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# Organocatalytic asymmetric synthesis of 3,3-disubstituted oxindoles featuring two heteroatoms at C3 position

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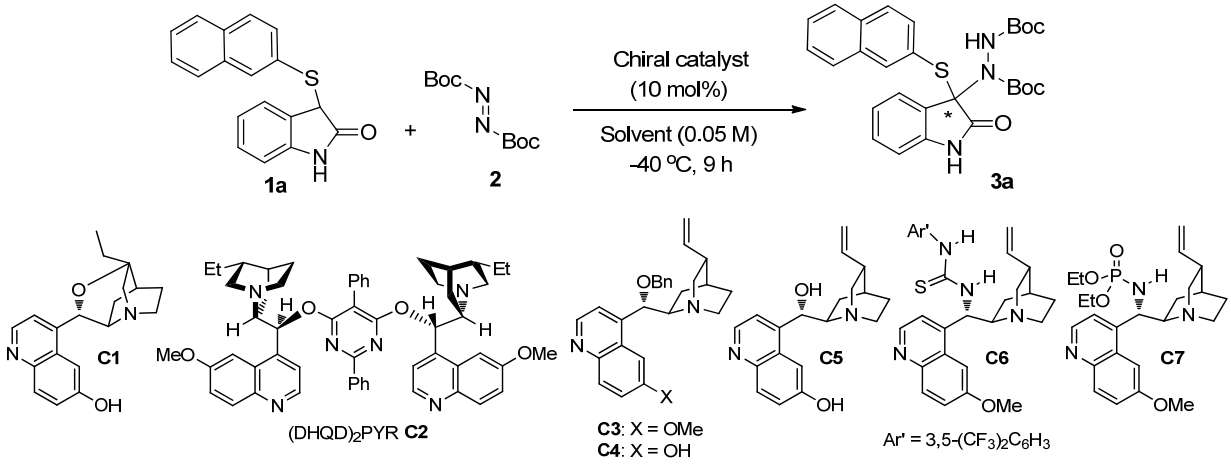
**1. General**: Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products was carried out by flash chromatography on silica gel. Chemical yields refered to pure isolated substances. $^{1}H$ and $^{13}C$ NMR spectra were obtained using a Bruker DPX-400 spectrometer. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet, br = broad.

Anhydrous ether, THF and toluene were prepared by distillation over sodium-benzophenone ketyl prior to use. Anhydrous acetone was distilled over anhydrous $CaSO_4$ and stored over MS 4Å. Anhydrous halogenated solvents and $CH_3CN$ were prepared by first distillation over $P_2O_5$ and then from $CaH_2$. β-ICD were purchased from TCI and $(DHQ)_2PHAL$ from Aldrich. Catalysts **C4-C5**[1]and **C7**[2] were prepared using literature methods. Di-*tert*-butyl azodicarboxylate (DBAD) was recrystallized from petroleum ether and stored under nitrogen.

[1] X. Liu, H. Li, L. Deng, *Org. Lett.* **2005**, *7*, 167.

[2] B.Vakulya, S. Varga, A. Csámpai, T. Soós, *Org. Lett.* **2005**, *7*, 1967.

## 2. Condition optimization for the amination of 3-thiooxyindoles.

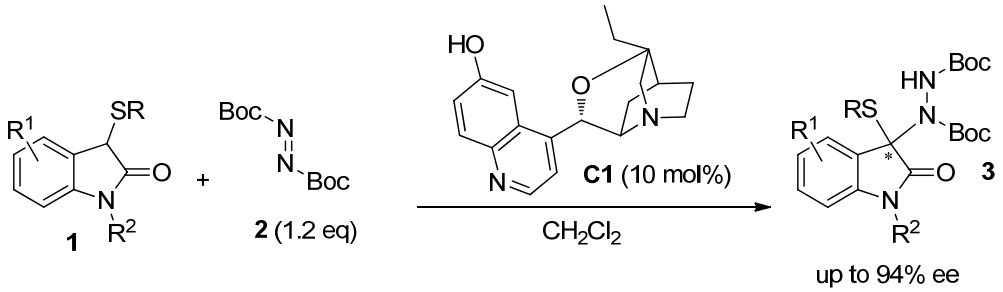



| Entry[a] | Cat. | Solvent | T (°C) | Yield[b] (%) | Ee[c] (%) |
|---|---|---|---|---|---|
| 1 | **C1** | $CH_2Cl_2$ | -40 | 97 | 92 |
| 2 | **C2** | $CH_2Cl_2$ | -40 | 57 | 40 |
| 3 | **C3** | $CH_2Cl_2$ | -40 | 61 | 30 |
| 4 | **C4** | $CH_2Cl_2$ | -40 | 46 | 78 |
| 5 | **C5** | $CH_2Cl_2$ | -40 | 85 | 33 |
| 6 | **C6** | $CH_2Cl_2$ | -40 | 52 | 46 |
| 7 | **C7** | $CH_2Cl_2$ | -40 | 33 | 15 |
| 8 | **C1** | THF | -40 | 97 | 86 |
| 9 | **C1** | Toluene | -40 | 87 | 82 |
| 10 | **C1** | Acetone | -40 | 97 | 76 |
| 11 | **C1** | $CH_3CN$ | -40 | 96 | 76 |
| 12 | **C1** | EtOAc | -40 | 94 | 80 |
| 13 | **C1** | EtOH | -40 | 89 | 24 |
| 14[d] | **C1** | $CH_2Cl_2$ | -80 | 95 | 92 |

[a] 0.1 mmol scale. [b] Isolated yield. [c] Determined by chiral HPLC analysis. [d] 12 h.

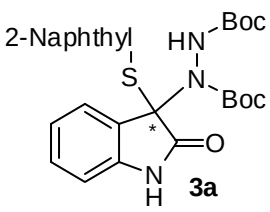
The reaction of 3-(naphthalen-2-ylthio)indolin-2-one **1a** and di-*tert*-butyl azodicarboxylate (DBAD) **2** was chosen for optimization, using $CH_2Cl_2$ as the solvent at -10 °C in the presence of 10 mol% catalyst. The reaction could finish within 9 hours when using cinchona alkaloid derivatives as the catalyst (entries 1-7).The Hatakeyama's catalyst β-ICD **C1** could afford the desired product **3a** in 97% yield with 92% ee (entry 1). The solvent effects were then studied. Of several typical solvents we tried, $CH_2Cl_2$ turned out to be the best one (entry 1 vs entries 8-13). Lowering the temperature to -80 °C had no beneficial effect on the ee (entry 14 vs 1).

**3. General procedure for the amination of 3-thiooxyindoles using DBAD.**



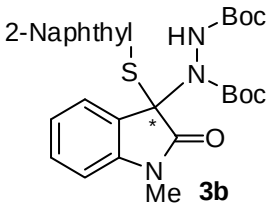

To a 10 mL vial were added catalyst **C1** (7.8 mg, 0.025 mmol) and 3-thiooxindoles **1** (0.25 mmol), followed by the addition of 5.0 mL of anhydrous $CH_2Cl_2$. The reaction mixture was stirred vigorously at room temperature until full dissolution of 3-thiooxindoles **1**, and then cooled to -40 $^oC$ and kept stirring for about 30 min before DBAD **2** (69.0 mg, 0.30 mmol) was added. After the full conversion of 3-thiooxindoles **1** by TLC analysis, the mixture was directly subjected to column chromatography using $CH_2Cl_2$/EtOAc (from 15:1 to 10:1) as the eluent, affording the desired product **3**.

**It should be noted that due to the distinct presence of rotameric isomers, the $^1$H NMR and $^{13}$C NMR contained extra peaks, as reported in the related work.[3]**



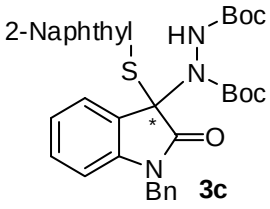

Compound **3a** was obtained in 97% yield as white solid, Mp: 115-117 $^oC$. IR (neat): 1731, 1699, 1618, 1473, 1246, 1153 $cm^{-1}$. HPLC analysis (Chiralcel IC, 10% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 13.77 min, $t_r$ (minor) = 8.43 min) gave the isomeric composition of the product: 92% ee. $[\alpha]_D^{20}$ = +54.8 (c = 0.89, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$): δ = 7.76 (d, *J* = 8.0 Hz, 1H), 7.68-7.66 (m, 2H), 7.54 (d, *J* = 4.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.42-7.34 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.06-6.97 (m, 2H), 6.92 (s, 1H), 6.36 (d, *J* = 4.0 Hz, 1H), 1.54 (s, 9H), 1.15 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 176.04, 155.39, 152.37, 139.33, 137.95, 133.39, 133.07, 132.94, 129.05, 128.04, 127.57, 127.38, 127.20, 126.12, 125.78, 122.82, 109.67, 83.17, 81.43, 76.19, 28.30, 27.66. MS (EI): 521 ($M^+$, 1), 57 (100), 160 (82), 206 (73), 162 (46), 115 (39), 161 (30), 159 (18). HRMS (EI): Exact mass calcd for $C_{28}H_{31}N_3O_5S$ $[M]^+$: 521.1984, Found: 521.1987.

[3] a) R. Matsubara, S. Kobayashi, *Angew. Chem.* **2006**, *118*, 8161; *Angew. Chem. Int. Ed.* **2006**, *45*, 7993; b) T. B. Poulsen, C. Alemparte, K. A. Jørgensen, *J. Am. Chem. Soc.* **2005**, *127*, 11614; c) S. Saaby, M. Bella, K. A. Jørgensen, *J. Am. Chem. Soc.* **2004,** *126*, 8120.



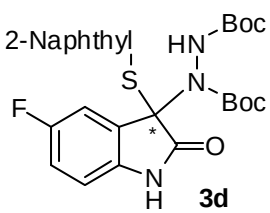
**3b**

Compound **3b** was obtained in 96% yield as white solid, Mp: 90-92 $^{o}$C. IR (neat): 1729, 1692, 1612, 1472, 1246, 1148 cm$^{-1}$. HPLC analysis (Chiralcel OD-H, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 5.67 min, $t_r$ (minor) = 12.75 min) gave the isomeric composition of the product: 82% ee. $[\alpha]_D^{20}$ = +20.4 (c = 1.14, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$): δ = 7.93 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.60-7.54 (m, 3H), 7.48-7.42 (m, 2H), 7.14-7.09 (m, 3H), 6.96 (s, 1H), 6.23-6.21 (m, 1H), 2.66 (s, 3H), 1.60 (s, 9H), 1.15 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.40, 155.35, 152.06, 141.69, 137.70, 133.23, 133.01, 132.75, 128.92, 127.86, 127.27, 127.11, 126.02, 125.43, 125.28, 122.90, 107.05, 82.69, 81.45, 75.85, 28.21, 27.62, 25.70. HRMS (ESI): Exact mass calcd for $C_{29}H_{33}N_3NaO_5S$ $[M+Na]^+$: 558.2039, Found: 558.2046.



**3c**

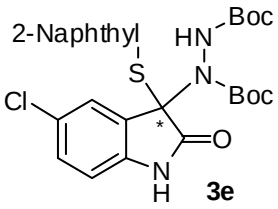
Compound **3c** was obtained in 92% yield as white solid, Mp: 91-93 $^{o}$C. IR (neat): 1700, 1612, 1486, 1392, 1245, 1159 cm$^{-1}$. HPLC analysis (Chiralcel OZ-H, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 10.21 min, $t_r$ (minor) = 7.77 min) gave the isomeric composition of the product: 79% ee. $[\alpha]_D^{20}$ = +11.5 (c = 1.30, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.71 (s, 1H), 7.57 (d, *J* = 16.0 Hz, 1H), 7.52-7.50 (m, 2H), 7.46-7.44 (m, 1H), 7.15-7.12 (m, 3H), 7.08-7.02 (m, 5H), 6.96 (s, 1H), 6.32 (d, *J* = 8.0 Hz, 1H), 4.59 (ABd, J = 16 Hz, 1H), 4.54 (ABd, J = 16 Hz, 1H), 1.61 (s, 9H), 1.18 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.60, 155.28, 152.22, 141.33, 137.80, 133.39, 132.97, 132.95, 128.90, 128.35, 128.01, 127.50, 127.41, 127.18, 127.02, 126.14, 108.46, 82.64, 81.38, 75.69, 44.07, 28.27, 27.72. HRMS (ESI): Exact mass calcd for $C_{35}H_{37}N_3NaO_5S$ $[M+Na]^+$: 634.2352, Found: 634.2356.



**3d**

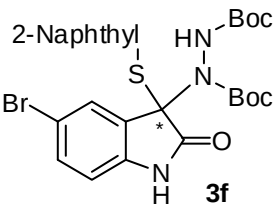
Compound **3d** was obtained in 95% yield as white solid, Mp: 123-125 $^{o}$C. IR (neat): 1732, 1700, 1482, 1246, 1148 cm$^{-1}$. HPLC analysis (Chiralcel OZ-H, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 14.00 min, $t_r$ (minor) = 16.44 min) gave the isomeric composition of the product: 94% ee. $[\alpha]_D^{20}$ = +46.2 (c = 1.26, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.82-7.73 (m, 2H), 7.69 (d, *J* = 4.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.50-7.39 (m, 3H), 7.23 (d, *J* =

8.0 Hz, 1H), 6.96-6.94 (m, 1H), 6.82-6.81 (m, 1H), 6.35-6.32 (m, 1H), 1.60 (s, 9H), 1.25 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.92, 160.36, 157.97, 155.39, 152.40, 138.02, 133.49, 132.99, 128.05, 127.76, 127.46, 127.39, 126.30, 125.01, 115.62, 115.38, 113.87, 113.62, 110.26, 110.18, 83.46, 81.68, 76.22, 28.30, 27.75. HRMS (ESI): Exact mass calcd for $C_{28}H_{30}FN_3NaO_5S$ $[M+Na]^+$: 562.1788, Found: 562.1762.



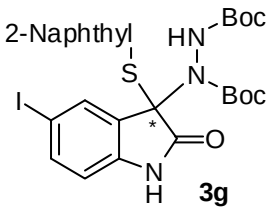
**3e**

Compound **3e** was obtained in 82% yield as white solid, Mp: 120-122 °C. IR (neat): 1730, 1699, 1619, 1475, 1247, 1146 $cm^{-1}$. HPLC analysis (Chiralcel IC, 10% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 10.65 min, $t_r$ (minor) = 7.45 min) gave the isomeric composition of the product: 91% ee. $[\alpha]_D^{20}$ = -73.7 (c = 1.04, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.85 (s, 1H), 7.76-7.74 (m, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.51-7.45 (m, 2H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.09-7.07 (m, 1H), 6.93 (s, 1H), 6.34 (d, *J* = 8.0 Hz, 1H), 1.61 (s, 9H), 1.26 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.59, 155.30, 152.47, 138.12, 137.87, 133.48, 132.97, 129.02, 128.11, 128.06, 127.78, 127.43, 126.31, 126.14, 124.97, 110.67, 83.50, 81.64, 76.02, 28.30, 27.76. HRMS (ESI): Exact mass calcd for $C_{28}H_{30}ClN_3NaO_5S$ $[M+Na]^+$: 578.1492, Found: 578.1497.



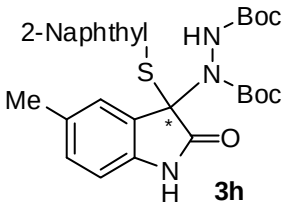
**3f**

Compound **3f** was obtained in 89% yield as white solid, Mp: 124-126 °C. IR (neat): 1731, 1616, 1473, 1367, 1247, 1155 $cm^{-1}$. HPLC analysis (Chiralcel IC, 10% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 12.20 min, $t_r$ (minor) = 7.94 min) gave the isomeric composition of the product: 92% ee. $[\alpha]_D^{20}$ = -88.8 (c = 1.07, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.95 (s, 1H), 7.79-7.75 (m, 2H), 7.66-7.58 (m, 2H), 7.51-7.45 (m, 3H), 7.23-7.21 (m, 2H), 6.92 (s, 1H), 6.30 (d, *J* = 8.0 Hz, 1H), 1.61 (s, 9H), 1.26 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.43, 155.24, 152.48, 138.33, 138.16, 133.49, 132.97, 131.91, 128.88, 128.08, 127.78, 127.43, 126.32, 125.00, 115.35, 111.14, 83.52, 81.64, 75.97, 28.31, 27.77. HRMS (ESI): Exact mass calcd for $C_{28}H_{30}BrN_3NaO_5S$ $[M+Na]^+$: 622.0987, Found: 622.0986.



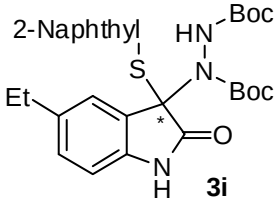

**3g**

Compound **3g** was obtained in 78% yield as white solid, Mp: 128-130 $^{o}$C. IR (neat): 1801, 1699, 1612, 1473, 1248, 1160 cm$^{-1}$. HPLC analysis (Chiralcel IC, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 14.23 min, $t_r$ (minor) = 8.39 min) gave the isomeric composition of the product: 91% ee. $[\alpha]_D^{20}$ = -130.0 (c = 1.12, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$):see below. $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.33, 155.28, 152.64, 139.05, 138.33, 137.95, 134.53, 133.58, 133.05, 131.34, 128.22, 127.86, 127.54, 126.41, 125.15, 111.80, 85.19, 83.60, 81.69, 76.01, 28.42, 27.88. HRMS (ESI): Exact mass calcd for $C_{28}H_{30}IN_3NaO_5S$ $[M+Na]^+$: 670.0849, Found: 670.0854.




**3h**

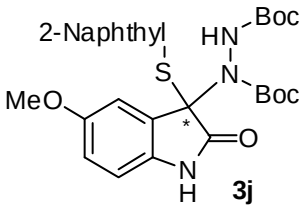
Compound **3h** was obtained in 98% yield as white solid, Mp: 114-116 $^{o}$C. IR (neat): 1800, 1686, 1492, 1394, 1247, 1152 cm$^{-1}$. HPLC analysis (Chiralcel IC, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 22.69 min, $t_r$ (minor) = 10.29 min) gave the isomeric composition of the product: 93% ee. $[\alpha]_D^{20}$ = -10.1 (c = 1.09, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.74 (s, 2H), 7.63-7.56 (m, 2H), 7.53-7.43 (m, 3H), 7.23 (d, *J* = 8.0 Hz, 1H), 6.93-6.91 (m, 2H), 6.36 (d, *J* = 8.0 Hz, 1H), 2.28 (s, 3H), 1.61 (s, 9H), 1.23 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 176.02, 155.32, 152.50, 138.05, 136.78, 133.43, 133.17, 132.96, 132.34, 129.43, 128.06, 127.52, 127.40, 127.21, 126.14, 125.76, 109.44 83.15, 81.35, 76.35, 28.36, 27.72, 21.18. MS (EI): 535 ($M^+$, 1), 220 (100), 160 (82), 57 (66), 176 (65), 115 (42), 159 (39), 175 (33). HRMS (EI): Exact mass calcd for $C_{29}H_{33}N_3O_5S$ $[M]^+$: 535.2141, Found: 535.2139.




**3i**

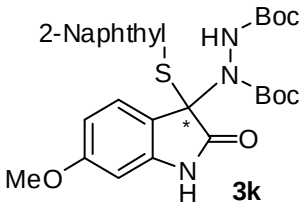
Compound **3i** was obtained in 98% yield as white solid, Mp: 109-111 $^{o}$C. IR (neat): 1722, 1626, 1529, 1366, 1231, 1151 cm$^{-1}$. HPLC analysis (Chiralcel IC, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 20.77 min, $t_r$ (minor) = 10.24 min) gave the isomeric composition of the product: 92% ee. $[\alpha]_D^{20}$ = -9.9 (c = 1.13, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.74-7.72 (m, 2H), 7.61-7.53 (m, 3H), 7.48-7.40 (m, 2H), 7.26-7.23 (m, 2H), 6.96-6.91 (m, 2H), 6.38 (d, *J* = 8.0 Hz, 1H), 2.59-2.45 (m, 2H), 1.61 (s, 9H), 1.21 (s, 9H), 1.13 (t, *J* = 8.0 Hz, 3H). $^{13}$C NMR (100

MHz, $CDCl_3$): δ 176.31, 155.24, 152.56 138.89, 138.04, 133.39, 133.17, 132.94, 128.21, 128.03, 127.51, 127.37, 127.17, 126.09, 125.77, 125.19, 109.52, 83.07, 81.24, 76.49, 28.47, 28.33, 27.67, 15.91. HRMS (ESI): Exact mass calcd for $C_{30}H_{35}N_3NaO_5S$ $[M+Na]^+$: 572.2195, Found: 572.2200.



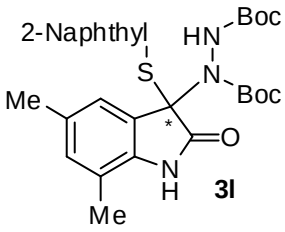
**3j**

Compound **3j** was obtained in 98% yield as white solid, Mp: 115-117 $^oC$. IR (neat): 1719, 1702, 1489, 1283, 1247, 1155 $cm^{-1}$. HPLC analysis (Chiralcel IC, 10% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 17.56 min, $t_r$ (minor) = 9.45 min) gave the isomeric composition of the product: 91% ee. $[\alpha]_D^{20}$ = -16.5 (c = 1.21, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.76-7.72 (m, 2H), 7.63-7.55 (m, 2H), 7.48-7.40 (m, 3H), 7.26-7.23 (m, 1H), 7.00 (s, 1H), 6.69-6.66 (m, 1H), 6.39 (d, *J* = 8.0 Hz, 1H), 3.69 (s, 3H), 1.60 (s, 9H), 1.23 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.97, 155.83, 155.30, 152.43, 138.01, 133.40, 133.14, 132.95, 130.10, 128.04, 127.57, 127.38, 127.23, 126.16, 114.91, 111.87, 110.23, 83.18, 81.33, 55.57, 28.28, 27.71. MS (EI): 551 ($M^+$, 1), 236 (100), 160 (76), 192 (75), 57 (67), 191 (48), 115 (37), 292 (21). HRMS (EI): Exact mass calcd for $C_{29}H_{33}N_3O_6S$ $[M]^+$: 551.2090, Found: 551.2098.

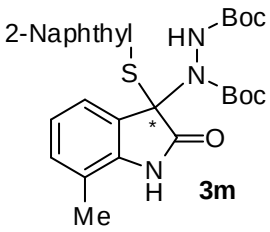


**3k**

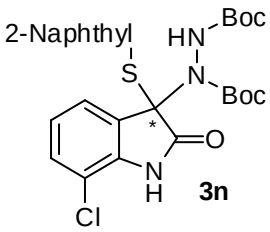
Compound **3k** was obtained in 95% yield as white solid, Mp: 113-115 $^oC$. IR (neat): 1727, 1703, 1626, 1503, 1246, 1153 $cm^{-1}$. HPLC analysis (Chiralcel IC, 10% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 19.29 min, $t_r$ (minor) = 10.94 min) gave the isomeric composition of the product: 83% ee. $[\alpha]_D^{20}$ = +29.5 (c = 1.12, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.96 (s, 1H), 7.76-7.71 (m, 3H), 7.61-7.54 (m, 2H), 7.46-7.39 (m, 2H), 7.26-7.23 (m, 1H), 6.95 (s, 1H), 6.58-6.56 (m, 1H), 6.04 (d, *J* = 4.0 Hz, 1H), 3.69 (s, 3H), 1.60 (s, 9H), 1.23 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 176.23, 160.77, 155.33, 152.41, 140.81, 137.84, 133.34, 133.10, 132.97, 128.04, 127.54, 127.38, 127.11, 126.85, 126.08, 125.80, 120.88, 108.06, 96.39, 83.01, 81.42, 76.15, 55.29, 28.30, 27.73. HRMS (ESI): Exact mass calcd for $C_{29}H_{33}N_3NaO_6S$ $[M+Na]^+$: 574.1988, Found: 574.1968.




Compound **3l** was obtained in 97% yield as white solid, Mp: 124-126 $^{o}$C. IR (neat): 1709, 1625, 1481, 1245, 1151 cm$^{-1}$. HPLC analysis (Chiralcel IC, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 25.01 min, $t_r$ (minor) = 9.59 min) gave the isomeric composition of the product: 92% ee. $[\alpha]_D^{20}$ = +41.8 (c = 1.17, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.75-7.73 (m, 2H), 7.63-7.56 (m, 2H), 7.49-7.38 (m, 3H), 7.29-7.27 (d, J = 8.0 Hz, 1H), 6.91 (s, 1H), 6.75 (s, 1H), 2.27 (s, 3H), 1.79 (s, 3H), 1.62 (s, 9H), 1.20 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 176.32, 155.24, 152.54, 137.79, 135.53, 133.37, 133.09, 132.90, 132.17, 130.84, 128.89, 127.99, 127.39, 127.32, 127.13, 126.07, 123.23, 118.73, 82.99, 81.23, 28.36, 27.63, 21.10, 15.61. MS (EI): 549 ($M^+$, 1), 234 (100), 190 (73), 57 (55), 160 (52), 189 (27), 115 (23), 290 (22). HRMS (EI): Exact mass calcd for $C_{30}H_{35}N_3O_5S$ $[M]^+$: 549.2297, Found: 549.2296.

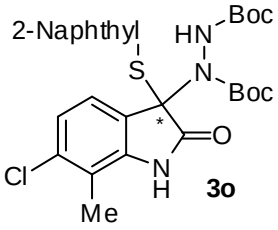



Compound **3m** was obtained in 98% yield as white solid, Mp: 120-122 $^{o}$C. IR (neat): 1720, 1708, 1245, 1149, 744 cm$^{-1}$. HPLC analysis (Chiralcel IC, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 15.56 min, $t_r$ (minor) = 8.32 min) gave the isomeric composition of the product: 92% ee. $[\alpha]_D^{20}$ = +88.1 (c = 1.06, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.75-7.72 (m, 2H), 7.66 (d, *J* = 4.0 Hz, 1H), 7.62-7.55 (m, 2H), 7.49-7.42 (m, 2H), 7.27 (d, *J* = 8.0 Hz, 1H),7.00-6.93 (m, 3H), 1.80 (s, 3H), 1.61 (s, 9H), 1.19 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 176.29, 155.30, 152.39, 138.02, 137.71, 133.37, 133.02, 132.91, 130.29, 128.93, 128.01, 127.48, 127.34, 127.16, 126.09, 125.88, 122.92, 122.76, 118.99, 83.05, 81.37, 76.52, 28.32, 27.61, 15.64. HRMS (ESI): Exact mass calcd for $C_{29}H_{33}N_3NaO_5S$ $[M+Na]^+$: 558.2039, Found: 558.2053.



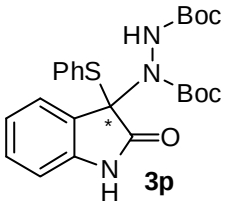

Compound **3n** was obtained in 68% yield as white solid, Mp: 99-101 $^{o}$C. IR (neat): 1729, 1701, 1619, 1476, 1149 cm$^{-1}$. HPLC analysis (Chiralcel IC, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 14.61 min, $t_r$ (minor) = 6.86 min) gave the isomeric composition of the product: 88% ee. $[\alpha]_D^{20}$ = +74.5 (c = 0.51, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.79-7.77 (m, 2H), 7.72 (d, *J* =

8.0 Hz, 1H), 7.67-7.61 (m, 2H), 7.52-7.45 (m, 2H), 7.24-7.22 (m, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 4.0 Hz, 1H), 1.61 (s, 9H), 1.23 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.35, 155.37, 152.23, 137.98, 133.58, 133.02, 132.87, 128.75, 128.03, 127.82, 127.50, 127.41, 126.30, 124.13, 114.64, 83.53, 81.69, 76.44, 28.33, 27.69. HRMS (ESI): Exact mass calcd for $C_{28}H_{30}ClN_3NaO_5S$ $[M+Na]^+$: 578.1492, Found: 578.1504.



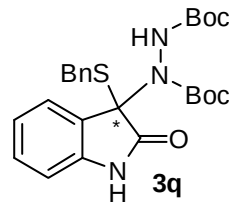
**3o**

Compound **3o** was obtained in 88% yield as white solid, Mp: 127-129 °C. IR (neat): 1800, 1697, 1247, 1150, 1004 $cm^{-1}$. HPLC analysis (Chiralcel IC, 10% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 8.01 min, $t_r$ (minor) = 6.15 min) gave the isomeric composition of the product: 92% ee. $[\alpha]_D^{20}$ = +81.5 (c = 1.03, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.77-7.73 (m, 2H), 7.63-7.58 (m, 3H), 7.51-7.43 (m, 2H), 7.31-7.26 (m, 2H), 7.08 (d, *J* = 8.0 Hz, 1H), 6.90 (br, 1H), 1.78 (s, 3H), 1.61 (s, 9H), 1.23 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 176.14, 155.34, 152.36, 139.28, 137.93, 135.00, 133.46, 132.93, 128.00, 127.74, 127.43, 127.39, 126.31, 125.46, 123.76, 123.31, 117.75, 83.30, 81.59, 76.45, 28.33, 27.70, 13.15. HRMS (ESI): Exact mass calcd for $C_{29}H_{32}ClN_3NaO_5S$ $[M+Na]^+$: 592.1649, Found: 592.1648.

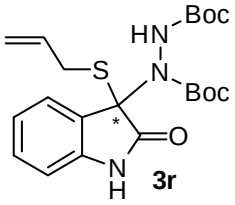


**3p**

Compound **3p** was obtained in 97% yield as white solid, Mp: 96-98 °C. IR (neat): 1726, 1698, 1620, 1473, 1245, 1151 $cm^{-1}$. HPLC analysis (Chiralcel IC, 5% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 22.11 min, $t_r$ (minor) = 16.30 min) gave the isomeric composition of the product: 90% ee. $[\alpha]_D^{20}$ = +47.8 (c =1.12, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$): δ = 8.00 (br, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.31-7.26 (m, 1H), 7.23-7.21 (m, 2H), 7.15-7.11 (m, 3H), 7.04-6.94 (m, 2H), 6.55 (d, *J* = 8.0 Hz, 1H), 1.59 (s, 9H), 1.22 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 176.16, 155.35, 152.38, 139.32, 137.38, 129.85, 129.11, 128.98, 128.24, 128.14, 125.80, 122.72, 109.58, 83.13, 81.37, 76.22, 28.27, 27.69. HRMS (ESI): Exact mass calcd for $C_{24}H_{29}N_3NaO_5S$ $[M+Na]^+$: 494.1726, Found: 494.1736.

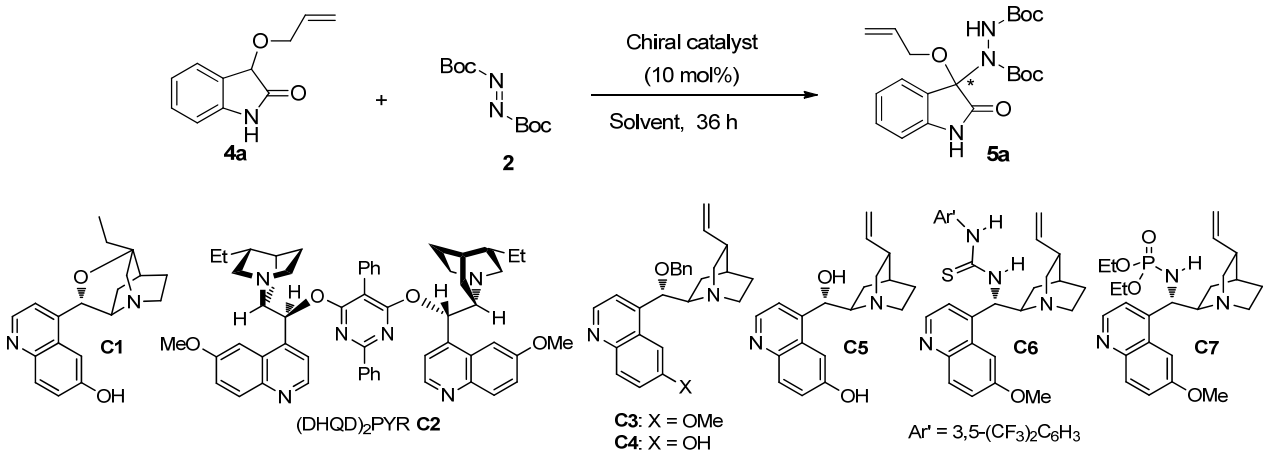



Compound **3q** was obtained in 88% yield as white solid, Mp: 109-111 $^{o}$C. IR (neat): 1725, 1619, 1473, 1367, 1244, 1153 cm$^{-1}$. HPLC analysis (Chiralcel OZ-H, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 11.06 min, $t_r$ (minor) = 16.89 min) gave the isomeric composition of the product: 56% ee. $[\alpha]_D^{20}$ = +17.6 (c = 0.91, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$): δ = 8.00 (br, 1H), 7.82 (d, *J* = 4.0 Hz, 1H), 7.33-7.31 (m, 2H), 7.30-7.26 (m, 2H), 7.24-7.21 (m, 2 H), 7.05 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.67 (s, 1H), 4.03 (ABd, *J* = 12.0 Hz, 1 H), 4.00 (ABd, *J* = 12.0 Hz, 1 H), 1.54 (s, 9H), 1.23 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.20, 155.67, 152.73, 138.88, 136.14, 129.46, 129.39, 129.09, 128.52, 127.31, 124.86, 122.99, 110.03, 83.11, 81.16, 73.17, 34.58, 28.26, 27.73. HRMS (ESI): Exact mass calcd for $C_{25}H_{31}N_3NaO_5S$ $[M+Na]^+$: 508.1882, Found: 508.1889.




Compound **3r** was obtained in 82% yield as white solid, Mp: 88-90 $^{o}$C. IR (neat): 1792, 1695, 1620, 1395, 1249, 1154 cm$^{-1}$. HPLC analysis (Chiralcel OZ-H, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 9.11 min, $t_r$ (minor) = 11.25 min) gave the isomeric composition of the product: 47% ee. $[\alpha]_D^{20}$ = +21.8 (c =1.01, $CHCl_3$). $^1$H NMR (400 MHz, $CDCl_3$): δ = 8.13 (br, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.23 (t, *J* = 8.0 Hz, 1H), 7.06 (t, *J* = 8.0 Hz, 1H), 6.94 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 5.84-5.74 (m, 1H), 5.21 (d, *J* = 16 Hz, 1H), 5.10 (d, *J* = 8.0 Hz, 1H), 3.51-3.41 (m, 2H), 1.56 (s, 9H), 1.22 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.56, 155.66, 152.75, 138.86, 132.51, 129.10, 128.86, 124.91, 122.97, 118.80, 110.02, 83.16, 81.23, 72.64, 32.74, 28.27, 27.72. MS (EI): 435 ($M^+$, 1), 57 (100), 206 (97), 162 (66), 204 (35), 145 (16), 161 (14), 262 (13). HRMS (EI): Exact mass calcd for $C_{21}H_{29}N_3O_5S$ $[M]^+$: 435.1828, Found: 435.1827.

## 4. Condition optimization for the amination of 3-alkoxyoxindoles

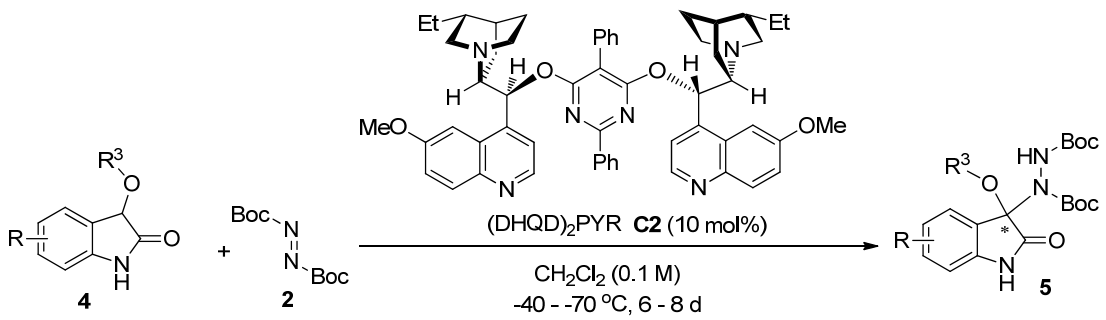



| Entry[a] | Cat. | Solvent | T (°C) | Yield[b] (%) | Ee[c] (%) |
|---|---|---|---|---|---|
| 1 | **C1** | $CH_2Cl_2$ | -10 | 60 | 25 |
| 2 | **C2** | $CH_2Cl_2$ | -10 | 77 | 83 |
| 3 | **C3** | $CH_2Cl_2$ | -10 | 42 | 36 |
| 4 | **C4** | $CH_2Cl_2$ | -10 | 31 | 16 |
| 5 | **C5** | $CH_2Cl_2$ | -10 | 54 | 21 |
| 6 | **C6** | $CH_2Cl_2$ | -10 | 32 | 48 |
| 7 | **C7** | $CH_2Cl_2$ | -10 | 19 | 25 |
| 8 | **C2** | THF | -10 | 57 | 20 |
| 9 | **C2** | Toluene | -10 | 72 | 59 |
| 10 | **C2** | Acetone | -10 | 82 | 20 |
| 11 | **C2** | $CH_3CN$ | -10 | 82 | 45 |
| 12 | **C2** | EtOAc | -10 | 72 | 31 |
| 13 | **C2** | EtOH | -10 | 79 | 10 |
| 14[d] | **C2** | $CH_2Cl_2$ | -40 | 77 | 90 |

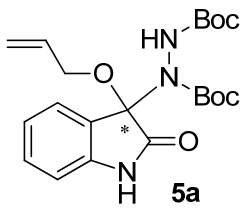
[a] 0.1 mmol scale. [b] Isolated yield. [c] Determined by chiral HPLC analysis. [d] 6 day.

Since catalyst **C1**, used for the the amination reaction of 3-thiooxindoles **1**, failed to achieve high ee in the reaction of 3-allyloxyoxindole **4a** and DBAD **2**, a variety of catalysts were further evaluated, and the results were summarized in the above Table (entries 1-7). Brønsted base catalyst **C2** turned out to be the most effective one, which could afford the product in 77% yield with 83% ee (entry 7). The solvent effect was further examined using catalyst **C2**, $CH_2Cl_2$ was found to be the best. Lowering the temperature to -40 °C could promote the reaction to 90% ee (entry 10).

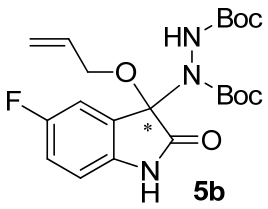
**5. General procedure for the amination of 3-alkoxyoxyindoles using DBAD.**




To a 5 mL vial were added catalyst **C2** (22.0 mg, 0.025 mmol) and 3-alkoxyoxyindoles **4** (0.25 mmol), followed by the addition of 2.5 mL of anhydrous $CH_2Cl_2$. The reaction mixture was stirred vigorously at room temperature until the full dissolution of 3-alkoxyoxyindoles **4**. The resulting mixture was stirred at indicated temperature for about 30 min before DBAD **2** (69.0 mg, 0.30 mmol) was added. After the full conversion of 3-alkoxyoxyindoles **4** by TLC analysis, the mixture was directly subjected to column chromatography using $CH_2Cl_2$/EtOAc (from 15:1 to 10:1) as the eluent, affording the desired product **5**.

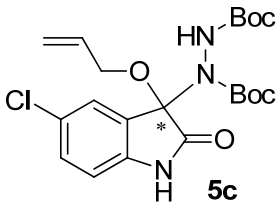



Compound **5a** was obtained in 77% yield as white solid, Mp: 79-81 °C. IR (neat): 1730, 1705, 1473, 1247, 1156 $cm^{-1}$. HPLC analysis (Chiralcel IC, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 19.22 min, $t_r$ (minor) = 15.65 min) gave the isomeric composition of the product: 90% ee. $[\alpha]_D^{20}$ = -8.9 (c = 0.80, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.91 (br, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.30-7.27 (m, 1H), 7.08 (t, *J* = 8.0 Hz, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.79(br, 1H), 5.86-5.78 (m, 1H), 5.25-5.21 (m, 1H), 5.13-5.10 (m, 1H), 4.20 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 4.06 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 1.54 (s, 9H), 1.26 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.62, 155.55, 152.95, 141.31, 133.35, 130.23, 126.34, 122.66, 117.00, 110.49, 88.73, 82.81, 81.08, 67.04, 28.21, 27.75. MS (EI): 419 ($M^+$, 1), 188 (100), 57 (82), 148 (38), 160 (35), 189 (20), 161 (10), 120 (9). HRMS (EI): Exact mass calcd for $C_{21}H_{29}N_3O_6$ $[M]^+$: 419.2056, Found: 419.2059.



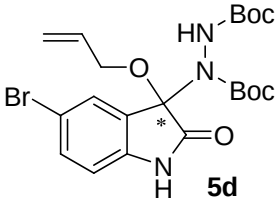
**5b**

Compound **5b** was obtained in 70% yield as white solid, Mp: 88-90 $^{o}$C. IR (neat): 1735, 1486, 1368, 1249, 1151 cm$^{-1}$. HPLC analysis (Chiralcel IC, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 16.42 min, $t_r$ (minor) = 14.05 min) gave the isomeric composition of the product: 92% ee. $[\alpha]_D^{20}$ = -6.7 (c = 1.03, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.09 (br, 1H), 7.60-7.58 (m, 1H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.77-6.75 (m, 2H), 5.85-5.79 (1H), 5.27-5.23 (m, 1H), 5.15-5.12 (m, 1H), 4.18 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 4.10 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 1.54 (s, 9H), 1.30 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.50, 160.26, 157.86, 155.58, 153.02, 137.24, 133.15, 128.05, 127.97, 117.32, 116.80, 116.56, 114.50, 114.25, 111.21, 111.14, 88.73, 83.17, 81.38, 67.09, 28.25, 27.89. MS (EI): 437 ($M^+$, 1), 57 (100), 206 (90), 166 (41), 178 (26), 207 (23), 138 (9), 116 (9). HRMS (EI): Exact mass calcd for $C_{21}H_{28}N_3O_6F$ $[M]^+$: 437.1962, Found: 437.1963.



**5c**

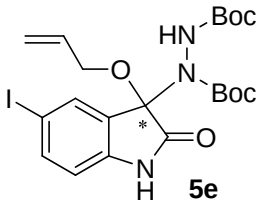
Compound **5c** was obtained in 80% yield as white solid, Mp: 90-92 $^{o}$C. IR (neat): 1733, 1708, 1476, 1367, 1152 cm$^{-1}$. HPLC analysis (Chiralcel IC, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 17.35 min, $t_r$ (minor) = 14.59 min) gave the isomeric composition of the product: 93% ee. $[\alpha]_D^{20}$ = -5.9 (c = 1.05, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.30-8.27 (m, 1H), 7.75 (s, 1H), 7.51-7.24 (m, 1H), 6.78-6.49 (m, 2H), 5.87-5.79 (m, 1H), 5.28-5.23 (m, 1H), 5.16-5.13 (m, 1H), 4.20 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 4.09 (dd, *J* = 12.0 Hz, *J* = 8.0 Hz, 1H), 1.54 (s, 9H), 1.31 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.13, 155.46, 153.11, 139.87, 133.10, 130.28, 128.10, 128.00, 126.56, 117.43, 111.65, 88.52, 83.24, 81.40, 67.11, 28.26, 27.91. MS (EI): 453 ($M^+$, 1), 57 (100), 222 (64), 182 (27), 224 (22), 223 (16), 194 (15), 184 (9). HRMS (EI): Exact mass calcd for $C_{21}H_{28}N_3O_6Cl$ $[M]^+$: 453.1667, Found: 453.1665.



**5d**

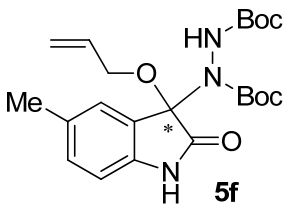
Compound **5d** was obtained in 86% yield as white solid, Mp: 99-101 $^{o}$C. IR (neat): 1734, 1708, 1475, 1367, 1156 cm$^{-1}$. HPLC analysis (Chiralcel IC, 5% $^{i}$PrOH/hexane, 0.8 mL/min, 230 nm; $t_r$ (major) = 17.98 min, $t_r$ (minor) = 15.12 min) gave the isomeric composition of the product: 93% ee. $[\alpha]_D^{20}$ = -6.2 (c = 1.02, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.48 (br, 1H),

7.86 (d, $J$ = 4.0 Hz, 1H), 7.40-7.37 (m, 1H), 6.82 (br, 1H), 6.73-6.69 (m, 1H), 5.87-5.79 (m, 1H), 5.28-5.23 (m, 1H), 5.16-5.13 (m, 1H), 4.21 (dd, $J$ = 12.0 Hz, $J$ = 4.0 Hz, 1H), 4.09 (dd, $J$ = 12.0 Hz, $J$ = 8.0 Hz, 1H), 1.54 (s, 9H), 1.30 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.95, 155.42, 153.16, 140.38, 133.19, 133.11, 129.22, 128.33, 117.45, 115.36, 112.16, 88.46, 83.26, 81.40, 67.10, 28.28, 27.92. MS (EI): 497 ($M^+$, 1), 57 (100), 266 (45), 268 (44), 226 (19), 228 (16), 267 (11), 269 (11). HRMS (EI): Exact mass calcd for $C_{21}H_{28}N_3O_6Br$ $[M]^+$: 497.1161, Found: 497.1165.



**5e**

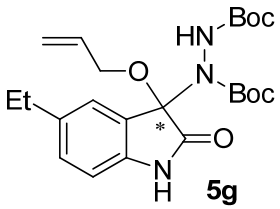
Compound **5e** was obtained in 67% yield as white solid, Mp: 98-100 °C. IR (neat): 1736, 1707, 1476, 1366, 1154 $cm^{-1}$. HPLC analysis (Chiralcel IC, 5% $^i$PrOH/hexane, 0.8 mL/min, 230 nm; $t_r$ (major) = 20.25 min, $t_r$ (minor) = 17.15 min) gave the isomeric composition of the product: 93% ee. $[\alpha]_D^{20}$ = -8.2 (c = 1.05, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.22 (br, 1H), 7.99 (m, 1H), 7.60-7.58 (m, 1H), 6.77 (s, 1H), 6.61 (d, $J$ = 8.0 Hz, 1H), 5.88-5.79 (m, 1H), 5.28-5.23 (m, 1H), 5.16-5.14 (m, 1H), 4.22 (dd, $J$ = 12.0 Hz, $J$ = 4.0 Hz, 1H), 4.08 (dd, $J$ = 12.0 Hz, $J$ = 8.0 Hz, 1H), 1.54 (s, 9H), 1.31 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.48, 155.23, 153.11, 140.87, 139.09, 134.62, 133.07, 128.50, 117.42, 112.58, 88.15, 85.14, 83.18, 81.34, 66.96, 28.22, 27.84. MS (EI): 545 ($M^+$, 1), 57 (100), 314 (77), 274 (25), 315 (20), 187 (16), 286 (12), 287 (11). HRMS (EI): Exact mass calcd for $C_{21}H_{28}N_3O_6I$ $[M]^+$: 545.1023, Found: 545.1024.



**5f**

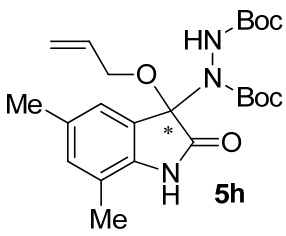
Compound **5f** was obtained in 79% yield as white solid, Mp: 88-90 °C. IR (neat): 1737, 1707, 1494, 1367, 1157 $cm^{-1}$. HPLC analysis (Chiralcel IC, 5% $^i$PrOH/hexane, 0.8 mL/min, 230 nm; $t_r$ (major) = 28.11 min, $t_r$ (minor) = 22.69 min) gave the isomeric composition of the product: 86% ee. $[\alpha]_D^{20}$ = -8.2 (c = 1.00, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.50-7.48 (m, 2H), 7.07 (d, $J$ = 8.0 Hz, 1H), 6.71-6.69 (m, 2H), 5.85-5.75 (m, 1H), 5.25-5.20 (m, 1H), 5.11-5.09 (m, 1H), 4.19 (dd, $J$ = 12.0 Hz, $J$ = 4.0 Hz, 1H), 4.03 (dd, $J$ = 12.0 Hz, $J$ = 4.0 Hz, 1H), 2.33 (s, 3H), 1.52 (s, 9H), 1.26 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.59, 155.45, 153.10, 138.75, 133.44, 132.14, 130.54, 126.77, 126.36, 117.00, 110.20, 88.81, 82.75, 80.99, 66.93, 28.23, 27.78,

21.11. MS (EI): 433 ($M^+$, 1), 202 (100), 57 (65), 174 (37), 162 (34), 203 (18), 132 (13), 146 (12). HRMS (EI): Exact mass calcd for $C_{22}H_{31}N_3O_6$ $[M]^+$: 433.2213, Found: 433.2214.



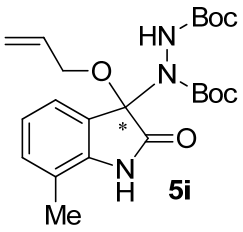
**5g**

Compound **5g** was obtained in 71% yield as white solid, Mp: 77-79 $^oC$. IR (neat): 1728, 1707, 1491, 1367, 1155 $cm^{-1}$. HPLC analysis (Chiralcel ADH, 10% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 10.16 min, $t_r$ (minor) = 13.83 min) gave the isomeric composition of the product: 86% ee. $[\alpha]_D^{20}$ = -5.5 (c = 0.98, $CHCl_3$). $^1H$ NMR (400 MHz, $DCl_3$): δ = 7.66 (br, 1H), 7.53 (br, 1H), 7.09 (d, *J* = 4.0 Hz, 1H), 6.74-6.72 (m, 2H), 5.85-5.75 (m, 1H), 5.24-5.20 (m, 1H), 5.11-5.08 (m, 1H), 4.23-4.18 (m, 1H), 4.06-4.01 (m, 1H), 2.66-2.62 (m, 2H), 1.52 (s, 9H), 1.24-1.19 (m, 12H). $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 174.61, 155.39, 153.17, 138.91, 138.81, 133.48, 129.34, 126.43, 125.80, 117.00, 110.25, 88.84, 82.73, 80.97, 66.94, 28.48, 28.25, 27.77, 15.86. MS (EI): 447 ($M^+$, 1), 216 (100), 57 (68), 188 (35), 176 (31), 217 (18), 146 (15), 174 (14). HRMS (EI): Exact mass calcd for $C_{23}H_{33}N_3O_6$ $[M]^+$: 447.2369, Found: 447.2368.



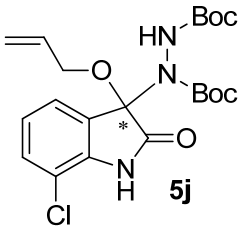
**5h**

Compound **5h** was obtained in 50% yield as white solid, Mp: 97-99 $^oC$. IR (neat): 1731, 1689, 1484, 1247, 1157 $cm^{-1}$. HPLC analysis (Chiralcel IC, 5% $^i$PrOH/hexane, 0.8 mL/min, 230 nm; $t_r$ (major) = 23.93 min, $t_r$ (minor) = 21.11 min) gave the isomeric composition of the product: 88% ee. $[\alpha]_D^{20}$ = -6.5 (c = 0.98, $CHCl_3$). $^1H$ NMR (400 MHz, $DCl_3$): δ = 7.78 (s, 1H), 7.34 (s, 1H), 6.91 (s, 1H), 6.71 (s, 1H), 5.85-5.76 (m, 1H), 5.25-5.20 (m, 1H), 5.11-5.09 (m, 1H), 4.19 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 4.02 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 2.30 (s, 3H), 2.17 (s, 3H), 1.52 (s, 9H), 1.23 (s, 9H). $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 175.19, 155.42, 153.09, 137.37, 133.52, 132.08, 132.03, 126.13, 124.15, 119.22, 117.00, 89.22, 82.71, 80.96, 67.01, 28.24, 27.71, 21.05, 15.99. MS (EI): 447 ($M^+$, 1), 216 (100), 57 (54), 188 (40), 176 (31), 146 (18), 217 (17), 160 (12). HRMS (EI): Exact mass calcd for $C_{23}H_{33}N_3O_6$ $[M]^+$: 447.2369, Found: 447.2366.



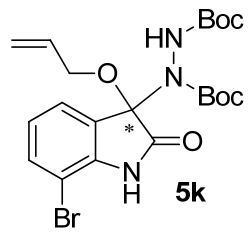
**5i**

Compound **5i** was obtained in 73% yield as white solid, Mp: 88-90 $^{o}$C. IR (neat): 1726, 1392, 1367, 1247, 1153 cm$^{-1}$. HPLC analysis (Chiralcel IC, 5% $^{i}$PrOH/hexane, 0.8 mL/min, 230 nm; $t_r$ (major) = 19.79 min, $t_r$ (minor) = 17.22 min) gave the isomeric composition of the product: 90% ee. $[\alpha]_D^{20}$ = -10.5 (c = 1.07, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.36 (br, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.98 (t, *J* = 8.0 Hz, 1H), 6.74 (s, 1H), 5.84-5.75 (m, 1H), 5.24-5.23 (m, 1H), 5.11-5.08 (m, 1H), 4.18 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 4.03 (dd, *J* = 12.0 Hz, *J* = 4.0 Hz, 1H), 2.22 (s, 3H), 1.52 (s, 9H), 1.22 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.28, 155.50, 152.90, 139.90, 133.43, 131.57, 126.12, 123.75, 122.58, 119.55, 117.00, 89.13, 82.75, 81.04, 67.12, 28.21, 27.68, 16.04. MS (EI): 433 ($M^+$, 1), 202 (100), 57 (70), 174 (37), 162 (36), 203 (18), 132 (11). HRMS (EI): Exact mass calcd for $C_{22}H_{31}N_3O_6$ $[M]^+$: 433.2213, Found: 433.2212.



**5j**

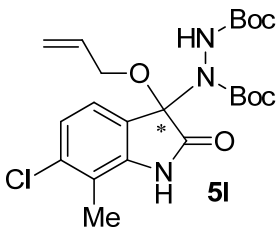
Compound **5j** was obtained in 97% yield as white solid, Mp: 85-87 $^{o}$C. IR (neat): 1736, 1621, 1476, 1246, 1150 cm$^{-1}$. HPLC analysis (Chiralcel ODH, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 4.58 min, $t_r$ (minor) = 4.07 min) gave the isomeric composition of the product: 89% ee. $[\alpha]_D^{20}$ = +10.3 (c = 1.02, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.74-7.71 (m, 2H), 7.30-7.28 (m, 1H), 7.05 (t, *J* = 8.0 Hz, 1H), 6.70 (s, 1H), 5.86-5.76 (m, 1H), 5.26-5.22 (m, 1H), 5.15-5.12 (m, 1H), 4.22-4.17 (m, 1H), 4.10-4.06 (m, 1H), 1.54 (s, 9H), 1.27 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.68, 155.60, 152.69, 138.87, 133.13, 130.11, 128.35, 124.64, 123.69, 117.32, 115.49, 89.04, 83.28, 81.31, 67.24, 28.26, 27.76. MS (EI): 453 ($M^+$, 1), 57 (100), 222 (71), 182 (39), 194 (25), 224 (25). HRMS (EI): Exact mass calcd for $C_{21}H_{28}N_3O_6Cl$ $[M]^+$: 453.1667, Found: 453.1666.



**5k**

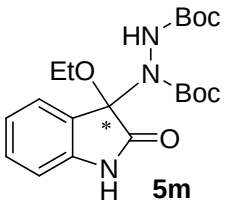
Compound **5k** was obtained in 96% yield as white solid, Mp: 87-89 $^{o}$C. IR (neat): 1738, 1617, 1474, 1247, 1146 cm$^{-1}$. HPLC analysis (Chiralcel ODH, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 4.67 min, $t_r$ (minor) = 4.13 min) gave the isomeric composition of the product: 89% ee. $[\alpha]_D^{20}$ = +14.3 (c = 1.07, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.76 (d, *J* = 8.0 Hz, 1H), 7.62 (br, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.00 (t, *J* = 8.0 Hz, 1H), 6.68 (s, 1H), 5.86-5.76 (m, 1H),

5.26-5.22 (m, 1H), 5.15-5.13 (m, 1H), 4.19 (dd, $J$ = 12.0 Hz , $J$ = 4.0 Hz, 1H), 4.07 (dd, $J$ = 12.0 Hz , $J$ = 8.0 Hz, 1H), 1.54 (s, 9H), 1.27 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.44, 155.60, 152.66, 140.44, 133.12, 132.89, 128.45, 125.20, 124.10, 117.33, 103.47, 99.98, 89.32, 83.32, 81.32, 67.25, 28.26, 27.78. MS (EI): 497 ($M^+$, 1), 57 (100), 266 (43), 268 (42), 226 (24), 228 (21), 240 (16). HRMS (EI): Exact mass calcd for $C_{21}H_{28}N_3O_6Br[M]^+$: 497.1161, Found: 497.1158.



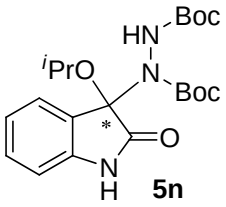
**5l**

Compound **5l** was obtained in 92% yield as white solid, Mp: 101-103 °C. IR (neat): 1731, 1709, 1368, 1248, 1152 $cm^{-1}$. HPLC analysis (Chiralcel IC, 5% $^i$PrOH/hexane, 0.8 mL/min, 230 nm; $t_r$ (major) = 11.26 min, $t_r$ (minor) = 9.70 min) gave the isomeric composition of the product: 88% ee. $[\alpha]_D^{20}$ = +7.2 (c = 0.95, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.81 (s, 1H), 7.55 (d, $J$ = 8.0 Hz, 1H), 7.08 (d, $J$ = 8.0 Hz, 1H), 6.75 (s, 1H), 5.85-5.74 (m, 1H), 5.24-5.23 (m, 1H), 5.12-5.09 (m, 1H), 4.15 (dd, $J$ = 12.0 Hz , $J$ = 8.0 Hz, 1H), 4.03 (dd, $J$ = 12.0 Hz , $J$ = 8.0 Hz, 1H), 2.24 (s, 3H), 1.52 (s, 9H), 1.26 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.23, 155.49, 152.81, 141.22, 136.29, 133.20, 124.58, 124.49, 123.18, 118.33, 117.20, 88.94, 82.98, 81.23, 67.11, 28.19, 27.75, 13.57. MS (EI): 467 ($M^+$, 1), 57 (100), 236 (99), 238 (34), 196 (30), 208 (22), 237 (18), 209 (11). HRMS (EI): Exact mass calcd for $C_{22}H_{30}N_3O_6Cl[M]^+$: 467.1823, Found: 467.1819.



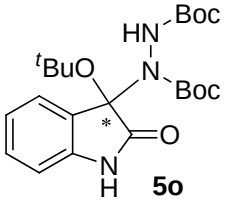
**5m**

Compound **5m** was obtained in 97% yield as white solid, Mp: 74-76 °C. IR (neat): 1726, 1691, 1472, 1244, 1155 $cm^{-1}$. HPLC analysis (Chiralcel IC, 5% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 19.15 min, $t_r$ (minor) = 15.67 min) gave the isomeric composition of the product: 81% ee. $[\alpha]_D^{20}$ = -1.5 (c = 0.76, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.86-7.82 (m, 1H), 7.74 (d, $J$ = 8.0 Hz, 1H), 7.28-7.24 (m, 1H), 7.06 (t, $J$ = 8.0 Hz, 1H), 6.81 (d, $J$ = 8.0 Hz, 1H), 6.74 (br, 1H), 3.71-3.63 (m, 1H), 3.55-3.47 (m, 1H), 1.53 (s, 9H), 1.23 (s, 9H), 1.14 (t, $J$ = 8.0 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.75, 155.53, 152.96, 141.16, 130.12, 126.59, 126.43, 122.67, 110.33, 88.85, 82.72, 81.04, 62.13, 28.23, 27.78, 15.13. MS (EI): 407 ($M^+$, 1), 148 (100), 176 (88), 57 (40), 177 (26), 149 (10), 146 (6), 120 (5). HRMS (EI): Exact mass calcd for $C_{20}H_{29}N_3O_6$ $[M]^+$: 407.2056, Found: 407.2058.



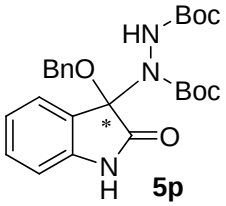
**5n**

Compound **5n** was obtained in 92% yield as white solid, Mp: 75-77 $^{o}$C. IR (neat): 1703, 1619, 1474, 1246, 1159 cm$^{-1}$. HPLC analysis (Chiralcel ADH, 10% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 13.20 min, $t_r$ (minor) = 9.78 min) gave the isomeric composition of the product: 86% ee. $[\alpha]_D^{20}$ = -9.9 (c = 1.09, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.87-7.85 (m, 2H), 7.29-7.25 (m, 1H), 7.06 (t, *J* = 8.0 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.74 (br, 1H), 4.10-4.04 (m, 1H), 1.54 (s, 9H), 1.23 (s, 9H), 1.14 (d, *J* = 4.0 Hz, 3H), 0.84 (d, *J* = 4.0 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 175.79, 155.53, 152.63, 141.33, 130.06, 127.10, 126.46, 122.70, 110.29, 89.03, 82.54, 80.92, 69.65, 28.23, 27.76, 23.52, 23.21. MS (EI): 421 ($M^+$, 1), 148 (100), 57 (32), 190 (15), 149 (13), 120 (10), 191 (7), 146 (6). HRMS (EI): Exact mass calcd for $C_{21}H_{31}N_3O_6$ $[M]^+$: 421.2213, Found: 421.2212.



**5o**

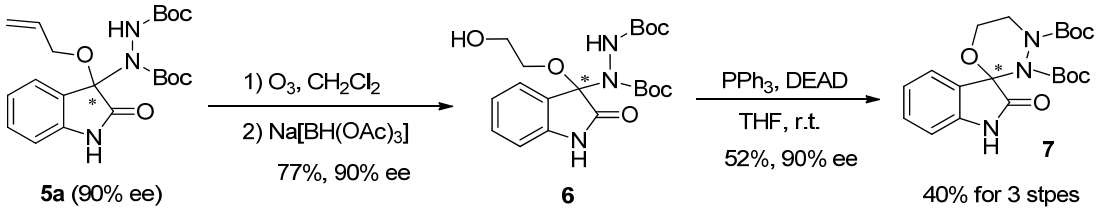
Compound **5o** was obtained in 96% yield as white solid, Mp: 89-91 $^{o}$C. IR (neat): 1731, 1709, 1473, 1248, 1160 cm$^{-1}$. HPLC analysis (Chiralcel ADH, 15% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 6.83 min, $t_r$ (minor) = 5.61 min) gave the isomeric composition of the product: 88% ee. $[\alpha]_D^{20}$ = -22.9 (c = 0.84, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 7.87 (d, *J* = 8.0 Hz, 1H), 7.75 (br, 1H), 7.26-7.24 (m, 1H), 7.03 (t, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 4.0 Hz, 1H), 6.69 (br, 1H), 1.54 (s, 9H), 1.24 (s, 9H), 1.14 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 177.29, 155.50, 152.44, 141.76, 130.29, 128.40 127.66, 122.49, 110.19, 87.47, 82.16, 80.50, 79.18, 29.77, 28.31, 27.86. MS (EI): 435 ($M^+$, 1), 148 (100), 57 (52), 149 (15), 232 (15), 120 (15), 176 (13), 132 (12). HRMS (EI): Exact mass calcd for $C_{22}H_{33}N_3O_6$ $[M]^+$: 435.2369, Found: 435.2368.



**5p**

Compound **5p** was obtained in 83% yield as white solid, Mp: 78-80 $^{o}$C. IR (neat): 1732, 1708, 1473, 1247, 1154 cm$^{-1}$. HPLC analysis (Chiralcel IC, 5% $^{i}$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 18.99 min, $t_r$ (minor) = 13.96 min) gave the isomeric composition of the product: 91% ee. $[\alpha]_D^{20}$ = -21.7 (c = 1.01, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.15 (br, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.28-7.22 (m, 6H), 7.08 (t, *J* = 8.0 Hz, 1H), 6.83-6.81 (m, 2H), 4.64 (ABd, *J* = 12.0 Hz, 1H), 4.56 (ABd, *J* = 12.0 Hz, 1H), 1.47 (s, 9H), 1.25 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.59, 155.55, 152.92, 141.38, 136.96, 130.32, 128.07, 127.55, 127.45, 126.46, 126.31, 122.81, 110.49, 88.91, 82.85, 81.09, 67.71, 28.14, 27.75. MS (EI): 469 ($M^+$, 1), 91 (100), 57 (56), 166 (33), 148 (28), 238 (19), 92 (12), 146 (11). HRMS (EI): Exact mass calcd for $C_{25}H_{31}N_3O_6$ $[M]^+$: 469.2213, Found: 469.2215.

## 7. Transformation of Adduct 12a[4].




**5a** (90% ee) **6** 40% for 3 stpes

An stream of ozone was bubbled through a solution of **5a** (42.0 mg, 0.1 mmol) in $CH_2Cl_2$ (2 mL) at -78 °C until it turned light blue. Excess ozone was removed by flushing the solution with $O_2$, and then $Na[BH(OAc)_3]$ (110.0 mg, 0.5 mmol) was added. The mixture was vigorously stirred and warm to room temperature naturally. After 3 h, the reaction was quenched by the addition of aqueous NaOH (2 N, 0.2 mL), followed by dehydration using anhydrous $Na_2SO_4$. The solvent was removed under reduced pressure, and the residue was purified by column chromatography (hexanes/ethyl acetate 1:1), affording compound **6** in 32.7 mg (77% yield) as white solid, Mp: 59-61 °C. IR (neat): 1697, 1622, 1474, 1393, 1250, 1154 $cm^{-1}$. HPLC analysis (Chiralcel IC, 15% $^i$PrOH/hexane, 1.0 mL/min, 230 nm; $t_r$ (major) = 10.61 min, $t_r$ (minor) = 25.01 min) gave the isomeric composition of the product: 90% ee. $[\alpha]_D^{20}$ = +7.7 (c = 1.01, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): δ = 8.77-8.71 (m, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.49-7.33 (m, 1H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.06-7.01 (m, 1H), 6.83-6.81 (m, 1H), 3.72-3.61 (m, 4H), 2.28 (br, 1H), 1.52 (s, 9H), 1.25 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$): δ 174.38, 155.61, 152.92, 141.16, 130.45, 126.44, 126.00, 122.89, 110.55, 88.67, 82.88, 81.22, 67.49, 61.46, 28.22, 27.83. MS (EI): 423 ($M^+$, 1), 148 (100), 57 (54), 192 (33), 193 (14), 149 (10), 176 (9), 132 (8). HRMS (EI): Exact mass calcd for $C_{20}H_{29}N_3O_7[M]^+$: 423.2006, Found: 423.2003.

To a stirred solution of **6** (30.0 mg, 0.07 mmol) and $Ph_3P$ (39.3 mg, 0.15mmol) in THF (3 mL) was added diethyl azodicarboxylate (DBAD) (24 μL, 0.15 mmol) at room temperature. After 3 h, the solvent was removed under reduced pressure. The residue was purified by column chromatography (hexanes/ethyl acetate 1:1), giving compound **7** in 15.4 mg (52% yield) as white solid. Mp: 57-59 °C. IR (neat): 1799, 1700, 1624, 1473, 1394, 1260, 1149 $cm^{-1}$. HPLC analysis (Chiralcel ADH, 10% $^i$PrOH/hexane, 1.0 mL/min, 215 nm; $t_r$ (major) = 10.49 min, $t_r$ (minor) = 13.78 min) gave the isomeric composition of the product: 90% ee. $[\alpha]_D^{20}$ = -7.3 (c = 0.71, $CHCl_3$). $^1$H NMR (400 MHz, $DCl_3$): see below. $^{13}$C NMR (100 MHz, $CDCl_3$): see below. MS (EI): 405 ($M^+$, 1), 57 (100), 177 (73), 221 (39), 148 (26), 249 (21), 175 (16), 119 (13). HRMS (EI): Exact mass calcd for $C_{20}H_{27}N_3O_6[M]^+$: 405.1900, Found: 405.1901.

[4] H. Bittermann, P. Gmeiner, *J. Org. Chem.* **2006**, *71*, 97.

## 8. Single-Crystal X-ray Crystallography of product 3a[5]

Data intensity of **3a** was collected using a Bruker SMART APEX II (Mo radiation). The X-ray condition of was 50 kV × 30 mA. Data collection and reduction were done by using the Bruker ApexII software package. The structure was solved by direct methods and refined by full-matrix least-squares on $F^2$ with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically idea positions and refined isotropically. Crystal data for **3a**: $C_{28}H_{31}N_3O_5S$, M = 521.62, T = 296(2) K, λ = 0.71073 Å, monoclinic, space group P2(1)/n, a = 13.8796(10) Å, b = 23.1960(17) Å, c = 8.6991(6) Å, V = 2785.3(3) Å$^3$, z = 4, $d_{calc}$ = 1.244 mg/m$^3$, 32345 reflections measured, 4920 unique [$R_{int}$ = 0.0604], $R_1$ = 0.0865, $wR_2$ = 0.2238 ($I > 2\sigma(I)$, final), $R_1$ = 0.1233, $wR_2$ = 0.2563 (all data), GOF = 1.054, and 334 parameters.

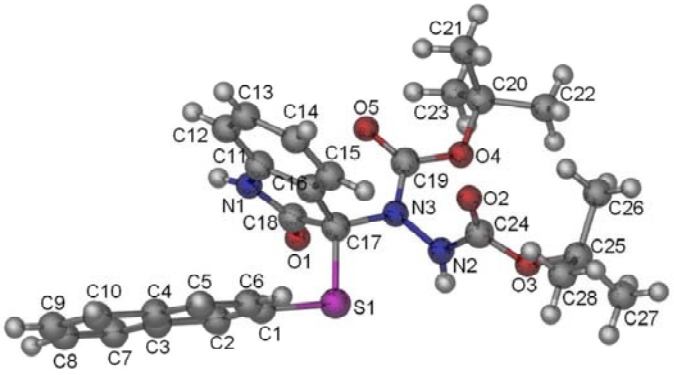



Table 1. Crystal data and structure refinement for z.

| | |
|---|---|
| Identification code | z |
| Empirical formula | C28 H31 N3 O5 S |
| Formula weight | 521.62 |
| Temperature | 296(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Monoclinic, P2(1)/c |
| Unit cell dimensions | a = 13.8796(10) A alpha = 90 deg. |
| | b = 23.1960(17) A beta = 96.000(2) deg. |
| | c = 8.6991(6) A gamma = 90 deg. |

[5] CCDC number: 910674.

| | |
|---|---|
| Volume | 2785.3(3) A^3 |
| Z, Calculated density | 4, 1.244 Mg/m^3 |
| Absorption coefficient | 0.157 mm^-1 |
| F(000) | 1104 |
| Crystal size | 0.44 x 0.23 x 0.11 mm |
| Theta range for data collection | 1.48 to 25.01 deg. |
| Limiting indices | -16<=h<=16, -27<=k<=27, -10<=l<=9 |
| Reflections collected / unique | 32345 / 4920 [R(int) = 0.0604] |
| Completeness to theta = 25.01 | 99.8 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9829 and 0.9341 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4920 / 11 / 334 |
| Goodness-of-fit on F^2 | 1.054 |
| Final R indices [I>2sigma(I)] | R1 = 0.0865, wR2 = 0.2238 |
| R indices (all data) | R1 = 0.1233, wR2 = 0.2563 |
| Largest diff. peak and hole | 1.048 and -0.757 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for z. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| S(1) | 34501(1) | 8733(1) | -14456(1) | 60(1) |
| O(1) | 34364(3) | 10027(2) | -13002(5) | 73(1) |
| O(2) | 37448(3) | 8479(2) | -13727(4) | 70(1) |
| O(3) | 37462(3) | 8772(2) | -16215(4) | 61(1) |

| | | | | |
|---|---|---|---|---|
| O(4) | 37452(2) | 9841(2) | -13233(4) | 61(1) |
| O(5) | 36464(2) | 9843(2) | -11317(4) | 62(1) |
| N(1) | 34409(3) | 9463(2) | -10844(4) | 51(1) |
| N(2) | 36365(3) | 9124(2) | -14864(4) | 47(1) |
| N(3) | 36094(3) | 9317(2) | -13466(4) | 48(1) |
| C(11) | 34877(3) | 8956(2) | -10286(5) | 45(1) |
| C(12) | 34886(4) | 8715(2) | -8854(6) | 63(1) |
| C(13) | 35396(5) | 8205(3) | -8599(7) | 77(2) |
| C(14) | 35882(4) | 7958(2) | -9713(6) | 71(2) |
| C(15) | 35894(4) | 8216(2) | -11158(6) | 55(1) |
| C(16) | 35385(3) | 8721(2) | -11431(5) | 42(1) |
| C(17) | 35222(3) | 9095(2) | -12841(5) | 43(1) |
| C(18) | 34614(3) | 9602(2) | -12267(6) | 51(1) |
| C(19) | 36671(3) | 9686(2) | -12572(6) | 50(1) |
| C(20) | 38206(4) | 10203(3) | -12385(7) | 72(2) |
| C(21) | 38572(5) | 9917(4) | -10874(9) | 107(2) |
| C(22) | 38978(5) | 10209(4) | -13476(10) | 113(3) |
| C(23) | 37788(6) | 10796(3) | -12156(9) | 98(2) |
| C(24) | 37143(3) | 8760(2) | -14827(6) | 50(1) |
| C(25) | 38305(4) | 8422(2) | -16557(7) | 67(2) |
| C(26) | 39177(4) | 8579(3) | -15432(9) | 95(2) |
| C(27) | 38436(6) | 8607(3) | -18178(8) | 104(2) |
| C(28) | 38056(5) | 7790(2) | -16474(8) | 82(2) |
| C(1) | 33514(4) | 8502(4) | -13462(7) | 101(3) |
| C(2) | 32730(5) | 8807(5) | -13223(9) | 161(6) |
| C(3) | 32000(6) | 8456(4) | -12315(8) | 96(2) |
| C(4) | 32214(6) | 7897(4) | -11805(9) | 120(3) |
| C(5) | 32979(8) | 7566(5) | -12087(13) | 239(10) |

| | | | | |
|---|---|---|---|---|
| C(6) | 33540(8) | 7946(5) | -12889(11) | 170(6) |
| C(7) | 31232(8) | 8787(5) | -12101(13) | 299(14) |
| C(8) | 30639(9) | 8433(6) | -11312(15) | 197(8) |
| C(9) | 30717(6) | 7885(5) | -10684(10) | 141(4) |
| C(10) | 31500(7) | 7562(6) | -10912(11) | 162(5) |

Table 3. Bond lengths [A] and angles [deg] for z.

| | |
|---|---|
| S(1)-C(1) | 1.778(6) |
| S(1)-C(17) | 1.840(4) |
| O(1)-C(18) | 1.206(6) |
| O(2)-C(24) | 1.198(6) |
| O(3)-C(24) | 1.328(5) |
| O(3)-C(25) | 1.481(6) |
| O(4)-C(19) | 1.329(5) |
| O(4)-C(20) | 1.477(6) |
| O(5)-C(19) | 1.213(5) |
| N(1)-C(18) | 1.338(6) |
| N(1)-C(11) | 1.405(6) |
| N(2)-C(24) | 1.369(6) |
| N(2)-N(3) | 1.385(5) |
| N(3)-C(19) | 1.360(6) |
| N(3)-C(17) | 1.470(5) |
| C(11)-C(12) | 1.365(7) |
| C(11)-C(16) | 1.390(6) |
| C(12)-C(13) | 1.384(8) |
| C(13)-C(14) | 1.363(8) |
| C(14)-C(15) | 1.395(7) |

| | |
|---|---|
| C(15)-C(16) | 1.376(6) |
| C(16)-C(17) | 1.499(6) |
| C(17)-C(18) | 1.560(6) |
| C(20)-C(22) | 1.504(9) |
| C(20)-C(21) | 1.512(9) |
| C(20)-C(23) | 1.514(9) |
| C(25)-C(27) | 1.503(8) |
| C(25)-C(28) | 1.508(8) |
| C(25)-C(26) | 1.520(9) |
| C(1)-C(2) | 1.333(8) |
| C(1)-C(6) | 1.381(9) |
| C(2)-C(3) | 1.575(8) |
| C(3)-C(7) | 1.342(9) |
| C(3)-C(4) | 1.392(8) |
| C(4)-C(5) | 1.354(9) |
| C(4)-C(10) | 1.533(8) |
| C(5)-C(6) | 1.409(9) |
| C(7)-C(8) | 1.394(10) |
| C(8)-C(9) | 1.383(9) |
| C(9)-C(10) | 1.351(9) |
| C(1)-S(1)-C(17) | 98.7(2) |
| C(24)-O(3)-C(25) | 121.0(4) |
| C(19)-O(4)-C(20) | 120.3(4) |
| C(18)-N(1)-C(11) | 112.6(4) |
| C(24)-N(2)-N(3) | 117.7(4) |
| C(19)-N(3)-N(2) | 120.5(4) |
| C(19)-N(3)-C(17) | 117.8(4) |
| N(2)-N(3)-C(17) | 121.4(4) |

| | |
|---|---|
| C(12)-C(11)-C(16) | 122.4(4) |
| C(12)-C(11)-N(1) | 128.2(4) |
| C(16)-C(11)-N(1) | 109.4(4) |
| C(11)-C(12)-C(13) | 116.9(5) |
| C(14)-C(13)-C(12) | 121.9(5) |
| C(13)-C(14)-C(15) | 120.9(5) |
| C(16)-C(15)-C(14) | 117.9(5) |
| C(15)-C(16)-C(11) | 120.0(4) |
| C(15)-C(16)-C(17) | 131.6(4) |
| C(11)-C(16)-C(17) | 108.4(4) |
| N(3)-C(17)-C(16) | 116.4(4) |
| N(3)-C(17)-C(18) | 110.4(4) |
| C(16)-C(17)-C(18) | 102.4(3) |
| N(3)-C(17)-S(1) | 106.3(3) |
| C(16)-C(17)-S(1) | 112.6(3) |
| C(18)-C(17)-S(1) | 108.6(3) |
| O(1)-C(18)-N(1) | 127.6(4) |
| O(1)-C(18)-C(17) | 125.6(4) |
| N(1)-C(18)-C(17) | 106.8(4) |
| O(5)-C(19)-O(4) | 126.1(4) |
| O(5)-C(19)-N(3) | 121.5(4) |
| O(4)-C(19)-N(3) | 112.4(4) |
| O(4)-C(20)-C(22) | 101.8(5) |
| O(4)-C(20)-C(21) | 109.9(5) |
| C(22)-C(20)-C(21) | 110.8(6) |
| O(4)-C(20)-C(23) | 108.7(5) |
| C(22)-C(20)-C(23) | 112.5(6) |
| C(21)-C(20)-C(23) | 112.5(6) |

| | |
|---|---|
| O(2)-C(24)-O(3) | 128.0(4) |
| O(2)-C(24)-N(2) | 124.5(4) |
| O(3)-C(24)-N(2) | 107.5(4) |
| O(3)-C(25)-C(27) | 102.0(5) |
| O(3)-C(25)-C(28) | 109.5(4) |
| C(27)-C(25)-C(28) | 111.9(6) |
| O(3)-C(25)-C(26) | 109.4(5) |
| C(27)-C(25)-C(26) | 111.6(6) |
| C(28)-C(25)-C(26) | 111.9(6) |
| C(2)-C(1)-C(6) | 115.5(8) |
| C(2)-C(1)-S(1) | 126.8(7) |
| C(6)-C(1)-S(1) | 117.7(6) |
| C(1)-C(2)-C(3) | 112.5(9) |
| C(7)-C(3)-C(4) | 129.4(9) |
| C(7)-C(3)-C(2) | 109.7(9) |
| C(4)-C(3)-C(2) | 120.9(8) |
| C(5)-C(4)-C(3) | 128.1(9) |
| C(5)-C(4)-C(10) | 111.4(9) |
| C(3)-C(4)-C(10) | 120.4(8) |
| C(4)-C(5)-C(6) | 102.6(10) |
| C(1)-C(6)-C(5) | 140.2(11) |
| C(3)-C(7)-C(8) | 104.5(11) |
| C(9)-C(8)-C(7) | 135.2(12) |
| C(10)-C(9)-C(8) | 118.8(9) |
| C(9)-C(10)-C(4) | 111.5(9) |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for z.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| S(1) | 52(1) | 87(1) | 43(1) | -6(1) | 8(1) | -12(1) |
| O(1) | 78(3) | 63(2) | 83(3) | 23(2) | 23(2) | 27(2) |
| O(2) | 72(2) | 79(3) | 61(2) | 19(2) | 18(2) | 24(2) |
| O(3) | 67(2) | 67(2) | 54(2) | 5(2) | 28(2) | 13(2) |
| O(4) | 51(2) | 67(2) | 68(2) | -8(2) | 19(2) | -12(2) |
| O(5) | 59(2) | 66(2) | 64(2) | -17(2) | 19(2) | -4(2) |
| N(1) | 51(2) | 52(2) | 53(2) | -3(2) | 19(2) | 7(2) |
| N(2) | 45(2) | 57(2) | 41(2) | 2(2) | 9(2) | 4(2) |
| N(3) | 45(2) | 53(2) | 46(2) | -3(2) | 13(2) | -3(2) |
| C(11) | 44(2) | 47(3) | 45(2) | -1(2) | 9(2) | 1(2) |
| C(12) | 71(3) | 74(4) | 46(3) | 1(3) | 16(2) | 3(3) |
| C(13) | 97(4) | 82(4) | 54(3) | 23(3) | 18(3) | 13(4) |
| C(14) | 85(4) | 62(3) | 67(3) | 18(3) | 9(3) | 19(3) |
| C(15) | 62(3) | 48(3) | 58(3) | 2(2) | 12(2) | 8(2) |
| C(16) | 42(2) | 45(2) | 40(2) | -1(2) | 8(2) | -2(2) |
| C(17) | 39(2) | 48(2) | 43(2) | 1(2) | 9(2) | 2(2) |
| C(18) | 45(3) | 52(3) | 56(3) | 4(2) | 11(2) | 5(2) |
| C(19) | 48(3) | 47(3) | 57(3) | -1(2) | 14(2) | 0(2) |
| C(20) | 52(3) | 69(4) | 95(4) | -6(3) | 8(3) | -18(3) |
| C(21) | 73(4) | 121(6) | 122(6) | 13(5) | -12(4) | 2(4) |
| C(22) | 66(4) | 129(7) | 147(7) | -11(5) | 33(4) | -40(4) |
| C(23) | 106(5) | 65(4) | 123(6) | -14(4) | 6(5) | -19(4) |
| C(24) | 50(3) | 50(3) | 55(3) | -1(2) | 18(2) | 1(2) |

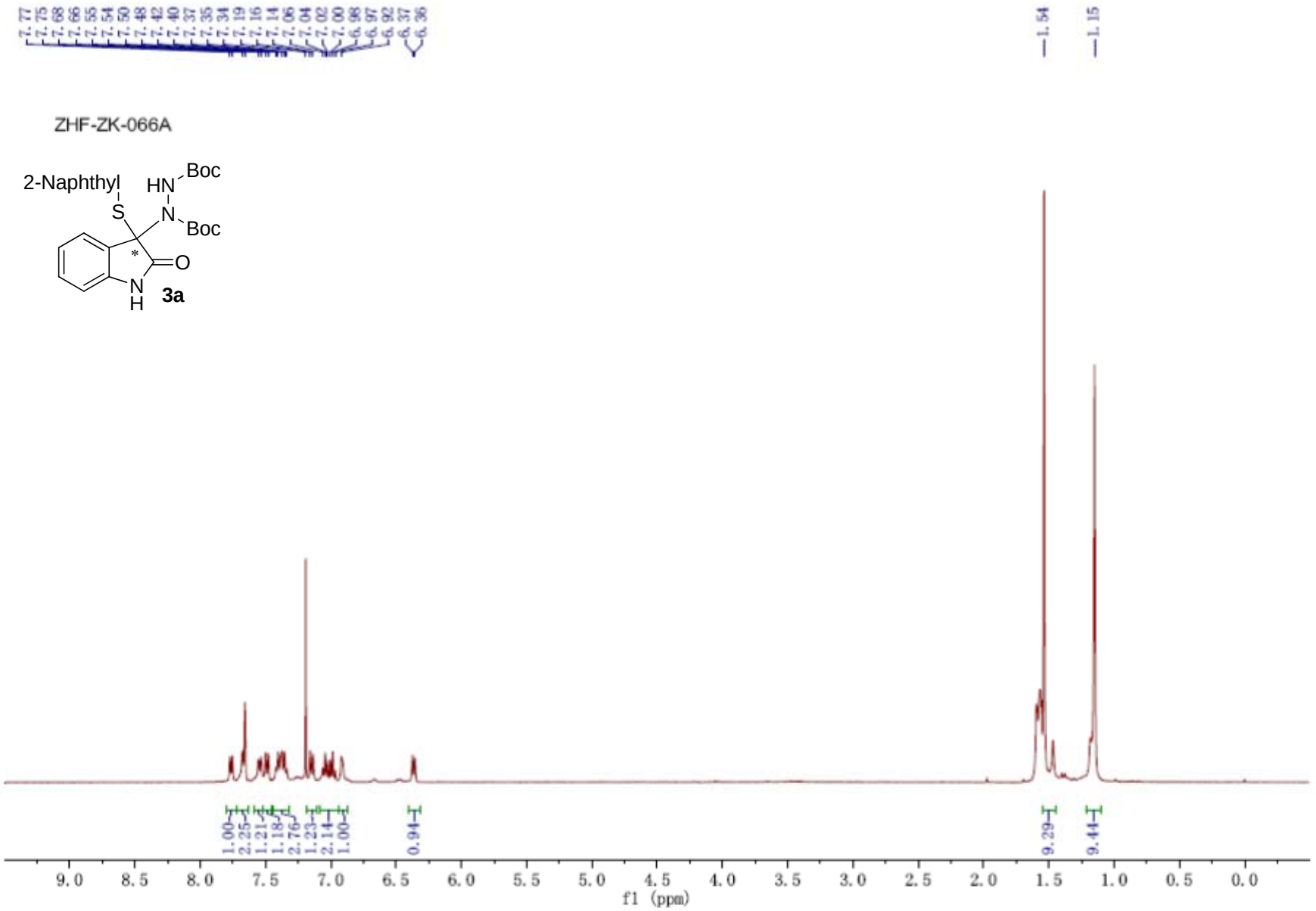
| | | | | | | |
|---|---|---|---|---|---|---|
| C(25) | 60(3) | 67(3) | 80(4) | -9(3) | 34(3) | 4(3) |
| C(26) | 56(4) | 101(5) | 132(6) | -30(4) | 27(4) | -10(3) |
| C(27) | 119(6) | 113(6) | 92(5) | 3(4) | 65(5) | 10(5) |
| C(28) | 80(4) | 61(4) | 107(5) | -12(3) | 22(4) | 2(3) |
| C(1) | 67(4) | 188(8) | 49(3) | -27(4) | 8(3) | -59(5) |
| C(2) | 48(4) | 333(16) | 105(6) | -106(8) | 21(4) | -39(6) |
| C(3) | 97(5) | 118(6) | 70(4) | -22(4) | -13(4) | 1(5) |
| C(4) | 87(5) | 148(8) | 115(6) | -45(6) | -37(5) | 17(5) |
| C(5) | 340(20) | 146(11) | 199(14) | -63(10) | -146(15) | 115(13) |
| C(6) | 175(10) | 245(14) | 91(6) | 19(7) | 8(6) | -157(11) |
| C(7) | 360(20) | 244(17) | 243(18) | -166(15) | -225(18) | 165(18) |
| C(8) | 166(11) | 289(19) | 139(10) | 5(11) | 26(8) | -151(13) |
| C(9) | 107(7) | 231(12) | 89(6) | 2(7) | 26(5) | -106(8) |
| C(10) | 85(6) | 289(16) | 112(7) | 7(8) | 15(5) | -65(9) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for z.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 34032 | 9663 | -10326 | 61 |
| H(2B) | 36055 | 9229 | -15726 | 57 |
| H(12A) | 34565 | 8885 | -8085 | 75 |
| H(13A) | 35408 | 8026 | -7641 | 92 |
| H(14A) | 36210 | 7612 | -9506 | 85 |
| H(15A) | 36235 | 8053 | -11914 | 66 |
| H(21A) | 38829 | 9544 | -11077 | 160 |
| H(21B) | 38047 | 9876 | -10245 | 160 |

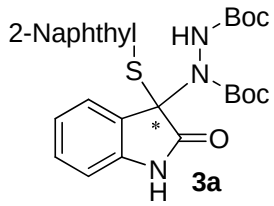
| | | | | |
|---|---|---|---|---|
| H(21C) | 39071 | 10151 | -10340 | 160 |
| H(22A) | 39219 | 9825 | -13584 | 169 |
| H(22B) | 39498 | 10457 | -13072 | 169 |
| H(22C) | 38708 | 10350 | -14467 | 169 |
| H(23A) | 37566 | 10960 | -13144 | 147 |
| H(23B) | 38279 | 11040 | -11639 | 147 |
| H(23C) | 37254 | 10765 | -11542 | 147 |
| H(26A) | 39312 | 8983 | -15517 | 143 |
| H(26B) | 39730 | 8361 | -15672 | 143 |
| H(26C) | 39042 | 8493 | -14396 | 143 |
| H(27A) | 37874 | 8501 | -18856 | 156 |
| H(27B) | 38997 | 8421 | -18507 | 156 |
| H(27C) | 38520 | 9018 | -18204 | 156 |
| H(28A) | 37506 | 7707 | -17204 | 123 |
| H(28B) | 37905 | 7698 | -15451 | 123 |
| H(28C) | 38599 | 7563 | -16716 | 123 |
| H(2A) | 32625 | 9185 | -13555 | 193 |
| H(5A) | 33103 | 7183 | -11818 | 287 |
| H(6A) | 34109 | 7765 | -13101 | 205 |
| H(7A) | 31121 | 9167 | -12410 | 359 |
| H(8A) | 30050 | 8606 | -11174 | 237 |
| H(9A) | 30239 | 7741 | -10116 | 169 |
| H(10B) | 31594 | 7184 | -10570 | 194 |

Table 6. Torsion angles [deg] for z.

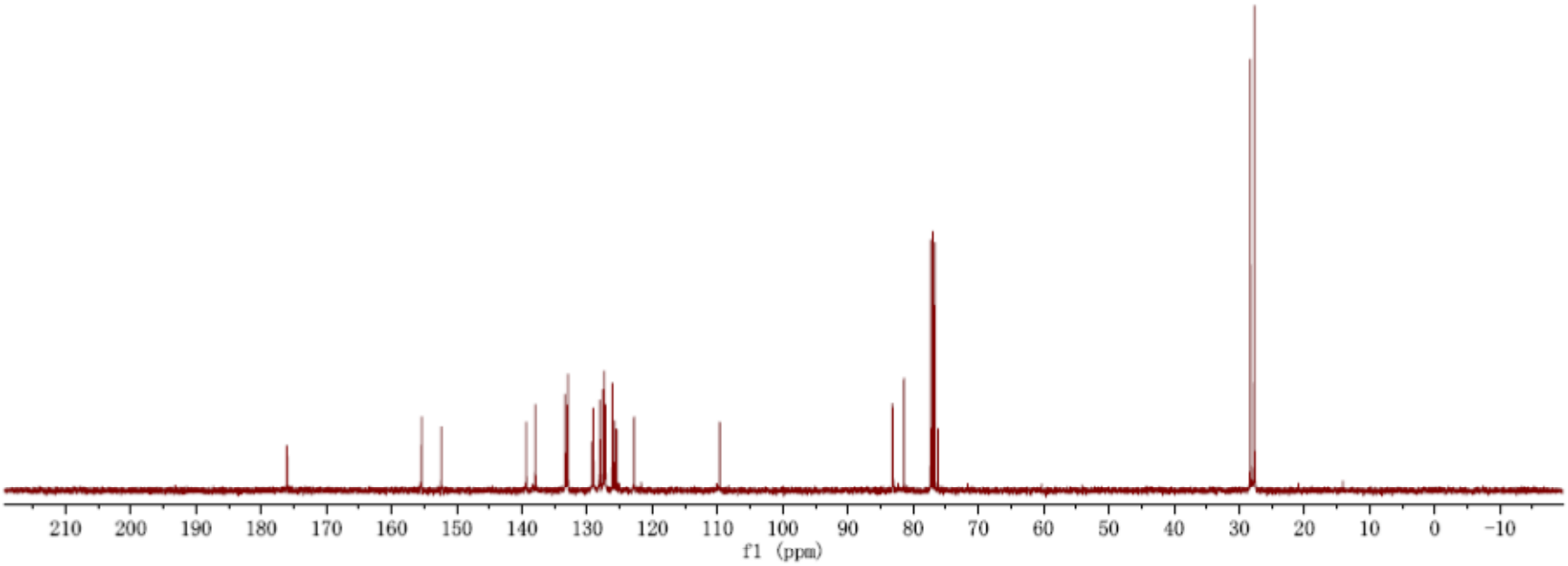


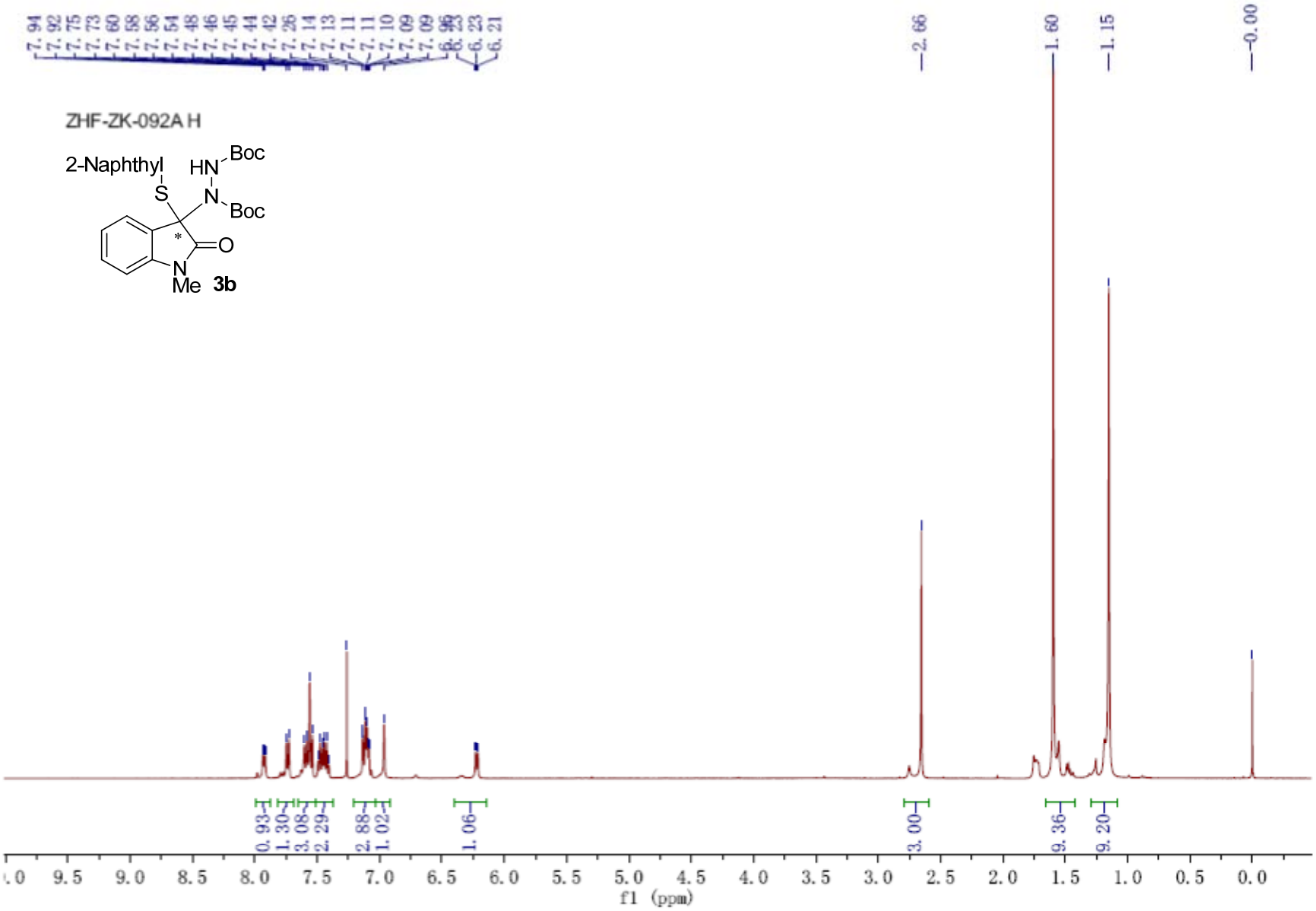
zhf-zk-089A
zhf-zk-089A C

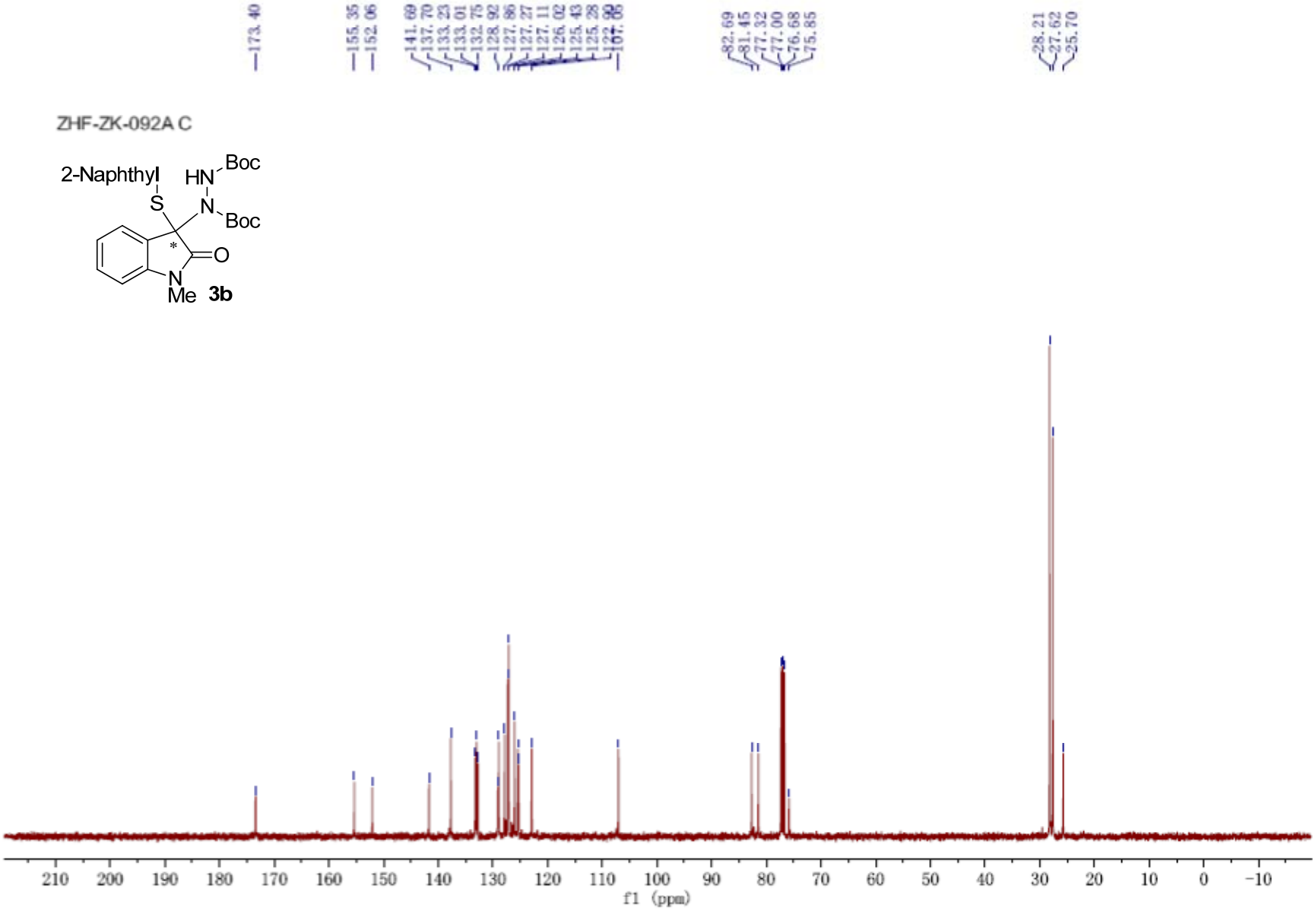
176.04
155.39
152.37
139.33
137.95
133.39
133.07
132.94
129.05
128.04
127.57
127.38
127.20
126.12
125.78
83.17
81.43
77.32
77.00
76.68
76.19
28.30
27.66

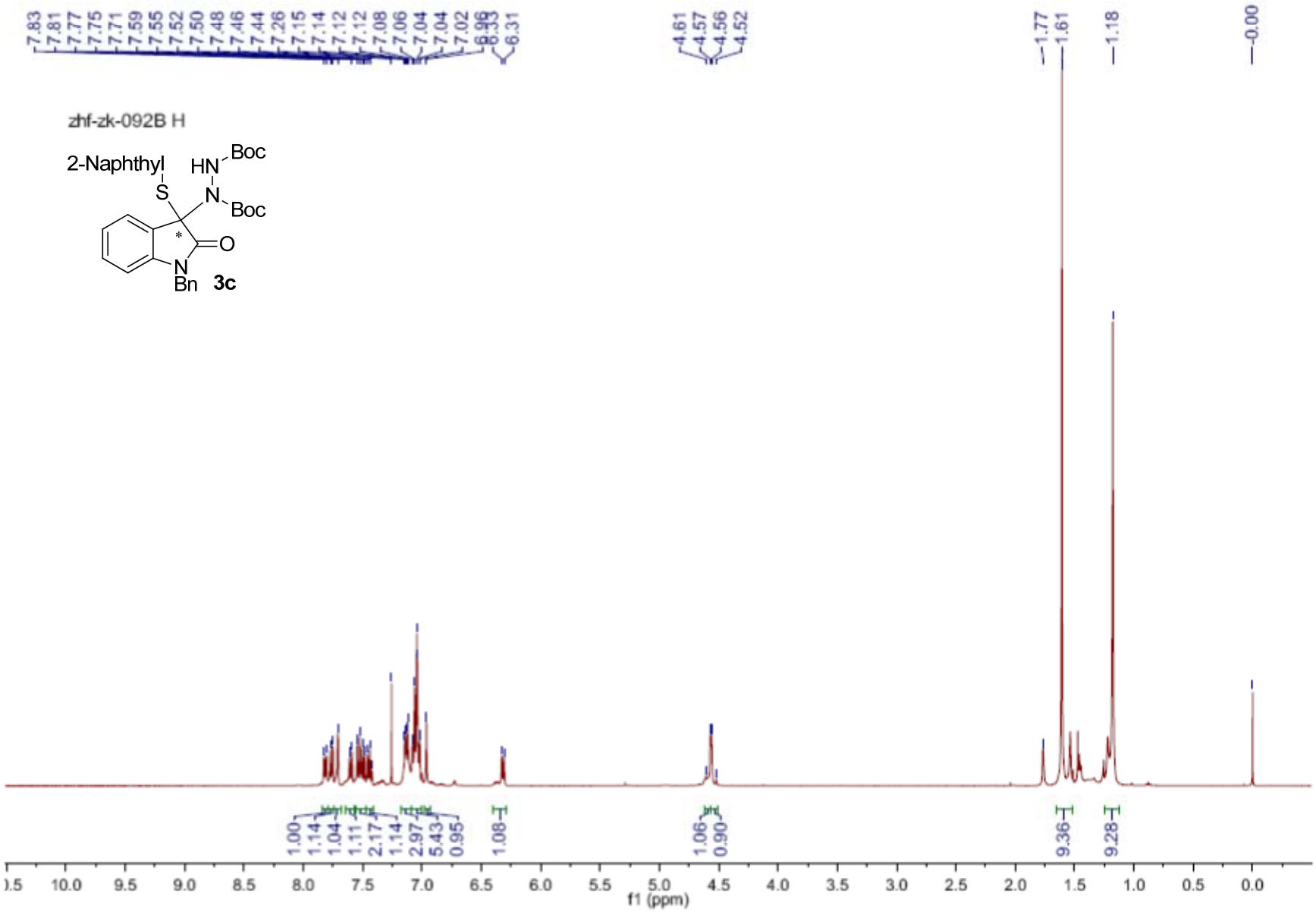



**3a**

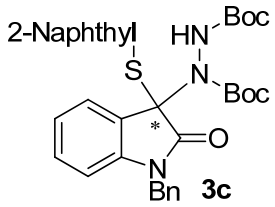




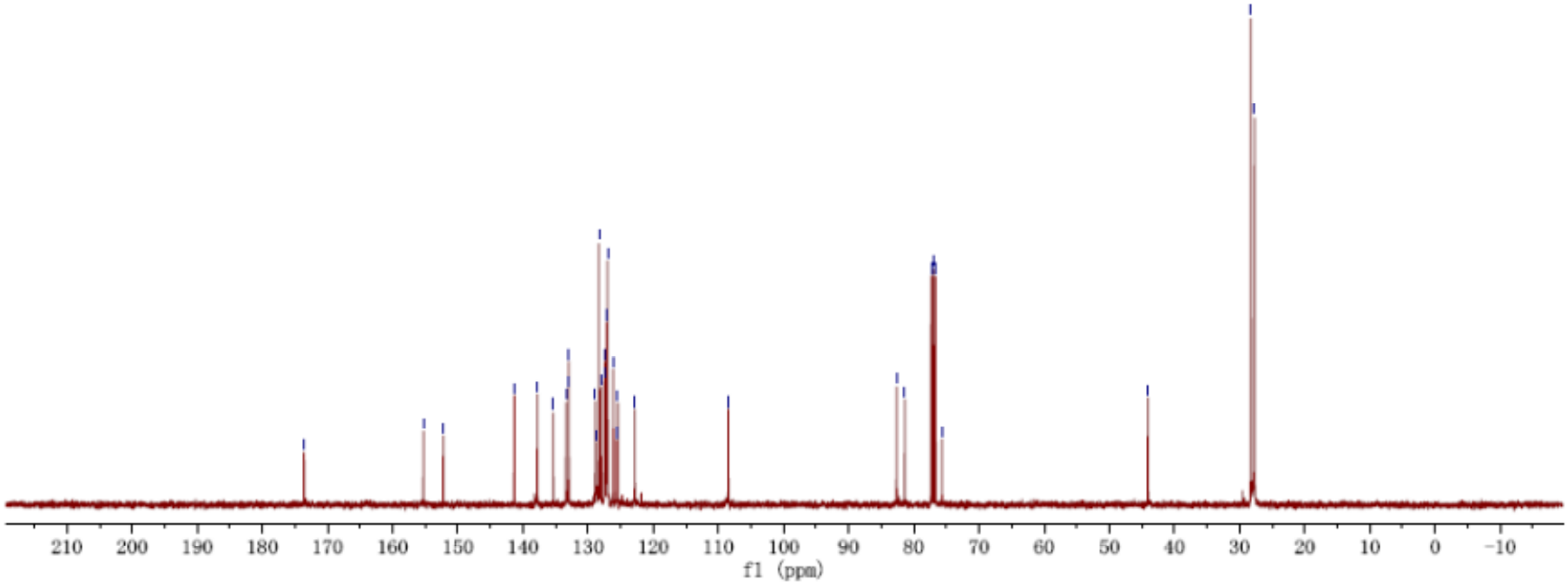


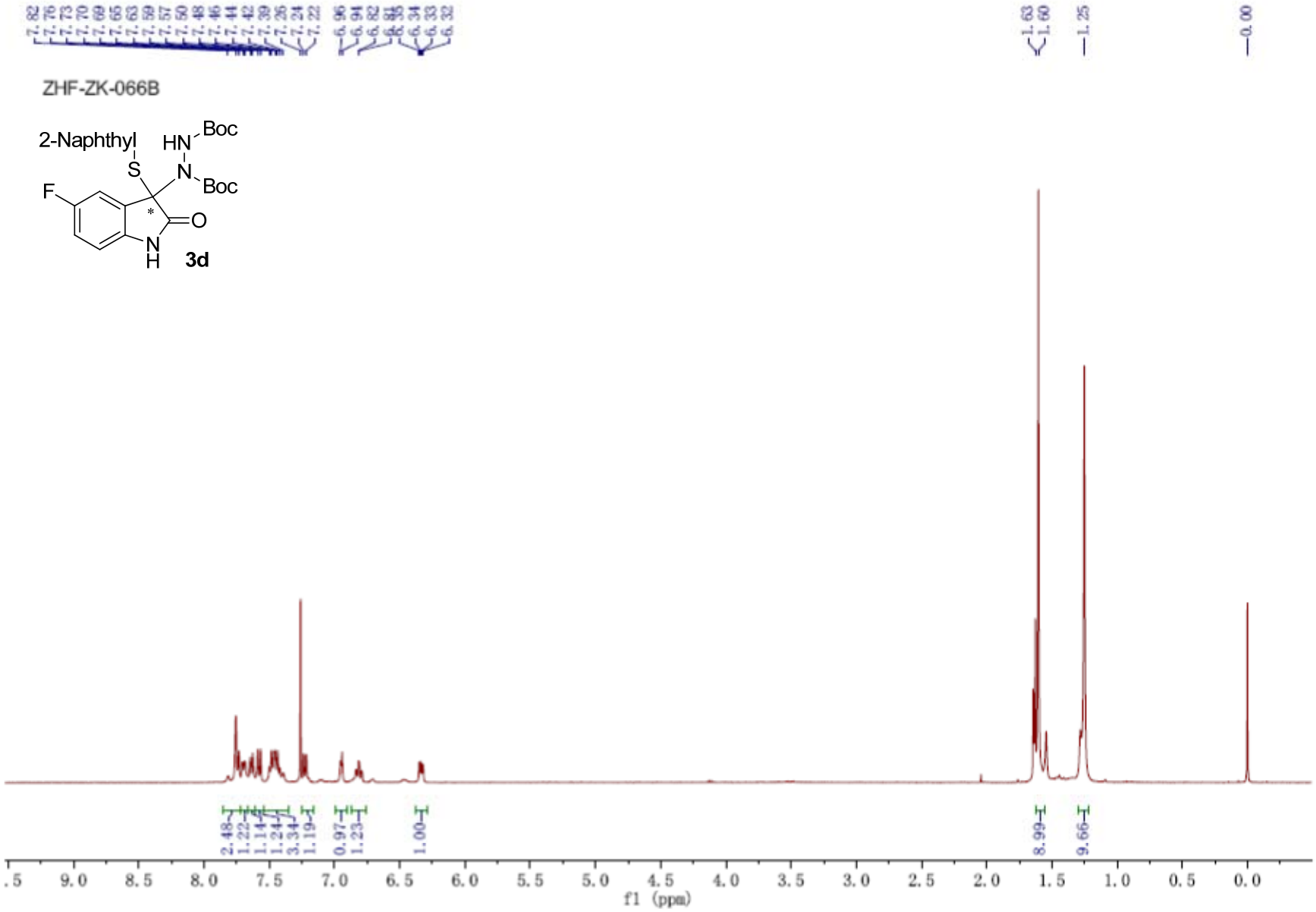



ZHF-ZK-092B C



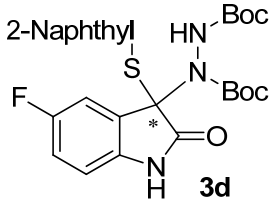

**3c**



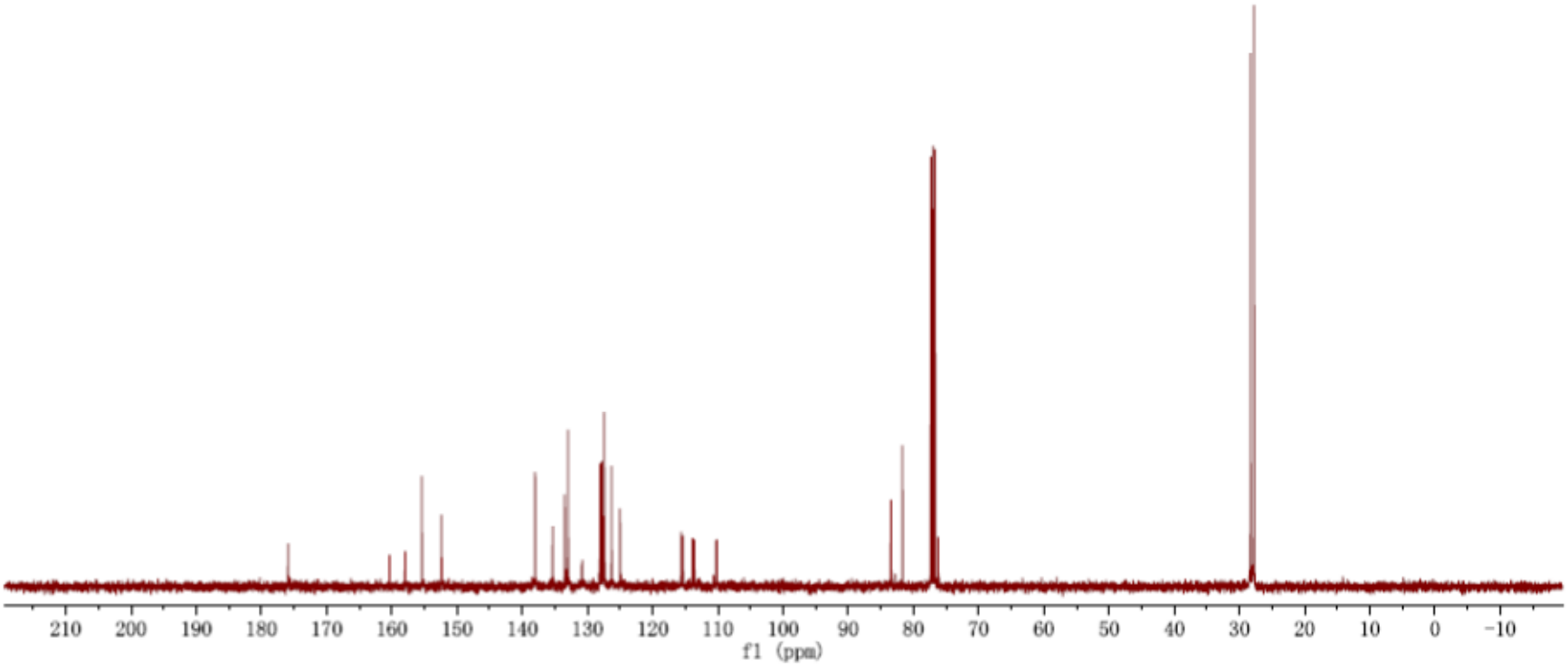


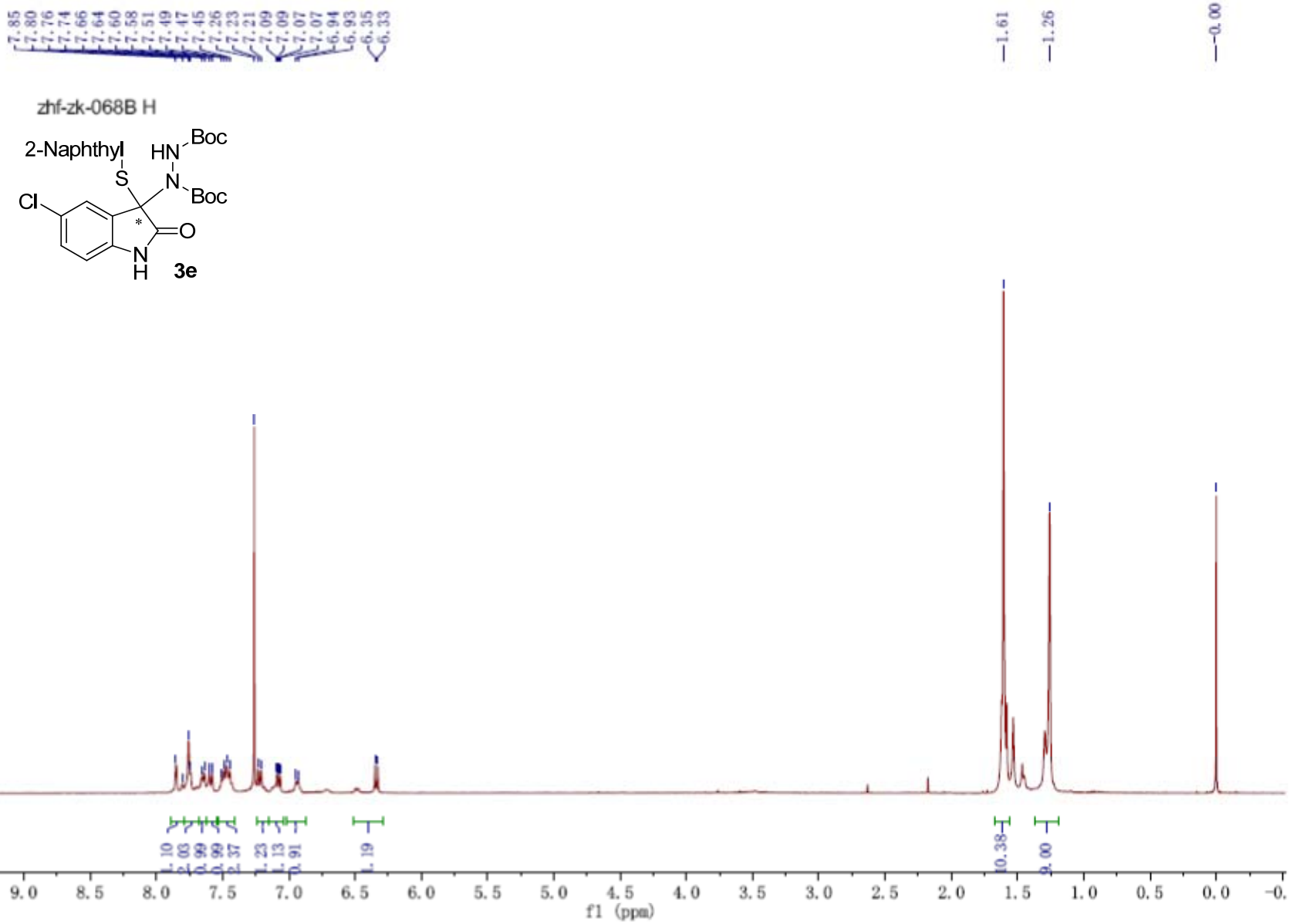
zhf-zk-089B
zhf-zk-089B C

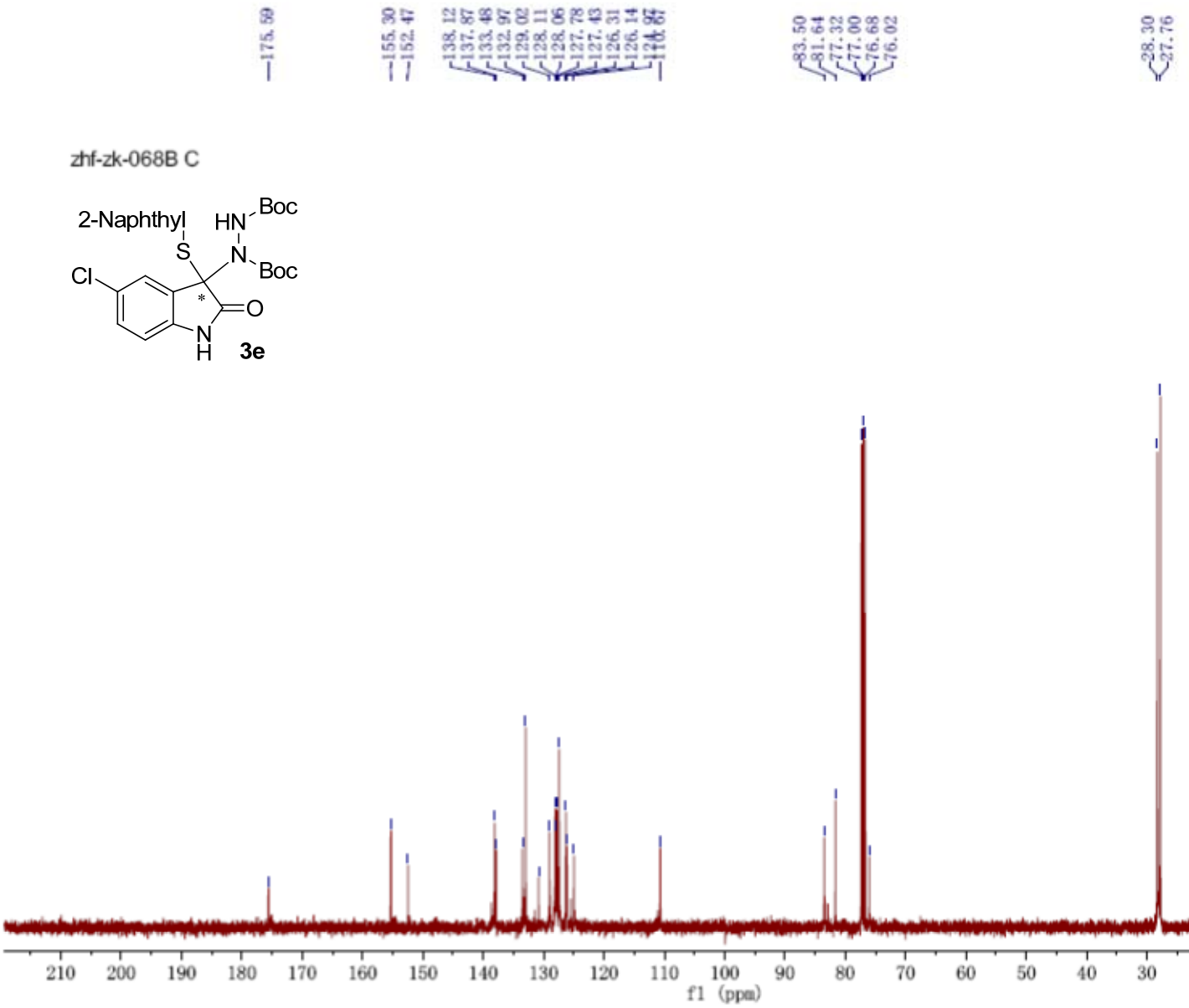
175.92
160.36
157.97
155.39
152.40
138.02
133.49
132.99
128.05
127.76
127.46
127.39
126.30
115.38
113.87
113.62
110.26
110.18
83.46
81.68
77.32
77.00
76.68
76.22
28.30
27.75

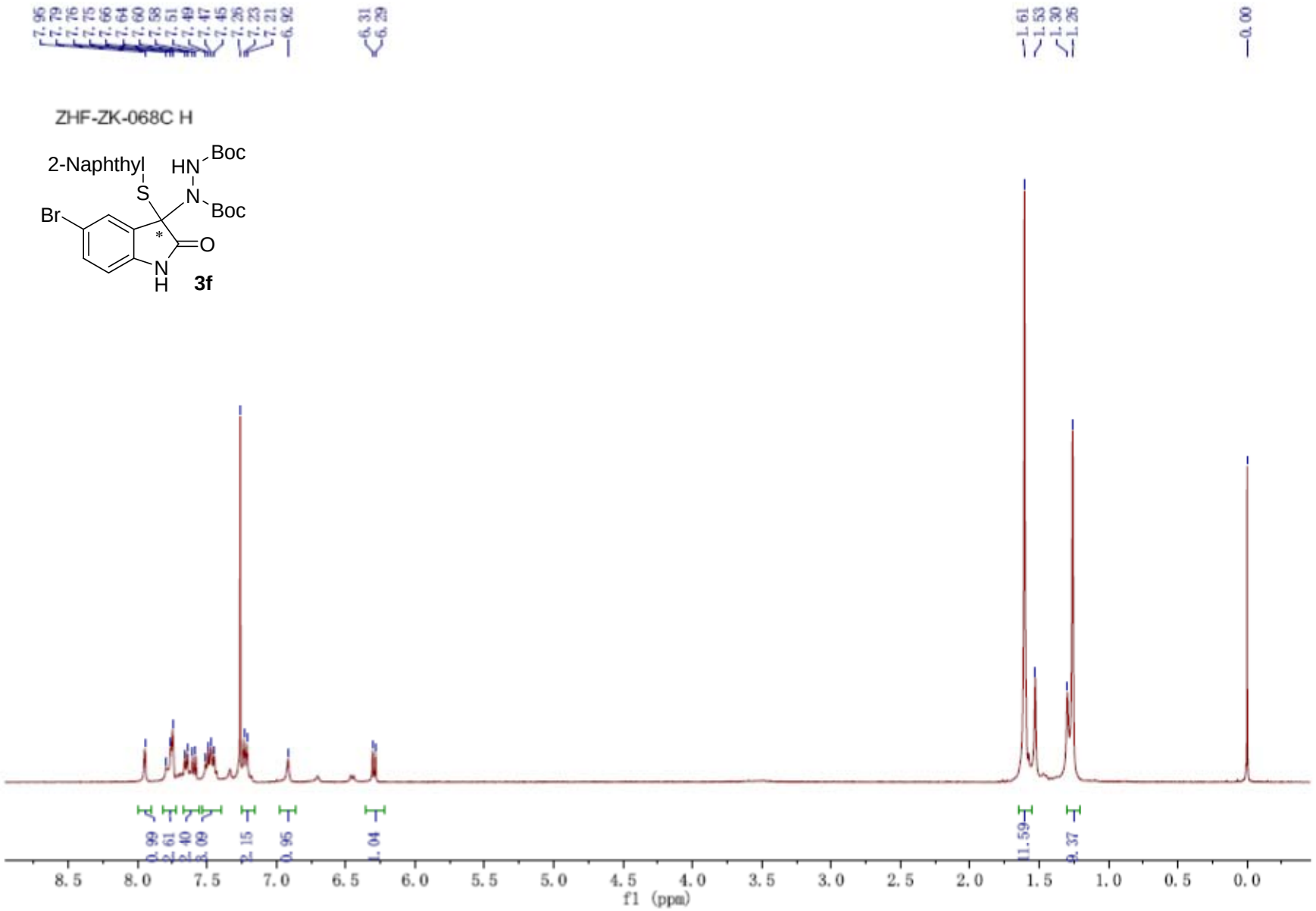



**3d**









zhf-zk-068C C
zhf-zk-068C C

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155.24
152.48
138.33
138.16
133.49
132.97
131.91
131.11
128.88
128.08
127.78
127.43
126.32
125.00
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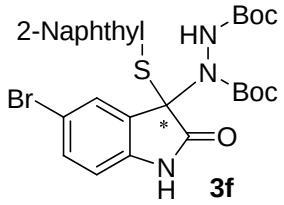
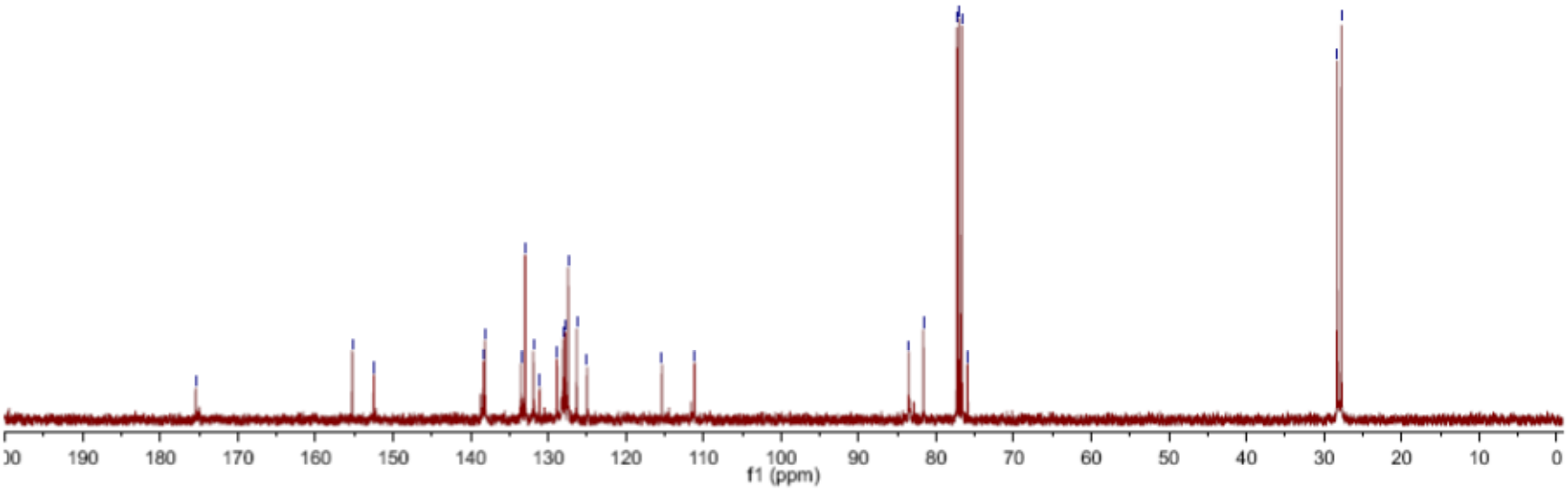
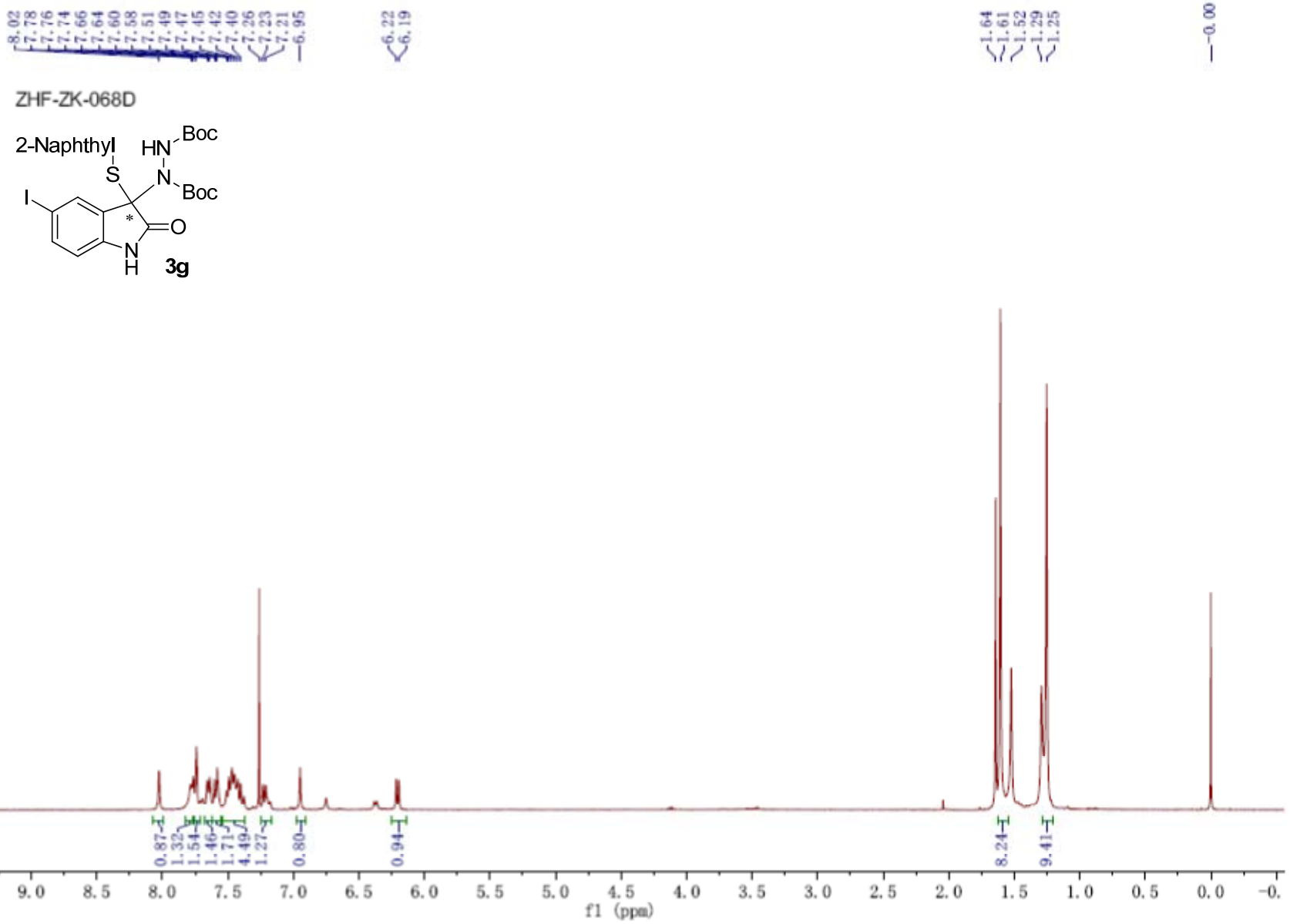
111.14
83.52
81.64
77.32
77.00
76.68
75.97
28.31
27.77




**3f**





zhf-zk-089E
zhf-zk-089E C

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155.28
152.64
139.05
138.33
137.95
134.53
133.58
133.05
131.34
128.22
127.86
127.54
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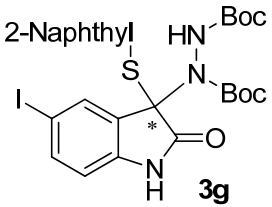
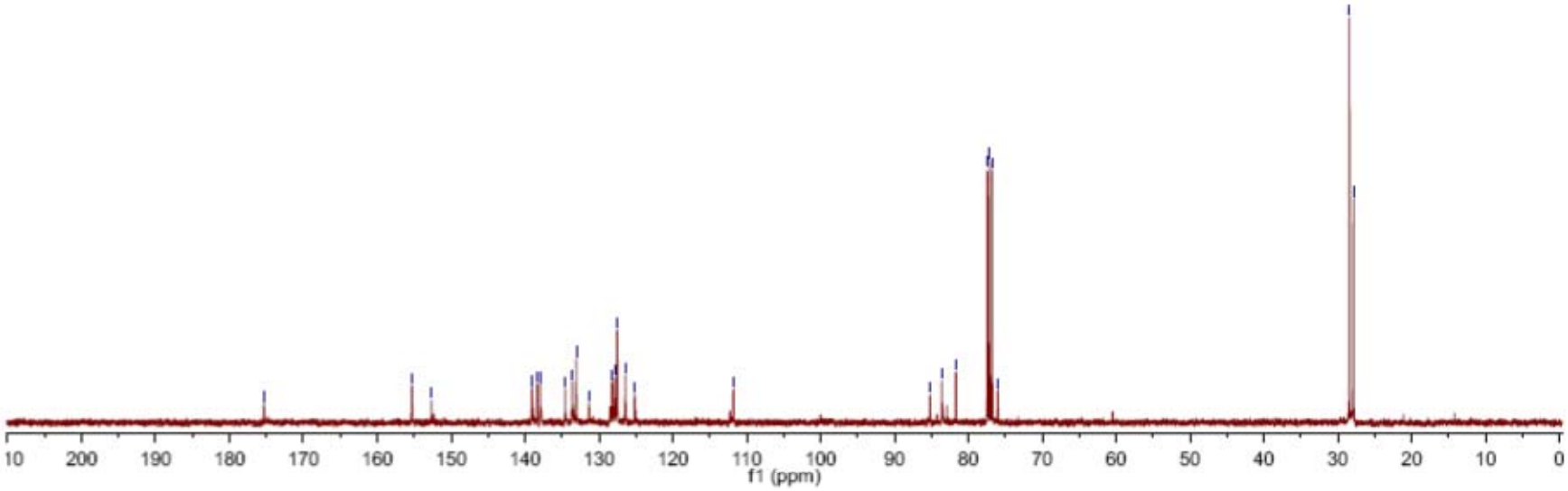
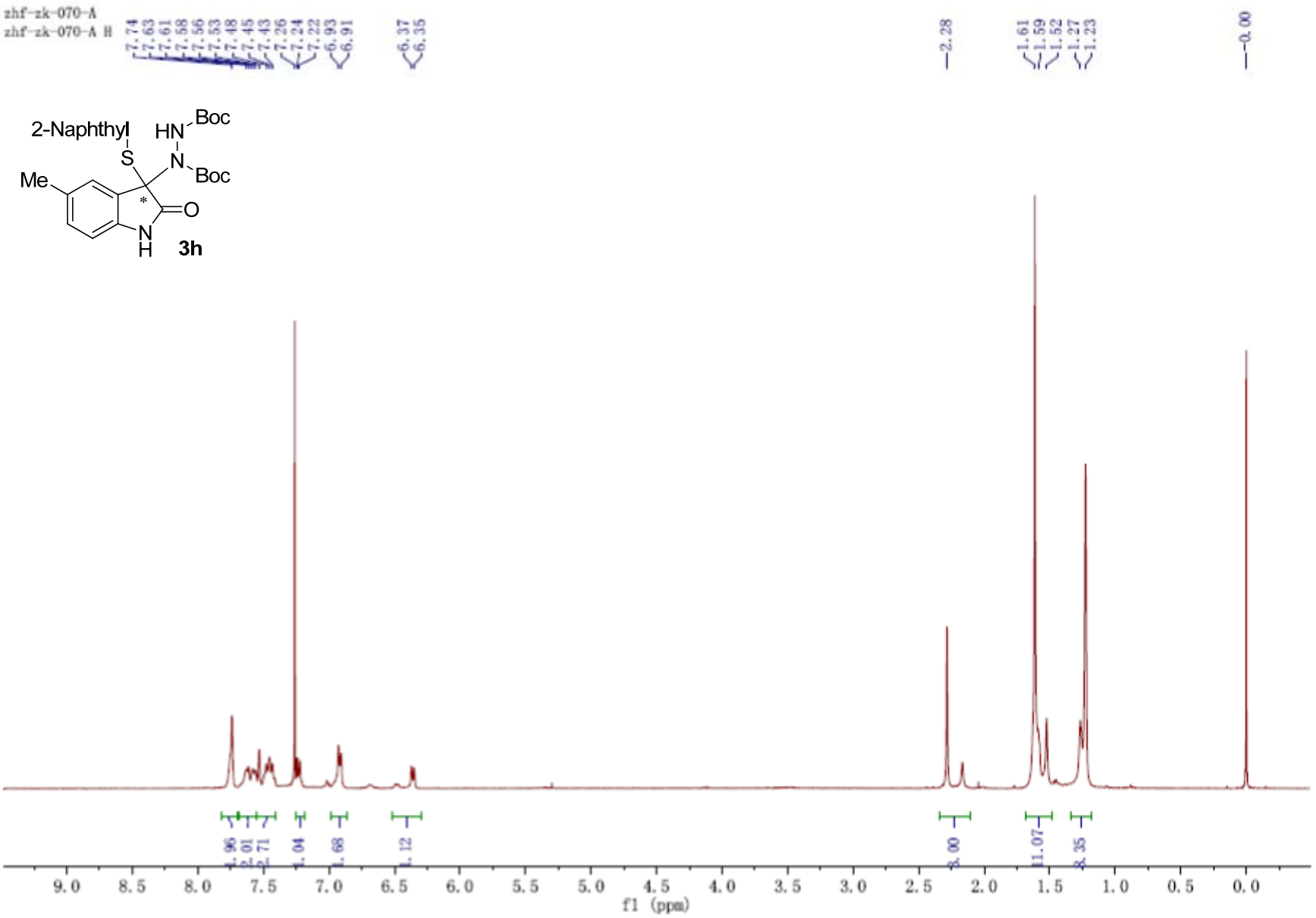
83.60
81.69
77.42
77.10
76.78
76.01
28.42
27.88




**3g**





zhf-zk-070-A C
zhf-zk-070-A C

176.02
155.32
152.50
138.05
136.78
133.43
133.17
132.96
132.34
129.43
128.06
127.52
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77.00
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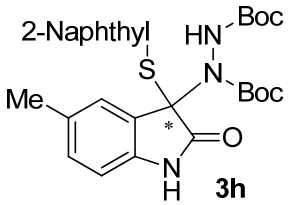
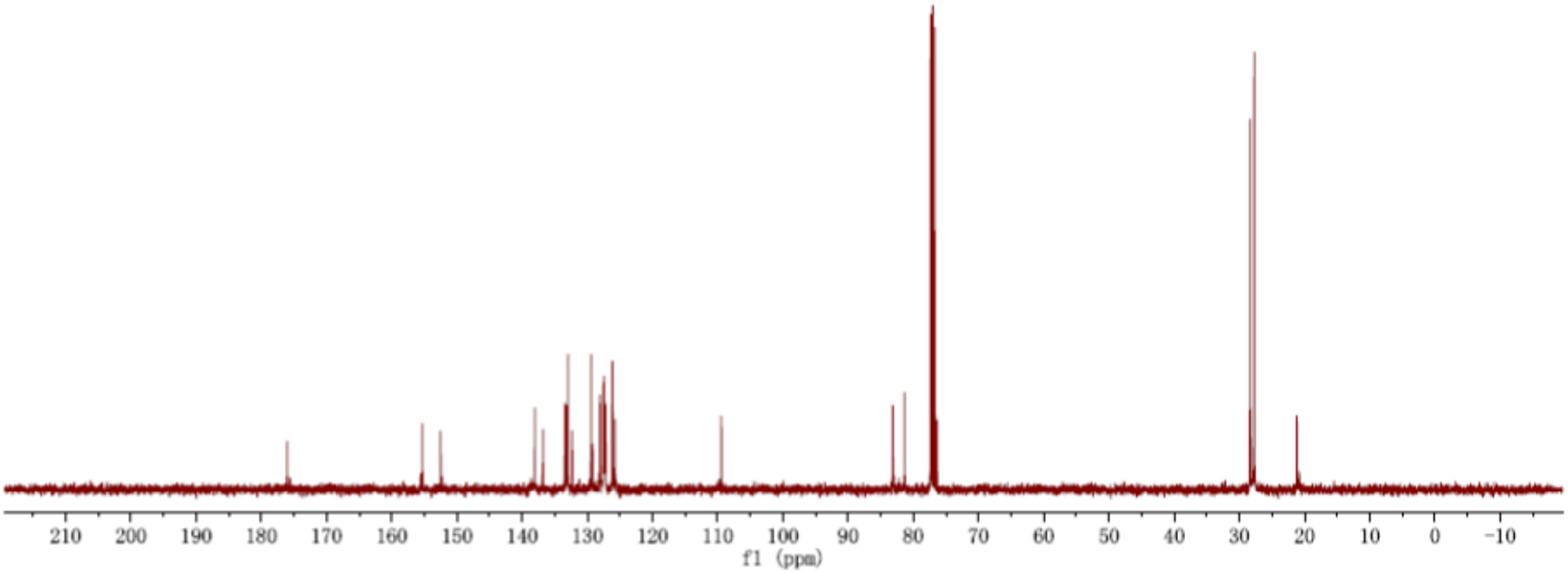
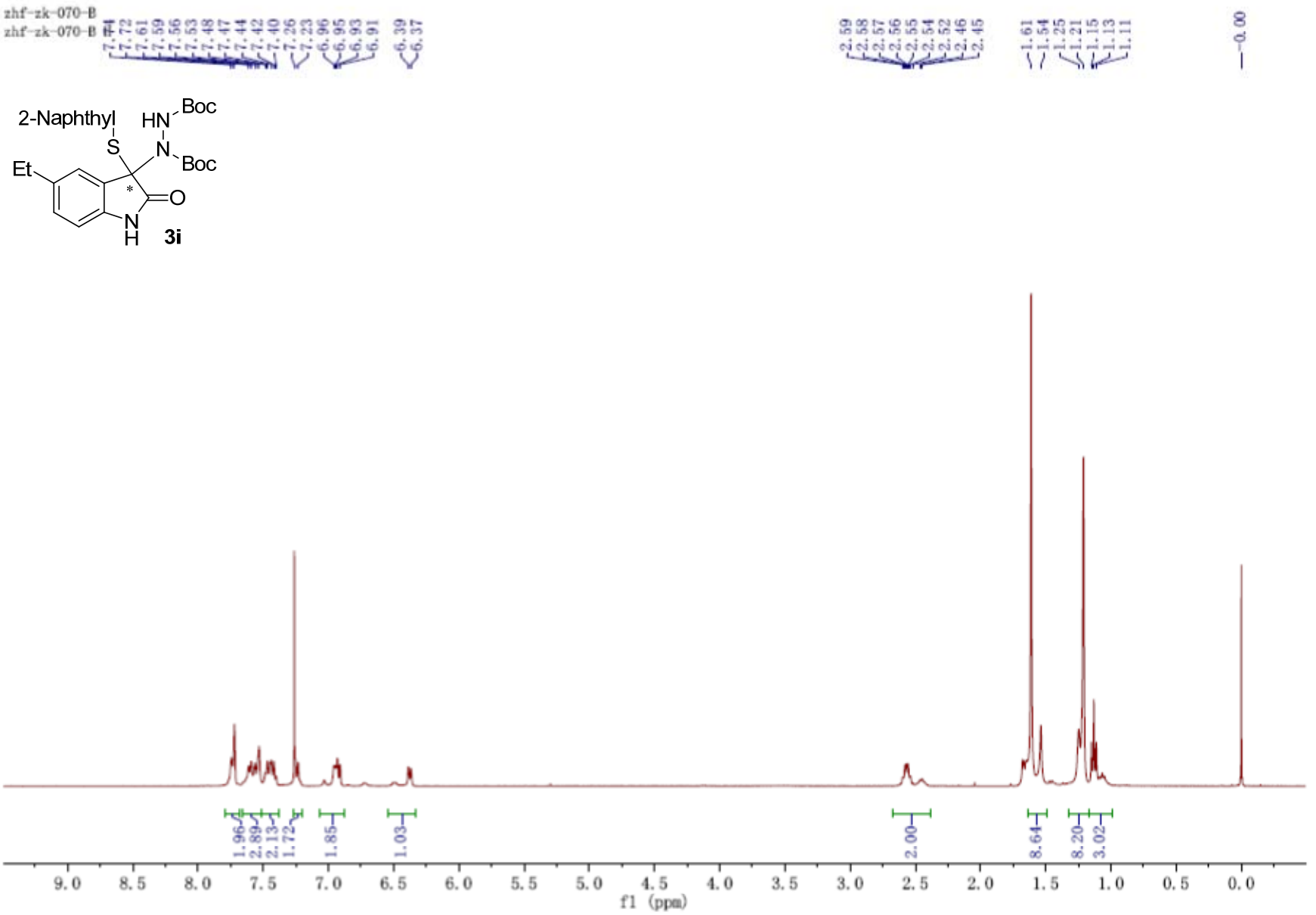
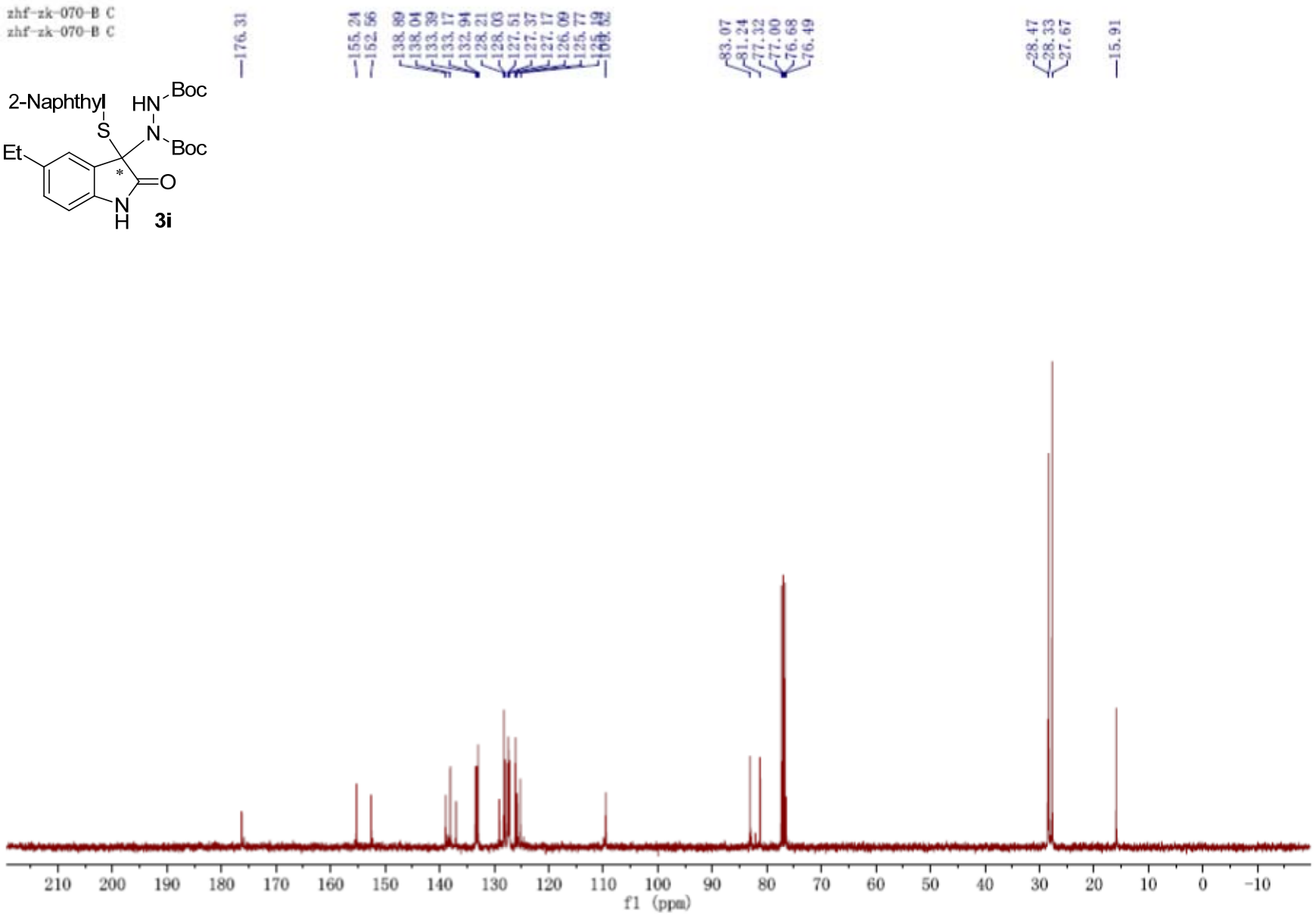
27.72
21.18

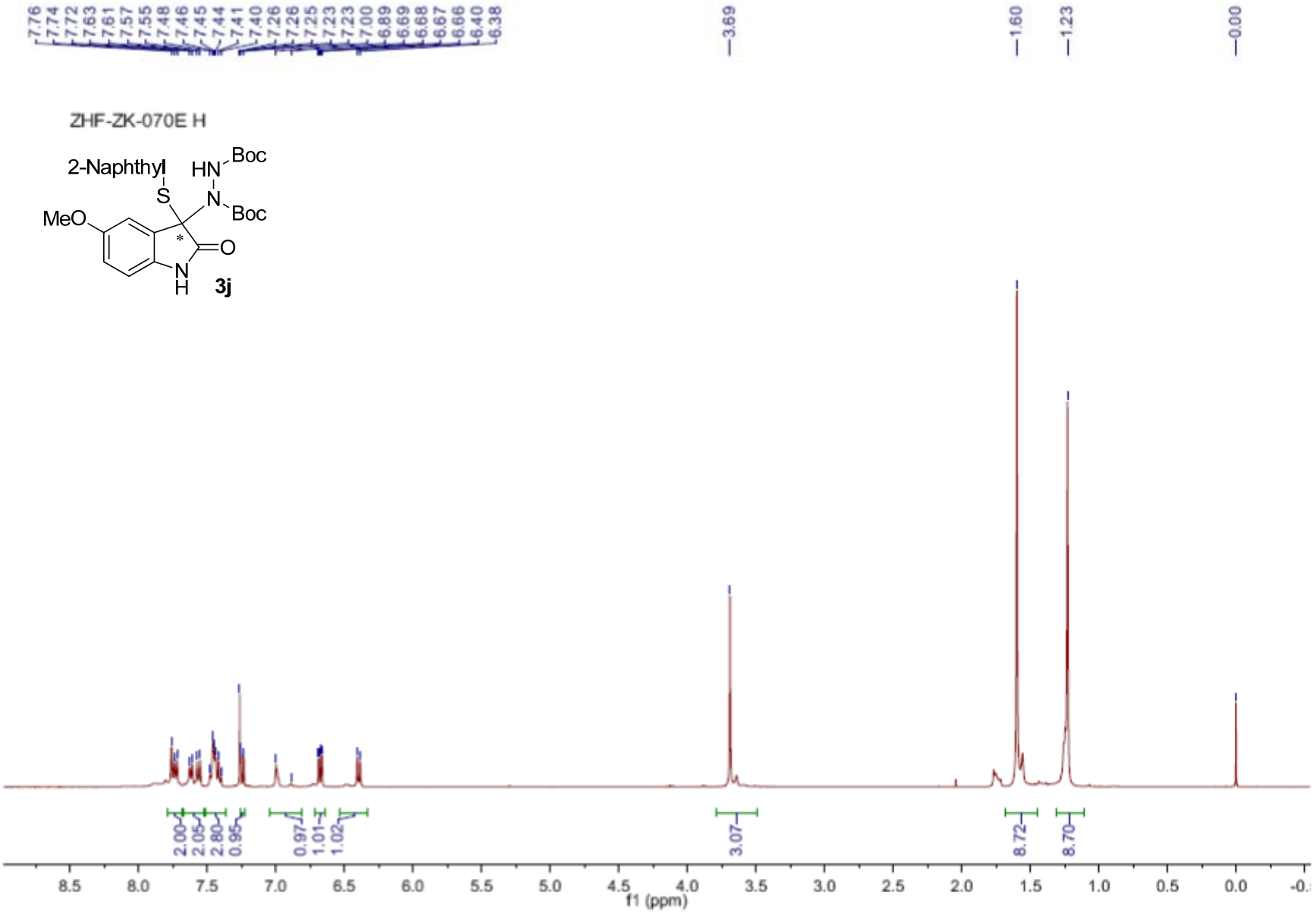


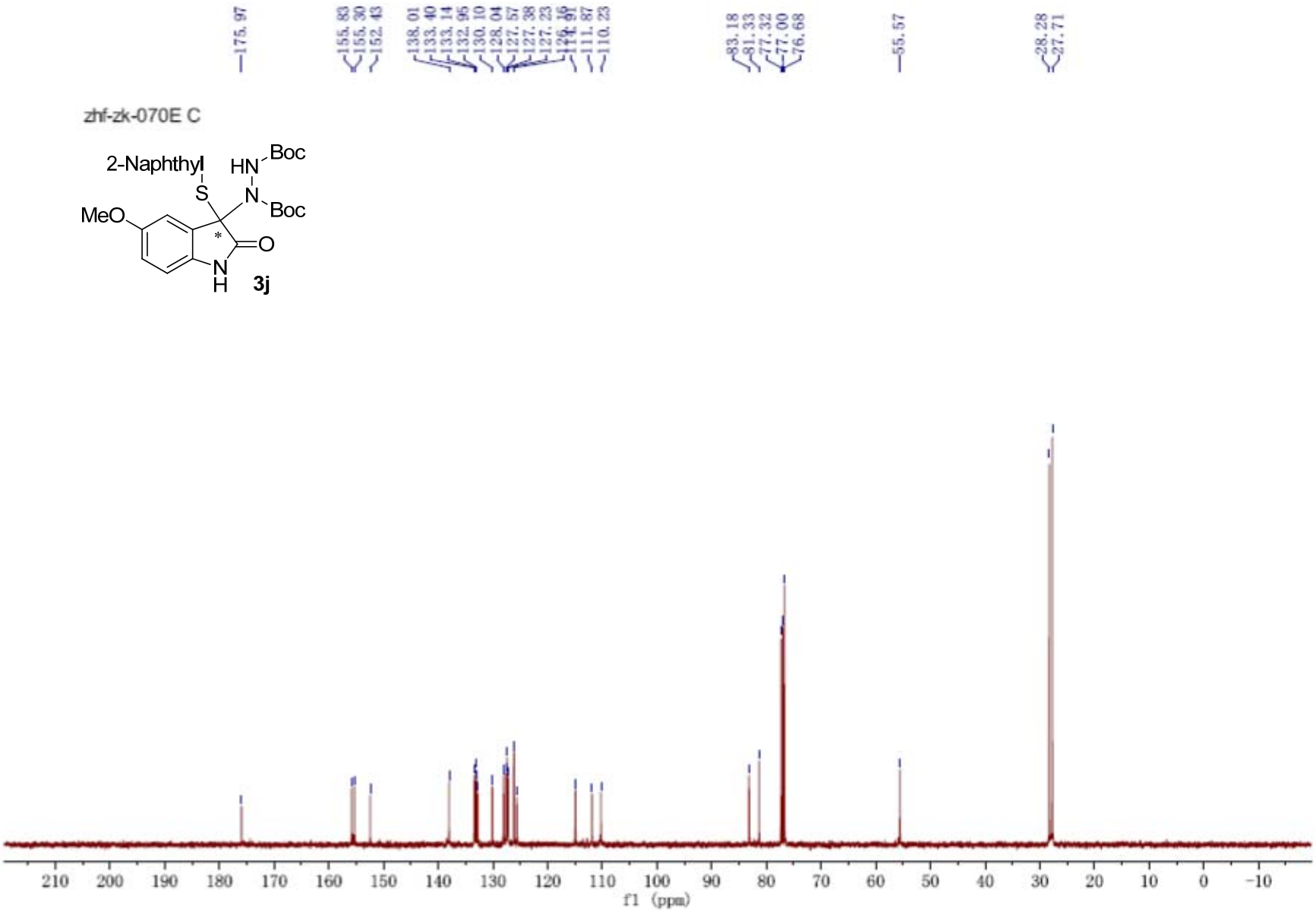

**3h**

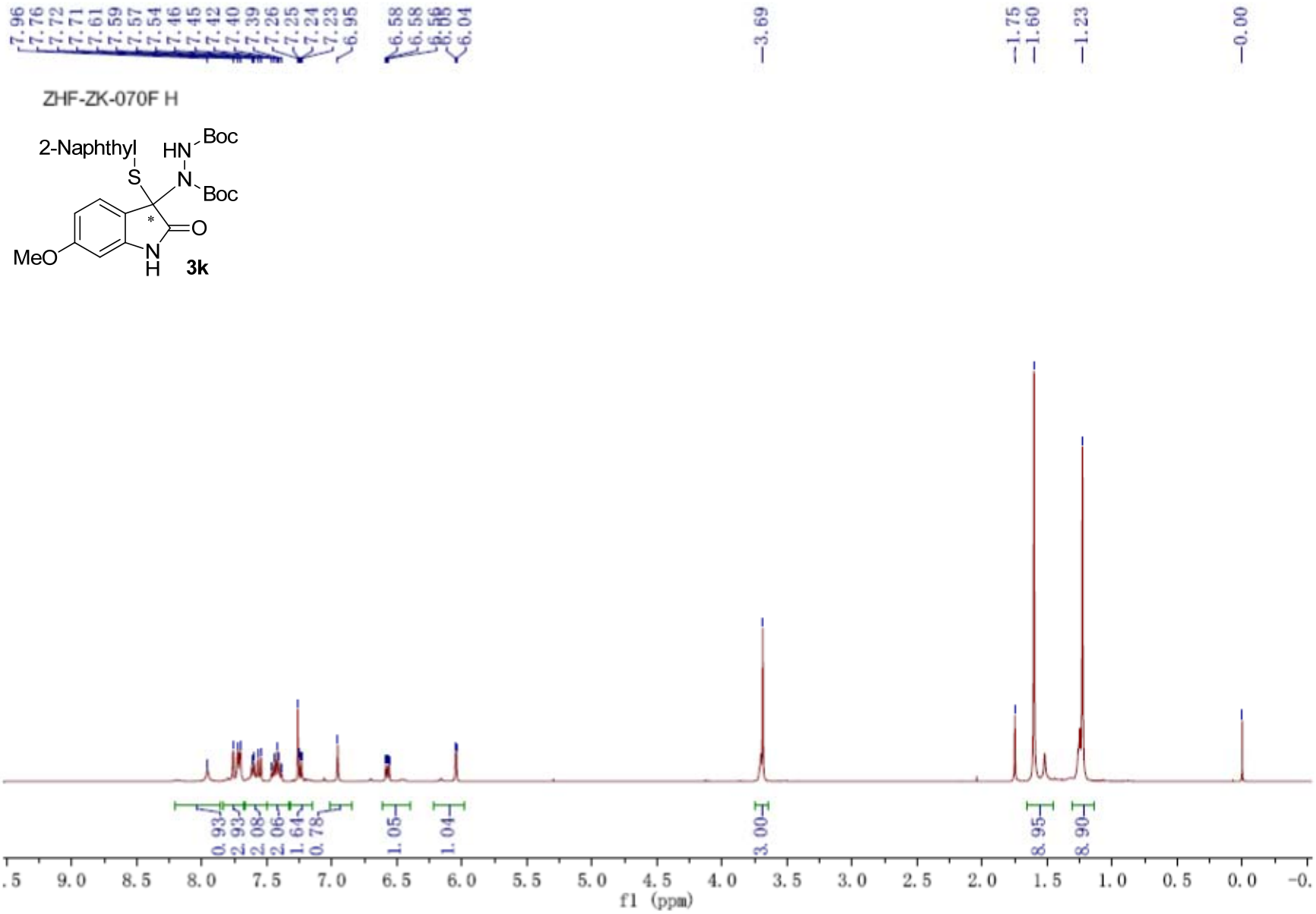




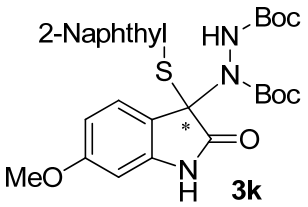




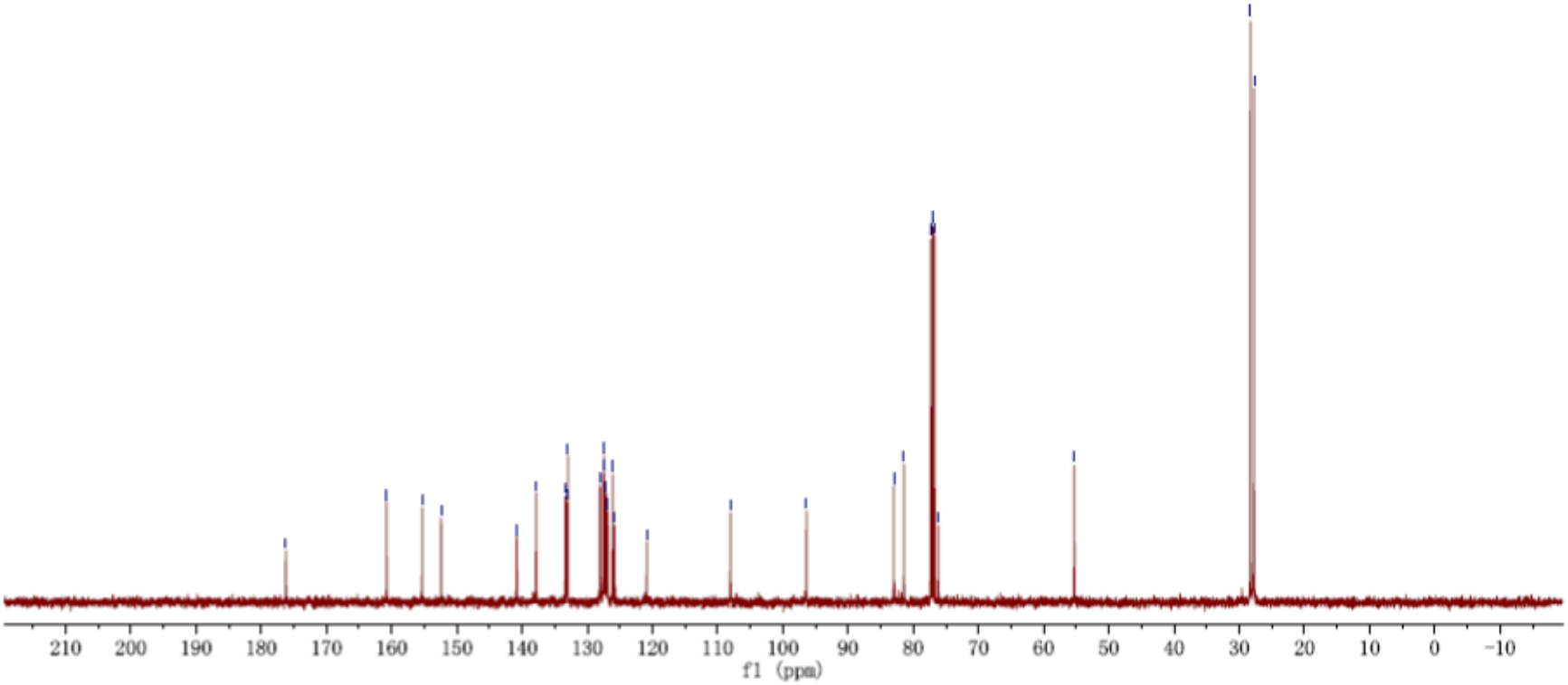





ZHF-ZK-070F C

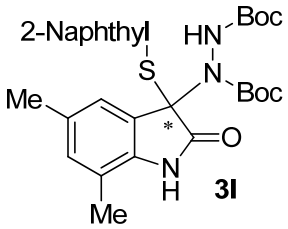



**3k**

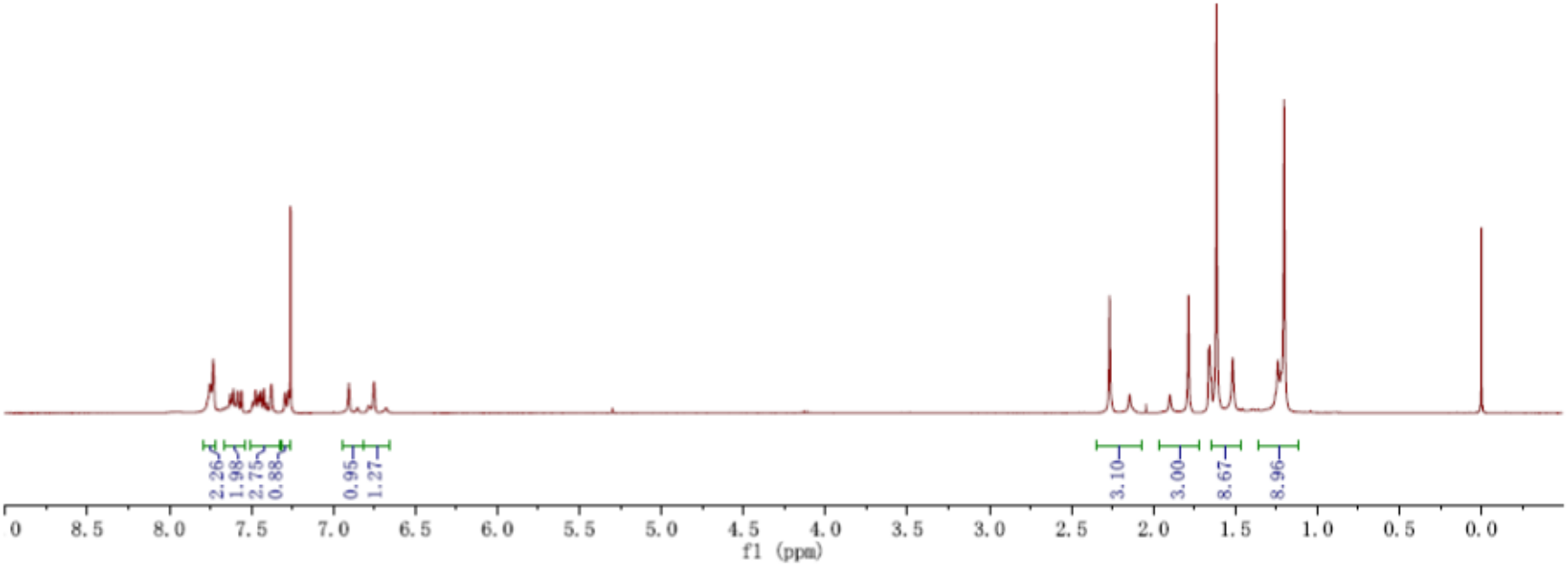




ZHF-ZK-070-C




**3l**



zhf-zk-070-C C
zhf-zk-070-C C

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155.24
152.54
137.79
135.53
133.37
133.09
132.90
132.17
130.84
128.89
127.99
127.39
127.32
127.13
126.07
123.23
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77.00
76.68
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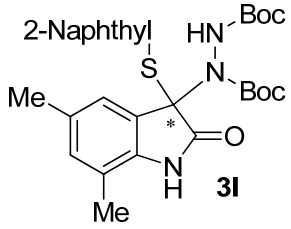
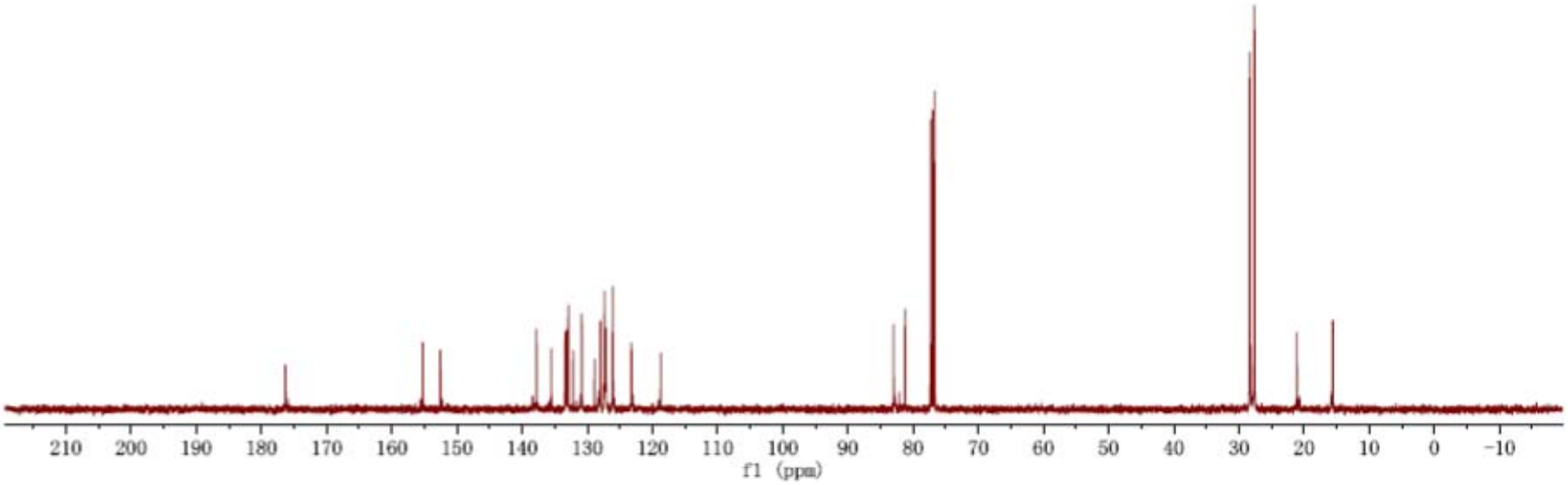
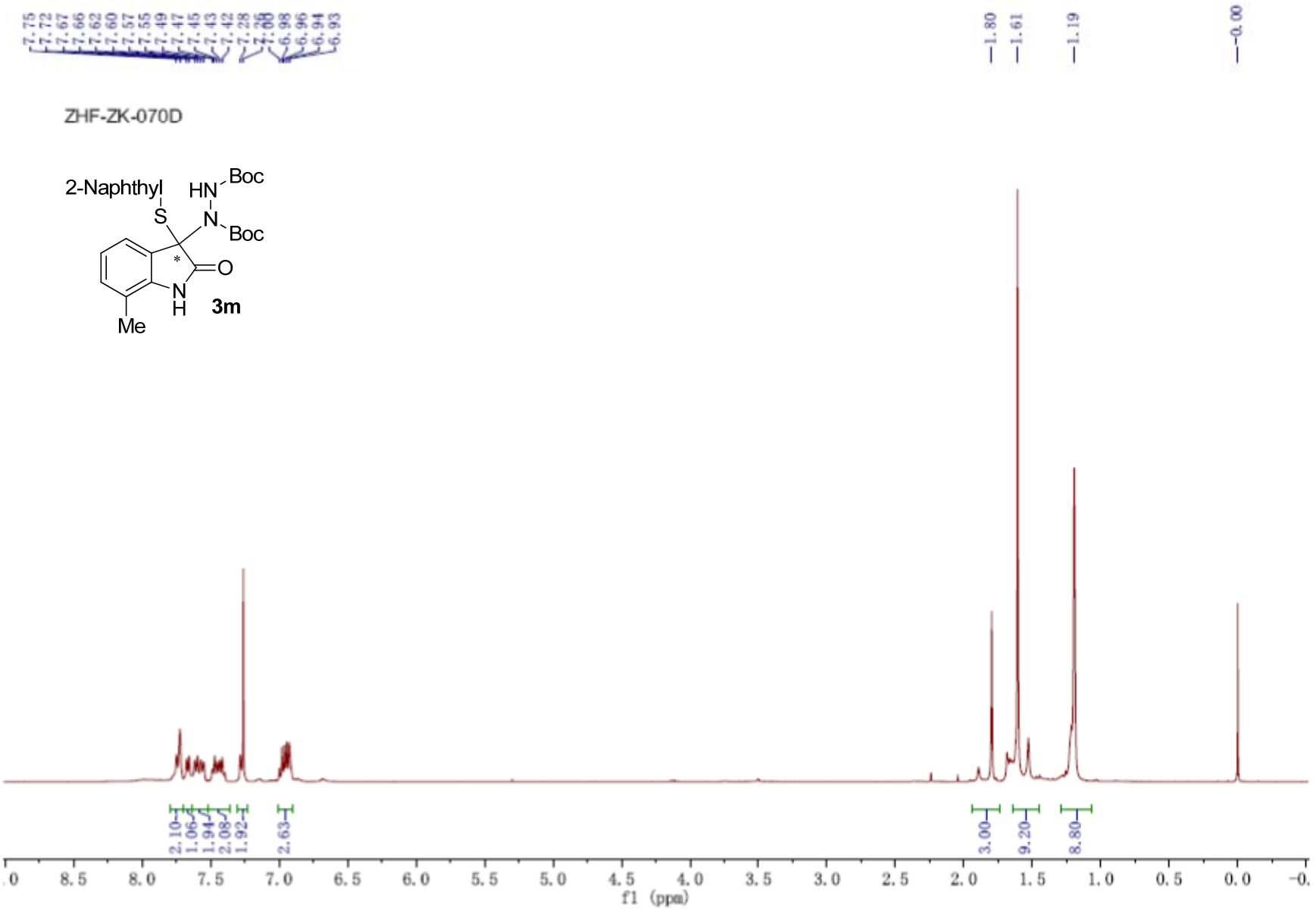
27.63
21.10
15.61




**3l**





zhf-zk-070-D C
zhf-zk-070-D C

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155.30
152.39
138.02
137.71
133.37
133.02
132.91
130.29
128.93
128.01
127.48
127.34
127.16
126.09
125.88
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77.00
76.68
76.52
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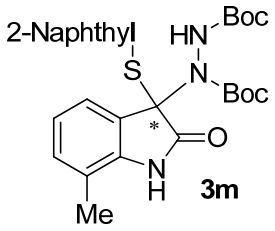
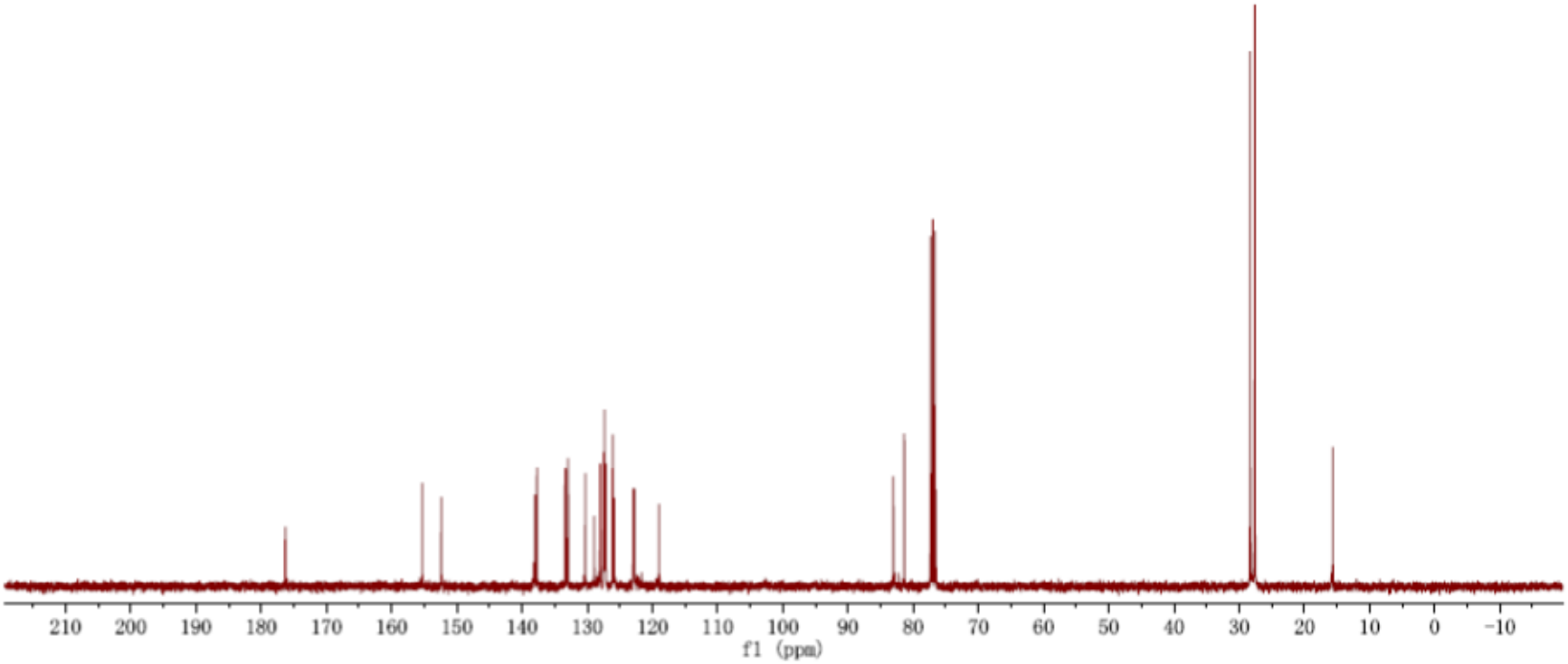
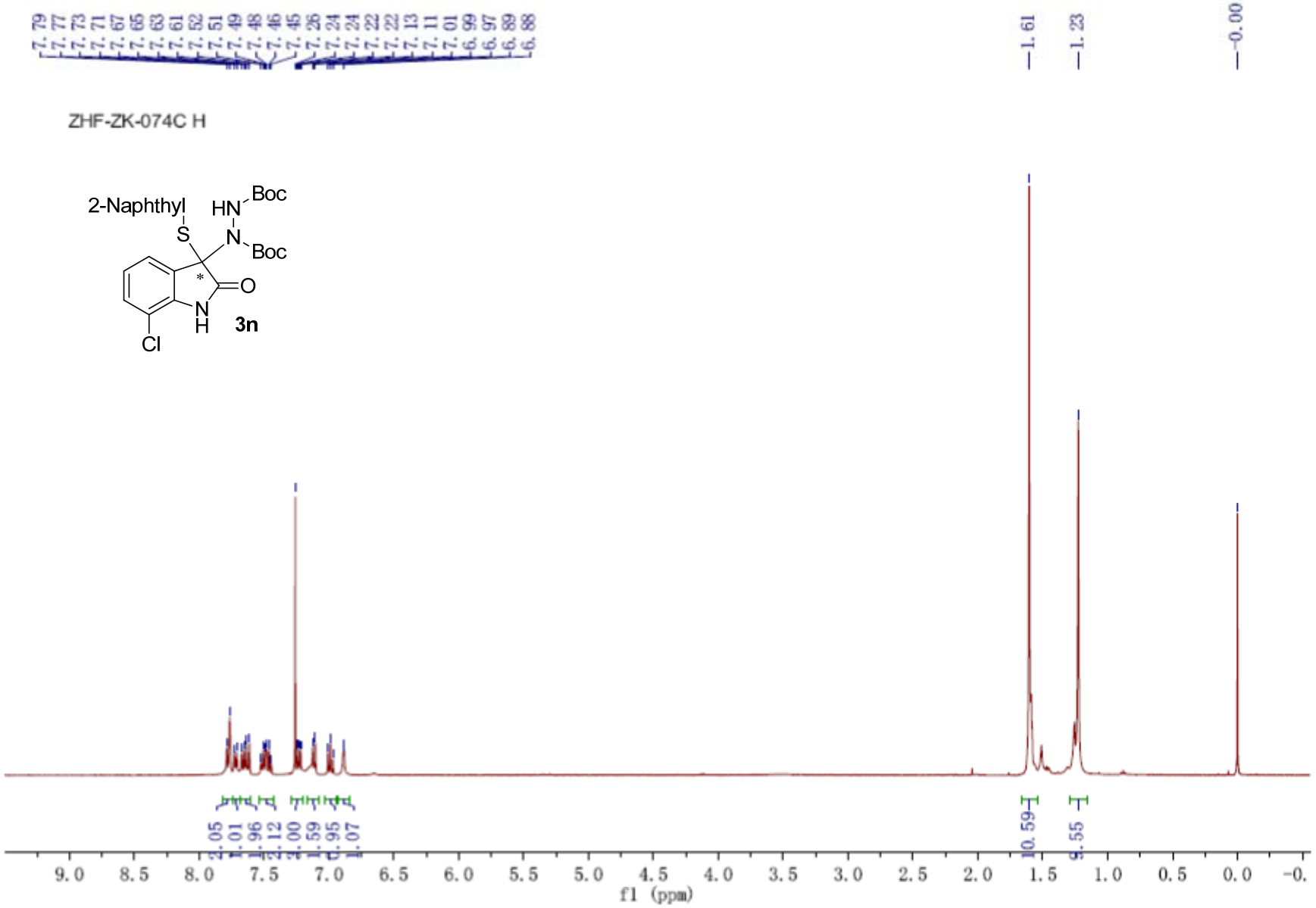
27.61
15.64

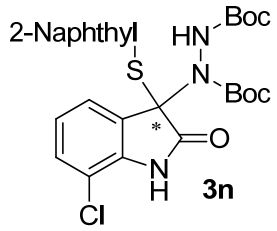



**3m**

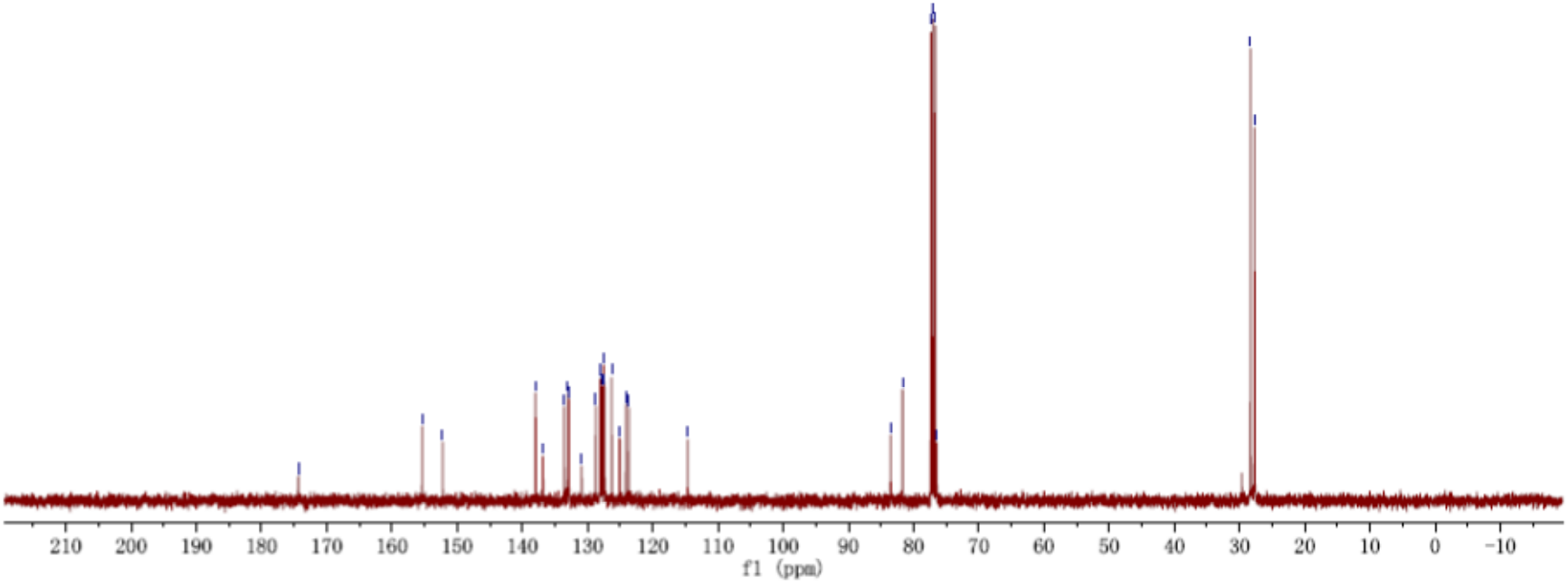


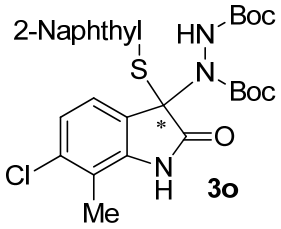


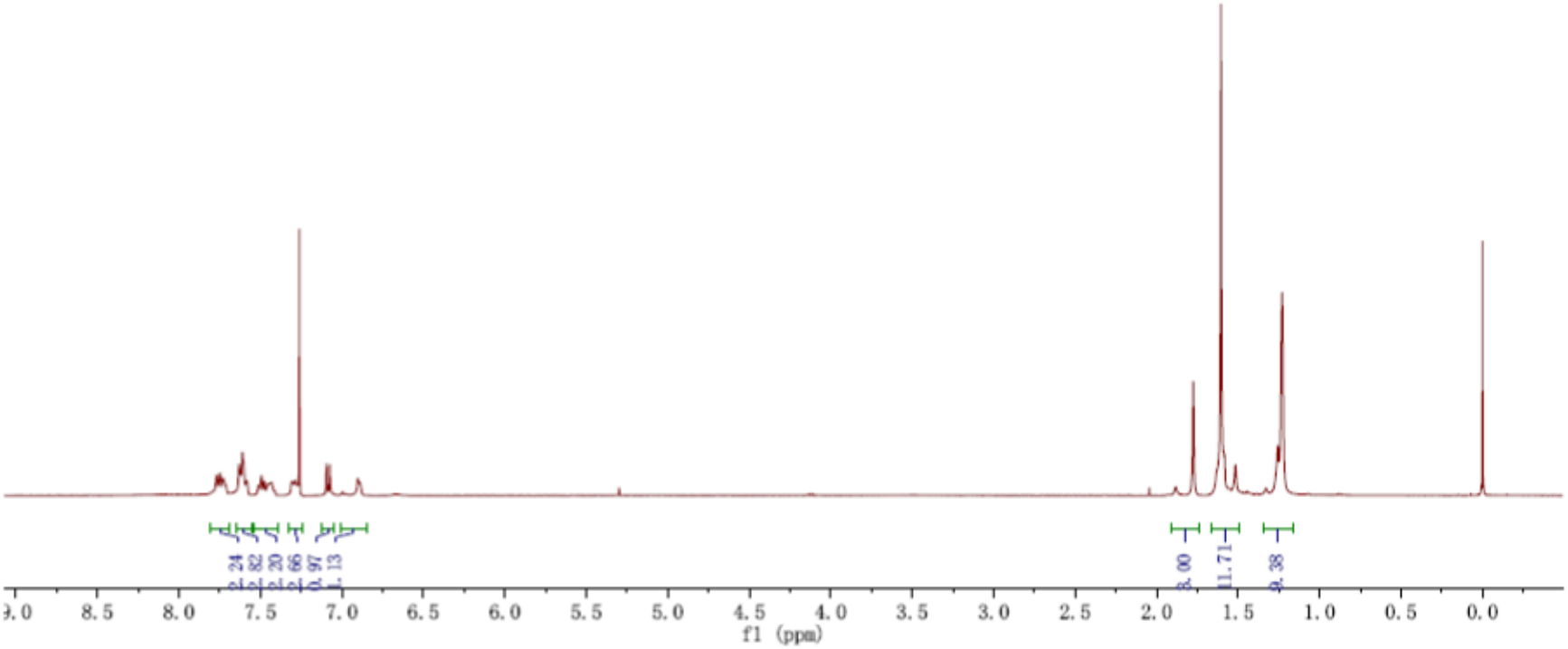

ZHF-ZK-074C




**3n**



zhf-zk-096 C4
zhf-zk-096 C

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152.36
139.28
137.93
135.00
133.46
132.93
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126.31
125.46
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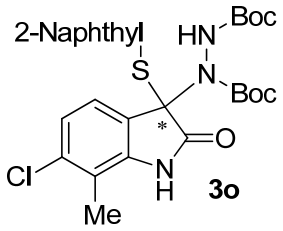
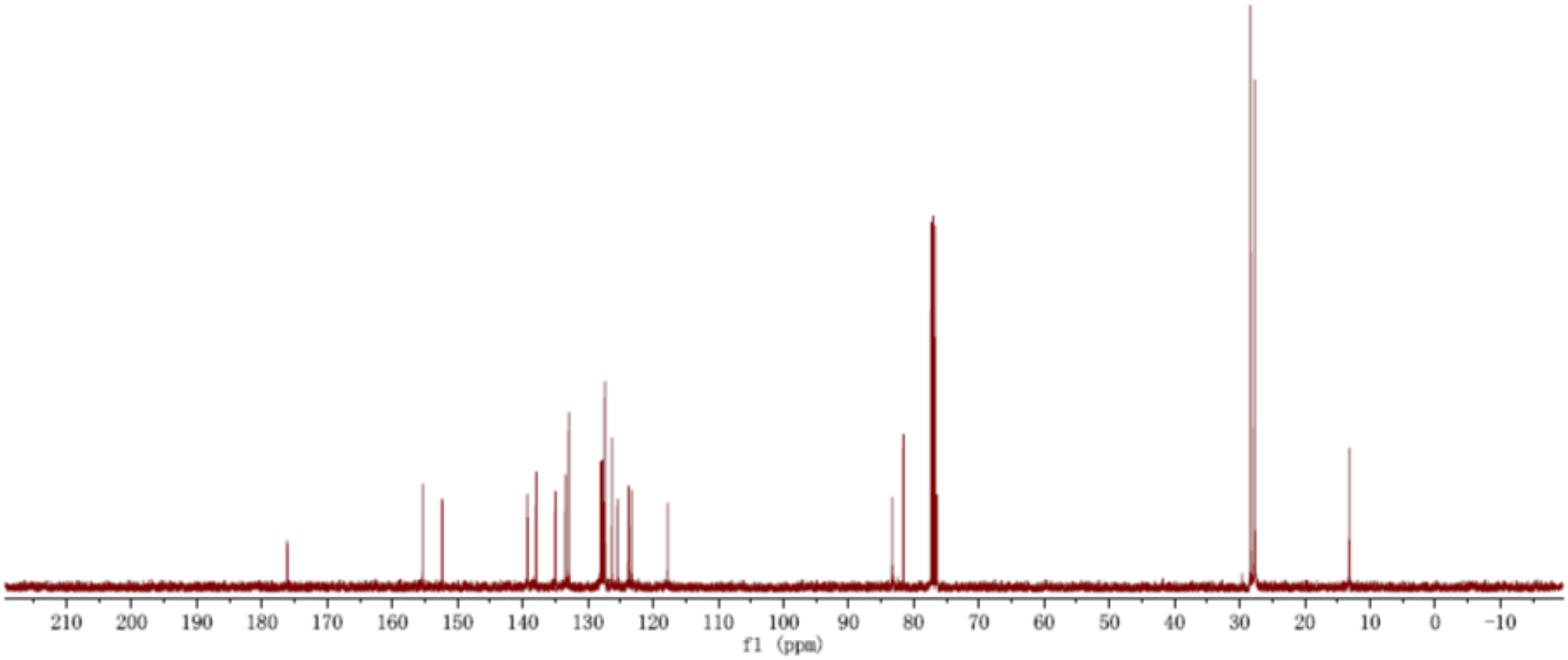
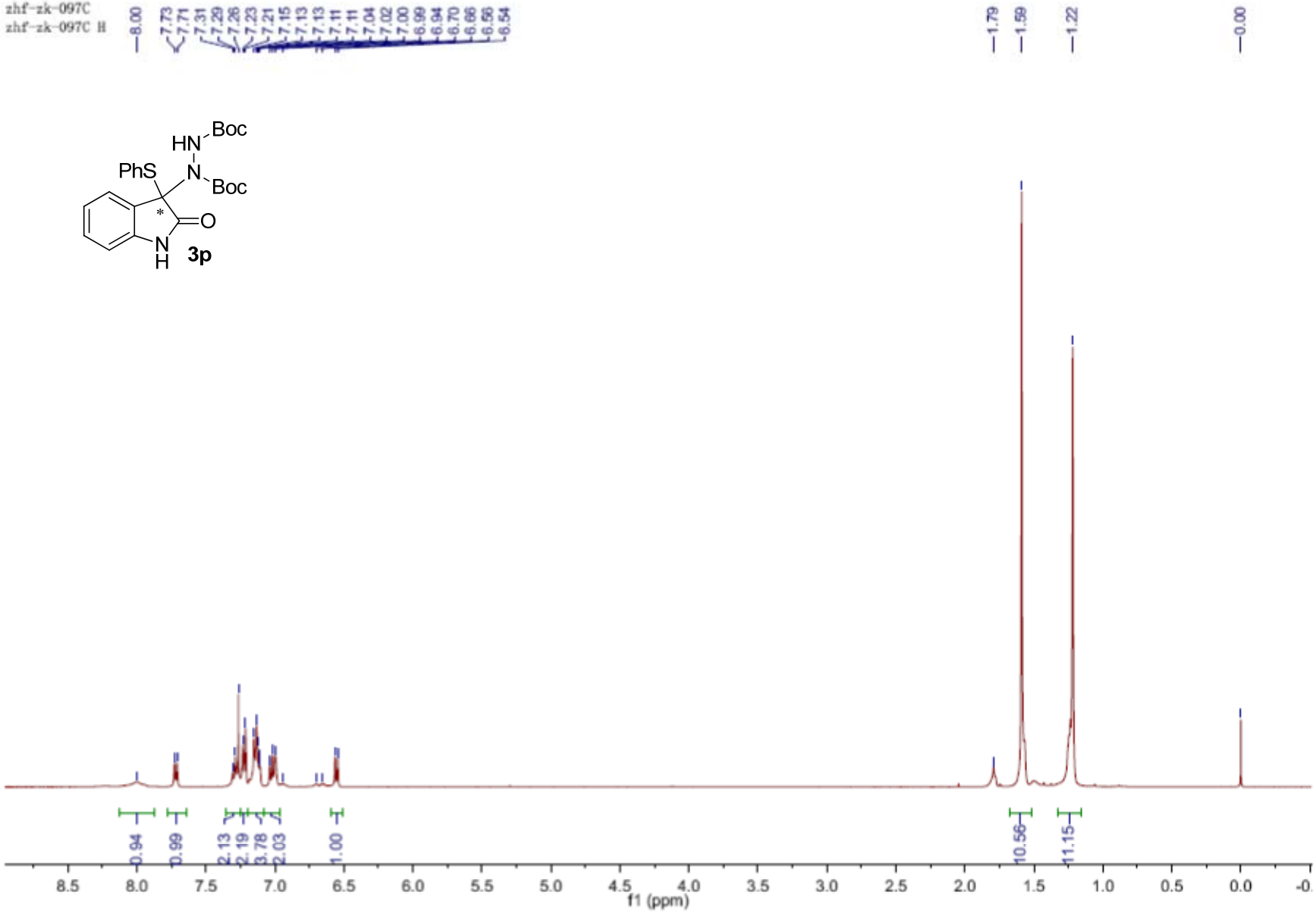
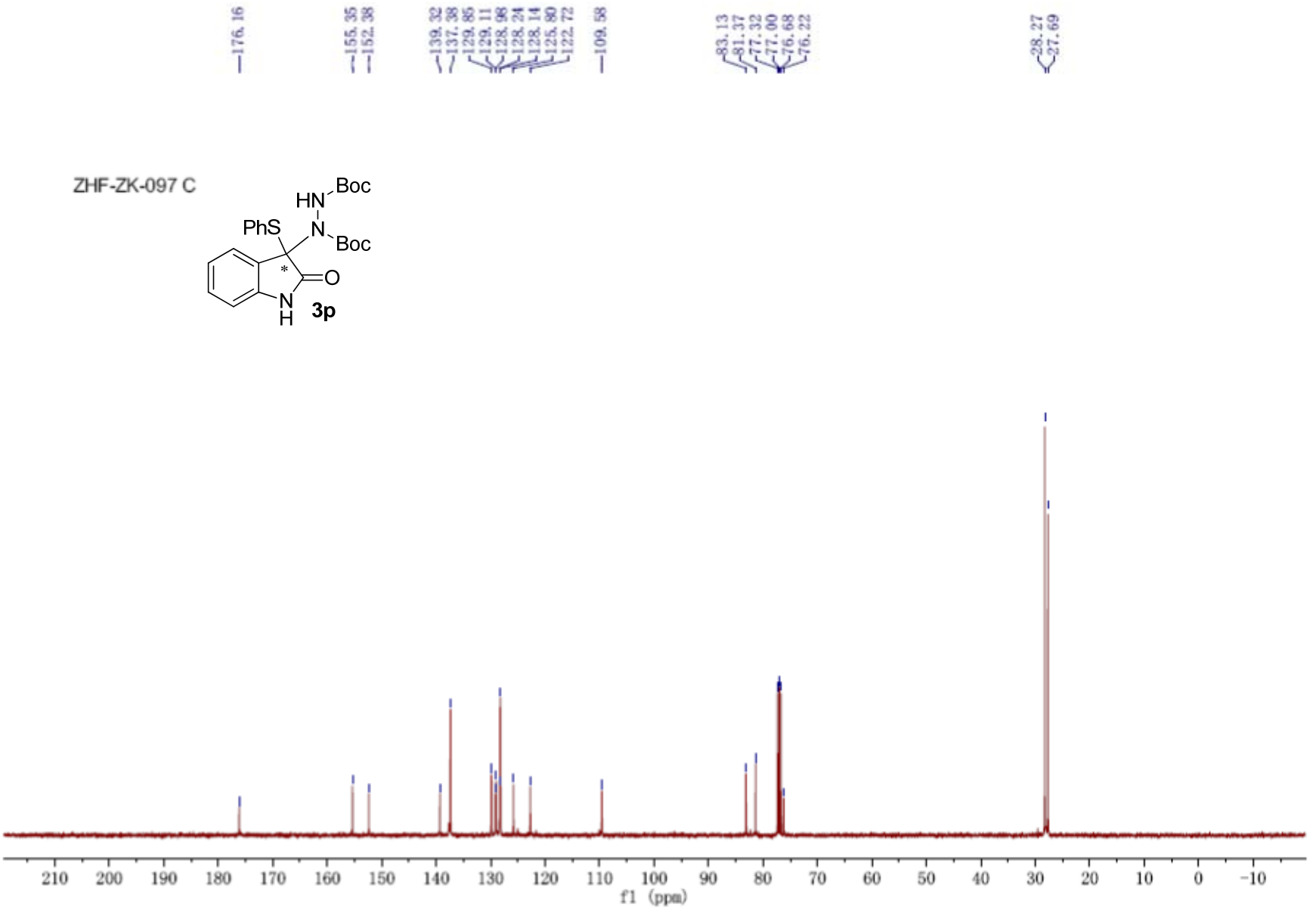
77.00
76.68
76.45
28.33
27.70
13.15

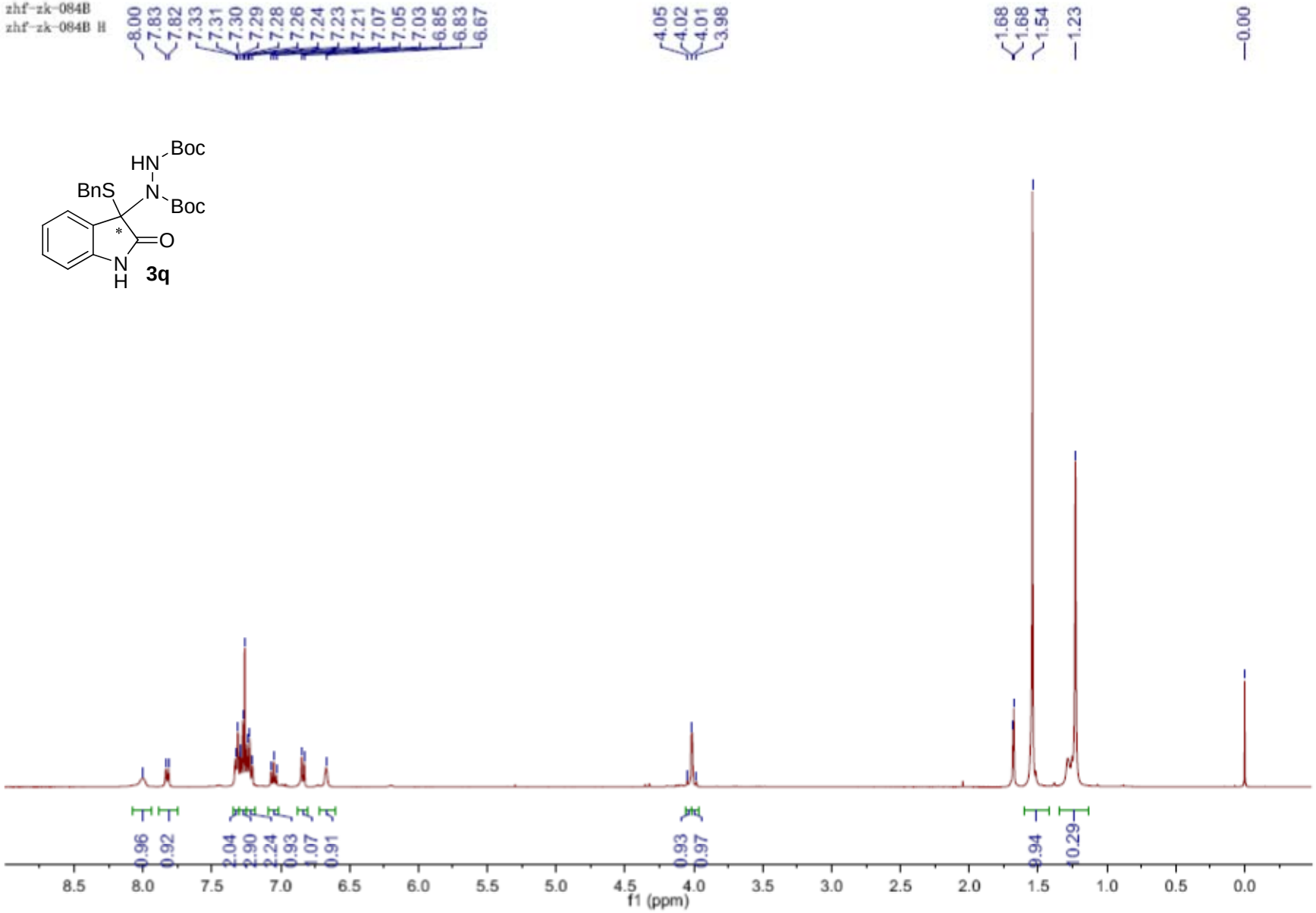


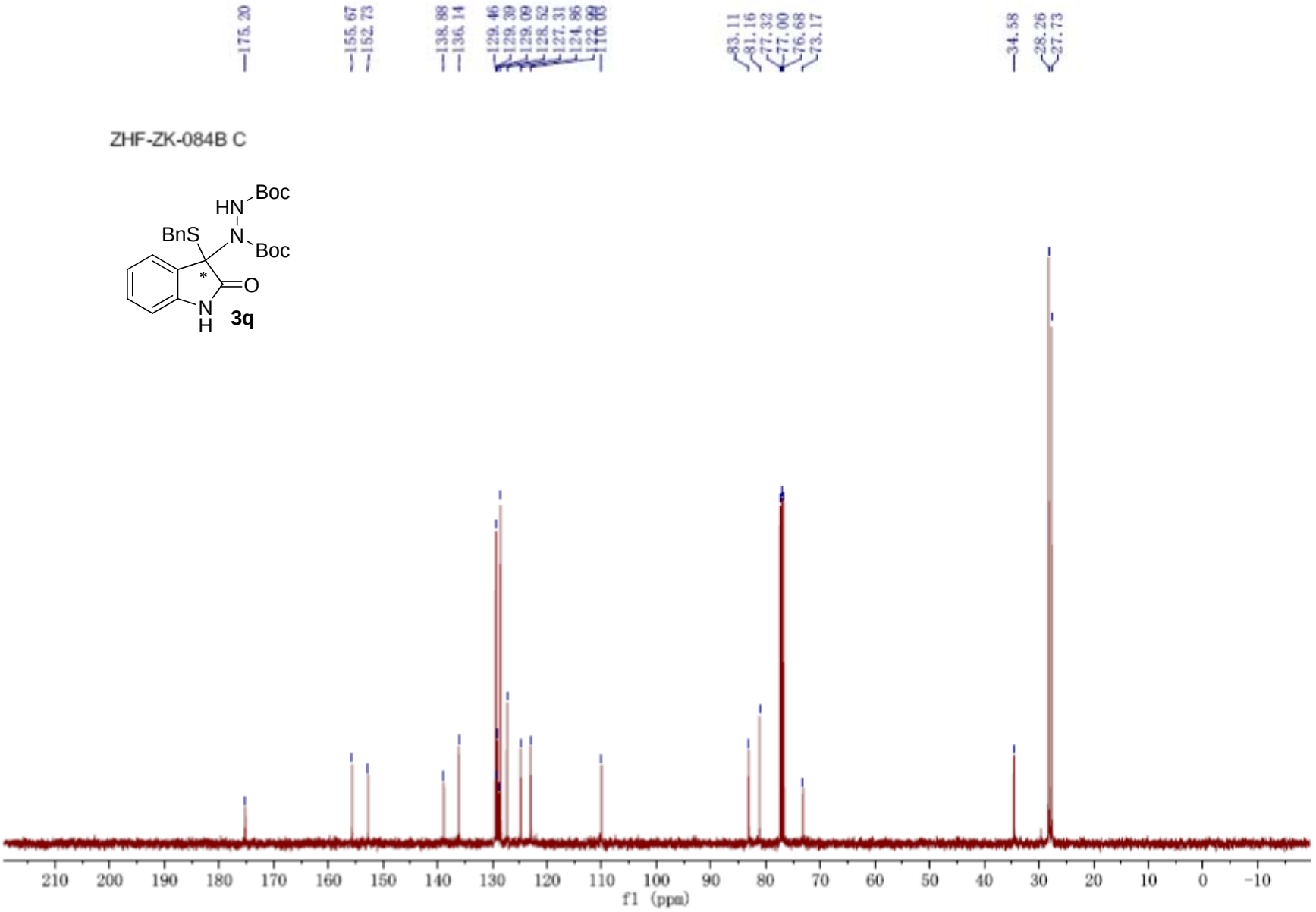

**3o**

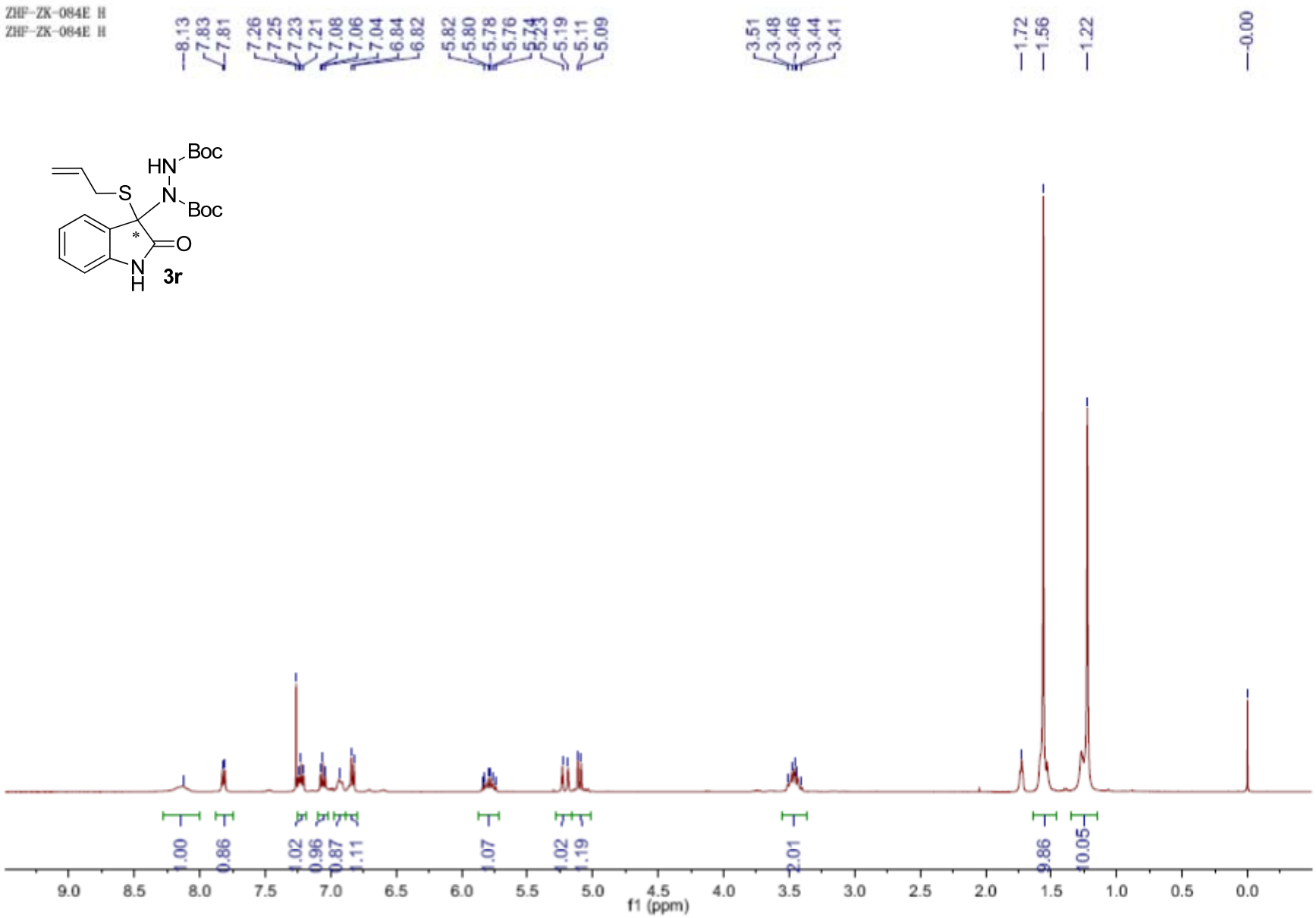


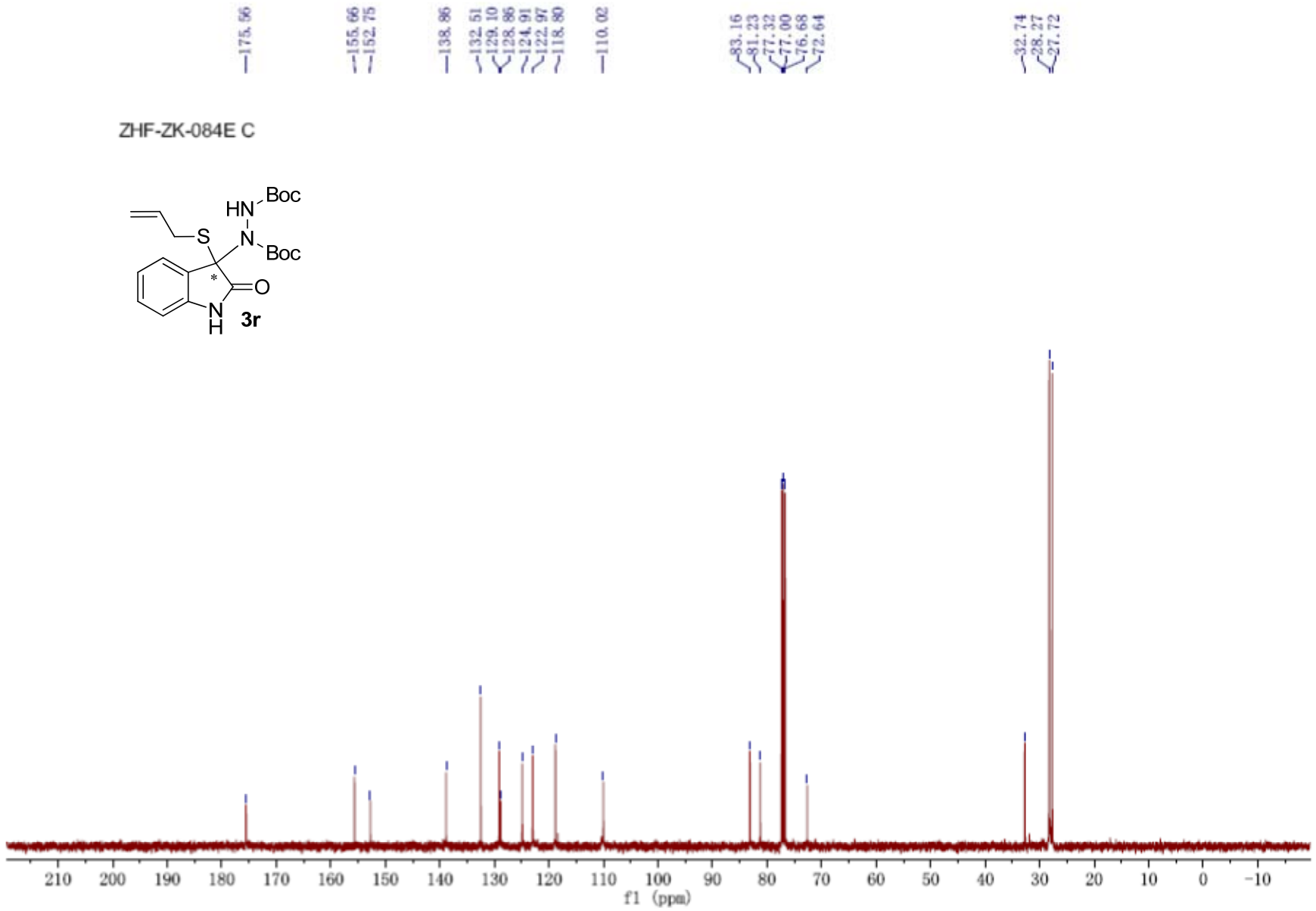


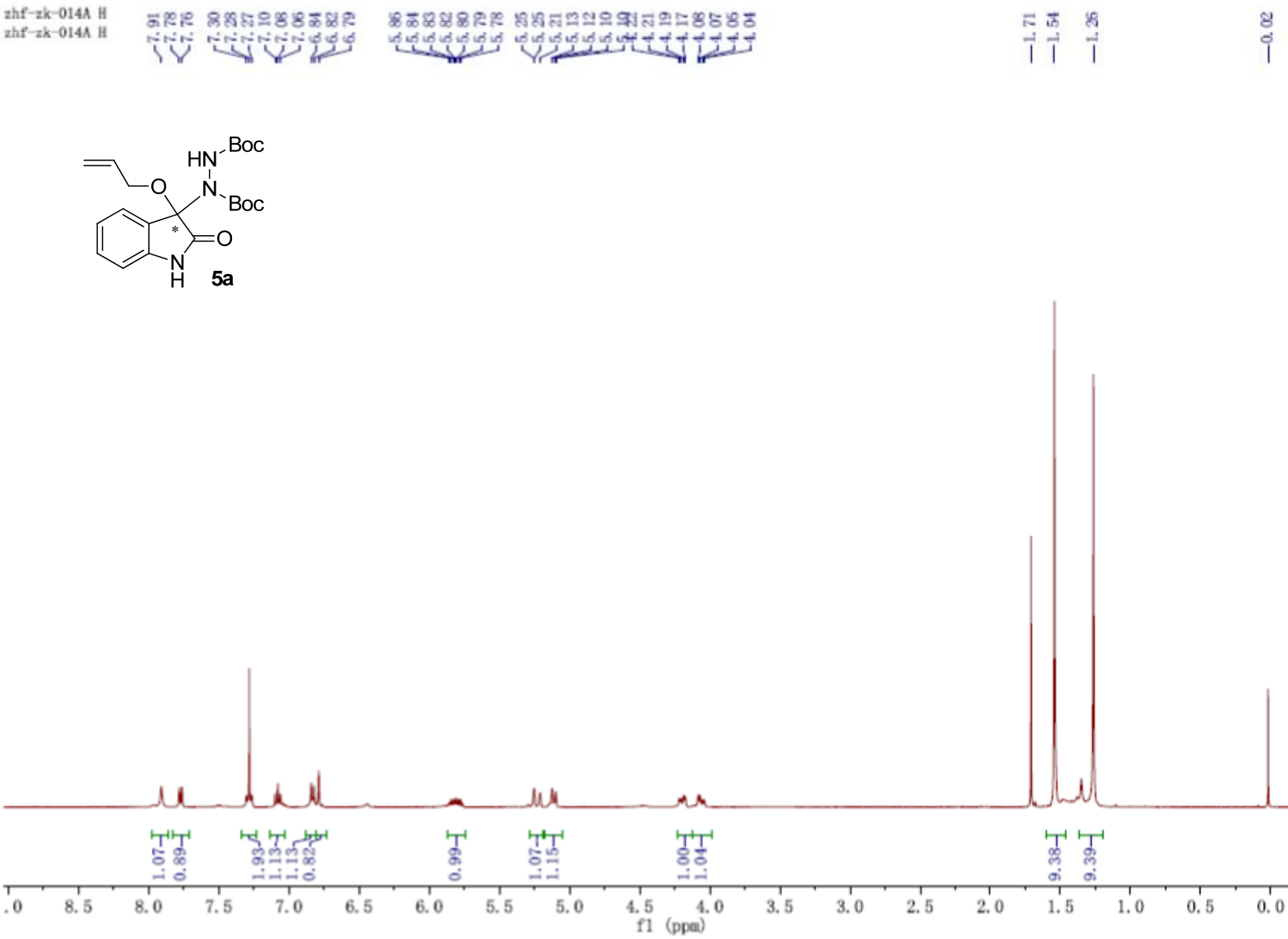


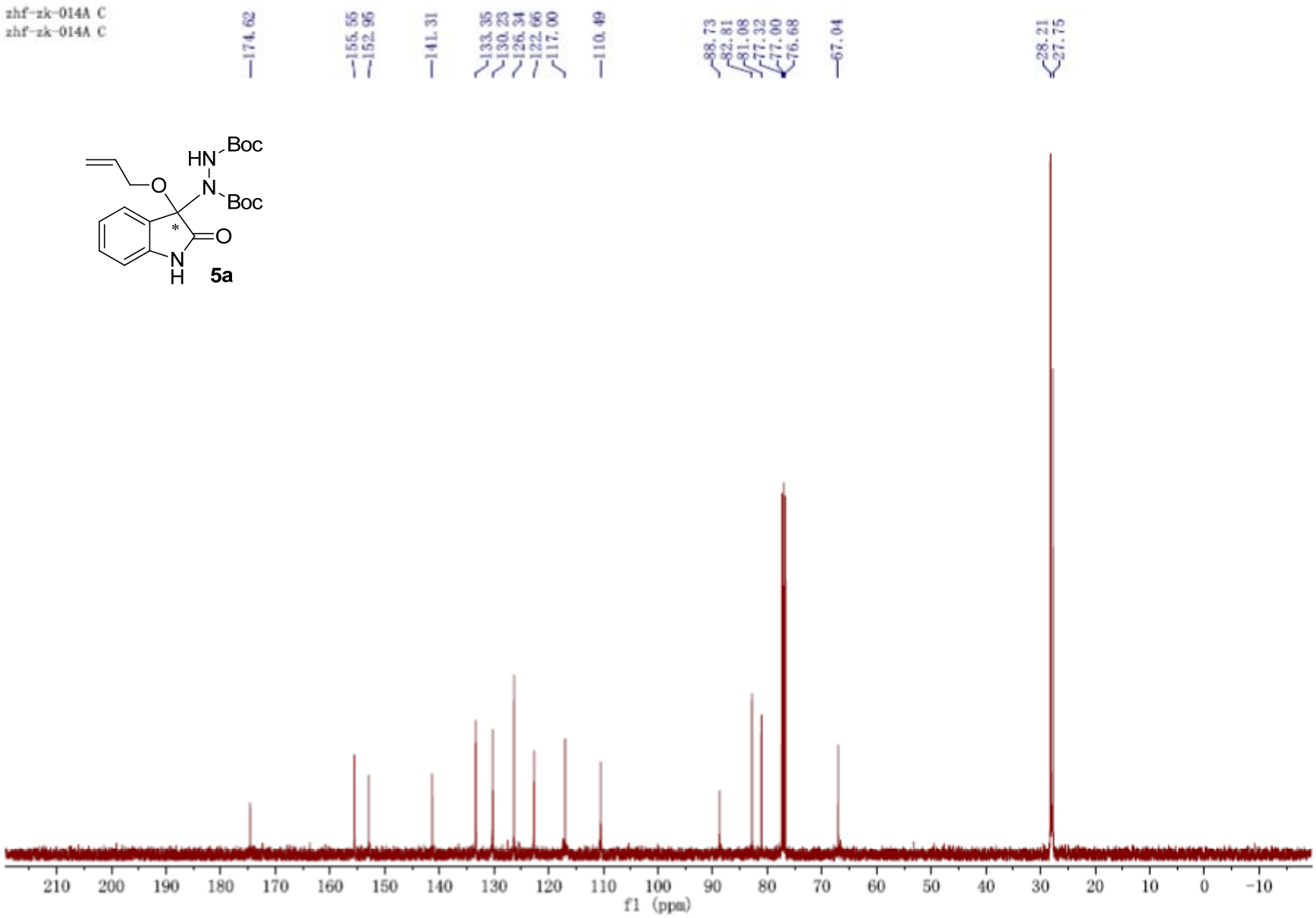


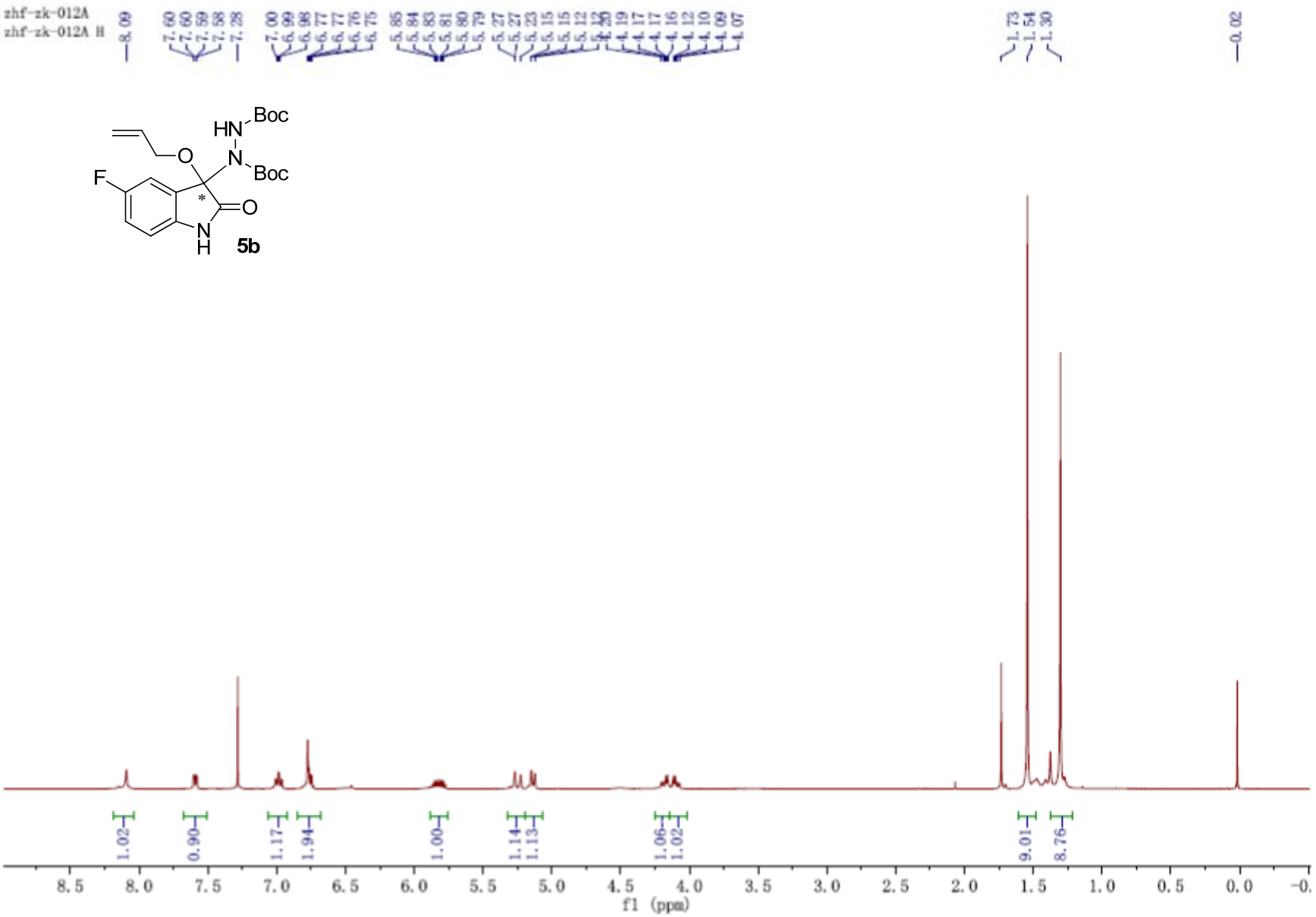












zhf-zk-012 A C
zhf-zk-012 A C

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133.15
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127.97
117.32
116.80
116.56
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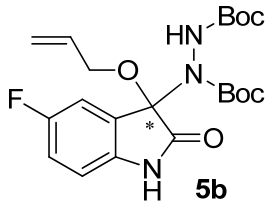
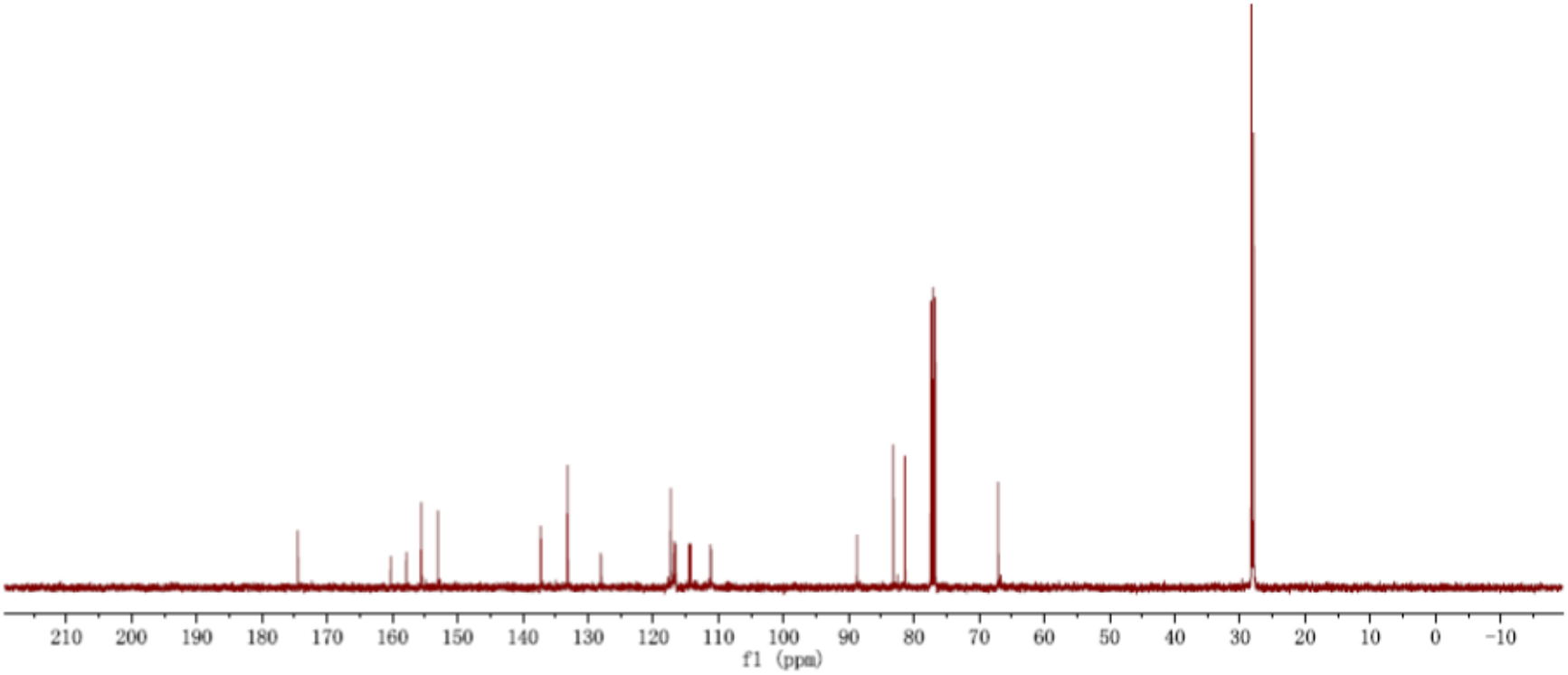
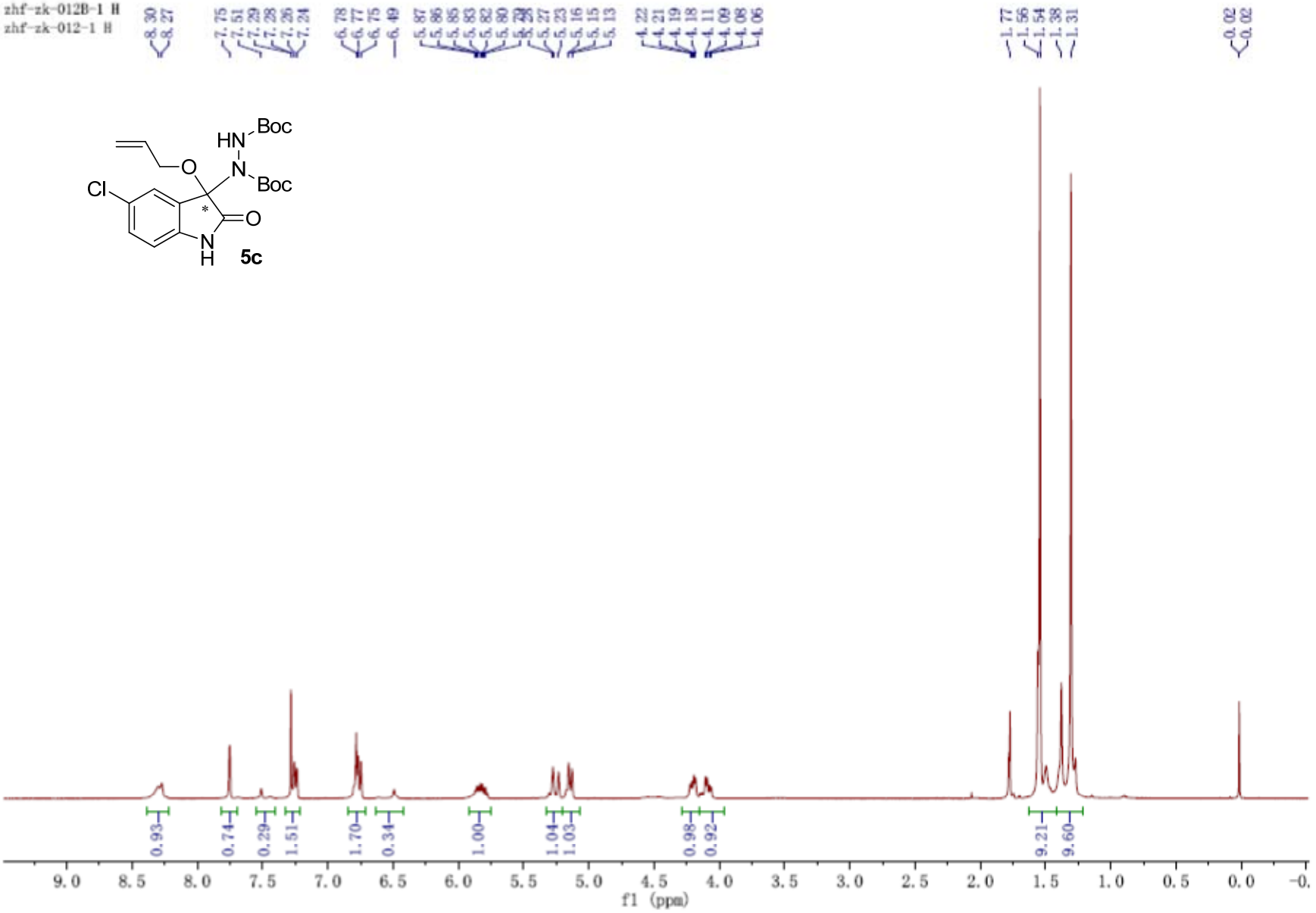
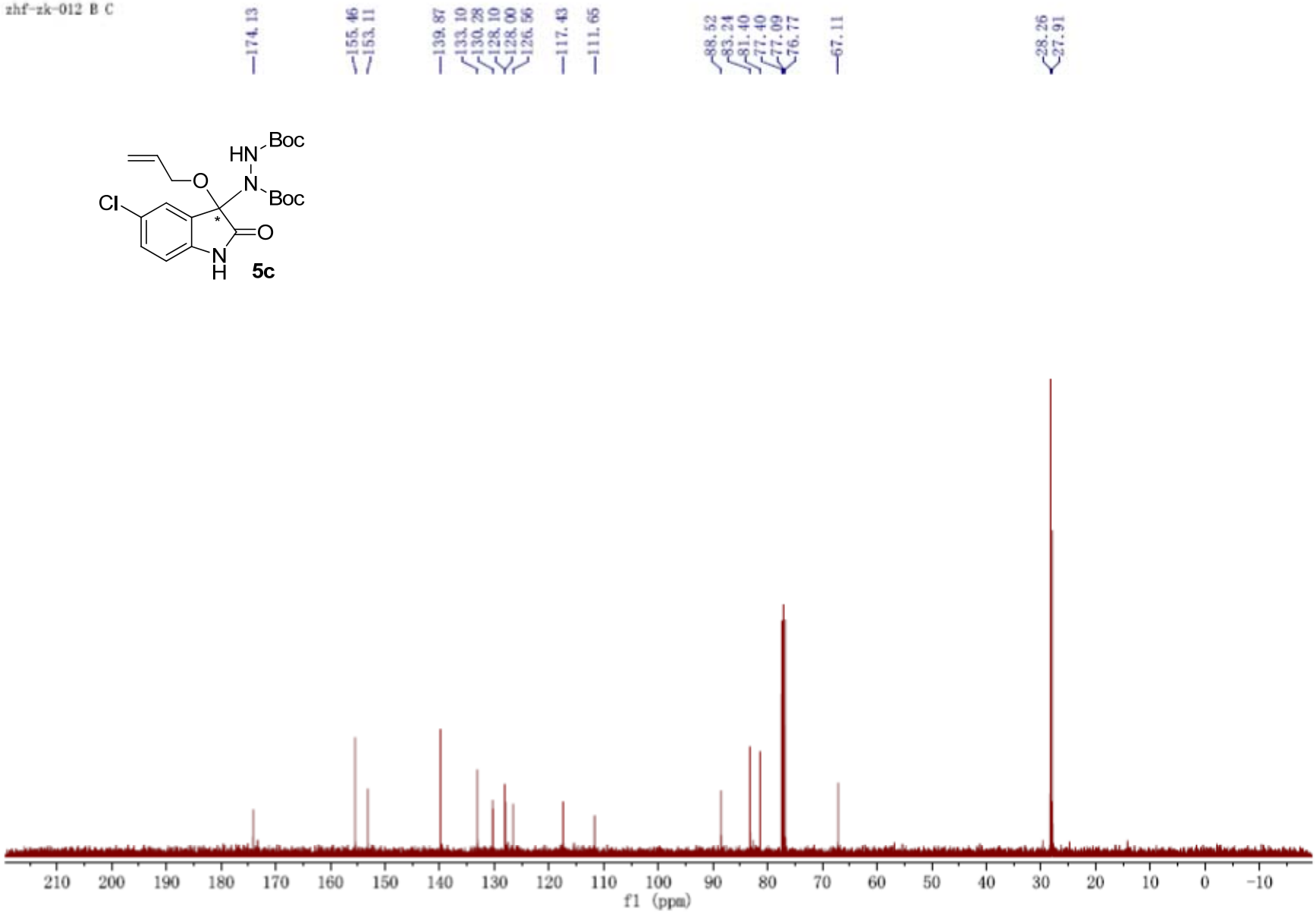
28.25
27.89

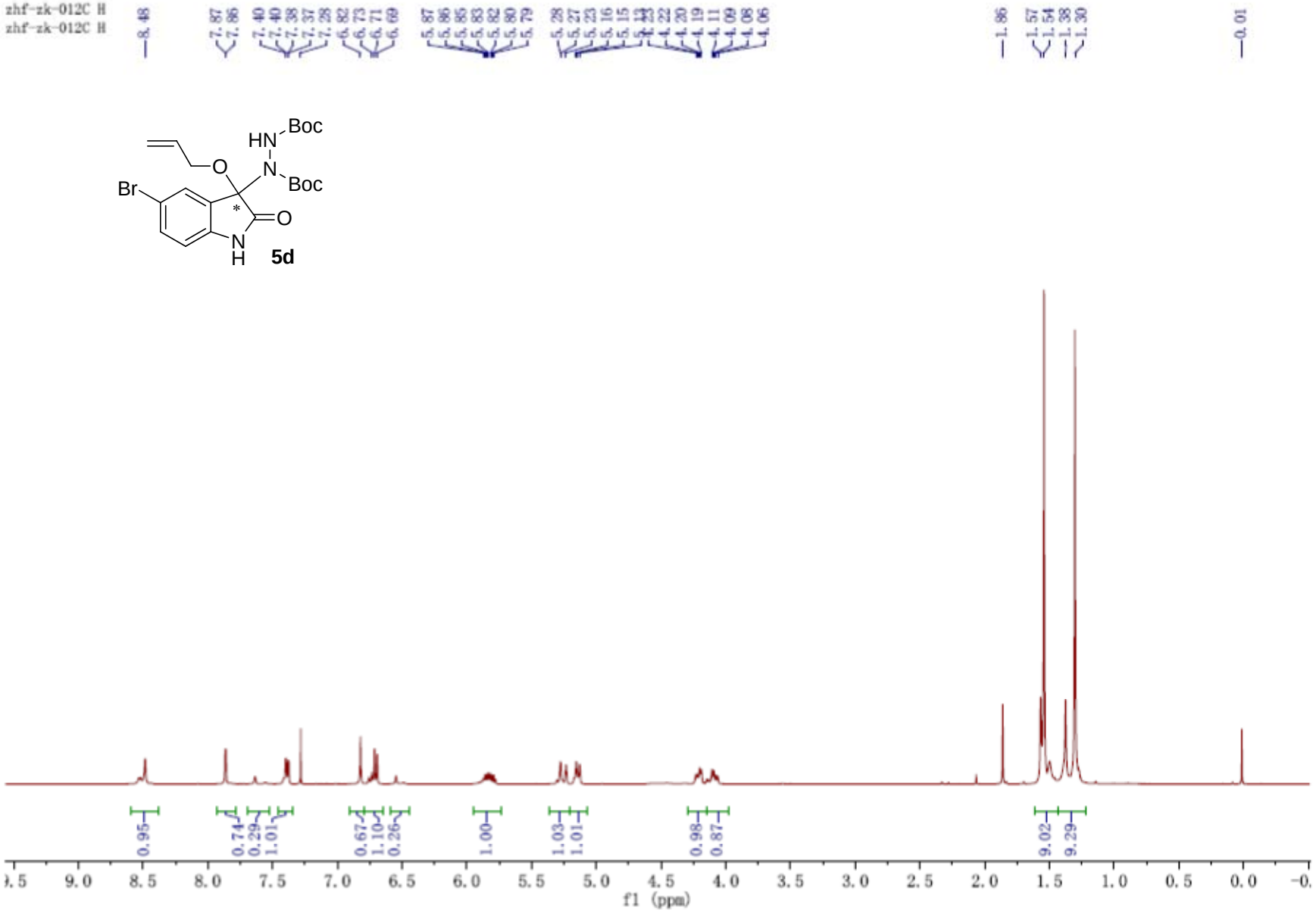


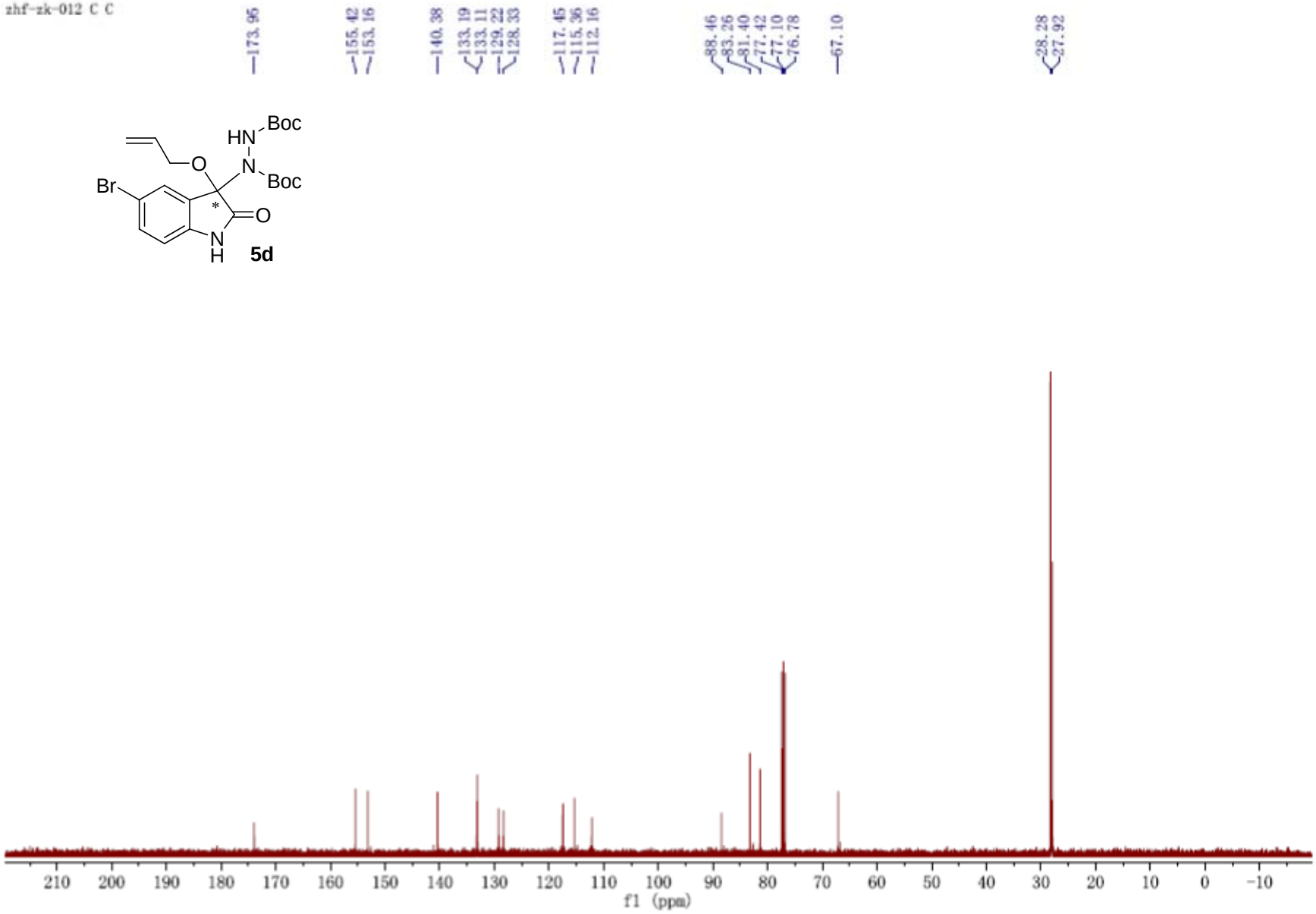

**5b**

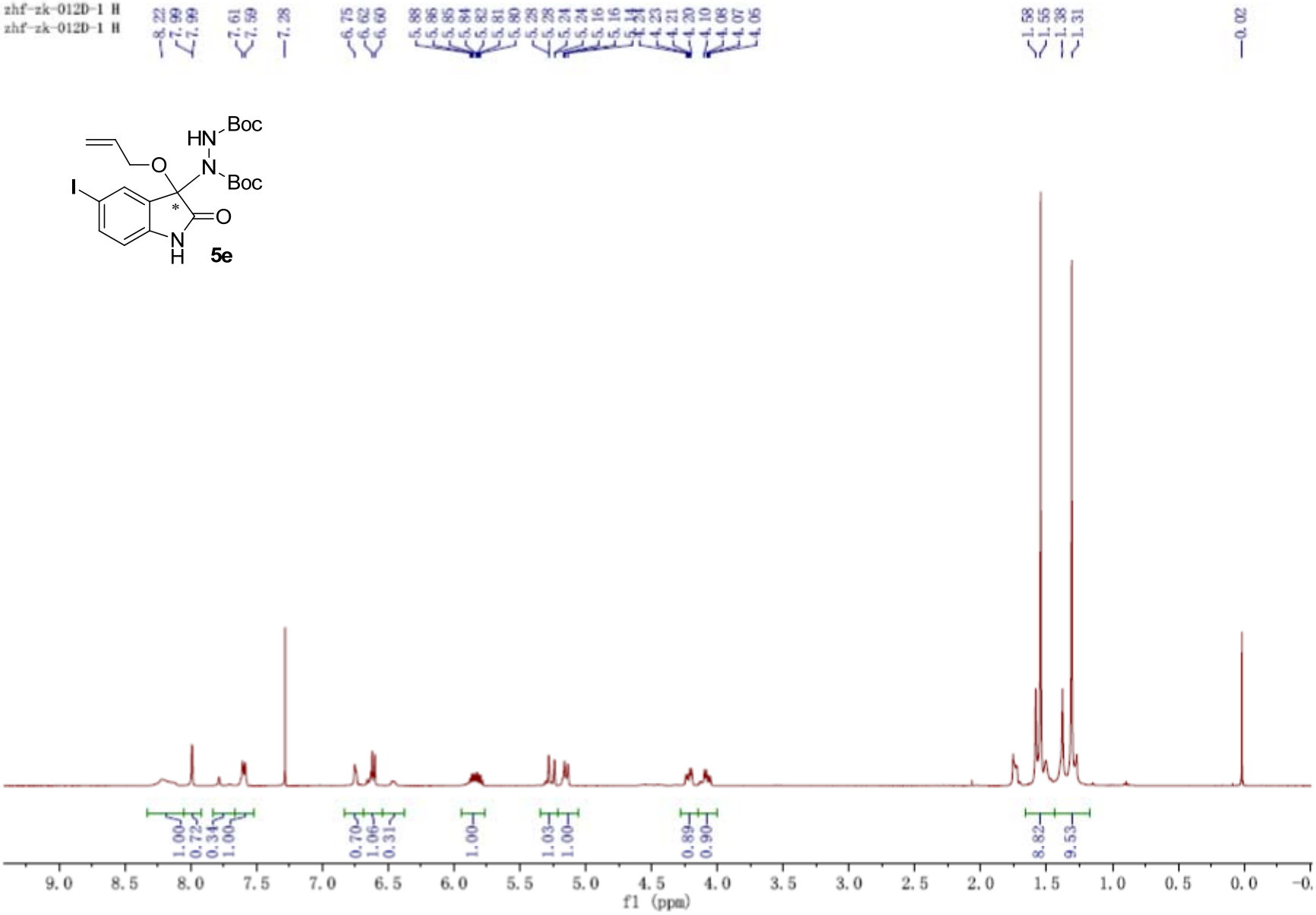












zhf-zk-012D-1 C
zhf-zk-012D-1 C

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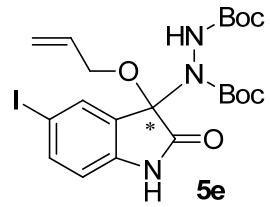
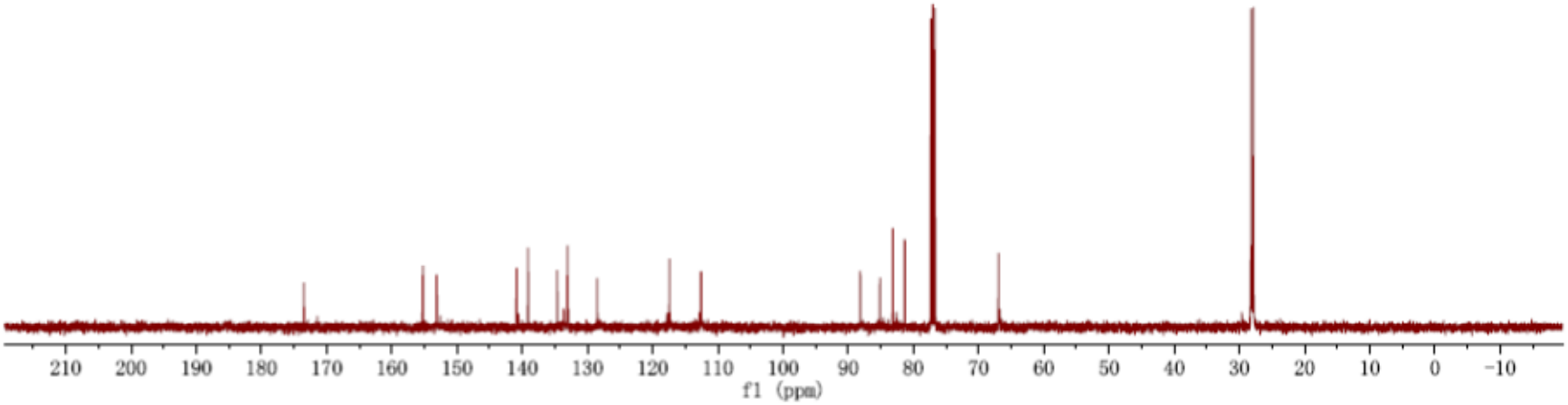
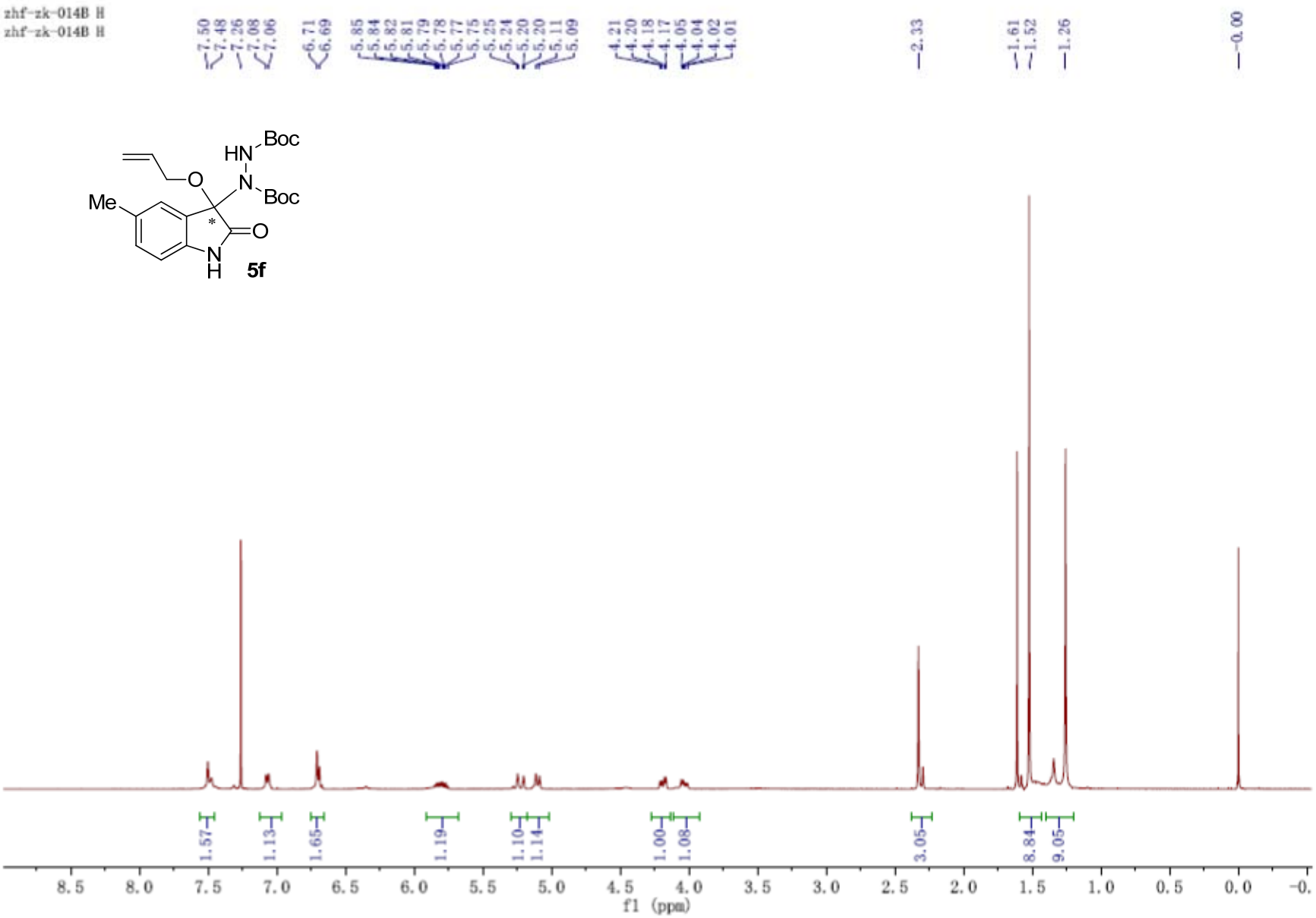



**5e**





zhf-zk-014B C
zhf-zk-014B C

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130.54
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126.36
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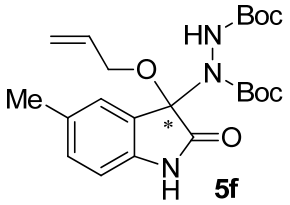
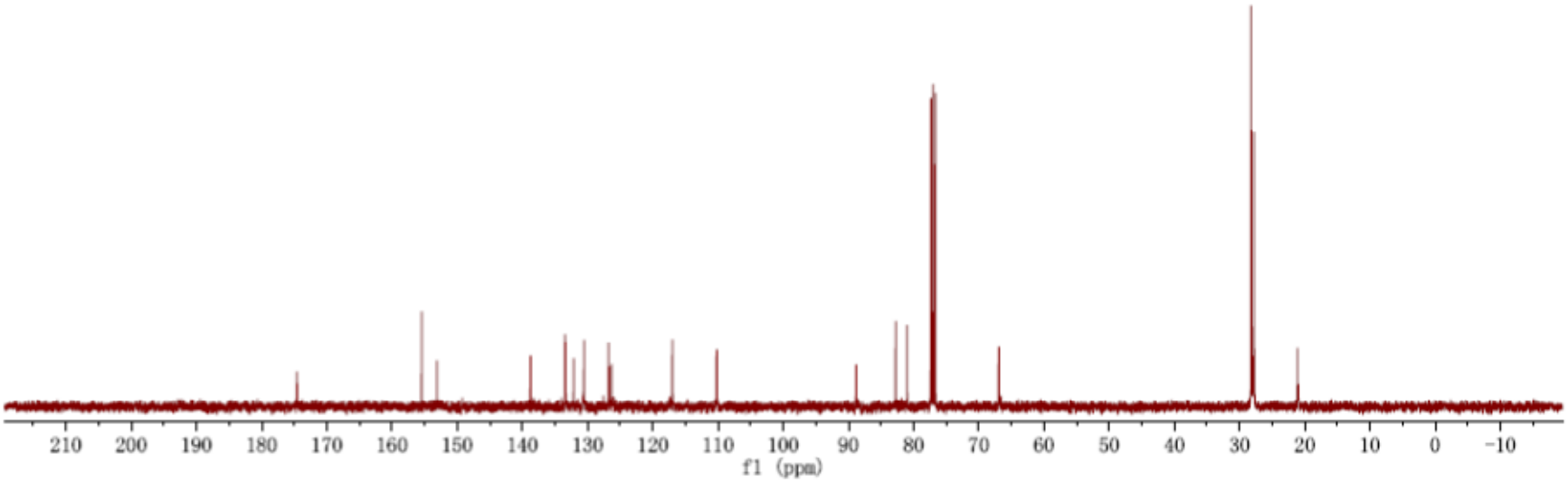
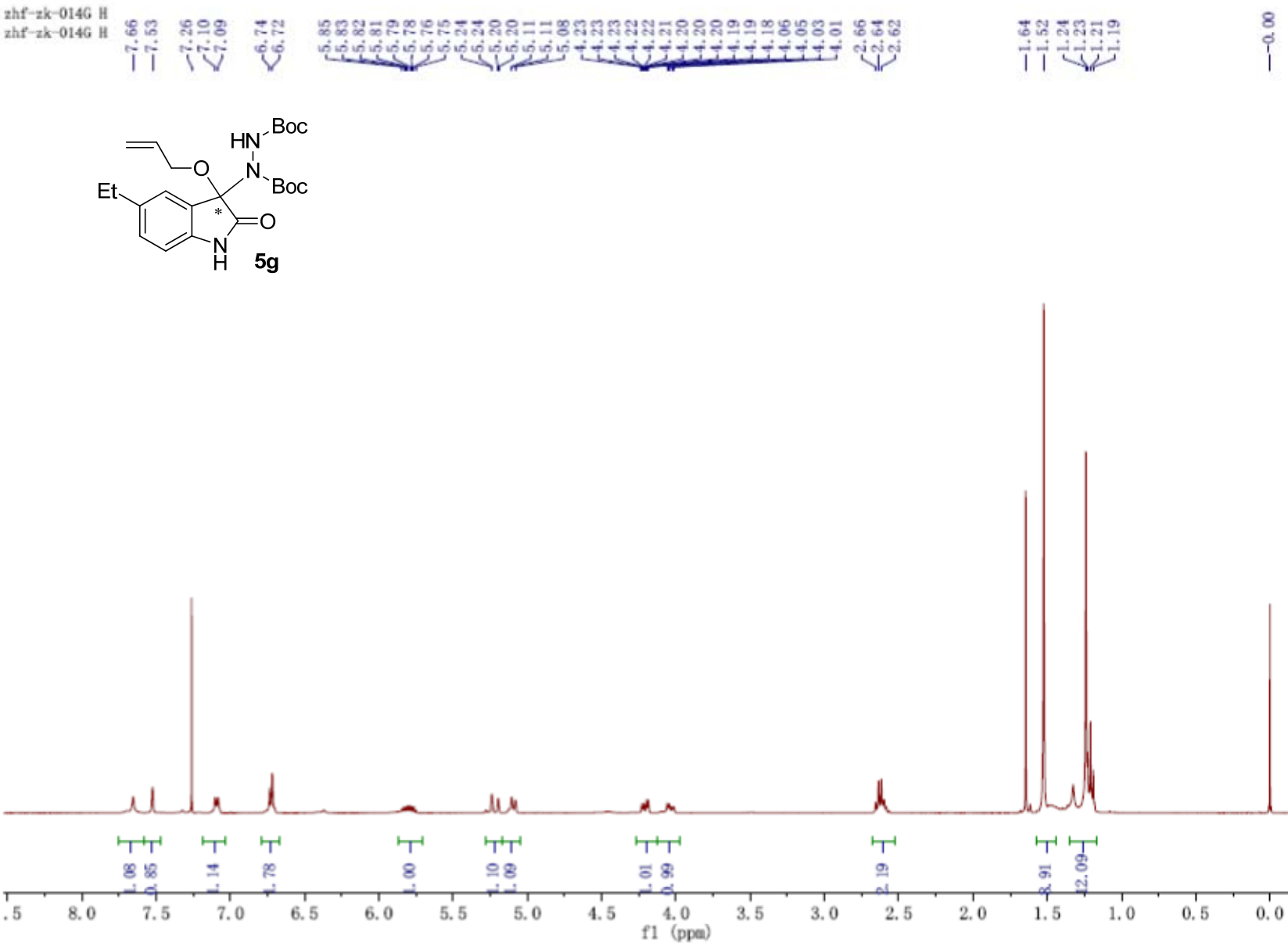
21.11




**5f**





zhf-zk-014G C
zhf-zk-014G C

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138.91
138.81
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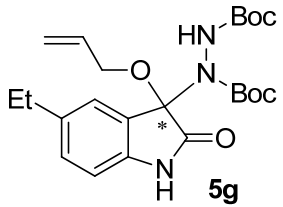
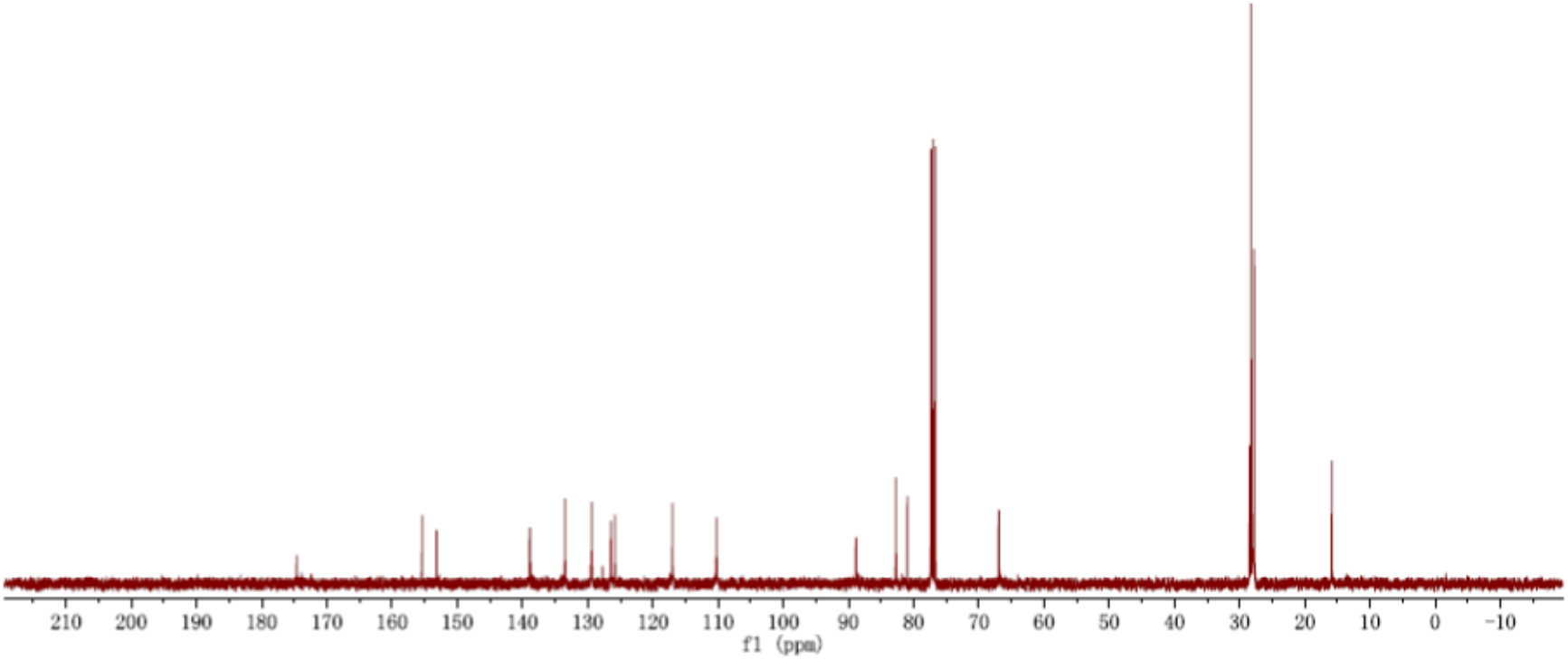
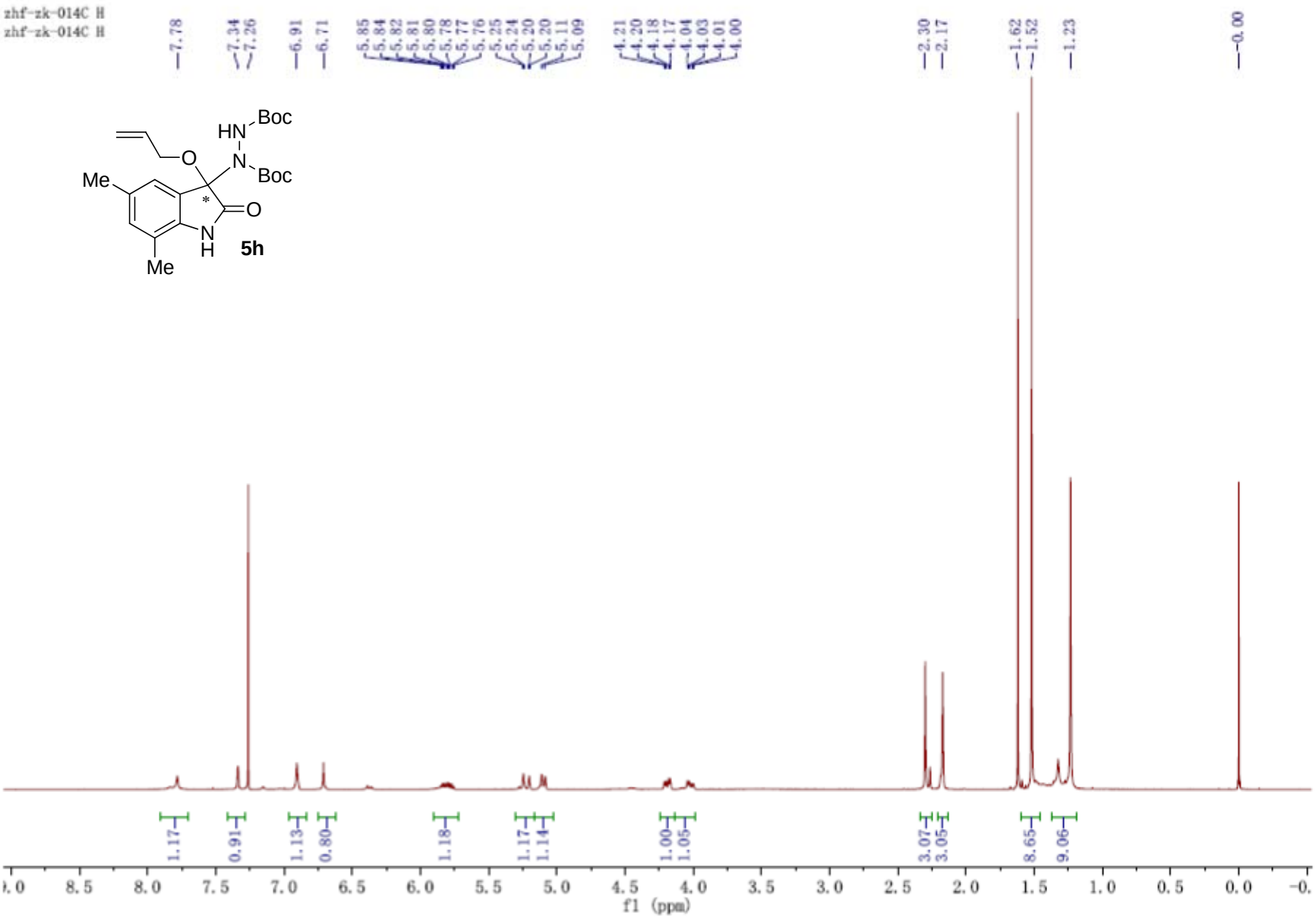
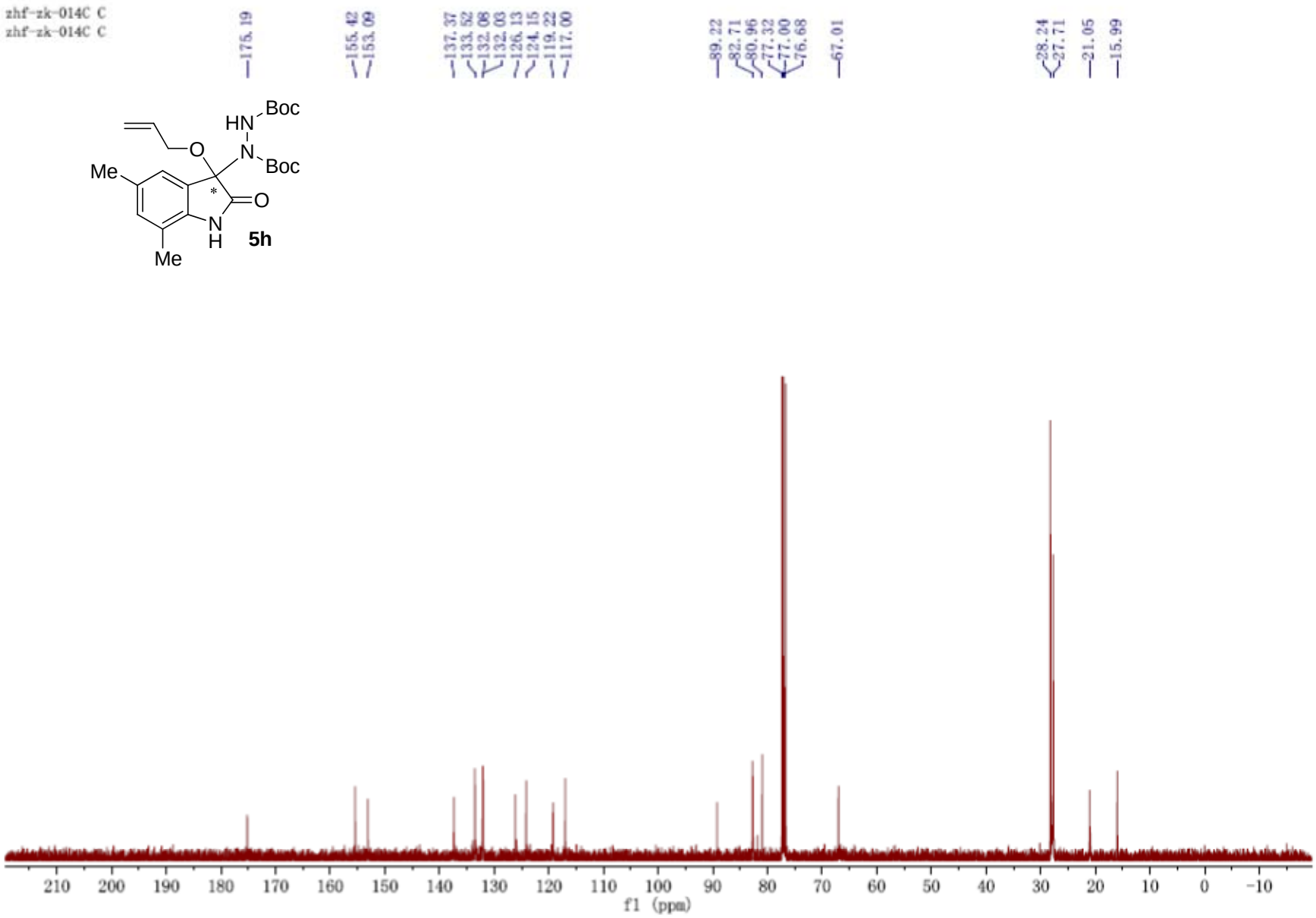
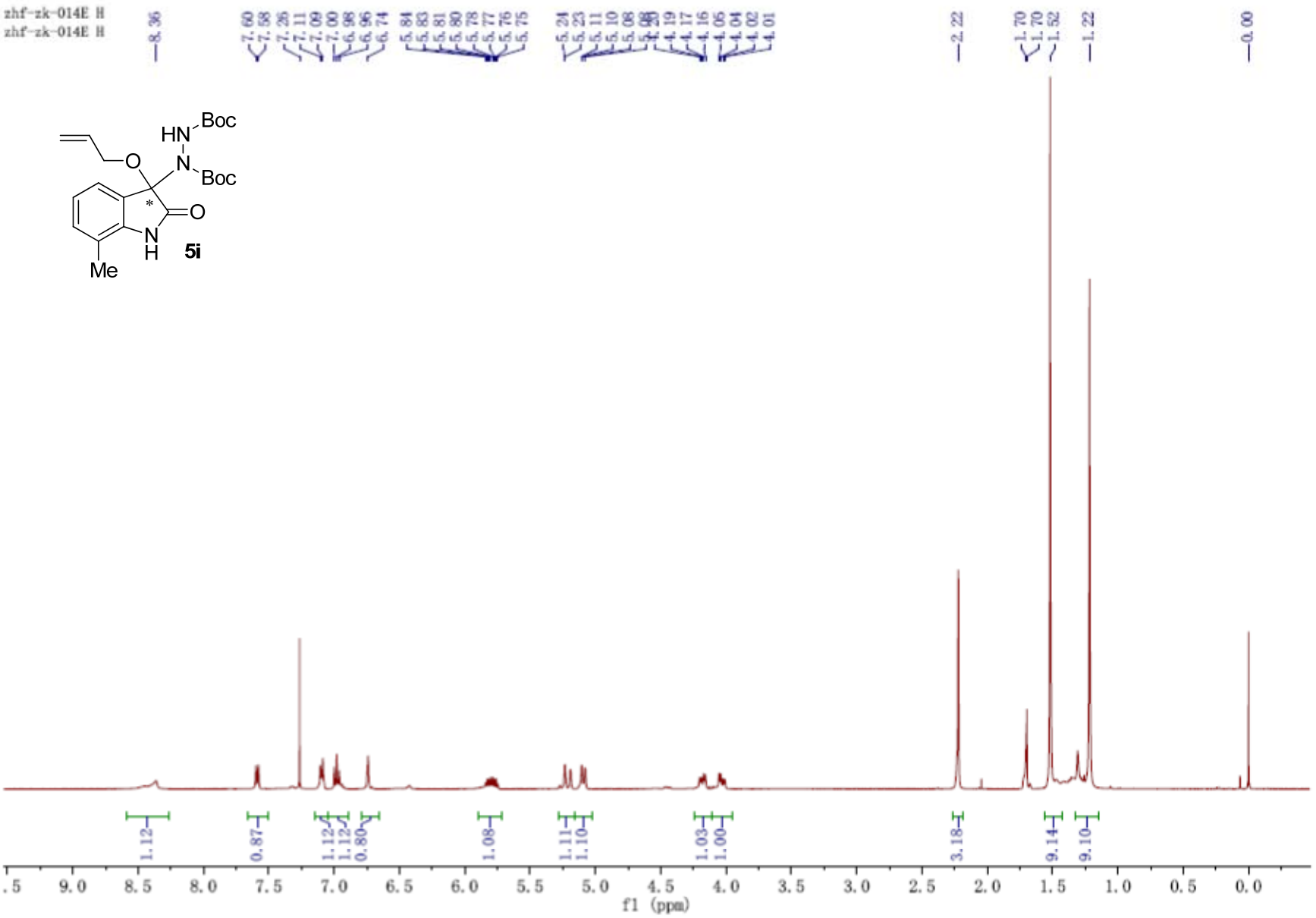



**5g**









zhf-zk-014E C
zhf-zk-014E C

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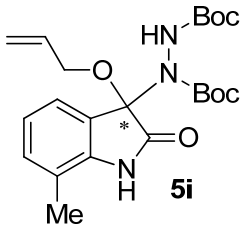
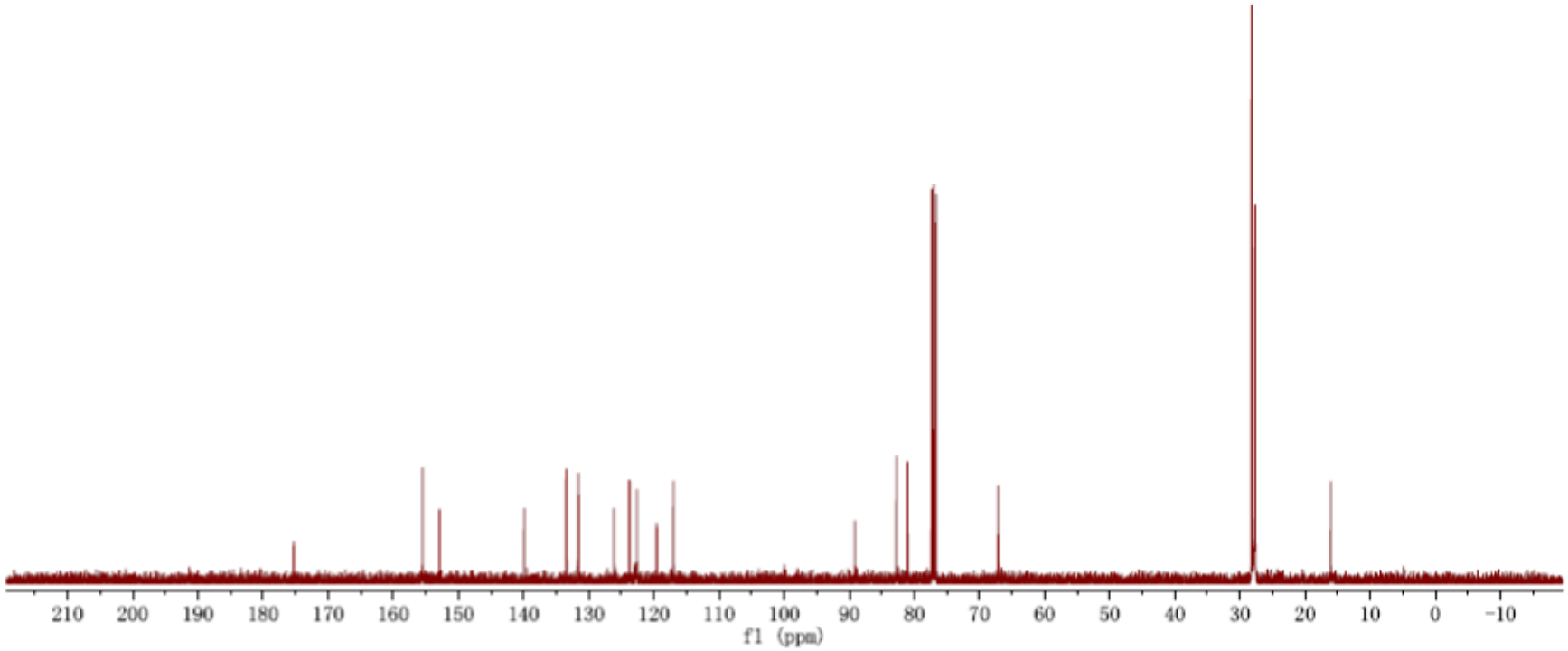
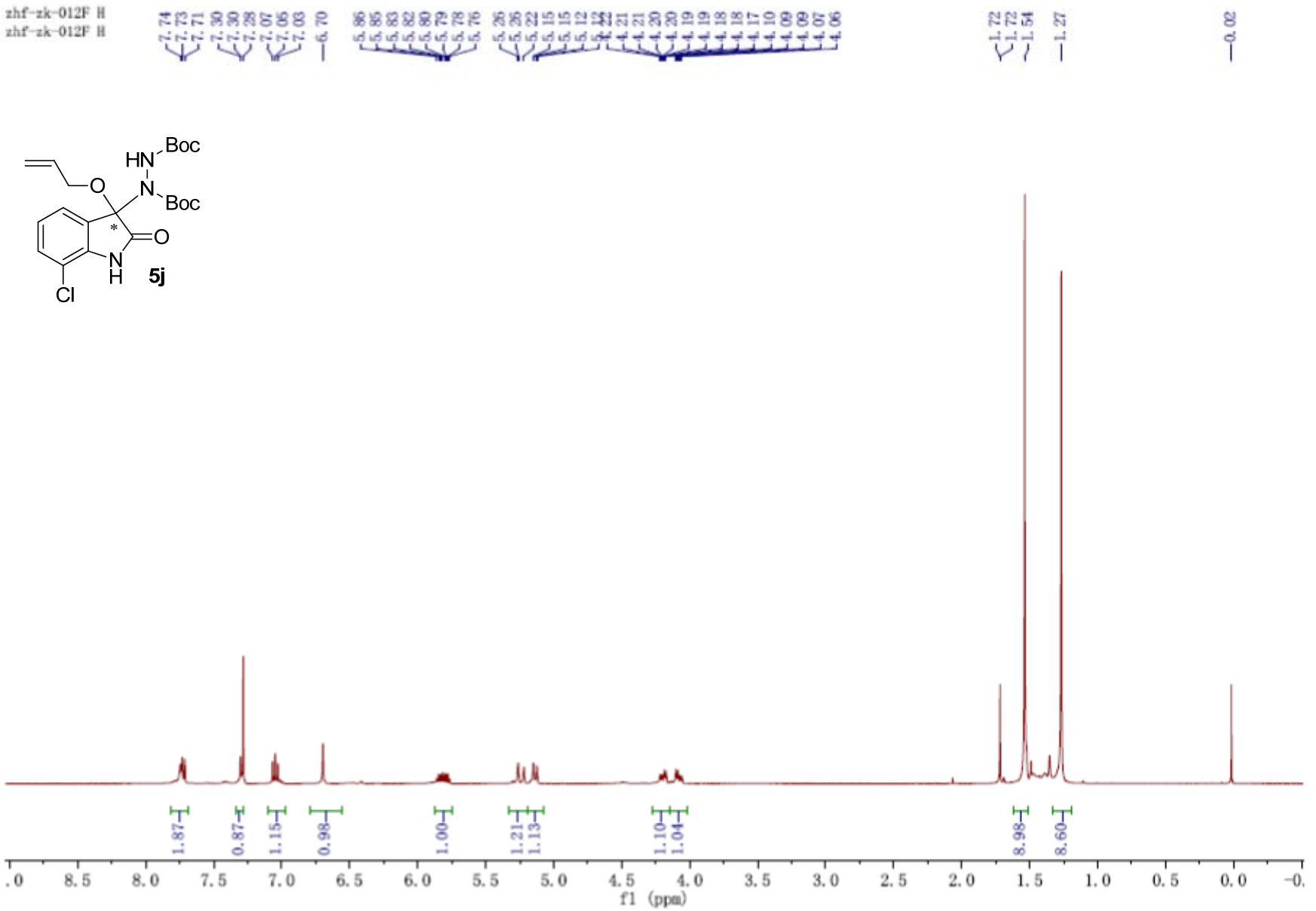
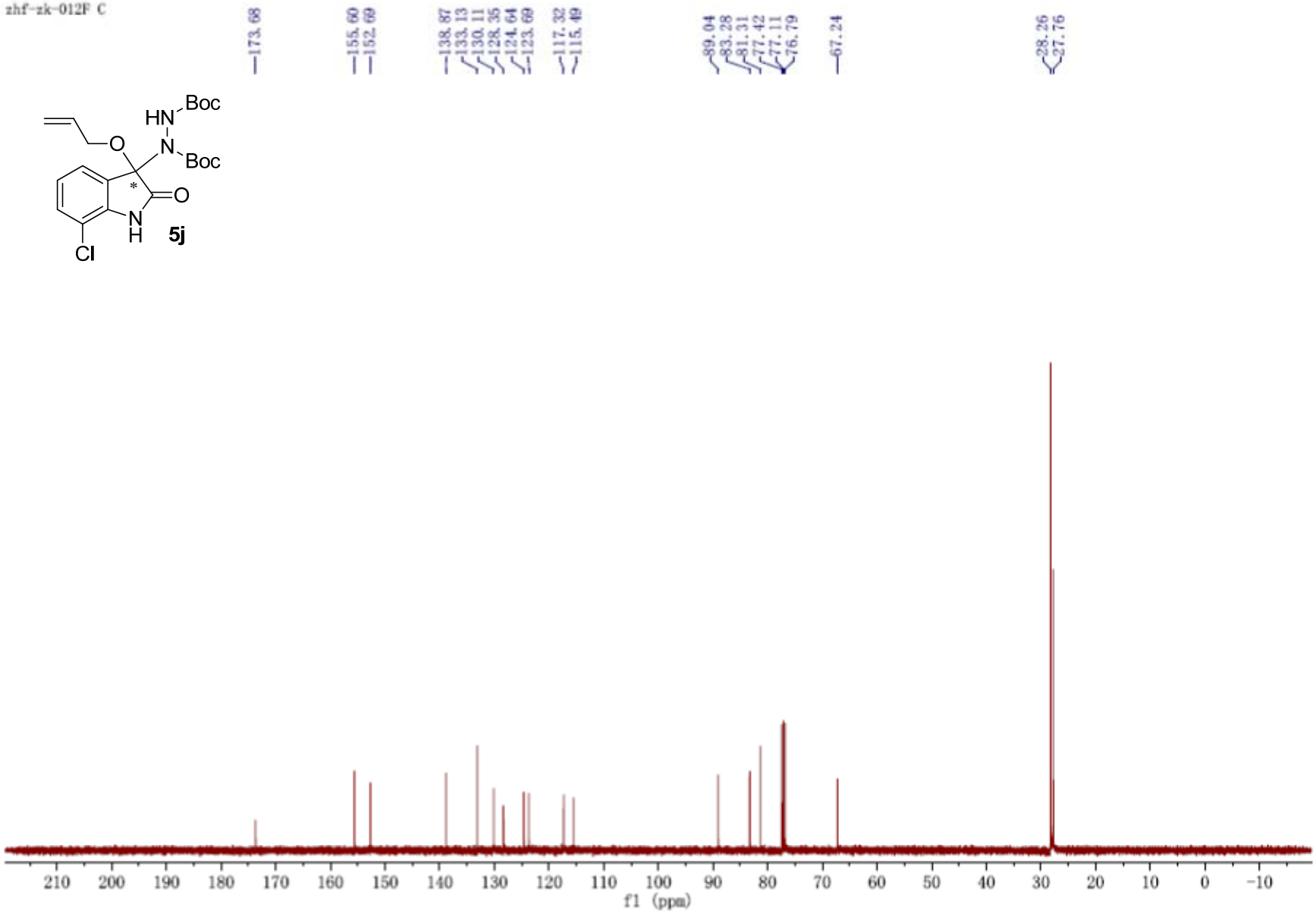
27.68
16.04

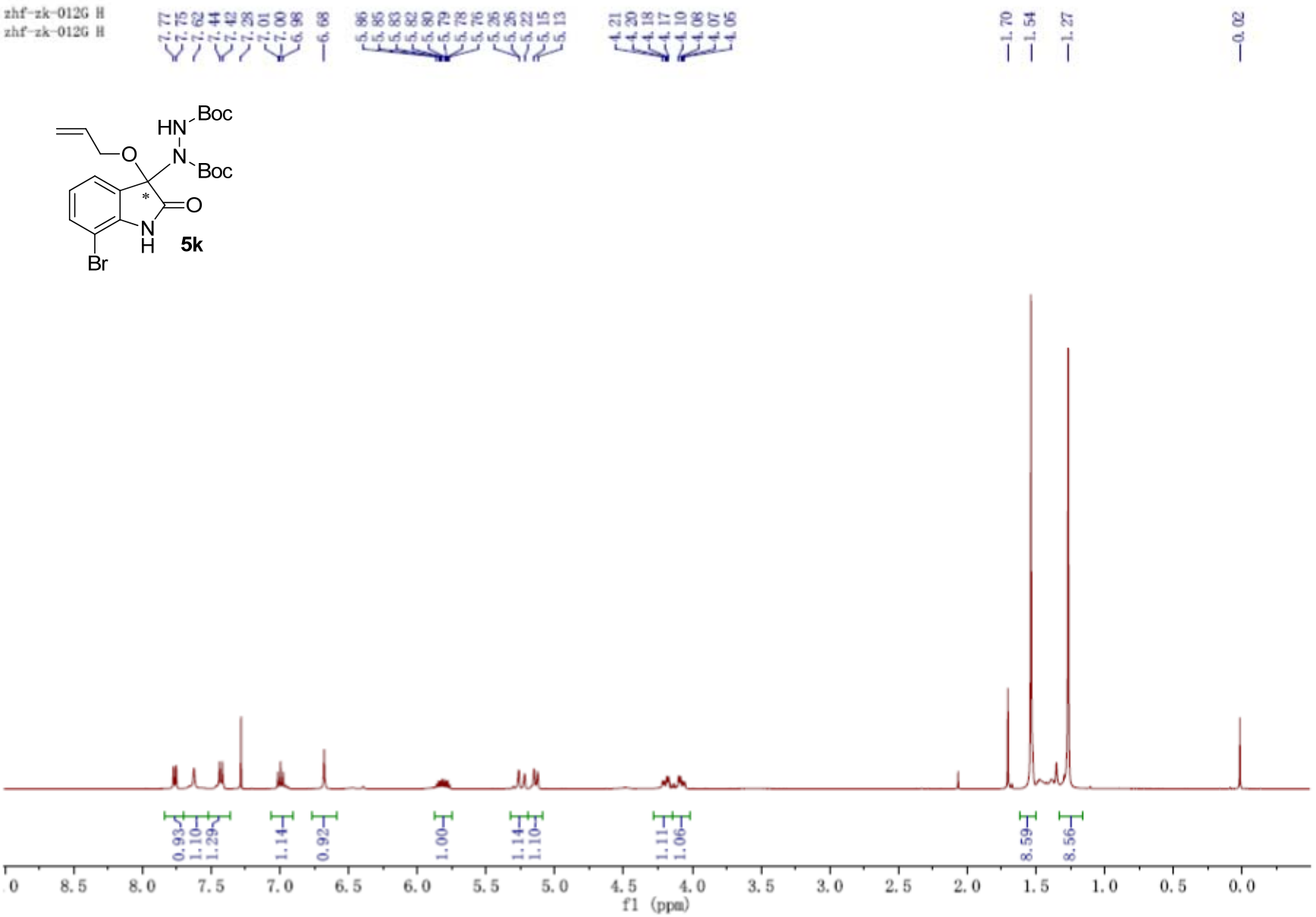


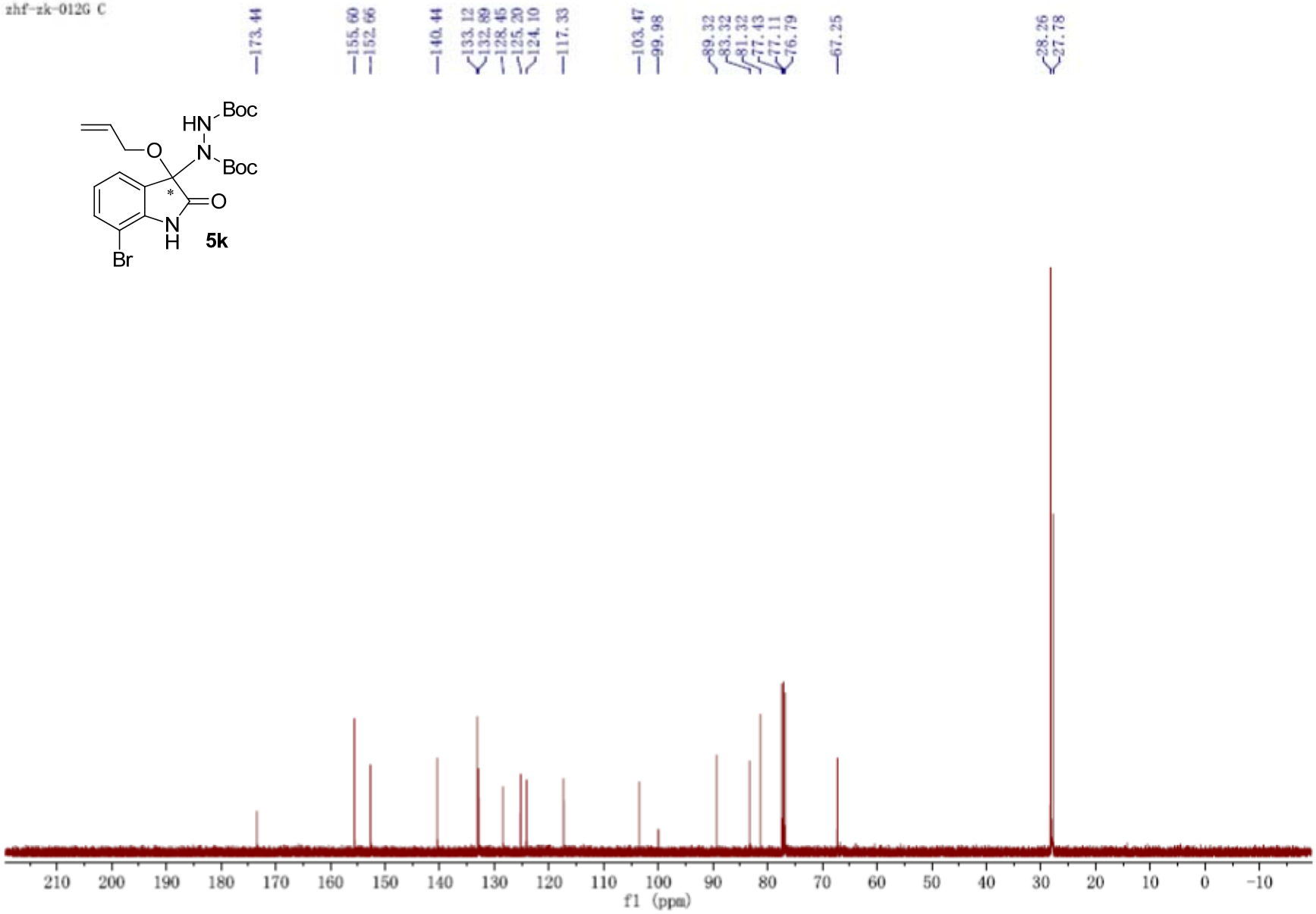

**5i**

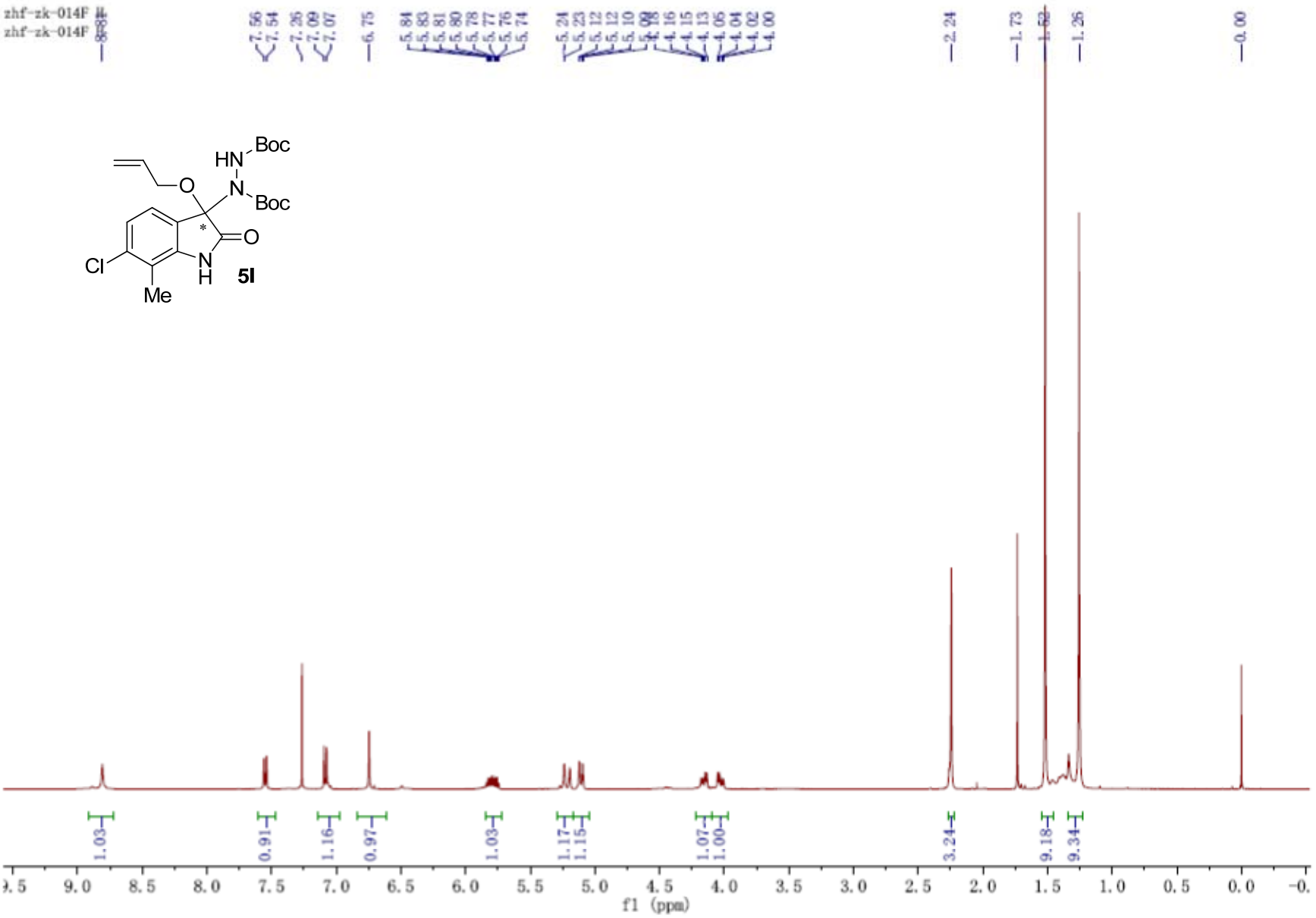


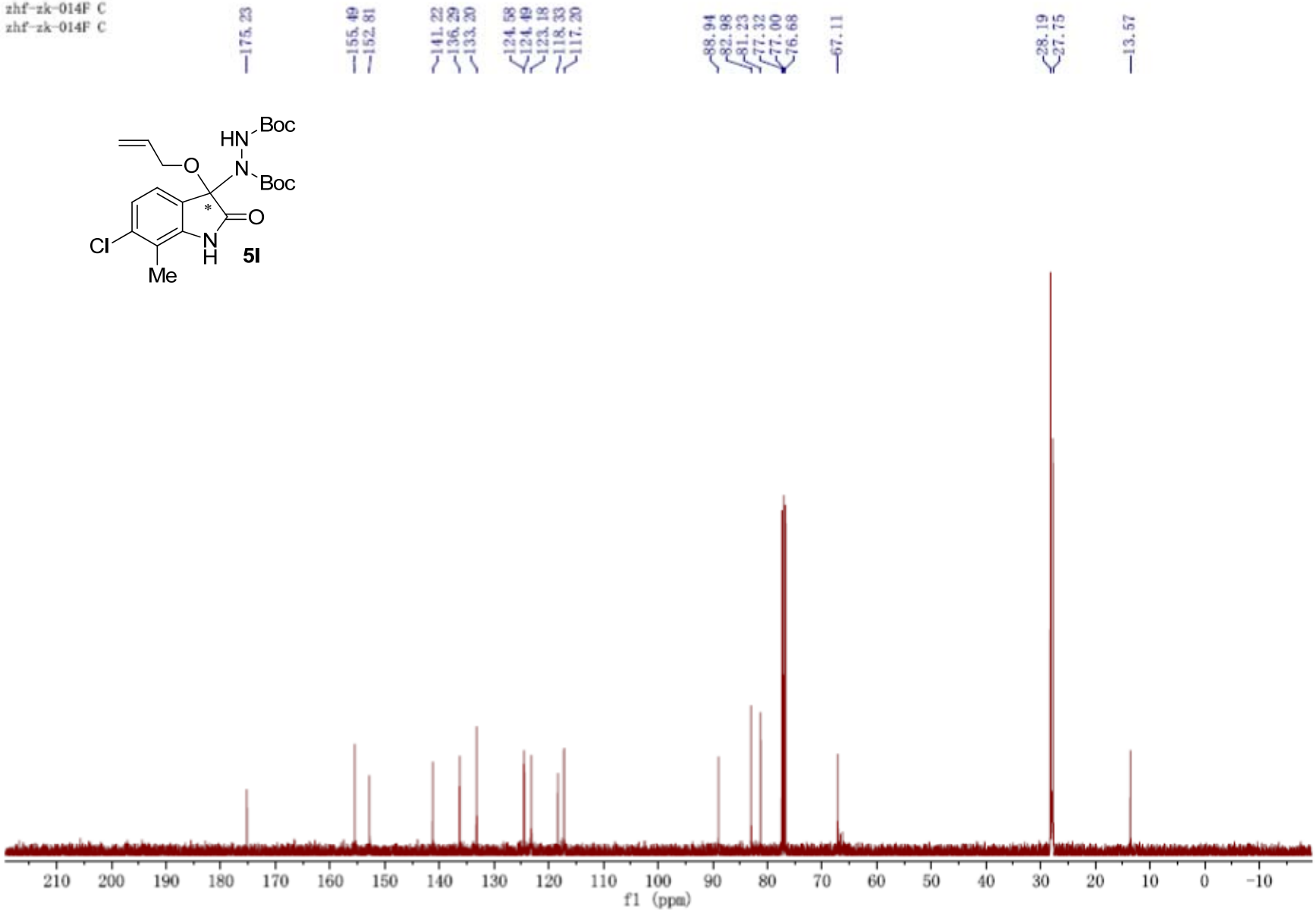


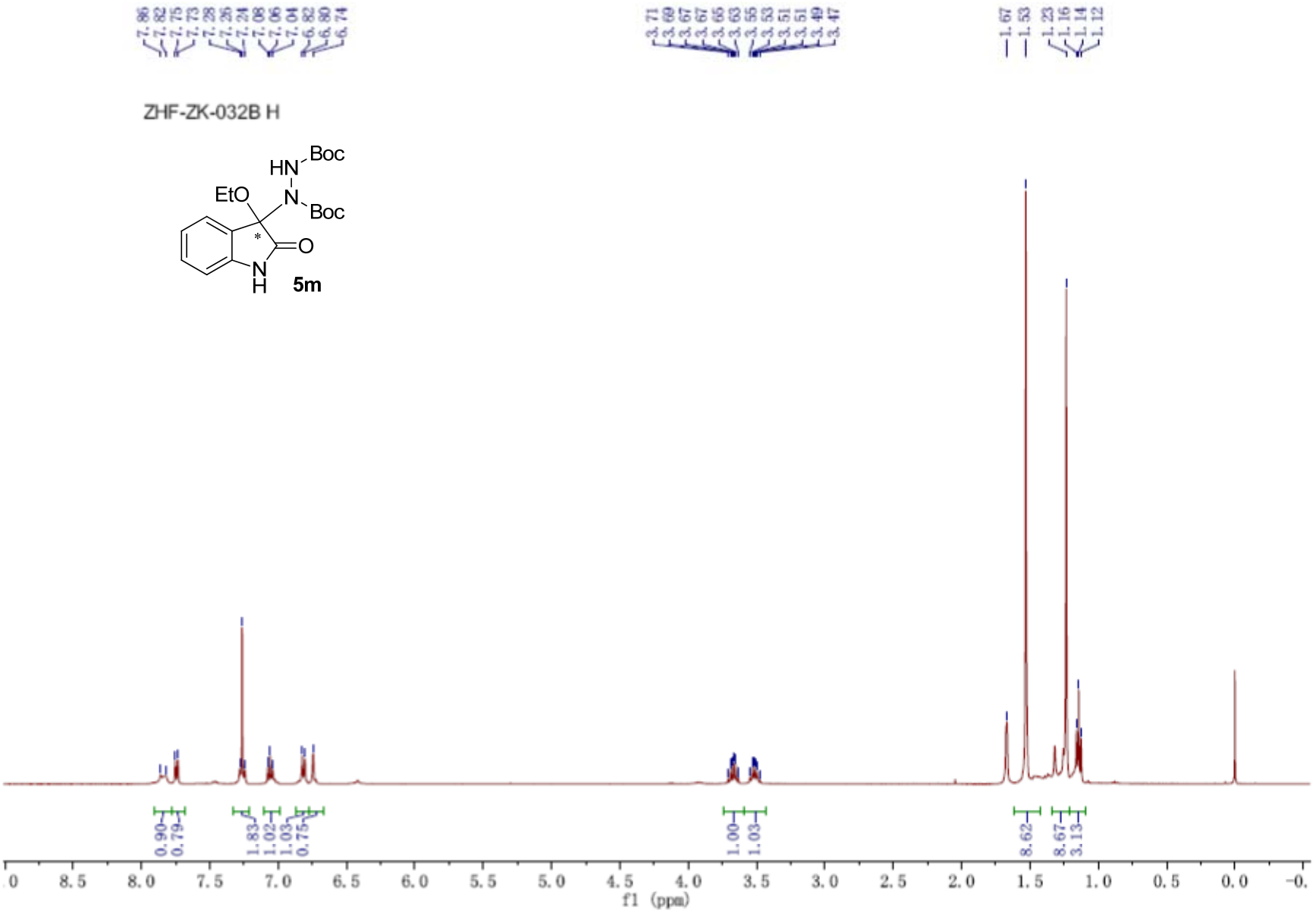


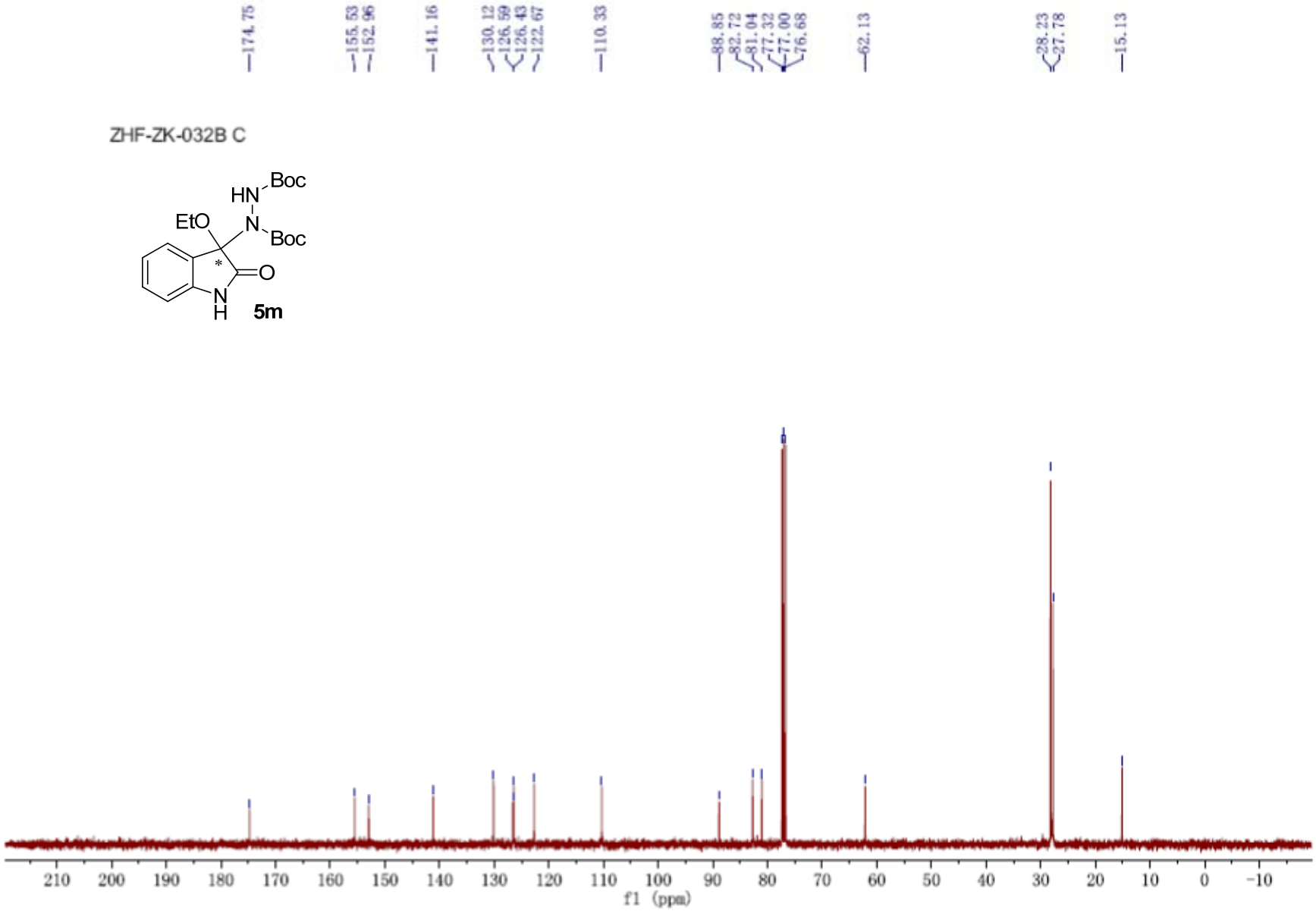


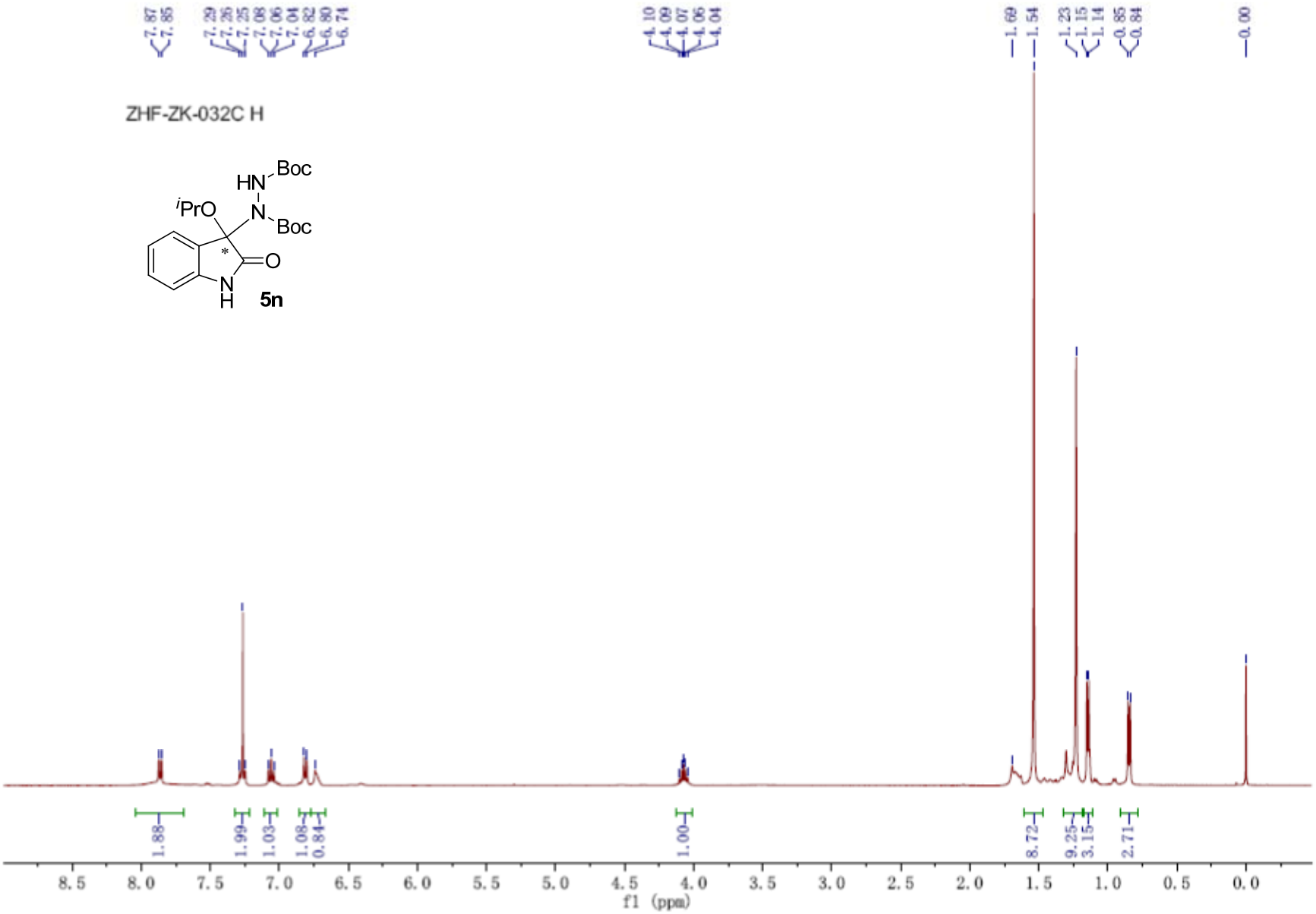


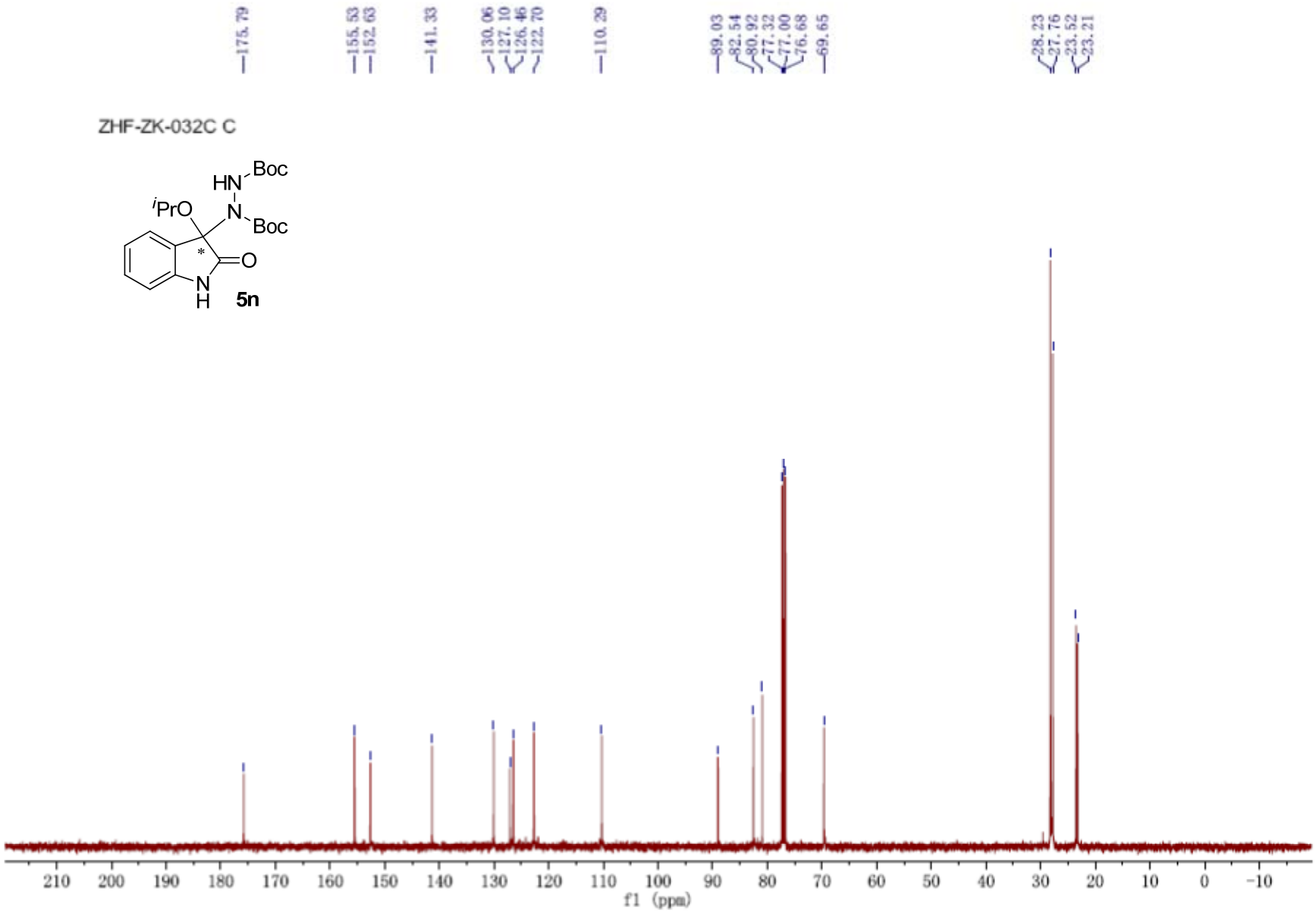


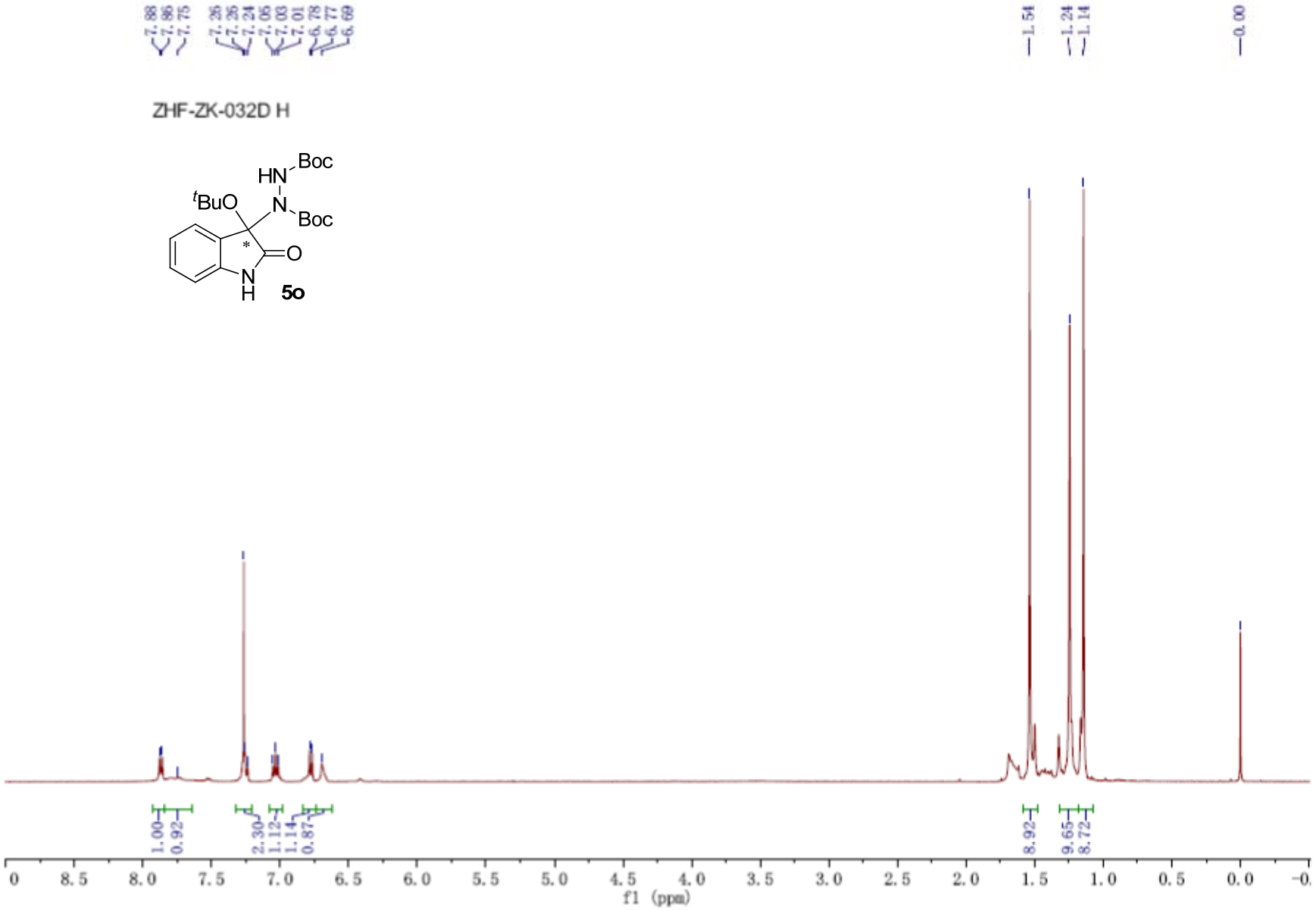


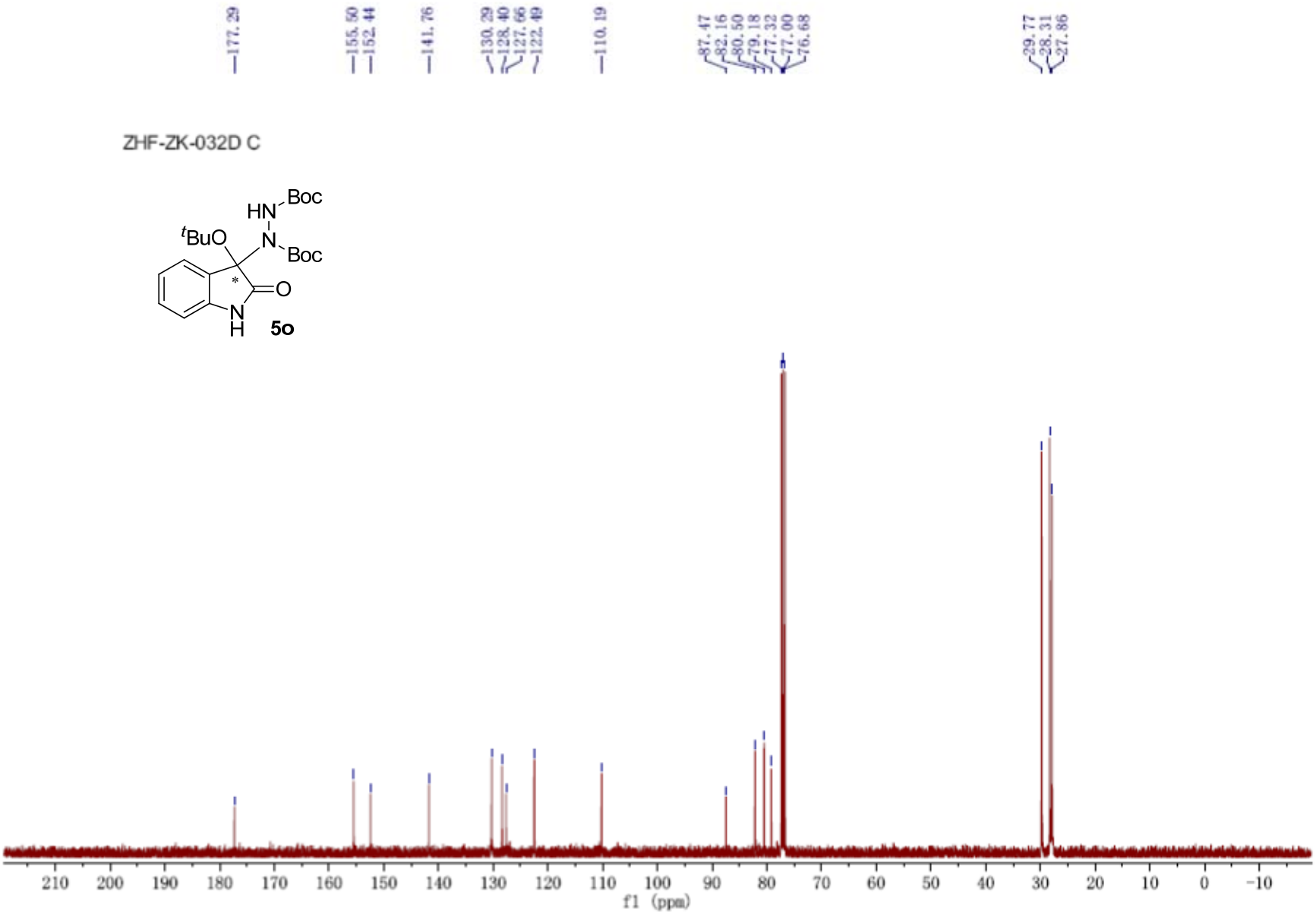


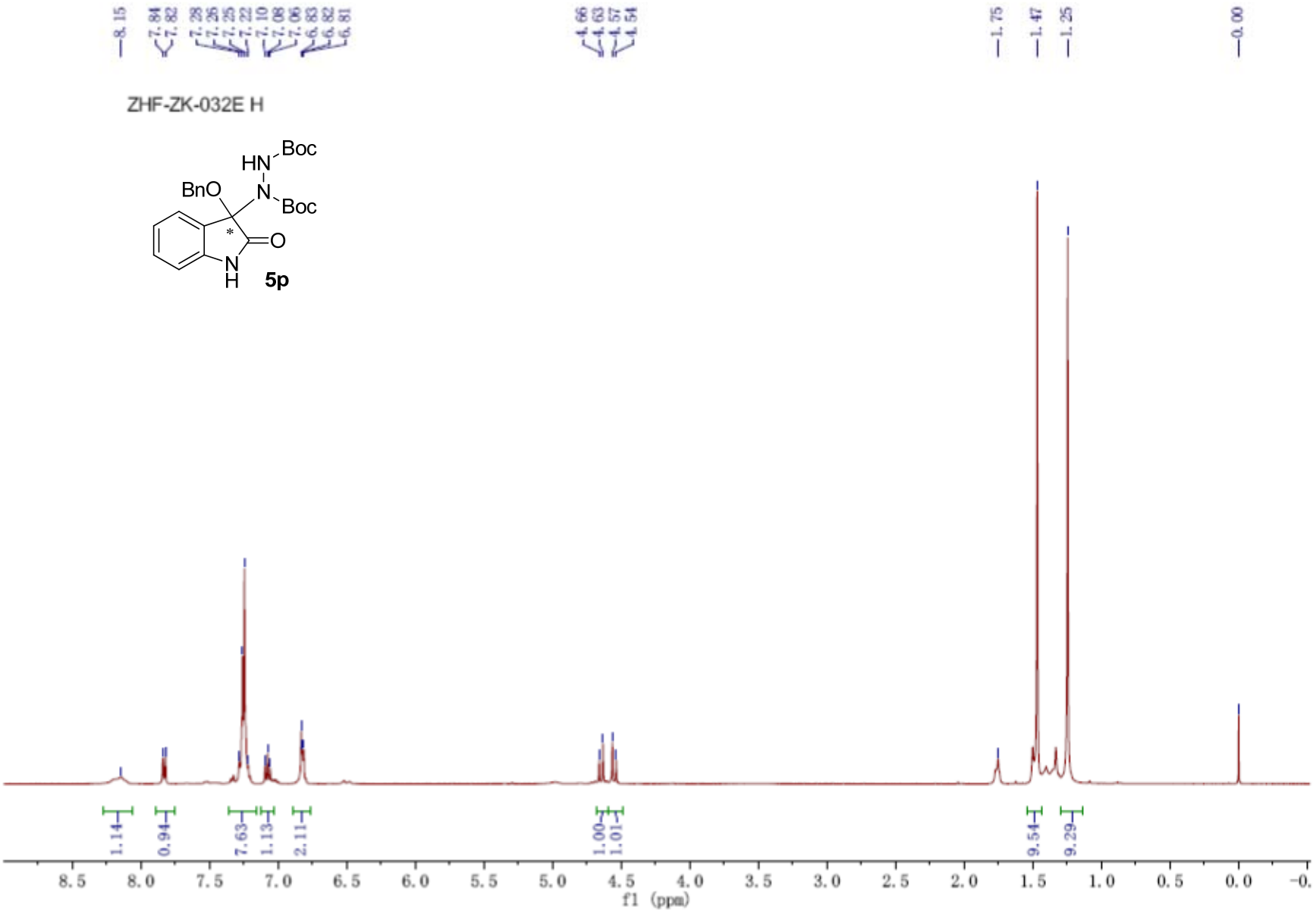


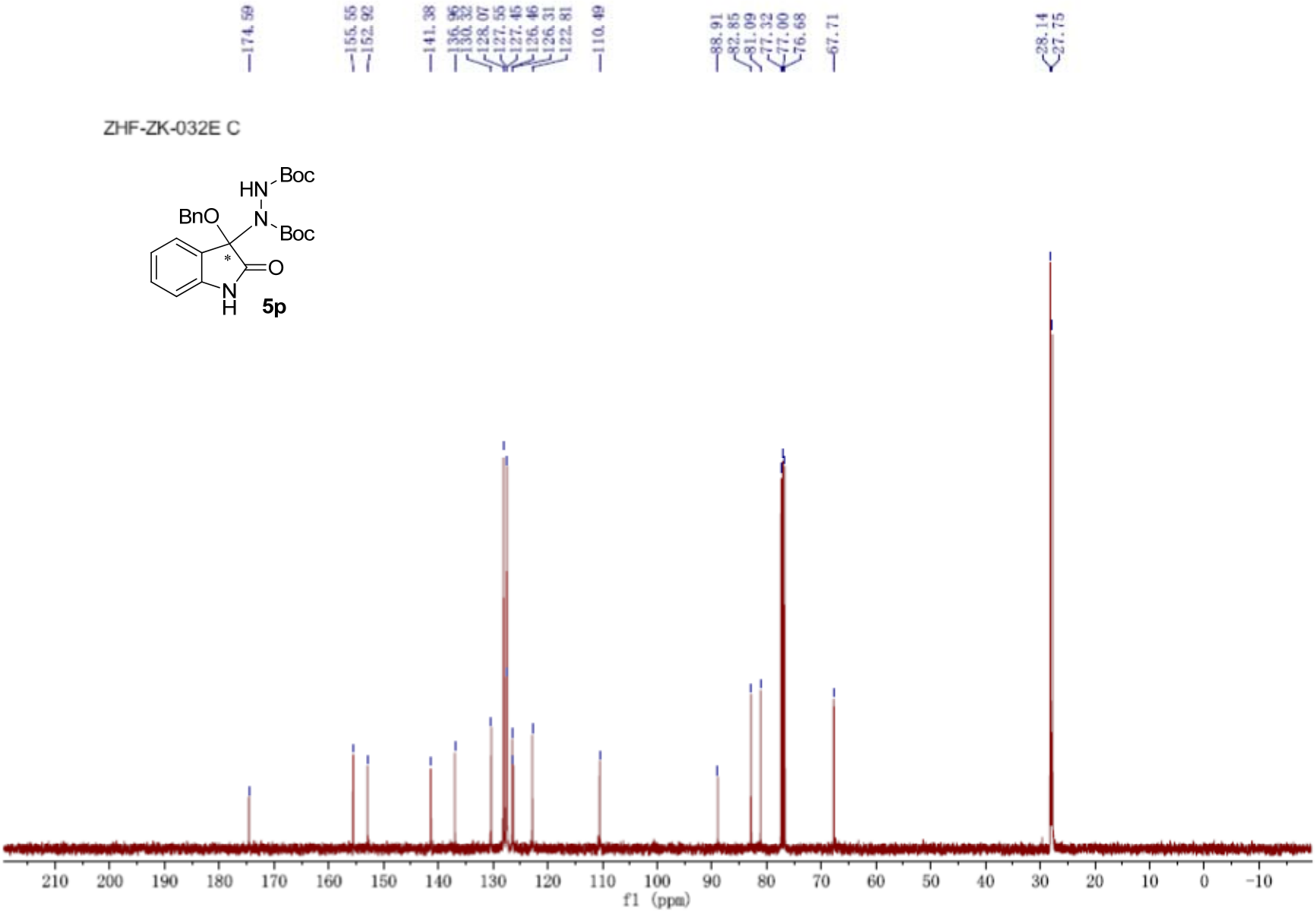


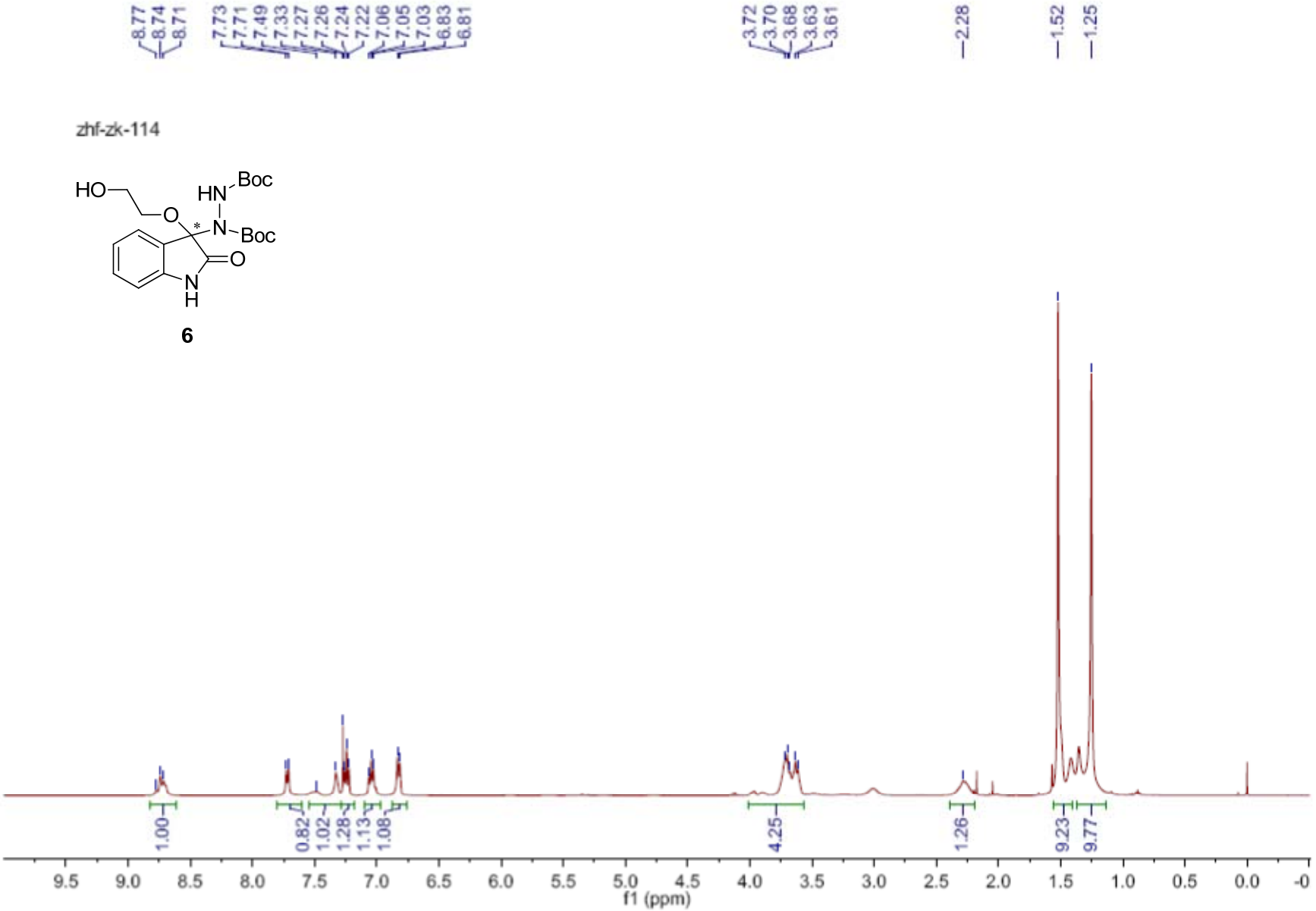


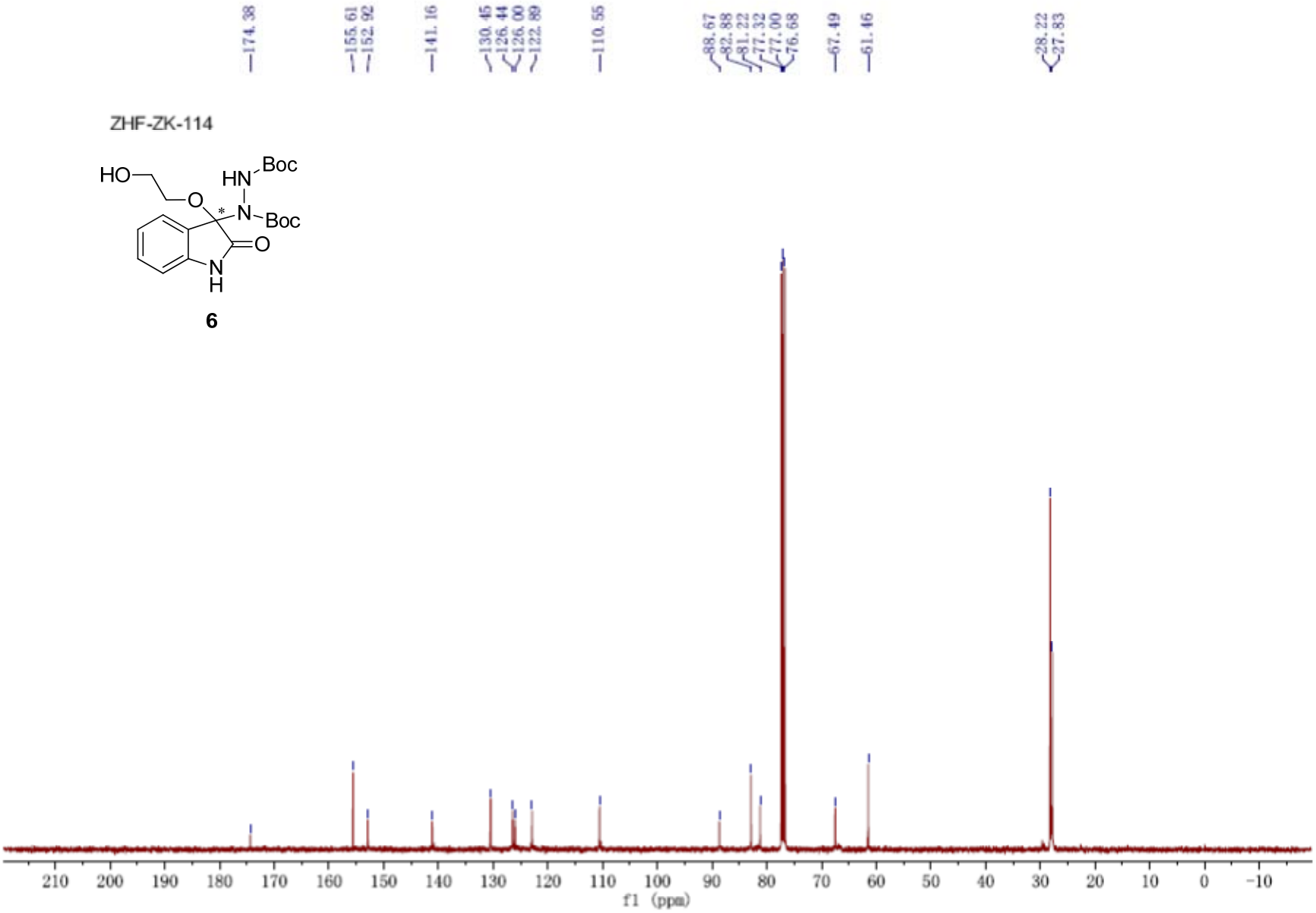




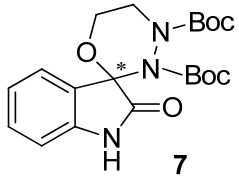




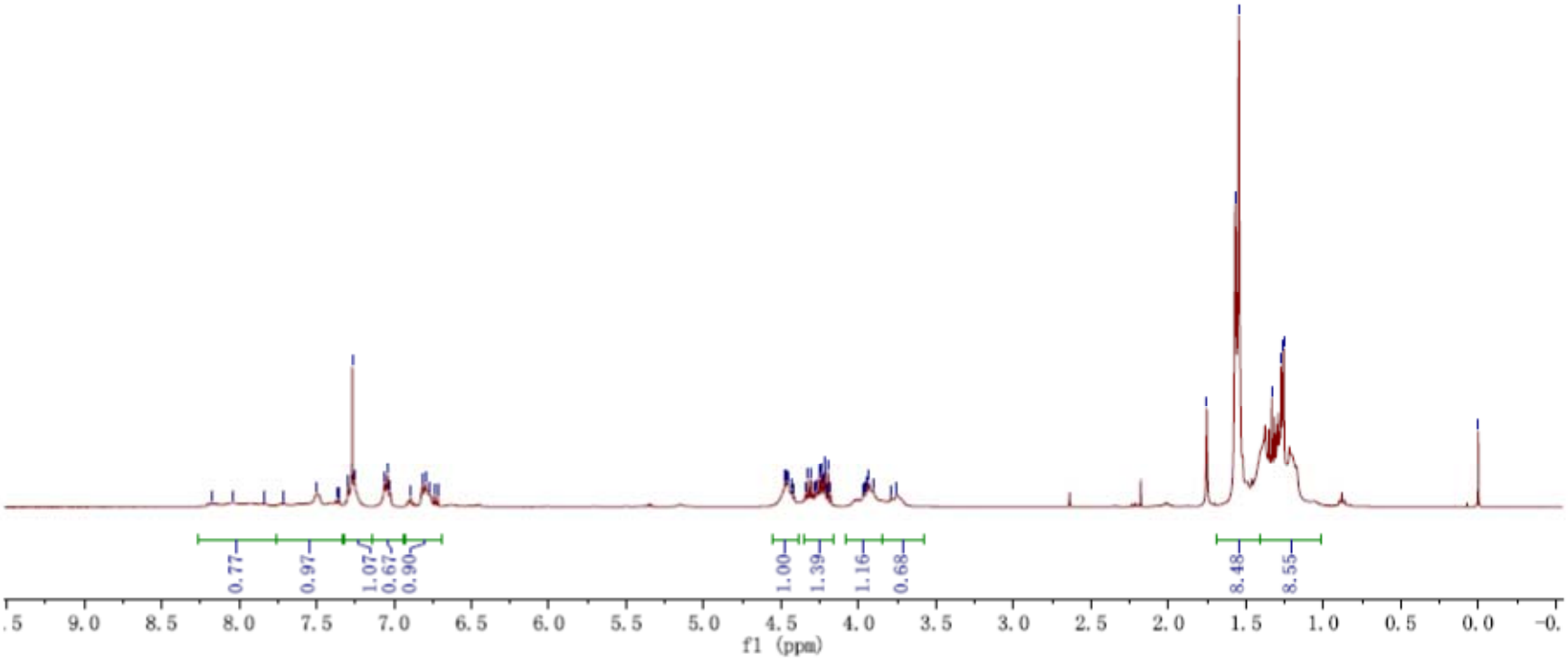





ZHF-ZK-118




**7**



zhf-z1-012
zhf-z1-012 C

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110.45
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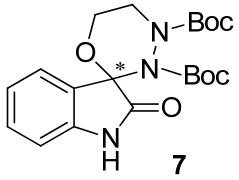
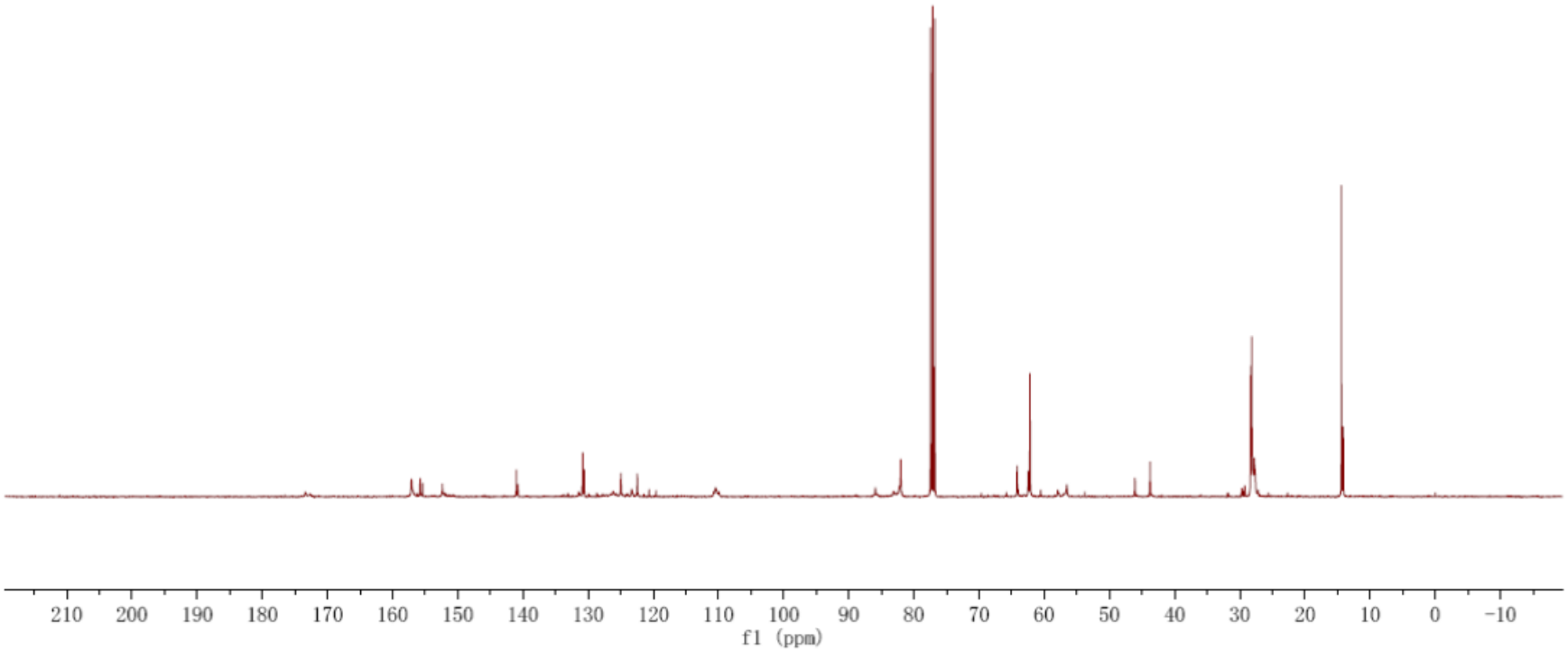
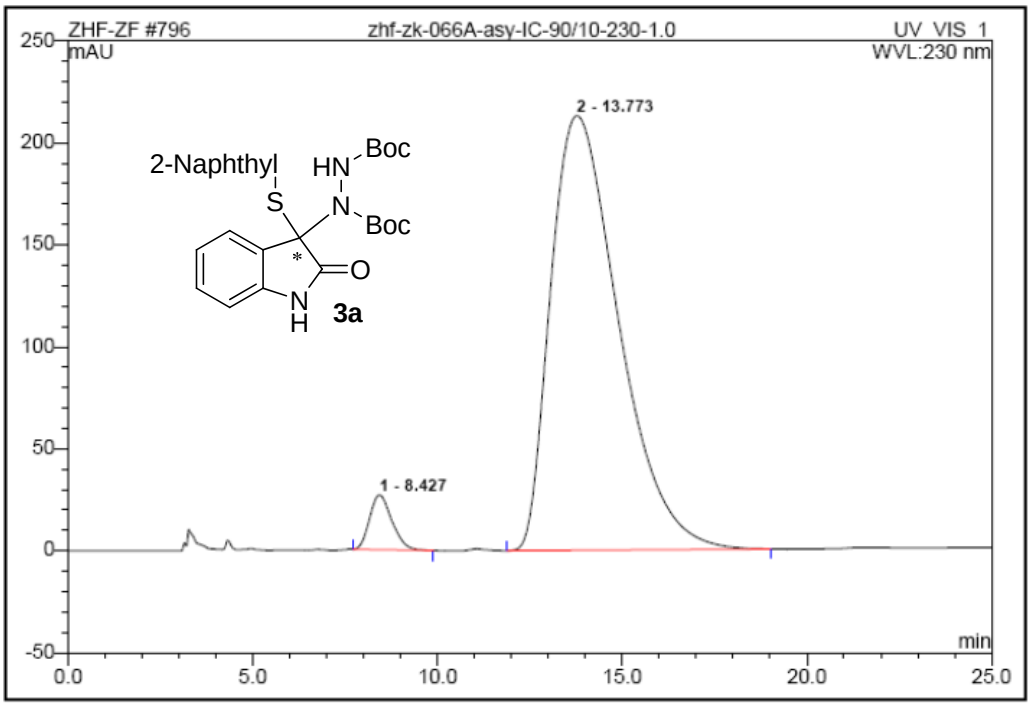
14.11

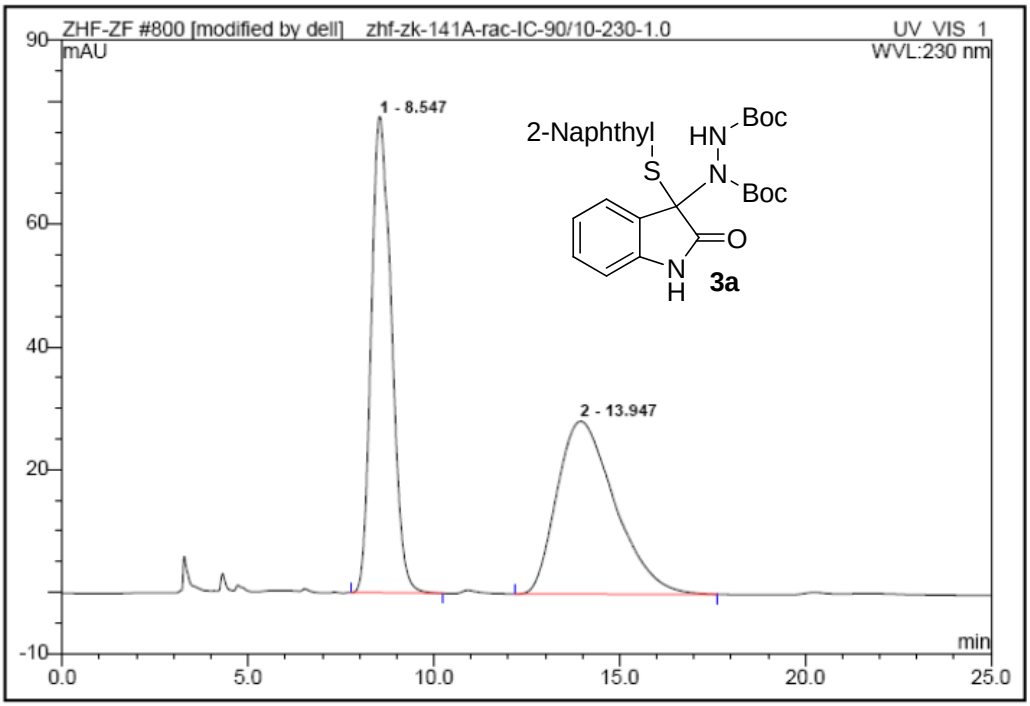



**7**

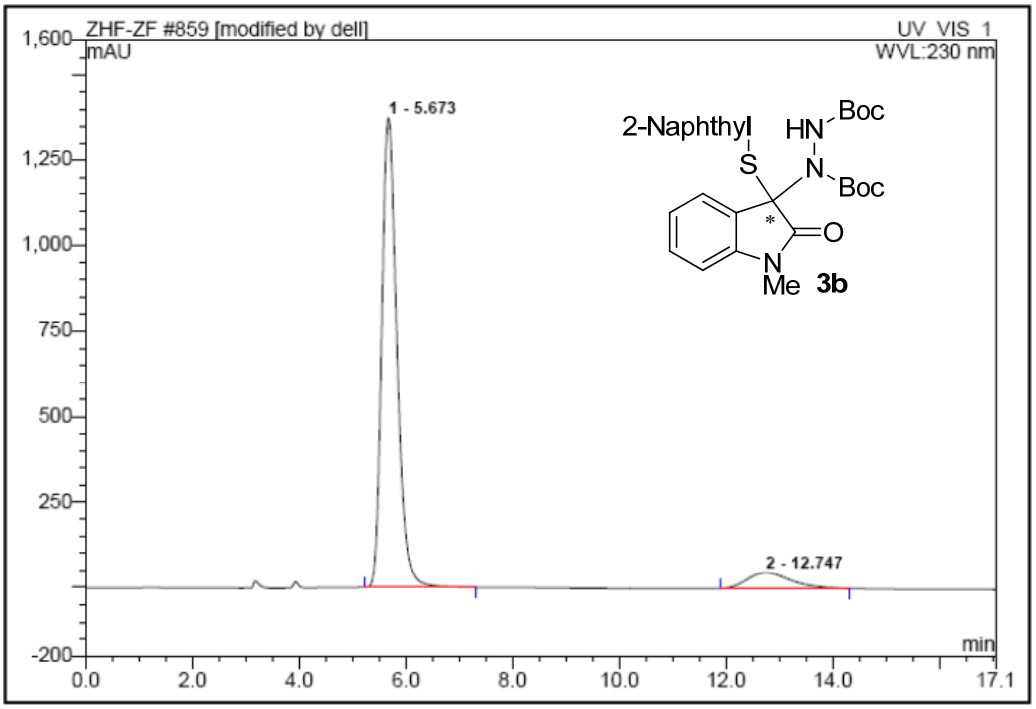




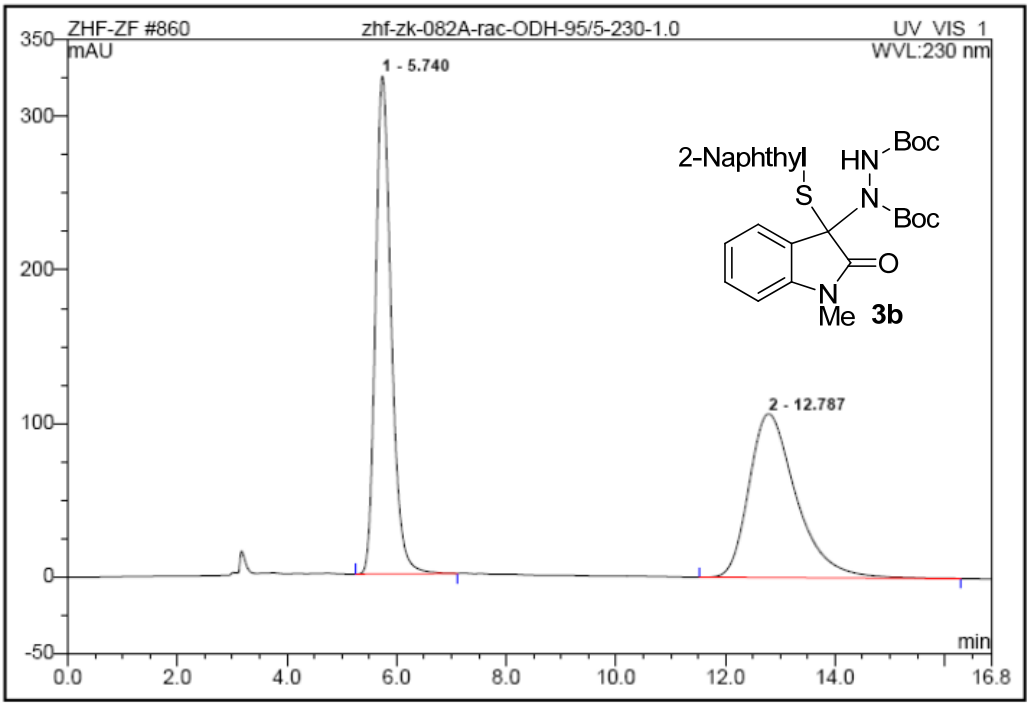

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 8.43 | n.a. | 26.808 | 18.724 | 3.96 | n.a. | BMB |
| 2 | 13.77 | n.a. | 213.023 | 454.582 | 96.04 | n.a. | BMB |
| Total: | | | 239.831 | 473.306 | 100.00 | 0.000 | |



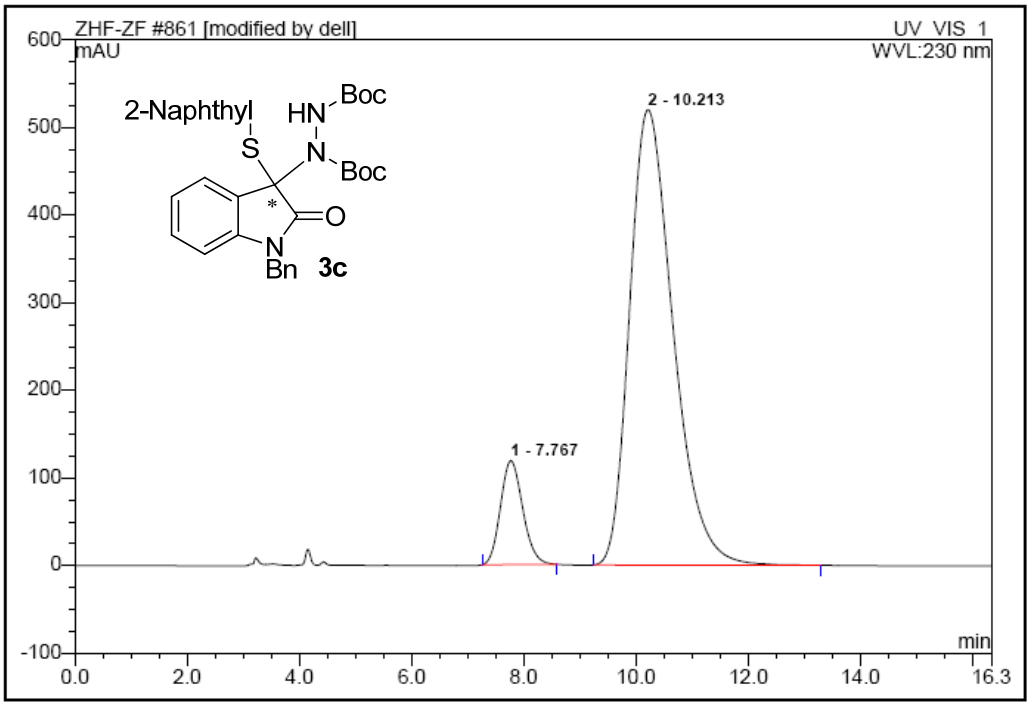

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 8.55 | n.a. | 77.683 | 49.103 | 49.05 | n.a. | BMB |
| 2 | 13.95 | n.a. | 28.189 | 50.997 | 50.95 | n.a. | BMB |
| Total: | | | 105.872 | 100.100 | 100.00 | 0.000 | |



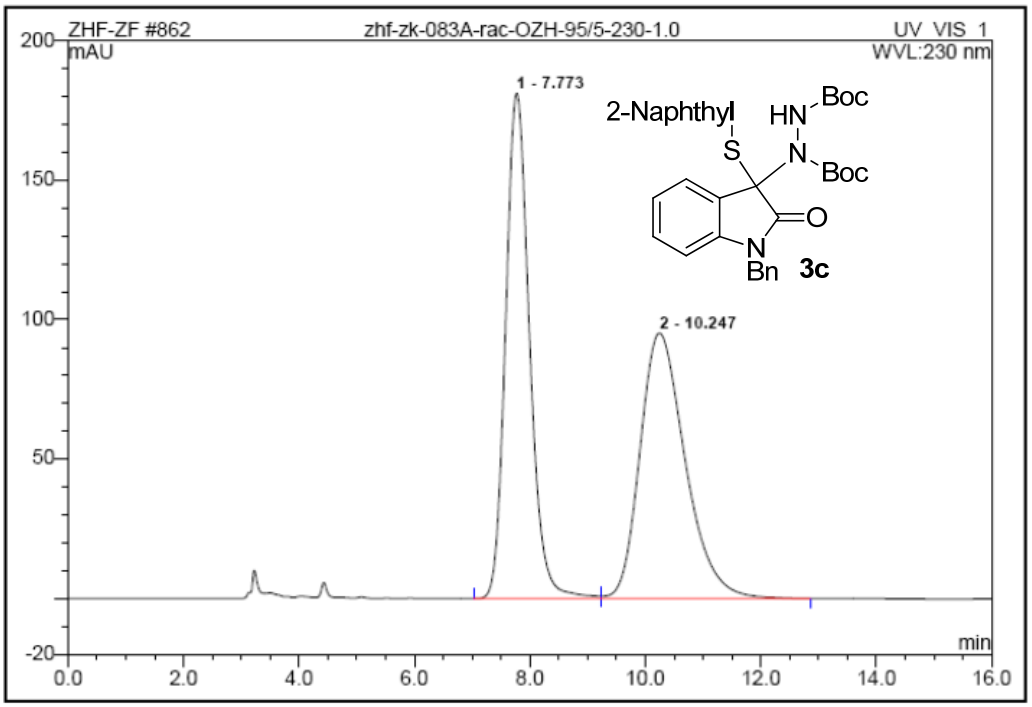

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 5.67 | n.a. | 1375.106 | 452.928 | 91.14 | n.a. | BMB* |
| 2 | 12.75 | n.a. | 46.229 | 44.008 | 8.86 | n.a. | BMB* |
| Total: | | | 1421.335 | 496.936 | 100.00 | 0.000 | |



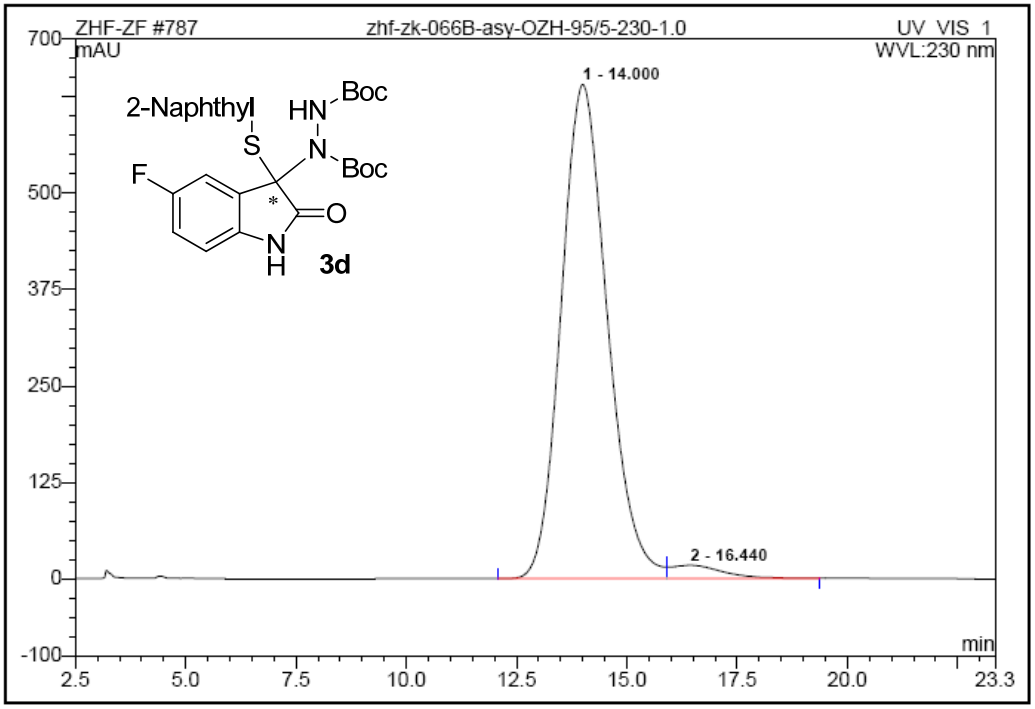

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 5.74 | n.a. | 324.558 | 107.970 | 50.27 | n.a. | BMB |
| 2 | 12.79 | n.a. | 106.774 | 106.814 | 49.73 | n.a. | BMB |
| Total: | | | 431.332 | 214.784 | 100.00 | 0.000 | |



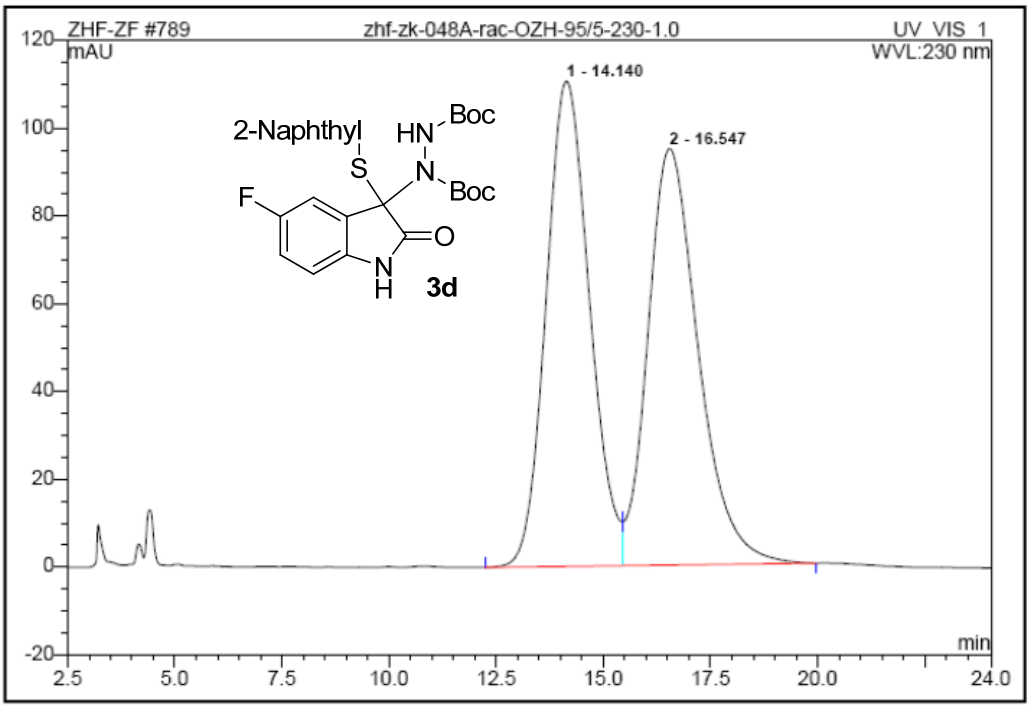

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.77 | n.a. | 118.465 | 54.425 | 10.44 | n.a. | BMB* |
| 2 | 10.21 | n.a. | 519.780 | 466.701 | 89.56 | n.a. | BMB* |
| Total: | | | 638.245 | 521.126 | 100.00 | 0.000 | |



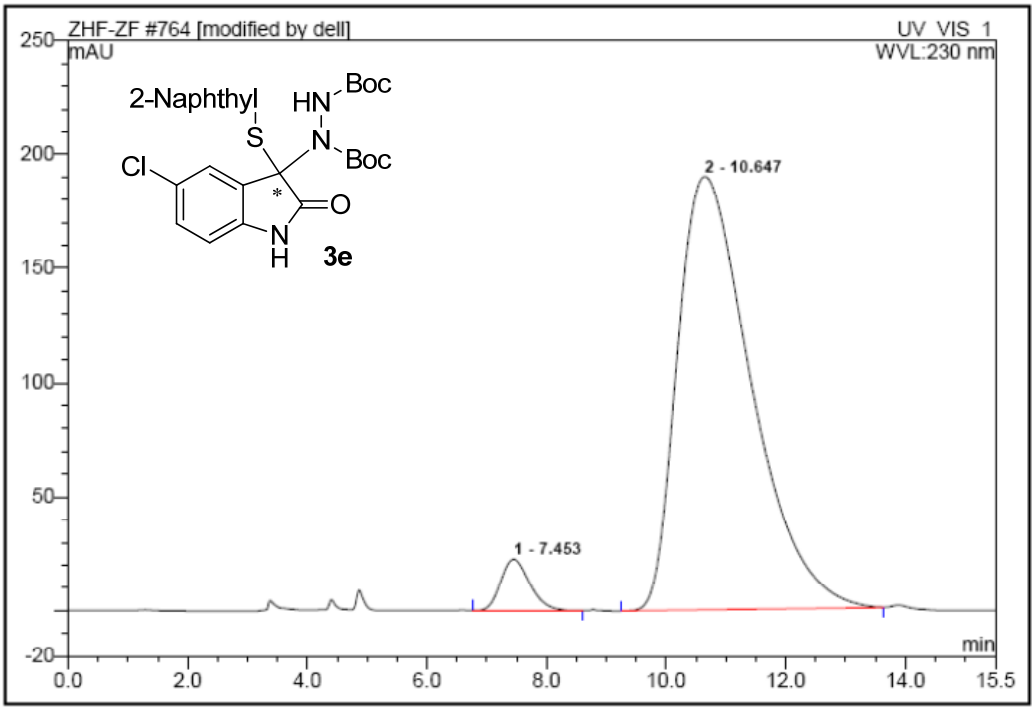

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.77 | n.a. | 181.227 | 86.768 | 50.10 | n.a. | BM |
| 2 | 10.25 | n.a. | 95.226 | 86.412 | 49.90 | n.a. | MB |
| Total: | | | 276.453 | 173.180 | 100.00 | 0.000 | |



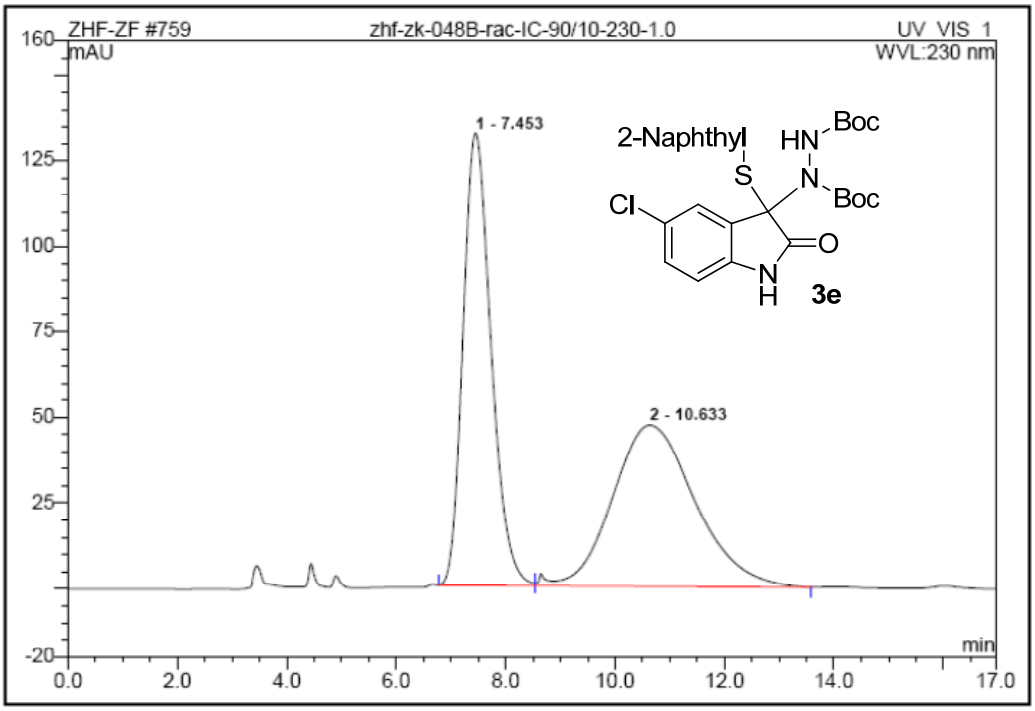

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 14.00 | n.a. | 641.072 | 777.698 | 97.18 | n.a. | BM |
| 2 | 16.44 | n.a. | 16.962 | 22.552 | 2.82 | n.a. | MB |
| Total: | | | 658.034 | 800.250 | 100.00 | 0.000 | |



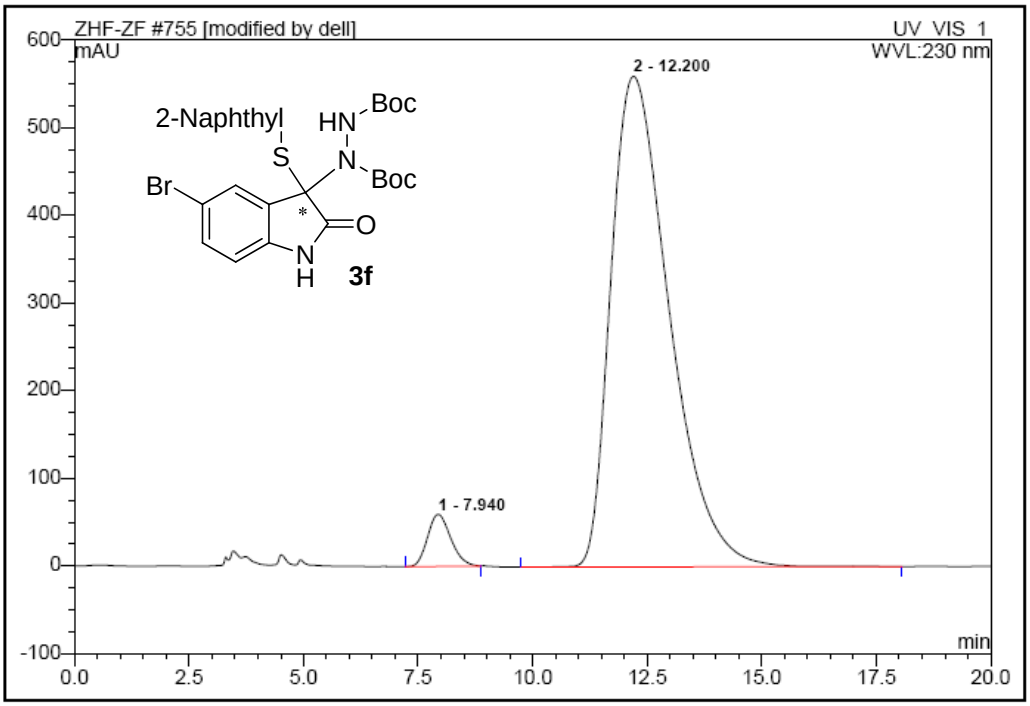

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 14.14 | n.a. | 110.636 | 129.840 | 49.99 | n.a. | BM |
| 2 | 16.55 | n.a. | 94.949 | 129.881 | 50.01 | n.a. | MB |
| Total: | | | 205.584 | 259.721 | 100.00 | 0.000 | |



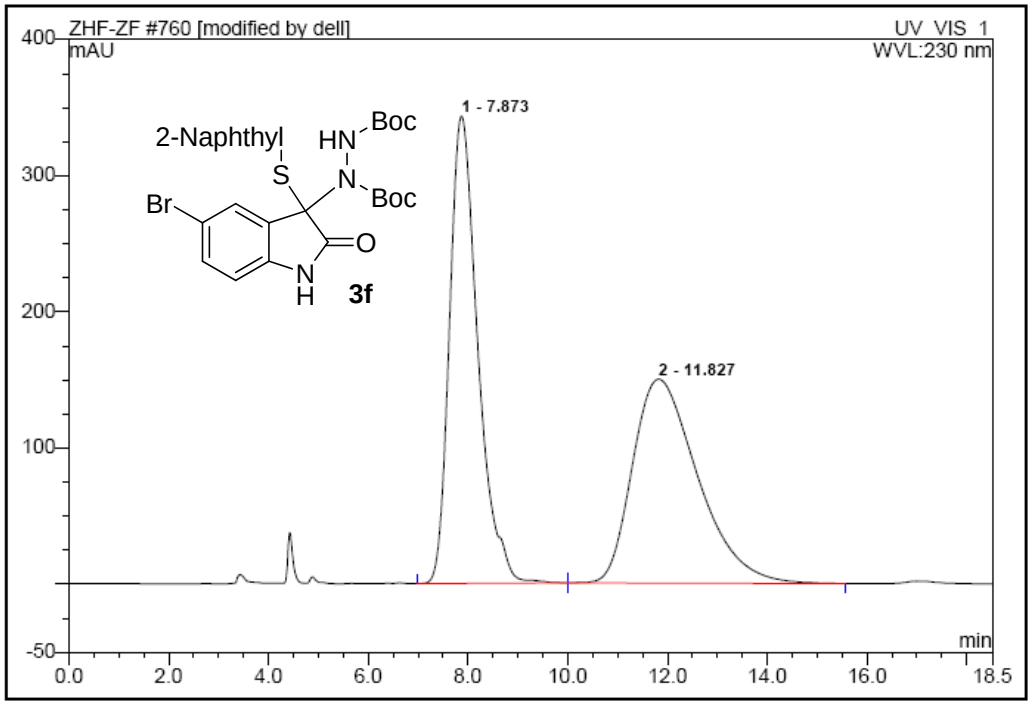

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.45 | n.a. | 22.661 | 12.728 | 4.48 | n.a. | BMB |
| 2 | 10.65 | n.a. | 189.942 | 271.358 | 95.52 | n.a. | BMB |
| Total: | | | 212.603 | 284.086 | 100.00 | 0.000 | |



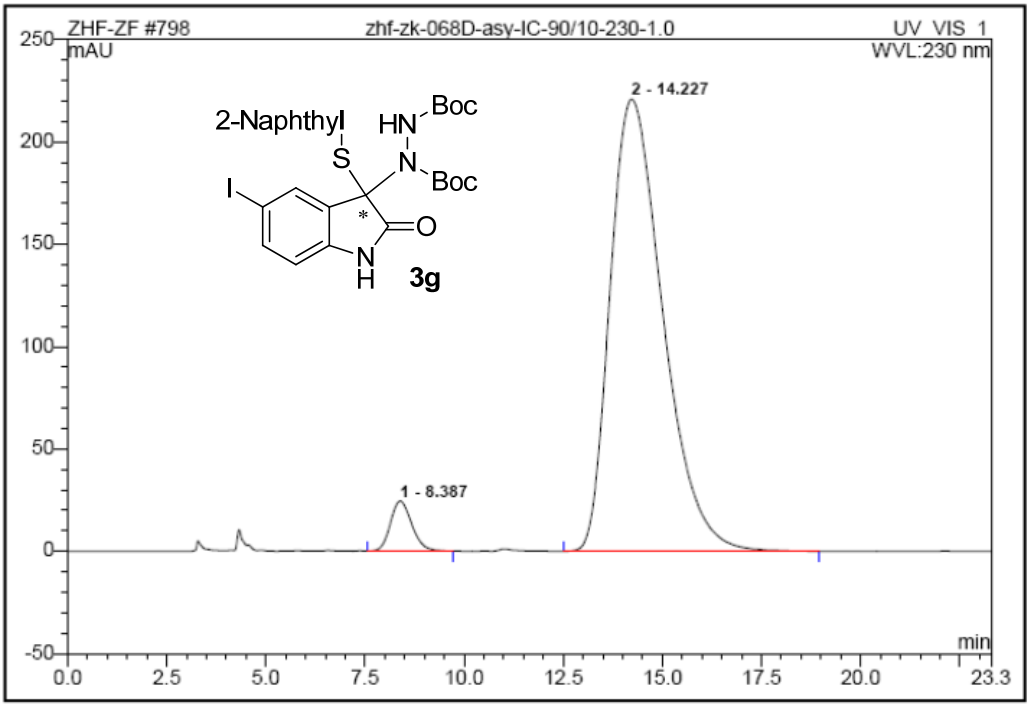

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.45 | n.a. | 131.898 | 78.248 | 48.72 | n.a. | BM |
| 2 | 10.63 | n.a. | 46.964 | 82.356 | 51.28 | n.a. | MB |
| Total: | | | 178.863 | 160.604 | 100.00 | 0.000 | |



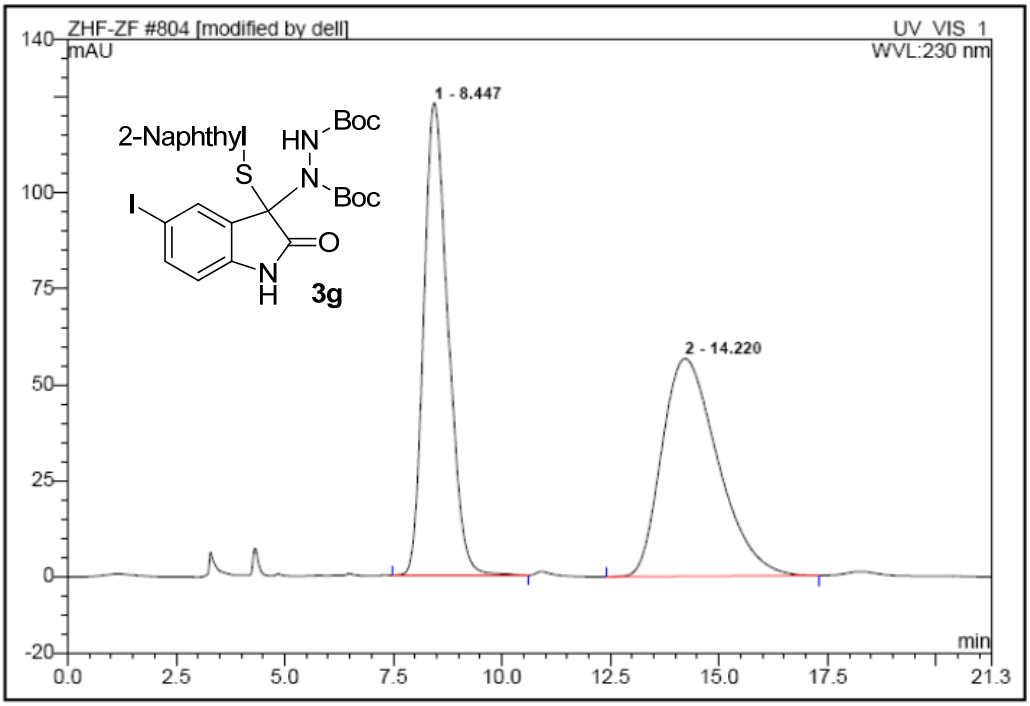

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.94 | n.a. | 59.396 | 34.898 | 4.04 | n.a. | BMB |
| 2 | 12.20 | n.a. | 559.854 | 828.154 | 95.96 | n.a. | BMB |
| Total: | | | 619.249 | 863.051 | 100.00 | 0.000 | |



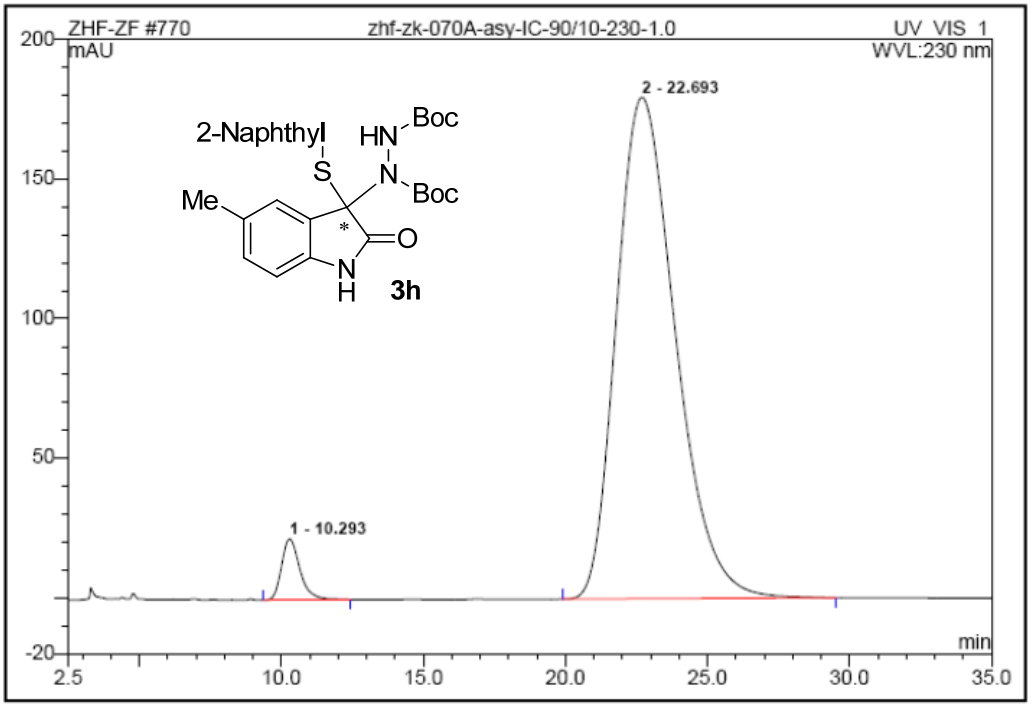

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.87 | n.a. | 343.172 | 225.922 | 49.88 | n.a. | BMb* |
| 2 | 11.83 | n.a. | 149.720 | 227.011 | 50.12 | n.a. | bMB |
| Total: | | | 492.892 | 452.933 | 100.00 | 0.000 | |



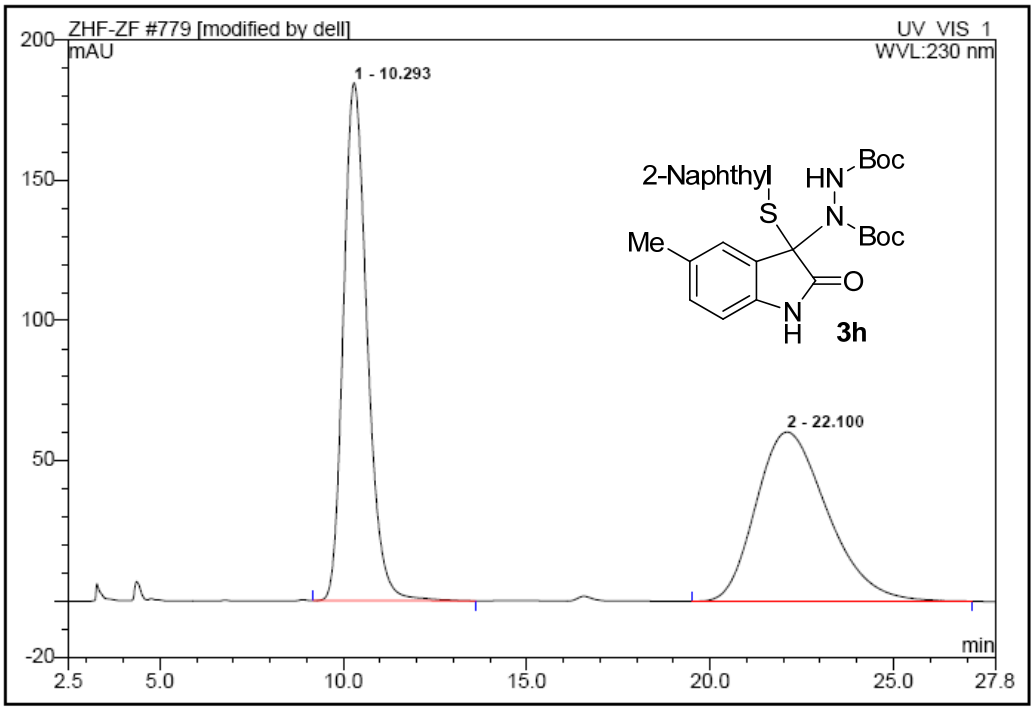

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 8.39 | n.a. | 24.416 | 15.226 | 4.29 | n.a. | BMB |
| 2 | 14.23 | n.a. | 220.730 | 339.572 | 95.71 | n.a. | BMB |
| Total: | | | 245.146 | 354.798 | 100.00 | 0.000 | |



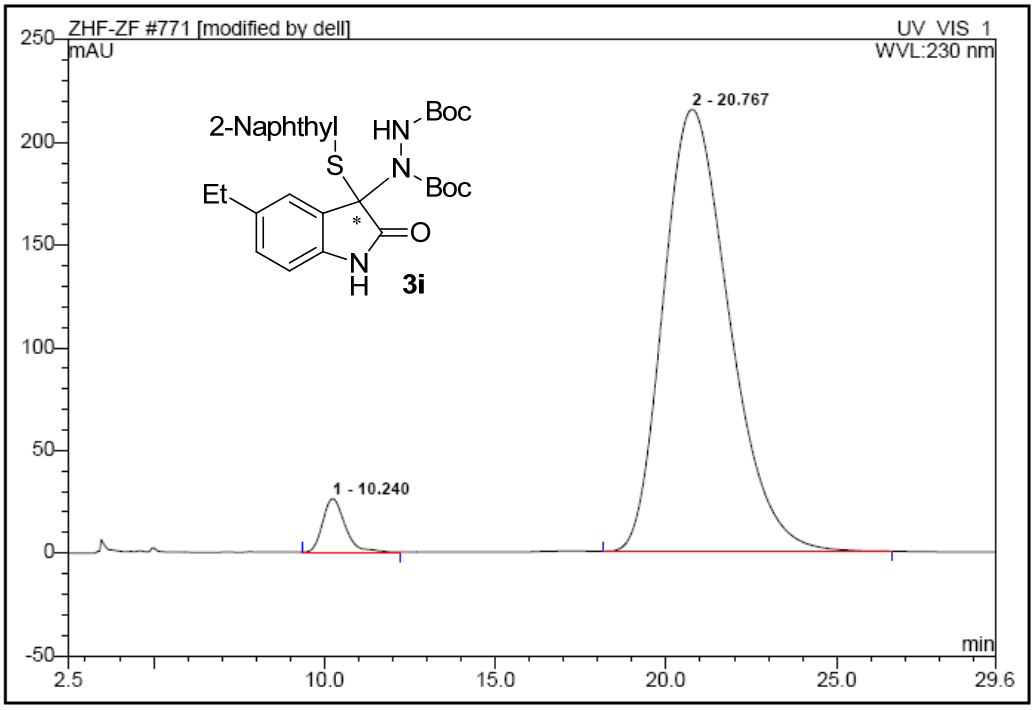

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 8.45 | n.a. | 123.318 | 79.928 | 48.43 | n.a. | BMB |
| 2 | 14.22 | n.a. | 56.803 | 85.125 | 51.57 | n.a. | BMB* |
| Total: | | | 180.121 | 165.052 | 100.00 | 0.000 | |



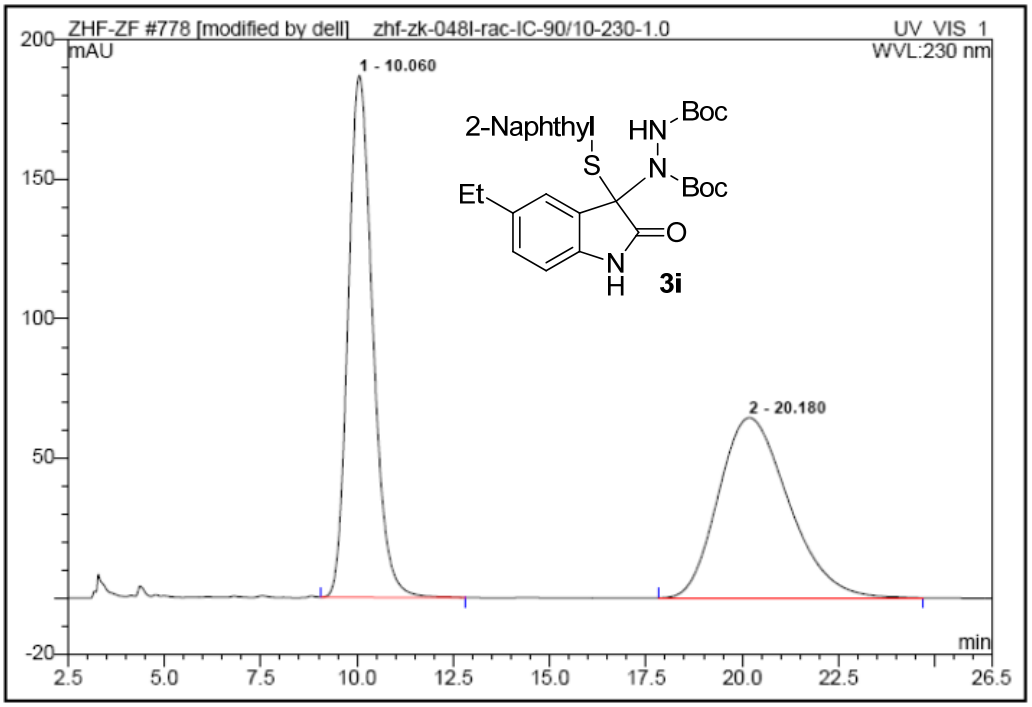

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.29 | n.a. | 21.773 | 16.281 | 3.64 | n.a. | BMB |
| 2 | 22.69 | n.a. | 179.636 | 430.853 | 96.36 | n.a. | BMB |
| Total: | | | 201.409 | 447.134 | 100.00 | 0.000 | |



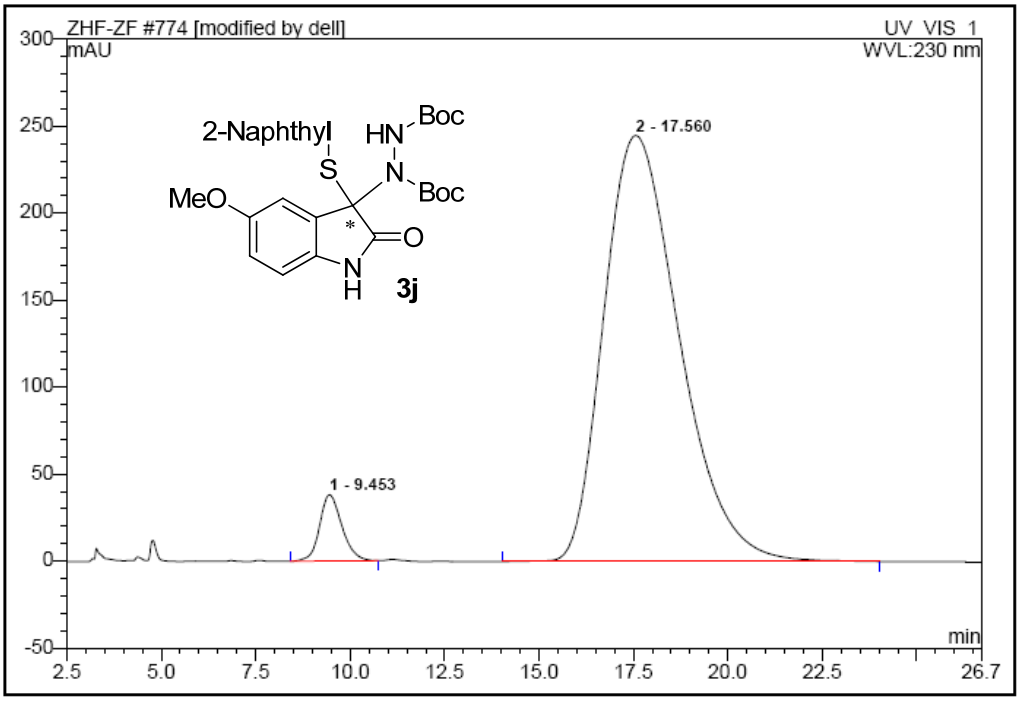

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.29 | n.a. | 184.645 | 138.666 | 50.36 | n.a. | BMB |
| 2 | 22.10 | n.a. | 60.396 | 136.694 | 49.64 | n.a. | BMB |
| Total: | | | 245.042 | 275.361 | 100.00 | 0.000 | |



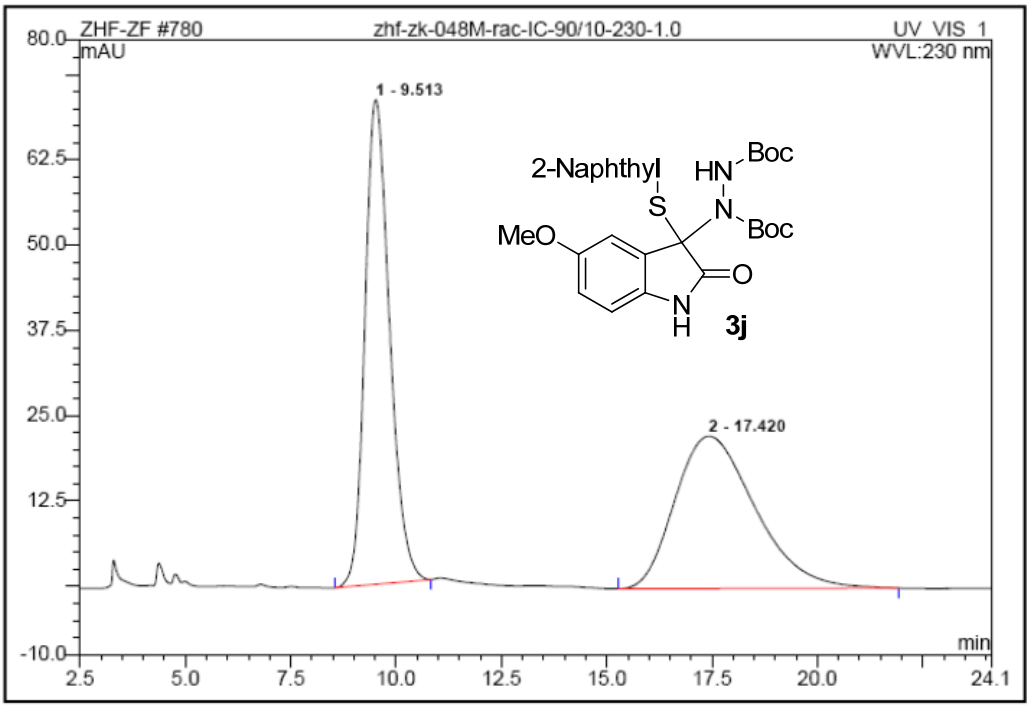

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.24 | n.a. | 26.021 | 19.739 | 3.94 | n.a. | BMB |
| 2 | 20.77 | n.a. | 215.172 | 481.320 | 96.06 | n.a. | BMB |
| Total: | | | 241.193 | 501.059 | 100.00 | 0.000 | |



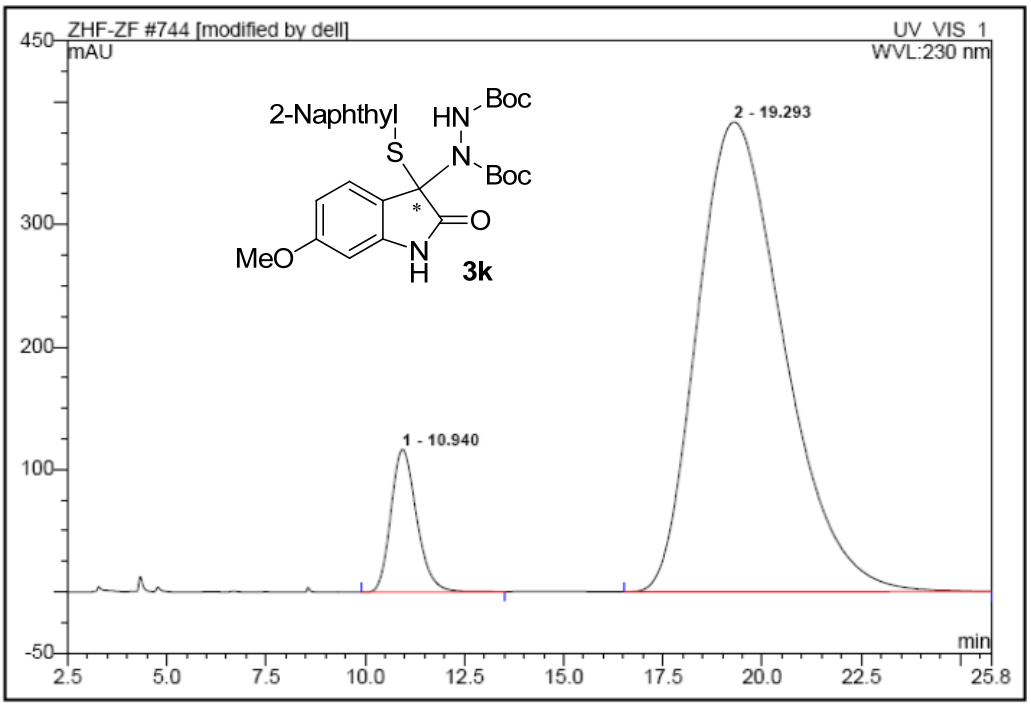

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.06 | n.a. | 186.972 | 138.288 | 50.37 | n.a. | BMB |
| 2 | 20.18 | n.a. | 64.497 | 136.275 | 49.63 | n.a. | BMB |
| Total: | | | 251.469 | 274.563 | 100.00 | 0.000 | |



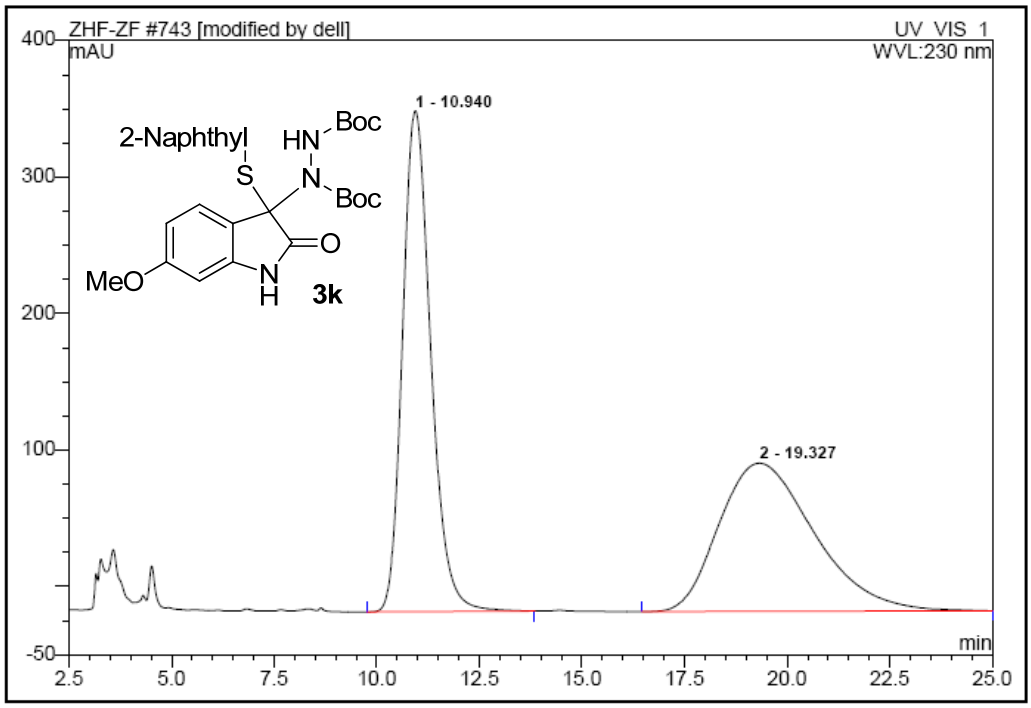

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.45 | n.a. | 38.033 | 26.081 | 4.40 | n.a. | BMB |
| 2 | 17.56 | n.a. | 244.801 | 566.069 | 95.60 | n.a. | BMB |
| Total: | | | 282.833 | 592.150 | 100.00 | 0.000 | |



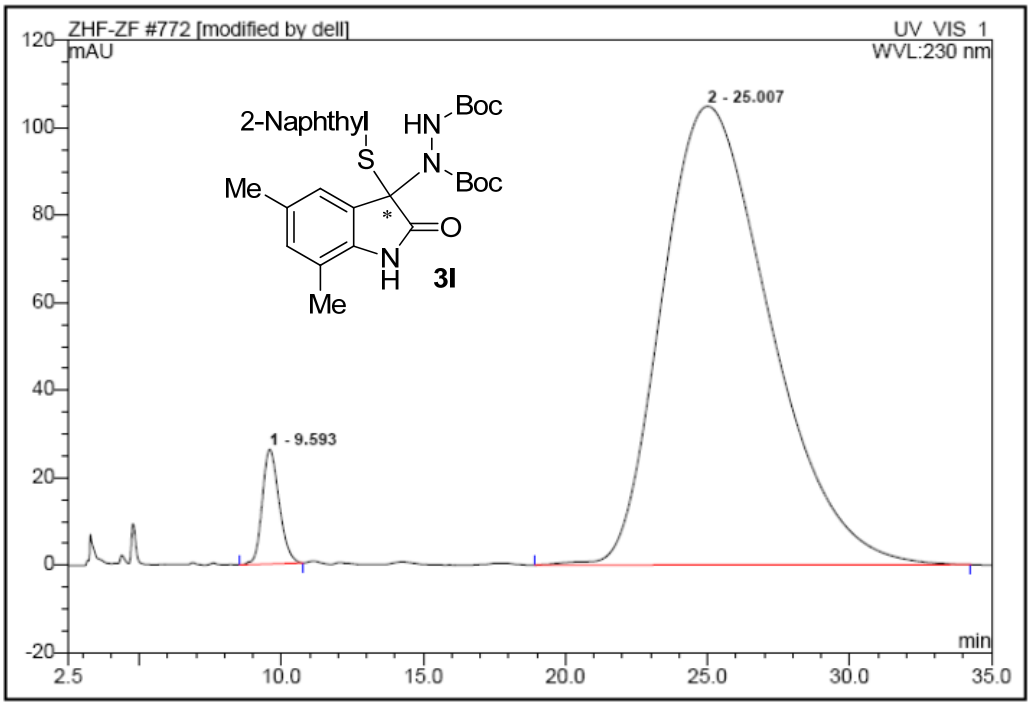

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.51 | n.a. | 71.010 | 48.154 | 49.49 | n.a. | BMB |
| 2 | 17.42 | n.a. | 22.319 | 49.154 | 50.51 | n.a. | BMB |
| Total: | | | 93.329 | 97.308 | 100.00 | 0.000 | |



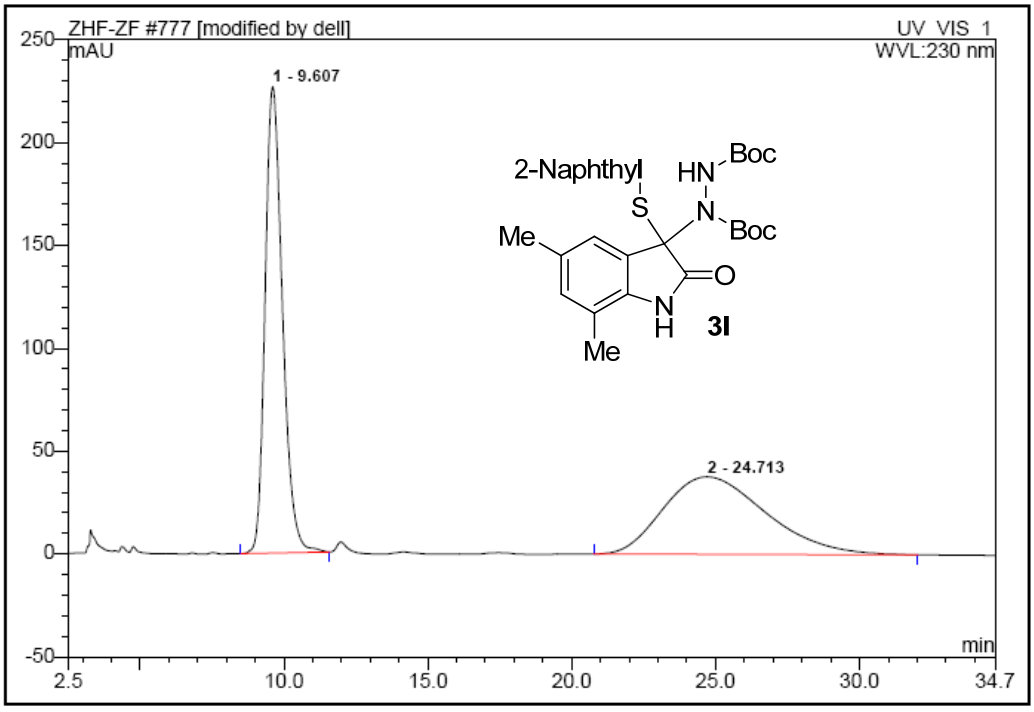

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.94 | n.a. | 116.683 | 88.399 | 8.36 | n.a. | BMB |
| 2 | 19.29 | n.a. | 383.640 | 968.903 | 91.64 | n.a. | BMB |
| Total: | | | 500.322 | 1057.301 | 100.00 | 0.000 | |



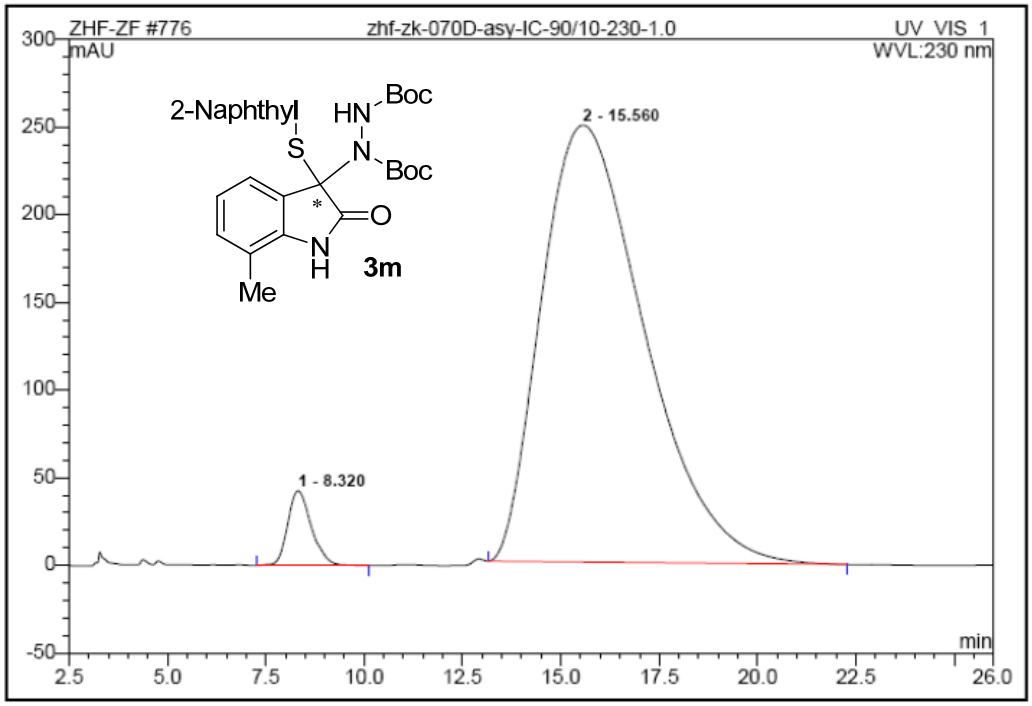

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.94 | n.a. | 366.915 | 292.086 | 50.04 | n.a. | BMB |
| 2 | 19.33 | n.a. | 108.552 | 291.675 | 49.96 | n.a. | BMB |
| Total: | | | 475.467 | 583.761 | 100.00 | 0.000 | |



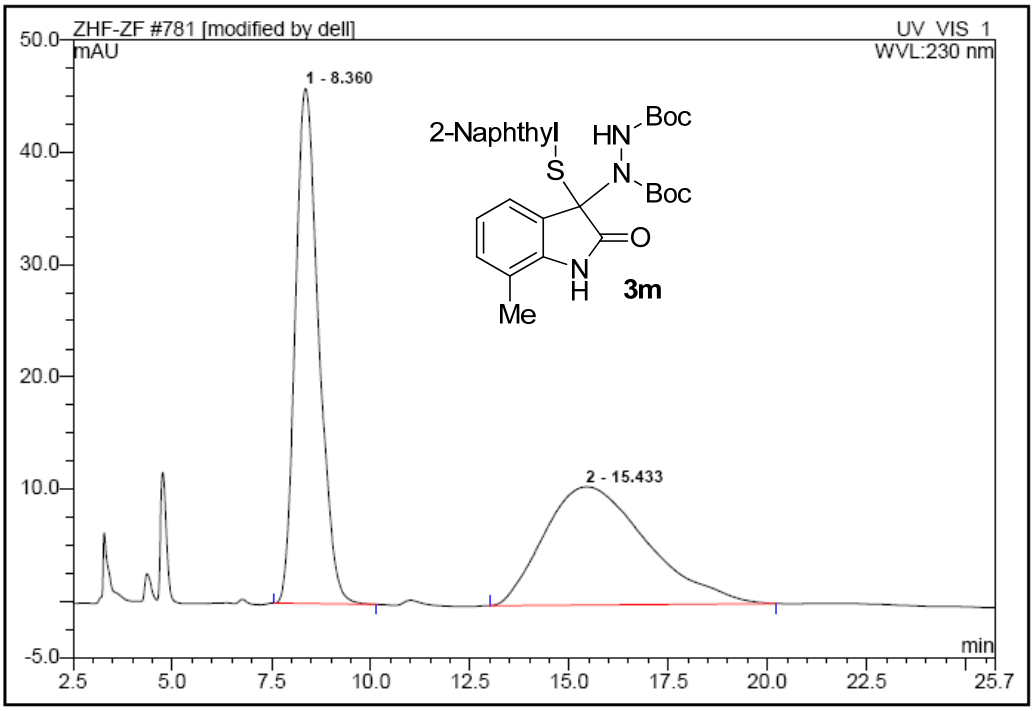

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.59 | n.a. | 26.203 | 18.141 | 3.77 | n.a. | BMB |
| 2 | 25.01 | n.a. | 104.913 | 462.798 | 96.23 | n.a. | BMB |
| Total: | | | 131.117 | 480.939 | 100.00 | 0.000 | |



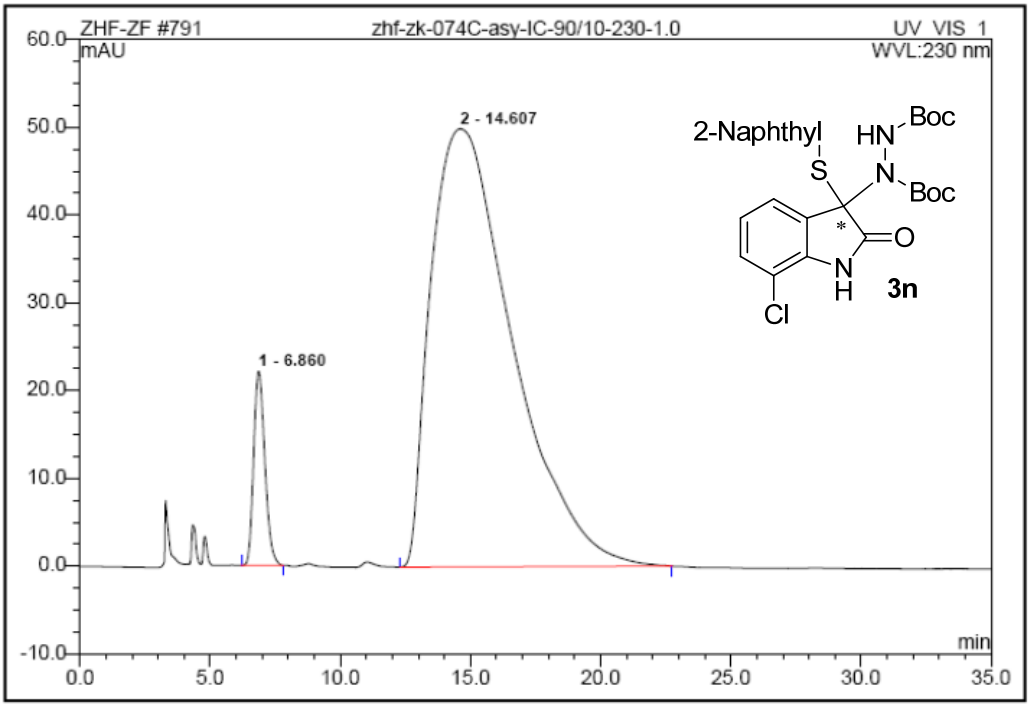

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.61 | n.a. | 226.627 | 158.621 | 50.54 | n.a. | BMB* |
| 2 | 24.71 | n.a. | 37.606 | 155.261 | 49.46 | n.a. | BMB |
| Total: | | | 264.233 | 313.881 | 100.00 | 0.000 | |



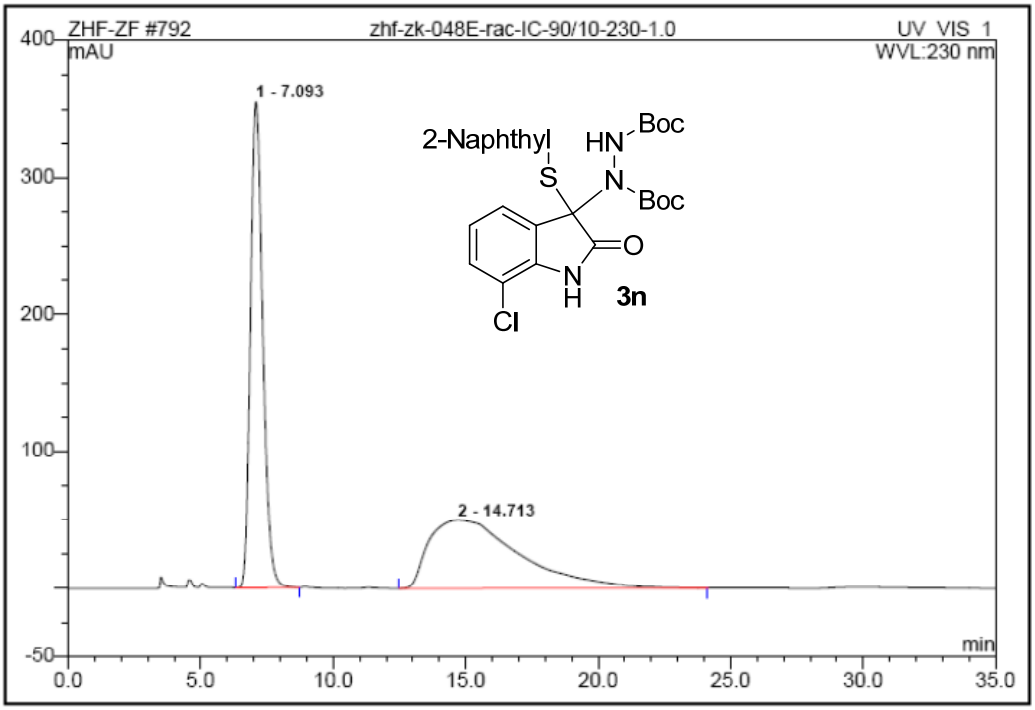

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 8.32 | n.a. | 42.564 | 29.709 | 3.78 | n.a. | BMB |
| 2 | 15.56 | n.a. | 249.240 | 755.841 | 96.22 | n.a. | BMB |
| Total: | | | 291.804 | 785.549 | 100.00 | 0.000 | |



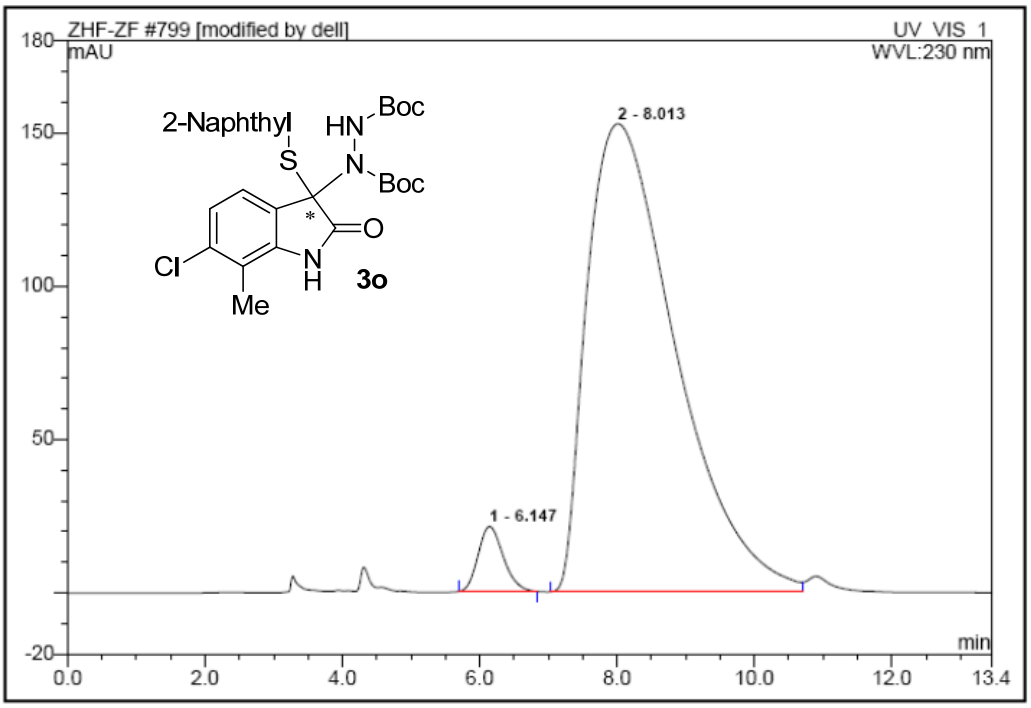

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 8.36 | n.a. | 45.895 | 31.400 | 49.74 | n.a. | BMB |
| 2 | 15.43 | n.a. | 10.528 | 31.734 | 50.26 | n.a. | BMB |
| Total: | | | 56.424 | 63.134 | 100.00 | 0.000 | |



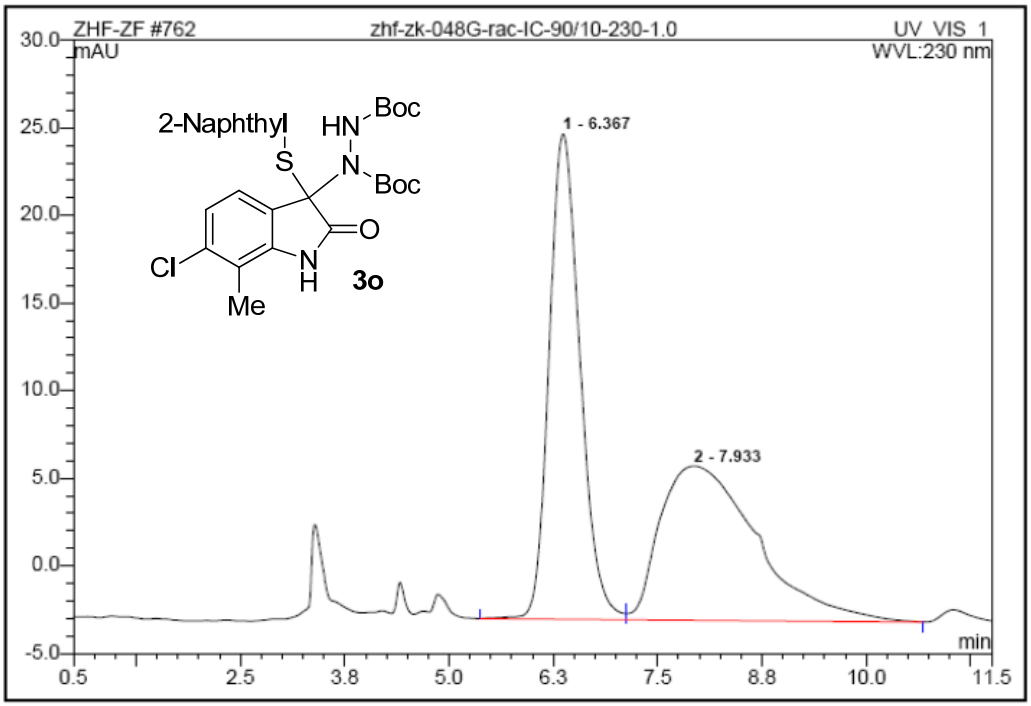

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 6.86 | n.a. | 22.143 | 11.089 | 5.76 | n.a. | BMB |
| 2 | 14.61 | n.a. | 49.930 | 181.405 | 94.24 | n.a. | BMB |
| Total: | | | 72.073 | 192.494 | 100.00 | 0.000 | |



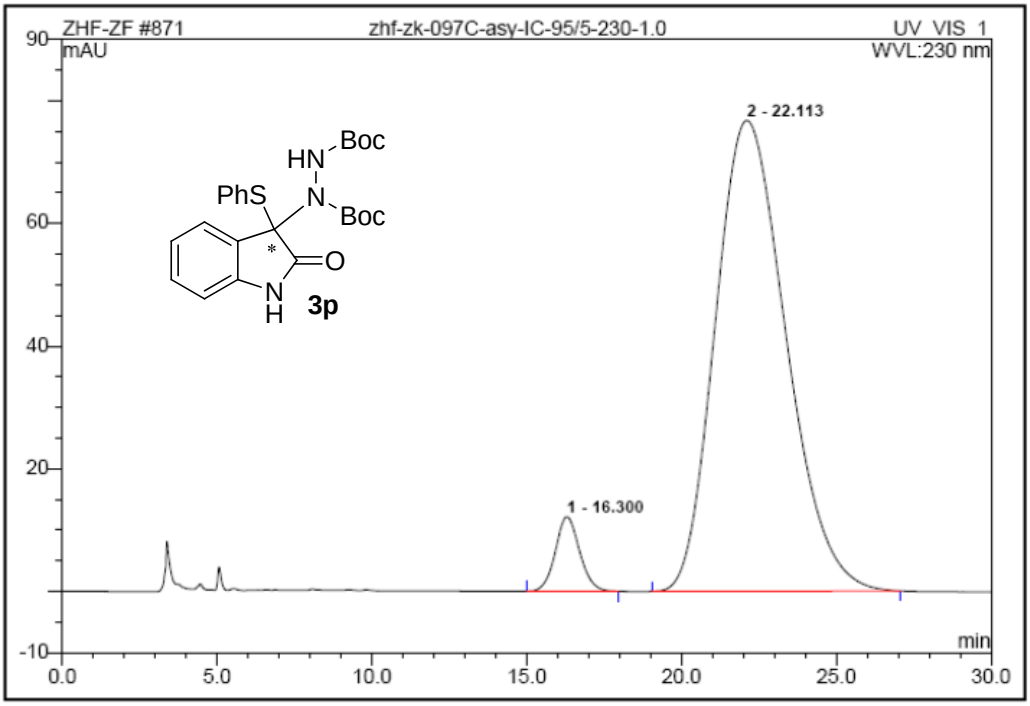

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 7.09 | n.a. | 354.812 | 191.068 | 49.16 | n.a. | BMB |
| 2 | 14.71 | n.a. | 49.776 | 197.599 | 50.84 | n.a. | BMB |
| Total: | | | 404.588 | 388.667 | 100.00 | 0.000 | |



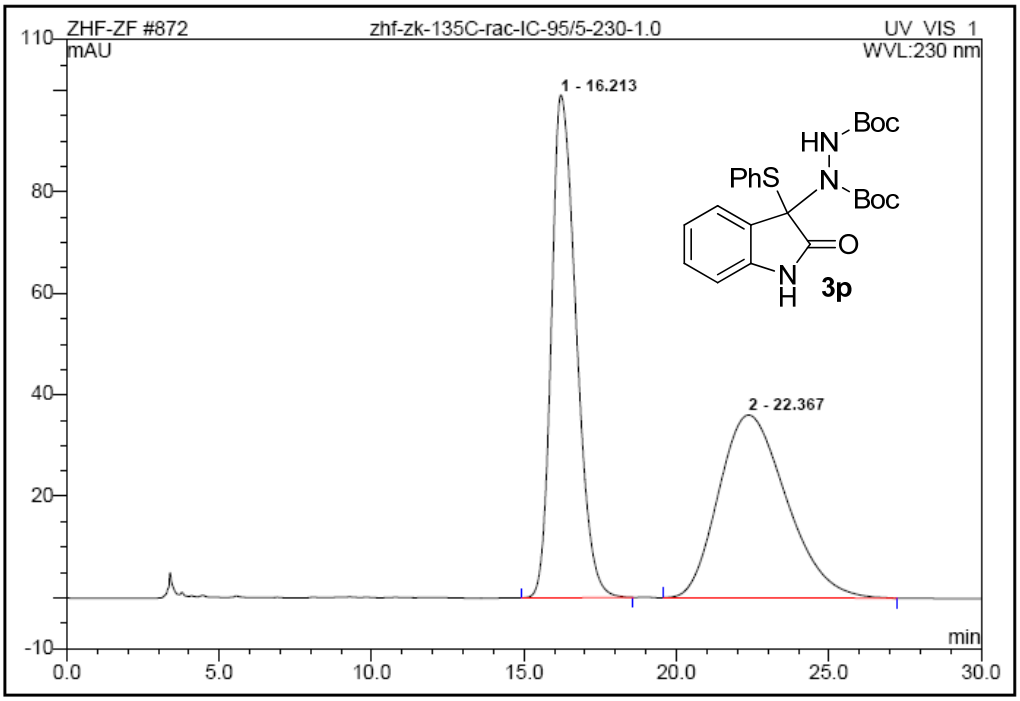

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 6.15 | n.a. | 21.147 | 8.995 | 3.79 | n.a. | BMB* |
| 2 | 8.01 | n.a. | 152.657 | 228.457 | 96.21 | n.a. | BM * |
| Total: | | | 173.804 | 237.453 | 100.00 | 0.000 | |



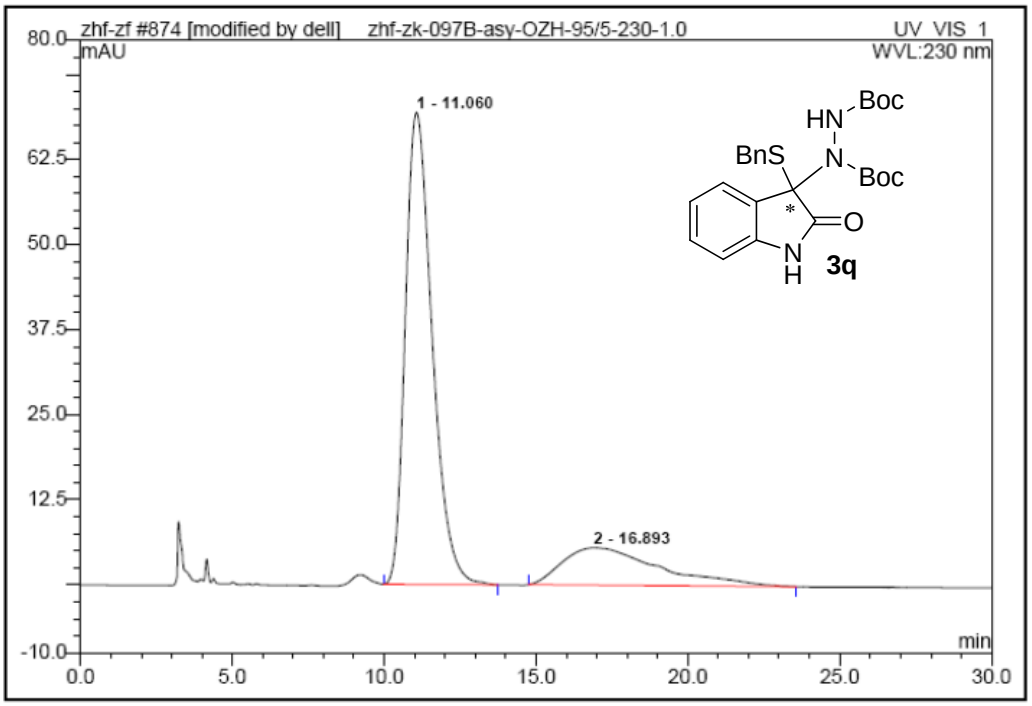

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 6.37 | n.a. | 27.704 | 11.877 | 50.09 | n.a. | BM |
| 2 | 7.93 | n.a. | 8.798 | 11.837 | 49.91 | n.a. | MB |
| Total: | | | 36.502 | 23.714 | 100.00 | 0.000 | |



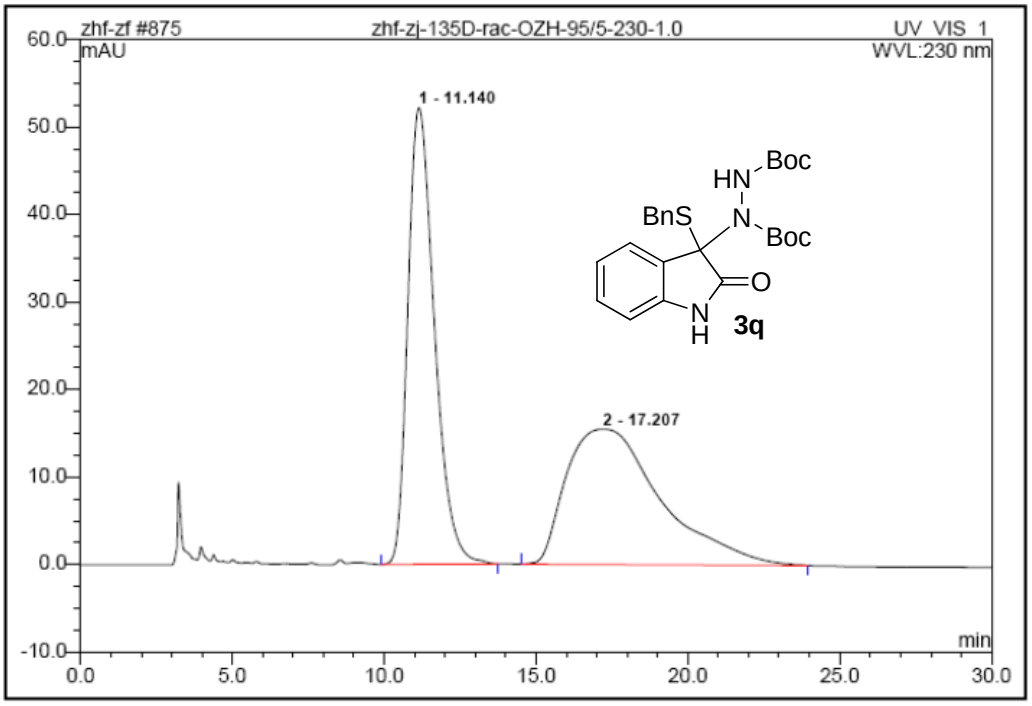

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 16.30 | n.a. | 12.148 | 11.084 | 5.18 | n.a. | BMB |
| 2 | 22.11 | n.a. | 76.786 | 203.035 | 94.82 | n.a. | BMB |
| Total: | | | 88.934 | 214.119 | 100.00 | 0.000 | |



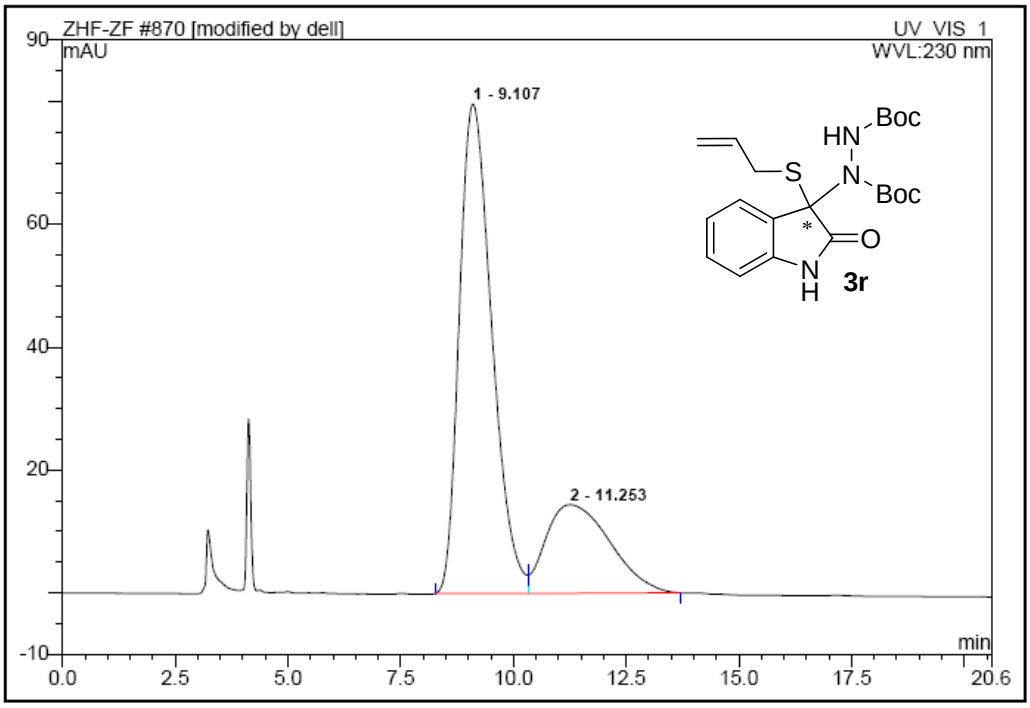

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 16.21 | n.a. | 99.063 | 93.402 | 50.07 | n.a. | BMB |
| 2 | 22.37 | n.a. | 36.042 | 93.148 | 49.93 | n.a. | BMB |
| Total: | | | 135.104 | 186.551 | 100.00 | 0.000 | |



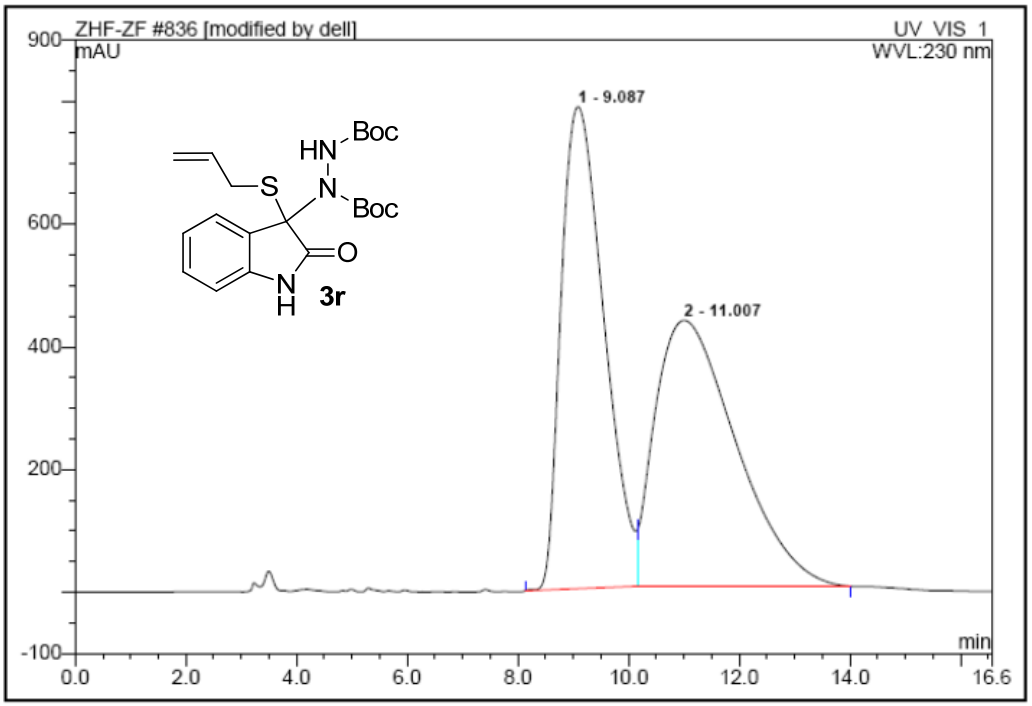

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 11.06 | n.a. | 69.373 | 70.927 | 77.89 | n.a. | BMB* |
| 2 | 16.89 | n.a. | 5.477 | 20.132 | 22.11 | n.a. | BMB* |
| Total: | | | 74.850 | 91.059 | 100.00 | 0.000 | |



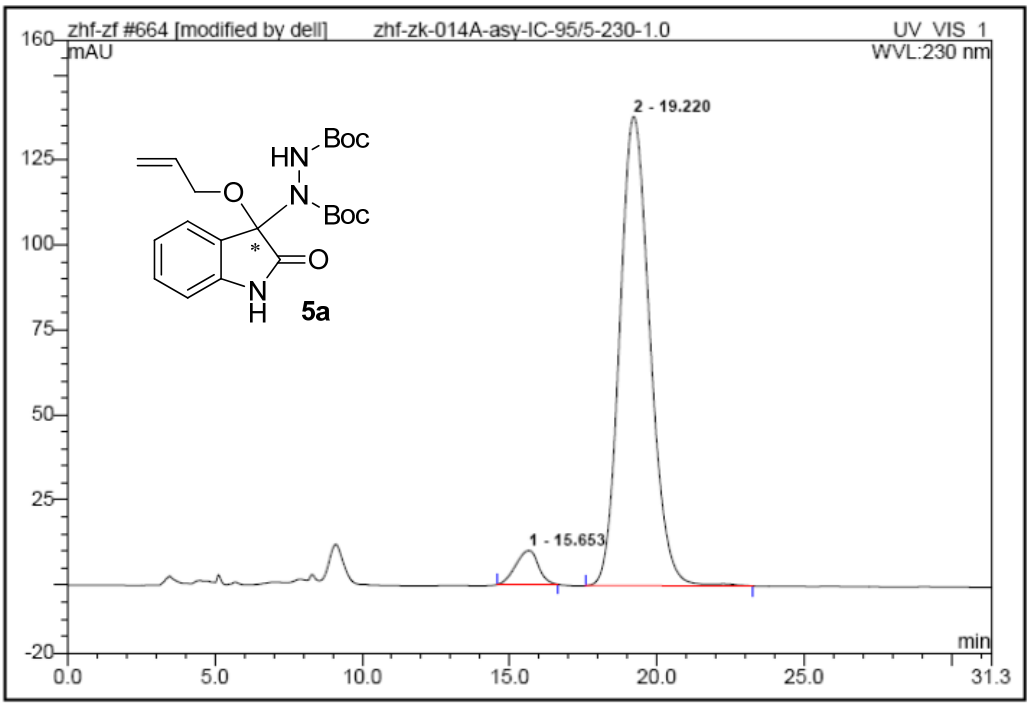

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 11.14 | n.a. | 52.204 | 52.850 | 48.63 | n.a. | BMB |
| 2 | 17.21 | n.a. | 15.499 | 55.823 | 51.37 | n.a. | BMB |
| Total: | | | 67.703 | 108.673 | 100.00 | 0.000 | |



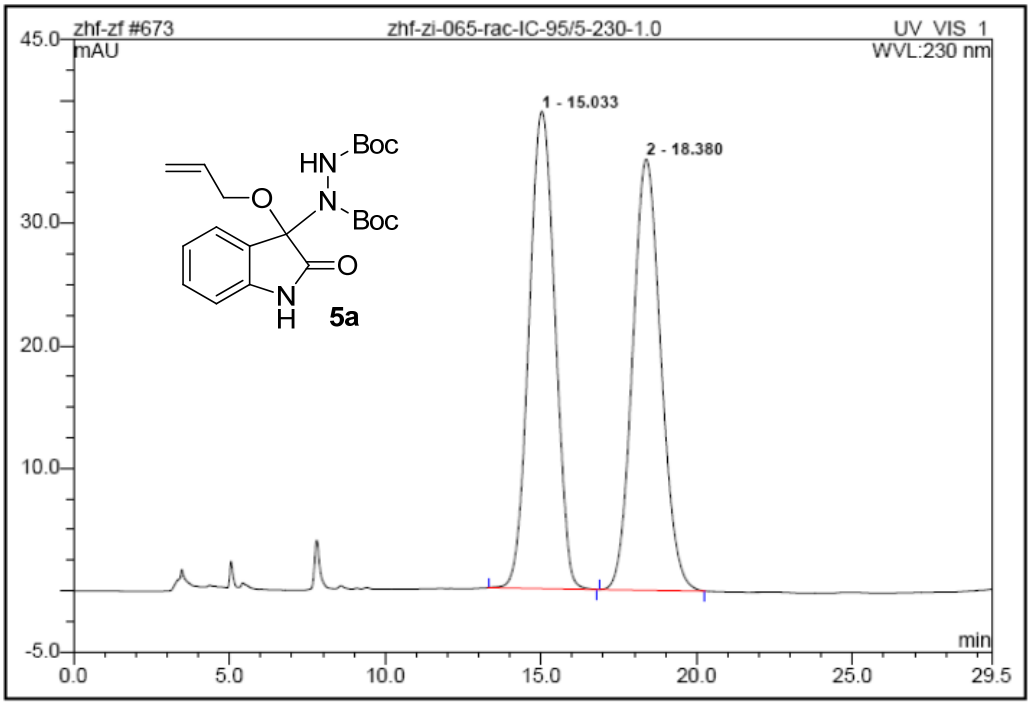

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.11 | n.a. | 79.682 | 66.658 | 73.68 | n.a. | BM * |
| 2 | 11.25 | n.a. | 14.422 | 23.806 | 26.32 | n.a. | MB* |
| Total: | | | 94.104 | 90.464 | 100.00 | 0.000 | |



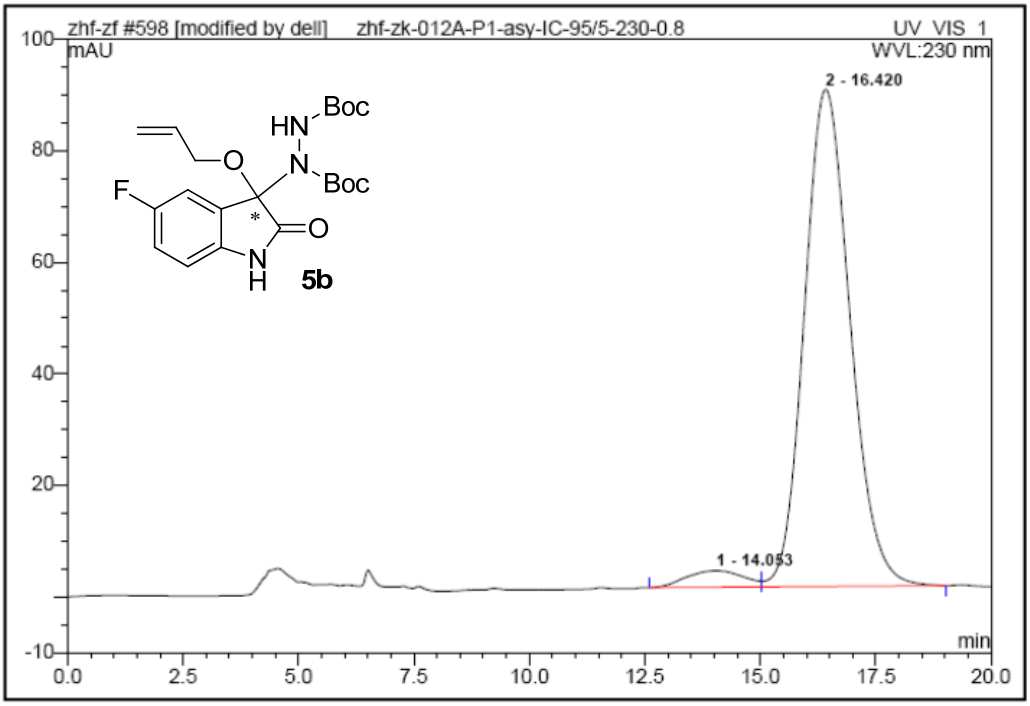

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.09 | n.a. | 786.134 | 706.011 | 49.01 | n.a. | BM * |
| 2 | 11.01 | n.a. | 433.740 | 734.436 | 50.99 | n.a. | MB* |
| Total: | | | 1219.875 | 1440.447 | 100.00 | 0.000 | |



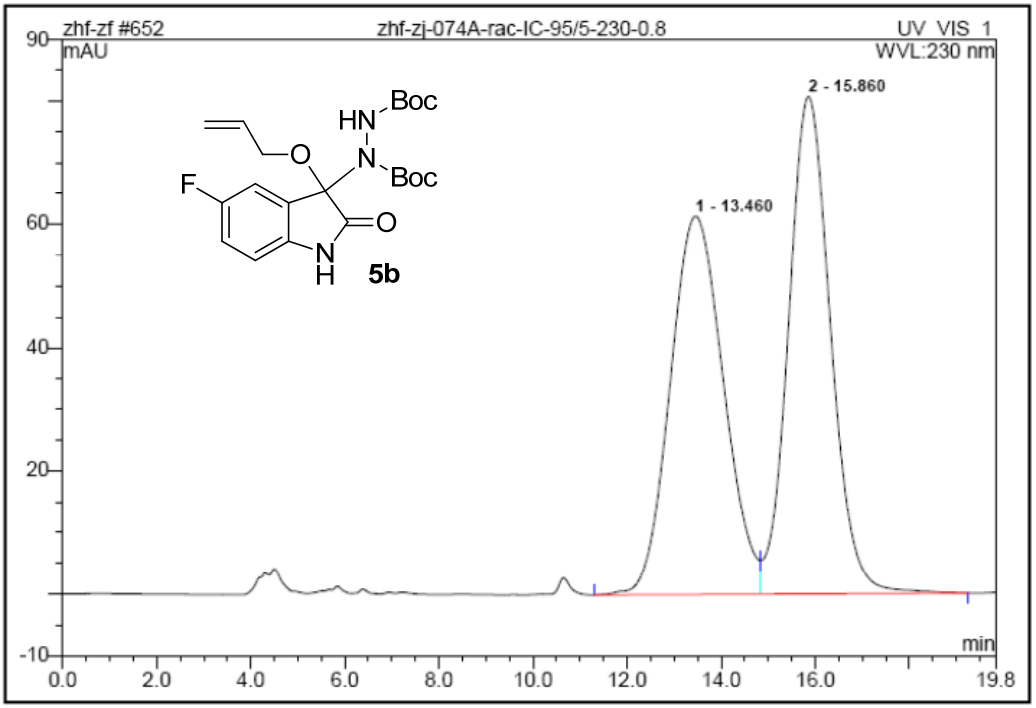

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 15.65 | n.a. | 9.953 | 8.903 | 5.15 | n.a. | BMB* |
| 2 | 19.22 | n.a. | 138.019 | 163.864 | 94.85 | n.a. | BMB* |
| Total: | | | 147.972 | 172.767 | 100.00 | 0.000 | |



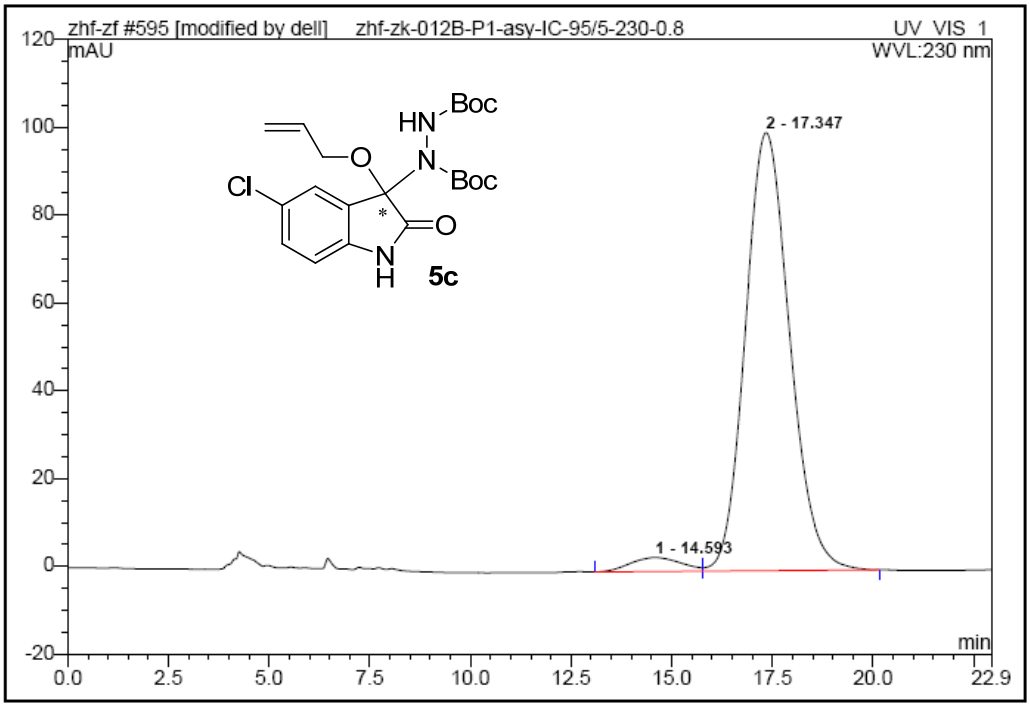

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 15.03 | n.a. | 38.969 | 37.667 | 50.42 | n.a. | BMB |
| 2 | 18.38 | n.a. | 35.205 | 37.041 | 49.58 | n.a. | BMB |
| Total: | | | 74.174 | 74.708 | 100.00 | 0.000 | |



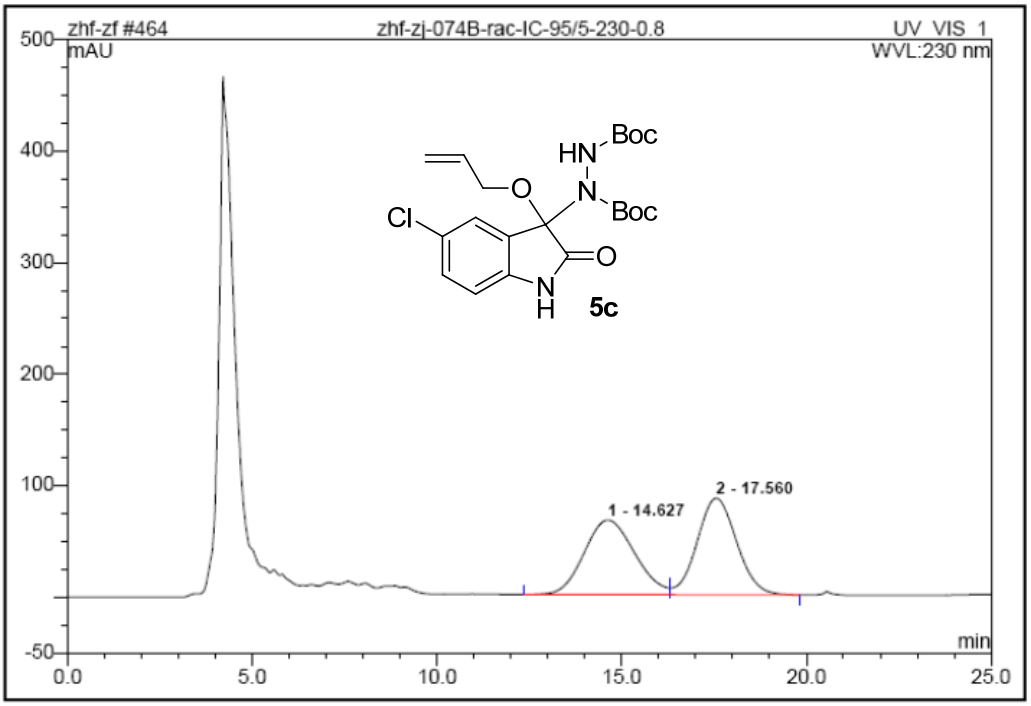

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 14.05 | n.a. | 2.926 | 4.181 | 3.93 | n.a. | BM |
| 2 | 16.42 | n.a. | 89.161 | 102.324 | 96.07 | n.a. | MB |
| Total: | | | 92.087 | 106.505 | 100.00 | 0.000 | |



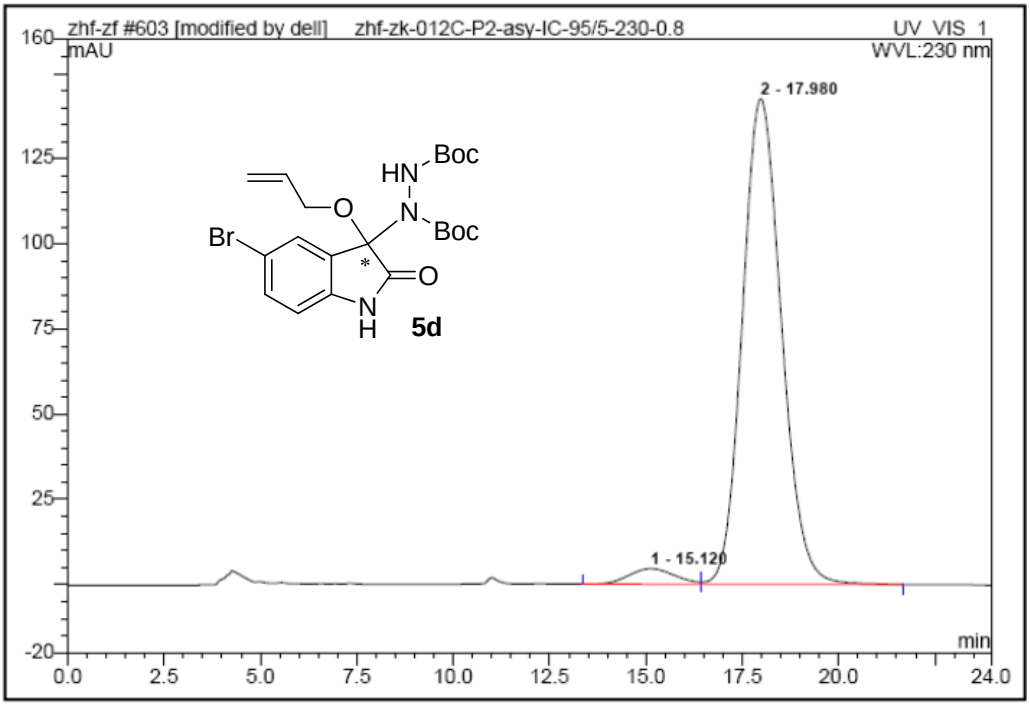

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 13.46 | n.a. | 61.414 | 80.735 | 49.08 | n.a. | BM |
| 2 | 15.86 | n.a. | 80.729 | 83.766 | 50.92 | n.a. | MB |
| Total: | | | 142.143 | 164.500 | 100.00 | 0.000 | |



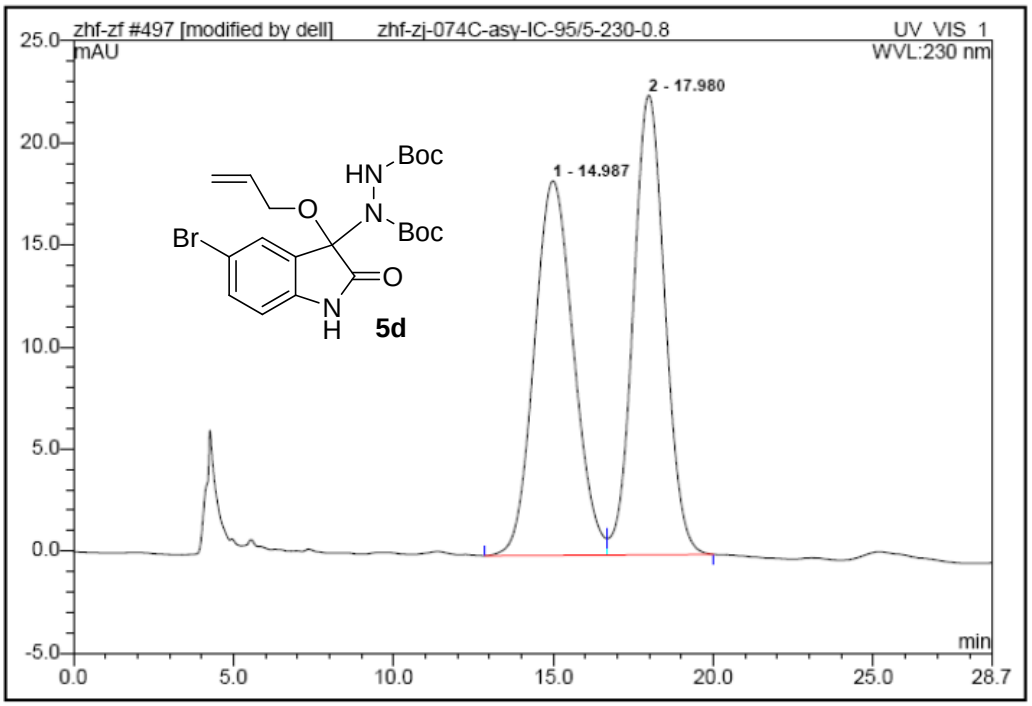

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 14.59 | n.a. | 3.164 | 4.593 | 3.48 | n.a. | BM |
| 2 | 17.35 | n.a. | 99.768 | 127.459 | 96.52 | n.a. | MB |
| Total: | | | 102.932 | 132.052 | 100.00 | 0.000 | |



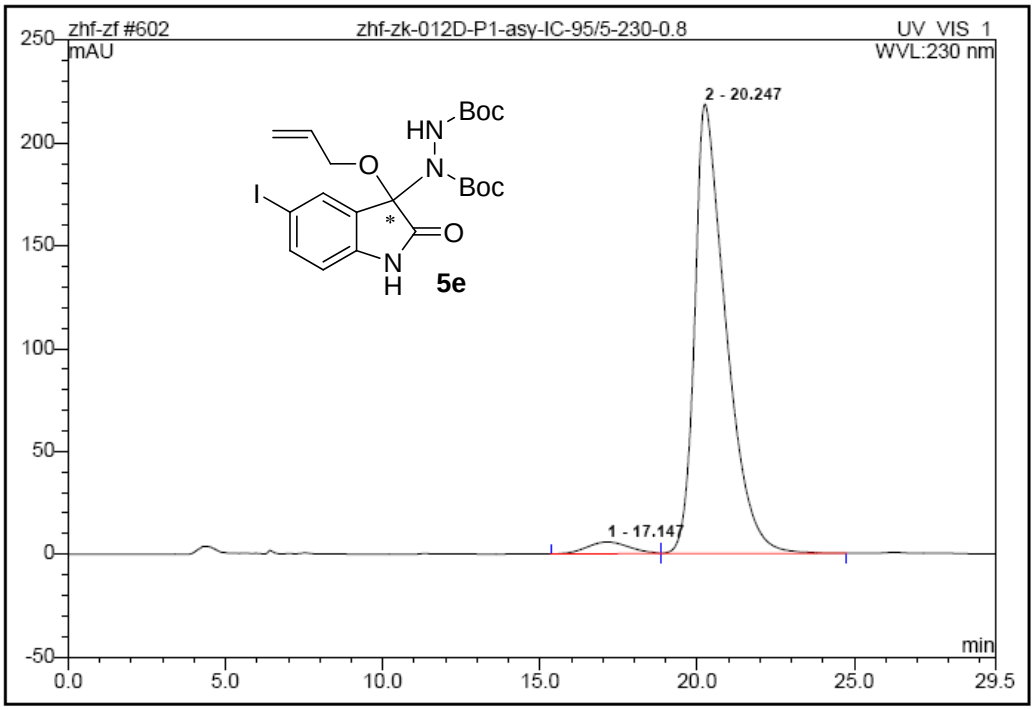

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 14.63 | n.a. | 67.034 | 106.367 | 49.72 | n.a. | BM |
| 2 | 17.56 | n.a. | 86.621 | 107.552 | 50.28 | n.a. | MB |
| Total: | | | 153.655 | 213.918 | 100.00 | 0.000 | |



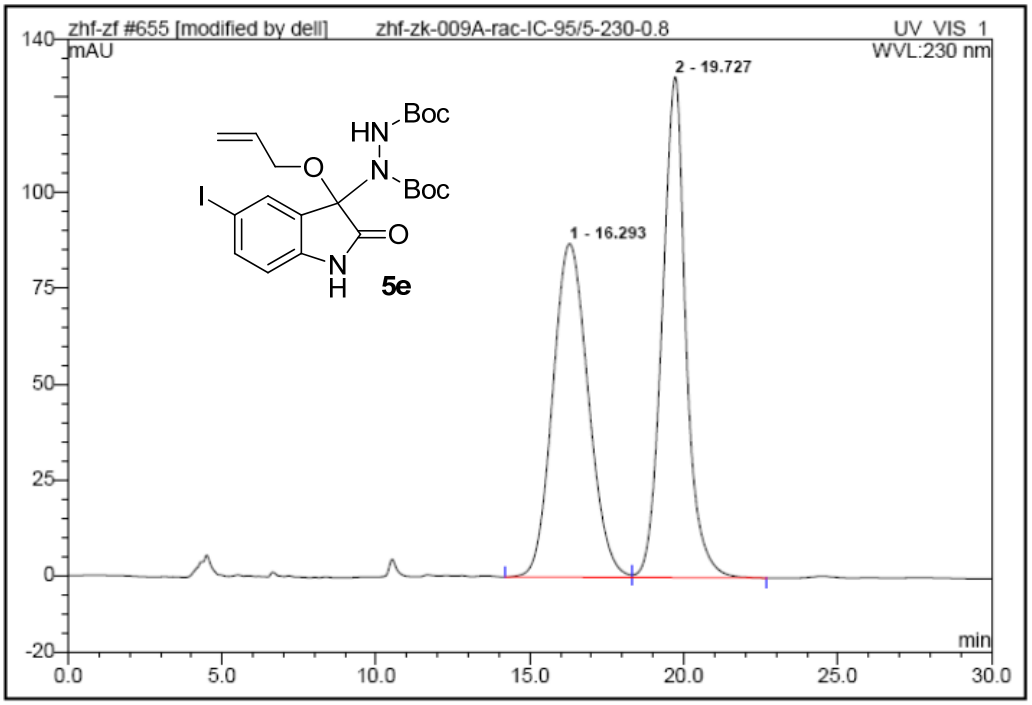

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 15.12 | n.a. | 4.554 | 6.292 | 3.63 | n.a. | BM |
| 2 | 17.98 | n.a. | 142.574 | 167.083 | 96.37 | n.a. | MB |
| Total: | | | 147.128 | 173.375 | 100.00 | 0.000 | |



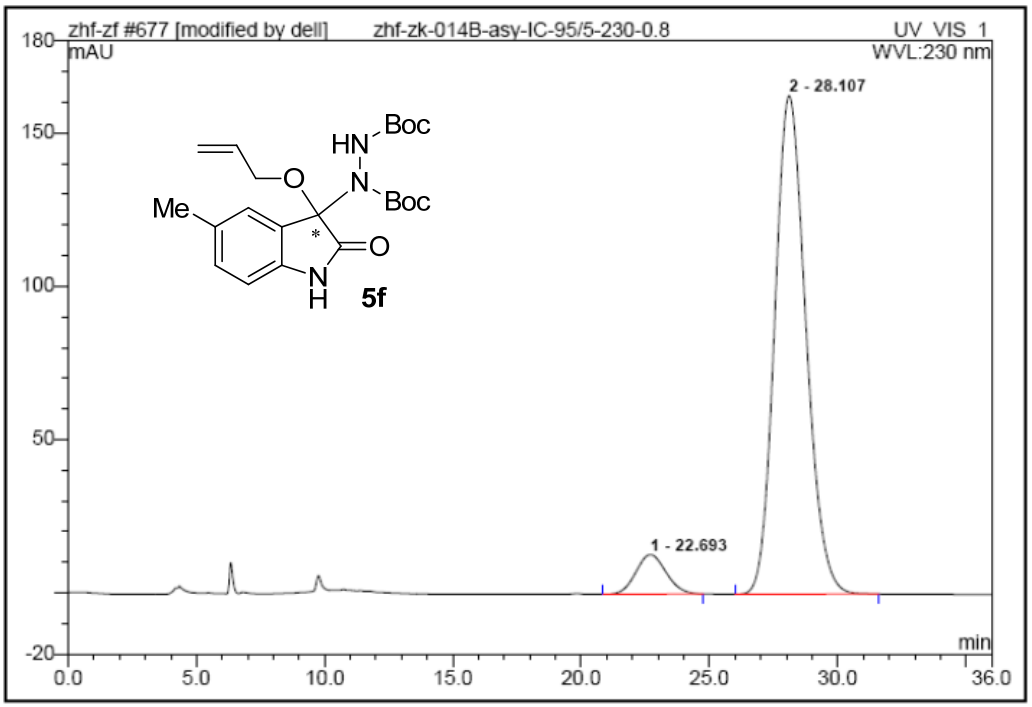

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 14.99 | n.a. | 18.341 | 26.067 | 50.25 | n.a. | BM |
| 2 | 17.98 | n.a. | 22.516 | 25.808 | 49.75 | n.a. | MB |
| Total: | | | 40.858 | 51.874 | 100.00 | 0.000 | |



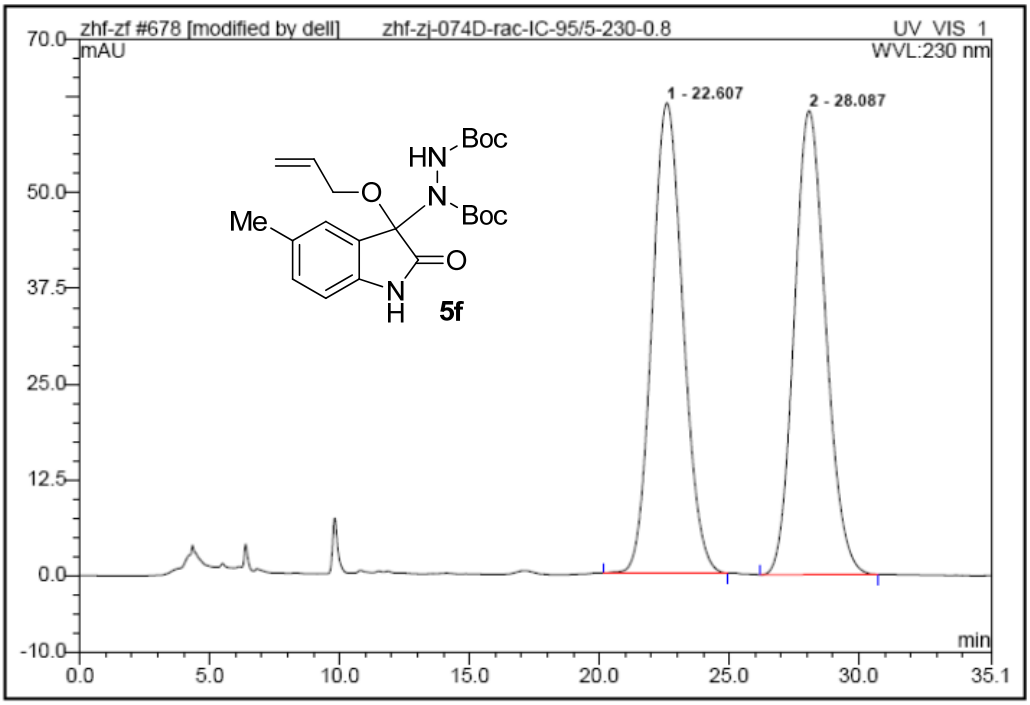

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 17.15 | n.a. | 5.745 | 9.004 | 3.45 | n.a. | BM |
| 2 | 20.25 | n.a. | 218.540 | 252.067 | 96.55 | n.a. | MB |
| Total: | | | 224.284 | 261.071 | 100.00 | 0.000 | |



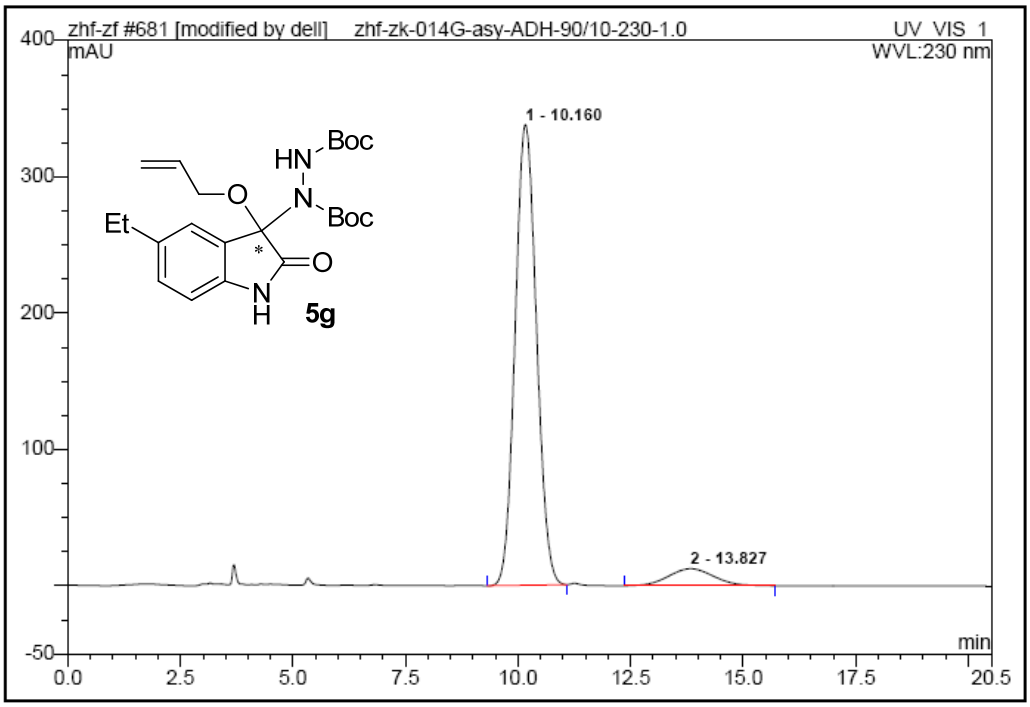

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 16.29 | n.a. | 87.152 | 116.580 | 49.91 | n.a. | BM |
| 2 | 19.73 | n.a. | 130.914 | 117.005 | 50.09 | n.a. | MB |
| Total: | | | 218.066 | 233.585 | 100.00 | 0.000 | |



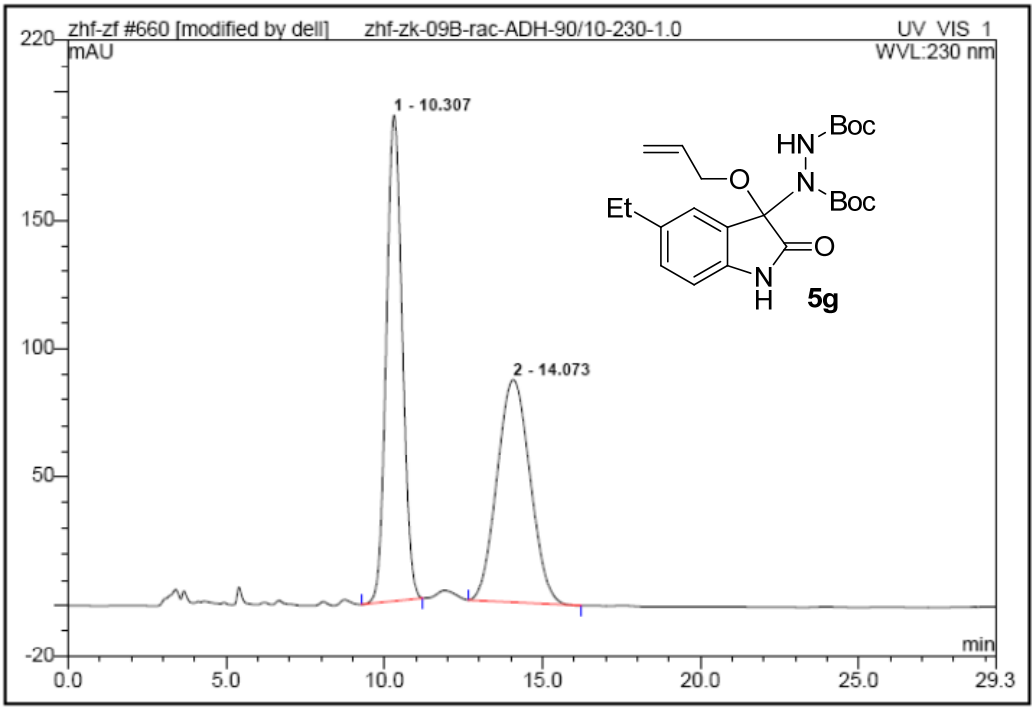

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 22.69 | n.a. | 12.899 | 17.693 | 7.17 | n.a. | BMB |
| 2 | 28.11 | n.a. | 162.572 | 229.054 | 92.83 | n.a. | BMB |
| Total: | | | 175.471 | 246.747 | 100.00 | 0.000 | |



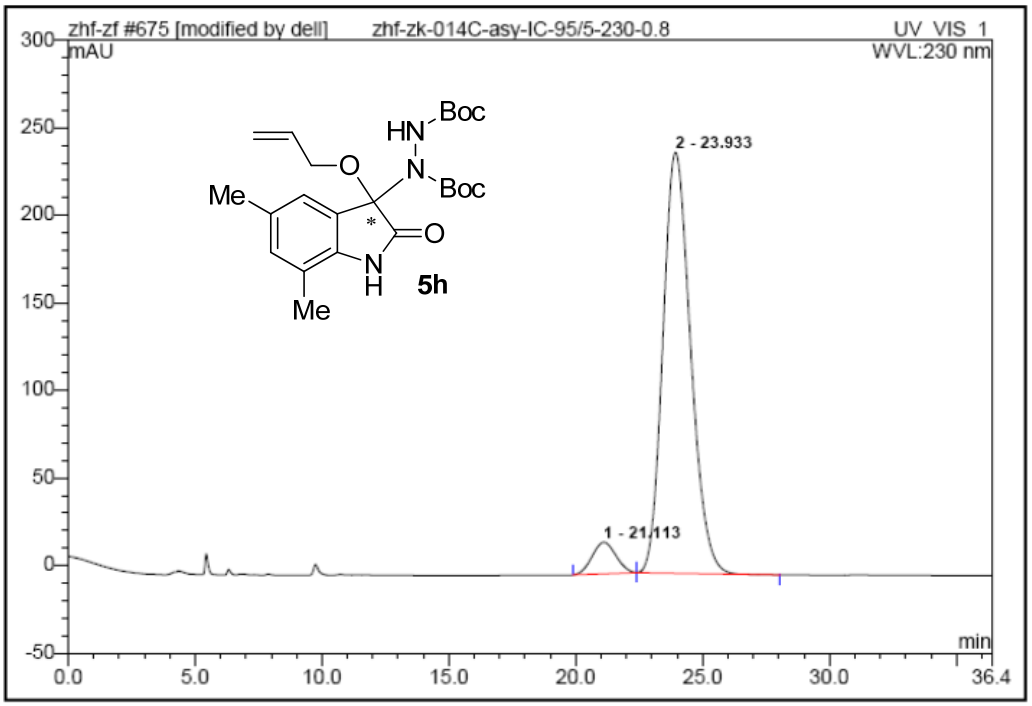

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 22.61 | n.a. | 61.443 | 84.971 | 49.91 | n.a. | BMB |
| 2 | 28.09 | n.a. | 60.623 | 85.264 | 50.09 | n.a. | BMB |
| Total: | | | 122.066 | 170.236 | 100.00 | 0.000 | |



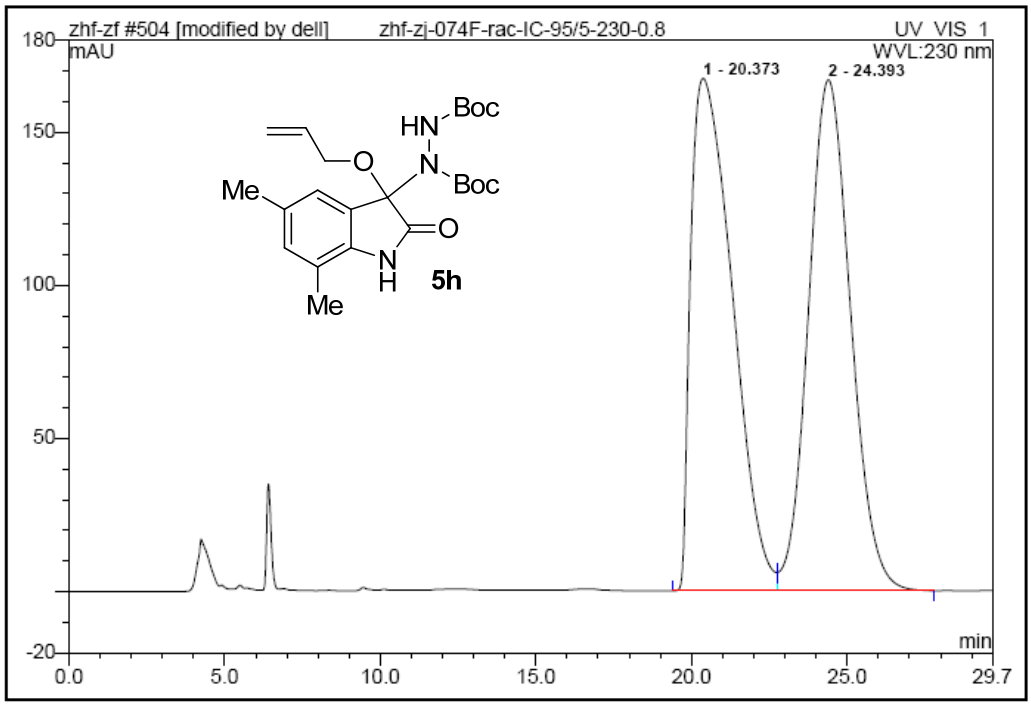

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.16 | n.a. | 337.846 | 185.775 | 92.79 | n.a. | BMB |
| 2 | 13.83 | n.a. | 12.404 | 14.430 | 7.21 | n.a. | BMB |
| Total: | | | 350.250 | 200.205 | 100.00 | 0.000 | |



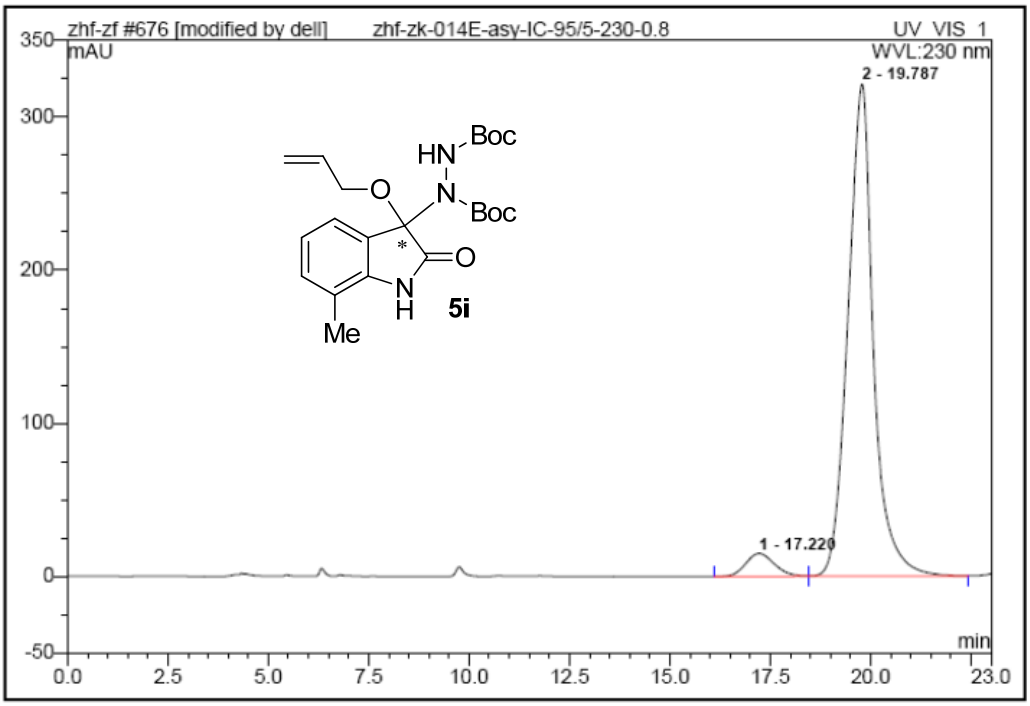

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.31 | n.a. | 189.332 | 110.144 | 51.13 | n.a. | BMB* |
| 2 | 14.07 | n.a. | 86.731 | 105.275 | 48.87 | n.a. | BMB* |
| Total: | | | 276.064 | 215.420 | 100.00 | 0.000 | |



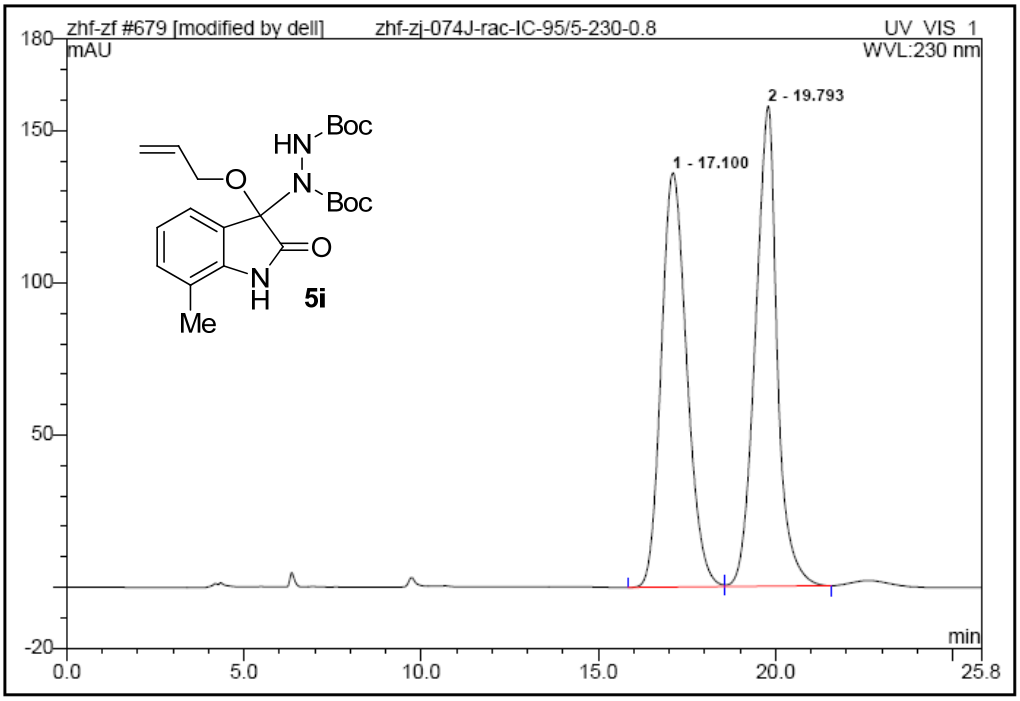

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 21.11 | n.a. | 17.981 | 19.545 | 6.05 | n.a. | BMb* |
| 2 | 23.93 | n.a. | 240.372 | 303.596 | 93.95 | n.a. | bMB* |
| Total: | | | 258.352 | 323.141 | 100.00 | 0.000 | |



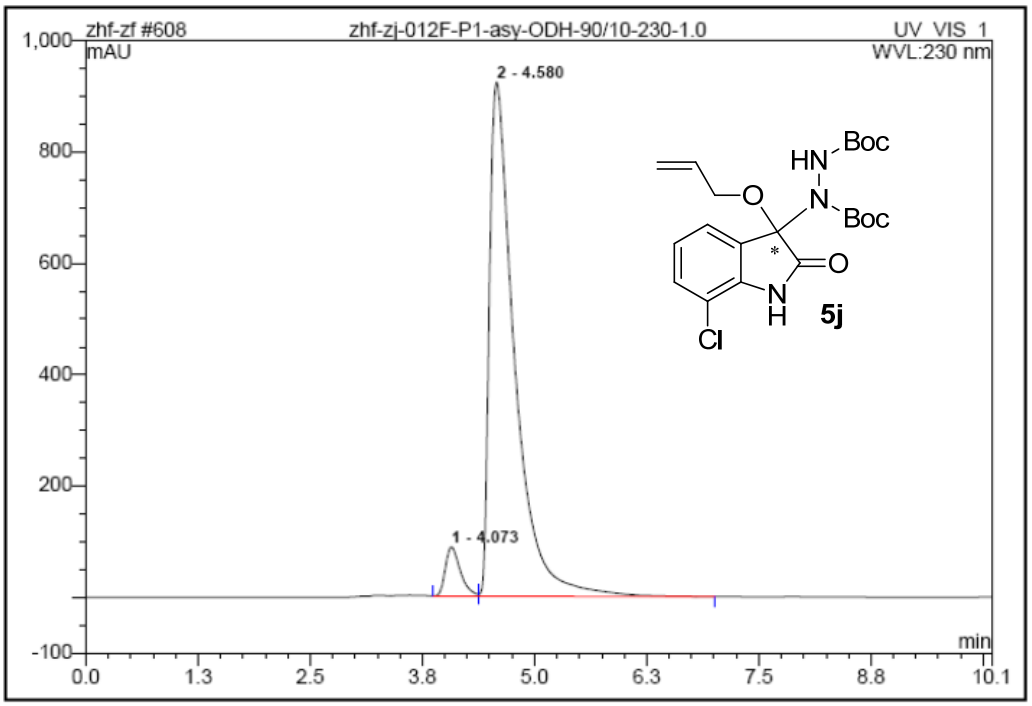

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 20.37 | n.a. | 167.356 | 259.171 | 49.72 | n.a. | BM |
| 2 | 24.39 | n.a. | 166.843 | 262.087 | 50.28 | n.a. | MB |
| Total: | | | 334.200 | 521.258 | 100.00 | 0.000 | |



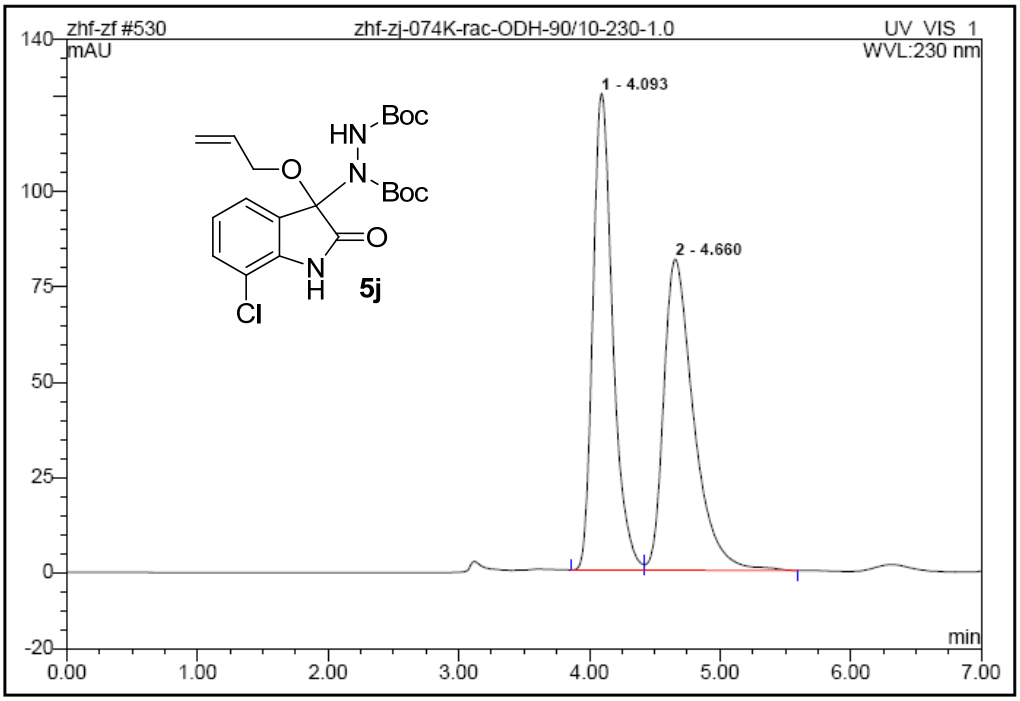

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 17.22 | n.a. | 15.062 | 12.449 | 5.02 | n.a. | BM |
| 2 | 19.79 | n.a. | 321.465 | 235.739 | 94.98 | n.a. | MB |
| Total: | | | 336.527 | 248.188 | 100.00 | 0.000 | |



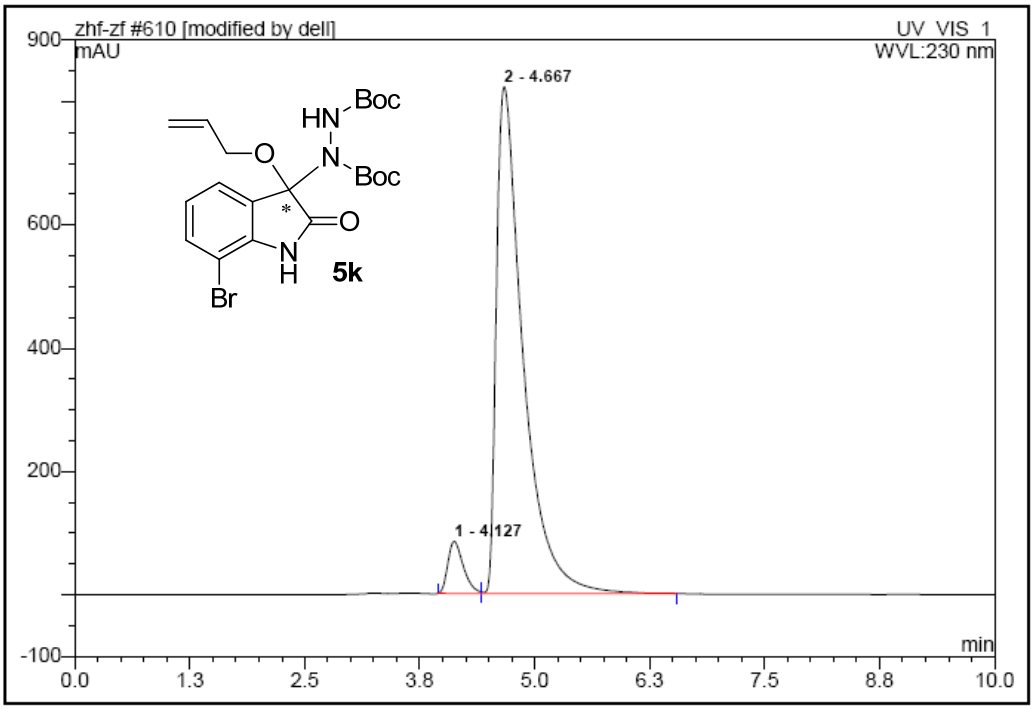

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 17.10 | n.a. | 136.017 | 113.611 | 50.17 | n.a. | BM * |
| 2 | 19.79 | n.a. | 157.763 | 112.828 | 49.83 | n.a. | MB* |
| Total: | | | 293.780 | 226.439 | 100.00 | 0.000 | |



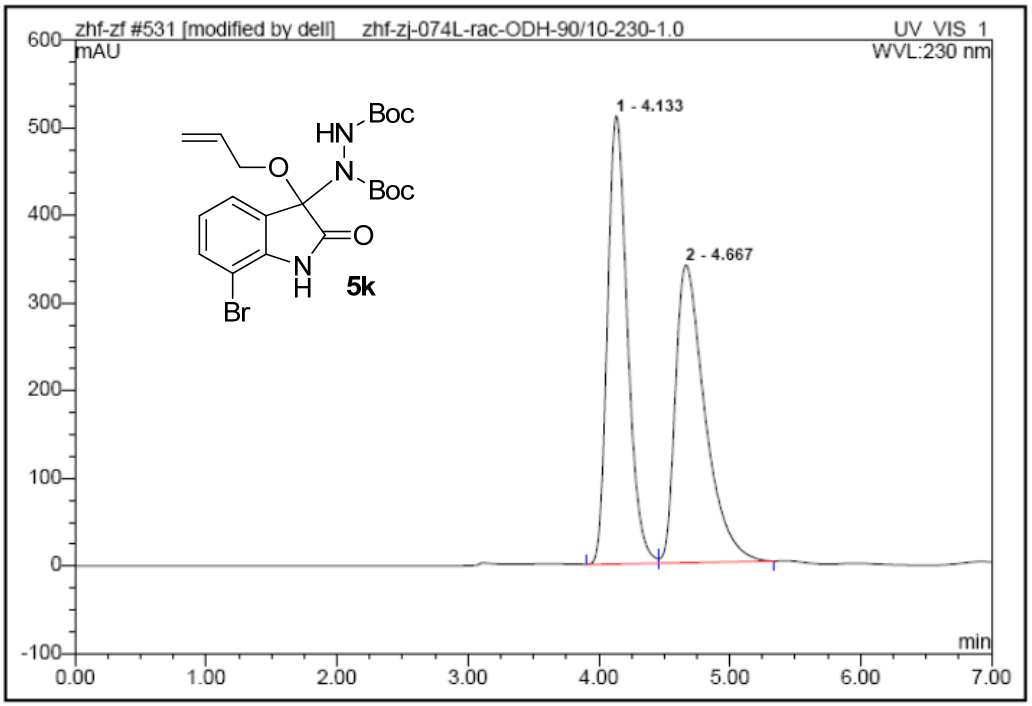

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 4.07 | n.a. | 87.851 | 17.009 | 5.33 | n.a. | BM |
| 2 | 4.58 | n.a. | 923.112 | 301.848 | 94.67 | n.a. | MB |
| Total: | | | 1010.963 | 318.857 | 100.00 | 0.000 | |



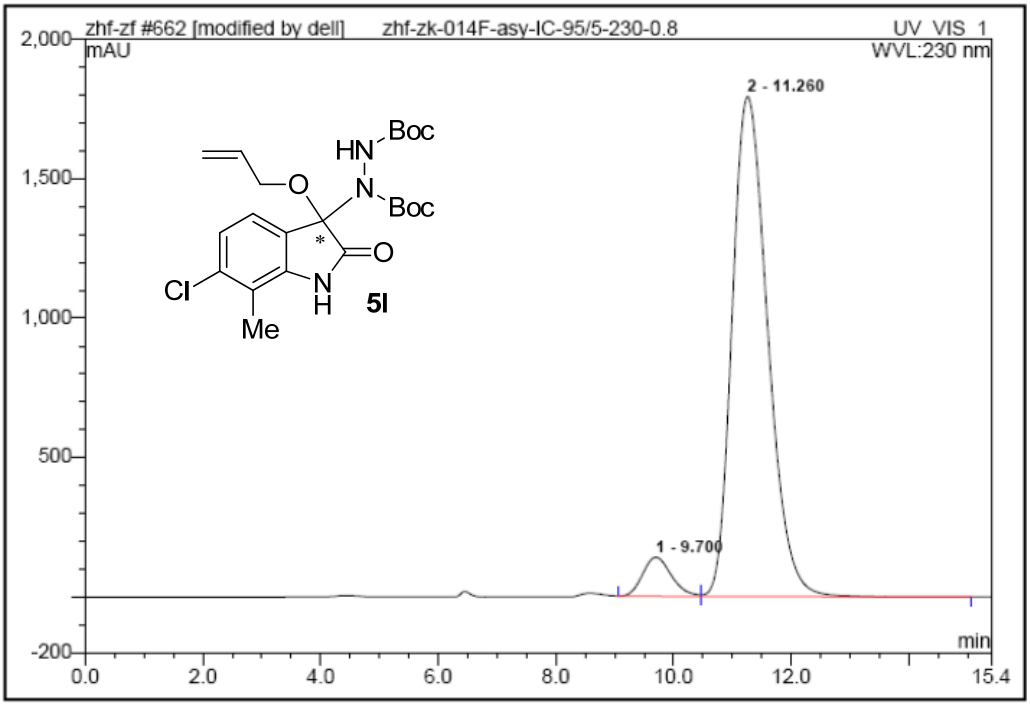

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 4.09 | n.a. | 125.245 | 22.056 | 50.33 | n.a. | BM |
| 2 | 4.66 | n.a. | 81.705 | 21.763 | 49.67 | n.a. | MB |
| Total: | | | 206.950 | 43.818 | 100.00 | 0.000 | |



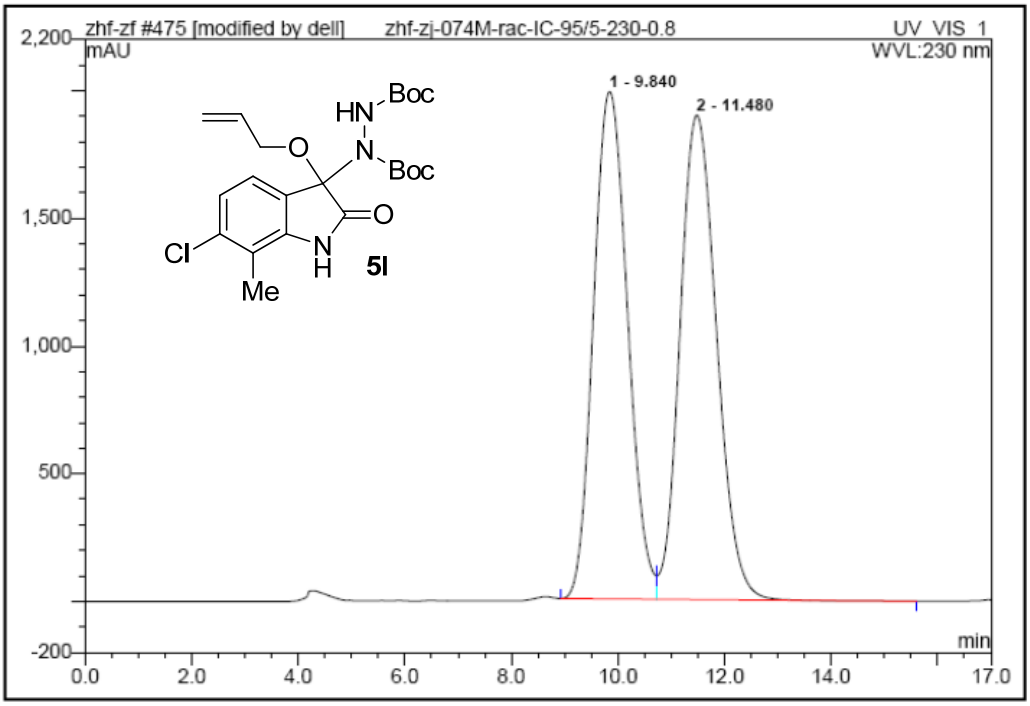

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 4.13 | n.a. | 84.437 | 16.538 | 5.64 | n.a. | BM * |
| 2 | 4.67 | n.a. | 822.473 | 276.938 | 94.36 | n.a. | MB* |
| Total: | | | 906.911 | 293.476 | 100.00 | 0.000 | |



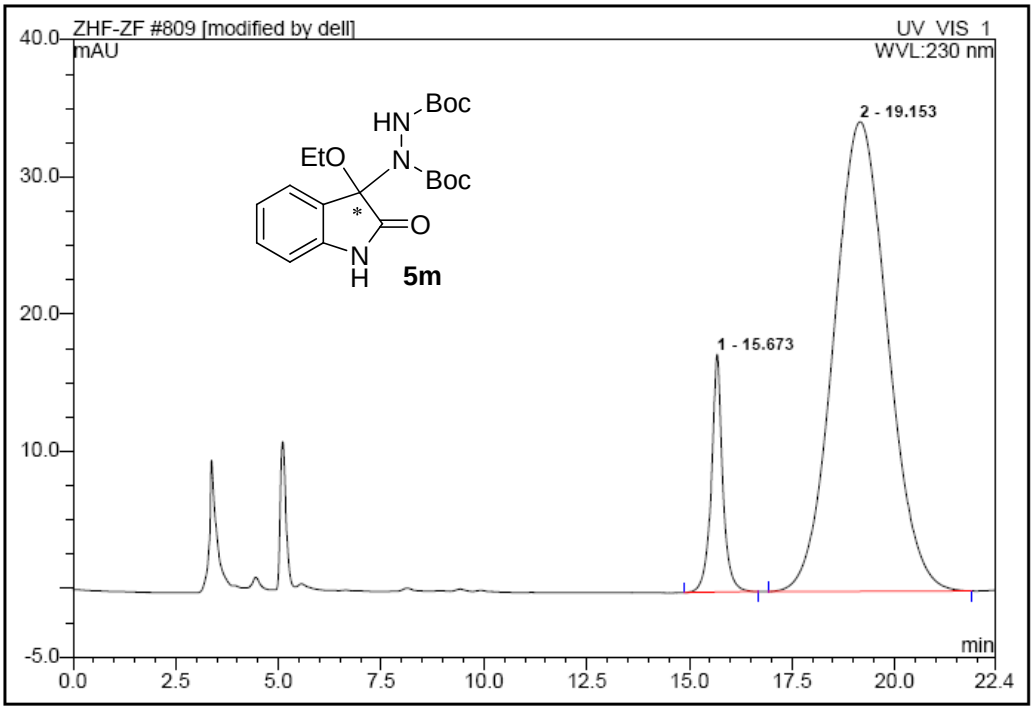

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 4.13 | n.a. | 512.001 | 90.207 | 50.34 | n.a. | BM |
| 2 | 4.67 | n.a. | 339.882 | 88.985 | 49.66 | n.a. | MB |
| Total: | | | 851.883 | 179.193 | 100.00 | 0.000 | |



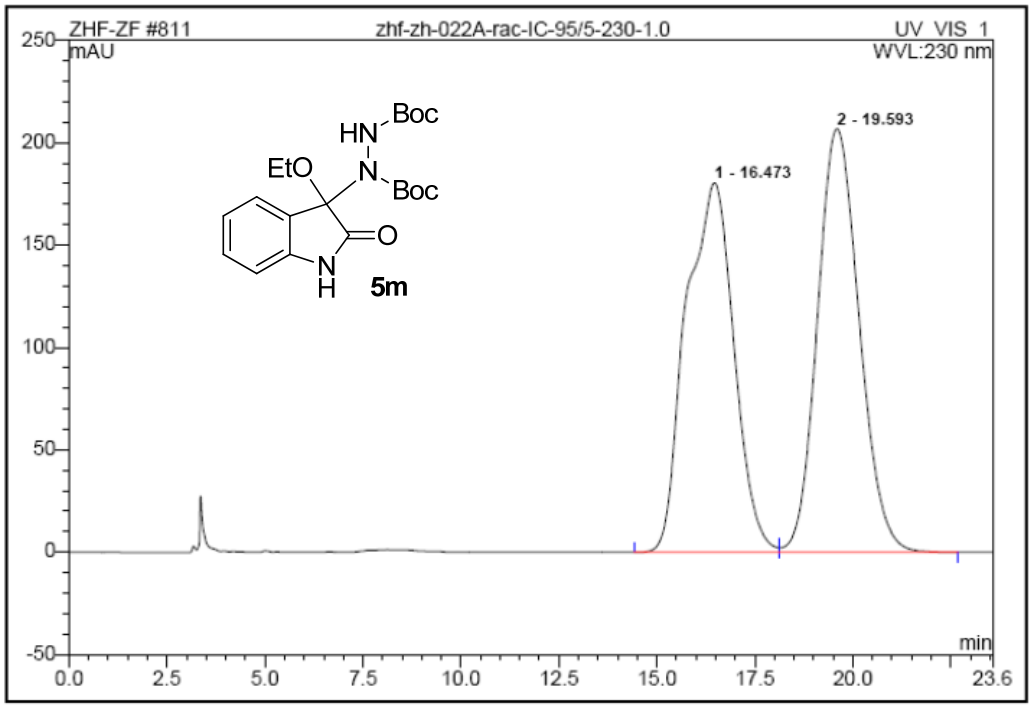

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.70 | n.a. | 140.106 | 79.294 | 5.95 | n.a. | BM * |
| 2 | 11.26 | n.a. | 1793.995 | 1252.548 | 94.05 | n.a. | MB* |
| Total: | | | 1934.101 | 1331.842 | 100.00 | 0.000 | |



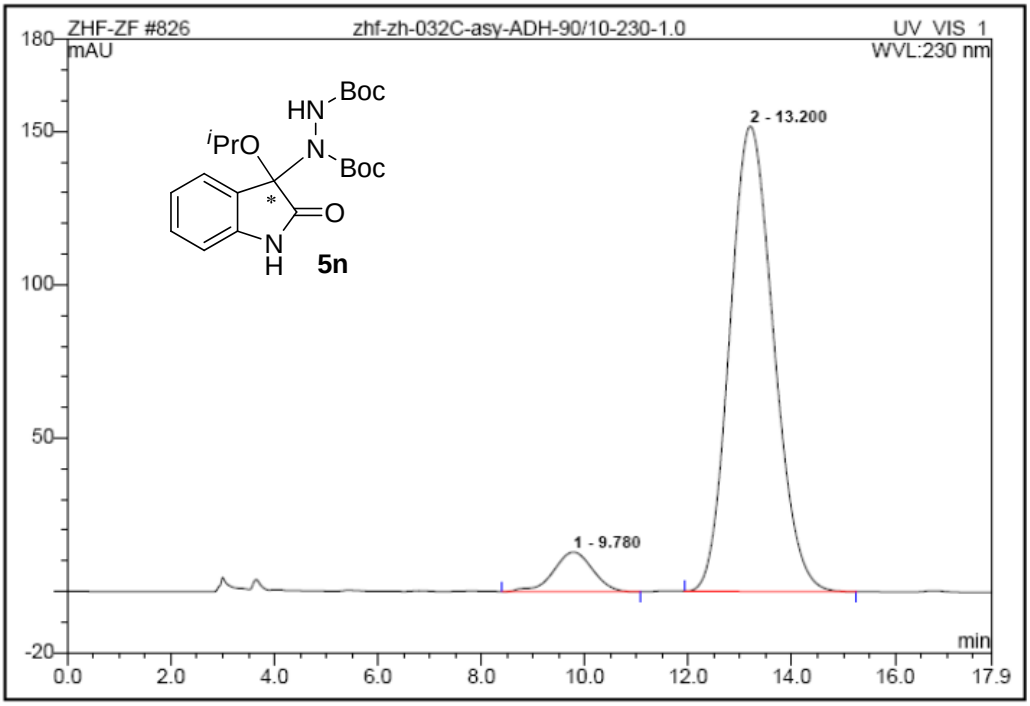

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.84 | n.a. | 1986.804 | 1475.331 | 49.42 | n.a. | BM * |
| 2 | 11.48 | n.a. | 1896.891 | 1510.250 | 50.58 | n.a. | MB* |
| Total: | | | 3883.695 | 2985.582 | 100.00 | 0.000 | |



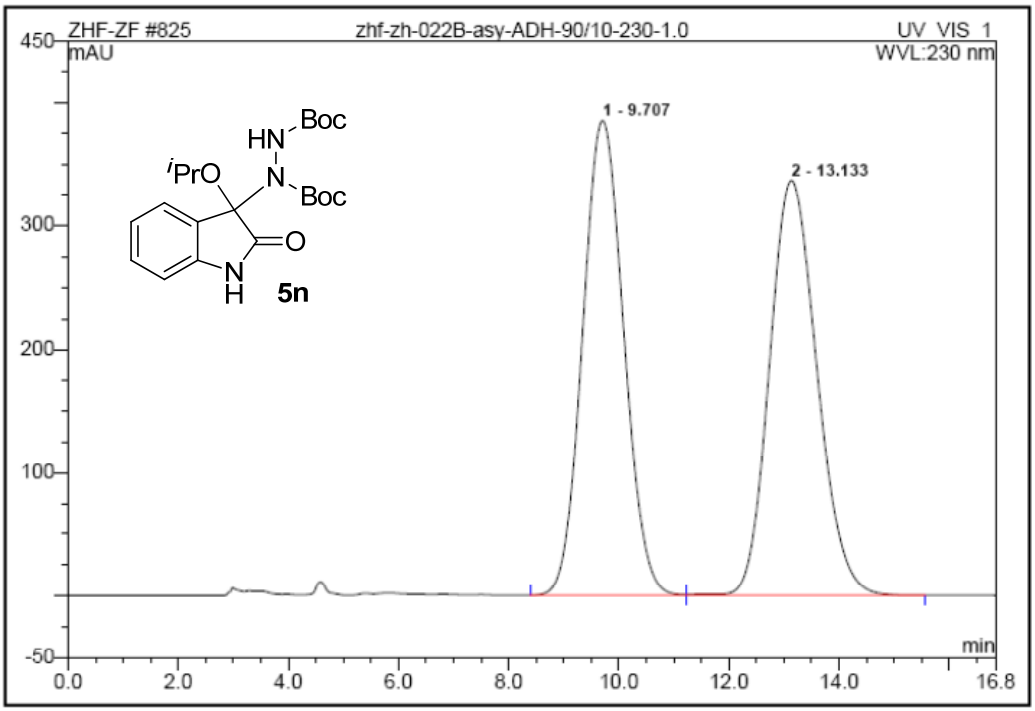

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 15.67 | n.a. | 17.343 | 5.529 | 9.62 | n.a. | BMB |
| 2 | 19.15 | n.a. | 34.234 | 51.946 | 90.38 | n.a. | BMB |
| Total: | | | 51.577 | 57.476 | 100.00 | 0.000 | |



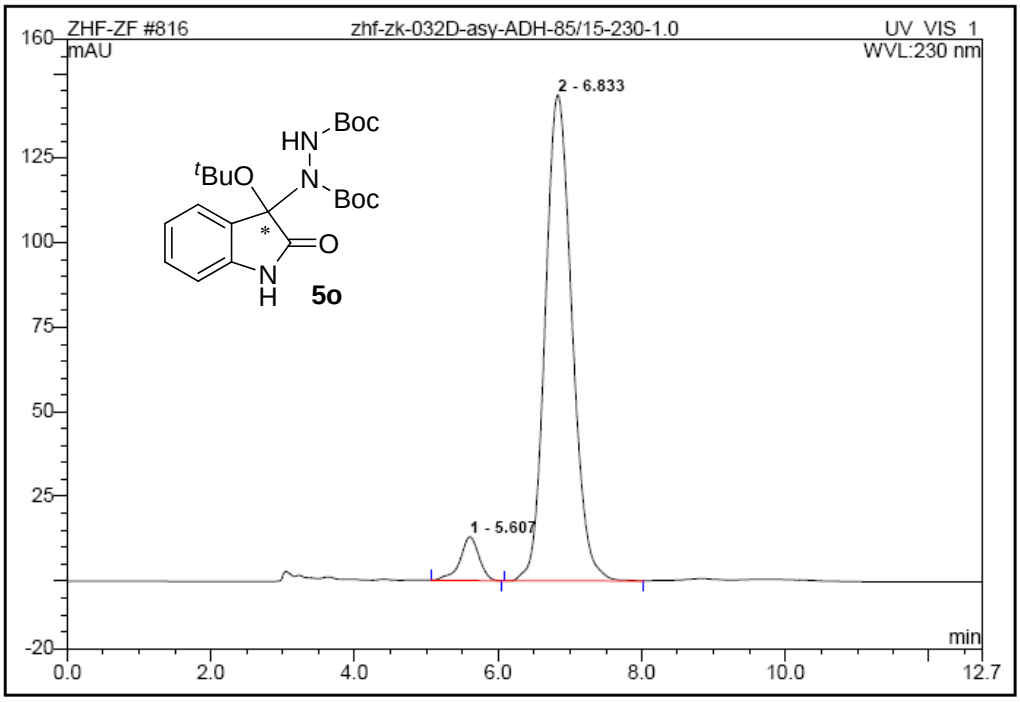

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 16.47 | n.a. | 180.407 | 255.628 | 49.98 | n.a. | BM |
| 2 | 19.59 | n.a. | 206.856 | 255.804 | 50.02 | n.a. | MB |
| Total: | | | 387.263 | 511.432 | 100.00 | 0.000 | |



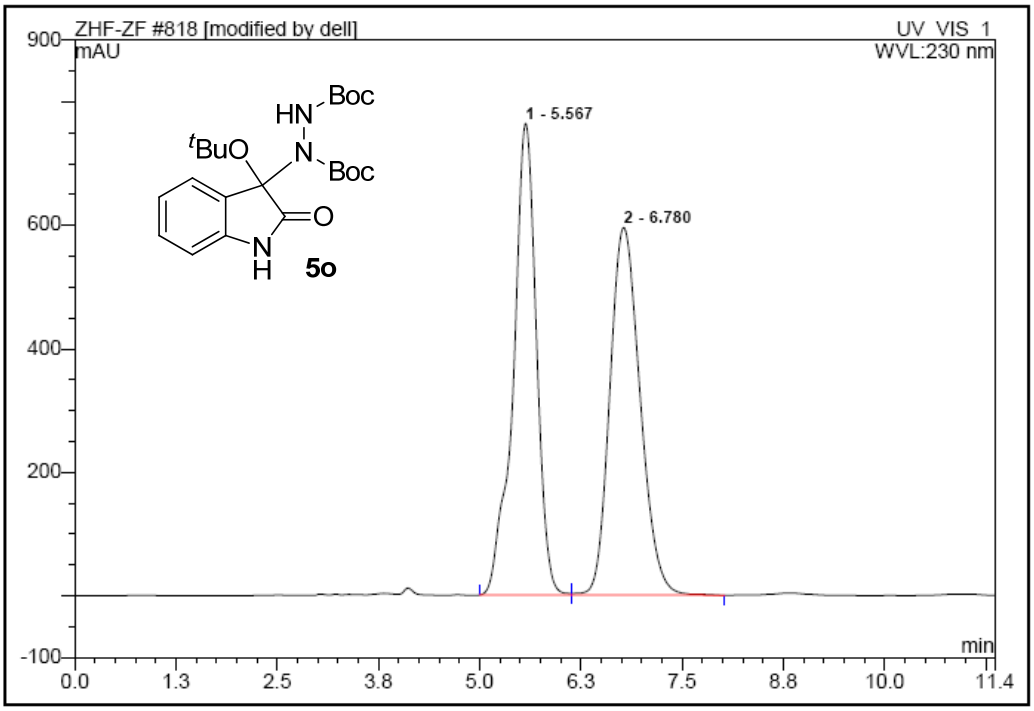

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.78 | n.a. | 12.907 | 11.376 | 7.10 | n.a. | BMB |
| 2 | 13.20 | n.a. | 151.748 | 148.788 | 92.90 | n.a. | BMB |
| Total: | | | 164.654 | 160.164 | 100.00 | 0.000 | |



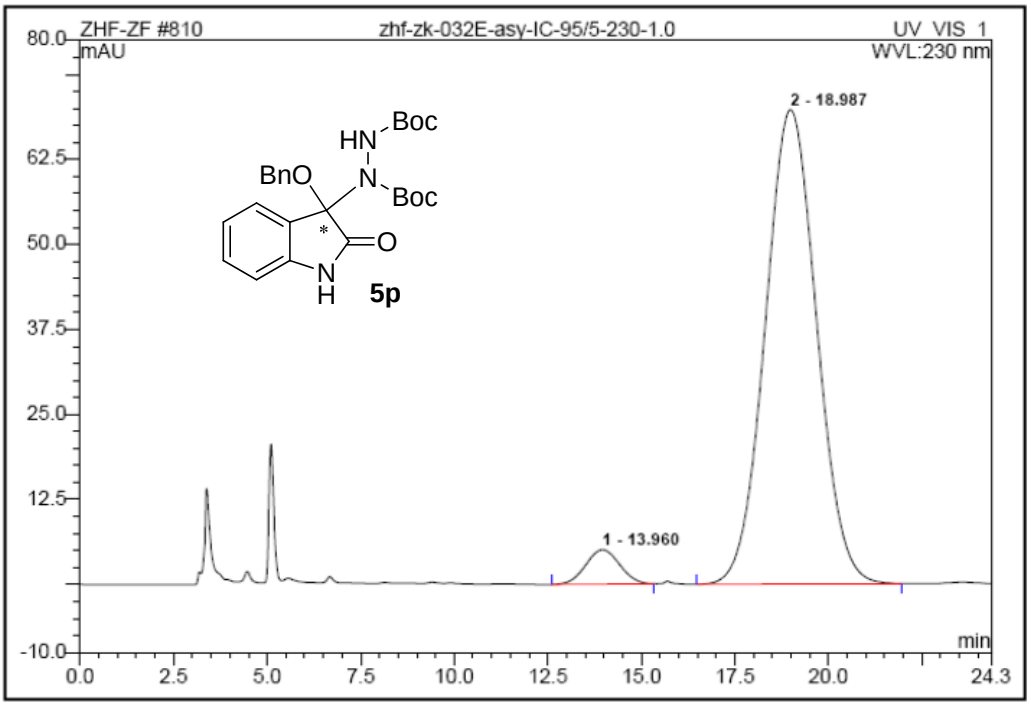

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 9.71 | n.a. | 385.170 | 332.516 | 49.75 | n.a. | BM |
| 2 | 13.13 | n.a. | 336.530 | 335.917 | 50.25 | n.a. | MB |
| Total: | | | 721.700 | 668.433 | 100.00 | 0.000 | |



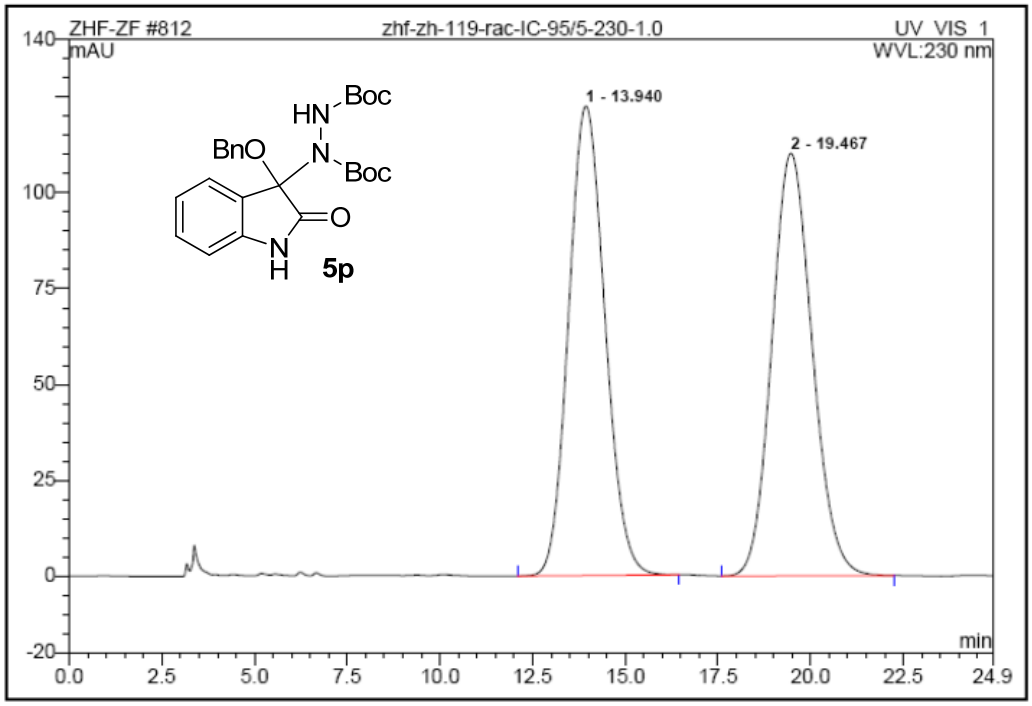

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 5.61 | n.a. | 12.922 | 4.002 | 6.08 | n.a. | BMB |
| 2 | 6.83 | n.a. | 143.632 | 61.868 | 93.92 | n.a. | BMB |
| Total: | | | 156.553 | 65.869 | 100.00 | 0.000 | |



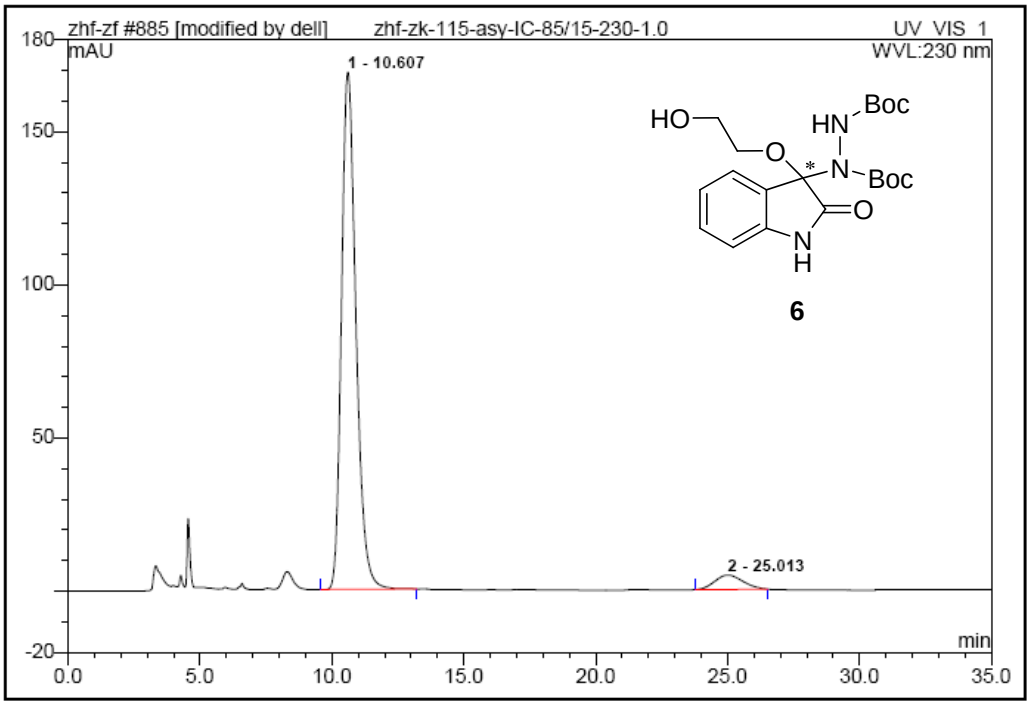

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 5.57 | n.a. | 764.115 | 252.556 | 49.45 | n.a. | BM |
| 2 | 6.78 | n.a. | 595.397 | 258.216 | 50.55 | n.a. | MB |
| Total: | | | 1359.512 | 510.773 | 100.00 | 0.000 | |



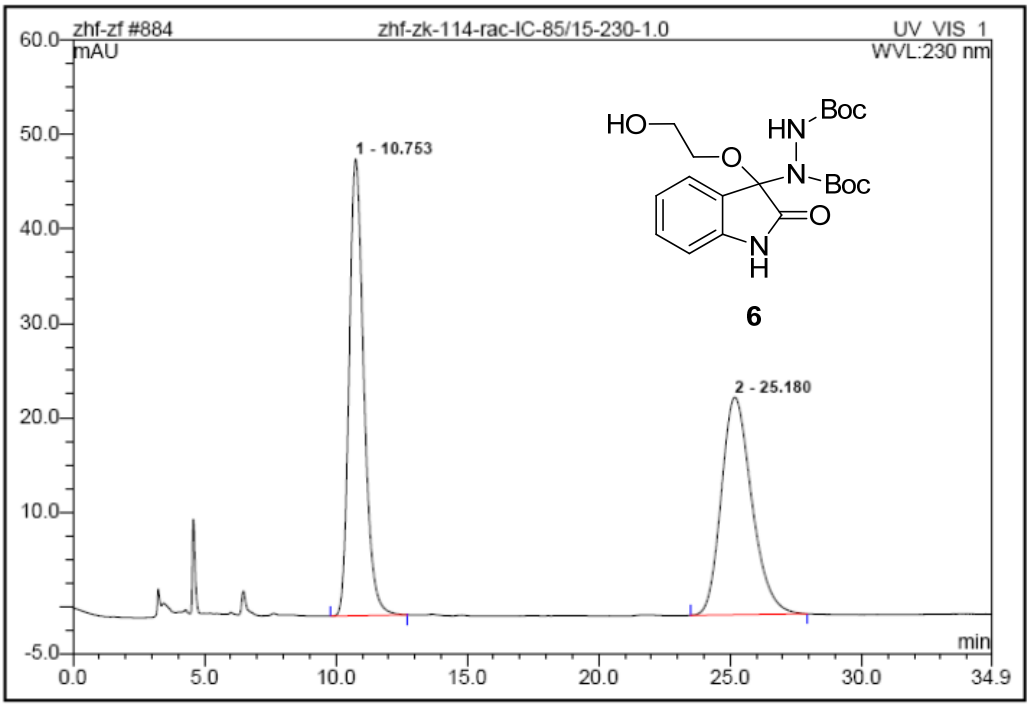

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 13.96 | n.a. | 5.050 | 5.328 | 4.58 | n.a. | BMB |
| 2 | 18.99 | n.a. | 69.719 | 110.890 | 95.42 | n.a. | BMB |
| Total: | | | 74.769 | 116.218 | 100.00 | 0.000 | |



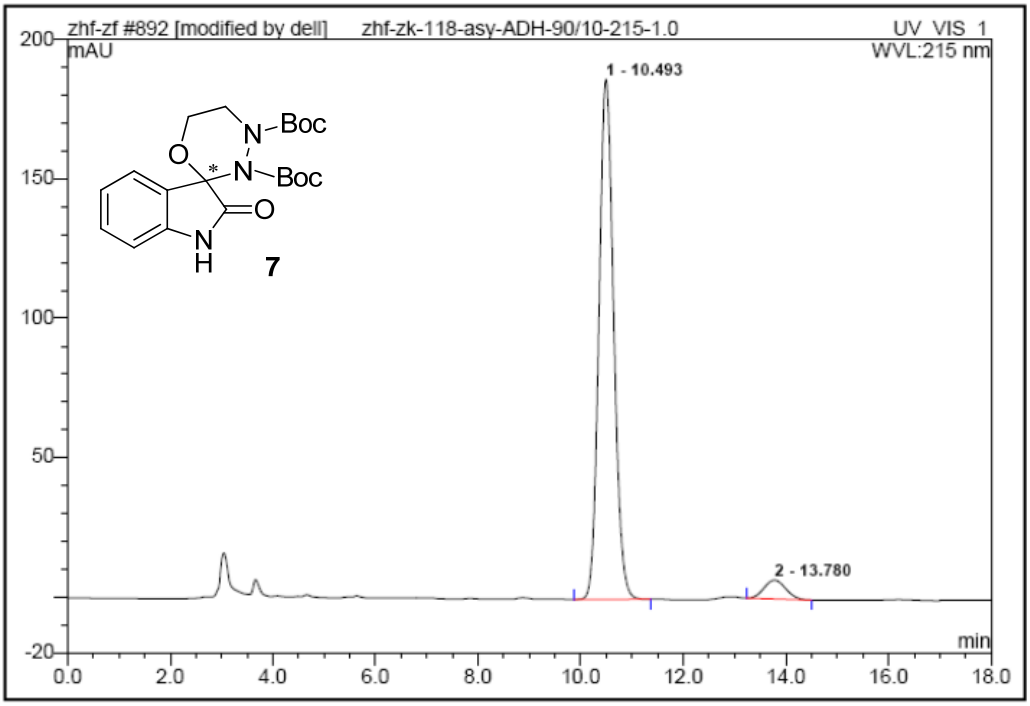

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 13.94 | n.a. | 122.578 | 139.197 | 49.95 | n.a. | BMB |
| 2 | 19.47 | n.a. | 110.320 | 139.449 | 50.05 | n.a. | BMB |
| Total: | | | 232.898 | 278.646 | 100.00 | 0.000 | |



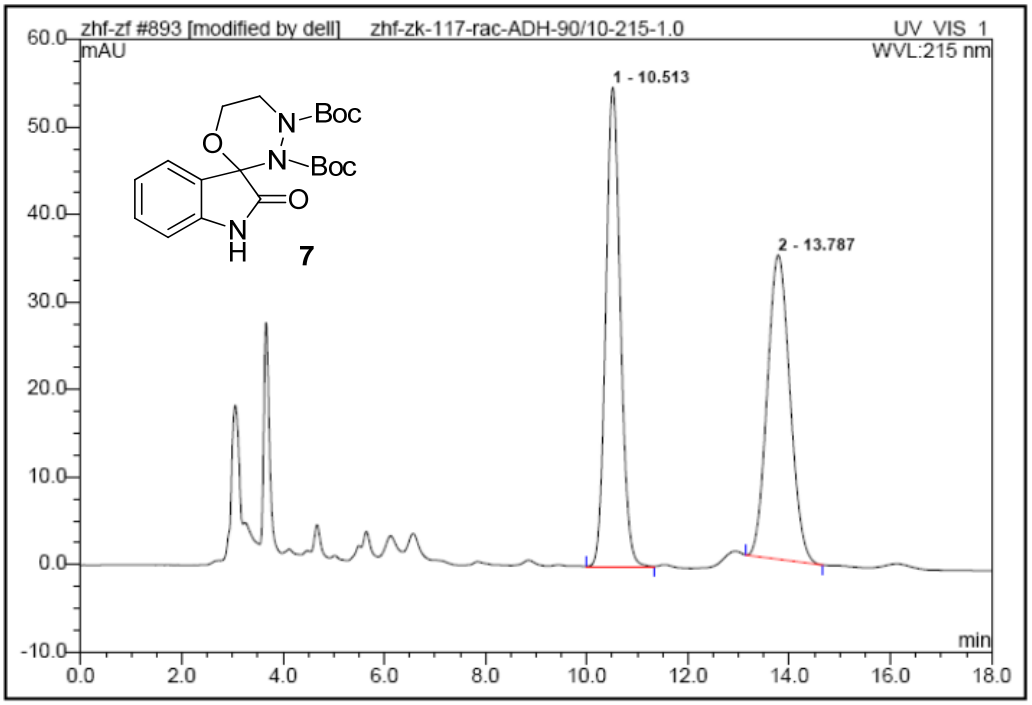

| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.61 | n.a. | 168.933 | 107.250 | 94.89 | n.a. | BMB* |
| 2 | 25.01 | n.a. | 4.675 | 5.774 | 5.11 | n.a. | BMB* |
| Total: | | | 173.608 | 113.024 | 100.00 | 0.000 | |




| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.75 | n.a. | 48.419 | 31.454 | 50.34 | n.a. | BMB |
| 2 | 25.18 | n.a. | 23.063 | 31.035 | 49.66 | n.a. | BMB |
| Total: | | | 71.482 | 62.490 | 100.00 | 0.000 | |




| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.49 | n.a. | 186.661 | 62.169 | 94.90 | n.a. | BMB |
| 2 | 13.78 | n.a. | 6.786 | 3.341 | 5.10 | n.a. | BMB |
| Total: | | | 193.448 | 65.510 | 100.00 | 0.000 | |




| No. | Ret.Time min | Peak Name | Height mAU | Area mAU*min | Rel.Area % | Amount | Type |
|---|---|---|---|---|---|---|---|
| 1 | 10.51 | n.a. | 54.772 | 18.320 | 50.40 | n.a. | BMB |
| 2 | 13.79 | n.a. | 34.784 | 18.032 | 49.60 | n.a. | BMB |
| Total: | | | 89.557 | 36.351 | 100.00 | 0.000 | |