Supporting Information

Chiral CNN Pincer Palladium(II) Complexes with 2-Aryl -6-(Oxazolinyl)pyridine Ligands: Synthesis, Characterization, and Application to Enantioselective Allylation of Isatins and Suzuki-Miyaura Coupling Reaction

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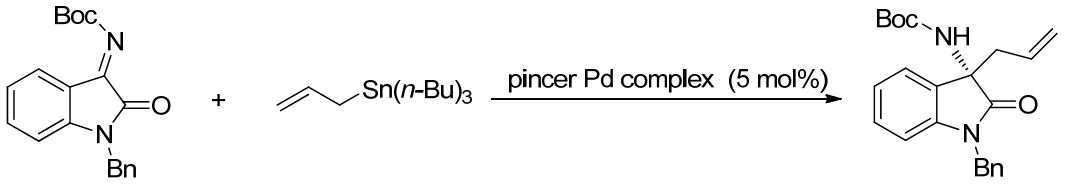
Table S1. **Summary of Crystallographic Details for Complexes 3c-f**

	3c	**3d**	**3e**·(n-hexane)	(2 x **3f**)·CH_2Cl_2
formula	$C_{20}H_{15}ClN_2OPd$	$C_{21}H_{17}ClN_2OPd$	$C_{32}H_{33}ClN_2OPd$	$C_{49}H_{36}Cl_4N_4O_2Pd_2$
Mr	441.19	455.22	603.45	1067.42
temp (K)	291(2)	291(0)	291(2)	291(2)
cryst syst	orthorhombic	monoclinic	monoclinic	orthorhombic
space group	$P2_12_12_1$	$P2_1$	$P2_1$	$P2_12_12_1$
cryst size (mm)	0.24 x 0.20 x 0.20	0.24 x 0.22 x 0.20	0.5272 x 0.3018 x 0.1313	0.20 x 0.20 x 0.18
a (Å)	10.100(2)	7.1915(2)	6.0672(6)	12.8040(4)
b (Å)	11.2001(12)	21.4390(7)	17.9824(12)	13.5812(4)
c (Å)	15.725(2)	12.2763(3)	12.2022(9)	24.3928(5)
α (deg)	90.00	90.00	90.00	90.00
β (deg)	90.00	101.495(3)	100.610(8)	90.00
γ (deg)	90.00	90.00	90.00	90.00
V ($Å^3$)	1778.9(5)	1854.79(9)	1308.54(19)	4241.75(19)
Z	4	4	2	4
D_{calcd} (g cm^{-3})	1.647	1.630	1.532	1.671
μ (mm^{-1})	1.203	1.156	0.840	1.147
θ range (deg)	3.01-26.37	3.04-26.39	3.4-26.37	3.0-26.37
index range	$-12 \le h \le 6$, $-14 \le k \le 12$, $-10 \le l \le 19$	$-8 \le h \le 8$, $-26 \le k \le 26$, $-8 \le l \le 15$	$-7 \le h \le 7$, $-22 \le k \le 22$, $-15 \le l \le 14$	$-16 \le h \le 15$, $-16 \le k \le 16$, $-28 \le l \le 30$
no. of data collected	7100	8473	11301	18581
no. of unique data	3625	6363	5355	8666
final R indices ($I > 2\sigma(I)$) R1	0.0268	0.0388	0.0442	0.0437
wR2	0.0486	0.0784	0.1121	0.0570
R indices (all data) R1	0.0311	0.0463	0.0512	0.0702
wR2	0.0504	0.0835	0.1186	0.0633
F(000)	880	912	620	2136
peak/hole ($e·Å^{-3}$)	0.243/-0.307	0.484/-0.464	0.736/-0.325	0.680/-0.458

Additional Catalytical Results on the Allylation of a Ketimine Derived from N-benzyl Isatin.

Table S2. The Asymmetric Allylation of a Ketimine Derived from N-benzyl Isatin Catalyzed by the Chiral CNN Pincer Pd(II) Complexes 3[a]

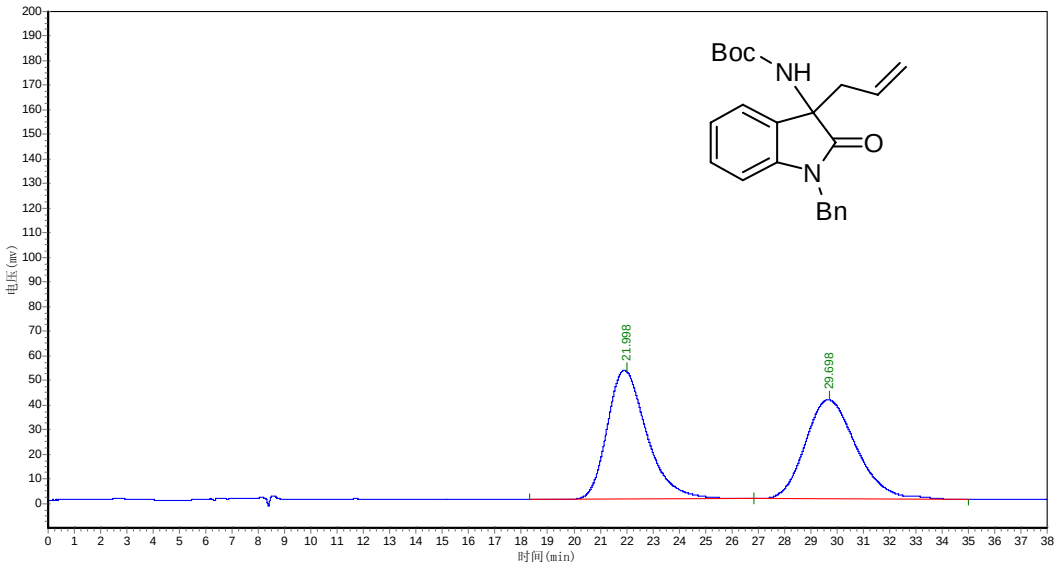


Entry	Cat.	Solvent	Temp. (°C)	Yield (%)[b]	*ee* (%)[c,d]
1	**3b**	CH_2Cl_2	-60	0	--
2	**3b**	CH_2Cl_2	RT	98	39
3	**3b**	CH_2Cl_2	-10	77	51
4	**3b**	THF	-10	85	0
5[e]	**3b**	CH_2Cl_2	-30	80	58
6[e]	**3e**	CH_2Cl_2	-30	84	69
7[e,f]	**3e**	CH_2Cl_2	-30	81	9
8[e]	**3e**	CH_2Cl_2	-40	53	72
9[e]	**3e**	CH_2Cl_2	-50	37	72

[a]Reaction conditions: ketimine (0.20 mmol), allyltributyltin (0.30 mmol), cat. **3** (5 mol %), solvent (1 mL), 12 h. [b]Isolated yields. [c]Determined by chiral HPLC. [d]The absolute configuration of the product was assigned to be *S* by comparison of optical rotation with that in the literature (*Chem. Eur. J.* **2013**, *19*, 7304). [e]36 h. [f]Allyltrimethylsilane (0.30 mmol) as the allyl source in the presence of AgF (0.20 mmol) as an additive.

(*S*)-tert-Butyl (3-allyl-1-benzyl-2-oxoindolin-3-yl)carbamate: White solid (40.1 mg, 0.106 mmol; 53%). The enantiomeric excess was determined on a Daicel Chiralpak AS-H column with hexane/2-propanol = 90/10, flow = 0.5 mL/min, and detected at a UV wave length of 254 nm. Retention times: 22.2 min (major), 29.4 min, 72% *ee*. $[\alpha]_D^{20}$ = -8.5 (*c* 1.000, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (d, *J* = 7.3 Hz, 2H, ArH), 7.30 (t, *J* = 7.3 Hz, 2H, ArH), 7.25 (d, *J* = 6.6 Hz, 2H, ArH), 7.16 (t, *J* = 7.5 Hz, 1H, ArH), 7.02 (t, *J* = 7.4 Hz, 1H, ArH), 6.70 (d, *J* = 7.7 Hz, 1H, ArH), 5.76-5.65 (m, 1H, CH_2CH=CH_2),

5.25-5.17 (m, 4H, NCH_2, CH_2CH=CH_2), 4.76 (br s, 1H, NH), 2.66-2.61 (m, 1H, CH_2CH=CH_2), 2.52-2.47 (m, 1H, CH_2CH=CH_2), 1.26 (s, 9H, $C(CH_3)_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 176.8, 153.8, 142.3, 135.9, 130.1, 128.7, 128.6, 127.5, 127.4, 122.7, 122.5, 121.5, 109.2, 80.4, 60.9, 44.1, 42.3, 42.0, 28.1.



PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
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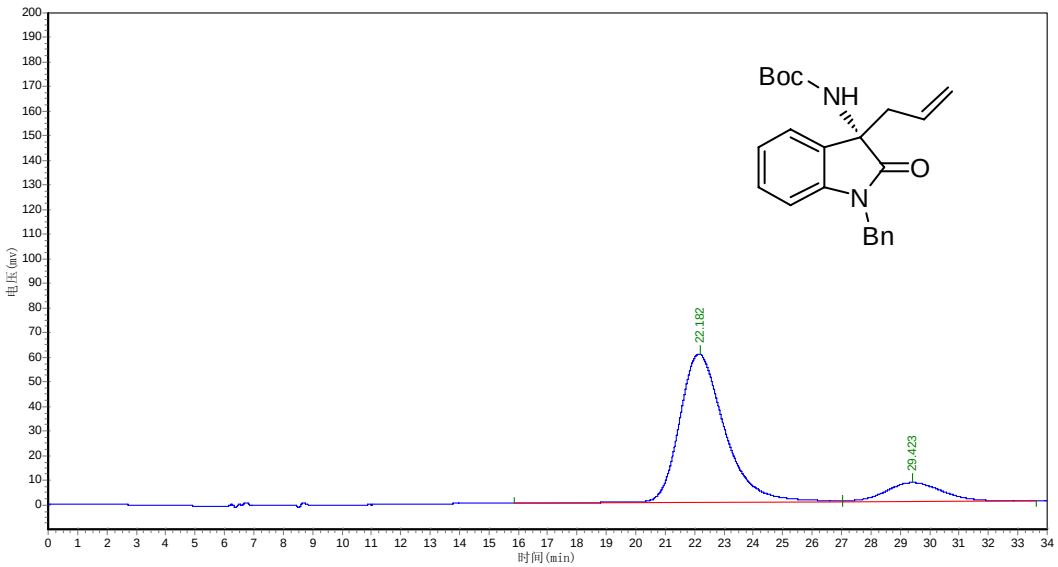
2	29.698	40321.773	5447492.500	49.6497



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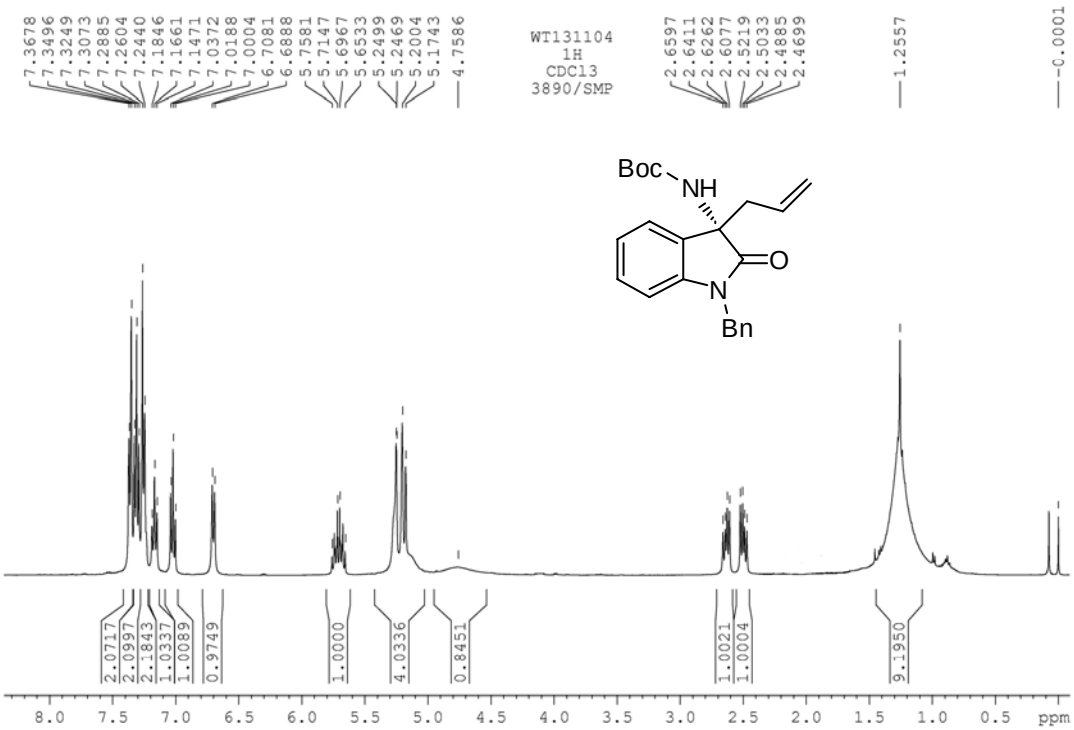
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7.1661
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7.0188
7.0004
6.7081
6.6888
5.7581
5.7147
5.6967
5.6533
5.2499
5.2469
5.2004
5.1743
4.7586
WT131104
1H
CDCl3
3890/SMP
2.6597
2.6411
2.6262
2.6077
2.5219
2.5033
2.4885
2.4699
1.2557
0.0001
Boc
NH
O
N
Bn
2.0717
2.0997
2.1843
1.0337
1.0089
0.9749
1.0000
4.0336
0.8451
1.0021
1.0004
9.1950
8.0
7.5
7.0
6.5
6.0
5.5
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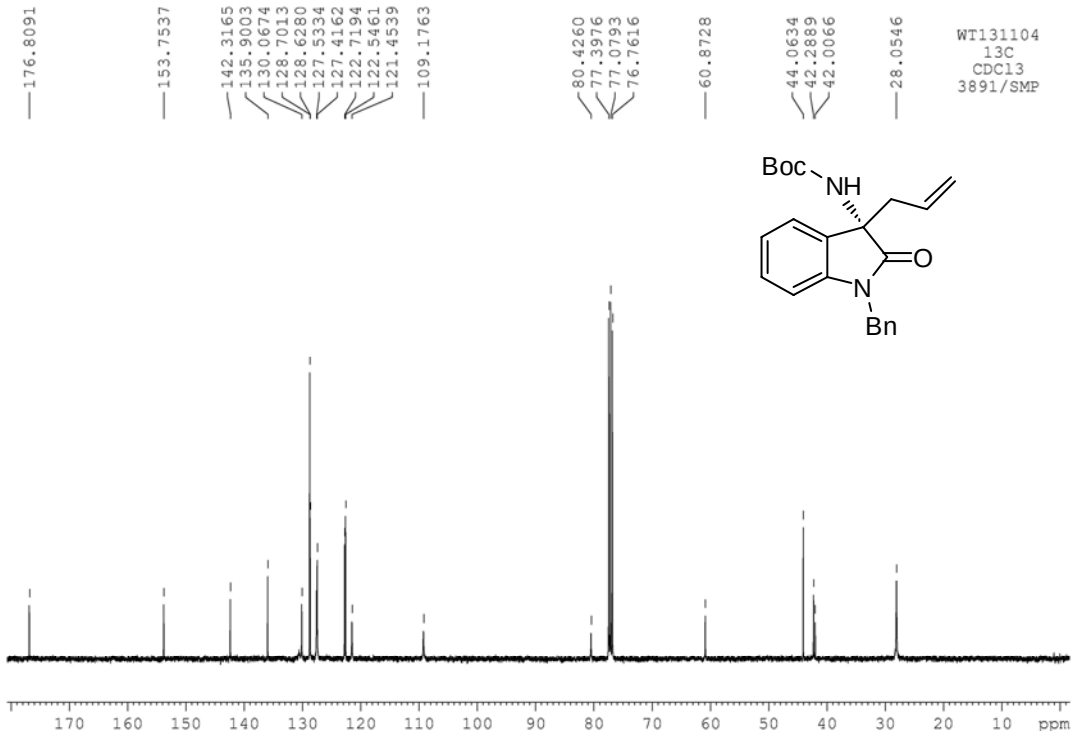
3.0
2.5
2.0
1.5
1.0
0.5
ppm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135.9003
130.0674
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128.6280
127.5334
127.4162
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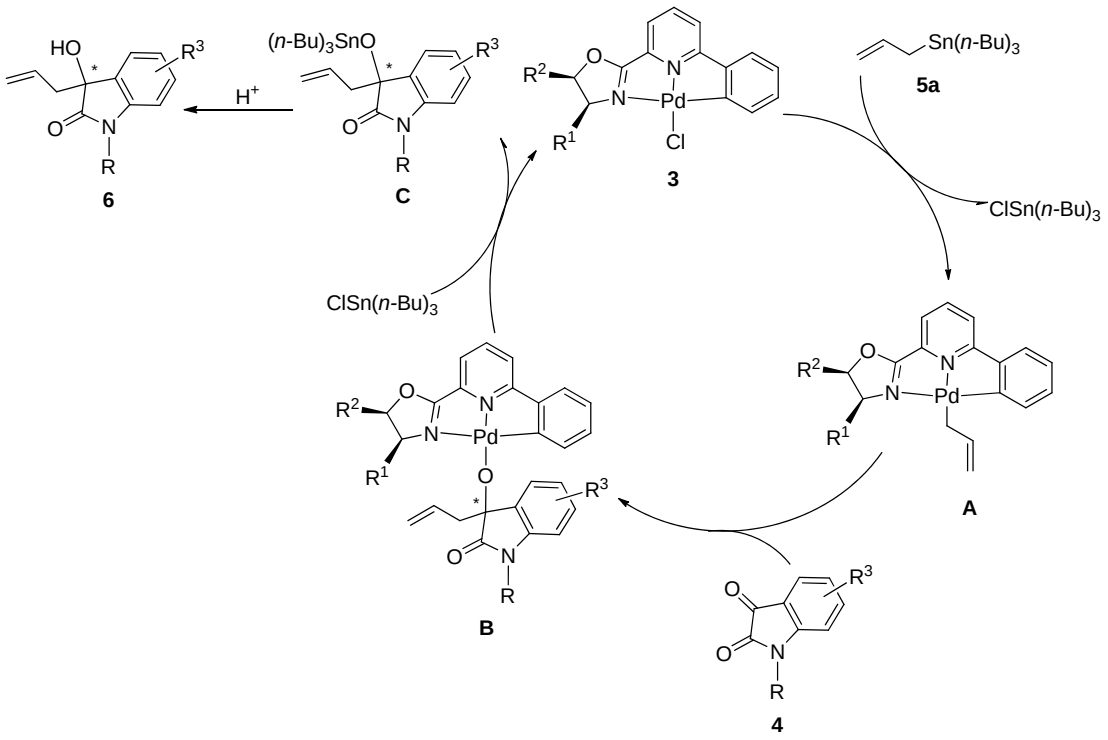
122.5461
121.4539
109.1763
80.4260
77.3976
77.0793
76.7616
60.8728
44.0634
42.2889
42.0066
28.0546
WT131104
13C
CDCl3
3891/SMP
Boc
NH
O
N
Bn
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Proposed Reaction Cycle for the Asymmetric Allylation of Isatins Catalyzed by the Chiral CNN Pincer Pd(II) Complexes 3. A catalytic cycle (Scheme S1) for the allylation of isatins with allyltributyltin catalyzed by the chiral CNN pincer Pd(II) complexes **3** is proposed based on the related literature reports.[1] The chloride on the Pd(II) complex **3** reacts with allyltributyltin to give an η^1-allyl palladium(II) complex **A**. Then the nucleophilic reaction of allyl-palladium species **A** with isatin results in the intermediate **B**, which subsequently undergoes transmetallation with chlorotributyltin giving complex **C** and regenerating the pincer Pd(II) catalyst **3**. Finally, further acidification of the complex **C** affords the 3-allyl-3-hydroxyoxindole product **6**.

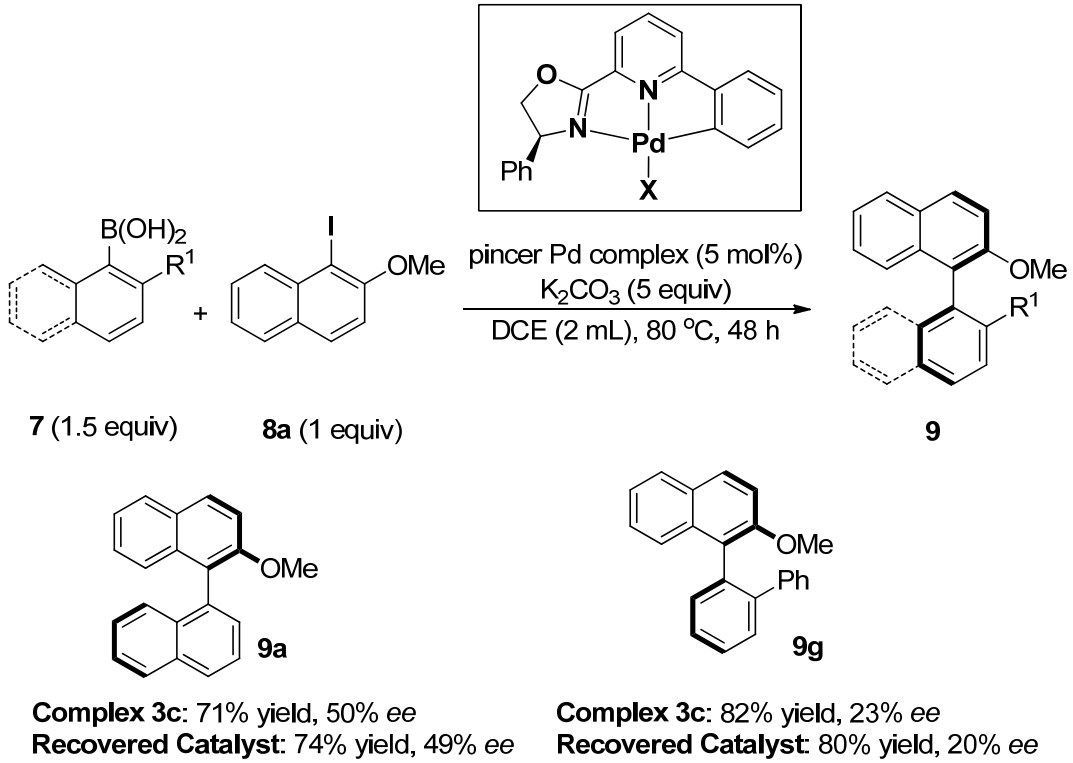


Scheme S1. Proposed Reaction Cycle for the Asymmetric Allylation of Isatins Catalyzed by the Chiral CNN Pincer Pd(II) Complexes 3

References

(1) (a) Nakamura, S.; Hyodo, K.; Nakamura, M.; Nakane, D.; Masuda, H. *Chem. Eur. J.* **2013**, *19*, 7304. (b) Li, J.; Minnaard, A. J.; Klein Gebbink, R. J. M.; van Koten, G. *Tetrahedron Lett.* **2009**, *50*, 2232. (c) Aydin, J.; Kumar, K. S.; Sayah, M. J.; Wallner, O. A.; Szabó, K. J. *J. Org. Chem*. **2007**, *72*, 4689. (d) Yao, Q.; Sheets, M. *J. Org. Chem.* **2006**, *71*, 5384. (e) Solin, N.; Kjellgren, J.; Szabó, K. J. *J. Am. Chem. Soc*. **2004**, *126*, 7026.

Proposed Mechanism of Asymmetric Suzuki-Miyaura Reaction. To gain some insights into the mechanism of Suzuki-Miyaura reaction catalyzed by the chiral CNN pincer Pd(II) complexes **3**, the recycling of the catalyst was investigated. It was found that the catalyst could be recovered when preparative TLC on silica gel plates was performed to isolate the axially chiral biaryl products. In the couplings of 1-iodo-2-methoxynaphthalene with 1-naphthaleneboronic acid and 2-phenylbenzeneboronic acid, the recovered catalyst exhibited comparable activity and enantioselectivities (Scheme S2). The NMR spectra of the recovered catalyst are very similar to those of the CNN-PdCl complex **3c**, but not the same. Although satisfactory elemental analysis of the recovered catalyst was not obtained (ESI-MS did not provide useful information, either), it was tentatively identified as the corresponding CNN-PdI complex on the basis of the NMR spectra and literature report.[2] In addition, palladium blacking out was not observed throughout the reaction process. The above results suggest that the current asymmetric Suzuki-Miyaura reaction may include a Pd(II)-Pd(IV) catalytic cycle instead of a Pd(0)-Pd(II) cycle, as reported by Iwasa and Nishiyama in the NCN bis(oxazolinyl)phenyl pincer Pd(II)-catalyzed Suzuki-Miyaura reaction.[2]

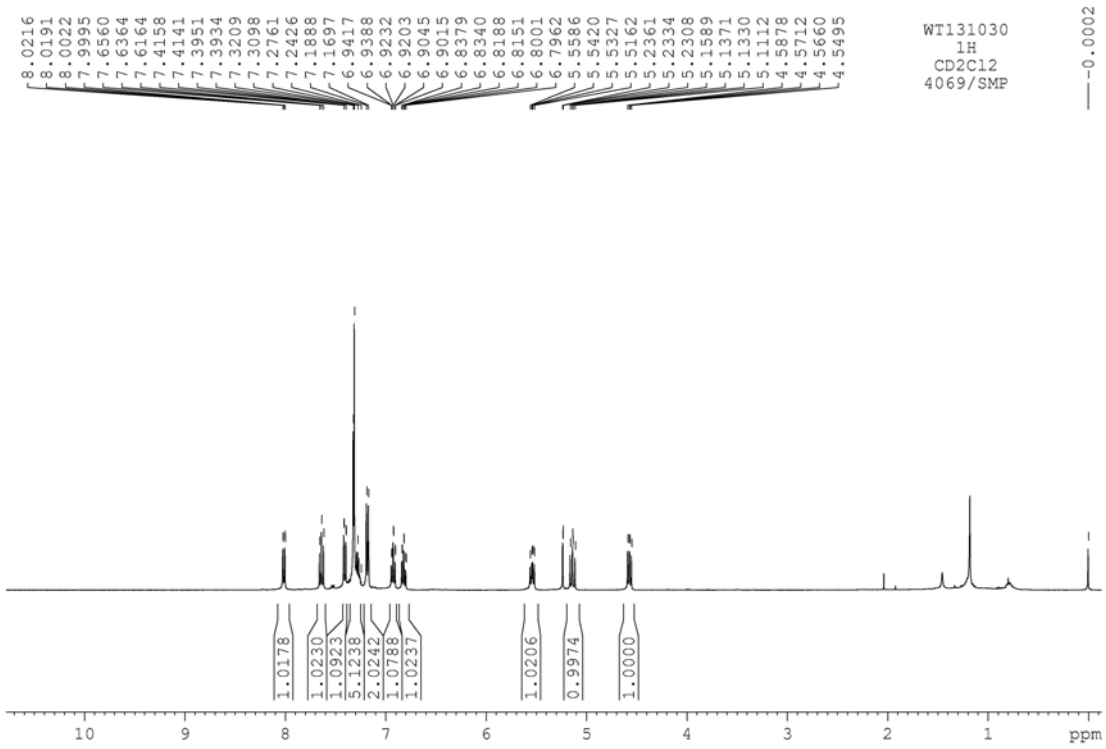


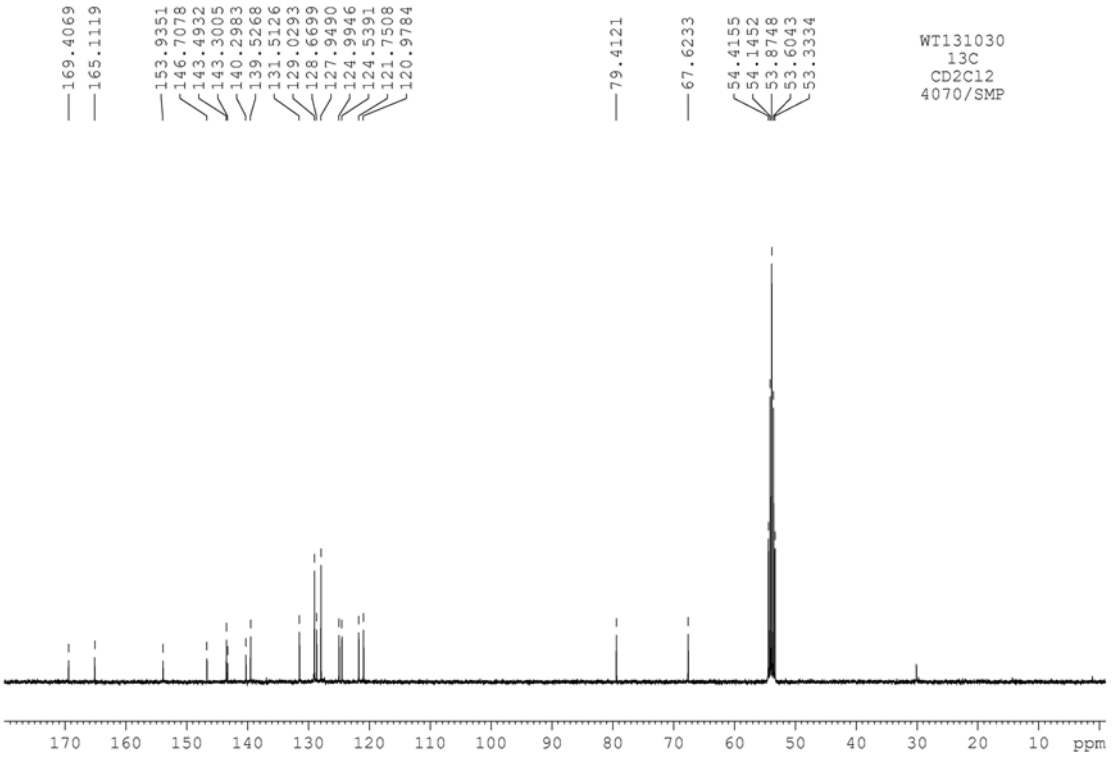
Scheme S2.

Reference

(2) Takemoto, T.; Iwasa, S.; Hamada, H.; Shibatomi, K.; Kameyama, M.; Motoyama, Y.; Nishiyama, H. *Tetrahedron Lett.* **2007**, *48*, 3397.

Recovered catalyst: ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.01 (dd, *J* = 1.0, 7.8 Hz, 1H, ArH), 7.64 (t, *J* = 7.8 Hz, 1H, ArH), 7.40 (dd, *J* = 0.7, 8.3 Hz, 1H, ArH), 7.32-7.24 (m, 5H, ArH), 7.18 (d, *J* = 7.6 Hz, 2H, ArH), 6.92 (dt, *J* = 1.2, 7.4 Hz, 1H, ArH), 6.82 (dt, *J* = 1.6, 7.6 Hz, 1H, ArH), 5.54 (dd, *J* = 6.6, 10.4 Hz, 1H, OxH), 5.13 (dd, *J* = 8.7, 10.4 Hz, 1H, OxH), 4.57 (dd, *J* = 6.6, 8.7 Hz, 1H, OxH). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 169.4, 165.1, 153.9, 146.7, 143.4, 143.3, 140.3, 139.5, 131.5, 129.0, 128.7, 127.9, 125.0, 124.5, 121.8, 121.0, 79.4, 67.6.





Characterization Data of the Known Catalysis Products

(*S*)-3-Allyl-1-benzyl-3-hydroxyindolin-2-one (6a): White solid (52.5 mg, 0.188 mmol; 94%). M.p.: 147-149 ^{o}C. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 0.8 mL/min, and detected at a UV wave length of 254 nm. Retention times: 13.5 min, 21.6 min (major), 78% *ee*. $[\alpha]_D^{20}$ = -1.4 (*c* 0.908, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (dd, *J* = 0.6, 7.3 Hz, 1H, ArH), 7.31-7.24 (m, 5H, ArH), 7.21-7.16 (m, 1H, ArH), 7.07-7.03 (m, 1H, ArH), 6.68 (d, *J* = 7.8 Hz, 1H, ArH), 5.65-5.54 (m, 1H, CH_2CH=CH_2), 5.14-5.05 (m, 2H, CH_2CH=CH_2), 5.01 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 4.70 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 3.76 (br s, 1H, OH), 2.85-2.81 (m, 1H, CH_2CH=CH_2), 2.74-2.69 (m, 1H, CH_2CH=CH_2).

(*S*)-3-Allyl-3-hydroxyindolin-2-one (6d): White solid (34.1 mg, 0.180 mmol; 90%). M.p.: 124-125 ^{o}C. The enantiomeric excess was determined on a Daicel Chiralcel OD-H column

with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 9.4 min (major), 12.0 min, 60% *ee*. $[\alpha]_D^{20}$ = +99.7 (*c* 0.464, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70 (br s, 1H, NH), 7.35 (d, *J* = 7.3 Hz, 1H, ArH), 7.26-7.22 (m, 1H, ArH), 7.08-7.04 (m, 1H, ArH), 6.87 (d, *J* = 7.8 Hz, 1H, ArH), 5.69-5.58 (m, 1H, CH_2CH=CH_2), 5.11-5.07 (m, 2H, CH_2CH=CH_2), 3.82 (br s, 1H, OH), 2.77-2.72 (m, 1H, CH_2CH=CH_2), 2.63-2.58 (m, 1H, CH_2CH=CH_2).

(*S*)-3-Allyl-3-hydroxy-1-methylindolin-2-one (6e): White solid (36.6 mg, 0.180 mmol; 90%). M.p.: 150-152 ^{o}C. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 95/5, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 16.2 min, 17.8 min (major), 82% *ee*. $[\alpha]_D^{20}$ = -17.5 (*c* 0.634, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, *J* = 7.3 Hz, 1H, ArH), 7.31 (t, *J* = 7.7 Hz, 1H, ArH), 7.09 (t, *J* = 7.5 Hz, 1H, ArH), 6.81 (d, *J* = 7.8 Hz, 1H, ArH), 5.66-5.56 (m, 1H, CH_2CH=CH_2), 5.10-5.05 (m, 2H, CH_2CH=CH_2), 3.70 (br s, 1H, OH), 3.15 (s, 3H, CH_3), 2.78-2.73 (m, 1H, CH_2CH=CH_2), 2.65-2.59 (m, 1H, CH_2CH=CH_2).

(*S*)-3-Allyl-1-benzyl-3-hydroxy-5-methylindolin-2-one (6j): White solid (55.7 mg, 0.190 mmol; 95%). M.p.: 148-150 ^{o}C. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 8.2 min, 14.7 min (major), 86% *ee*. $[\alpha]_D^{20}$ = -10.4 (*c* 0.432, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.22 (m, 6H, ArH), 6.98 (dd, *J* = 0.9, 8.0 Hz, 1H, ArH), 6.57 (d, *J* = 8.0 Hz, 1H, ArH), 5.67-5.56 (m, 1H, CH_2CH=CH_2), 5.17-5.07 (m, 2H, CH_2CH=CH_2), 4.98 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 4.69 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 3.40 (br s, 1H, OH), 2.83-2.78 (m, 1H, CH_2CH=CH_2), 2.73-2.68 (m, 1H, CH_2CH=CH_2), 2.30 (s, 3H, CH_3).

(*S*)-3-Allyl-3-hydroxy-1,5-dimethylindolin-2-one (6l): White solid (40.8 mg, 0.188 mmol; 94%). M.p.: 145-147 ^{o}C. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 7.3 min, 10.9 min (major), 85% *ee*. $[\alpha]_D^{20}$ = -5.9 (*c* 0.732, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (s, 1H, ArH), 7.11 (d, *J* = 7.8 Hz, 1H, ArH), 6.70 (d, *J* = 7.9 Hz, 1H, ArH), 5.66-5.56 (m, 1H, CH_2CH=CH_2), 5.12-5.05 (m, 2H, CH_2CH=CH_2), 3.64 (br s, 1H, OH), 3.13 (s, 3H, NCH_3), 2.76-2.71 (m, 1H, CH_2CH=CH_2), 2.65-2.59 (m, 1H, CH_2CH=CH_2), 2.34 (s, 3H, CH_3).

(*S*)-3-Allyl-1-benzyl-3-hydroxy-5-methoxyindolin-2-one (6m): White solid (56.9 mg, 0.184 mmol; 92%). M.p.: 150-151 ^{o}C. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 14.8 min, 20.9 min (major), 81% *ee*. $[\alpha]_D^{20}$ = -3.5 (*c* 0.958, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.21 (m, 5H, ArH), 7.02 (d, *J* = 2.5 Hz, 1H, ArH), 6.69 (dd, *J* = 2.6, 8.5 Hz, 1H, ArH), 6.56 (d, *J* = 8.5 Hz, 1H, ArH), 5.64-5.54 (m, 1H, CH_2CH=CH_2), 5.15-5.05 (m, 2H, CH_2CH=CH_2), 4.96 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 4.65 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 4.04 (br s, 1H, OH), 3.73 (s, 3H, OCH_3), 2.85-2.80 (m, 1H, CH_2CH=CH_2), 2.75-2.70 (m, 1H, CH_2CH=CH_2).

(*S*)-3-Allyl-1-benzyl-5-fluoro-3-hydroxyindolin-2-one (6n): White solid (56.5 mg, 0.190 mmol; 95%). M.p.: 126-127 ^{o}C. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 10.7 min, 14.3 min (major), 76% *ee*. $[\alpha]_D^{20}$ = -5.5 (*c* 0.930, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.23 (m, 5H, ArH), 7.14 (dd, *J* = 2.6, 7.6 Hz, 1H, ArH), 6.89-6.84 (m, 1H, ArH), 6.58 (dd, *J* = 4.0, 8.6 Hz, 1H,

ArH), 5.63-5.53 (m, 1H, CH_2CH=CH_2), 5.15-5.07 (m, 2H, CH_2CH=CH_2), 4.97 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 4.67 (d, *J* = 15.8 Hz, 1H, CH_2Ph), 4.15 (br s, 1H, OH), 2.85-2.80 (m, 1H, CH_2CH=CH_2), 2.74-2.69 (m, 1H, CH_2CH=CH_2).

(*S*)-3-Allyl-1-benzyl-5-chloro-3-hydroxyindolin-2-one (6o): White solid (57.7 mg, 0.184 mmol; 92%). M.p.: 117-119 ^oC. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 9.8 min, 14.8 min (major), 80% *ee*. $[\alpha]_D^{20}$ = -14.5 (*c* 0.408, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (d, *J* = 2.0 Hz, 1H, ArH), 7.32-7.23 (m, 5H, ArH), 7.15 (dd, *J* = 2.1, 8.3 Hz, 1H, ArH), 6.59 (d, *J* = 8.3 Hz, 1H, ArH), 5.66-5.55 (m, 1H, CH_2CH=CH_2), 5.17-5.10 (m, 2H, CH_2CH=CH_2), 4.98 (d, *J* = 15.8 Hz, 1H, CH_2Ph), 4.70 (d, *J* = 15.8 Hz, 1H, CH_2Ph), 3.57 (br s, 1H, OH), 2.82-2.78 (m, 1H, CH_2CH=CH_2), 2.72-2.67 (m, 1H, CH_2CH=CH_2).

(*S*)-3-Allyl-1-benzyl-5-bromo-3-hydroxyindolin-2-one (6q): White solid (63.8 mg, 0.178 mmol; 89%). M.p.: 121-123 ^oC. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 11.4 min, 17.7 min (major), 80% *ee*. $[\alpha]_D^{20}$ = -12.4 (*c* 0.696, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (d, *J* = 1.9 Hz, 1H, ArH), 7.31-7.22 (m, 6H, ArH), 6.54 (d, *J* = 8.3 Hz, 1H, ArH), 5.63-5.52 (m, 1H, CH_2CH=CH_2), 5.16-5.09 (m, 2H, CH_2CH=CH_2), 4.96 (d, *J* = 15.7 Hz, 1H, CH_2Ph), 4.66 (d, *J* = 15.8 Hz, 1H, CH_2Ph), 3.83 (br s, 1H, OH), 2.83-2.78 (m, 1H, CH_2CH=CH_2), 2.73-2.68 (m, 1H, CH_2CH=CH_2).

(*S*)-3-Allyl-1-benzyl-6-bromo-3-hydroxyindolin-2-one (6r): White solid (65.9 mg, 0.184 mmol; 92%). M.p.: 152-155 ^oC. The enantiomeric excess was determined on a Daicel

Chiralpak AD-H column with hexane/2-propanol = 95/5, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 24.3 min, 27.6 min (major), 70% *ee*. $[\alpha]_D^{20}$ = -3.0 (*c* 0.968, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.23 (m, 6H, ArH), 7.18 (dd, *J* = 1.6, 7.9 Hz, 1H, ArH), 6.81 (d, *J* = 1.5 Hz, 1H, ArH), 5.60-5.50 (m, 1H, CH_2CH=CH_2), 5.14-5.05 (m, 2H, CH_2CH=CH_2), 4.95 (d, *J* = 15.8 Hz, 1H, CH_2Ph), 4.62 (d, *J* = 15.8 Hz, 1H, CH_2Ph), 4.00 (br s, 1H, OH), 2.82-2.77 (m, 1H, CH_2CH=CH_2), 2.71-2.65 (m, 1H, CH_2CH=CH_2).

(*S*)-2-Methoxy-1,1'-binaphthalene (9a): White solid (40.4 mg, 0.142 mmol; 71%). M.p.: 118-119 °C. The enantiomeric excess was determined on a Daicel Chiralpak AD-H column with hexane/2-propanol = 98/2, flow = 0.25 mL/min, and detected at a UV wave length of 254 nm. Retention times: 20.9 min, 24.4 min (major), 52% *ee*. $[\alpha]_D^{20}$ = +24.4 (*c* 0.446, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 9.0 Hz, 1H, ArH), 7.93 (dd, *J* = 4.2, 8.2 Hz, 2H, ArH), 7.86 (d, *J* = 8.2 Hz, 1H, ArH), 7.61 (dd, *J* = 7.0, 8.2 Hz, 1H, ArH), 7.47-7.42 (m, 3H, ArH), 7.34-7.14 (m, 5H, ArH), 3.75 (s, 3H, OCH_3).

(*S*)-2-Ethoxy-1,1'-binaphthalene (9b): White solid (46.5 mg, 0.156 mmol; 78%). M.p.: 113-114 °C. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 90/10, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 7.3 min (major), 11.5 min, 54% *ee*. $[\alpha]_D^{20}$ = +44.9 (*c* 0.406, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (dd, *J* = 3.9, 9.1 Hz, 3H, ArH), 7.85 (d, *J* = 8.2 Hz, 1H, ArH), 7.59 (dd, *J* = 7.0, 8.2 Hz, 1H, ArH), 7.46-7.39 (m, 3H, ArH), 7.34-7.16 (m, 5H, ArH), 4.07-3.95 (m, 2H, OC$H_2$$CH_3$), 1.02 (t, *J* = 7.0 Hz, 3H, OCH_2CH_3).

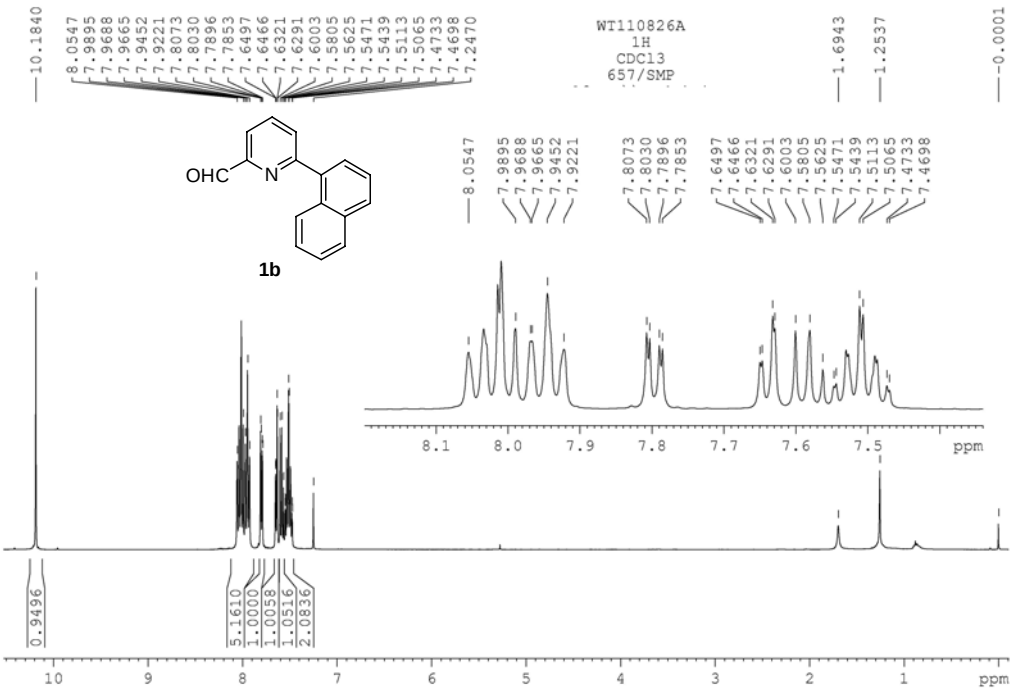
(*S*)-2-(Benzyloxy)-1,1'-binaphthalene (9c): White solid (53.3 mg, 0.148 mmol; 74%). M.p.: 78-79 °C. The enantiomeric excess was determined on a Daicel Chiralpak AD-H

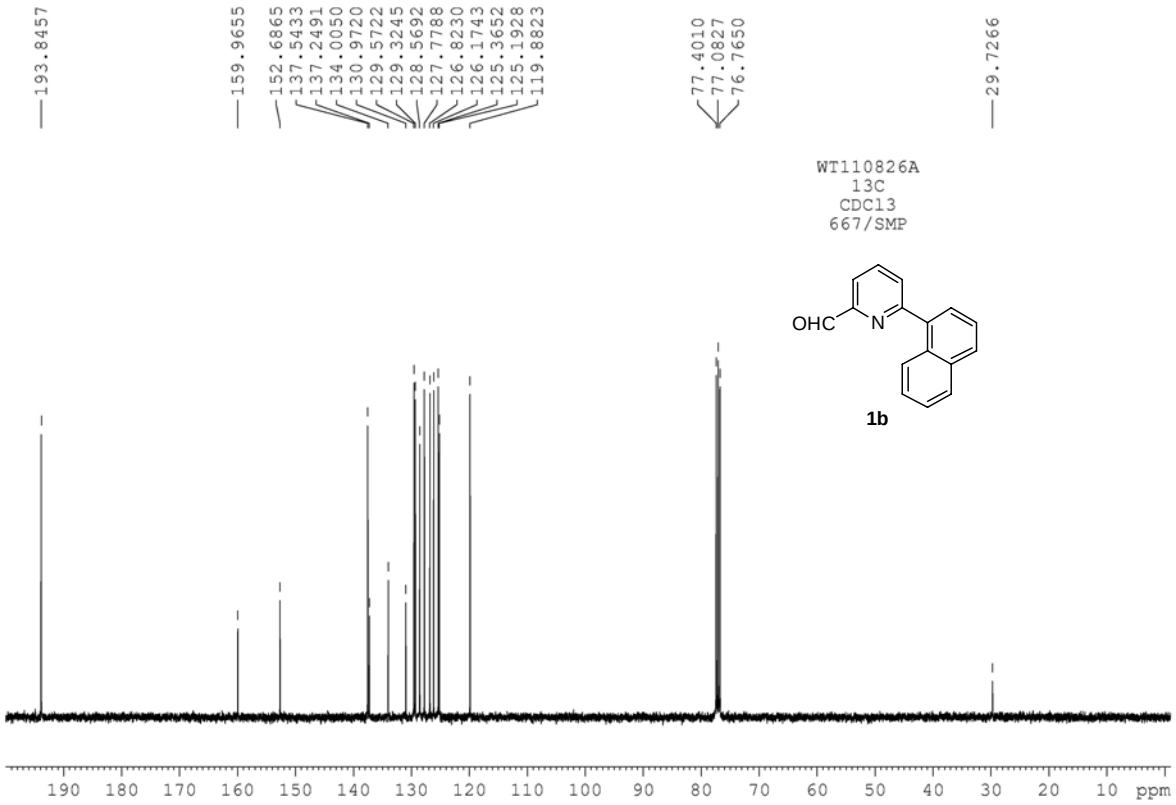
column with hexane/2-propanol = 98/2, flow = 0.5 mL/min, and detected at a UV wave length of 254 nm. Retention times: 20.8 min, 32.2 min (major), 51% *ee*. $[\alpha]_D^{20}$ = +38.7 (*c* 0.350, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ 7.95 (dd, *J* = 1.5, 8.1 Hz, 2H, ArH), 7.91 (d, *J* = 9.0 Hz, 1H, ArH), 7.85 (d, *J* = 8.1 Hz, 1H, ArH), 7.61 (dd, *J* = 7.0, 8.1 Hz, 1H, ArH), 7.48-7.41 (m, 3H, ArH), 7.37-7.25 (m, 3H, ArH), 7.23-7.22 (m, 2H, ArH), 7.15-7.10 (m, 3H, ArH), 6.95-6.92 (m, 2H, ArH), 5.05 (d, *J* = 12.5 Hz, 1H, OC*H*HC_6H_5), 5.00 (d, *J* = 12.5 Hz, 1H, OCH*H*C_6H_5).

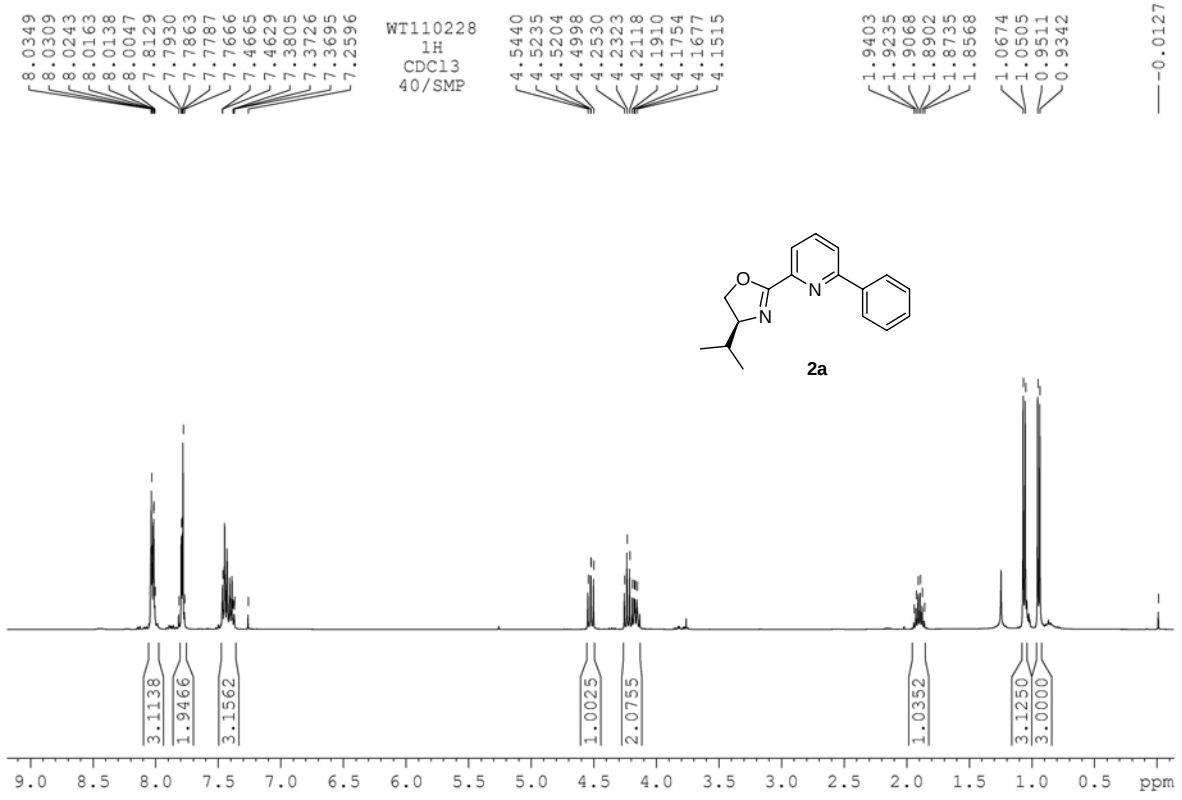
(*S*)-2-Methoxy-1-(o-tolyl)naphthalene (9d): White solid (45.2 mg, 0.182 mmol; 91%). M.p.: 89-90 ^oC. The enantiomeric excess was determined on a Daicel Chiralcel OJ-H column with hexane/2-propanol = 98/2, flow = 1.0 mL/min, and detected at a UV wave length of 254 nm. Retention times: 9.0 min (major), 14.0 min, 23% *ee*. $[\alpha]_D^{20}$ = +14.2 (*c* 0.774, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 9.0 Hz, 1H, ArH), 7.83-7.80 (m, 1H, ArH), 7.37-7.33 (m, 3H, ArH), 7.32-7.24 (m, 4H, ArH), 7.20-7.17 (m, 1H, ArH), 3.82 (s, 3H, OCH_3), 1.99 (s, 3H, CH_3).

(*R*)-1-([1,1'-Biphenyl]-2-yl)-2-methoxynaphthalene (9g): White solid (50.9 mg, 0.164 mmol; 82%). M.p.: 93-95 ^oC. The enantiomeric excess was determined on a Daicel Chiralpak AD-H column with hexane/2-propanol = 98/2, flow = 0.8 mL/min, and detected at a UV wave length of 254 nm. Retention times: 6.0 min, 6.6 min (major), 23% *ee*. $[\alpha]_D^{20}$ = -9.5 (*c* 0.970, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.8 Hz, 2H, ArH), 7.54-7.43 (m, 4H, ArH), 7.34-7.26 (m, 3H, ArH), 7.08 (d, *J* = 9.0 Hz, 1H, ArH), 7.05-6.99 (m, 5H, ArH), 3.48 (s, 3H, OCH_3).

Copies of the ^{1}H and ^{13}C NMR Spectra of New Compounds 1-3



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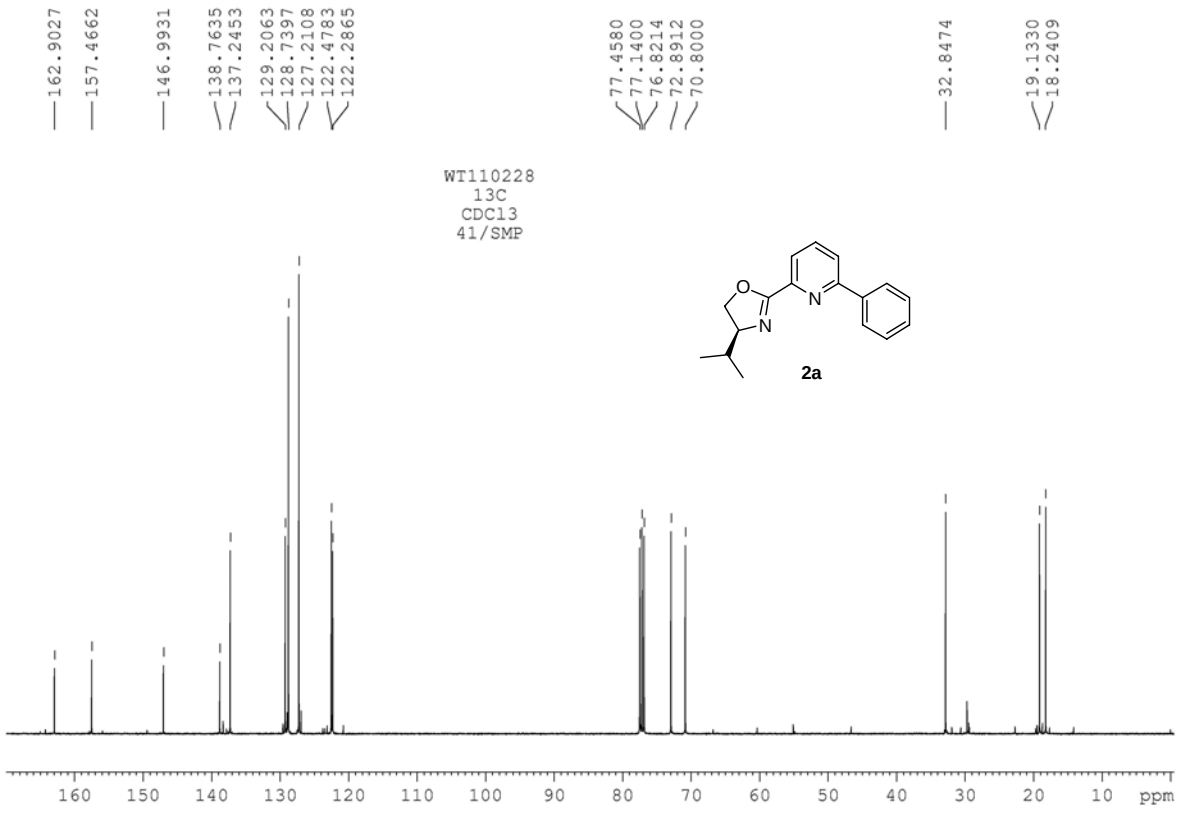
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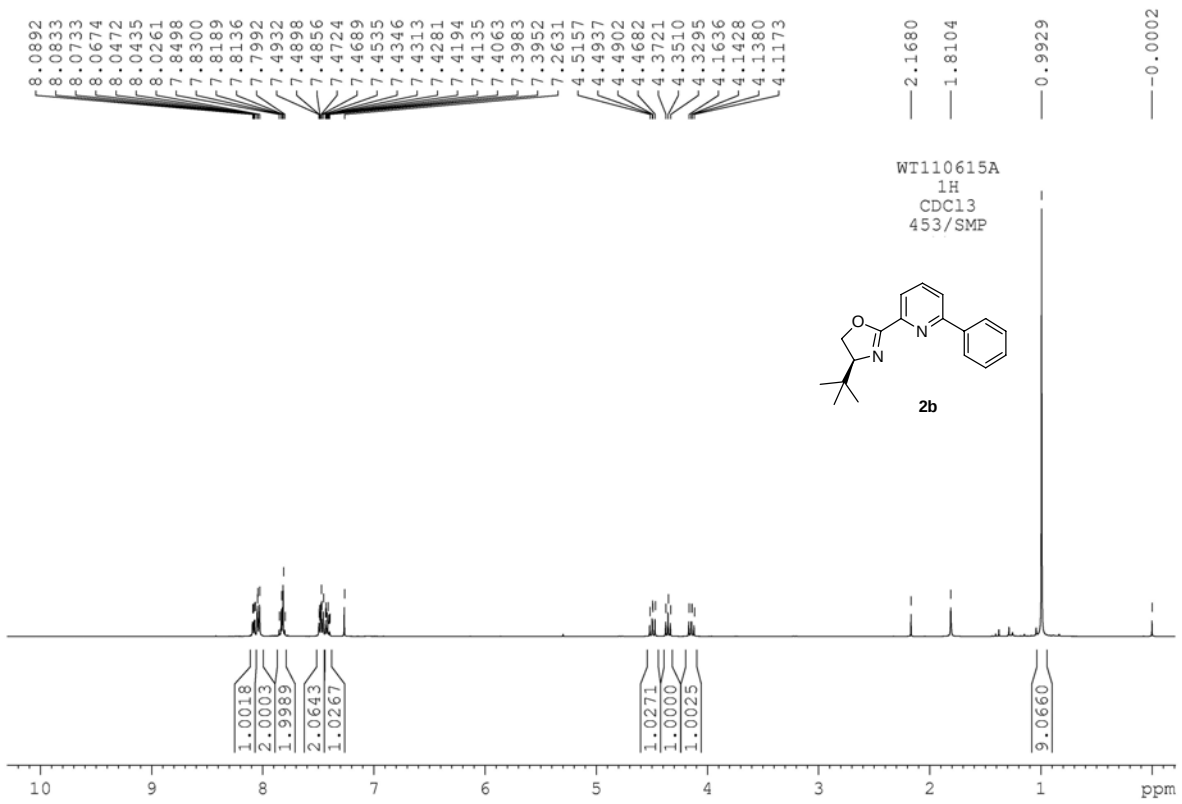
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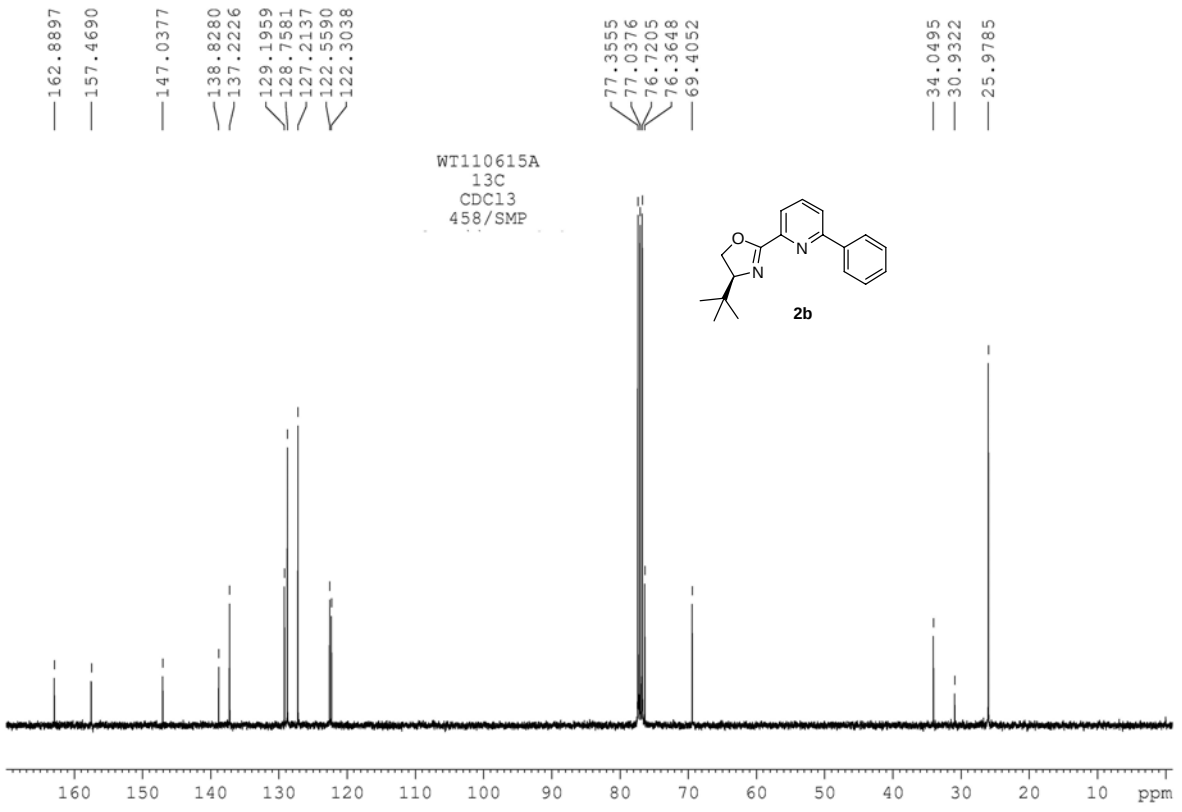
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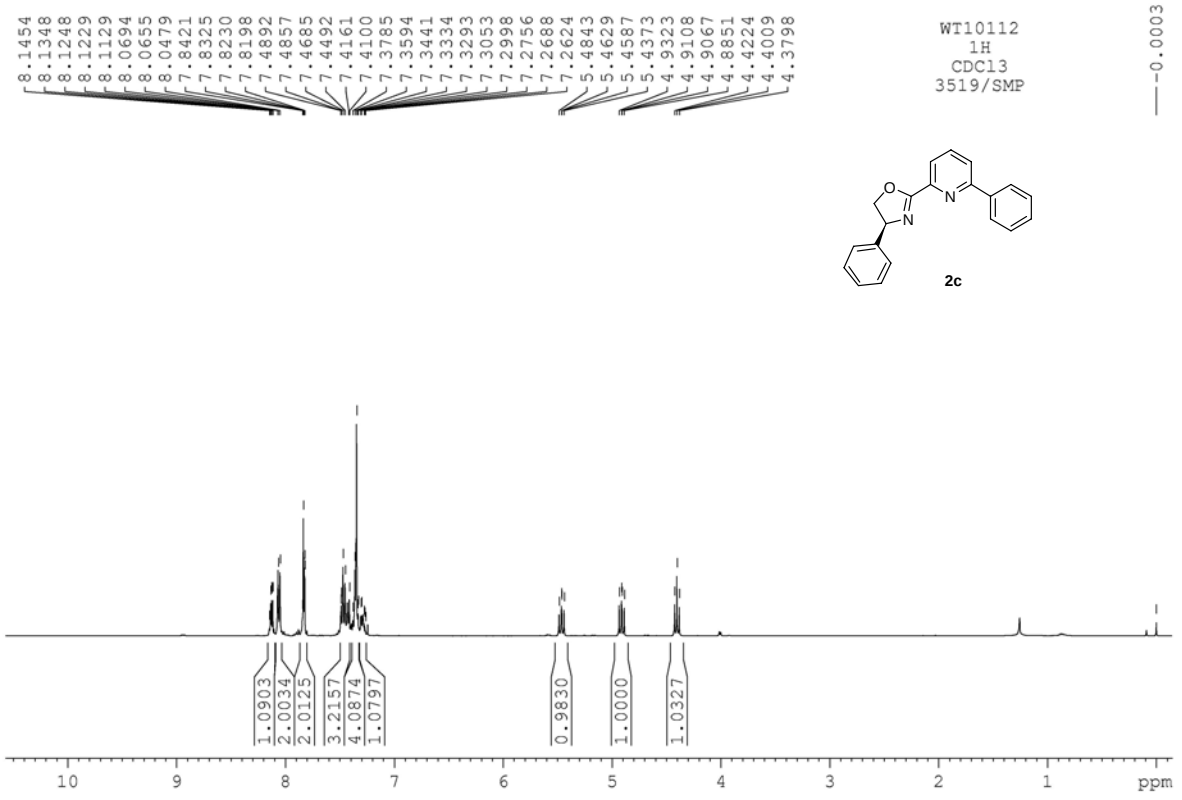
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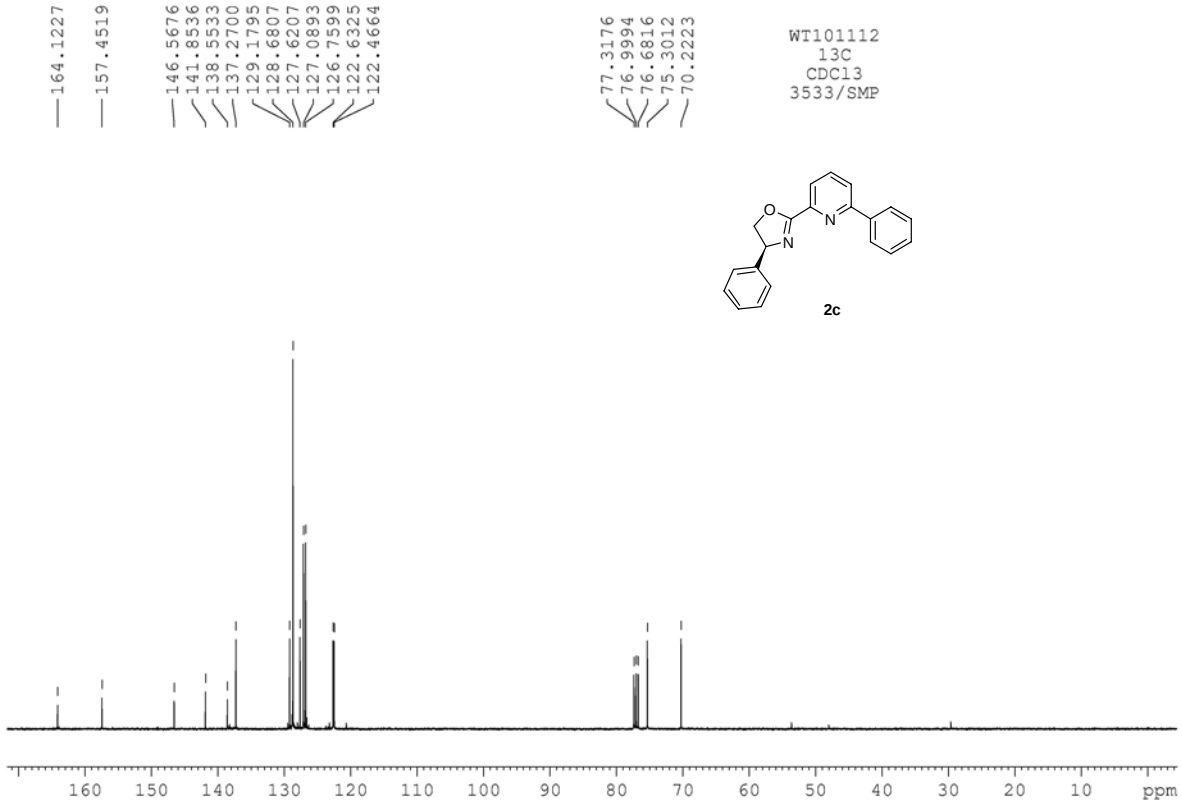
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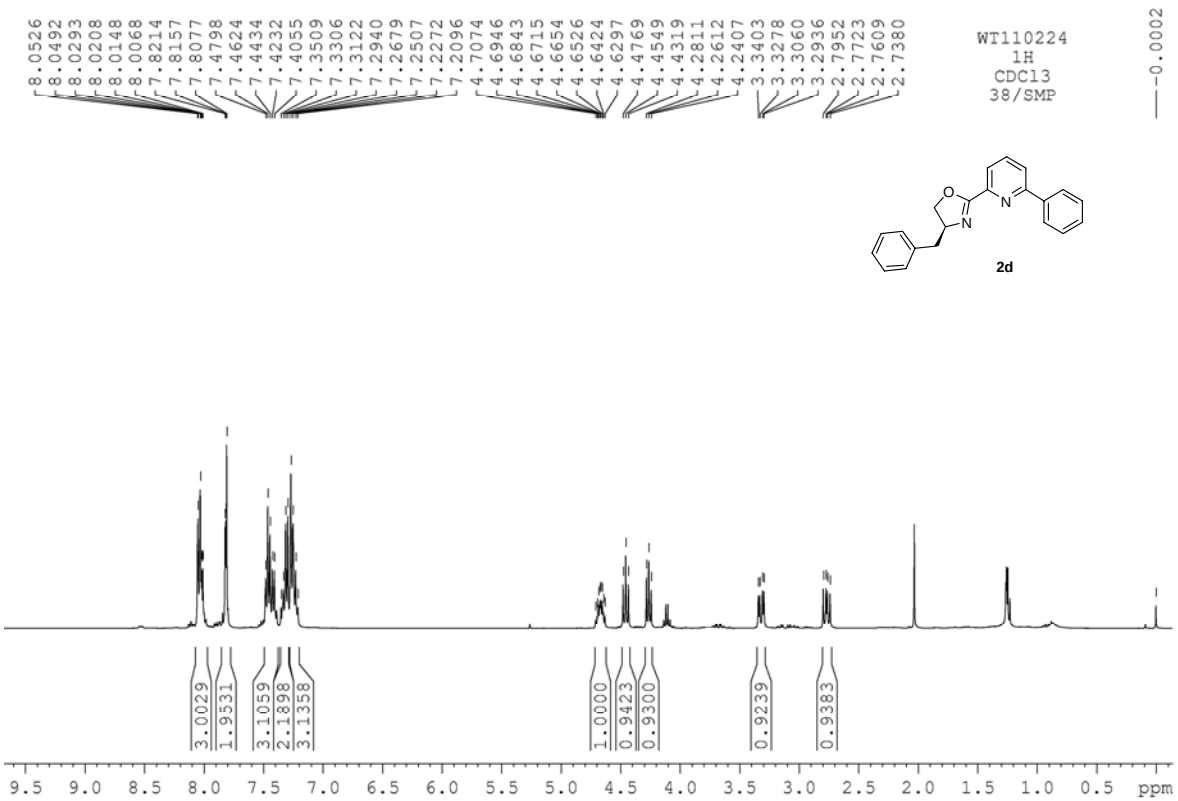
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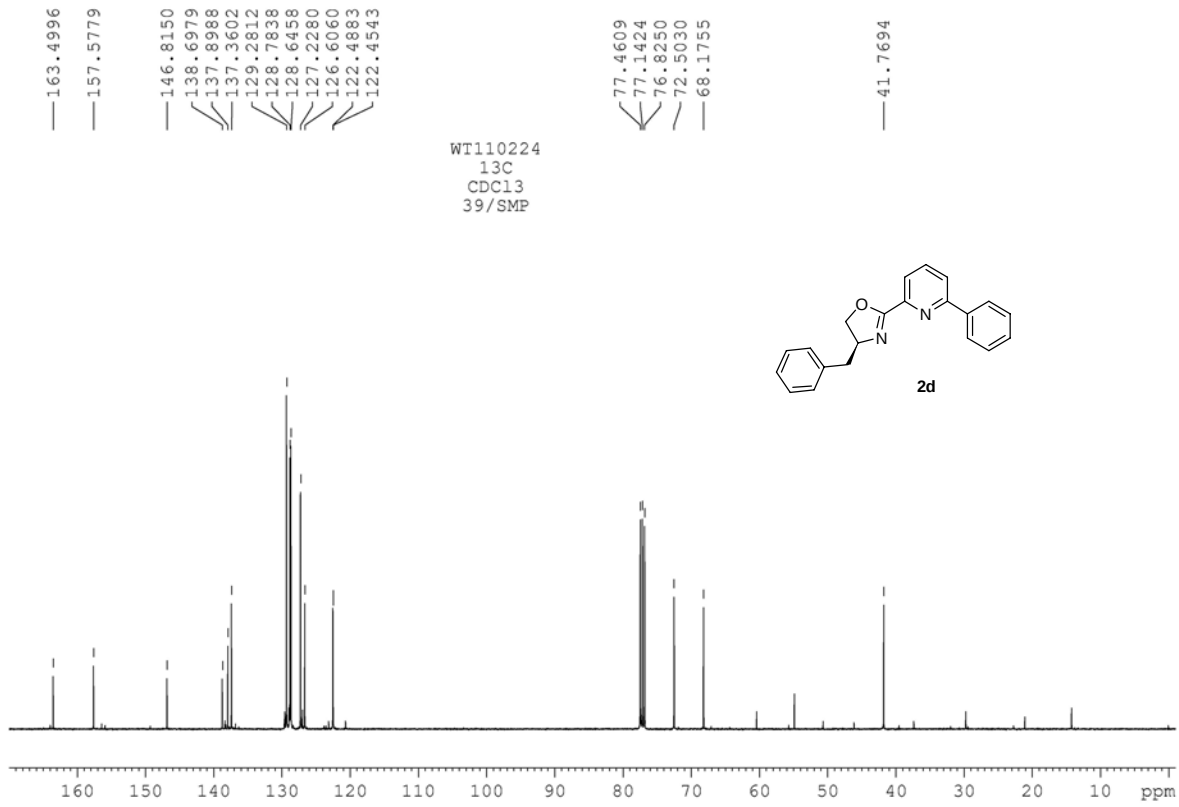
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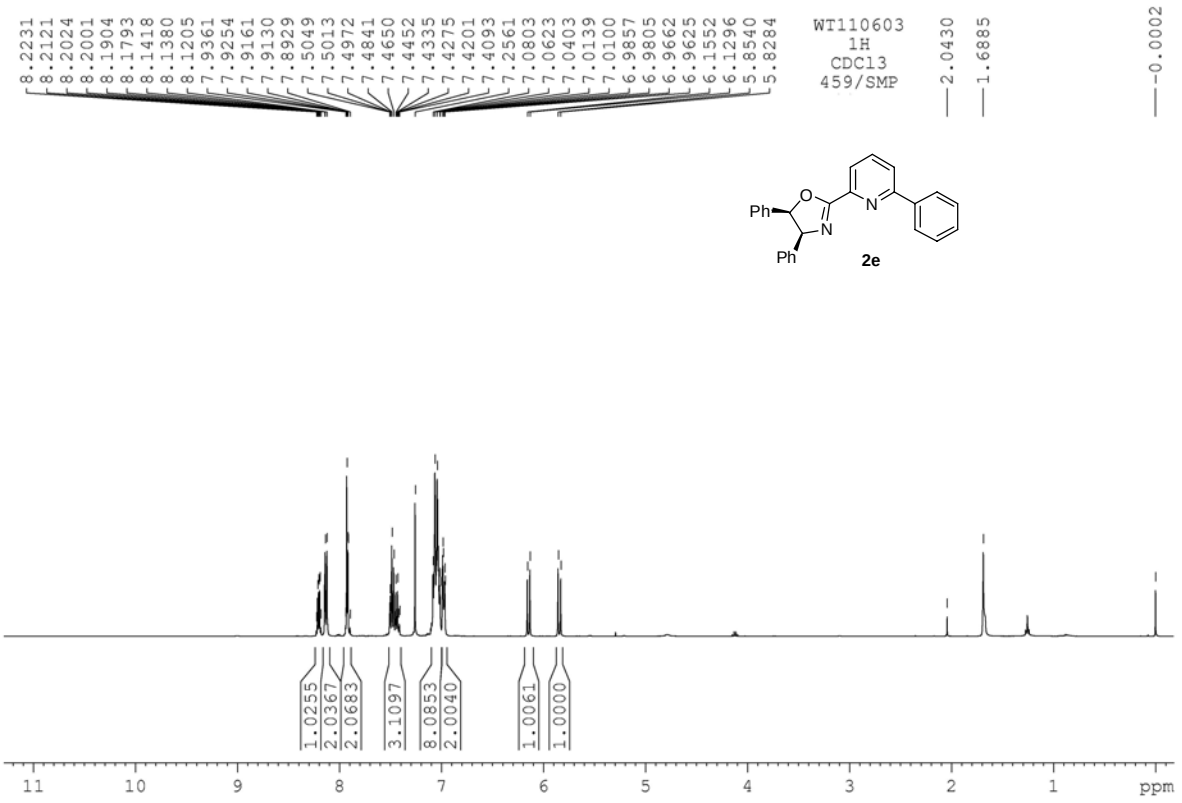
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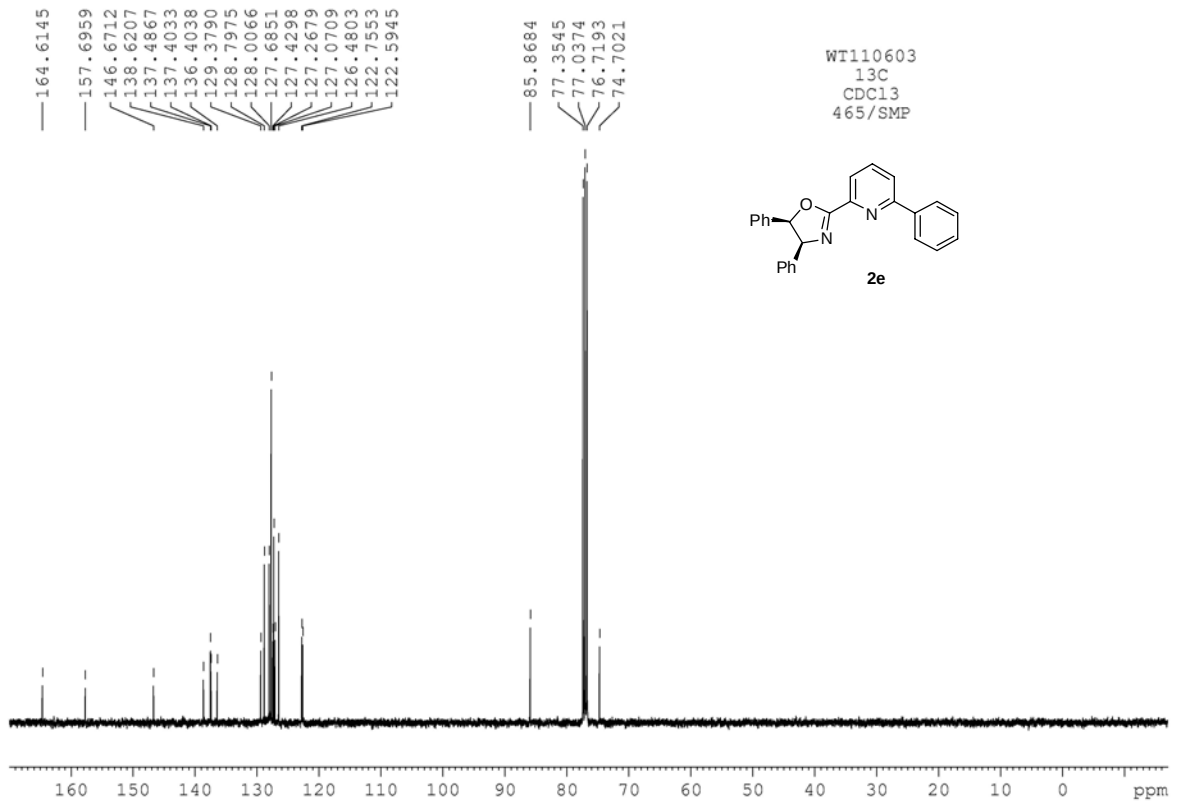
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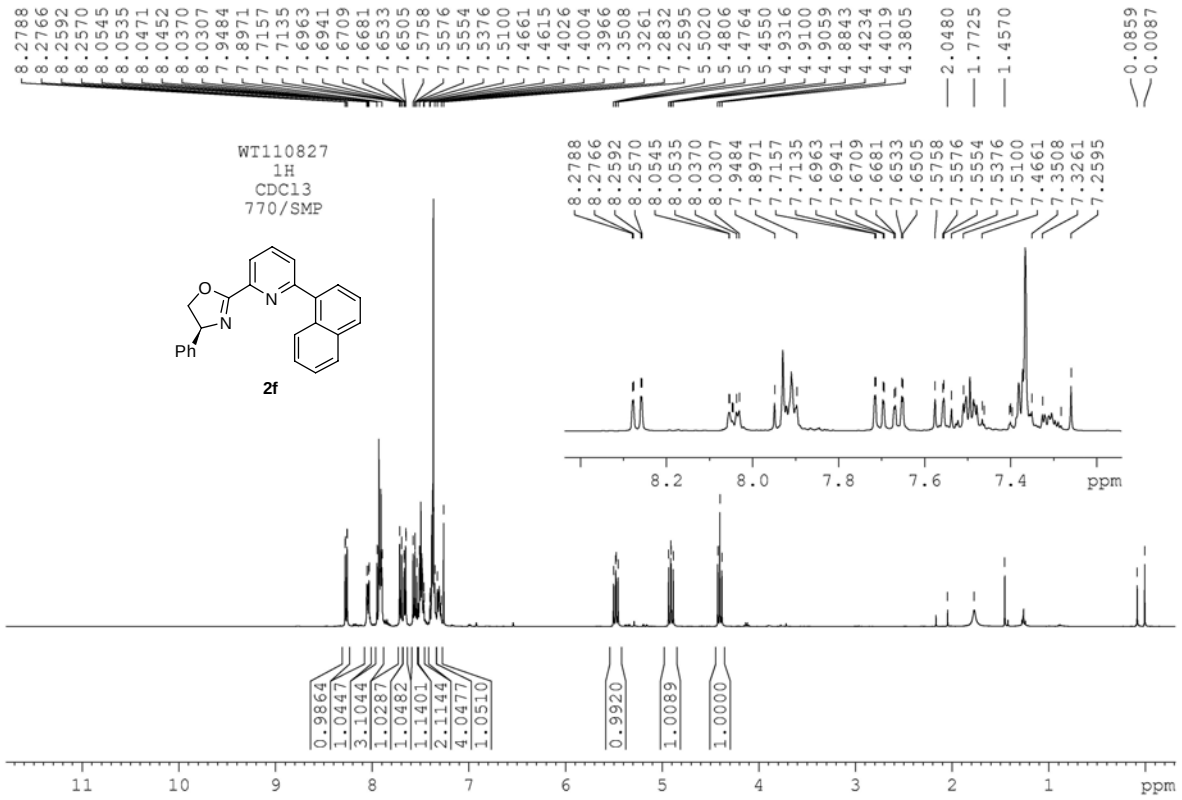
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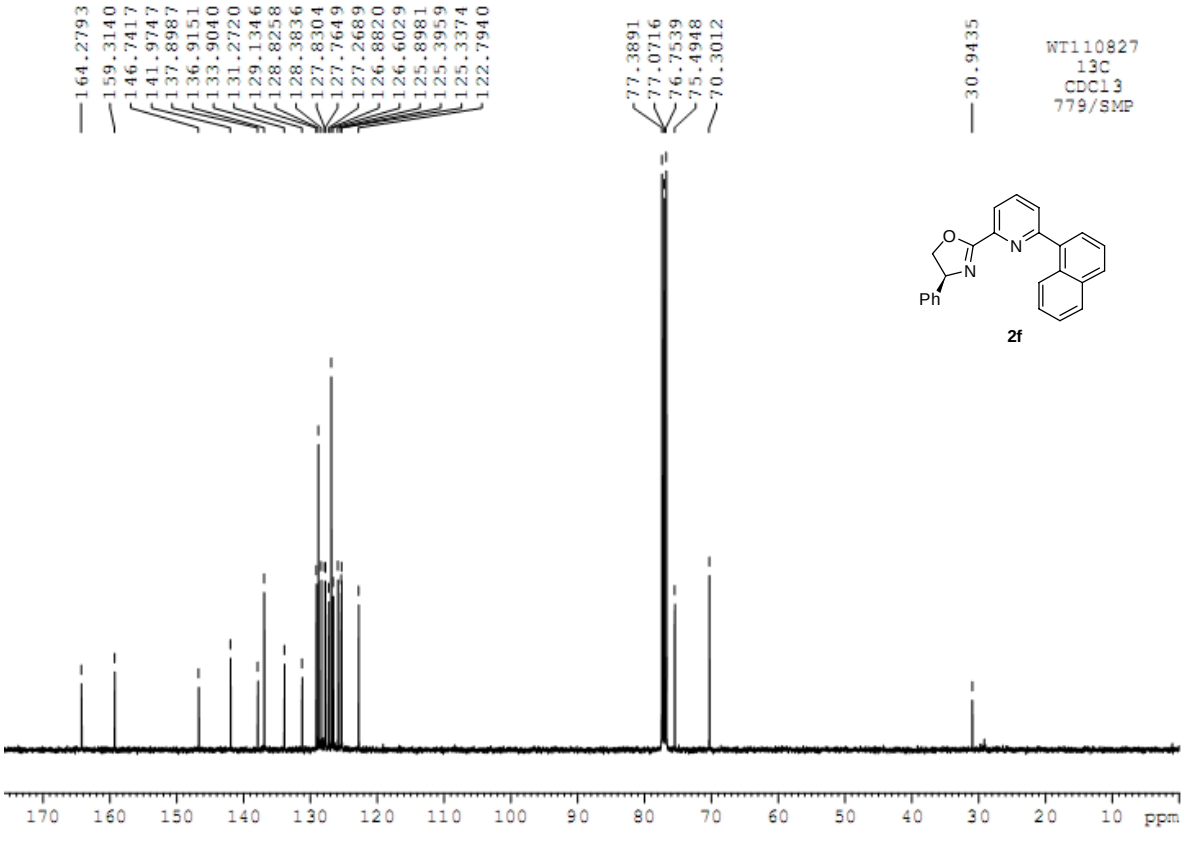
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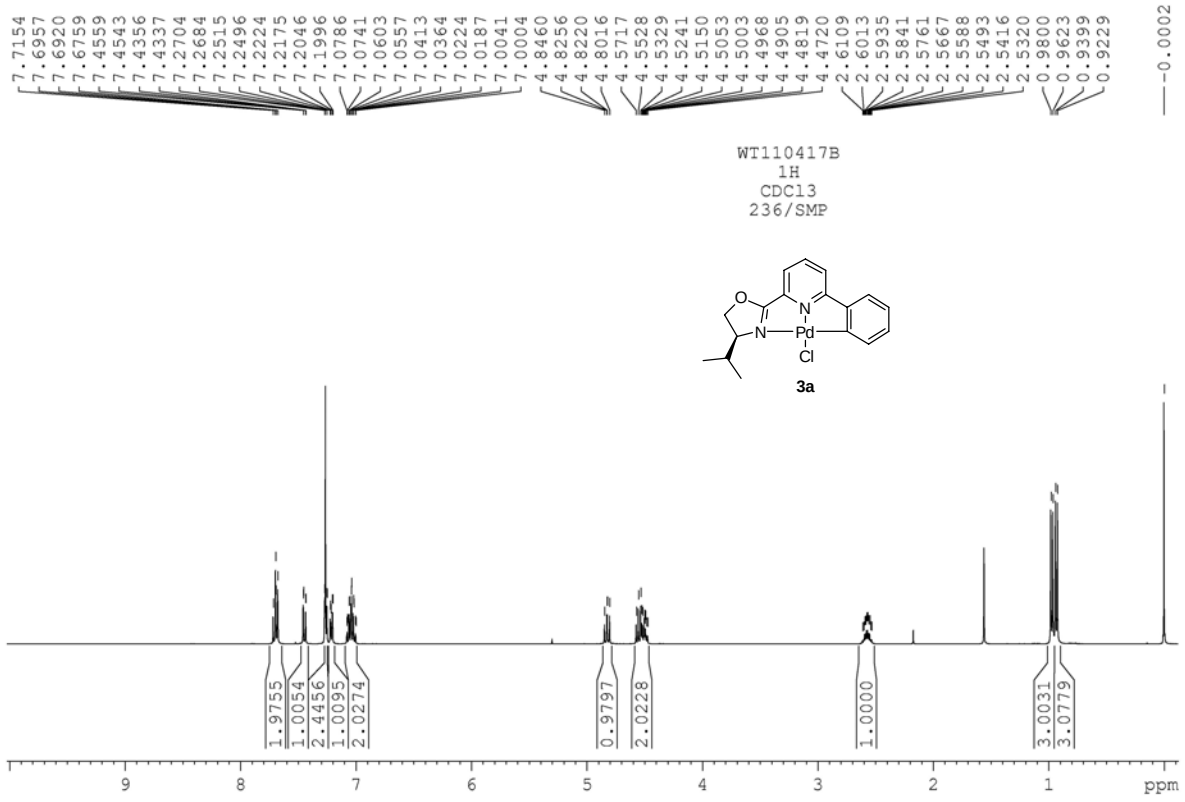
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7.0557
7.0413
7.0364
7.0224
7.0187
7.0041
7.0004
4.8460
4.8256
4.8220
4.8016
4.5717
4.5528
4.5329
4.5241
4.5150
4.5053
4.5003
4.4968
4.4905
4.4819
4.4720
2.6109
2.6013
2.5935
2.5841
2.5761
2.5667
2.5588
2.5493
2.5416
2.5320
0.9800
0.9623
0.9399
0.9229
-0.0002
WT110417B
1H
CDCl3
236/SMP
O
N
N
Pd
Cl
3a
1.9755
1.0054
2.4456
1.0095
2.0274
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1.0000
3.0031
3.0779
9
8
7
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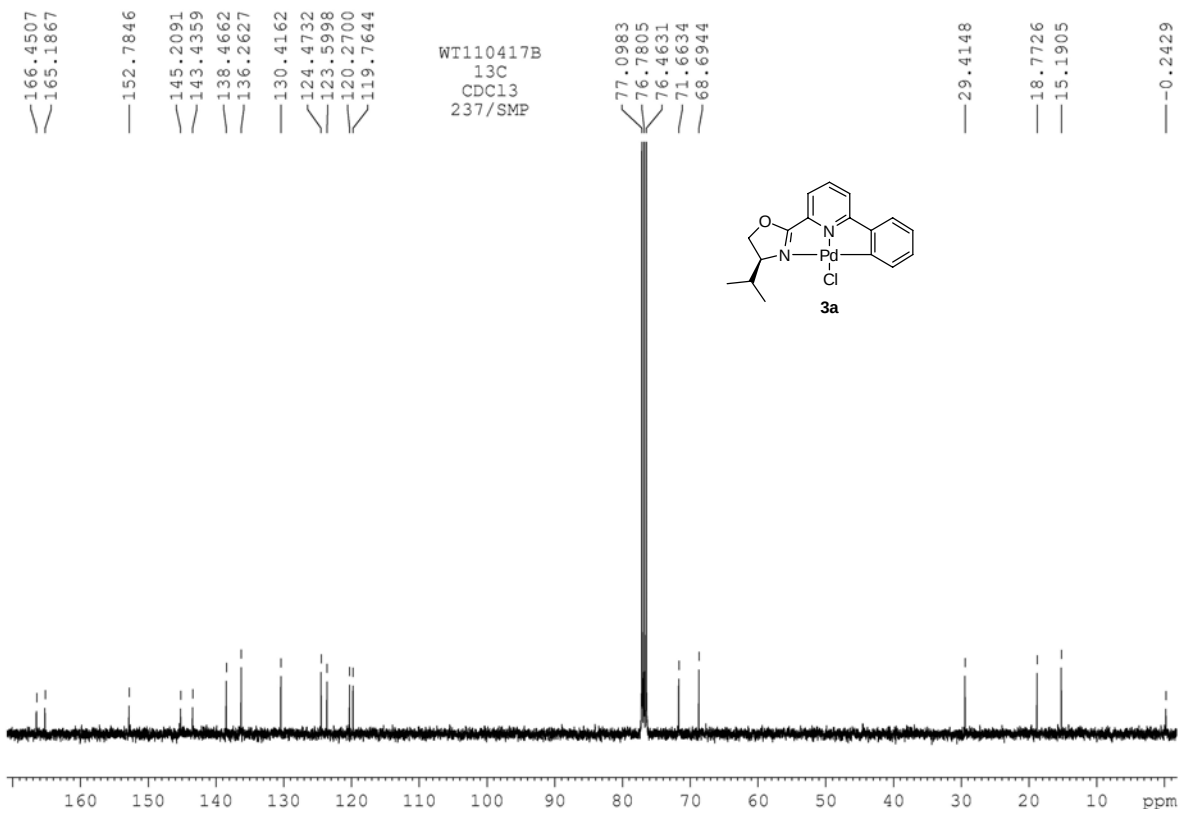
5
4
3
2
1
ppm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152.7846
145.2091
143.4359
138.4662
136.2627
130.4162
124.4732
123.5998
120.2700
119.7644
WT110417B
13C
CDCl3
237/SMP
77.0983
76.7805
76.4631
71.6634
68.6944
29.4148
18.7726
15.1905
-0.2429
O
N
N
Pd
Cl
3a
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150
140
130
120
110
100
90
80
70
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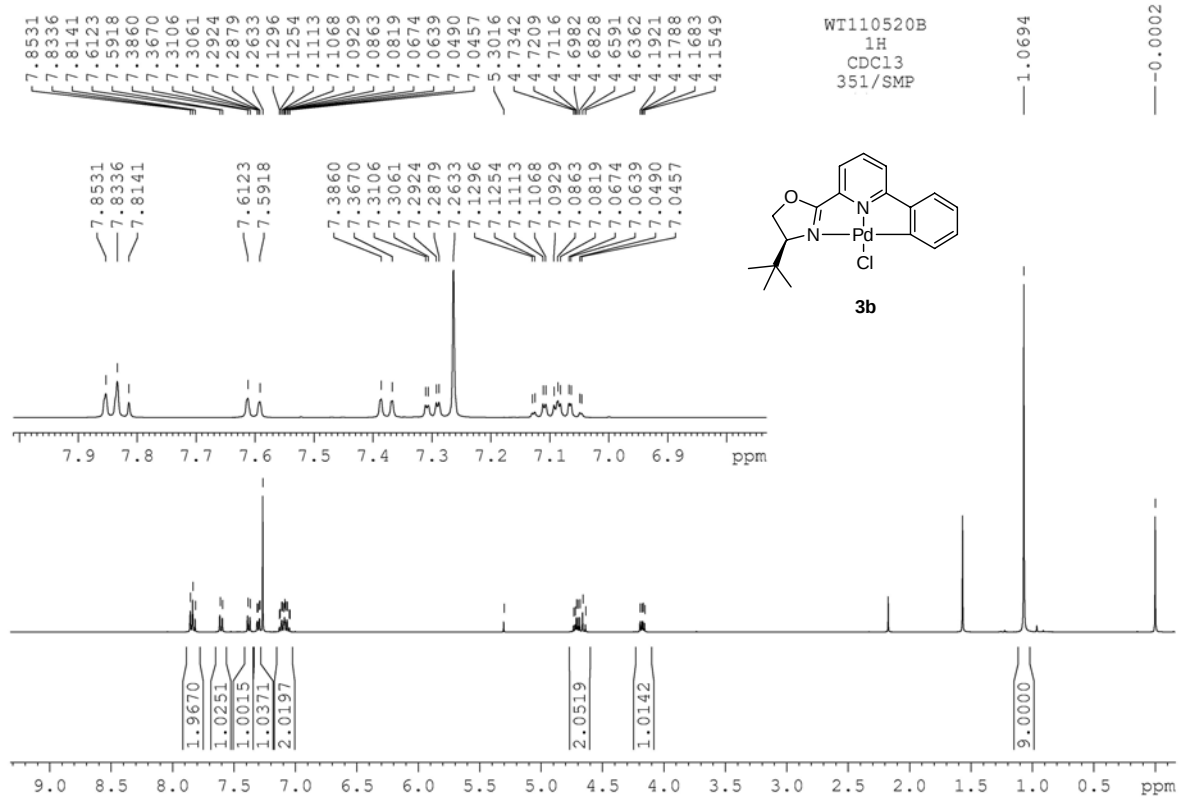
10
ppm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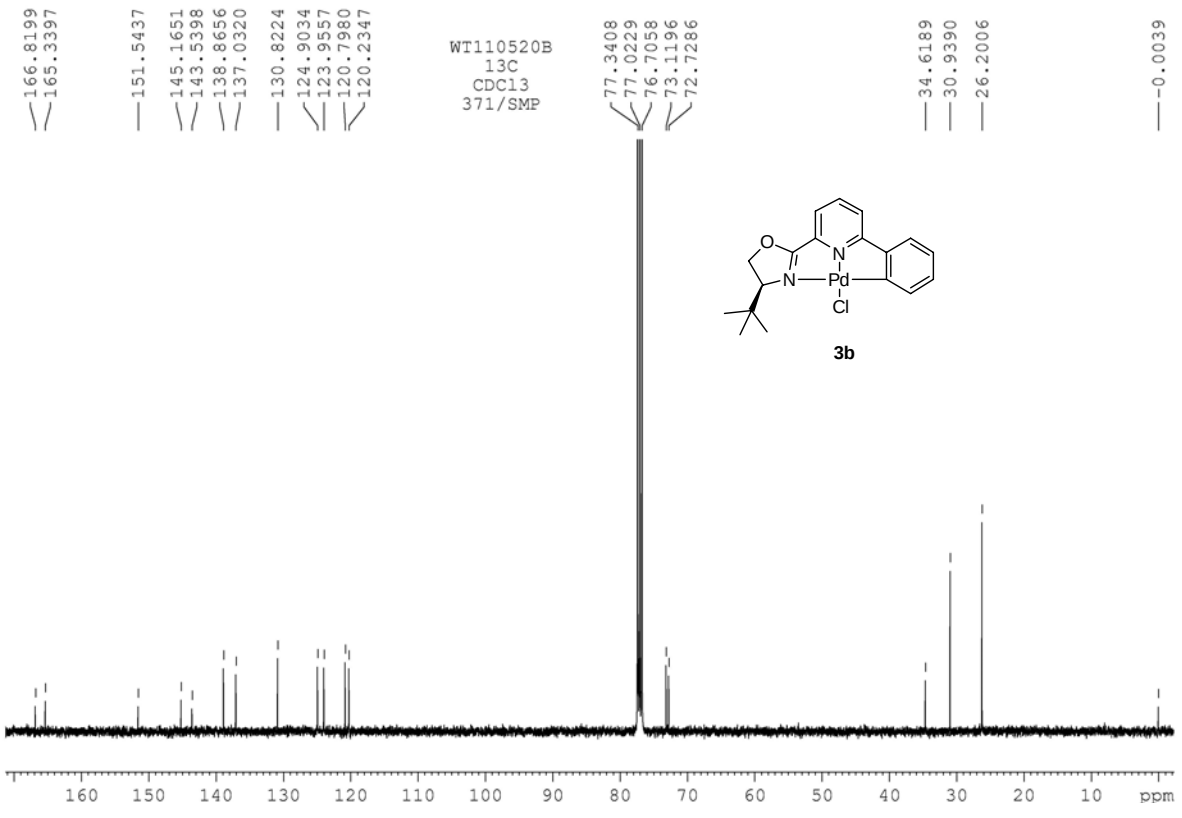
1H
CDCl3
351/SMP
3b
ppm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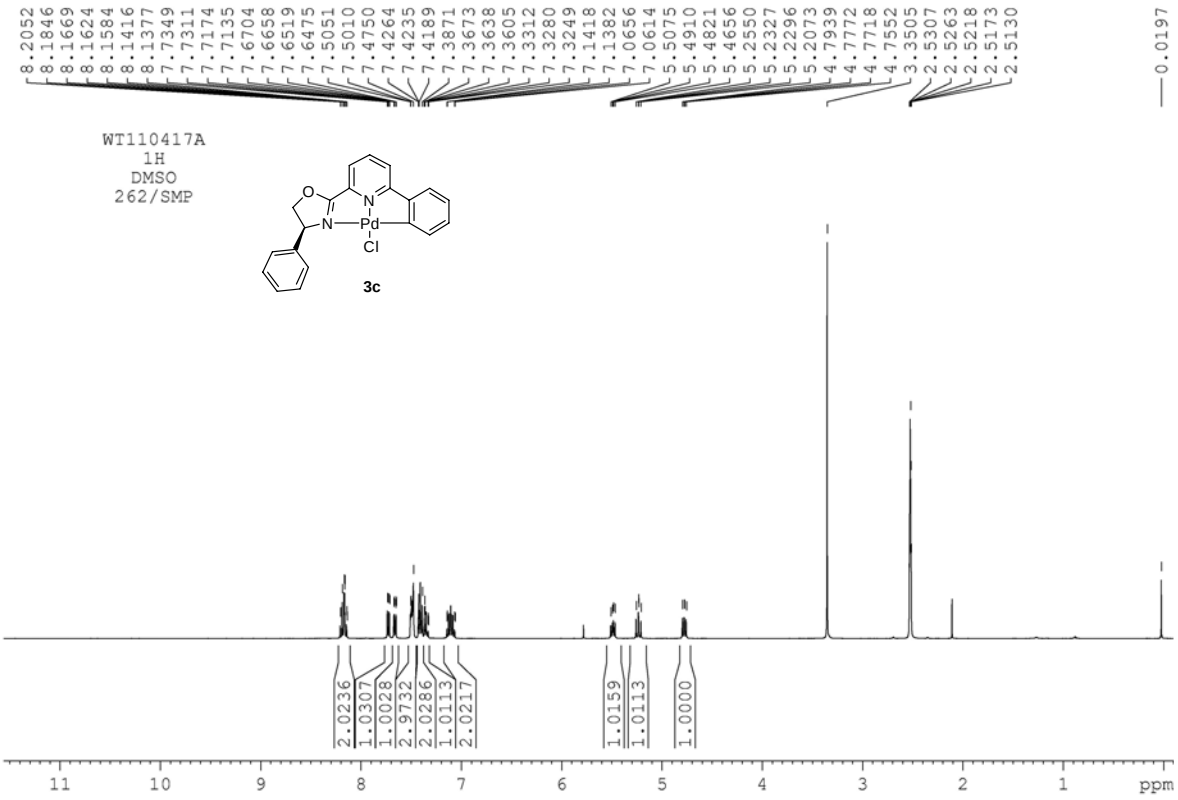
13C
CDCl3
371/SMP
3b
ppm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8.1624
8.1584
8.1416
8.1377
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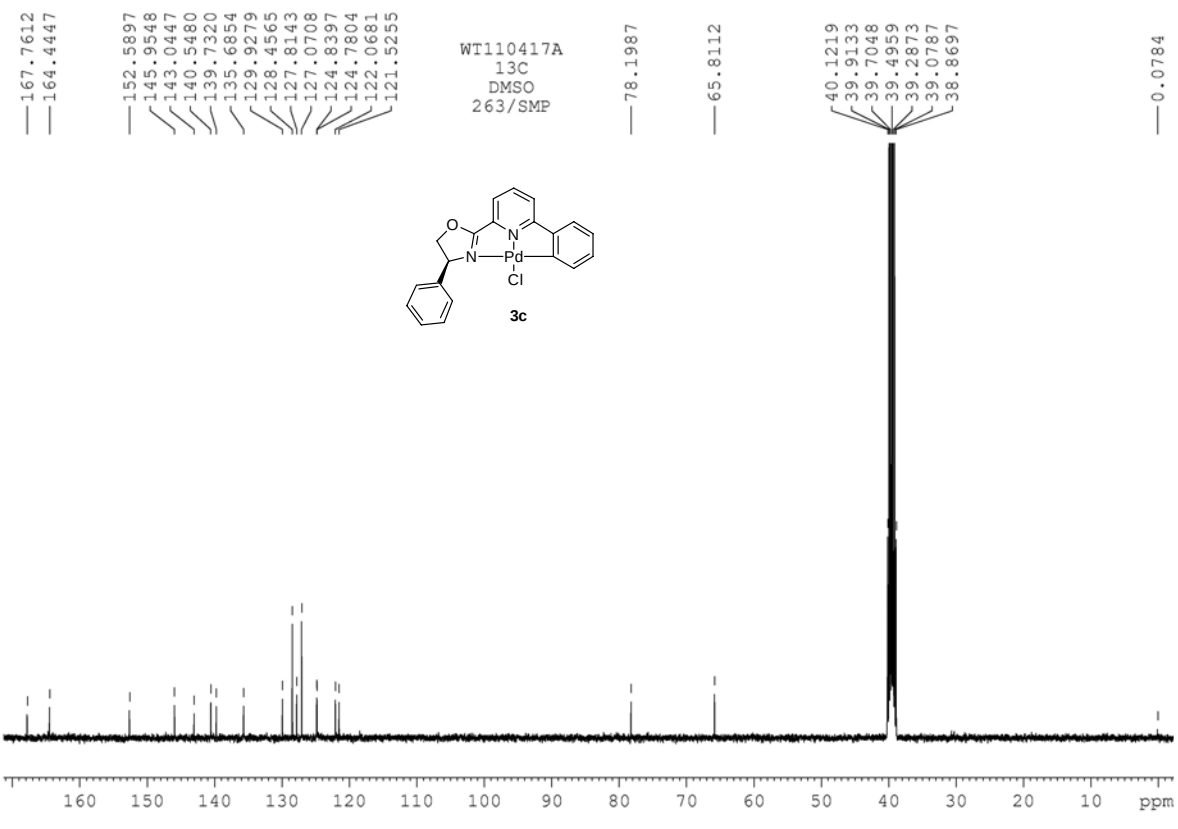
7.7311
7.7174
7.7135
7.6704
7.6658
7.6519
7.6475
7.5051
7.5010
7.4750
7.4264
7.4235
7.4189
7.3871
7.3673
7.3638
7.3605
7.3312
7.3280
7.3249
7.1418
7.1382
7.0656
7.0614
5.5075
5.4910
5.4821
5.4656
5.2550
5.2327
5.2296
5.2073
4.7939
4.7772
4.7718
4.7552
3.3505
2.5307
2.5263
2.5218
2.5173
2.5130
0.0197
WT110417A
1H
DMSO
262/SMP
3c
2.0236
1.0307
1.0028
2.9732
2.0286
1.0113
2.0217
1.0159
1.0113
1.0000
11
10
9
8
7
6
5
4
3
2
1
ppm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152.5897
145.9548
143.0447
140.5480
139.7320
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129.9279
128.4565
127.8143
127.0708
124.8397
124.7804
122.0681
121.5255
WT110417A
13C
DMSO
263/SMP
78.1987
65.8112
40.1219
39.9133
39.7048
39.4959
39.2873
39.0787
38.8697
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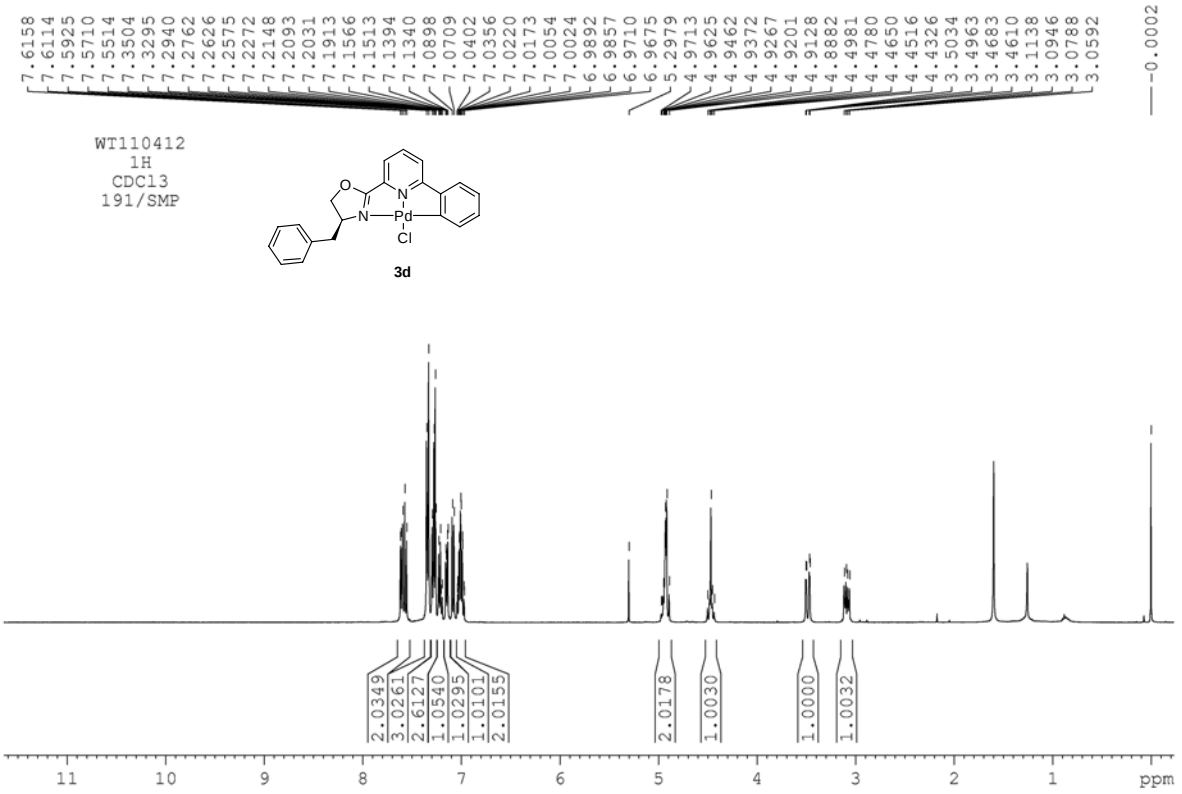
3c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.6114
7.5925
7.5710
7.5514
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7.3295
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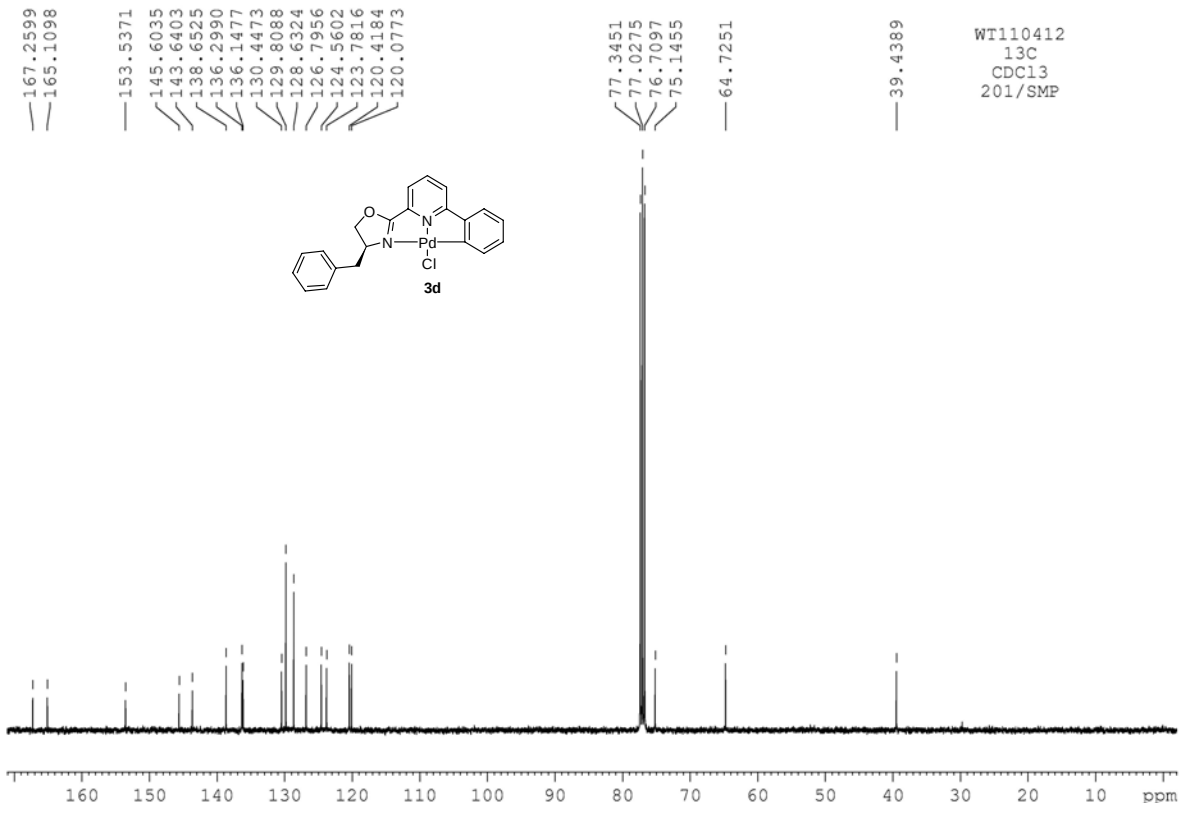
7.2762
7.2626
7.2575
7.2272
7.2148
7.2093
7.2031
7.1913
7.1566
7.1513
7.1394
7.1340
7.0898
7.0709
7.0402
7.0356
7.0220
7.0173
7.0054
7.0024
6.9892
6.9857
6.9710
6.9675
5.2979
4.9713
4.9625
4.9462
4.9372
4.9267
4.9201
4.9128
4.8882
4.4981
4.4780
4.4650
4.4516
4.4326
3.5034
3.4963
3.4683
3.4610
3.1138
3.0946
3.0788
3.0592
-0.0002
WT110412
1H
CDCl3
191/SMP
O
N
N
Pd
Cl
3d
2.0349
3.0261
2.6127
1.0540
1.0295
1.0101
2.0155
2.0178
1.0030
1.0000
1.0032
11
10
9
8
7
6
5
4
3
2
1
ppm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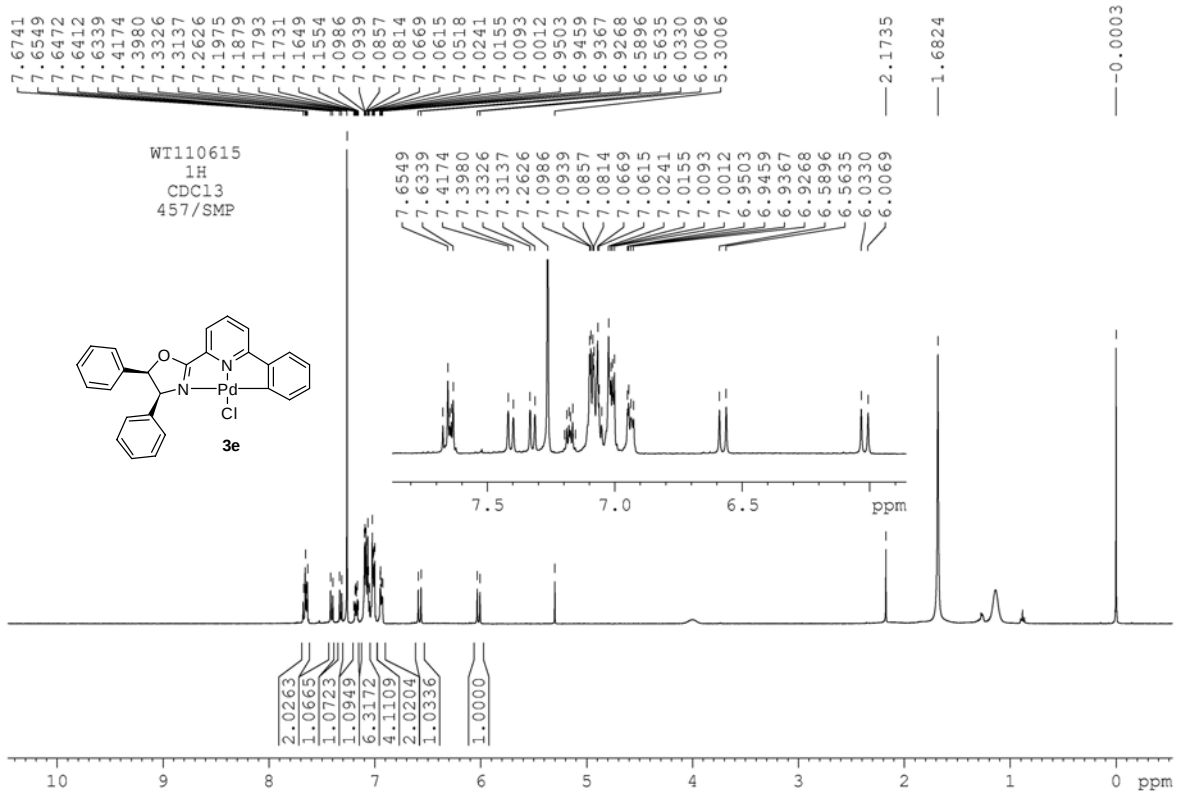
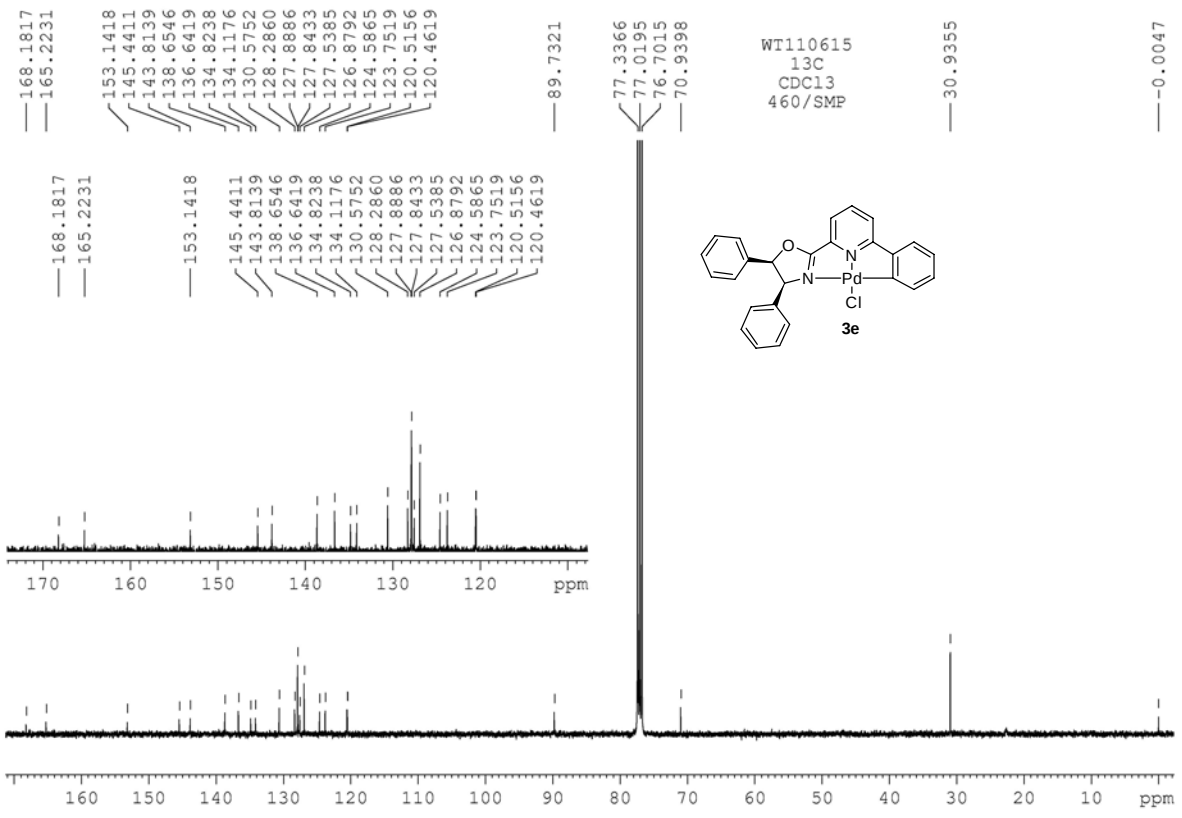
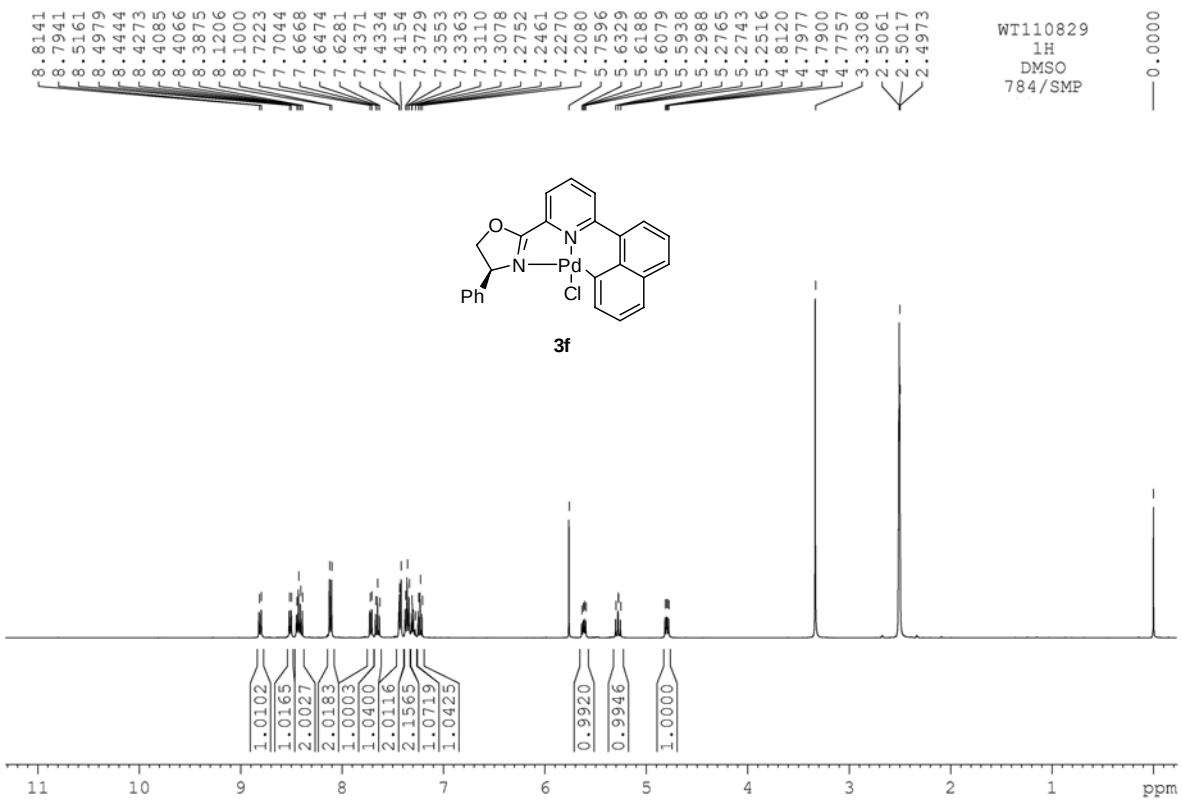
165.1098
153.5371
145.6035
143.6403
138.6525
136.2990
136.1477
130.4473
129.8088
128.6324
126.7956
124.5602
123.7816
120.4184
120.0773
77.3451
77.0275
76.7097
75.1455
64.7251
39.4389
WT110412
13C
CDCl3
201/SMP
O
N
N
Pd
Cl
3d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


WT110615
1H
CDCl3
457/SMP
3e
ppm


WT110615
13C
CDCl3
460/SMP
3e
ppm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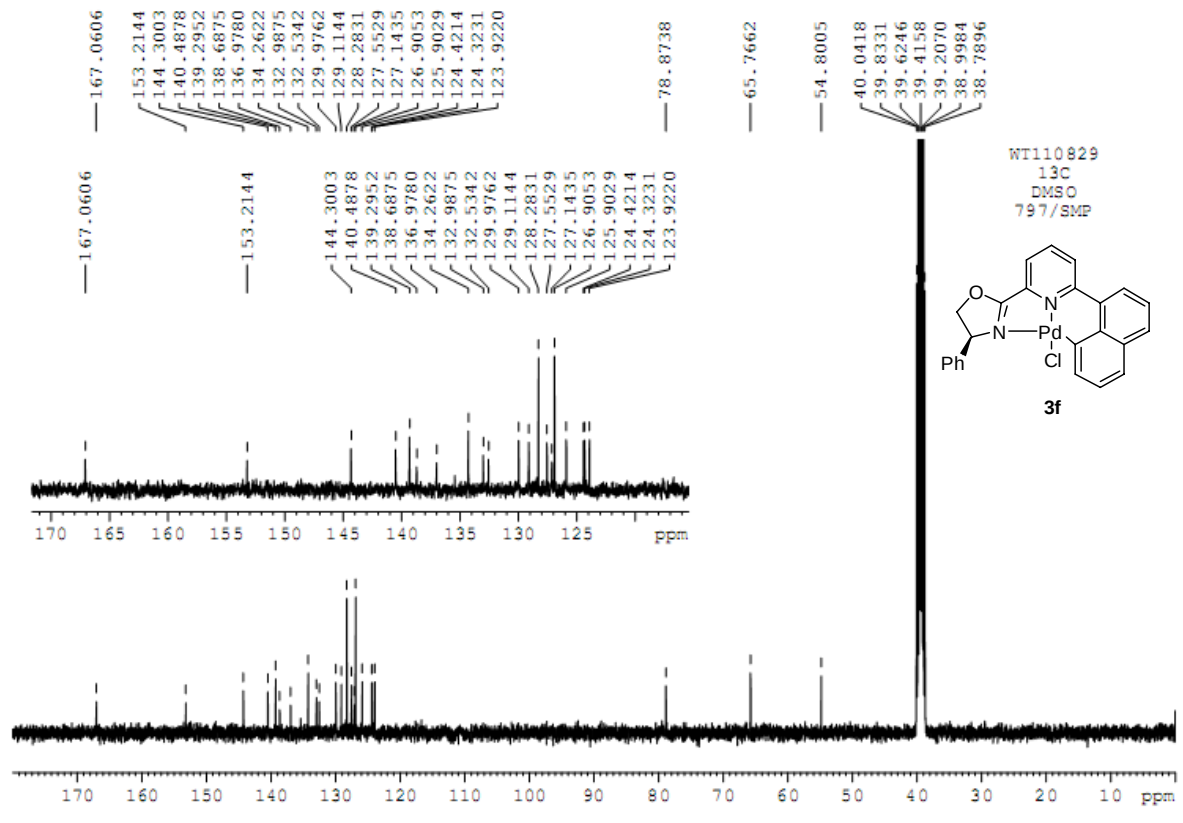
8.7941
8.5161
8.4979
8.4444
8.4273
8.4085
8.4066
8.3875
8.1206
8.1000
7.7223
7.7044
7.6668
7.6474
7.6281
7.4371
7.4334
7.4154
7.3729
7.3553
7.3363
7.3110
7.3078
7.2752
7.2461
7.2270
7.2080
5.7596
5.6329
5.6188
5.6079
5.5938
5.2988
5.2765
5.2743
5.2516
4.8120
4.7977
4.7900
4.7757
3.3308
2.5061
2.5017
2.4973
WT110829
1H
DMSO
784/SMP
0.0000
O
N
N
Pd
Cl
Ph
1.0102
1.0165
2.0027
2.0183
1.0003
1.0400
2.0116
2.1565
1.0719
1.0425
0.9920
0.9946
1.0000
11
10
9
8
7
6
5
4
3
2
1
ppm

3f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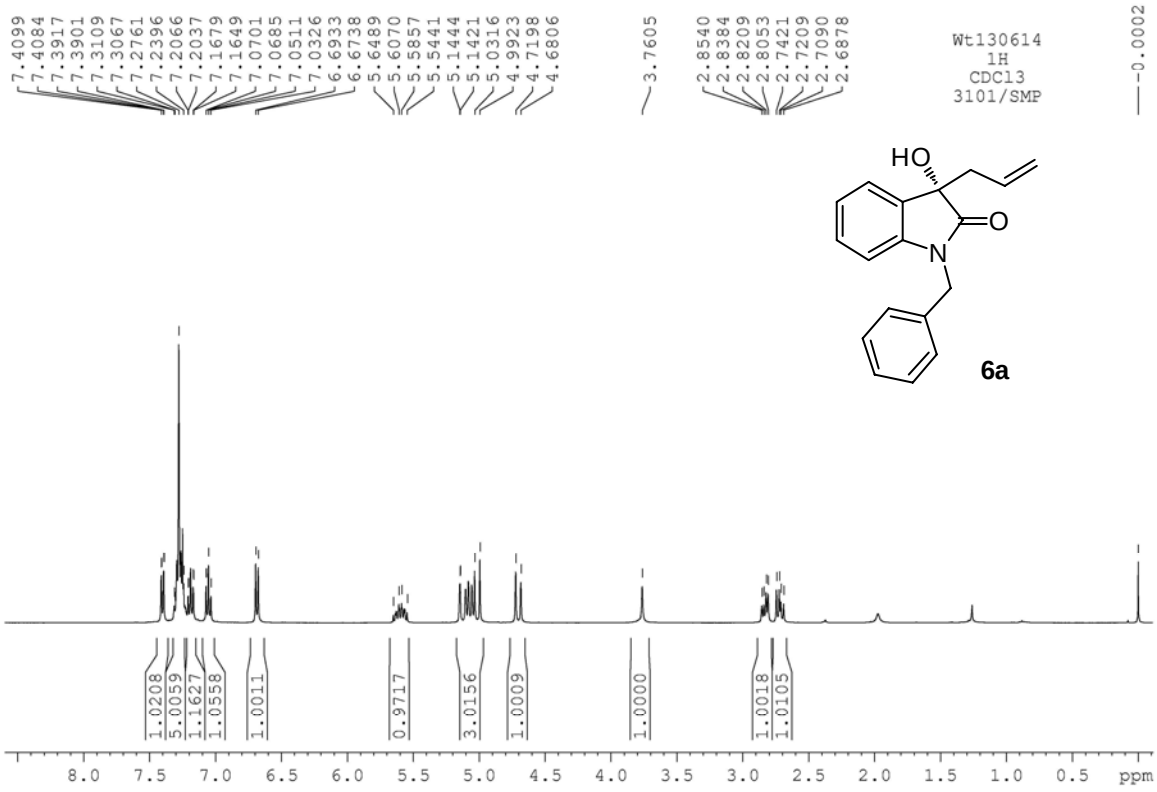
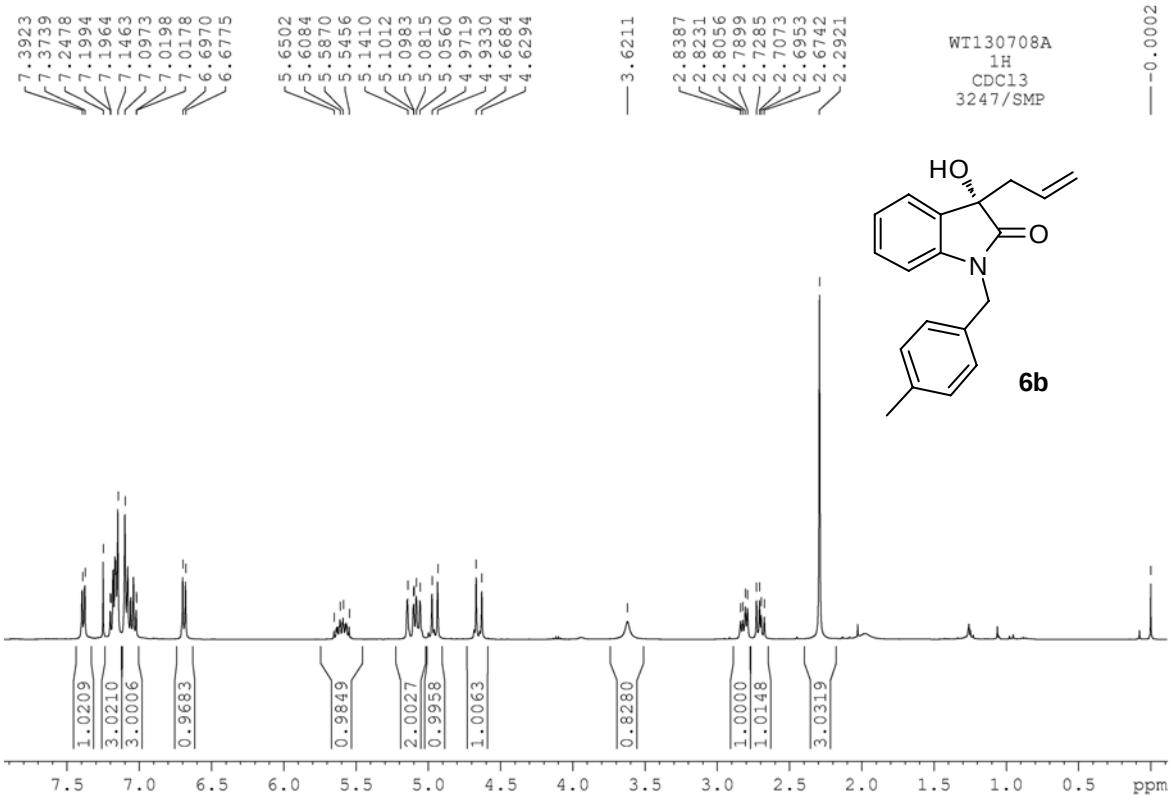
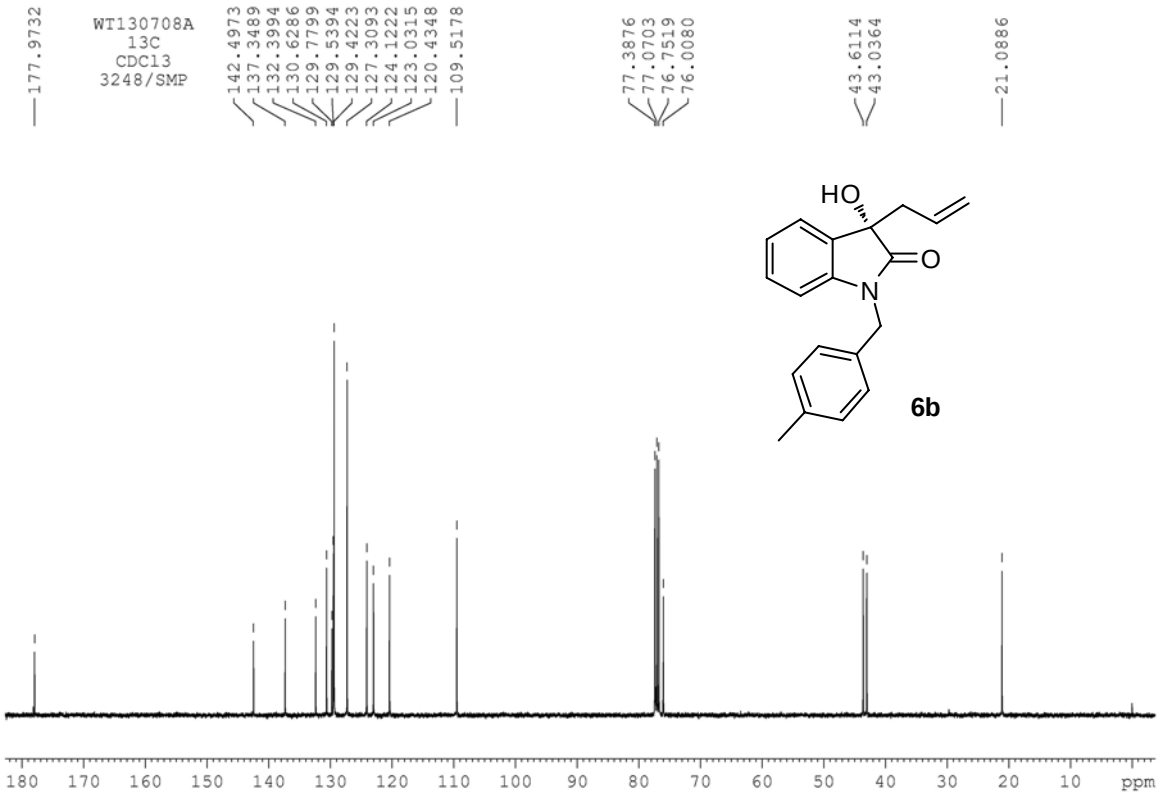
144.3003
140.4878
139.2952
138.6875
136.9780
134.2622
132.9875
132.5342
129.9762
129.1144
128.2831
127.5529
127.1435
126.9053
125.9029
124.4214
124.3231
123.9220
78.8738
65.7662
54.8005
40.0418
39.8331
39.6246
39.4158
39.2070
38.9984
38.7896
WT110829
13C
DMSO
797/SMP
O
N
N
Pd
Cl
Ph
170
165
160
155
150
145
140
135
130
125
ppm
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3f

Copies of the NMR Spectra of the Catalysis Products



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13C
CDCl3
3248/SMP
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137.3489
132.3994
130.6286
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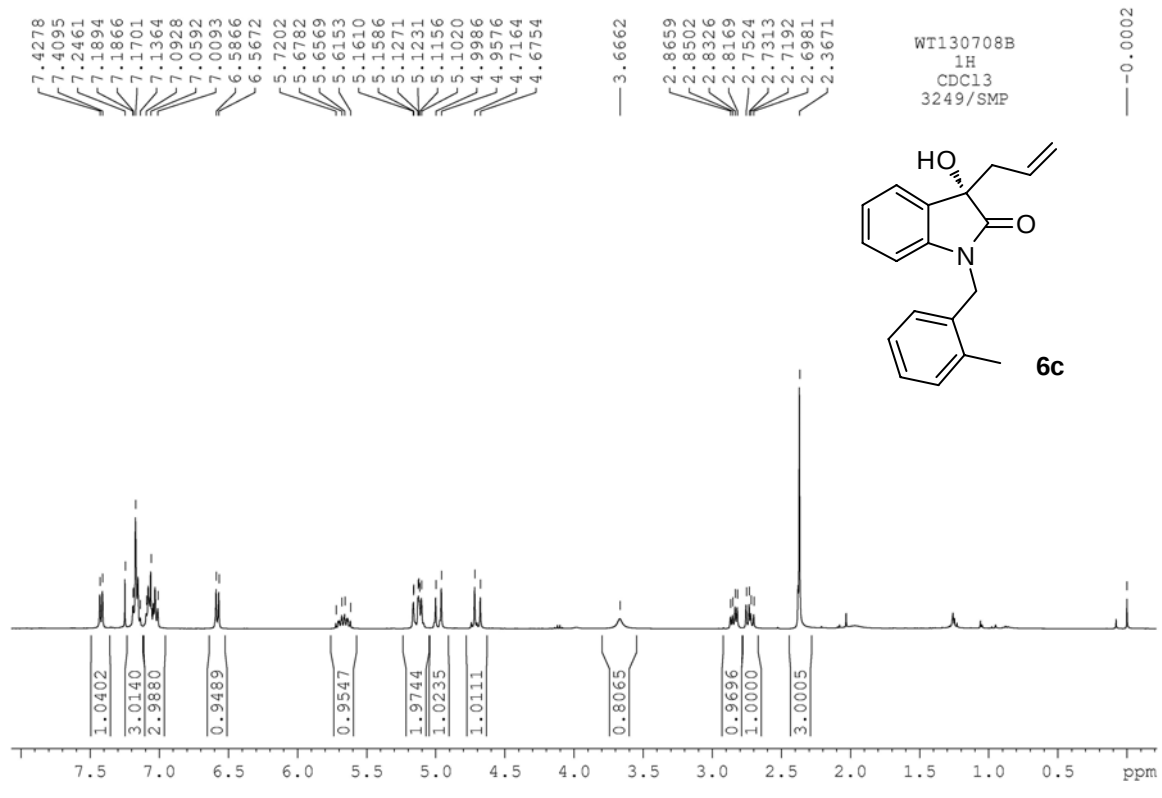
129.5394
129.4223
127.3093
124.1222
123.0315
120.4348
109.5178
77.3876
77.0703
76.7519
76.0080
43.6114
43.0364
21.0886
HO
O
N
6b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.4095
7.2461
7.1894
7.1866
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7.1364
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7.0592
7.0093
6.5866
6.5672
5.7202
5.6782
5.6569
5.6153
5.1610
5.1586
5.1271
5.1231
5.1156
5.1020
4.9986
4.9576
4.7164
4.6754
3.6662
2.8659
2.8502
2.8326
2.8169
2.7524
2.7313
2.7192
2.6981
2.3671
WT130708B
1H
CDCl3
3249/SMP
-0.0002
HO
O
N
6c
1.0402
3.0140
2.9880
0.9489
0.9547
1.9744
1.0235
1.0111
0.8065
0.9696
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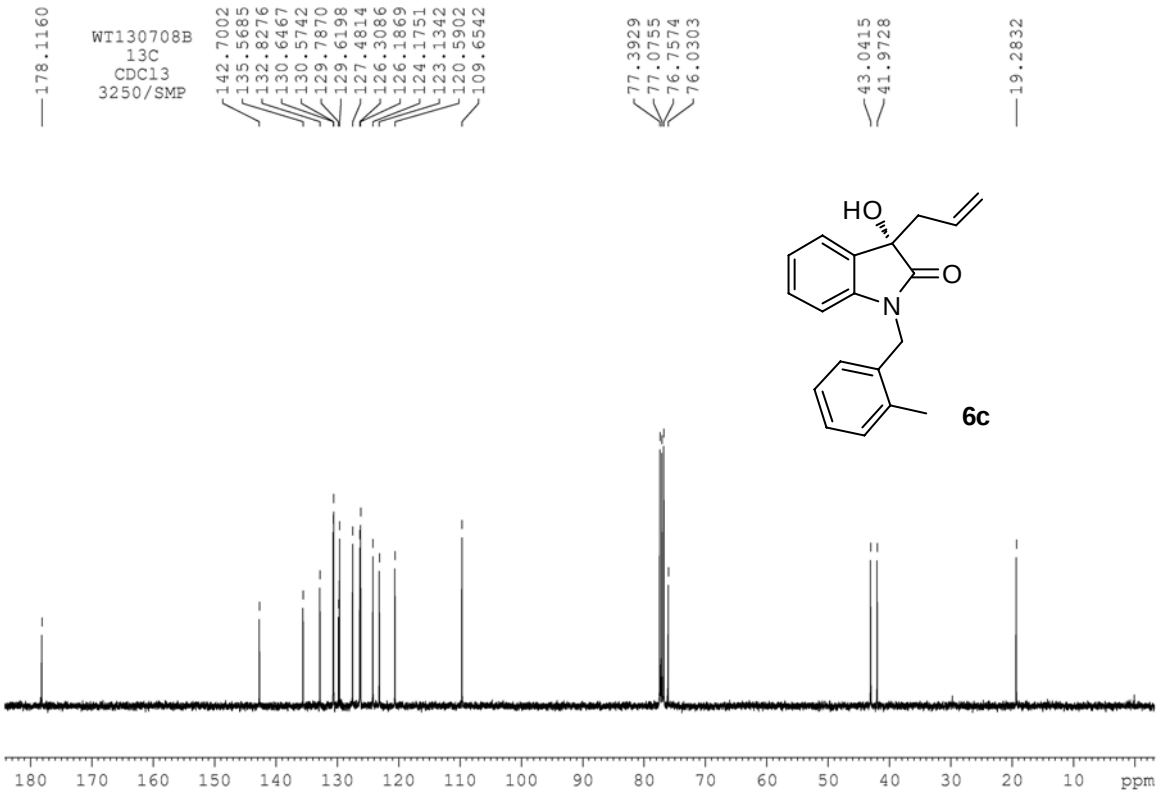
3.0005
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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13C
CDCl3
3250/SMP
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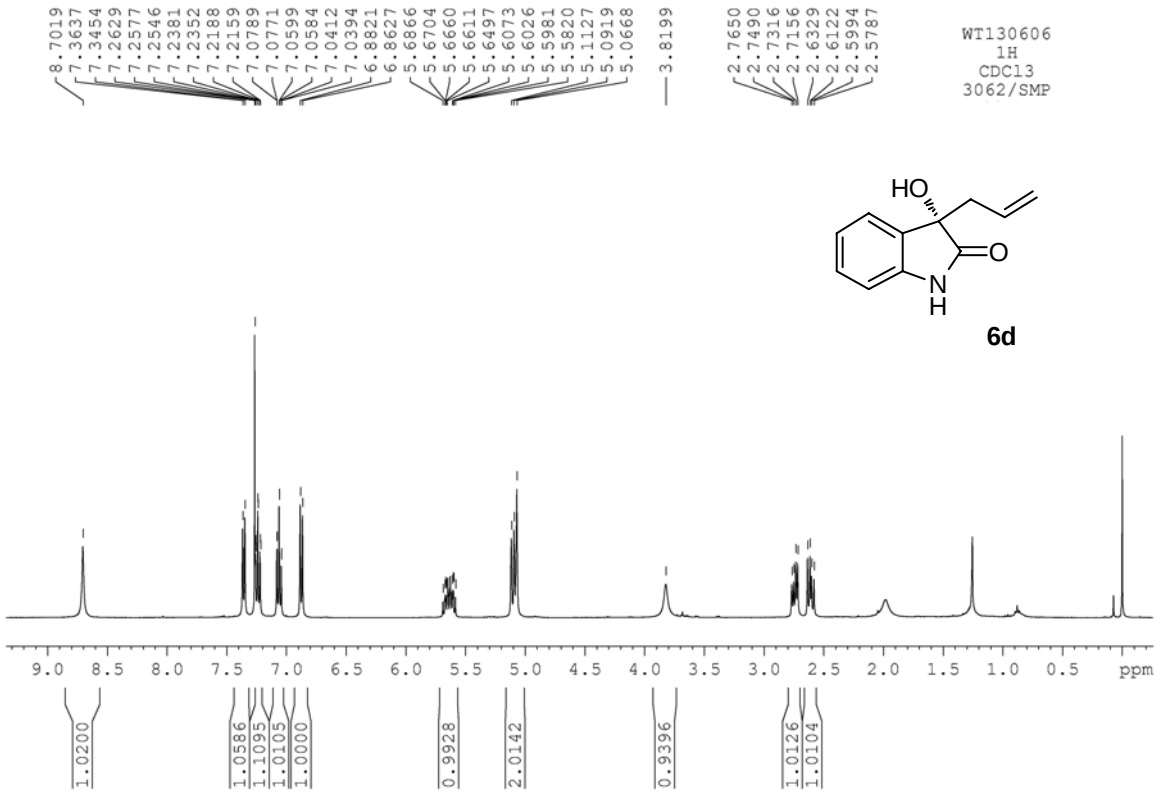
130.5742
129.7870
129.6198
127.4814
126.3086
126.1869
124.1751
123.1342
120.5902
109.6542
77.3929
77.0755
76.7574
76.0303
43.0415
41.9728
19.2832
HO
O
N
6c
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.0789
7.0771
7.0599
7.0584
7.0412
7.0394
6.8821
6.8627
5.6866
5.6704
5.6660
5.6611
5.6497
5.6073
5.6026
5.5981
5.5820
5.1127
5.0919
5.0668
3.8199
2.7650
2.7490
2.7316
2.7156
2.6329
2.6122
2.5994
2.5787
WT130606
1H
CDCl3
3062/SMP
HO
O
N
H
6d
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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1.1095
1.0105
1.0000
0.9928
2.0142
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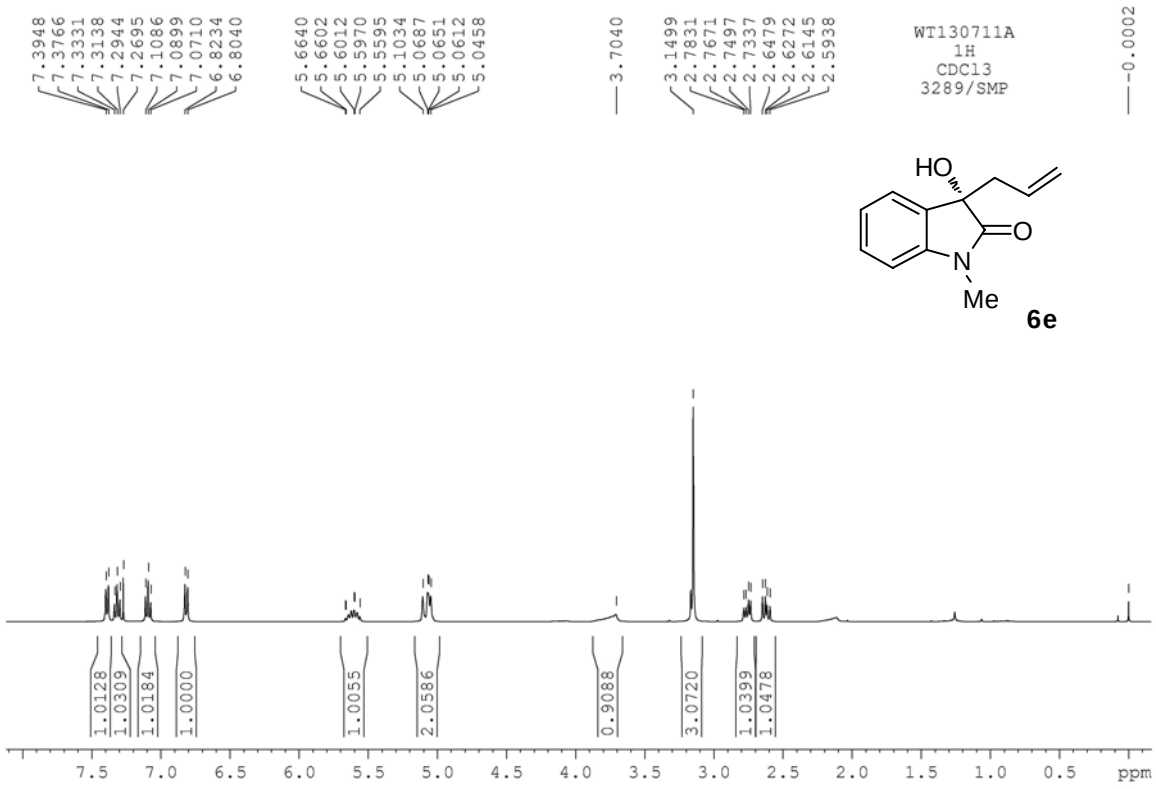
1.0126
1.0104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7.1086
7.0899
7.0710
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6.8040
5.6640
5.6602
5.6012
5.5970
5.5595
5.1034
5.0687
5.0651
5.0612
5.0458
3.7040
3.1499
2.7831
2.7671
2.7497
2.7337
2.6479
2.6272
2.6145
2.5938
WT130711A
1H
CDCl3
3289/SMP
-0.0002
HO
O
N
Me
6e
1.0128
1.0309
1.0184
1.0000
1.0055
2.0586
0.9088
3.0720
1.0399
1.0478
7.5
7.0
6.5
6.0
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4.5
4.0
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3.0
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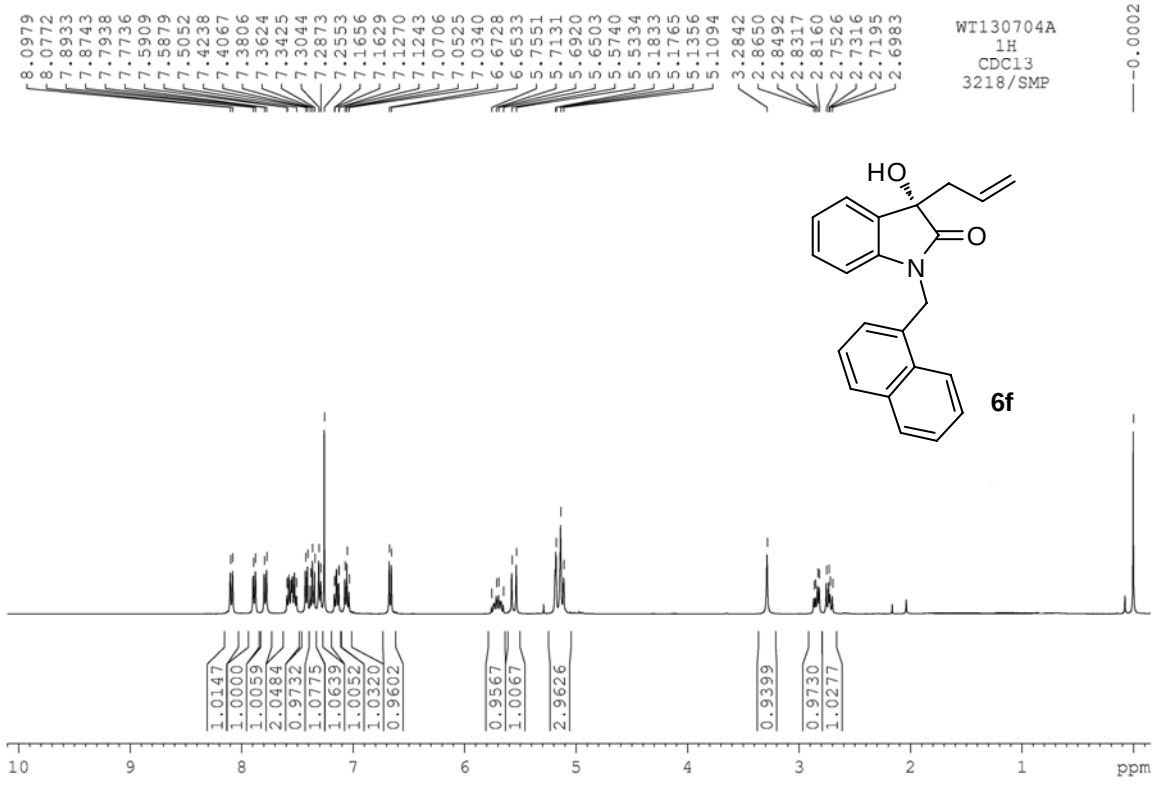
2.0
1.5
1.0
0.5
ppm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7.7736
7.5909
7.5879
7.5052
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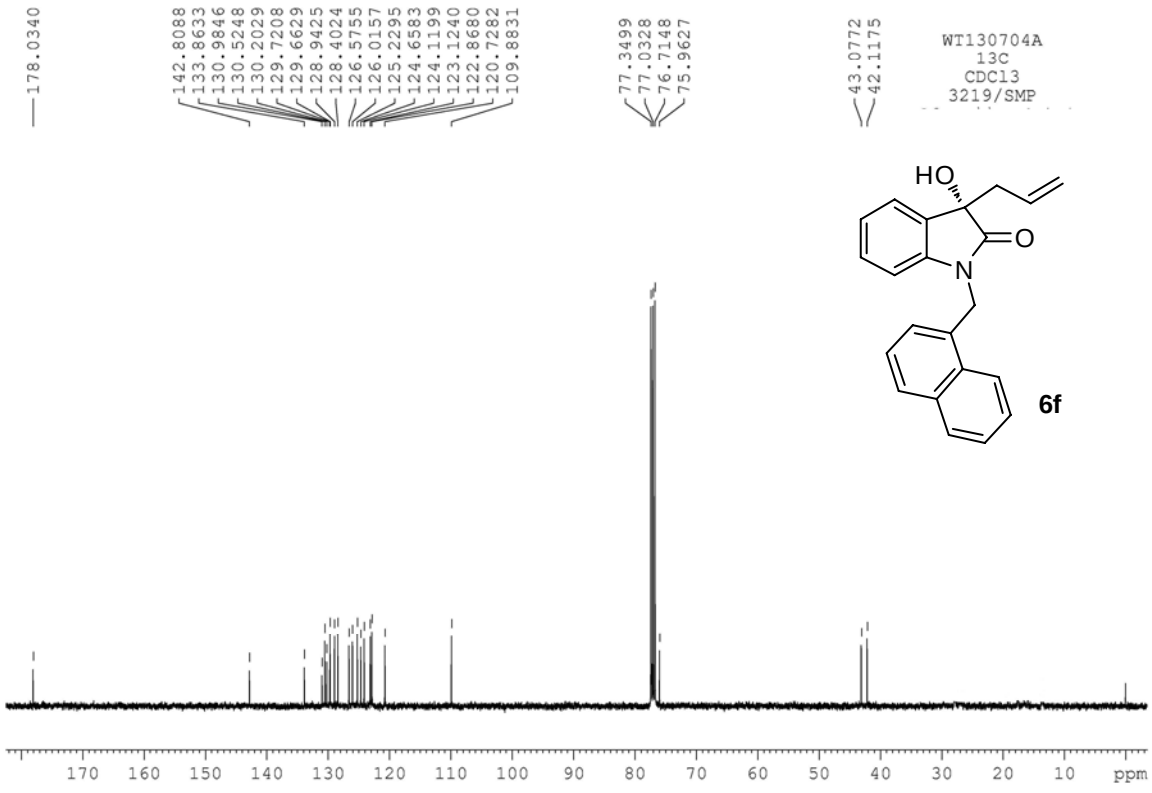
7.4067
7.3806
7.3624
7.3425
7.3044
7.2873
7.2553
7.1656
7.1629
7.1270
7.1243
7.0706
7.0525
7.0340
6.6728
6.6533
5.7551
5.7131
5.6920
5.6503
5.5740
5.5334
5.1833
5.1765
5.1356
5.1094
3.2842
2.8650
2.8492
2.8317
2.8160
2.7526
2.7316
2.7195
2.6983
WT130704A
1H
CDCl3
3218/SMP
-0.0002
HO
O
N
6f
1.0147
1.0000
1.0059
2.0484
0.9732
1.0775
1.0639
1.0052
1.0320
0.9602
0.9567
1.0067
2.9626
0.9399
0.9730
1.0277
10
9
8
7
6
5
4
3
2
1
ppm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130.5248
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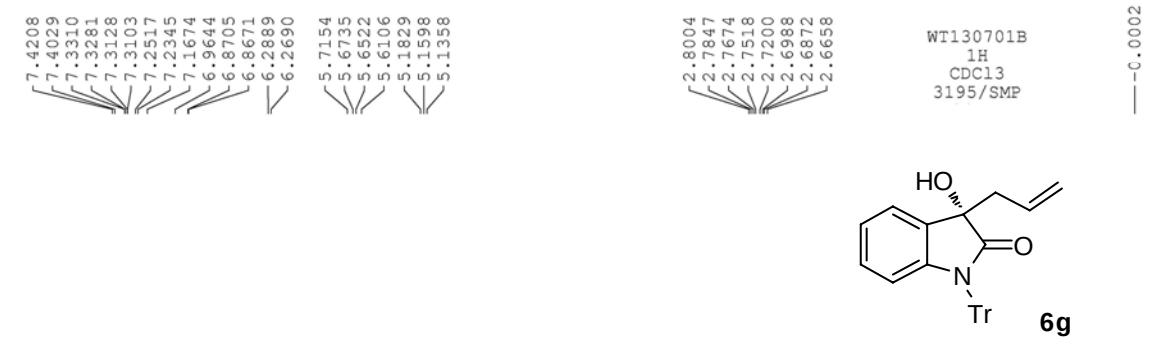
129.7208
129.6629
128.9425
128.4024
126.5755
126.0157
125.2295
124.6583
124.1199
123.1240
122.8680
120.7282
109.8831
77.3499
77.0328
76.7148
75.9627
43.0772
42.1175
WT130704A
13C
CDCl3
3219/SMP
HO
O
N
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

6f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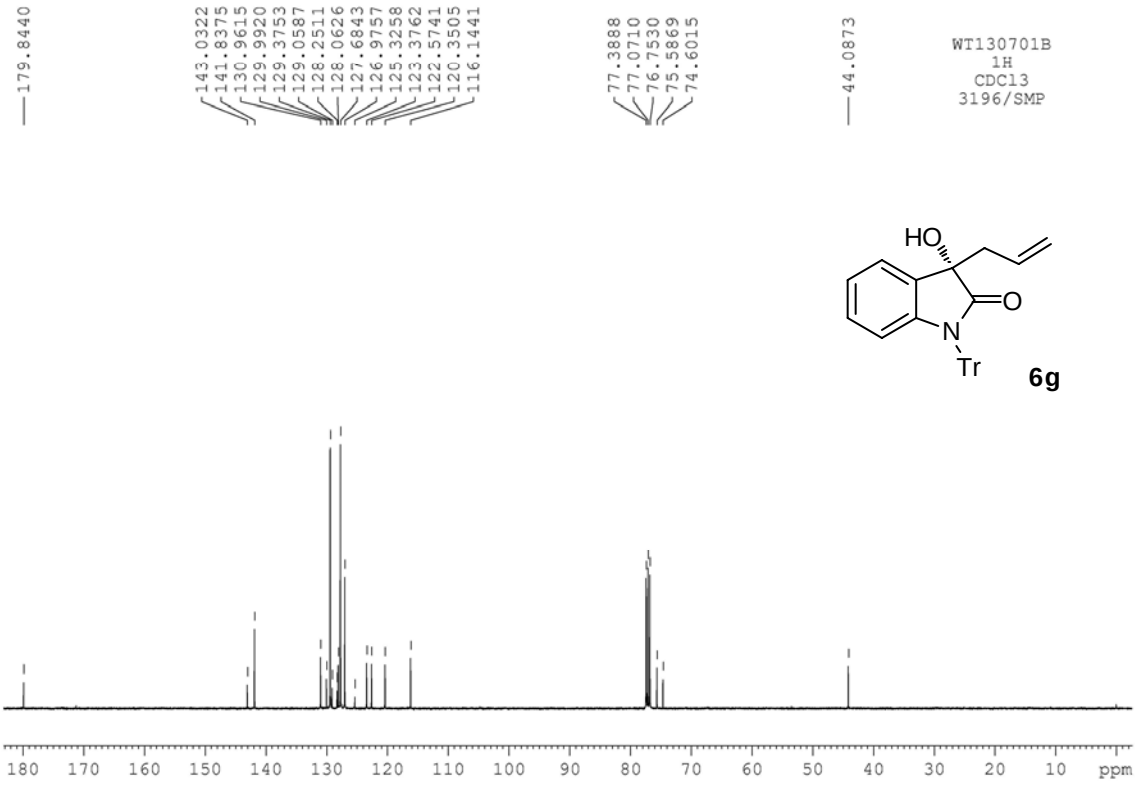
7.3128
7.3103
7.2517
7.2345
7.1674
6.9644
6.8705
6.8671
6.2889
6.2690
5.7154
5.6735
5.6522
5.6106
5.1829
5.1598
5.1358
2.8004
2.7847
2.7674
2.7518
2.7200
2.6988
2.6872
2.6658
WT130701B
1H
CDCl3
3195/SMP
-0.0002
6.0768
1.1278
10.3601
2.0655
1.0000
1.0081
1.0130
0.9899
1.0625
1.0859
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

6g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143.0322
141.8375
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129.9920
129.3753
129.0587
128.2511
128.0626
127.6843
126.9757
125.3258
123.3762
122.5741
120.3505
116.1441
77.3888
77.0710
76.7530
75.5869
74.6015
44.0873
WT130701B
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CDCl3
3196/SMP
HO
O
N
Tr
6g
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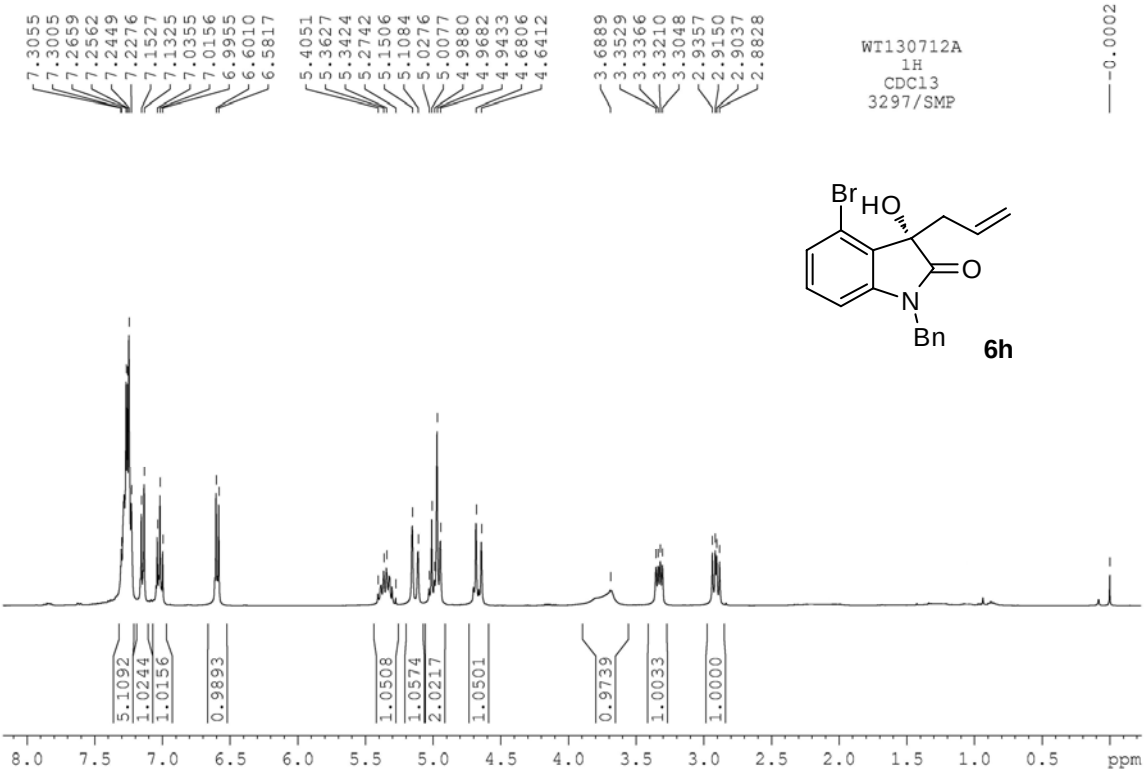
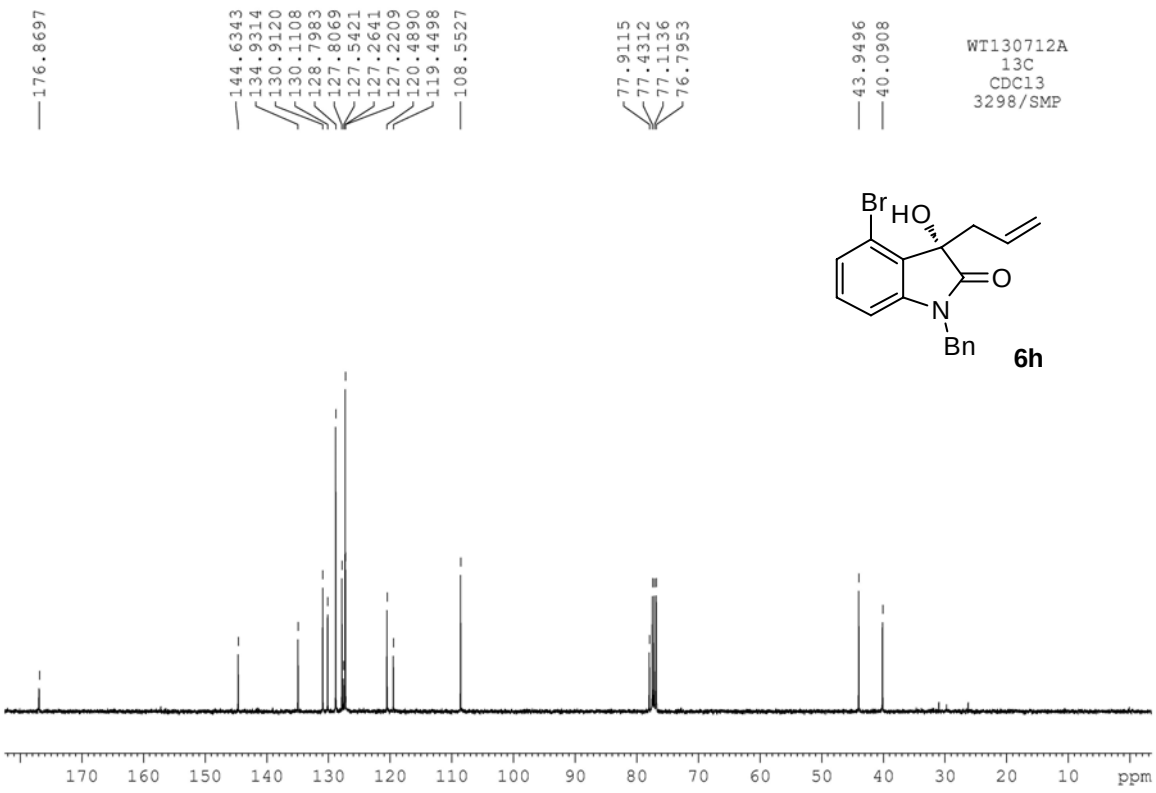

7.3055
7.3005
7.2659
7.2562
7.2449
7.2276
7.1527
7.1325
7.0355
7.0156
6.9955
6.6010
6.5817
5.4051
5.3627
5.3424
5.2742
5.1506
5.1084
5.0276
5.0077
4.9880
4.9682
4.9433
4.6806
4.6412
3.6889
3.3529
3.3366
3.3210
3.3048
2.9357
2.9150
2.9037
2.8828
WT130712A
1H
CDCl3
3297/SMP
-0.0002
Br
HO
O
N
Bn
6h
5.1092
1.0244
1.0156
0.9893
1.0508
1.0574
2.0217
1.0501
0.9739
1.0033
1.0000
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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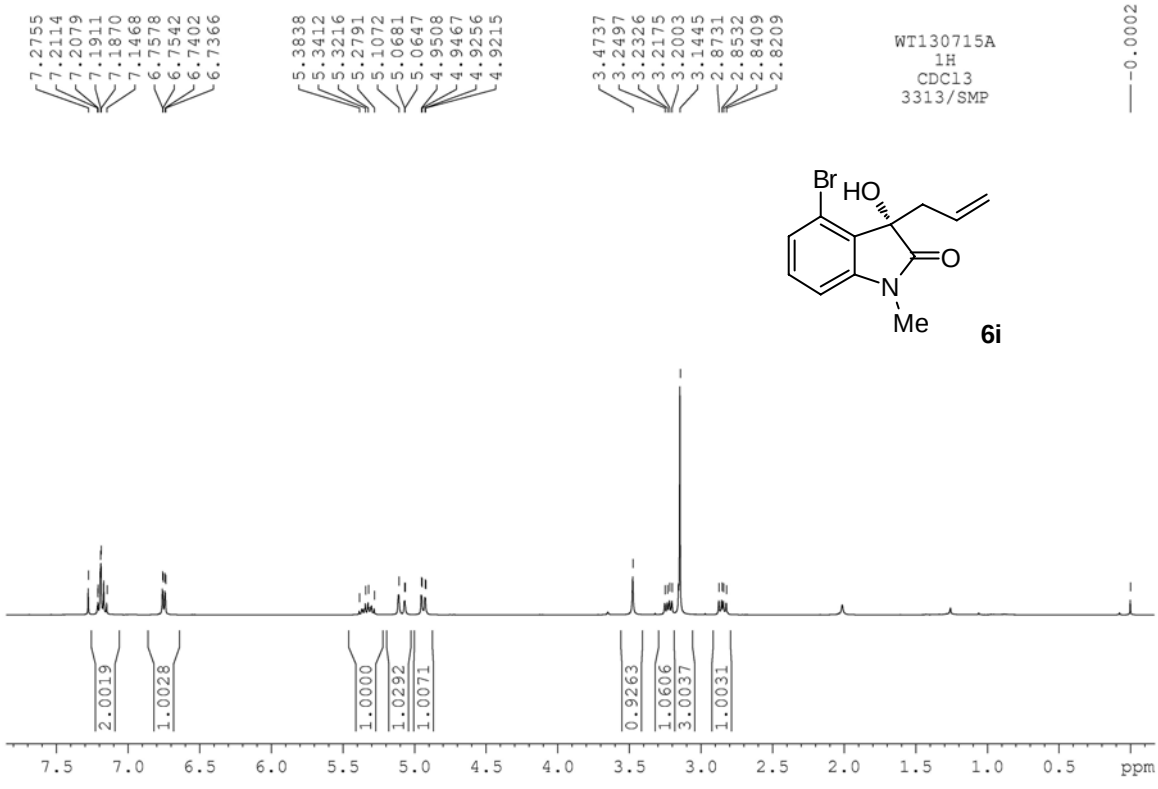
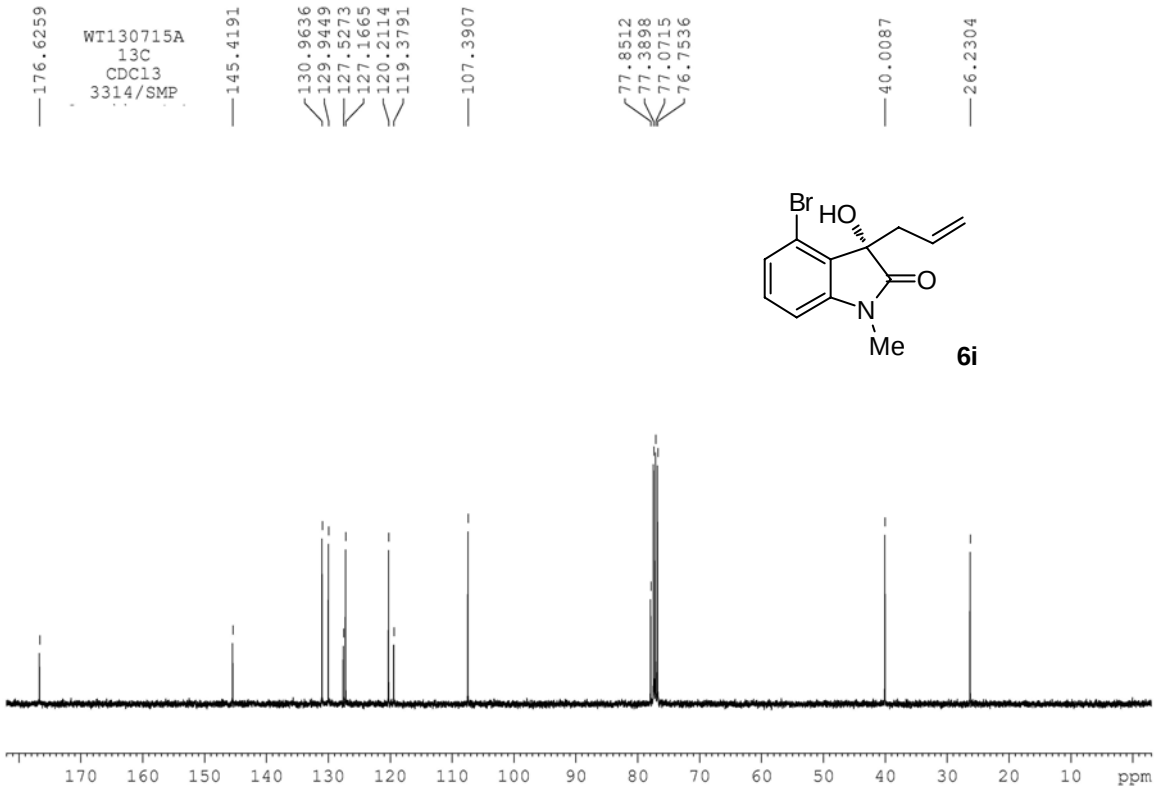
134.9314
130.9120
130.1108
128.7983
127.8069
127.5421
127.2641
127.2209
120.4890
119.4498
108.5527
77.9115
77.4312
77.1136
76.7953
43.9496
40.0908
WT130712A
13C
CDCl3
3298/SMP
Br
HO
O
N
Bn
6h
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.2755
7.2114
7.2079
7.1911
7.1870
7.1468
6.7578
6.7542
6.7402
6.7366
5.3838
5.3412
5.3216
5.2791
5.1072
5.0681
5.0647
4.9508
4.9467
4.9256
4.9215
3.4737
3.2497
3.2326
3.2175
3.2003
3.1445
2.8731
2.8532
2.8409
2.8209
WT130715A
1H
CDCl3
3313/SMP
0.0002
Br
HO
O
N
Me
6i
2.0019
1.0028
1.0000
1.0292
1.0071
0.9263
1.0606
3.0037
1.0031
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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13C
CDCl3
3314/SMP
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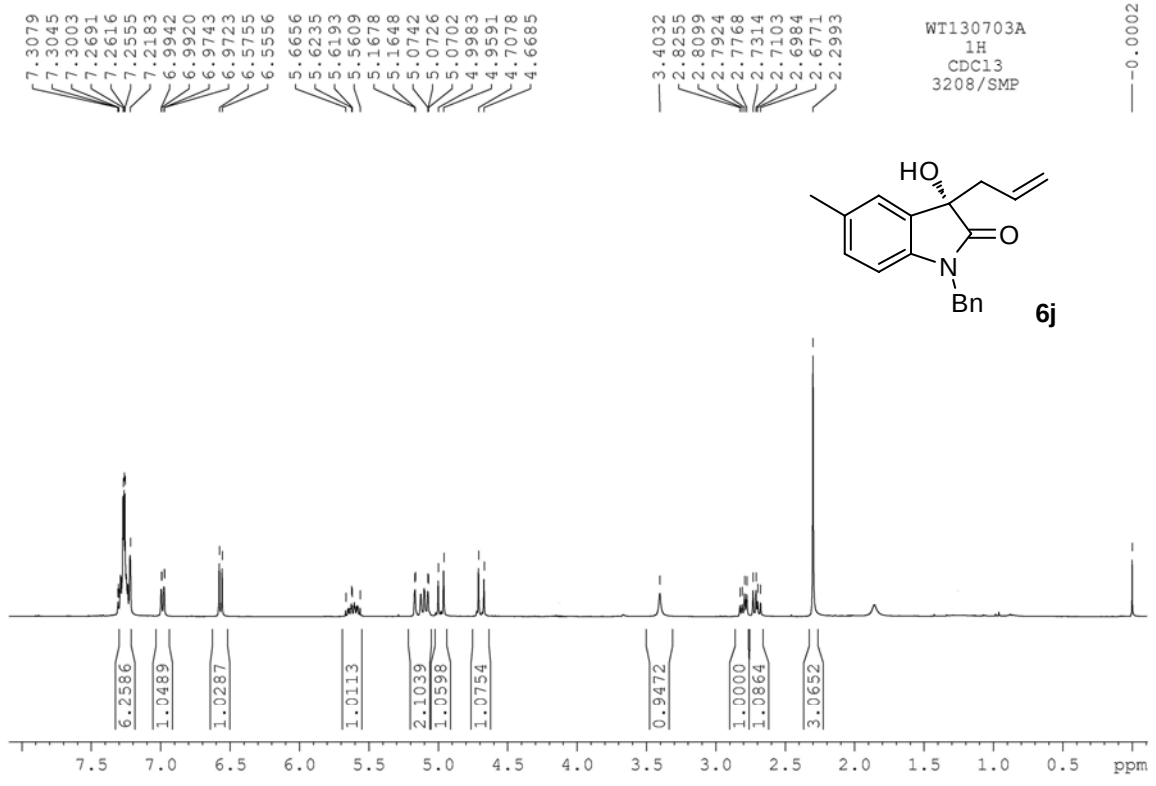
130.9636
129.9449
127.5273
127.1665
120.2114
119.3791
107.3907
77.8512
77.3898
77.0715
76.7536
40.0087
26.2304
Br
HO
O
N
Me
6i
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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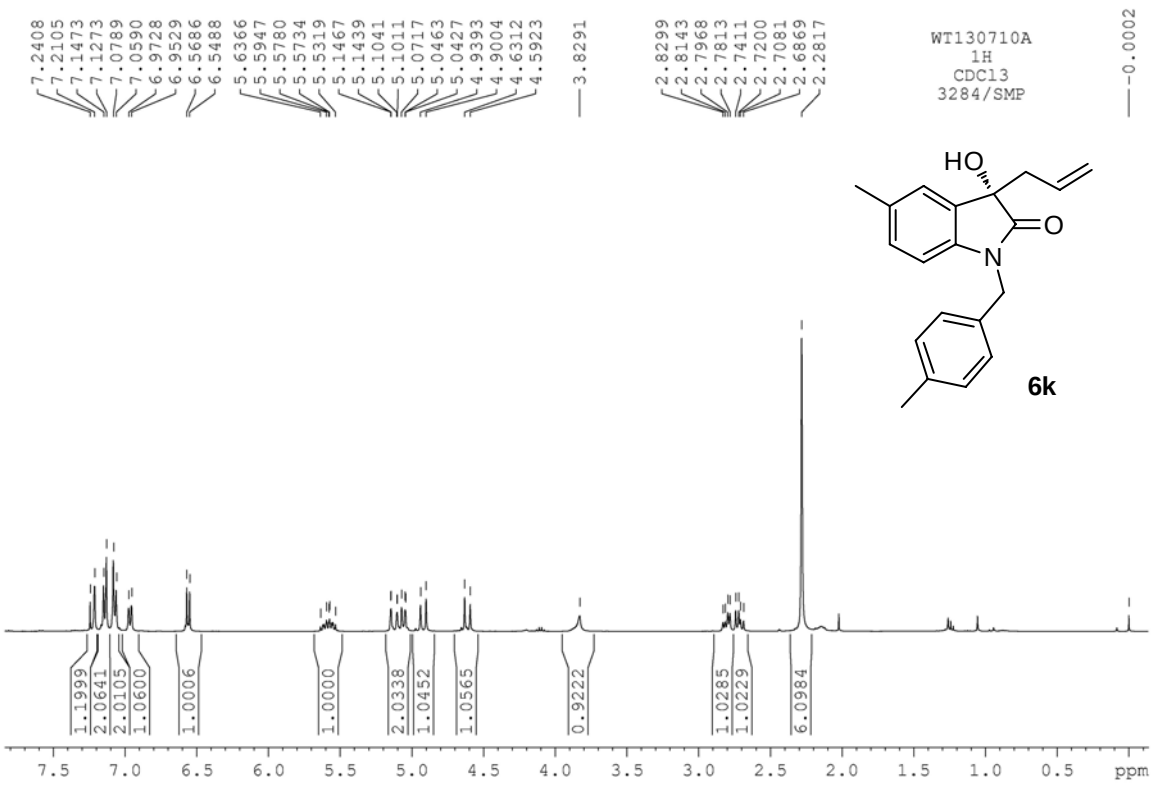
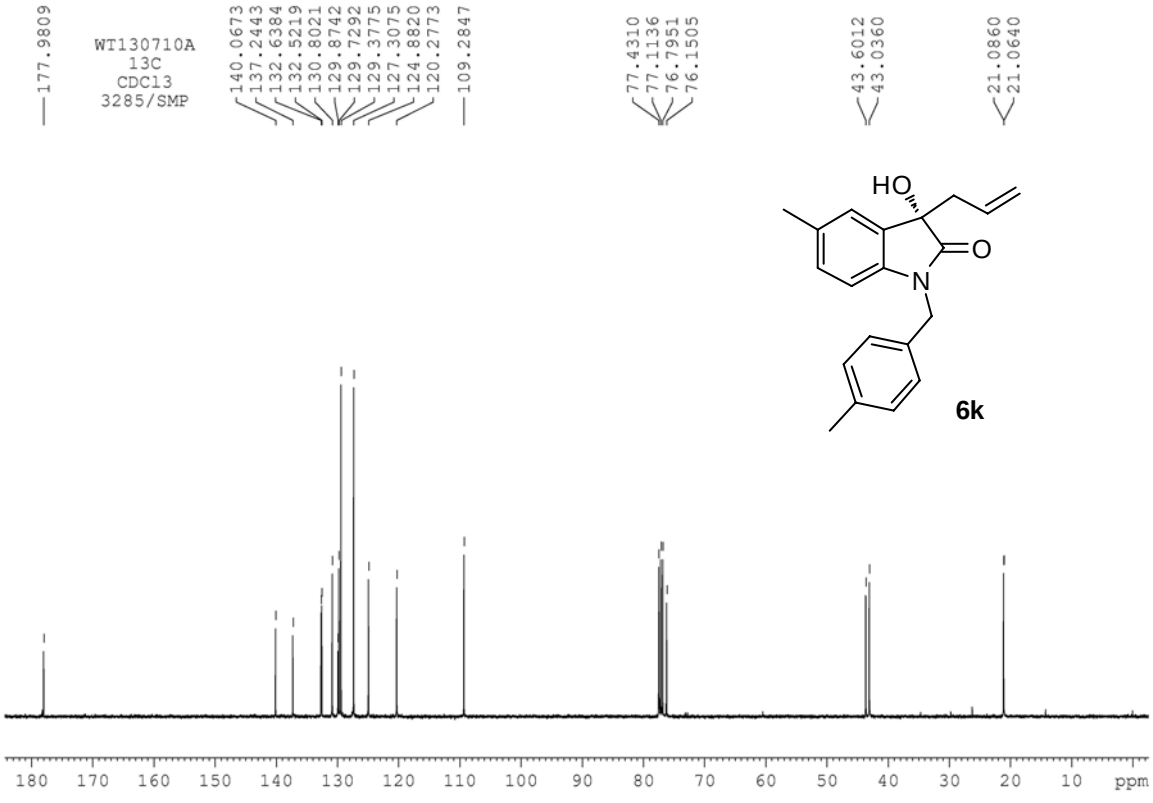
7.3045
7.3003
7.2691
7.2616
7.2555
7.2183
6.9942
6.9920
6.9743
6.9723
6.5755
6.5556
5.6656
5.6235
5.6193
5.5609
5.1678
5.1648
5.0742
5.0726
5.0702
4.9983
4.9591
4.7078
4.6685
3.4032
2.8255
2.8099
2.7924
2.7768
2.7314
2.7103
2.6984
2.6771
2.2993
WT130703A
1H
CDCl3
3208/SMP
0.0002
HO
O
N
Bn
6j
6.2586
1.0489
1.0287
1.0113
2.1039
1.0598
1.0754
0.9472
1.0000
1.0864
3.0652
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


7.2408
7.2105
7.1473
7.1273
7.0789
7.0590
6.9728
6.9529
6.5686
6.5488
5.6366
5.5947
5.5780
5.5734
5.5319
5.1467
5.1439
5.1041
5.1011
5.0717
5.0463
5.0427
4.9393
4.9004
4.6312
4.5923
3.8291
2.8299
2.8143
2.7968
2.7813
2.7411
2.7200
2.7081
2.6869
2.2817
WT130710A
1H
CDCl3
3284/SMP
-0.0002
HO
O
N
6k
1.1999
2.0641
2.0105
1.0600
1.0006
1.0000
2.0338
1.0452
1.0565
0.9222
1.0285
1.0229
6.0984
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm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WT130710A
13C
CDCl3
3285/SMP
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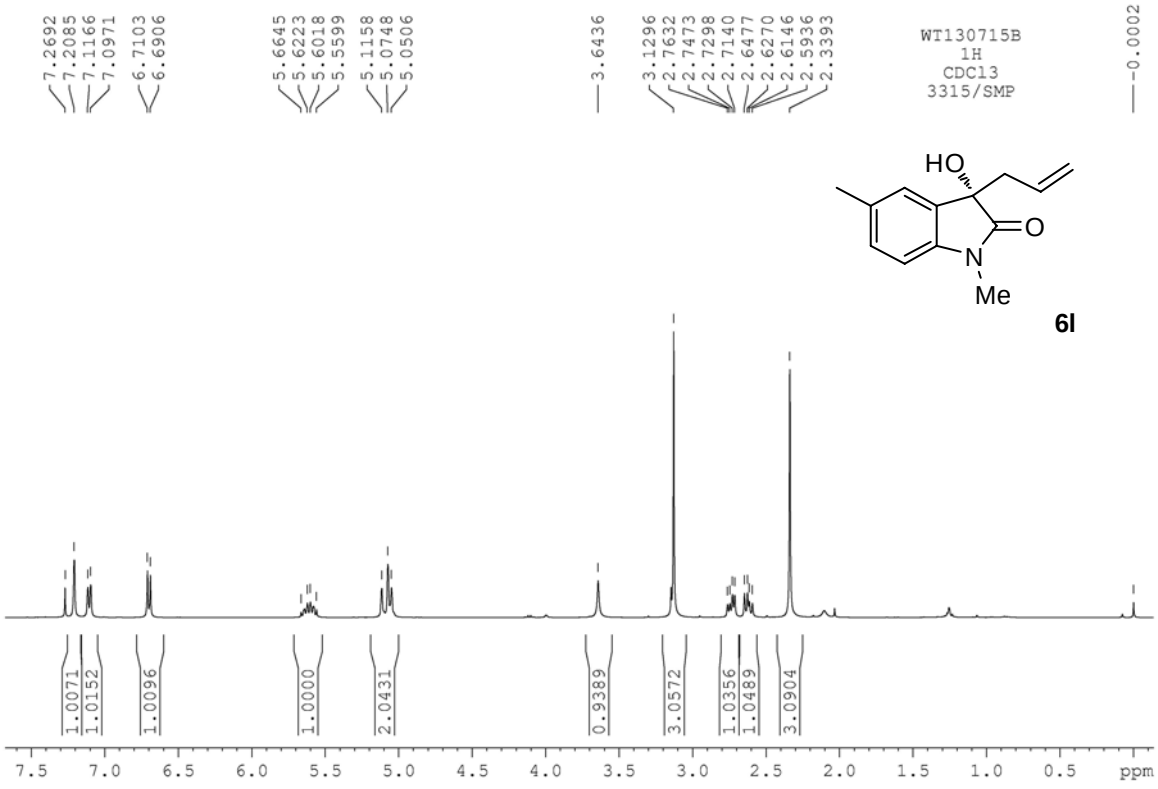
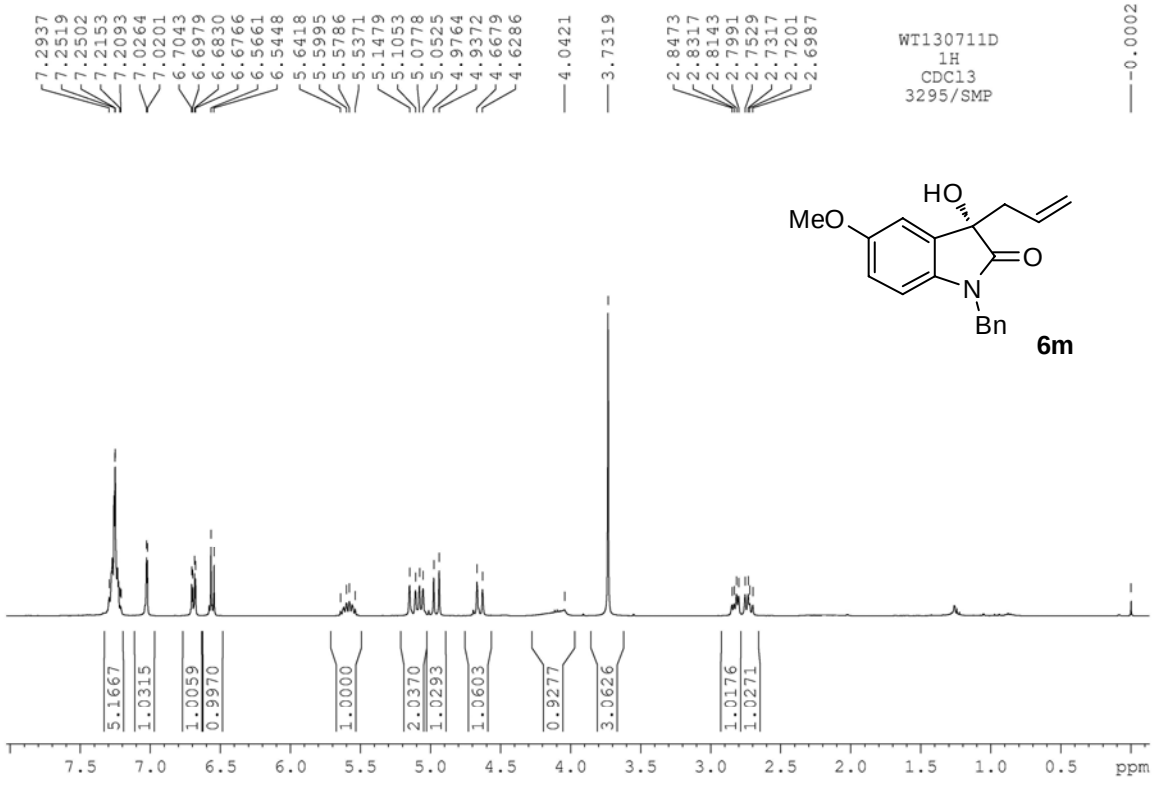
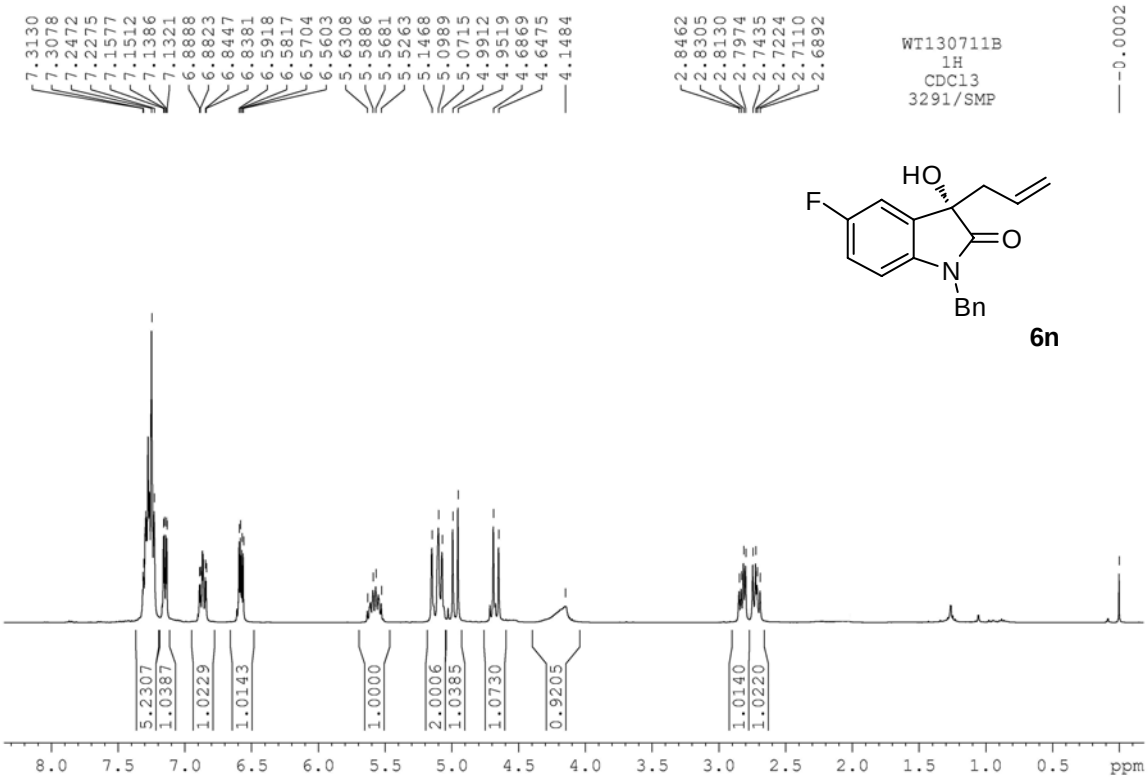
137.2443
132.6384
132.5219
130.8021
129.8742
129.7292
129.3775
127.3075
124.8820
120.2773
109.2847
77.4310
77.1136
76.7951
76.1505
43.6012
43.0360
21.0860
21.0640
HO
O
N
6k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.2692
7.2085
7.1166
7.0971
6.7103
6.6906
5.6645
5.6223
5.6018
5.5599
5.1158
5.0748
5.0506
3.6436
3.1296
2.7632
2.7473
2.7298
2.7140
2.6477
2.6270
2.6146
2.5936
2.3393
WT130715B
1H
CDCl3
3315/SMP
-0.0002
HO
O
N
Me
1.0071
1.0152
1.0096
1.0000
2.0431
0.9389
3.0572
1.0356
1.0489
3.0904
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

6l


7.2937
7.2519
7.2502
7.2153
7.2093
7.0264
7.0201
6.7043
6.6979
6.6830
6.6766
6.5661
6.5448
5.6418
5.5995
5.5786
5.5371
5.1479
5.1053
5.0778
5.0525
4.9764
4.9372
4.6679
4.6286
4.0421
3.7319
2.8473
2.8317
2.8143
2.7991
2.7529
2.7317
2.7201
2.6987
WT130711D
1H
CDCl3
3295/SMP
-0.0002
HO
MeO
O
N
Bn
5.1667
1.0315
1.0059
0.9970
1.0000
2.0370
1.0293
1.0603
0.9277
3.0626
1.0176
1.0271
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

6m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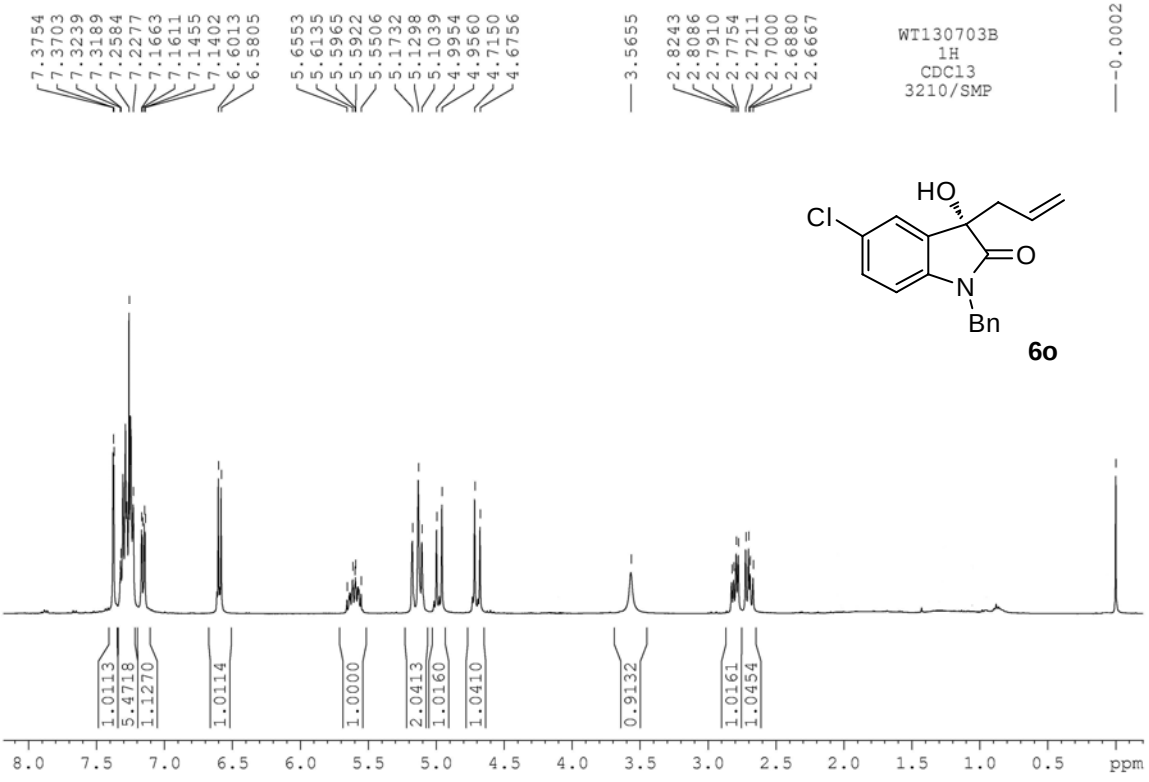
7.3078
7.2472
7.2275
7.1577
7.1512
7.1386
7.1321
6.8888
6.8823
6.8447
6.8381
6.5918
6.5817
6.5704
6.5603
5.6308
5.5886
5.5681
5.5263
5.1468
5.0989
5.0715
4.9912
4.9519
4.6869
4.6475
4.1484
2.8462
2.8305
2.8130
2.7974
2.7435
2.7224
2.7110
2.6892
WT130711B
1H
CDCl3
3291/SMP
-0.0002
HO
F
O
N
Bn
5.2307
1.0387
1.0229
1.0143
1.0000
2.0006
1.0385
1.0730
0.9205
1.0140
1.0220
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

6n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7.3239
7.3189
7.2584
7.2277
7.1663
7.1611
7.1455
7.1402
6.6013
6.5805
5.6553
5.6135
5.5965
5.5922
5.5506
5.1732
5.1298
5.1039
4.9954
4.9560
4.7150
4.6756
3.5655
2.8243
2.8086
2.7910
2.7754
2.7211
2.7000
2.6880
2.6667
WT130703B
1H
CDCl3
3210/SMP
-0.0002
HO
Cl
O
N
Bn
1.0113
5.4718
1.1270
1.0114
1.0000
2.0413
1.0160
1.0410
0.9132
1.0161
1.0454
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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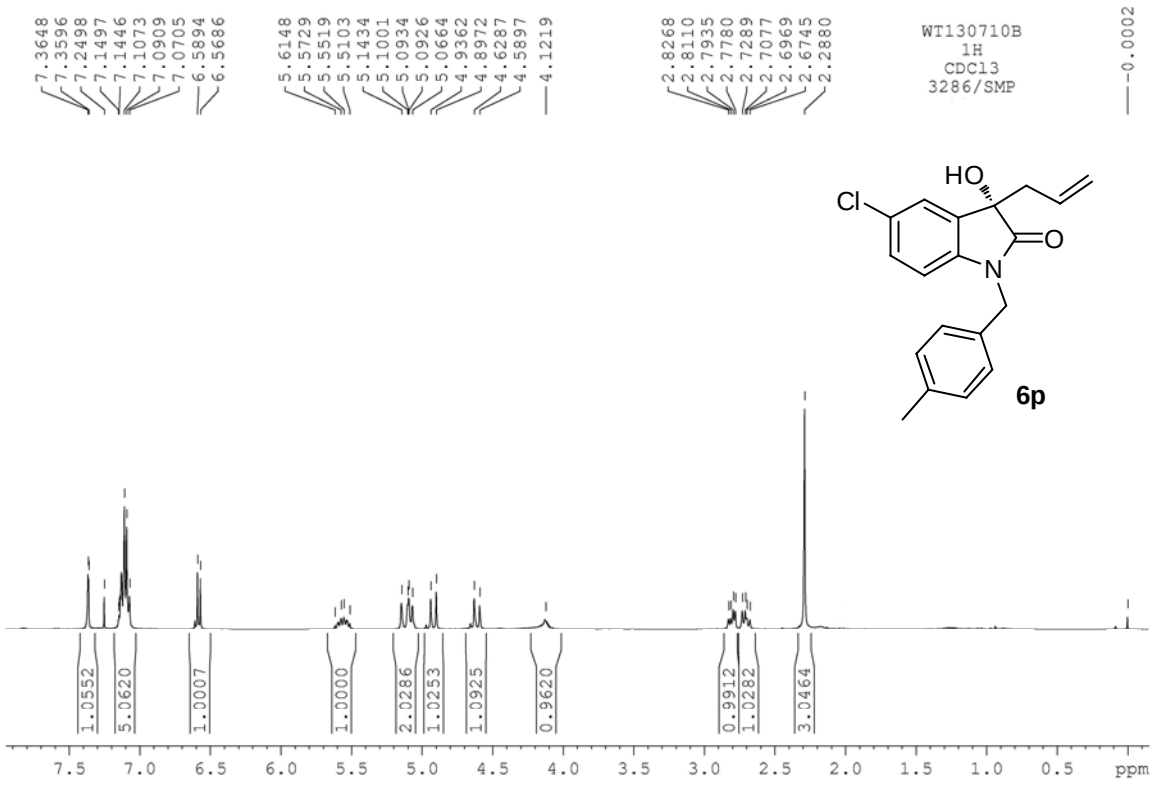
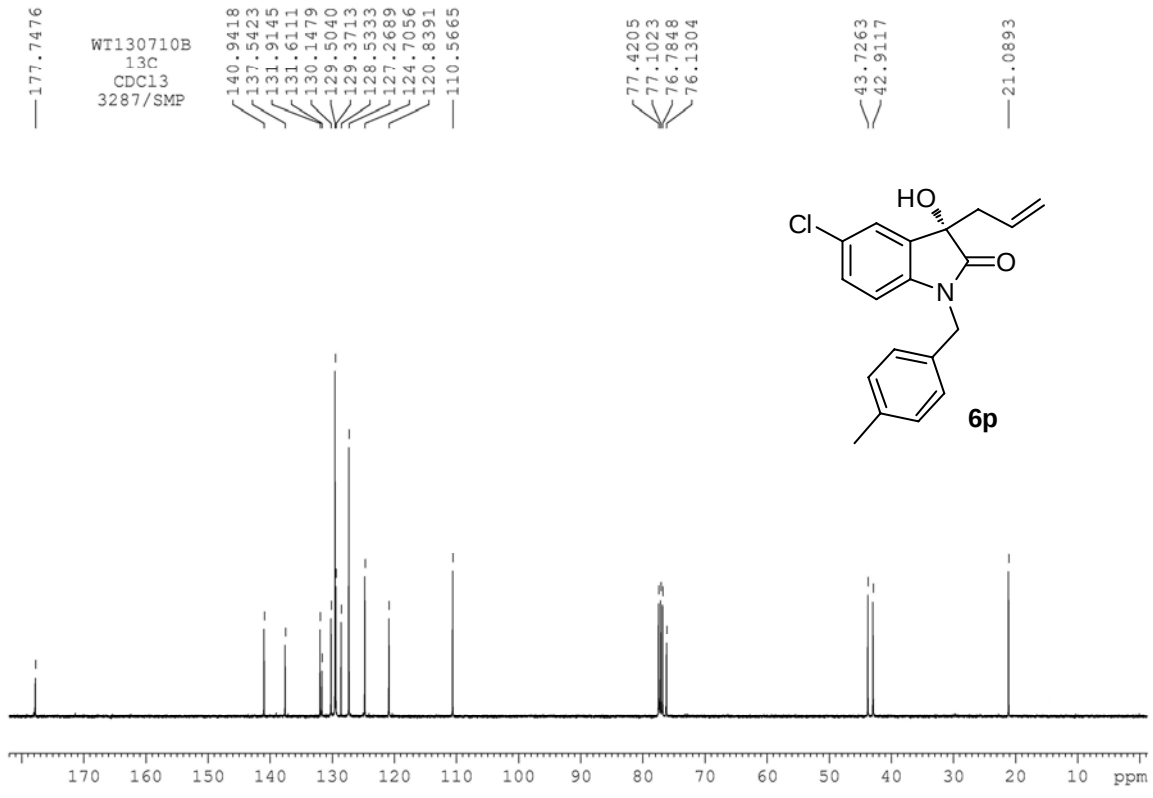
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

6o


7.3648
7.3596
7.2498
7.1497
7.1446
7.1073
7.0909
7.0705
6.5894
6.5686
5.6148
5.5729
5.5519
5.5103
5.1434
5.1001
5.0934
5.0926
5.0664
4.9362
4.8972
4.6287
4.5897
4.1219
2.8268
2.8110
2.7935
2.7780
2.7289
2.7077
2.6969
2.6745
2.2880
WT130710B
1H
CDCl3
3286/SMP
-0.0002
HO
Cl
O
N
6p
1.0552
5.0620
1.0007
1.0000
2.0286
1.0253
1.0925
0.9620
0.9912
1.0282
3.0464
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


177.7476
WT130710B
13C
CDCl3
3287/SMP
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137.5423
131.9145
131.6111
130.1479
129.5040
129.3713
128.5333
127.2689
124.7056
120.8391
110.5665
77.4205
77.1023
76.7848
76.1304
43.7263
42.9117
21.0893
HO
Cl
O
N
6p
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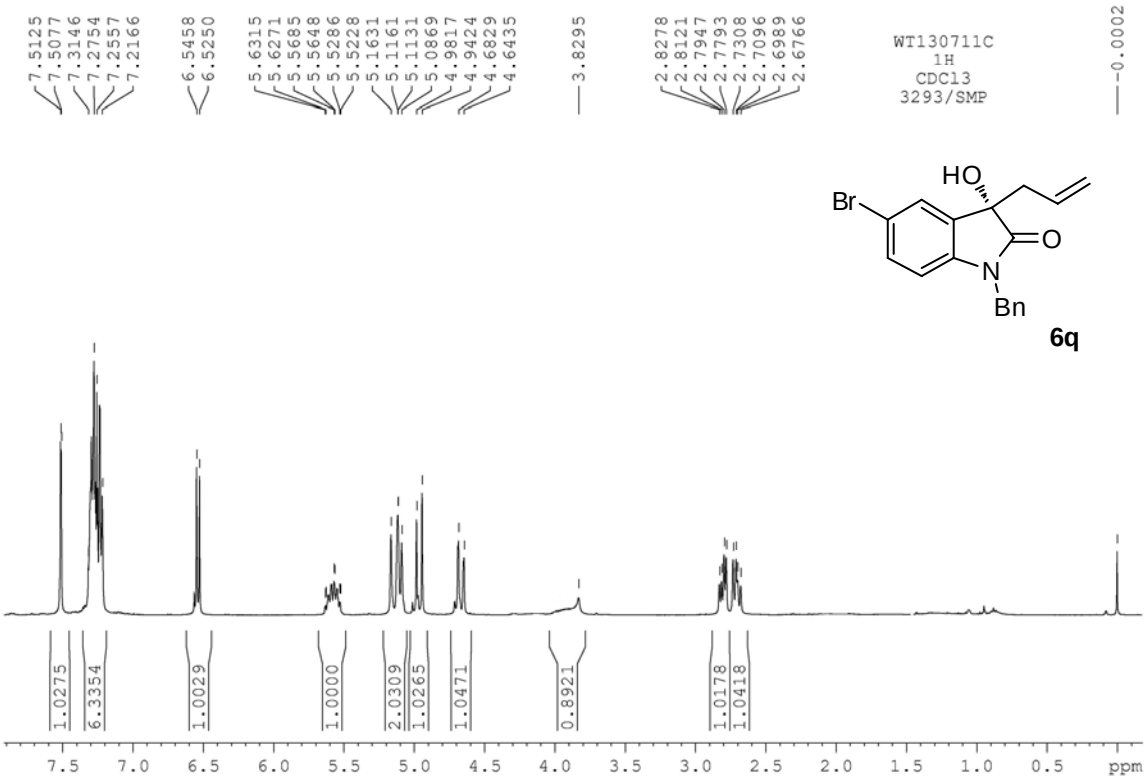
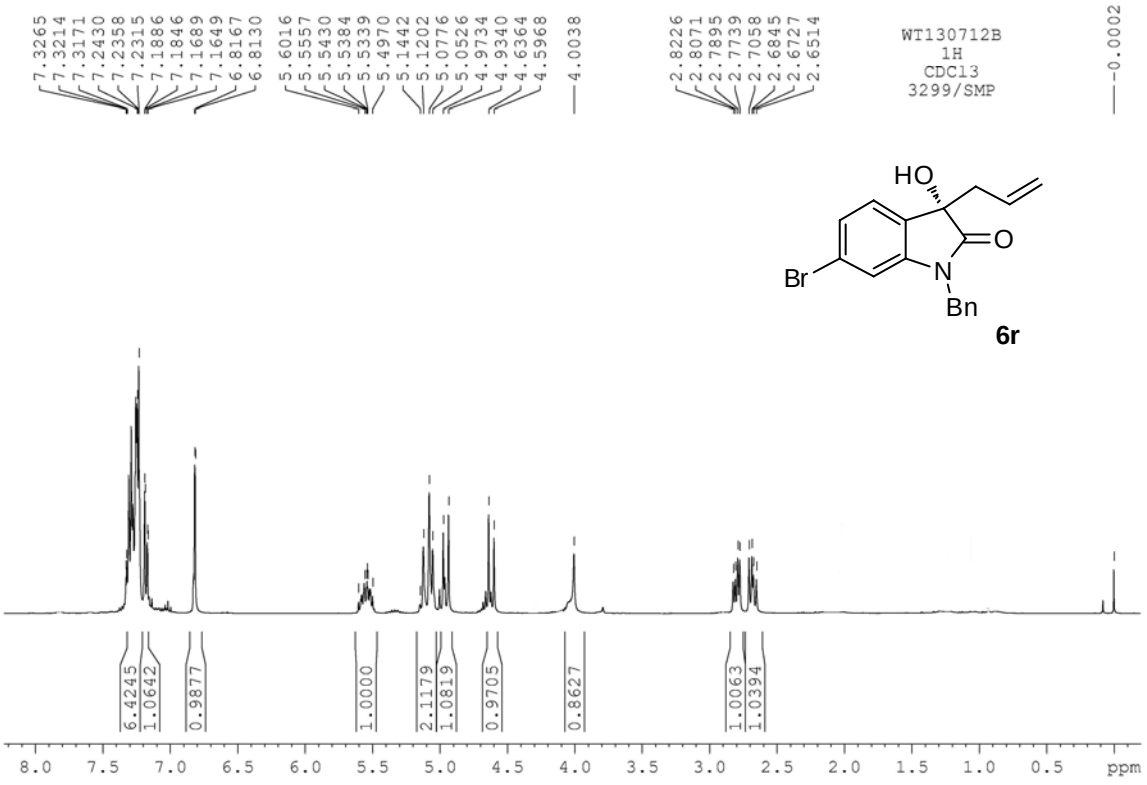
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.5125
7.5077
7.3446
7.2754
7.2557
7.2166
6.5458
6.5250
5.6315
5.6271
5.5685
5.5648
5.5286
5.5228
5.1631
5.1161
5.1131
5.0869
4.9817
4.9424
4.6829
4.6435
3.8295
2.8278
2.8121
2.7947
2.7793
2.7308
2.7096
2.6989
2.6766
WT130711C
1H
CDCl3
3293/SMP
-0.0002
HO
Br
O
N
Bn
6q
1.0275
6.3354
1.0029
1.0000
2.0309
1.0265
1.0471
0.8921
1.0178
1.0418
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


7.3265
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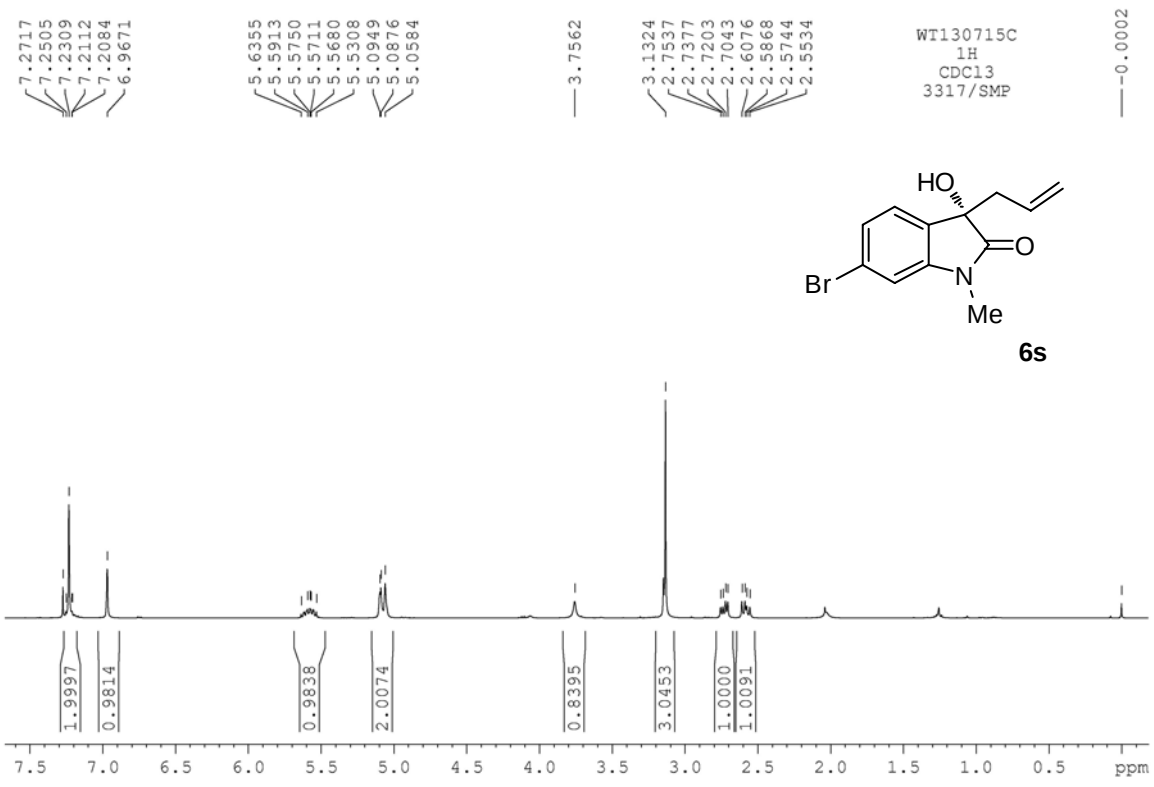
7.3171
7.2430
7.2358
7.2315
7.1886
7.1846
7.1689
7.1649
6.8167
6.8130
5.6016
5.5557
5.5430
5.5384
5.5339
5.4970
5.1442
5.1202
5.0776
5.0526
4.9734
4.9340
4.6364
4.5968
4.0038
2.8226
2.8071
2.7895
2.7739
2.7058
2.6845
2.6727
2.6514
WT130712B
1H
CDCl3
3299/SMP
-0.0002
HO
O
Br
N
Bn
6r
6.4245
1.0642
0.9877
1.0000
2.1179
1.0819
0.9705
0.8627
1.0063
1.0394
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm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7.2505
7.2309
7.2112
7.2084
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5.5750
5.5711
5.5680
5.5308
5.0949
5.0876
5.0584
3.7562
3.1324
2.7537
2.7377
2.7203
2.7043
2.6076
2.5868
2.5744
2.5534
WT130715C
1H
CDCl3
3317/SMP
0.0002
HO
O
Br
N
Me
1.9997
0.9814
0.9838
2.0074
0.8395
3.0453
1.0000
1.0091
7.5
7.0
6.5
6.0
5.5
5.0
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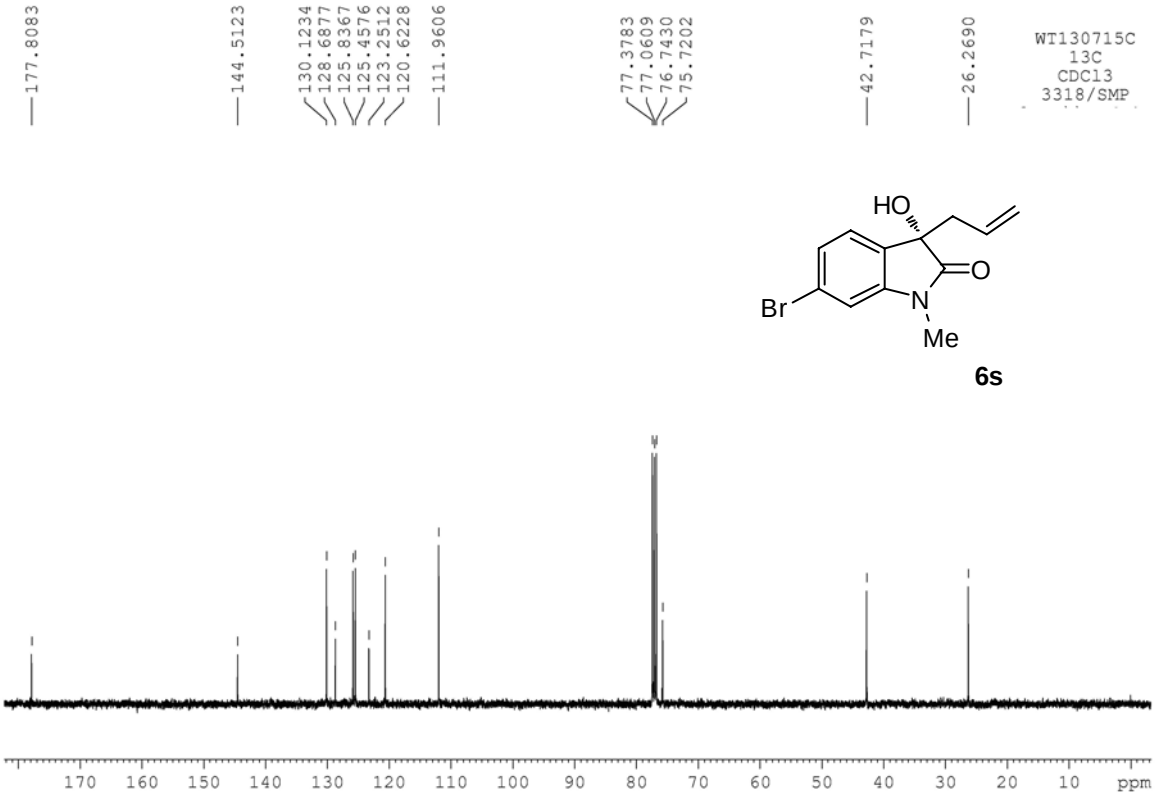
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

6s


177.8083
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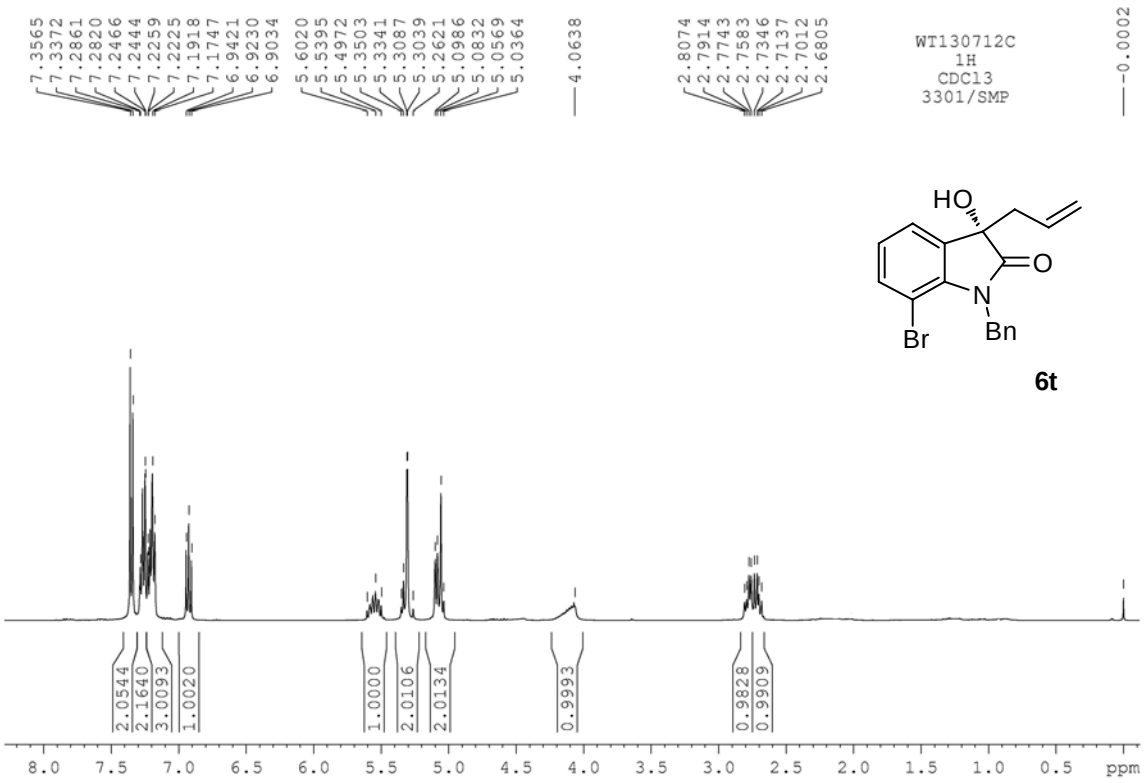
130.1234
128.6877
125.8367
125.4576
123.2512
120.6228
111.9606
77.3783
77.0609
76.7430
75.7202
42.7179
26.2690
WT130715C
13C
CDCl3
3318/SMP
HO
O
Br
N
Me
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

6s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7.1918
7.1747
6.9421
6.9230
6.9034
5.6020
5.5395
5.4972
5.3503
5.3341
5.3087
5.3039
5.2621
5.0986
5.0832
5.0569
5.0364
4.0638
2.8074
2.7914
2.7743
2.7583
2.7346
2.7137
2.7012
2.6805
WT130712C
1H
CDCl3
3301/SMP
-0.0002
HO
O
N
Bn
Br
2.0544
2.1640
3.0093
1.0020
1.0000
2.0106
2.0134
0.9993
0.9828
0.9909
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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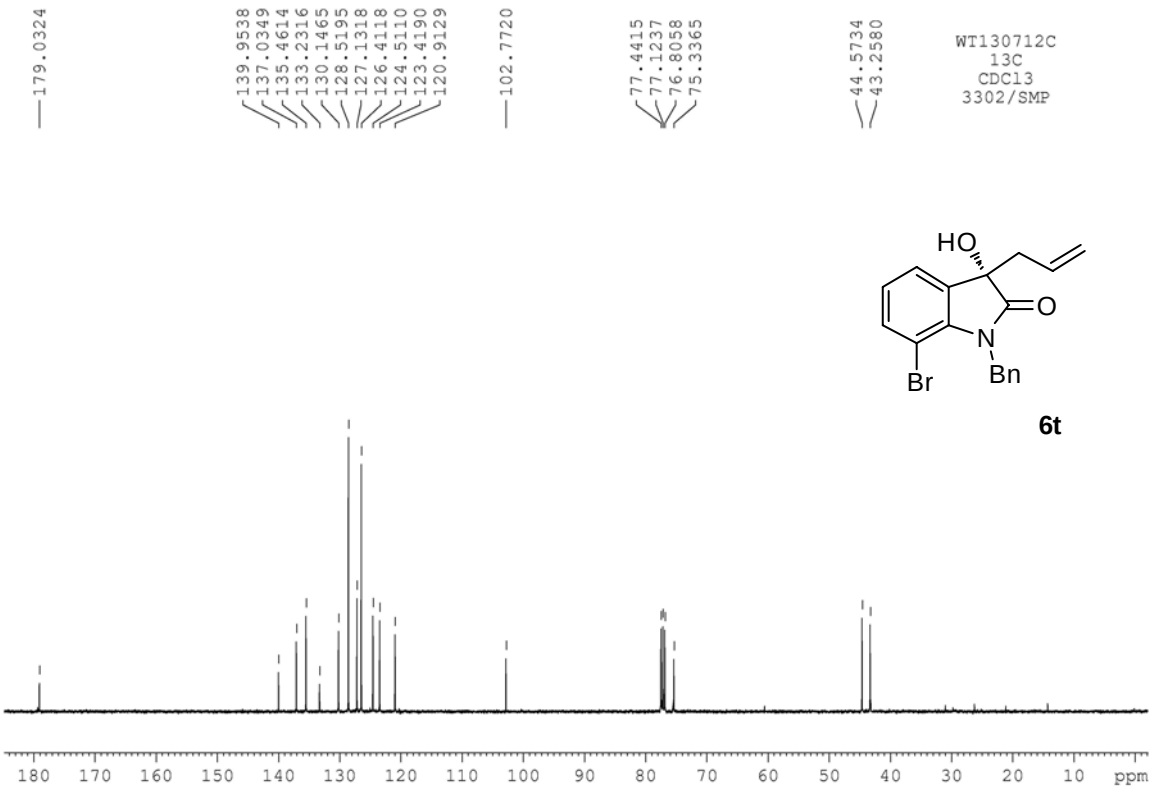
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

6t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124.5110
123.4190
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102.7720
77.4415
77.1237
76.8058
75.3365
44.5734
43.2580
WT130712C
13C
CDCl3
3302/SMP
HO
O
N
Bn
Br
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140
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80
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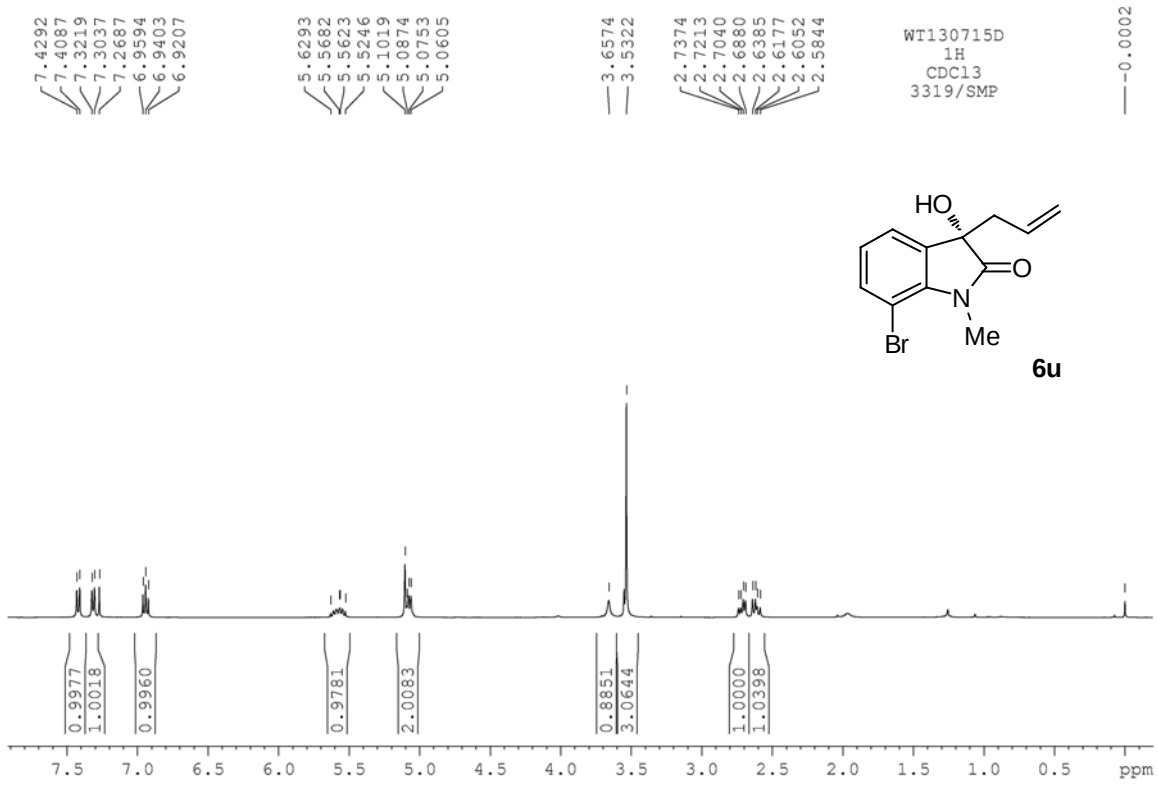
20
10
ppm

6t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5.5623
5.5246
5.1019
5.0874
5.0753
5.0605
3.6574
3.5322
2.7374
2.7213
2.7040
2.6880
2.6385
2.6177
2.6052
2.5844
WT130715D
1H
CDCl3
3319/SMP
-0.0002
HO
O
N
Me
Br
6u
0.9977
1.0018
0.9960
0.9781
2.0083
0.8851
3.0644
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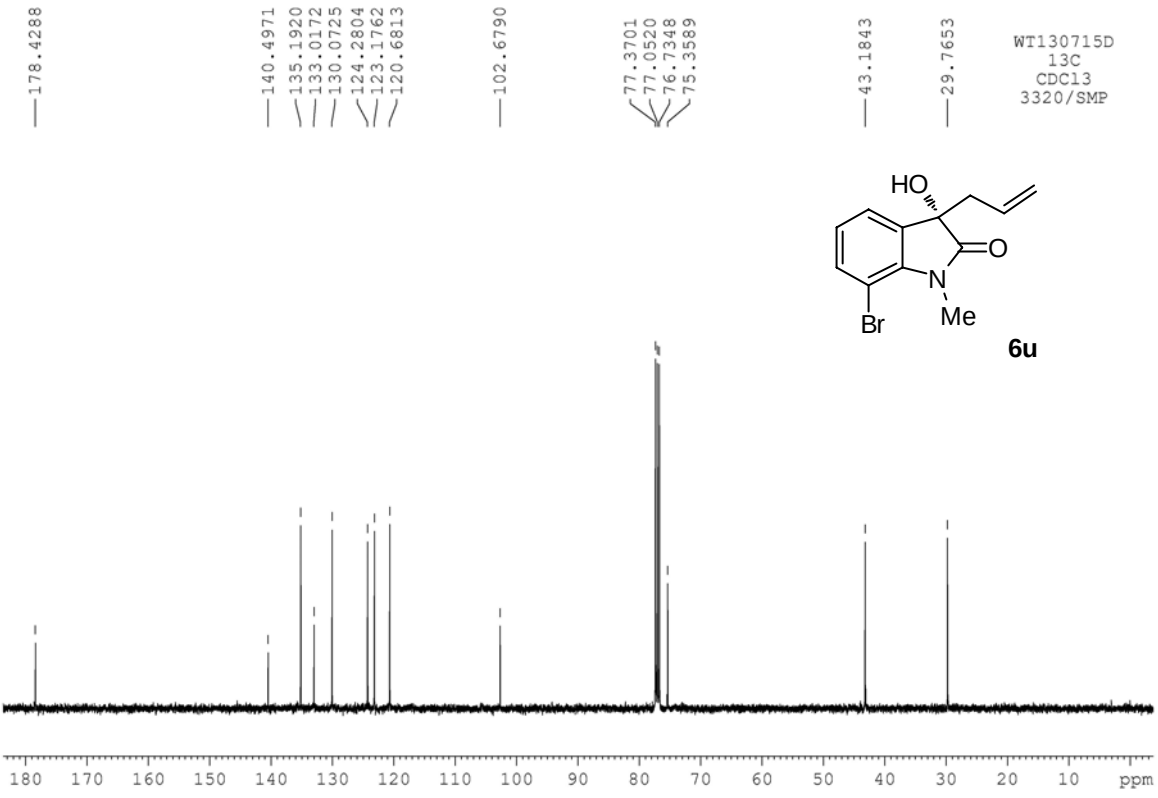
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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76.7348
75.3589
43.1843
29.7653
WT130715D
13C
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3320/SMP
HO
O
N
Me
Br
6u
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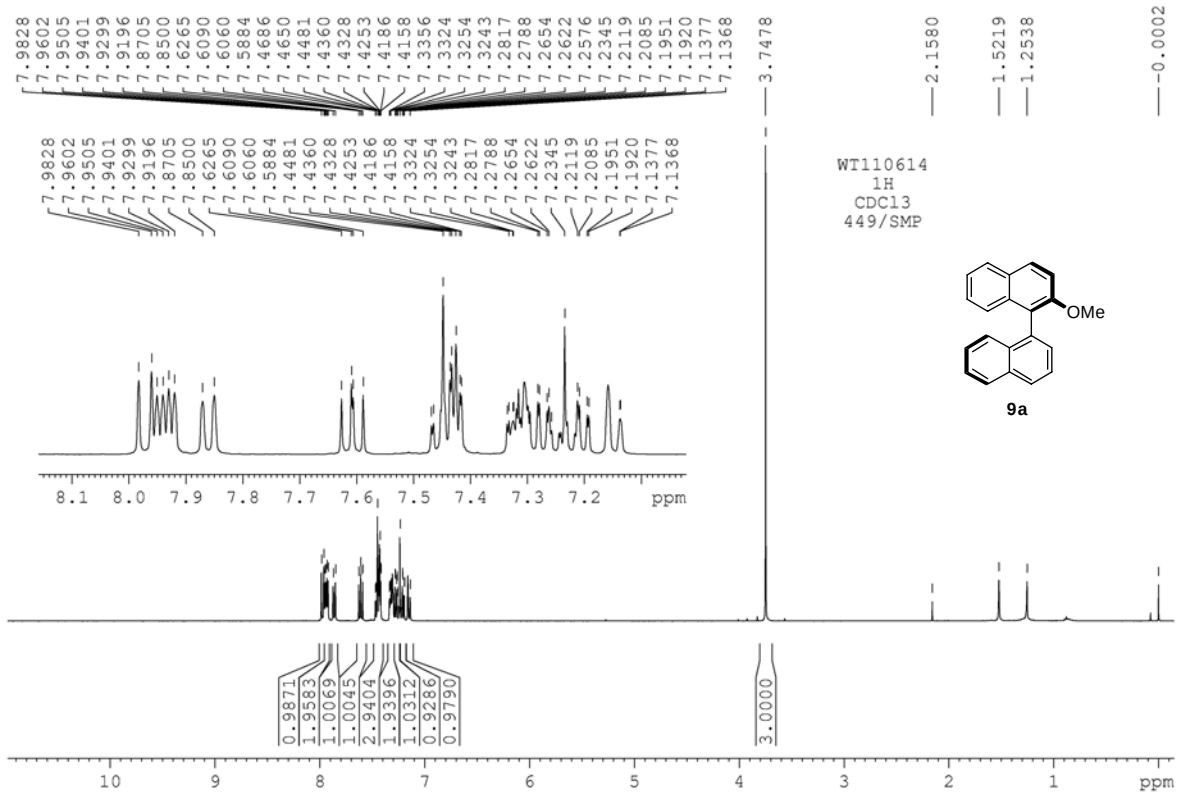
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OMe
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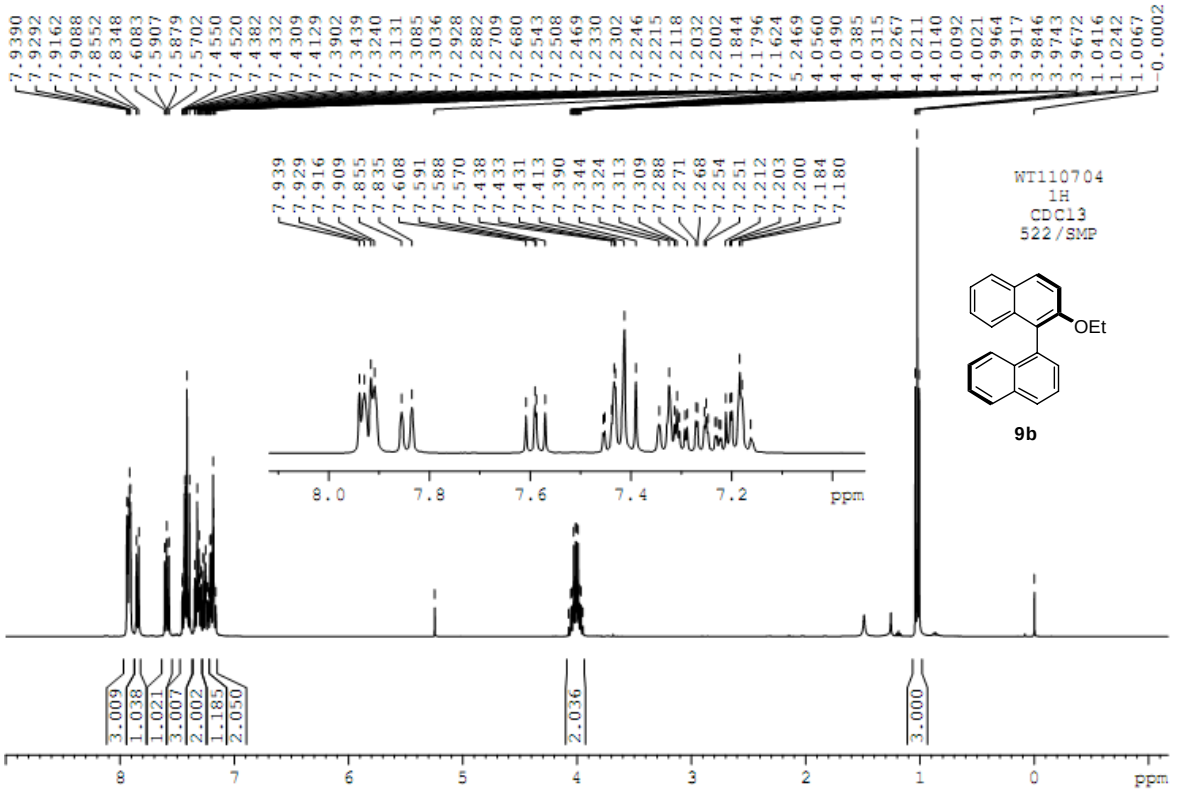
ppm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522/SMP
OEt
9b
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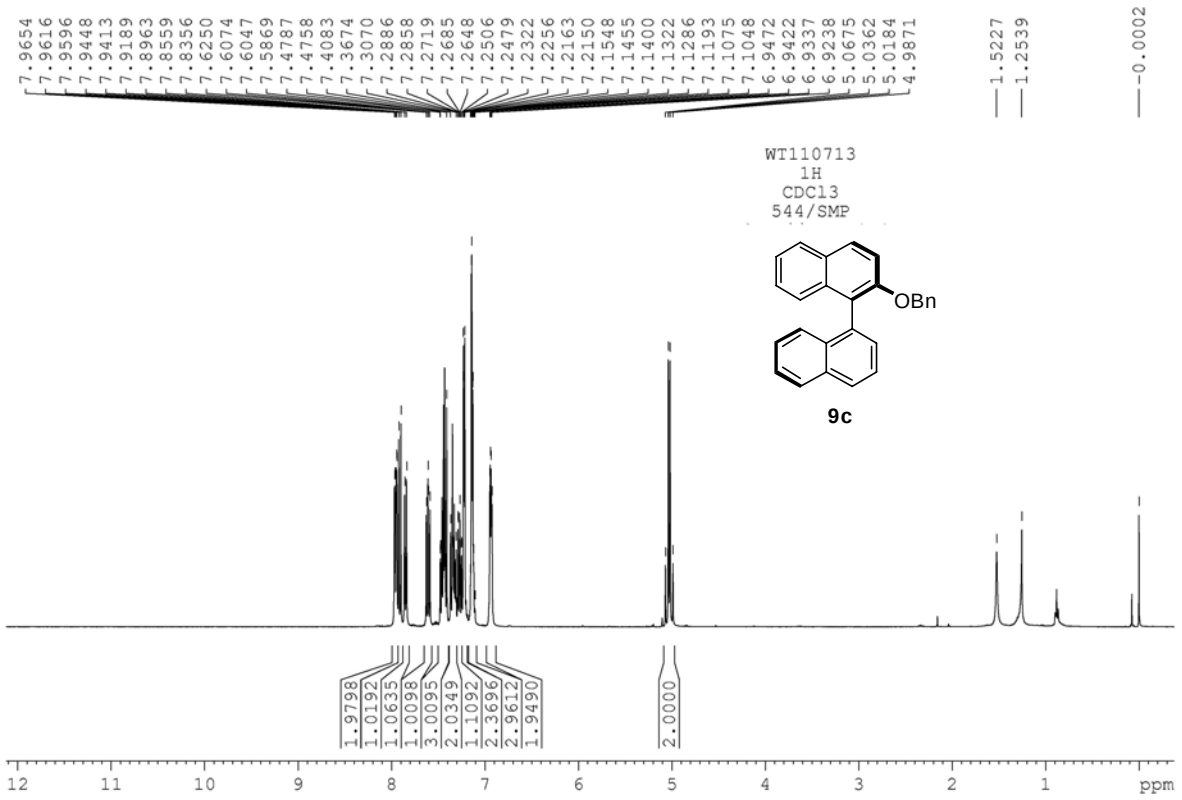
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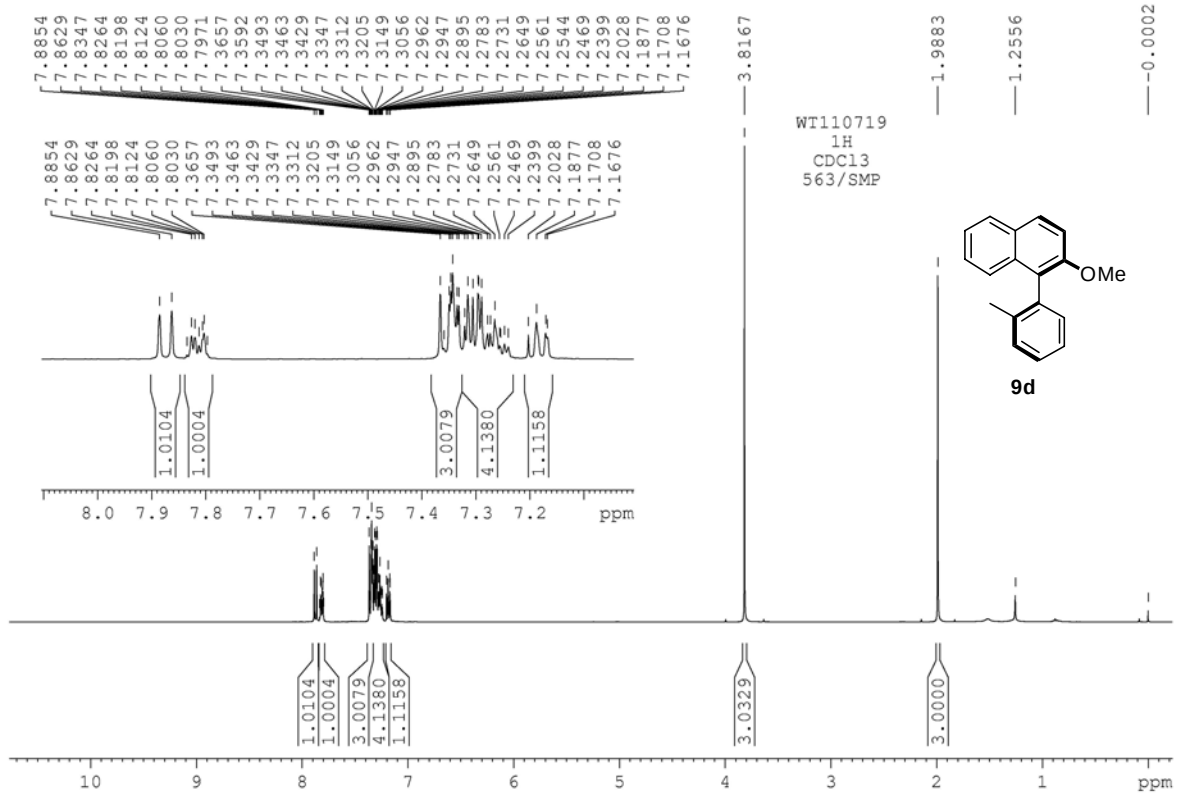
OBn
9c
ppm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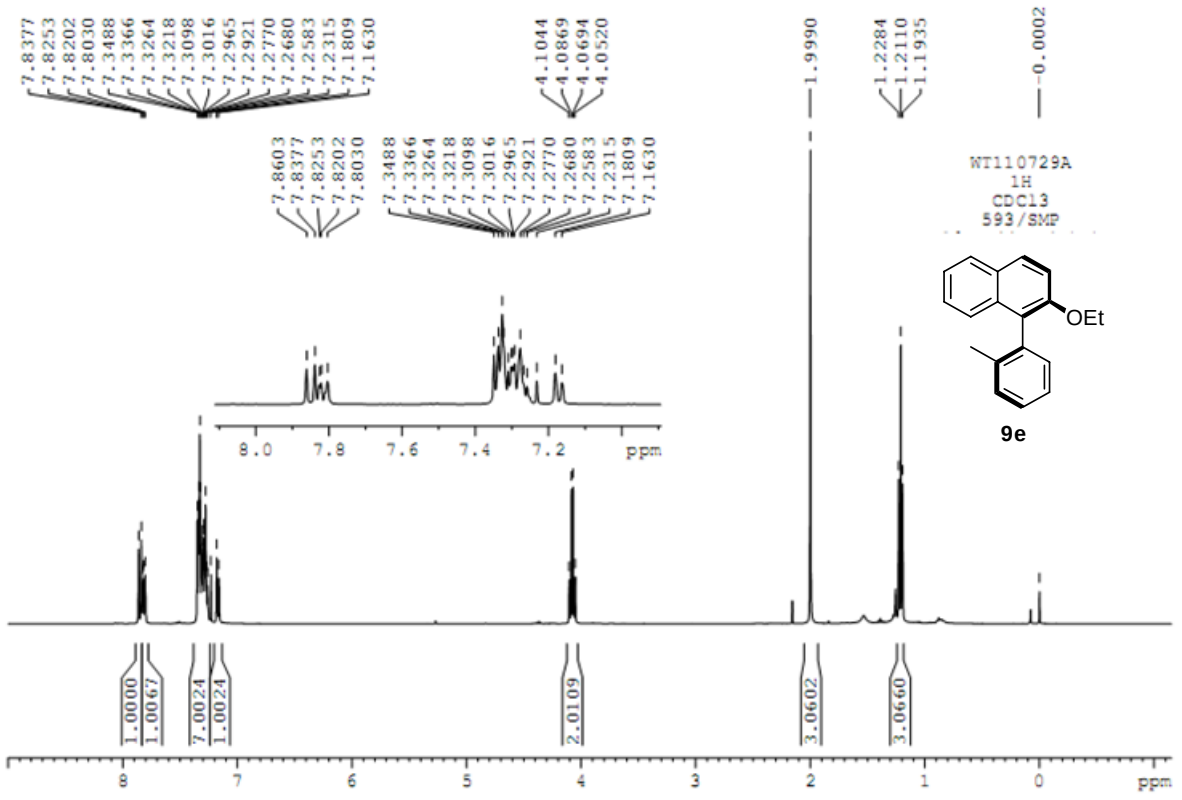
CDCl3
563/SMP
OMe
9d
ppm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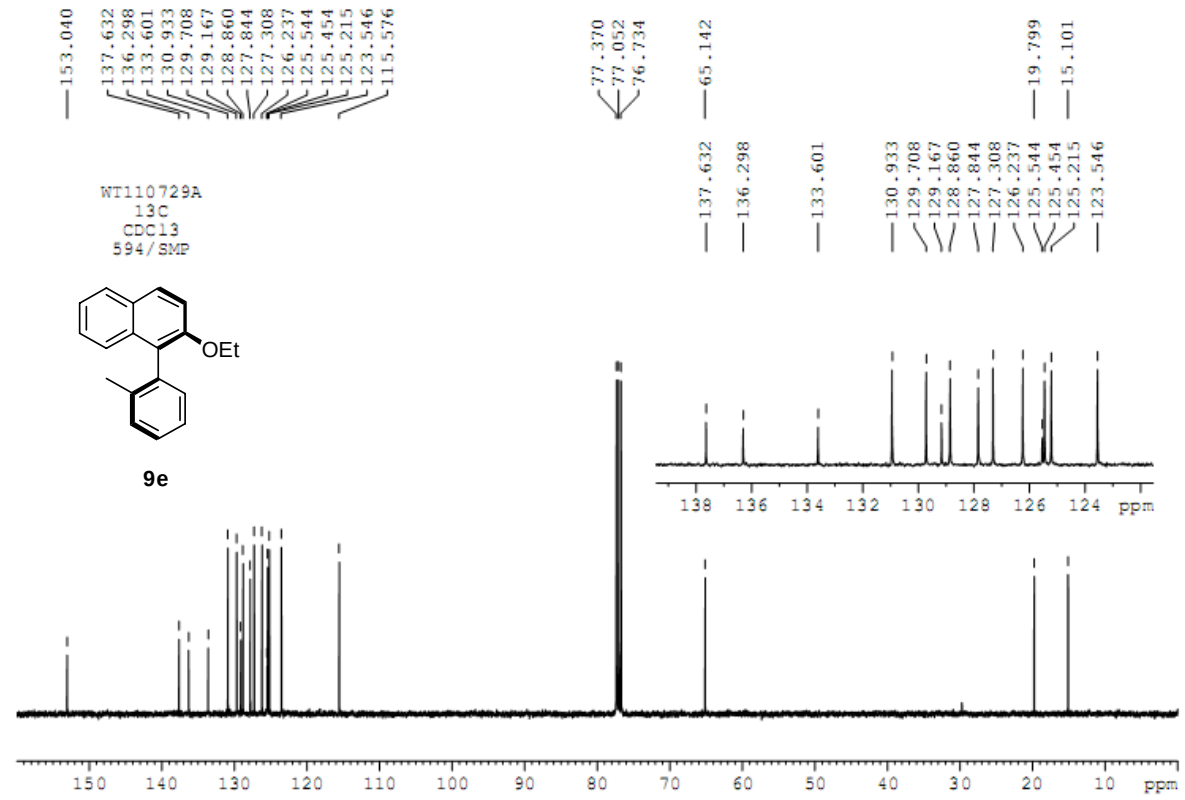
OEt
9e
ppm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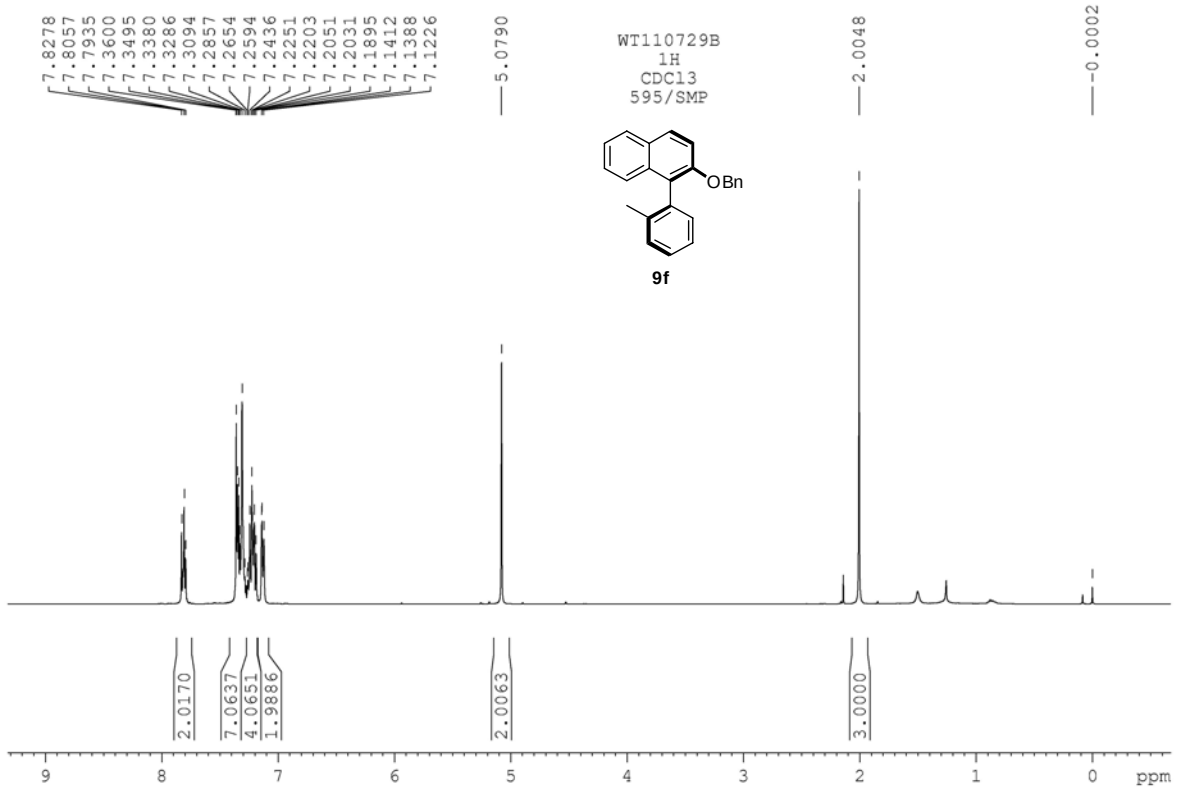
13C
CDCl3
594/SMP
OEt
9e
ppm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7.3286
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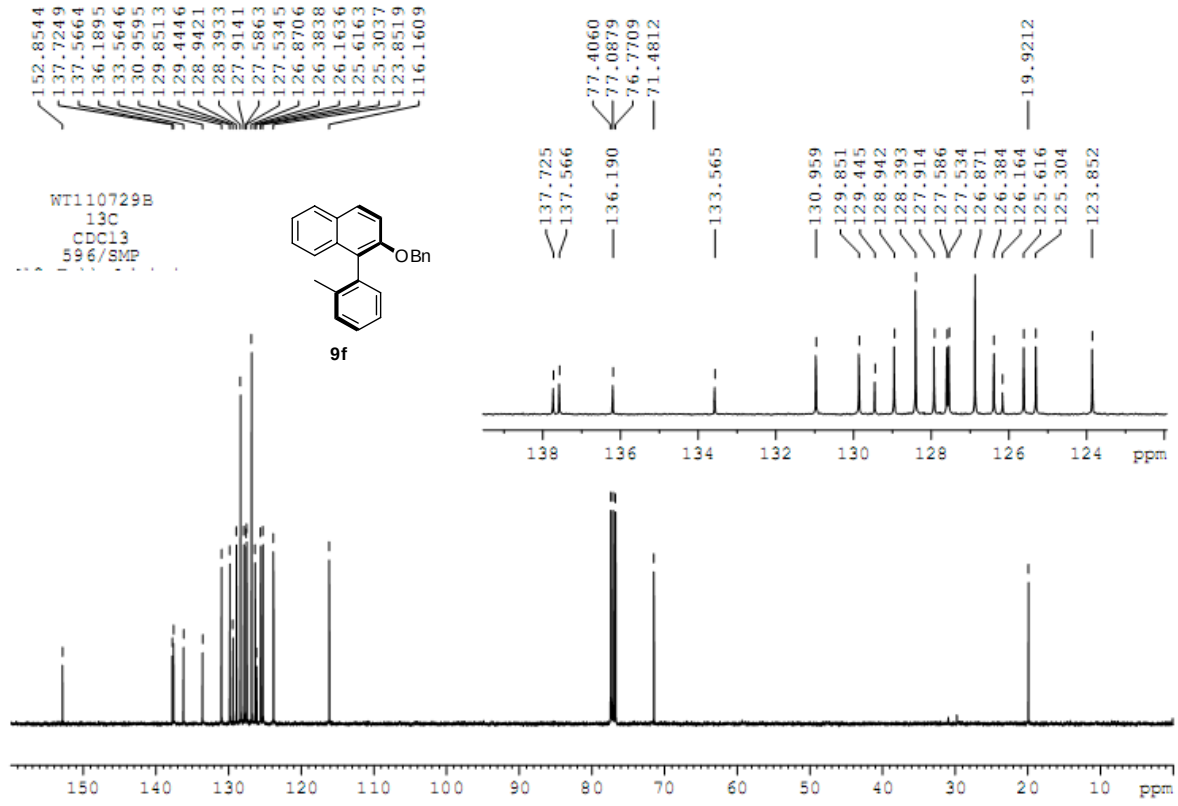
7.2654
7.2594
7.2436
7.2251
7.2203
7.2051
7.2031
7.1895
7.1412
7.1388
7.1226
5.0790
2.0048
0.0002
WT110729B
1H
CDCl3
595/SMP
OBn
9f
2.0170
7.0637
4.0651
1.9886
2.0063
3.0000
9
8
7
6
5
4
3
2
1
0
ppm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127.5863
127.5345
126.8706
126.3838
126.1636
125.6163
125.3037
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116.1609
77.4060
77.0879
76.7709
71.4812
19.9212
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137.566
136.190
133.565
130.959
129.851
129.445
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127.914
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127.534
126.871
126.384
126.164
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125.304
123.852
WT110729B
13C
CDCl3
596/SMP
OBn
9f
138
136
134
132
130
128
126
124
ppm
150
140
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120
110
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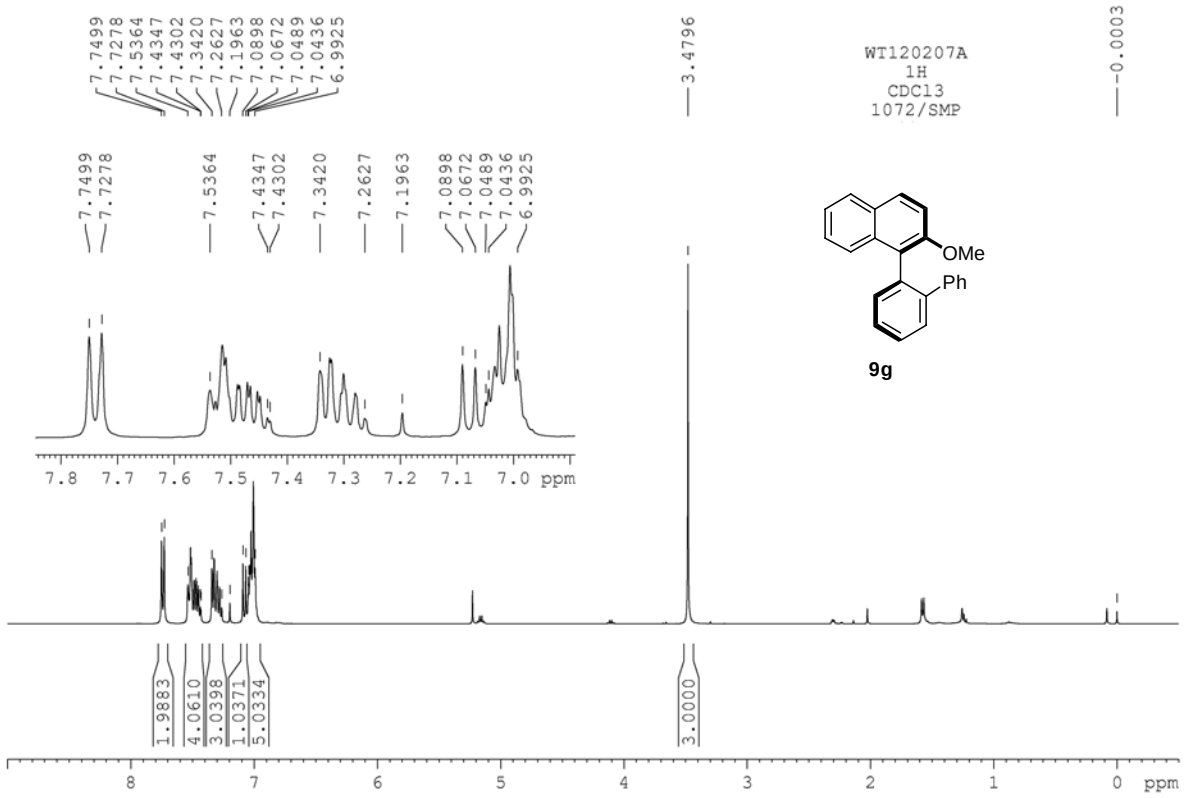
80
70
60
50
40
30
20
10
ppm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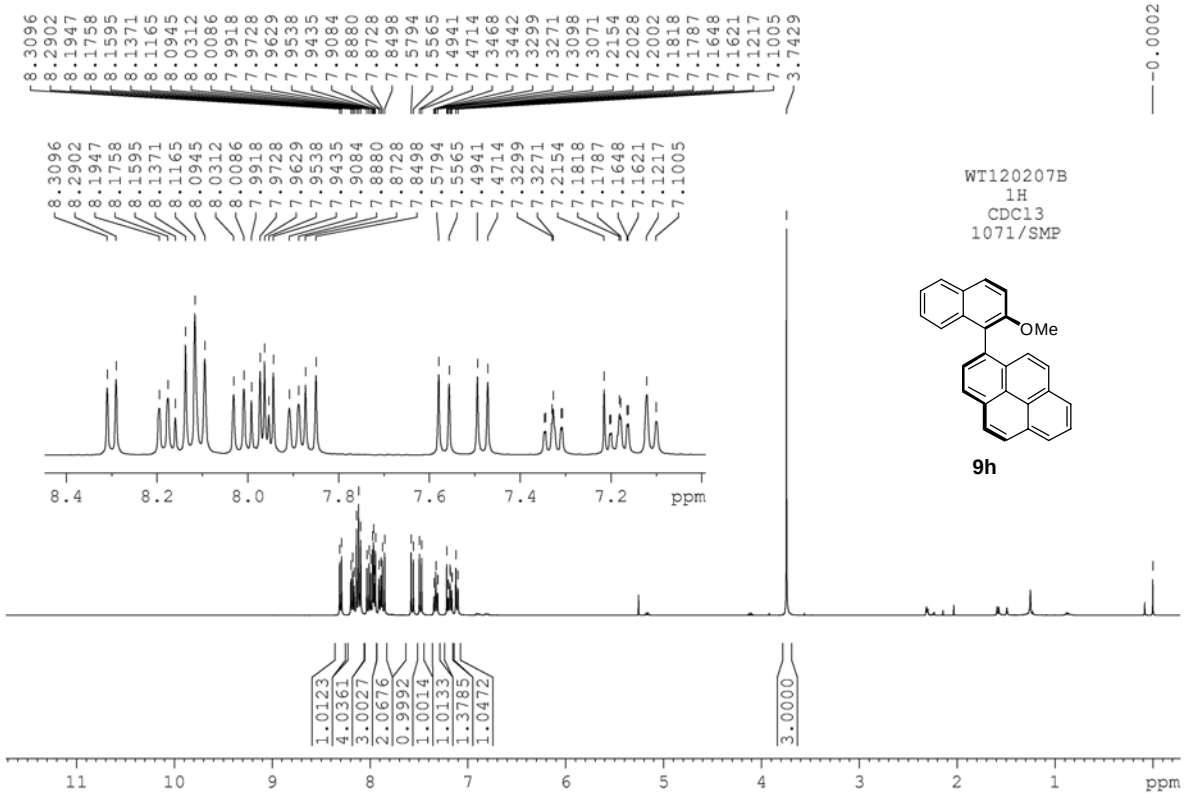
CDCl3
1072/SMP
OMe
Ph
9g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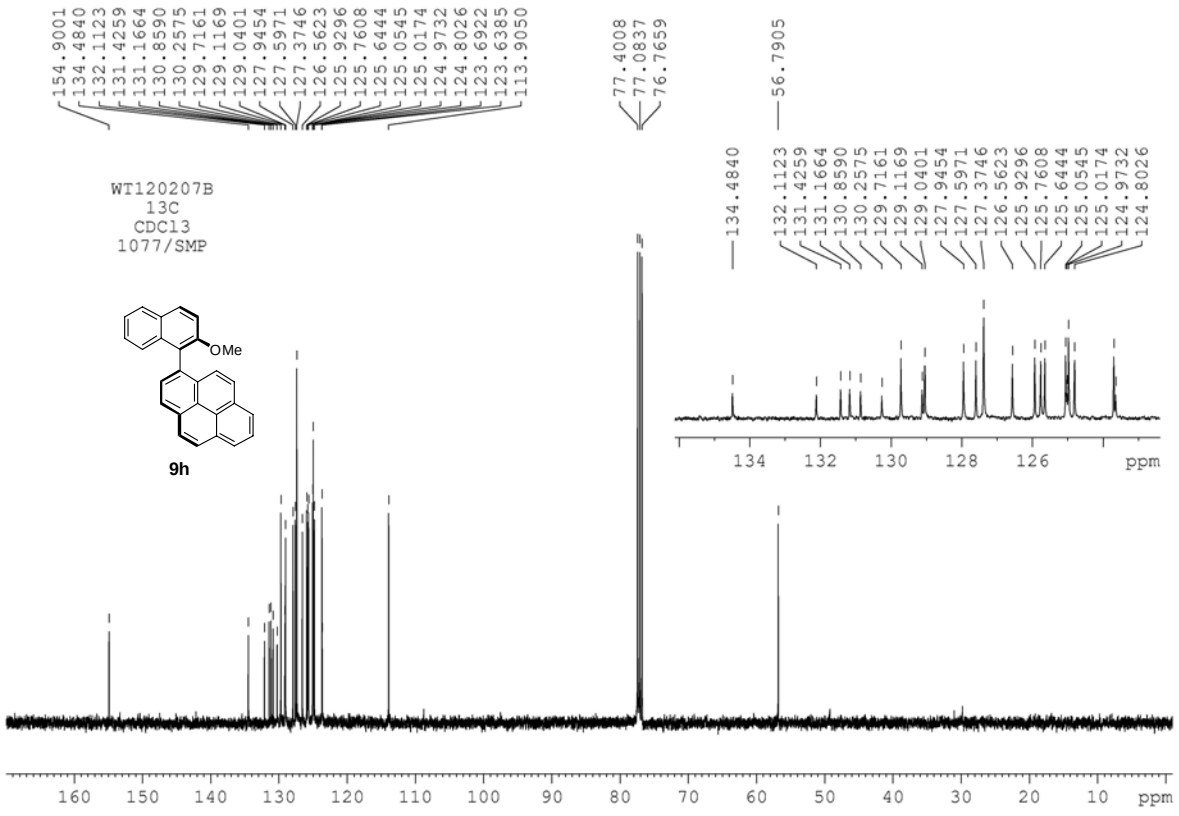
CDCl3
1071/SMP
OMe
9h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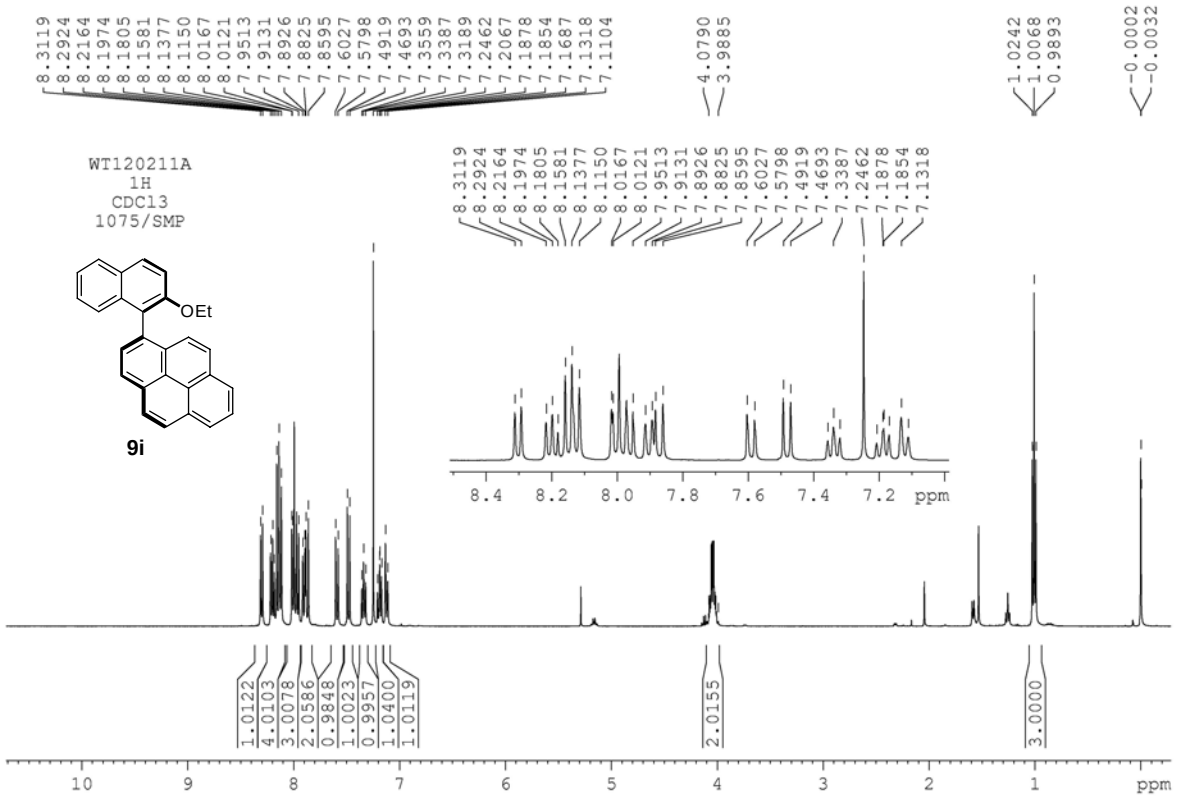
OMe
9h
ppm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CDCl3
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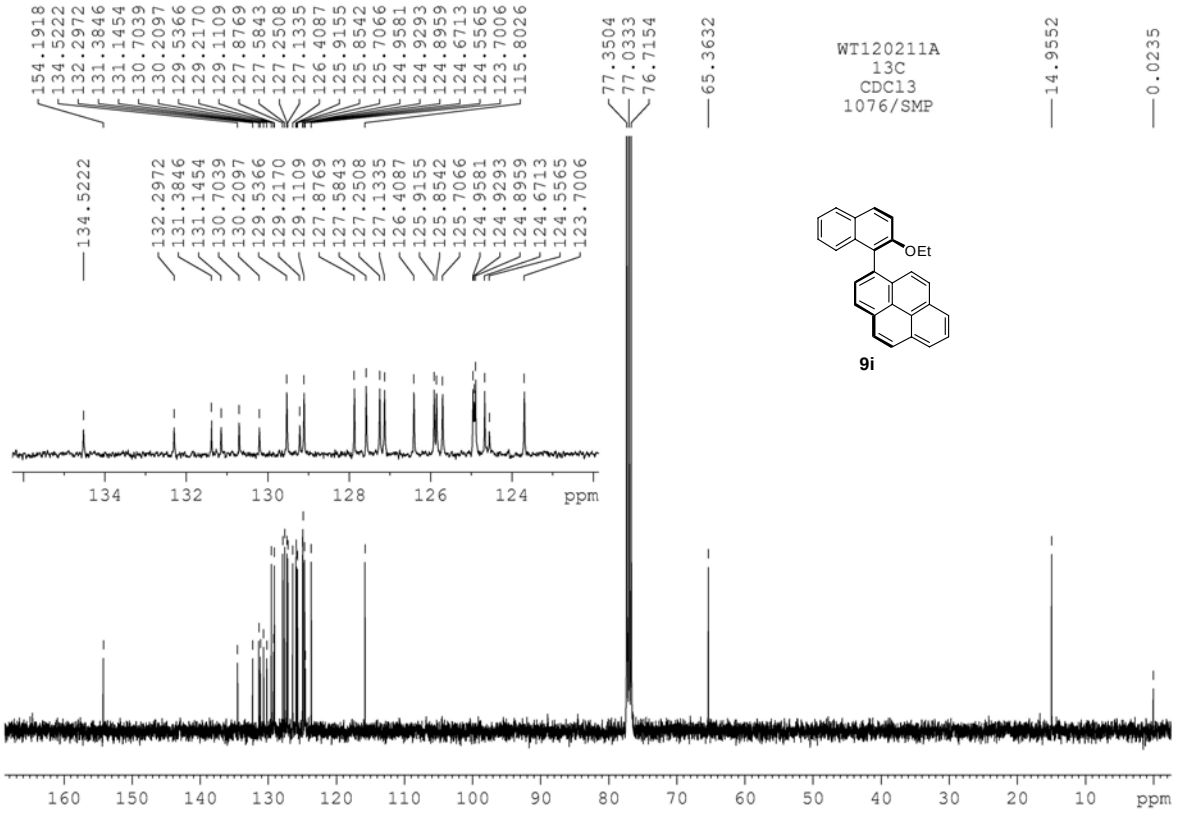
OEt
9i
ppm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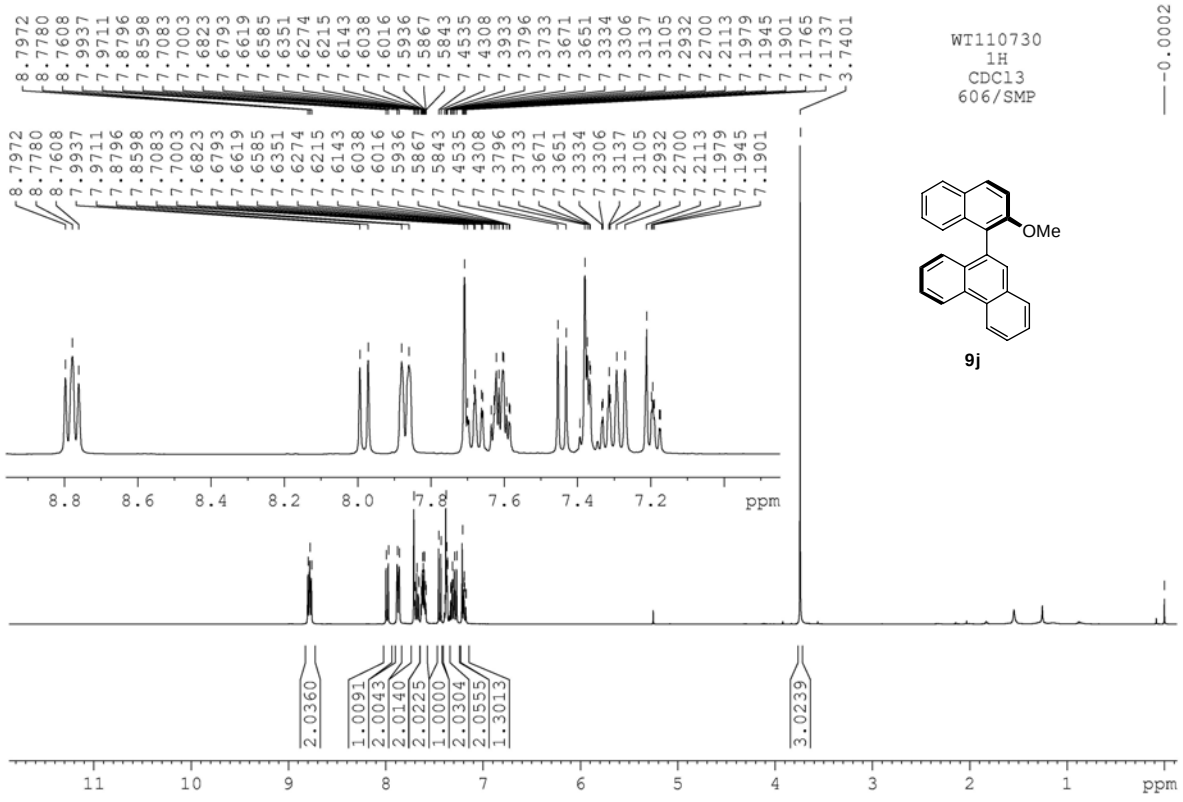
13C
CDCl3
1076/SMP
OEt
9i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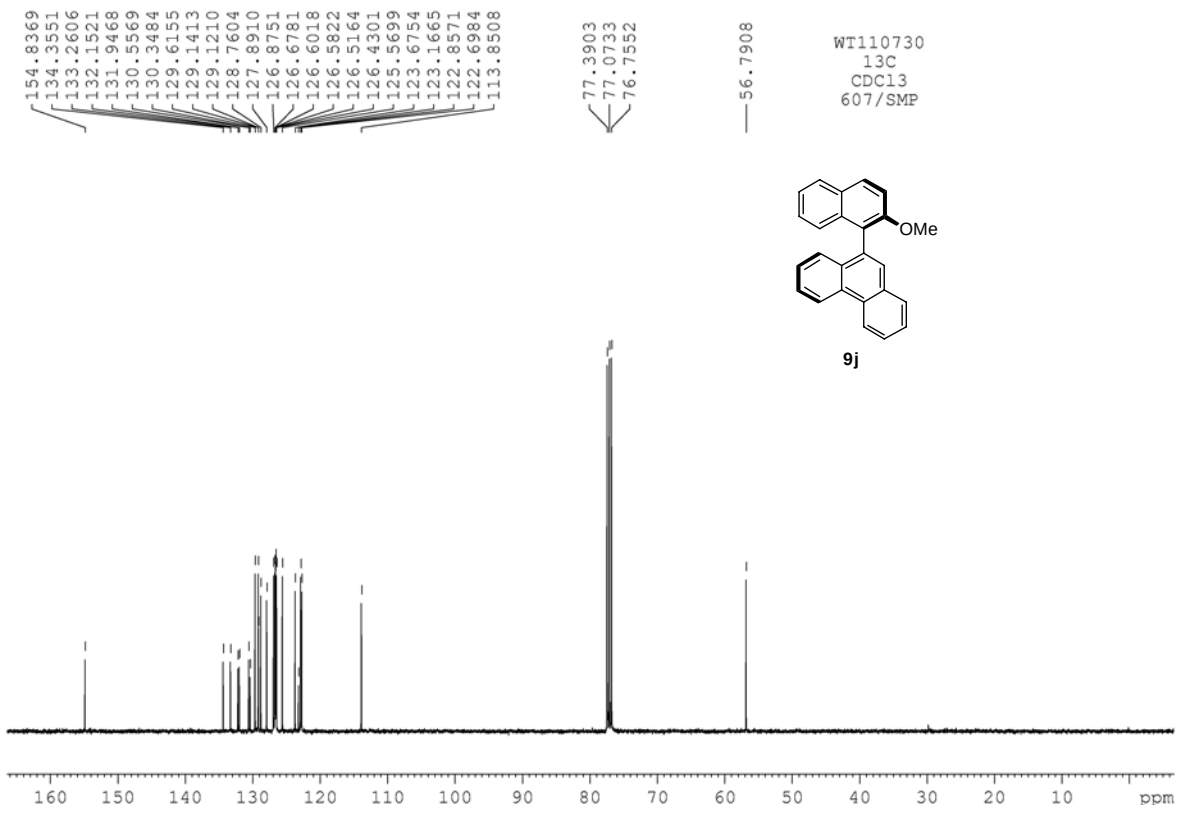
CDCl3
606/SMP
OMe
9j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126.6018
126.5822
126.5164
126.4301
125.5699
123.6754
123.1665
122.8571
122.6984
113.8508
77.3903
77.0733
76.7552
56.7908
WT110730
13C
CDCl3
607/SMP
OMe
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80
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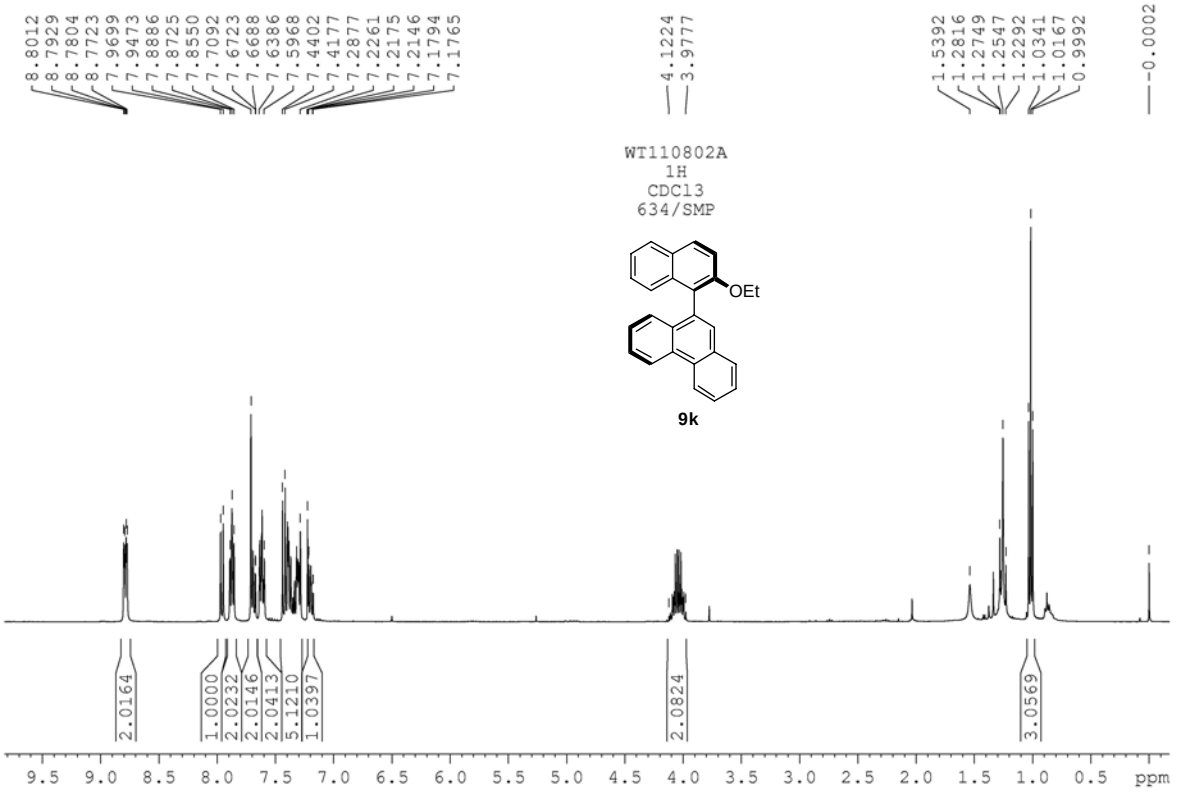
10
ppm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7.6723
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7.6386
7.5968
7.4402
7.4177
7.2877
7.2261
7.2175
7.2146
7.1794
7.1765
4.1224
3.9777
1.5392
1.2816
1.2749
1.2547
1.2292
1.0341
1.0167
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-0.0002
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1H
CDCl3
634/SMP
OEt
9k
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2.0146
2.0413
5.1210
1.0397
2.0824
3.0569
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8.5
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7.5
7.0
6.5
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1.0
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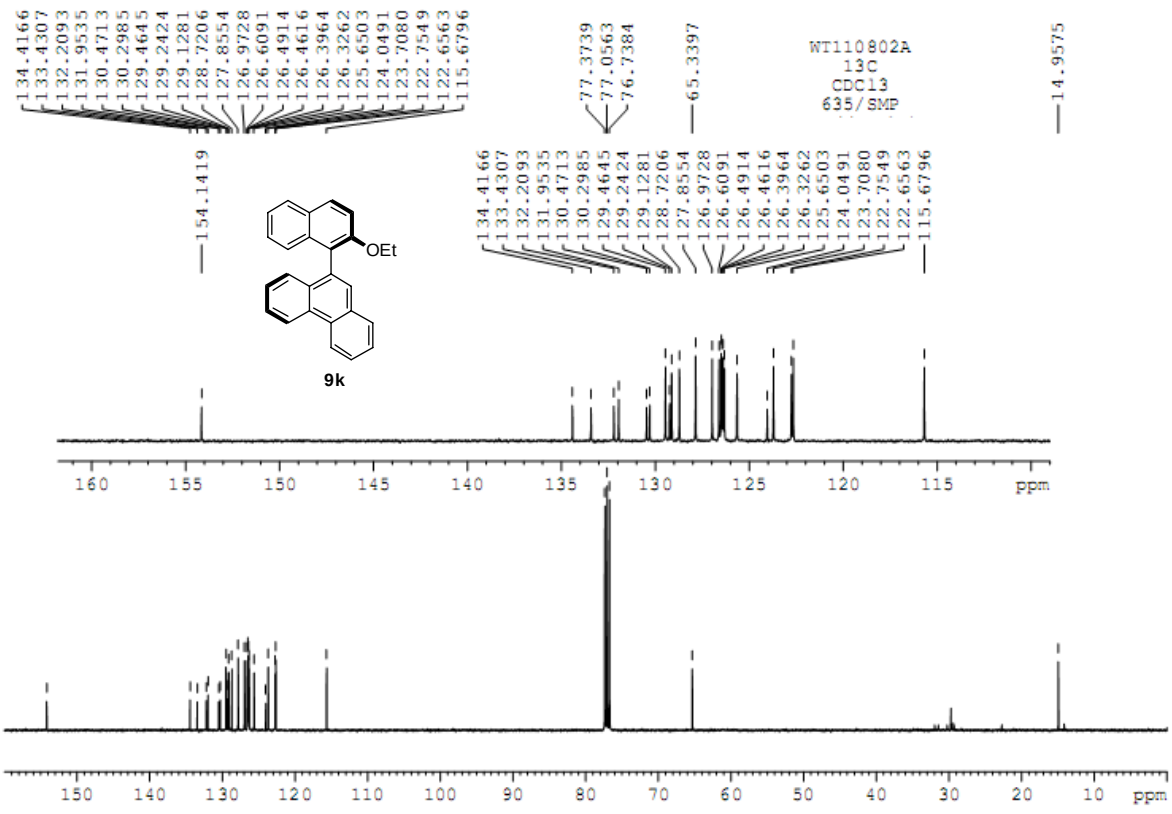
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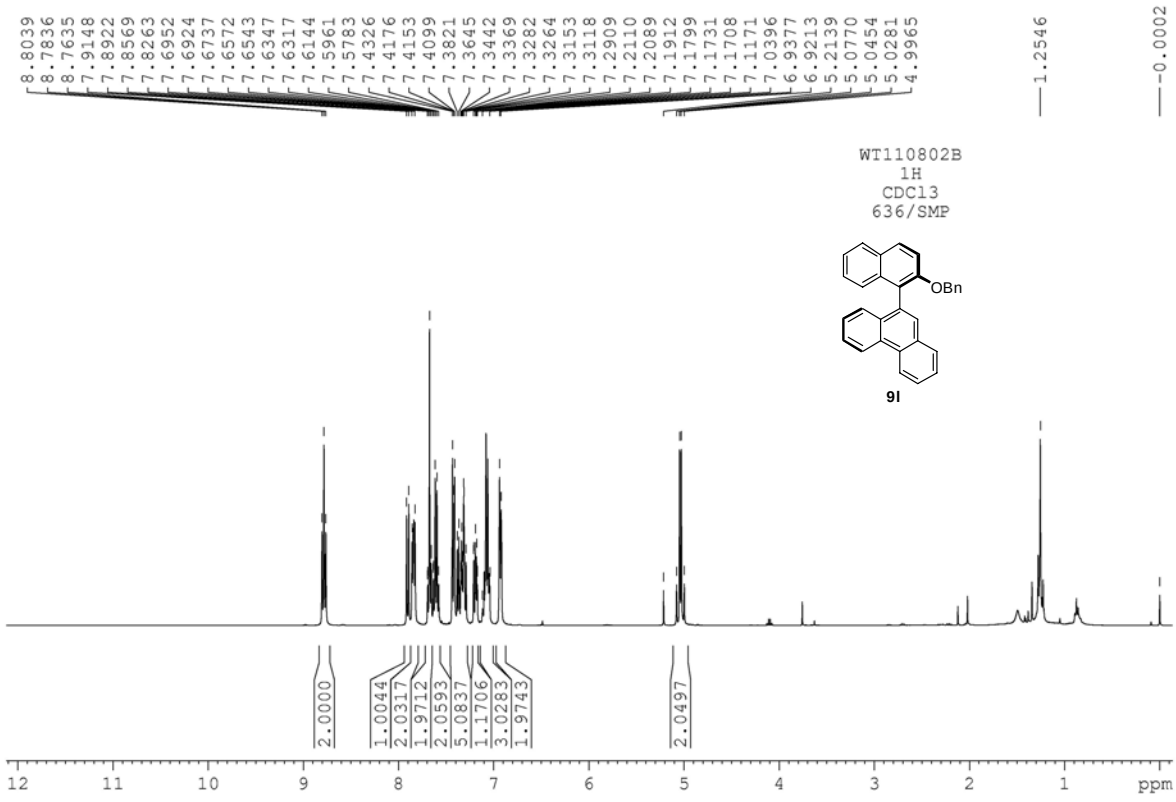
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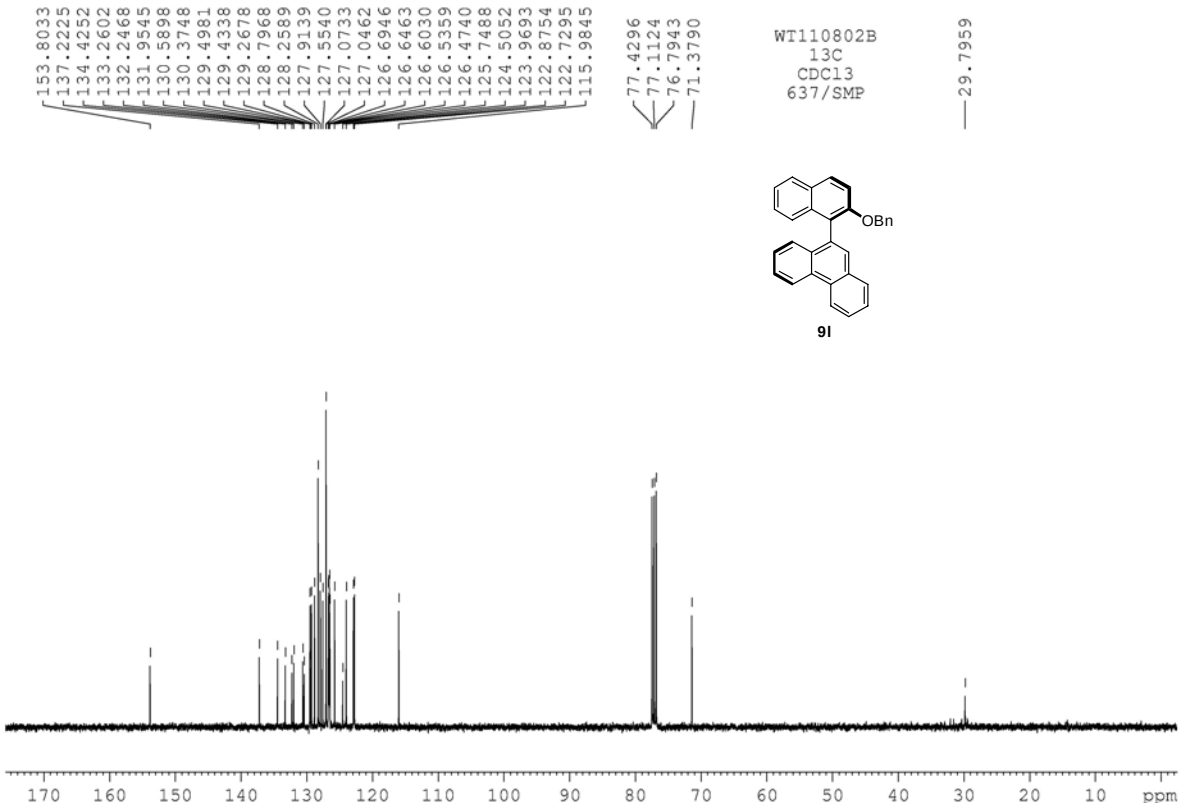
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128.2589
127.9139
127.5540
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127.0462
126.6946
126.6463
126.6030
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125.7488
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71.3790
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13C
CDCl3
637/SMP
29.7959
OBn
9l
170
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100
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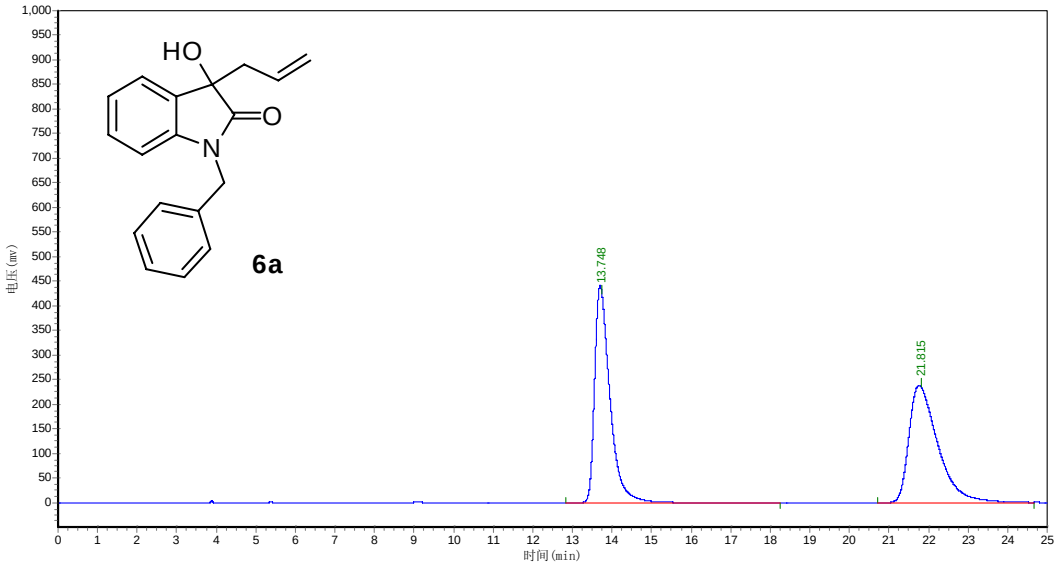
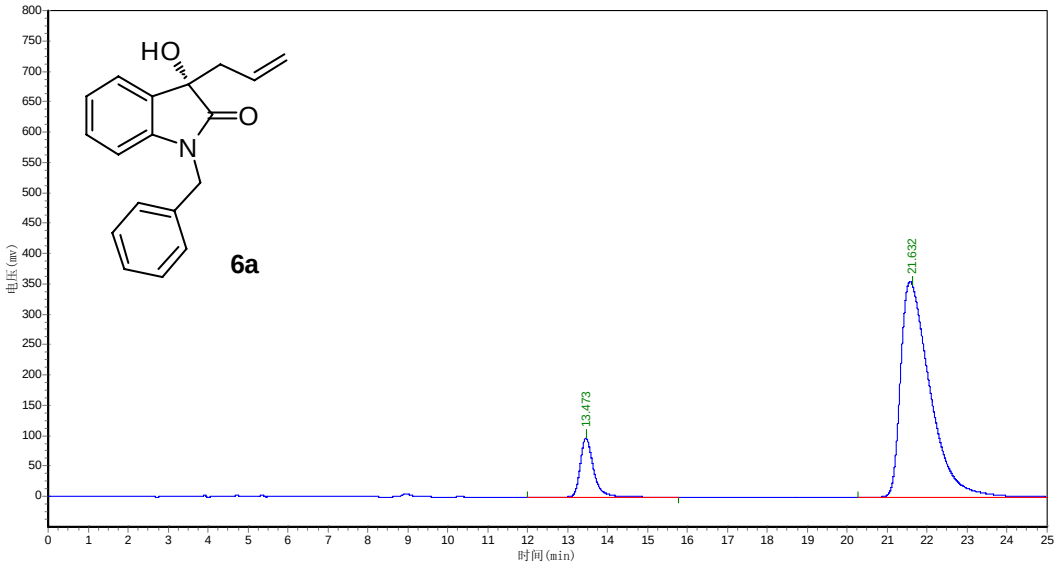
40
30
20
10
ppm

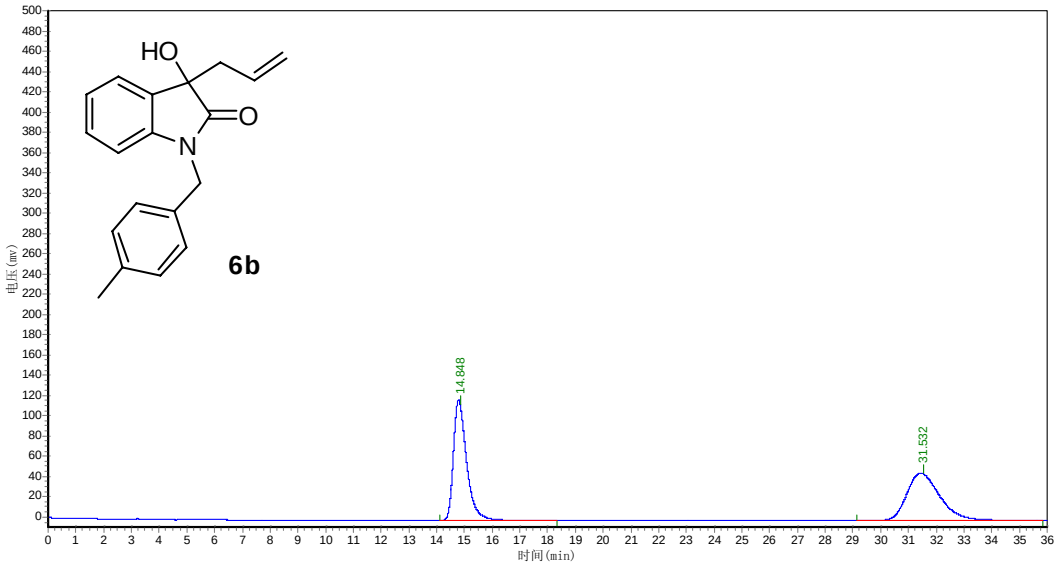
HPLC Spectra of the Catalysis Products



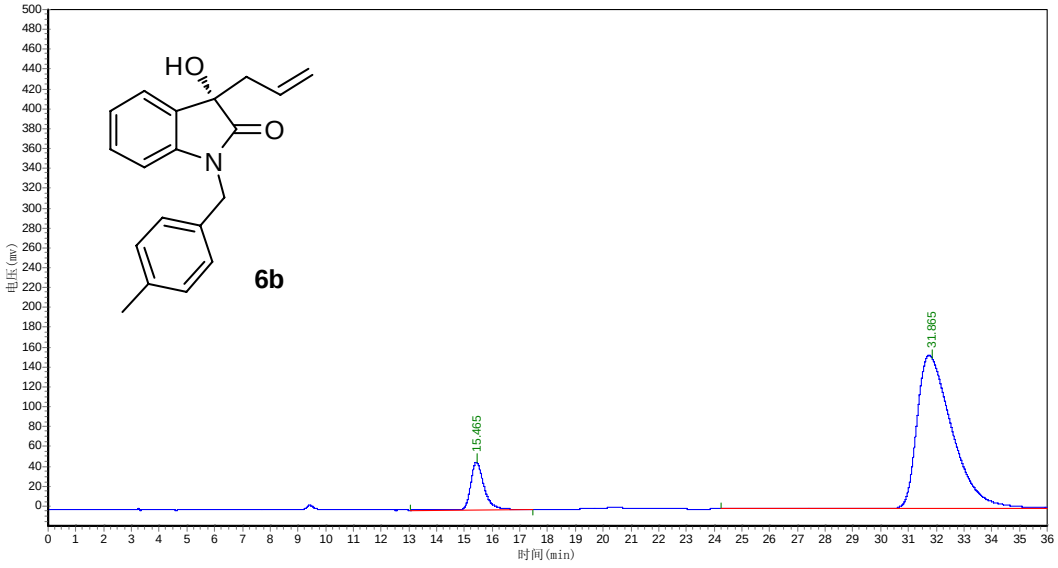
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	13.748	435453.031	11848680.000	49.5216
2	21.815	237599.609	12077611.000	50.4784



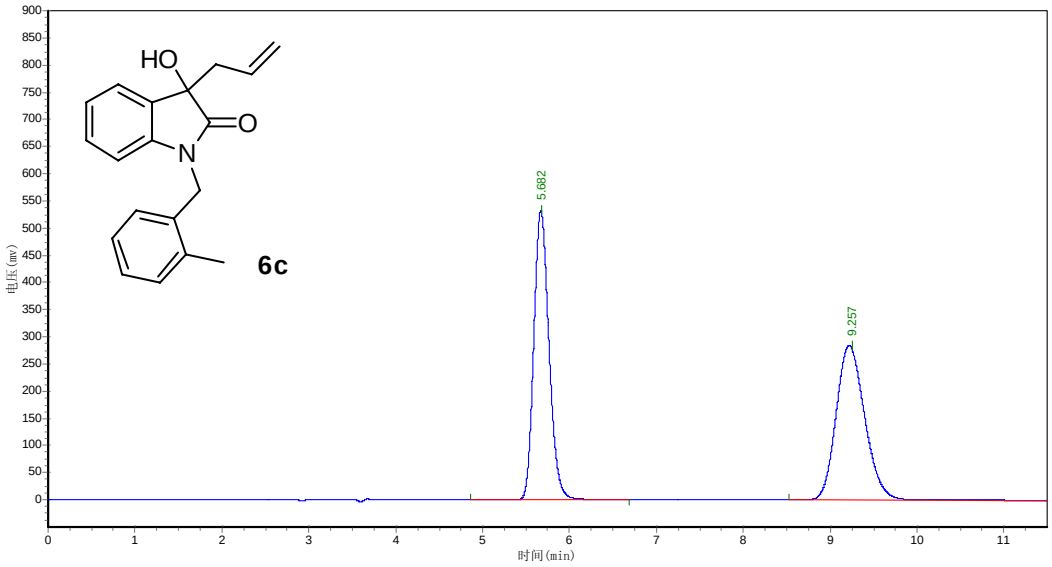
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	13.473	93414.125	2220433.500	10.9524
2	21.632	353226.313	18053064.000	89.0476



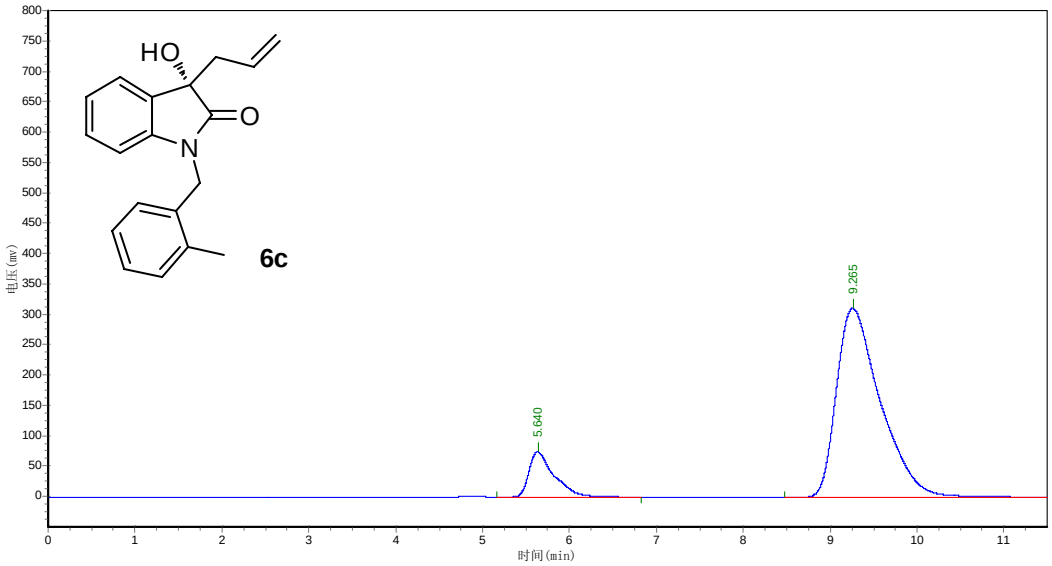
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	14.848	117938.258	3939534.500	50.2363
2	31.532	46845.848	3902468.000	49.7637



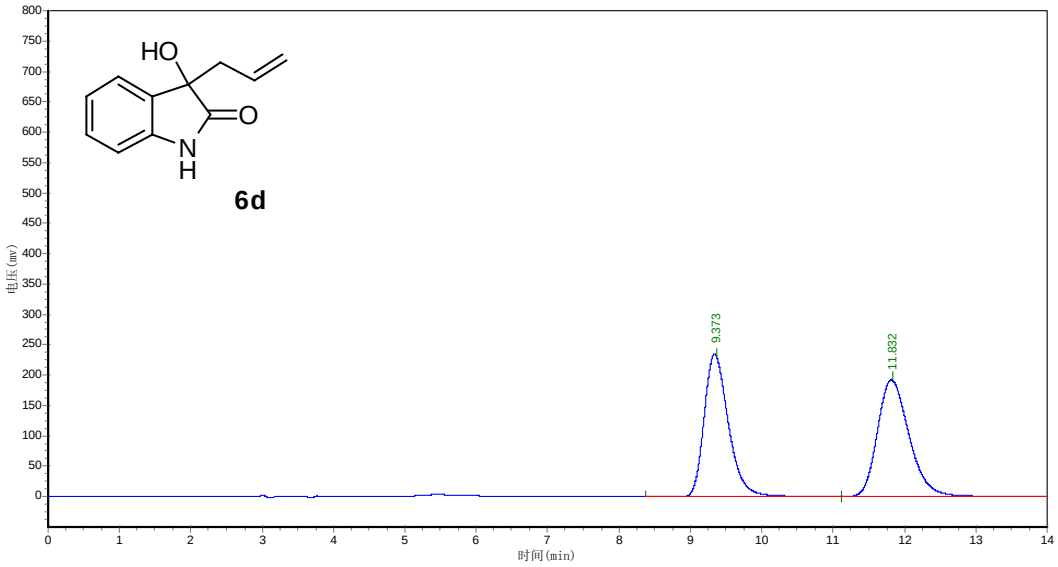
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	15.465	46419.547	1567856.375	10.3593
2	31.865	152968.516	13566866.000	89.6407



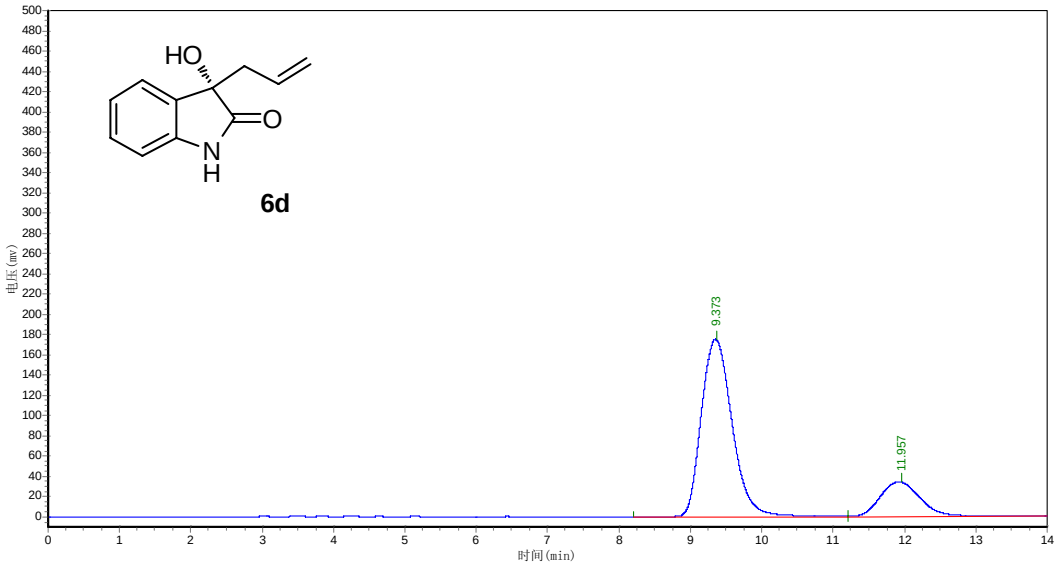
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	5.682	457612.156	6502315.000	49.9723
2	9.257	279133.781	6509526.000	50.0277



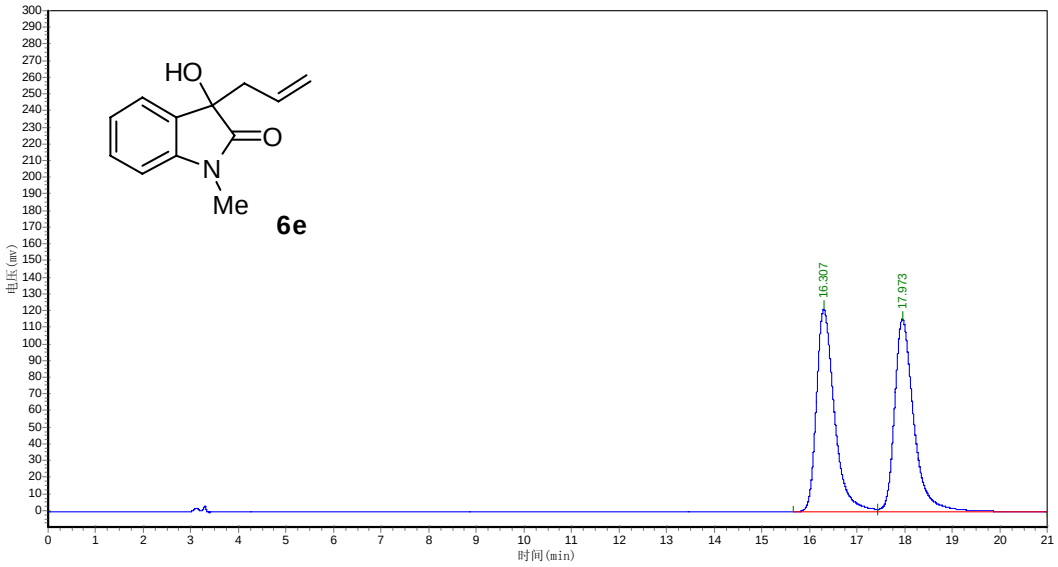
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	5.640	74274.617	1486815.750	11.9485
2	9.265	311061.063	10956707.000	88.0515



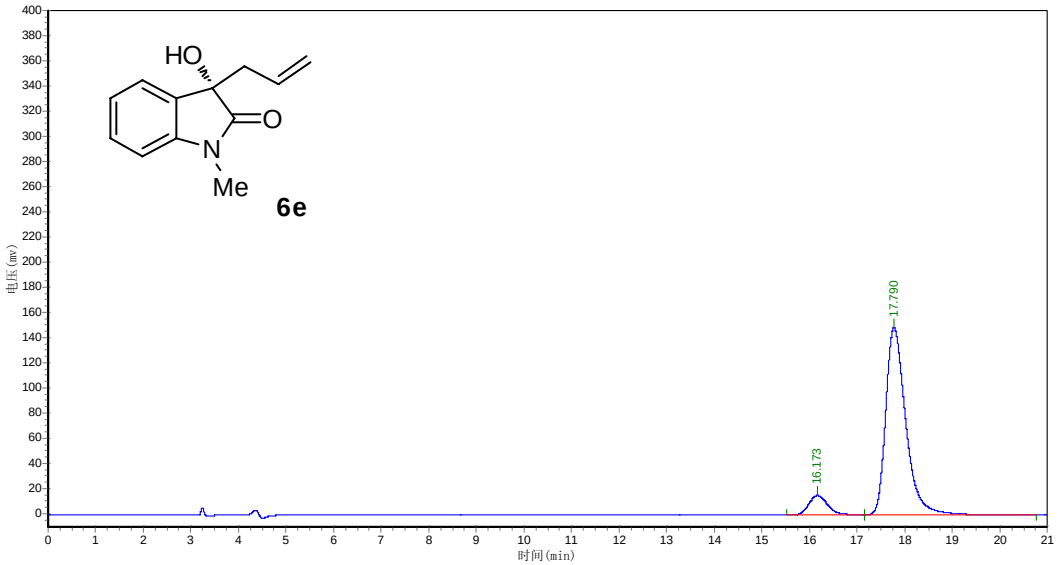
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	9.373	232818.719	5581357.500	48.1657
2	11.832	191994.297	6006461.000	51.8343



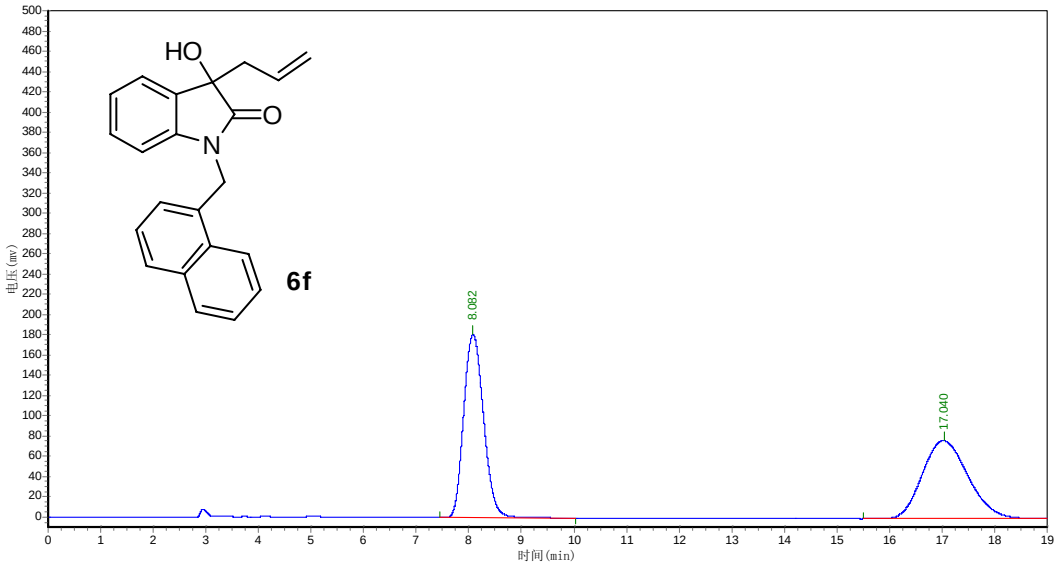
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	9.373	174935.938	5258504.500	79.7376
2	11.957	34188.531	1336254.125	20.2624



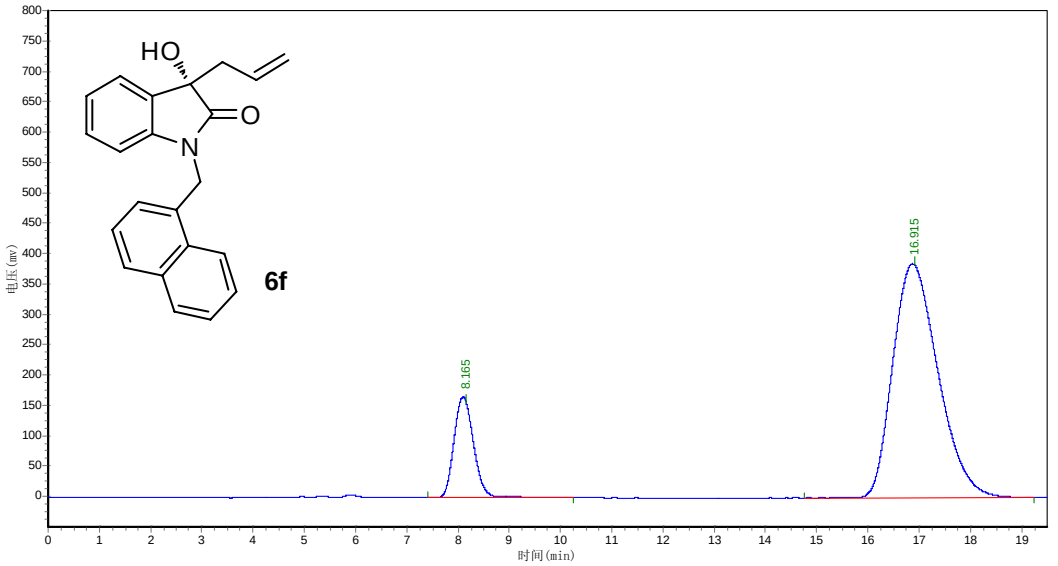
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	16.307	121310.266	3188576.750	49.5872
2	19.973	115365.078	3241659.750	50.4128



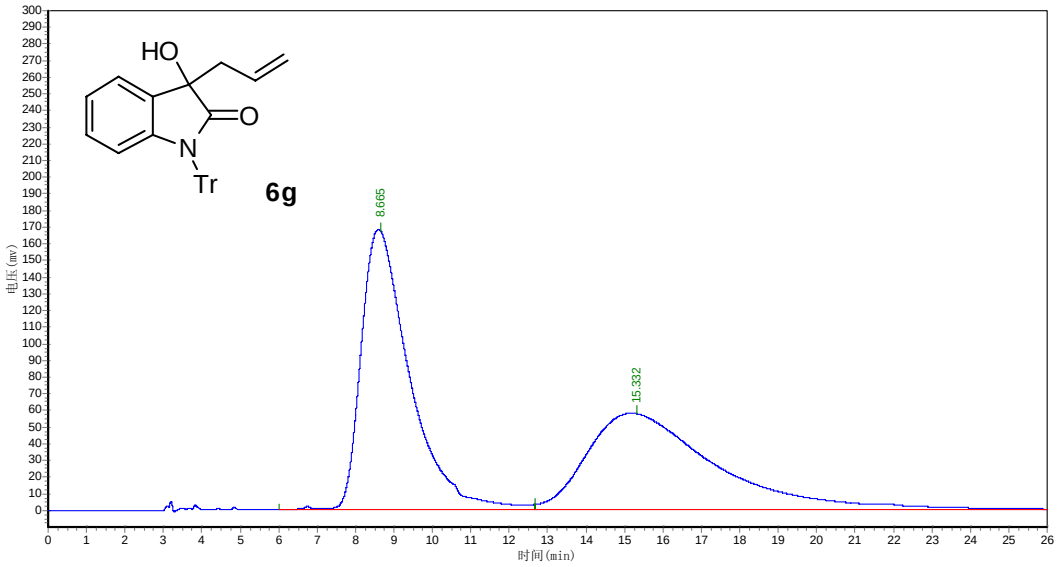
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	16.173	15706.481	445244.844	9.2049
2	17.790	148909.203	4391781.500	90.7951



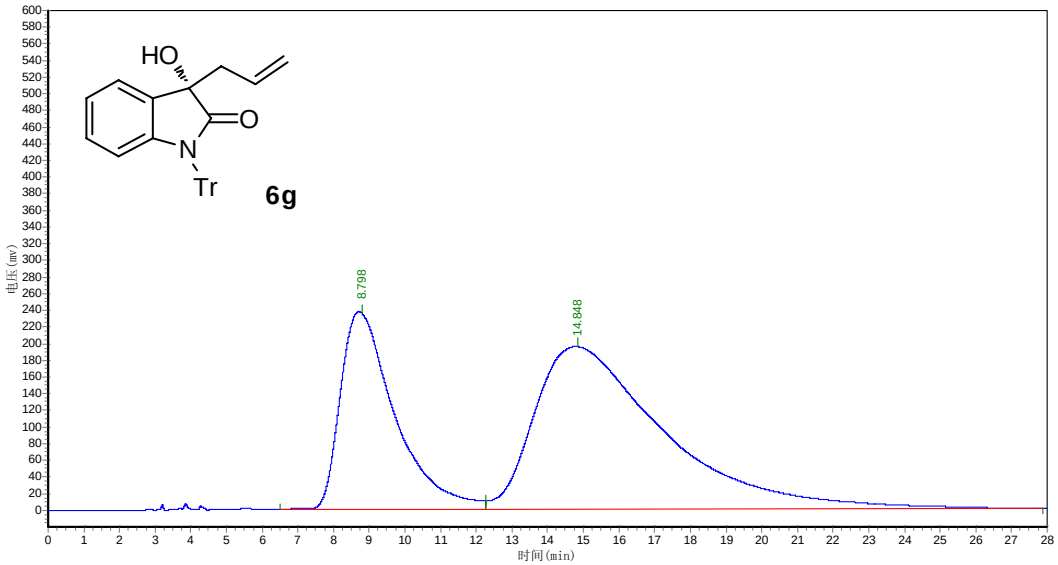
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	8.082	179941.906	4776146.500	50.5080
2	17.040	77113.508	4680072.500	49.4920



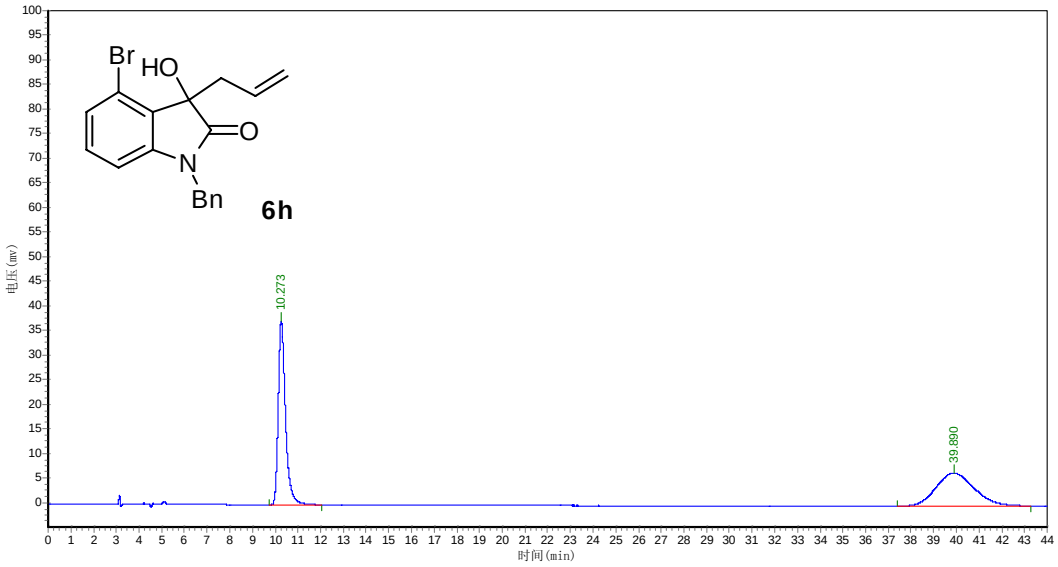
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	8.165	162826.859	4420632.000	15.7954
2	16.915	384297.125	23566120.000	84.2046



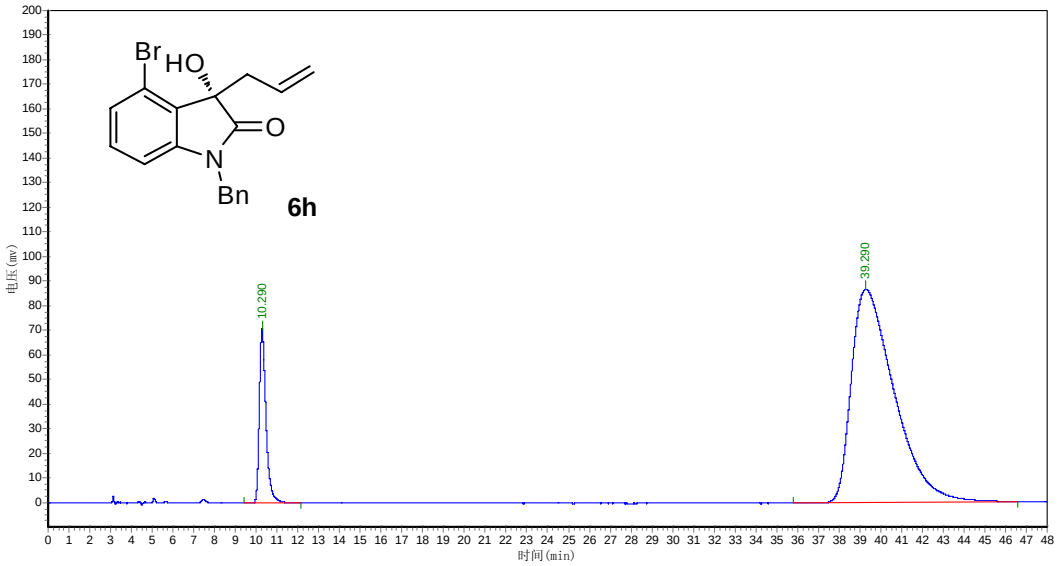
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	8.665	161888.703	14796688.000	52.7314
2	15.332	57601.969	13263776.000	47.2686



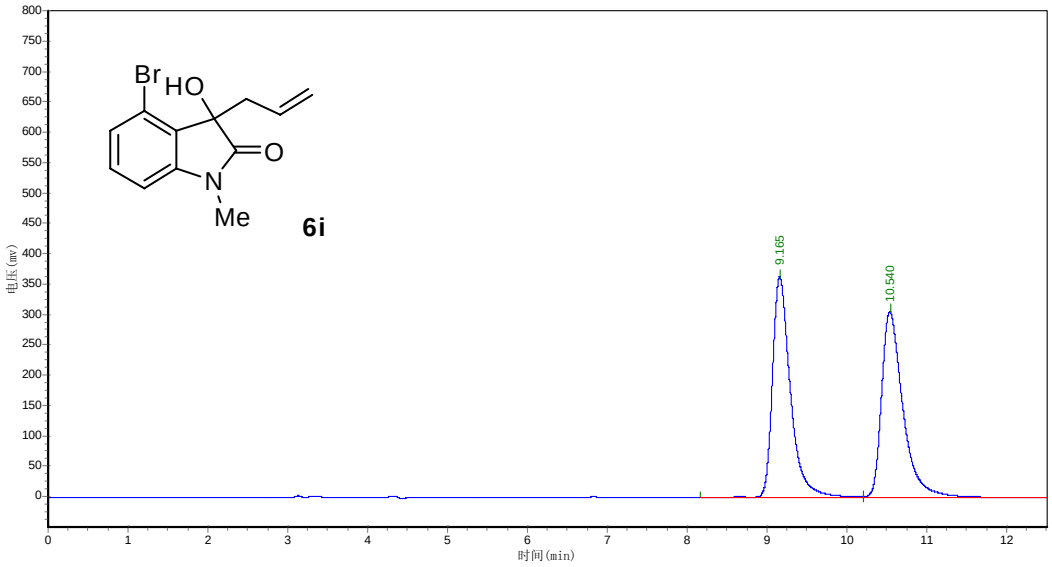
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	8.798	237231.781	25359674.000	33.9400
2	14.848	195366.219	49359464.000	66.0600



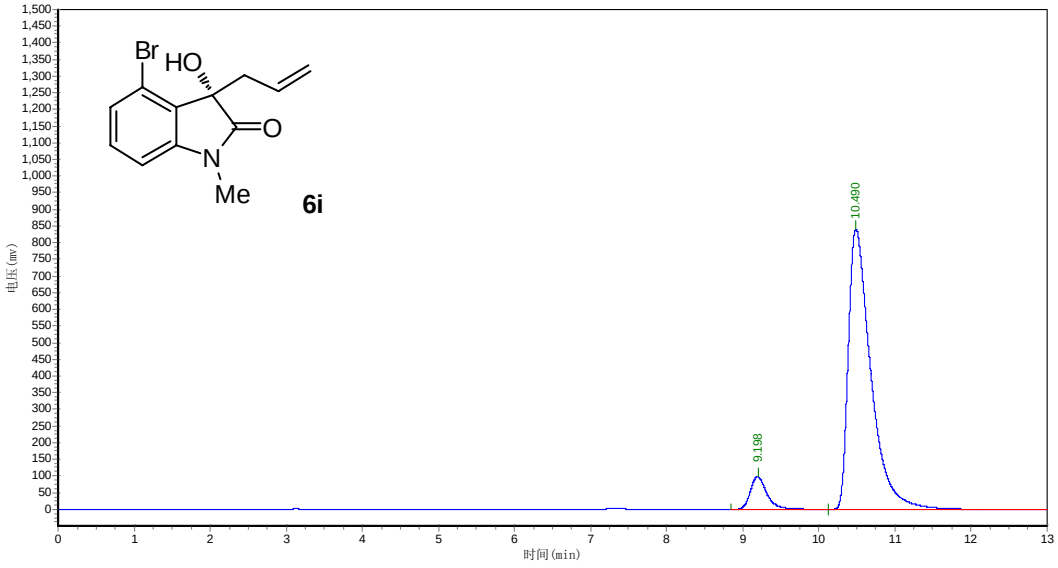
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.273	37374.000	836698.500	51.0917
2	39.890	6742.313	800942.875	48.9083



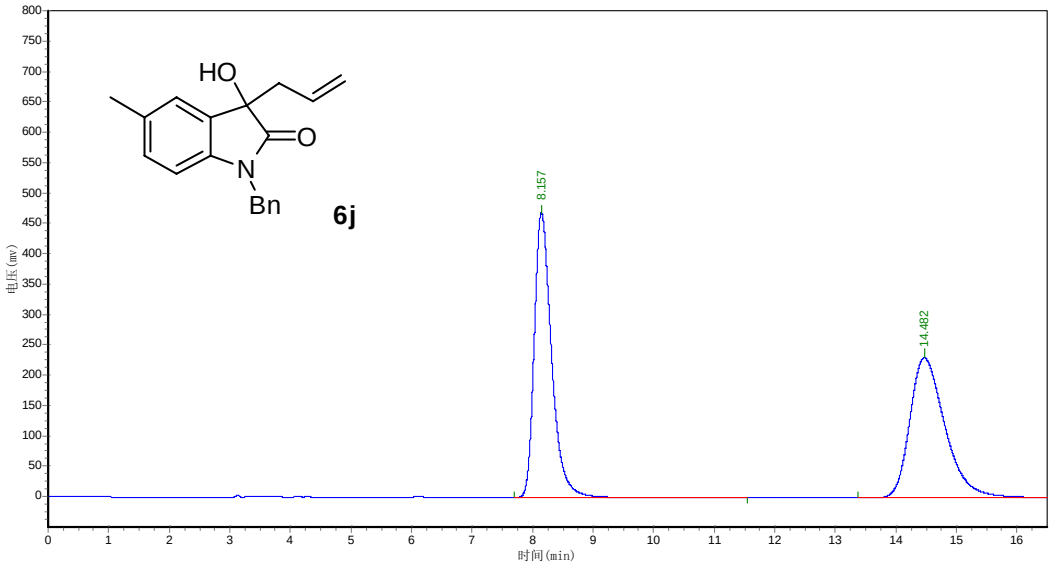
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.290	70323.711	1586164.000	11.3357
2	39.290	86800.375	12406421.000	88.6643



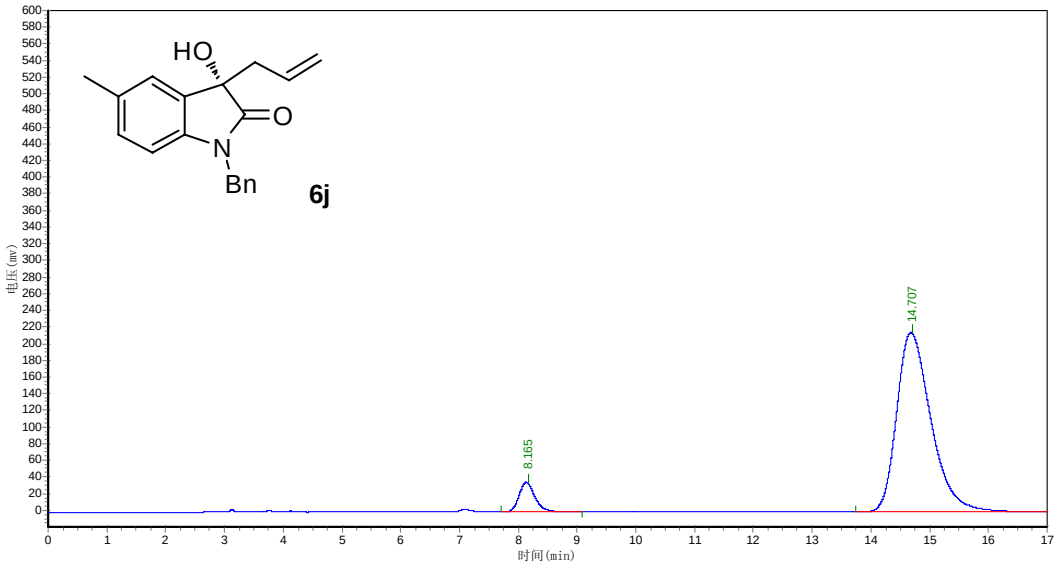
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	9.165	358324.188	5674352.500	49.9648
2	10.540	302539.594	5682345.000	50.0352



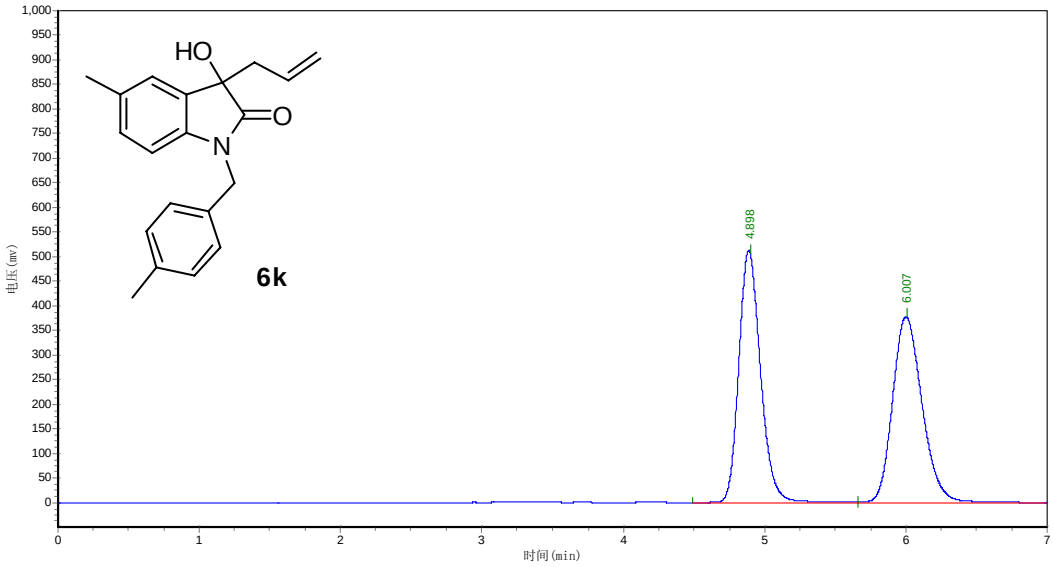
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	9.198	98180.859	1501473.000	7.9798
2	10.490	841130.188	17314460.000	92.0202



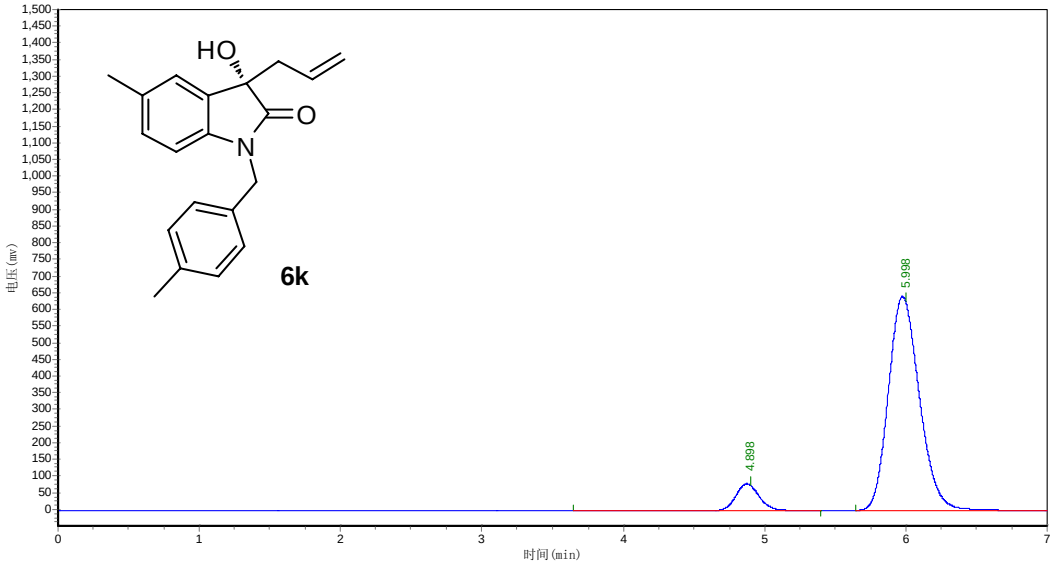
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	8.157	435905.781	9323303.000	50.0332
2	14.482	226776.141	9309918.000	49.9668



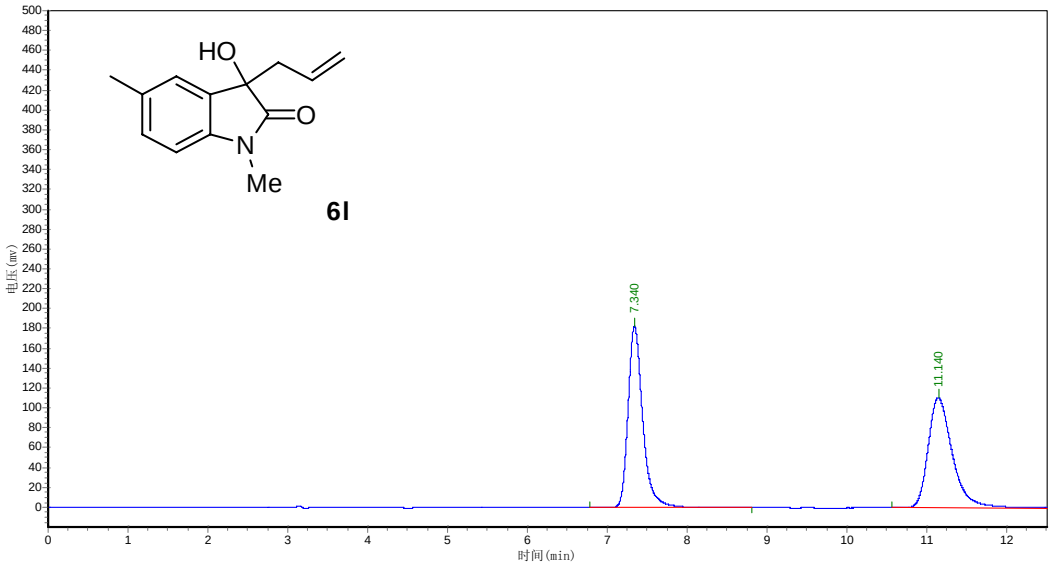
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	8.165	35064.000	667083.375	7.0799
2	14.707	215273.672	8755143.000	92.9201



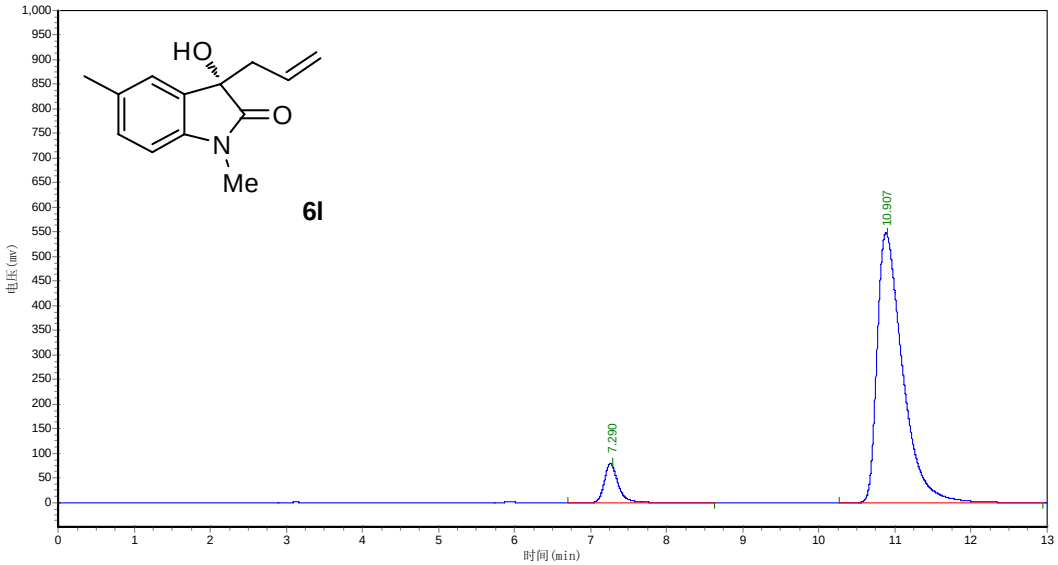
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	4.898	479798.875	5468246.500	49.9338
2	6.007	360839.438	5482753.000	50.0662



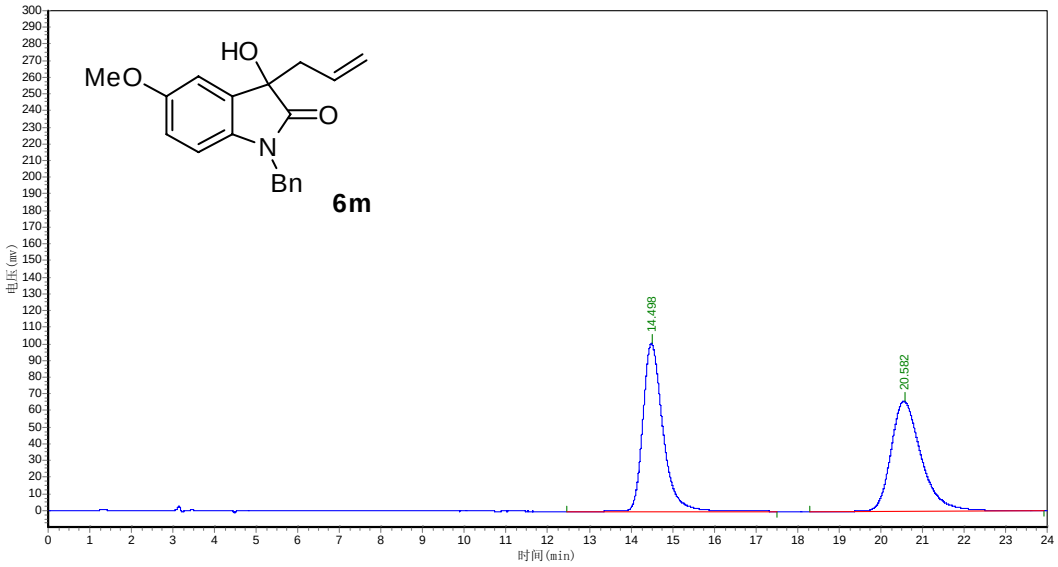
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	4.898	79057.953	960973.563	8.8983
2	5.998	635712.813	9838487.000	91.1016



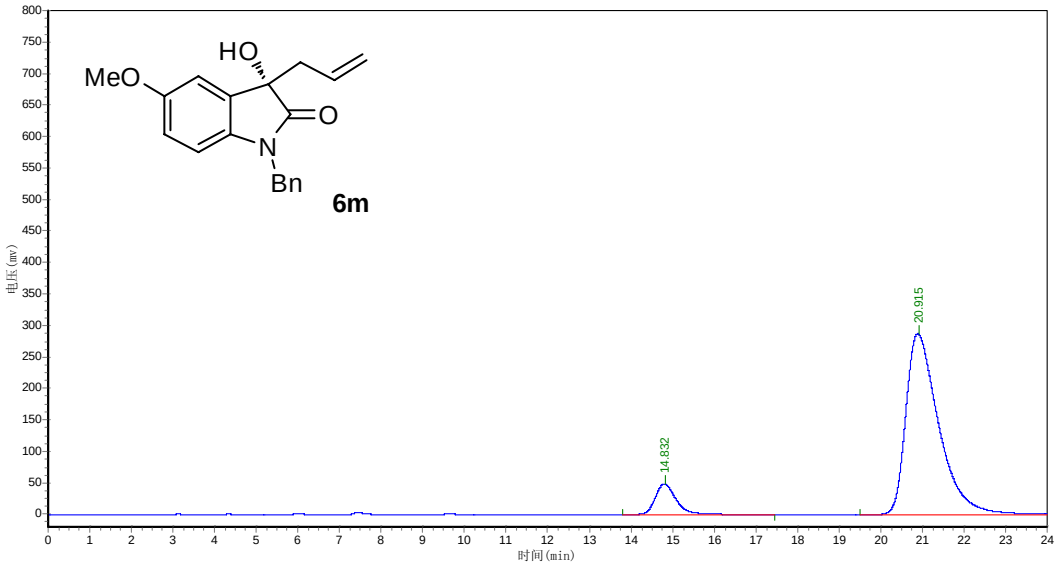
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	7.340	182888.375	2345038.250	50.0488
2	11.140	110971.047	2340468.250	49.9512



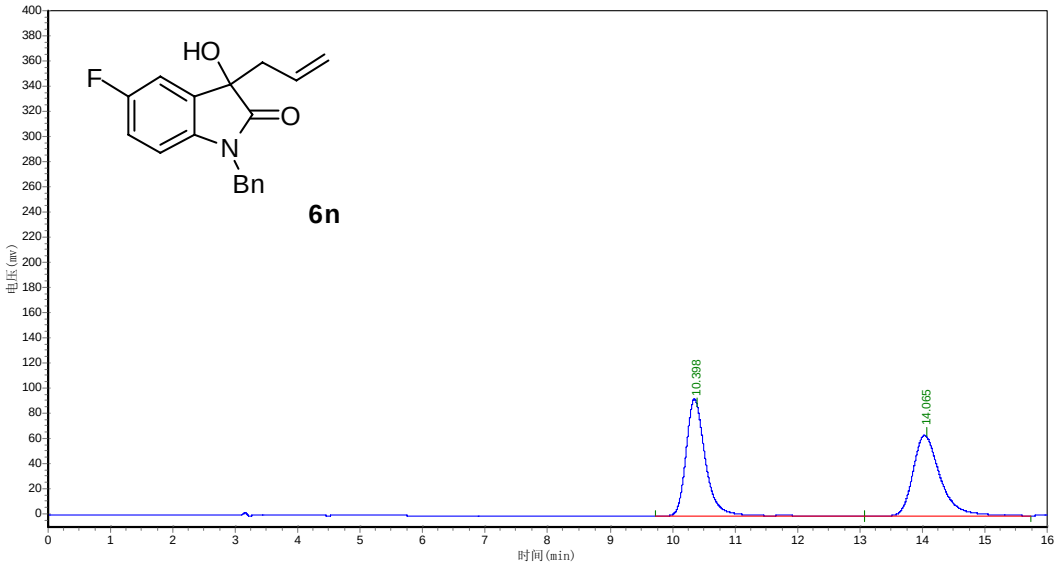
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	7.290	77879.094	1011647.563	7.3505
2	10.907	544764.563	12751247.000	92.6495



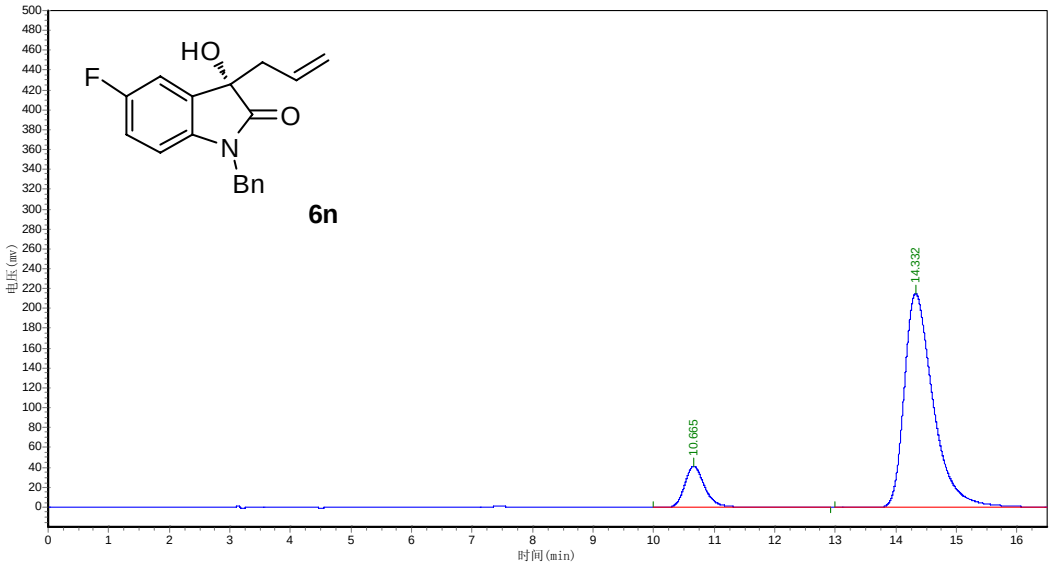
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	14.498	100314.609	3345486.500	50.0534
2	20.582	65947.039	3338350.000	49.9466



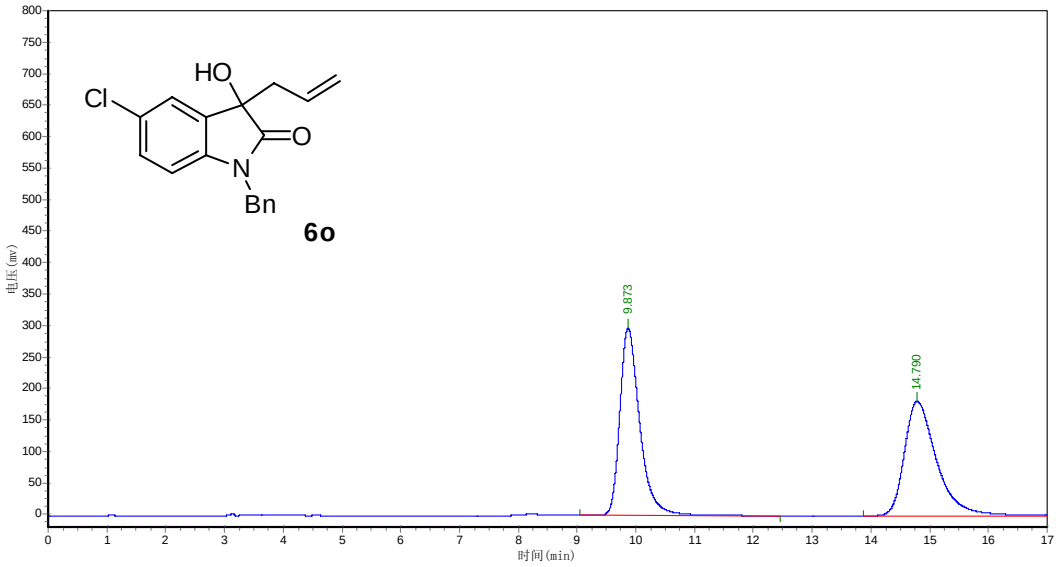
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	14.832	48379.602	1684058.625	9.6608
2	20.915	286879.000	15747899.000	90.3392



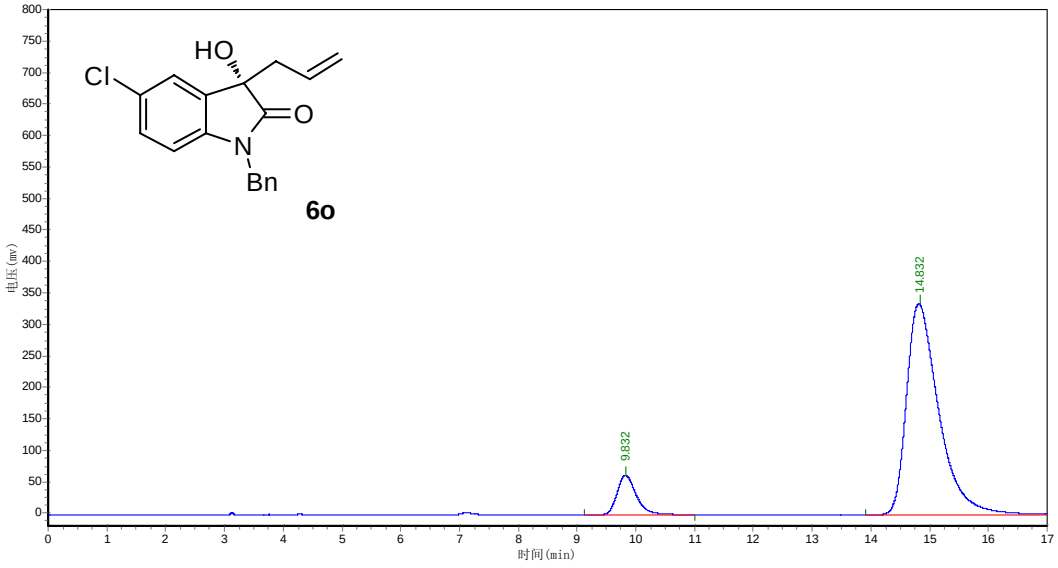
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.398	91169.000	1993330.375	50.7155
2	14.065	63442.000	1937088.750	49.2845



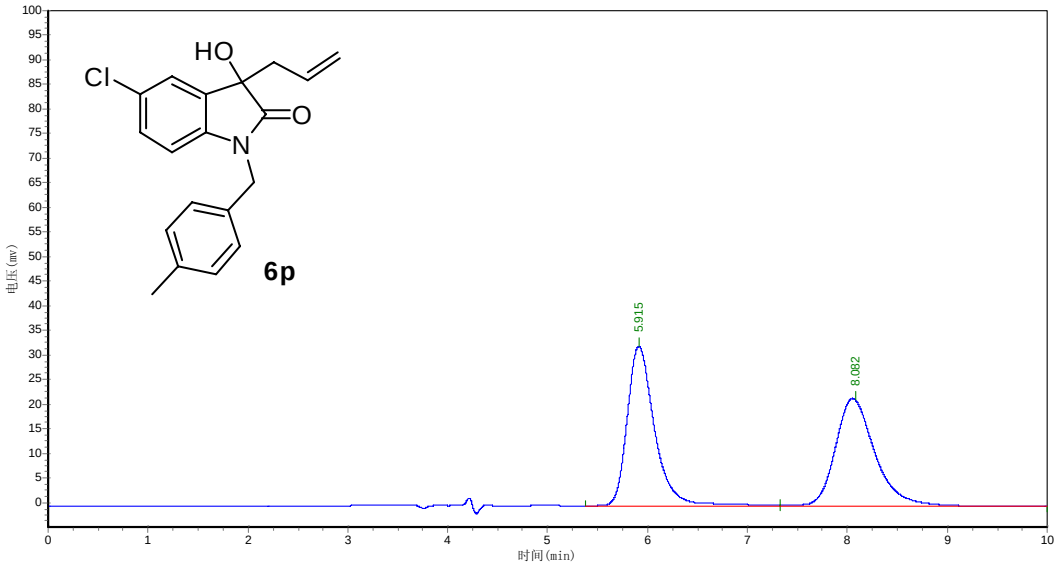
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.665	41068.086	970142.500	11.8760
2	14.332	214600.750	7198789.000	88.1240



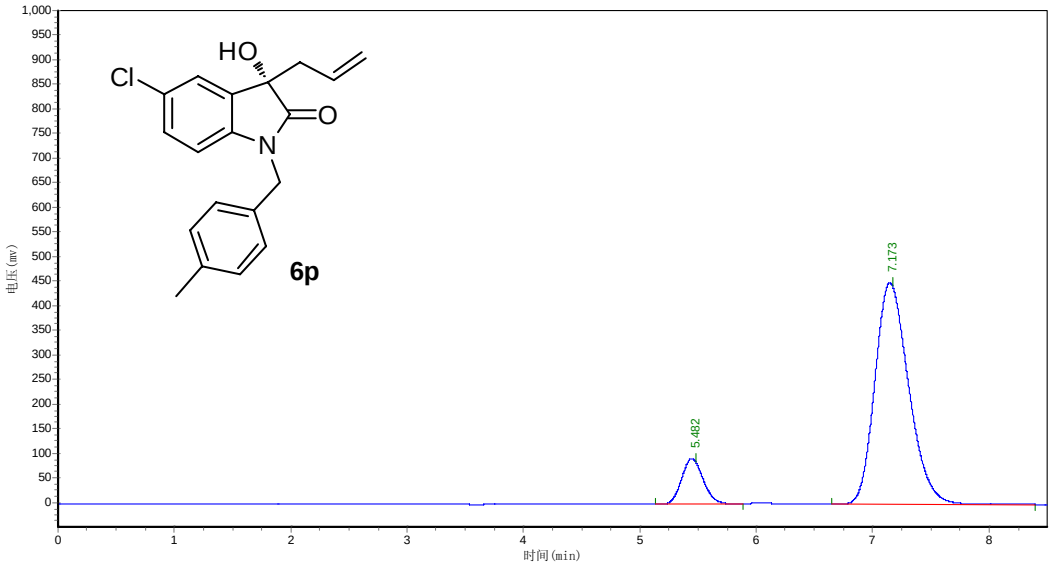
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	9.873	294339.719	6985419.500	50.1838
2	14.790	180632.500	6934243.500	49.8162



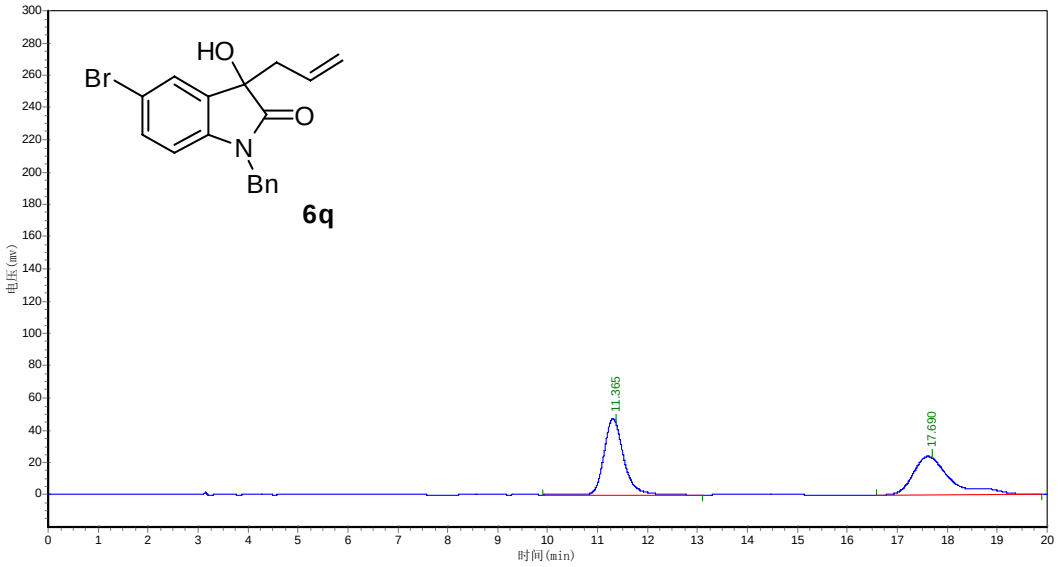
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	9.832	62636.777	1437535.375	10.0646
2	14.832	335039.000	12845596.000	89.9354



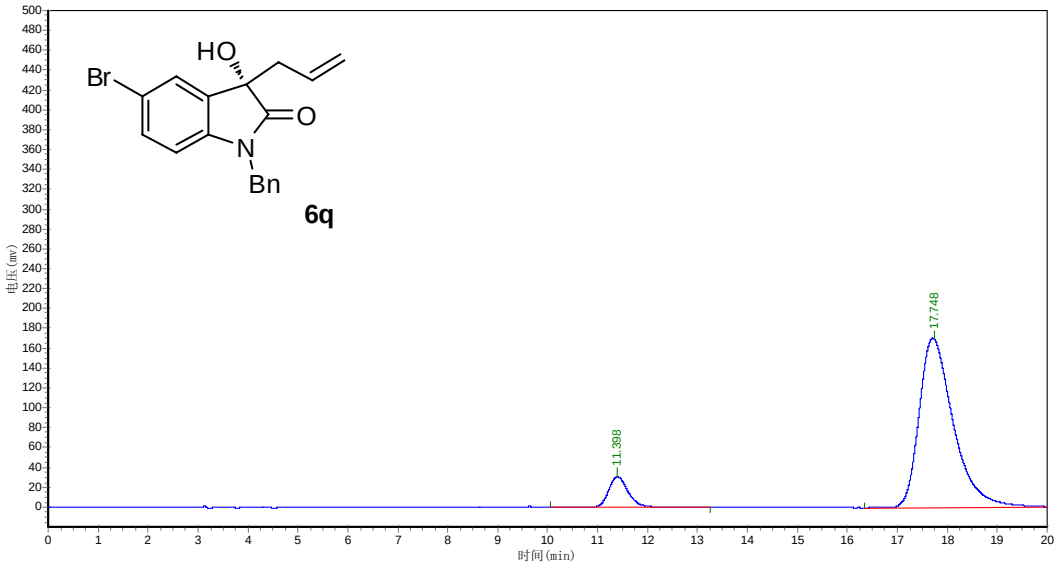
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	5.915	32010.783	631603.625	50.8768
2	8.082	21863.918	609834.625	49.1232



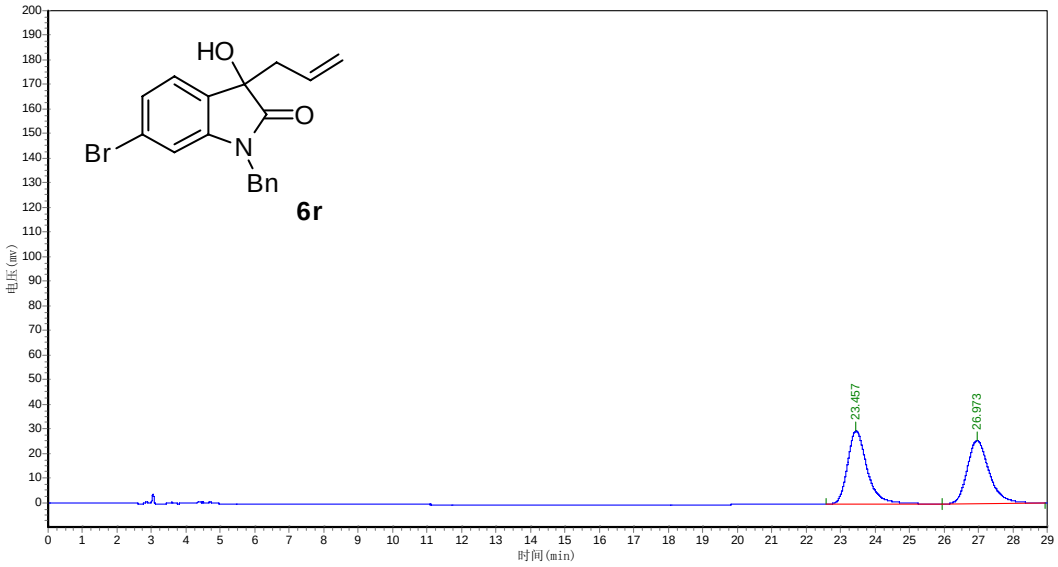
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	5.482	90607.766	1193568.000	11.6055
2	7.173	447060.594	9090935.000	88.3945



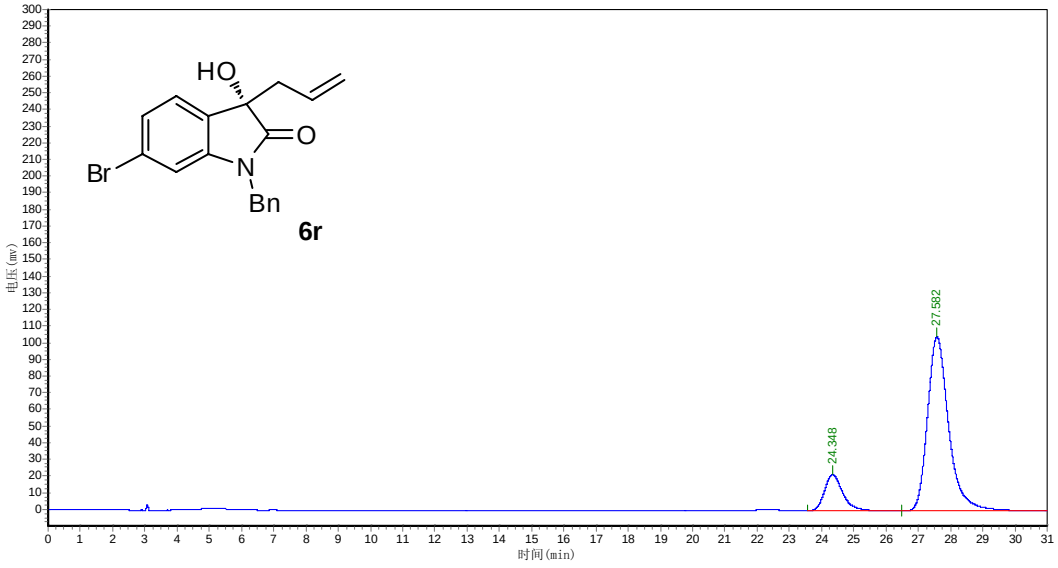
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	11.365	46536.086	1286158.000	50.9487
2	17.690	23590.000	1238258.125	49.0513



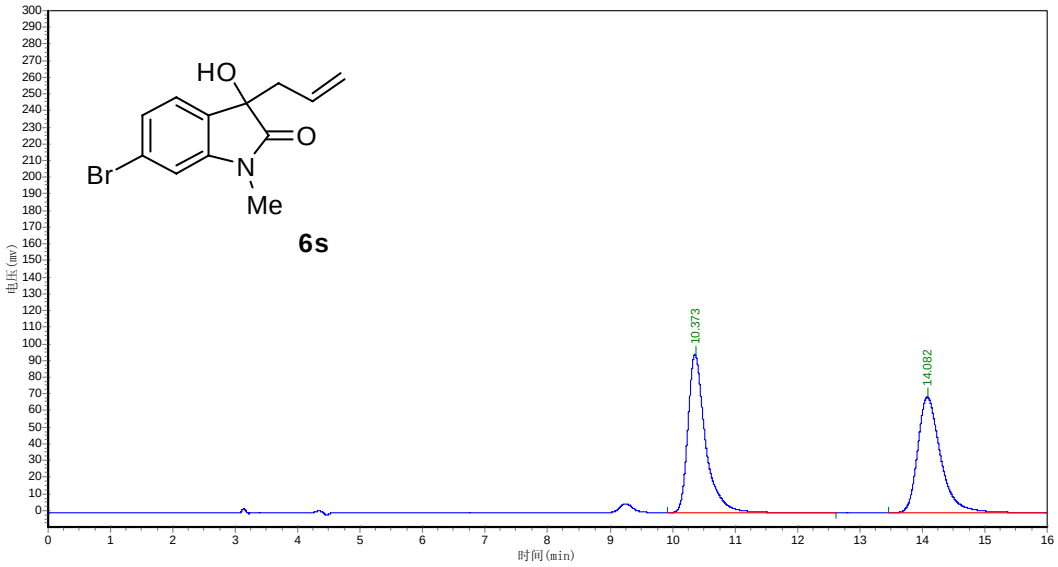
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	11.398	30748.344	868963.375	9.5887
2	17.748	170258.859	8193376.000	90.4113



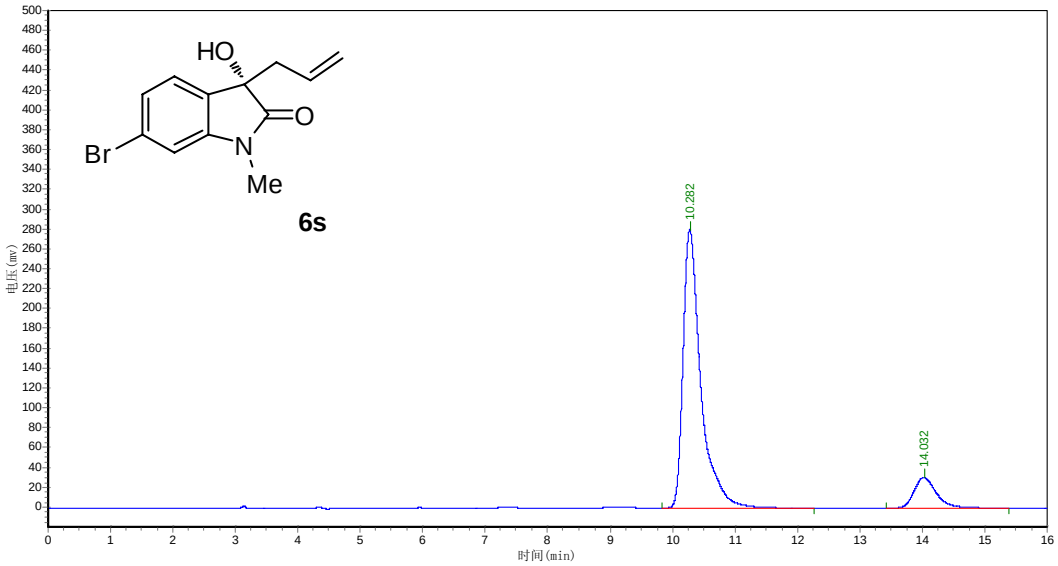
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	23.457	29760.367	1176750.500	50.8366
2	26.973	25693.797	1138212.250	49.1634



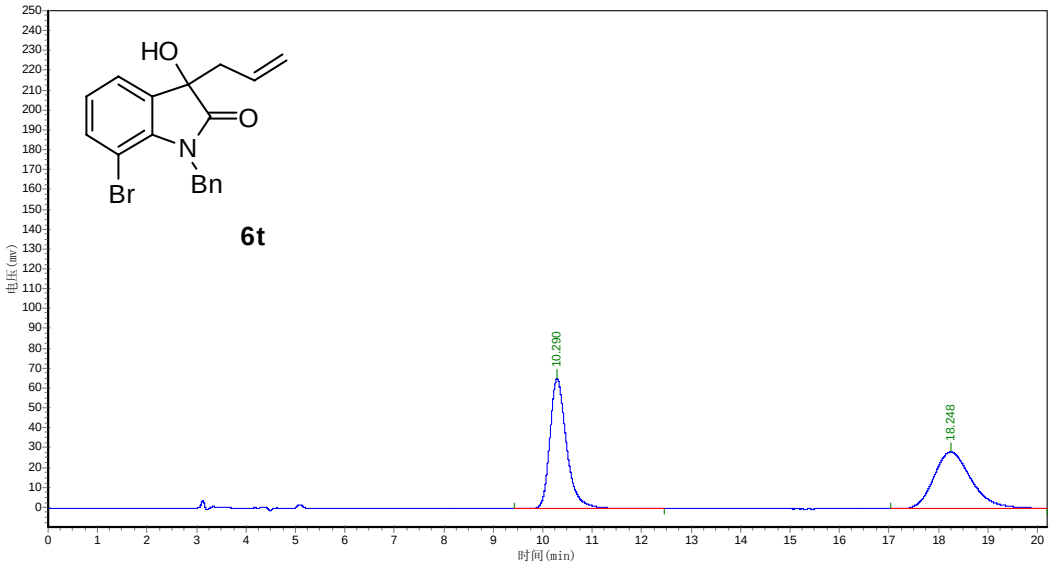
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	24.348	21652.305	858483.875	15.1748
2	27.582	104353.813	4798808.500	84.8252



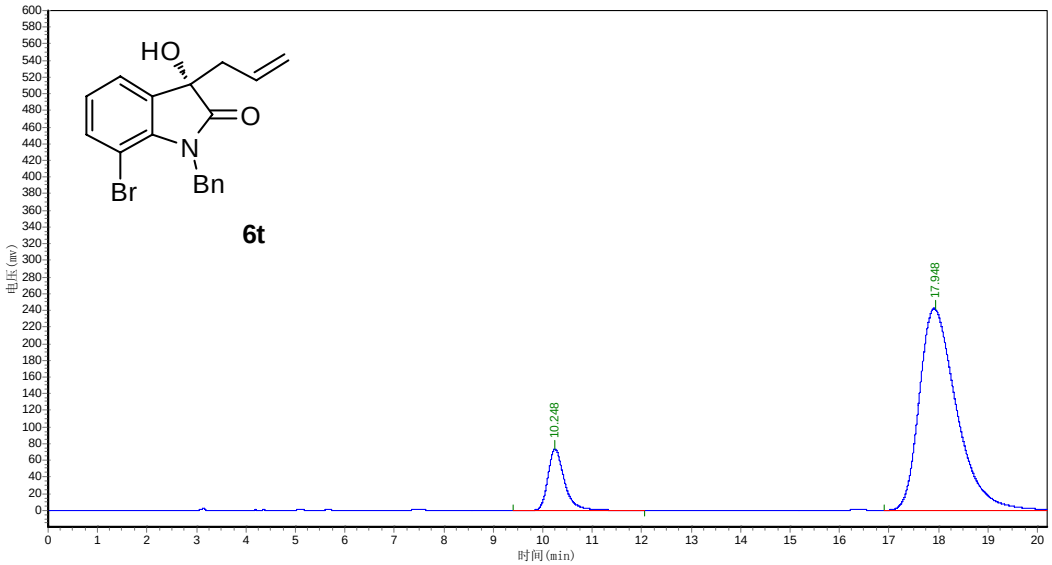
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.373	94354.859	1861904.500	51.1402
2	14.082	68676.156	1778883.000	48.8598



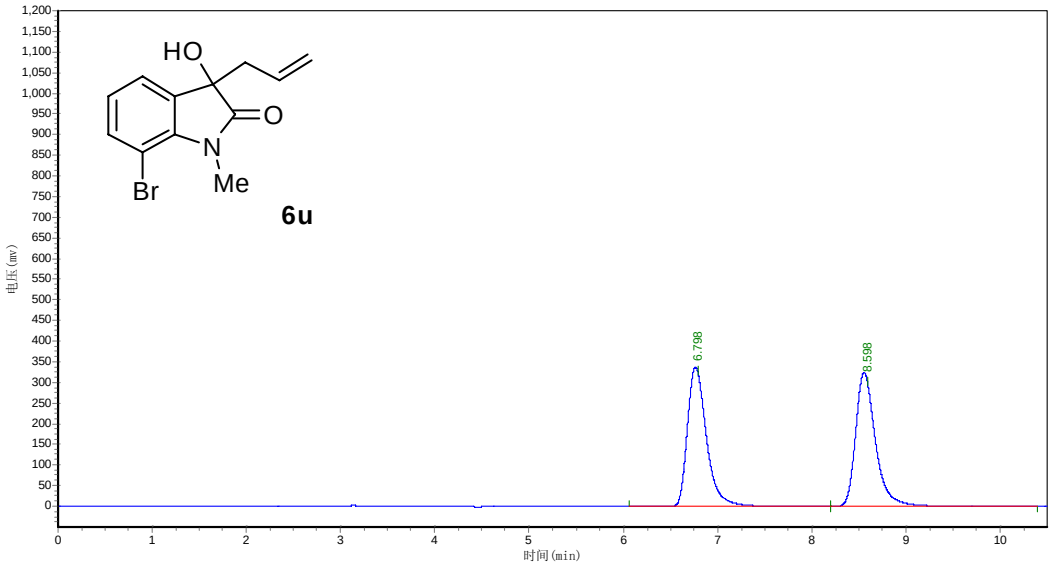
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.282	280275.563	5549502.000	87.8031
2	14.032	30788.014	770893.500	12.1969



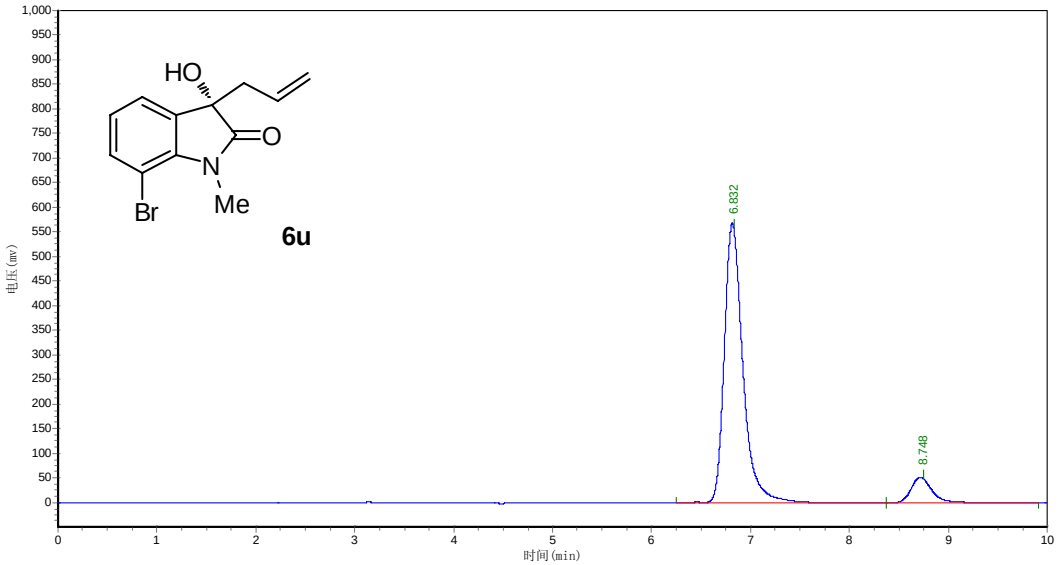
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.290	64529.590	1545542.500	50.8803
2	18.248	28454.408	1492064.125	49.1197



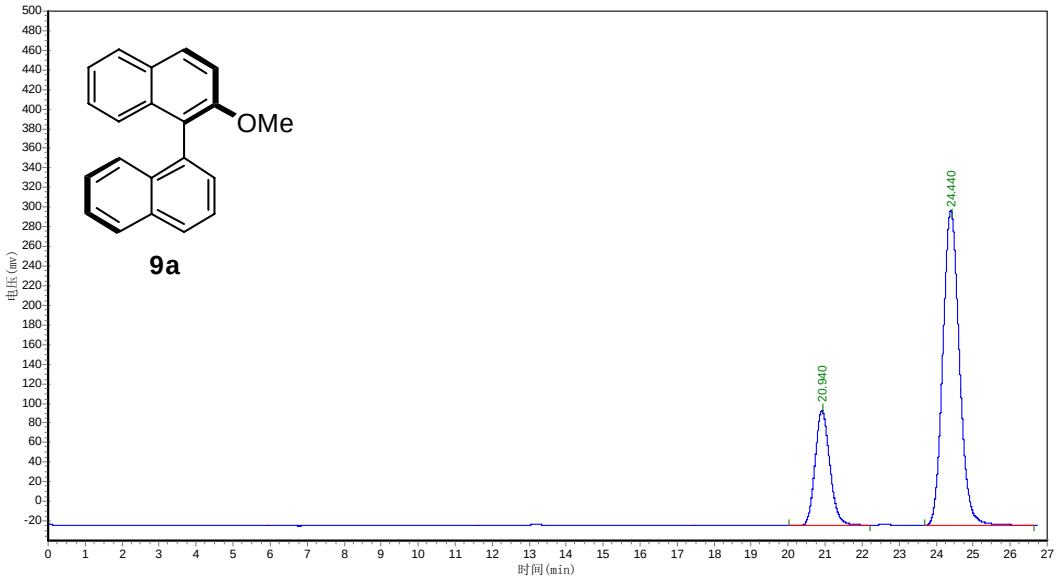
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	10.248	72021.719	1697211.000	11.8081
2	17.948	242865.047	12676030.000	88.1919



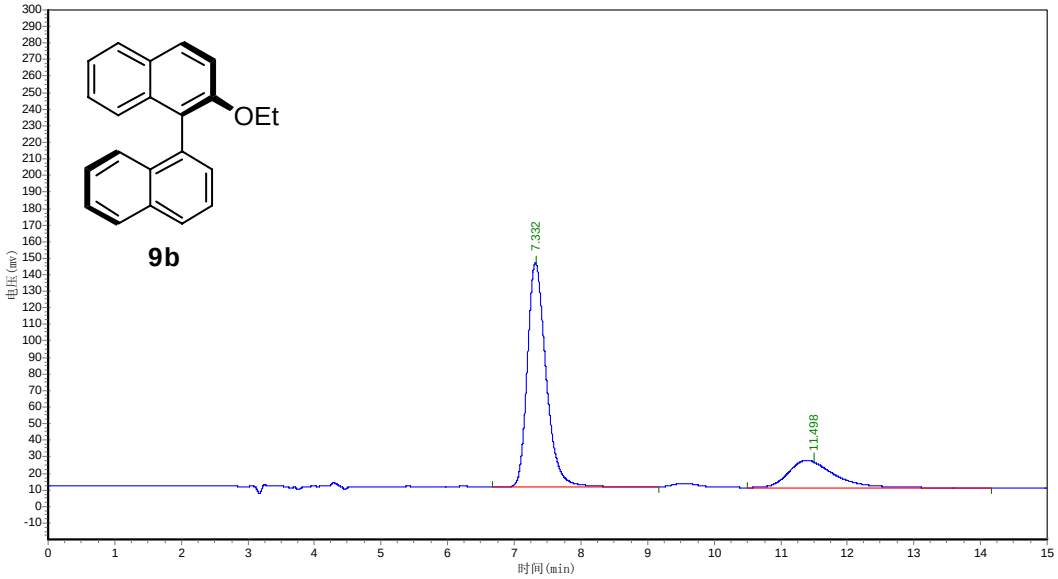
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	6.798	329890.813	4792507.500	50.546
2	8.598	316043.406	4782059.500	49.9454



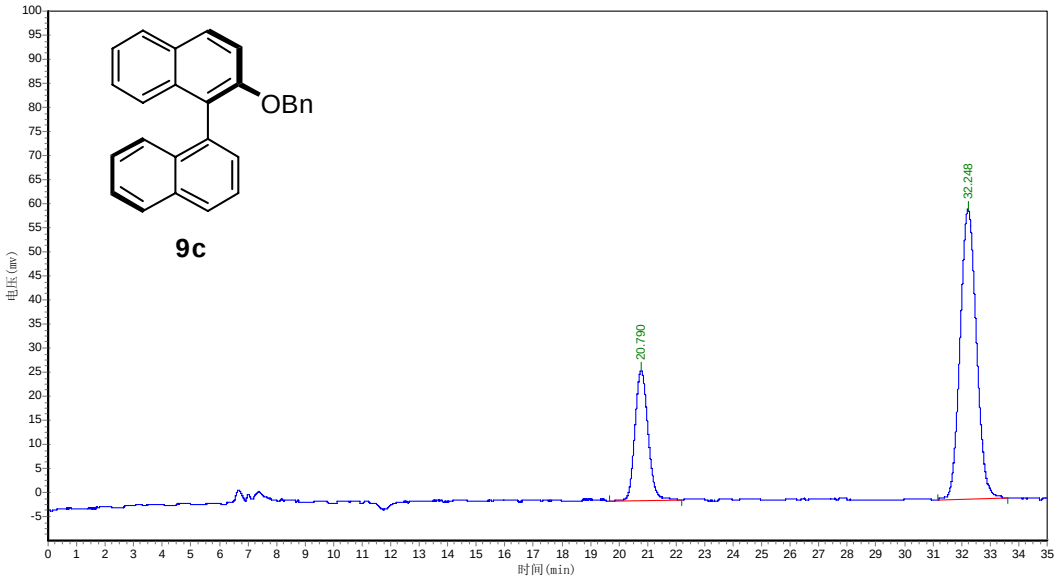
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	6.832	560885.000	7461302.000	90.5709
2	8.748	51464.953	776780.188	9.4291



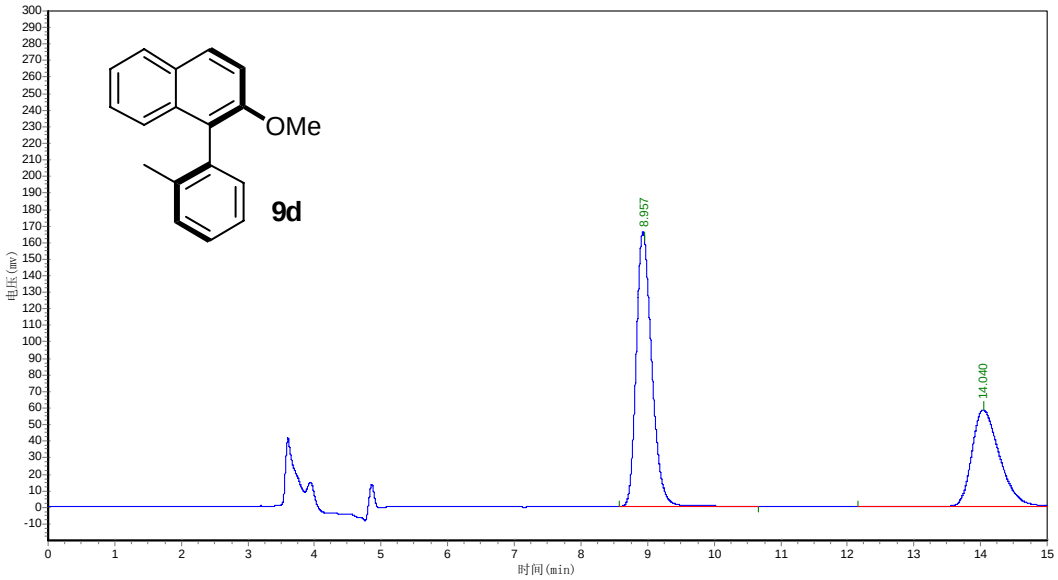
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	20.940	113030.000	3240603.000	24.4637
2	24.440	309526.375	10005961.000	75.5363



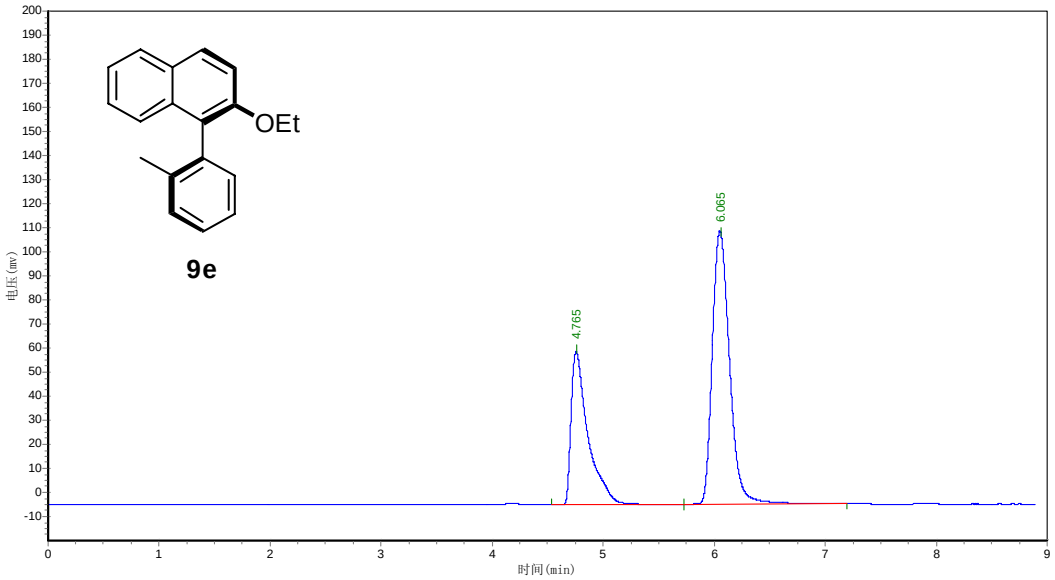
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	7.332	135253.109	2665170.500	75.7229
2	11.498	16414.688	783910.750	22.2725



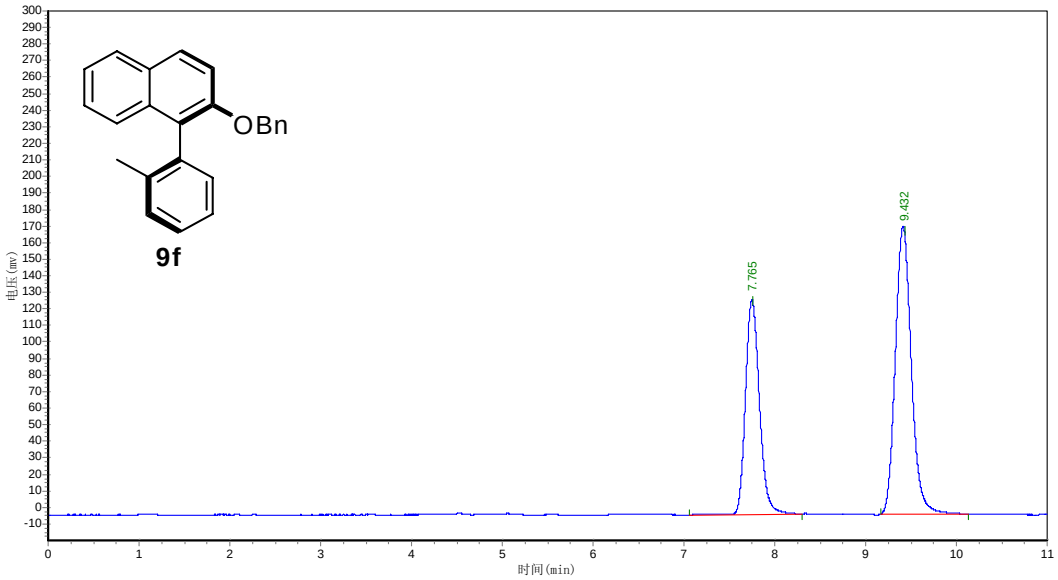
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	20.790	26889.443	866877.063	24.4957
2	32.248	60158.680	2404885.250	75.5043



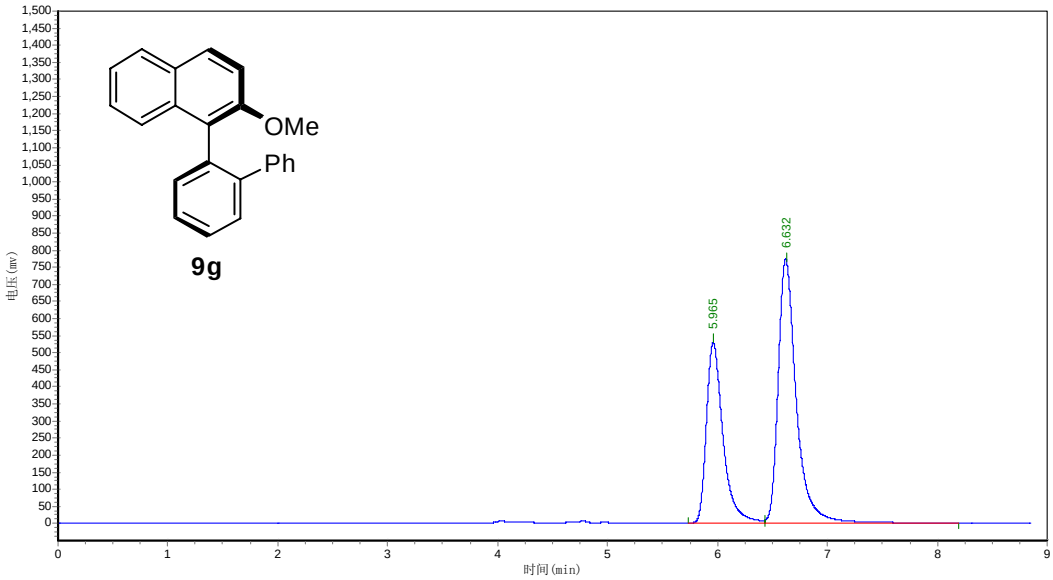
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	8.957	163812.078	2688827.500	61.5748
2	14.040	58177.691	1677937.250	38.4252



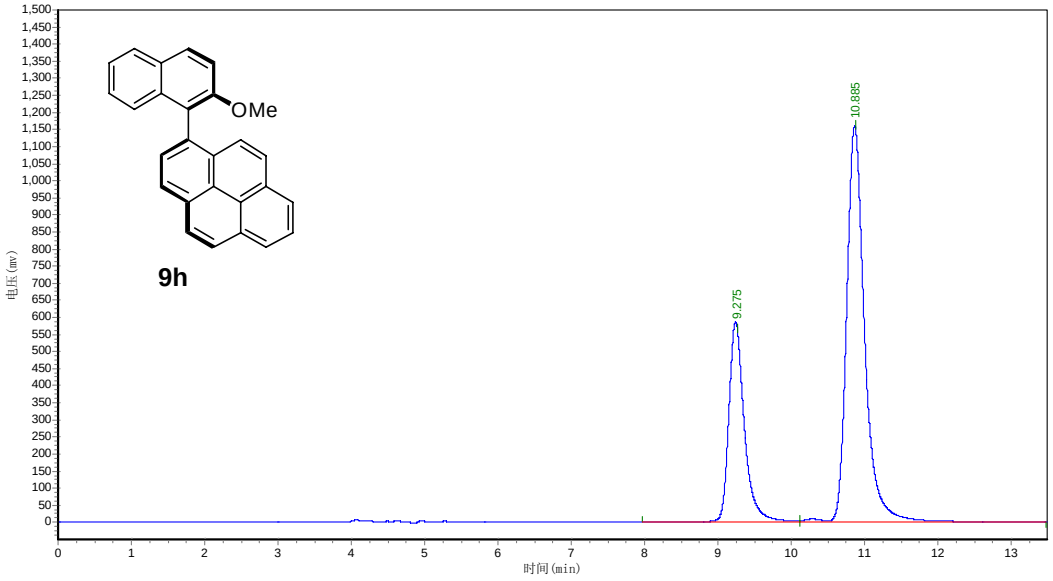
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	4.765	59606.332	677907.375	35.4598
2	6.065	106107.336	1233857.000	64.5402



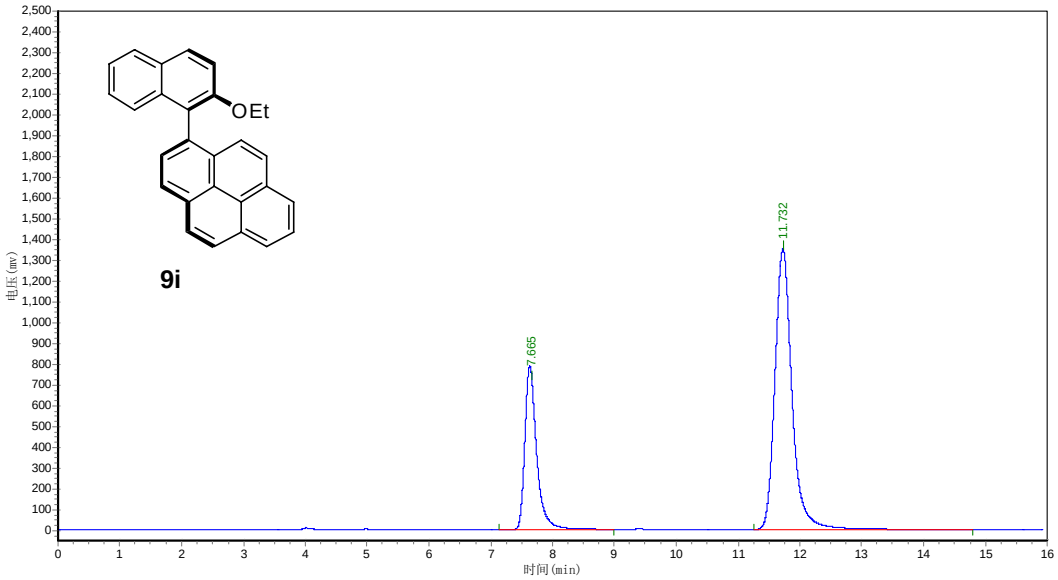
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	7.765	122264.805	1413330.125	39.5027
2	9.432	167760.375	2164474.750	60.4973



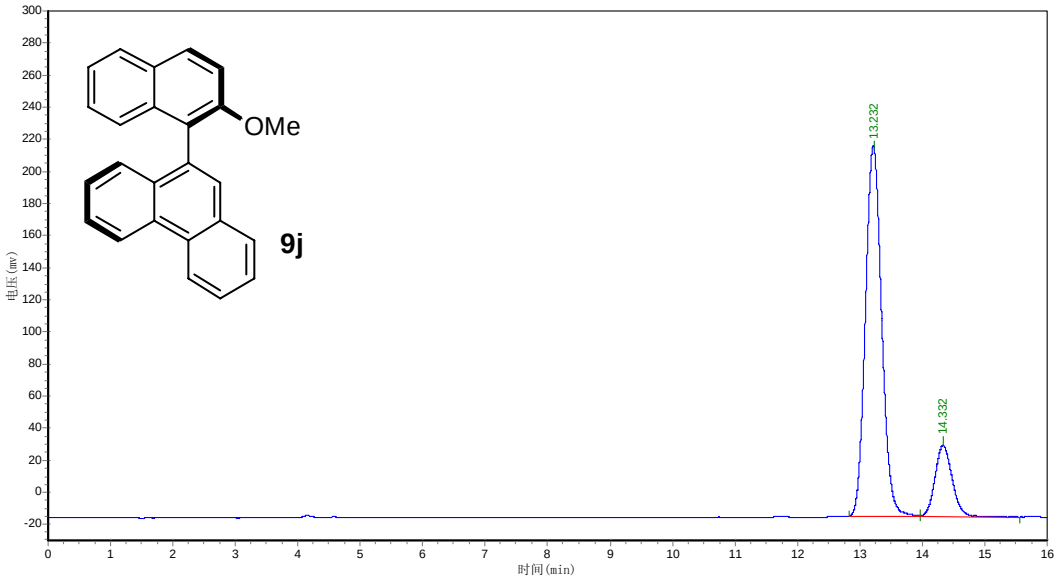
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	5.965	496668.438	5525764.500	38.3598
2	6.632	749708.438	8879322.000	61.6402



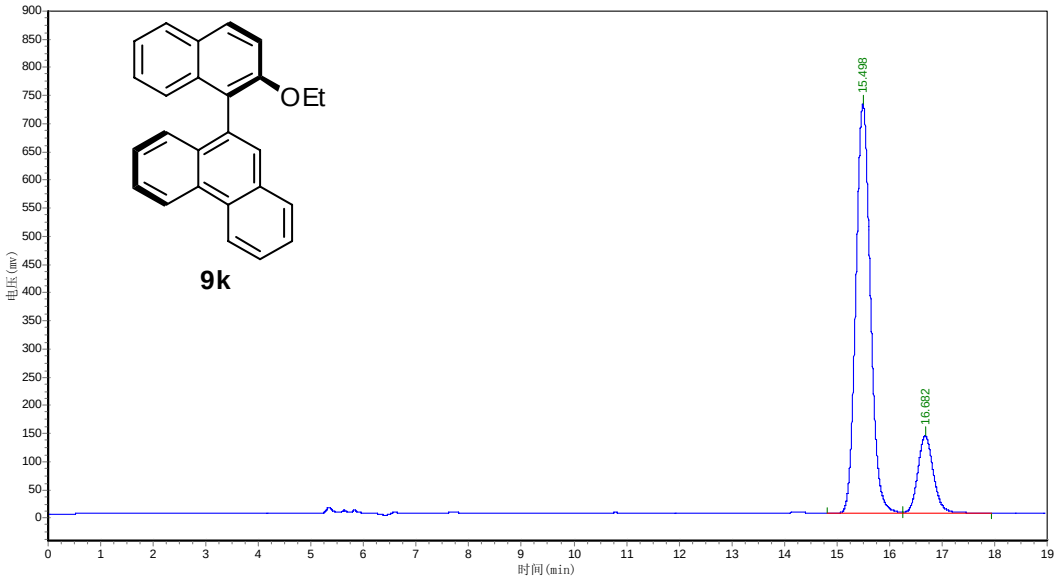
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	9.275	526645.313	8663389.000	30.3546
2	10.885	1047565.188	19877228.000	69.6454



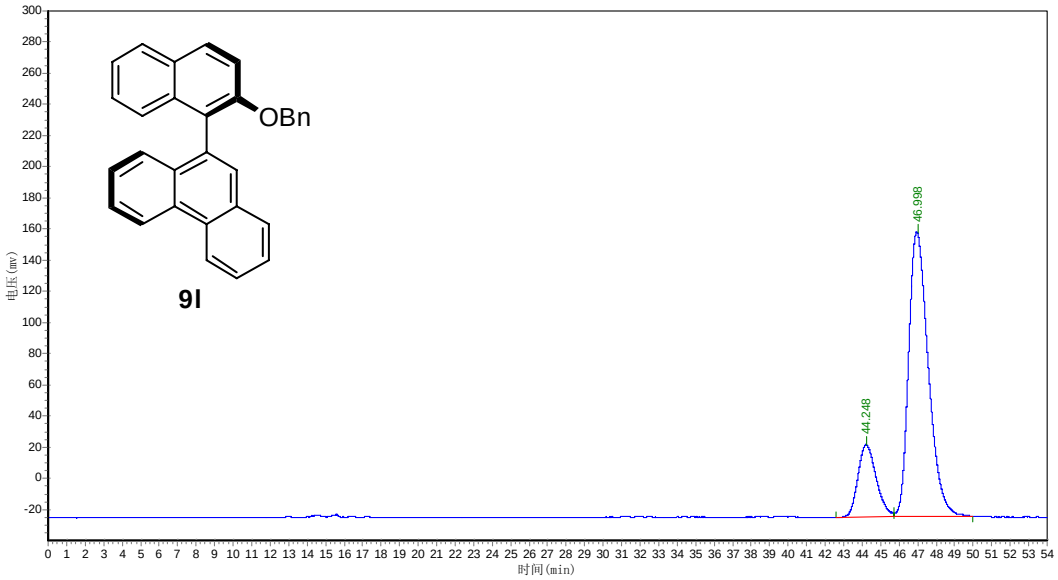
PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	7.665	643408.000	10396649.000	28.6495
2	11.732	1223090.625	25892460.000	71.3505



PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	13.232	230307.609	4192408.750	83.6917
2	14.332	44062.535	871393.000	16.3083



PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	15.498	726574.125	13942462.000	83.7169
2	16.682	137071.453	2811909.250	16.2831



PeakNO.	Ret.Time	PeakHeight	PeakArea	Area%
1	44.248	46322.242	3189235.750	19.0490
2	46.998	182892.156	13553059.000	80.9510