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Supporting Information for

Enantioselective Synthesis of *N*-Allylindoles *via* Palladium-Catalyzed Allylic Amination/Oxidation of Indolines

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General Methods. Unless stated otherwise, all reactions were carried out in flame-dried glassware under argon atmosphere. All solvents were purified and dried according to standard methods prior to use.

^{1}H NMR spectra were obtained at 300 MHz or 400 MHz and recorded relative to tetramethylsilane signal (0 ppm) or residual protio-solvent. ^{13}C NMR spectra were obtained at 75 MHz or 100 MHz, and chemical shifts were recorded relative to the solvent resonance ($CDCl_3$, 77.0 ppm). Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, coupling constant(s) in Hz, integration). Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm).

The phosphinooxazoline ligands[1], the substituted (*E*)-1,3-diphenylallyl acetates[2], and the substituted indolines[3] were prepared according to known procedures.

Reference:

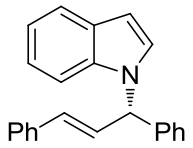
1. (a) G. Helmchen and A. Pfaltz, *Acc. Chem. Res.* 2000, **33**, 336; (b) G. C. Lloyd-Jones and A. Pfaltz, *Angew. Chem. Int. Ed. Engl.* 1995, **34**, 462; (c) C. García-Yebra, J. P. Janssen, F. Rominger and G. Helmchen, *Organometallics* 2004, **23**, 5459.

2. (a) T. Hayashi, A. Yamamoto, Y. Ito, E. Nishioka, H. Miura and K. Yanagi, *J. Am. Chem. Soc.* 1989, **111**, 6301; (b) H. Ji, L. Li, X.-L. Xu, S. Ham, L. A. Hammad and D. M. Birney, *J. Am. Chem. Soc.* 2009, **131**, 528; (c) J. W. Faller, J. C. Wilt and J. Parr, *Org. Lett.* 2004, **6**, 1301.

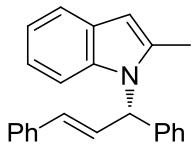
3. E. M. Santangelo, I. Liblikas, A. Mudalige, K. W. Törnroos, P.-O. Norrby, C. R. Unelius, *Eur. J. Org. Chem.* 2008, 5915.

General Procedure for the Palladium-Catalyzed Asymmetric Allylic Amination/Oxidation:

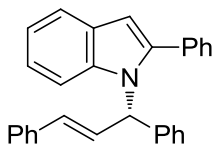
A flame dried Schlenk tube was cooled to room temperature and filled with argon. To this flask were added $[Pd(C_3H_5)Cl]_2$ (3.65 mg, 0.01 mmol, 5 mol%), Phox ligand (*S*)-**L1** (8.52 mg, 0.022 mmol, 11 mol%), and THF (1 mL). The reaction mixture was stirred at room temperature for about 10 min. After that, (*E*)-1,3-diphenylallyl acetate derivative **2** (0.20 mmol), indoline derivative **1** (0.24 mmol), Na_2CO_3 (42.4 mg, 0.4 mmol) and THF (1 mL) were added. The reaction mixture was stirred at room temperature for 12 hours. After the reaction was complete (monitored by TLC), the crude reaction mixture was filtrated with celite and washed with DCM. The solvents were removed under reduced pressure. Then THF (4 mL) and DDQ (90.8 mg, 0.4 mmol) were added to the crude reaction mixture. The reaction mixture was stirred at room temperature for about 10 min. After the reaction was complete (monitored by TLC), the solvents were removed under reduced pressure. Then the crude residue was purified by silica gel column chromatography to give the desired product **4** (eluents: hexanes/ethyl acetate). The characterization data of **4** are summarized below.



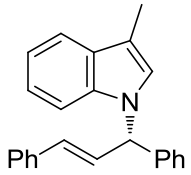
4aa. White solid, m.p. = 88-89 ^{o}C, 80% yield, 95% *ee* [Daicel Chiralcel OD-H, hexane/2-propanol = 98/2, *v* = 0.5 mL·min^{-1}, λ = 254 nm, t (minor) = 6.82 min, t (major) = 11.72 min]; $[\alpha]_D^{20}$ -67.7 (*c* 1.00, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.2 Hz, 1H), 7.37-7.10 (m, 14H), 6.7 (dd, *J* = 6.3, 15.9 Hz, 1H), 6.55 (d, *J* = 3.3 Hz, 1H), 6.39 (d, *J* = 15.9 Hz, 1H), 6.28 (d, *J* = 6.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.5, 136.1, 133.7, 128.9, 128.8, 128.6, 128.1, 127.9, 127.6, 127.5, 126.7, 126.3, 121.6, 120.9, 119.7, 110.2, 101.6, 61.5; IR (thin film): ν_{max} (cm^{-1}) = 3100, 3058, 2924, 1609, 1573, 1507, 1205, 968, 740, 690; HRMS (EI) calcd for $C_{23}H_{19}N$ (M^+): 309.1517. Found: 309.1519.



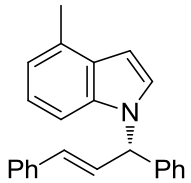
4ba. White solid, m.p. = 62-63 ^{o}C, 81% yield, 96% *ee* [Daicel Chiralcel AD-H, hexane/2-propanol = 90/10, *v* = 1 mL·min^{-1}, λ = 254 nm, t (minor) = 5.70 min, t (major) = 6.02 min]; $[\alpha]_D^{20}$ +54.2 (*c* 1.00, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 2H), 7.32-7.19 (m, 8H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.05-6.95 (m, 2H), 6.87 (dd, *J* = 6.8, 15.6 Hz, 1H), 6.49 (d, *J* = 16.0 Hz, 1H), 6.32 (d, *J* = 6.4 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 136.8, 136.3, 136.2, 133.7, 128.64, 128.60, 128.56, 128.0, 127.5, 126.9, 126.7, 126.6, 120.5, 119.7, 119.3, 111.2, 101.4, 59.9, 14.0; IR (thin film): ν_{max} (cm^{-1}) = 3027, 2974, 2918, 1600, 1449, 1307, 1263, 1088, 1018, 744, 693; HRMS (ESI) calcd for $C_{24}H_{22}N$ $[M+H]^+$: 324.1674. Found: 324.1746.



4ca. White solid, m.p. = 129-130 ^{o}C, 53% yield, 96% *ee* [Daicel Chiralpak AD-H, hexane/2-propanol = 90/10, *v* = 1 mL·min^{-1}, λ = 254 nm, t (minor) = 5.46 min, t (major) = 7.69 min]; $[\alpha]_D^{20}$ +40.6 (*c* 1.00, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.1 Hz, 1H), 7.54-7.22 (m, 15H), 7.10-6.97 (m, 3H), 6.88 (dd, *J* = 6.9, 15.9 Hz, 1H), 6.63 (s, 1H), 6.42 (d, *J* = 15.6 Hz, 1H), 6.33 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.2, 139.8, 136.2, 136.1, 133.8, 133.1, 129.5, 129.0, 128.6, 128.2, 128.0, 127.4, 126.8, 126.6, 126.4, 121.4, 120.6, 119.9, 113.2, 102.9, 60.7; IR (thin film): ν_{max} (cm^{-1}) = 3052, 3025, 2918, 2849, 1647, 1489, 1454, 1347, 1026, 965, 737, 687; HRMS (EI) calcd for $C_{29}H_{23}N$ (M^+): 385.1830. Found: 385.1828.

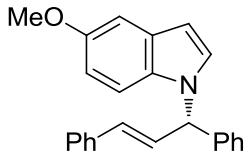


4da. White solid, m.p. = 43-44 ^{o}C, 72% yield, 97% *ee* [Daicel Chiralpak OD-H, hexane/2-propanol = 90/10, *v* = 1.0 mL·min^{-1}, λ = 254 nm, t (minor) = 5.41 min, t (major) = 7.26 min]; $[\alpha]_D^{20}$ -71.4 (*c* 1.00, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.37-7.10 (m, 13H), 6.95 (s, 1H), 6.68 (dd, *J* = 6.3, 15.9 Hz, 1H), 6.38 (d, *J* = 16.2 Hz, 1H), 6.22 (d, *J* = 6.0 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.8, 136.4, 136.2, 133.4, 129.1, 128.9, 128.7, 128.6, 128.0, 127.9, 127.8, 127.5, 126.6, 123.8, 121.5, 119.0, 118.9, 110.8, 109.9, 61.3, 9.8; IR (thin film): ν_{max} (cm^{-1}) = 3027, 2918, 1611, 1494, 1452, 1354, 968, 737, 697; MS-EI: 323; HRMS (EI) calcd for $C_{24}H_{21}N$ (M^+): 323.1674. Found: 323.1676.

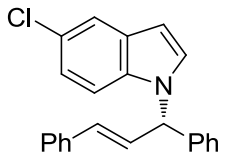


4ea. White solid, m.p. = 66-68 ^{o}C, 77% yield, 95% *ee* [Daicel Chiralpak OD-H, hexane/2-propanol = 90/10, *v* = 1.0 mL·min^{-1}, λ = 254 nm, t (minor) = 5.25 min, t (major) = 6.93 min]; $[\alpha]_D^{20}$ -67.7 (*c* 1.00, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-7.03 (m, 13H), 6.91 (d, *J* = 6.6 Hz, 1H), 6.69 (dd, *J* = 6.3, 15.6 Hz, 1H), 6.57 (d,

J = 3.0 Hz, 1H), 6.38 (d, *J* = 15.9 Hz, 1H), 6.25 (d, *J* = 6.3 Hz, 2H), 2.56 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.6, 136.1, 135.8, 133.6, 130.4, 128.7, 128.6, 128.0, 127.9, 127.6, 127.4, 126.6, 125.6, 121.7, 119.9, 107.8, 100.1, 61.6, 18.7; IR (thin film): ν_{max} (cm^{-1}) = 3028, 2922, 2856, 1699, 1489, 1451, 1231, 970, 745, 695; HRMS (EI) calcd for $C_{24}H_{21}N$ (M^+): 323.1674. Found: 323.1671.

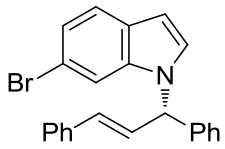


4fa. Colourless oil, 72% yield, 61% *ee* [Daicel Chiralpak AD-H, hexane/2-propanol = 90/10, *v* = 1.0 mL · min^{-1}, λ = 254 nm, t (major) = 11.36 min, t (minor) = 11.93 min]; $[\alpha]_D^{20}$ -34.8 (*c* 1.00, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.16 (m, 12H), 7.11 (d, *J* = 2.0 Hz, 1H), 6.80 (dd, *J* = 2.4, 9.2 Hz, 1H), 6.68 (dd, *J* = 6.4, 15.6 Hz, 1H), 6.47 (d, *J* = 3.2 Hz, 1H), 6.38 (d, *J* = 16.0 Hz, 1H), 6.21 (d, *J* = 6.4 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 139.6, 136.1, 133.6, 131.4, 129.4, 129.3, 128.7, 128.6, 128.2, 128.1, 127.9, 127.6, 127.4, 126.8, 126.6, 111.8, 110.9, 102.5, 101.1, 61.8, 55.8; IR (thin film): ν_{max} (cm^{-1}) = 3058, 3028, 2926, 1575, 1476, 1448, 1233, 1150, 1030, 834, 747, 693; HRMS (ESI) calcd for $C_{24}H_{22}NO$ $[M+H]^+$: 340.1623. Found: 340.1690.

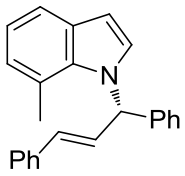


4ga. Colourless oil, 75% yield, 97% *ee* [Daicel Chiralpak OD-H, hexane/2-propanol = 90/10, *v* = 1.0 mL · min^{-1}, λ = 254 nm, t (major) = 6.63 min, t (minor) = 7.13 min]; $[\alpha]_D^{20}$ -55.3 (*c* 1.00, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 1.2 Hz, 1H), 7.40-7.08 (m, 13H), 6.70 (dd, *J* = 6.3, 15.6 Hz, 1H), 6.51 (d, *J* = 3.0 Hz, 1H), 6.39 (d, *J* = 15.9 Hz, 1H), 6.25 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.1, 135.9, 134.4, 133.9, 129.9, 128.9, 128.7, 128.2, 128.1, 127.6, 127.4, 127.1, 126.7, 125.4, 121.9, 120.3, 111.2, 101.3, 61.9; IR (thin film): ν_{max} (cm^{-1}) = 3027, 2927, 2855, 1450,

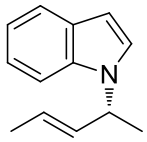
1204, 968, 794, 751, 695; HRMS (EI) calcd for $C_{23}H_{18}NCl$ (M^+): 343.1128. Found: 343.1125.



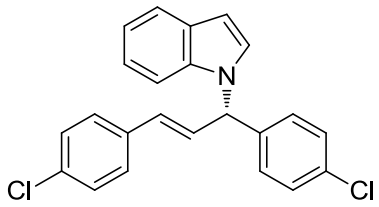
4ha. Colorless oil, 73% yield, 96% *ee* [Daicel Chiralpak AD-H, hexane/2-propanol = 90/10, v = 0.8 mL·min^{-1}, λ = 254 nm, t (minor) = 6.48 min, t (major) = 7.36 min]; $[\alpha]_D^{20}$ -77.3 (*c* 1.00, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.4 Hz, 1H), 7.45-7.18 (m, 12H), 7.14 (d, *J* = 3.2 Hz, 1H), 6.64 (dd, *J* = 6.0, 15.6 Hz, 1H), 6.51 (d, *J* = 3.2 Hz, 1H), 6.35 (d, *J* = 16.0 Hz, 1H), 6.19 (d, *J* = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 136.9, 135.9, 133.9, 128.9, 128.6, 128.2, 128.1, 127.7, 127.4, 127.1, 126.9, 126.7, 123.0, 122.2, 115.3, 113.0, 101.9, 61.5; IR (thin film): ν_{max} (cm^{-1}) = 3083, 3059, 3028, 1601, 1449, 1308, 1206, 968, 803, 743, 694; HRMS (EI) calcd for $C_{23}H_{18}NBr$ (M^+): 387.0623. Found: 387.0627.



4ia. White solid, m.p. = 114-115 ^{o}C 82% yield, 93% *ee* [Daicel Chiralcel AD-H, hexane/2-propanol = 90/10, v = 0.8 mL·min^{-1}, λ = 254 nm, t (minor) = 6.23 min, t (major) = 13.34 min]; $[\alpha]_D^{20}$ -105.9 (*c* 1.00, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.6 Hz, 1H), 7.35-7.23 (m, 8H), 7.14-7.11 (m, 3H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 7.2 Hz, 1H), 6.83 (d, *J* = 9.6 Hz, 1H), 6.71 (dd, *J* = 5.6, 15.6 Hz, 1H), 6.53 (d, *J* = 3.6 Hz, 1H), 6.21 (dd, *J* = 1.2, 7.6 Hz, 1H), 2.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 136.1, 135.2, 133.4, 129.6, 129.1, 128.8, 128.6, 128.0, 127.8, 127.4, 127.0, 126.6, 124.9, 120.9, 119.8, 119.2, 102.1, 62.3, 20.5; IR (thin film): ν_{max} (cm^{-1}) = 2972, 2903, 1464, 1335, 1244, 1155, 970, 783, 746, 695; HRMS (EI) calcd for $C_{24}H_{21}N$ (M^+): 323.1674. Found: 323.1670.

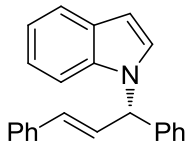


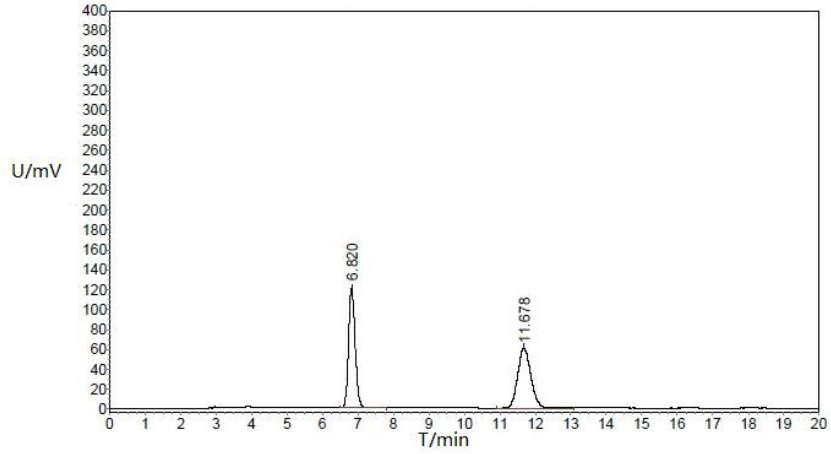
4ab. Colorless oil, 48% yield, 39% *ee* [Daicel Chiralpak OD-H, hexane/2-propanol = 98/2, v = 0.5 mL · min^{-1}, λ = 254 nm, t (major) = 13.13 min, t (minor) = 14.86 min]; $[\alpha]_D^{20}$ -24.8 (*c* 0.50, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, J = 8.1 Hz, 1H), 7.37 (d, J = 8.1 Hz, 1H), 7.24-7.06 (m, 3H), 6.51 (d, J = 3.0 Hz, 1H), 5.71-5.52 (m, 2H), 5.04-4.98 (m, 1H), 1.68 (d, J = 6.0 Hz, 3H), 1.60 (d, J = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 135.6, 131.8, 128.6, 126.6, 124.6, 121.1, 120.9, 119.2, 109.8, 101.1, 52.6, 20.4, 17.6; IR (thin film): ν_{max} (cm^{-1}) = 3051, 3030, 2963, 2919, 2852, 1459, 1259, 1012, 794, 736; HRMS (EI) calcd for $C_{13}H_{15}N$ (M^+): 185.1204. Found: 185.1202.



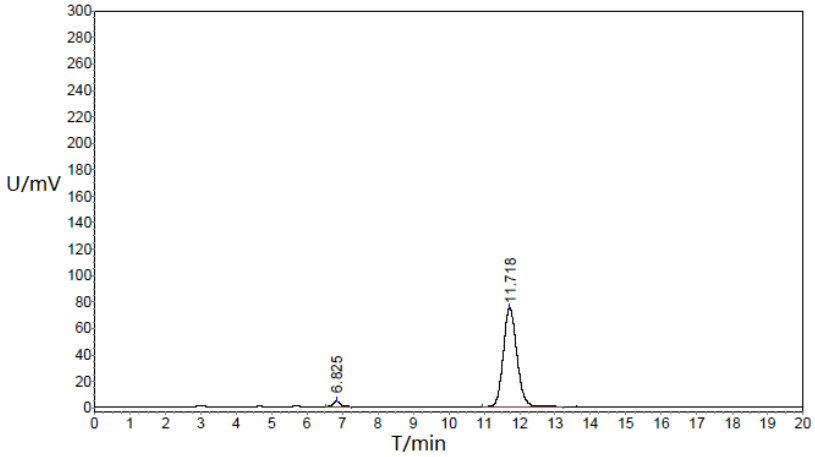
4ac. White solid, m.p. = 58-59 ^{o}C, 91% yield, 97% *ee* [Daicel Chiralpak AD-H, hexane/2-propanol = 90/10, v = 1.0 mL · min^{-1}, λ = 254 nm, t (minor) = 7.17 min, t (major) = 8.64 min]; $[\alpha]_D^{20}$ -43.6 (*c* 1.00, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.64 (m, 1H), 7.30-7.09 (m, 12H), 6.62 (dd, J = 6.4, 15.6 Hz, 1H), 6.56 (dd, J = 0.8, 3.2 Hz, 1H), 6.30 (dd, J = 1.6, 16.0 Hz, 1H) 6.21 (d, J = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 135.9, 134.3, 133.92, 133.86, 132.8, 129.0, 128.9, 128.8, 128.7, 127.9, 127.6, 125.9, 121.8, 121.1, 119.9, 110.0, 102.1, 60.8; IR (thin film): ν_{max} (cm^{-1}) = 3084, 3027, 1488, 1458, 1332, 1213, 1088, 1012, 980, 740, 608; HRMS (EI) calcd for $C_{23}H_{17}NCl_2$ (M^+): 377.0738. Found: 377.0733.

NMR and HPLC spectra of 4

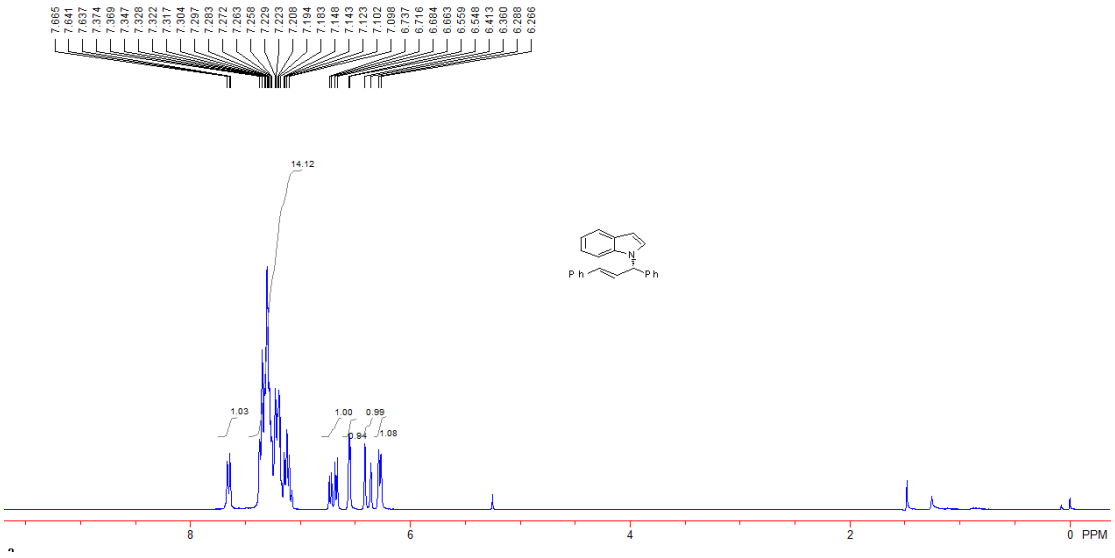




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	6.820	119582.727	1562986.500	49.9751
2	11.678	60384.566	1564542.625	50.0249
Total		179967.293	3127529.125	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	6.825	3851.073	51695.598	2.5645
2	11.718	74514.047	1964106.375	97.4355
Total		78365.119	2015801.973	100.0000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7.374
7.369
7.347
7.328
7.322
7.317
7.304
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7.272
7.263
7.258
7.229
7.223
7.208
7.194
7.183
7.148
7.143
7.123
7.102
7.098
6.737
6.716
6.684
6.663
6.559
6.548
6.413
6.360
6.288
6.266
14.12
1.03
1.00
0.99
0.84
1.08
Ph
Ph
8
6
4
2
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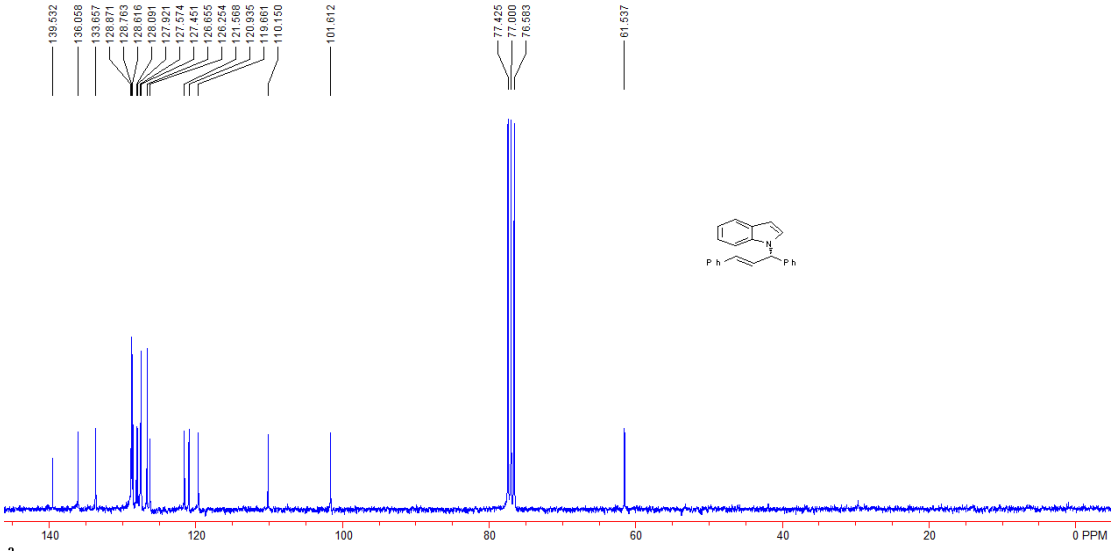
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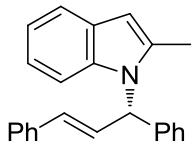
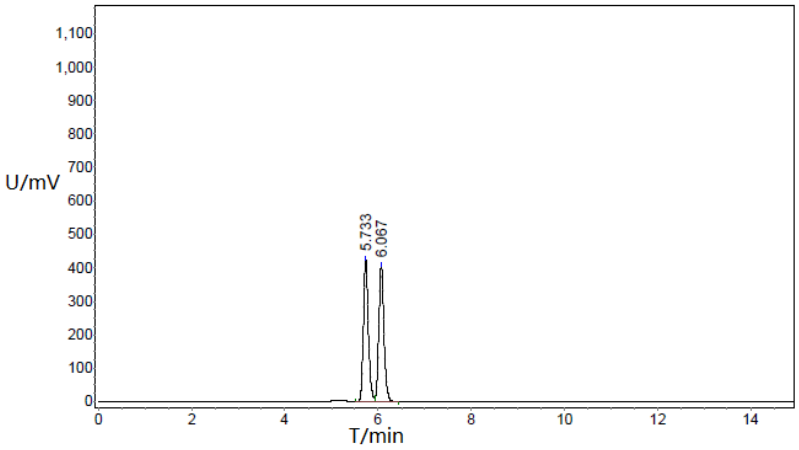
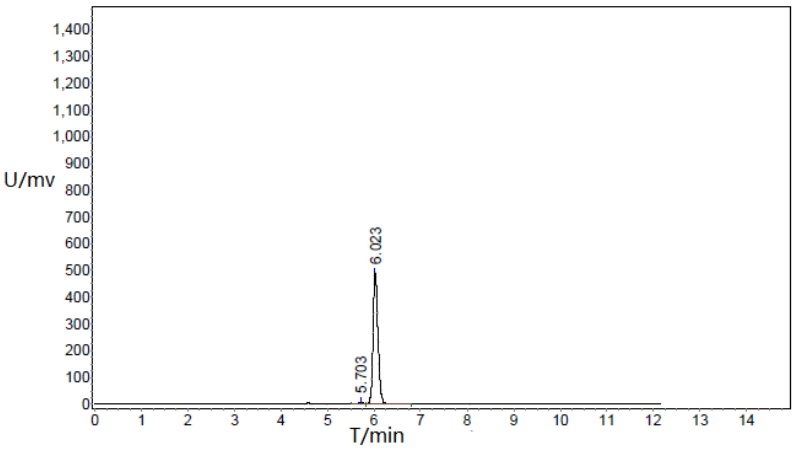
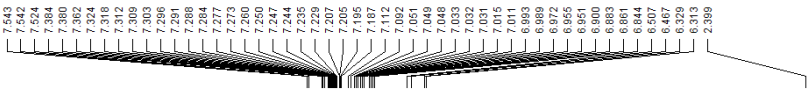




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.733	422779.563	3108393.750	50.0992
2	6.067	405066.813	3096078.250	49.9008
Total		827846.375	6204472.000	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.703	9822.784	68470.281	1.8384
2	6.023	491314.031	3656069.750	98.1616
Total		501136.815	3724540.031	100.0000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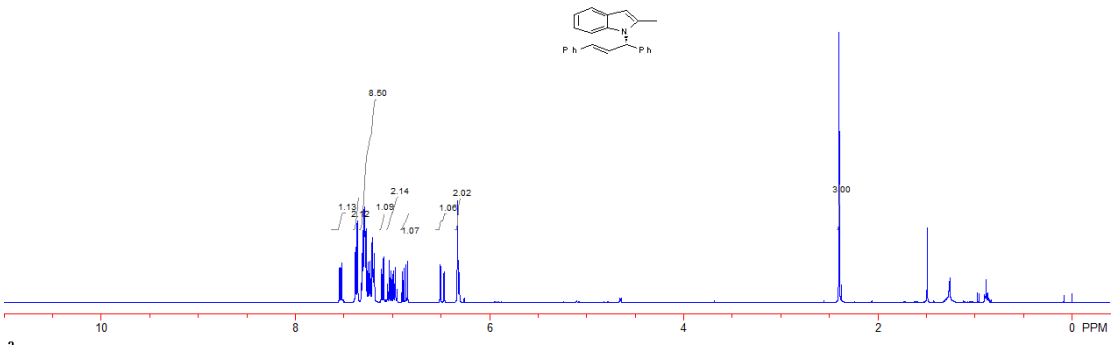
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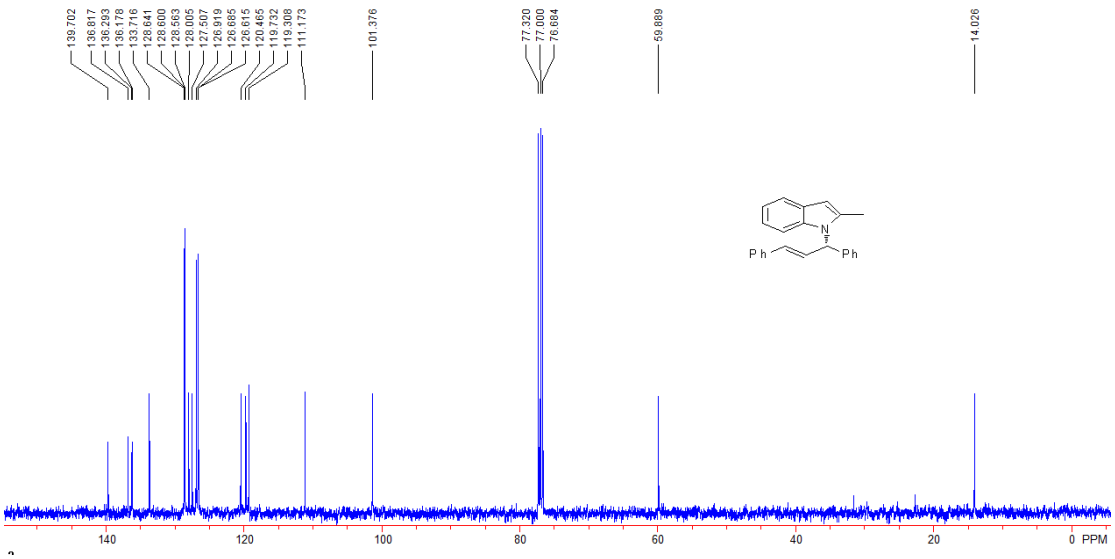
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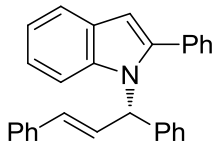
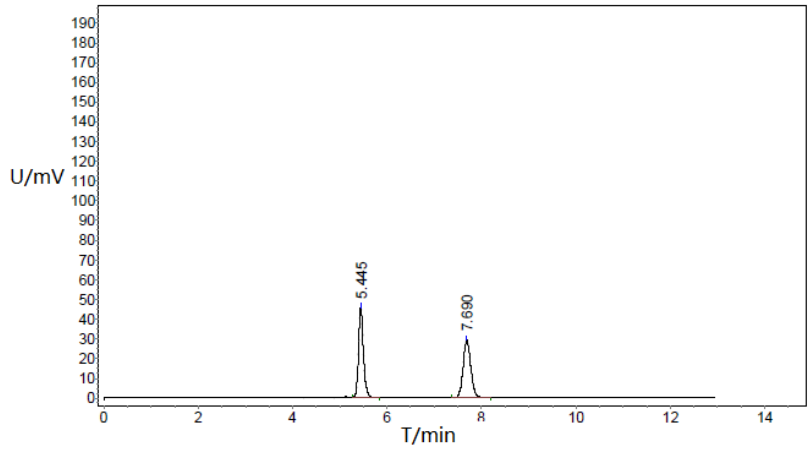
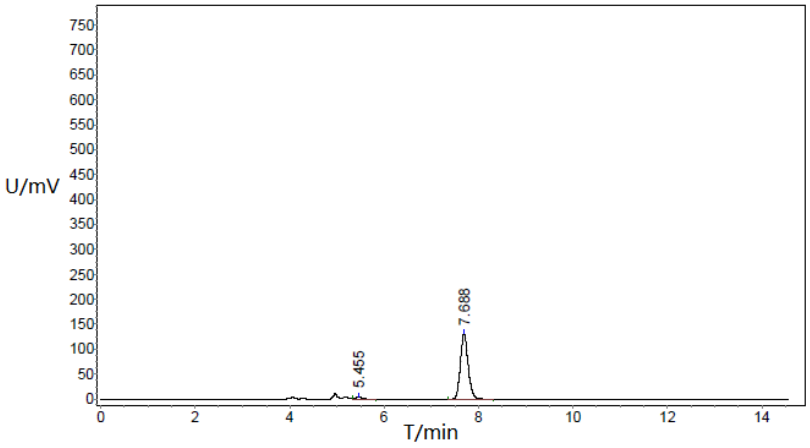
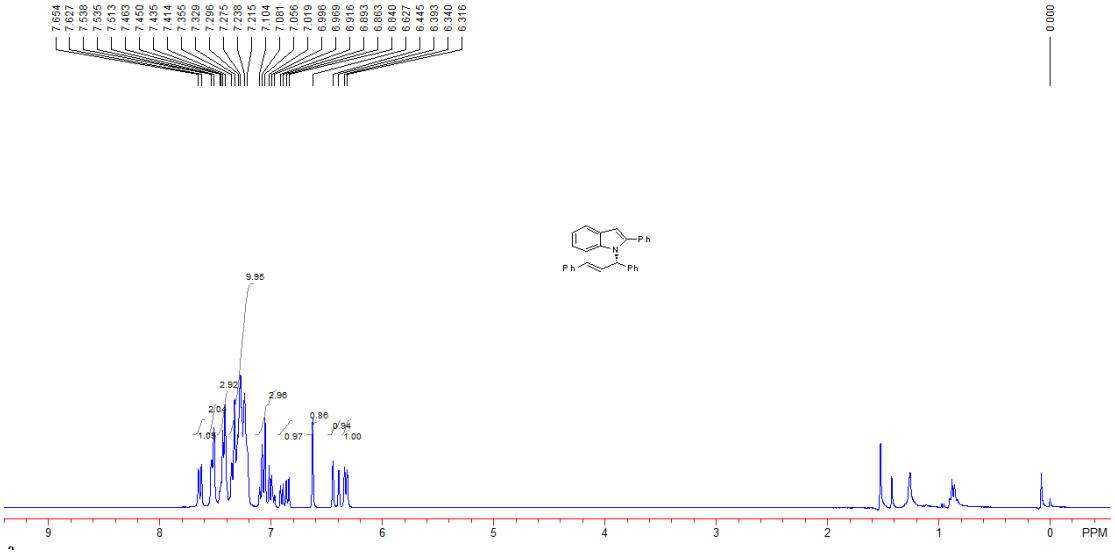




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.445	45580.648	328653.813	50.1882
2	7.690	29104.102	326188.656	49.8118
Total		74684.750	654842.469	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.455	4247.690	33462.441	2.2462
2	7.688	130160.047	1456254.500	97.7538
Total		134407.737	1489716.941	100.0000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6.393
6.340
6.316
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Ph
Ph
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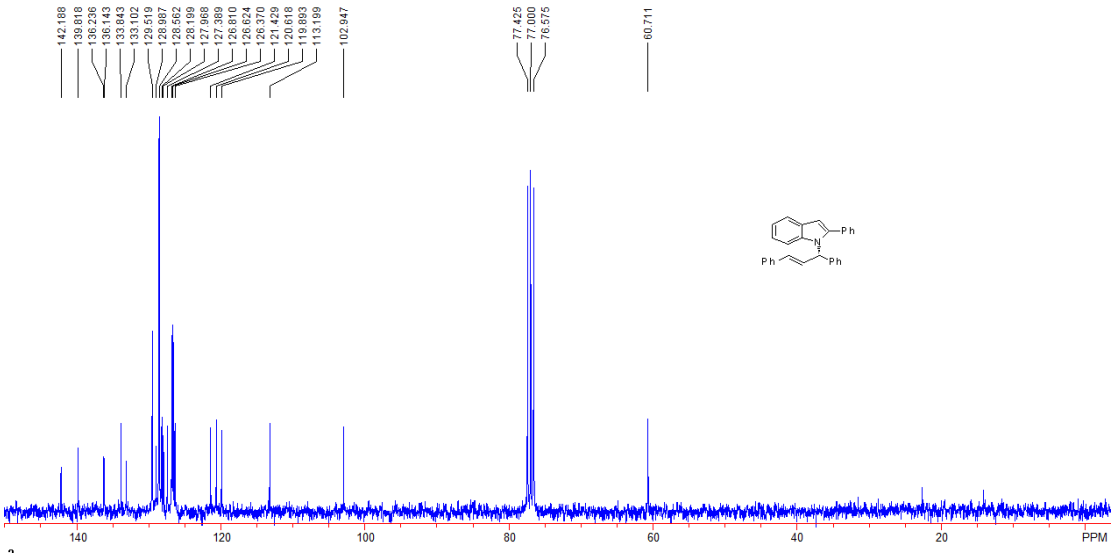
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120.618
119.893
113.199
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60
40
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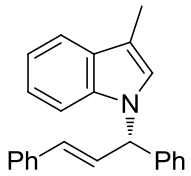
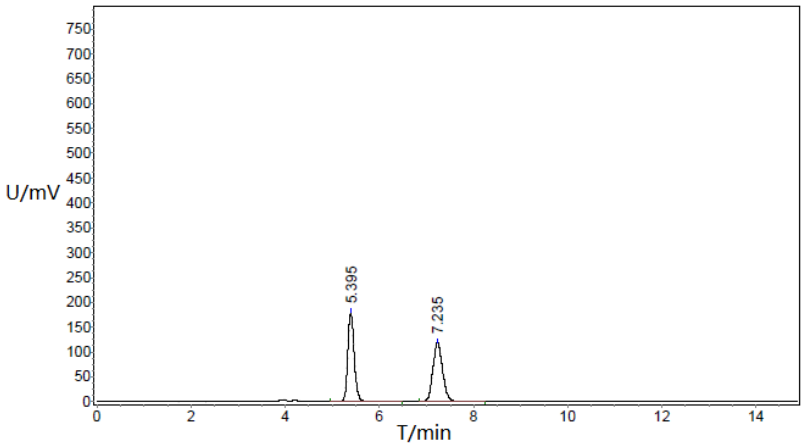
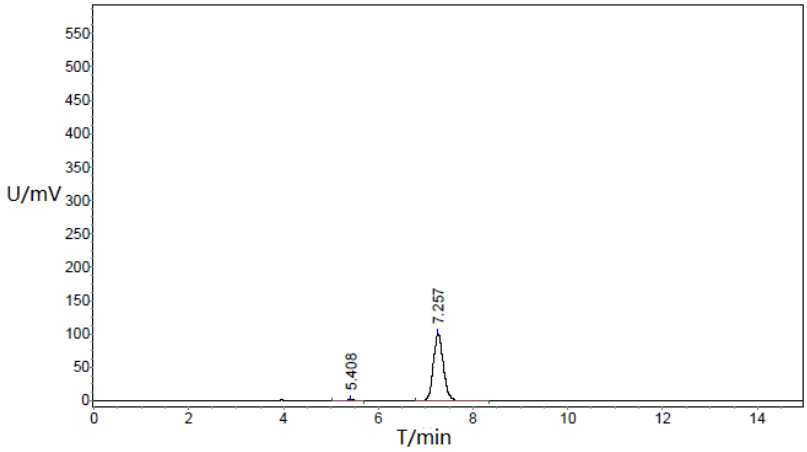
PPM

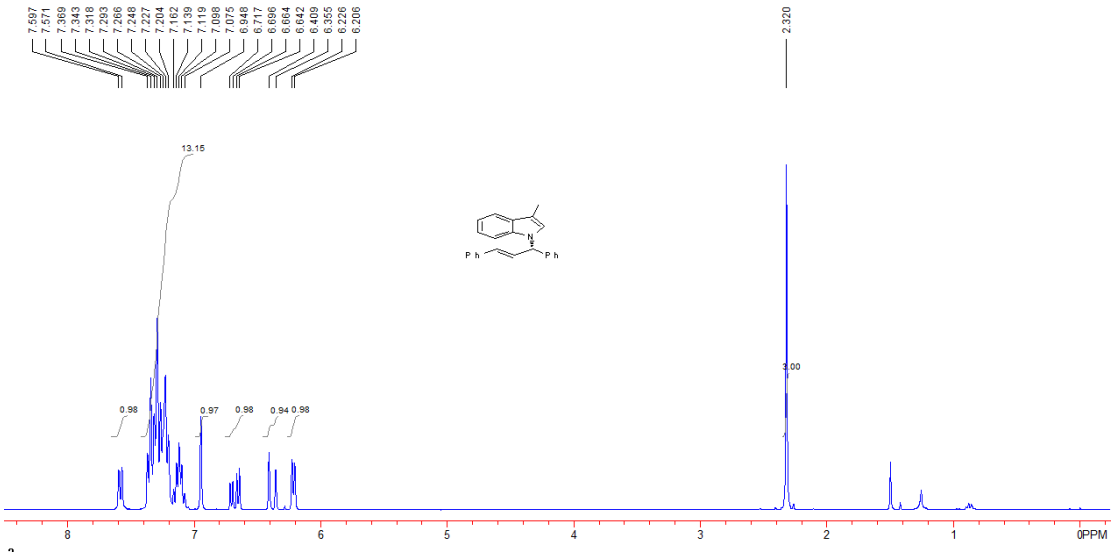




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.395	179473.750	1697569.250	49.9809
2	7.235	118559.914	1698869.875	50.0191
Total		298033.664	3396439.125	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percet
1	5.408	2197.931	21125.100	1.4332
2	7.257	100466.836	1452903.875	98.5668
Total		102664.767	1474028.975	100.0000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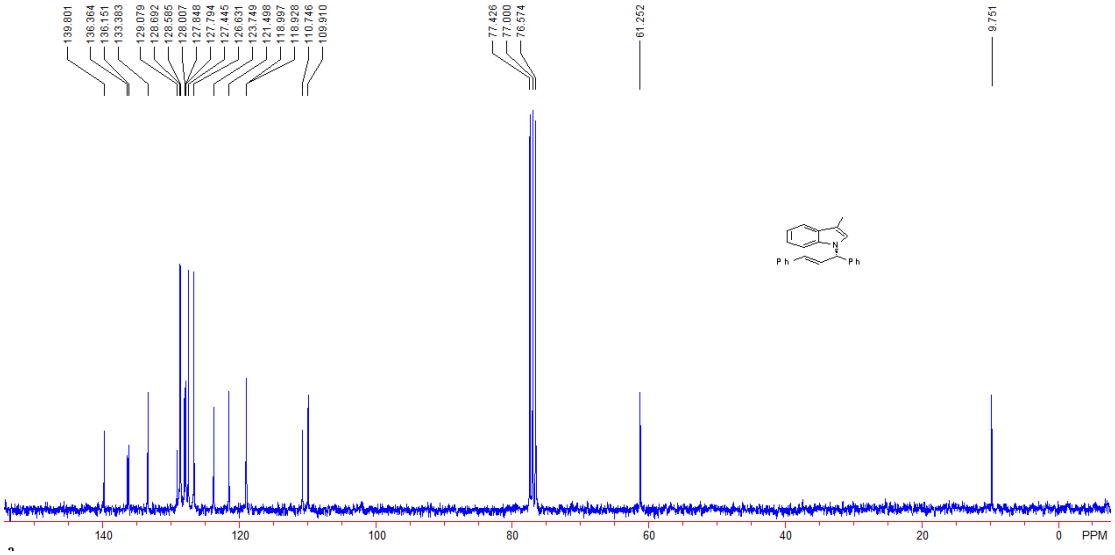
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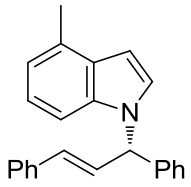
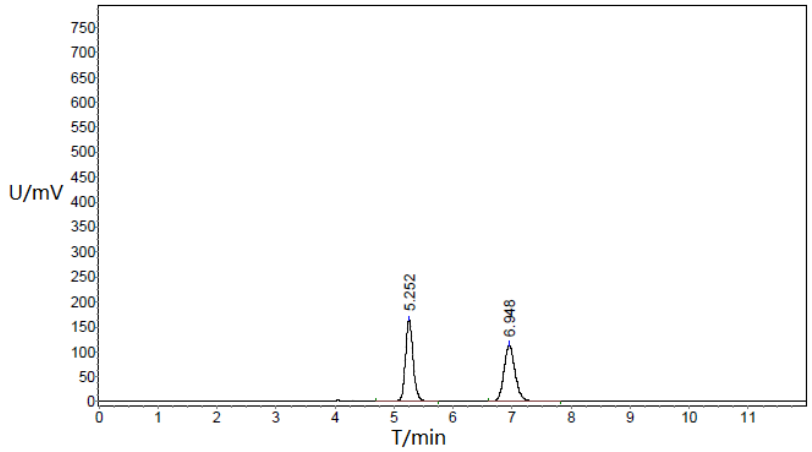
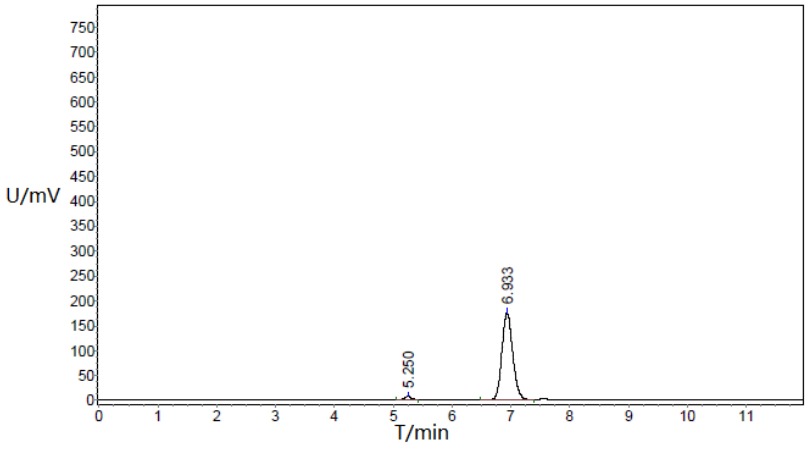
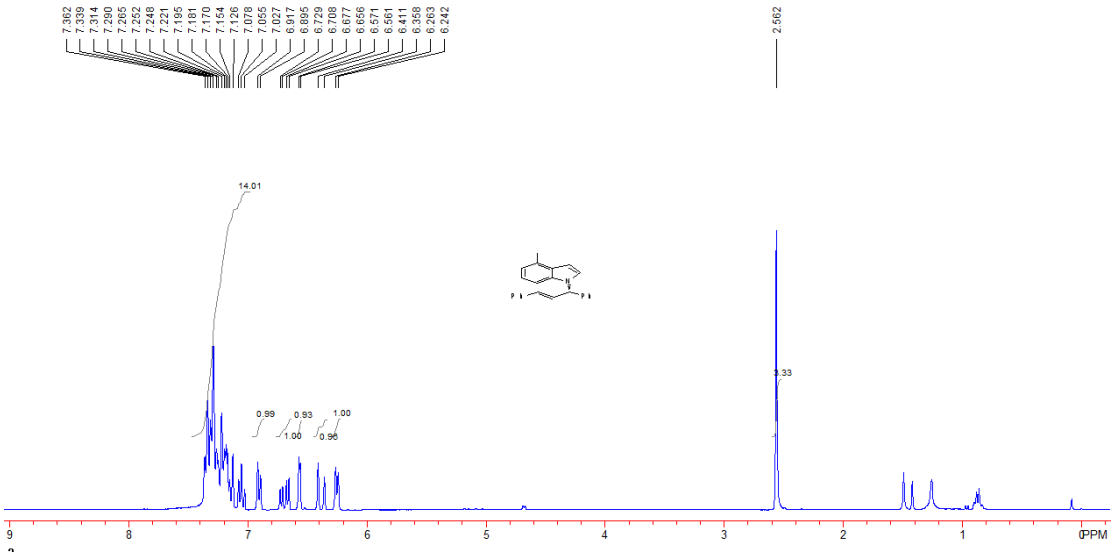




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.252	162392.281	1472011.500	50.1939
2	6.948	112150.180	1460637.000	49.8061
Total		274542.461	2932648.500	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.250	6742.496	60162.727	2.6014
2	6.933	175561.516	2252517.500	97.3986
Total		182304.011	2312680.227	100.0000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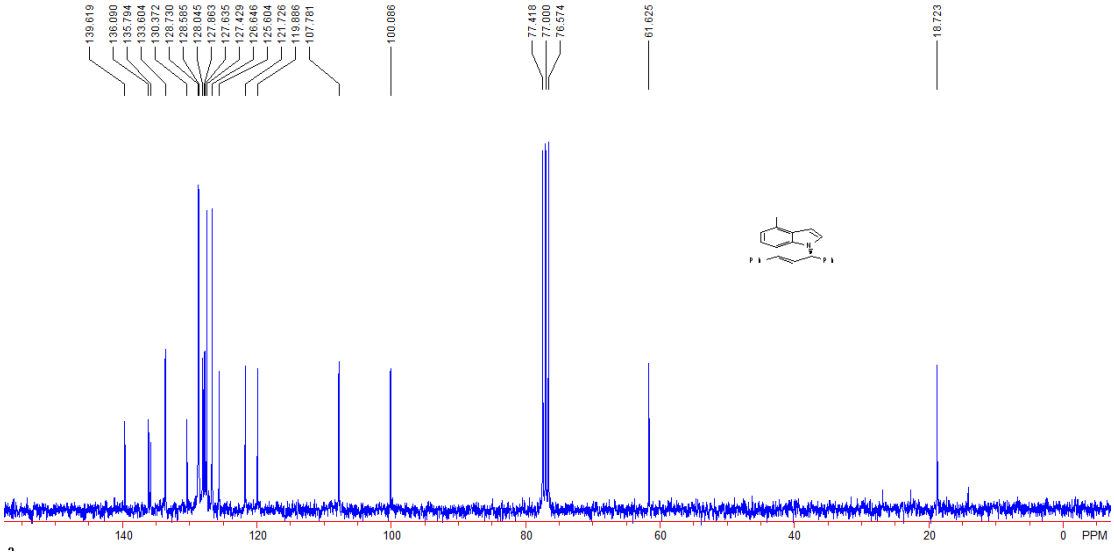
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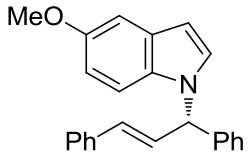
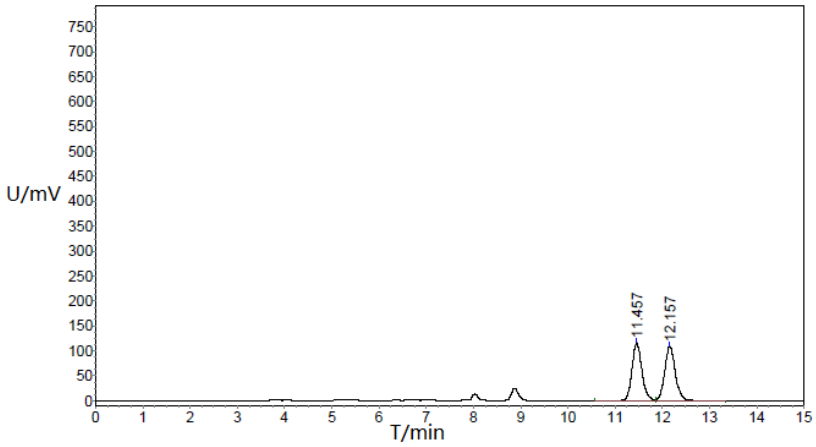
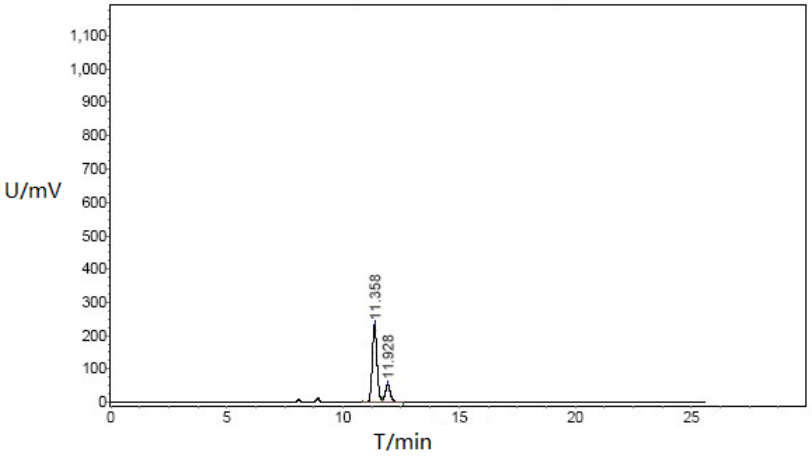
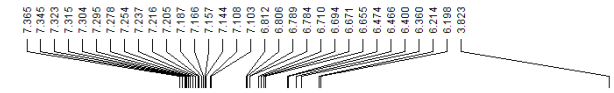




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	11.457	115970.813	1669731.375	49.8214
2	12.157	108718.523	1681705.250	50.1786
Total		224689.336	3351436.625	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	11.358	234797.250	3350075.500	80.4959
2	11.928	53603.230	811723.125	19.5041
Total		288400.480	4161798.625	100.0000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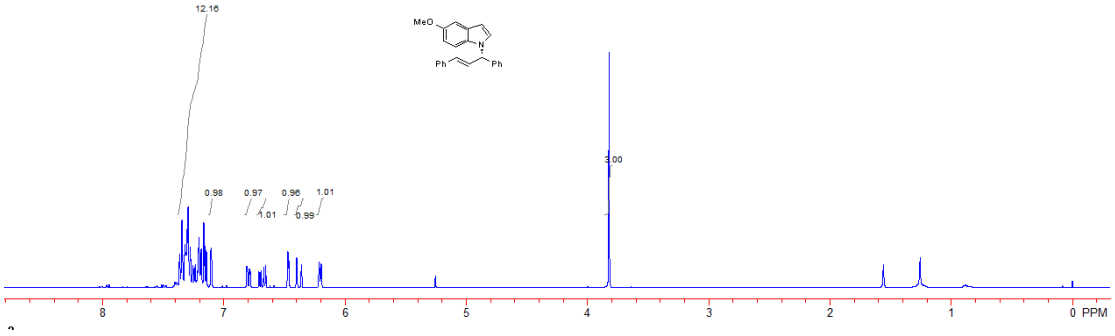
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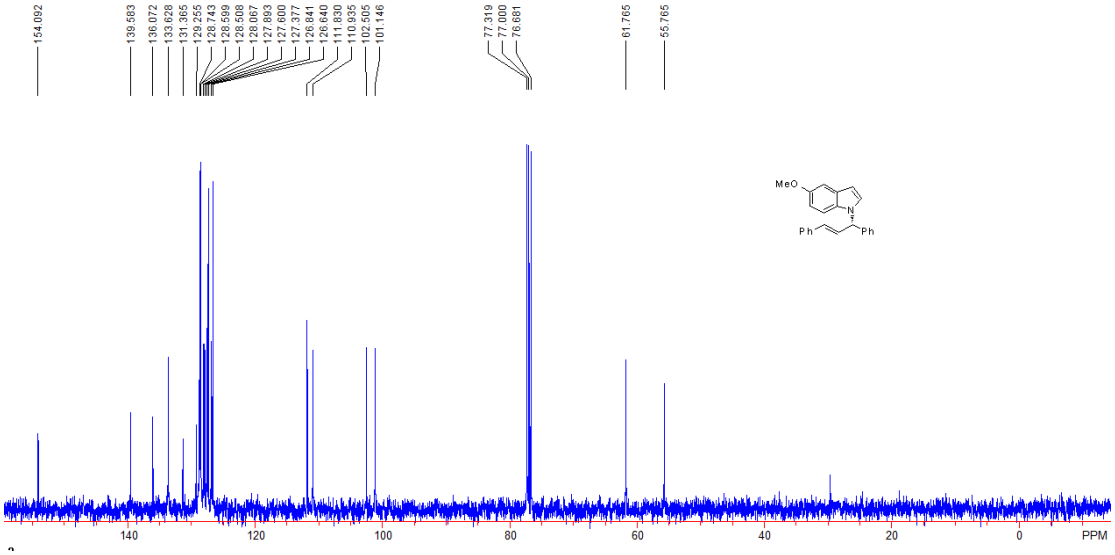
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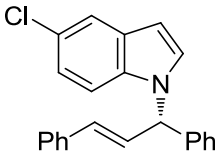
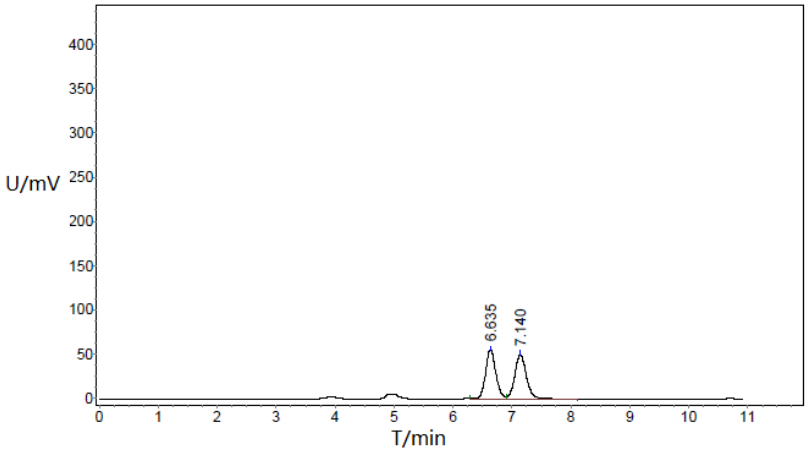
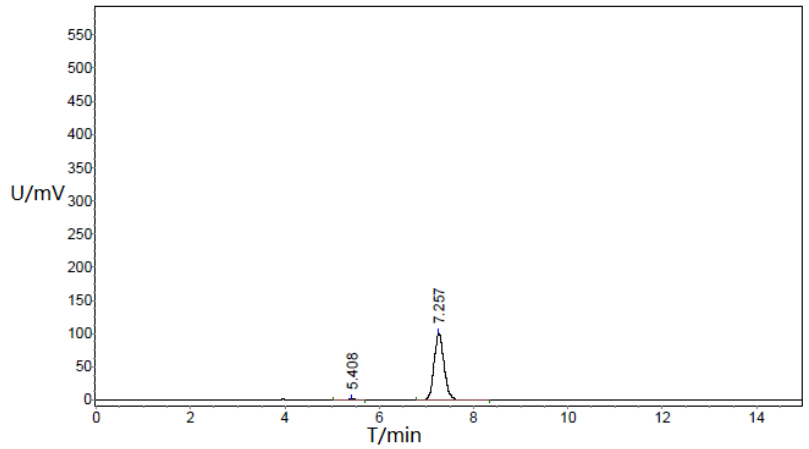
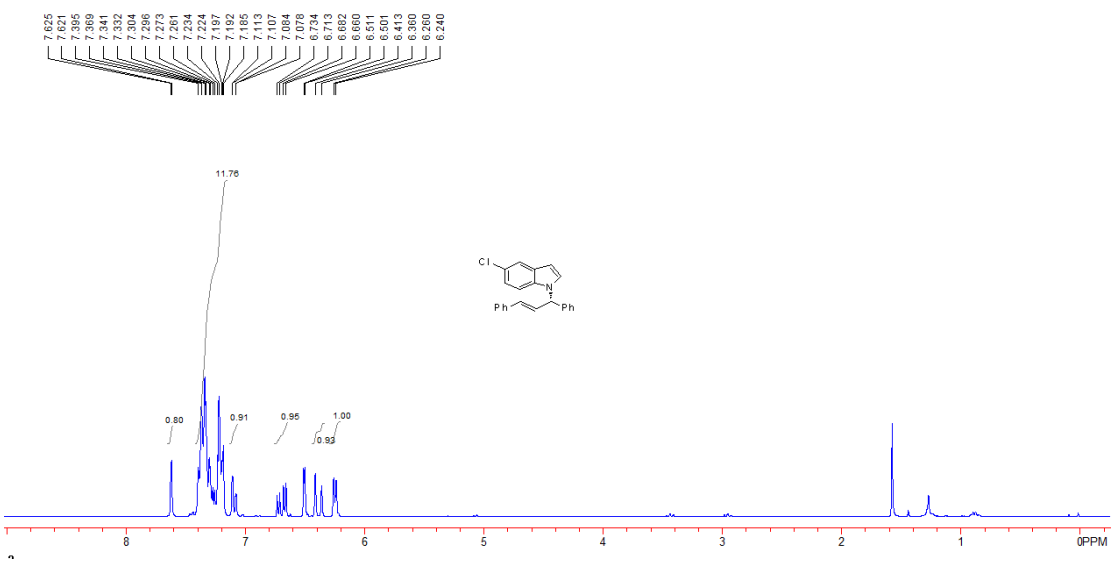




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	6.635	55066.379	658793.813	49.7502
2	7.140	49666.645	665409.375	50.2498
Total		104733.023	1324203.188	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.408	2197.931	21125.100	1.4332
2	7.257	100466.836	1452903.875	98.5668
Total		102664.767	1474028.975	100.0000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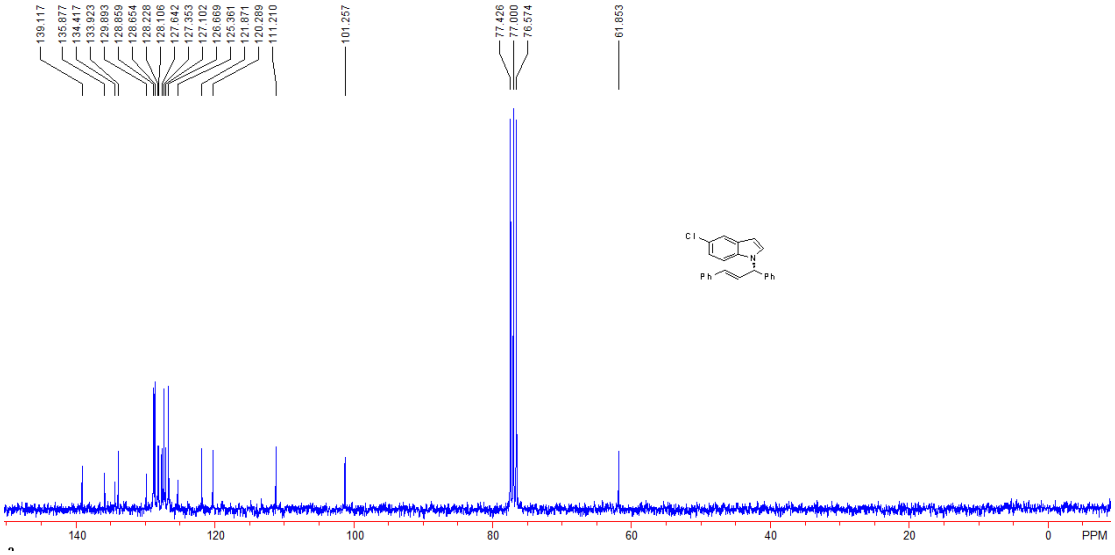
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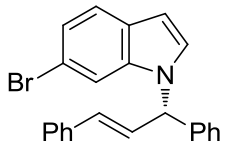
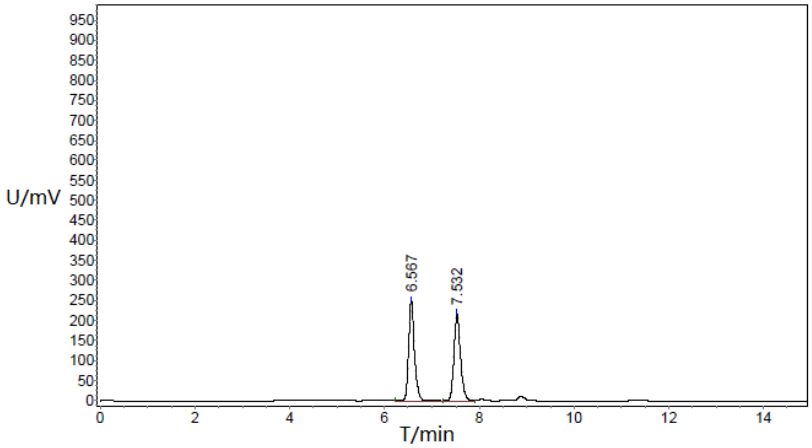
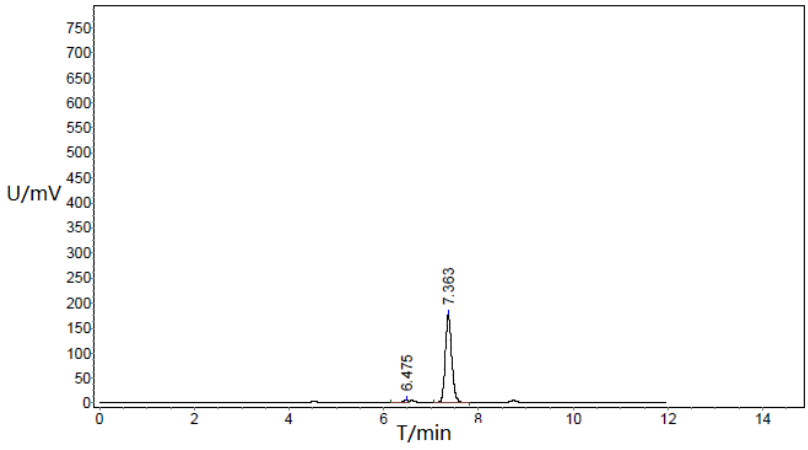
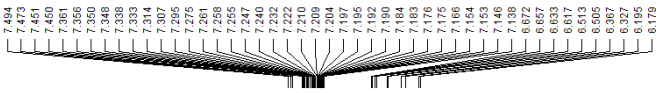




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	6.567	250514.906	2126169.500	50.0282
2	7.532	217948.219	2123775.750	49.9718
Total		468463.125	4249945.250	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	6.475	4637.729	37421.785	2.2117
2	7.363	176069.172	1654558.125	97.7883
Total		180706.901	1691979.910	100.0000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7.275
7.261
7.258
7.255
7.247
7.240
7.232
7.222
7.210
7.209
7.204
7.197
7.195
7.192
7.190
7.184
7.183
7.176
7.175
7.166
7.154
7.153
7.146
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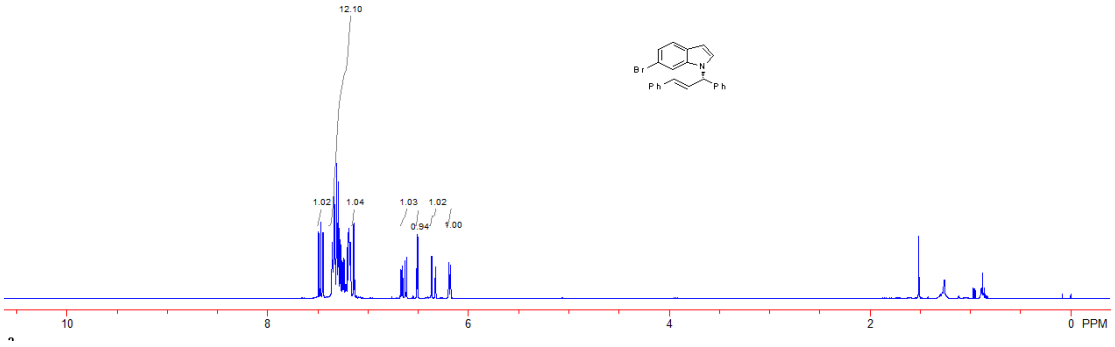
6.633
6.617
6.513
6.505
6.367
6.327
6.195
6.179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1.04
1.03
0.94
1.02
4.00
Br
N
Ph
Ph
10
8
6
4
2
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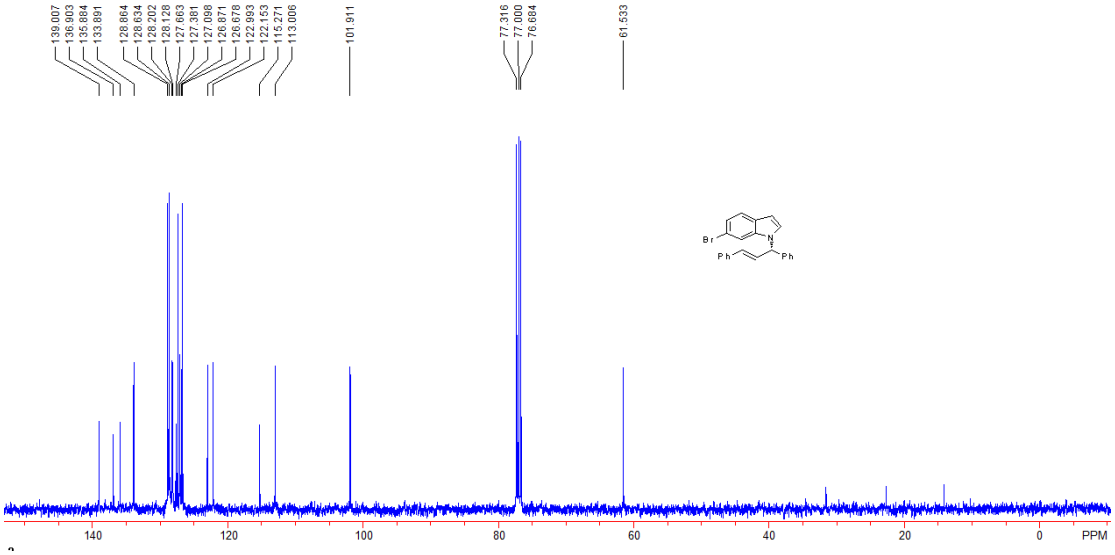
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128.128
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127.381
127.098
126.871
126.678
122.993
122.153
115.271
113.006
101.911
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61.533
Br
N
Ph
Ph
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80
60
40
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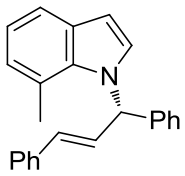
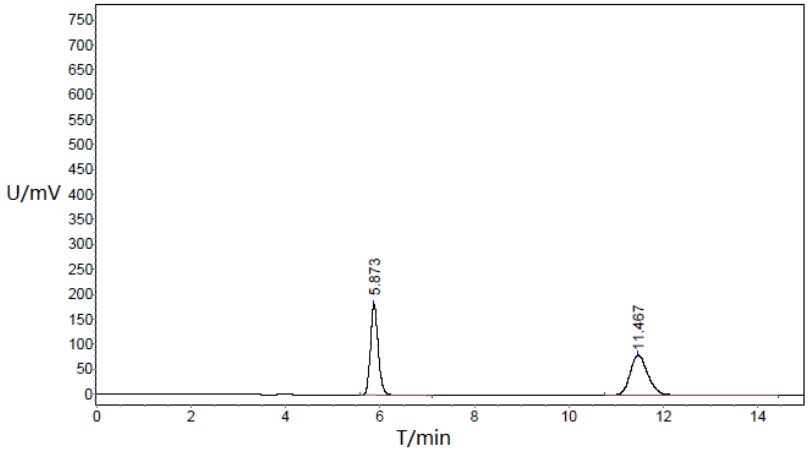
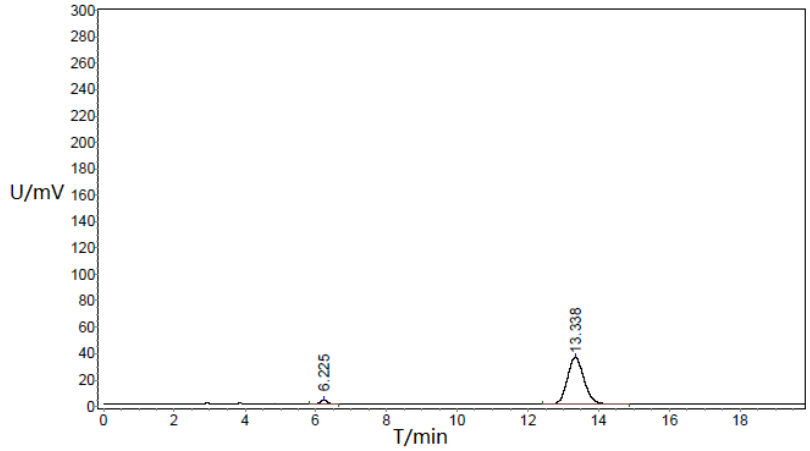
PPM

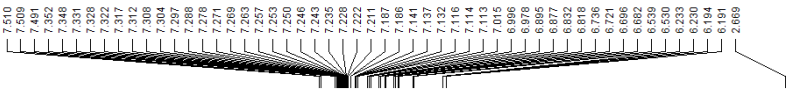




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	5.873	182517.547	2086852.500	49.6626
2	11.467	80373.156	2115204.000	50.3374
Total		262890.703	4202056.500	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	6.225	3115.276	40569.352	3.4176
2	13.338	35428.332	1146510.375	96.5824
Total		38543.608	1187079.727	100.0000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7.322
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7.288
7.278
7.271
7.269
7.263
7.257
7.253
7.250
7.246
7.243
7.235
7.228
7.222
7.211
7.187
7.186
7.141
7.137
7.132
7.116
7.114
7.113
7.015
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6.978
6.895
6.877
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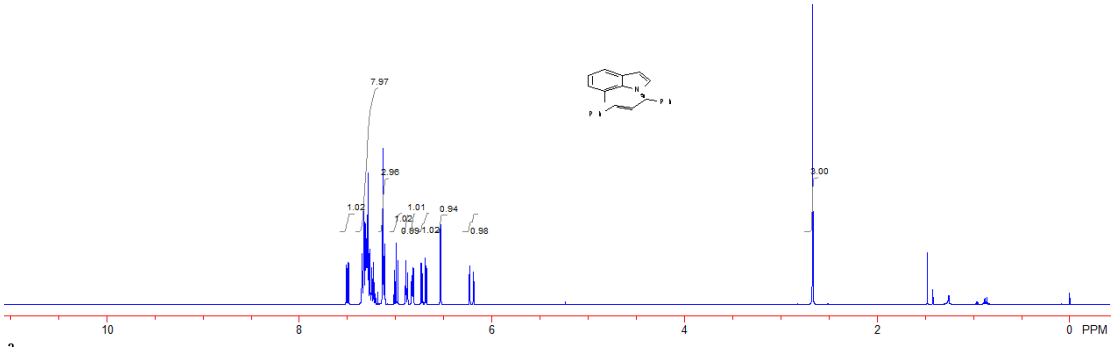
6.191
2.669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1.02
0.94
0.98
3.00
10
8
6
4
2
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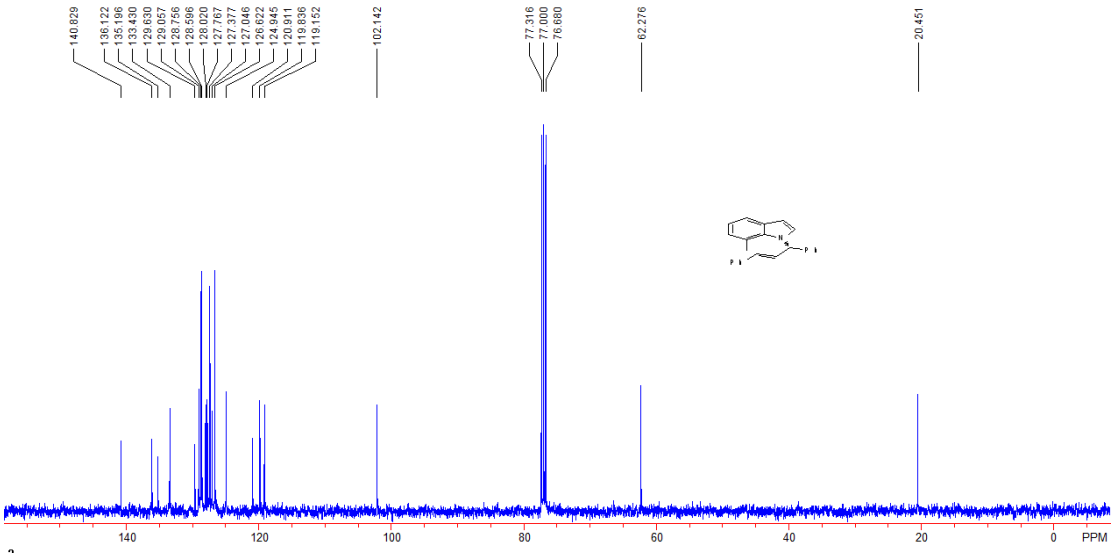
PPM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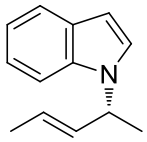
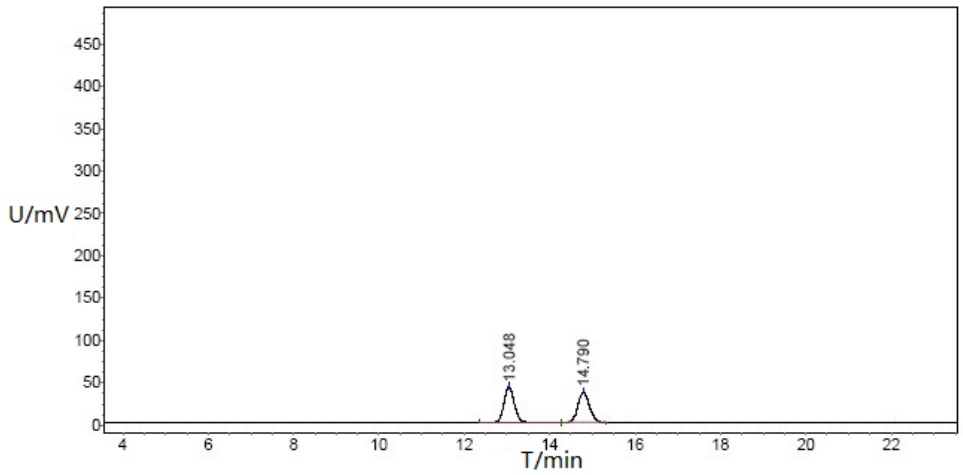
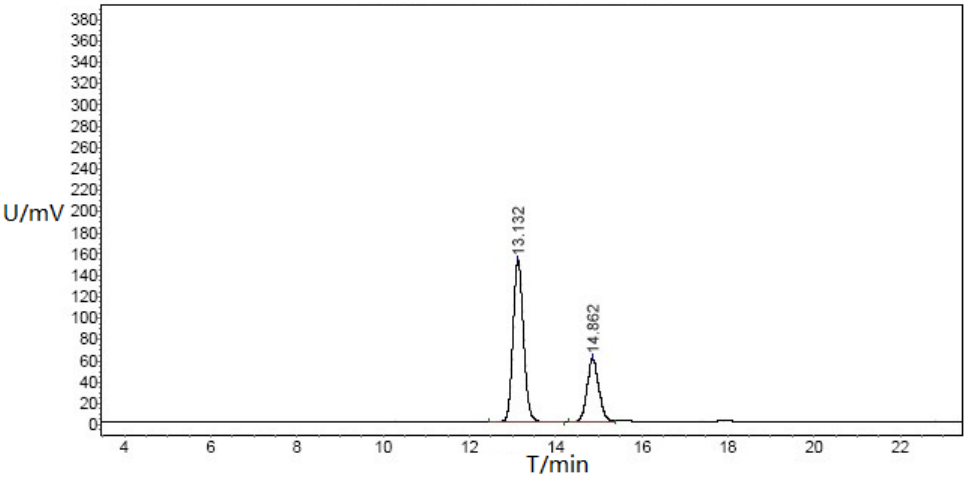
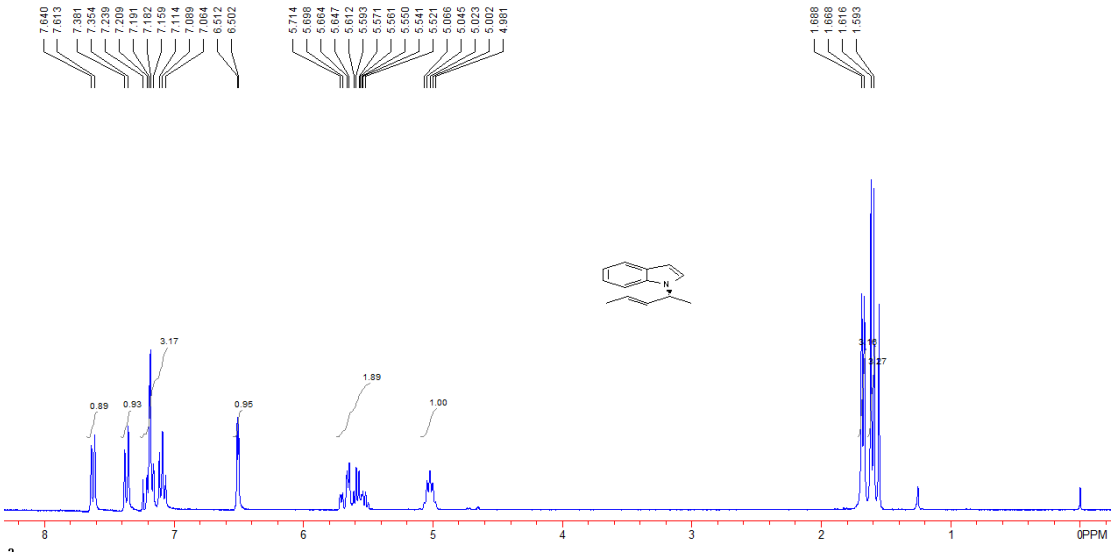




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	13.048	42050.504	706191.875	51.4354
2	14.790	35843.055	666777.188	48.5646
Total		77893.559	1372969.063	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	13.132	151359.078	2533865.250	69.4511
2	14.862	58981.035	1114552.750	30.5489
Total		210340.113	3648418.000	100.0000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7.239
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7.191
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7.159
7.114
7.089
7.064
6.512
6.502
5.714
5.698
5.664
5.647
5.612
5.593
5.571
5.561
5.550
5.541
5.521
5.066
5.045
5.023
5.002
4.981
1.688
1.668
1.616
1.593
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0.93
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6
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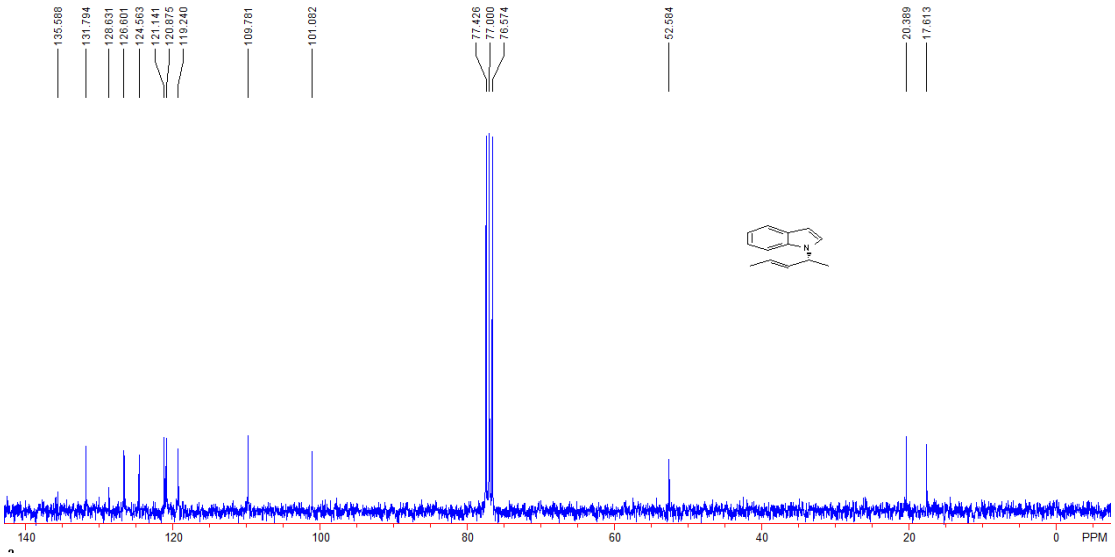
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40
20
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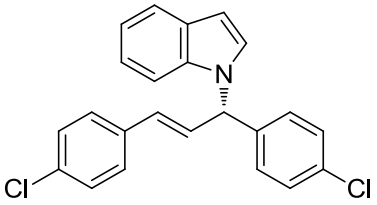
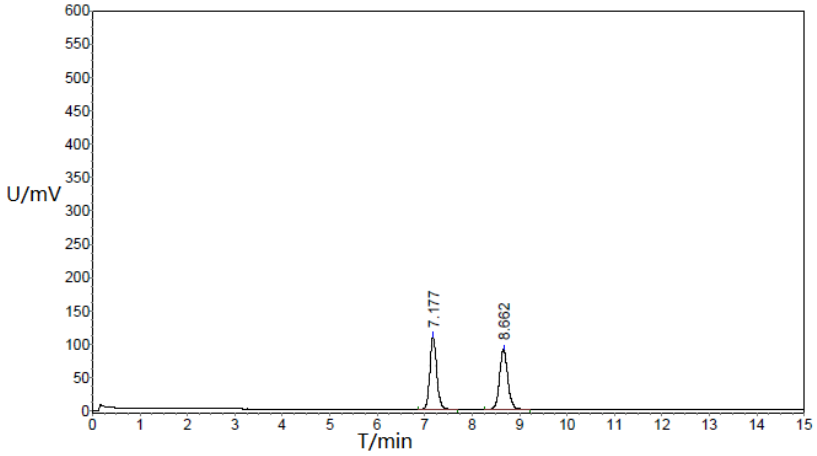
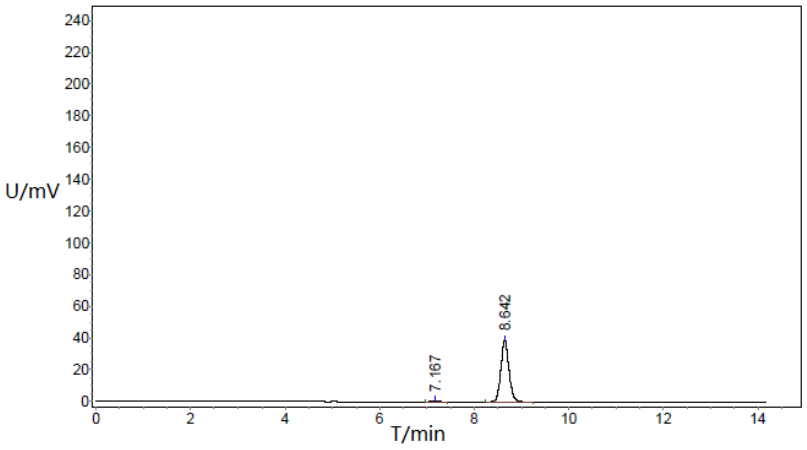
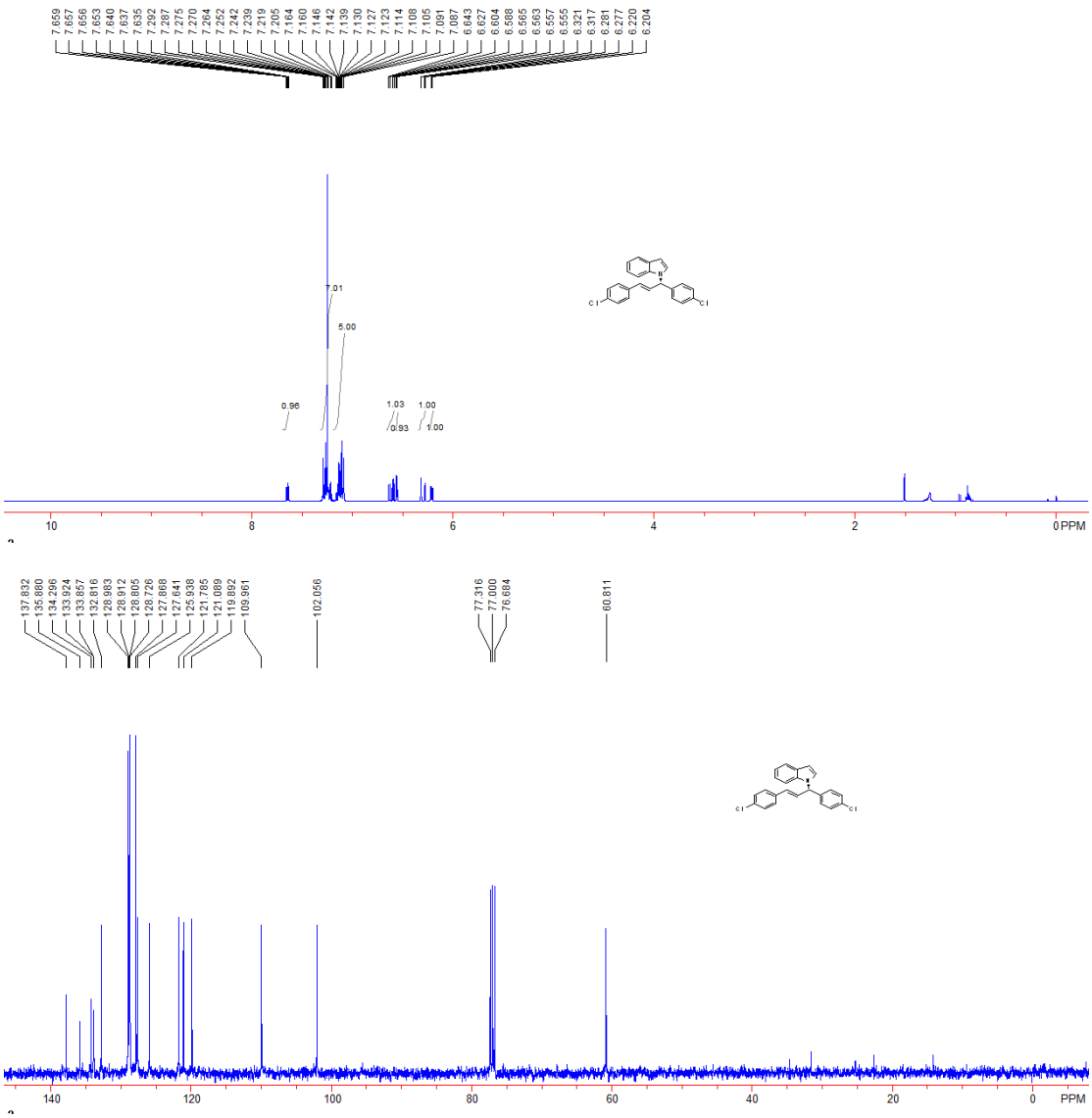




Peak No.	R. Time	Peak Height	Peak Area	Percent
1	7.177	108962.242	1080164.500	49.9959
2	8.662	90504.375	1080339.625	50.0041
Total		199466.617	2160504.125	100.0000



Peak No.	R. Time	Peak Height	Peak Area	Percent
1	7.167	790.484	7467.500	1.5921
2	8.642	38977.656	461565.000	98.4079
Total		39768.140	469032.500	100.0000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7.252
7.242
7.239
7.219
7.205
7.164
7.160
7.146
7.142
7.139
7.130
7.127
7.123
7.114
7.108
7.105
7.091
7.087
6.643
6.627
6.604
6.588
6.585
6.563
6.557
6.555
6.321
6.317
6.281
6.277
6.220
6.204
7.01
5.00
0.96
1.03
0.93
1.00
1.00
Cl
Cl
10
8
6
4
2
0 PPM
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135.880
134.296
133.924
133.857
132.816
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128.912
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128.726
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77.000
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Cl
Cl
140
120
100
80
60
40
20
0
PPM

X-ray crystal structure of (*S*)-4aa

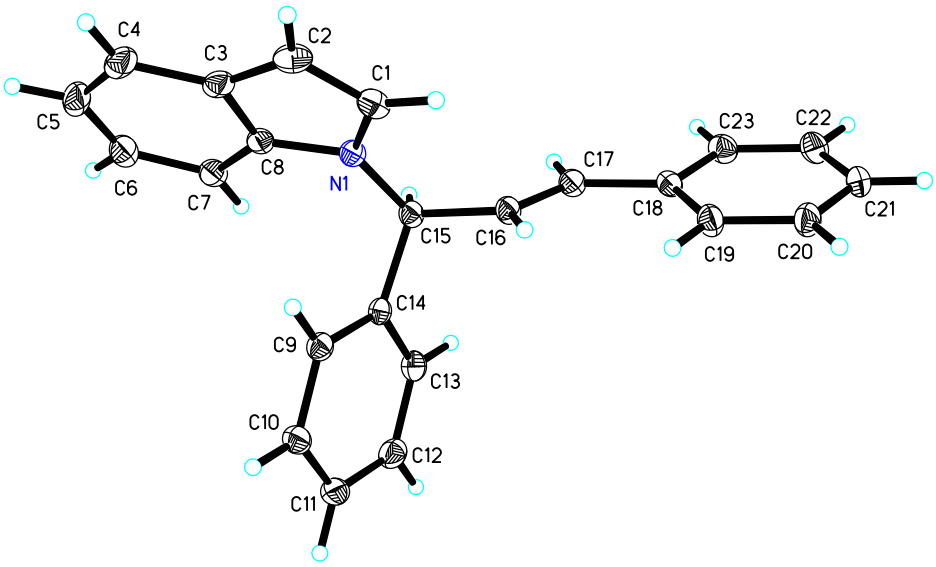

Table 1. Crystal data and structure refinement for cu_dm12452_0m.

Identification code	cu_dm12452_0m
Empirical formula	C23 H19 N
Formula weight	309.39
Temperature	173(2) K
Wavelength	1.54178 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 8.5200(2) A alpha = 90 deg. b = 5.8727(2) A beta = 98.145(2) deg. c = 16.9410(5) A gamma = 90 deg.
Volume	839.10(4) A^3
Z, Calculated density	2, 1.225 Mg/m^3
Absorption coefficient	0.537 mm^-1

F(000)	328
Crystal size	0.20 x 0.15 x 0.02 mm
Theta range for data collection	5.24 to 69.93 deg.
Limiting indices	-9<=h<=10, -7<=k<=7, -20<=l<=20
Reflections collected / unique	8656 / 2875 [R(int) = 0.0400]
Completeness to theta = 69.93	97.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9893 and 0.9002
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2875 / 1 / 217
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0895
R indices (all data)	R1 = 0.0367, wR2 = 0.0907
Absolute structure parameter	0.1(6)
Largest diff. peak and hole	0.165 and -0.201 e.A^-3