 28.4, 14.43. IR (cm^{-1}, neat) 3025.6, 2976.2, 2929.7, 1727.3, 1599.2, 1492.8, 1455.6, 1392.8, 1365.0, 1116.0, 964.5, 842.0, 743.6, 694.9. GC-MS (EI): calcd for $C_{29}H_{29}NO_2$ [M]: 423.2; Found: 323.2, 291.1, 246.1, 218.1, 191.1, 144.1, 116.1.



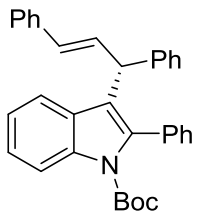
6c

(*R*,*E*)-tert-butyl-5-bromo-3-(1,3-diphenylallyl)-1H-indole-1-carboxylate (6c): White solid, 152-153 ^{o}C. 78% yield, 94% *ee*. $[\alpha]_D^{25}$ = -28.8 (*c* = 0.8, $CDCl_3$). HPLC conditions: chiralcel OJ-H, n-hexane/2-propanol = 99/1, 0.5 mL/min, 254 nm. minor enantiomer: t_R = 11.75 min (S); major enantiomer: t_R = 12.77 min (R). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09-7.95(m, 1H), 7.51-7.47 (m, 1H), 7.44-7.37 (m, 4H), 7.37-7.28 (m, 7H), 7.27-7.22(m, 1H), 6.71-6.64 (m, 1H), 6.44 (d, J = 15.5 Hz, 1H), 5.01 (d, J = 7.5 Hz, 1H), 1.68 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.5, 141.6, 137.1, 131.6, 131.5, 130.8, 128.7, 128.6, 128.4, 127.5, 127.3, 126.9, 126.4, 124.9, 122.6, 122.4, 116.7, 115.9, 84.2, 45.7, 28.4. IR (cm^{-1}, neat) 3025.8, 2977.0, 1732.1, 1600.1, 1447.4, 1367.1, 1275.5, 1150.5, 1028.5, 786.5, 695.7. GC-MS (EI): calcd for $C_{28}H_{26}BrNO_2$ [M]: 487.1; Found: 389.1, 310.0, 284.0, 255.1, 230.1, 191.0, 154.0, 115.0.



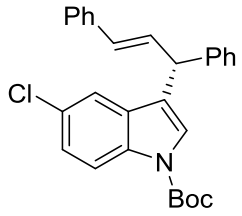
6d

(*R,E*)-tert-butyl-3-(1,3-diphenylallyl)-5-methoxy-1H-indole-1-carboxylate (6d): White solid, 124-126 ^{o}C. 77% yield, 98% *ee*. $[\alpha]_D^{25}$ = -41.1 (*c* = 0.56, $CDCl_3$). HPLC conditions: chiralcel OD-H, n-hexane/2-propanol = 99/1, 0.7 mL/min, 254 nm. minor enantiomer: t_R = 10.25 min (S); major enantiomer: t_R = 11.89 min (R). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03(s, 1H), 7.43-7.30 (m, 9H), 7.30-7.22 (m, 2H), 6.96-6.91 (m, 1H), 6.83-6.79 (m, 1H), 6.75-6.68 (m, 1H), 6.48 (d, J = 15.5 Hz, 1H), 5.03 (d, J = 7.0 Hz, 1H), 3.74 (s, 3H), 1.69 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 149.9, 142.0, 137.2, 131.4, 131.1, 128.6, 128.5, 128.4, 127.4, 126.7, 126.4, 124.5, 122.8, 115.9, 112.8, 103.1, 83.5, 55.6, 46.0, 28.3. IR (cm^{-1}, neat) 2974.3, 2010.0, 1730.7, 1474.7, 1445.0, 1372.0, 1253.0, 1150.8, 1072.6, 968.6, 917.8, 699.8. GC-MS (EI): calcd for $C_{29}H_{29}NO_3$ [M]: 439.2; Found: 339.2, 308.2, 262.1, 218.1, 191.0, 160.0, 115.0.



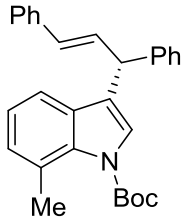
6e

(*R,E*)-tert-butyl-3-(1,3-diphenylallyl)-2-phenyl-1H-indole-1-carboxylate (6e): White solid, mp: 153-155 ^{o}C. 78% yield, 95% *ee*. $[\alpha]_D^{25}$ = -22.2 (*c* = 0.87, $CDCl_3$). HPLC conditions: chiralcel AD-H, n-hexane/2-propanol = 99/1, 1.0 mL/min, 254 nm. minor nantiomer: t_R = 3.74 min (S) ; major enantiomer: t_R = 9.16 min (R). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35-8.30 (m, 1H), 7.49-7.39 (m, 5H), 7.38-7.26 (m, 10H), 7.25-7.18 (m, 2H), 7.17-7.11 (m, 1H), 6.83-6.75 (m, 1H), 6.35 (d, J = 16.0 Hz, 1H), 4.89 (d, J = 5.5 Hz, 1H), 1.28-1.25 (m, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.2, 142.6, 137.4, 137.0, 136.6, 134.3, 131.6, 130.7, 130.1, 128.5, 128.3, 128.1, 128.0, 127.8, 127.3, 126.4, 126.3, 124.3, 122.6, 121.3, 120.9, 115.4, 83.1, 44.9, 27.5. IR (cm^{-1}, neat) 3027.0, 2921.2, 2850.8, 1719.4, 1454.0, 1325.7, 1150.1, 1027.1, 964.9, 830.7, 748.1, 693.7.



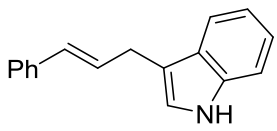
6f

(*R*,*E*)-tert-butyl-5-chloro-3-(1,3-diphenylallyl)-1H-indole-1-carboxylate (6f): White solid, mp: 54-56 ^{o}C. 75% yield, 92% *ee*. $[\alpha]_D^{25}$ = -14.6 (*c* = 0.7, $CDCl_3$). HPLC conditions: chiralcel OD-H, n-hexane/2-propanol = 99/1, 0.5 mL/min, 254 nm. minor nantiomer: t_R = 10.07 min (S) ; major enantiomer: t_R = 10.98 min (R). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.46-7.26 (m, 13H), 6.70 (dd, J = 7.5 Hz, 16.0 Hz, H), 6.47 (d, J = 15.5 Hz, 1H), 5.03 (d, J = 7.0 Hz, 1H), 1.70 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.6, 141.7, 137.1, 131.6, 131.1, 130.8, 128.8, 128.6, 128.2, 127.5, 127.0, 126.5, 125.1, 124.6, 122.5, 119.7, 116.4, 84.2, 45.8, 28.2. IR (cm^{-1}, neat) 3027.4, 2976.4, 2927.4, 1735.1, 1491.7, 1332.6, 1243.1, 1030.5, 842.1, 754.5, 694.6.



6g

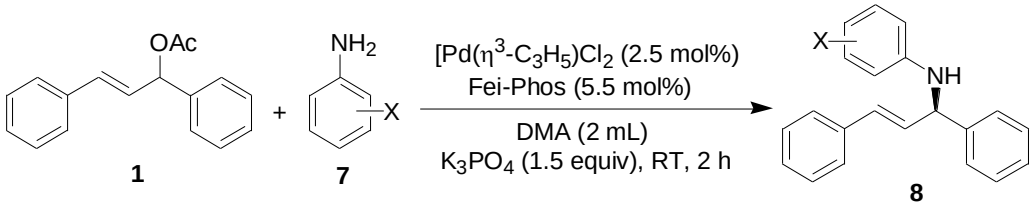
(*R*,*E*)-tert-butyl-3-(1,3-diphenylallyl)-7-methyl-1H-indole-1-carboxylate (6g): White solid, mp: 123-125 ^{o}C. 76% yield, 91% *ee*. HPLC conditions: chiralcel OD-H, n-hexane/2-propanol = 97/3, 0.7 mL/min, 254 nm. minor nantiomer: t_R = 6.22 min (S) ; major enantiomer: t_R = 6.73 min (R). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51-7.33 (m, 12H), 7.24-7.18 (m, 2H), 6.85 (dd, J = 7.5 Hz, 16.0 Hz, H), 6.59 (d, J = 15.5 Hz, 1H), 5.17 (d, J = 7.5 Hz, 1H), 2.80 (s, 3H), 1.75 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.9, 142.3, 137.4, 135.6, 131.5, 131.3, 128.7, 128.6, 127.9, 127.5, 126.8, 126.2, 125.5, 123.1, 122.8, 117.9, 83.5, 28.2, 22.4.



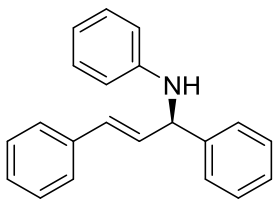
3-cinnamyl-1H-indole (6h), white solid, Yield: 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.37 – 7.08 (m, 8H), 6.53 (d, *J* = 15.9 Hz, 1H), 6.45 (dt, *J* = 15.7, 6.2 Hz, 1H), 3.67 (d, *J* = 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.09, 135.80, 129.79, 128.65, 127.83, 126.82, 126.29, 125.46, 121.40, 121.12,

118.70, 118.47, 113.96, 110.45, 76.70, 76.38, 76.06, 28.31. HRMS (ESI) calcd. for $C_{17}H_{16}N[M+H]^+$: 234.1277, Found: 234.1125.

3.5 General procedures for Pd-catalyzed asymmetric allylic amination of aniline

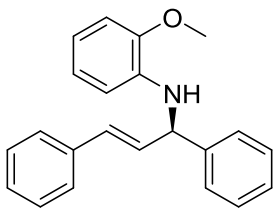


A flame-dried Schlenk tube was charged with $[Pd(\eta^3\text{-allyl})Cl]_2$ (4.5 mg, 0.0125 mmol, 2.5 mol%) and (2*S*,3*S*,5*R*,6*R*)-Fei-Phos (18.9 mg, 0.0275 mmol, 5.5 mol%) under an N_2 atmosphere, and the mixture was dissolved in dry *N*,*N*-dimethylacetamide (2.0 mL). The solution was stirred at room temperature for 30 min and then adding (*E*)-1,3-diphenyl-2-propenyl acetate (0.5 mmol), The mixture solution was further stirred for 10 minutes at room temperature, and anhydrous K_3PO_4 (160 mg, 0.75 mmol) was added in to the vial followed by aniline (0.75 mmol). The reaction mixture was stirred at room temperature for 2 h. The solution was quenched with EtOAc and saturated aqueous NH_4Cl solution. The mixture was then extracted twice with EtOAc (20×3 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude product was purified by flash column chromatography to afford the product **8**.

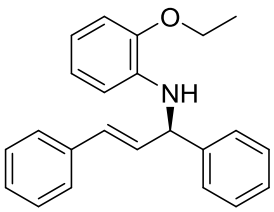


(*R*)-*N*-(1,3-diphenylallyl)aniline (8a), yellow oil, Yield: 97%. $[\alpha]_D^{25}$ = -31.3(c = 5.25, $CHCl_3$), 83% *ee*[determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 95:5, 1.0 mL/min, 254 nm; t_R (major) = 10.00 min; t_R (minor)

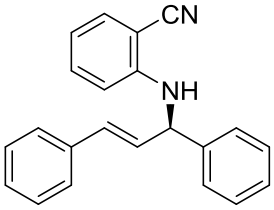
=12.23 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.1 Hz, 2H), 7.27 – 7.01 (m, 10H), 6.61 (t, *J* = 7.3 Hz, 1H), 6.55–6.49 (m, 3H), 6.29 (dd, *J* = 15.8, 6.2 Hz, 1H), 4.98 (d, *J* = 6.2 Hz, 1H), 4.15 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.08, 142.00, 136.66, 131.18, 130.67, 129.14, 128.81, 128.53, 127.66, 127.53, 127.23, 126.52, 117.87, 113.77, 60.77. IR (neat, cm^{-1}) 3408, 3081, 3054, 3028, 1600, 1501, 1449, 1426, 1384, 1313, 1260, 1179, 967, 746, 692. HRMS (ESI) calcd. for $C_{21}H_{19}N[M+H]^+$: 286.1590, Found:286.1621.



(*R*)-N-(1,3-diphenylallyl)-2-methoxyaniline (8b), white solid, Yield: 95%. $[\alpha]_D^{25}$=-29.6(c = 70.6, $CHCl_3$), 77% *ee*[determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 98:2, 1.0 mL/min, 254 nm; t_R (minor) = 7.96 min; t_R (major) =9.12 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (t, *J* = 5.7 Hz, 2H), 7.38 – 7.14 (m, 9H), 6.80 – 6.72 (m, 2H), 6.70 – 6.55 (m, 3H), 6.47 – 6.38 (m, 1H), 5.08 (d, *J* = 5.8 Hz, 1H), 4.90 (s, 1H), 3.84 (d, *J* = 4.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.04, 142.24, 137.05, 136.86, 131.11, 131.05, 128.82, 128.57, 127.66, 127.48, 127.31, 126.61, 121.26, 117.14, 111.65, 109.52, 60.73, 55.50. IR (neat, cm^{-1}) 3434, 3024, 1637, 1600, 1507, 1447, 1421, 1236, 1219, 1178, 1139, 1048, 1024, 967, 741, 698. HRMS (ESI) calcd. for $C_{22}H_{21}NO[M+H]^+$: 316.1696, Found: 316.1703.

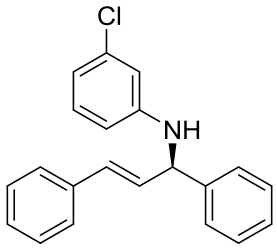


(*R*)-N-(1,3-diphenylallyl)-2-ethoxyaniline (8c), orange oil, Yield: 97%. $[\alpha]_D^{25}$ = -33.9(c = 73.3, $CHCl_3$), 81% *ee*[determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 95:5, 1.0 mL/min, 254 nm; t_R (major) = 12.98 min; t_R (minor) =18.45 min].^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, J=7.5 Hz, 2H), 7.36 – 7.17 (m, 9H), 6.72 (d, J = 8.7 Hz, 2H), 6.64 – 6.57 (m, 3H), 6.40 (dd, J = 15.8, 6.3 Hz, 1H), 5.00 (d, J = 6.3 Hz, 1H), 3.92 (q, J = 6.9 Hz, 2H), 1.34 (t, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.97, 142.04, 140.82, 136.74, 131.24, 130.87, 128.81, 128.55, 128.30, 127.66, 127.55, 127.34, 126.77, 126.56, 115.66, 115.52, 64.06, 62.06, 15.01. IR (neat, cm^{-1}) 3545, 3057, 3026, 1619, 1509, 1478, 1449, 1385, 1235, 1117, 1049, 921, 817, 745, 699. HRMS (ESI) calcd. for $C_{23}H_{23}NO[M+Na]^+$: 352.1672, Found:352.1693.

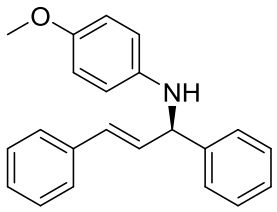


(*R*)-2-((1,3-diphenylallyl)amino)benzonitrile (8d), white solid, Yield: 86%. $[\alpha]_D^{25}$ = -44.7(c = 58.5, $CHCl_3$), 85% *ee*[determined by HPLC analysis using a Chiralcel OJ-H column; *n*-Hex / *i*-PrOH = 95:5, 1.0 mL/min, 254 nm; t_R (major) = 20.26 min; t_R (minor) =22.88 min].^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.38 (m, 7H), 7.37 – 7.24 (m, 5H), 6.76 – 6.58 (m, 3H), 6.42 (dd, *J* = 15.9, 6.2 Hz, 1H), 5.23 (d, *J* = 6.1 Hz, 1H), 5.06 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.10, 140.57, 136.15, 134.12, 132.70, 132.08, 129.12, 129.07, 128.60, 128.01, 127.98, 127.01, 126.62, 117.13, 112.18, 96.41, 59.99. IR (neat, cm^{-1}) 3406, 3333, 3081, 3025, 2854, 2213, 1633, 1575, 1506,

1450, 1321, 1274, 961, 745, 699. HRMS (ESI) calcd. for $C_{22}H_{18}N_2[M+Na]^+$: 333.1362, Found:333.1368.

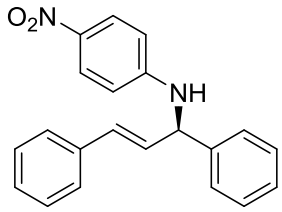


(*R*)-3-chloro-N-(1,3-diphenylallyl)aniline (8e), yellow oil, Yield: 92%. $[\alpha]_D^{25}$=-34.4(c = 74.3, $CHCl_3$), 83% *ee*[determined by HPLC analysis using a Chiralcel OD-H column; *n*-Hex / *i*-PrOH = 90:10, 1.0 mL/min, 254 nm; t_R (minor) = 12.52 min; t_R (major) =21.00 min].^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.21 (m, 13H), 7.02 (t, *J* = 8.0 Hz, 1H), 6.68 – 6.56 (m, 3H), 6.49 (dd, *J* = 8.1, 1.8 Hz, 1H), 6.36 (dd, *J* = 15.8, 6.2 Hz, 1H), 5.05 (d, *J* = 6.2 Hz, 1H), 4.33 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.30, 141.53, 136.56, 134.94, 131.52, 130.18, 130.10, 128.98, 128.64, 127.86, 127.80, 127.24, 126.62, 117.78, 113.54, 111.90, 60.53. IR (neat, cm^{-1}) 3416, 3059, 3026, 2960, 1598, 1494, 1450, 1417, 1322, 1279, 1166, 1091, 1074, 1028, 966, 913, 838, 746, 698. HRMS (ESI) calcd. for $C_{21}H_{18}ClN[M+H]^+$: 320.1201, Found: 320.1200.

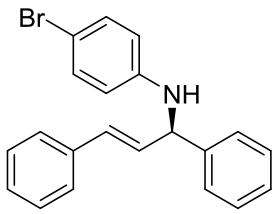


(*R*)-N-(1,3-diphenylallyl)-4-methoxyaniline (8f), white solid, Yield: 95%. $[\alpha]_D^{25}$ = -35.9(c = 68.5, $CHCl_3$), 81% *ee*[determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 95:5, 1.0 mL/min, 254 nm; t_R (major) = 15.19 min; t_R (minor) =20.84 min].^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.5 Hz, 2H), 7.36 –

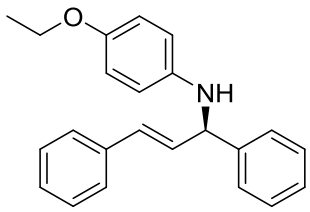
7.15 (m, 8H), 6.72 (d, *J* = 6.5 Hz, 2H), 6.63 – 6.55 (m, 3H), 6.37 (dd, *J* = 15.8, 6.2 Hz, 1H), 4.99 (d, *J* = 5.4 Hz, 1H), 4.00 (s, 1H), 3.69 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ=152.42, 142.27, 141.30, 136.74, 131.03, 128.79, 128.54, 127.63, 127.47, 127.24, 126.52, 115.15, 114.80, 61.71, 55.73. IR (neat, cm^{-1}) 3440, 3024, 2835, 1636, 1509, 1448, 1312, 1248, 1180, 1032, 964, 825, 745, 697. HRMS (ESI) calcd. for $C_{22}H_{21}NO[M+Na]^+$: 338.1515, Found:338.1524.



(*R*)-N-(1,3-diphenyallyl)-4-nitroaniline (8g), yellow solid, Yield: 93%. $[\alpha]_D^{25}$ = -74.1(c = 70.4, $CHCl_3$), 86% *ee*[determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 80:20, 1.0 mL/min, 254 nm; t_R (major) = 11.94 min; t_R (minor) =13.63 min].^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 9.2 Hz, 2H), 7.41 – 7.28 (m, 10H), 6.63 – 6.56 (m, 3H), 6.37 (dd, *J* = 15.9, 6.1 Hz, 1H), 5.20 (d, *J* = 5.9 Hz, 1H), 4.84 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.29, 140.39, 138.48, 136.12, 132.31, 129.18, 128.71, 128.18, 128.15, 127.16, 126.65, 126.26, 113.39, 112.19, 60.08. IR (neat, cm^{-1}) 3447, 3208, 2916, 1630, 1502, 1468, 1384, 1309, 1182, 1111, 965, 831, 744, 695. HRMS (ESI) calcd. for $C_{21}H_{18}N_2O_2[M+Na]^+$: 353.1260, Found:353.1270.



(*R*)-4-bromo-N-(1,3-diphenylallyl)aniline (8h), yellow oil, Yield: 84%. $[\alpha]_D^{25}$=-37.4(c = 72.5, $CHCl_3$), 82% *ee*[determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 90:10, 1.0 mL/min, 254 nm; t_R (major) = 9.52 min; t_R (minor) =11.94 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.27 (m, 9H), 7.25 – 7.17 (m, 4H), 6.57 (dd, *J* = 27.1, 12.3 Hz, 3H), 6.37 (dd, *J* = 15.8, 6.3 Hz, 1H), 5.03 (d, *J* = 6.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.91, 141.44, 136.51, 131.90, 131.58, 130.07, 128.95, 128.62, 127.85, 127.77, 127.23, 126.58, 115.51, 109.76, 60.87. IR (neat, cm^{-1}) 3417, 3083, 2850, 1594, 1492, 1449, 1384, 1313, 1258, 1178, 1122, 967, 812, 746, 698. HRMS (ESI) calcd. for $C_{21}H_{18}BrN[M+H]^+$: 364.0695, Found: 364.0683.



(*R*)-N-(1,3-diphenylallyl)-4-ethoxyaniline (8i), yellow oil, Yield: 94%. $[\alpha]_D^{25}$= -33.5(c = 79.7, $CHCl_3$), 75% *ee*[determined by HPLC analysis using a Chiralcel AD-H column; *n*-Hex / *i*-PrOH = 95:5, 1.0 mL/min, 254 nm; t_R (major) = 12.97 min; t_R (minor) =18.66 min].^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, J = 7.1 Hz, 2H), 7.36–7.17 (m, 9H), 6.72 (d, J = 8.9 Hz, 2H), 6.61 (dd, J = 12.2, 3.2 Hz, 3H), 6.40 (dd, J = 15.8, 6.4 Hz, 1H), 4.99 (d, J = 6.3 Hz, 1H), 3.92 (q, J = 7.0 Hz, 2H), 1.34 (t, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.96, 142.00, 136.71, 131.22, 130.82, 128.79, 128.53, 128.27, 127.64, 127.53, 127.32, 126.53, 115.62, 115.50, 64.03, 62.05, 14.99. HRMS (ESI) calcd. for $C_{23}H_{23}NO[M+Na]^+$: 352.1672, Found:352.1635.

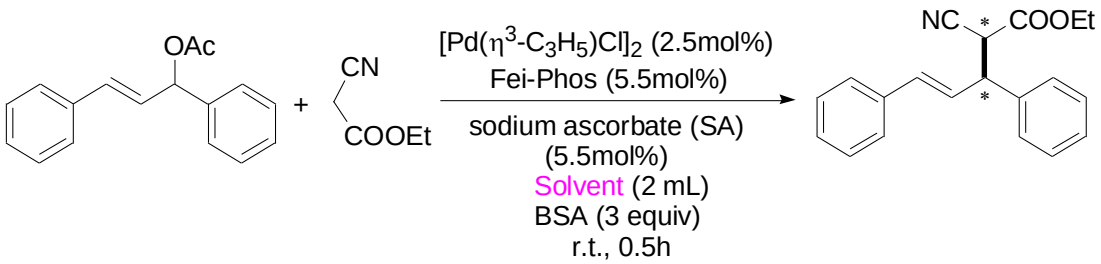
References

[1] a) Auburn, P. R.; Mackenzie, P. B.; Bosnich, B. *J. Am. Chem. Soc.* **1985**, *107*, 2033; b) Müller, C. A.; Pfaltz, A. *Angew. Chem. Int. Ed.* **2008**, *47*, 3363; c) Jiang, Z. Y.; Zhang, C. H.; Gu, F. L.; Yang, K. F.; Lai, G. Q.; Xu, L. W.; Xia, C. G. *Synlett* **2010**, 1251; d) Troshin, K.; Mayr, H. *J. Org. Chem.* **2013**, *78*, 2649.

[2] Ye, F.; Zheng, Z. J.; Li, L.; Yang, K. F.; Xia, C. G.; Xu, L. W. *Chem. Eur. J.* **2013**, *19*, 15452-15457

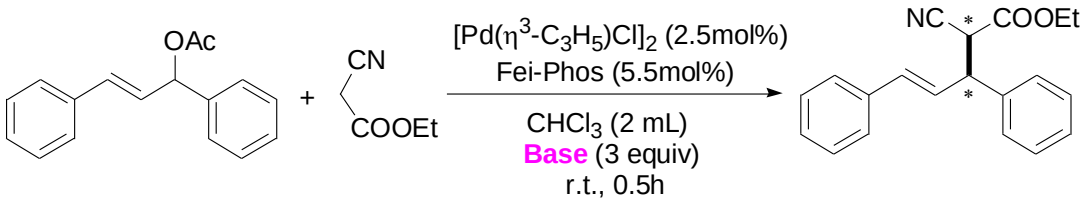
[3] Deng, W. H.; Ye, F.; Bai, X. F.; Zheng, Z. J.; Cui, Y. M.; Xu, L. W. *ChemCatChem* **2015**, 7, 75-79

Table S1. Effect of the solvent on the catalytic asymmetric allylic alkylation of ethyl 2-cyanoacetate



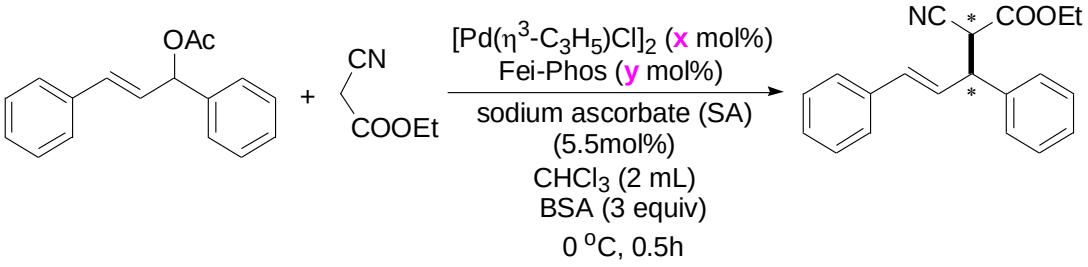
Entry	solvent	conv.(%)	*Ee* (%)
1	THF	>99	60
2	$CHCl_3$	>99	88
3	CH_3CN	>99	67
4	DMA	59	67
5	Toluene	>99	45
6	CH_2Cl_2	>99	79
7	DME	>99	86

Table S2. Effect of the base on the catalytic asymmetric allylic alkylation of ethyl 2-cyanoacetate



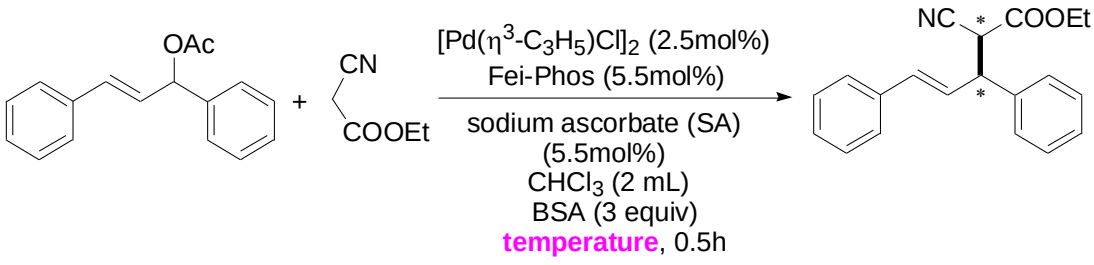
Entry	Base	conv.(%)	*Ee* (%)
1	-	66.7	63
2	SA (5.5mol%) BSA	>99	88
3	KOAc (5.5mol%) BSA	>99	76
4	LiOAc (5.5mol%) BSA	>99	86
5	TMEDA	>99	87
6	K_3PO_4	>99	87
7	Cs_2CO_3	>99	87
8	K_2CO_3	>99	87

Table S3. Effect of the dosage of catalyst on the catalytic asymmetric allylic alkylation of ethyl 2-cyanoacetate



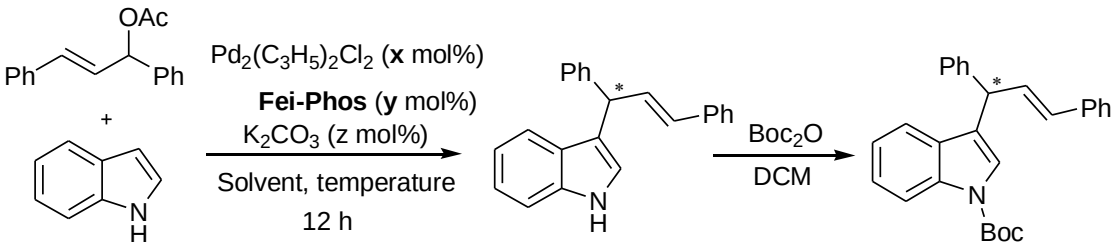
entry	x	y	conv.(%)	ee(%)
1	2	4.4	>99	88.1
2	2.5	5.5	>99	89
3	3	6.6	>99	88.5

Table S4. Effect of the temperature on the catalytic AAA of ethyl 2-cyanoacetate



entry	Temperature (°C)	conv.(%)	*Ee* (%)
1	r.t.	>99	88
2	10	>99	89
3	0	>99	89
4	-20	98	91
5	-30	93	87

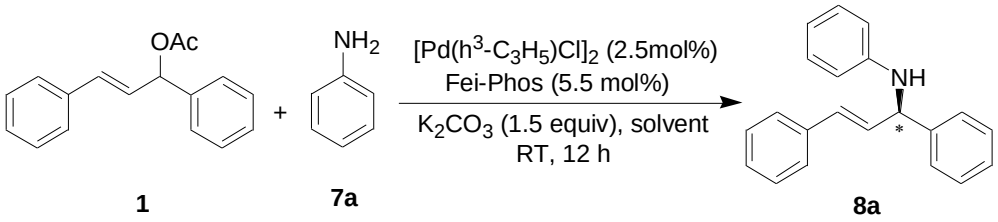
Table S5. Optimization of reaction conditions for catalytic AAA of indole.



Entry	[Pd] (x mol%)	**Fei-Phos** (y mol%)	Solvent	K_2CO_3	Temperature	Total Yield %	Ee %
1	4	5	toluene (2.5M)	2 eq.	rt.	65	96
2	2	2.2	DCM (3.75 M)	2 eq.	rt. For 12h and 50 °C for 12h	70	95
3	2	2.2	Et_2O (3.75 M)	2 eq.	rt.	70	93
4	2	2.2	toluene (5 M)	3 eq.	rt.	75	90
5	4	6	toluene (5 M)	2 eq.	rt.	70	87
6	4	5	DCM (5 M)	2 eq.	50 °C	70	88
7	2	2.2	toluene (5 M)	2 eq.	50 °C	65	94
8	8	12	toluene (5 M)	2 eq.	rt.	65	86
9	4	6	DCM (5 M)	2 eq.	rt.	70	92

10	4	6	Et_2O (5 M)	2 eq.	rt.	70	83
11	4	6	EA (5 M)	2 eq.	rt.	75	83
12	4	4	toluene (5 M)	2 eq.	rt.	70	85
13	4	3.2	toluene (5 M)	2 eq.	rt.	70	90
14	4	2	toluene (5 M)	2 eq.	rt.	70	85

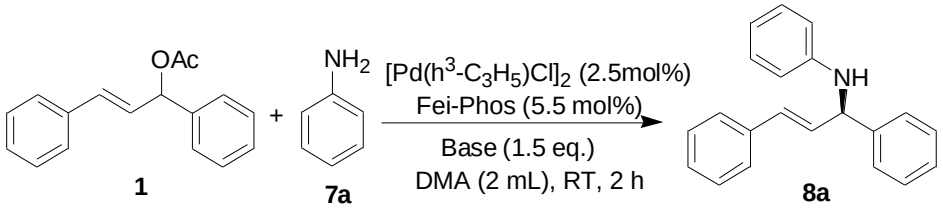
Table S6. Effect of the solvents on palladium-catalyzed asymmetric allylic amination of 1,3-diphenyl-2-propenyl acetate with aniline.



Entry	solvent	conv.(%)	*Ee* (%)
1	Toluene	>99	0
2	DCM	>99	23
3	THF	>99	68
4	DMF	>99	77
5	NMP	>99	70
6	DMSO	>99	51
7	CH_3CN	>99	63
8	DMA	>99	80

Unless otherwise noted, all the reactions were performed with 0.5 mmol of (E)-1,3-diphenyl-2-propenyl acetate and 0.75 mmol of aniline in 2 mL of the specified solvent for 24 h, in the presence of 0.75 mmol of the specified base, using 0.0125 mmol of [Pd] as the catalyst and 0.0125 mmol of Fei-Phos as chiral ligand. The conversion rate of product is determined by GC on an achiral stationary phase. The *ee* value (*ee* %) of product was determined by chiral HPLC with a Chiracel AD-H column.

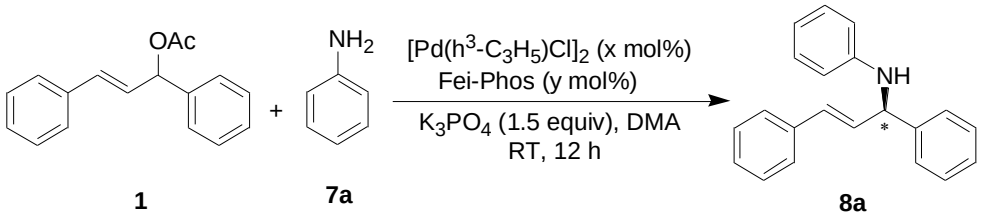
Table S7. Effect of the bases on palladium-catalyzed asymmetric allylic amination of 1,3-diphenyl-2-propenyl acetate with aniline.



Entry	base	conv.(%)	*Ee* (%)
1	-	84	73
2	BSA	86	57
3	DBU	trace	-
5	CsF	93	81
6	TMEDA	85	80
7	Cs_2CO_3	trace	-
8	K_2CO_3	>99	80
9	LiOAc	87	75
10	NaOAc	>99	67
11	KOAc	>99	80
12	KH_2PO_4	>99	70
13	K_2HPO_4	>99	40
14	*t*-BuOK	trace	-
15	K_3PO_4	>99	83
16[a]	K_3PO_4	>99	80
17[b]	K_3PO_4	>99	81

[a] Aniline (3 eq.), K_3PO_4 (3 eq.). [b] Aniline (1.5 eq.), K_3PO_4 (3 eq.).

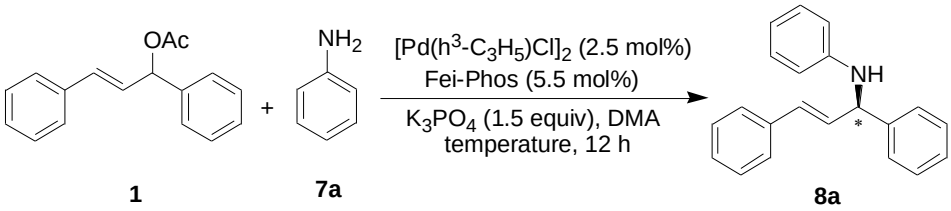
Table S8. Effect of the dosage of catalyst on palladium-catalyzed asymmetric allylic amination of 1,3-diphenyl-2-propenyl acetate with aniline.



1 **7a** **8a**

Entry	x	y	conv.(%)	*Ee* (%)
1	2	4.4	>99	82
2	2.5	5.5	>99	83
3	3	6.3	>99	81

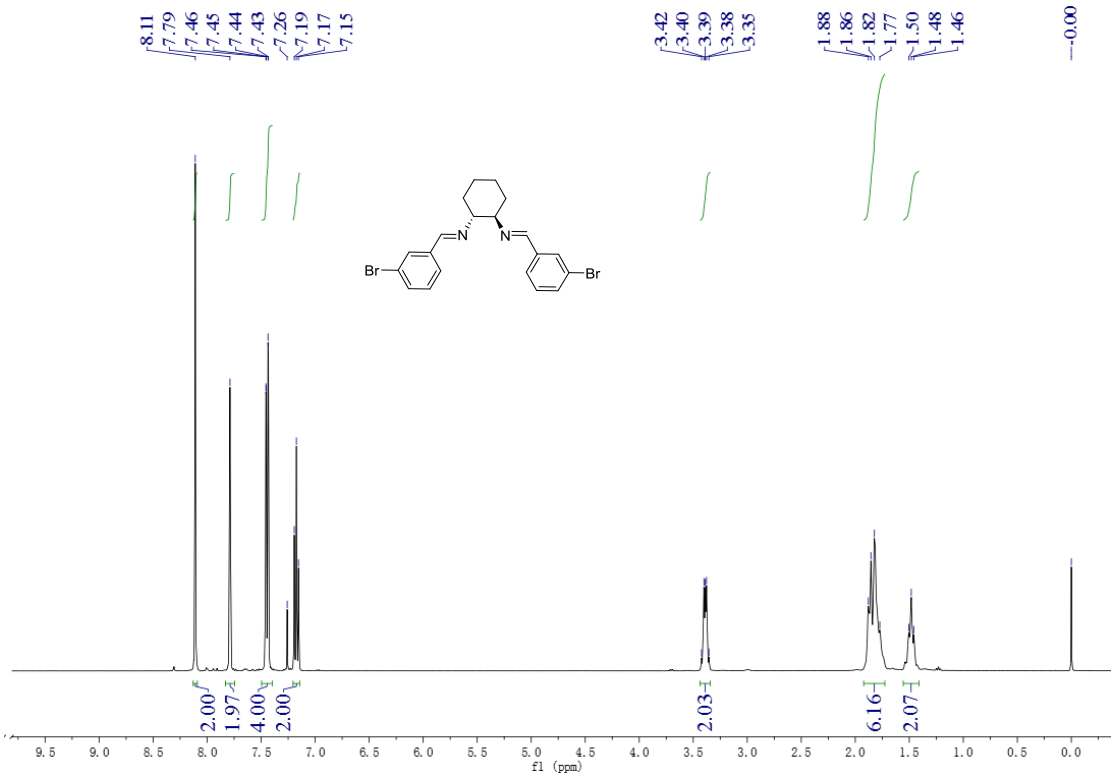
Table S9. Effect of the temperature on palladium-catalyzed asymmetric allylic amination of 1,3-diphenyl-2-propenyl acetate with aniline.

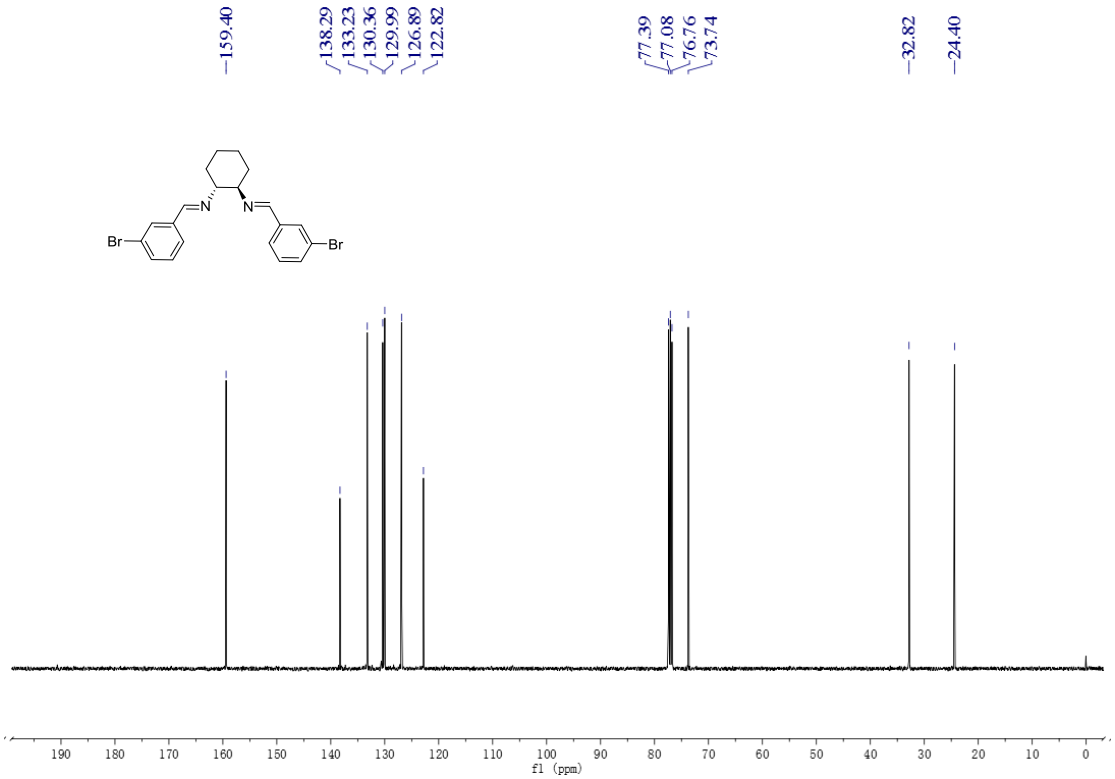


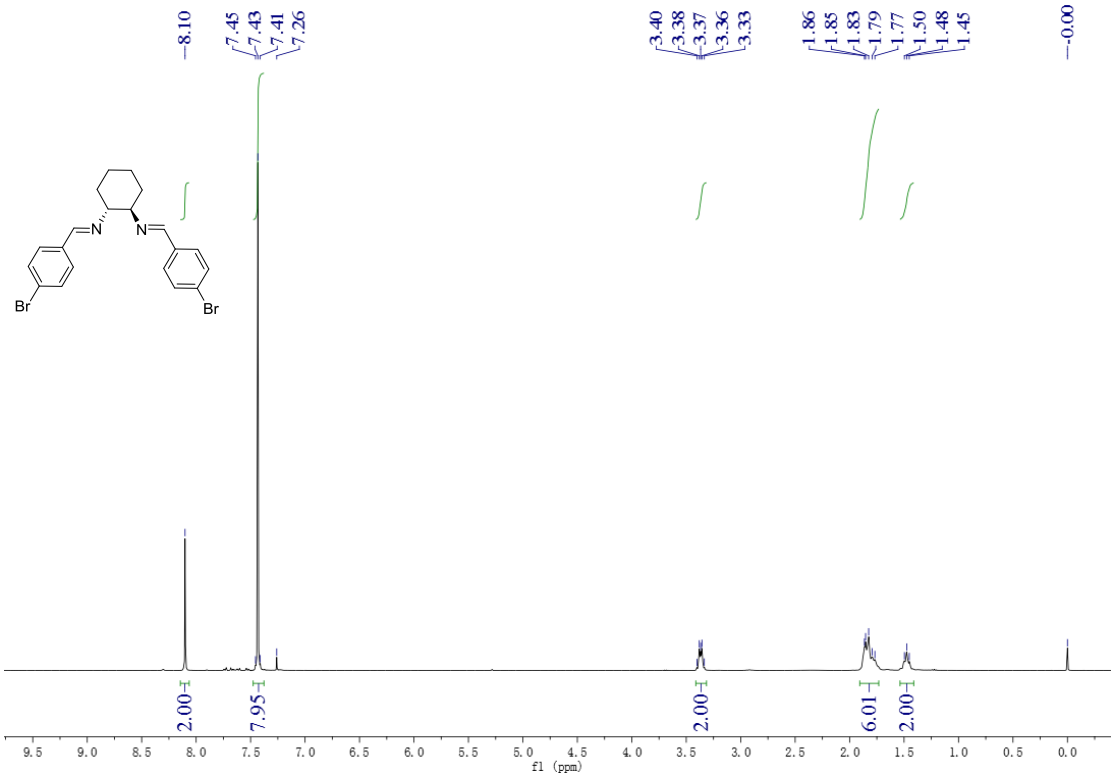
1 **7a** **8a**

Entry	T/^{o}C	conv.(%)	*Ee* (%)
1	25	>99	83
2	-5	>99	81
3	-18	>99	82

4. NMR Spectra of products: ^{1}H, ^{13}C, ^{31}P NMR



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1.79
1.77
1.50
1.48
1.45
0.00
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Br
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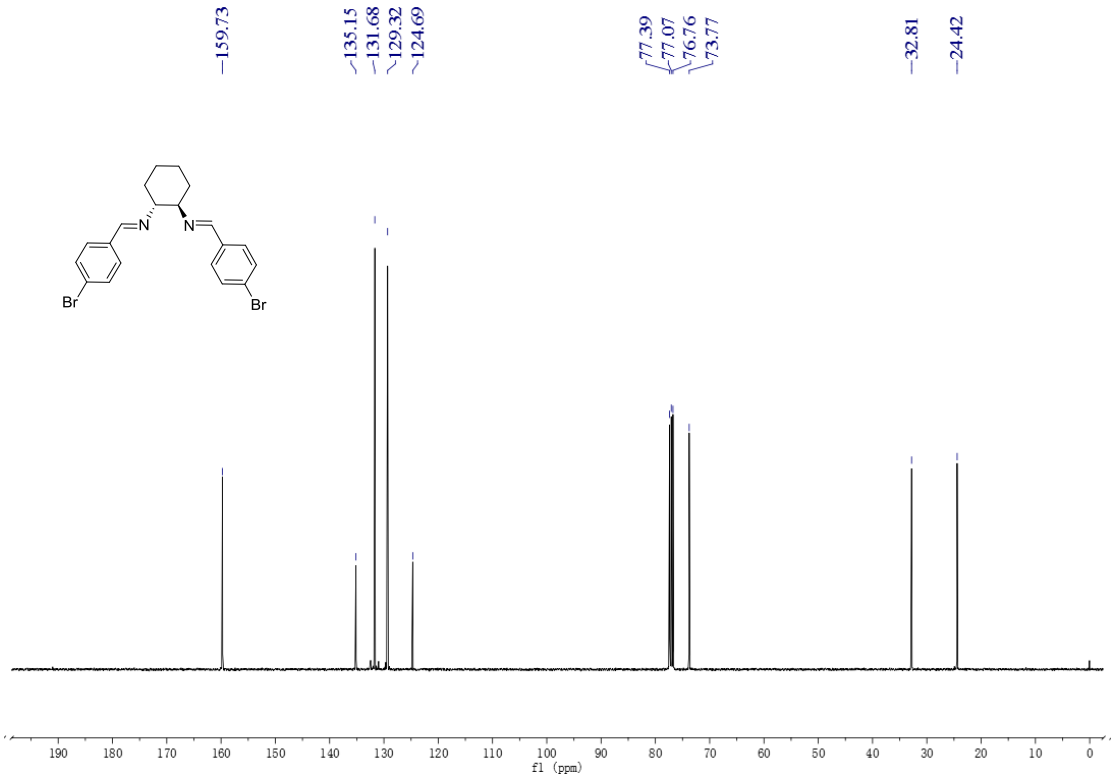
2.00
6.01
2.00
f1 (ppm)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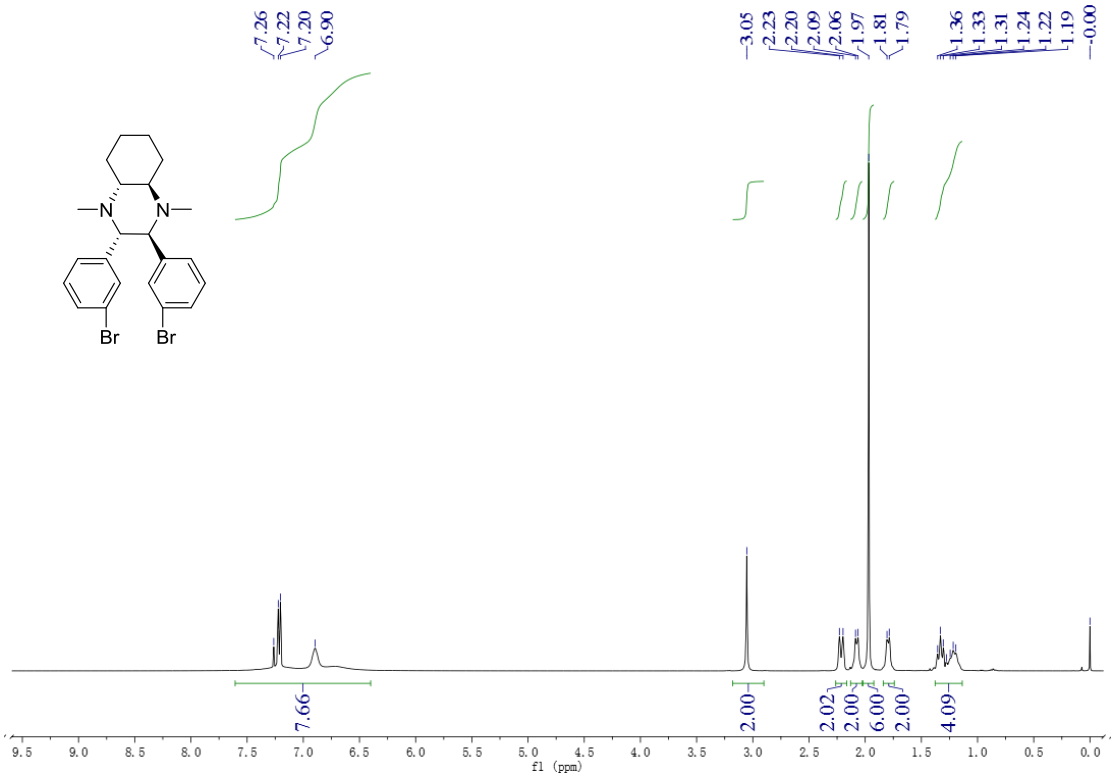
f1 (ppm)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1.36
1.33
1.31
1.24
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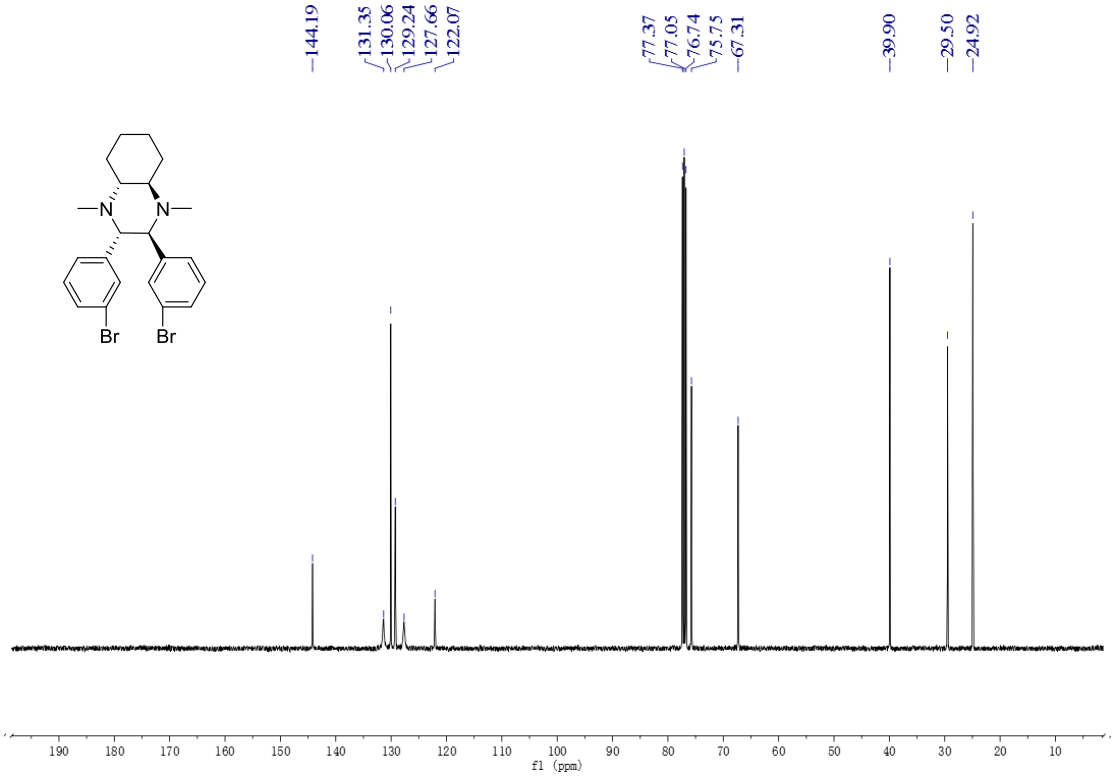
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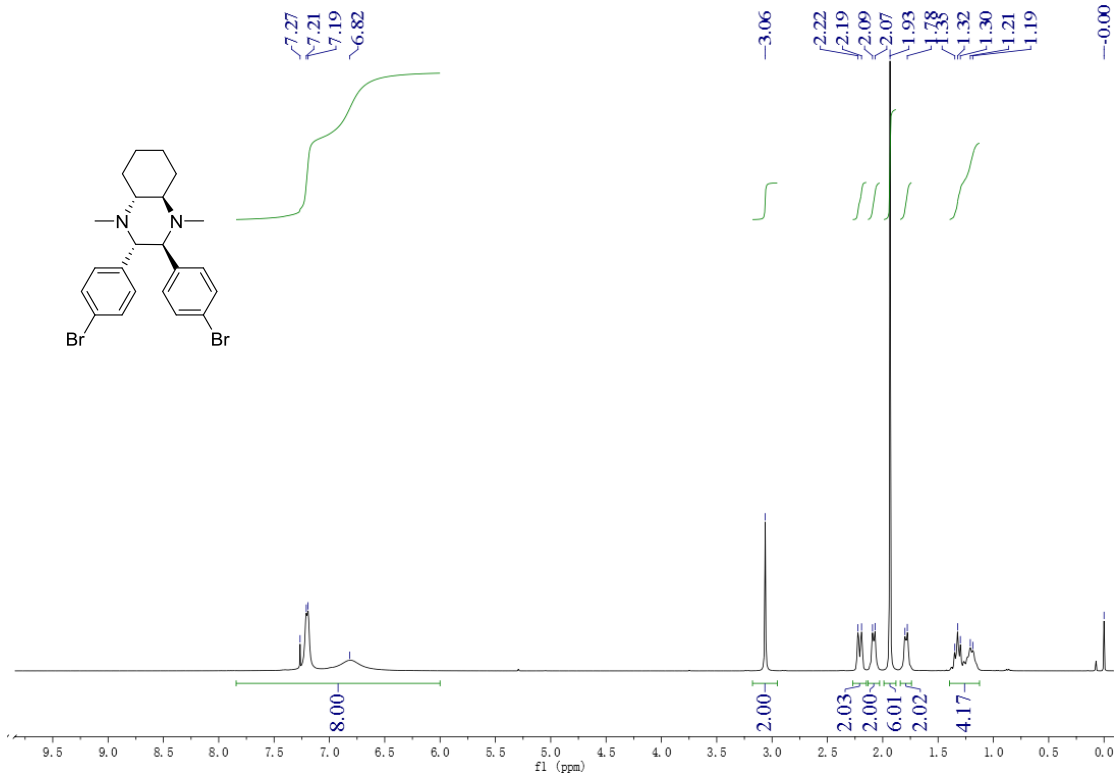
Br
f1 (ppm)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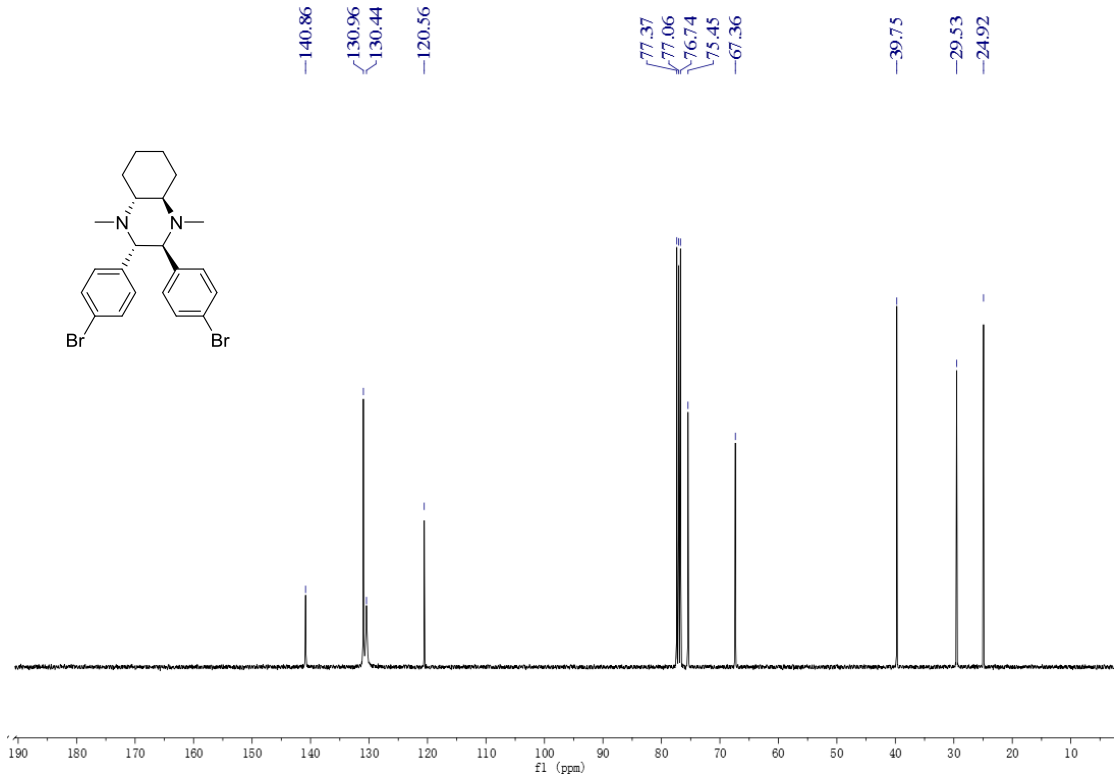
f1 (ppm)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Br
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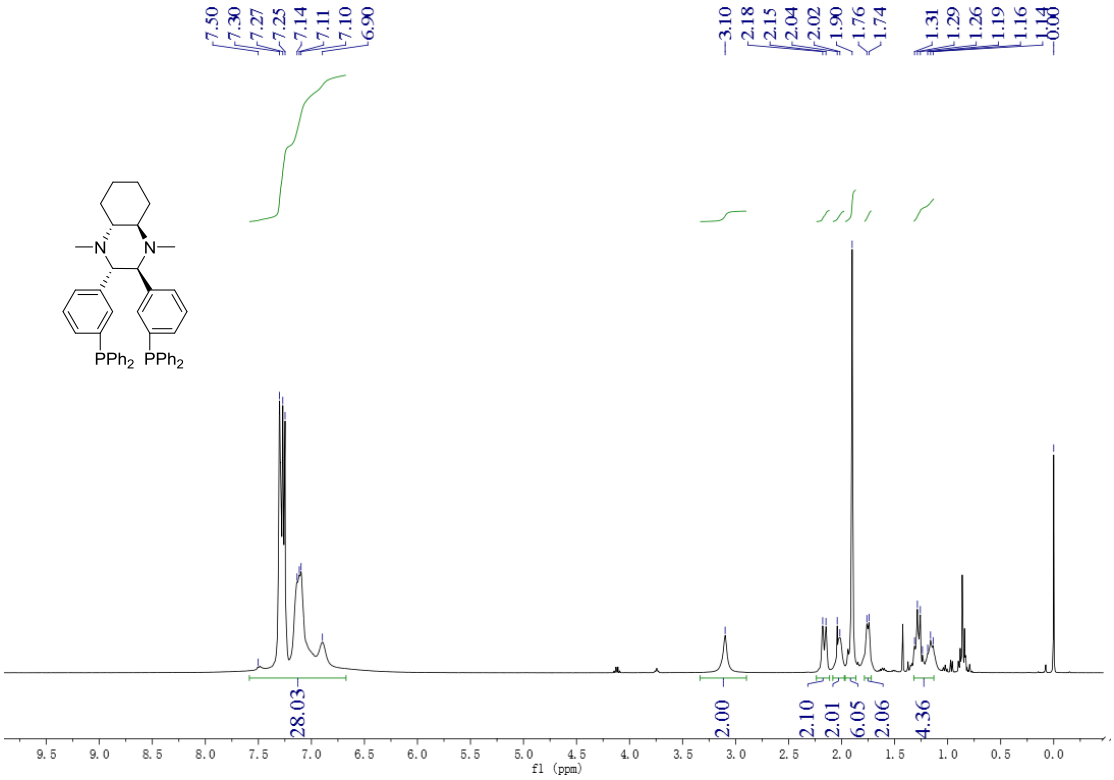
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1.76
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1.29
1.26
1.19
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2.01
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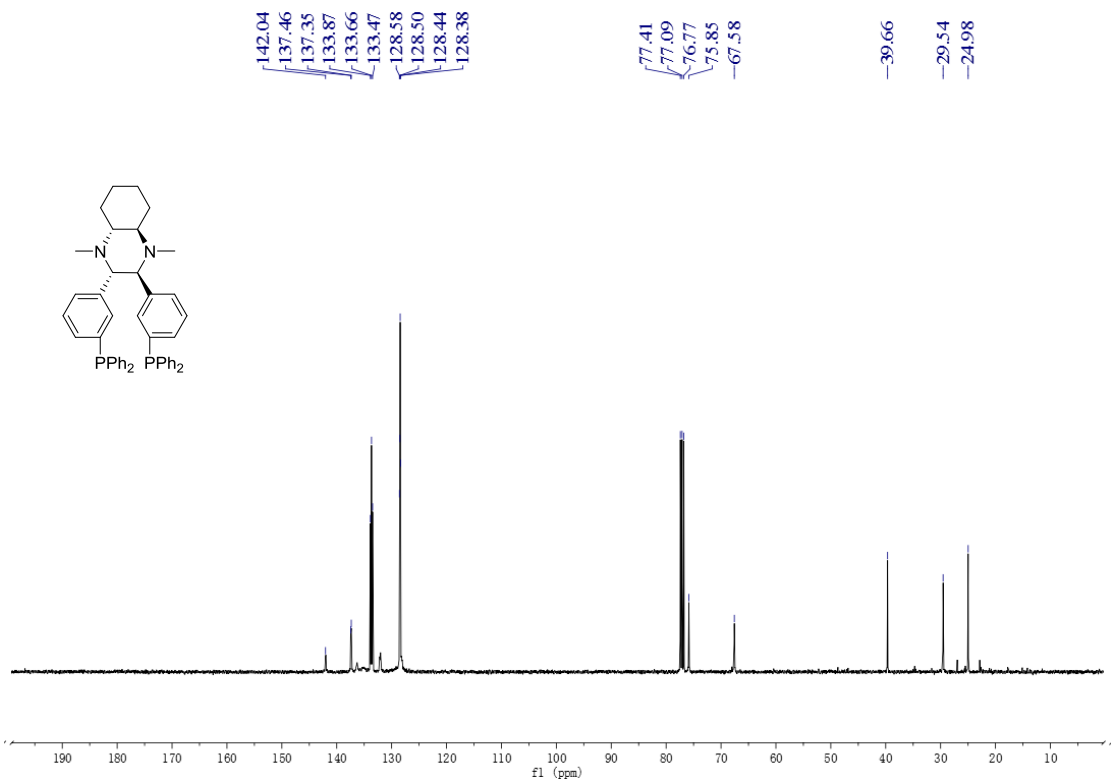
4.36
f1 (ppm)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29.54
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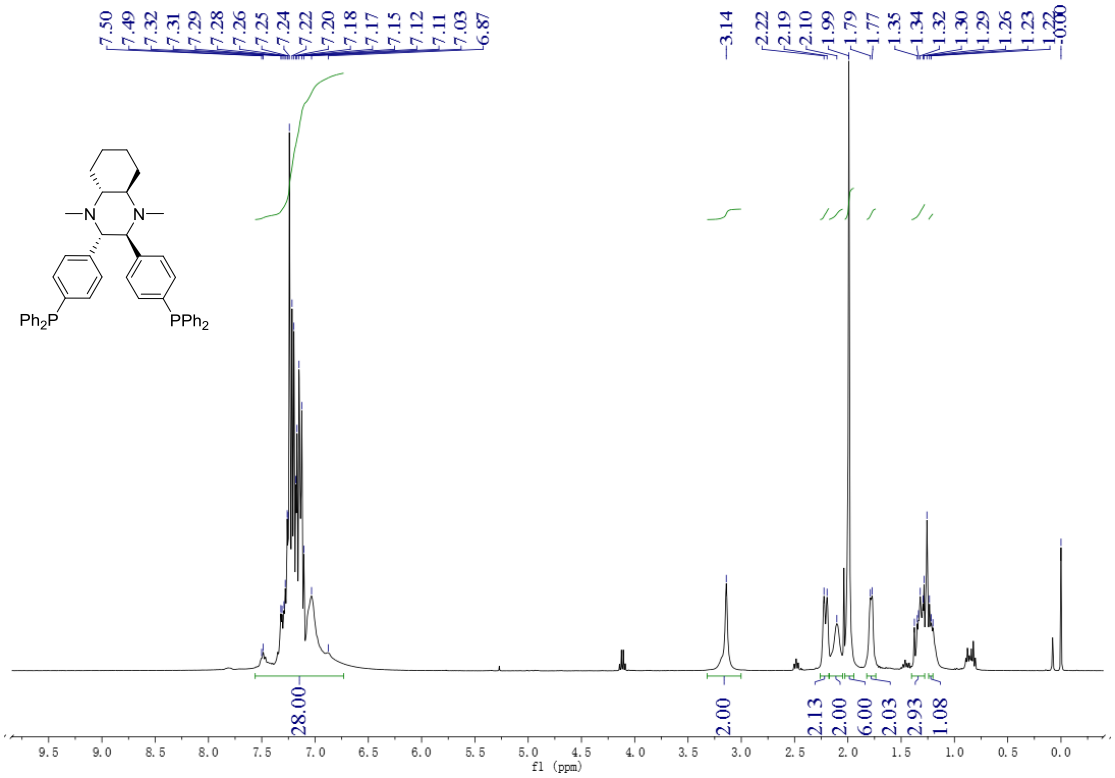
PPh2 PPh2
f1 (ppm)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7.12
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1.77
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1.30
1.29
1.26
1.23
1.22
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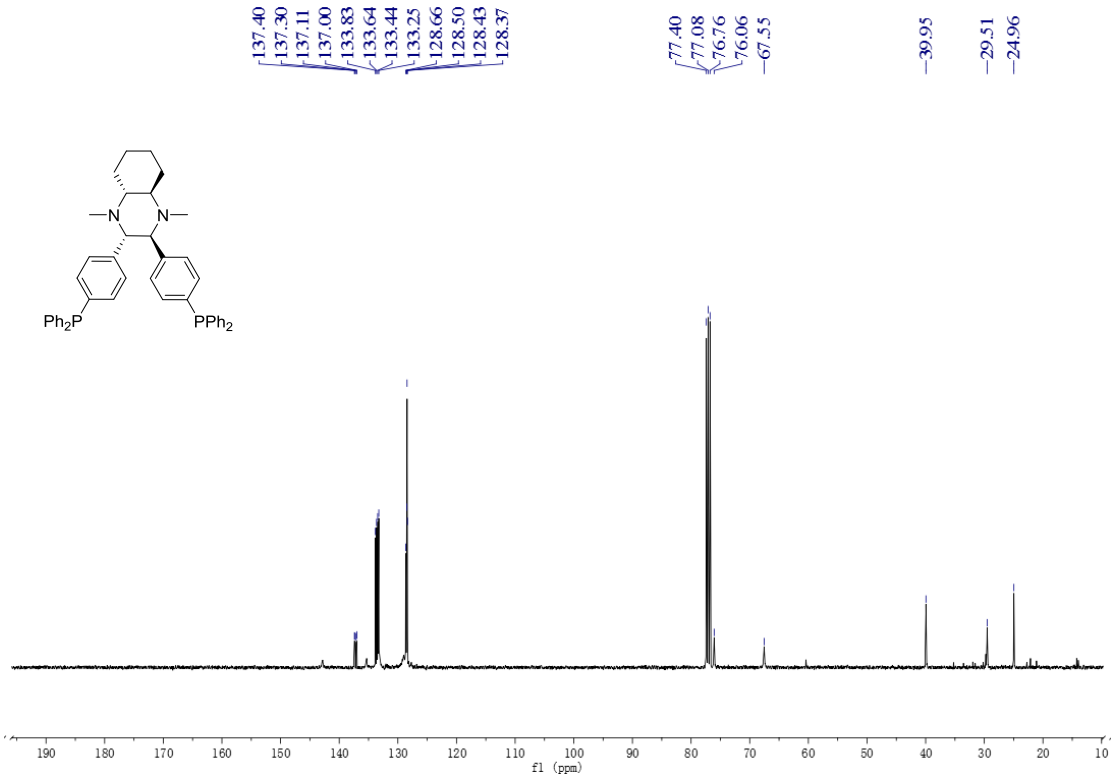
2.93
1.08
f1 (ppm)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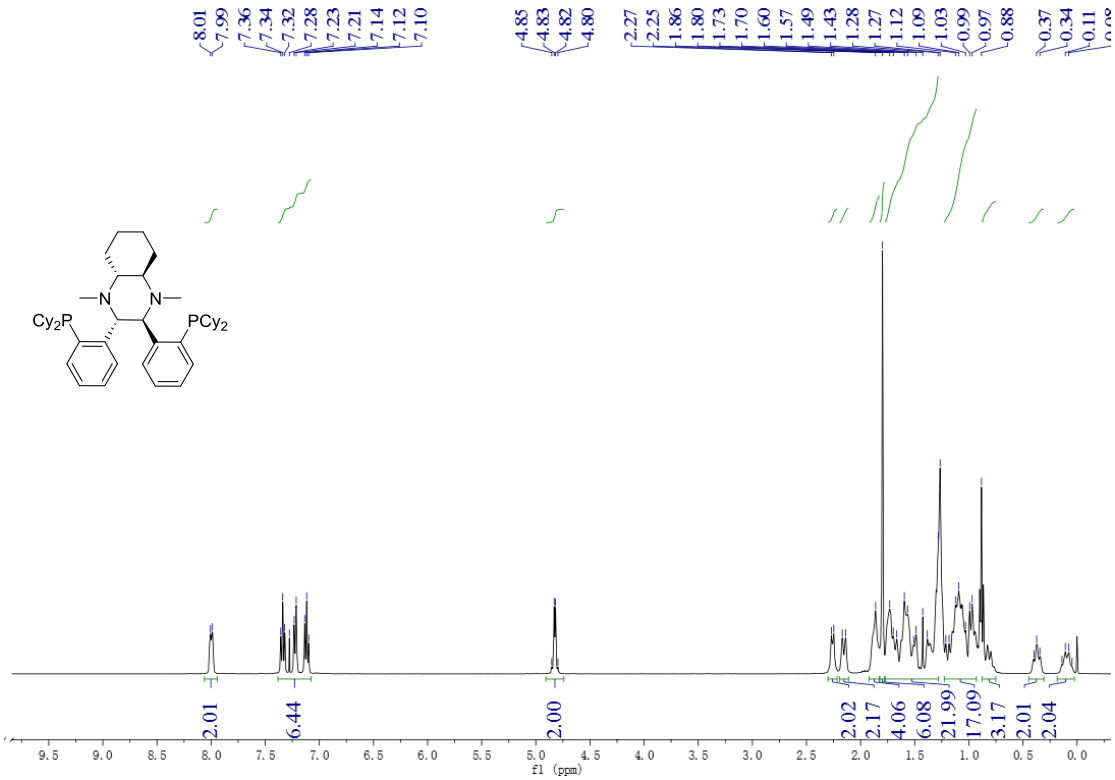
76.76
76.06
67.55
39.95
29.51
24.96
Ph2P
PPh2
f1 (ppm)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7.99
7.36
7.34
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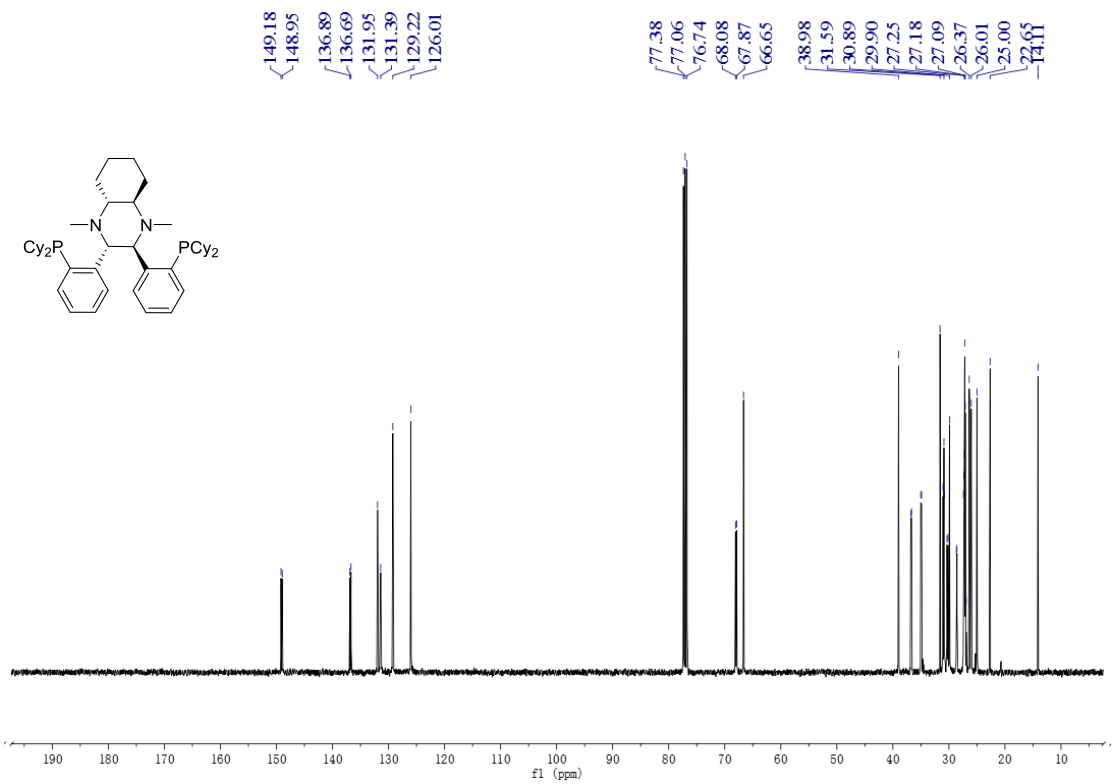
7.28
7.23
7.21
7.14
7.12
7.10
4.85
4.83
4.82
4.80
2.27
2.25
1.86
1.80
1.73
1.70
1.60
1.57
1.49
1.43
1.28
1.27
1.12
1.09
1.03
0.99
0.97
0.88
0.37
0.34
0.11
Cy2P
PCy2
2.01
6.44
2.00
2.02
2.17
4.06
6.08
21.99
17.09
3.17
2.01
2.04
f1 (ppm)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131.39
129.22
126.01
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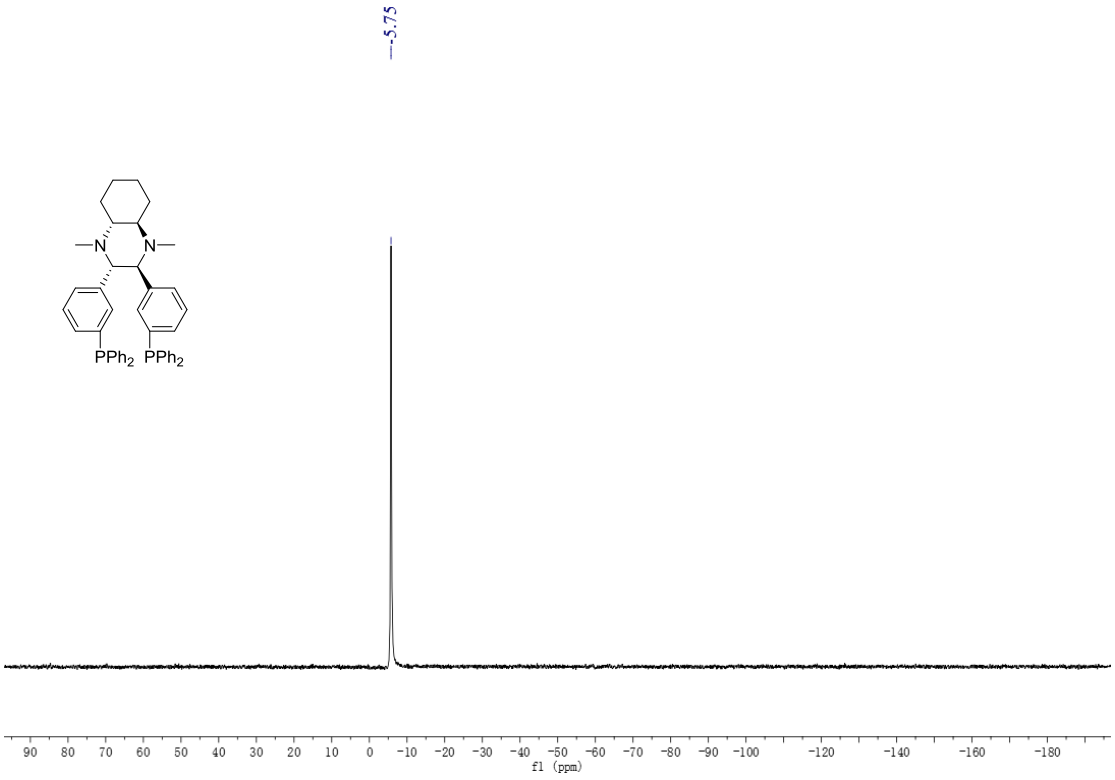
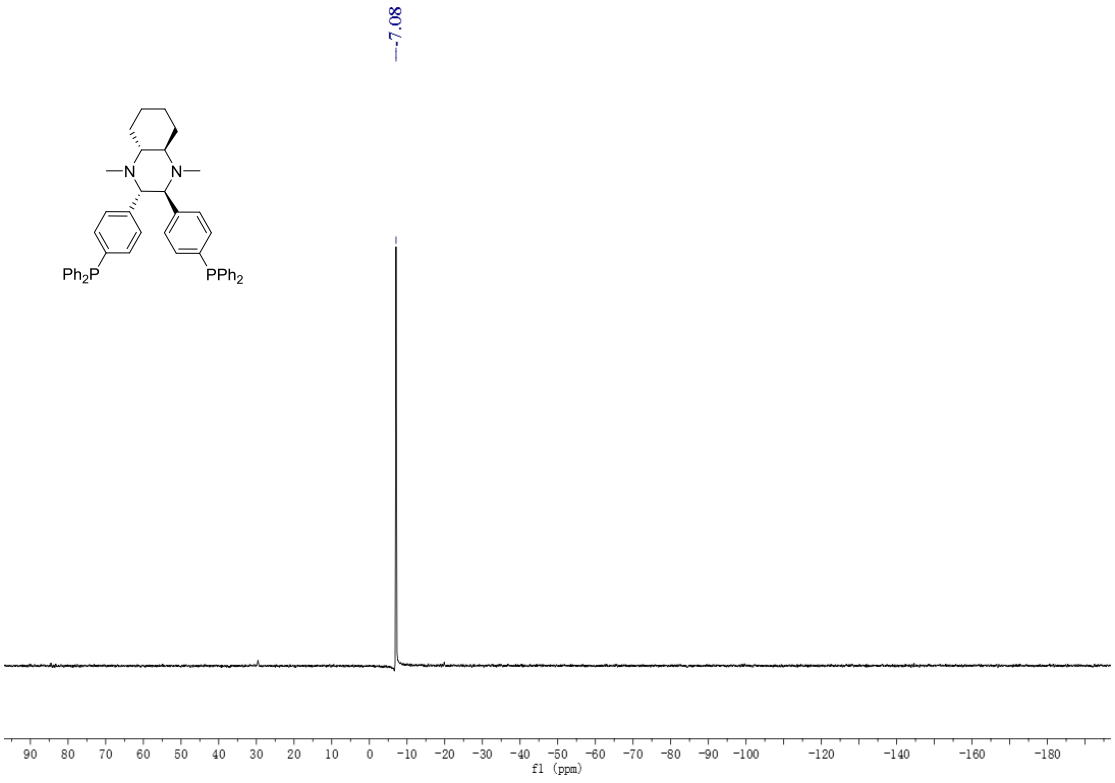
77.06
76.74
68.08
67.87
66.65
38.98
31.59
30.89
29.90
27.25
27.18
27.09
26.37
26.01
25.00
22.65
14.11
Cy2P
PCy2
f1 (ppm)

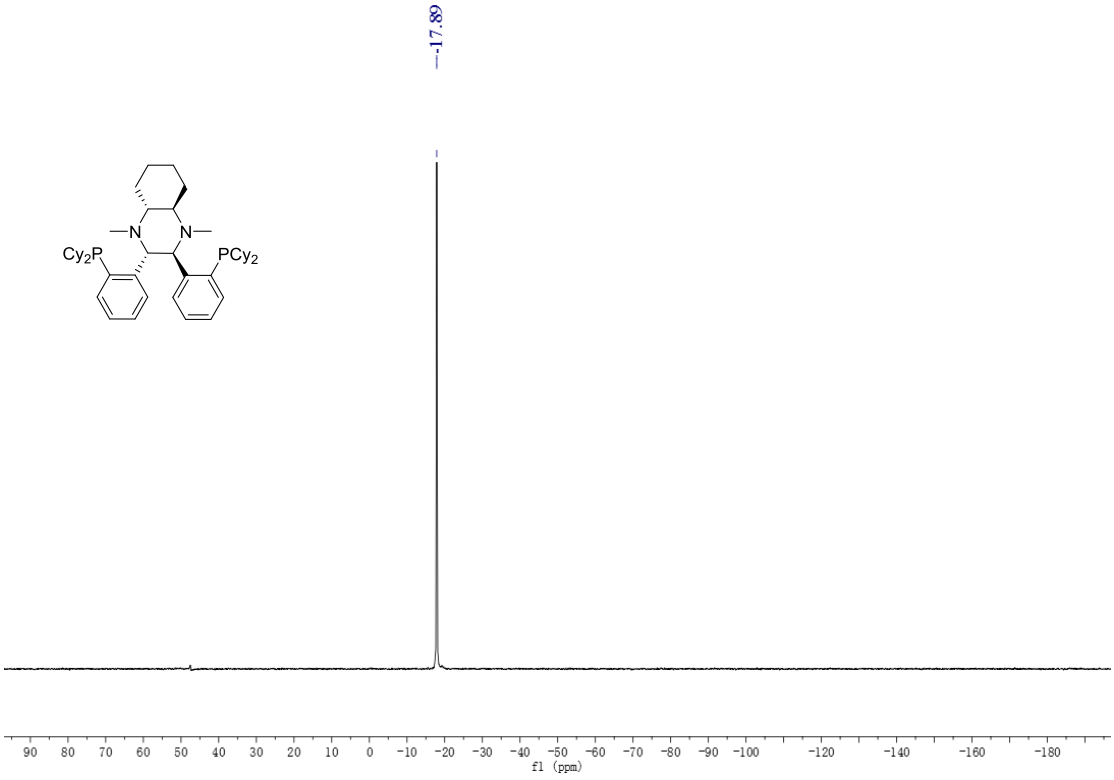
^{31}P NMR of L1a

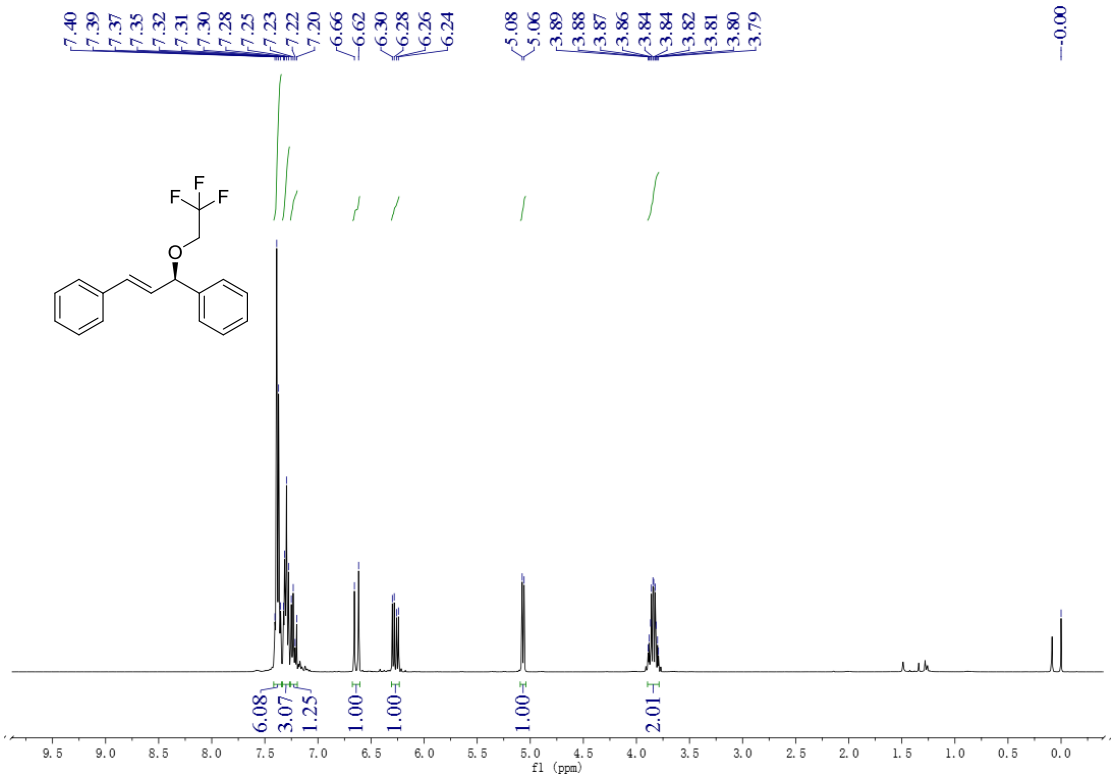


^{31}P NMR of L1b



^{31}P NMR of L2


-17.89
Cy2P
PCy2
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180
f1 (ppm)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7.35
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7.30
7.28
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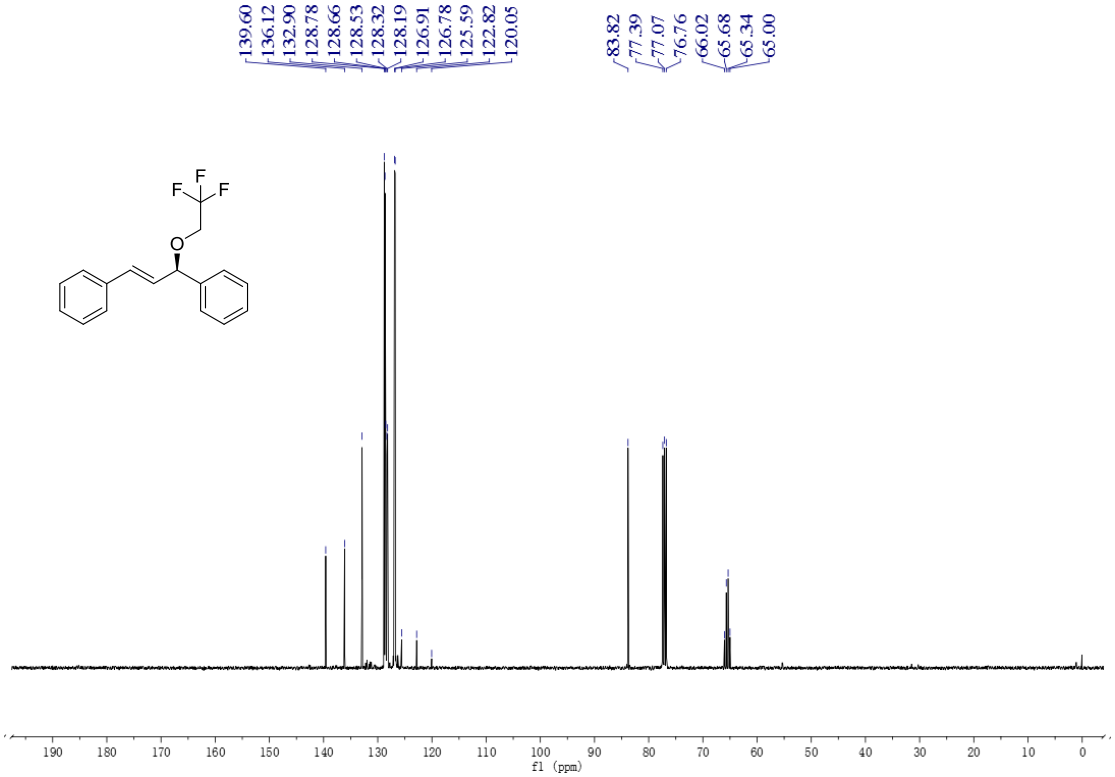
7.23
7.22
7.20
6.66
6.62
6.30
6.28
6.26
6.24
5.08
5.06
3.89
3.88
3.87
3.86
3.84
3.84
3.82
3.81
3.80
3.79
-0.00
F
F
F
O
6.08
3.07
1.25
1.00
1.00
1.00
2.01
f1 (ppm)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128.53
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128.19
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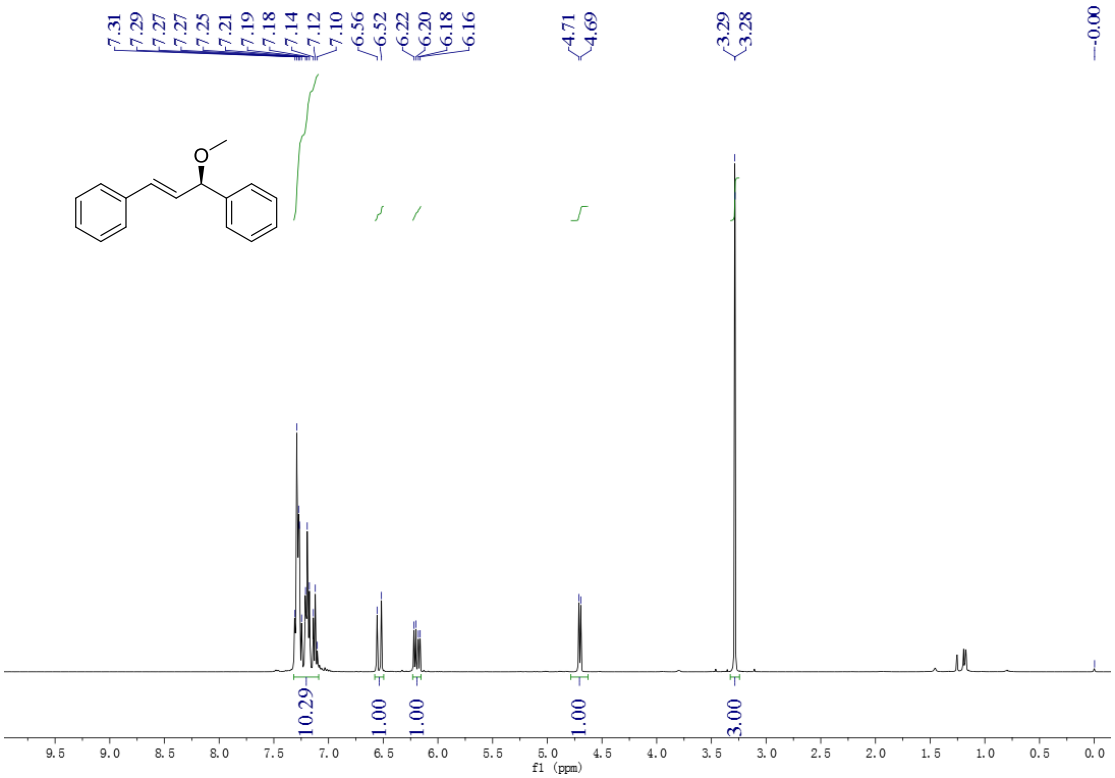
126.78
125.59
122.82
120.05
83.82
77.39
77.07
76.76
66.02
65.68
65.34
65.00
F
F
F
O
f1 (ppm)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6.52
6.22
6.20
6.18
6.16
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4.69
3.29
3.28
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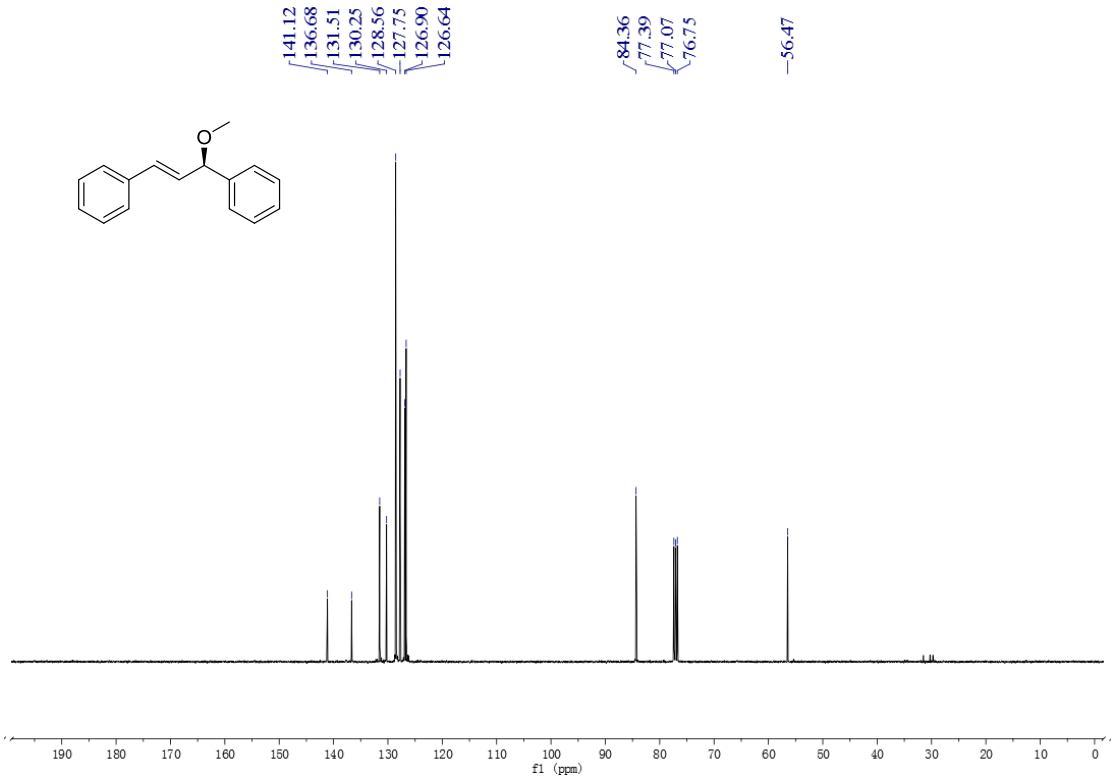
O
10.29
1.00
1.00
1.00
3.00
f1 (ppm)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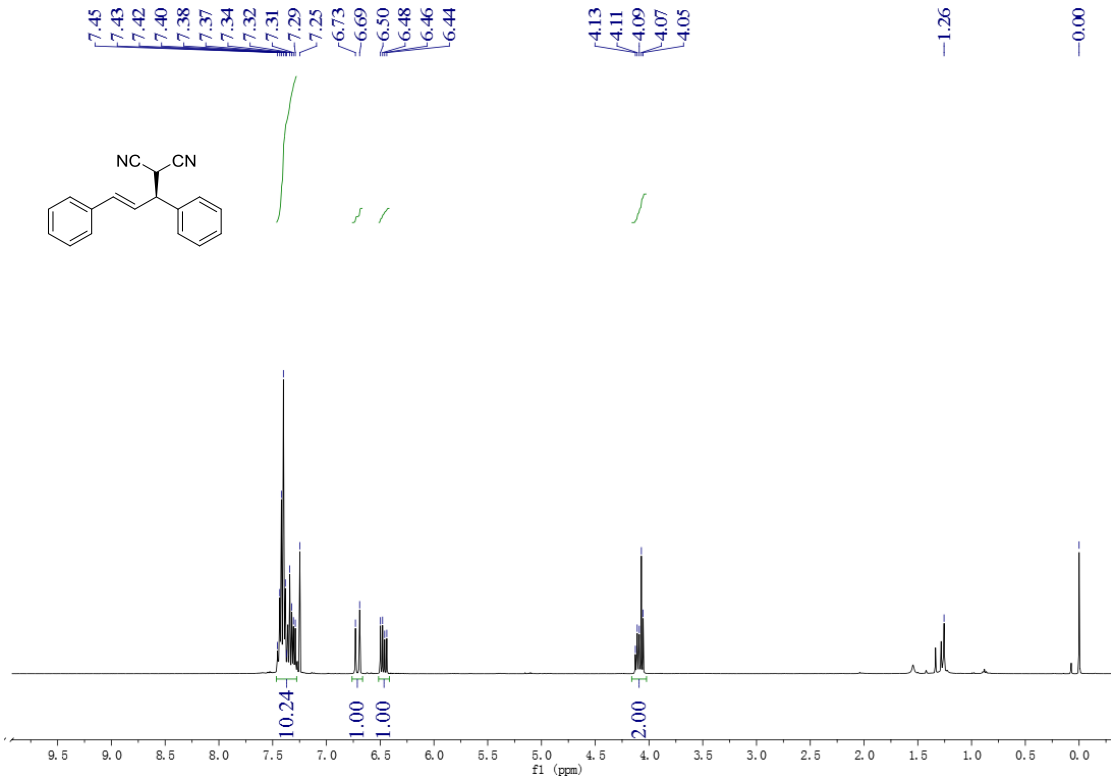
126.90
126.64
84.36
77.39
77.07
76.75
56.47
O
f1 (ppm)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7.37
7.34
7.32
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7.29
7.25
6.73
6.69
6.50
6.48
6.46
6.44
4.13
4.11
4.09
4.07
4.05
1.26
0.00
NC
CN
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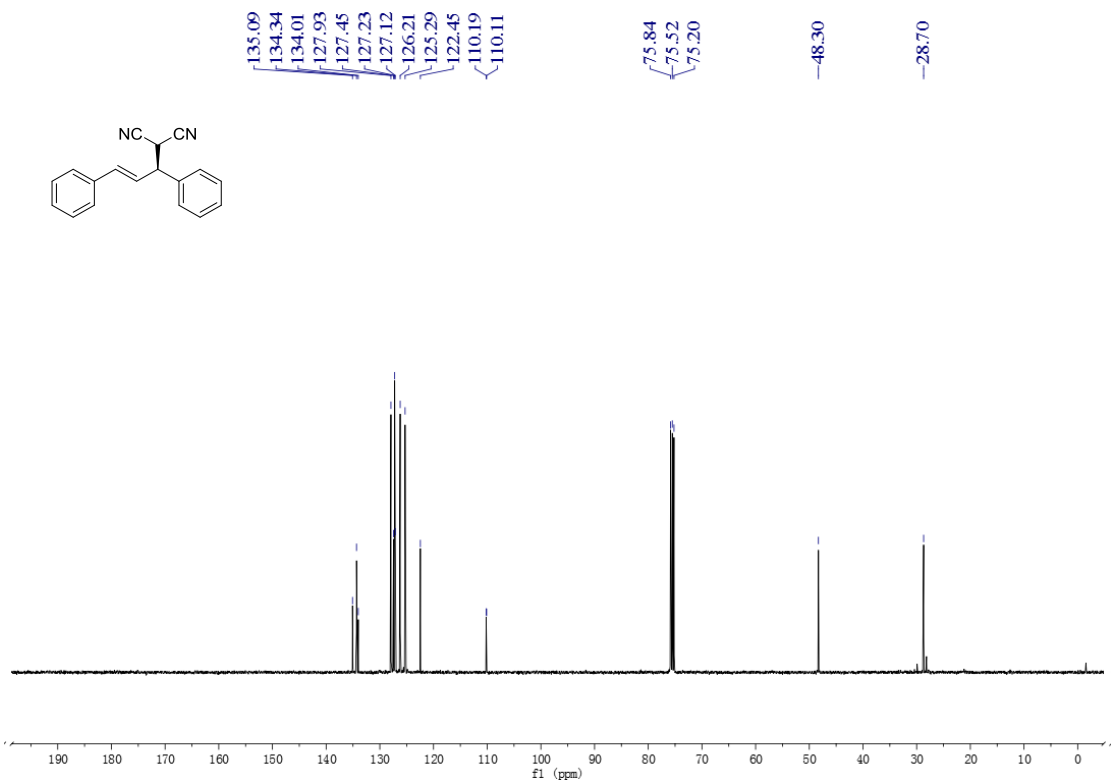
1.00
1.00
2.00
f1 (ppm)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110.11
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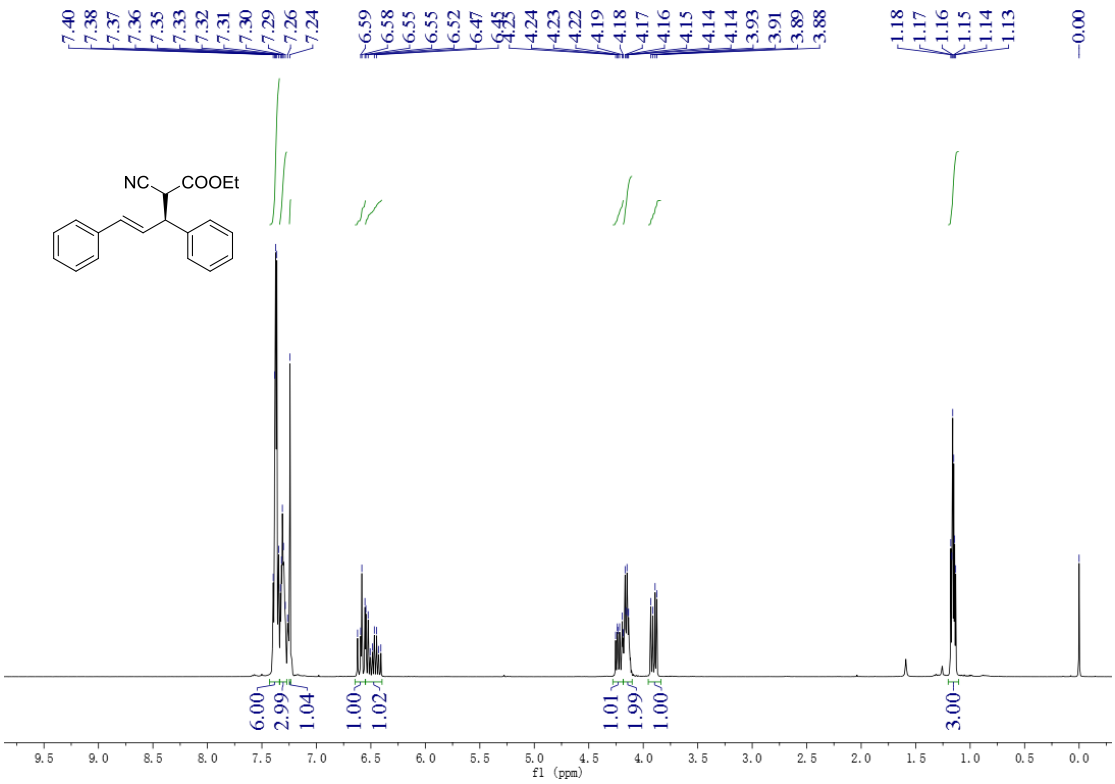
75.52
75.20
48.30
28.70
NC
CN
f1 (ppm)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6.58
6.55
6.55
6.52
6.47
6.45
4.25
4.24
4.23
4.22
4.19
4.18
4.17
4.16
4.15
4.14
4.14
3.93
3.91
3.89
3.88
1.18
1.17
1.16
1.15
1.14
1.13
0.00
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COOEt
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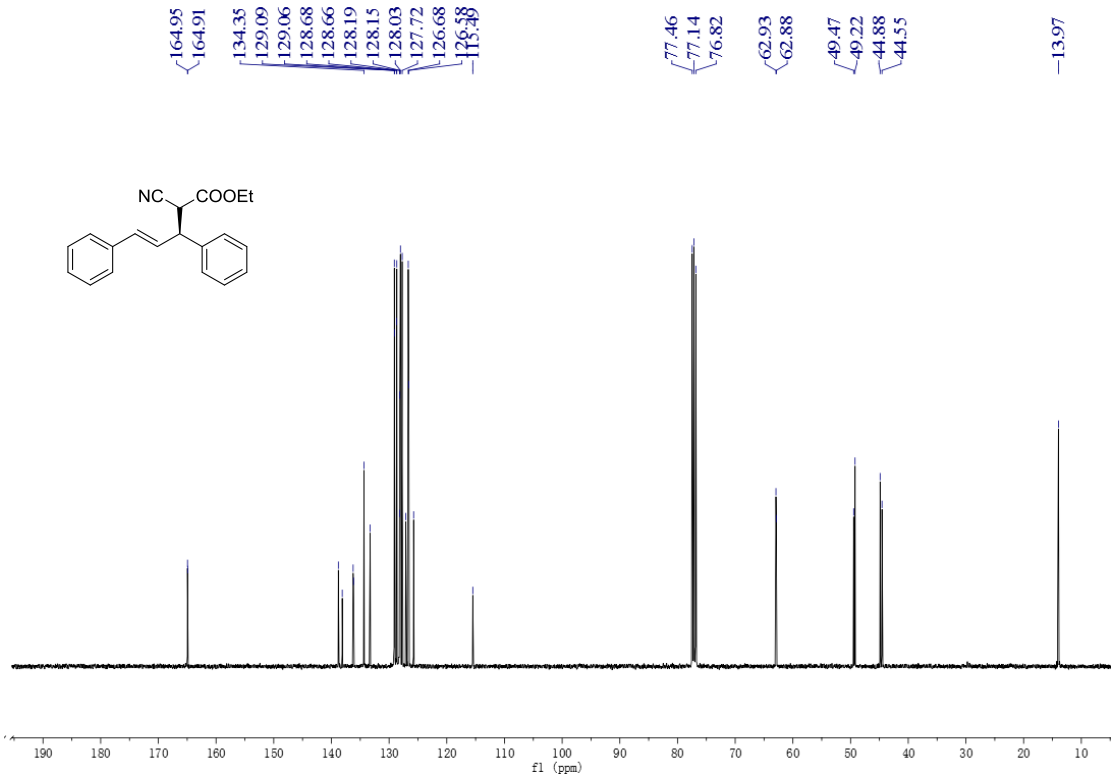
1.00
1.02
1.01
1.99
1.00
3.00
f1 (ppm)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115.40
77.46
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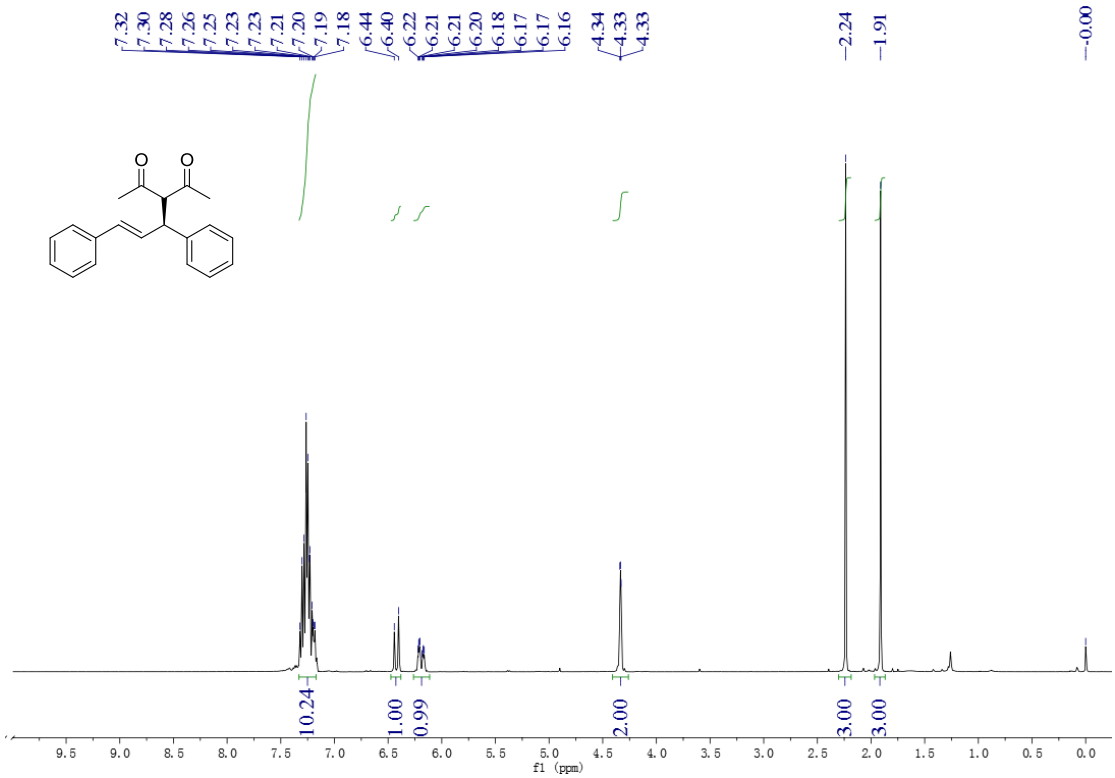
62.88
49.47
49.22
44.88
44.55
13.97
NC
COOEt
f1 (ppm)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6.40
6.22
6.21
6.21
6.20
6.18
6.17
6.17
6.16
4.34
4.33
4.33
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1.91
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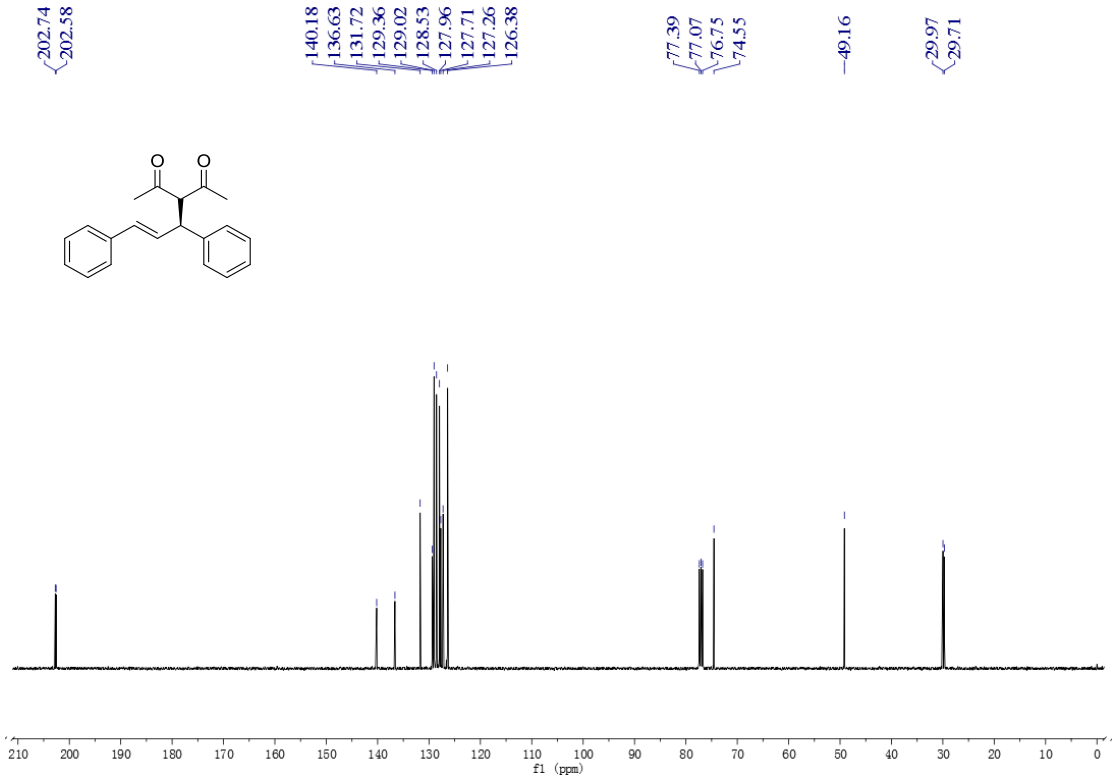
10.24
1.00
0.99
2.00
3.00
3.00
f1 (ppm)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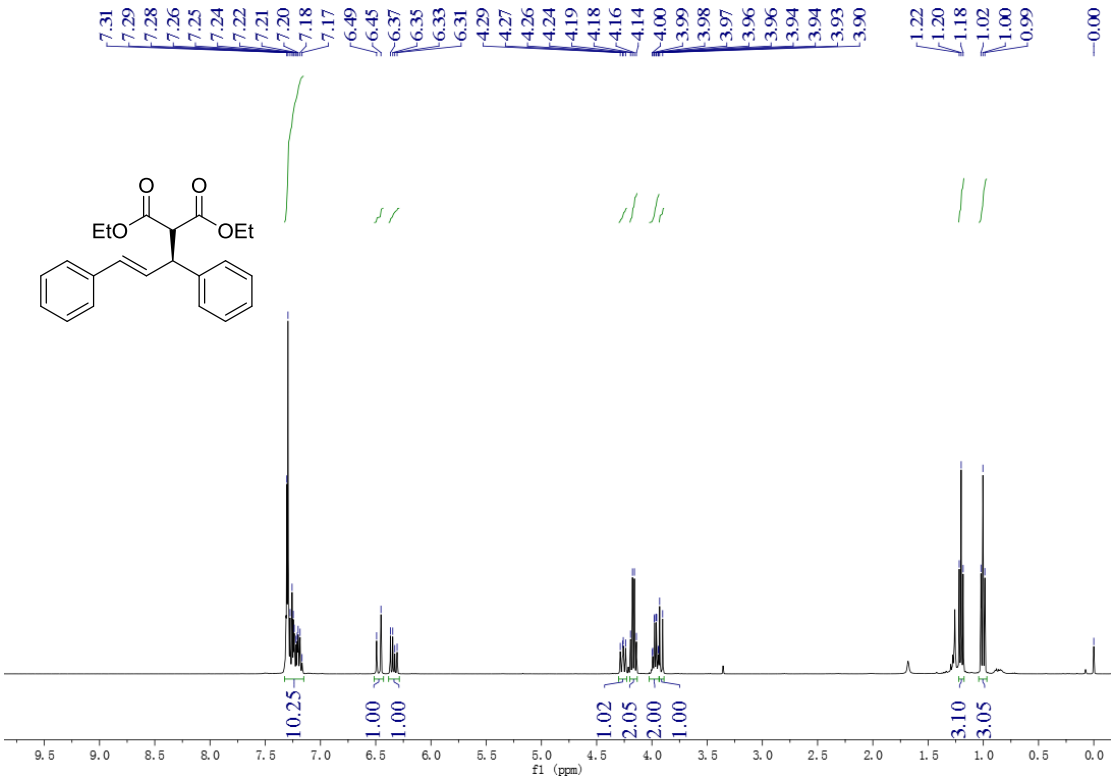
77.07
76.75
74.55
49.16
29.97
29.71
f1 (ppm)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6.35
6.33
6.31
4.29
4.27
4.26
4.24
4.19
4.18
4.16
4.14
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3.99
3.98
3.97
3.96
3.96
3.94
3.94
3.93
3.90
1.22
1.20
1.18
1.02
1.00
0.99
0.00
EtO
OEt
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1.00
1.02
2.05
2.00
1.00
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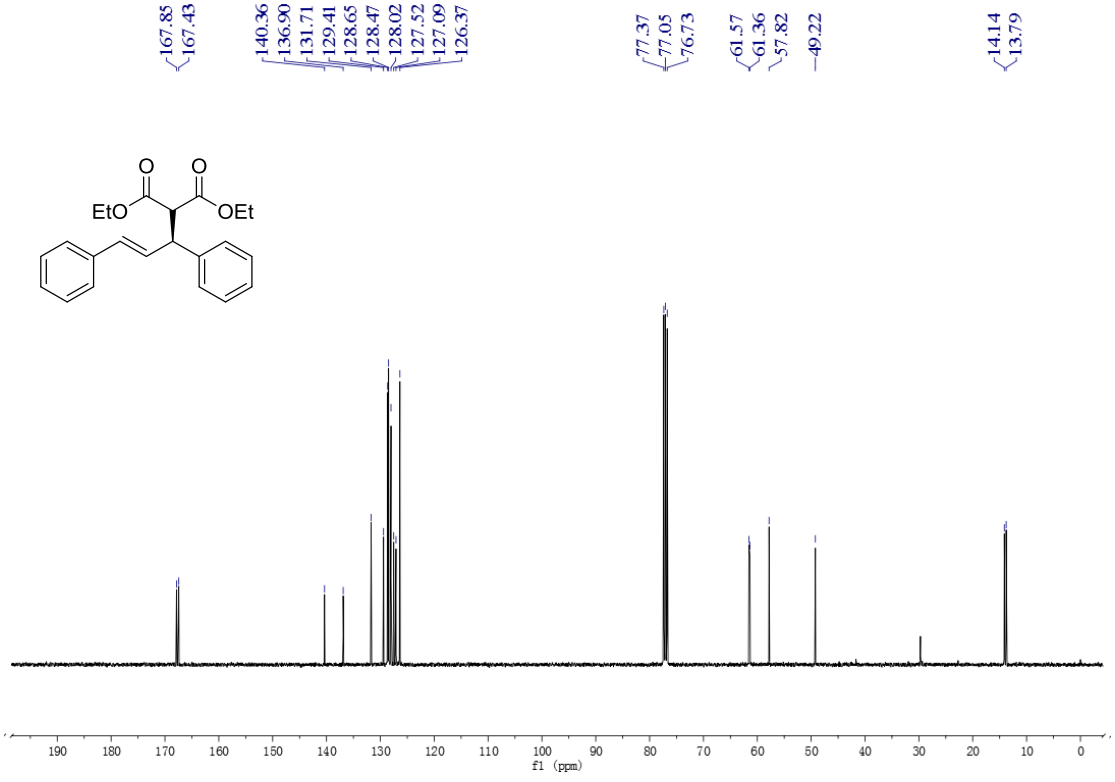
3.05
f1 (ppm)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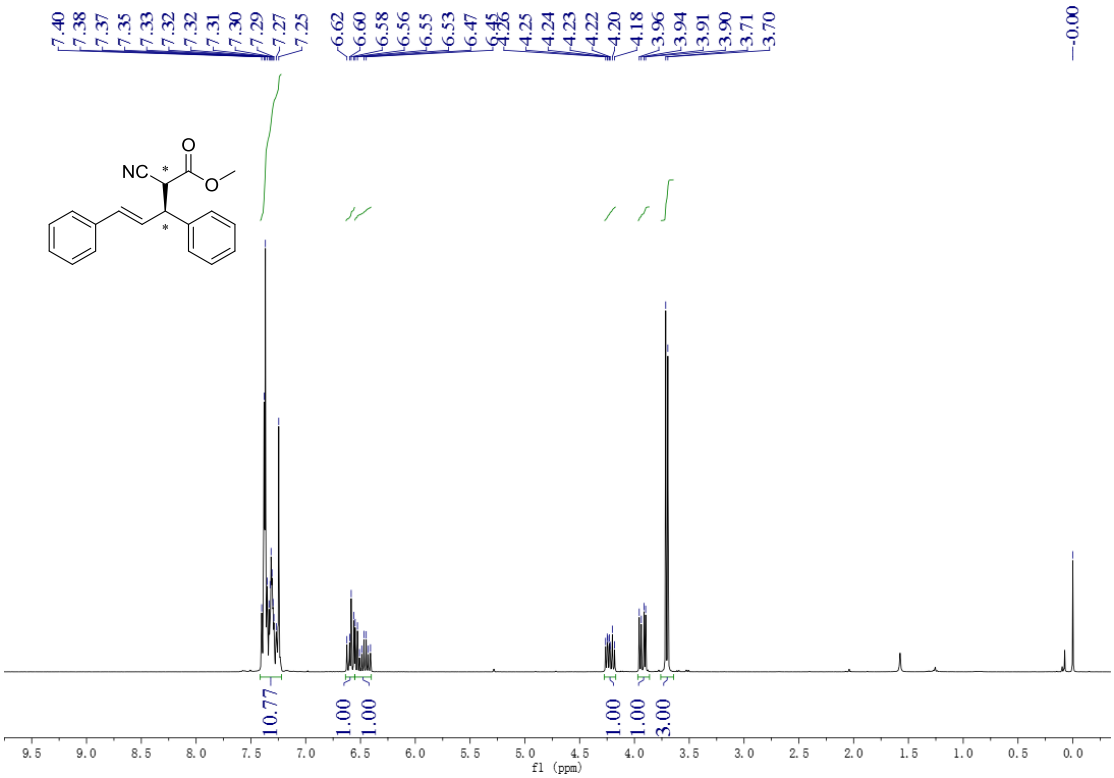
14.14
13.79
EtO
OEt
f1 (ppm)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6.60
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6.56
6.55
6.53
6.47
4.25
4.24
4.23
4.22
4.20
4.18
3.96
3.94
3.91
3.90
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O
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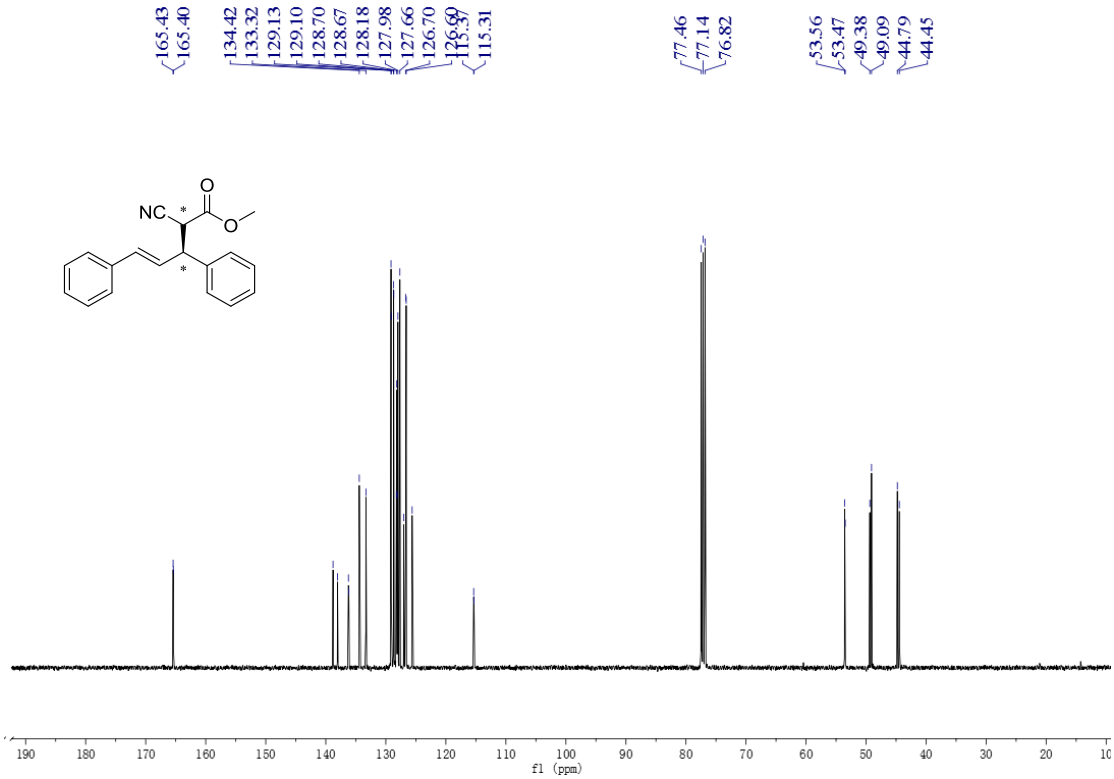
f1 (ppm)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49.38
49.09
44.79
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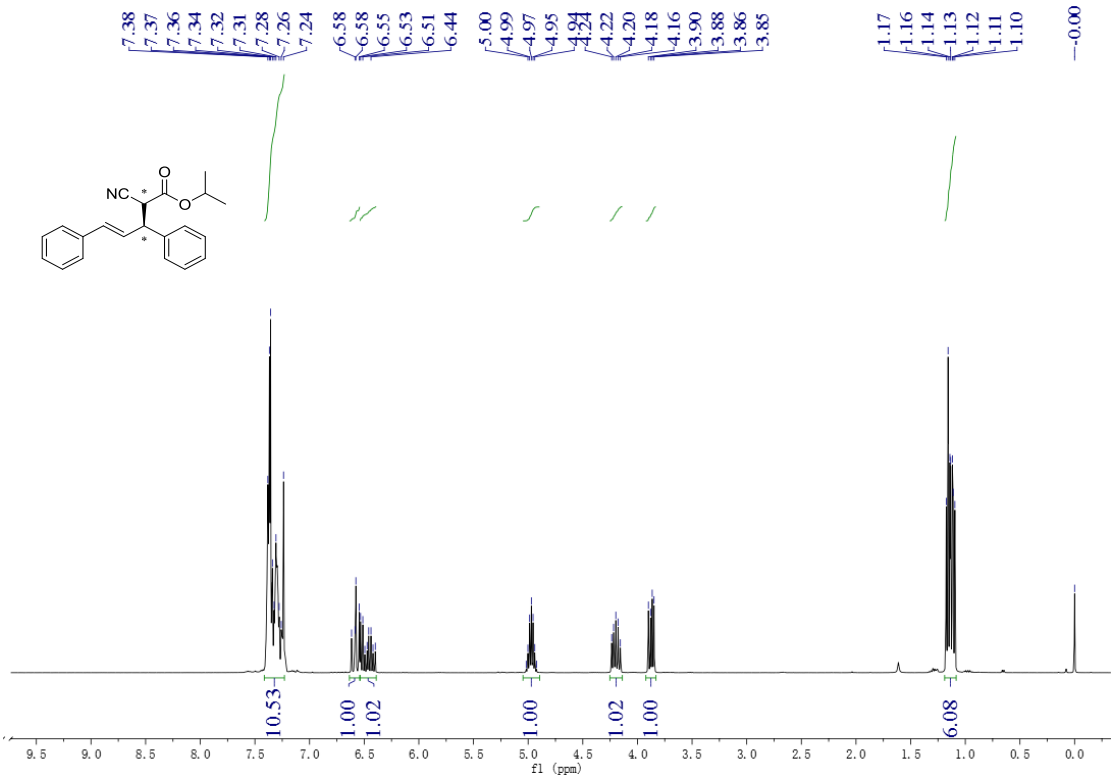
O
O
f1 (ppm)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6.53
6.51
6.44
5.00
4.99
4.97
4.95
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4.22
4.20
4.18
4.16
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3.88
3.86
3.85
1.17
1.16
1.14
1.13
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1.11
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1.02
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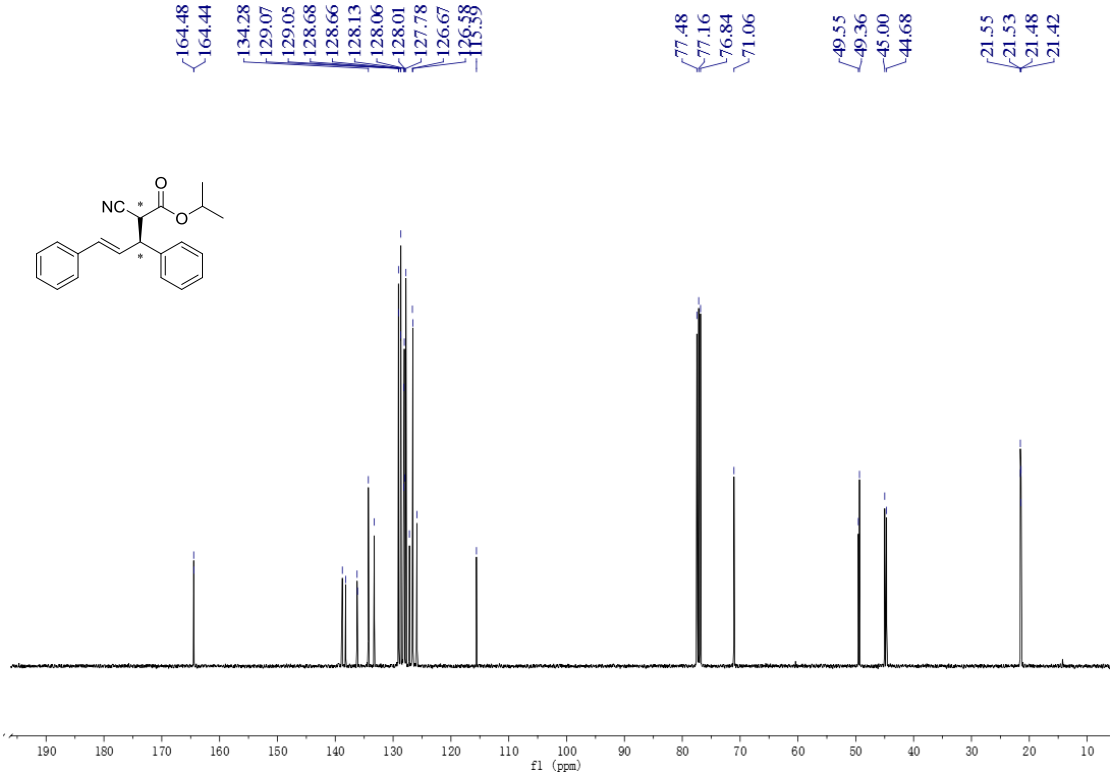
6.08
f1 (ppm)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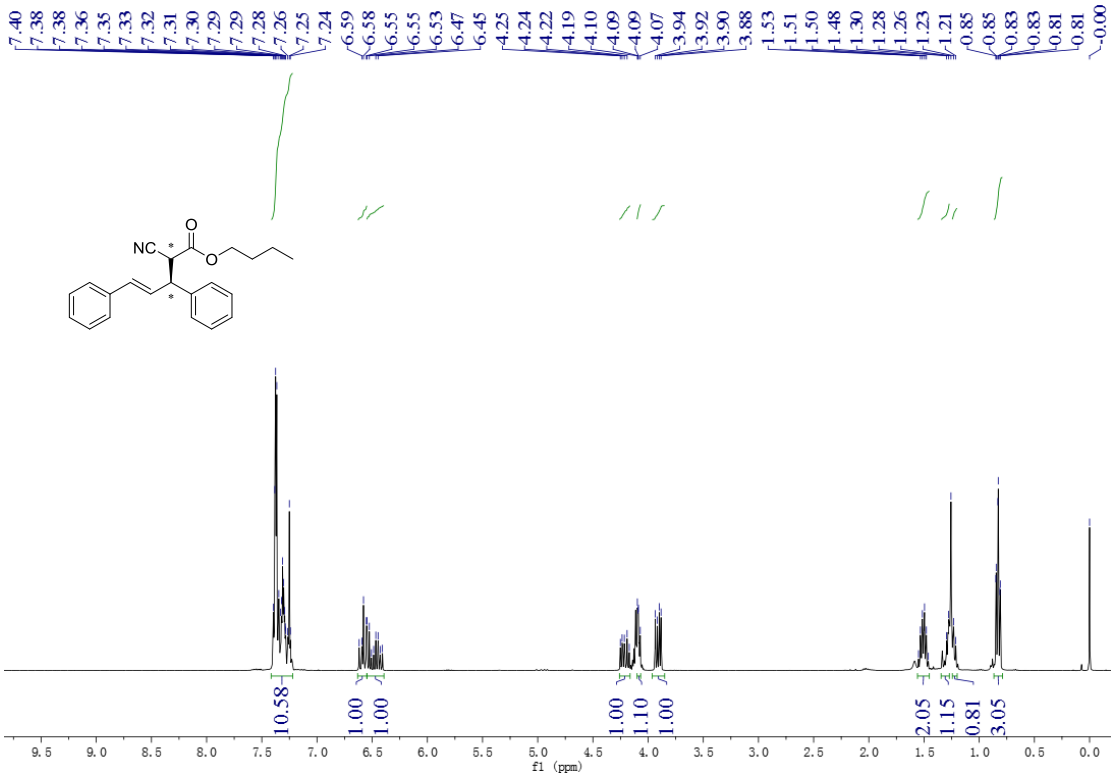
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6.58
6.55
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4.07
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3.90
3.88
1.53
1.51
1.50
1.48
1.30
1.28
1.26
1.23
1.21
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0.85
0.83
0.83
0.81
0.81
-0.00
NC
O
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1.10
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3.05
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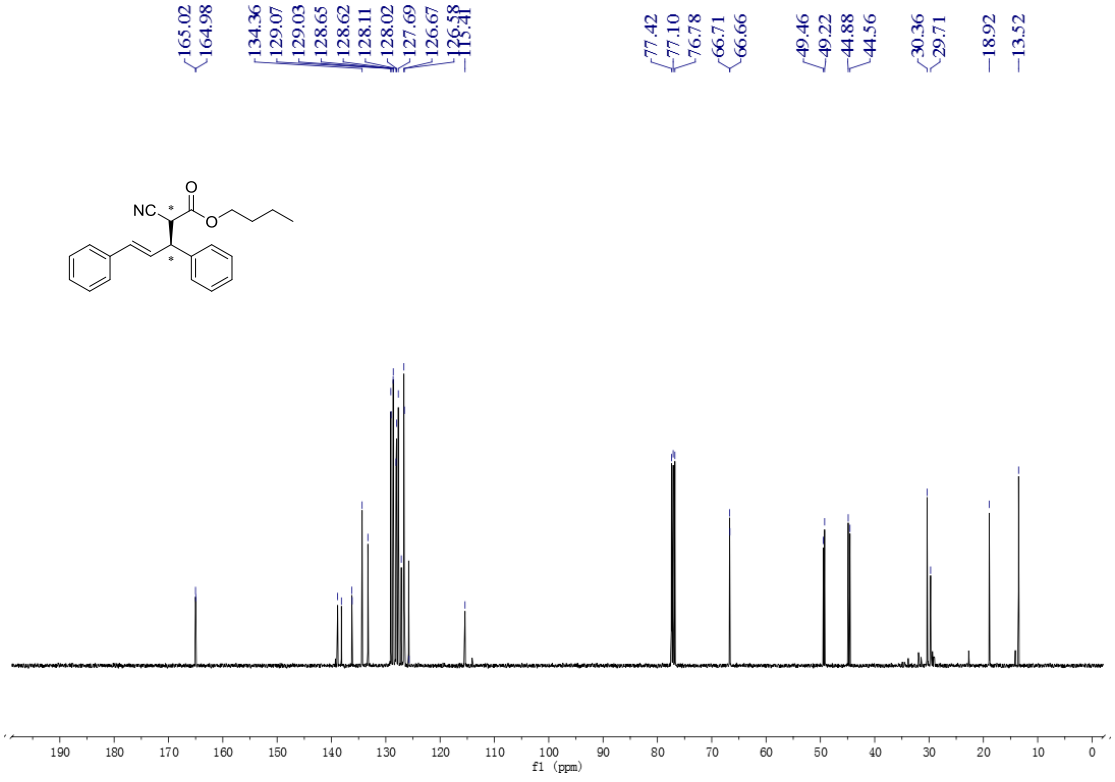
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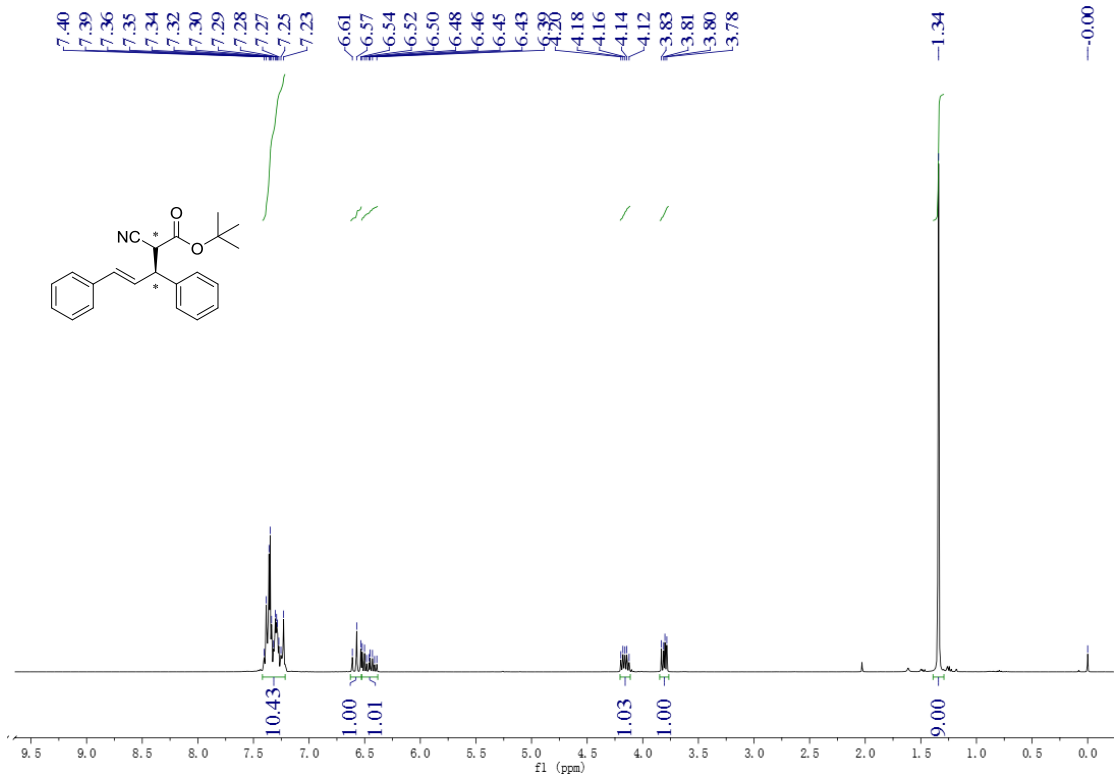
f1 (ppm)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6.57
6.54
6.52
6.50
6.48
6.46
6.45
6.43
4.18
4.16
4.14
4.12
3.83
3.81
3.80
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O
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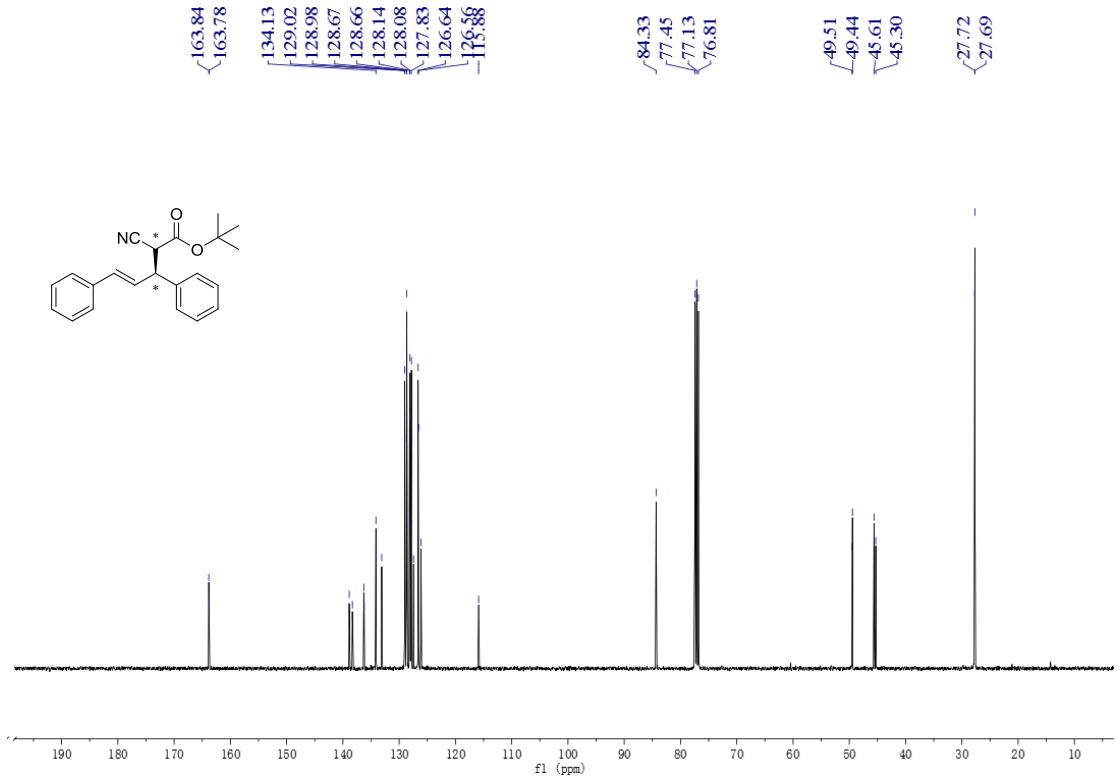
1.03
1.00
9.00
f1 (ppm)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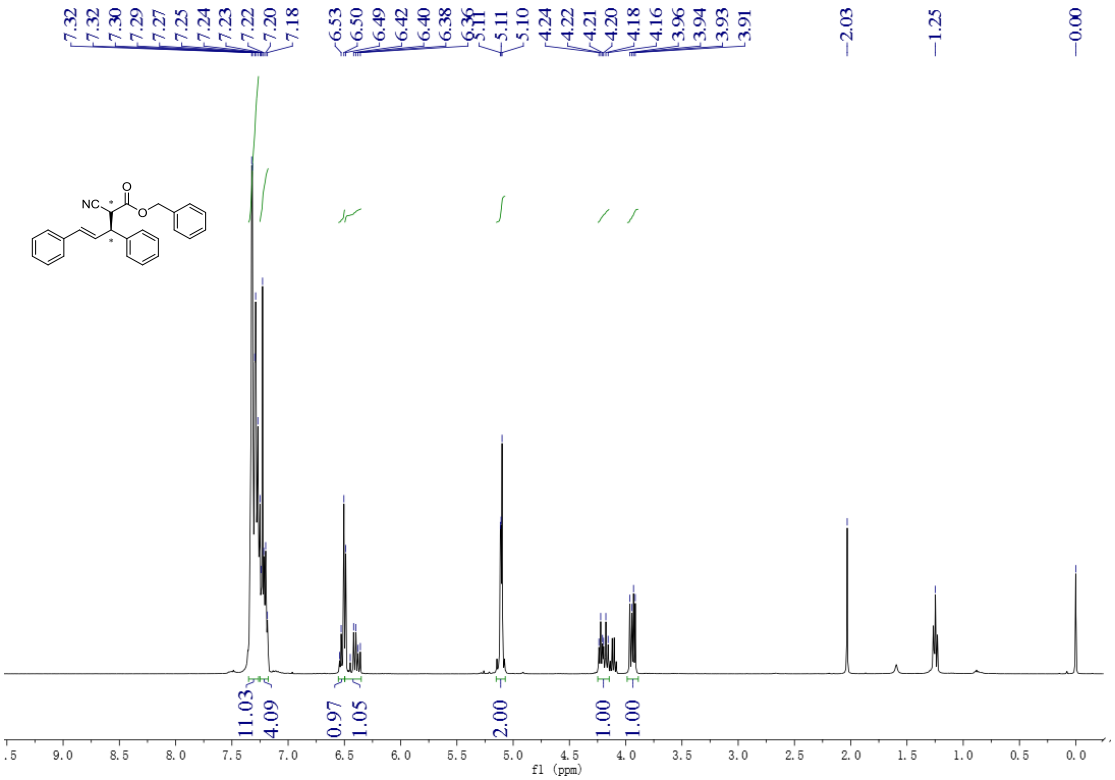
45.61
45.30
27.72
27.69
NC
O
O
f1 (ppm)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6.50
6.49
6.42
6.40
6.38
6.36
5.11
5.10
4.24
4.22
4.21
4.20
4.18
4.16
3.96
3.94
3.93
3.91
2.03
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O
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4.09
0.97
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2.00
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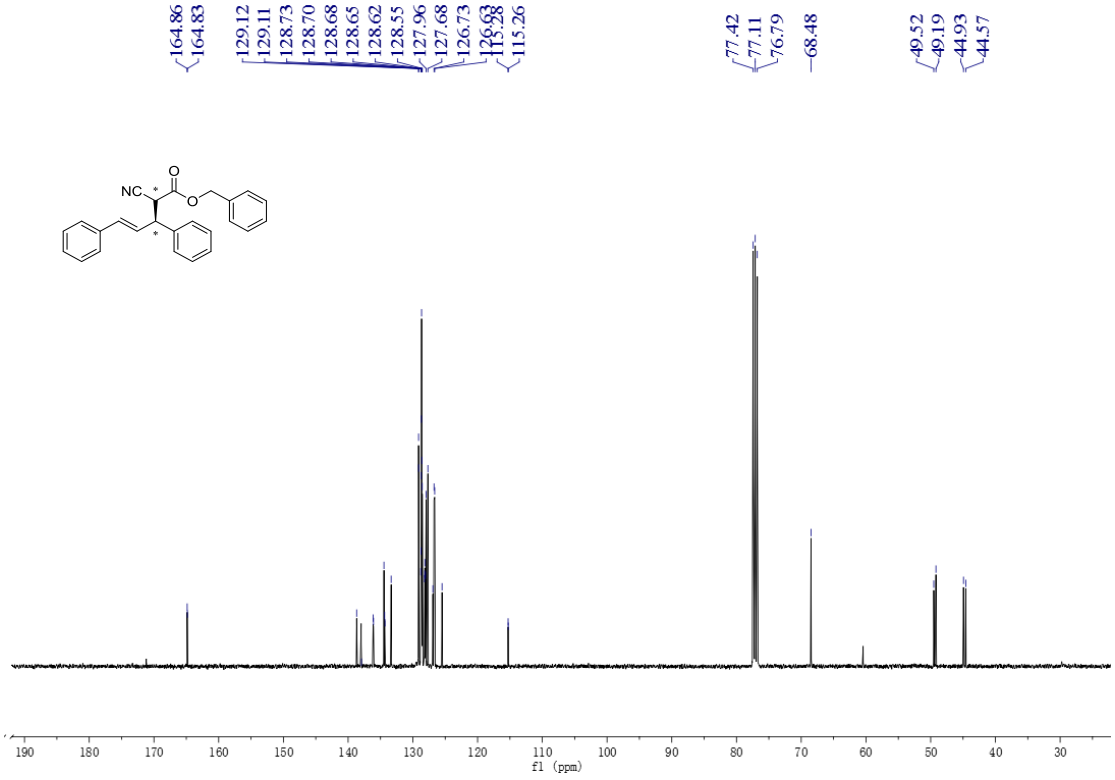
1.00
f1 (ppm)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49.52
49.19
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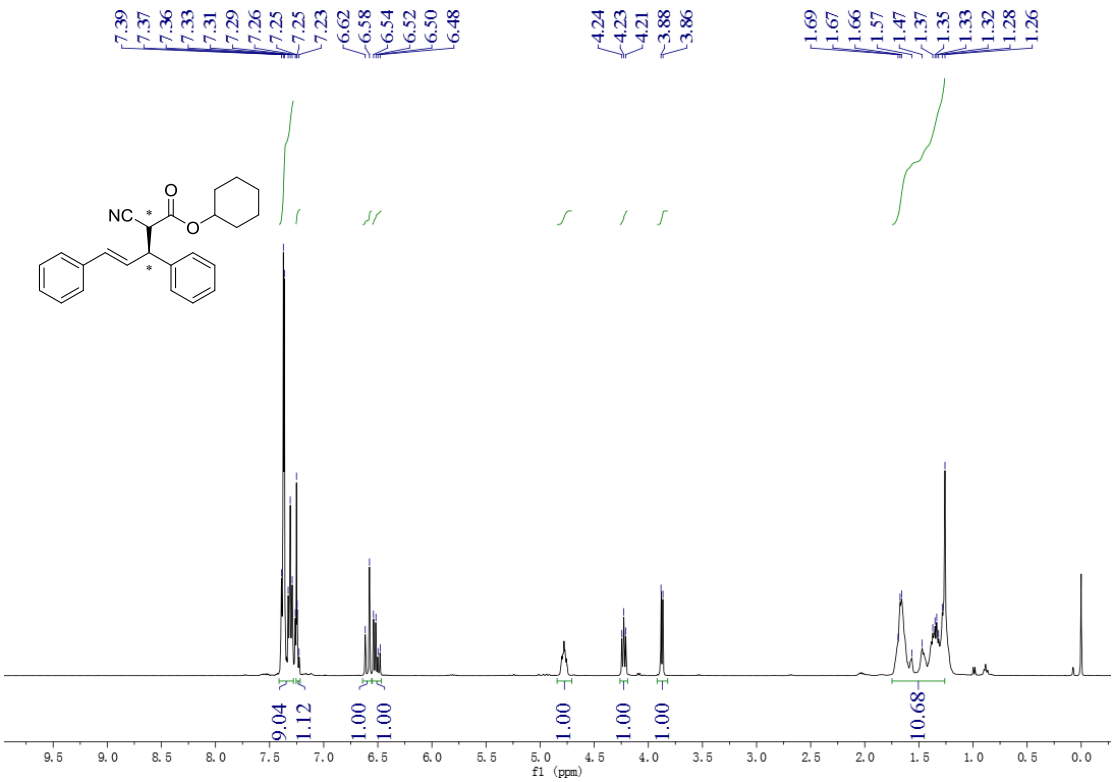
NC
O
O
f1 (ppm)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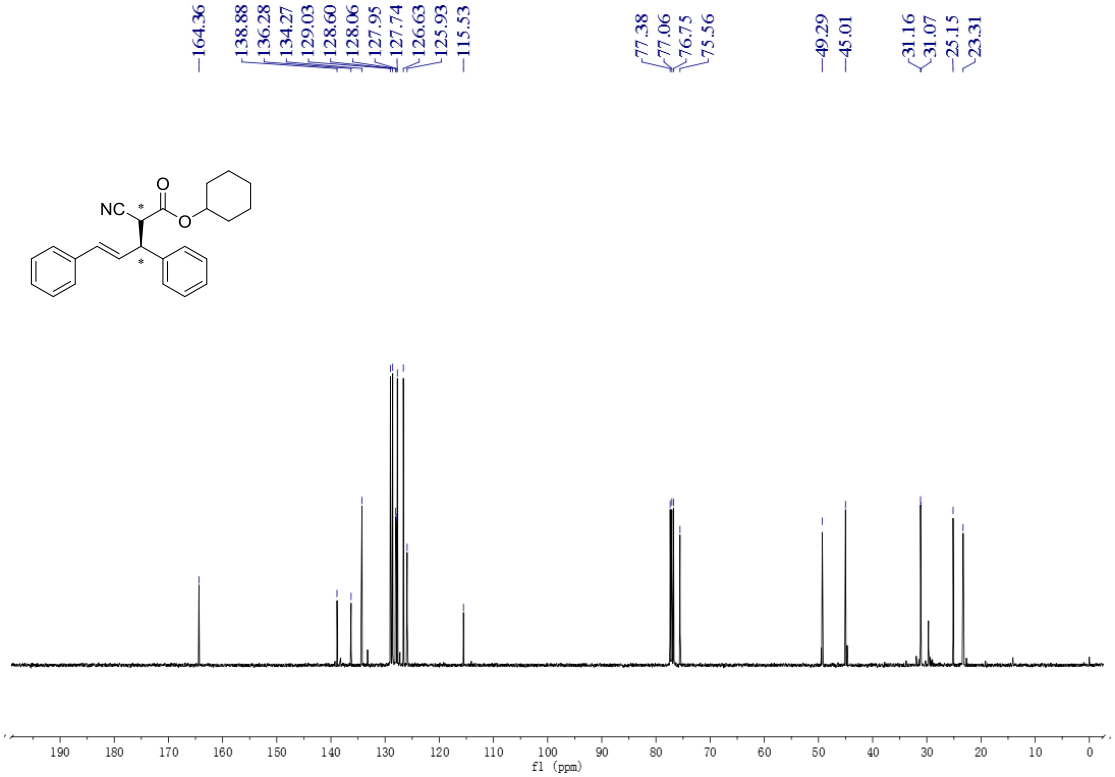
4.24
4.23
4.21
3.88
3.86
1.69
1.67
1.66
1.57
1.47
1.37
1.35
1.33
1.32
1.28
1.26
NC
O
O
9.04
1.12
1.00
1.00
1.00
1.00
1.00
10.68
f1 (ppm)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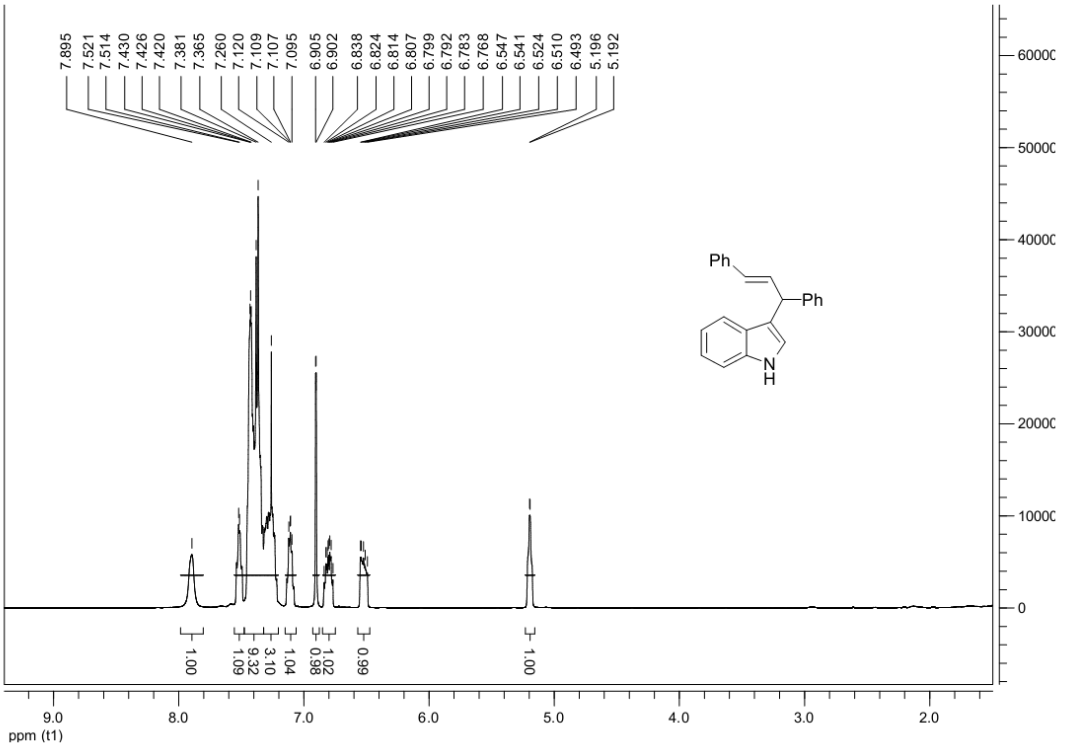
136.28
134.27
129.03
128.60
128.06
127.95
127.74
126.63
125.93
115.53
77.38
77.06
76.75
75.56
49.29
45.01
31.16
31.07
25.15
23.31
NC
O
O
f1 (ppm)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7.521
7.514
7.430
7.426
7.420
7.381
7.365
7.260
7.120
7.109
7.107
7.095
6.905
6.902
6.838
6.824
6.814
6.807
6.799
6.792
6.783
6.768
6.547
6.541
6.524
6.510
6.493
5.196
5.192
Ph
Ph
N
H
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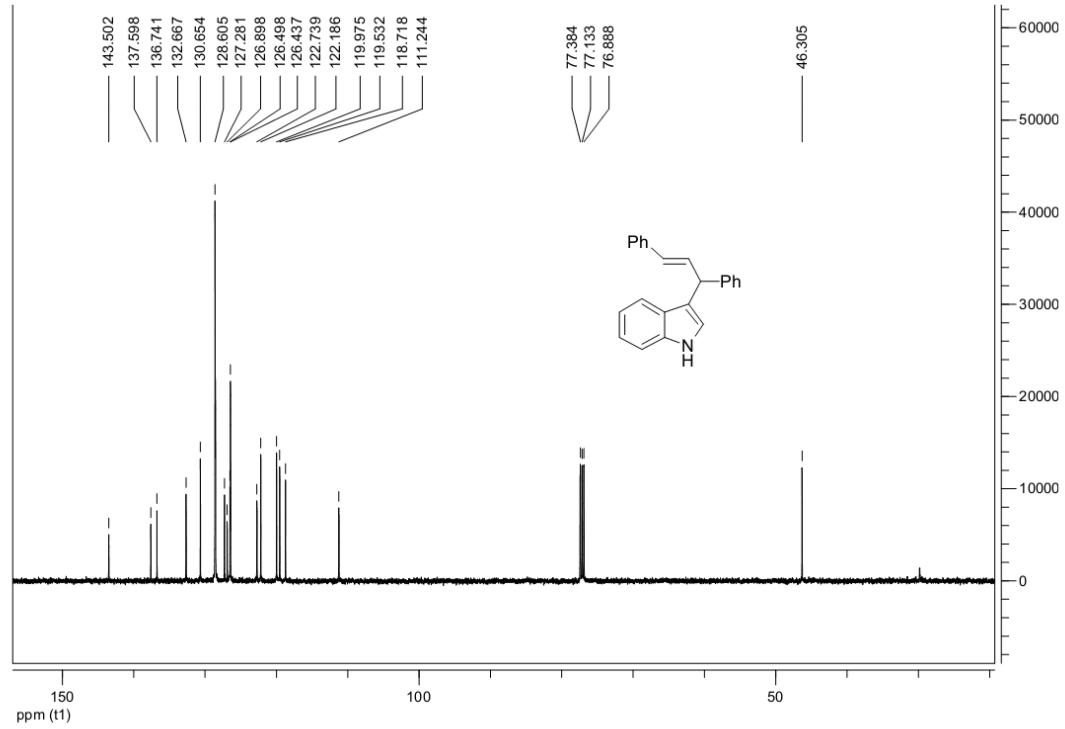
1.09
8.22
3.10
1.04
0.98
1.02
0.99
1.00
ppm (t1)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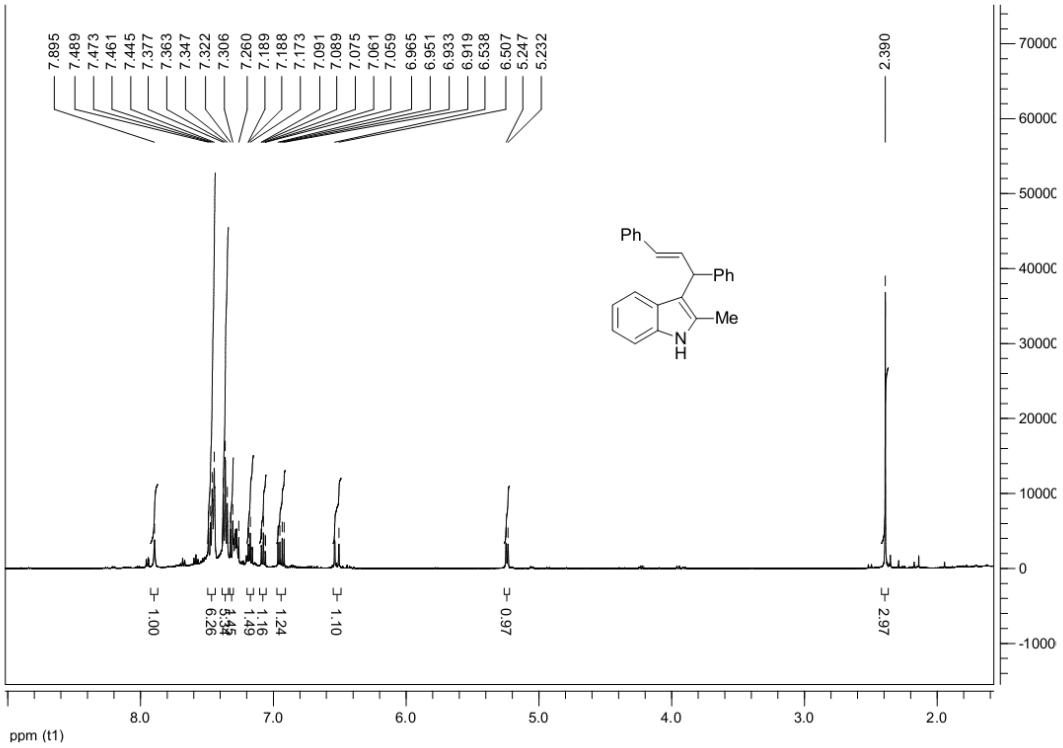
137.598
136.741
132.667
130.654
128.605
127.281
126.898
126.498
126.437
122.739
122.186
119.975
119.532
118.718
111.244
77.384
77.133
76.888
46.305
Ph
Ph
N
H
ppm (t1)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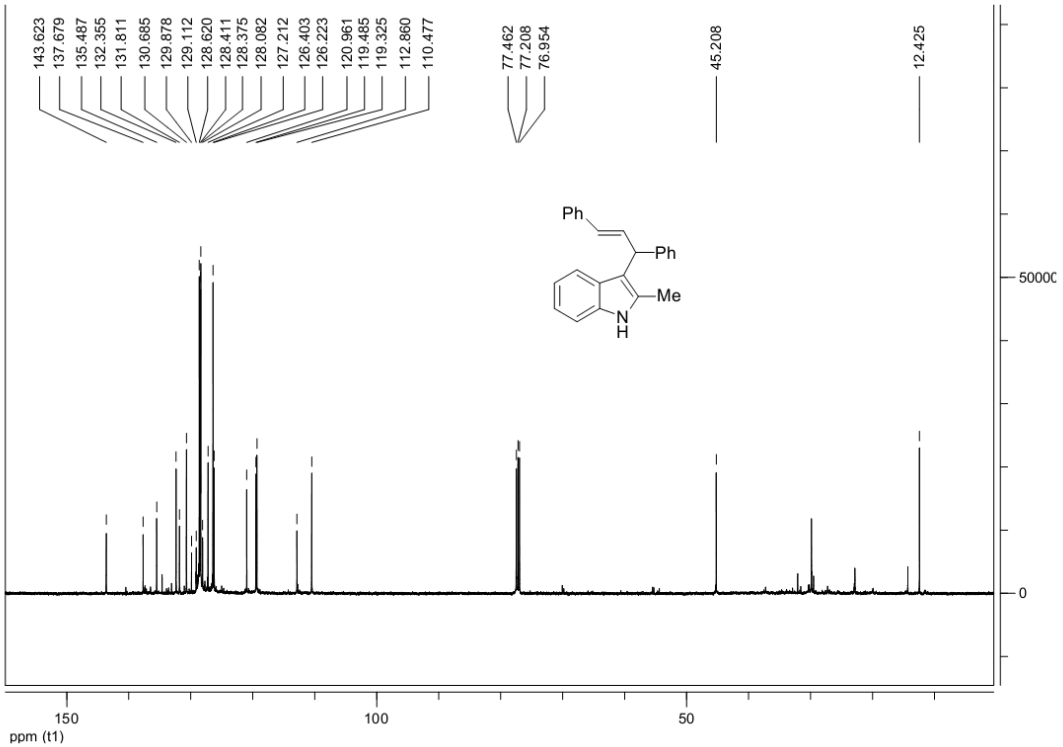
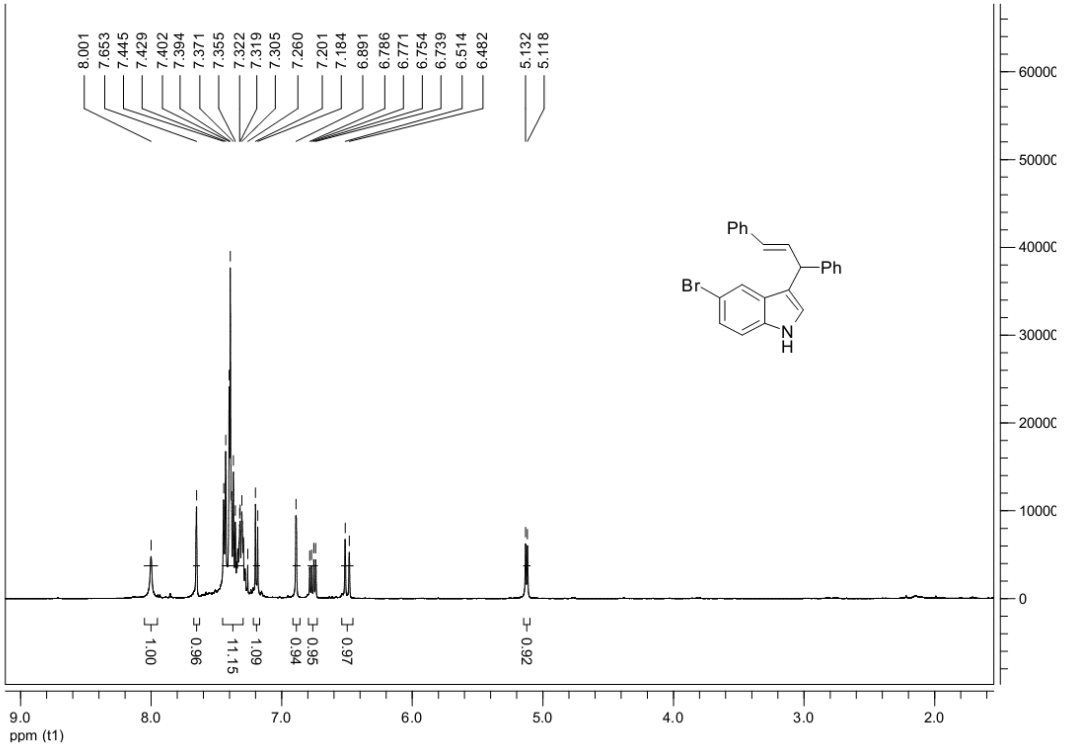
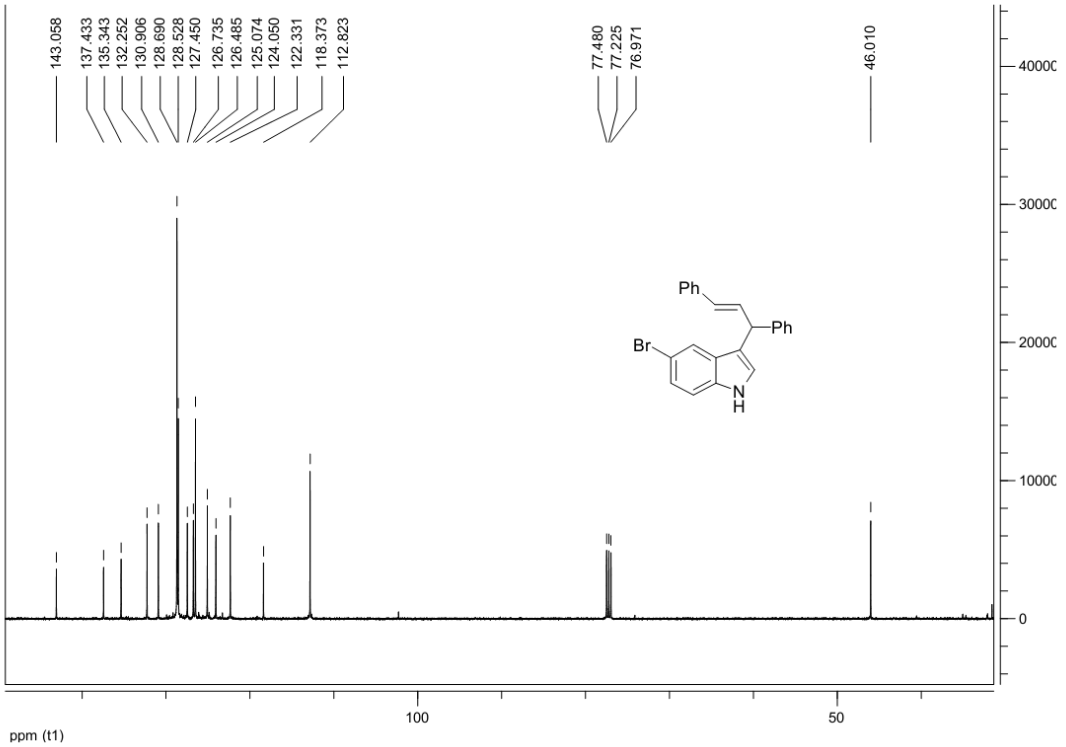
7.473
7.461
7.445
7.377
7.363
7.347
7.322
7.306
7.260
7.189
7.188
7.173
7.091
7.089
7.075
7.061
7.059
6.965
6.951
6.933
6.919
6.538
6.507
5.247
5.232
2.390
Ph
Ph
Me
N
H
1.00
6.26
1.49
1.16
1.24
1.10
0.97
2.97
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)


143.623
137.679
135.487
132.355
131.811
130.685
129.878
129.112
128.620
128.411
128.375
128.082
127.212
126.403
126.223
120.961
119.485
119.325
112.860
110.477
77.462
77.208
76.954
45.208
12.425
Ph
Ph
Me
N
H
150
100
50
ppm (t1)


8.001
7.653
7.445
7.429
7.402
7.394
7.371
7.355
7.322
7.319
7.305
7.260
7.201
7.184
6.891
6.786
6.771
6.754
6.739
6.514
6.482
5.132
5.118
Ph
Ph
Br
N
H
1.00
0.96
11.15
1.60
0.94
0.95
0.97
0.92
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)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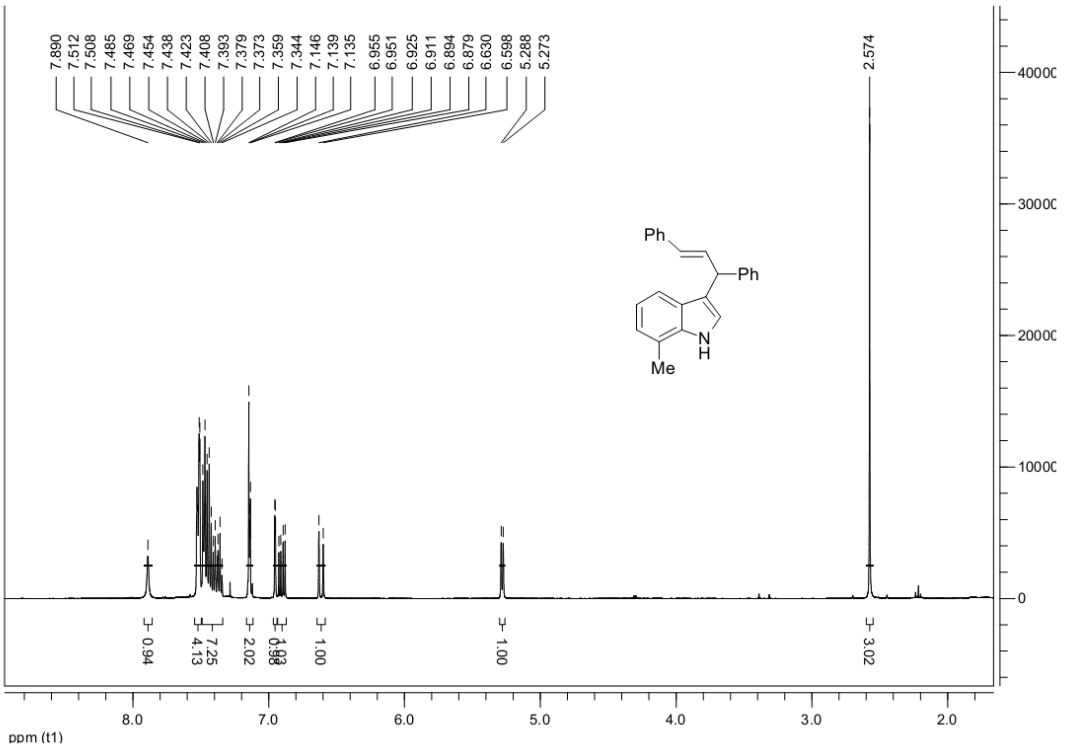
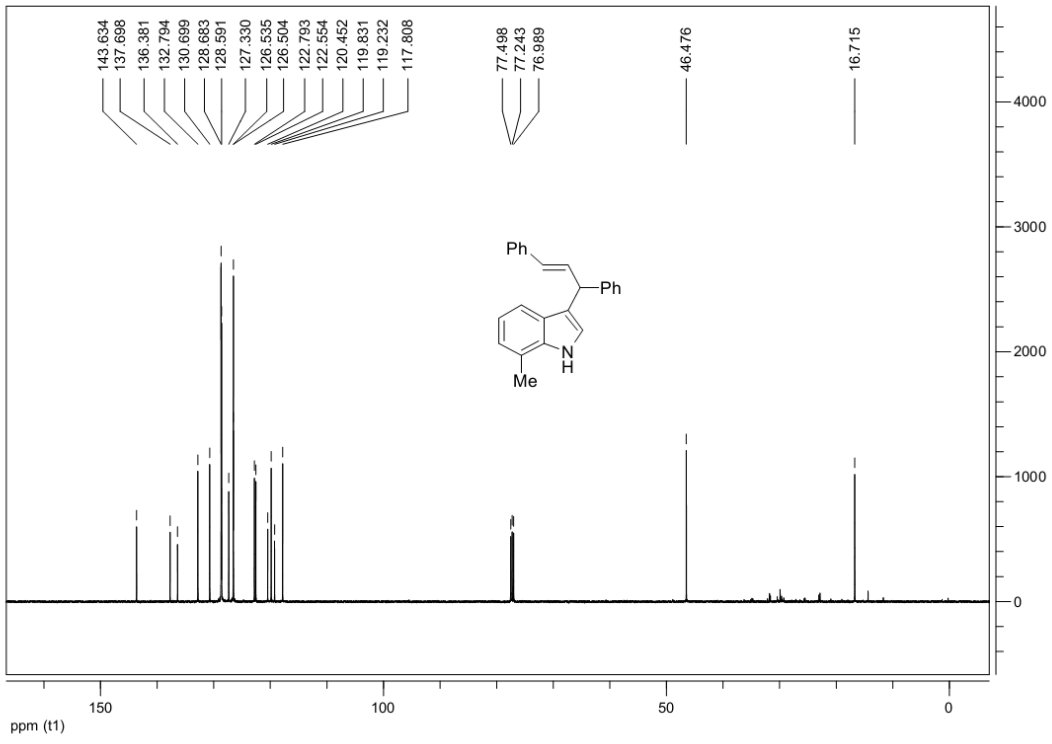
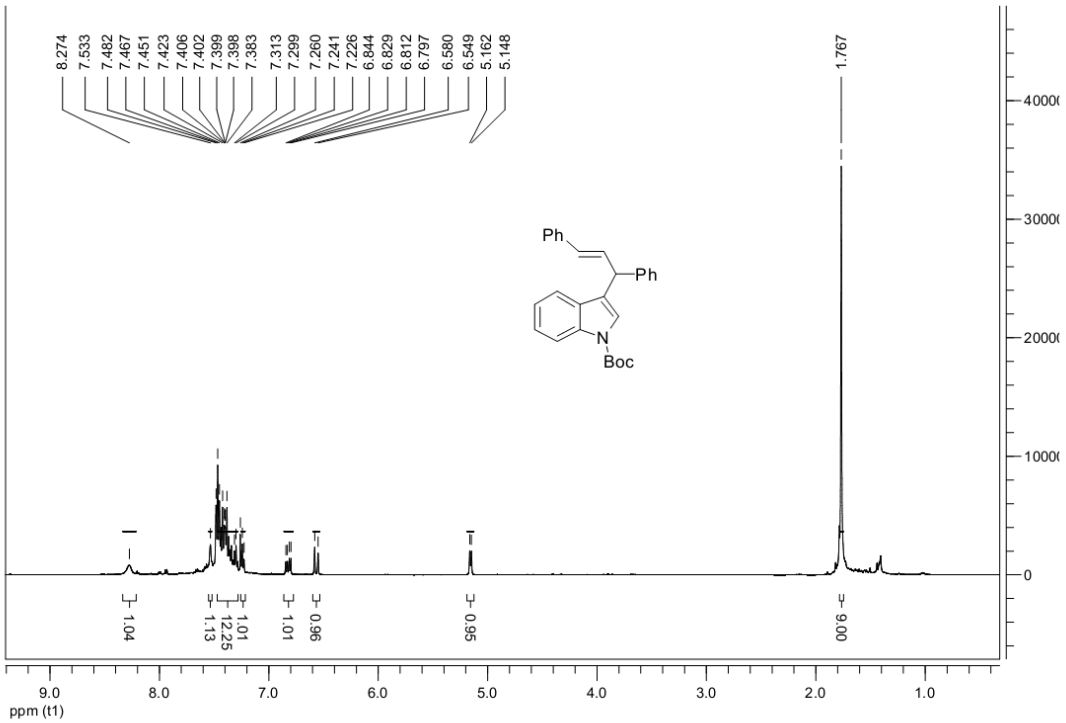
137.433
135.343
132.252
130.906
128.690
128.528
127.450
126.735
126.485
125.074
124.050
122.331
118.373
112.823
77.480
77.225
76.971
46.010
Ph
Ph
Br
N
H
100
50
ppm (t1)


7.890
7.512
7.506
7.485
7.469
7.454
7.438
7.423
7.408
7.393
7.379
7.373
7.359
7.344
7.146
7.139
7.135
6.955
6.951
6.925
6.911
6.894
6.879
6.630
6.598
5.288
5.273
2.574
Ph
Ph
N
H
Me
0.94
4.13
7.25
2.02
1.03
1.00
1.00
3.02
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)


143.634
137.698
136.381
132.794
130.699
128.683
128.591
127.330
126.535
126.504
122.793
122.554
120.452
119.831
119.232
117.808
77.498
77.243
76.989
46.476
16.715
Ph
Ph
N
H
Me
150
100
50
0
ppm (t1)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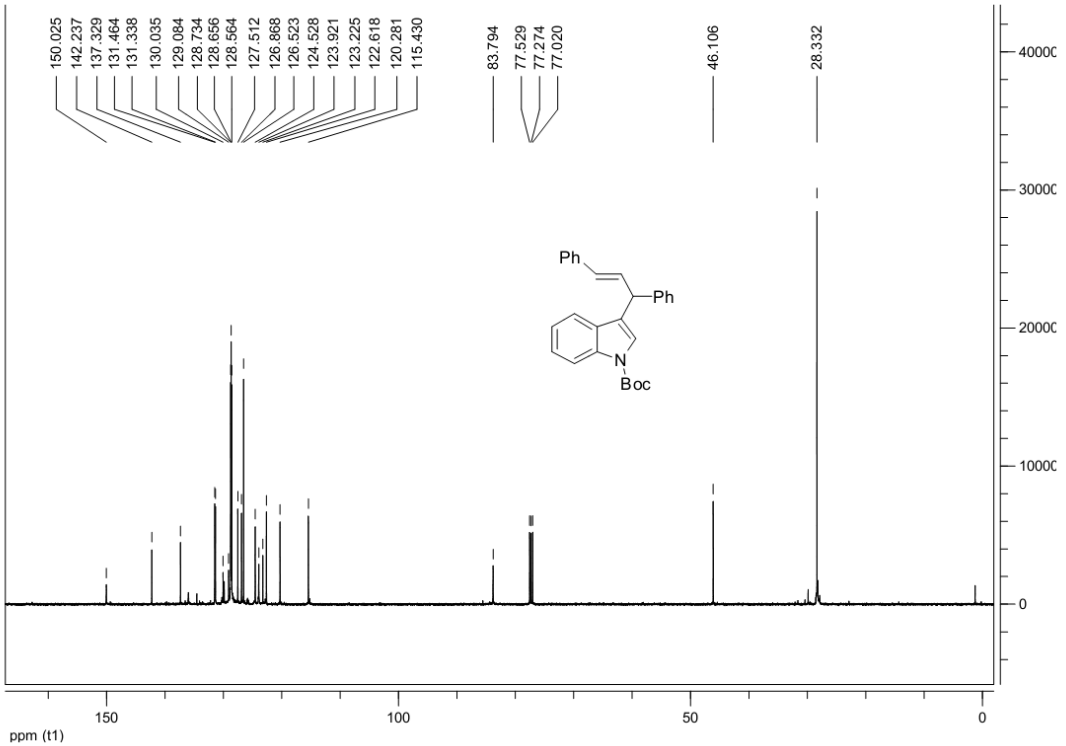
7.533
7.482
7.467
7.451
7.423
7.406
7.402
7.399
7.398
7.383
7.313
7.299
7.260
7.241
7.226
6.844
6.829
6.812
6.797
6.580
6.549
5.162
5.148
1.767
Ph
Ph
N
Boc
1.04
1.13
1.25
1.01
1.01
0.96
0.95
9.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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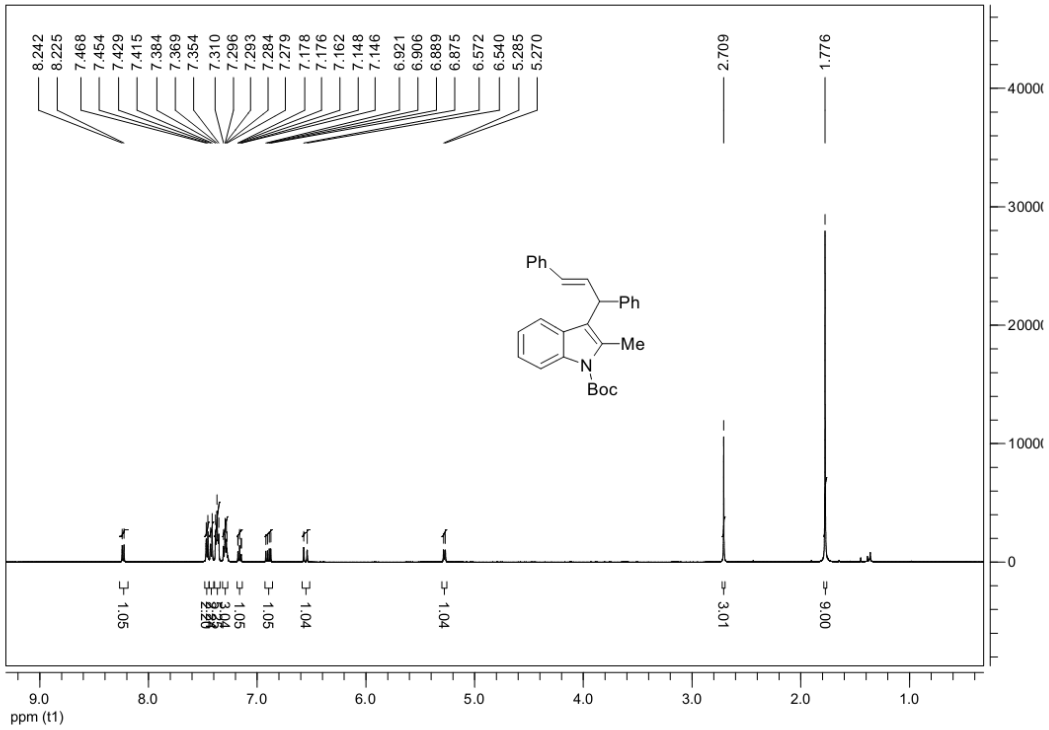
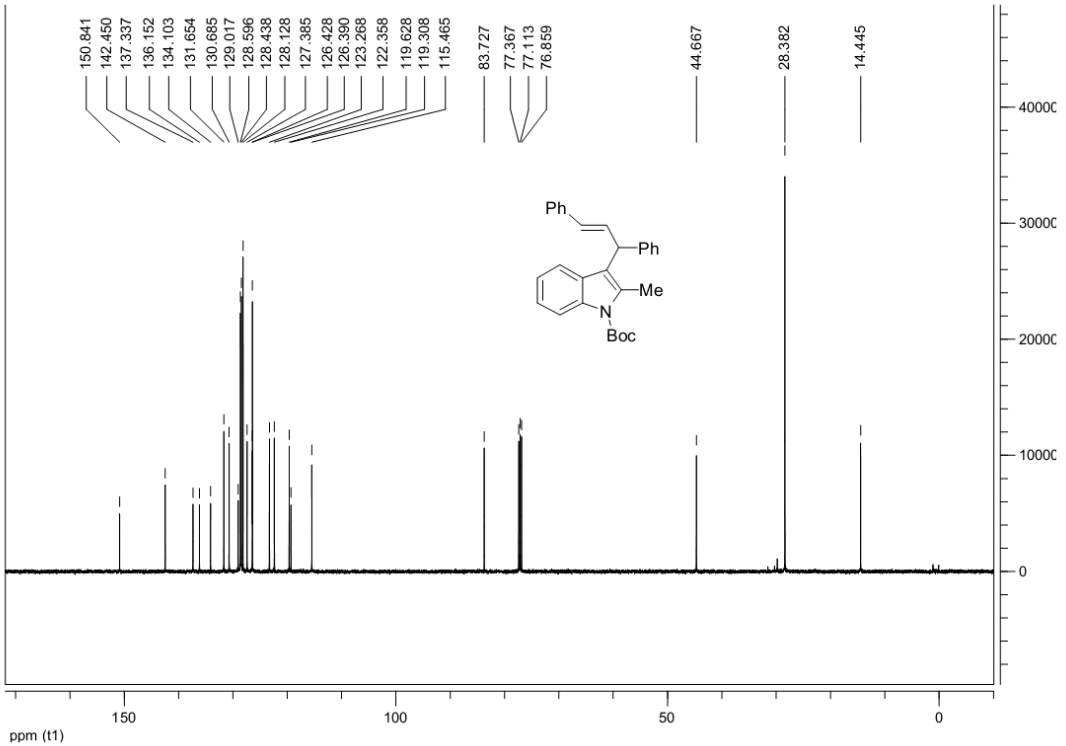
142.237
137.329
131.464
131.338
130.035
129.084
128.734
128.656
128.564
127.512
126.868
126.523
124.528
123.921
123.225
122.618
120.281
115.430
83.794
77.529
77.274
77.020
46.106
28.332
Ph
Ph
N
Boc
150
100
50
0
ppm (t1)


8.242
8.225
7.468
7.454
7.429
7.415
7.384
7.369
7.354
7.310
7.296
7.293
7.284
7.279
7.178
7.176
7.162
7.148
7.146
6.921
6.906
6.889
6.875
6.572
6.540
5.285
5.270
2.709
1.776
Ph
Ph
Me
N
Boc
1.05
1.05
1.04
1.04
3.01
9.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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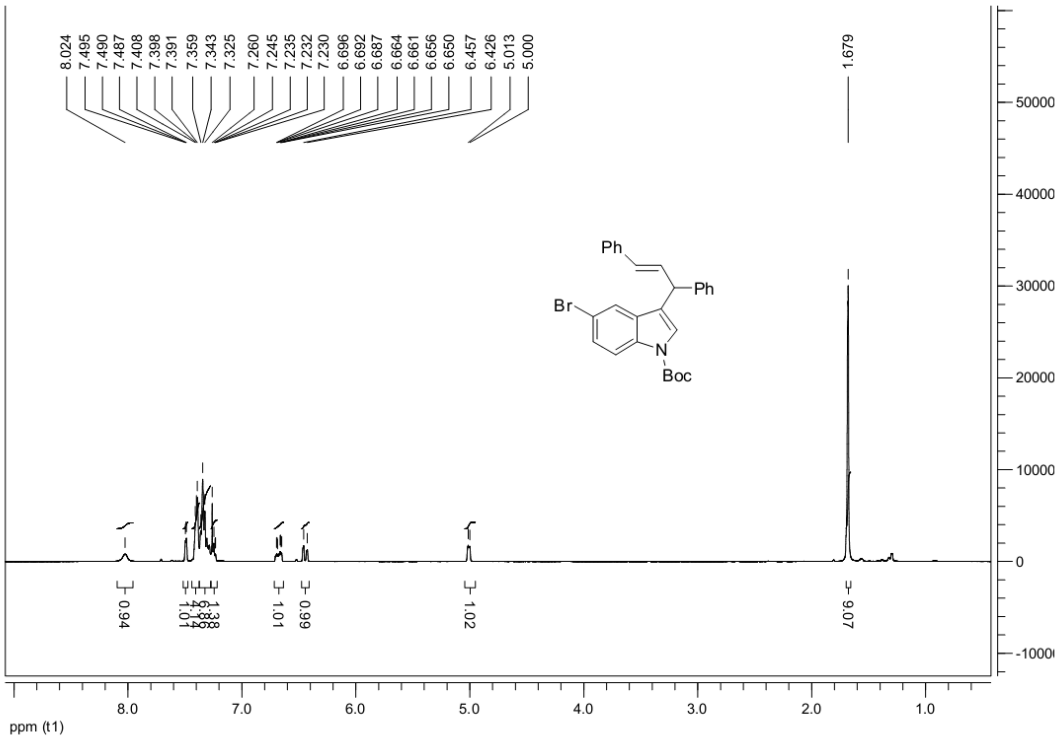
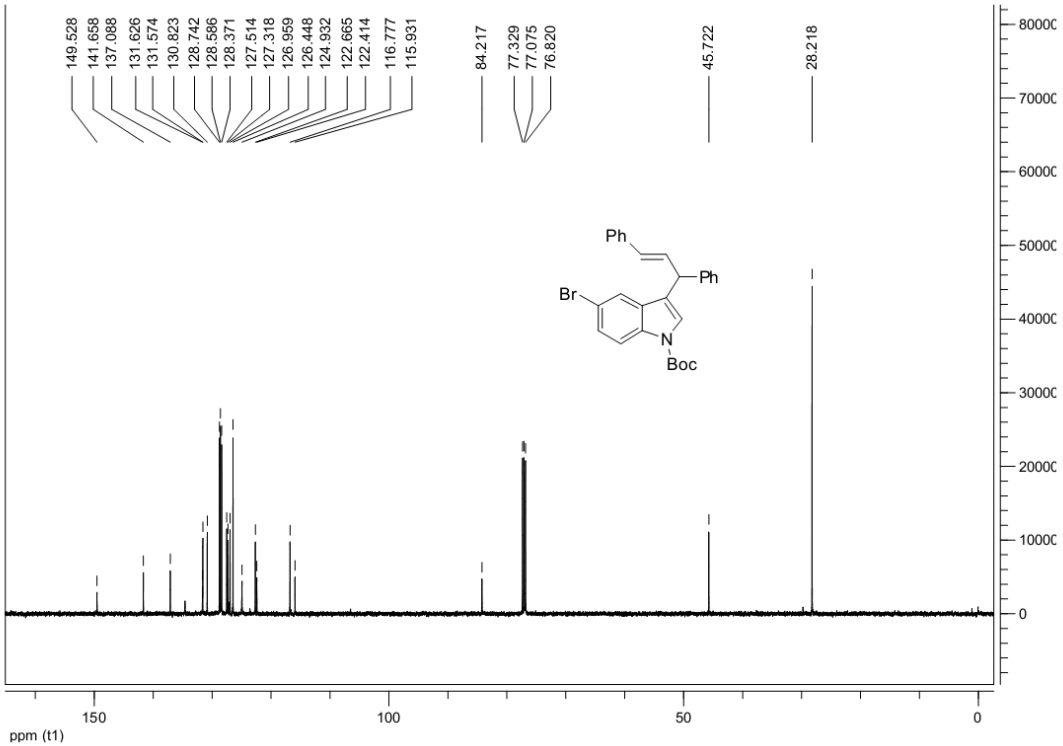
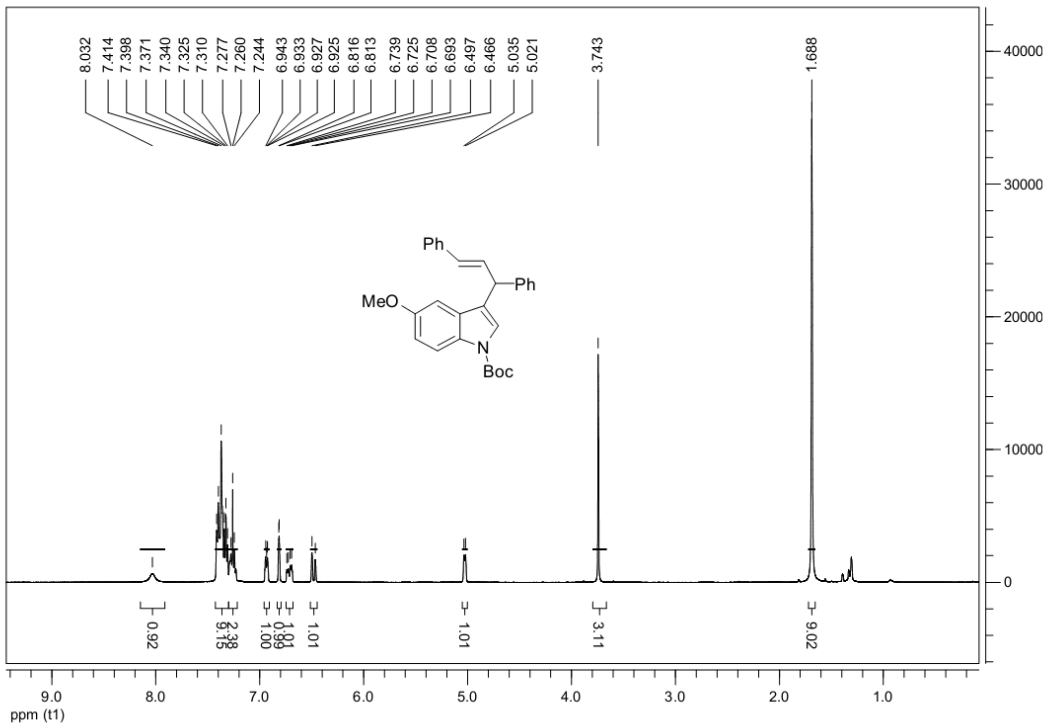
137.337
136.152
134.103
131.654
130.685
129.017
128.596
128.438
128.128
127.385
126.428
126.390
123.268
122.358
119.628
119.308
115.465
83.727
77.367
77.113
76.859
44.667
28.382
14.445
Ph
Ph
Me
N
Boc
150
100
50
0
ppm (t1)


8.024
7.495
7.490
7.487
7.408
7.398
7.391
7.359
7.343
7.325
7.260
7.245
7.235
7.232
7.230
6.696
6.692
6.687
6.664
6.661
6.656
6.650
6.457
6.426
5.013
5.000
1.679
Ph
Ph
Br
N
Boc
0.94
1.01
1.01
0.99
1.02
9.07
ppm (t1)


149.528
141.658
137.088
131.626
131.574
130.823
128.742
128.586
128.371
127.514
127.318
126.959
126.448
124.932
122.665
122.414
116.777
115.931
84.217
77.329
77.075
76.820
45.722
28.218
Ph
Ph
Br
N
Boc
ppm (t1)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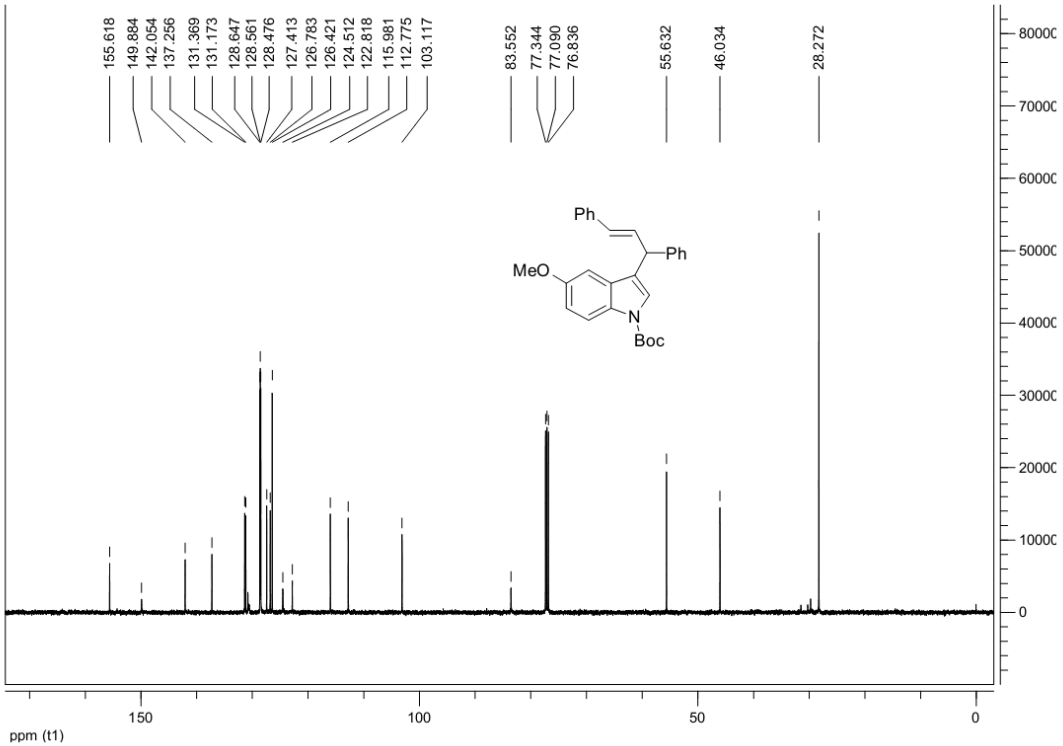
7.398
7.371
7.340
7.325
7.310
7.277
7.260
7.244
6.943
6.933
6.927
6.925
6.816
6.813
6.739
6.725
6.708
6.693
6.497
6.466
5.035
5.021
3.743
1.688
Ph
Ph
MeO
N
Boc
0.92
2.38
2.15
1.00
1.01
1.01
3.11
9.02
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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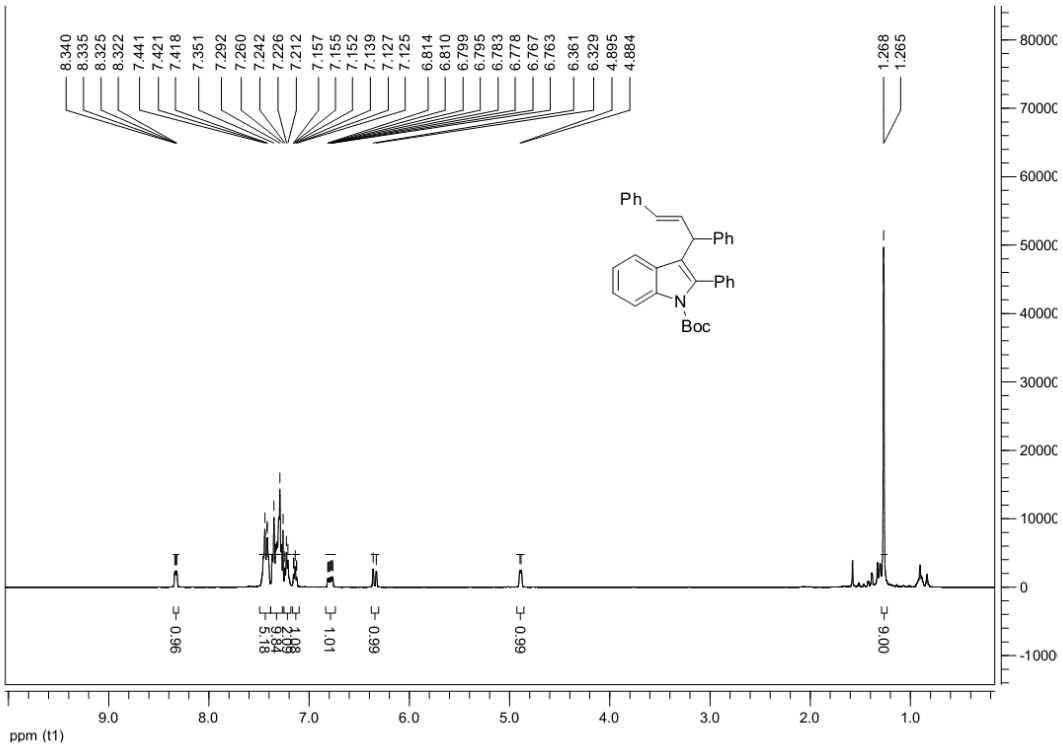
142.054
137.256
131.369
131.173
128.647
128.561
128.476
127.413
126.783
126.421
124.512
122.818
115.981
112.775
103.117
83.552
77.344
77.090
76.836
55.632
46.034
28.272
Ph
Ph
MeO
N
Boc
150
100
50
0
ppm (t1)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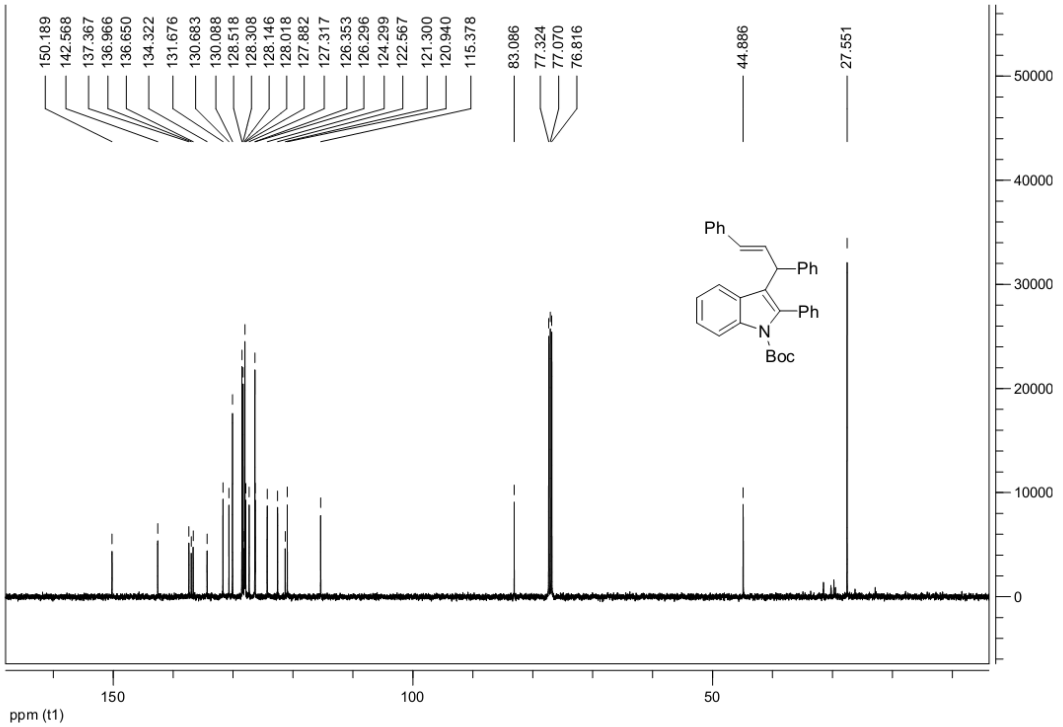
8.335
8.325
8.322
7.441
7.421
7.418
7.351
7.292
7.260
7.242
7.226
7.212
7.157
7.155
7.152
7.139
7.127
7.125
6.814
6.810
6.799
6.795
6.783
6.778
6.767
6.763
6.361
6.329
4.895
4.884
1.268
1.265
Ph
Ph
Ph
N
Boc
0.96
5.18
1.01
0.99
0.99
9.00
ppm (t1)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134.322
131.676
130.683
130.088
128.518
128.308
128.146
128.018
127.882
127.317
126.353
126.296
124.299
122.567
121.300
120.940
115.378
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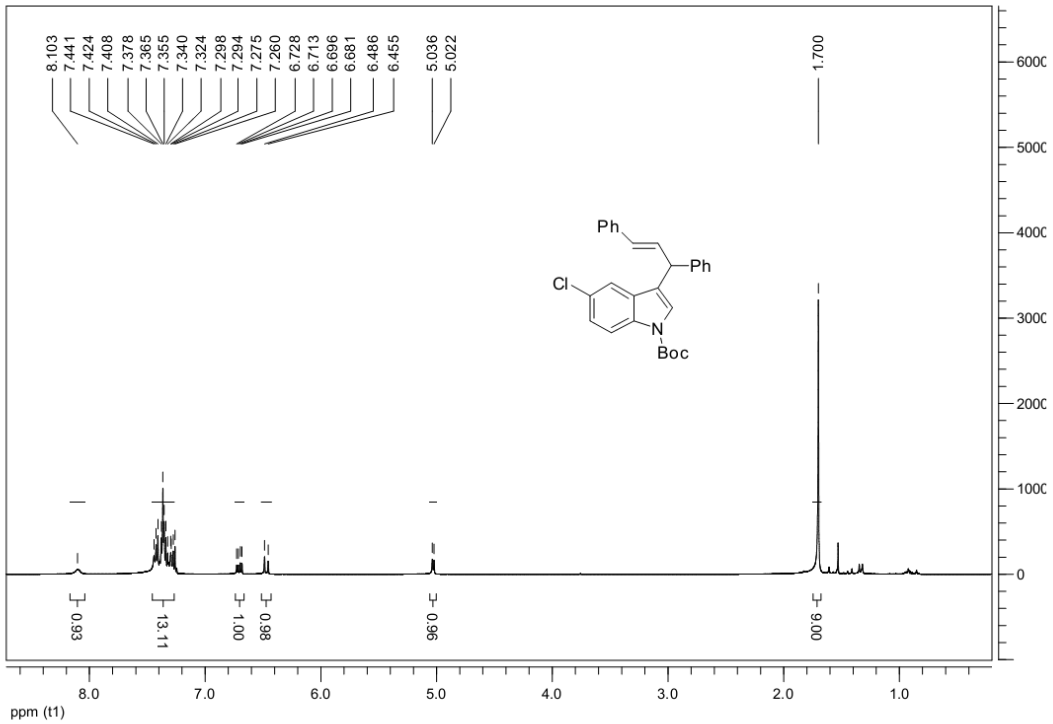
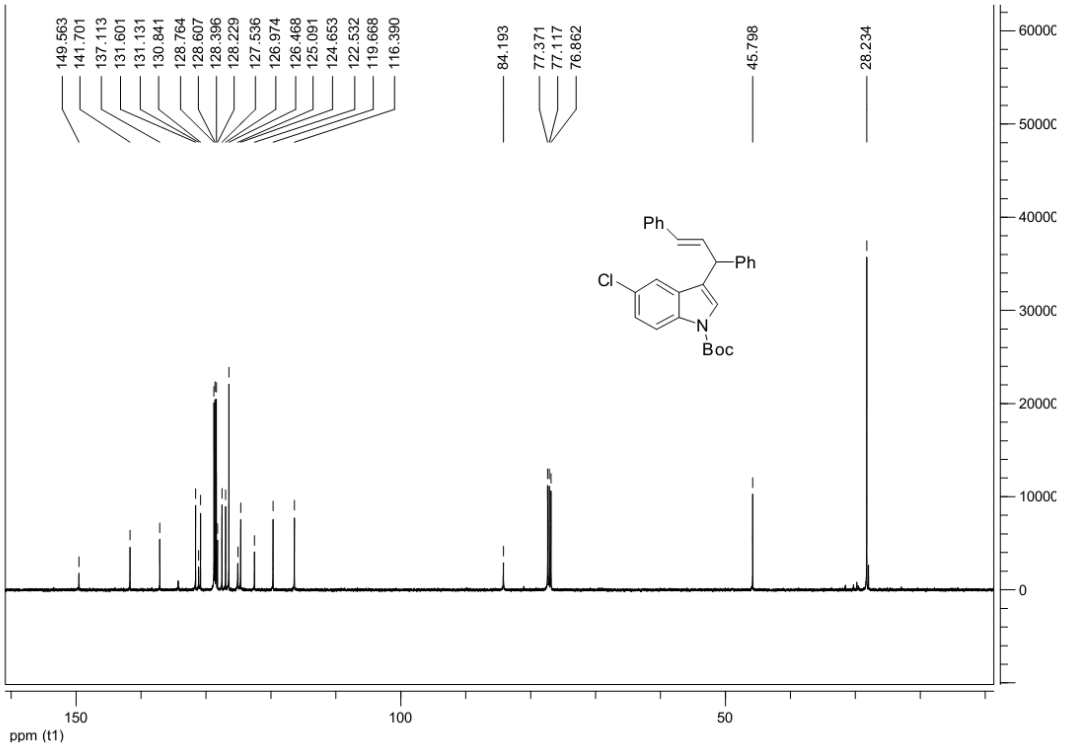
77.324
77.070
76.816
44.886
27.551
Ph
Ph
Ph
N
Boc
ppm (t1)


8.103
7.441
7.424
7.408
7.378
7.365
7.355
7.340
7.324
7.298
7.294
7.275
7.260
6.728
6.713
6.696
6.681
6.486
6.455
5.036
5.022
1.700
Ph
Ph
Cl
N
Boc
0.93
13.11
1.00
0.98
0.96
9.00
ppm (t1)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141.701
137.113
131.601
131.131
130.841
128.764
128.607
128.396
128.229
127.536
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126.468
125.091
124.653
122.532
119.668
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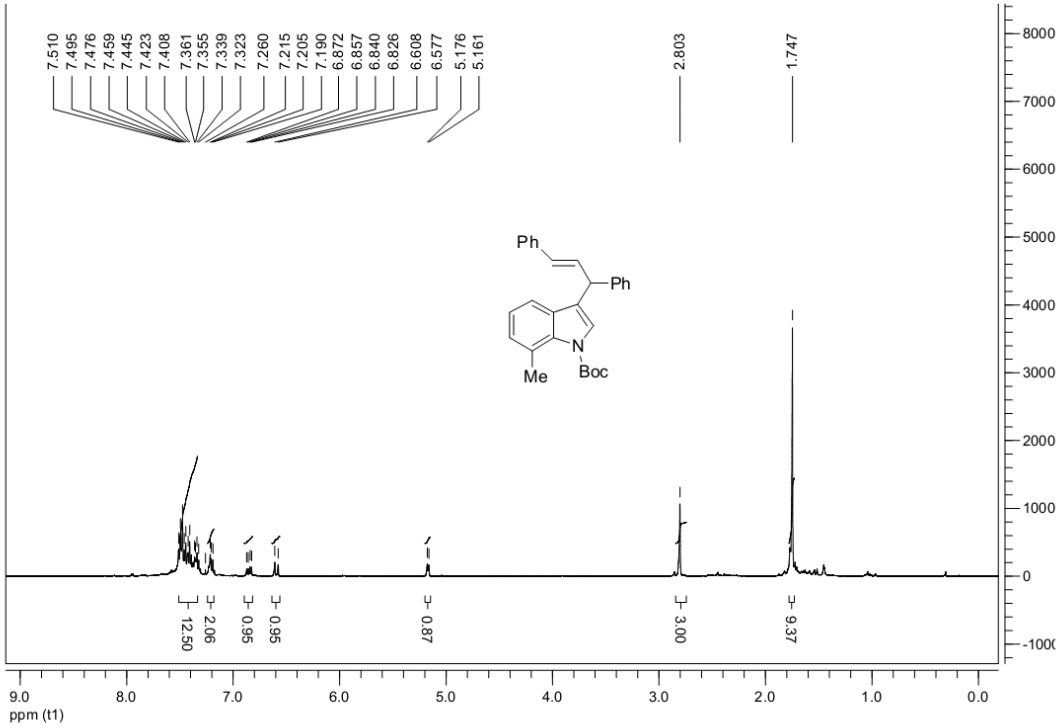
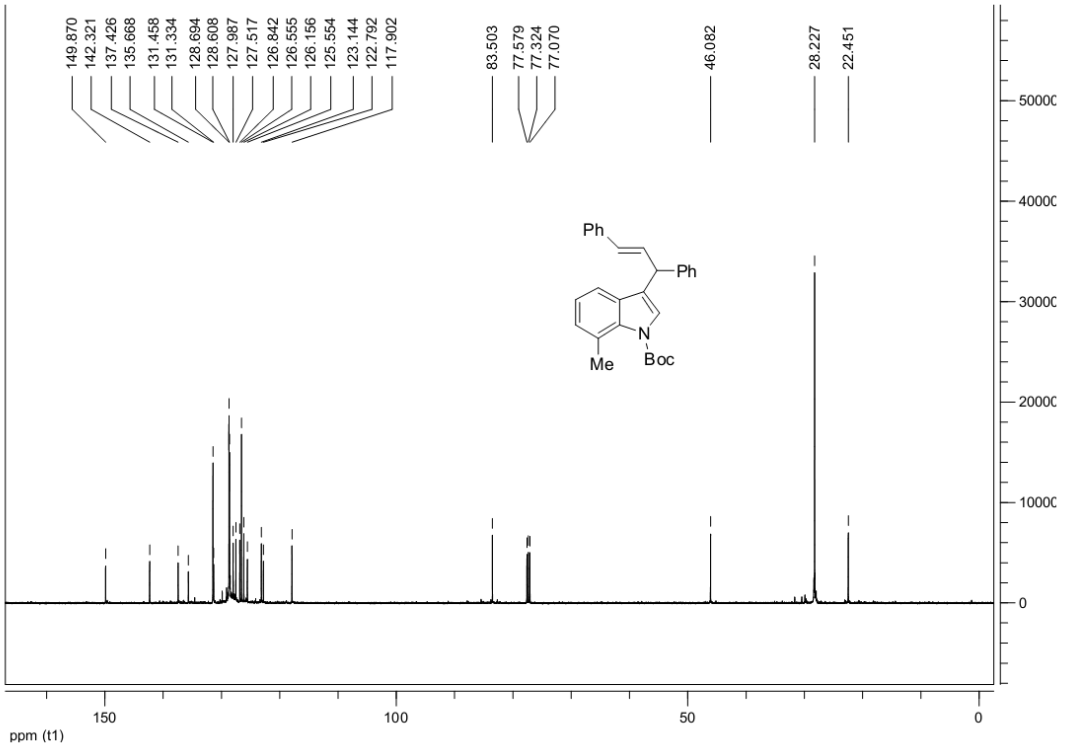
77.371
77.117
76.862
45.798
28.234
Ph
Ph
Cl
N
Boc
ppm (t1)


7.510
7.495
7.476
7.459
7.445
7.423
7.408
7.361
7.355
7.339
7.323
7.260
7.215
7.205
7.190
6.872
6.857
6.840
6.826
6.608
6.577
5.176
5.161
2.803
1.747
Ph
Ph
N
Boc
Me
12.50
2.06
0.95
0.95
0.87
3.00
9.37
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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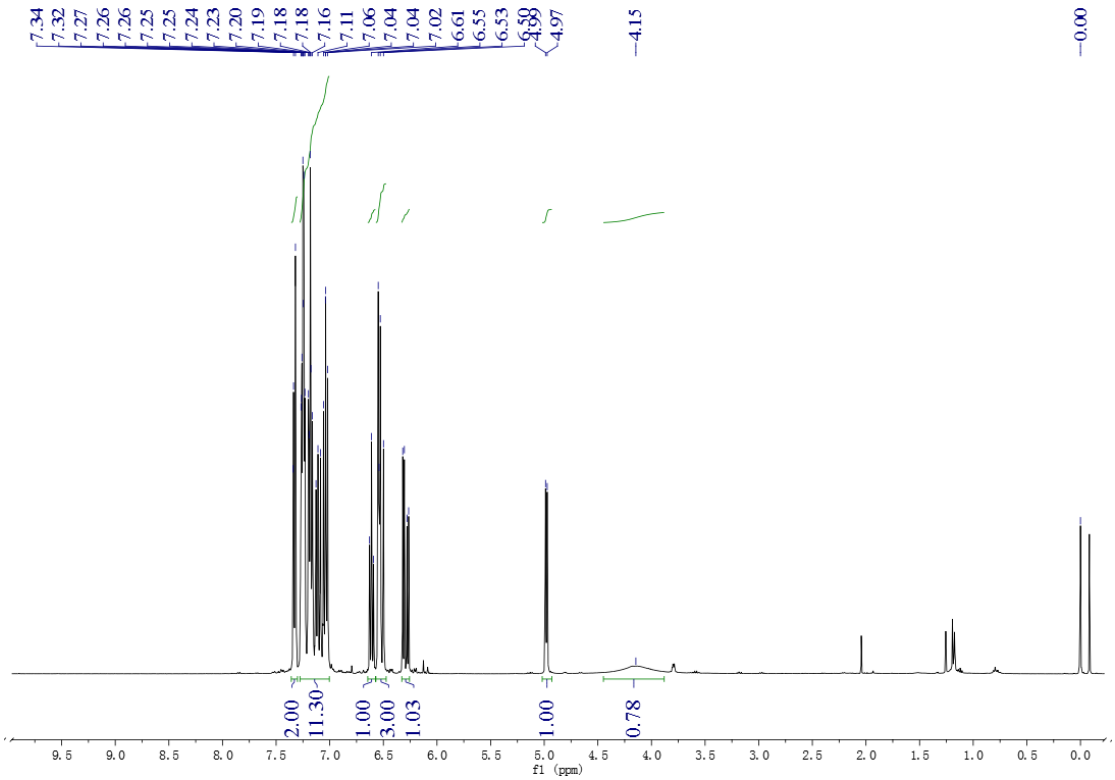
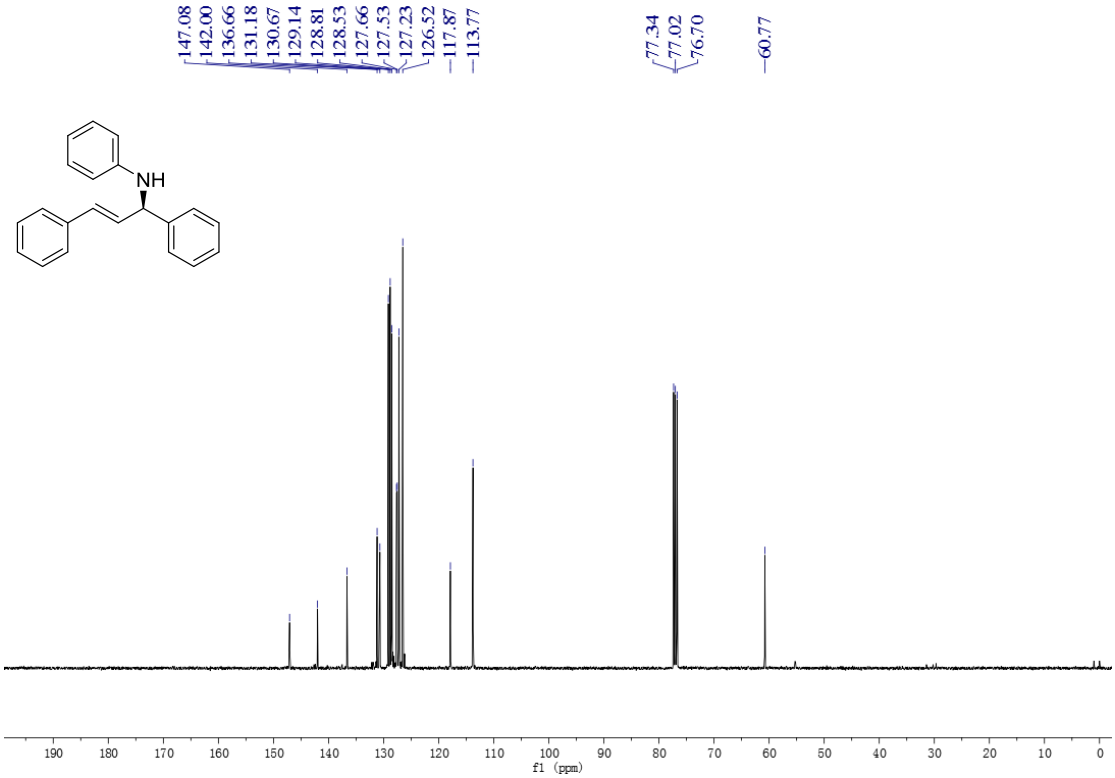
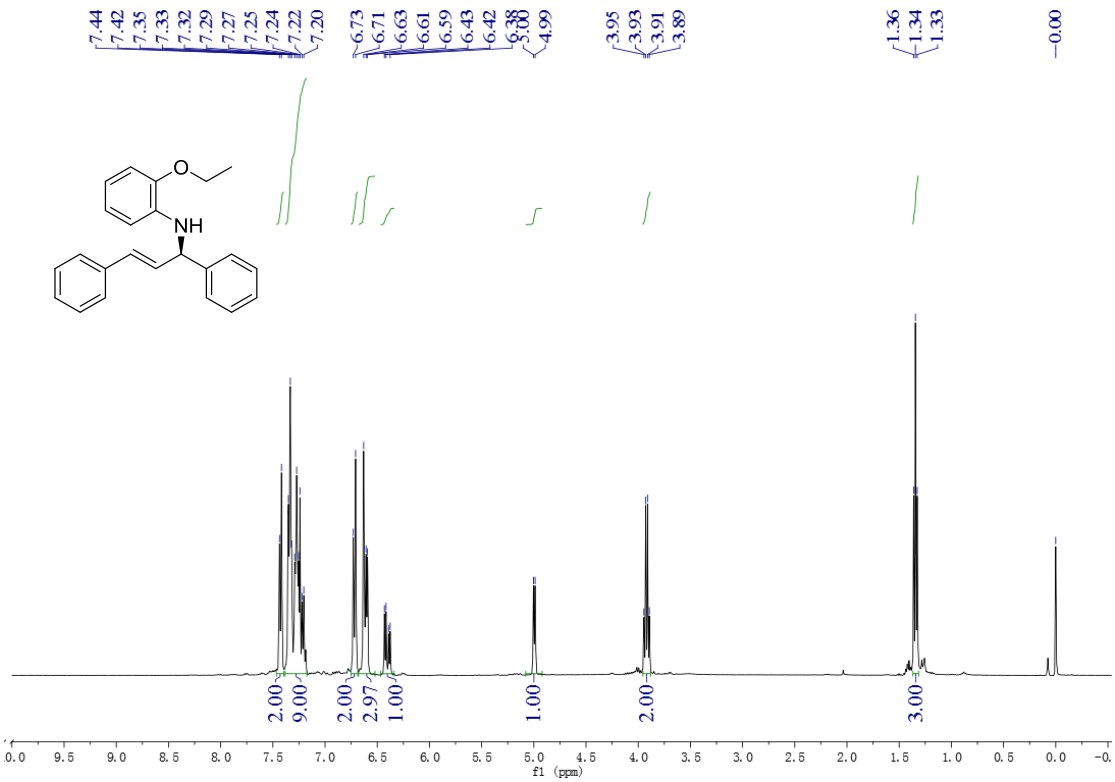
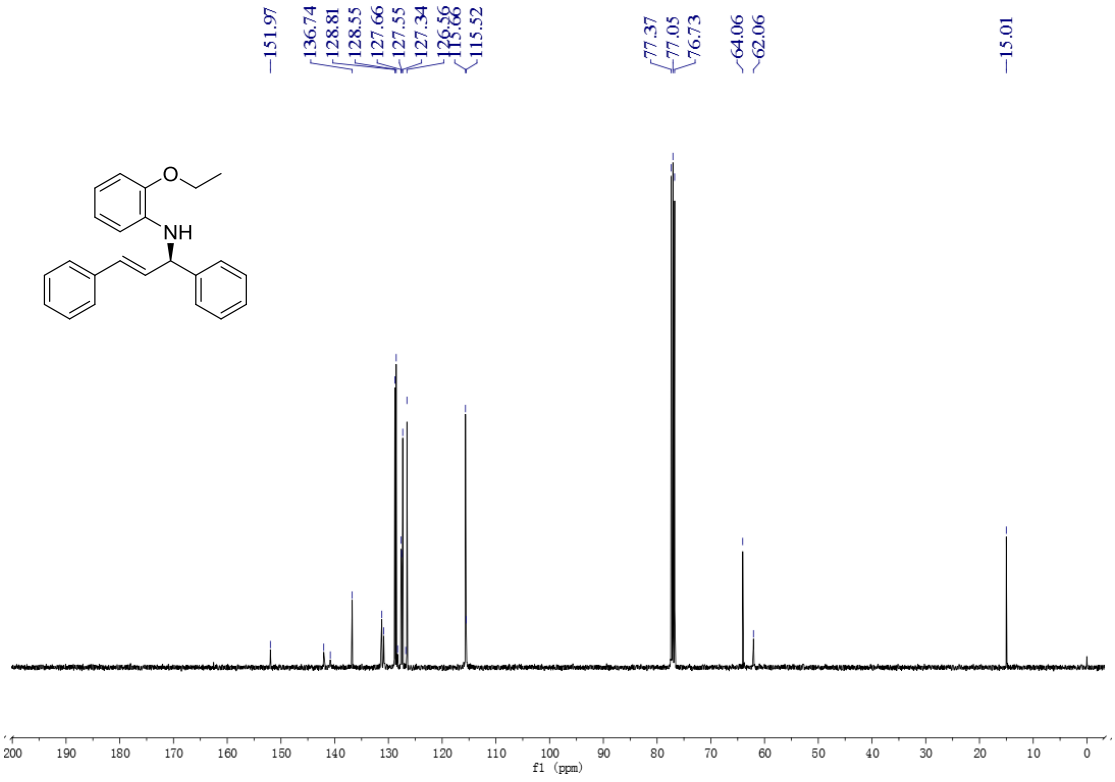
131.458
131.334
128.694
128.608
127.987
127.517
126.842
126.555
126.156
125.554
123.144
122.792
117.902
83.503
77.579
77.324
77.070
46.082
28.227
22.451
Ph
Ph
N
Boc
Me
150
100
50
0
ppm (t1)


7.34
7.32
7.27
7.26
7.26
7.25
7.25
7.24
7.23
7.20
7.19
7.18
7.18
7.16
7.11
7.06
7.04
7.04
7.02
6.61
6.55
6.53
4.99
4.97
4.15
0.00
2.00
11.30
1.00
3.00
1.03
1.00
0.78
f1 (ppm)


147.08
142.00
136.66
131.18
130.67
129.14
128.81
128.53
127.66
127.53
127.23
126.52
117.87
113.77
77.34
77.02
76.70
60.77
NH
f1 (ppm)


7.44
7.42
7.35
7.33
7.32
7.29
7.27
7.25
7.24
7.22
7.20
6.73
6.71
6.63
6.61
6.59
6.43
6.42
6.38
5.00
4.99
3.95
3.93
3.91
3.89
1.36
1.34
1.33
0.00
O
NH
2.00
9.00
2.00
2.97
1.00
1.00
2.00
3.00
f1 (ppm)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127.55
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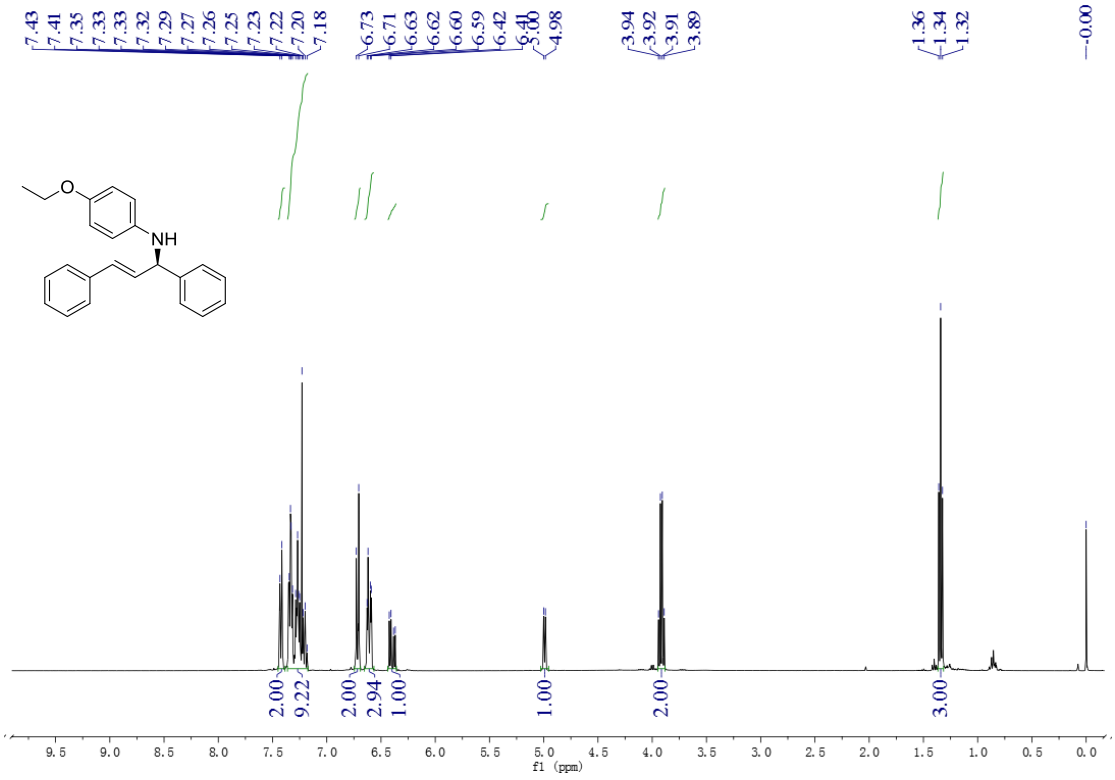
115.52
77.37
77.05
76.73
64.06
62.06
15.01
O
NH
f1 (ppm)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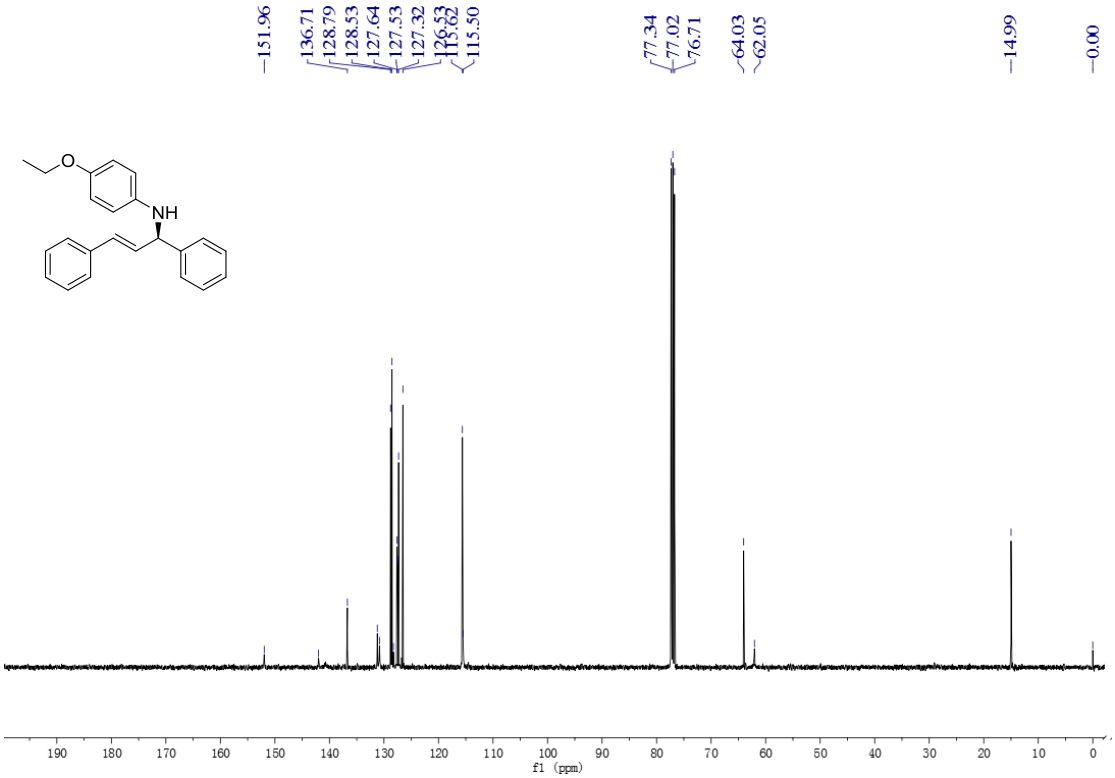
7.33
7.33
7.32
7.29
7.27
7.26
7.25
7.23
7.22
7.20
7.18
6.73
6.71
6.63
6.62
6.60
6.59
6.42
6.41
5.00
4.98
3.94
3.92
3.91
3.89
1.36
1.34
1.32
0.00
O
NH
2.00
9.22
2.00
2.94
1.00
1.00
2.00
3.00
f1 (ppm)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76.71
64.03
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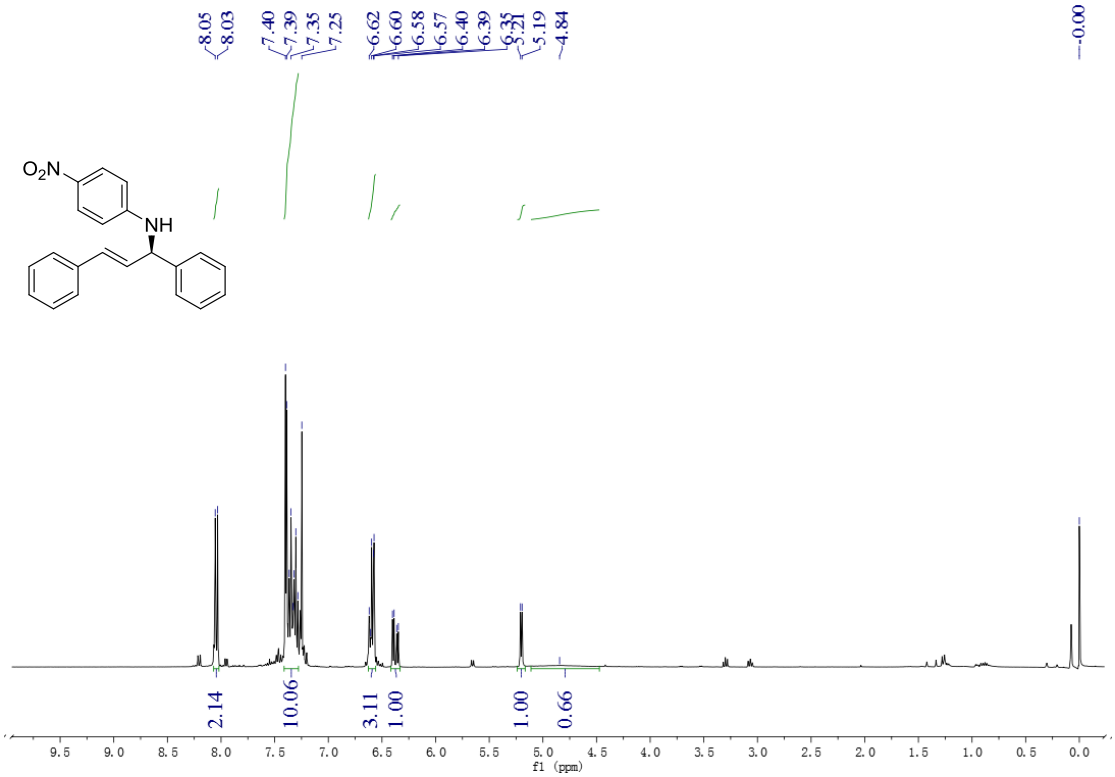
14.99
0.00
O
NH
f1 (ppm)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7.35
7.25
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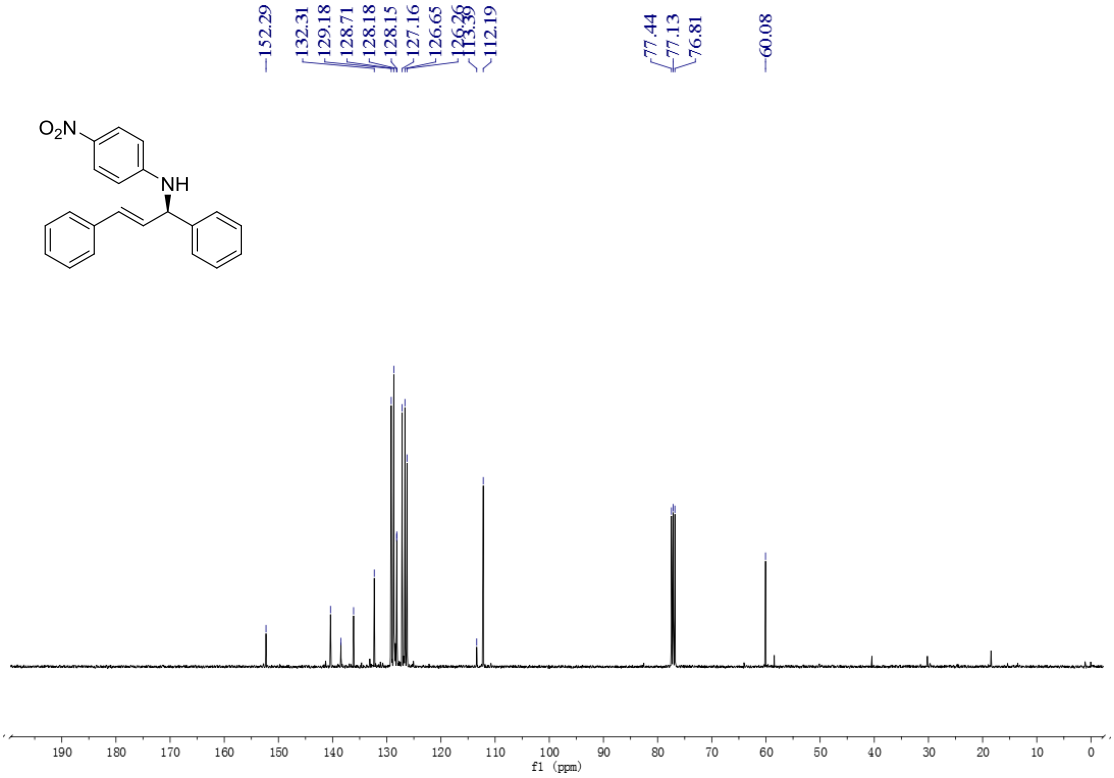
6.60
6.58
6.57
6.40
6.39
6.35
5.21
5.19
4.84
0.00
O2N
NH
2.14
10.06
3.11
1.00
1.00
0.66
f1 (ppm)


152.29
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127.16
126.65
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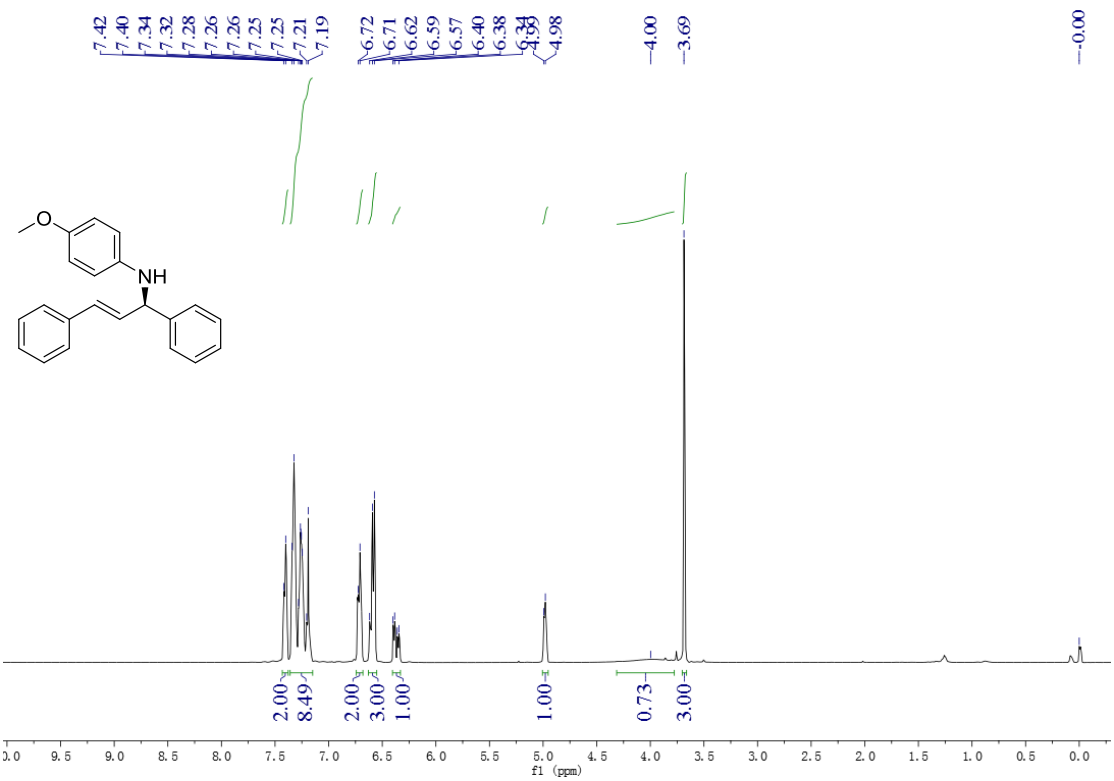
77.13
76.81
60.08
O2N
NH
f1 (ppm)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7.34
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7.26
7.26
7.25
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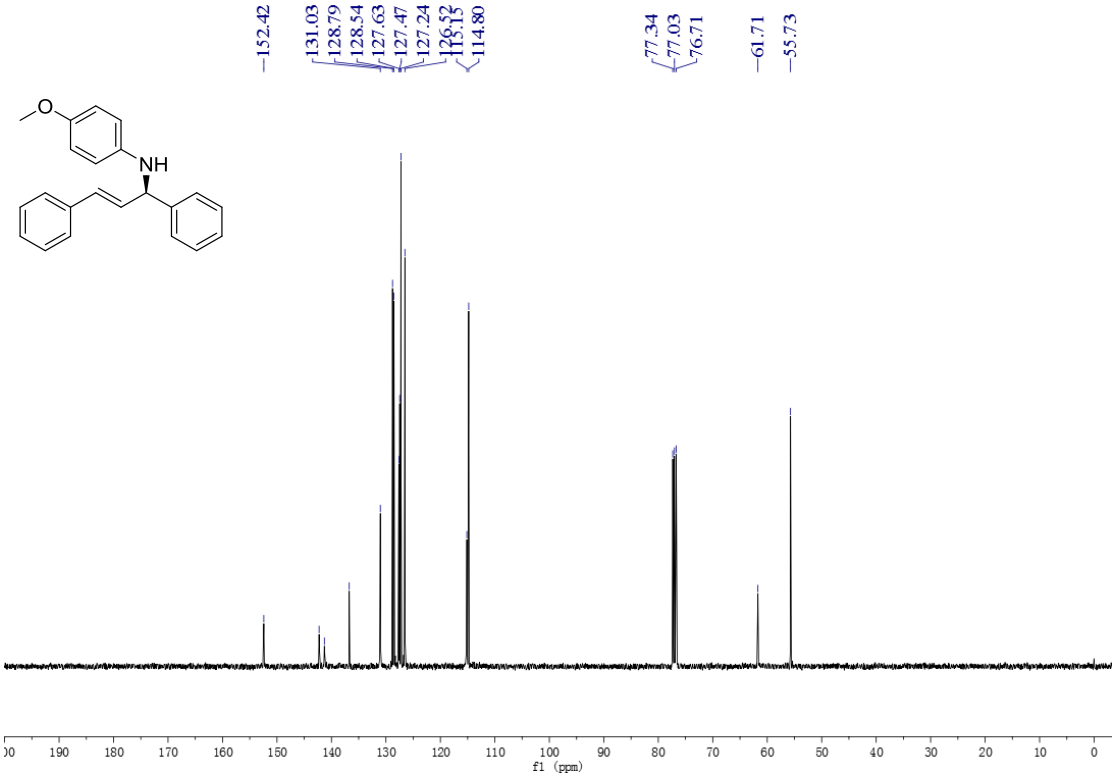
7.21
7.19
6.72
6.71
6.62
6.59
6.57
6.40
6.38
4.98
4.00
3.69
0.00
O
NH
2.00
8.49
2.00
3.00
1.00
1.00
0.73
3.00
f1 (ppm)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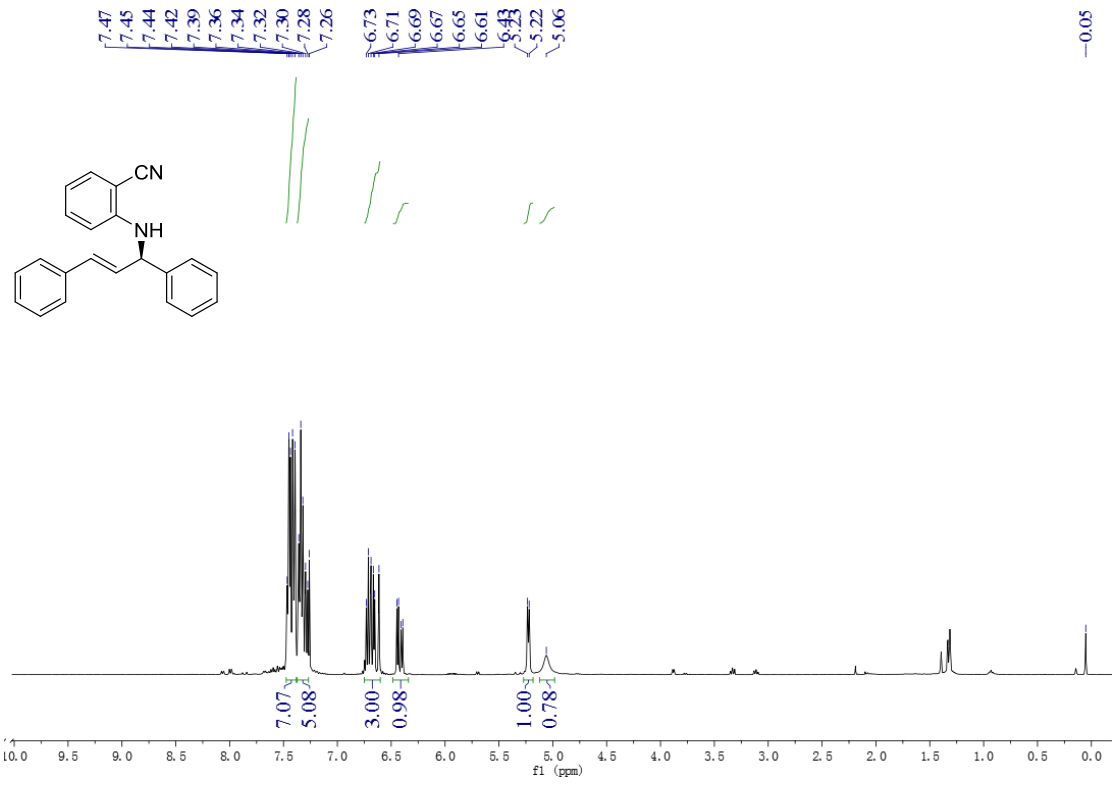
115.15
114.80
77.34
77.03
76.71
61.71
55.73
O
NH
f1 (ppm)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7.32
7.30
7.28
7.26
6.73
6.71
6.69
6.67
6.65
6.61
5.22
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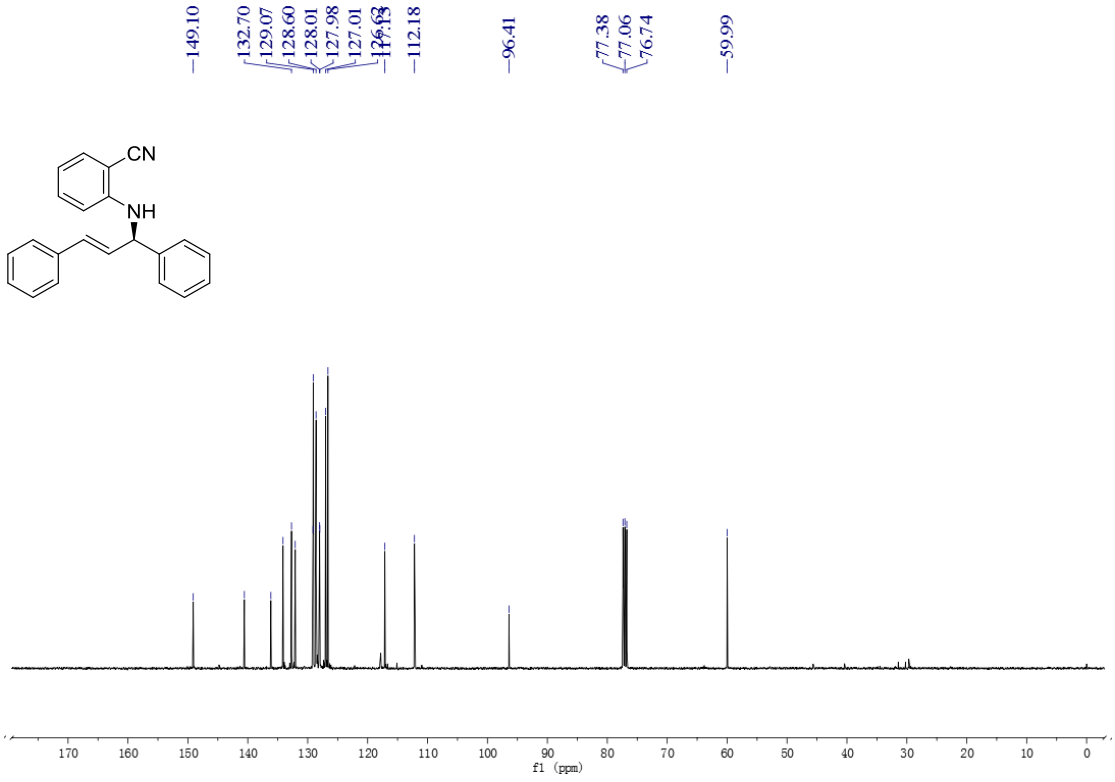
0.05
CN
NH
7.07
5.08
3.00
0.98
1.00
0.78
f1 (ppm)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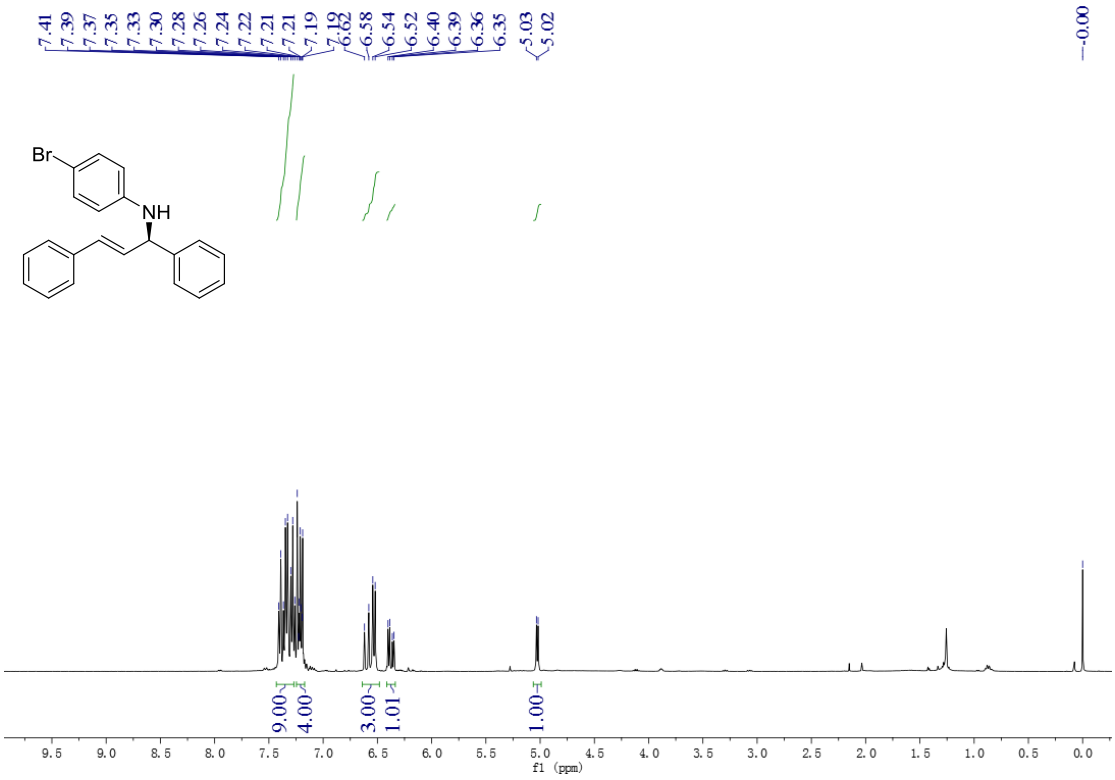
127.98
127.01
112.18
96.41
77.38
77.06
76.74
59.99
CN
NH
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.37
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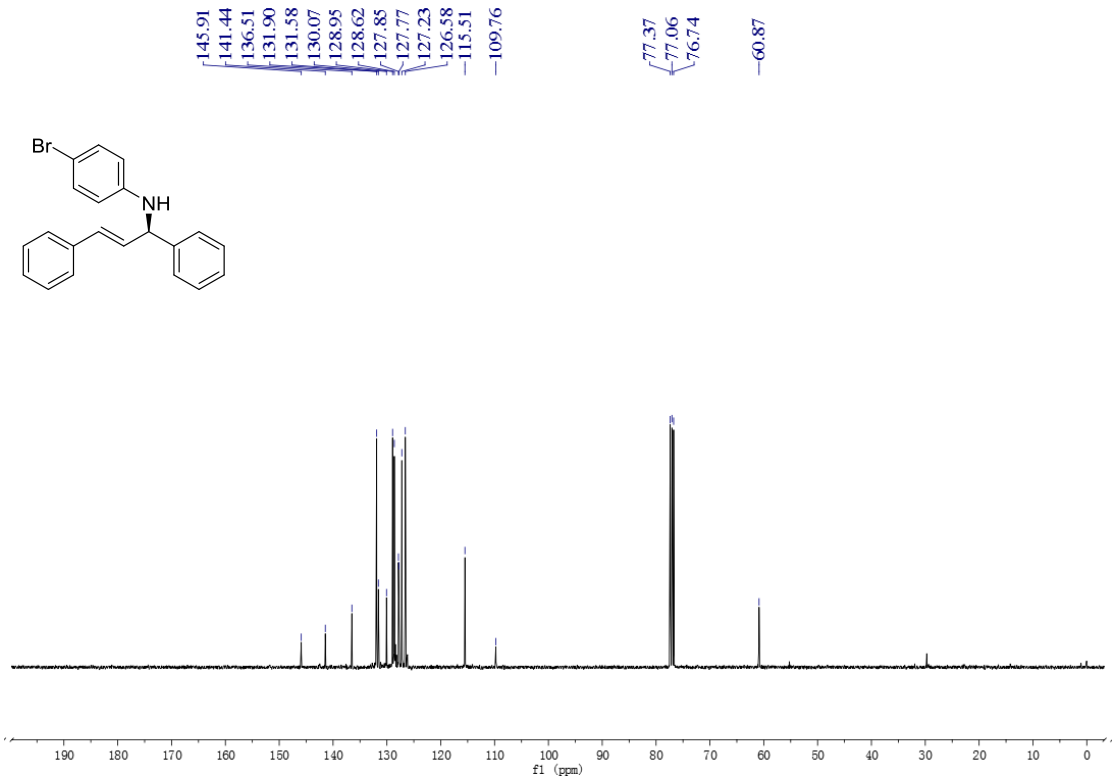
7.33
7.30
7.28
7.26
7.24
7.22
7.21
7.21
7.19
6.62
6.58
6.54
6.52
6.40
6.39
6.36
6.35
5.03
5.02
-0.00
Br
NH
9.00
4.00
3.00
1.01
1.00
f1 (ppm)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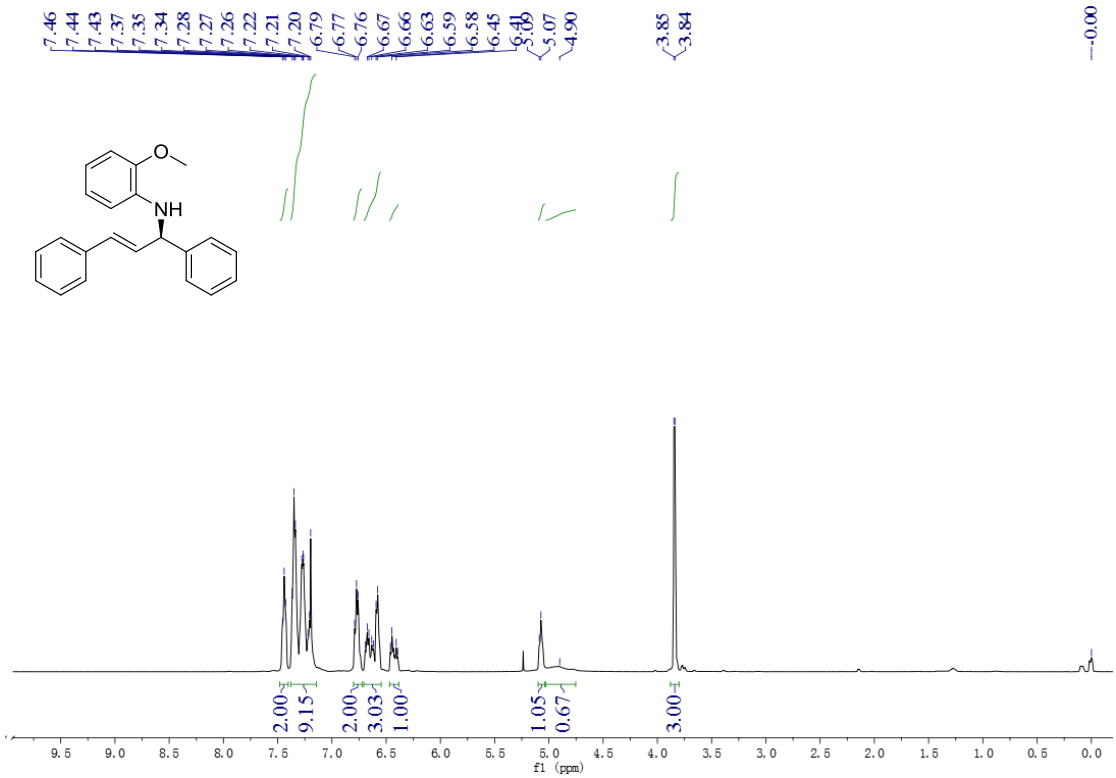
109.76
77.37
77.06
76.74
60.87
Br
NH
f1 (ppm)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7.43
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7.34
7.28
7.27
7.26
7.22
7.21
7.20
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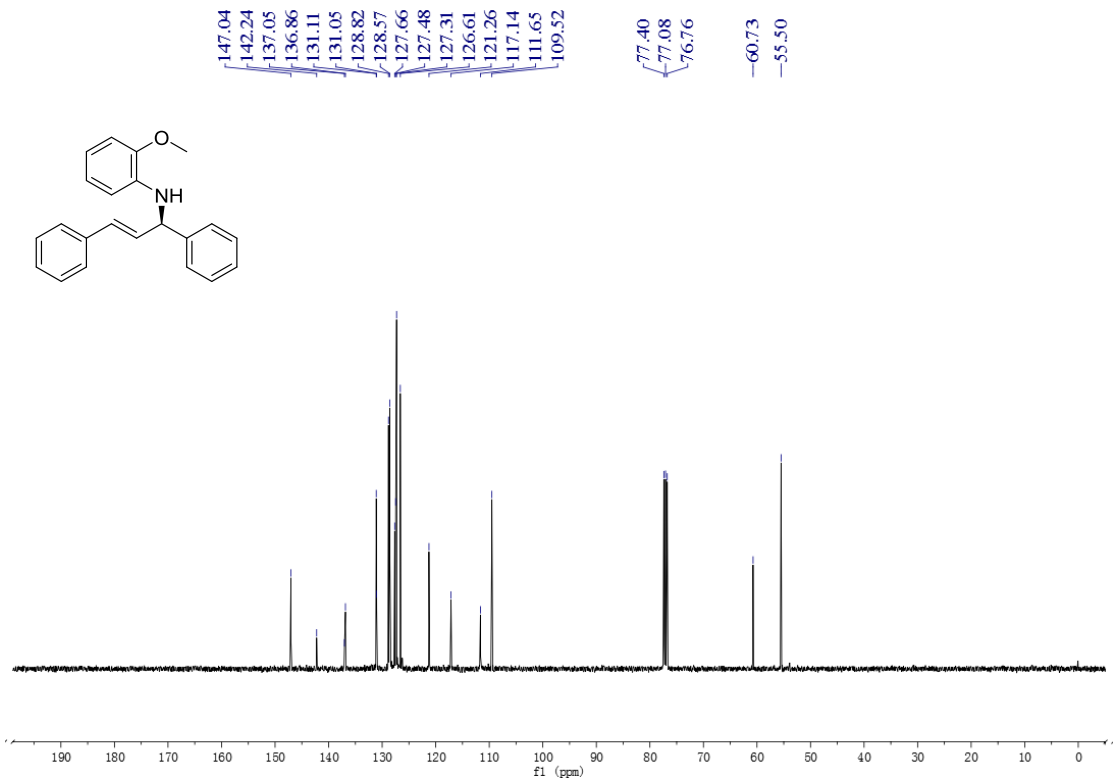
6.77
6.76
6.67
6.66
6.63
6.59
6.58
6.45
6.41
5.08
5.07
4.90
3.85
3.84
-0.00
O
NH
2.00
9.15
2.00
3.03
1.00
1.05
0.67
3.00
f1 (ppm)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128.57
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127.48
127.31
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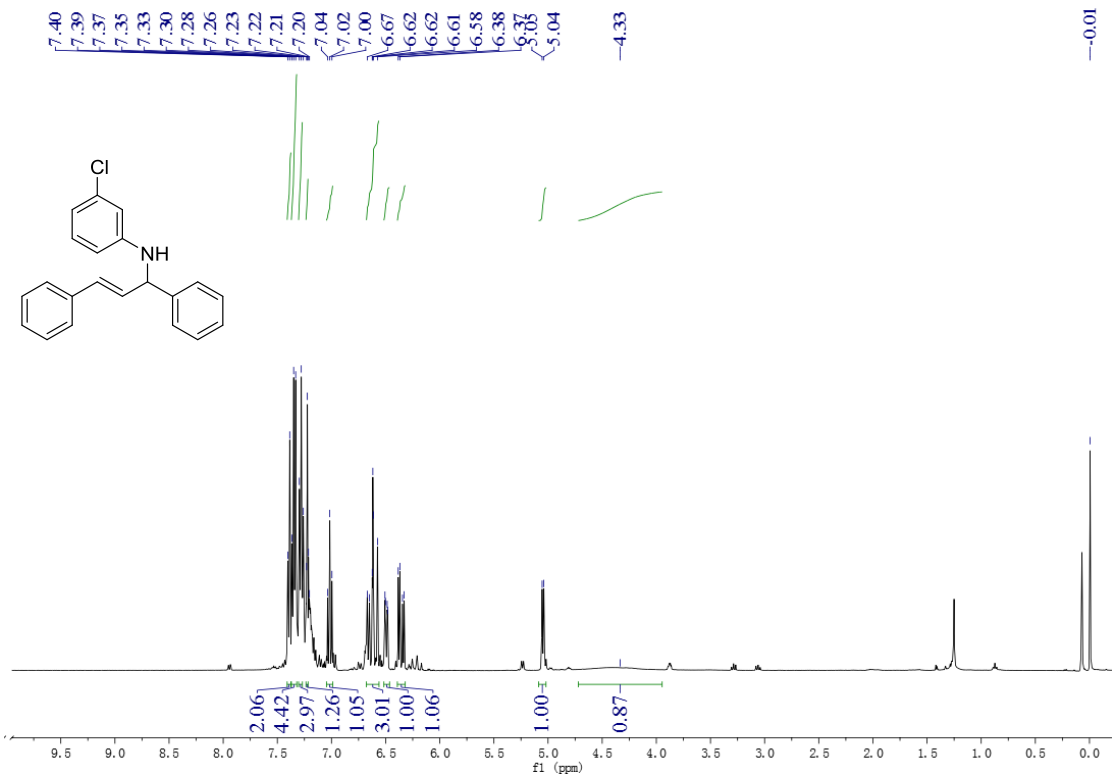
111.65
109.52
77.40
77.08
76.76
60.73
55.50
O
NH
f1 (ppm)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7.33
7.30
7.28
7.26
7.23
7.22
7.21
7.20
7.04
7.02
7.00
6.67
6.62
6.62
6.61
6.58
6.38
6.37
5.05
5.04
4.33
0.01
Cl
NH
2.06
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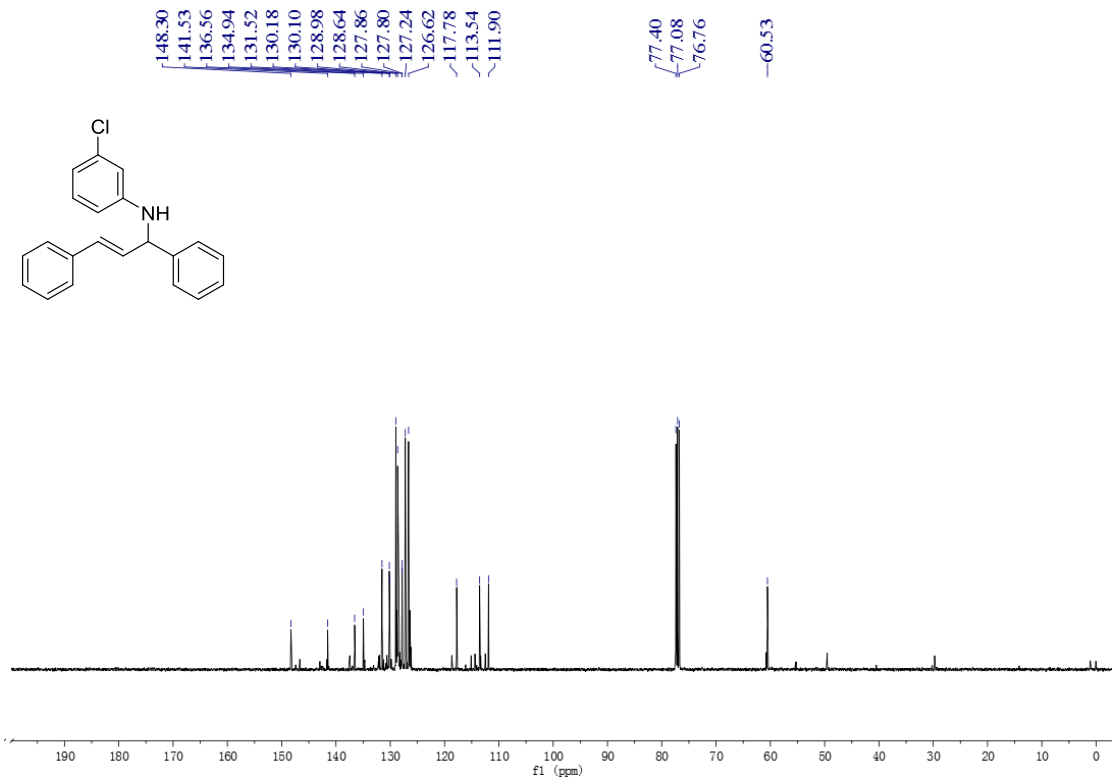
2.97
1.26
1.05
3.01
1.00
1.06
1.00
0.87
f1 (ppm)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128.98
128.64
127.86
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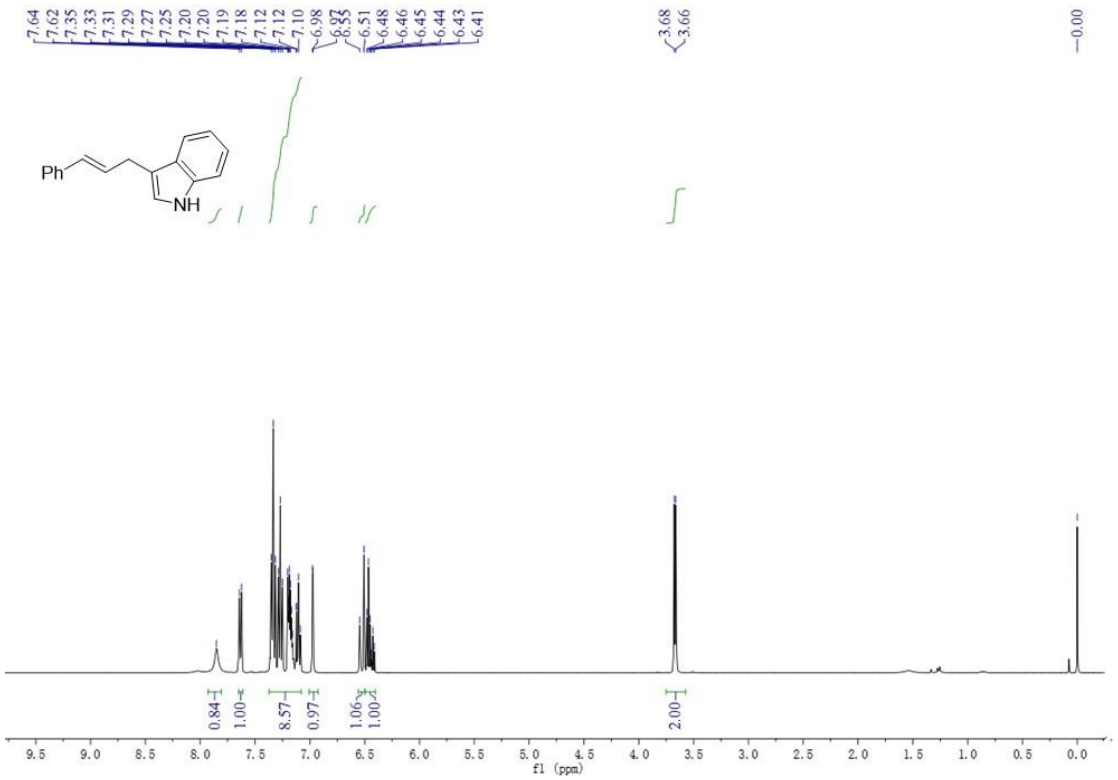
77.08
76.76
60.53
Cl
NH
f1 (ppm)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7.19
7.18
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6.46
6.45
6.44
6.43
6.41
3.68
3.66
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Ph
NH
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1.00
8.57
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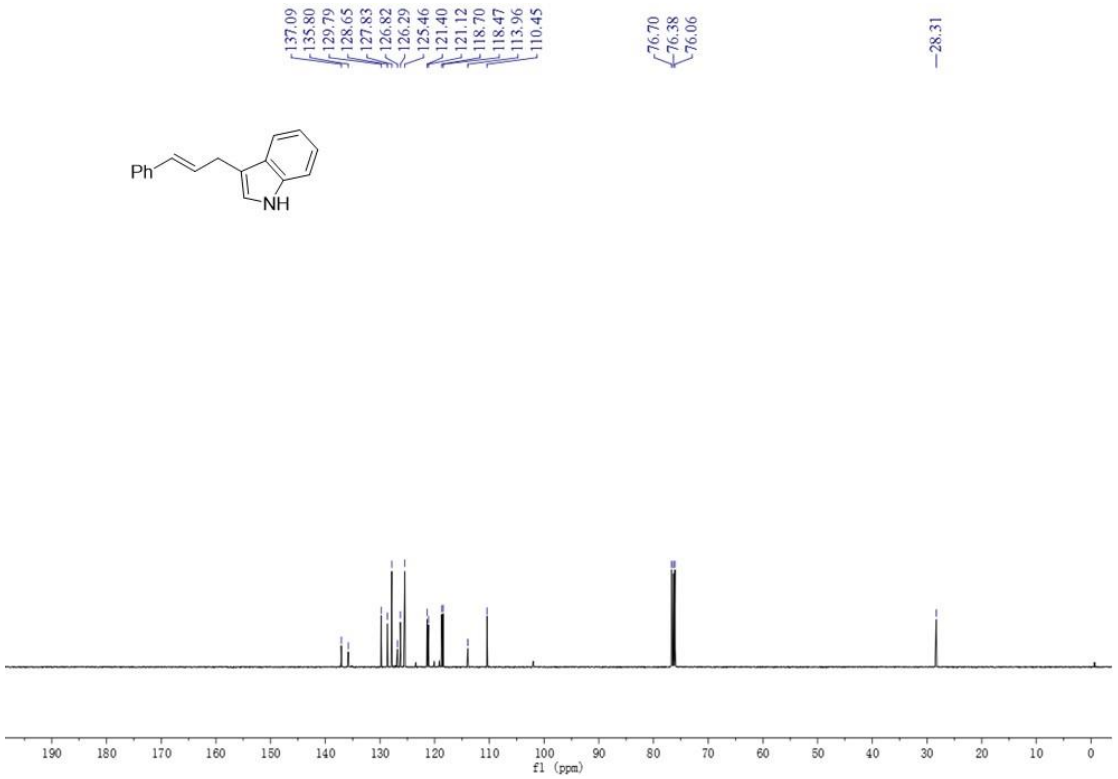
1.06
1.00
2.00
f1 (ppm)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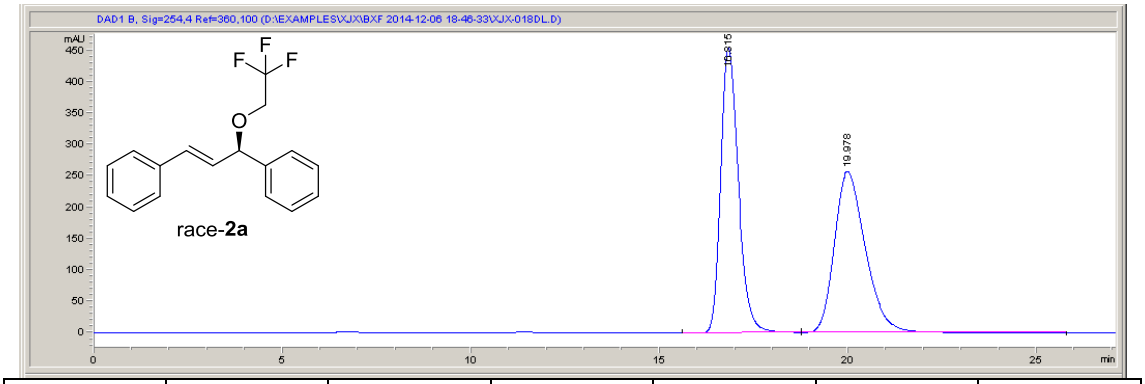
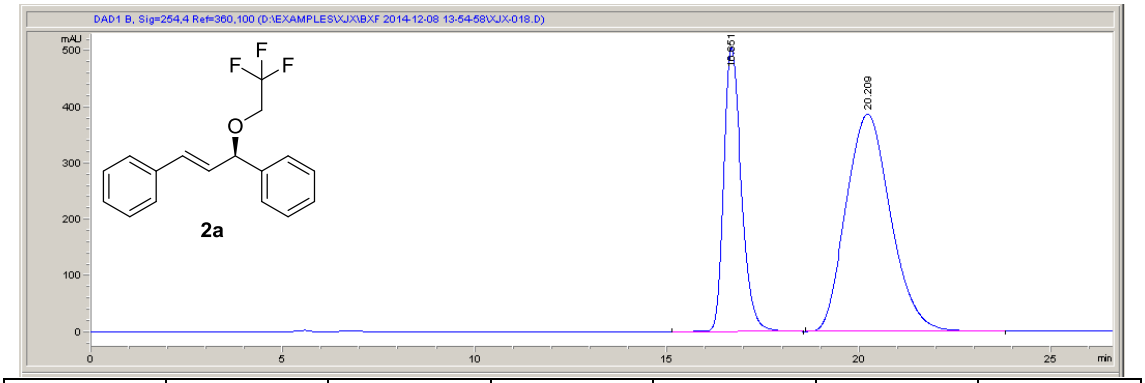
126.82
126.29
125.46
121.40
121.12
118.70
118.47
113.96
110.45
76.70
76.38
76.06
28.31
Ph
NH
f1 (ppm)

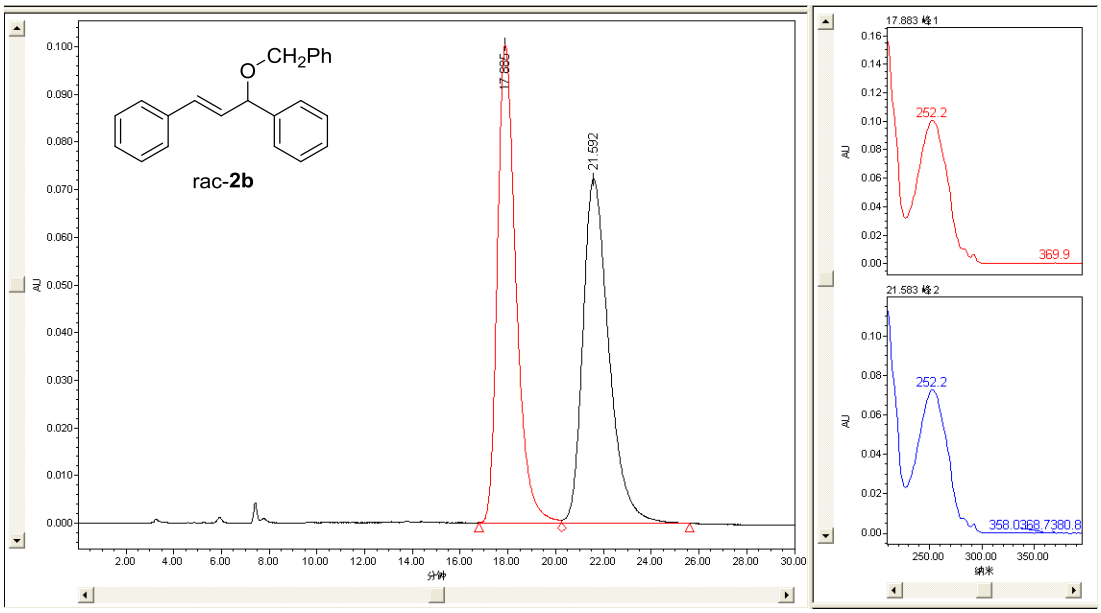
5. HPLC Spectra of products: Determination of *ee* values



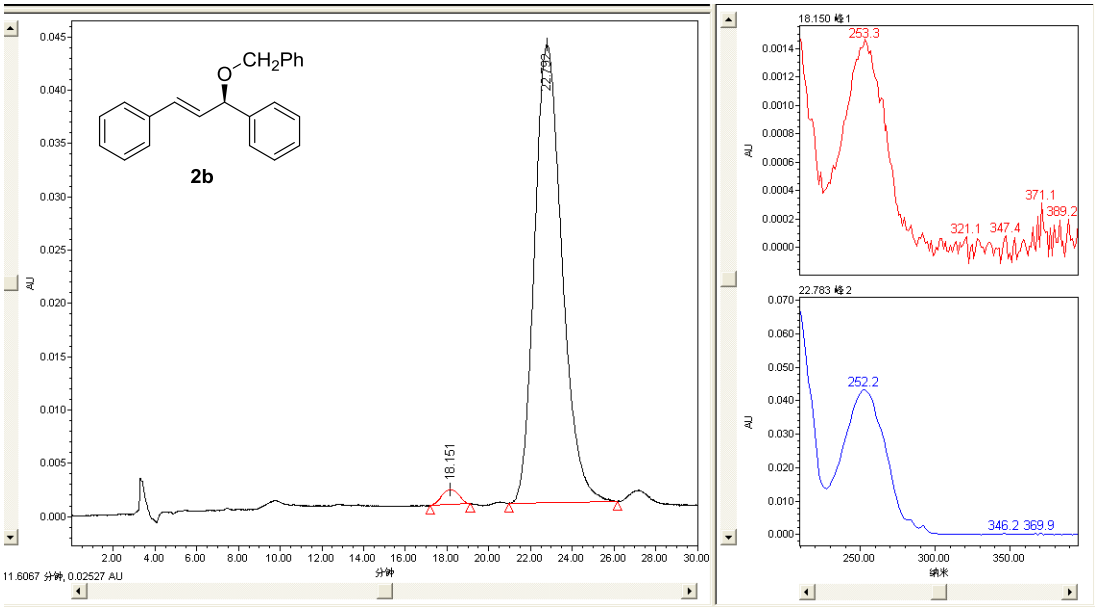
#	Time	Area	Height	Width	Symmetry	Area %
1	16.815	14710.1	453.7	0.4982	0.701	49.929
2	19.978	14752	257	0.8816	0.695	50.071



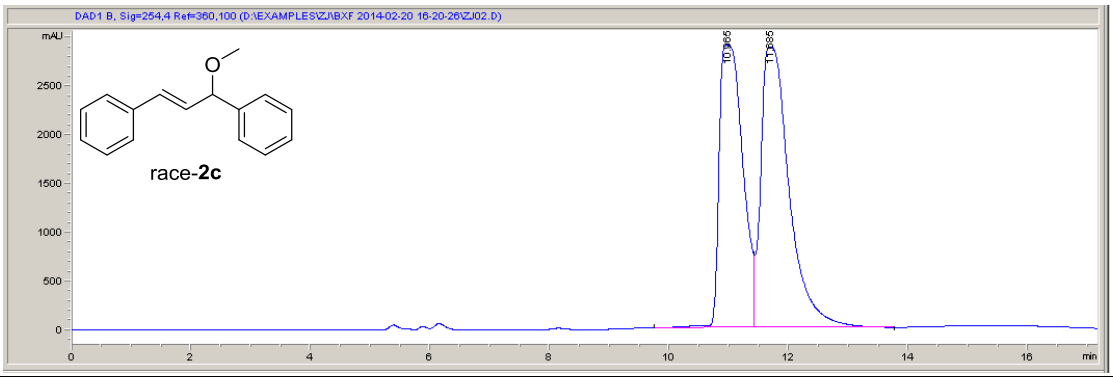
#	Time	Area	Height	Width	Symmetry	Area %
1	16.651	16473.9	505.1	0.5045	0.693	34.648
2	20.209	31072.4	386.4	1.2661	0.893	65.352



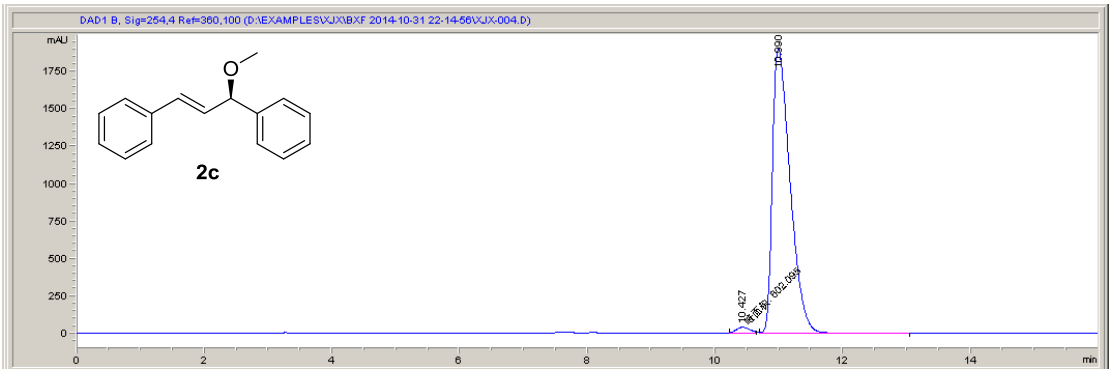
#	Time	Area	Height	Area %
1	17.885	5450629	100303	49.95
2	21.592	5461961	72293	50.05



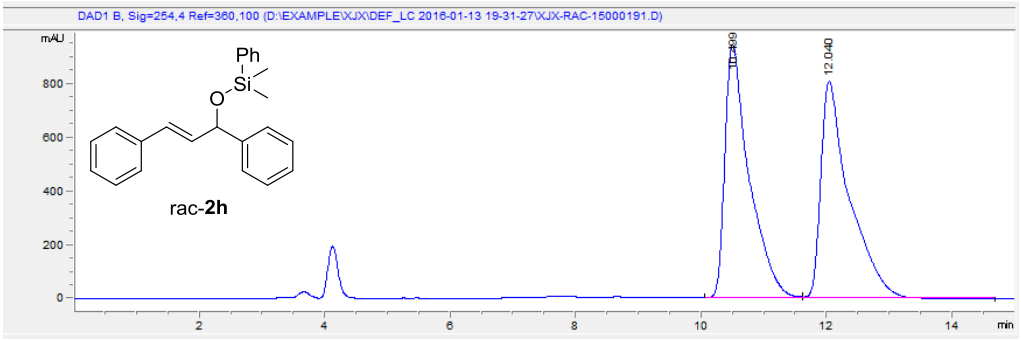
#	Time	Area	Height	Area %
1	18.151	81168	1448	2.02
2	22.792	3945386	42966	97.98



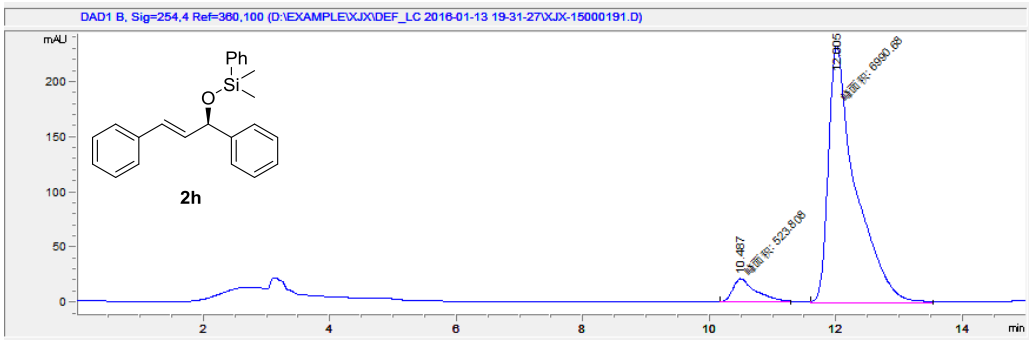
#	Time	Area	Height	Width	Symmetry	Area %
1	10.965	79209	2902.3	0.4264	0.506	45.491
2	11.685	94910.4	2881.7	0.4962	0.461	54.509



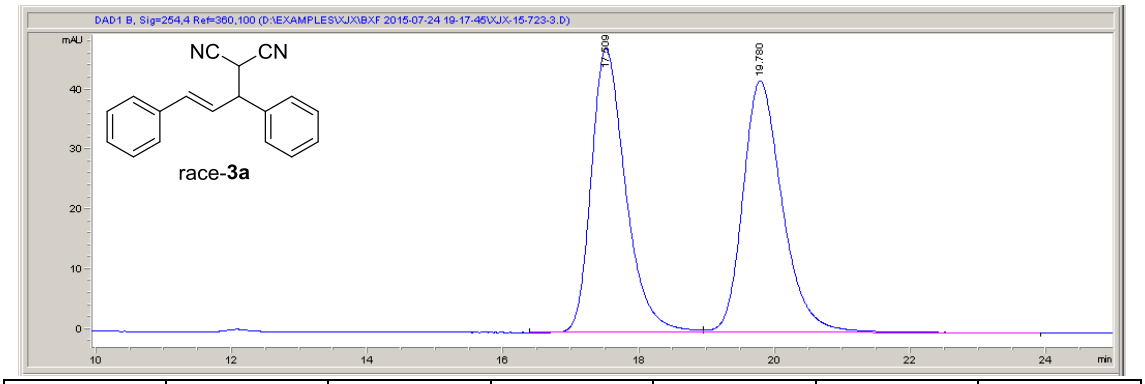
#	Time	Area	Height	Width	Symmetry	Area %
1	10.427	602.1	39.7	0.2526	0.885	1.613
2	10.99	36731.4	1900.7	0.2975	0.496	98.387



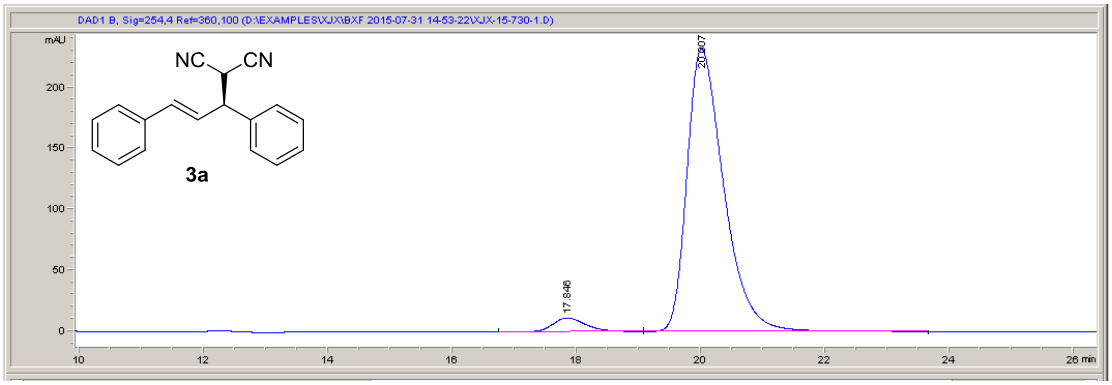
#	Time	Area	Height	Width	Symmetry	Area %
1	10.499	25380.1	942	0.3863	0.426	49.895
2	12.04	25486.7	807.8	0.4441	0.378	50.105



#	Time	Area	Height	Width	Symmetry	Area %
1	10.487	523.8	20.8	0.4188	0.491	6.917
2	12.005	6990.7	233	0.5	0.419	93.029

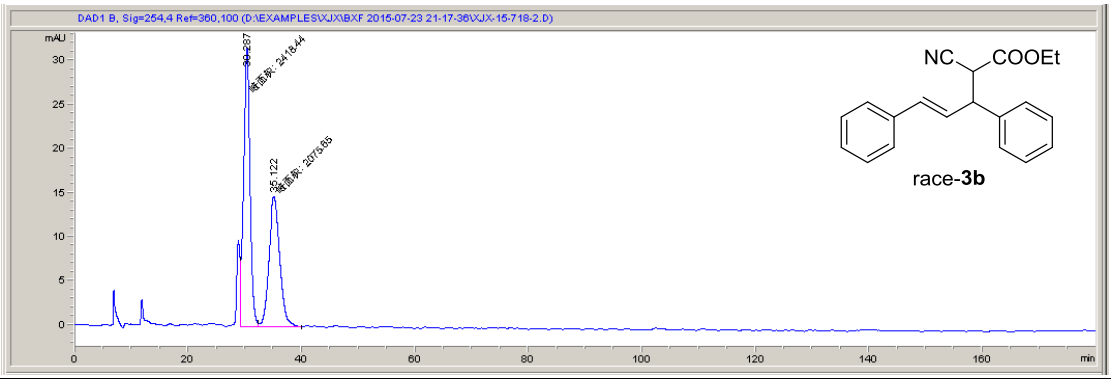


#	Time	Area	Height	Width	Symmetry	Area %
1	17.509	1671.4	47.4	0.5353	0.694	49.420
2	19.78	1710.6	42.1	0.6182	0.718	50.580

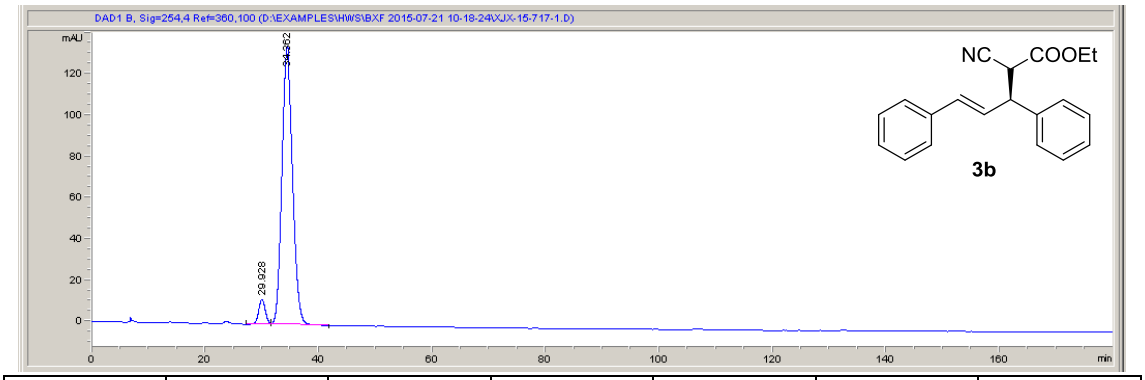


#	Time	Area	Height	Width	Symmetry	Area %

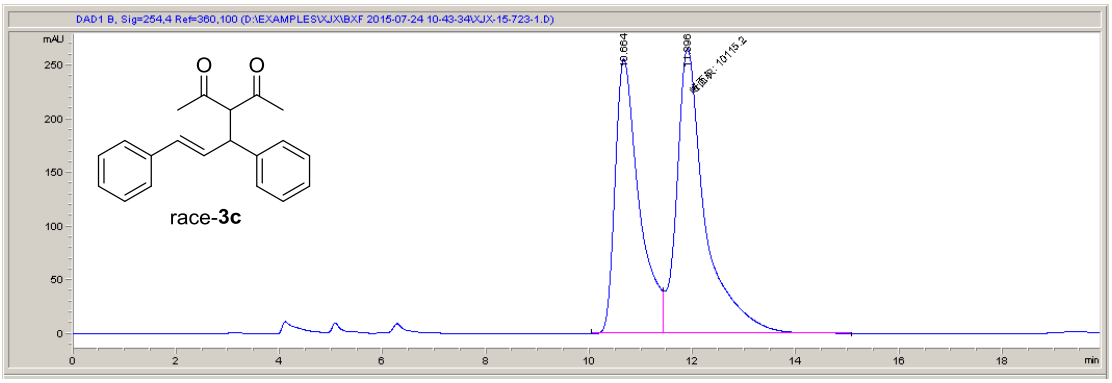
1	17.846	421.3	11.4	0.5688	0.725	4.215
2	20.007	9573.3	232.2	0.629	0.613	95.785



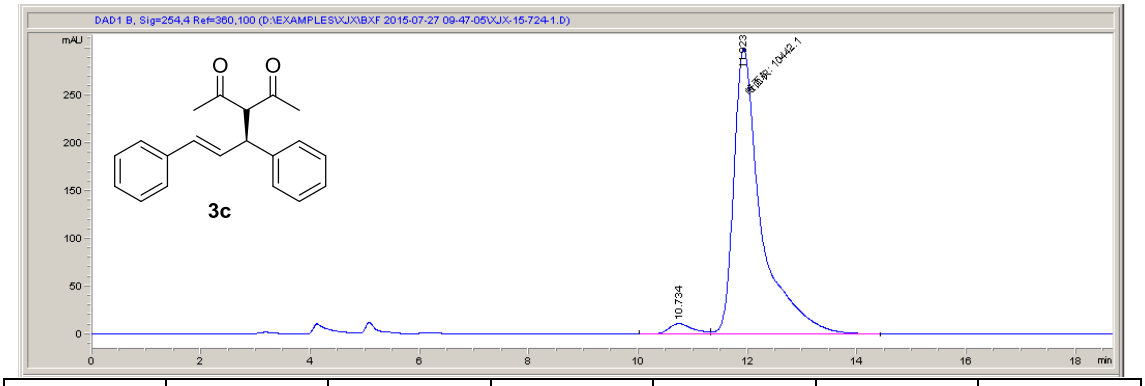
#	Time	Area	Height	Width	Symmetry	Area %
1	30.287	2418.4	31.8	1.2681	1.03	53.814
2	35.122	2075.6	14.9	2.329	0.878	46.186



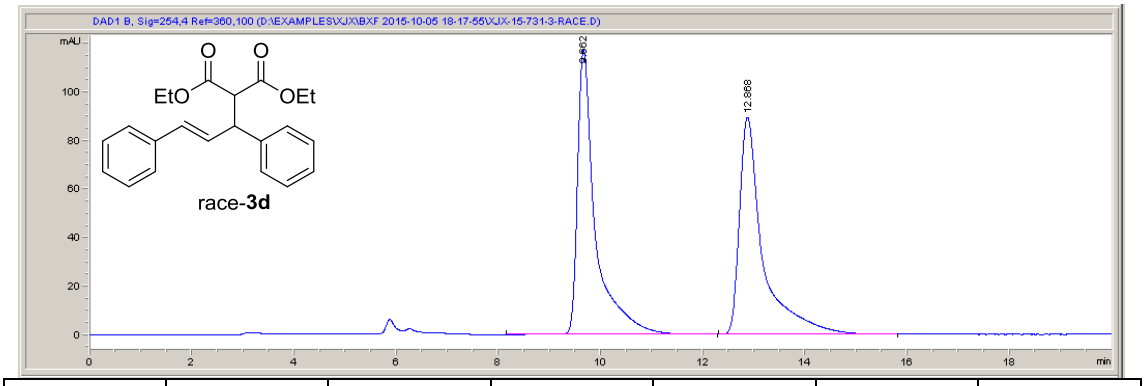
#	Time	Area	Height	Width	Symmetry	Area %
1	29.928	1010.6	12.2	1.2664	0.922	5.140
2	34.362	18650	134.8	2.1739	0.856	94.860



#	Time	Area	Height	Width	Symmetry	Area %
1	10.664	8330.3	255.8	0.4799	0.531	45.162
2	11.896	10115.2	266.1	0.6335	0.57	54.838

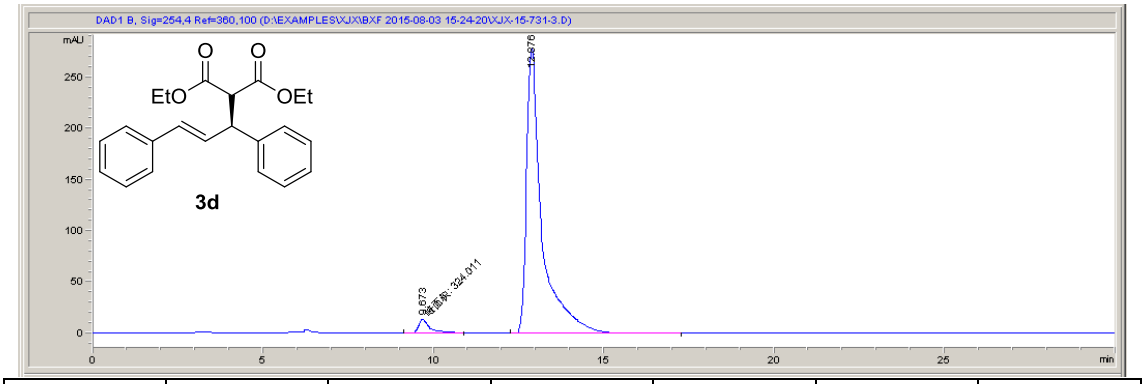


#	Time	Area	Height	Width	Symmetry	Area %
1	10.734	327.1	10.8	0.4545	0.634	3.037
2	11.923	10442.1	299.3	0.5814	0.544	96.963

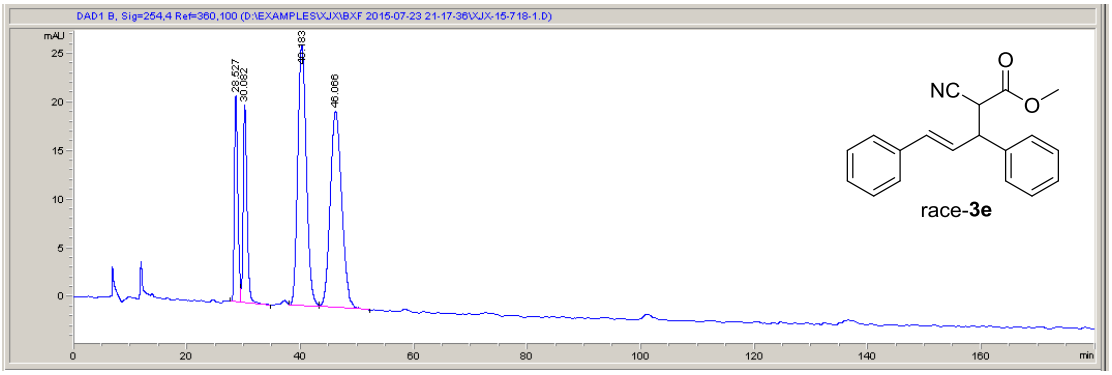


#	Time	Area	Height	Width	Symmetry	Area %
1	9.662	2856.1	117.1	0.3525	0.46	50.236

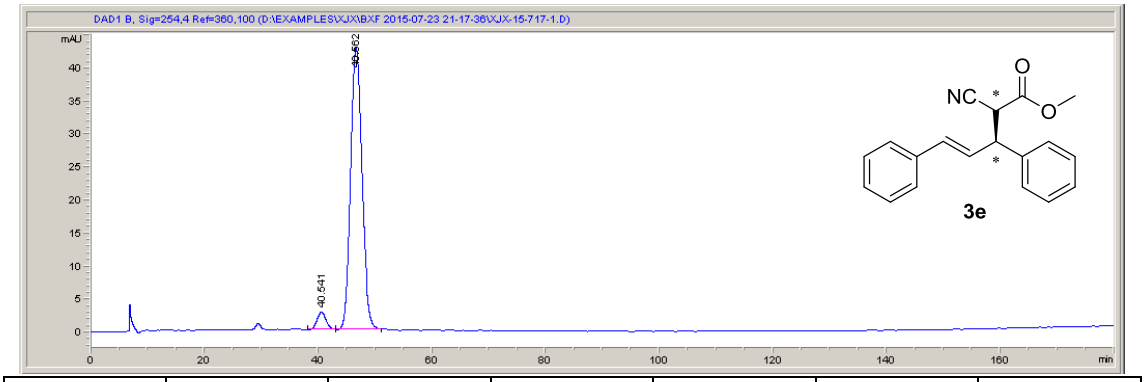
2	12.868	2829.2	89.3	0.4575	0.453	49.764



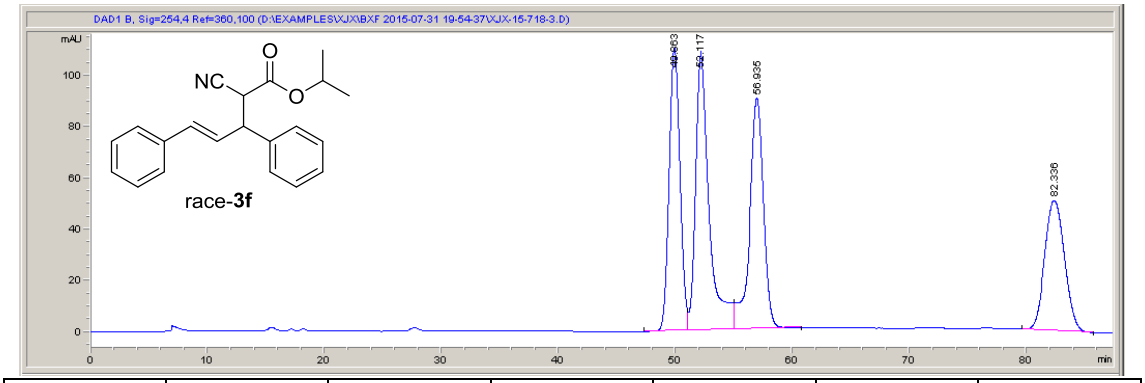
#	Time	Area	Height	Width	Symmetry	Area %
1	9.673	324	13.8	0.3913	0.477	3.586
2	12.876	8711.3	278	0.4496	0.439	96.414



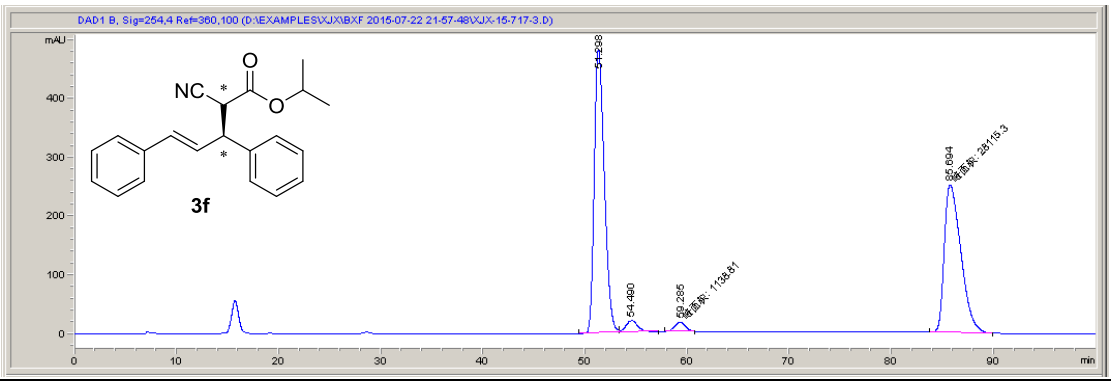
#	Time	Area	Height	Width	Symmetry	Area %
1	28.527	882.5	21.1	0.6477	0.647	11.818
2	30.082	924.5	20.3	0.6954	0.623	12.380
3	40.183	2803.2	26.9	1.6245	0.825	37.538
4	46.066	2857.4	20.2	2.0445	0.819	38.264



#	Time	Area	Height	Width	Symmetry	Area %
1	40.541	285.3	2.7	1.2941	0.937	4.551
2	46.562	5983.6	42.6	2.1459	0.856	95.449

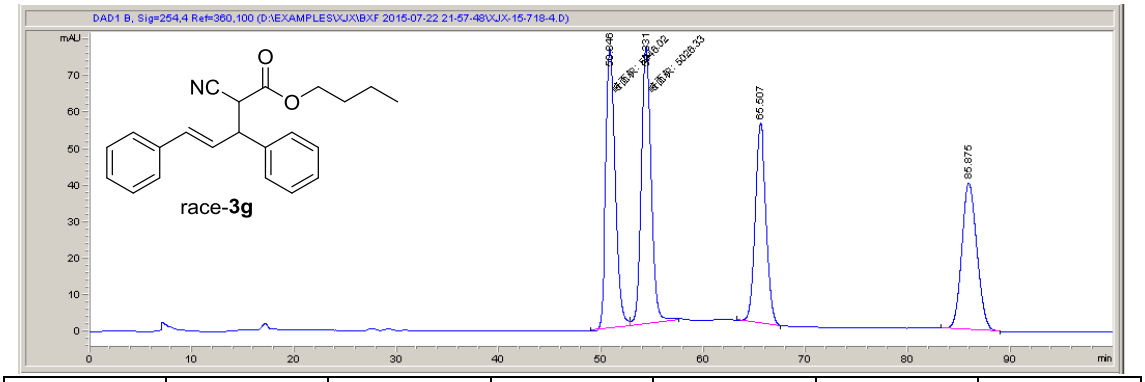


#	Time	Area	Height	Width	Symmetry	Area %
1	49.863	7015.2	110.3	0.9939	0.904	23.784
2	52.117	9072.2	108.5	1.2512	0.577	30.758
3	56.935	7449.9	89.8	1.2596	1.139	25.258
4	82.336	5958.2	50.8	1.8368	0.906	20.200

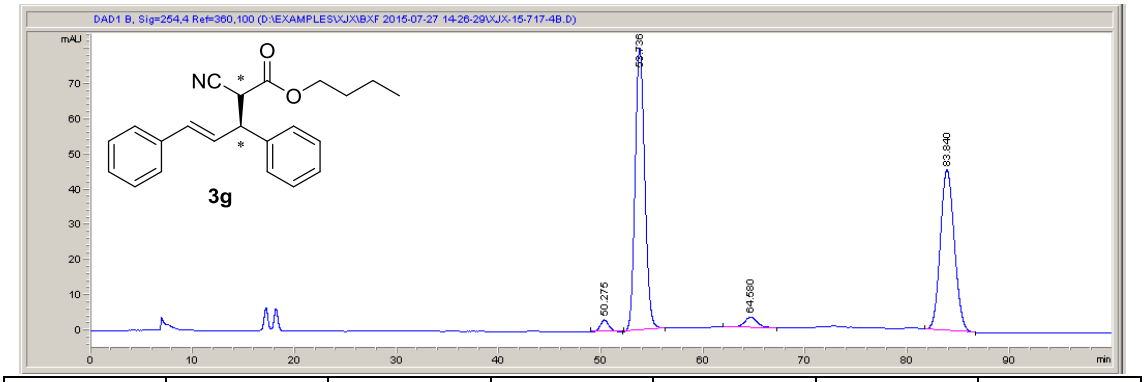


#	Time	Area	Height	Width	Symmetry	Area %

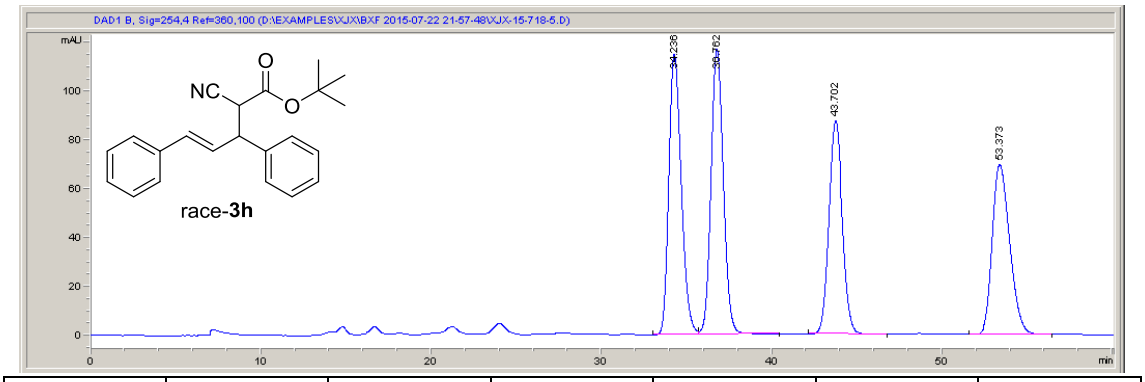
1	51.298	32740.8	483.5	1.0541	0.668	51.467
2	54.49	1620.6	19.9	1.2445	0.858	2.547
3	59.285	1138.8	15.4	1.2315	1.012	1.790
4	85.694	28115.3	251.4	1.8639	0.529	44.196



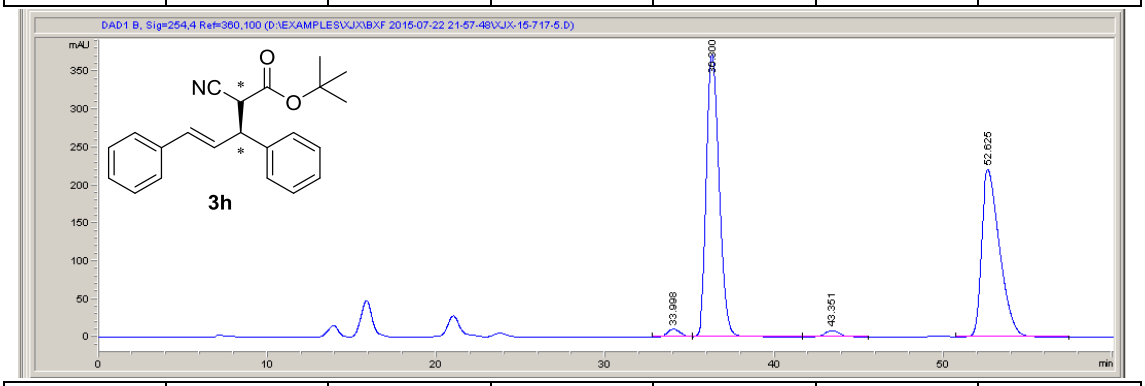
#	Time	Area	Height	Width	Symmetry	Area %
1	50.846	5046	76.3	1.1019	0.775	27.490
2	54.331	5026.3	75.8	1.1048	0.862	27.382
3	65.507	4211.1	54.7	1.2027	0.883	22.941
4	85.875	4072.6	40.1	1.5839	0.832	22.187



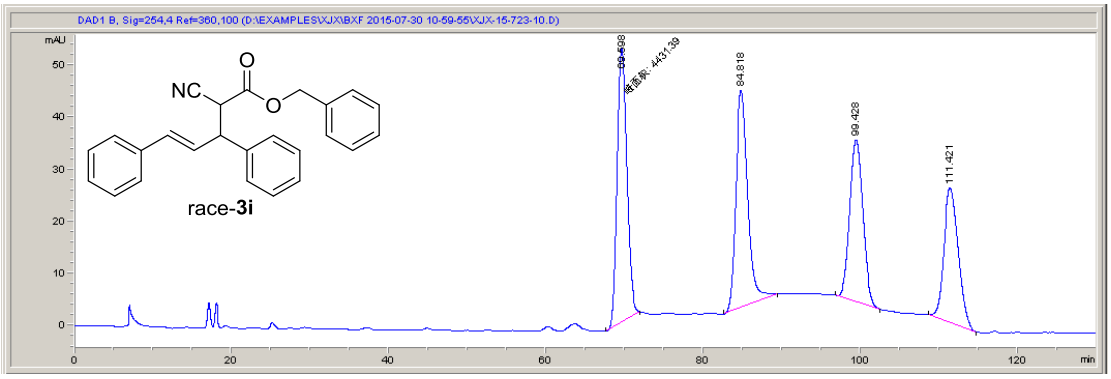
#	Time	Area	Height	Width	Symmetry	Area %
1	50.275	211.3	3.4	0.9328	0.914	2.119
2	53.736	5189.1	80.2	1.0105	0.846	52.039
3	64.58	266.6	2.9	1.3002	1.018	2.637
4	83.84	4304.6	45.6	1.4802	0.864	43.169



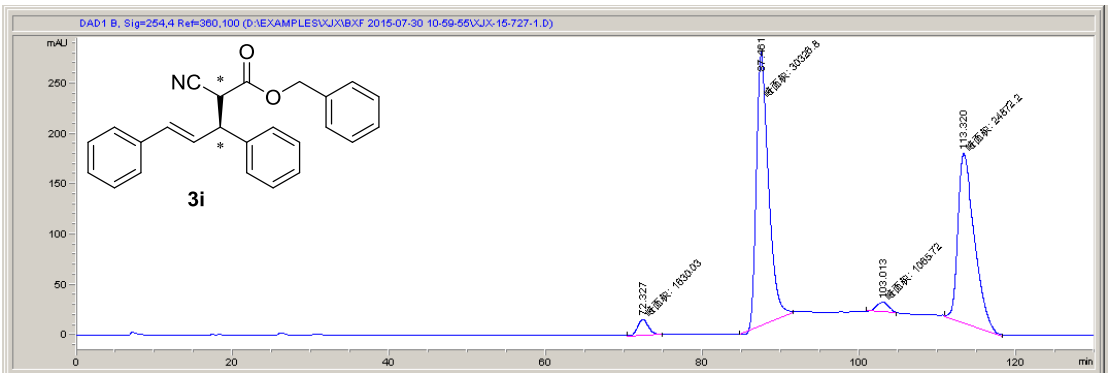
#	Time	Area	Height	Width	Symmetry	Area %
1	34.236	5759.9	114.8	0.7771	0.738	26.920
2	36.762	5825.5	117	0.773	0.856	27.227
3	43.702	4920	87.5	0.8802	0.887	22.995
4	53.373	4890.9	69.6	1.0835	0.718	22.858



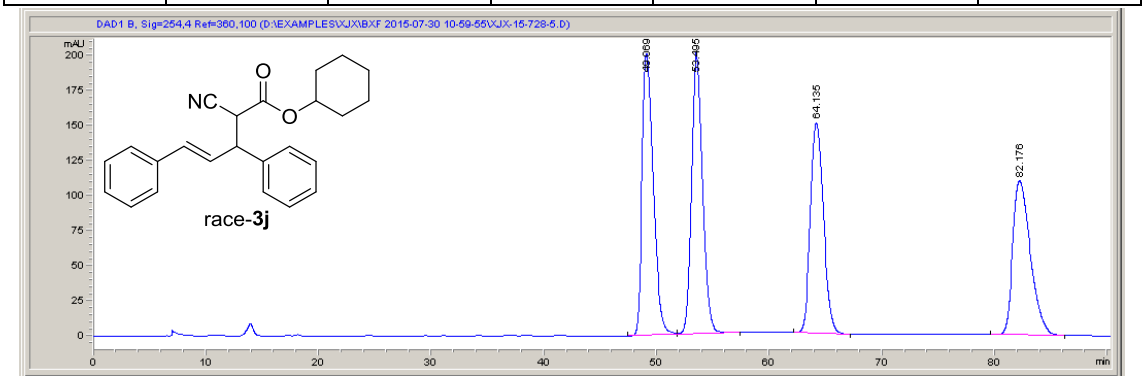
#	Time	Area	Height	Width	Symmetry	Area %
1	39.998	562.6	10.6	0.8221	0.877	1.509
2	36.3	19594.5	373.2	0.8205	0.758	52.563
3	43.351	479.4	8.1	0.9251	0.894	1.286
4	52.625	16641.4	220.4	1.161	0.55	44.641



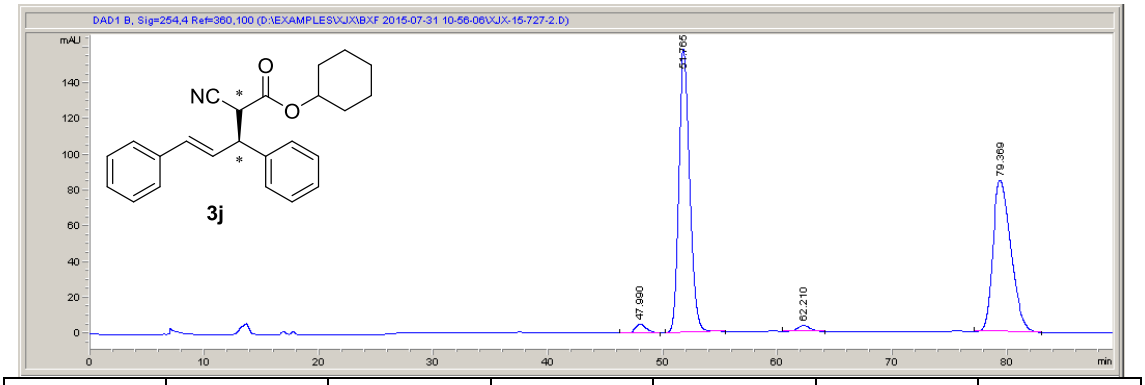
#	Time	Area	Height	Width	Symmetry	Area %
1	69.598	4431.4	52.6	1.4045	0.822	28.203
2	84.818	4416.8	41.7	1.6389	0.772	28.110
3	99.428	3577.3	31	1.7643	0.885	22.768
4	111.421	3286.9	25.8	1.9693	0.773	20.919



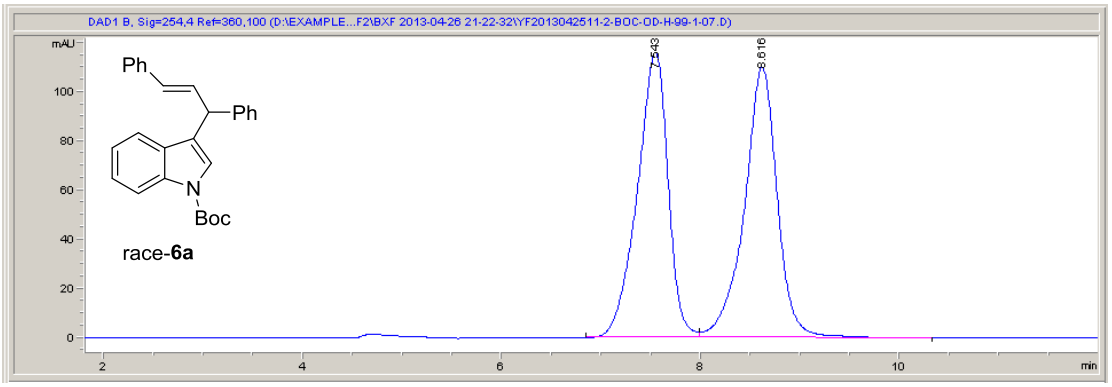
#	Time	Area	Height	Width	Symmetry	Area %
1	72.327	1630	16.5	1.6492	0.795	2.816
2	87.461	30326.8	272.6	1.8538	0.65	52.383
3	103.013	1065.7	9.8	1.8215	0.765	1.841
4	113.32	24872.2	168.2	2.4648	0.503	42.961



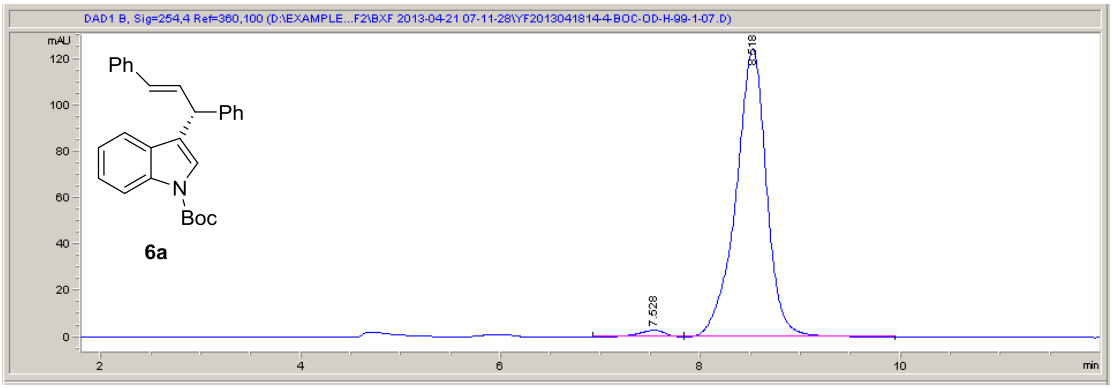
#	Time	Area	Height	Width	Symmetry	Area %
1	49.069	13881.3	200.9	1.066	0.632	26.851
2	53.495	13847	200.6	1.0732	0.787	26.785
3	64.135	12049	150	1.2491	0.791	23.307
4	82.176	11920.1	110	1.6608	0.604	23.057



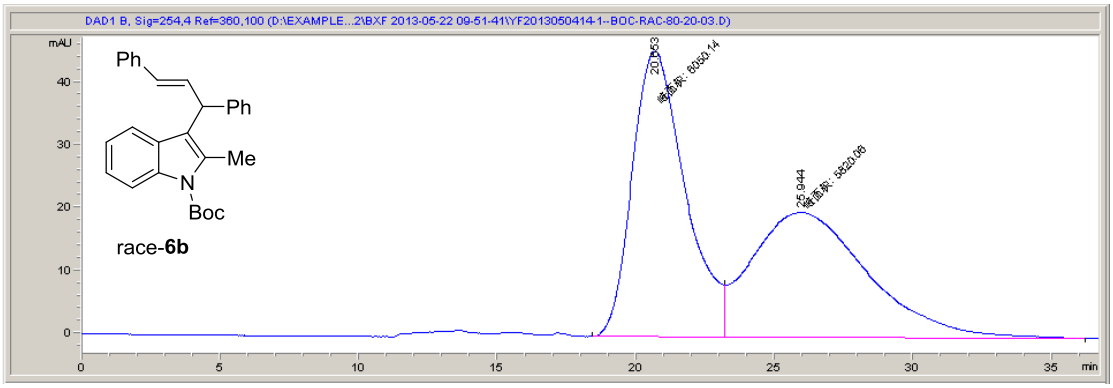
#	Time	Area	Height	Width	Symmetry	Area %
1	47.99	319.3	4.9	1.0188	0.84	1.550
2	51.765	10728.2	158.5	1.0535	0.789	52.069
3	62.21	263.8	3.4	1.1171	0.938	1.280
4	79.369	9292.7	85	1.6917	0.661	45.101



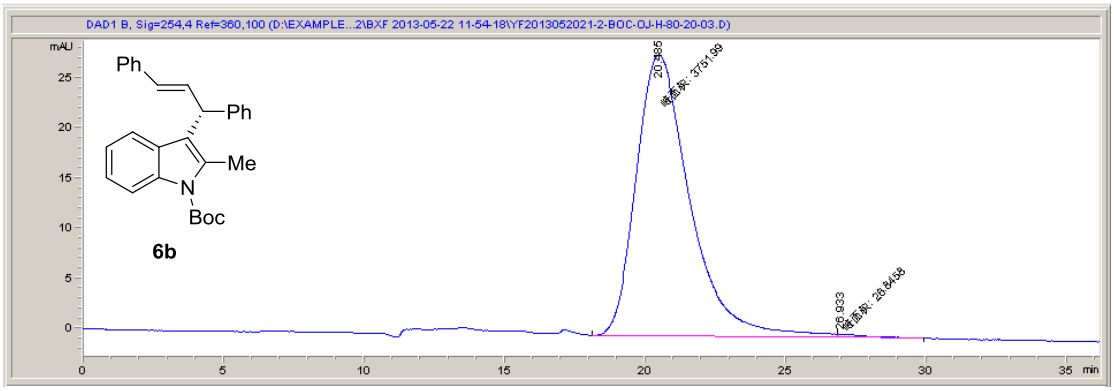
#	Time	Area	Height	Width	Symmetry	Area %
1	7.543	2493.5	116	0.3227	1.395	49.567
2	8.616	2537.1	110	0.3432	1.151	50.433



#	Time	Area	Height	Width	Symmetry	Area %
1	7.528	55.3	2.9	0.2751	1.433	2.040
2	8.518	2657.1	124.2	0.3196	1.175	97.960

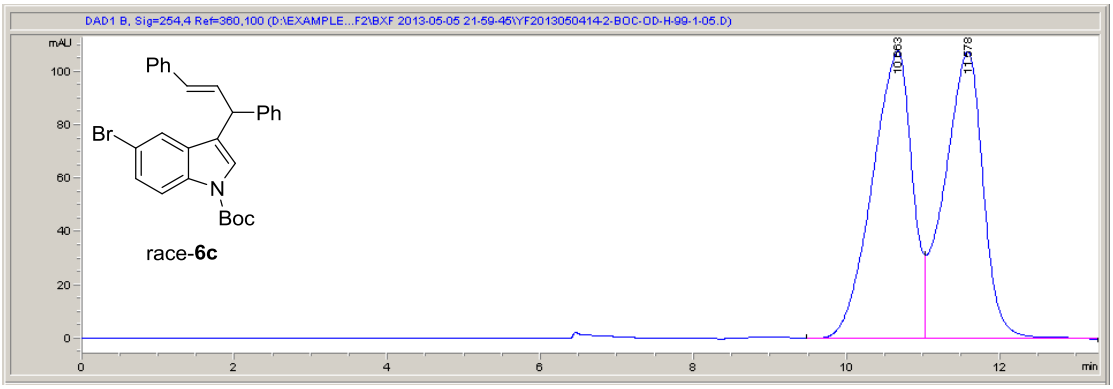


#	Time	Area	Height	Width	Symmetry	Area %
1	20.653	6050.1	45.4	2.219	0.698	50.969
2	25.944	5820.1	19.9	4.8682	0.704	49.031

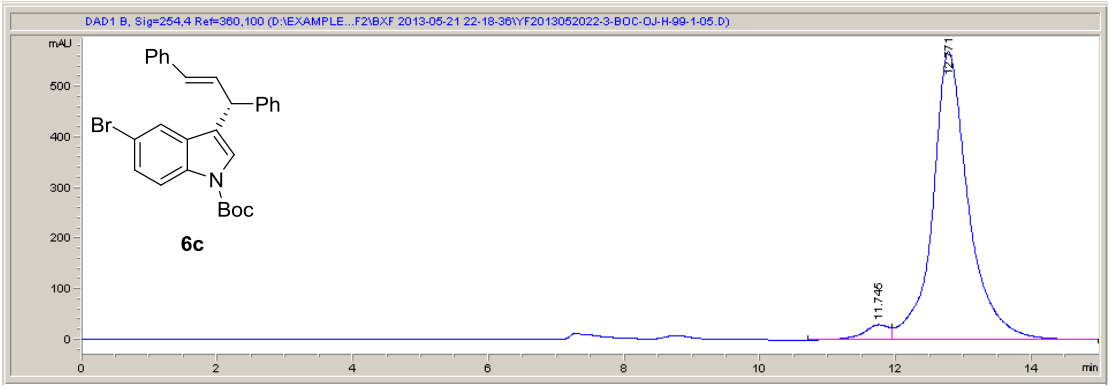


#	Time	Area	Height	Width	Symmetry	Area %

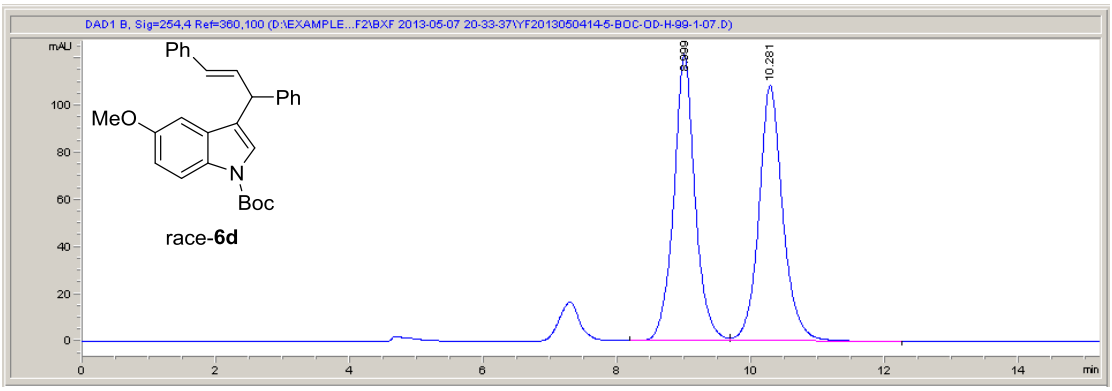
1	20.485	3752	28.1	2.2246	0	99.290
2	26.933	26.8	3.7E-1	1.2048	6.02E-2	0.710



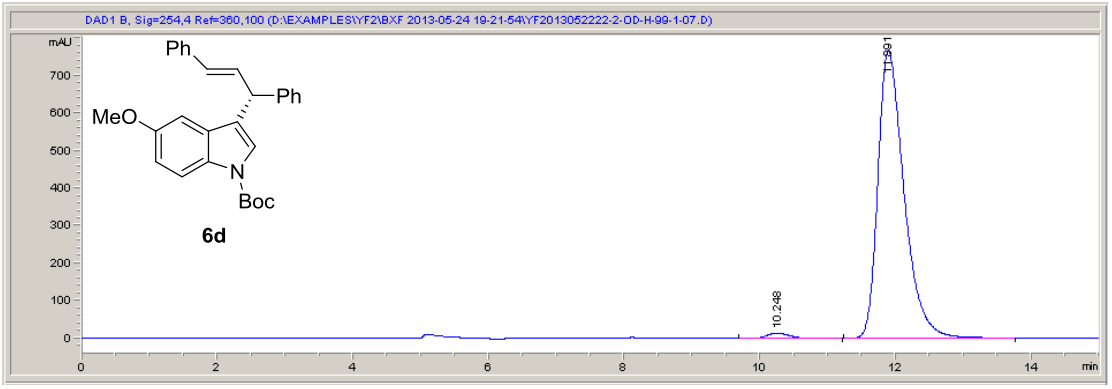
#	Time	Area	Height	Width	Symmetry	Area %
1	10.663	3921.2	107.7	0.5667	1.671	51.046
2	11.578	3760.5	107.6	0.5359	1.392	48.954



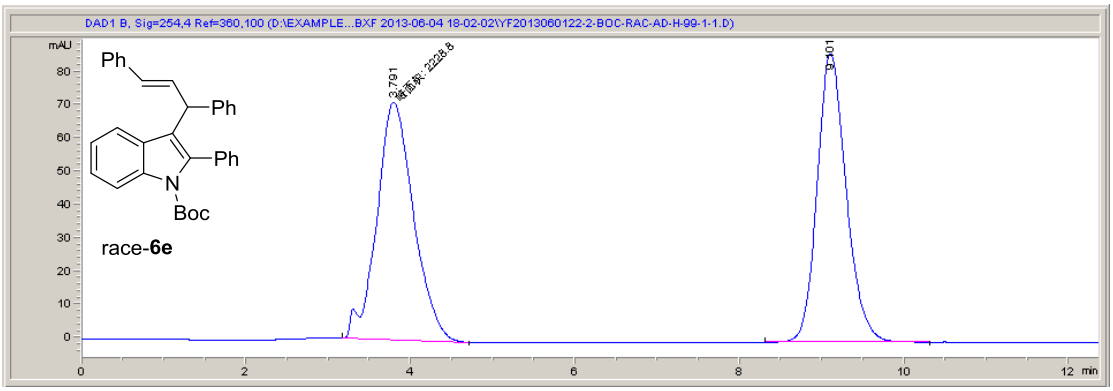
#	Time	Area	Height	Width	Symmetry	Area %
1	11.745	807.5	29.6	0.3999	1.546	3.728
2	12.771	20849.8	568.8	0.5377	0.765	96.272



#	Time	Area	Height	Width	Symmetry	Area %
1	8.999	2686.3	121.3	0.3244	0.945	49.899
2	10.281	2697.2	108.3	0.3686	0.842	50.101

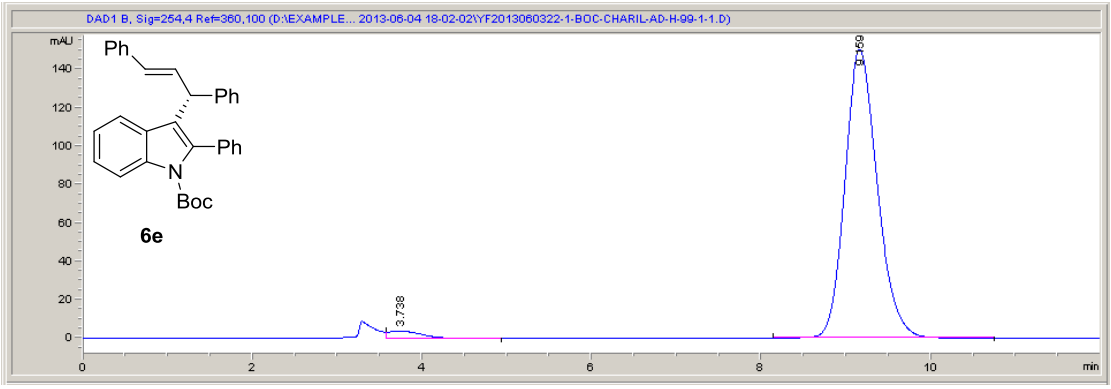


#	Time	Area	Height	Width	Symmetry	Area %
1	10.248	344.2	14.7	0.359	0.76	1.644
2	11.891	20595.3	767.6	0.409	0.623	98.356

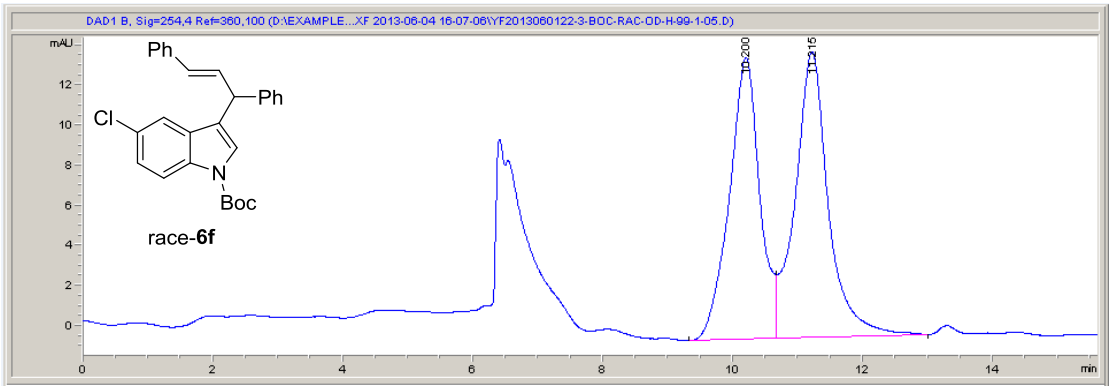


#	Time	Area	Height	Width	Symmetry	Area %

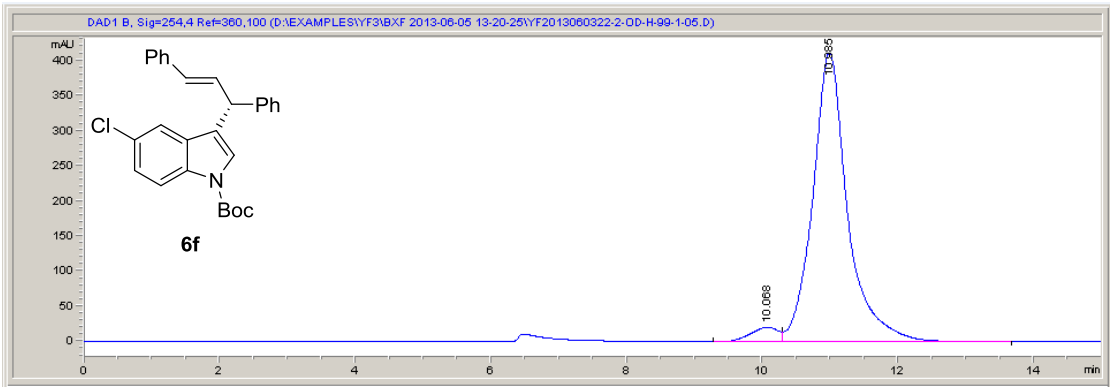
1	3.791	2228.8	71.5	0.5193	0.831	51.102
2	9.101	2132.6	86.7	0.3769	0.806	48.898



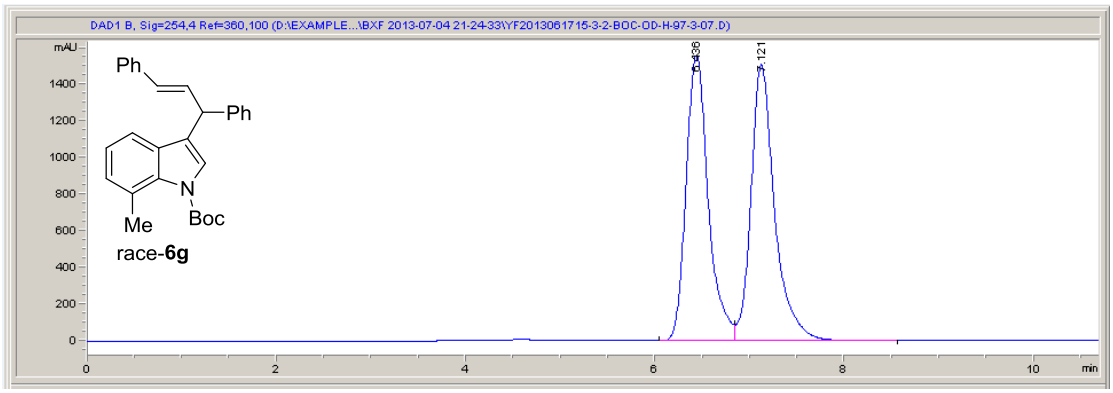
#	Time	Area	Height	Width	Symmetry	Area %
1	3.738	108.2	3.9	0.4009	0.465	2.636
2	9.159	3998.9	150.5	0.406	0.808	97.364



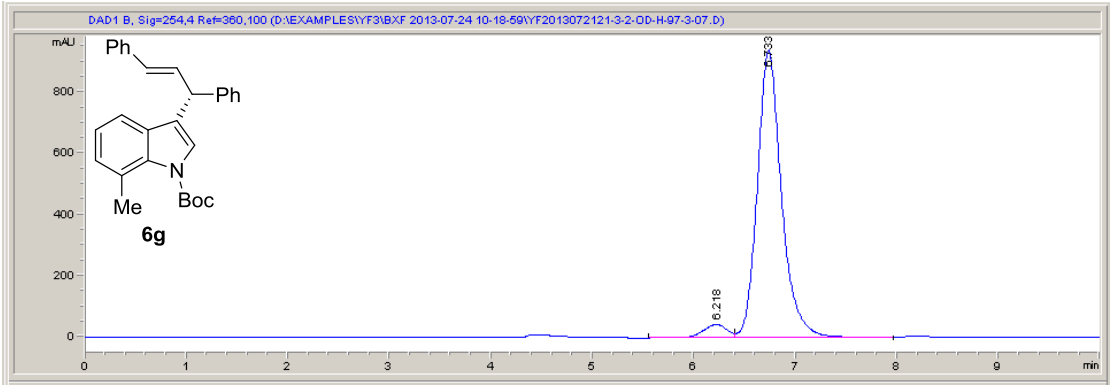
#	Time	Area	Height	Width	Symmetry	Area %
1	10.2	457.2	14.1	0.471	1.168	49.324
2	11.215	508.9	14.3	0.5096	0.939	50.676



#	Time	Area	Height	Width	Symmetry	Area %
1	10.068	601.4	20.8	0.434	1.594	3.932
2	10.985	14693.7	411.6	0.5185	0.845	96.068



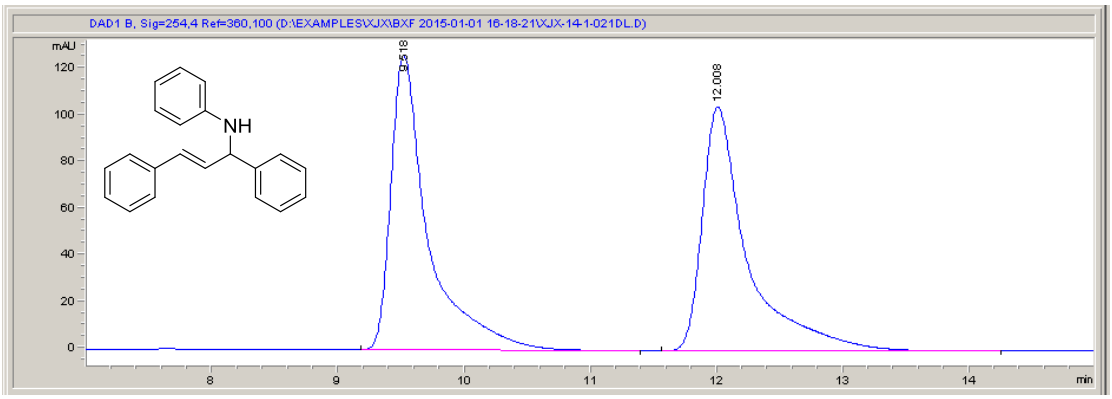
#	Time	Area	Height	Width	Symmetry	Area %
1	6.436	25382	1558.6	0.25	0.828	49.285
2	7.121	26118.9	1508.7	0.258	0.719	50.715



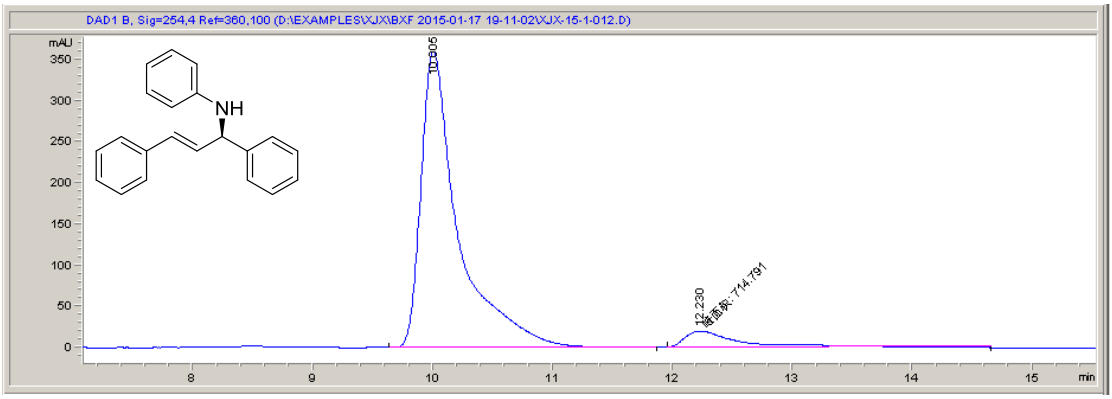
#	Time	Area	Height	Width	Symmetry	Area %

1	6.218	708.8	43.5	0.2481	1.242	4.376
2	6.733	15490.6	937.1	0.2469	0.807	95.624

(R, E)-N-(1,3-diphenylallyl)aniline (**8a**)

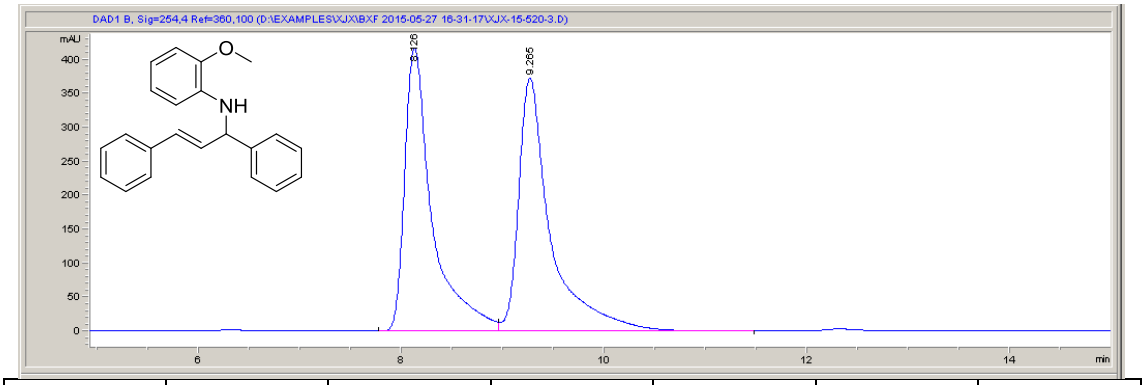


#	Time	Area	Height	Width	Symmetry	Area %
1	9.518	2598.1	126.5	0.2957	0.465	49.946
2	12.008	2603.7	104.7	0.3582	0.466	50.054

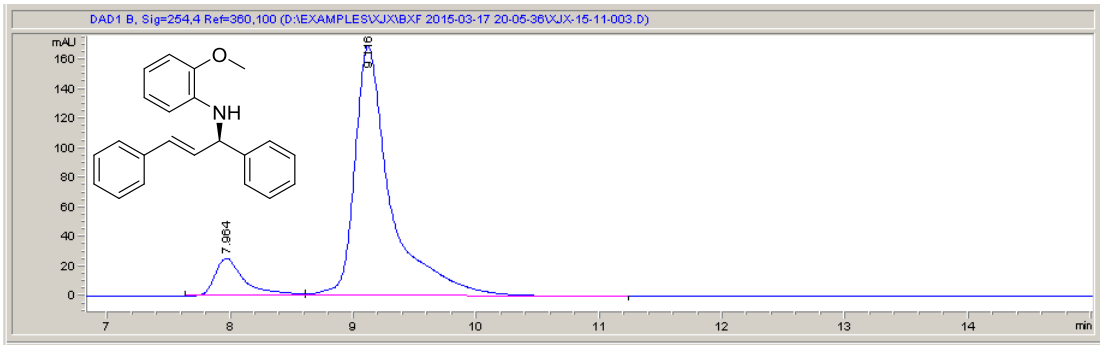


#	Time	Area	Height	Width	Symmetry	Area %
1	10.005	7796.2	359.9	0.3127	0.444	91.602
2	12.23	714.8	20.7	0.5753	0.357	8.398

8b:

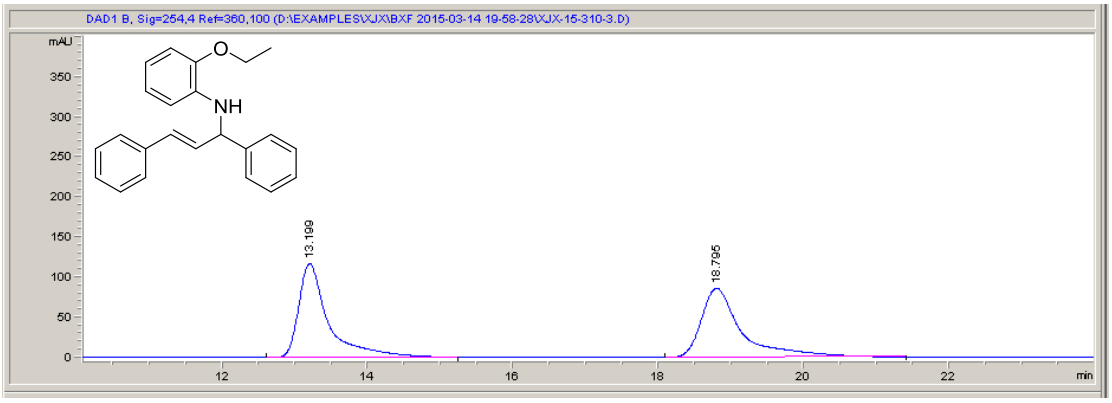


#	Time	Area	Height	Width	Symmetry	Area %
1	8.126	7857.8	416.9	0.2759	0.496	49.046
2	9.265	8163.4	372.1	0.32	0.483	50.954

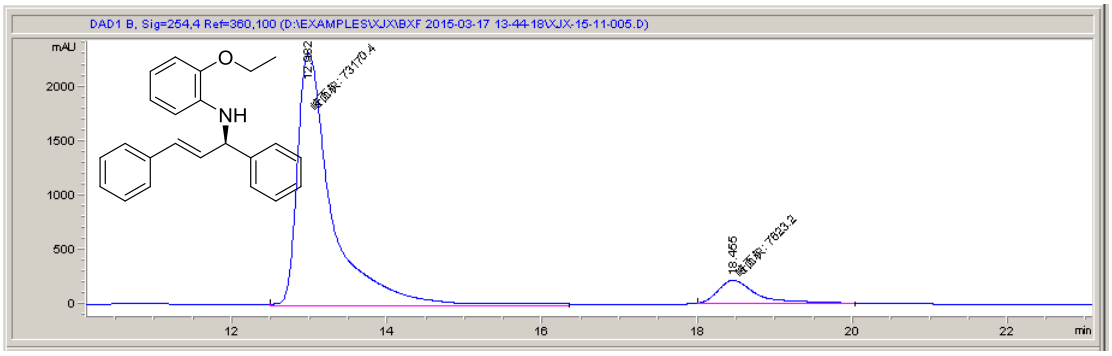


#	Time	Area	Height	Width	Symmetry	Area %
1	7.964	435.7	25.5	0.2494	0.537	11.153
2	9.116	3471	169.1	0.2975	0.526	88.847

8c:

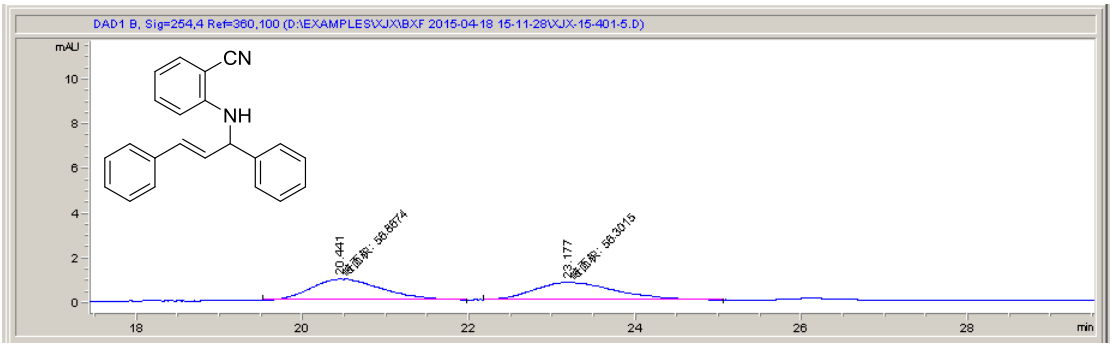


#	Time	Area	Height	Width	Symmetry	Area %
1	13.199	3327.7	117	0.414	0.515	49.813
2	18.795	3352.6	86.2	0.5619	0.529	50.187

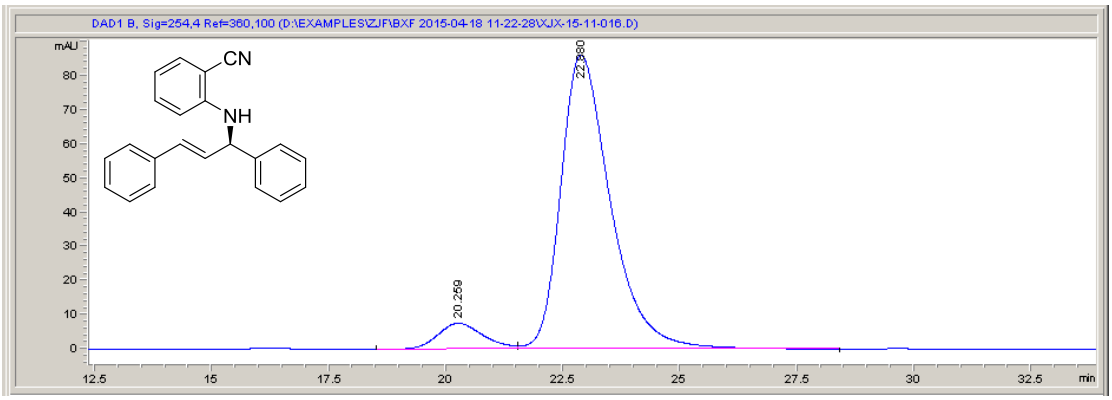


#	Time	Area	Height	Width	Symmetry	Area %
1	12.982	73170.4	2322.5	0.5251	0.45	90.565
2	18.455	7623.2	214	0.5936	0.6	9.435

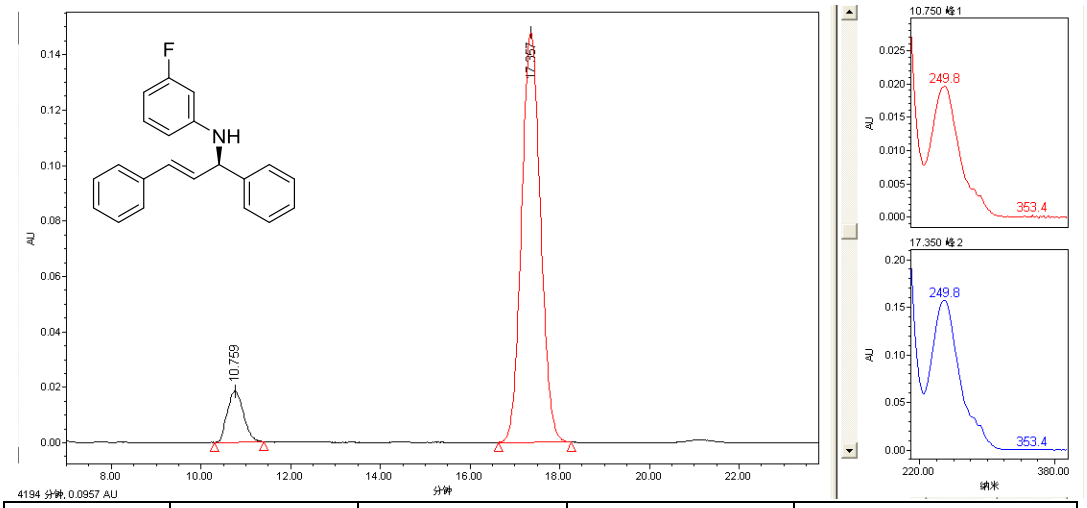
8d:



#	Time	Area	Height	Width	Symmetry	Area %
1	20.441	56.9	0.95	1.0009	0.68	50.250
2	23.177	56.3	0.79	1.1862	0.668	49.750

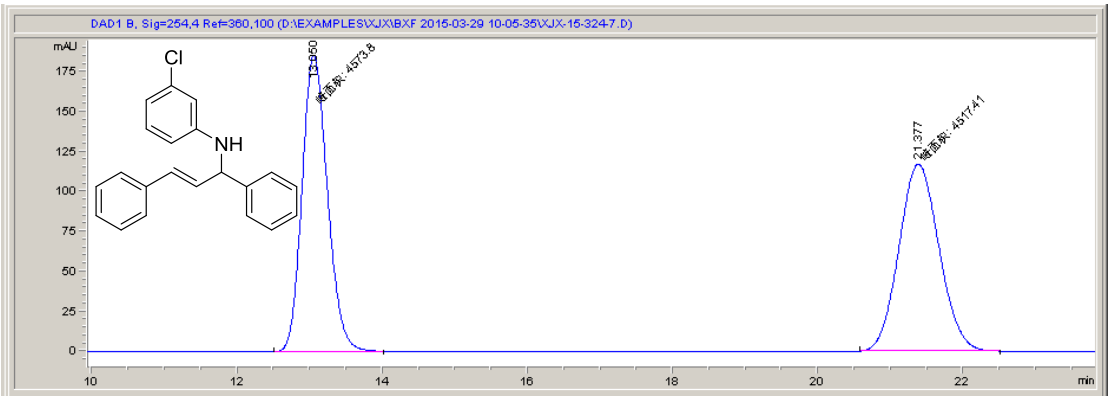


#	Time	Area	Height	Width	Symmetry	Area %
1	20.259	520.5	7.6	1.0133	0.794	7.529
2	22.88	6393	86.4	1.1245	0.636	92.471

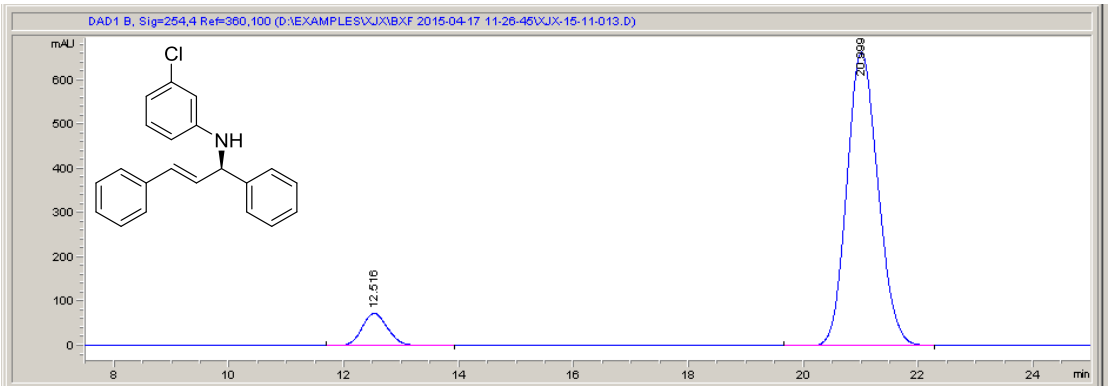


#	Time	Area	Height	Area %
1	10.759	461148	18458	9.60
2	17.357	4341330	147794	90.40

8e:

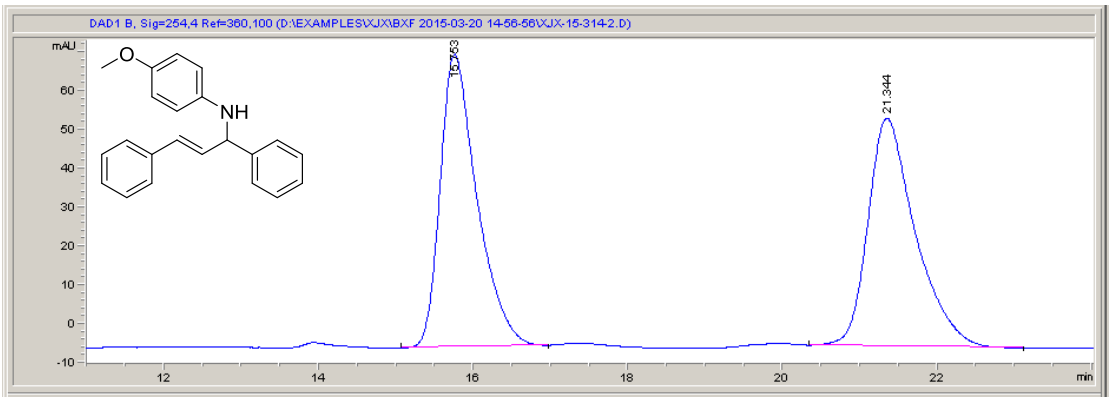


#	Time	Area	Height	Width	Symmetry	Area %
1	13.05	4573.8	186.5	0.4088	0.803	50.310
2	21.377	4517.4	117.4	0.6414	0.912	49.690

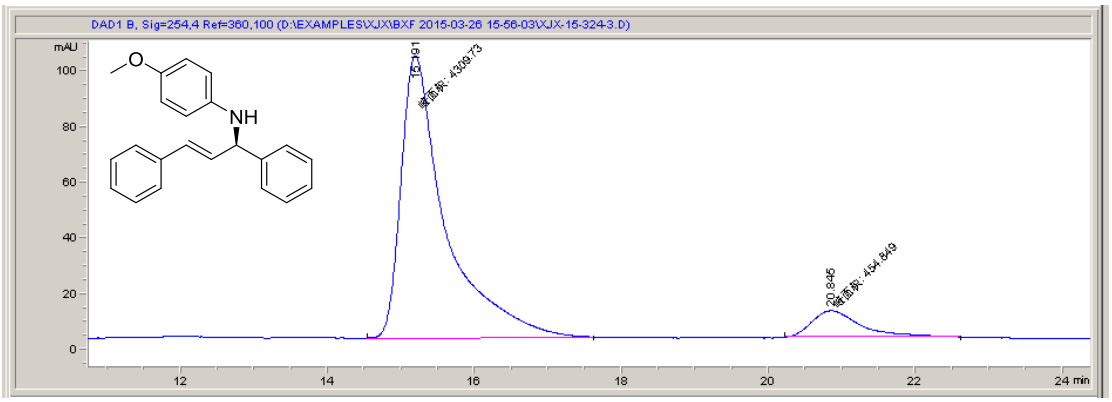


#	Time	Area	Height	Width	Symmetry	Area %
1	12.516	2261.3	72.9	0.4819	0.86	8.326
2	20.999	24896.3	662.1	0.5867	0.841	91.674

8f:

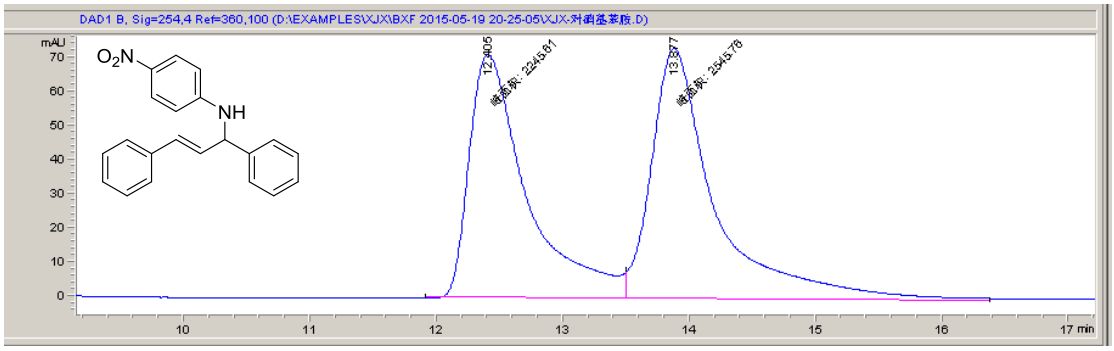


#	Time	Area	Height	Width	Symmetry	Area %
1	15.753	2490.1	75.3	0.4878	0.607	49.819
2	21.344	2508.3	58.7	0.6204	0.633	50.181

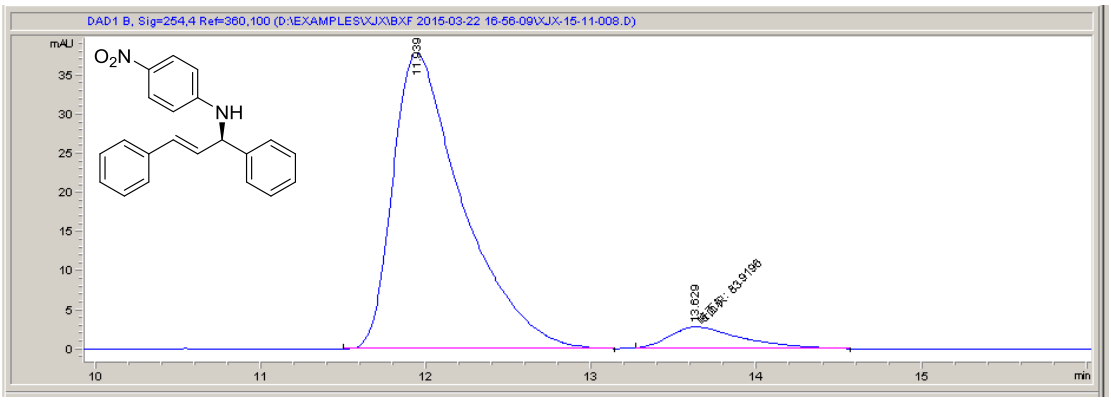


#	Time	Area	Height	Width	Symmetry	Area %
1	15.191	4309.7	101.9	0.705	0.461	90.454
2	20.845	454.8	9.5	0.7961	0.596	9.546

(R,E)-N-(1,3-Diphenyallyl)-4-nitroaniline (**8g**)

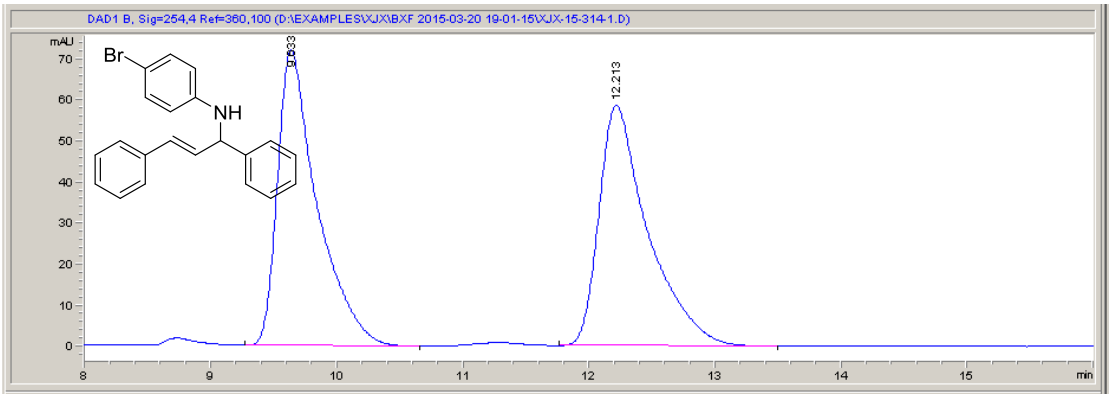


#	Time	Area	Height	Width	Symmetry	Area %
1	12.405	2245.6	71.1	0.5264	0	46.868
2	13.877	2545.8	73	0.581	0.528	53.132

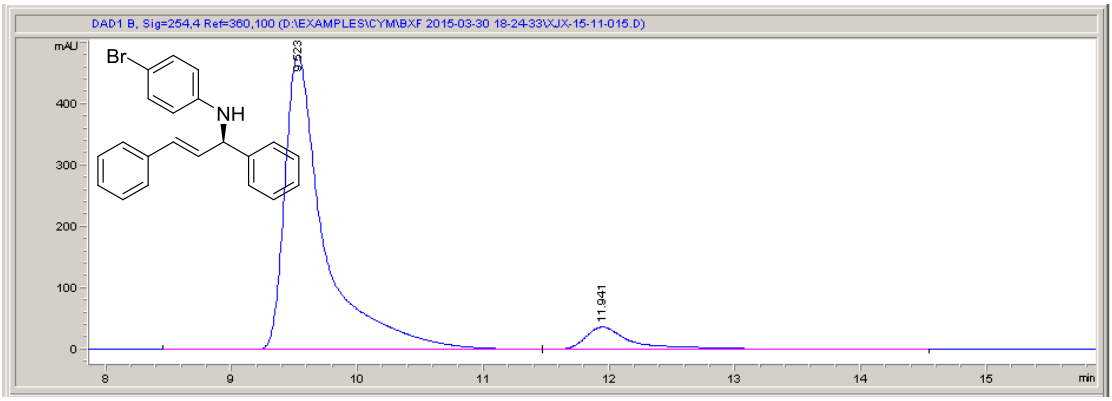


#	Time	Area	Height	Width	Symmetry	Area %
1	11.939	1113.5	37.9	0.4348	0.473	92.991
2	13.629	83.9	2.8	0.5085	0.524	7.009

8h:

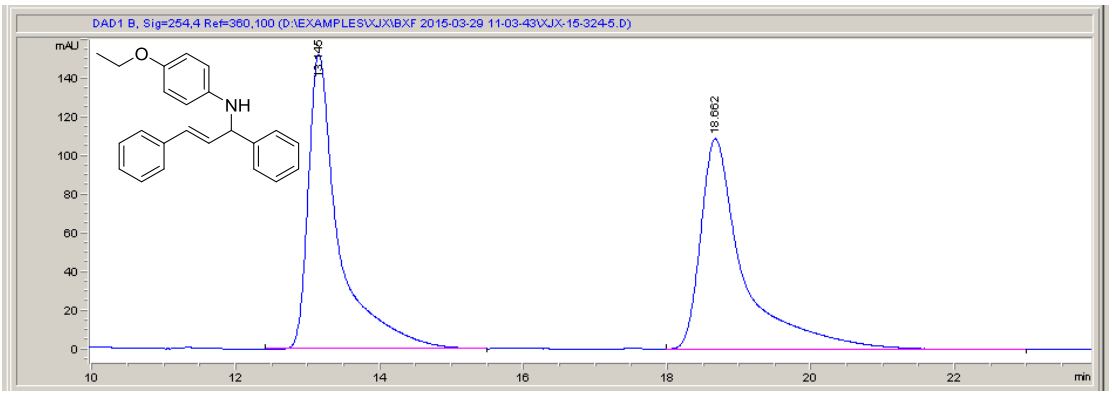


#	Time	Area	Height	Width	Symmetry	Area %
1	9.633	1573.6	71.9	0.3152	0.484	49.877
2	12.213	1581.4	58.6	0.3888	0.507	50.123

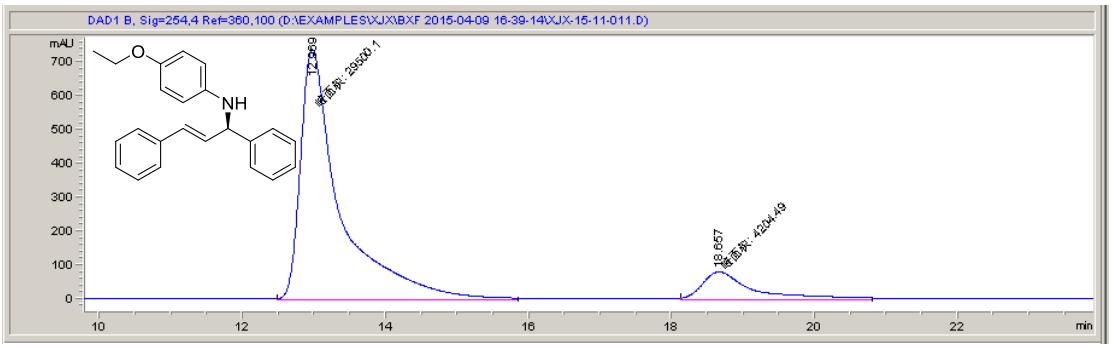


#	Time	Area	Height	Width	Symmetry	Area %
1	9.523	10522.8	480.1	0.3157	0.435	91.376
2	11.941	993.1	36.7	0.3919	0.465	8.624

8i:



#	Time	Area	Height	Width	Symmetry	Area %
1	13.145	4508.6	152.2	0.4257	0.457	49.712
2	18.662	4560.8	108.8	0.6009	0.457	50.288



#	Time	Area	Height	Width	Symmetry	Area %
1	12.969	29500.1	743.8	0.661	0.392	87.525
2	18.657	4204.5	82.3	0.851	0.456	12.475