Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

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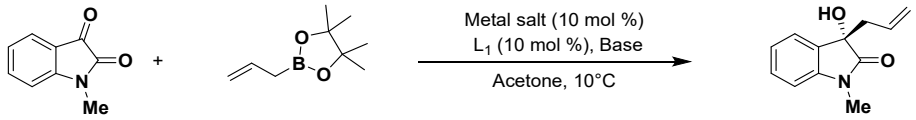
Part I Experimental Section

1.1 General information

^{1}H NMR and ^{13}C NMR were recorded on Bruker-400 MHz Spectrometer (^{1}H NMR: 400MHz, ^{13}C NMR: 100MHz, ^{19}F NMR: 376MHz) and Bruker-500 MHz Spectrometer (^{1}H NMR: 500MHz, ^{13}C NMR: 125MHz, ^{19}F NMR: 470MHz) using TMS as internal reference. The chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz respectively. HPLC analysis was carried out on Agilent 1260 series HPLC with a multiple wavelength detector. Chiralpak IC, AS-H, OD-H, OJ-H, AD-H were purchased form Daicel Chemical Industries, LTD. Optical rotations were measured on a PerKinElmer^{TM} Polarimeter (Model 343). Commercially available compounds were used without further purification. All solvents were purified according to the standard procedures unless otherwise noted. Ligands **L**[1] and isatins[2] were prepared according to the literature procedures.

1.2 Optimization of reaction conditions

Table 1. Optimization of reaction conditions of allylation of isatins[a]

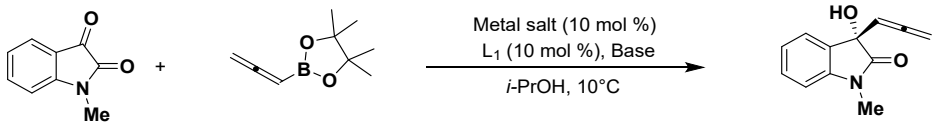


1a 2a 3aa

Entry	Metal salt	Base	Amount of base	Yield[b] (%)	*ee*[c] (%)
1	**Cu(OTf)$_2$**	Et_3N	10%	Trace	--
2	**Zn(OTf)$_2$**	Et_3N	10%	98	73
3	**Zn(OTf)$_2$**	Li_2CO_3	10%	98	24
4	**Zn(OTf)$_2$**	Cs_2CO_3	10%	98	83
5	**Zn(OTf)$_2$**	Na_2CO_3	10%	99	32
6	**Zn(OTf)$_2$**	*t*-BuOK	10%	99	39
7	**Zn(OTf)$_2$**	DABCO	10%	98	63
8	**Zn(OTf)$_2$**	DIPEA	10%	97	32
9	**Zn(OTf)$_2$**	DBU	10%	98	51
10	**Zn(OTf)$_2$**	N-Ethylmorfolin	10%	98	52
11	**Zn(OTf)$_2$**	Cs_2CO_3	5%	99	79
12	**Zn(OTf)$_2$**	Cs_2CO_3	15%	99	75
13	**Zn(OTf)$_2$**	Cs_2CO_3	20%	99	68

[a]Unless otherwise noted, the reaction of **1a** (0.1 mmol) and **2a** (0.25 mmol) was performed in the presence of $\mathbf{L_1}$ (10 mol %), base, metal salt (10 mol %) in acetone (1.0 mL). [b]Isolated yield. [c]Determined by chiral HPLC analysis.

Table 2. Optimization of reaction conditions of allenylation of isatins[a]

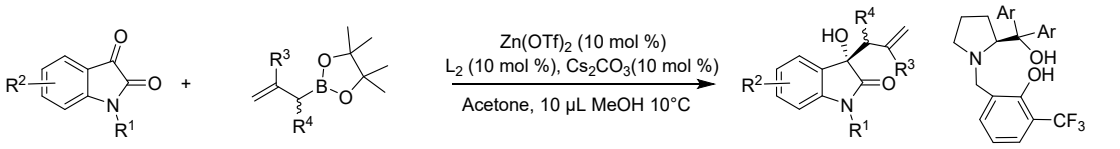


1a 2b 3ba

Entry	Metal salt	Base	Yield[b] (%)	*ee*[c] (%)
1	**$Cu(OTf)_2$**	Et_3N	Trace	--
2	**$Zn(OTf)_2$**	Et_3N	97	75
3	**$Zn(OTf)_2$**	Li_2CO_3	99	35
4	**$Zn(OTf)_2$**	Cs_2CO_3	98	86
5	**$Zn(OTf)_2$**	Na_2CO_3	99	62
6	**$Zn(OTf)_2$**	*t*-BuOK	98	58
7	**$Zn(OTf)_2$**	DABCO	98	64
8	**$Zn(OTf)_2$**	DIPEA	98	37
9	**$Zn(OTf)_2$**	DBU	98	54
10	**$Zn(OTf)_2$**	N-Ethylmorfolin	98	57

[a]Unless otherwise noted, the reaction of **1a** (0.1 mmol) and **2b** (0.25 mmol) was performed in the presence of $\mathbf{L_1}$ (10 mol %), base (10 mol %), metal salt (10 mol %) in *i*-PrOH (1.0 mL). [b]Isolated yield. [c]Determined by chiral HPLC analysis.

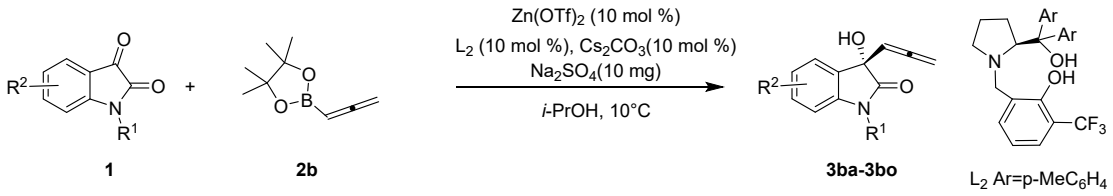
1.3 General working procedure



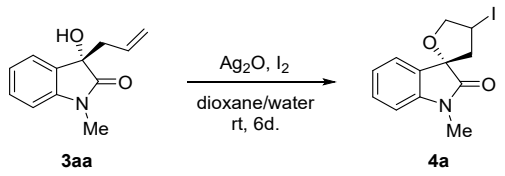
1 2a 3aa-3av

L_2 Ar=*p*-MeC_6H_4

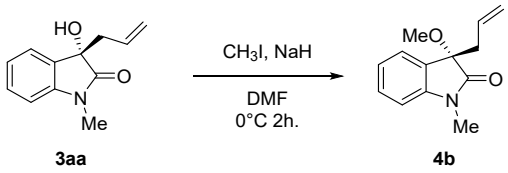
A mixture of $Zn(OTf)_2$ (3.6 mg, 0.01 mmol) and the ligand $\mathbf{L_2}$ (4.6 mg, 0.01 mmol) in acetone (1 mL) with Cs_2CO_3 (3.3 mg, 0.01 mmol) was stirred at room temperature for 2 h. MeOH (10 μL) and isatin **1** (0.1 mmol) were then added and the resulting mixture was cooled to 10℃. After stirring the mixture for 0.5 h, allylborate **2a** (0.25 mmol) was added in one portion. After the reaction was completed (monitored by TLC), the reaction mixture was evaporated in vacuo. Purification of the residue by column chromatography afforded the desired product **3aa-3av.**



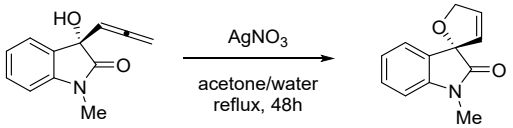
A mixture of $Zn(OTf)_2$ (3.6 mg, 0.01 mmol), the ligand (**L_2**, 4.6 mg, 0.01 mmol), and Na_2SO_4 (10 mg) in *i*-PrOH (1 mL) with Cs_2CO_3 (3.3 mg, 0.01 mmol) was stirred at room temperature for 2 h. Isatins **1** (0.1 mmol) were then added and the resulting mixture was cooled to 10℃. After stirring the mixture for 0.5 h, allenylborate **2b** (0.25 mmol) was added in one portion. After the reaction was completed (monitored by TLC), the reaction mixture was evaporated in vacuo. Purification of the residue by column chromatography afforded the desired product **3ba-3bo.**



To a solution of **3aa** (60.9 mg, 0.3 mmol) in 1,4-Dioxane/H_2O(2.8 mL/0.4 mL), Ag_2O (104 mg, 0.45 mmol) and I_2 (114.3 mg, 0.45 mmol) was added, and the resulting solution was stirred for 6 days at room temperature. The resulting mixture was extracted with CH_2Cl_2 (3 x 10 mL). The organic layer was washed with brine, dried over Na_2SO_4 and removed the solvent in vacuo. Purification of the residue by column chromatography afforded the white solid **4a** (37.5 mg, 38% yield)**.**

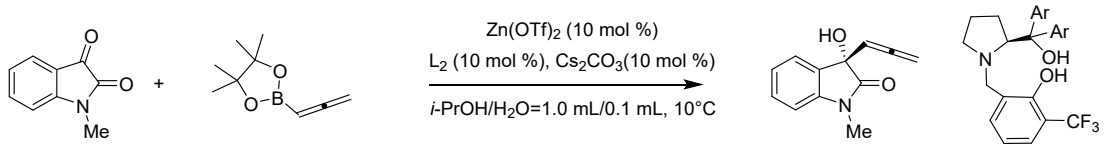


To a solution of **3aa** (20.6 mg, 0.2 mmol) in DMF (4.0 mL), NaH (12 mg, 0.5 mmol) was added at 0℃, and the resulting solution was stirred for 30 minutes. CH_3I (18.8 μL, 0.3 mmol) was added and the solution was then warmed up slowly from 0℃ to room temperature and stirred for 2 hours. The reaction was then re-cooled to 0℃ and quenched by addition of aqueous NH_4Cl solution. The resulting mixture was extracted with CH_2Cl_2 (3×10 mL), and the organic layer was washed with brine, dried over Na_2SO_4 and the solvent was removed in vacuo. Purification of the residue by column chromatography afforded the yellow oil **4b** (35.6mg, 82% yield)**.**



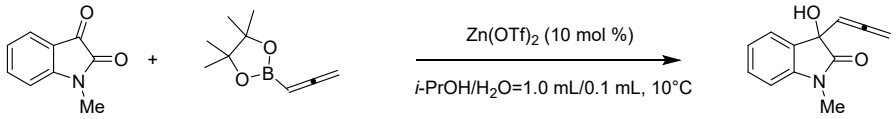
3ba **4c**

To a solution of **3ba** (20.1 mg, 0.1 mmol) in acetone/H_2O(1 mL/1 mL), $AgNO_3$(17 mg, 0.1 mmol) was added, and the resulting solution was refluxed for 48 hours. The resulting mixture was extracted with CH_2Cl_2 (3×10 mL). The organic layer was washed with brine, dried over Na_2SO_4 and removed the solvent in vacuo. Purification of the residue by column chromatography afforded the white solid **4c** (17.5 mg, 87% yield)**.**



1a **2b** **3ba** 98% yield, 48% *ee* L_2 Ar=p-MeC_6H_4

A mixture of $Zn(OTf)_2$ (3.6 mg, 0.01 mmol), the ligand (**L_2**, 4.6 mg, 0.01 mmol) in *i*-PrOH/H_2O (1.0 mL/0.1mL) with Cs_2CO_3 (3.3 mg, 0.01 mmol) was stirred at room temperature for 2 h. Isatins **1a** (0.1 mmol) were then added and the resulting mixture was cooled to 10℃. After stirring the mixture for 0.5 h, allenylborate **2b** (0.25 mmol) was added in one portion. After the reaction was completed (monitored by TLC), the reaction mixture was evaporated in vacuo. Purification of the residue by column chromatography afforded the desired product **3ba** with 98% yield and 48% *ee*.

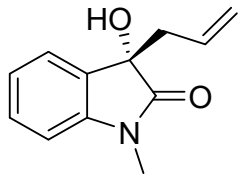


1a **2b** **3ba** racemic

A mixture of $Zn(OTf)_2$ (3.6 mg, 0.01 mmol) and isatins **1a** (0.1 mmol) in *i*-PrOH/H_2O (1.0 mL/0.1mL) was stirred at 10℃ for 0.5 h. Allenylborate **2b** (0.25 mmol) was added in one portion. After the reaction was stirred for 12 h, the reaction mixture was evaporated in vacuo. Purification of the residue by column chromatography afforded the desired product racemic **3ba** (8.3 mg, 41% yield).

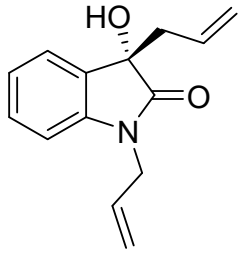
1.4 Experimental date of products

(*S*)-3-allyl-3-hydroxy-1-methylindolin-2-one（3aa）[3], [4]



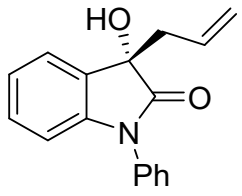
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (19.9 mg, 98% yield). $[\alpha]_D^{20}$ = -40.7 (*c* = 0.5, $CHCl_3$, 93% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.4 min (minor), t_R = 10.5 min (major); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 7.4, 0.8 Hz, 1H), 7.32 (ddd, *J* = 7.8, 6.3, 1.2 Hz, 1H), 7.09 (td, *J* = 7.6, 0.9 Hz, 1H), 6.82 (d, *J* = 7.8 Hz, 1H), 5.72 – 5.54 (m, 1H), 5.16 – 5.02 (m, 2H), 3.63 (s, 1H), 3.16 (s, 3H), 2.83 – 2.72 (m, 1H), 2.62 (dd, *J* = 13.4, 8.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.9, 143.2, 130.6, 129.8, 129.7, 124.1, 123.1, 120.3, 108.4, 76.0, 42.9, 26.2.

(*S*)-1,3-diallyl-3-hydroxyindolin-2-one（3ab）[3]



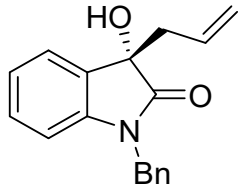
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (22.6 mg, 99% yield). $[\alpha]_D^{20}$ = -37.8 (*c* = 0.6, $CHCl_3$, 97% *ee*); HPLC: Daicel Chiralpak AS-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 230 nm, t_R = 8.0 min (minor), t_R = 12.5 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.3 Hz, 1H), 7.33 – 7.23 (m, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.81 (d, *J* = 7.8 Hz, 1H), 5.89 – 5.72 (m, 1H), 5.69 – 5.53 (m, 1H), 5.30 – 5.17 (m, 2H), 5.16 – 5.00 (m, 2H), 4.48 – 4.33 (m, 1H), 4.24 – 4.12 (m, 1H), 3.37 (s, 1H), 2.78 (dd, *J* = 13.3, 6.3 Hz, 1H), 2.66 (dd, *J* = 13.2, 8.4 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.5, 141.4, 130.1, 129.5, 128.6, 128.5, 123.1, 122.0, 119.5, 116.6, 108.3, 74.9, 42.0, 41.3.

(*S*)-3-allyl-3-hydroxy-1-phenylindolin-2-one（3ac）[3]



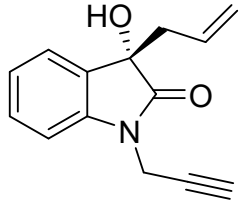
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (25.7 mg, 97% yield). $[\alpha]_D^{20}$ = -49.0 (*c* = 0.6, $CHCl_3$, 89% *ee*); HPLC: Daicel Chiralpak AS-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.1 min (minor), t_R = 9.5 min (major); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.34 (m, 6H), 7.25 (t, *J* = 7.7 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 7.9 Hz, 1H), 5.79 – 5.56 (m, 1H), 5.24 – 5.07 (m, 2H), 3.26 (s, 1H), 2.92 – 2.66 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.2, 143.3, 134.0, 130.4, 129.7, 129.6, 129.3, 128.3, 126.5, 124.4, 123.6, 120.7, 109.7, 76.1, 43.5.

(*S*)-3-allyl-1-benzyl-3-hydroxyindolin-2-one（3ad）[3]



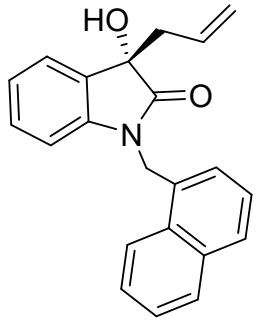
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (27.6 mg, 99% yield). $[\alpha]_D^{20}$ = -15.5 (*c* = 0.3, $CHCl_3$, 95% *ee*); HPLC: Daicel Chiralpak AS-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 230 nm, t_R = 14.6 min (minor), t_R = 17.8 min (major); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.2 Hz, 1H), 7.33 – 7.22 (m, 5H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 7.8 Hz, 1H), 5.71 – 5.54 (m, 1H), 5.20 – 4.95 (m, 3H), 4.71 (d, *J* = 15.7 Hz, 1H), 3.39 (s, 1H), 2.82 (dd, *J* = 13.3, 6.2 Hz, 1H), 2.71 (dd, *J* = 13.3, 8.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.9, 142.5, 135.4, 130.6, 129.7, 129.6, 128.8, 127.7, 127.3, 124.2, 123.1, 120.6, 109.5, 76.0, 43.8, 43.1.

(*S*)-3-allyl-3-hydroxy-1-(prop-2-yn-1-yl)indolin-2-one（3ae）[5]



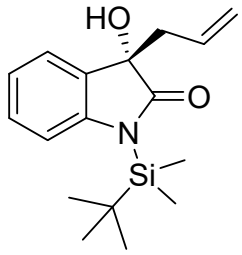
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (22.2 mg, 98% yield). $[\alpha]_D^{20}$ = -41.8 (*c* = 0.6, $CHCl_3$, 95% *ee*); HPLC: Daicel Chiralpak AS-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 230 nm, t_R = 10.9 min (minor), t_R = 16.7 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.3 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 1H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 5.63 – 5.49 (m, 1H), 5.02 (dd, *J* = 12.8, 10.0 Hz, 2H), 4.45 (dd, *J* = 17.7, 2.2 Hz, 1H), 4.30 (dd, *J* = 17.7, 2.1 Hz, 1H), 3.24 (s, 1H), 2.68 (dd, *J* = 13.3, 6.3 Hz, 1H), 2.55 (dd, *J* = 13.3, 8.3 Hz, 1H), 2.16 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.8, 140.3, 129.2, 128.6, 128.5, 123.2, 122.4, 119.6, 108.4, 75.5, 74.8, 71.5, 41.9, 28.3.

(*S*)-3-allyl-3-hydroxy-1-(naphthalen-1-ylmethyl)indolin-2-one（3af）[6]



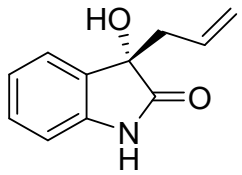
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (32.6 mg, 99% yield). $[\alpha]_D^{20}$ = +1.9 (*c* = 0.7, $CHCl_3$, 90% *ee*); HPLC: Daicel Chiralpak AS-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 230 nm, t_R = 15.9 min (major), t_R = 22.5 min (minor); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.9 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.41 (m, 2H), 7.34 (d, *J* = 7.3 Hz, 1H), 7.28 (td, *J* = 7.9, 2.6 Hz, 1H), 7.21 (d, *J* = 6.9 Hz, 1H), 7.05 (ddd, *J* = 7.7, 5.0, 1.7 Hz, 1H), 6.97 (td, *J* = 7.5, 2.3 Hz, 1H), 6.57 (dd, *J* = 7.8, 2.2 Hz, 1H), 5.73 – 5.56 (m, 1H), 5.47 (d, *J* = 16.2 Hz, 1H), 5.13 – 4.98 (m, 3H), 3.32 (s, 1H), 2.77 (dd, *J* = 13.0, 6.0 Hz, 1H), 2.66 (dd, *J* = 13.2, 8.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.1, 142.8, 133.7, 131.0, 130.6, 130.2, 129.8, 129.7, 129.0, 128.4, 126.6, 126.0, 125.3, 124.6, 124.2, 123.2, 122.9, 120.8, 109.9, 76.0, 43.1, 42.1.

(*S*)-3-allyl-1-(tert-butyldimethylsilyl)-3-hydroxyindolin-2-one（3ag）[7]



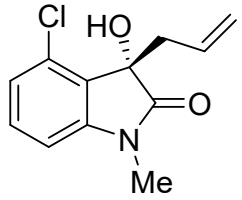
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as pale yellow oil (30.0 mg, 99% yield). $[\alpha]_D^{20}$ = -26.9 (*c* = 0.6, $CHCl_3$, 94% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 95:5, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 4.1 min (minor), t_R =5.5 min (major); ^{1}H NMR (500 MHz, Acetone) δ 7.35 (dd, *J* = 7.3, 0.9 Hz, 1H), 7.25 – 7.19 (m, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 5.51 – 5.40 (m, 1H), 4.99 – 4.89 (m, 3H), 2.70 (dd, *J* = 13.0, 6.3 Hz, 1H), 2.60 (dd, *J* = 13.0, 8.3 Hz, 1H), 0.99 (s, 9H), 0.51 (s, 3H), 0.50 (s, 3H). ^{13}C NMR (125 MHz, Acetone) δ 184.5, 145.8, 132.8, 131.8, 128.8, 124.2, 122.0, 118.5, 112.7, 75.8, 43.2, 26.0, 19.4, -3.9, -4.1.

(*S*)-3-allyl-3-hydroxyindolin-2-one（3ah）[8]



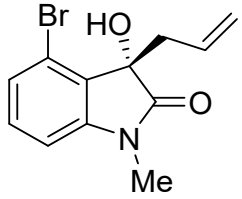
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (18.5 mg, 98% yield). $[\alpha]_D^{20}$ = -8.5 (*c* = 2.0, MeOH, 87% *ee*); HPLC: Daicel Chiralpak OD-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 6.7 min (major), t_R = 7.9 min (minor); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.37 (d, *J* = 7.4 Hz, 1H), 7.29 – 7.23 (m, 1H), 7.12 – 7.04 (m, 1H), 6.88 (d, *J* = 7.8 Hz, 1H), 5.82 – 5.51 (m, 1H), 5.18 – 5.04 (m, 2H), 3.34 (s, 1H), 2.75 (dd, *J* = 13.4, 6.4 Hz, 1H), 2.62 (dd, *J* = 13.4, 8.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.0, 140.2, 130.3, 130.1, 129.7, 124.5, 123.1, 120.7, 110.3, 76.2, 42.8.

(*S*)-3-allyl-4-chloro-3-hydroxy-1-methylindolin-2-one（3ai）[9]



The title compound was prepared according to the general working procedure and purified by column chromatography(ethyl acetate/petroleum ether) to give the product as white solid (23.2 mg, 98% yield). $[\alpha]_D^{20}$ = +2.9 (*c* = 0.6, $CHCl_3$, 94% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.2 min (minor), t_R = 9.7 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (dd, *J* = 12.4, 4.2 Hz, 1H), 7.03 (dd, *J* = 8.2, 0.7 Hz, 1H), 6.72 (dd, *J* = 7.8, 0.6 Hz, 1H), 5.44 – 5.31 (m, 1H), 5.15 – 5.05 (m, 1H), 4.98 – 4.91 (m, 1H), 3.25 (s, 1H), 3.19 – 3.11 (m, 4H), 2.88 (dd, *J* = 12.9, 8.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.5, 144.2, 130.5, 129.8, 129.0, 124.7, 123.1, 119.3, 105.8, 76.3, 39.2, 25.3.

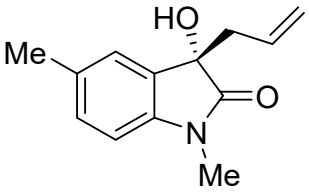
(*S*)-3-allyl-4-bromo-3-hydroxy-1-methylindolin-2-one（3aj）[4]



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (27.5 mg, 98% yield). $[\alpha]_D^{20}$ = +2.1 (*c* = 0.35, $CHCl_3$, 93% *ee*);

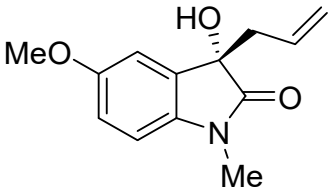
HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.6 min (minor), t_R = 10.2 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 – 7.15 (m, 2H), 6.75 (dd, *J* = 7.2, 1.1 Hz, 1H), 5.43 – 5.28 (m, 1H), 5.10 (d, *J* = 17.0 Hz, 1H), 4.96 (dd, *J* = 10.1, 1.0 Hz, 1H), 3.21 (dd, *J* = 12.9, 6.9 Hz, 1H), 3.16 (s, 3H), 2.85 (dd, *J* = 12.9, 8.1 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.5, 145.5, 131.0, 129.9, 127.5, 127.2, 120.3, 119.4, 107.4, 77.8, 40.1, 26.3.

(*S*)-3-allyl-3-hydroxy-1,5-dimethylindolin-2-one（3ak）[4]



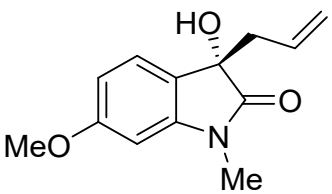
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (21.3 mg, 98% yield). $[\alpha]_D^{20}$ = -29.8 (*c* = 0.4, $CHCl_3$, 90% *ee*); HPLC: Daicel Chiralpak OJ-H, hexane: 2-propanol = 90:10, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.2 min (minor), t_R = 10.9 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (s, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 5.73 – 5.58 (m, 1H), 5.11 (t, *J* = 13.2 Hz, 2H), 3.15 (s, 3H), 2.73 (dd, *J* = 13.4, 6.3 Hz, 1H), 2.61 (dd, *J* = 13.4, 8.4 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.6, 139.9, 131.7, 129.6, 128.8, 128.6, 123.8, 119.3, 107.1, 74.9, 41.9, 25.2, 20.1.

(S)-3-allyl-3-hydroxy-5-methoxy-1-methylindolin-2-one（3al）[9]



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (23.1 mg, 99% yield). $[\alpha]_D^{20}$ = -8.6 (*c* = 1.33, $CHCl_3$, 90% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 12.5 min (minor), t_R = 19.1 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.02 (d, *J* = 2.5 Hz, 1H), 6.84 (dd, *J* = 8.4, 2.5 Hz, 1H), 6.73 (d, *J* = 8.5 Hz, 1H), 5.74 – 5.54 (m, 1H), 5.19 – 5.01 (m, 2H), 3.81 (s, 3H), 3.43 (s, 1H), 3.15 (s, 3H), 2.74 (dd, *J* = 13.4, 6.3 Hz, 1H), 2.61 (dd, *J* = 13.4, 8.4 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.5, 155.3, 135.5, 129.9, 129.5, 119.3, 113.1, 110.2, 107.8, 75.2, 54.8, 42.0, 25.2. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{13}H_{15}NNaO_3$ 256.0944, found 256.0938.

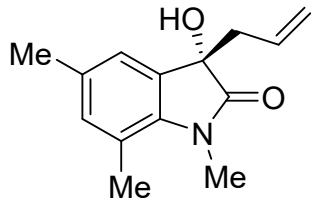
(*S*)-3-allyl-3-hydroxy-6-methoxy-1-methylindolin-2-one（3am）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (22.6 mg, 97% yield). MP: 76-78°C； $[\alpha]_D^{20}$ = -33.1 (*c* = 0.8, $CHCl_3$, 97% *ee*); HPLC: Daicel Chiralpak OD-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 6.5 min (minor), t_R = 8.3 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 1H), 6.65 – 6.51 (m, 1H), 6.40 (d, *J* = 1.9 Hz, 1H), 5.74 –

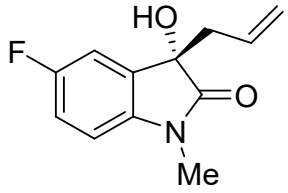
5.56 (m, 1H), 5.17 – 5.01 (m, 2H), 3.83 (s, 3H), 3.14 (s, 3H), 2.73 (dd, *J* = 13.3, 6.3 Hz, 1H), 2.58 (dd, *J* = 13.3, 8.4 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.2, 160.3, 143.7, 129.7, 123.9, 120.6, 119.2, 105.4, 95.5, 74.5, 54.5, 41.8, 25.1. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{13}H_{15}NNaO_3$ 256.0944, found 256.0942.

(*S*)-3-allyl-3-hydroxy-1,5,7-trimethylindolin-2-one（3an）



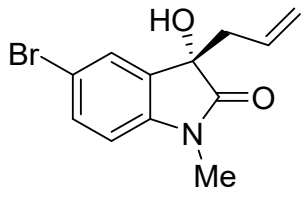
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (22.4 mg, 97% yield). MP: 139-142℃; $[\alpha]_D^{20}$ = -14.1 (*c* = 0.5, $CHCl_3$, 91% *ee*); HPLC: Daicel Chiralpak OJ-H, hexane: 2-propanol = 90:10, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 9.5 min (major), t_R = 11.6 min (minor); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.04 (s, 1H), 6.85 (s, 1H), 5.70 – 5.55 (m, 1H), 5.17 – 5.04 (m, 2H), 3.41 (s, 3H), 2.68 (dd, *J* = 13.3, 6.3 Hz, 1H), 2.60 (dd, *J* = 13.3, 8.4 Hz, 1H), 2.50 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.4, 138.4, 133.8, 132.6, 130.8, 130.5, 122.6, 120.2, 119.7, 75.2, 43.2, 29.5, 20.8, 18.8. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{14}H_{17}NNaO_2$ 254.1151, found 254.1146.

(*S*)-3-allyl-5-fluoro-3-hydroxy-1-methylindolin-2-one（3ao）[10]



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (21.9 mg, 99% yield). MP: 135-137℃ $[\alpha]_D^{20}$ -30.7 (*c* = 0.5, $CHCl_3$, 90% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.1 min (minor), t_R = 8.7 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (dd, *J* = 7.6, 2.4 Hz, 1H), 7.02 (td, *J* = 8.8, 2.4 Hz, 1H), 6.75 (dd, *J* = 8.4, 3.9 Hz, 1H), 5.72 – 5.52 (m, 1H), 5.15 – 5.04 (m, *J* = 17.3, 6.7 Hz, 2H), 3.67 (s, 1H), 3.18 (s, 3H), 2.74 (dd, *J* = 13.4, 6.4 Hz, 1H), 2.60 (dd, *J* = 13.4, 8.4 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.7, 159.5 (d, *J* = 241.8 Hz), 139.1, 131.4 (d, *J* = 7.6 Hz), 130.1, 120.7, 115.8 (d, *J* = 23.4 Hz), 112.4 (d, *J* = 24.9 Hz), 109.0 (d, *J* = 8.1 Hz), 76.1, 42.9, 26.3. ^{19}F NMR (470 MHz, $CDCl_3$) δ -119.7.

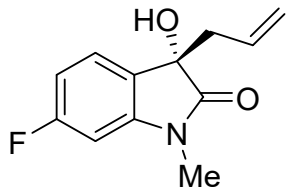
(*S*)-3-allyl-5-bromo-3-hydroxy-1-methylindolin-2-one（3ap）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (27.5 mg, 98% yield). MP: 140-144℃; $[\alpha]_D^{20}$ -5.4 (*c* = 0.6, $CHCl_3$, 95% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 6.9 min (minor), t_R = 10.0 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (d, *J* = 2.0 Hz, 1H), 7.30 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.75 (dd, *J* = 8.3, 3.7 Hz, 1H), 5.69 – 5.53 (m, 1H), 5.16 – 5.05 (m, 2H), 3.65 (s, 1H), 3.15 (s, 3H), 2.74 (dd, *J* = 13.4,

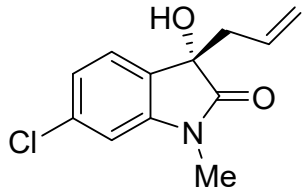
6.4 Hz, 1H), 2.61 (dd, *J* = 13.4, 8.3 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.5, 140.7, 130.4, 128.9, 128.5, 127.5, 123.7, 119.8, 108.4, 74.9, 41.8, 25.3. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{12}BrNNaO_2$ 303.9944, found 303.9943.

(*S*)-3-allyl-6-fluoro-3-hydroxy-1-methylindolin-2-one（3aq）



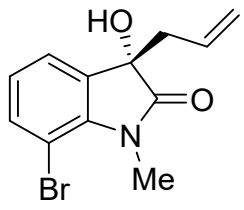
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (21.4 mg, 97% yield). MP: 114-117℃ $[\alpha]_D^{20}$ -23.3 (*c* = 0.5, $CHCl_3$, 90% *ee*); HPLC: Daicel Chiralpak OJ-H, hexane: 2-propanol = 90:10, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 11.5 min (major), t_R = 14.9 min (minor); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 8.2, 5.4 Hz, 1H), 6.77 (ddd, *J* = 9.6, 8.2, 2.3 Hz, 1H), 6.57 (dd, *J* = 8.8, 2.2 Hz, 1H), 5.70 – 5.51 (m, 1H), 5.16 – 5.02 (m, 2H), 3.16 (s, 3H), 2.74 (dd, *J* = 13.4, 6.4 Hz, 1H), 2.59 (dd, *J* = 13.4, 8.3 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.2, 162.9 (d, *J* = 246.7 Hz), 143.9 (d, *J* = 11.3 Hz), 129.2, 124.4 (d, *J* = 10.0 Hz), 124.1 (d, *J* = 2.7 Hz), 119.6, 108.0 (d, *J* = 22.6 Hz), 96.3 (d, *J* = 27.6 Hz), 74.5, 41.8, 25.3. ^{19}F NMR (470 MHz, $CDCl_3$) δ -109.9. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{12}FNNaO_2$ 244.0744, found 244.0740.

(*S*)-3-allyl-6-chloro-3-hydroxy-1-methylindolin-2-one（3ar）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (23.2 mg, 98% yield). MP: 63-68°C. $[\alpha]_D^{20}$ -31.3 (*c* = 0.5, $CHCl_3$, 95% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 6.9 min (minor), t_R = 8.1 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.9 Hz, 1H), 7.07 (dd, *J* = 7.9, 1.4 Hz, 1H), 6.82 (d, *J* = 1.4 Hz, 1H), 5.67 – 5.52 (m, 1H), 5.15 – 5.01 (m, 2H), 3.49 (s, 1H), 3.15 (s, 3H), 2.73 (dd, *J* = 13.4, 6.4 Hz, 1H), 2.59 (dd, *J* = 13.3, 8.4 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.9, 144.5, 135.5, 130.1, 128.1, 125.1, 122.9, 120.7, 109.2, 75.6, 42.8, 26.3. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{12}ClNNaO_2$ 260.0449, found 260.0446.

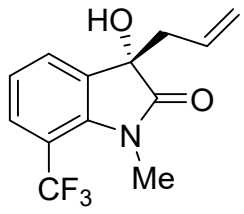
(*S*)-3-allyl-7-bromo-3-hydroxy-1-methylindolin-2-one（3as）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (27.3 mg, 97% yield). MP: 74-78°C. $[\alpha]_D^{20}$ = -23.6 (*c* = 0.5, $CHCl_3$, 91% *ee*); HPLC: Daicel Chiralpak OJ-H, hexane: 2-propanol = 90:10, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.7 min (major), t_R = 8.3 min (minor); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.31 (dd, *J* = 7.3, 1.1 Hz, 1H), 6.97 – 6.92 (m, 1H), 5.66 –

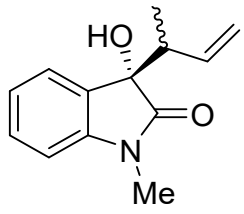
5.51 (m, 1H), 5.15 – 5.04 (m, 2H), 3.54 (s, 3H), 2.71 (dd, *J* = 13.4, 6.4 Hz, 1H), 2.61 (dd, *J* = 13.4, 8.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.4, 140.5, 135.2, 133.0, 130.1, 124.3, 123.2, 120.8, 102.7, 75.3, 43.2, 29.8. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{12}BrNNaO_2$ 303.9944, found 303.9935.

(*S*)-3-allyl-3-hydroxy-1-methyl-7-(trifluoromethyl)indolin-2-one（3at）



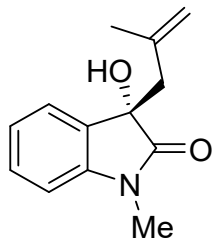
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as amorphous solid (25.7 mg, 95% yield). $[\alpha]_D^{20}$ = -34.3 (*c* = 0.4, $CHCl_3$, 87% *ee*); HPLC: Daicel Chiralpak AS-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 3.9 min (minor), t_R = 5.3 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.17 (t, *J* = 7.7 Hz, 1H), 5.66 – 5.50 (m, 1H), 5.17 – 5.03 (m, 2H), 3.37 (s, 3H), 2.73 (dd, *J* = 13.3, 6.3 Hz, 1H), 2.62 (dd, *J* = 13.3, 8.4 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.8, 140.1, 131.3, 128.7, 126.5, 126.4, 122.4 (q, *J* = 271.5 Hz), 121.5, 119.9, 111.9 (q, *J* = 33.2 Hz), 73.1, 42.2, 27.8 (q, *J* = 6.4 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ -53.4. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{13}H_{12}F_3NNaO_2$ 294.0712, found 294.0711.

(S)-3-(but-3-en-2-yl)-3-hydroxy-1-methylindolin-2-one（3au）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as amorphous solid (21.3 mg, 98% yield). $[\alpha]_D^{20}$ = -79.4 (*c* = 1.0, $CHCl_3$, 1:1 *dr*, 92% *ee*/87% *ee*); HPLC: Daicel Chiralpak OD-H, hexane: 2-propanol = 95:5, flow rate = 1.1 mL/min, T = 30°C, UV = 254 nm, t_R = 10.5 min (minor), t_R = 11.6 min (minor), t_R = 12.8 min (major), t_R = 13.8 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.29 (m, 2H), 7.15 – 7.03 (m, 1H), 6.88 – 6.76 (m, 1H), 6.12 – 6.02 (m, 0.5H), 5.70 – 5.58 (m, 0.5H), 5.29 – 5.06 (m, 2H), 3.19 (s, 1.5H), 3.15 (s, 1.5H), 3.09 (s, 0.5H), 3.03 (s, 0.5H), 2.90 – 2.82 (m, 0.5H), 2.80 – 2.72 (m, 0.5H), 1.02 (d, *J* = 6.9 Hz, 1.5H), 0.77 (d, *J* = 6.8 Hz, 1.5H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.7, 177.6, 144.0, 143.9, 137.1, 136.8, 129.7, 129.6, 128.7, 128.3, 124.8, 124.1, 122.9, 122.8, 118.6, 118.0, 108.2, 108.2, 78.3, 78.1, 46.9, 44.8, 26.2, 26.0, 14.0, 13.2. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{13}H_{15}NNaO_2$ 240.0995, found 240.1007.

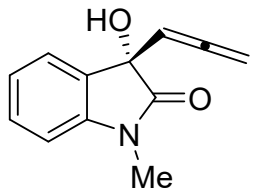
(*S*)-3-hydroxy-1-methyl-3-(2-methylallyl)indolin-2-one（3av）



The title compound was prepared according to the general working procedure and 0.5 mmol β-methyl branch allylboronic acid pinacol ester was used. Purified by column chromatography (ethyl acetate/petroleum ether) to give the product as amorphous solid (20.8 mg, 96% yield). $[\alpha]_D^{20}$ = -31.5 (*c* = 1.0, $CHCl_3$, 70% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 90:10, flow rate

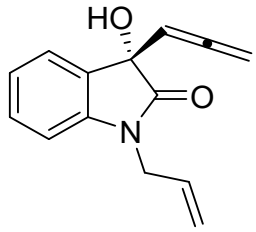
= 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 15.5 min (minor), t_R = 20.7 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.31 (td, *J* = 7.7, 1.3 Hz, 1H), 7.09 (td, *J* = 7.5, 1.0 Hz, 1H), 6.81 (d, *J* = 7.7 Hz, 1H), 4.74 (dp, *J* = 6.6, 1.6 Hz, 1H), 4.63 – 4.59 (m, 1H), 3.43 (s, 1H), 3.15 (s, 3H), 2.71 (s, 2H), 1.51 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 178.1, 143.5, 139.2, 129.8, 129.7, 124.4, 122.9, 115.9, 108.4, 76.4, 46.1, 26.1, 23.9. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{13}H_{15}NNaO_2$ 240.0995, found 240.0987.

(*S*)-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3ba）



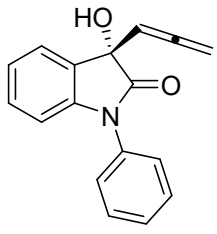
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (19.9 mg, 99% yield). MP: 135-138°C. $[\alpha]_D^{20}$ = -36.0 (*c* = 0.2, $CHCl_3$, 97% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 12.7 min (minor), t_R = 16.2 min (major); ^{1}H NMR (500 MHz, Acetone) δ 7.38 – 7.31 (m, 2H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 7.8 Hz, 1H), 5.55 (t, *J* = 6.6 Hz, 1H), 5.28 (s, 1H), 4.85 (dd, *J* = 11.5, 6.7 Hz, 1H), 4.76 (dd, *J* = 11.5, 6.6 Hz, 1H), 3.14 (s, 3H). ^{13}C NMR (125 MHz, Acetone) δ 205.3, 175.6, 143.4, 130.3, 129.4, 124.7, 122.2, 108.3, 92.9, 77.9, 74.2, 25.3. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{11}NNaO_2$ 224.0682, found 224.0678.

(*S*)-1-allyl-3-hydroxy-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bb）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (22.2 mg, 98% yield). MP: 106-109°C. $[\alpha]_D^{20}$ = -47.5 (*c* = 0.4, $CHCl_3$, 92% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 10.3 min (minor), t_R = 13.1 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.1 Hz, 1H), 7.33 – 7.27 (m, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 5.90 – 5.76 (m, 1H), 5.54 (t, *J* = 6.6 Hz, 1H), 5.26 – 5.17 (m, 2H), 5.00 – 4.92 (m, 2H), 4.43 – 4.35 (m, 1H), 4.27 – 4.20 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 207.6, 176.3, 142.2, 131.0, 129.8, 129.4, 124.8, 123.1, 117.7, 109.5, 92.9, 80.1, 74.5, 42.4. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{14}H_{13}NNaO_2$ 250.0838, found 250.0834.

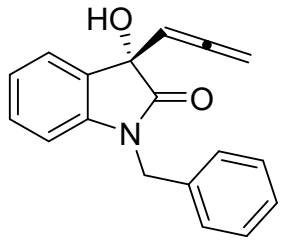
(*S*)-3-hydroxy-1-phenyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bc）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (25.5 mg, 97% yield). MP: 75-77°C. $[\alpha]_D^{20}$ = -38.7 (*c* = 0.4, $CHCl_3$, 97% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate

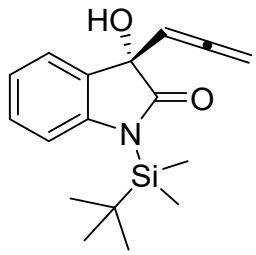
= 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 12.9 min (major), t_R = 18.8 min (minor); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.45 (m, 3H), 7.44 – 7.38 (m, 3H), 7.25 (t, *J* = 7.7 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 6.82 (d, *J* = 7.9 Hz, 1H), 5.62 (t, *J* = 6.5 Hz, 1H), 5.08 – 4.93 (m, 2H), 3.77 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.8, 174.9, 142.0, 132.9, 128.7, 128.6, 128.1, 127.2, 125.4, 124.0, 122.6, 108.8, 91.9, 79.1, 73.6. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{17}H_{13}NNaO_2$ 286.0838, found 286.0839.

(*S*)-1-benzyl-3-hydroxy-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bd）



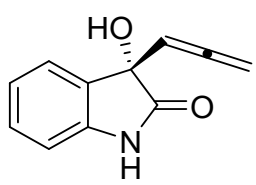
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (27.4 mg, 99% yield). MP: 124-126°C. $[\alpha]_D^{20}$ = -54.3 (*c* = 0.4, $CHCl_3$, 97% *ee*); HPLC: Daicel Chiralpak OD-H, hexane: 2-propanol = 70:30, flow rate = 1.2 mL/min, T = 30°C, UV = 254 nm, t_R = 5.4 min (major), t_R = 7.1 min (minor); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.2 Hz, 1H), 7.32 – 7.17 (m, 6H), 7.06 (t, *J* = 7.4 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 5.60 (t, *J* = 6.4 Hz, 1H), 5.07 – 4.90 (m, 3H), 4.77 (d, *J* = 15.7 Hz, 1H), 3.88 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 207.7, 176.8, 142.1, 135.3, 129.8, 129.6, 128.8, 127.7, 127.2, 124.8, 123.2, 109.6, 92.9, 80.1, 74.7, 43.9. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{18}H_{15}NNaO_2$ 300.0995, found 300.0993.

(S)-1-(tert-butyldimethylsilyl)-3-hydroxy-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3be）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as pale yellow oil (29.5 mg, 98% yield). $[\alpha]_D^{20}$ = -23.6 (*c* = 0.125, $CHCl_3$, 90% *ee*); HPLC: Daicel Chiralpak OD-H, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 3.7 min (major), t_R = 4.1 min (minor); ^{1}H NMR (500 MHz, Acetone) δ 7.34 (d, *J* = 7.3 Hz, 1H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 5.53 (t, *J* = 6.7 Hz, 1H), 5.25 (s, 1H), 4.83 (dd, *J* = 11.4, 6.7 Hz, 1H), 4.76 (dd, *J* = 11.4, 6.6 Hz, 1H), 0.99 (s, 9H), 0.54 (s, 3H), 0.53 (s, 3H). ^{13}C NMR (125 MHz, Acetone) δ 207.5, 183.2, 145.4, 132.6, 129.0, 124.9, 122.0, 112.8, 93.8, 77.9, 74.6, 26.0, 19.5, -3.8, -4.0. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{17}H_{23}NNaO_2Si$ 324.1390, found 324.1384.

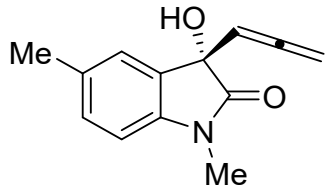
(*S*)-3-hydroxy-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bf）[7]



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid

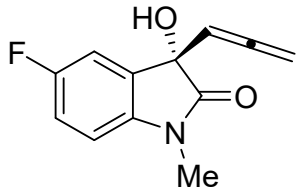
(18.1 mg, 97% yield). $[\alpha]_D^{20}$ = -34.7 (*c* = 0.15, MeOH, 94% *ee*); HPLC: Daicel Chiralpak AS-H, hexane: 2-propanol = 70:30, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 30.1 min (major), t_R = 49.1 min (minor); ^{1}H NMR (500 MHz, DMSO) δ 10.27 (s, 1H), 7.26 – 7.17 (m, 2H), 7.00 – 6.92 (m, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 6.34 (s, 1H), 5.48 (t, *J* = 6.6 Hz, 1H), 4.89 (dd, *J* = 11.7, 6.6 Hz, 1H), 4.82 (dd, *J* = 11.7, 6.6 Hz, 1H). ^{13}C NMR (125 MHz, DMSO) δ 207.4, 177.9, 141.7, 131.6, 129.6, 125.3, 122.0, 110.1, 93.6, 79.0, 74.6.

(*S*)-3-hydroxy-1,5-dimethyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bg）



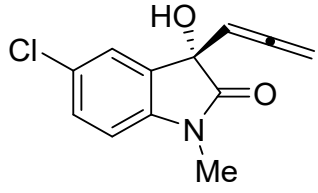
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (21.3 mg, 99% yield). MP: 145-148°C. $[\alpha]_D^{20}$ = +20.9 (*c* = 0.6, $CHCl_3$, 94% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 12.6 min (minor), t_R = 15.8 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (s, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.73 (d, *J* = 7.9 Hz, 1H), 5.48 (t, *J* = 6.6 Hz, 1H), 5.03 – 4.90 (m, 2H), 3.55 (s, 1H), 3.18 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.5, 175.4, 139.6, 131.8, 129.1, 128.3, 124.5, 107.3, 91.8, 79.1, 73.4, 25.4, 20.1. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{13}H_{13}NNaO_2$ 238.0838, found 238.0835.

(*S*)-5-fluoro-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bh）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (21.0 mg, 96% yield). MP: 143-145°C. $[\alpha]_D^{20}$ = -34.5 (*c* = 0.3, $CHCl_3$, 91% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.7 min (minor), t_R = 10.8 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 7.6, 2.6 Hz, 1H), 7.03 (td, *J* = 8.9, 2.6 Hz, 1H), 6.77 (dd, *J* = 8.5, 4.0 Hz, 1H), 5.53 (t, *J* = 6.6 Hz, 1H), 5.04 – 4.88 (m, 2H), 3.98 (s, 1H), 3.19 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.7, 175.5, 158.5 (d, *J* = 242.1 Hz), 137.9, 129.9 (d, *J* = 7.8 Hz), 115.0 (d, *J* = 23.8 Hz), 112.1 (d, *J* = 25.2 Hz), 108.1 (d, *J* = 8.1 Hz), 91.3, 79.2, 73.6, 25.5. ^{19}F NMR (470 MHz, $CDCl_3$) δ -119.5. HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{12}H_{11}FNO_2$ 220.0768, found 220.0763.

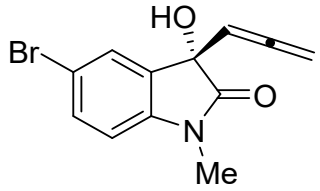
(*S*)-5-chloro-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bi）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the

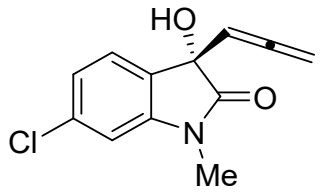
product as white solid (22.3 mg, 95% yield). MP: 121-124℃ $[\alpha]_D^{20}$ = -42.9 (*c* = 0.2, $CHCl_3$, 96% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.6 min (minor), t_R = 16.0 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 1.8 Hz, 1H), 7.46 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.73 (d, *J* = 8.3 Hz, 1H), 5.48 (t, *J* = 6.5 Hz, 1H), 5.10 – 4.90 (m , 2H), 3.63 (s, 1H), 3.18 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.6, 175.0, 141.1, 131.7, 130.2, 127.1, 114.8, 109.1, 91.3, 79.5, 73.3, 25.5. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{10}ClNNaO_2$ 258.0292, found 258.0279.

(*S*)-5-bromo-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bj）



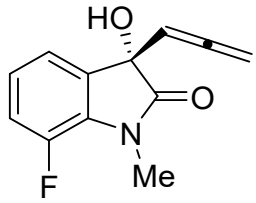
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (27.2 mg, 97% yield). MP: 123-125℃ $[\alpha]_D^{20}$ = -46.6 (*c* = 0.6, $CHCl_3$, 93% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.2 min (minor), t_R = 12.2 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 1.9 Hz, 1H), 7.30 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 5.51 (t, *J* = 6.5 Hz, 1H), 5.06 – 4.91 (m, 2H), 3.91 (s, 1H), 3.18 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 207.7, 176.3, 141.6, 131.0, 129.7, 128.6, 125.4, 109.6, 92.3, 80.4, 74.4, 26.5. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{10}BrNNaO_2$ 301.9787, found 301.9779.

(*S*)-6-chloro-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bk）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (22.1 mg, 94% yield). MP: 144-147℃ $[\alpha]_D^{20}$ = -33.2 (*c* = 0.5, $CHCl_3$, 93% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.9 min (minor), t_R = 10.3 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.9 Hz, 1H), 7.08 (dd, *J* = 7.9, 1.7 Hz, 1H), 6.85 (d, *J* = 1.6 Hz, 1H), 5.49 (t, *J* = 6.5 Hz, 1H), 5.03 – 4.90 (m, 2H), 3.60 (s, 1H), 3.18 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.7, 175.5, 143.3, 134.7, 126.5, 124.8, 122.0, 108.4, 91.3, 79.2, 73.1, 25.5. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{10}ClNNaO_2$ 258.0292, found 258.0289.

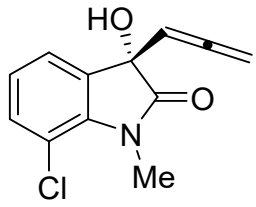
(S)-7-fluoro-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bl）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (20.1 mg, 92% yield). MP: 81-83℃ $[\alpha]_D^{20}$ = -49.4 (*c* = 0.3,

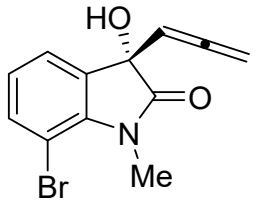
$CHCl_3$, 94% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.0 min (minor), t_R = 7.9 min (major); ^{1}H NMR (500 MHz, Acetone) δ 7.20 (d, *J* = 7.2 Hz, 1H), 7.17 – 7.10 (m, 1H), 7.10 – 7.01 (m, 1H), 5.54 (t, *J* = 6.6 Hz, 1H), 5.46 (s, 1H), 4.87 (dd, *J* = 11.6, 6.7 Hz, 1H), 4.79 (dd, *J* = 11.6, 6.6 Hz, 1H), 3.33 (s, 3H). ^{13}C NMR (125 MHz, Acetone) δ 207.7, 175.4, 147.5 (d, *J* = 241.7 Hz), 133.4 (d, *J* = 2.7 Hz), 129.7 (d, *J* = 8.3 Hz), 123.1 (d, *J* = 6.3 Hz), 120.9 (d, *J* = 3.0 Hz), 117.1 (d, *J* = 19.4 Hz), 92.7, 78.2, 74.2, 27.84 (d, *J* = 5.7 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ -138.3. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{10}FNNaO_2$ 242.0588, found 242.0586.

(*S*)-7-chloro-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bm）



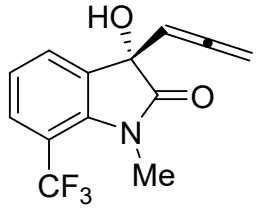
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (22.1 mg, 94% yield). MP: 120-124℃ $[\alpha]_D^{20}$ = -35.3 (*c* = 0.25, $CHCl_3$, 95% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.3 min (minor), t_R = 8.1 min (major); ^{1}H NMR (500 MHz, Acetone) δ 7.35 – 7.27 (m, 2H), 7.06 (t, *J* = 7.8 Hz, 1H), 5.54 (t, *J* = 6.6 Hz, 1H), 5.45 (s, 1H), 4.88 (dd, *J* = 11.6, 6.7 Hz, 1H), 4.80 (dd, *J* = 11.7, 6.6 Hz, 1H), 3.49 (s, 3H). ^{13}C NMR (125 MHz, Acetone) δ 207.7, 176.0, 139.1, 133.4, 131.4, 123.7, 123.5, 114.8, 92.7, 78.3, 73.8, 28.8. HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{12}H_{11}ClNO_2$ 236.0473, found 236.0471.

(S)-7-bromo-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)indolin-2-one（3bn）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (26.6 mg, 95% yield). MP: 124-126℃ $[\alpha]_D^{20}$ -58.5 (*c* = 0.4, $CHCl_3$, 93% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 7.2 min (minor), t_R = 8.0 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 – 7.41 (m, 1H), 7.33 (dd, *J* = 7.3, 1.2 Hz, 1H), 6.99 – 6.92 (m, 1H), 5.48 (t, *J* = 6.6 Hz, 1H), 5.00 – 4.93 (m, 2H), 3.71 (s, 1H), 3.57 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.6, 176.0, 139.3, 134.4, 131.4, 123.4, 122.9, 101.7, 91.6, 79.3, 72.8, 29.0. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{12}H_{10}BrNNaO_2$ 301.9787, found 301.9779.

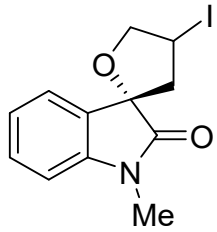
(*S*)-3-hydroxy-1-methyl-3-(2γ^5-propa-1,2-dien-1-yl)-7-(trifluoromethyl)indolin-2-one（3bo）



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid

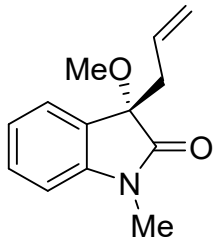
(24.5 mg, 91% yield). MP: 66-68℃ $[\alpha]_D^{20}$ = -37.8 (*c* = 0.25, $CHCl_3$, 92% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 80:20, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 4.9 min (minor), t_R = 5.2 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.54 (m, 2H), 7.19 (t, *J* = 7.7 Hz, 1H), 5.50 (t, *J* = 6.5 Hz, 1H), 5.06 – 4.90 (m, 2H), 3.75 (s, 1H), 3.40 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 207.7, 177.5, 141.0, 131.9, 128.4, 127.7 (q, *J* = 6.1 Hz), 123.4(q, *J* = 270.1 Hz), 122.6, 113.1 (q, *J* = 32.9 Hz), 92.5, 80.5, 72.7, 29.1 (q, *J* = 6.3 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ -53.3. HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_{13}H_{10}F_3NNaO_2$ 292.0556, found 292.0558.

(*2S*)-4-iodo-1'-methyl-4,5-dihydro-3H-spiro[furan-2,3'-indolin]-2'-one (4a) [11]



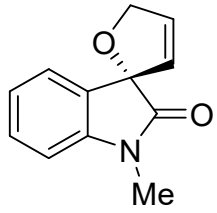
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (37.5 mg, 38% yield). $[\alpha]_D^{20}$ = -5.0 (*c* = 0.35, $CHCl_3$, 90% *ee*, 4:1 *dr*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 70:30, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.9 min (minor), t_R = 13.6 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 0.8H), 7.47 – 7.43 (m, 0.2H), 7.38 – 7.34 (m, 0.2H), 7.32 – 7.28 (m, 0.8H), 7.15 – 7.11 (m, 0.2H), 7.10 – 7.05 (m, 0.8H), 6.88 – 6.84 (m, 0.2H), 6.81 – 6.77 (m, 0.8H), 4.94 – 4.76 (m, 1H), 4.37 (dd, *J* = 9.6, 3.8 Hz, 1H), 4.15 (d, *J* = 9.6 Hz, 1H), 3.20 (s, 0.6H), 3.15 (s, 2.4H), 2.72 – 2.69 (m, 0.2H), 2.67 – 2.62 (m, 0.8H), 2.21 – 2.17 (m, 0.8H), 2.17 – 2.15 (m, 0.2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.8, 142.6, 129.1, 128.8, 124.3, 122.3, 107.2, 81.9, 76.5, 72.0, 42.9, 25.1.

(*S*)-3-allyl-3-methoxy-1-methylindolin-2-one (4b) [12]



The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as yellow oil (35.6 mg, 82% yield). $[\alpha]_D^{20}$ = -17.9 (*c* = 0.35, $CHCl_3$, 90% *ee*); HPLC: Daicel Chiralpak IC, hexane: 2-propanol = 90:10, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 12.6 min (minor), t_R = 13.9 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.30 (m, 2H), 7.22 – 7.06 (m, 1H), 6.85 (d, *J* = 7.5 Hz, 1H), 5.76 – 5.47 (m, 1H), 5.22 – 4.97 (m, 2H), 3.21 (s, 3H), 3.03 (s, 3H), 2.75 (dd, *J* = 12.6, 5.8 Hz, 1H), 2.61 (dd, *J* = 12.8, 8.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.7, 142.9, 129.6, 128.8, 125.7, 123.5, 121.9, 118.6, 107.2, 81.5, 76.4, 76.0, 75.8, 52.0, 40.9, 25.0.

(*S*)-1'-methyl-5H-spiro[furan-2,3'-indolin]-2'-one (4c)



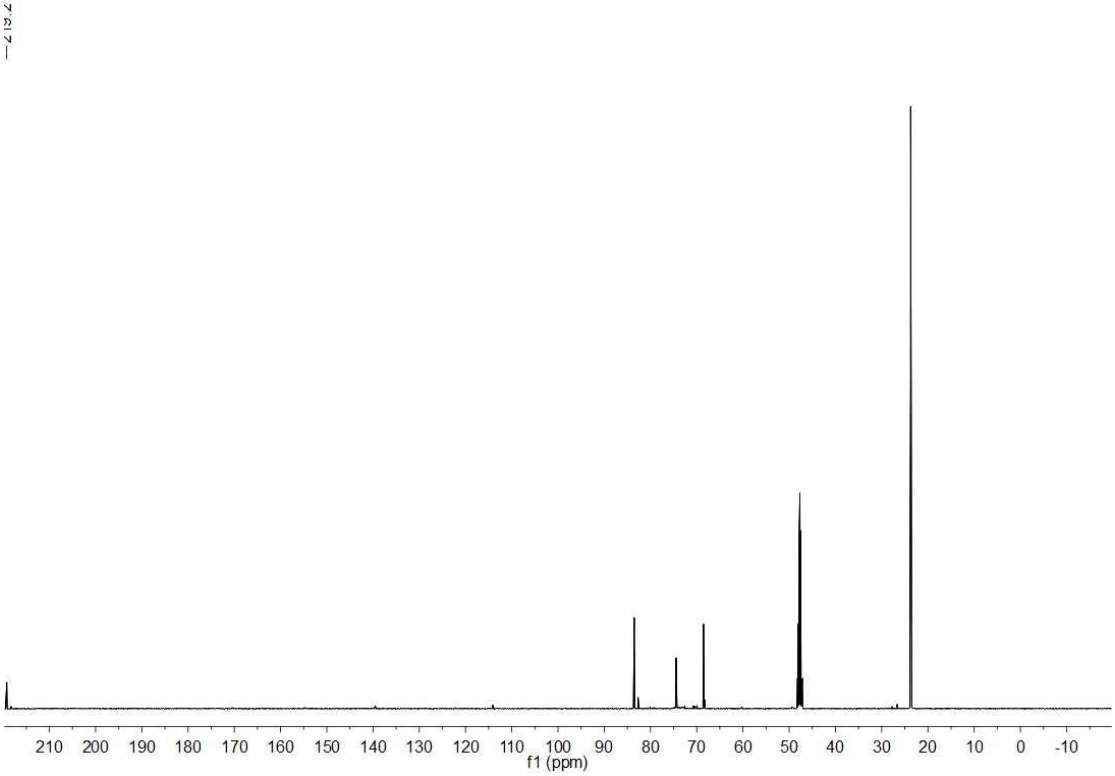
The title compound was prepared according to the general working procedure and purified by column chromatography (ethyl acetate/petroleum ether) to give the product as white solid (17.5

mg, 87% yield). MP: 68-71°C $[\alpha]_D^{20}$ = -15.9 (*c* = 0.7, $CHCl_3$, 91% *ee*); HPLC: Daicel Chiralpak AD-H, hexane: 2-propanol = 90:10, flow rate = 1.0 mL/min, T = 30°C, UV = 254 nm, t_R = 8.3 min (minor), t_R = 10.2 min (major); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (t, *J* = 7.7 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.06 (t, *J* = 7.3 Hz, 1H), 6.82 (d, *J* = 7.7 Hz, 1H), 6.40 (d, *J* = 6.0 Hz, 1H), 5.66 – 5.60 (m, 1H), 5.10 (dd, *J* = 13.0, 1.2 Hz, 1H), 4.99 (dd, *J* = 12.9, 1.5 Hz, 1H), 3.19 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.5, 142.6, 130.3, 129.2, 127.9, 125.9, 123.8, 122.1, 107.4, 89.7, 76.2, 25.3. HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{12}H_{12}NO_2$ 202.0863, found 202.0864.

1.5 NMR experiment and DFT calculations

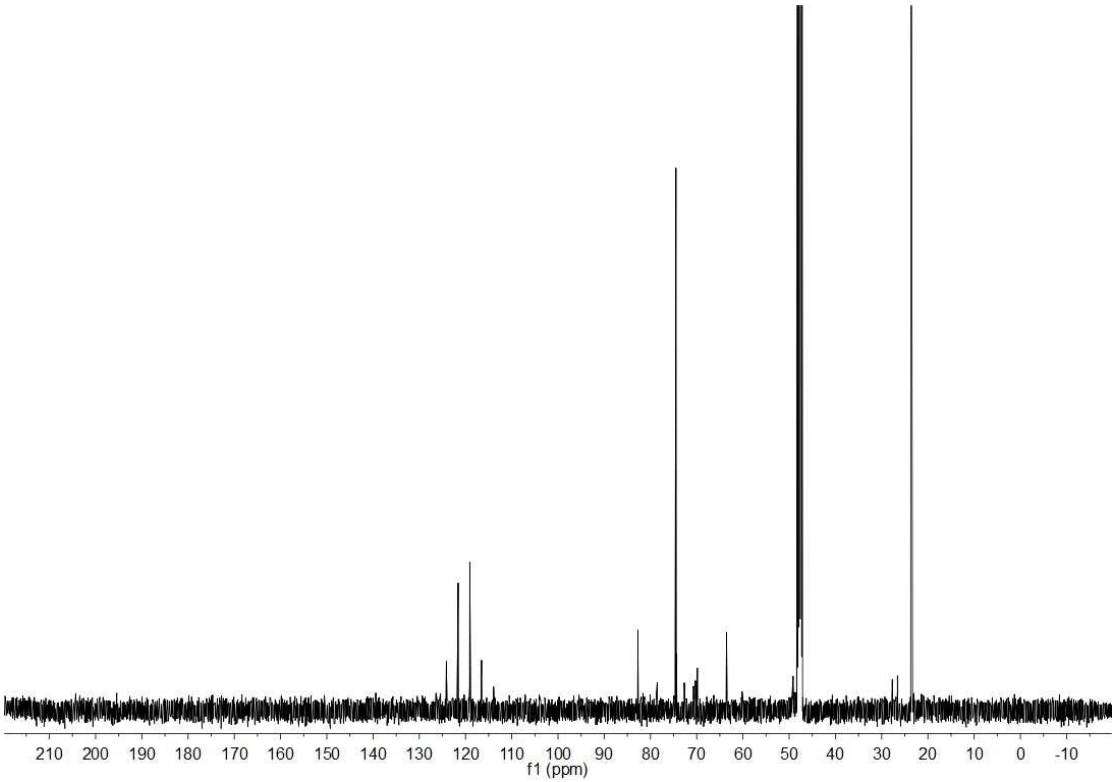
NMR experiment, ^{13}C NMR (125 MHz)

^{13}C NMR of **2b**（MeOD）



A mixture of $Zn(OTf)_2$ (36 mg, 0.1 mmol), the ligand (**L_2**, 46 mg, 0.1 mmol) in MeOD (1 mL) with Cs_2CO_3 (33 mg, 0.1 mmol) was stirred at room temperature for 2 h. Allenylborate **2b** (0.1 mmol) was added in one portion and was stired at 10℃ for 2 h. The reaction mixture was directly characterized by NMR experiment.

^{13}C NMR of reaction mixture（MeOD）



According to the results of NMR experiment, we found that when allenylborate **2b** was mixed with **L-Zn**, the signal peak of 219.4 ppm in the ^{13}C NMR disappeared. It means that the structure of allene has changed.

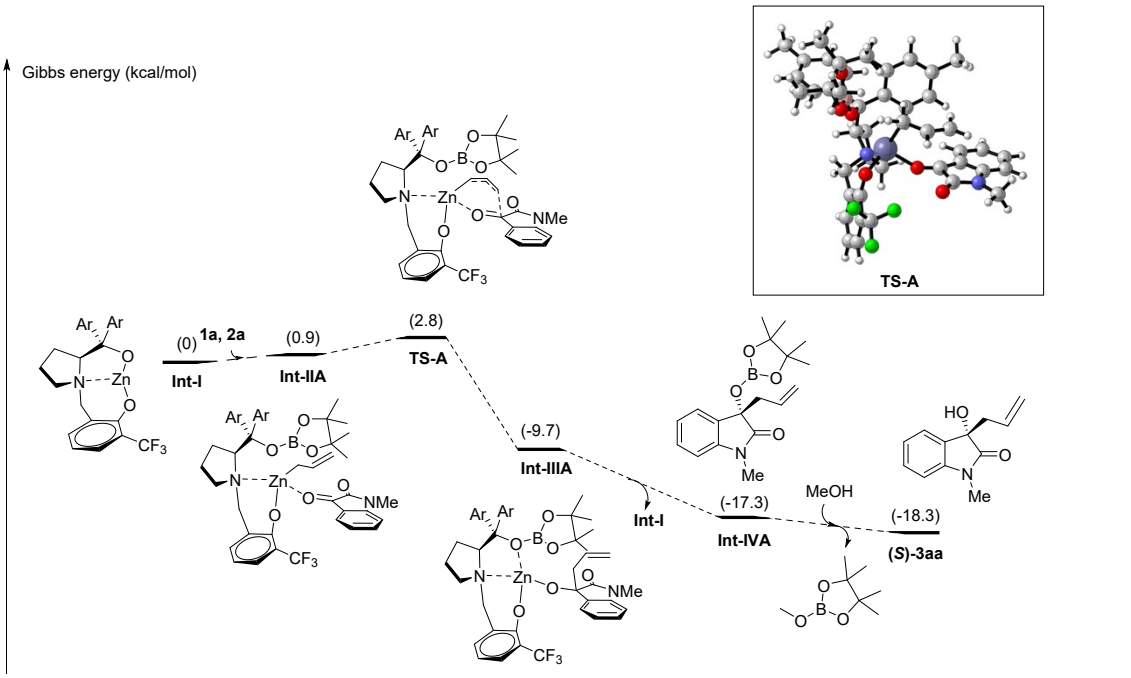
DFT calculations

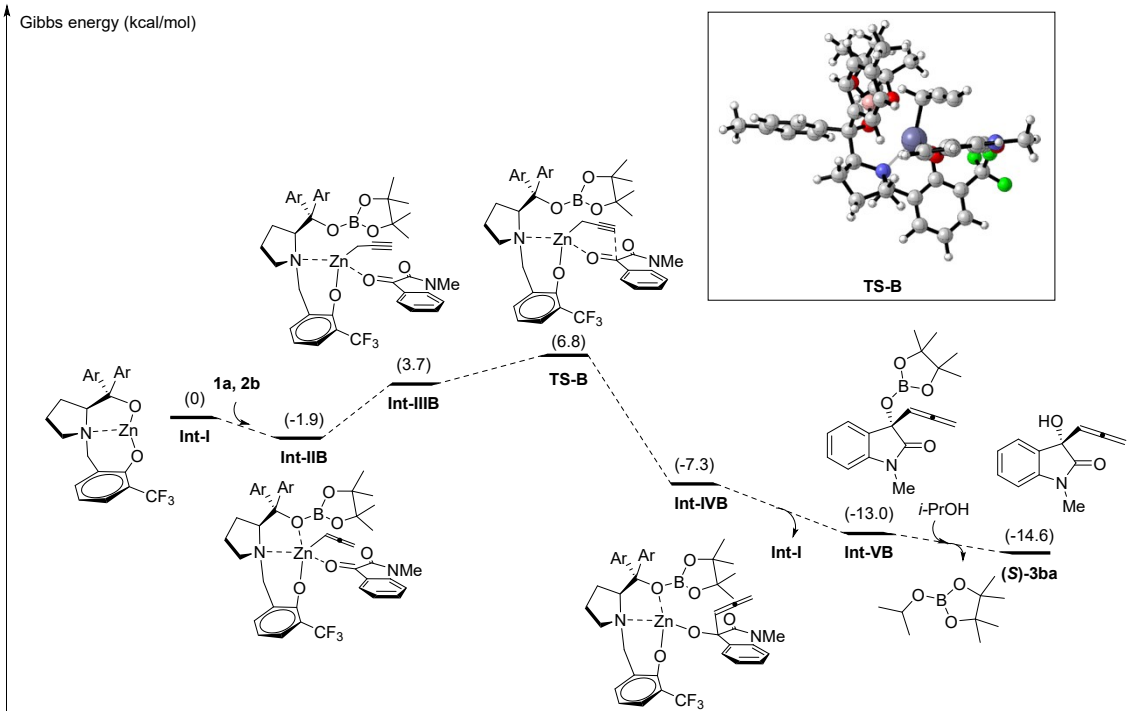
All the calculations were performed using Gaussian 16 software packages.[13] The geometry of all reactants and transition states were optimized using the (U)B3LYP[14]-D3(Becke-Johnson damping function)[15] in acetone or isopropyl alcohol (using PCM solvation model). In these geometry optimizations, a mixed basis set of SDD[16] for Zn, while 6-31G(d)[17] for all the other atoms was used. Vibrational frequency analysis was calculated at the same level of theory to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and thermal corrections at 298 K. For each transition state, the intrinsic reaction coordinate (IRC) analysis was conducted to ensure that it connects the right reactant and product.[18] To obtain more accurate energies, solution-phase single point energy calculations were performed at the (U)B3LYP-D3(BJ)/6-311+G(d,p).

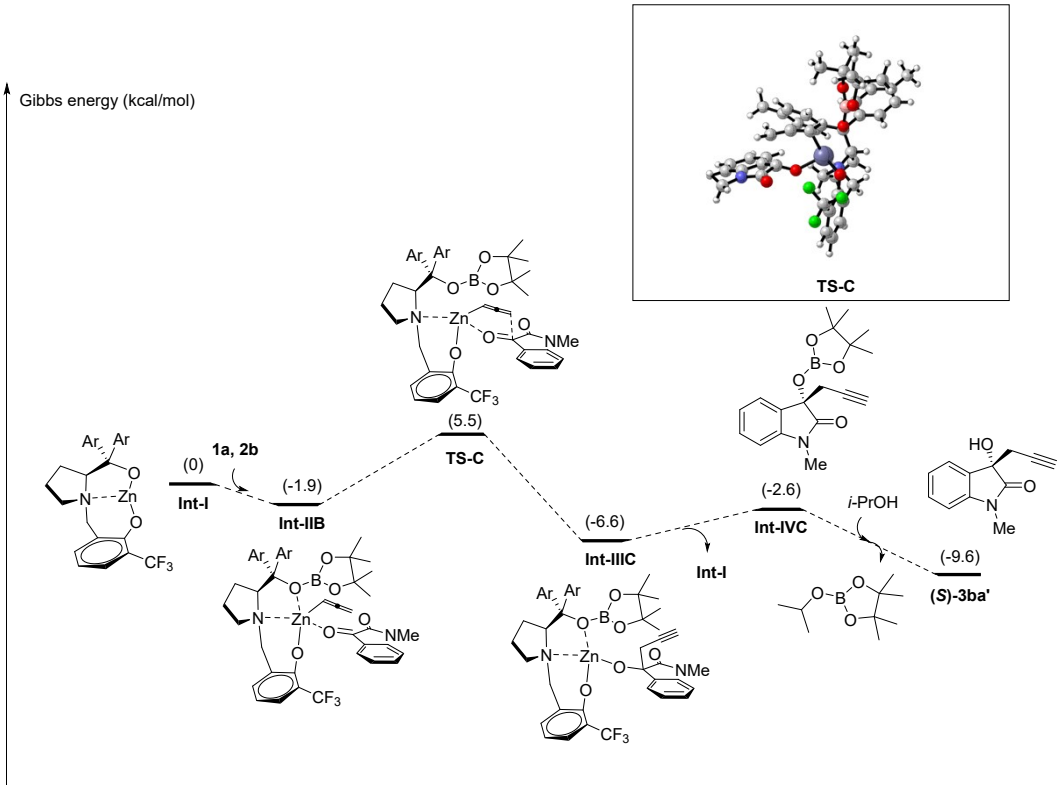
Table 3. Thermal correction of Gibbs free energy (TCG, hartree) and single point energies (SP, hartree) in solvent for all species involved in this study

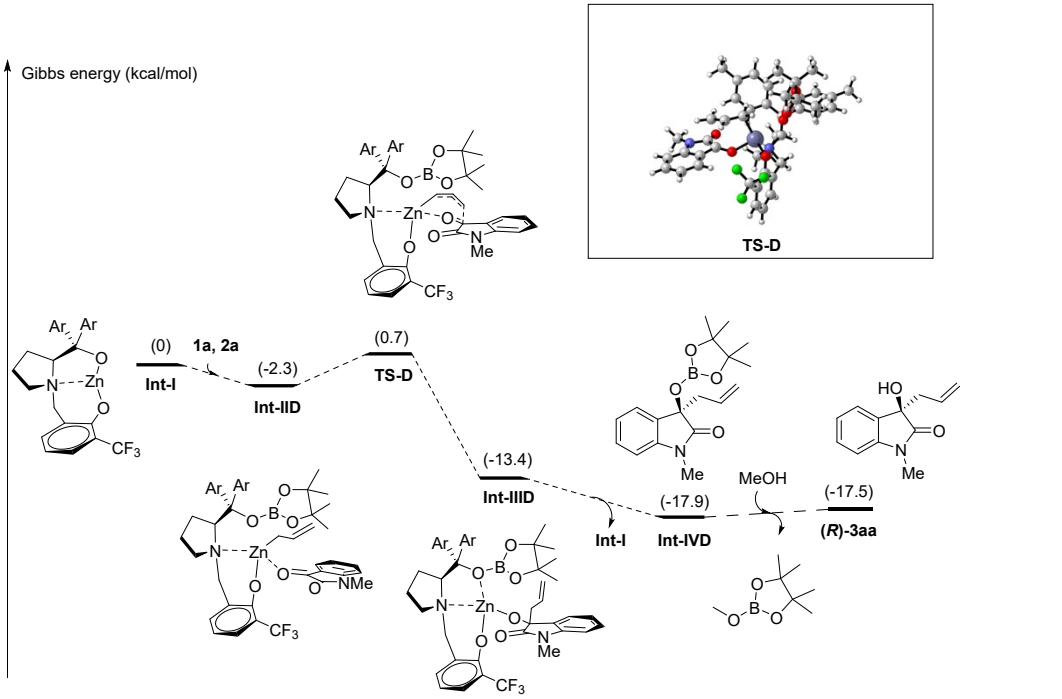
Compounds	TCG (acetone)	SP(acetone)	Compounds	TCG (*i*-PrOH)	SP (*i*-PrOH)
Int-I	0.415232	1777.059207	**Int-I**	0.412343	-1777.053494

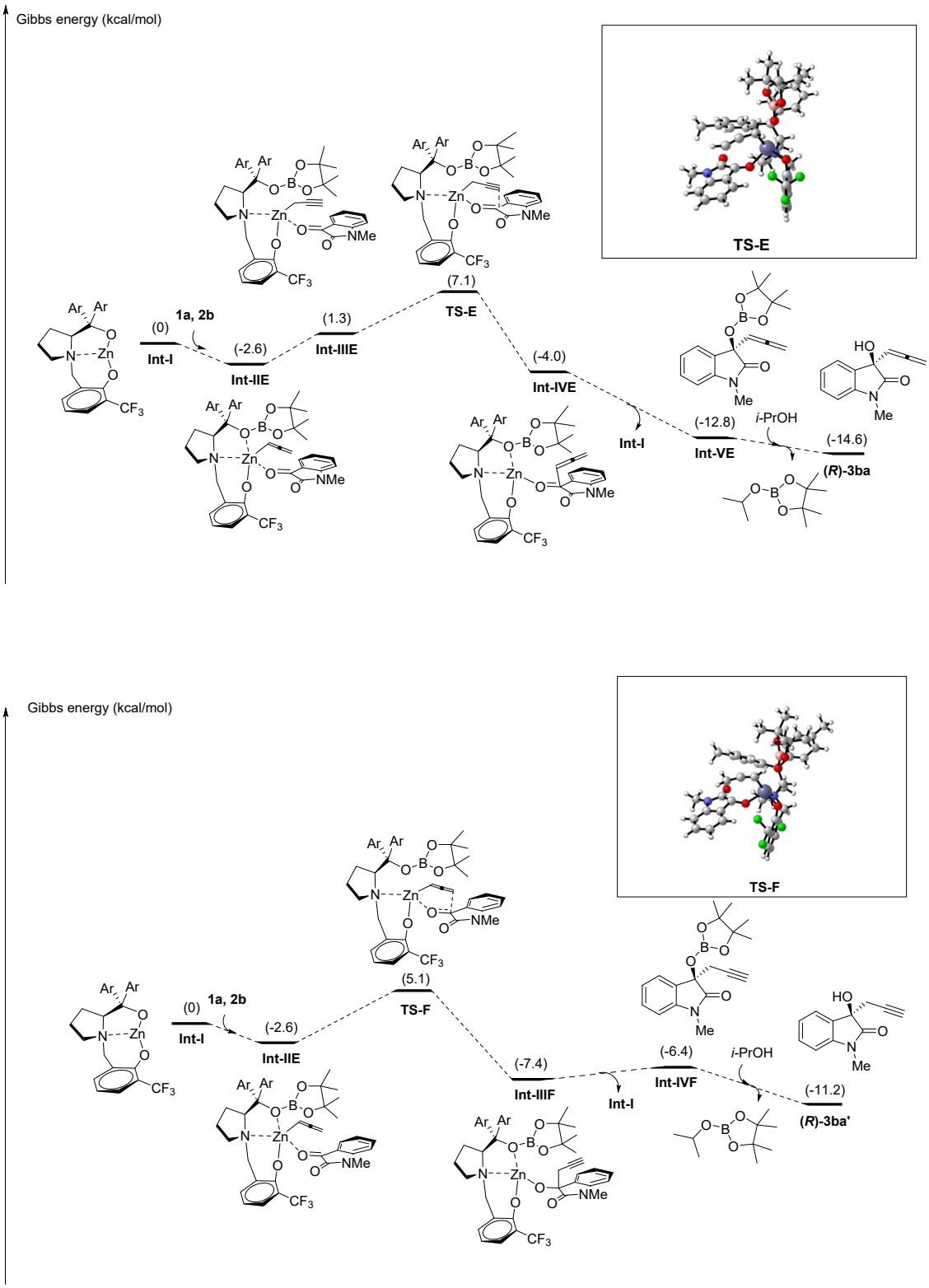
1a	0.109157	-552.580272	**1a**	0.109155	-552.580196
2a	0.212617	-528.796929	**2b**	0.190918	-527.554852
Int-IIA	0.787645	-2858.485677	**Int-IIB**	0.763119	-2857.24235
TS-A	0.790444	-2858.485427	**IntIIIB**	0.763214	-2857.233471
Int-IIIA	0.79265	-2858.507444	**TS-B**	0.765756	-2857.231035
Int-IVA	0.349374	-1081.432443	**Int-IVB**	0.765215	-2857.252993
(*S*)-**3aa**	0.188321	-670.551132	**Int-VB**	0.324663	-1080.180322
Int-IID	0.787925	-2858.491008	**(*S*)-3ba**	0.162685	-669.298379
TS-D	0.789956	-2858.488174	**TS-C**	0.766829	-2857.234215
Int-IIID	0.792297	-2858.512996	**Int-IIIC**	0.76899	-2857.25556
Int-IVD	0.348914	-1081.432854	**Int-IVC**	0.325249	-1080.164429
(*R*)-**3aa**	0.18859	-670.550172	(*S*)-**3ba'**	0.164318	-669.292119
			Int-IIE	0.762789	-2857.243025
			Int-IIIE	0.762779	-2857.236824
			TS-E	0.765342	-2857.230146
			Int-IVE	0.767475	-2857.249998
			Int-VE	0.324586	-1080.179922
			(*R*)-**3ba**	0.162687	-669.298379
			TS-F	0.765489	-2857.233518
			Int-IIIF	0.768939	-2857.256886
			Int-IVF	0.325494	-1080.170594
			(*R*)-**3ba'**	0.164217	-669.294551


Gibbs energy (kcal/mol)
TS-A
(0)
1a, 2a
Int-I
(0.9)
Int-IIA
(2.8)
TS-A
(-9.7)
Int-IIIA
Int-I
(-17.3)
Int-IVA
MeOH
(-18.3)
(S)-3aa


Gibbs energy (kcal/mol)
TS-B
(0)
1a, 2b
Int-I
(-1.9)
Int-IIB
(3.7)
Int-IIIB
(6.8)
TS-B
(-7.3)
Int-IVB
Int-I
(-13.0)
Int-VB
i-PrOH
(-14.6)
(S)-3ba


Gibbs energy (kcal/mol)
TS-C
(0)
Int-I
1a, 2b
(-1.9)
Int-IIB
(5.5)
TS-C
(-6.6)
Int-IIIC
Int-I
(-2.6)
Int-IVC
i-PrOH
(-9.6)
(S)-3ba'


Gibbs energy (kcal/mol)
TS-D
(0)
Int-I
1a, 2a
(-2.3)
Int-IID
(0.7)
TS-D
(-13.4)
Int-IIID
Int-I
(-17.9)
Int-IVD
MeOH
(-17.5)
(R)-3aa



Scheme1. Gibbs energy profiles for the zinc-catalyzed enantioselective allylation and allenylation of **1a** with **2**. Free energies in solution (in kcal/mol) at the (U)B3LYP-D3(BJ)/6-311+G(d,p)SDD/PCM//(U)B3LYP-D3(BJ)/6-31G(d)-SDD/PCM level are displayed. (b) 3D structures were generated by CYLview, key bond distances shown in units of Å [19].

From the calculation results, the energy barrier of **TS-B** involving propargylzinc

(3.1 kcal/mol) is smaller than that of **TS-C** involving allenylzinc (7.4 kcal/mol). Therefore, the allenylation product of isatin is easier to obtain and it is consistent with our experimental results.

The energy barrier of **TS-A** (1.9 kcal/mol) leading to (*S*)-**3aa** is smaller than that of **TS-D** (3.0 kcal/mol) leading to (*R*)-**3aa**. Therefore, the (*S*)-**3aa** is easier to obtain and it is consistent with our experimental results.

The energy barrier of **TS-B** (3.1 kcal/mol) leading to (*S*)-**3ba** is smaller than that of **TS-E** (5.8 kcal/mol) leading to (*R*)-**3ba**. Therefore, the (*S*)-**3ba** is easier to obtain and it is consistent with our experimental results.

Int-I (acetone)

N	0.28973300	-0.42937300	1.02903100
C	-1.14808300	-0.82715000	1.02077100
H	-1.18390700	-1.90080100	0.83003400
C	-1.65427500	-0.51320100	2.44269200
H	-1.58059800	-1.42130500	3.04826000
H	-2.70621300	-0.22418600	2.45367300
C	-0.69904400	0.57523900	2.99808700
H	-0.23483600	0.23959400	3.92971400
H	-1.21581100	1.51404800	3.21019100
C	0.36221400	0.77953600	1.89325300
H	1.37855300	0.89074500	2.27377300
H	0.12866200	1.65282400	1.28452600
C	-1.87887300	-0.19832700	-0.24169500
C	-3.26695600	-0.86077900	-0.34282600
C	-4.48016800	-0.17305100	-0.25686100
C	-3.32324600	-2.24624900	-0.57477200
C	-5.70146600	-0.84457000	-0.37513000
H	-4.48991500	0.90007500	-0.11188600
C	-4.53801300	-2.91316300	-0.68924000
H	-2.39929800	-2.80285200	-0.69151200
C	-5.75646900	-2.22376700	-0.58609000
H	-6.62657300	-0.27690400	-0.30719500
H	-4.54426000	-3.98562600	-0.87105200
C	-1.96787700	1.34234300	-0.19409700
C	-1.42652900	2.09187800	-1.24466900
C	-2.57885500	2.06016100	0.84891600
C	-1.43634500	3.48854400	-1.23010500
H	-1.00009400	1.56646700	-2.09043500
C	-2.58943700	3.45295200	0.86397300
H	-3.06324300	1.53984000	1.66442000

C	-2.00399300	4.19844400	-0.16881300
H	-0.99830300	4.03235500	-2.06395700
H	-3.06610900	3.96981100	1.69362400
C	2.64788000	-1.13977700	1.37233100
C	3.46251600	-1.11613200	2.50643800
C	4.58305900	-0.48198200	0.05204000
C	4.81957200	-0.79723000	2.43854300
H	3.01597300	-1.35913200	3.46787700
C	5.37389200	-0.47763000	1.20238900
H	5.43058300	-0.79147700	3.33498800
H	6.42300900	-0.21596900	1.12363200
C	5.17894500	-0.11469600	-1.27220500
O	2.52180100	-0.84279300	-1.03868600
F	5.10714900	-1.11766200	-2.18181700
F	4.57079400	0.96046700	-1.83784100
F	6.49328300	0.20762500	-1.16639200
C	1.19224400	-1.51352400	1.51571800
H	0.96112400	-2.40545900	0.92215100
H	0.97729400	-1.76083900	2.56363300
C	3.20717500	-0.82066500	0.10259100
Zn	0.68308800	-0.49243700	-1.06129800
O	-1.14649700	-0.60500600	-1.38102300
C	-7.07274900	-2.95327000	-0.69997000
H	-7.24363700	-3.60320400	0.16777300
H	-7.91173200	-2.25329500	-0.76138200
H	-7.09843400	-3.59396700	-1.58918400
C	-1.98583800	5.70666400	-0.12780000
H	-1.21564100	6.07416800	0.56287700
H	-1.77178100	6.12933600	-1.11442100
H	-2.94472900	6.10941500	0.21690200

1a (acetone)

C	2.91503600	0.51239500	0.00007400
C	2.73939300	-0.87674200	0.00010100
C	1.46637000	-1.46710300	0.00003300
C	0.37036600	-0.61726300	-0.00015100
C	0.53380400	0.78377400	-0.00013100
C	1.80220800	1.35689100	0.00000800
N	-0.99444800	-0.96342800	-0.00024900
C	-1.78680100	0.16048100	0.00007400
O	-3.00383300	0.20778400	0.00023000
H	3.91633700	0.92959000	0.00014200
H	3.61249400	-1.52227400	0.00021300
H	1.35265900	-2.54521300	0.00013400

H	1.91098700	2.43700000	-0.00000800
C	-1.50171700	-2.32261600	-0.00000600
H	-1.16566100	-2.85785100	0.89363700
H	-2.59056600	-2.26644800	-0.00260400
H	-1.16144100	-2.85950000	-0.89103200
C	-0.80268600	1.37832000	-0.00006900
O	-1.16235500	2.53970000	-0.00002100

2a

C	4.06398100	-0.46053200	0.61136000
C	2.31146200	0.31176900	-1.03630000
B	0.80495200	0.16638200	-0.59424600
C	-1.17681700	-0.81923600	-0.04526000
C	-1.25669500	0.72926700	0.20674000
O	0.14713300	1.12776600	0.13148600
C	-1.80448400	1.13107500	1.57028800
C	-1.98639300	1.48700800	-0.90533400
C	-2.34311300	-1.40578900	-0.82998900
C	-0.93065300	-1.62741900	1.23136700
H	4.64513000	-0.31151800	1.51760700
H	4.23358600	-1.38860100	0.06847800
H	2.41325400	1.20731800	-1.66674300
H	2.61901000	-0.55359700	-1.63347700
H	-1.80585300	2.22188200	1.65979500
H	-2.83502600	0.77979400	1.68807900
H	-1.20104000	0.72197900	2.38325200
H	-3.06263700	1.29167500	-0.88129500
H	-1.82775500	2.56062600	-0.76690800
H	-1.60360000	1.20948400	-1.89228700
H	-2.18839900	-2.47994600	-0.97172400
H	-3.28159400	-1.26778100	-0.28274700
H	-2.44131900	-0.94165800	-1.81354200
H	-1.81558300	-1.63729000	1.87462600
H	-0.69121100	-2.65938900	0.95808100
H	-0.08919800	-1.22132200	1.80130800
C	3.18656300	0.44986900	0.18340700
H	3.04448400	1.36186500	0.76414000
O	0.03785200	-0.94045400	-0.85062200

Int-IIA

N	0.13624500	0.35560800	2.03554400
C	1.51940200	-0.24901000	2.22366900
H	2.13477800	0.55874400	2.62300200
C	1.40798100	-1.33199200	3.31490600

H	2.29170200	-1.32351900	3.95637700
H	1.33141400	-2.33233100	2.88372100
C	0.12017600	-0.95910300	4.06379500
H	0.32249000	-0.18915400	4.81641100
H	-0.33783900	-1.81083500	4.57413200
C	-0.77278800	-0.40459400	2.95345300
H	-1.56824800	0.25667200	3.29771200
H	-1.25169700	-1.20405200	2.39106000
C	2.26254800	-0.64374200	0.91739200
C	3.73976300	-0.74763500	1.30523300
C	4.32247600	-1.97916000	1.61807200
C	4.50685500	0.41204900	1.47331300
C	5.64404000	-2.04978000	2.06057400
H	3.74583900	-2.89176500	1.51541100
C	5.82769600	0.33673400	1.90628000
H	4.07092700	1.38383200	1.26504900
C	6.42408000	-0.89689000	2.20264800
H	6.07434800	-3.01968100	2.29670100
H	6.40474000	1.25114100	2.01879800
C	1.77497000	-1.88365000	0.16401500
C	2.53516600	-2.35893900	-0.91738100
C	0.56940000	-2.53588800	0.43664900
C	2.08618700	-3.41360900	-1.70714300
H	3.47833700	-1.88526100	-1.15320900
C	0.12699900	-3.60230200	-0.34615300
H	-0.05857700	-2.20756800	1.24998300
C	0.86735100	-4.05215000	-1.44276100
H	2.69473300	-3.74591400	-2.54448400
H	-0.81719800	-4.08089900	-0.10530800
C	-1.05021700	2.57573700	2.39835200
C	-1.72716000	3.02620200	3.53022300
C	-2.65802200	3.75853900	1.00823900
C	-2.86498900	3.83257300	3.42376100
H	-1.34877100	2.75201700	4.51310600
C	-3.31683700	4.20127200	2.15762300
H	-3.38262400	4.17670400	4.31316600
H	-4.19004600	4.83675500	2.05532400
C	-3.12209400	4.17451800	-0.35007100
O	-0.89727700	2.48304900	0.02712700
F	-2.19090000	4.91157600	-1.01364400
F	-3.41966100	3.12785900	-1.15714900
F	-4.24238200	4.94337400	-0.29545100
C	0.22629600	1.79590500	2.49690600
H	0.98983700	2.25424700	1.86343500

H	0.59061400	1.80933500	3.53150300
C	-1.51694100	2.91986800	1.10038500
Zn	-0.54470700	0.55036600	-0.03364200
C	-3.53816100	-4.59186200	1.30311100
C	-4.71217800	-4.93458900	0.62137700
C	-5.39215100	-4.01043200	-0.18490000
C	-4.85264200	-2.73610400	-0.29818800
C	-3.64956900	-2.38512600	0.35696400
C	-3.00338500	-3.30663400	1.17691900
N	-5.36014400	-1.64506900	-1.01309000
C	-4.54074200	-0.53767100	-0.87675100
C	-3.37182600	-0.98634200	0.02869300
O	-2.54086500	-0.20757000	0.51486700
O	-4.74343000	0.57318400	-1.33583000
H	-3.04439500	-5.32469200	1.93258300
H	-5.11632400	-5.93699300	0.72517700
H	-6.30957100	-4.28460200	-0.69381900
H	-2.10102800	-3.03158400	1.71030500
C	-6.56999200	-1.66311100	-1.81056000
H	-7.43366800	-1.93446000	-1.19517000
H	-6.71198200	-0.65918400	-2.21193900
H	-6.47921500	-2.37657300	-2.63663800
O	2.02036300	0.52343700	0.07847800
C	7.86567800	-0.97697300	2.64056300
H	8.05928800	-1.89074000	3.21108900
H	8.54010300	-0.98183300	1.77426600
H	8.14264400	-0.11817600	3.26101700
C	0.35295900	-5.16028200	-2.32639500
H	-0.27207700	-4.75331000	-3.13216400
H	1.17290100	-5.71263500	-2.79611800
H	-0.26362300	-5.86751600	-1.76245700
O	3.81175300	0.32544700	-1.58429900
O	2.20110600	1.95619000	-1.78510500
C	3.20905500	2.25487200	-2.79703900
C	4.09151200	3.36748000	-2.22651000
C	2.50174400	2.72280100	-4.06137100
H	4.60790800	3.03737100	-1.31949400
H	4.84016200	3.69540400	-2.95377700
H	3.46071900	4.22357400	-1.96952900
H	1.75526400	1.99855500	-4.39430000
H	1.99503900	3.67351800	-3.86878800
H	3.22450200	2.87959000	-4.86894600
C	3.95956300	0.88039800	-2.92897000
C	3.26886100	-0.09470000	-3.88601000

C	5.44454800	0.98459200	-3.24582400
H	2.20191800	-0.18653200	-3.66054300
H	3.38086100	0.22491900	-4.92615400
H	3.72473100	-1.08329600	-3.77793500
H	5.97937000	1.55049000	-2.48028200
H	5.88080100	-0.01775300	-3.29931900
H	5.59496900	1.47331500	-4.21406800
B	2.68102000	0.89456900	-1.05906700
C	-2.37225400	-1.74215200	-2.40521600
H	-1.86256300	-2.62132800	-2.02234500
H	-3.34775200	-1.89157700	-2.85421400
C	-1.75036200	-0.53441100	-2.44717300
H	-2.32418700	0.30860200	-2.83426200
C	-0.43624800	-0.23166400	-1.92524700
H	0.23120200	-1.09016100	-1.86237100
H	0.04542200	0.61810100	-2.41671400

TS-A

N	-0.14597800	0.43417200	-2.02937300
C	-1.53188300	-0.16103100	-2.22870500
H	-2.14942100	0.66125800	-2.59442000
C	-1.43038400	-1.19852900	-3.36247200
H	-2.33369800	-1.18800500	-3.97599600
H	-1.31356400	-2.21212200	-2.97263000
C	-0.17499800	-0.76255500	-4.13054000
H	-0.41288800	0.04812600	-4.82828100
H	0.27713200	-1.57535500	-4.70549700
C	0.74416600	-0.26556900	-3.01489500
H	1.52455000	0.42280600	-3.34162300
H	1.24209000	-1.09404800	-2.51241700
C	-2.26471800	-0.60271800	-0.93399700
C	-3.74575700	-0.68385300	-1.31511800
C	-4.33076600	-1.89449800	-1.69831900
C	-4.51382000	0.48336600	-1.40869800
C	-5.65500900	-1.93893800	-2.13568200
H	-3.75357400	-2.81152100	-1.65525500
C	-5.83762000	0.43369500	-1.83706000
H	-4.07616700	1.44142700	-1.14759400
C	-6.43608100	-0.77978400	-2.20311700
H	-6.08661000	-2.89306100	-2.42728000
H	-6.41506100	1.35315200	-1.89125100
C	-1.77429500	-1.87661500	-0.24364400
C	-2.54667400	-2.42320300	0.79445600
C	-0.55490100	-2.49618600	-0.53445800

C	-2.10315000	-3.52295600	1.52345400
H	-3.49610500	-1.97034000	1.04503900
C	-0.12357400	-3.61262900	0.18237500
H	0.08852700	-2.11204300	-1.31134100
C	-0.87845000	-4.13824200	1.23462800
H	-2.72197100	-3.91112300	2.32855800
H	0.82500000	-4.07379500	-0.07332100
C	1.01217800	2.69135900	-2.30611400
C	1.60525200	3.23237600	-3.44579800
C	2.63363500	3.88099900	-0.93991600
C	2.71022200	4.08371400	-3.35718400
H	1.18035500	2.99714200	-4.41960500
C	3.20568600	4.41455500	-2.09769600
H	3.16279300	4.49757200	-4.25229000
H	4.04489300	5.09543600	-2.00578600
C	3.14284600	4.28381200	0.40712400
O	1.00910400	2.44335500	0.06209500
F	2.18837900	4.89306200	1.16012600
F	3.59900600	3.24376100	1.14368500
F	4.17358700	5.16712100	0.32035900
C	-0.25741000	1.89873000	-2.39347600
H	-0.99794300	2.31041300	-1.70269000
H	-0.66447000	1.97555200	-3.40924800
C	1.53965300	2.97751700	-1.01681300
Zn	0.61293200	0.52034800	0.02635200
C	3.75809300	-4.67679300	-1.37780700
C	4.95800400	-4.92971100	-0.70189900
C	5.54883900	-3.97117500	0.13495000
C	4.89119500	-2.75748900	0.28642500
C	3.65912200	-2.50565500	-0.35746100
C	3.10337200	-3.45191200	-1.21292400
N	5.29387000	-1.63545800	1.02121000
C	4.37952900	-0.60088300	0.89403400
C	3.25218900	-1.14648900	0.00127200
O	2.38337300	-0.43885700	-0.54813600
O	4.48831100	0.51995200	1.36511400
H	3.33838700	-5.43171300	-2.03456900
H	5.45519200	-5.88557500	-0.83673200
H	6.49053800	-4.17202200	0.63398100
H	2.18229700	-3.23752400	-1.74475300
C	6.50491200	-1.55013500	1.81199700
H	7.38767200	-1.71971500	1.18691200
H	6.54907200	-0.54627600	2.23564100
H	6.49198800	-2.28740400	2.62185000

O	-2.01199300	0.52701800	-0.05010300
C	-7.88040000	-0.83426700	-2.63597400
H	-8.07329800	-1.70230200	-3.27422100
H	-8.54847400	-0.91058100	-1.76808600
H	-8.16646100	0.06830500	-3.18609700
C	-0.37131000	-5.30186800	2.04822200
H	0.25412500	-4.94909400	2.87888900
H	-1.19481600	-5.87858100	2.48078200
H	0.24340600	-5.97533200	1.44239000
O	-3.76527800	0.22615500	1.63537600
O	-2.18355100	1.88033500	1.87346000
C	-3.17545200	2.11392400	2.91850400
C	-4.08963300	3.23392600	2.41676400
C	-2.45000800	2.53838300	4.18800300
H	-4.61840200	2.93518000	1.50602100
H	-4.82918300	3.51415700	3.17270200
H	-3.48025100	4.11290000	2.18672000
H	-1.68508500	1.81332200	4.47406000
H	-1.96297600	3.50522400	4.02741700
H	-3.15837800	2.64715100	5.01598200
C	-3.89856800	0.72075100	3.00431600
C	-3.17456200	-0.28200000	3.90666800
C	-5.37939100	0.78332200	3.35099800
H	-2.11006000	-0.34401000	3.66108000
H	-3.27548700	-0.01091500	4.96162700
H	-3.61399000	-1.27323400	3.76126200
H	-5.93833300	1.37123100	2.62008800
H	-5.79603800	-0.22861400	3.36837800
H	-5.52147400	1.22682600	4.34198000
B	-2.65707200	0.83988900	1.11263100
C	2.28589500	-1.89166900	2.24807200
H	1.74218400	-2.72003200	1.80730600
H	3.23627400	-2.11740500	2.71769500
C	1.68357800	-0.67507000	2.42327600
H	2.28060800	0.10972400	2.88738400
C	0.39552700	-0.29511900	1.92859100
H	-0.31326800	-1.10907500	1.79062100
H	-0.04643100	0.57655100	2.41390200

Int-IIIA

N	-0.10627200	0.29524500	-2.05891900
C	-1.46740500	-0.37056000	-2.21053200
H	-2.10232800	0.39803000	-2.65670800
C	-1.31504000	-1.47401500	-3.27061400

H	-2.24354400	-1.59654300	-3.83225800
H	-1.07107600	-2.44026600	-2.82427900
C	-0.15119600	-0.96281300	-4.12854000
H	-0.49955000	-0.19530900	-4.82927200
H	0.33245600	-1.75318500	-4.70893600
C	0.78509300	-0.36275000	-3.08097200
H	1.48641900	0.37939600	-3.46799600
H	1.36522200	-1.13721100	-2.57678000
C	-2.22829900	-0.73347300	-0.90367800
C	-3.69866000	-0.83583200	-1.33421600
C	-4.27233300	-2.06367100	-1.67703700
C	-4.46021000	0.32511300	-1.51700000
C	-5.58007600	-2.12990700	-2.15999800
H	-3.69925500	-2.97774900	-1.56720000
C	-5.76714800	0.25484300	-1.99095500
H	-4.03039700	1.29476900	-1.28808600
C	-6.35518300	-0.97552400	-2.31574900
H	-6.00284800	-3.09749500	-2.41831300
H	-6.33963400	1.17087700	-2.11360600
C	-1.78052500	-1.97277300	-0.12531500
C	-2.61578600	-2.44412300	0.90504700
C	-0.56541300	-2.63203900	-0.32602900
C	-2.24476600	-3.51750300	1.70555100
H	-3.56017600	-1.95049500	1.08835200
C	-0.21038500	-3.72803300	0.46646000
H	0.14483100	-2.29155300	-1.06693000
C	-1.03205800	-4.18938400	1.49580100
H	-2.91021300	-3.84335700	2.50123300
H	0.73486400	-4.22799800	0.28884500
C	0.87988600	2.65988200	-2.27372200
C	1.38400100	3.32362000	-3.39194600
C	2.32901900	4.01225800	-0.86331900
C	2.36062300	4.31562800	-3.27068100
H	0.98328700	3.07629700	-4.37266400
C	2.80760900	4.67004200	-1.99995000
H	2.74415600	4.82364000	-4.14933500
H	3.53493300	5.46558900	-1.88169100
C	2.77056600	4.44603600	0.49959800
O	0.96981300	2.28579000	0.08343000
F	1.72463500	4.83076900	1.27737700
F	3.42365900	3.48423700	1.19099000
F	3.61326800	5.51175000	0.44521800
C	-0.31400500	1.75443100	-2.39159900
H	-1.08760800	2.09333600	-1.69875600

H	-0.71773100	1.82259700	-3.40954500
C	1.38789800	2.95719400	-0.97889100
Zn	0.96953600	0.37177500	-0.20521200
C	4.36961100	-4.89020800	-0.72322700
C	5.72358600	-4.70975000	-0.43590000
C	6.19778000	-3.49667100	0.08653500
C	5.26665700	-2.49246200	0.32325900
C	3.89665800	-2.67146300	0.07936400
C	3.44832200	-3.86111200	-0.46729200
N	5.50372400	-1.18058800	0.77003900
C	4.34019000	-0.44126900	0.77308700
C	3.14901500	-1.40790600	0.47477200
O	2.28772700	-0.95844100	-0.50122500
O	4.27259100	0.75747000	1.01147300
H	4.02642900	-5.82748300	-1.15067800
H	6.42868600	-5.51215800	-0.63261000
H	7.25461700	-3.34819000	0.28212400
H	2.40217700	-3.98583400	-0.72188100
C	6.81702700	-0.62446200	1.02444300
H	7.44561900	-0.68797100	0.12905100
H	6.68308800	0.42191000	1.30051700
H	7.30960900	-1.15946600	1.84295100
O	-2.00331800	0.43107800	-0.06605200
C	-7.78263700	-1.05016000	-2.79877900
H	-7.96215200	-1.96387600	-3.37395600
H	-8.48436900	-1.05045500	-1.95442000
H	-8.03612900	-0.19114300	-3.42902900
C	-0.63842000	-5.37145900	2.34502300
H	-0.79274500	-5.16325300	3.40966500
H	-1.24334100	-6.25326400	2.09858300
H	0.41277000	-5.63615300	2.19642300
O	-3.86980500	0.26636000	1.51383000
O	-2.20125800	1.81467400	1.83828100
C	-3.25052100	2.14390000	2.79640500
C	-4.04140300	3.31133200	2.20140400
C	-2.59684100	2.55205900	4.10983500
H	-4.51864800	3.02633100	1.25837100
H	-4.81495400	3.66219300	2.89089000
H	-3.35474900	4.13909900	2.00129000
H	-1.91148000	1.78356000	4.47376300
H	-2.02955900	3.47688400	3.96629200
H	-3.35741700	2.73440100	4.87627300
C	-4.07539000	0.80721100	2.85427800
C	-3.50185800	-0.21543400	3.83863000

C	-5.57142300	0.98217800	3.07712000
H	-2.42768300	-0.35803900	3.68766100
H	-3.66984300	0.09407800	4.87428000
H	-3.99663600	-1.17836300	3.68150000
H	-6.02649200	1.58523400	2.28872900
H	-6.05917200	0.00240300	3.08390200
H	-5.76125600	1.46342000	4.04217200
B	-2.69058000	0.79677000	1.05374000
C	2.41585600	-1.63367200	1.85288000
H	1.72659900	-2.47191000	1.72388500
H	3.15775600	-1.91115400	2.61207300
C	1.66802100	-0.40718700	2.27330400
H	2.26607800	0.46508100	2.52968900
C	0.32541000	-0.31070600	2.28774200
H	-0.30232900	-1.16753500	2.05767700
H	-0.17677900	0.60590300	2.58080100

Int-IVA

C	-1.42433400	-2.56840100	-2.26678200
C	-1.58403000	-3.43764500	-1.18618200
C	-1.70886200	-2.95695000	0.12661900
C	-1.66635300	-1.58133400	0.31019200
C	-1.51106700	-0.69903100	-0.76717700
C	-1.38990300	-1.18008500	-2.05864400
N	-1.72813700	-0.86058100	1.51538000
C	-1.52020000	0.48269800	1.30415300
C	-1.48633300	0.71597200	-0.23721000
O	-0.32509700	1.44623400	-0.63653400
O	-1.40494000	1.33596000	2.17102600
H	-1.32484800	-2.96658400	-3.27160400
H	-1.61015000	-4.50954700	-1.35857800
H	-1.82402300	-3.63900100	0.96217900
H	-1.25508500	-0.49668400	-2.89222400
C	-1.72777800	-1.47043300	2.82976900
H	-0.82553900	-2.07671500	2.96998200
H	-1.74376800	-0.66803500	3.56748800
H	-2.61006200	-2.10438000	2.95768300
O	2.03950400	1.38374700	-0.96392600
O	1.12283300	-0.06202800	0.57933300
C	2.48411400	-0.53197400	0.35000200
C	2.37724900	-1.71036500	-0.62176400
C	3.07152800	-0.98407200	1.67944300
H	1.95896800	-1.39560800	-1.58264600
H	3.35267000	-2.17291500	-0.79868400

H	1.70680700	-2.46109600	-0.19316700
H	3.00949100	-0.19737300	2.43414300
H	2.51975600	-1.85537900	2.04618600
H	4.12076000	-1.27253100	1.55771600
C	3.16238400	0.73941000	-0.28214800
C	3.67208500	1.72997900	0.76631300
C	4.24416200	0.43955800	-1.31062000
H	2.90287000	1.94453400	1.51460700
H	4.55957600	1.34664300	1.27851300
H	3.93841300	2.66766000	0.26969200
H	3.85196700	-0.14317600	-2.14679200
H	4.64958100	1.37658600	-1.70480700
H	5.06562900	-0.11861200	-0.84934400
B	0.90593300	0.93661900	-0.33771800
C	-2.71734800	1.52523500	-0.69603600
H	-2.71341100	1.53121400	-1.79202500
H	-3.60979400	0.96908500	-0.37902600
C	-2.75983900	2.93235300	-0.16930500
H	-2.76650800	3.03906100	0.91283900
C	-2.78864900	4.01461700	-0.94697800
H	-2.77089900	3.93822000	-2.03255200
H	-2.83447600	5.01710700	-0.52969800

(*S*)-3aa

C	-2.60847500	-2.12628500	-0.00487500
C	-3.40139000	-0.99795100	-0.22263100
C	-2.84509100	0.28948300	-0.25776600
C	-1.47368400	0.39830500	-0.06740600
C	-0.66457100	-0.72740600	0.14429000
C	-1.22288900	-1.99335700	0.17820400
N	-0.68879000	1.56640800	-0.03901900
C	0.63070700	1.27036500	0.21212300
C	0.76852300	-0.27783700	0.27105400
O	1.53341300	2.08240000	0.36368600
H	-3.06476800	-3.11081300	0.02305300
H	-4.47174400	-1.11298900	-0.36605700
H	-3.46709300	1.16273200	-0.42264000
H	-0.59979200	-2.86633000	0.34978100
C	-1.21126400	2.91337900	-0.15301500
H	-1.94183300	3.11153100	0.63849200
H	-0.37150100	3.60177800	-0.05419900
H	-1.69114800	3.05825300	-1.12621800
C	1.64173900	-0.78815100	-0.90981100
H	1.58065900	-1.88200900	-0.89468700

H	1.19828700	-0.44136300	-1.85033000
C	3.07289900	-0.34358900	-0.78761100
H	3.29243200	0.68121300	-1.07669300
C	4.04255300	-1.11253800	-0.28293300
H	3.85331000	-2.14003900	0.02182100
H	5.06179400	-0.75150500	-0.17610200
O	1.31646200	-0.68502400	1.51404000
H	2.26959000	-0.48083600	1.46737200

Int-I (in *i*-PrOH)

N	0.40758000	-0.50632000	1.03153400
C	-1.07393300	-0.79869900	0.99385400
H	-1.16128800	-1.86141900	0.75655300
C	-1.60380300	-0.55163500	2.42533000
H	-2.31017600	-1.32901300	2.72418900
H	-2.12624500	0.40647000	2.48226900
C	-0.34514800	-0.52266900	3.30589300
H	-0.05617000	-1.53756900	3.60180800
H	-0.47535200	0.06602000	4.21850800
C	0.71075900	0.07378400	2.37217800
H	1.73857100	-0.16392900	2.64817200
H	0.63049200	1.16222500	2.33069200
C	-1.84423600	-0.07653600	-0.19595600
C	-3.04763600	-0.99775500	-0.45642300
C	-4.14563100	-1.03029300	0.41604300
C	-3.03151900	-1.89105800	-1.52836400
C	-5.18987300	-1.93013900	0.21845600
H	-4.19296000	-0.33655600	1.24957300
C	-4.08232800	-2.79073600	-1.72645100
H	-2.18615500	-1.87368200	-2.20626600
C	-5.17867100	-2.82870800	-0.85899900
H	-6.03011700	-1.93372400	0.90922900
H	-4.04733000	-3.47526300	-2.57104200
C	-2.31442600	1.36974900	0.05750700
C	-3.44872300	1.85602300	-0.60990900
C	-1.56653800	2.29813100	0.79353100
C	-3.82716100	3.19489400	-0.52459300
H	-4.04389000	1.17844500	-1.21196200
C	-1.94363800	3.63833000	0.88191200
H	-0.66334500	1.98855500	1.30161100
C	-3.08768700	4.11322600	0.23097700
H	-4.71250600	3.53259900	-1.05854600
H	-1.33585300	4.32371800	1.46801100
C	2.70038200	-1.49280200	0.78372600

C	3.52299800	-2.14686800	1.70447000
C	4.68767400	-0.41675200	-0.12072500
C	4.90630800	-1.96467800	1.72475600
H	3.06093300	-2.81905300	2.42367600
C	5.48291300	-1.09200200	0.80617600
H	5.52118300	-2.48881600	2.44868600
H	6.55410600	-0.92518800	0.80659600
C	5.31221500	0.53082900	-1.09851300
O	2.59010700	0.04708800	-1.09266400
F	5.11938700	0.16064100	-2.38888100
F	4.82786800	1.79436000	-0.98507100
F	6.65558400	0.62468600	-0.92800100
C	1.21333400	-1.75476700	0.81386500
H	0.87230200	-2.19782500	-0.13000900
H	0.98779400	-2.48788100	1.59941900
C	3.28224700	-0.60357800	-0.16283900
Zn	0.74870900	0.32246100	-0.92433600
O	-1.02179400	-0.04028000	-1.34393500
C	-6.32225800	-3.79031500	-1.07548900
H	-6.55724600	-4.34458700	-0.15918800
H	-7.23683200	-3.26135400	-1.37267700
H	-6.08867400	-4.51631600	-1.86038500
C	-3.51872600	5.55411600	0.35394700
H	-2.66049400	6.21604400	0.50984000
H	-4.05212300	5.88878300	-0.54190900
H	-4.19640200	5.69354200	1.20669600

1a (in *i*-PrOH)

C	2.91503900	0.51236900	0.00007400
C	2.73940200	-0.87676100	0.00010100
C	1.46637900	-1.46711000	0.00003200
C	0.37036000	-0.61727400	-0.00015100
C	0.53380800	0.78375800	-0.00013000
C	1.80220300	1.35686100	0.00000900
N	-0.99442900	-0.96342700	-0.00024900
C	-1.78683900	0.16052900	0.00007300
O	-3.00383600	0.20773300	0.00023100
H	3.91634100	0.92956700	0.00014100
H	3.61250400	-1.52229700	0.00021100
H	1.35266000	-2.54522200	0.00013400
H	1.91095700	2.43697300	-0.00000700
C	-1.50175200	-2.32257500	-0.00000700
H	-1.16575000	-2.85785000	0.89364400
H	-2.59060000	-2.26633000	-0.00261300

H	-1.16151500	-2.85950300	-0.89103100
C	-0.80270500	1.37835500	-0.00006900
O	-1.16228300	2.53973500	-0.00002300

2b

C	4.35170600	0.51176400	0.17225000
C	2.30042300	-1.06722800	-0.22682400
B	0.84113200	-0.55372900	-0.11815000
C	-1.43151900	-0.61967100	0.03048400
C	-0.93193400	0.87022100	0.00090200
O	0.49961100	0.72355600	0.25075900
C	-1.52400100	1.76793900	1.08000500
C	-1.07152700	1.52729900	-1.37482900
C	-2.56392900	-0.93776900	-0.93770300
C	-1.77812900	-1.11349800	1.43750100
H	4.80287600	1.07314100	-0.64344500
H	4.78246500	0.64318800	1.16281900
H	2.47964600	-2.11495200	-0.47566500
H	-1.10539100	2.77526000	0.99113500
H	-2.61056600	1.84052200	0.96468700
H	-1.30322700	1.39296500	2.08152300
H	-2.11943300	1.73002000	-1.61530100
H	-0.52829900	2.47694100	-1.37172700
H	-0.64935100	0.89462600	-2.16166400
H	-2.82952500	-1.99655100	-0.85842000
H	-3.45289300	-0.34590100	-0.69549900
H	-2.27928500	-0.73309700	-1.97185600
H	-2.70084100	-0.65438400	1.80469000
H	-1.92029600	-2.19790100	1.40882300
H	-0.97313300	-0.89271600	2.14515500
C	3.33630700	-0.28407600	-0.02874200
O	-0.23995900	-1.35510700	-0.38735500

Int-IIB

N	0.12121400	0.74089800	1.91307800
C	1.49262100	0.13588500	2.18464100
H	2.12626900	0.97955800	2.46185500
C	1.36168400	-0.77315000	3.42299300
H	2.24387300	-0.68104500	4.05993400
H	1.27445400	-1.82495700	3.14333400
C	0.07724800	-0.27854700	4.10392000
H	0.28714900	0.58808400	4.74048100
H	-0.39588900	-1.04229100	4.72726300
C	-0.80227600	0.12406900	2.92070200

H	-1.59332400	0.83327300	3.16464800
H	-1.28169900	-0.74144500	2.46692800
C	2.22726100	-0.45494800	0.95257100
C	3.69343800	-0.58296700	1.37807100
C	4.21984300	-1.80173300	1.81501200
C	4.50656000	0.55555100	1.44963900
C	5.53044300	-1.88303300	2.28795900
H	3.60748600	-2.69604200	1.78583400
C	5.81587900	0.46885800	1.91348300
H	4.11623100	1.51852500	1.13641300
C	6.35522200	-0.75409200	2.33718100
H	5.91653000	-2.84284200	2.62170900
H	6.42955600	1.36552400	1.94925700
C	1.69254700	-1.75572500	0.34840800
C	2.41700300	-2.35077400	-0.69856800
C	0.50550600	-2.37633800	0.74161300
C	1.95257400	-3.49439500	-1.33783000
H	3.35154000	-1.90777800	-1.01674800
C	0.05084700	-3.53624700	0.11352800
H	-0.09905700	-1.95963100	1.53199900
C	0.75507600	-4.10912600	-0.94652600
H	2.53332800	-3.92082000	-2.15234300
H	-0.87811800	-3.98868100	0.44635400
C	-1.03355900	2.99967200	2.09067000
C	-1.56391800	3.62921600	3.21643900
C	-2.83492900	3.94607900	0.76218200
C	-2.71615100	4.41579500	3.13819200
H	-1.05643000	3.50828400	4.17134200
C	-3.34191700	4.57185900	1.90299700
H	-3.11503000	4.90158500	4.02259000
H	-4.23494000	5.18153000	1.81836900
C	-3.51554100	4.11138900	-0.55829600
O	-1.19204100	2.54589700	-0.24614500
F	-2.70938700	4.66217700	-1.50189200
F	-3.95566900	2.93652000	-1.07210100
F	-4.60551200	4.92039700	-0.47463200
C	0.24929500	2.22854000	2.17344600
H	0.96532200	2.59088000	1.43008900
H	0.69492500	2.37408600	3.16471400
C	-1.67062800	3.13473700	0.82741000
Zn	-0.56677400	0.69320500	-0.14828000
C	-3.53579700	-4.42679000	1.92889100
C	-4.54611400	-4.98060400	1.13132200
C	-5.12835900	-4.27098800	0.07113700

C	-4.65955400	-2.98761900	-0.17465800
C	-3.62283300	-2.42676100	0.60517400
C	-3.07040700	-3.13602000	1.66949200
N	-5.08800100	-2.08543000	-1.15737600
C	-4.36270900	-0.91142600	-1.09992900
C	-3.36740900	-1.09015500	0.08260600
O	-2.62541000	-0.20361200	0.49458600
O	-4.50285000	0.07086900	-1.80445800
H	-3.11705300	-5.00196200	2.74760400
H	-4.89734800	-5.98627500	1.34139900
H	-5.91671500	-4.71292400	-0.52757100
H	-2.29234600	-2.69215600	2.28100200
C	-6.09997900	-2.36528400	-2.15719900
H	-7.05673800	-2.60126800	-1.68133100
H	-6.21057400	-1.47031300	-2.77016300
H	-5.79448600	-3.20536700	-2.78998000
O	2.05422700	0.61173900	-0.02198200
C	7.78489600	-0.84889600	2.81004000
H	7.93941900	-1.73080400	3.43948400
H	8.47601100	-0.92601100	1.96051100
H	8.07556300	0.03818500	3.38288400
C	0.23469100	-5.32894800	-1.66414100
H	-0.21826200	-5.04969700	-2.62426300
H	1.03783700	-6.04168200	-1.88111600
H	-0.53160700	-5.84212700	-1.07483000
O	3.90423700	0.22760500	-1.58565000
O	2.23056700	1.72571700	-2.08712100
C	3.26075000	1.91859000	-3.10233600
C	4.05761700	3.15870100	-2.69152600
C	2.57954200	2.13664500	-4.44651000
H	4.55136900	3.00984100	-1.72591800
H	4.81818200	3.40957500	-3.43683400
H	3.37175000	4.00587900	-2.59857100
H	1.88507500	1.32670000	-4.67956400
H	2.01667300	3.07495800	-4.42559800
H	3.32347100	2.20322500	-5.24724500
C	4.09125500	0.58689300	-2.98984800
C	3.51389200	-0.56072800	-3.82249700
C	5.58412900	0.73514700	-3.25073800
H	2.44613200	-0.70108500	-3.62872000
H	3.65334900	-0.38288700	-4.89269500
H	4.02963700	-1.48855100	-3.55754100
H	6.04419800	1.44315800	-2.55847400
H	6.07620900	-0.23452400	-3.12673500

H	5.76232200	1.07853400	-4.27507700
B	2.73286300	0.81864100	-1.18700600
C	-2.08598600	-2.30407400	-2.40079200
H	-1.95122700	-3.31446100	-2.02370700
C	-1.21326600	-1.34726300	-2.13162300
C	-0.39872000	-0.40399400	-1.78983400
H	0.47383600	-0.18969900	-2.40624400
H	-2.93377300	-2.13127700	-3.05864800

Int-IIIB

N	0.19073600	0.24311100	2.03631700
C	1.56473000	-0.38274600	2.23073000
H	2.17718100	0.39695800	2.68800700
C	1.41035000	-1.51464500	3.26174000
H	2.30090000	-1.59168700	3.88897000
H	1.26664300	-2.48255800	2.77524300
C	0.15281900	-1.10874500	4.04106300
H	0.39592100	-0.35677500	4.80016500
H	-0.32798900	-1.95083900	4.54639400
C	-0.73257700	-0.51119600	2.94831400
H	-1.51005600	0.16356100	3.30748300
H	-1.23179800	-1.29279600	2.37794700
C	2.33218800	-0.72661100	0.92519700
C	3.80362300	-0.82715500	1.33029700
C	4.37531900	-2.05562800	1.67625800
C	4.57322600	0.33149000	1.48797200
C	5.68905700	-2.12411400	2.14054500
H	3.79523000	-2.96713200	1.58159900
C	5.88710900	0.25804800	1.94355900
H	4.14454700	1.30076100	1.25588000
C	6.47260100	-0.97180500	2.27294800
H	6.11079100	-3.09129000	2.40213300
H	6.46663900	1.17182700	2.04820200
C	1.85245700	-1.94136500	0.12953500
C	2.66358200	-2.45534500	-0.89233900
C	0.57547100	-2.49599200	0.28132100
C	2.19915100	-3.45442100	-1.74675300
H	3.65499800	-2.05001600	-1.04129300
C	0.11618200	-3.49868800	-0.56773400
H	-0.09317900	-2.13385100	1.04727100
C	0.91274000	-3.98659800	-1.60911900
H	2.84732500	-3.81756800	-2.54026000
H	-0.88847100	-3.88674500	-0.43578500
C	-0.96199900	2.48371500	2.40137300

C	-1.62985400	2.94449600	3.53458300
C	-2.51718200	3.73996800	1.01614600
C	-2.73900700	3.78967400	3.43174300
H	-1.26401500	2.64944700	4.51610600
C	-3.16624000	4.19209100	2.16772000
H	-3.25000700	4.14125800	4.32204000
H	-4.01178600	4.86415700	2.06812200
C	-2.95193100	4.20922700	-0.33534900
O	-0.80398700	2.40246700	0.02890300
F	-1.97309800	4.89519700	-0.98421500
F	-3.31920500	3.20223400	-1.16288400
F	-4.01835900	5.05047700	-0.26555200
C	0.29846100	1.67812100	2.50568300
H	1.07705900	2.12743300	1.88421400
H	0.65156600	1.67921800	3.54435600

TS-B

N	0.11048200	0.27450900	2.03191600
C	1.48444600	-0.34989100	2.22496900
H	2.09299100	0.42687900	2.69256100
C	1.32853400	-1.48932400	3.24672300
H	2.22209100	-1.57729300	3.86822600
H	1.17488800	-2.45239300	2.75365800
C	0.07821500	-1.07960500	4.03532000
H	0.33024900	-0.32987100	4.79384500
H	-0.40274600	-1.92049300	4.54241700
C	-0.81160600	-0.47679700	2.94925400
H	-1.58240700	0.20257500	3.31473300
H	-1.31846800	-1.25398300	2.37883000
C	2.25812400	-0.68054100	0.91967800
C	3.72899100	-0.76699400	1.33053300
C	4.31101200	-1.99024300	1.67704000
C	4.48576100	0.39918700	1.49573100
C	5.62295200	-2.04652400	2.14847700
H	3.74080000	-2.90746700	1.57778300
C	5.79757400	0.33800100	1.95838000
H	4.04856300	1.36479800	1.26413600
C	6.39383400	-0.88683500	2.28802100
H	6.05291000	-3.00997200	2.41025900
H	6.36706800	1.25740200	2.06865200
C	1.79433900	-1.89717800	0.11777700
C	2.61962300	-2.40282400	-0.89733200
C	0.51762300	-2.45735300	0.25250100
C	2.17096100	-3.40206800	-1.75967500

H	3.60998900	-1.99077700	-1.03424800
C	0.07399800	-3.45965900	-0.60618500
H	-0.16248800	-2.10016800	1.01153800
C	0.88632900	-3.94257000	-1.63770500
H	2.83039000	-3.75941500	-2.54642800
H	-0.92992400	-3.85352300	-0.48800800
C	-1.03464800	2.52640300	2.37164800
C	-1.69694700	3.00283100	3.50196800
C	-2.57216600	3.79567300	0.97907900
C	-2.79473600	3.86152100	3.39424500
H	-1.33410100	2.70985000	4.48512400
C	-3.21494800	4.26353400	2.12798000
H	-3.30139700	4.22472500	4.28232900
H	-4.05026800	4.94748700	2.02408900
C	-2.99887200	4.26906600	-0.37377400
O	-0.88127100	2.42407500	-0.00333600
F	-2.01086000	4.94489900	-1.01946600
F	-3.37427300	3.26653800	-1.20201200
F	-4.05618900	5.12163600	-0.30645000
C	0.22083900	1.71352800	2.48721500
H	1.00317500	2.15341400	1.86389100
H	0.57026400	1.72298000	3.52705700
C	-1.48065400	2.89271600	1.07189700
Zn	-0.58490700	0.49231800	-0.02125800
C	-3.72770400	-4.66608600	1.18808500
C	-4.98172700	-4.87699100	0.60443100
C	-5.62026400	-3.87872700	-0.14621200
C	-4.95678200	-2.66859400	-0.30318300
C	-3.67585100	-2.45545000	0.25134100
C	-3.06785200	-3.44370400	1.01703900
N	-5.39989600	-1.51683900	-0.96797400
C	-4.47953900	-0.48668100	-0.85375800
C	-3.27677200	-1.08077200	-0.09402400
O	-2.40630200	-0.37788000	0.46705700
O	-4.62717200	0.66133500	-1.23771600
H	-3.26656500	-5.45176900	1.77760200
H	-5.48209800	-5.83073100	0.74252700
H	-6.60133700	-4.04701500	-0.57675900
H	-2.10014400	-3.27001500	1.47497000
C	-6.68104400	-1.38452100	-1.63237300
H	-7.50180600	-1.56211500	-0.92957600
H	-6.74715100	-0.36592800	-2.01604500
H	-6.76112600	-2.09347200	-2.46303900
O	2.00357500	0.50460700	0.10916500

C	7.82588800	-0.95188900	2.75856700
H	8.00641100	-1.84461700	3.36560200
H	8.51832900	-0.98874700	1.90736900
H	8.09083400	-0.07144600	3.35330500
C	0.37203100	-4.99083800	-2.59126900
H	-0.48638700	-4.60931100	-3.15806700
H	1.14192600	-5.29438500	-3.30660900
H	0.03141200	-5.88481900	-2.05583400
O	3.78923300	0.31738400	-1.55744600
O	2.13175000	1.89618600	-1.79062500
C	3.12792900	2.20386400	-2.81197000
C	3.96793300	3.36371600	-2.27286800
C	2.40163400	2.61135200	-4.08663700
H	4.49437700	3.07917800	-1.35622800
H	4.70539700	3.69786100	-3.00865000
H	3.30569900	4.20297000	-2.04087300
H	1.67970300	1.85267000	-4.39621300
H	1.86248400	3.54876100	-3.91868300
H	3.11584500	2.77023200	-4.90132500
C	3.93005800	0.85445400	-2.90997900
C	3.28917900	-0.16214400	-3.85791900
C	5.41419700	1.00732200	-3.21248200
H	2.22239100	-0.28593200	-3.64965800
H	3.40735700	0.14160300	-4.90212200
H	3.77556400	-1.13240000	-3.72233100
H	5.91938200	1.60520700	-2.45116300
H	5.88648600	0.02045500	-3.24287100
H	5.55907500	1.48404100	-4.18748800
B	2.64742100	0.86970600	-1.04152400
C	-2.56528100	-1.64287500	-2.23218400
H	-3.27949500	-2.29138600	-2.69514500
C	-1.50252200	-1.00646300	-2.25112200
C	-0.37795100	-0.23800400	-1.98398300
H	0.55333600	-0.80121400	-1.93879100
H	-0.28691300	0.69631500	-2.54162700

Int-IVB

N	0.11051000	0.27444200	2.03194500
C	1.48447800	-0.34994600	2.22498300
H	2.09300500	0.42682100	2.69260300
C	1.32857700	-1.48940700	3.24670600
H	2.22213900	-1.57739300	3.86819900
H	1.17492500	-2.45246300	2.75361700
C	0.07826600	-1.07970700	4.03532500

H	0.33030700	-0.32998800	4.79386200
H	-0.40268900	-1.92060600	4.54241000
C	-0.81156800	-0.47687700	2.94928100
H	-1.58236400	0.20249000	3.31478000
H	-1.31844000	-1.25405100	2.37884900
C	2.25818100	-0.68053400	0.91969200
C	3.72905400	-0.76682600	1.33055800
C	4.31117300	-1.98998500	1.67722100
C	4.48572000	0.39943700	1.49564000
C	5.62310500	-2.04609600	2.14870000
H	3.74104000	-2.90727000	1.57806600
C	5.79752600	0.33842000	1.95832900
H	4.04844200	1.36498400	1.26392900
C	6.39388300	-0.88632500	2.28813000
H	6.05313800	-3.00947700	2.41061100
H	6.36693600	1.25788400	2.06851200
C	1.79450800	-1.89722900	0.11781500
C	2.61989500	-2.40290800	-0.89719300
C	0.51779600	-2.45743000	0.25245900
C	2.17134600	-3.40223200	-1.75950200
H	3.61026100	-1.99084000	-1.03404800
C	0.07427900	-3.45981000	-0.60619700
H	-0.16239500	-2.10021200	1.01140900
C	0.88672300	-3.94277300	-1.63760500
H	2.83085800	-3.75961600	-2.54616800
H	-0.92964000	-3.85370000	-0.48807900
C	-1.03457900	2.52634200	2.37177500
C	-1.69680300	3.00278300	3.50213300
C	-2.57216600	3.79561200	0.97929600
C	-2.79458600	3.86148900	3.39447400
H	-1.33390000	2.70980400	4.48526900
C	-3.21487300	4.26349100	2.12823100
H	-3.30118900	4.22470500	4.28258600
H	-4.05020200	4.94743800	2.02438300
C	-2.99900200	4.26894100	-0.37353300
O	-0.88129800	2.42403800	-0.00321700
F	-2.01104800	4.94471800	-1.01937500
F	-3.37450900	3.26635700	-1.20165100
F	-4.05630000	5.12152900	-0.30615000
C	0.22089700	1.71345000	2.48727200
H	1.00321300	2.15334000	1.86392600
H	0.57036400	1.72287600	3.52710100
C	-1.48064500	2.89265800	1.07204800
Zn	-0.58489800	0.49228600	-0.02122800

C	-3.72772800	-4.66625400	1.18745700
C	-4.98179100	-4.87704500	0.60384700
C	-5.62034600	-3.87866000	-0.14661900
C	-4.95684300	-2.66852100	-0.30345900
C	-3.67587500	-2.45548600	0.25102000
C	-3.06785400	-3.44386400	1.01654300
N	-5.39996800	-1.51666100	-0.96806100
C	-4.47958400	-0.48653700	-0.85374300
C	-3.27678400	-1.08076600	-0.09416400
O	-2.40628900	-0.37796900	0.46699800
O	-4.62721700	0.66153800	-1.23752500
H	-3.26657500	-5.45203000	1.77683900
H	-5.48217900	-5.83079200	0.74184100
H	-6.60145000	-4.04686200	-0.57712900
H	-2.10011700	-3.27026400	1.47444300
C	-6.68114800	-1.38422200	-1.63237300
H	-7.50187600	-1.56189600	-0.92955800
H	-6.74725300	-0.36557400	-2.01590000
H	-6.76128900	-2.09305600	-2.46313400
O	2.00351300	0.50457500	0.10915600
C	7.82592600	-0.95119600	2.75873400
H	8.00651000	-1.84383800	3.36587700
H	8.51840100	-0.98808600	1.90756500
H	8.09077100	-0.07066100	3.35338200
C	0.37255400	-4.99114300	-2.59112500
H	-0.48582800	-4.60970200	-3.15803400
H	1.14252700	-5.29472200	-3.30636600
H	0.03192200	-5.88509200	-2.05564200
O	3.78913800	0.31745800	-1.55749800
O	2.13148900	1.89608100	-1.79070200
C	3.12759500	2.20379700	-2.81210900
C	3.96749800	3.36377300	-2.27311700
C	2.40120400	2.61112600	-4.08677400
H	4.49400700	3.07935200	-1.35647700
H	4.70489900	3.69794500	-3.00894900
H	3.30518500	4.20297300	-2.04115400
H	1.67934000	1.85234800	-4.39627000
H	1.86196200	3.54848900	-3.91885800
H	3.11536500	2.77002800	-4.90150200
C	3.92986400	0.85446500	-2.91006600
C	3.28906300	-0.16225800	-3.85792400
C	5.41397800	1.00746800	-3.21262200
H	2.22229600	-0.28615100	-3.64961800
H	3.40717200	0.14143700	-4.90215000

H	3.77555900	-1.13245400	-3.72229300
H	5.91912400	1.60545400	-2.45135600
H	5.88636700	0.02064800	-3.24296200
H	5.55877900	1.48414000	-4.18766300
B	2.64729300	0.86969600	-1.04156300
C	-2.56501100	-1.64314900	-2.23222000
H	-3.27911500	-2.29175100	-2.69522200
C	-1.50238200	-1.00652100	-2.25114200
C	-0.37787900	-0.23797300	-1.98398000
H	0.55344500	-0.80112300	-1.93878400
H	-0.28689600	0.69636000	-2.54160700

Int-VB

C	-1.72431600	-2.02871900	-2.50997900
C	-1.85044400	-3.06570400	-1.58339500
C	-1.87049700	-2.81543400	-0.20263000
C	-1.75627800	-1.49433600	0.20958700
C	-1.62905000	-0.44722900	-0.71210400
C	-1.61665800	-0.69939700	-2.07203100
N	-1.71560600	-0.99264500	1.52271400
C	-1.46654200	0.35907400	1.53436400
C	-1.49325500	0.85605100	0.04702300
O	-0.31255100	1.58197900	-0.27529000
O	-1.27262000	1.05410500	2.51667800
H	-1.71018700	-2.25076600	-3.57230300
H	-1.93478200	-4.09039500	-1.93305900
H	-1.96323600	-3.62758300	0.51031200
H	-1.51440200	0.11651100	-2.78162200
C	-1.65284800	-1.82276500	2.70911600
H	-0.76088100	-2.45921200	2.68355700
H	-1.60170400	-1.16106300	3.57392400
H	-2.54338900	-2.45375500	2.78190600
O	2.02375200	1.46087300	-0.74676800
O	1.09996600	-0.19374300	0.56501100
C	2.41774300	-0.68238200	0.17339100
C	2.19026200	-1.65673700	-0.98546500
C	3.04227300	-1.39816500	1.36244600
H	1.74739400	-1.15061700	-1.84861400
H	3.12502100	-2.13099200	-1.29862300
H	1.49472800	-2.43569800	-0.65968600
H	3.06593500	-0.76019100	2.24825000
H	2.45799700	-2.29290900	1.59948800
H	4.06464200	-1.71188200	1.12758200
C	3.13893400	0.64725900	-0.26031100

C	3.75942900	1.40327400	0.91592600
C	4.14738900	0.48610200	-1.38937400
H	3.04317700	1.51702500	1.73550900
H	4.64612500	0.88796100	1.29684600
H	4.05763600	2.40078800	0.58005900
H	3.67953300	0.08501600	-2.29088700
H	4.58719100	1.45801800	-1.63365100
H	4.95651700	-0.18631100	-1.08557100
B	0.89933300	0.96366600	-0.14425700
C	-2.68935500	1.76090500	-0.15433900
H	-3.66136500	1.29625800	0.00139600
C	-2.59947200	3.02094000	-0.49113500
C	-2.52337100	4.27765200	-0.83687900
H	-2.51512500	4.58221500	-1.88189900
H	-2.46028200	5.06972900	-0.09294800

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C	2.03301500	-2.51115000	-0.07889700
C	3.05430000	-1.58912500	0.15975100
C	2.79185400	-0.21397500	0.24759700
C	1.47541600	0.19663100	0.08307300
C	0.44171200	-0.71939900	-0.15780900
C	0.70806600	-2.07518500	-0.23350300
N	0.96307800	1.50877800	0.11812200
C	-0.39005600	1.51695200	-0.10883100
C	-0.86207900	0.03645800	-0.25996300
O	-1.11032500	2.49861300	-0.21220400
H	2.26404600	-3.56984400	-0.14146300
H	4.07520000	-1.93856600	0.28229000
H	3.58996800	0.49635700	0.43447000
H	-0.09563800	-2.78375500	-0.41023400
C	1.76873800	2.70458900	0.27101200
H	2.51017200	2.77353700	-0.53181500
H	1.09816800	3.56285700	0.22214600
H	2.28546800	2.69756300	1.23588900
C	-1.82027600	-0.31418800	0.86668300
H	-1.43247700	-0.22433000	1.88042000
C	-3.05183600	-0.69766200	0.65189400
C	-4.27947900	-1.08028400	0.42093700
H	-4.53365600	-2.13013000	0.28631700
H	-5.09680900	-0.36417100	0.35779400
O	-1.44167800	-0.13275900	-1.54249100
H	-2.20621800	0.47022100	-1.57676600

TS-C

N	-0.10537400	-0.67847200	-2.00716300
C	1.35937700	-0.50368300	-2.25251600
H	1.79048100	-1.50265200	-2.25452900
C	1.46912600	0.12557200	-3.65911800
H	1.64246000	-0.67101600	-4.38689300
H	2.32280200	0.79890600	-3.74288100
C	0.10247200	0.80773900	-3.91885700
H	-0.36459000	0.40355200	-4.82089600
H	0.19663600	1.88741400	-4.05980200
C	-0.73978300	0.50226700	-2.66457400
H	-1.78725000	0.27891700	-2.86686400
H	-0.70706400	1.32698400	-1.95905100
C	2.10857900	0.21071400	-1.08484200
C	3.61950000	0.07401600	-1.35192800
C	4.49005600	1.16134900	-1.44278100
C	4.16911500	-1.21634800	-1.44538500
C	5.86061300	0.96743700	-1.62869200
H	4.11385800	2.17162300	-1.34519700
C	5.53563900	-1.40549300	-1.62138300
H	3.53347900	-2.09058500	-1.34526700
C	6.41069900	-0.31398100	-1.72062500
H	6.51326900	1.83460000	-1.68810100
H	5.92999900	-2.41690800	-1.67765500
C	1.69046300	1.65109300	-0.76437300
C	1.33698500	2.02522800	0.53909000
C	1.76255500	2.67357400	-1.72315300
C	1.09150200	3.35533100	0.87262400
H	1.25242200	1.28065800	1.31395000
C	1.50549600	4.00376100	-1.38835300
H	2.05626800	2.45650300	-2.74062700
C	1.17812000	4.37571400	-0.08036100
H	0.83556200	3.60207400	1.89988300
H	1.57906500	4.76473700	-2.16058900
C	-1.95564900	-2.34497700	-2.43577500
C	-2.93062200	-2.34090900	-3.43037000
C	-3.57796100	-3.28458700	-0.88772400
C	-4.22746300	-2.79834000	-3.17436800
H	-2.66733300	-1.98593700	-4.42472000
C	-4.53853000	-3.27628300	-1.90272800
H	-4.97959000	-2.79092000	-3.95647100
H	-5.53700400	-3.64200700	-1.68847700
C	-3.90810100	-3.80773800	0.47271500
O	-1.35050800	-2.77998300	-0.17407200

F	-3.18138100	-4.91202200	0.79451200
F	-3.68335800	-2.90738500	1.45904200
F	-5.21337300	-4.17182000	0.57897900
C	-0.53544400	-1.94849500	-2.70443000
H	0.12951900	-2.73174900	-2.33052600
H	-0.36974900	-1.84686200	-3.78274800
C	-2.26539700	-2.80530400	-1.12628900
Zn	-0.68649900	-0.93652100	0.05869300
C	-2.39620500	4.79692800	-0.75698400
C	-3.57812500	5.30713600	-0.21260500
C	-4.43565000	4.50264600	0.55359500
C	-4.06435000	3.17914600	0.75652400
C	-2.86209100	2.66190200	0.23555800
C	-2.03005600	3.46233200	-0.53124600
N	-4.77212900	2.17242500	1.43432100
C	-4.11810000	0.95534500	1.35290600
C	-2.78172100	1.22715000	0.62790400
O	-2.24995500	0.31957000	-0.09839900
O	-4.52869200	-0.10981000	1.78708800
H	-1.75642800	5.43474500	-1.35839600
H	-3.84810700	6.34390600	-0.39076000
H	-5.35965800	4.90114500	0.95884700
H	-1.10638200	3.06946300	-0.93573600
C	-6.05883000	2.35563600	2.07396200
H	-6.80678900	2.69720000	1.35021700
H	-6.36296500	1.39046600	2.48057100
H	-5.98721600	3.08802100	2.88511800
O	1.77341200	-0.65478200	0.03530400
C	7.88936900	-0.52395300	-1.93108700
H	8.26636300	-1.34491600	-1.31152000
H	8.10528700	-0.78276700	-2.97570500
H	8.45887700	0.37853900	-1.68956300
C	0.90630200	5.81033700	0.29275300
H	1.13527800	6.48862500	-0.53466900
H	-0.14864800	5.94801000	0.55822600
H	1.50322400	6.11462700	1.16009400
C	-0.41500800	-0.69501400	2.16601300
H	0.26854000	-1.43813500	2.54143900
C	-1.01493400	0.35477400	2.48253300
O	3.55387200	0.02015100	1.56012600
O	2.41297000	-1.94796200	1.91899200
C	3.53851400	-1.95386900	2.85650400
C	4.61277800	-2.85115800	2.23761000
C	3.06138600	-2.51954700	4.18645200

H	4.96151600	-2.44987600	1.28092300
H	5.47230300	-2.95975700	2.90556800
H	4.18655400	-3.84278200	2.05895200
H	2.19366400	-1.97685500	4.56780900
H	2.78233100	-3.57030100	4.06174800
H	3.86162400	-2.46588900	4.93195400
C	3.94797900	-0.43623200	2.89126300
C	3.13384400	0.38871300	3.89098700
C	5.43863700	-0.17884700	3.06322000
H	2.05993300	0.21293000	3.77268600
H	3.41373000	0.15557000	4.92248100
H	3.32593600	1.45062100	3.71125700
H	6.01530300	-0.61877200	2.24686100
H	5.62680900	0.89913400	3.07331600
H	5.79352600	-0.59608000	4.01128100
B	2.58531000	-0.83910300	1.12862200
C	-1.78823800	1.49356800	2.47254100
H	-2.62399500	1.53389600	3.16636500
H	-1.26979900	2.44103700	2.34373900

Int-IIIC

N	-0.05590700	-0.44518500	-2.22580800
C	1.40466300	-0.15891300	-2.32656600
H	1.90148700	-1.12578700	-2.32688100
C	1.62338400	0.52470500	-3.69918100
H	2.05265400	-0.20352200	-4.39144600
H	2.34001600	1.34493800	-3.64080100
C	0.21427000	0.96178800	-4.17865100
H	-0.06955300	0.40529700	-5.07621000
H	0.16642900	2.02410500	-4.43458900
C	-0.72621300	0.63604900	-3.00283800
H	-1.71723100	0.29248700	-3.30699000
H	-0.85917400	1.48786500	-2.33774200
C	1.99860700	0.51984500	-1.05412100
C	3.52700300	0.44830400	-1.18637200
C	4.33134600	1.58970400	-1.19488500
C	4.15561000	-0.80269400	-1.30001900
C	5.71963500	1.48383000	-1.30277900
H	3.88287400	2.57136200	-1.10437300
C	5.53915800	-0.90416400	-1.39616900
H	3.56876600	-1.71643900	-1.28361100
C	6.35028500	0.24027400	-1.40061600
H	6.32095000	2.38922100	-1.30015800
H	5.99734300	-1.88729500	-1.46744500

C	1.54005900	1.92859300	-0.66986600
C	1.52234000	2.29484300	0.68468000
C	1.29819700	2.93784400	-1.60913000
C	1.28050900	3.60794600	1.07725800
H	1.72350700	1.55789800	1.44817100
C	1.05278100	4.25397800	-1.21226300
H	1.32139100	2.73163900	-2.66793300
C	1.04364400	4.61872400	0.13683800
H	1.28249300	3.85199800	2.13684100
H	0.86927400	5.00773500	-1.97325800
C	-1.66358000	-2.39129000	-2.52590800
C	-2.59116500	-2.66891200	-3.52776900
C	-3.04476200	-3.62517300	-0.94745000
C	-3.75121300	-3.40176200	-3.25919800
H	-2.38818300	-2.32720200	-4.54056600
C	-3.95439200	-3.89833300	-1.97367000
H	-4.46789000	-3.60948400	-4.04698000
H	-4.82624900	-4.50595600	-1.75771700
C	-3.22968500	-4.23572900	0.40707700
O	-1.06296500	-2.49810800	-0.21446600
F	-2.19445600	-5.05316800	0.74017300
F	-3.33398600	-3.33431600	1.40957300
F	-4.35091700	-5.00241100	0.46959600
C	-0.32202300	-1.79186700	-2.83991900
H	0.44396800	-2.45964600	-2.43598400
H	-0.17911400	-1.73748400	-3.92620400
C	-1.90108300	-2.82256400	-1.18918700
Zn	-0.74143800	-0.57492600	-0.18298900
C	-3.14438200	5.22824400	0.06211500
C	-4.50102600	5.25182800	0.39352800
C	-5.16251300	4.09480800	0.83396100
C	-4.41266700	2.92864000	0.93882000
C	-3.04456100	2.89896900	0.63649200
C	-2.40622000	4.03928200	0.18400000
N	-4.84968600	1.64132400	1.29859100
C	-3.82662600	0.72055400	1.19045100
C	-2.50635500	1.49833400	0.87222400
O	-1.80933900	0.99588300	-0.19796500
O	-3.95369000	-0.48683600	1.33525800
H	-2.65870600	6.13086600	-0.29686300
H	-5.06284100	6.17678600	0.29981500
H	-6.22110600	4.11362200	1.07126900
H	-1.35789100	4.00221600	-0.08645800
C	-6.22760200	1.28852700	1.57286200

H	-6.86926400	1.54021500	0.72090000
H	-6.26268100	0.21270900	1.74795000
H	-6.59238700	1.81619200	2.46033200
O	1.55120600	-0.41250600	-0.00660500
C	7.84888900	0.12615800	-1.52717700
H	8.23609200	-0.70676800	-0.93053300
H	8.14249300	-0.05839900	-2.56861200
H	8.34745700	1.04391400	-1.20114000
C	0.74813600	6.03140700	0.57204500
H	0.84148700	6.73448300	-0.26102000
H	-0.27506300	6.11045500	0.96164000
H	1.42393000	6.35207300	1.37226300
C	-0.51906500	-0.88575200	2.51219300
H	-0.07038700	-1.84905500	2.60622200
C	-1.01765200	0.21444600	2.40961500
O	3.30209200	-0.13057700	1.66873100
O	2.10906400	-2.09483200	1.58394500
C	3.19934600	-2.33298600	2.53270400
C	4.24811100	-3.16019800	1.78666400
C	2.64847600	-3.11447700	3.71771900
H	4.65241800	-2.61117900	0.93166300
H	5.07575200	-3.43776600	2.44589000
H	3.77893300	-4.07639400	1.41617800
H	1.81029800	-2.59871300	4.19098700
H	2.30305300	-4.09655200	3.38062100
H	3.42968200	-3.26785400	4.46933800
C	3.68274200	-0.87150000	2.86982400
C	2.92483900	-0.22893200	4.03314200
C	5.18684000	-0.72302500	3.05963800
H	1.84211100	-0.30113100	3.89313400
H	3.18882500	-0.69594600	4.98644600
H	3.19034000	0.83138700	4.08355000
H	5.73342600	-1.01629600	2.16098300
H	5.42624000	0.32193300	3.27916100
H	5.53117000	-1.33518600	3.89950900
B	2.32317800	-0.85250300	1.05040000
C	-1.64216100	1.51092700	2.18882000
H	-2.25318600	1.79995600	3.05187300
H	-0.86780500	2.27322900	2.05809800

Int-IVC

C	4.17802700	-2.19478800	-0.74647100
C	4.84711900	-1.09182500	-1.28059300
C	4.33135200	0.20659500	-1.15570000

C	3.12902600	0.35325800	-0.47566100
C	2.45496900	-0.74299900	0.07451000
C	2.96472000	-2.02235200	-0.06222400
N	2.40995200	1.53298000	-0.22180600
C	1.26811200	1.28757000	0.50993200
C	1.17973400	-0.26286800	0.72927200
O	0.08815400	-0.92035600	0.10860900
O	0.52264100	2.13938700	0.95936200
H	4.59629900	-3.18968700	-0.86139600
H	5.78610000	-1.23658600	-1.80661600
H	4.85384000	1.05846500	-1.57716300
H	2.43362700	-2.87660800	0.34752200
C	2.85906100	2.86267200	-0.58350000
H	2.95978700	2.95031500	-1.66999900
H	2.11157700	3.57159400	-0.22720700
H	3.82462900	3.08291700	-0.11597400
C	-1.17837900	0.00191800	3.41994700
H	-2.10501700	0.23976600	3.89320000
C	-0.12273500	-0.23453000	2.88273000
O	-2.09497800	-1.48813200	-0.53014300
O	-1.69660400	0.75019200	-0.16017600
C	-3.01647600	0.66858600	-0.77575900
C	-2.83644600	1.03422600	-2.25117500
C	-3.93305500	1.67078600	-0.08628300
H	-2.18155300	0.31946500	-2.75927000
H	-3.79581200	1.06200000	-2.77657300
H	-2.37783800	2.02538500	-2.31728600
H	-3.95053800	1.51914400	0.99492700
H	-3.58134000	2.68817900	-0.28361300
H	-4.95507100	1.58349400	-0.47014000
C	-3.39909800	-0.84023600	-0.55317200
C	-4.04515200	-1.10230400	0.81028800
C	-4.23488600	-1.45958000	-1.66596900
H	-3.44710900	-0.67097600	1.61877900
H	-5.05645700	-0.68809300	0.86164100
H	-4.10623200	-2.18289100	0.97117600
H	-3.72037100	-1.41451200	-2.62818900
H	-4.43710700	-2.51002700	-1.43417900
H	-5.19518600	-0.94117500	-1.75756200
B	-1.18852800	-0.52101800	-0.15493200
C	1.14618300	-0.57651700	2.24503400

(*S*)-3ba'

C	-2.82640300	-1.82512500	-0.05895900

C	-3.43966100	-0.59875900	-0.32333600
C	-2.70517900	0.59619100	-0.34836200
C	-1.34084900	0.51291500	-0.10146800
C	-0.71109000	-0.71325900	0.15514700
C	-1.44484700	-1.88733000	0.18043500
N	-0.40062500	1.55729300	-0.04402900
C	0.85092300	1.08821800	0.29217900
C	0.76862700	-0.47025400	0.34798500
O	1.83736600	1.77453500	0.50381000
H	-3.41981000	-2.73369600	-0.03887700
H	-4.50875500	-0.56274200	-0.51068500
H	-3.19006200	1.54554400	-0.54861200
H	-0.95942600	-2.83603800	0.39107100
C	-0.72383100	2.96300900	-0.18719900
H	-1.45523900	3.26968100	0.56822600
H	0.19835700	3.52845600	-0.05137400
H	-1.13322300	3.16267600	-1.18248300
C	4.22216500	-0.74448600	-0.70508100
H	5.28004000	-0.60783100	-0.66756400
C	3.02276900	-0.88240400	-0.73353300
C	1.57881300	-1.09274300	-0.81342700
H	1.18962100	-0.69907900	-1.75968300
H	1.36384000	-2.16841700	-0.80810200
O	1.31134900	-0.99505300	1.54734900
H	0.74069300	-0.71129900	2.28072900

Int-IID

N	0.21573600	-0.37872500	-2.02912200
C	1.65329800	0.07645300	-2.22687100
H	2.18929500	-0.80757700	-2.57593000
C	1.65603400	1.10960800	-3.37095400
H	2.53939700	0.98524700	-4.00104900
H	1.67168600	2.13098200	-2.98504200
C	0.34205500	0.83137000	-4.11502000
H	0.46990000	0.00890500	-4.82785300
H	-0.02173300	1.69960400	-4.67159600
C	-0.61054500	0.43133600	-2.98725200
H	-1.46373300	-0.16603400	-3.30955500
H	-1.00769800	1.30493300	-2.47149000
C	2.42398800	0.47197100	-0.93332700
C	3.90614000	0.35499300	-1.29966600
C	4.63096100	1.46481200	-1.74498600
C	4.53237000	-0.89726100	-1.31837000
C	5.95302600	1.32883700	-2.16949200

H	4.16469500	2.44376000	-1.75965500
C	5.85492900	-1.02750300	-1.73429700
H	3.98389000	-1.78068800	-1.00813100
C	6.59315000	0.08423800	-2.16220700
H	6.49490400	2.20745900	-2.51025200
H	6.32065800	-2.00980400	-1.72972200
C	2.08708100	1.81967500	-0.29181500
C	2.93424100	2.33462100	0.70446900
C	0.92591000	2.53968300	-0.58350500
C	2.61793400	3.50664000	1.38492700
H	3.83813100	1.80090600	0.96337900
C	0.61850700	3.72357700	0.08798700
H	0.21591300	2.19381900	-1.31689200
C	1.45332700	4.22835300	1.08774700
H	3.28954800	3.86749600	2.16031200
H	-0.30009900	4.23958900	-0.17193800
C	-1.17797500	-2.49055900	-2.28837500
C	-1.91259400	-2.90845300	-3.39517500
C	-2.87521000	-3.45874000	-0.83913500
C	-3.12546600	-3.59083600	-3.24852100
H	-1.52360900	-2.70673700	-4.39132900
C	-3.59267600	-3.87003500	-1.96611400
H	-3.68791500	-3.91056600	-4.11960500
H	-4.52343700	-4.41097400	-1.83260000
C	-3.36146500	-3.79304300	0.53165500
O	-0.98370400	-2.32128000	0.07357400
F	-2.49492800	-4.57800200	1.22033400
F	-3.56472700	-2.69420800	1.31878300
F	-4.54558900	-4.45571900	0.51285300
C	0.16545400	-1.83940700	-2.42747200
H	0.88622800	-2.34140400	-1.77683300
H	0.51948400	-1.93220300	-3.46154200
C	-1.65657100	-2.74080200	-0.97168700
Zn	-0.47850600	-0.40274200	0.01622100
C	-6.59948900	0.33229600	1.35628900
C	-7.11069600	1.63508100	1.32207200
C	-6.38459400	2.70145900	0.76791400
C	-5.12976000	2.41728900	0.25035300
C	-4.59919300	1.10895200	0.29027700
C	-5.33071700	0.05802400	0.83572100
N	-4.21949700	3.29881100	-0.35628400
C	-3.07736900	2.63549000	-0.74819000
C	-3.27981400	1.15974800	-0.33411600
O	-2.52352000	0.24195900	-0.65992800

O	-2.13341500	3.11047700	-1.36578600
H	-7.19104700	-0.46689100	1.79084400
H	-8.09677000	1.83192800	1.73201100
H	-6.79625200	3.70444200	0.74671400
H	-4.91290500	-0.94181200	0.86185300
C	-4.43716400	4.72024600	-0.53848200
H	-4.54159500	5.22098800	0.42969800
H	-3.56991000	5.12126700	-1.06381900
H	-5.33788500	4.89810400	-1.13429300
O	2.03284300	-0.58811700	-0.01032700
C	8.03599200	-0.05491900	-2.58107000
H	8.22398100	-1.02737600	-3.04794500
H	8.32347500	0.72860600	-3.28941300
H	8.70650000	0.02480700	-1.71530200
C	1.12518700	5.51158200	1.80912300
H	0.05593700	5.73801200	1.75074000
H	1.40896300	5.45857400	2.86562500
H	1.66610600	6.36046700	1.37076400
O	3.77931600	-0.38444900	1.69879200
O	1.99394600	-1.79945300	2.01394000
C	2.92481900	-2.07388700	3.10316400
C	3.69796400	-3.33650000	2.71622000
C	2.12317900	-2.30115100	4.37762400
H	4.27962400	-3.17949100	1.80227600
H	4.37927900	-3.64766700	3.51365400
H	2.98558200	-4.14662700	2.53432900
H	1.44826500	-1.46670900	4.57968300
H	1.52303300	-3.21083800	4.27720300
H	2.79246200	-2.42761900	5.23513100
C	3.81803600	-0.78062100	3.10541300
C	3.20585400	0.37297200	3.90441700
C	5.27079400	-1.00040400	3.50284800
H	2.16355400	0.54561300	3.61906500
H	3.24679400	0.17621700	4.97974700
H	3.76906800	1.28769300	3.69828200
H	5.76617800	-1.70907500	2.83589800
H	5.81228300	-0.05031800	3.45753800
H	5.33423800	-1.37944500	4.52818600
B	2.61012300	-0.88866100	1.19322700
C	-2.21586200	2.32392300	2.02896300
H	-1.55302200	3.11091300	1.68074700
H	-3.21765400	2.61162400	2.32811800
C	-1.77132300	1.05235900	2.18427800
H	-2.49173500	0.31533100	2.54580300

C	-0.46008400	0.53849900	1.82969600
H	0.31446200	1.30455700	1.77130900
H	-0.14214000	-0.29852800	2.45774000

TS-D

N	0.18220000	-0.25321200	-2.05148300
C	1.61433400	0.21977800	-2.22606500
H	2.15449500	-0.64009900	-2.62501200
C	1.60930500	1.31372700	-3.31227400
H	2.49382200	1.23071800	-3.94748100
H	1.61600500	2.31297900	-2.87216600
C	0.29743000	1.06439800	-4.07036700
H	0.43151800	0.27984100	-4.82367400
H	-0.07258600	1.95708200	-4.58223600
C	-0.65145400	0.60096400	-2.96429900
H	-1.50231700	0.01580400	-3.31477000
H	-1.05264800	1.44271100	-2.40034600
C	2.38596000	0.54994900	-0.91444800
C	3.86590200	0.43949700	-1.29176000
C	4.60008400	1.56509000	-1.67654600
C	4.47752800	-0.81679600	-1.38942800
C	5.91823100	1.43954800	-2.11755500
H	4.14505700	2.54836300	-1.63212800
C	5.79538600	-0.93708600	-1.82106800
H	3.92093000	-1.71131800	-1.12908900
C	6.54385200	0.19011400	-2.18794500
H	6.46763800	2.33063900	-2.41032800
H	6.24955400	-1.92315000	-1.87798000
C	2.05909200	1.86635600	-0.20685800
C	2.91663500	2.32734100	0.80826300
C	0.89602400	2.60108700	-0.44872700
C	2.60861700	3.46161200	1.55212200
H	3.82243100	1.77995700	1.02933200
C	0.59721400	3.74934500	0.28743700
H	0.17508800	2.29285900	-1.18990700
C	1.44194200	4.19973700	1.30396200
H	3.28803000	3.78029000	2.33906700
H	-0.32202400	4.27966400	0.06119500
C	-1.19323800	-2.37022900	-2.37798000
C	-1.95705500	-2.73848600	-3.48314800
C	-2.83744000	-3.43275400	-0.93257900
C	-3.15709000	-3.44306200	-3.33630200
H	-1.60131400	-2.47986800	-4.47846900
C	-3.58452600	-3.79361800	-2.05745700

H	-3.74195800	-3.72325200	-4.20619000
H	-4.50659300	-4.34948500	-1.92508900
C	-3.27804300	-3.83426900	0.43574100
O	-0.93022500	-2.32789500	-0.01405100
F	-2.39650600	-4.66426000	1.04847000
F	-3.43429200	-2.77560100	1.28544600
F	-4.47042000	-4.48070100	0.42632200
C	0.13846400	-1.69381300	-2.52034900
H	0.88023700	-2.21823200	-1.91266700
H	0.46718600	-1.73075300	-3.56611300
C	-1.63064100	-2.69840200	-1.06446600
Zn	-0.55703800	-0.39261300	-0.03507100
C	-6.50870600	0.15262200	1.36310000
C	-7.13980500	1.39688300	1.27465700
C	-6.47176200	2.52108500	0.76361800
C	-5.15672500	2.35234500	0.35355800
C	-4.50295400	1.10691700	0.45842200
C	-5.17707700	-0.00150500	0.95220000
N	-4.29183800	3.30457100	-0.21352700
C	-3.07966200	2.73756300	-0.55171500
C	-3.12582100	1.28872400	-0.05051400
O	-2.37981900	0.38948100	-0.53574700
O	-2.17385900	3.29153200	-1.16760800
H	-7.05407900	-0.70134800	1.75303000
H	-8.17088700	1.50057900	1.59957000
H	-6.97229500	3.48042900	0.68619500
H	-4.67959300	-0.96212400	1.01581000
C	-4.64869300	4.67954000	-0.49895400
H	-4.89834000	5.21253100	0.42435700
H	-3.78657600	5.15196900	-0.97095700
H	-5.50556100	4.72394700	-1.17958300
O	1.98458200	-0.54313200	-0.03250300
C	7.98152600	0.05801000	-2.62626200
H	8.13982200	-0.85872700	-3.20412000
H	8.29151100	0.90953300	-3.24005100
H	8.65470500	0.01509600	-1.76005000
C	1.12266600	5.44092000	2.09875900
H	0.07643300	5.73539800	1.97222700
H	1.31038300	5.28804100	3.16730800
H	1.74681700	6.28553400	1.77958500
O	3.79063700	-0.45297800	1.62245500
O	2.00050600	-1.86324900	1.92666800
C	2.97020000	-2.21085800	2.96111300
C	3.71042600	-3.45729300	2.47129800

C	2.21657400	-2.50317700	4.25129800
H	4.25806500	-3.25420700	1.54553800
H	4.41832900	-3.82093400	3.22199300
H	2.98100800	-4.24783300	2.27176500
H	1.56330800	-1.67382600	4.53070600
H	1.59944400	-3.39764900	4.12215500
H	2.91806100	-2.68911100	5.07135400
C	3.87975700	-0.93002300	3.00126000
C	3.31659900	0.18294700	3.88895300
C	5.34432100	-1.18862600	3.32553000
H	2.26636600	0.38531500	3.65699400
H	3.39689300	-0.07579600	4.94878500
H	3.88466600	1.10095700	3.71301900
H	5.80278800	-1.86183700	2.59824800
H	5.89605300	-0.24349000	3.31362800
H	5.44406800	-1.62832200	4.32332000
B	2.59988800	-0.91880400	1.13167400
C	-2.27107400	2.05444600	1.91779800
H	-1.61647500	2.84594400	1.56635100
H	-3.21601300	2.35822700	2.35129200
C	-1.71116400	0.83316200	2.26997800
H	-2.37936100	0.09260800	2.71247400
C	-0.41225300	0.40894100	1.93849500
H	0.33536000	1.18095900	1.76608500

Int-IIID

N	-0.13808900	-0.10175900	2.09625800
C	-1.58365200	0.34930600	2.25798200
H	-2.10058900	-0.51133300	2.68858500
C	-1.59486800	1.45405400	3.32631400
H	-2.52525900	1.42551800	3.89741100
H	-1.51093100	2.44898800	2.88403000
C	-0.35692100	1.12611500	4.17140000
H	-0.57723700	0.31417200	4.87386800
H	0.00576400	1.98067400	4.74881000
C	0.65354400	0.67399800	3.11751400
H	1.45514500	0.03851100	3.49961700
H	1.11667700	1.52542600	2.61653000
C	-2.36857500	0.61752200	0.94368000
C	-3.84571700	0.53760800	1.33896200
C	-4.58204100	1.68972000	1.62850800
C	-4.45409300	-0.70767100	1.54147200
C	-5.89910200	1.59829800	2.08144600
H	-4.12878400	2.66655900	1.50053400

C	-5.77026900	-0.79492600	1.98538800
H	-3.89658300	-1.61901500	1.35028700
C	-6.52072700	0.35747400	2.25854600
H	-6.45079000	2.50929000	2.29899600
H	-6.22226100	-1.77373600	2.12503300
C	-2.03812300	1.88873700	0.16365500
C	-2.86032100	2.25440500	-0.91872400
C	-0.89003000	2.64948400	0.38901200
C	-2.52586600	3.32105800	-1.74538500
H	-3.75542400	1.68283800	-1.12437700
C	-0.55498300	3.72186100	-0.44164600
H	-0.20351700	2.41128100	1.18596600
C	-1.36193900	4.07466900	-1.52439700
H	-3.17550500	3.56880100	-2.58158900
H	0.37603600	4.24823900	-0.25757600
C	1.20805500	-2.29471300	2.24677600
C	1.81066900	-2.90363900	3.34718400
C	2.75035000	-3.49086800	0.79243800
C	2.89090000	-3.77780400	3.19821300
H	1.40321000	-2.71337300	4.33777900
C	3.32629600	-4.09502100	1.91457100
H	3.35171500	-4.23981900	4.06488900
H	4.11566300	-4.82483100	1.77353900
C	3.13830300	-3.94877200	-0.57885100
O	1.25761200	-1.85526200	-0.10502400
F	2.06917100	-4.38998000	-1.28851500
F	3.72132000	-2.98965800	-1.35030400
F	4.02435000	-4.97528200	-0.54049600
C	-0.10700900	-1.57878600	2.40336900
H	-0.83455000	-2.02354700	1.72038000
H	-0.47340200	-1.72574200	3.42705200
C	1.72834200	-2.51514000	0.93933700
Zn	0.83879100	0.02062300	0.22366400
C	5.74398800	-0.67311800	-0.39199200
C	6.79416500	0.23072300	-0.22375100
C	6.55548200	1.61200700	-0.14040700
C	5.23776900	2.04148600	-0.24261900
C	4.17487800	1.14781300	-0.43557800
C	4.42087700	-0.21279300	-0.49491100
N	4.74391400	3.35626900	-0.14457300
C	3.37020700	3.38204200	-0.22053800
C	2.86990500	1.92797300	-0.49968100
O	1.93242000	1.55539300	0.44269600
O	2.68137100	4.38975700	-0.11126700

H	5.94083400	-1.73915000	-0.44602600
H	7.81454300	-0.13399700	-0.14684100
H	7.37167900	2.31174200	0.00699300
H	3.60944400	-0.91910900	-0.61157500
C	5.56317300	4.52346100	0.10975300
H	6.28993800	4.66638400	-0.69681800
H	4.89972200	5.38730900	0.16080500
H	6.10161300	4.41957800	1.05838500
O	-1.97414900	-0.51247800	0.11409600
C	-7.95707900	0.25866400	2.70992500
H	-8.11051000	-0.60430700	3.36656900
H	-8.26965900	1.15962300	3.24702800
H	-8.63158900	0.13676300	1.85230100
C	-0.99963800	5.23122500	-2.42249000
H	0.06154300	5.48308500	-2.33231000
H	-1.21273500	5.00309800	-3.47256800
H	-1.57603900	6.12902100	-2.16372100
O	-3.83093000	-0.60021000	-1.48257300
O	-1.97641500	-1.92855200	-1.77609200
C	-2.96722000	-2.39830300	-2.73879700
C	-3.60856300	-3.65046100	-2.13611400
C	-2.25597000	-2.73388700	-4.04265400
H	-4.12658200	-3.41853500	-1.20011400
H	-4.32510700	-4.10403100	-2.82721200
H	-2.82422100	-4.38231500	-1.92147700
H	-1.67093500	-1.88851800	-4.41113400
H	-1.57739600	-3.57786300	-3.88494100
H	-2.98120800	-3.01932500	-4.81187700
C	-3.95429800	-1.17752800	-2.81831000
C	-3.50641900	-0.10052500	-3.80982500
C	-5.41396600	-1.54387900	-3.04974600
H	-2.46156100	0.18146400	-3.64966500
H	-3.62155900	-0.44001700	-4.84331300
H	-4.12289700	0.79212800	-3.66911700
H	-5.79533000	-2.19055800	-2.25686200
H	-6.02223300	-0.63429100	-3.07240100
H	-5.53286900	-2.05677400	-4.00984000
B	-2.59918900	-0.97322700	-1.00857000
C	2.27385900	1.95833600	-1.95553500
H	1.52810700	2.75786300	-1.97664600
H	3.07578200	2.20442400	-2.66206800
C	1.64172300	0.65398500	-2.31349800
H	2.30942400	-0.18416400	-2.50802300
C	0.31212500	0.44860100	-2.34495200

H	-0.38469700	1.26879300	-2.18494200
H	-0.10961000	-0.52299400	-2.58233000

Int-IVD

C	2.52818000	0.98537900	2.67511800
C	2.67967600	2.25263100	2.11017000
C	2.37899800	2.48969000	0.76044400
C	1.93100600	1.41379200	0.00606500
C	1.79401000	0.12995400	0.55560300
C	2.08033700	-0.09071300	1.89228300
N	1.52632000	1.40929800	-1.34139000
C	1.03756800	0.17898600	-1.70640900
C	1.30939800	-0.80300900	-0.52895600
O	0.14267100	-1.54792600	-0.19015200
O	0.51953600	-0.11128800	-2.77384100
H	2.75552200	0.83001400	3.72508000
H	3.02939300	3.07706400	2.72452300
H	2.48275300	3.48037800	0.33096600
H	1.94815200	-1.07581900	2.32825700
C	1.39780600	2.59684900	-2.16186000
H	2.36873700	3.08612600	-2.28354600
H	1.02065200	2.28551200	-3.13623600
H	0.69407000	3.30286500	-1.70668300
O	-2.20975900	-1.58093000	0.19431700
O	-1.17379400	0.47210200	0.01609400
C	-2.60748000	0.73752400	-0.04654100
C	-2.95323700	0.92837200	-1.52515900
C	-2.89928800	2.00722700	0.74084200
H	-2.74578000	0.02163600	-2.10128500
H	-4.00565900	1.19562200	-1.65805600
H	-2.33606000	1.73559700	-1.93050900
H	-2.51483600	1.94464200	1.76092700
H	-2.42539200	2.86177600	0.24776700
H	-3.97756500	2.19323900	0.78222000
C	-3.20823800	-0.58008400	0.56803800
C	-3.25952500	-0.55711800	2.09731800
C	-4.55389500	-0.99748800	-0.00880300
H	-2.29767900	-0.25086400	2.52047900
H	-4.03310700	0.12579300	2.46073700
H	-3.48901300	-1.56326200	2.46037100
H	-4.49324800	-1.16791800	-1.08573200
H	-4.88865500	-1.92421400	0.46752700
H	-5.30719900	-0.22599300	0.18220100
B	-1.03866900	-0.89469900	0.00385500

C	2.37066200	-1.82055700	-1.00578100
H	1.93577800	-2.34591200	-1.86289900
H	3.23821200	-1.25368400	-1.36636700
C	2.79080700	-2.79227900	0.05935600
H	3.43985300	-2.39974200	0.84052200
C	2.41277200	-4.07019300	0.09760600
H	1.76439300	-4.49425300	-0.66613300
H	2.73921400	-4.73965100	0.88896700

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C	1.38514500	-2.78233000	0.18280600
C	2.59056700	-2.13317800	-0.08799900
C	2.65238500	-0.73749200	-0.21249000
C	1.46755500	-0.02882000	-0.06175200
C	0.24377000	-0.66671200	0.19154600
C	0.19870200	-2.04520000	0.32526800
N	1.28196900	1.36566600	-0.11165600
C	-0.02646600	1.70594700	0.13538100
C	-0.84010100	0.39090400	0.27259700
O	-0.47803700	2.83917300	0.19573700
H	1.36331100	-3.86281400	0.28505900
H	3.50162200	-2.71365600	-0.19950200
H	3.59319300	-0.23586000	-0.41241000
H	-0.73693500	-2.55061900	0.54411600
C	2.34162700	2.33117600	-0.32373700
H	2.81052500	2.17761700	-1.30101900
H	1.89464100	3.32486800	-0.28538500
H	3.10490500	2.24311700	0.45660900
C	-1.84831600	0.33920200	-0.90955000
H	-2.43578500	1.26217400	-0.85652700
H	-1.28925000	0.34253900	-1.85179600
C	-2.73930200	-0.86610600	-0.81832700
H	-2.32854800	-1.80664200	-1.18108700
C	-3.95727400	-0.84901300	-0.26674900
H	-4.40479000	0.07477700	0.09475000
H	-4.55924700	-1.74941500	-0.18229400
O	-1.52712700	0.43503200	1.51227900
H	-2.25587000	-0.20964700	1.44498500

Int-IIE

N	0.11413600	-1.10031300	-1.84984400
C	1.60741400	-1.24198000	-1.96904700
H	1.84998700	-2.23254300	-1.58977000
C	1.89888500	-1.14788700	-3.48024400

H	1.93303000	-2.15738100	-3.89761700
H	2.87428900	-0.70411500	-3.67992300
C	0.71859300	-0.34714700	-4.08382600
H	0.23716400	-0.91269400	-4.88636000
H	1.04470200	0.60582700	-4.50594100
C	-0.24778200	-0.10069800	-2.90667200
H	-1.30013400	-0.22775400	-3.16118400
H	-0.12362300	0.89439500	-2.49051800
C	2.40722400	-0.26719300	-1.04696400
C	3.89301500	-0.67091000	-1.06011800
C	4.93475100	0.23524700	-1.27397000
C	4.23588800	-1.99036300	-0.71895600
C	6.26784100	-0.16709700	-1.17966900
H	4.71670300	1.27352900	-1.48653100
C	5.56606100	-2.38703100	-0.61911200
H	3.46176100	-2.71505200	-0.48961300
C	6.61120400	-1.48304500	-0.85620200
H	7.05406800	0.56491300	-1.34599500
H	5.79605000	-3.41371600	-0.34563100
C	2.16020900	1.21340900	-1.34780400
C	1.45873500	2.03031000	-0.45285500
C	2.59390700	1.79713500	-2.54784300
C	1.16429100	3.35490900	-0.76242700
H	1.09832700	1.62964300	0.48230800
C	2.29439100	3.12424500	-2.85584900
H	3.17362300	1.22539300	-3.26107800
C	1.56133400	3.92658800	-1.97551300
H	0.58538300	3.94365700	-0.05779900
H	2.63524500	3.53691900	-3.80200300
C	-1.96381100	-2.57183800	-1.99873000
C	-2.86404000	-2.72091300	-3.04980400
C	-3.74215100	-3.12369200	-0.43015100
C	-4.20660000	-3.03812400	-2.81296500
H	-2.50532400	-2.61261100	-4.07137900
C	-4.62594200	-3.26971600	-1.50521100
H	-4.90247900	-3.14462100	-3.63854100
H	-5.64840700	-3.57408800	-1.30964800
C	-4.16678300	-3.51638100	0.94915400
O	-1.57138000	-2.46267500	0.34062200
F	-3.46704200	-4.58620900	1.40957000
F	-4.00105000	-2.54283400	1.88811900
F	-5.47754800	-3.86207100	1.00380000
C	-0.48599600	-2.43857200	-2.22109500
H	0.02297600	-3.17674700	-1.59493600

H	-0.24964400	-2.66230300	-3.26637100
C	-2.40200100	-2.70428600	-0.65016300
Zn	-0.59848000	-0.72813100	0.15069100
C	-5.57806900	0.34176100	1.71364900
C	-6.21874400	1.57047000	1.91731200
C	-5.72527700	2.77126300	1.37745200
C	-4.56458800	2.69966300	0.62164600
C	-3.91502600	1.46481900	0.41315000
C	-4.40944400	0.28421100	0.95071600
N	-3.86387100	3.73768400	-0.01657200
C	-2.74303600	3.25459900	-0.66094800
C	-2.73872000	1.71897100	-0.39650100
O	-1.92567400	0.94103600	-0.88348800
O	-1.95501000	3.89033800	-1.33842800
H	-5.98268700	-0.56590900	2.14821800
H	-7.12666900	1.60421800	2.51219100
H	-6.23759000	3.71080500	1.55160200
H	-3.88397100	-0.64561500	0.78571700
C	-4.25007600	5.13493900	0.00506600
H	-4.24511200	5.51974300	1.03012000
H	-3.52360500	5.68563700	-0.59331100
H	-5.24884300	5.26483700	-0.42352300
O	1.88680500	-0.62394000	0.25957900
C	8.05177000	-1.92183200	-0.77165500
H	8.72218200	-1.06640700	-0.64395200
H	8.20987900	-2.61135000	0.06457000
H	8.35723500	-2.44728600	-1.68580900
C	1.19346000	5.34946100	-2.31180900
H	1.49920000	5.61326200	-3.32888400
H	0.11017900	5.49192500	-2.22733700
H	1.66906500	6.05853300	-1.62271300
C	-0.61697200	0.25513300	1.89361800
H	-0.20511300	-0.30519900	2.73385700
C	-1.01640400	1.47342100	2.07322600
O	3.45961600	0.68585000	1.57740300
O	2.26091500	-1.01128000	2.57309700
C	3.25424700	-0.58206400	3.55560000
C	4.39537800	-1.60084200	3.49199700
C	2.60634900	-0.57824000	4.93294000
H	4.86043300	-1.61168000	2.50093400
H	5.16538800	-1.38522500	4.23866700
H	3.99169300	-2.59820800	3.69072000
H	1.69902700	0.02948300	4.94659000
H	2.33974600	-1.60069300	5.21817200

H	3.30231500	-0.18662600	5.68225300
C	3.66568700	0.83575900	3.01496500
C	2.72609000	1.95414300	3.47429600
C	5.12010700	1.21761700	3.25401000
H	1.67849300	1.69011100	3.29953100
H	2.86097000	2.17742300	4.53688800
H	2.94835200	2.85845400	2.89969300
H	5.80185600	0.50884200	2.77903500
H	5.31257900	2.21042500	2.83543600
H	5.33779000	1.25245700	4.32667100
B	2.53622700	-0.31113700	1.42746900
C	-1.43394300	2.72557900	2.16241200
H	-2.45658700	2.96688100	2.43992400
H	-0.74848200	3.56112200	2.03578000

Int-IIIE

N	0.13555600	-1.07124600	-1.87174600
C	1.62590500	-1.05557200	-2.05982000
H	1.97399800	-2.05715400	-1.81592600
C	1.83147400	-0.75498400	-3.55773000
H	1.90918300	-1.70148700	-4.09866500
H	2.76344500	-0.22219500	-3.74589500
C	0.56861000	0.02417900	-4.00203000
H	0.10553300	-0.45419700	-4.86959600
H	0.80320600	1.05329500	-4.28206400
C	-0.37257200	0.00914500	-2.77743900
H	-1.41302300	-0.20414500	-3.02027600
H	-0.35137900	0.95390200	-2.24121800
C	2.38096700	-0.12475700	-1.05851000
C	3.88853500	-0.42927700	-1.13715600
C	4.86825900	0.55363700	-1.29781700
C	4.31895300	-1.74877300	-0.91615400
C	6.22492300	0.22719700	-1.26972300
H	4.58433000	1.59094000	-1.41528800
C	5.67247800	-2.06999900	-0.88088200
H	3.59585600	-2.53615200	-0.73053500
C	6.65499800	-1.08721600	-1.06603100
H	6.96113500	1.01753900	-1.39234100
H	5.97045100	-3.09959800	-0.69956500
C	2.03289200	1.35814900	-1.20235400
C	1.30563800	2.03030700	-0.21548700
C	2.41012200	2.09557100	-2.33616200
C	0.94402900	3.36569500	-0.36388300
H	0.97981500	1.51643700	0.67555100
C	2.04184800	3.43175800	-2.48471200

H	3.00704000	1.64111900	-3.11608000
C	1.28974900	4.09109700	-1.50639600
H	0.35740500	3.83447700	0.42014300
H	2.34582600	3.96668500	-3.38094300
C	-1.80604400	-2.67832800	-2.11889200
C	-2.75126200	-2.75468500	-3.13684400
C	-3.53125000	-3.25879500	-0.50657100
C	-4.08603900	-3.07576600	-2.86228700
H	-2.43858600	-2.56935600	-4.16262100
C	-4.46379600	-3.33221200	-1.54608000
H	-4.81582700	-3.13333500	-3.66326100
H	-5.49284400	-3.58767800	-1.31648500
C	-3.94087500	-3.52543800	0.90269500
O	-1.28831900	-2.79314500	0.19352600
F	-3.25843400	-4.55000000	1.47052200
F	-3.74584400	-2.45184000	1.72993900
F	-5.25755400	-3.83511100	1.00978700
C	-0.35559100	-2.41309700	-2.37938500
H	0.24275400	-3.16608500	-1.85953200
H	-0.14630400	-2.48971400	-3.45115600
C	-2.17877900	-2.91542400	-0.76623900
Zn	-0.51682300	-0.94189700	0.16965600
C	-6.04416100	1.11781700	2.08035900
C	-6.30011400	2.49443900	2.05414100
C	-5.52926500	3.38005600	1.28464400
C	-4.49237400	2.83890100	0.53912500
C	-4.22412300	1.45301300	0.56028900
C	-4.99461700	0.58387100	1.32744200
N	-3.58567300	3.50821500	-0.30003900
C	-2.69772200	2.62194400	-0.87248000
C	-3.07466800	1.22169300	-0.30502400
O	-2.51458100	0.17954400	-0.61946300
O	-1.83467000	2.87854300	-1.69333600
H	-6.66274400	0.46658100	2.68897800
H	-7.11835700	2.89456800	2.64545800
H	-5.74186400	4.44324500	1.27932000
H	-4.76922800	-0.47622700	1.34162300
C	-3.58161500	4.93668900	-0.54548100
H	-3.39713300	5.48671100	0.38328500
H	-2.78113600	5.14591000	-1.25580600
H	-4.53802300	5.25849400	-0.96981800
O	1.91663600	-0.63492700	0.22090100
C	8.12086300	-1.44214700	-1.05227600
H	8.43327100	-1.86107900	-2.01769000

H	8.74238700	-0.56249300	-0.85867500
H	8.34129600	-2.19481700	-0.28771800
C	0.82120100	5.51099500	-1.69459200
H	1.42701500	6.04305600	-2.43485700
H	-0.21914300	5.52156300	-2.04497500
H	0.85262200	6.07243900	-0.75454900
C	-0.87217800	-0.12032700	1.98587000
H	0.00270100	-0.37364000	2.59244800
C	-1.16300600	1.28223700	2.03054800
O	3.48062400	0.61709500	1.60819300
O	2.28900100	-1.13629100	2.50910900
C	3.26967100	-0.74530900	3.52176600
C	4.42366900	-1.74550800	3.41670200
C	2.60939300	-0.81878300	4.89105700
H	4.89789200	-1.69933400	2.43095400
H	5.18418700	-1.55837400	4.18050700
H	4.03111500	-2.75654900	3.56063000
H	1.69491800	-0.22289600	4.92743200
H	2.35211000	-1.85737100	5.12103000
H	3.29415400	-0.45828700	5.66579800
C	3.66689000	0.70181700	3.05441900
C	2.70715500	1.78531100	3.55403900
C	5.11241400	1.09207600	3.32978500
H	1.66295700	1.52011000	3.35980800
H	2.82859900	1.96082300	4.62704400
H	2.92174800	2.71777000	3.02352800
H	5.80990700	0.41614300	2.83064900
H	5.29554800	2.10616200	2.96118000
H	5.31625900	1.07878300	4.40552400
B	2.56986900	-0.37992800	1.40055300
C	-1.43455400	2.46889700	2.02054800
H	-1.72501100	-0.70562600	2.34860400
H	-1.68114100	3.50423900	2.07245100

TS-E

N	0.05422300	-0.69188100	-1.91230600
C	1.53214900	-0.60594800	-2.15360900
H	1.90961300	-1.62470600	-2.09320200
C	1.67395400	-0.06620400	-3.59323100
H	1.78824800	-0.91197200	-4.27609300
H	2.57075200	0.54165100	-3.71519700
C	0.35836900	0.69545300	-3.88807000
H	-0.12250200	0.29939000	-4.78684100
H	0.52963000	1.76173700	-4.05394300

C	-0.52009200	0.48645500	-2.63758300
H	-1.56702800	0.28059200	-2.86021600
H	-0.48778600	1.34775400	-1.97441000
C	2.32610000	0.14741300	-1.04067100
C	3.82828800	-0.06266300	-1.31350400
C	4.74528800	0.98187100	-1.44395800
C	4.32480800	-1.37704200	-1.34614600
C	6.10670900	0.72388600	-1.61548100
H	4.41232900	2.00982600	-1.38320000
C	5.68302600	-1.63064600	-1.50857700
H	3.65344300	-2.21823800	-1.20599100
C	6.60308500	-0.58216200	-1.65185600
H	6.79557700	1.55993100	-1.70598700
H	6.03525700	-2.65907500	-1.51813400
C	1.93643300	1.61342400	-0.83297900
C	1.42745500	2.06517300	0.38951100
C	2.10532600	2.57003600	-1.84713000
C	1.07551900	3.39781300	0.58444400
H	1.28092400	1.37596500	1.20637800
C	1.75261900	3.90308200	-1.65003900
H	2.53210900	2.29151800	-2.80135800
C	1.21811500	4.34200700	-0.43382500
H	0.65936300	3.69584300	1.54290700
H	1.89396300	4.61209400	-2.46194200
C	-1.86121500	-2.31342100	-2.32472700
C	-2.80342700	-2.31245600	-3.34932600
C	-3.55777100	-3.16770500	-0.80532800
C	-4.12130100	-2.72606500	-3.12340000
H	-2.49911300	-1.99481900	-4.34464600
C	-4.48541300	-3.16211000	-1.85144400
H	-4.84714400	-2.72091600	-3.92992600
H	-5.49918300	-3.49810700	-1.66147300
C	-3.94724600	-3.64624100	0.55344700
O	-1.34933400	-2.67095400	-0.02962400
F	-3.21919900	-4.71388500	0.96586500
F	-3.78896800	-2.69673800	1.52422300
F	-5.24913800	-4.02280500	0.61573600
C	-0.41985300	-1.97610500	-2.56296200
H	0.20237400	-2.76857200	-2.13809500
H	-0.22167600	-1.92727500	-3.63896700
C	-2.22635300	-2.72283800	-1.01140300
Zn	-0.62683200	-0.82182100	0.10845100
C	-6.40271000	0.71914600	1.70728400
C	-6.80126600	2.05959600	1.67059800

C	-5.95505900	3.06465200	1.17702400
C	-4.69997900	2.67944400	0.72446100
C	-4.28382700	1.33316400	0.77125200
C	-5.13065500	0.34509900	1.25539200
N	-3.69146000	3.48134500	0.16600800
C	-2.60886900	2.71673200	-0.23634000
C	-2.91285600	1.27444500	0.22189600
O	-2.35009000	0.26660700	-0.27442000
O	-1.64932900	3.11450100	-0.87789100
H	-7.08364500	-0.03494200	2.08946500
H	-7.78980700	2.33440000	2.02669000
H	-6.27769600	4.09977800	1.14506300
H	-4.80308900	-0.68773700	1.28496000
C	-3.81341300	4.90195800	-0.09075800
H	-3.93205400	5.45622000	0.84603700
H	-2.90018100	5.22529700	-0.59161700
H	-4.67302900	5.10640000	-0.73817500
O	1.98218800	-0.62834400	0.13763900
C	8.07249300	-0.86130700	-1.84722400
H	8.28163900	-1.16720600	-2.88048500
H	8.67819700	0.02527200	-1.63636900
H	8.41320200	-1.67349900	-1.19584800
C	0.76031400	5.76491200	-0.24610100
H	1.28101300	6.45060700	-0.92220200
H	-0.31426300	5.84389600	-0.45573300
H	0.91811100	6.10687000	0.78225900
C	-0.54503500	-0.41125400	2.20673100
H	0.52870700	-0.37286200	2.37369900
C	-1.25951000	0.76139300	2.35741700
O	3.77335500	0.21577900	1.56167800
O	2.56250300	-1.63530200	2.20234100
C	3.68407800	-1.53825700	3.13768800
C	4.73004400	-2.55138500	2.66601600
C	3.18437600	-1.88407200	4.53317900
H	5.09015800	-2.30905300	1.66096900
H	5.58650100	-2.58516200	3.34580600
H	4.27333700	-3.54507500	2.63612500
H	2.33156500	-1.26476300	4.81922900
H	2.87269500	-2.93268500	4.56385000
H	3.98190500	-1.74448600	5.27046600
C	4.14507200	-0.04684000	2.94855800
C	3.35711600	0.94494600	3.80809500
C	5.64271900	0.18772000	3.09342600
H	2.27803100	0.78187400	3.72206500

H	3.63502300	0.86661500	4.86323400
H	3.57504000	1.96070600	3.46542200
H	6.20934200	-0.39215100	2.36189300
H	5.86449100	1.24766600	2.93492300
H	5.98026600	-0.08430700	4.09887700
B	2.77942500	-0.66979700	1.25168100
C	-2.01560200	1.73975800	2.20429700
H	-1.00034800	-1.30672200	2.63517600
H	-2.50639600	2.57317300	2.66625500

Int-IVE

N	0.06441700	-0.63553800	-1.96828700
C	1.54294100	-0.54291100	-2.17657800
H	1.92085300	-1.56221300	-2.13436300
C	1.71062600	0.03034800	-3.60118700
H	1.83914900	-0.80089900	-4.29925600
H	2.60828600	0.64216700	-3.69387800
C	0.39876300	0.79492800	-3.90587800
H	-0.06071400	0.41841700	-4.82401100
H	0.56962100	1.86530500	-4.04343500
C	-0.50571500	0.55280400	-2.68101900
H	-1.54535800	0.34123800	-2.92973200
H	-0.49939600	1.39812600	-1.99555600
C	2.31595100	0.18163700	-1.03017100
C	3.82079600	-0.02068600	-1.29809300
C	4.73537300	1.02903900	-1.40879800
C	4.31965200	-1.33229000	-1.36332900
C	6.09574800	0.77817700	-1.59352900
H	4.39988600	2.05446700	-1.32327400
C	5.67815400	-1.57916600	-1.53926500
H	3.65115600	-2.17841900	-1.23967800
C	6.59472400	-0.52630800	-1.66456500
H	6.78232100	1.61773800	-1.66807200
H	6.03230500	-2.60627000	-1.57427700
C	1.92466700	1.64067800	-0.78402200
C	1.42719500	2.06116700	0.45469500
C	2.08975600	2.62357000	-1.77315500
C	1.08257900	3.38933400	0.68793400
H	1.28415500	1.34980100	1.25437500
C	1.74322500	3.95193600	-1.53776000
H	2.50913700	2.36948700	-2.73727500
C	1.21950300	4.35966900	-0.30624400
H	0.67763500	3.66544400	1.65805900
H	1.88018200	4.68204100	-2.33147700

C	-1.84438000	-2.26366700	-2.37998100
C	-2.78860700	-2.24827500	-3.40375500
C	-3.53944500	-3.14233600	-0.87261100
C	-4.10516800	-2.66543500	-3.18295900
H	-2.48509300	-1.91633900	-4.39444100
C	-4.46713300	-3.12384600	-1.91839000
H	-4.83177600	-2.64866400	-3.98856900
H	-5.47938900	-3.46655900	-1.73347300
C	-3.92883700	-3.65345500	0.47540600
O	-1.33564800	-2.63507100	-0.07976900
F	-3.20589100	-4.73837500	0.85189500
F	-3.75989900	-2.73517800	1.47137100
F	-5.23237300	-4.02480800	0.52917400
C	-0.40419400	-1.91687000	-2.62561100
H	0.22457600	-2.70882400	-2.21013800
H	-0.21325000	-1.85918700	-3.70279100
C	-2.21114800	-2.68840300	-1.07152500
Zn	-0.74342700	-0.74959400	-0.02124300
C	-6.38406500	0.67600800	1.71448100
C	-6.84341900	1.98990600	1.60345600
C	-6.00508400	3.01744300	1.14327200
C	-4.69960600	2.67656900	0.80873200
C	-4.22011700	1.36519900	0.94011800
C	-5.05470500	0.35748500	1.38943900
N	-3.69288200	3.50658500	0.27814900
C	-2.56947400	2.77212600	-0.05424500
C	-2.72751300	1.34617000	0.59052000
O	-2.31640300	0.33500800	-0.22014000
O	-1.63838500	3.17857900	-0.72956600
H	-7.05627300	-0.10374200	2.06027900
H	-7.86983100	2.22533800	1.86707900
H	-6.36972700	4.03411800	1.04594000
H	-4.68671500	-0.65824700	1.47956500
C	-3.90434100	4.88019200	-0.13210300
H	-4.08259300	5.52344800	0.73999400
H	-3.00279500	5.21108400	-0.65520000
H	-4.76552300	4.95217500	-0.81101900
O	1.95815400	-0.62368100	0.12754000
C	8.06290400	-0.79394200	-1.88425100
H	8.28488500	-0.90856100	-2.95609100
H	8.67901800	0.03190700	-1.50777600
H	8.37889000	-1.71870700	-1.38501900
C	0.76245900	5.77692300	-0.07900600
H	1.28781900	6.48211600	-0.73085100

H	-0.31079200	5.86197400	-0.29248600
H	0.91431200	6.08770800	0.96005800
C	-0.50792900	-0.63576500	2.61230500
H	0.57233300	-0.66532100	2.55191900
C	-1.22949000	0.42807000	2.32983500
O	3.76467800	0.17477800	1.56118500
O	2.55359800	-1.68873900	2.16036500
C	3.68476900	-1.62188200	3.08890300
C	4.72110900	-2.62625100	2.57933000
C	3.19547800	-2.00474500	4.47832900
H	5.07436100	-2.35694400	1.57876600
H	5.58281800	-2.68394800	3.25068800
H	4.25876200	-3.61623900	2.52452500
H	2.34923900	-1.38946800	4.79133500
H	2.87866800	-3.05220600	4.48200000
H	4.00084700	-1.89041400	5.21137100
C	4.15023500	-0.12788100	2.93615200
C	3.37740500	0.84376300	3.83144000
C	5.65072900	0.09521800	3.07063700
H	2.29647600	0.68958800	3.75395200
H	3.66717400	0.73474900	4.88062500
H	3.59716200	1.86730700	3.51429900
H	6.20495700	-0.46184900	2.31231500
H	5.87592200	1.15884600	2.94554600
H	5.99954000	-0.21290400	4.06166600
B	2.76609300	-0.69841500	1.23332500
C	-2.02900200	1.39044200	1.97136300
H	-0.97979100	-1.52605000	3.03023000
H	-2.28852900	2.20007800	2.65038400

Int-VE

C	-2.59724300	-1.64366300	2.47405400
C	-2.77166600	-2.70103400	1.57882500
C	-2.49048500	-2.55628800	0.21190400
C	-2.02827000	-1.31963100	-0.21827400
C	-1.85058400	-0.25203900	0.67167300
C	-2.13673000	-0.39908600	2.01691000
N	-1.65957500	-0.93358400	-1.52062700
C	-1.15349900	0.34248700	-1.53785600
C	-1.35697900	0.94941100	-0.10565000
O	-0.15041000	1.51773200	0.38183300
O	-0.64521300	0.91260800	-2.48862800
H	-2.82059600	-1.78373800	3.52697600
H	-3.13181800	-3.65867900	1.94297100

H	-2.62423300	-3.38405200	-0.47613200
H	-1.99875400	0.43214100	2.70220800
C	-1.55728700	-1.84507400	-2.64302400
H	-2.52860000	-2.30165900	-2.85397700
H	-1.22814000	-1.26934300	-3.50815200
H	-0.82678600	-2.63397200	-2.43044500
C	-1.95644800	4.55100200	0.36771000
H	-1.64579400	5.25599800	-0.40123800
C	-2.17649800	3.29384000	0.09231000
O	1.07950200	-0.51521700	-0.07793500
O	2.21604600	1.36571300	0.62168200
C	3.18683200	0.27117200	0.62439700
C	3.31883300	-0.19843500	2.07464700
C	4.51682300	0.80143200	0.10725600
H	2.36824700	-0.58800300	2.45224700
H	4.07908900	-0.97889100	2.17348400
H	3.61321500	0.65098000	2.69800800
H	4.40581500	1.28047800	-0.86773600
H	4.91847000	1.53901000	0.80892800
H	5.24352000	-0.01280300	0.01718100
C	2.49469900	-0.79237000	-0.30587100
C	2.75231000	-0.55345000	-1.79538000
C	2.76764100	-2.24440300	0.06026600
H	2.55098500	0.48596300	-2.07113000
H	3.78432000	-0.79527700	-2.06575500
H	2.08196200	-1.19328900	-2.37673000
H	2.44110900	-2.47059000	1.07733500
H	2.22852300	-2.90345600	-0.62743400
H	3.83655100	-2.46660400	-0.02350400
B	1.00864900	0.79923700	0.31090400
C	-2.41083300	2.03588500	-0.17553100
H	-2.07057200	4.94242600	1.37700200
H	-3.40581700	1.70704400	-0.47004000

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C	-2.03231600	-2.51153600	-0.07907800
C	-3.05381400	-1.58981800	0.15985100
C	-2.79171500	-0.21461500	0.24785300
C	-1.47541500	0.19635300	0.08312100
C	-0.44150100	-0.71935600	-0.15806900
C	-0.70750800	-2.07520900	-0.23384800
N	-0.96339200	1.50864100	0.11842800
C	0.38969100	1.51719800	-0.10868900
C	0.86210700	0.03685700	-0.26011200

O	1.10971500	2.49905900	-0.21199800
H	-2.26307800	-3.57028500	-0.14172300
H	-4.07459400	-1.93955700	0.28253600
H	-3.58997500	0.49547700	0.43501200
H	0.09635700	-2.78354300	-0.41078600
C	-1.76943800	2.70425200	0.27096000
H	-2.28537000	2.69791800	1.23627100
H	-1.09926200	3.56275200	0.22075600
H	-2.51154800	2.77210900	-0.53132600
C	4.27947700	-1.08041400	0.42116400
H	5.09692500	-0.36442800	0.35811900
C	3.05187700	-0.69751900	0.65188300
C	1.82035900	-0.31378800	0.86650300
H	4.53349800	-2.13032000	0.28672600
H	1.43259800	-0.22374100	1.88024100
O	1.44170000	-0.13188900	-1.54266600
H	2.20605100	0.47133700	-1.57675300

TS-F

N	0.07276600	-0.44868600	-2.03586600
C	1.54856100	-0.32749300	-2.24710000
H	1.93804400	-1.34281500	-2.28333500
C	1.70266200	0.35356500	-3.62308200
H	1.81603000	-0.42294100	-4.38397000
H	2.60233400	0.96669000	-3.68296800
C	0.38799200	1.14163700	-3.84863200
H	-0.07876800	0.84736100	-4.79274700
H	0.55760600	2.22007200	-3.89188900
C	-0.50704500	0.79165800	-2.64084400
H	-1.54823300	0.59759800	-2.89953400
H	-0.49817800	1.57838200	-1.88951100
C	2.30535000	0.31365000	-1.04032100
C	3.81302200	0.10058900	-1.26573700
C	4.74391600	1.14057300	-1.28875800
C	4.29575300	-1.21414100	-1.38348900
C	6.10722300	0.87857400	-1.43862600
H	4.41891400	2.16538700	-1.16365300
C	5.65551200	-1.47208300	-1.52281500
H	3.61102300	-2.05478000	-1.33117500
C	6.59040800	-0.42739100	-1.55897600
H	6.80734600	1.71003400	-1.44625800
H	5.99696000	-2.50126100	-1.59991800
C	1.93279900	1.76096000	-0.70936500
C	1.44146700	2.11190900	0.55321400

C	2.11833900	2.80001000	-1.63516500
C	1.11709100	3.42969200	0.86517500
H	1.28868100	1.35718300	1.30804400
C	1.78420200	4.11624500	-1.32268300
H	2.54406500	2.60128000	-2.60921900
C	1.26136100	4.45617200	-0.07057000
H	0.73407200	3.65796000	1.85663100
H	1.93362500	4.89050000	-2.07088900
C	-1.81830900	-2.06609100	-2.53211100
C	-2.80840000	-1.98930800	-3.50729200
C	-3.42404000	-3.09888900	-1.02510900
C	-4.10620500	-2.45211000	-3.26140500
H	-2.55838500	-1.57059100	-4.48002600
C	-4.40146600	-3.01366900	-2.02144400
H	-4.87010700	-2.38599100	-4.02916500
H	-5.39948500	-3.38612400	-1.81696900
C	-3.74134000	-3.70996300	0.29919700
O	-1.18831400	-2.63403000	-0.30703500
F	-2.99349100	-4.80996900	0.56609800
F	-3.53126600	-2.85909000	1.34779600
F	-5.03836900	-4.09673000	0.39255500
C	-0.39744300	-1.66661800	-2.80092300
H	0.26022000	-2.48354100	-2.49185300
H	-0.25109800	-1.49810000	-3.87350100
C	-2.11229800	-2.60962300	-1.24954000
Zn	-0.57213600	-0.76740800	-0.02883100
C	-6.33819900	0.36098000	1.73063900
C	-6.84152900	1.66442300	1.73390000
C	-6.05695700	2.75138500	1.31645600
C	-4.75798800	2.48254300	0.90565000
C	-4.23420400	1.17642900	0.91910500
C	-5.02045500	0.10750200	1.31928600
N	-3.79779600	3.38225900	0.40857800
C	-2.65147400	2.72137700	0.00642700
C	-2.81972300	1.24916300	0.44365100
O	-2.26287900	0.30534500	-0.22044900
O	-1.71049700	3.22606100	-0.58867400
H	-6.97133600	-0.46221600	2.04764100
H	-7.86243800	1.84589000	2.05721800
H	-6.45881000	3.75913400	1.30708000
H	-4.61988400	-0.89950400	1.31313100
C	-4.03099100	4.79461400	0.18695300
H	-4.24527900	5.30304300	1.13273200
H	-3.12545900	5.21227500	-0.25476000

H	-4.87246300	4.94730600	-0.49800000
O	1.89203500	-0.56043700	0.04932300
C	8.06174700	-0.70982300	-1.73330500
H	8.37374800	-1.57597000	-1.13971700
H	8.29770700	-0.93507200	-2.78140800
H	8.67073600	0.14890400	-1.43494500
C	0.82433200	5.86316700	0.24459500
H	1.31940100	6.59498700	-0.40147400
H	-0.25833500	5.96344700	0.09265600
H	1.03235600	6.12564800	1.28744500
C	-0.42056900	-0.53901900	2.10476600
H	0.26429700	-1.27180300	2.49603800
C	-1.07707400	0.49046000	2.35562000
O	3.63795000	0.04877800	1.64014900
O	2.38673500	-1.85617900	1.97353000
C	3.47965000	-1.91086700	2.94755100
C	4.52933300	-2.86155400	2.36715500
C	2.93328300	-2.44608300	4.26319700
H	4.92576800	-2.48351500	1.41948000
H	5.36186700	-3.00544400	3.06204400
H	4.06295000	-3.83341900	2.18048300
H	2.08290100	-1.85868800	4.61632200
H	2.60533300	-3.48188700	4.13231200
H	3.71177700	-2.43022900	5.03295900
C	3.95945200	-0.41447900	2.98832000
C	3.14850600	0.45587300	3.95131200
C	5.45310000	-0.22678600	3.21552700
H	2.07253400	0.32709300	3.79649200
H	3.38109400	0.22051900	4.99399800
H	3.39424800	1.50625500	3.76963800
H	6.03872100	-0.70160000	2.42552000
H	5.69222500	0.84106300	3.22432800
H	5.75118700	-0.65096100	4.17999600
B	2.64641500	-0.76690300	1.17818000
C	-1.91124800	1.59000200	2.27889100
H	-2.78492300	1.58476800	2.92485100
H	-1.41810900	2.55824500	2.20634900

Int-IIIF

N	-0.03945000	-0.02932800	-2.23548200
C	1.44516600	-0.00920800	-2.37880300
H	1.76124900	-1.04641200	-2.46226200
C	1.72052500	0.73000400	-3.70696300
H	1.85652400	-0.01779100	-4.49258800

H	2.64392300	1.30986500	-3.67869400
C	0.45143100	1.57581500	-3.98866600
H	0.01532400	1.29829400	-4.95215800
H	0.66438100	2.64691200	-4.02720200
C	-0.50998000	1.25867500	-2.82364700
H	-1.55356900	1.14778900	-3.12539100
H	-0.46581700	2.01699800	-2.04433000
C	2.17643100	0.48110600	-1.08664600
C	3.66994300	0.16794100	-1.24647200
C	4.66071500	1.14530500	-1.13610300
C	4.07478900	-1.15932700	-1.46843200
C	6.01132000	0.80925300	-1.24587600
H	4.38690000	2.17544000	-0.94550500
C	5.42196300	-1.49107100	-1.56794900
H	3.33907700	-1.95523400	-1.53170300
C	6.41909300	-0.51045300	-1.46084900
H	6.76052700	1.59065700	-1.14921100
H	5.70388300	-2.52869400	-1.72755400
C	1.91016900	1.91686000	-0.63496600
C	1.57204200	2.19864600	0.69477000
C	2.06656600	3.00544100	-1.50374300
C	1.36084500	3.50420100	1.12391600
H	1.46197400	1.39844300	1.41095300
C	1.83873600	4.31242900	-1.07318700
H	2.38345400	2.85641800	-2.52582800
C	1.46723500	4.58705900	0.24609300
H	1.08240500	3.68284300	2.15806600
H	1.95401200	5.12932000	-1.78099200
C	-1.98399600	-1.62126500	-2.61400000
C	-3.04053700	-1.57971400	-3.51947500
C	-3.38900600	-2.87576500	-1.07175000
C	-4.27831500	-2.15609200	-3.21493700
H	-2.88470300	-1.11110900	-4.48885600
C	-4.43059000	-2.82835600	-2.00611500
H	-5.09758300	-2.11229700	-3.92490700
H	-5.36833400	-3.32134900	-1.77499100
C	-3.54346500	-3.72377100	0.15196200
O	-1.18647700	-2.16743200	-0.43194500
F	-2.84902900	-4.88931000	0.04899000
F	-3.11881500	-3.14750800	1.30416600
F	-4.84112400	-4.07108200	0.36799800
C	-0.59377200	-1.19798000	-3.00258000
H	0.07763100	-2.03753000	-2.80201900
H	-0.55263300	-0.98675500	-4.07778300

C	-2.15709200	-2.22240900	-1.33209700
Zn	-0.62719600	-0.29960300	-0.20003900
C	-5.44433800	-0.48151000	0.87800800
C	-6.35871100	0.56574500	0.75676900
C	-5.93744200	1.90511600	0.79467400
C	-4.57812000	2.14543900	0.95577000
C	-3.64817900	1.10396700	1.08418600
C	-4.07605800	-0.21057300	1.04338700
N	-3.91739800	3.38675100	1.01208000
C	-2.55911700	3.22627300	1.16919000
C	-2.24779300	1.69190700	1.18260000
O	-1.44070800	1.38808200	0.10192800
O	-1.75022000	4.13698200	1.28230000
H	-5.78205800	-1.51259000	0.83733800
H	-7.41536800	0.34880500	0.62789200
H	-6.65063800	2.71709900	0.69672700
H	-3.36702700	-1.02025000	1.13551100
C	-4.57366200	4.67384600	0.91602900
H	-5.30198200	4.79794000	1.72484800
H	-3.80424400	5.44240600	0.99760800
H	-5.09047300	4.77393900	-0.04473100
O	1.61414000	-0.44061900	-0.08362700
C	7.87749500	-0.87350000	-1.58743800
H	8.11475600	-1.77292600	-1.00862300
H	8.14145400	-1.08345800	-2.63182100
H	8.52200700	-0.06102900	-1.23899000
C	1.15327300	5.98618000	0.70841800
H	1.43511500	6.73182800	-0.04141200
H	0.07815200	6.08047800	0.90166400
H	1.67361200	6.22607500	1.64305300
C	-0.62607900	-1.11562700	2.46947900
H	-0.25636000	-2.11341500	2.40317300
C	-1.03064100	0.02342200	2.55664600
O	3.33881100	-0.28039500	1.63003800
O	2.05140900	-2.18218200	1.48243900
C	3.10135200	-2.48766600	2.45807300
C	4.12804200	-3.35558400	1.72793000
C	2.47814300	-3.25588600	3.61561700
H	4.57746400	-2.81740300	0.88868100
H	4.92483400	-3.67923200	2.40398700
H	3.62544900	-4.24473500	1.33563500
H	1.65289500	-2.70478800	4.07103500
H	2.09492200	-4.21532200	3.25461700
H	3.22851300	-3.45833300	4.38677000

C	3.64663100	-1.05650000	2.83025100
C	2.88432900	-0.39263900	3.97882500
C	5.14959100	-0.98610500	3.06641400
H	1.80385000	-0.41885900	3.80736500
H	3.10125200	-0.87941400	4.93422200
H	3.19331900	0.65474900	4.04712200
H	5.70761500	-1.29574600	2.18021800
H	5.43394400	0.04277500	3.30731800
H	5.43779100	-1.62518000	3.90736800
B	2.34155100	-0.94394200	0.98095900
C	-1.54715400	1.38495600	2.54532300
H	-2.24158500	1.54019300	3.37940600
H	-0.72540200	2.10052800	2.65590300

Int-IVF

C	-1.80731100	-2.89082900	0.77383100
C	-2.98761300	-2.95748500	0.03183100
C	-3.54439800	-1.80901100	-0.54642700
C	-2.86912000	-0.60921000	-0.36388000
C	-1.66646300	-0.52748800	0.35729800
C	-1.14148300	-1.66870500	0.94714700
N	-3.26443100	0.66611300	-0.80844500
C	-2.38715800	1.63054600	-0.39126700
C	-1.23856800	0.92687400	0.39715300
O	-0.05597600	1.28646900	-0.30892600
O	-2.47136000	2.83132000	-0.59359700
H	-1.39950700	-3.79131300	1.22253600
H	-3.49192400	-3.91081300	-0.09600300
H	-4.47181600	-1.85764800	-1.10671000
H	-0.22257800	-1.61430300	1.51441900
C	-4.46227300	0.93864200	-1.57823800
H	-5.35351100	0.62840300	-1.02320100
H	-4.50058000	2.01293500	-1.75936500
H	-4.43238100	0.40637400	-2.53420800
C	0.90071300	0.71095900	3.24879800
H	1.73755300	0.37055400	3.81714000
C	-0.05032300	1.08321700	2.60408200
O	2.19559600	1.25956700	-0.99088100
O	1.44764700	-0.59942400	0.14160600
C	2.77096500	-0.94112300	-0.36562100
C	2.55469000	-1.79125100	-1.61973000
C	3.50405700	-1.74110800	0.70304400
H	2.03290500	-1.22450300	-2.39708200
H	3.50405700	-2.15024800	-2.02809800

H	1.94038200	-2.65791200	-1.35799300
H	3.52586000	-1.20913500	1.65639900
H	2.99857000	-2.69971400	0.85665600
H	4.53355900	-1.94593300	0.39106100
C	3.38214800	0.47403500	-0.67213900
C	4.02597800	1.12665900	0.55436000
C	4.33257400	0.51624000	-1.86126600
H	3.34840200	1.10573900	1.41370600
H	4.95867900	0.62612700	0.83107100
H	4.25103700	2.17191300	0.32228400
H	3.84007600	0.19365900	-2.78099900
H	4.69608500	1.53822600	-2.00708800
H	5.19861200	-0.12977200	-1.68236500
B	1.14273000	0.64076900	-0.35624700
C	-1.18604800	1.54457700	1.81292700
H	-2.12787100	1.32157400	2.32856900
H	-1.13769100	2.63247200	1.68259400

(R)-3ba'

C	-0.65116000	2.94782900	0.23256800
C	-1.96401200	2.58579100	-0.07366300
C	-2.33062100	1.24162900	-0.23539700
C	-1.33614700	0.28592300	-0.07821900
C	-0.01013500	0.63533100	0.22190100
C	0.34075000	1.96584000	0.38136100
N	-1.45987900	-1.11580500	-0.17246100
C	-0.26095800	-1.72875900	0.07352000
C	0.80898000	-0.62822600	0.29434100
O	-0.04195800	-2.93164700	0.13314800
H	-0.39440200	3.99520200	0.35646200
H	-2.72148600	3.35550100	-0.18822800
H	-3.35317700	0.96554100	-0.46911300
H	1.36431200	2.23877700	0.61307100
C	-2.70487700	-1.82308300	-0.40245700
H	-3.12458100	-1.55237000	-1.37628700
H	-2.48667100	-2.89114100	-0.38305300
H	-3.43178500	-1.58373800	0.38047000
C	3.87101100	0.99220000	-0.57142800
H	4.67155400	1.69117300	-0.47164600
C	2.96691200	0.19918400	-0.68471500
C	1.87259600	-0.75609700	-0.82574300
H	1.38253100	-0.63011300	-1.79942100
H	2.25706700	-1.78437600	-0.79870400
O	1.38929900	-0.79029000	1.58060500

H	1.66303300	-1.72369400	1.64123700

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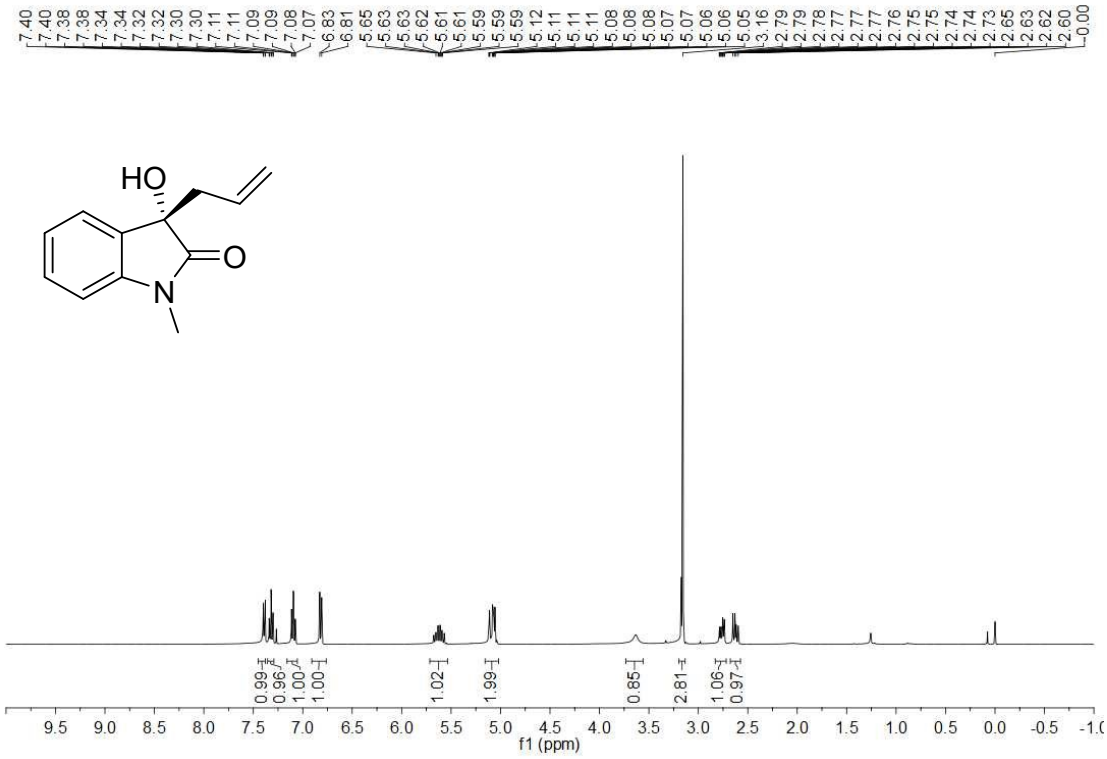
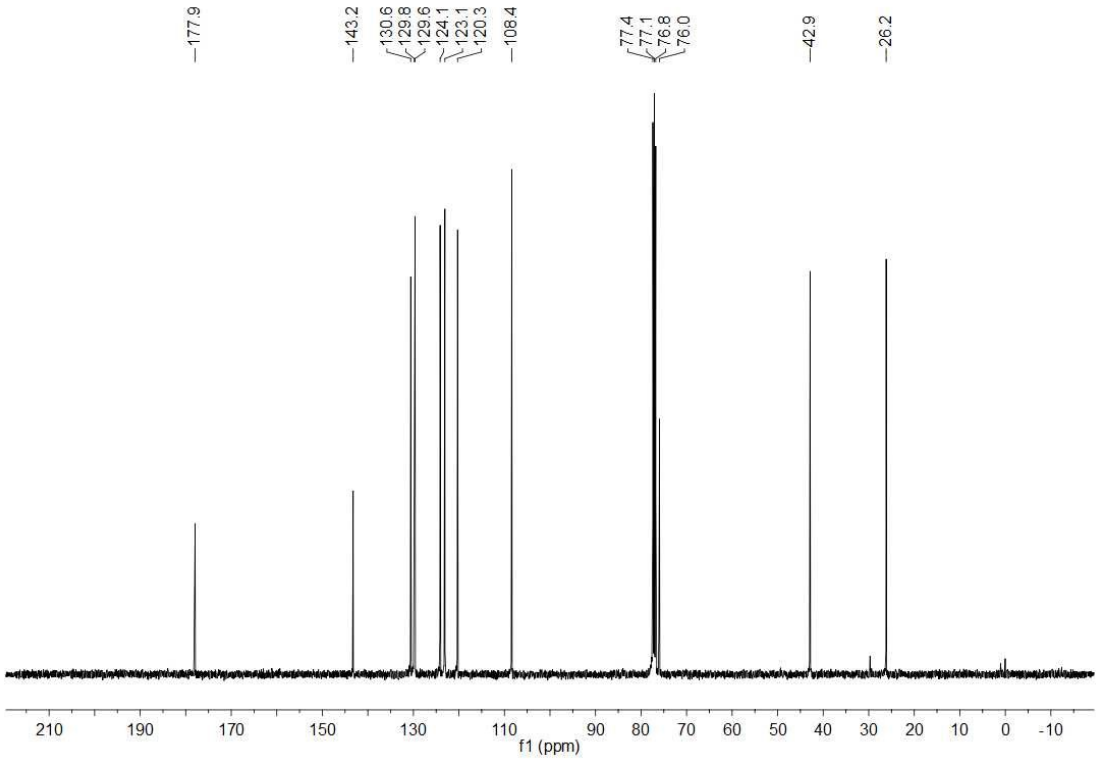
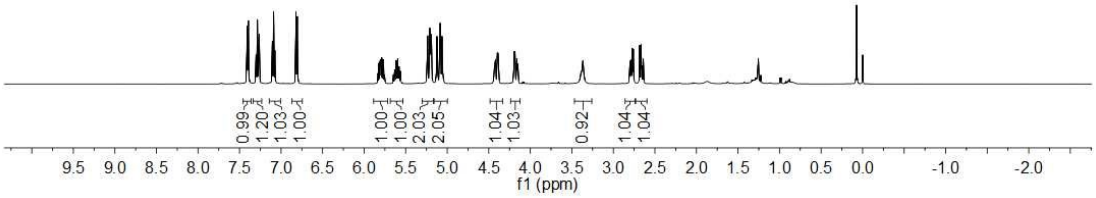
Part II NMR spectra

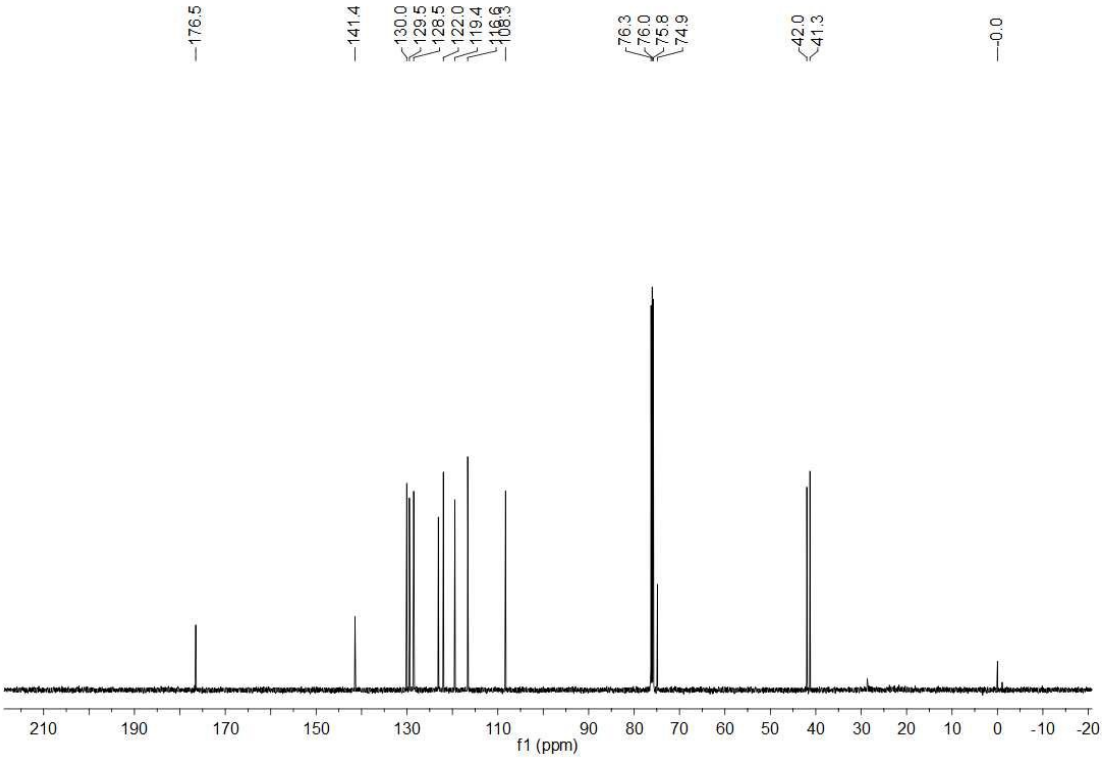
^{1}H NMR and ^{13}C NMR of **3aa**





^{1}H NMR and ^{13}C NMR of **3ab**





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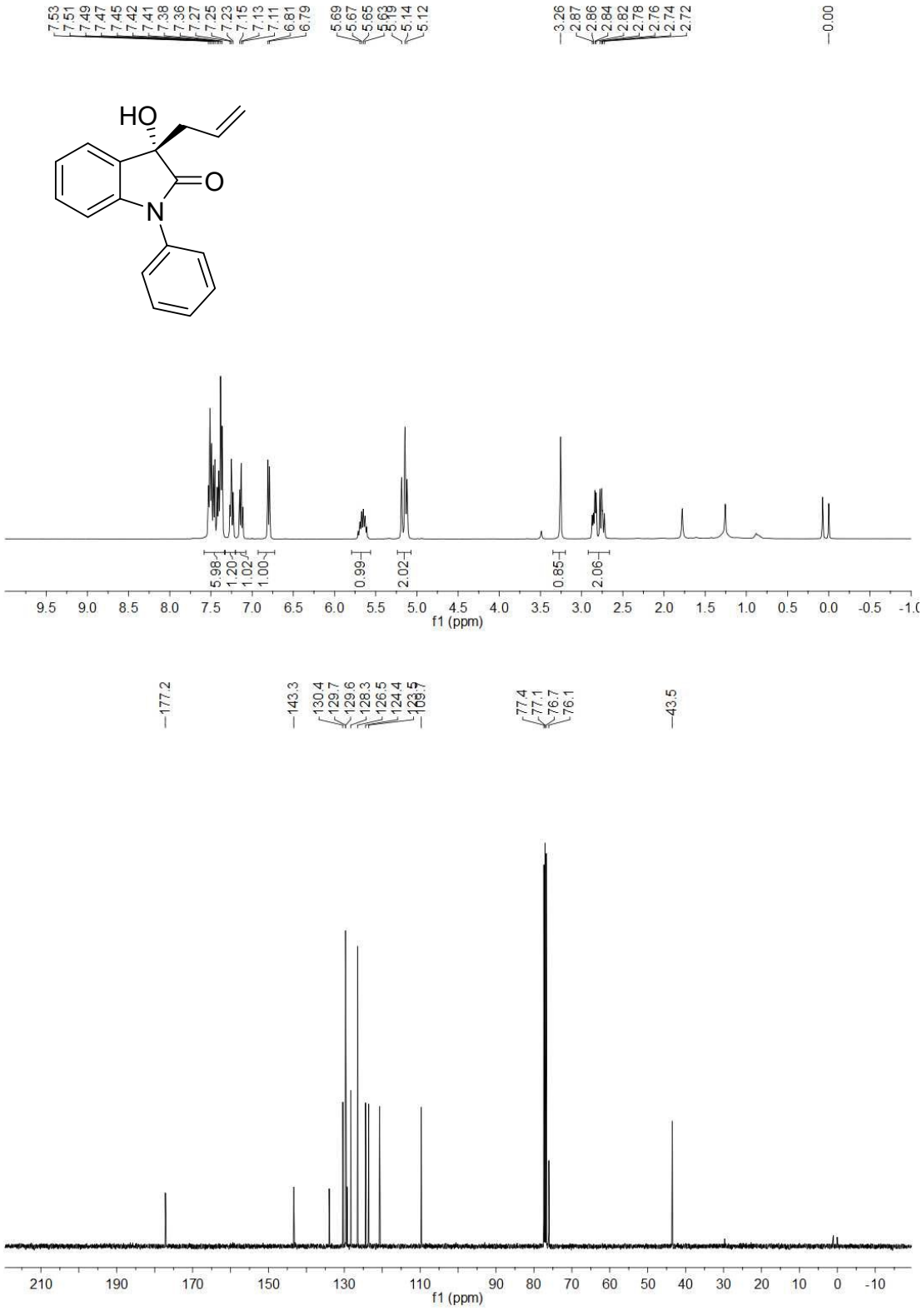

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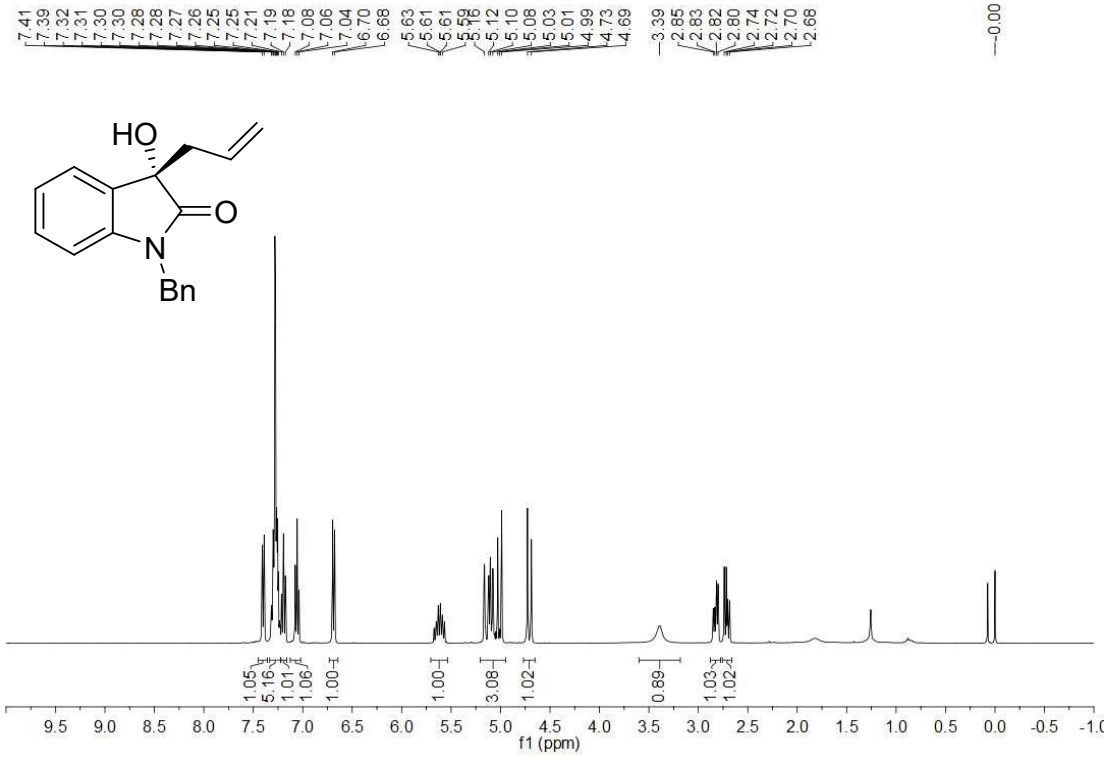

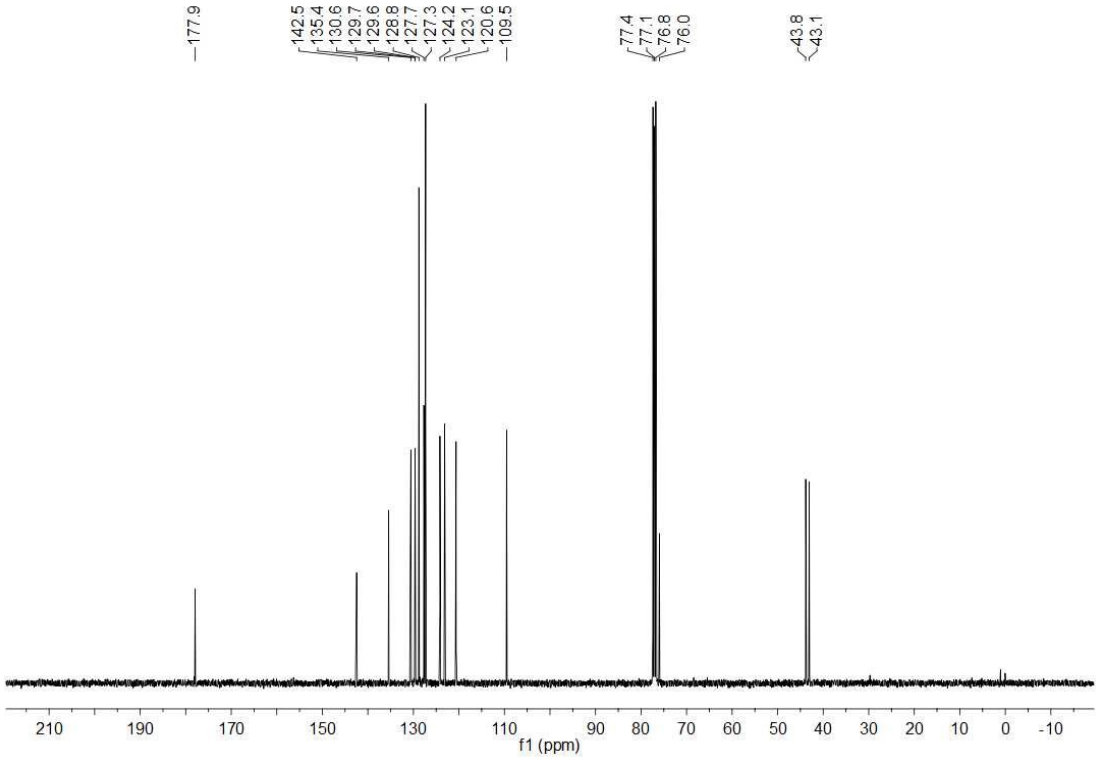

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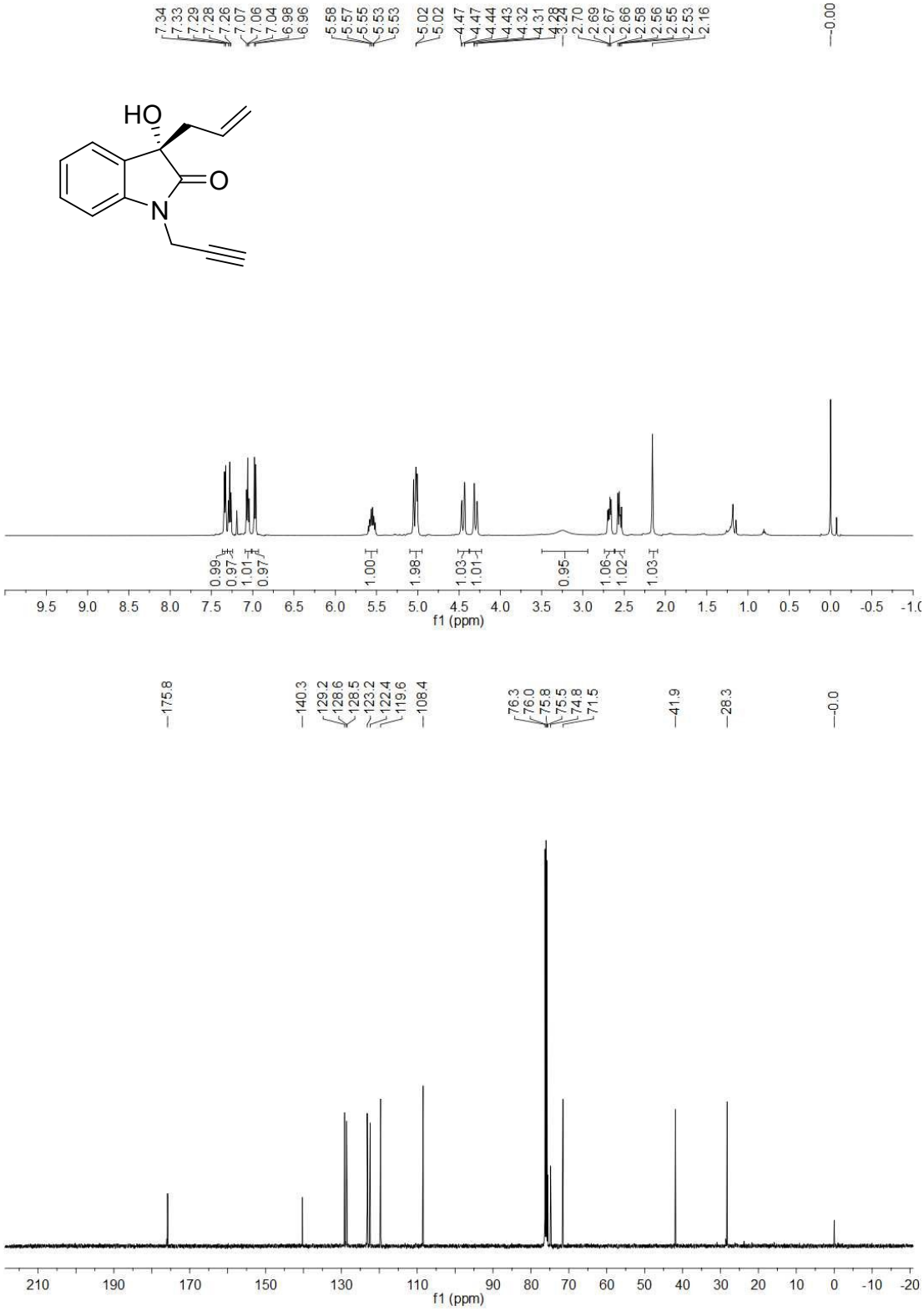

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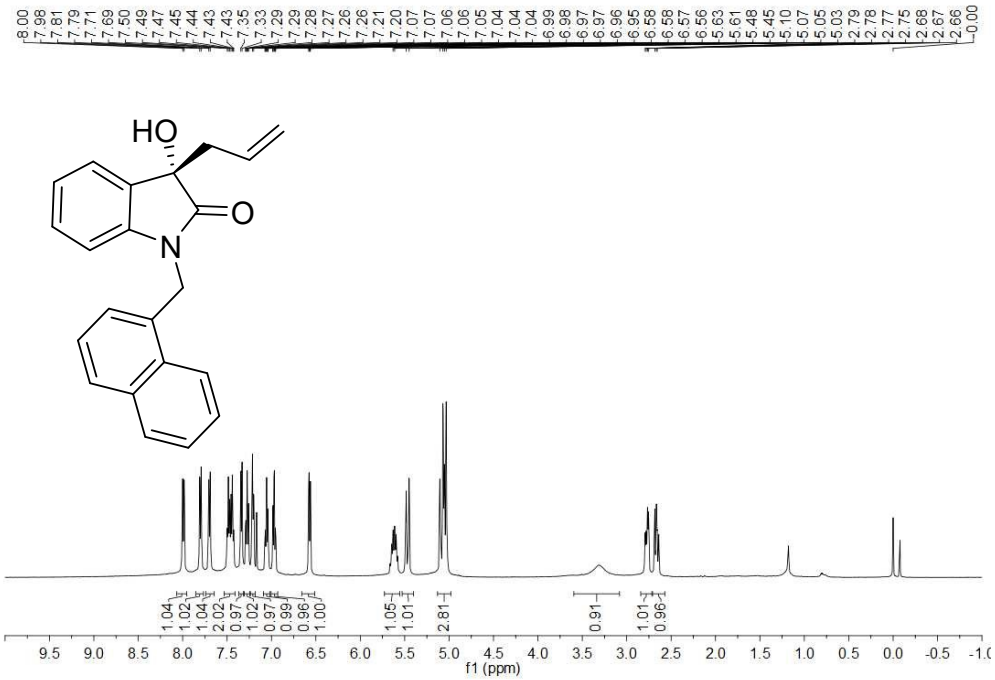

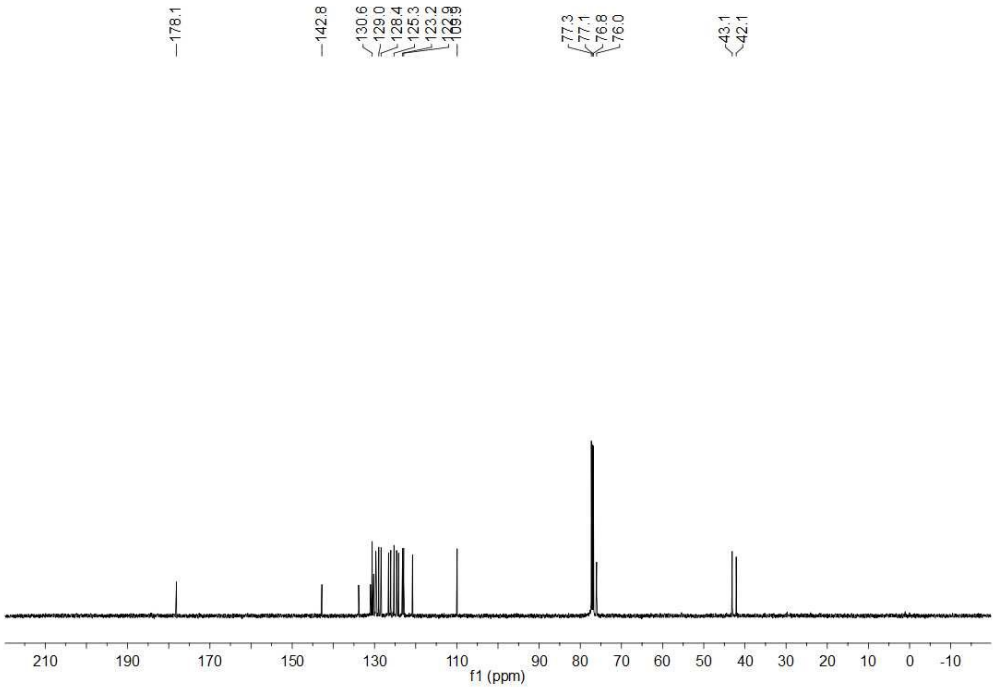

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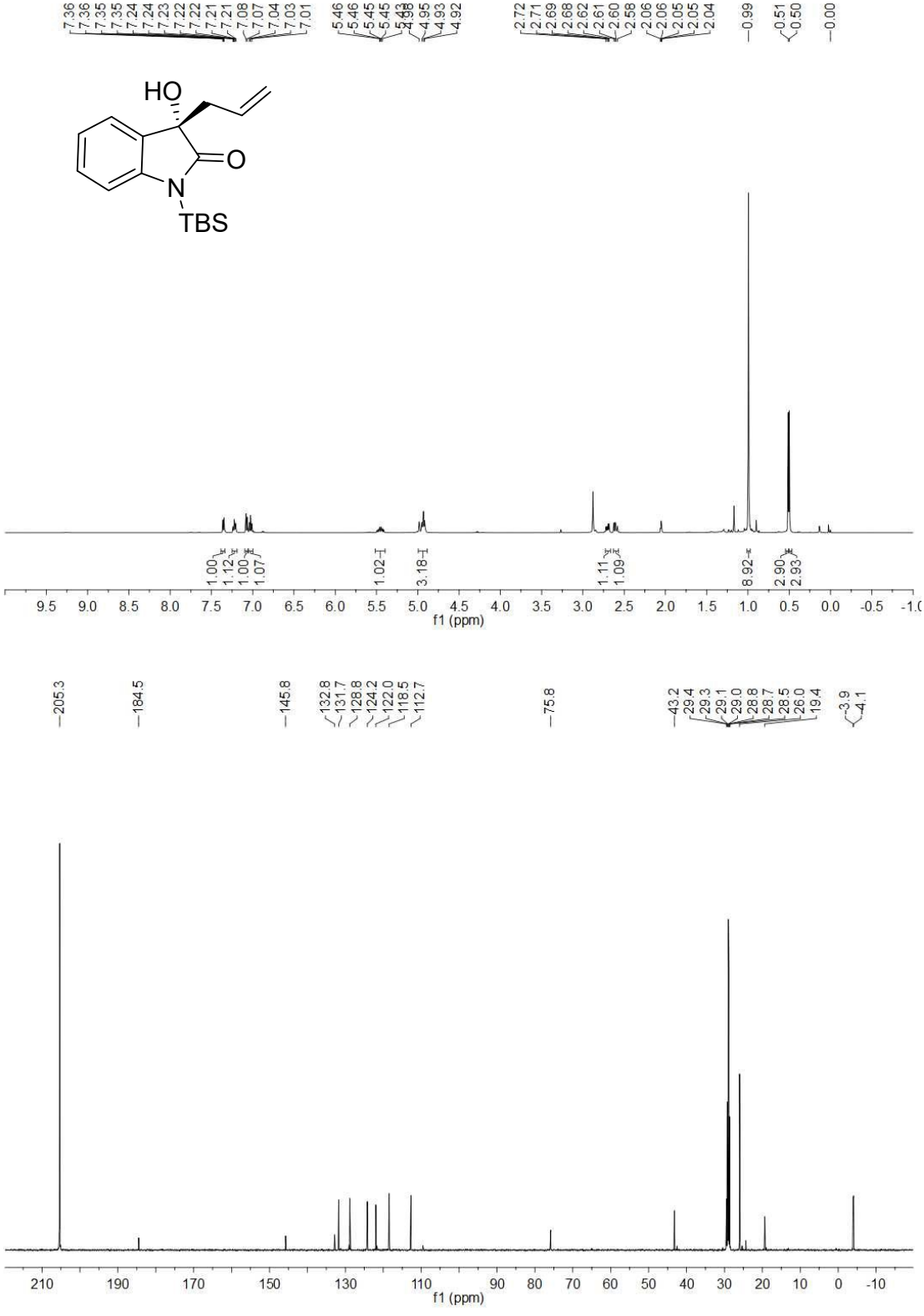

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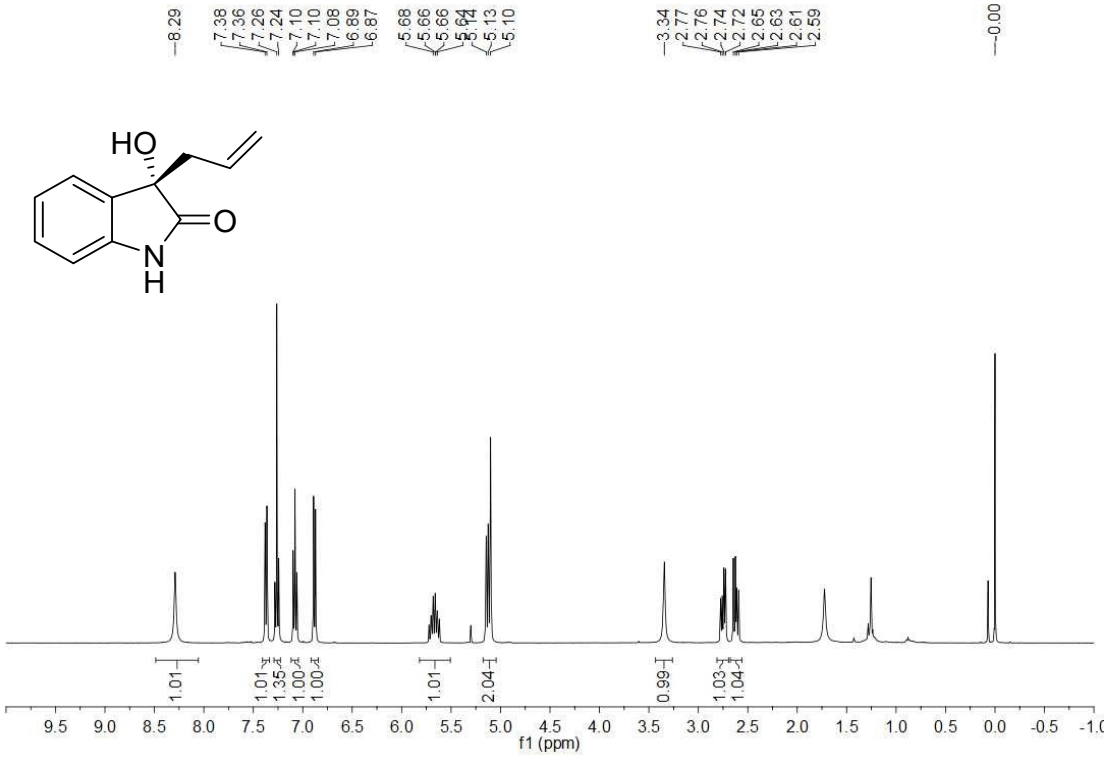

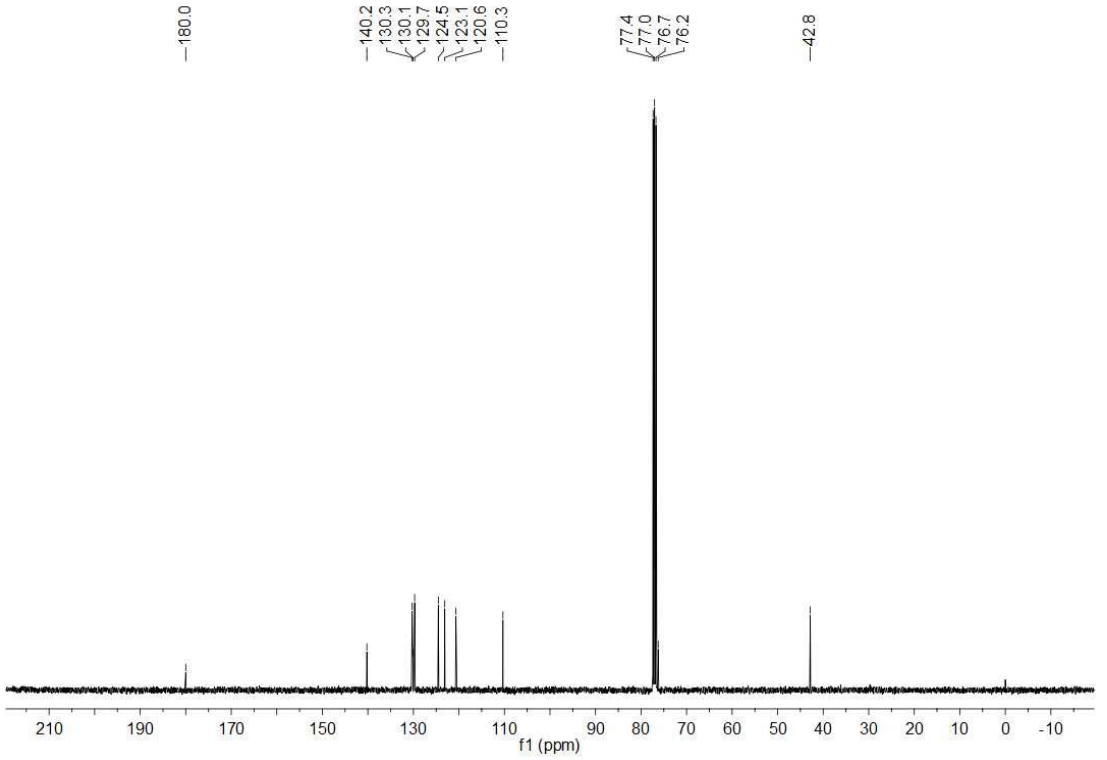

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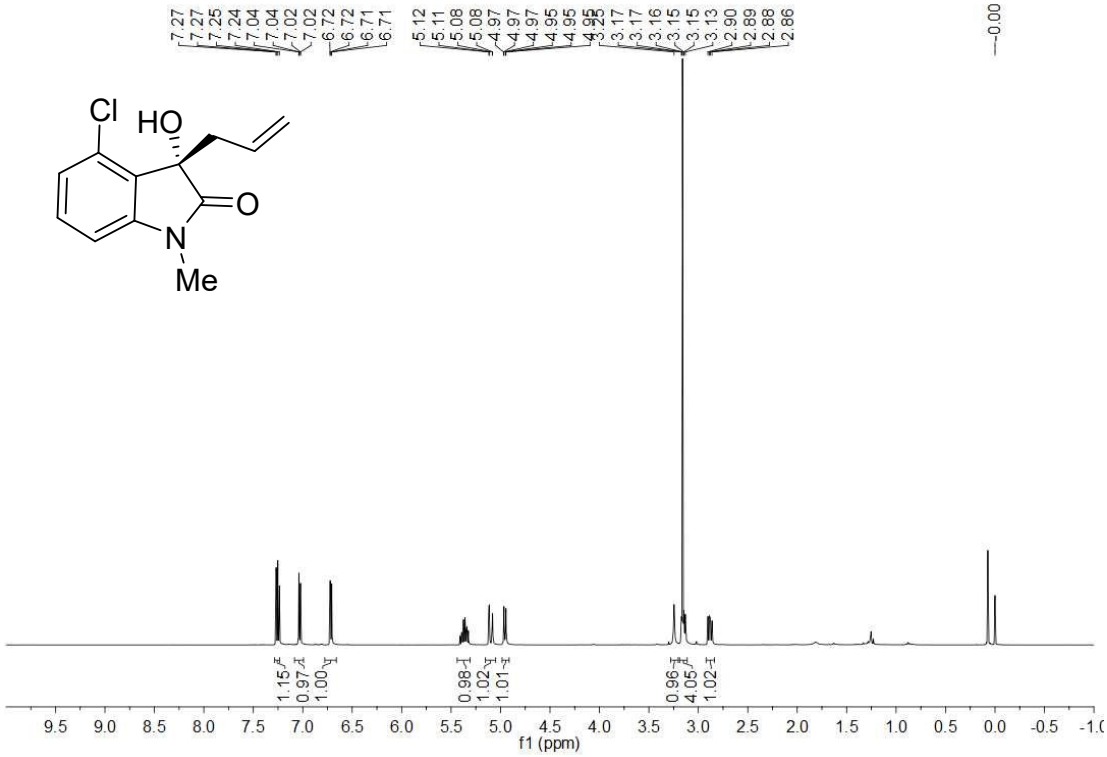

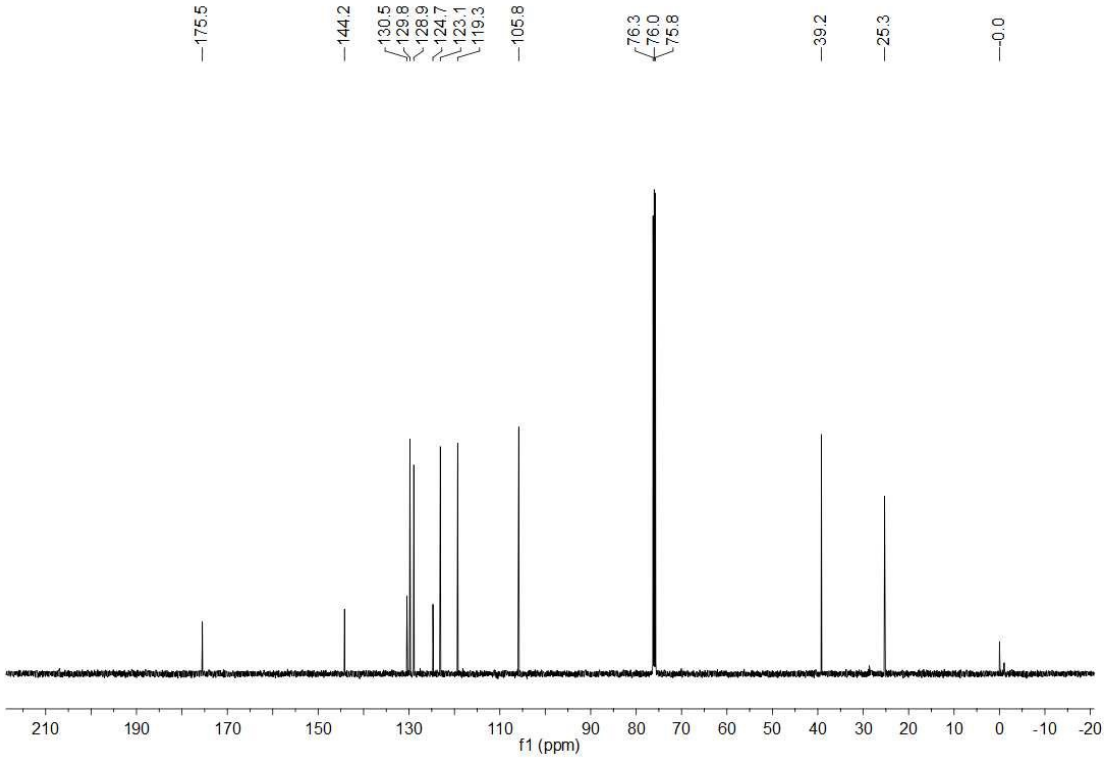

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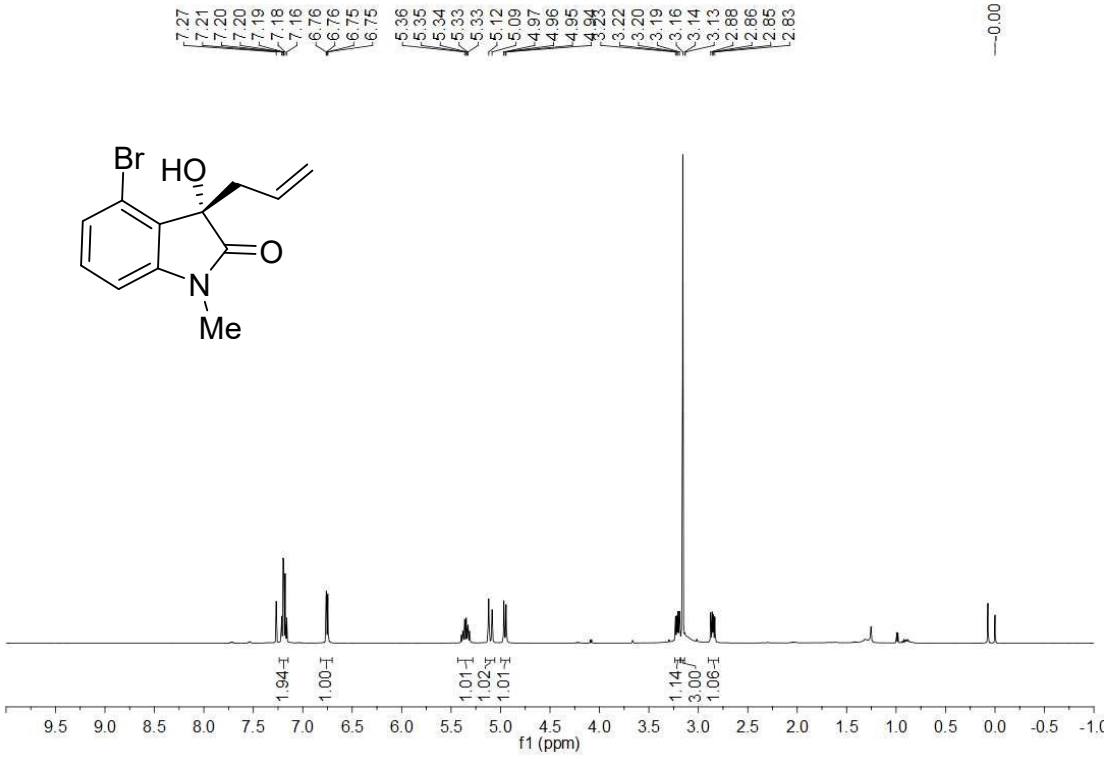
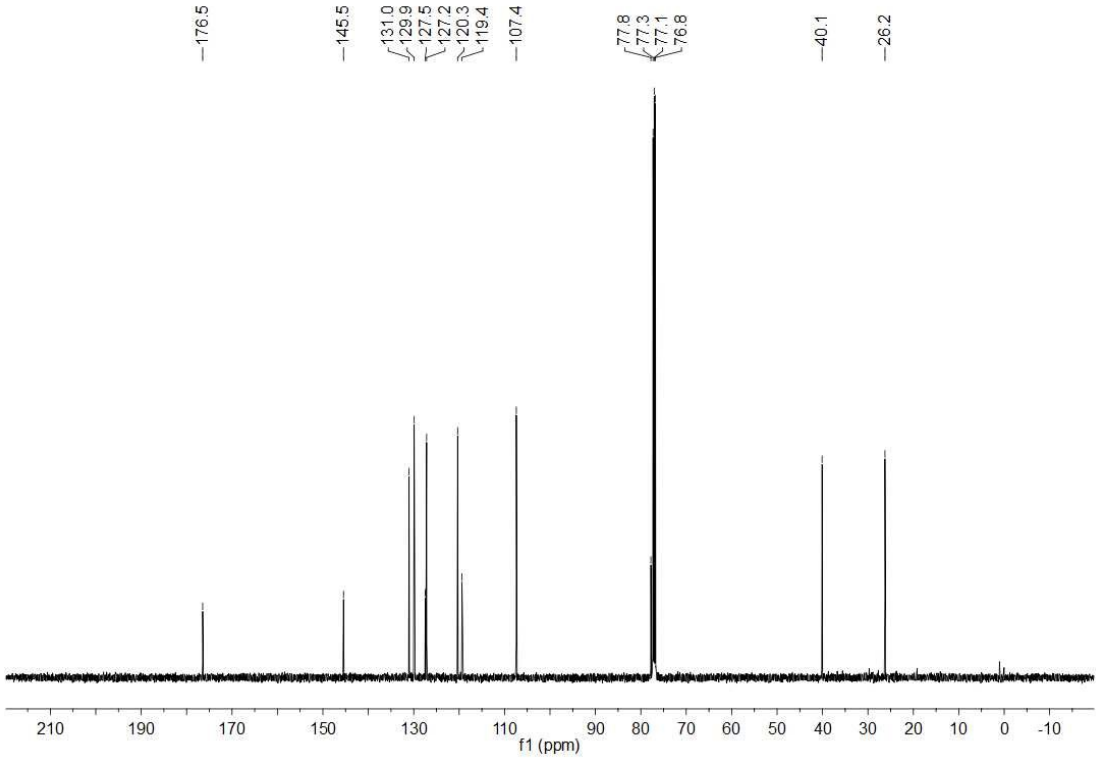
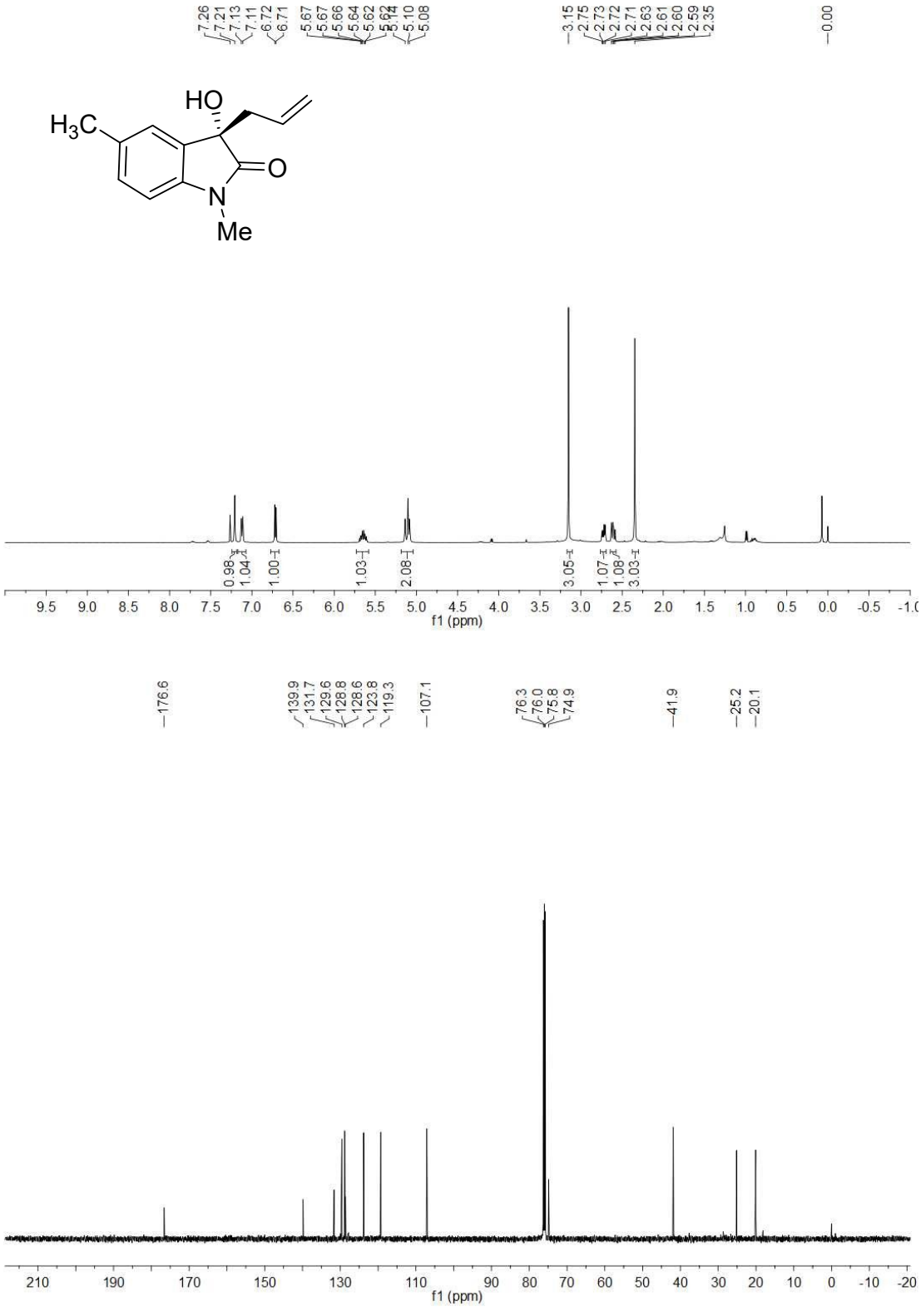
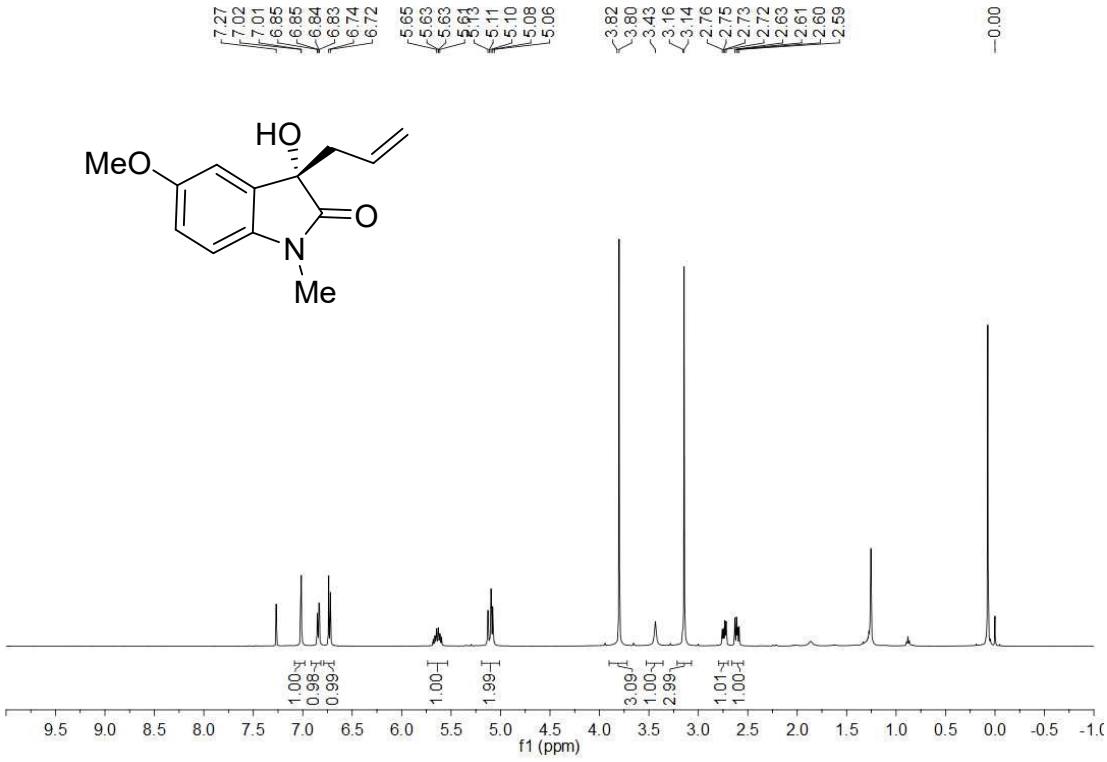


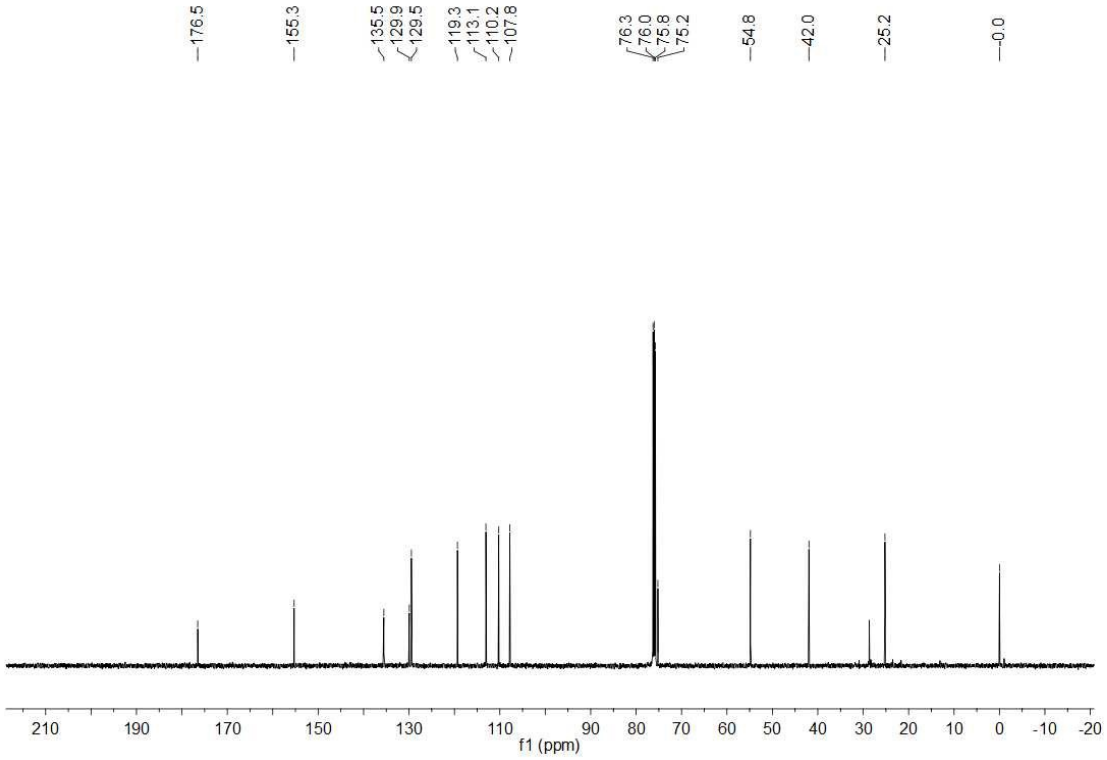


^{1}H NMR and ^{13}C NMR of **3ak**

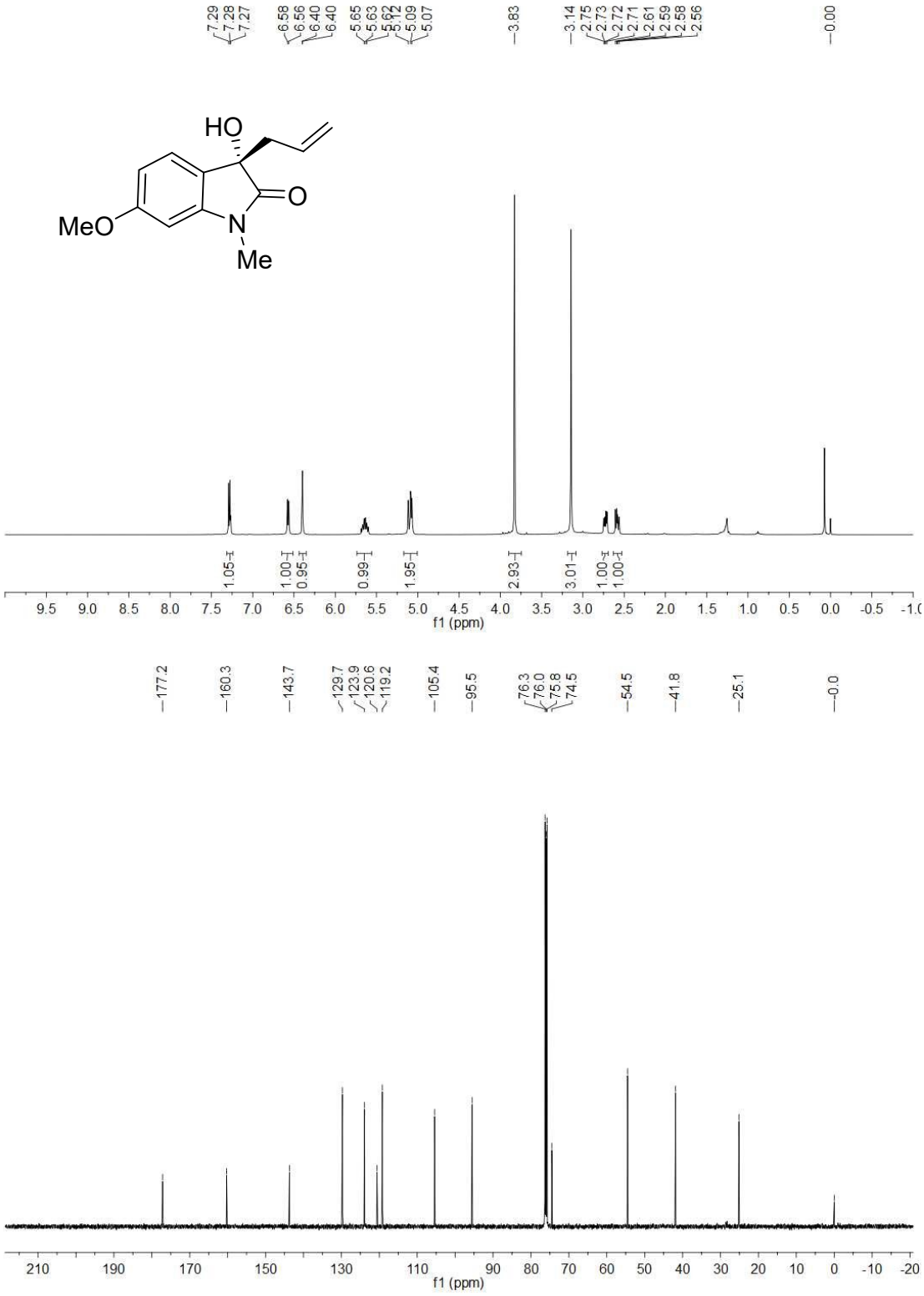


^{1}H NMR and ^{13}C NMR of **3al**





^{1}H NMR and ^{13}C NMR of **3am**



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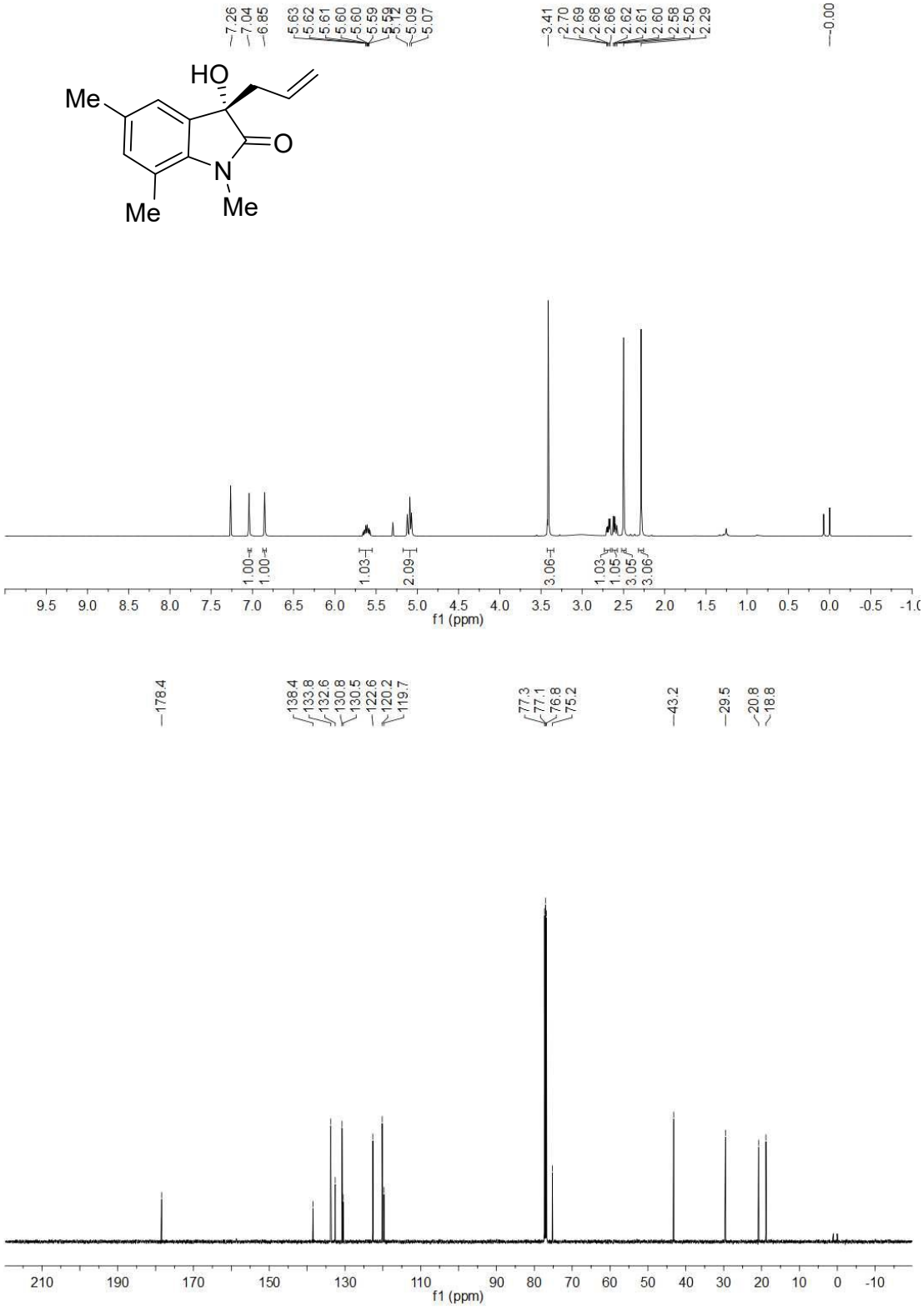

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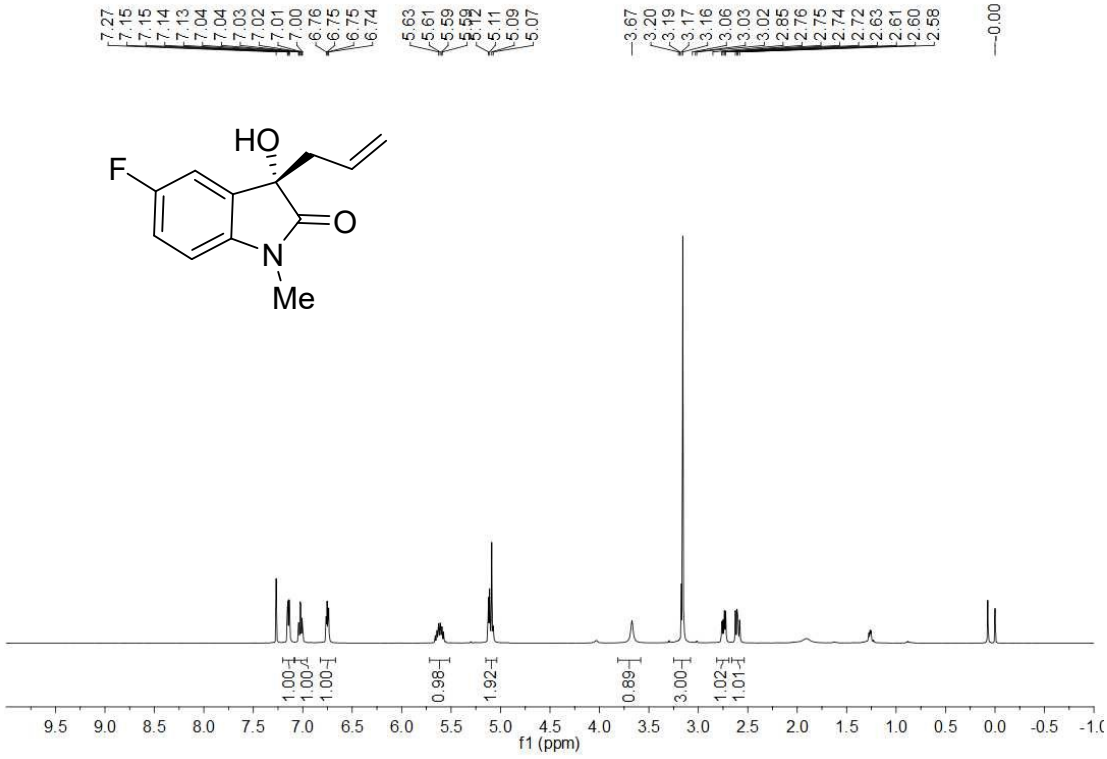
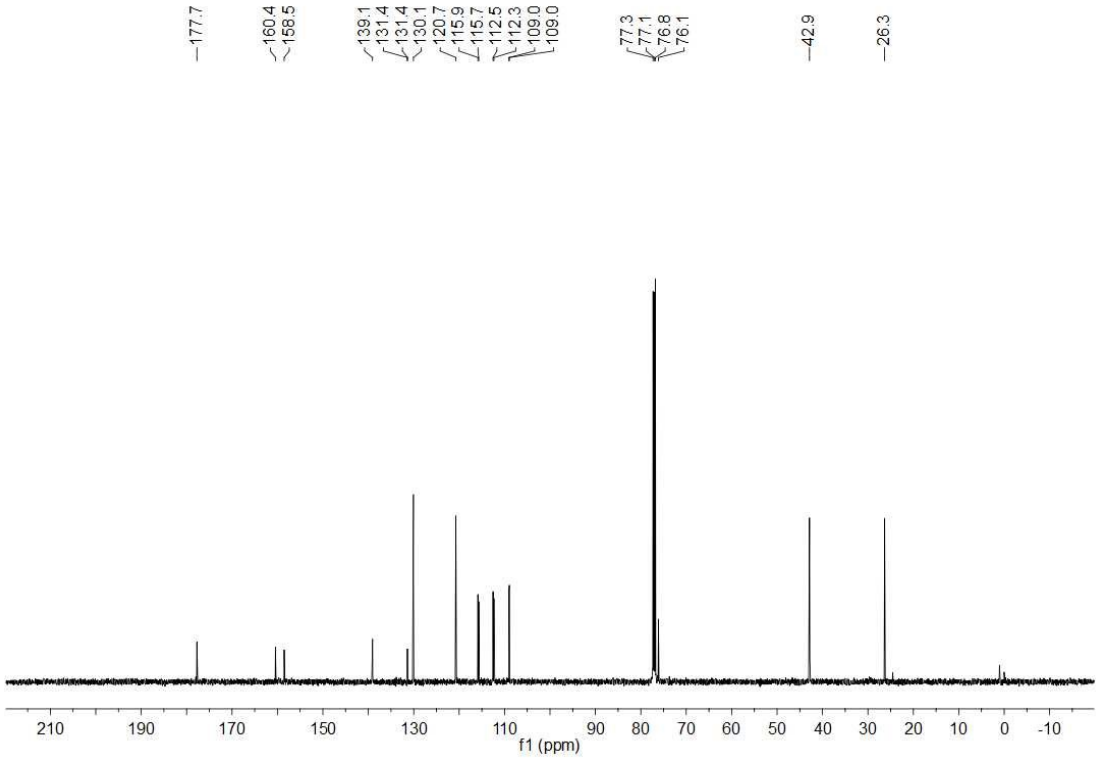
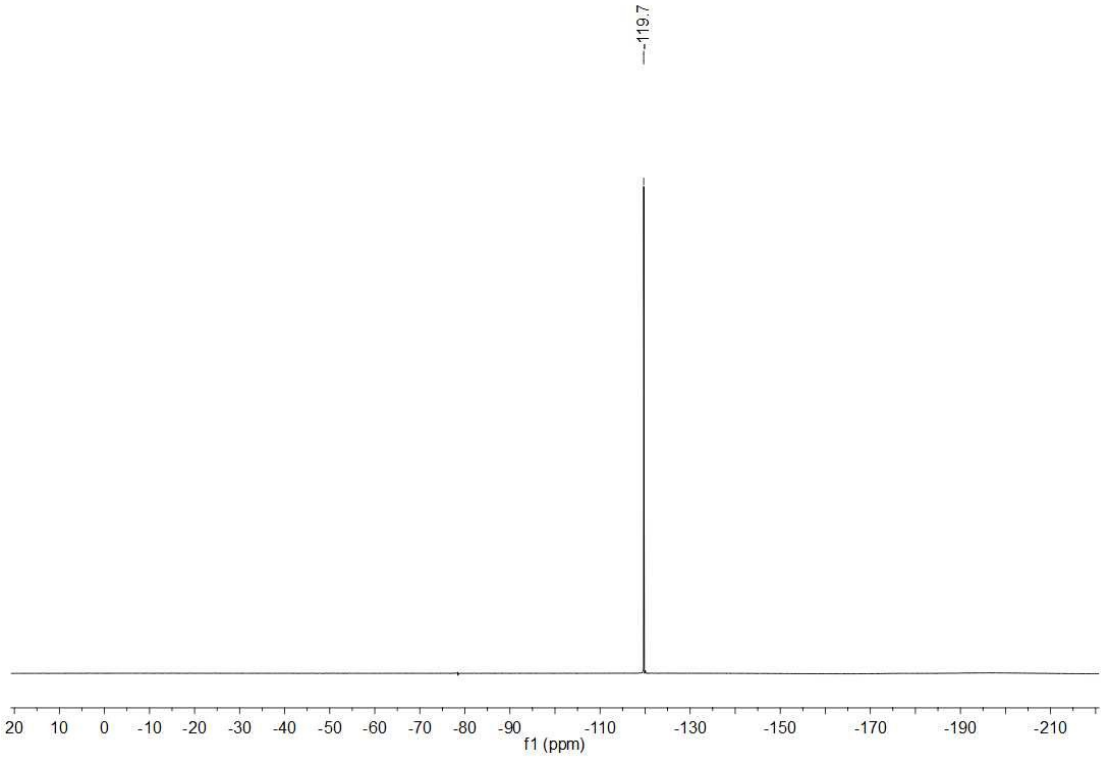
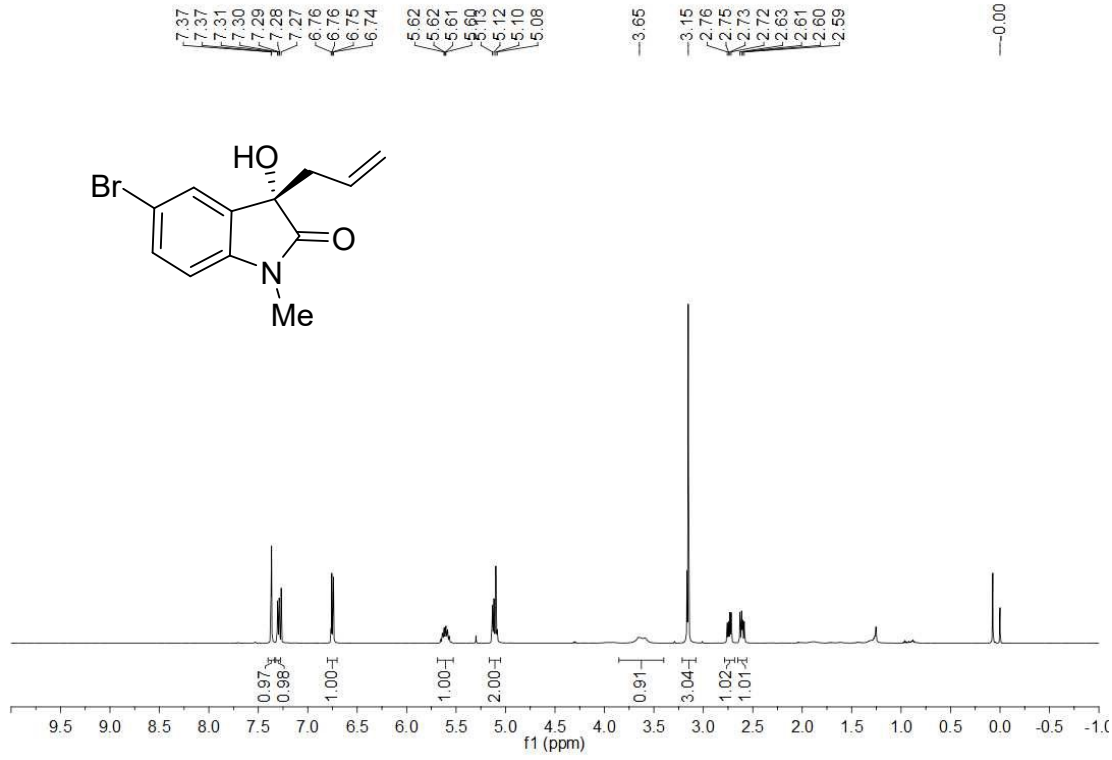
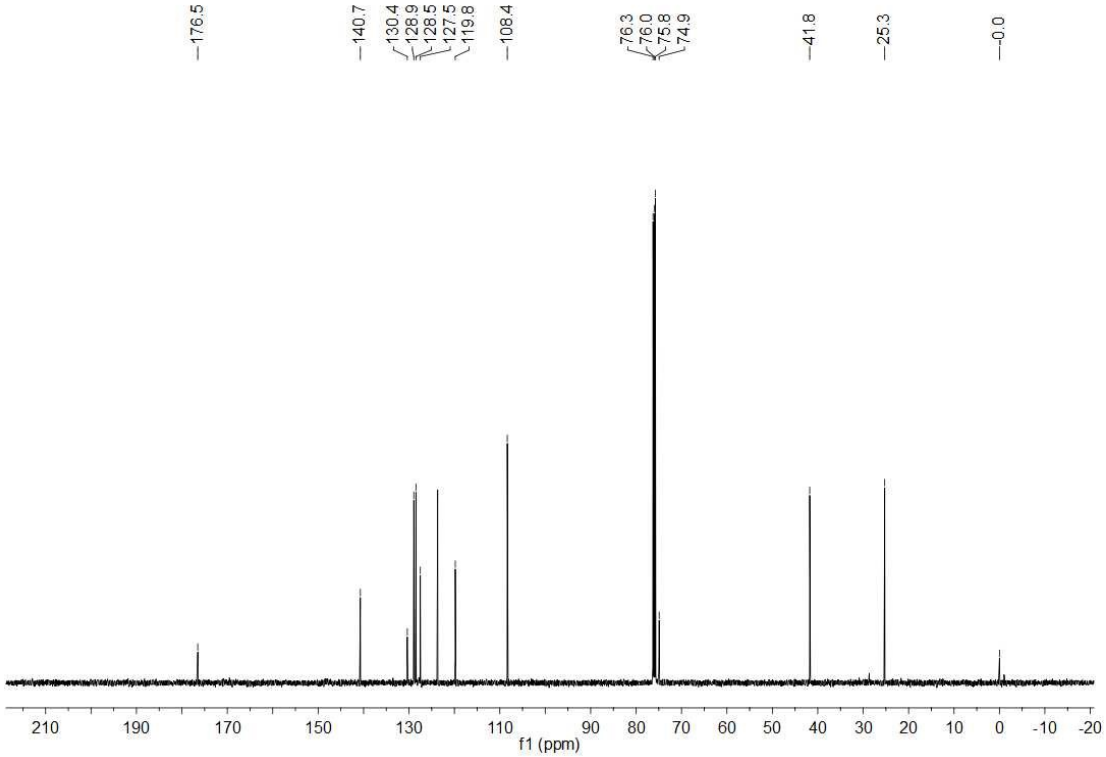




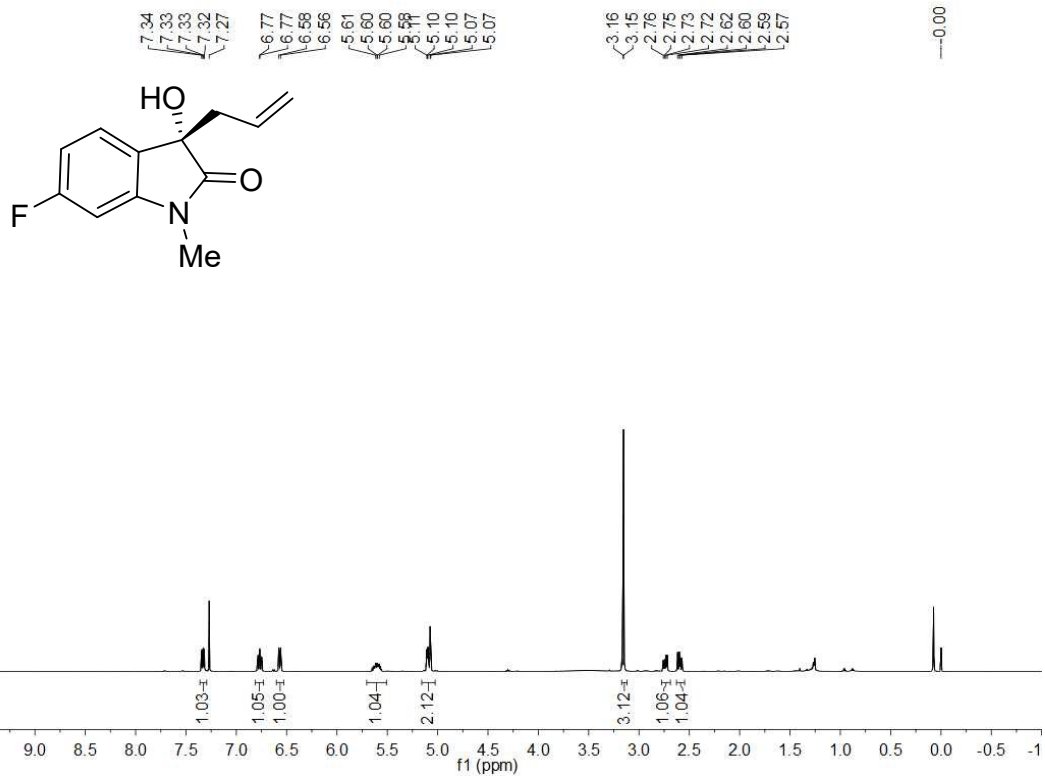


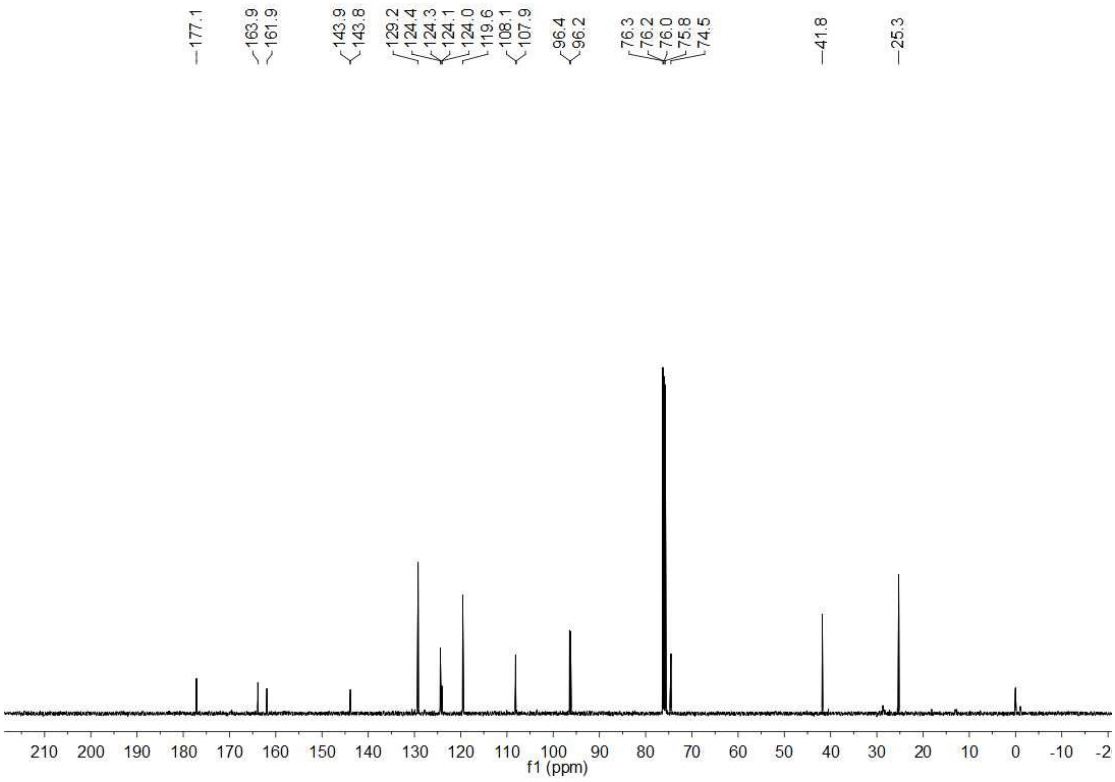
^{1}H NMR and ^{13}C NMR of **3ap**





^{1}H NMR, ^{13}C NMR and ^{19}F NMR of **3aq**

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163.9
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129.2
124.4
124.3
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124.0
119.6
108.1
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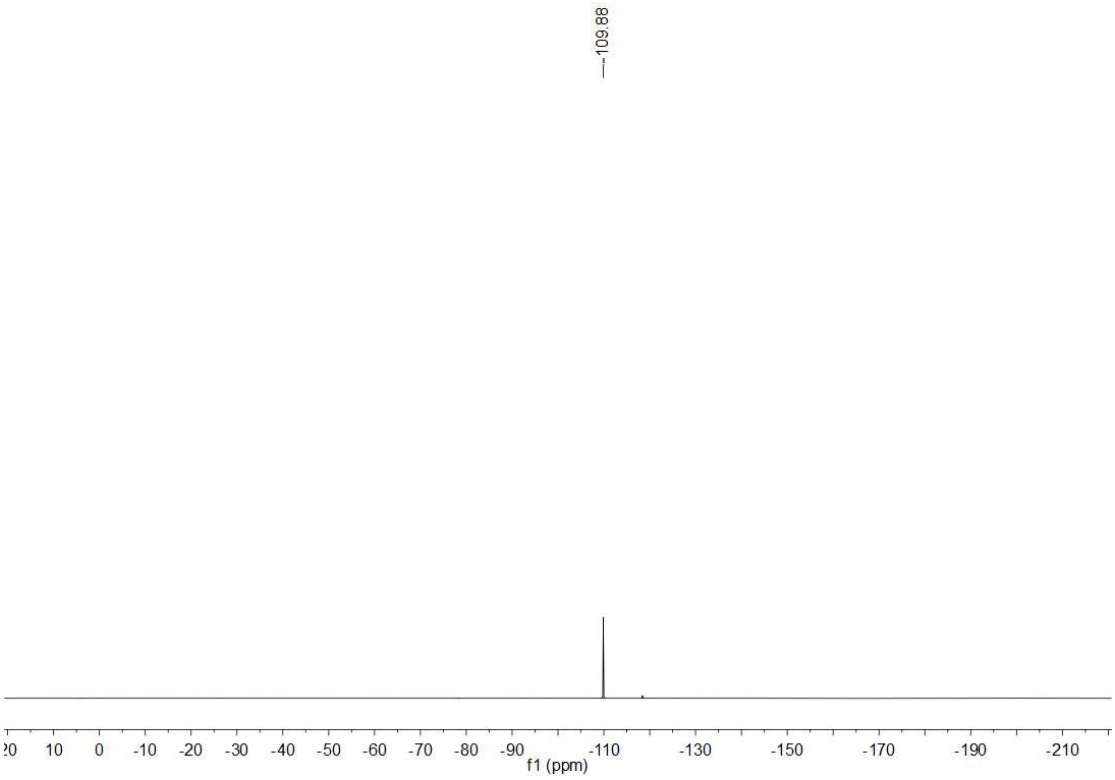
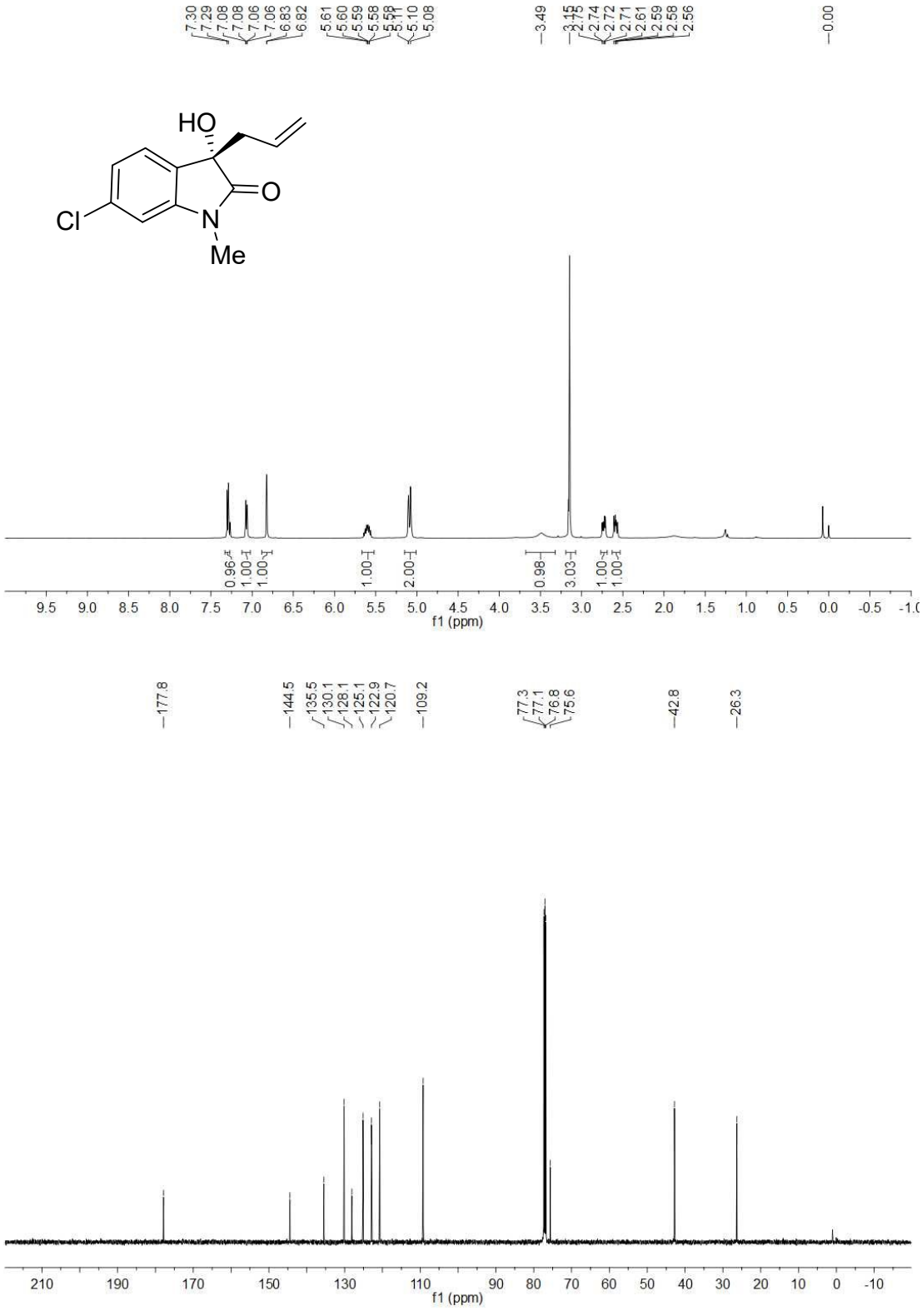
96.4
96.2
76.3
76.2
76.0
75.8
74.5
41.8
25.3
f1 (ppm)


109.88
f1 (ppm)

^{1}H NMR and ^{13}C NMR of **3ar**



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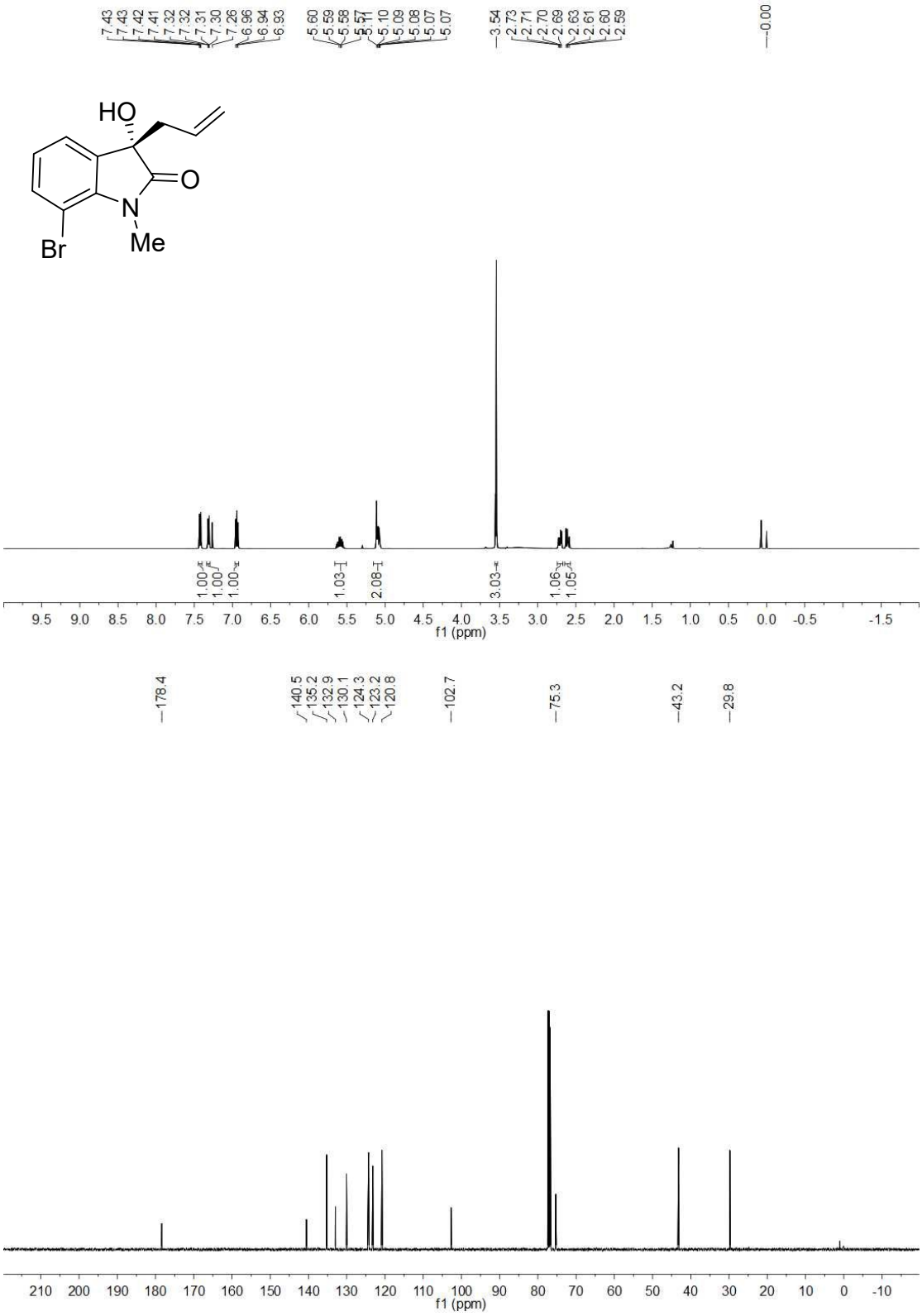
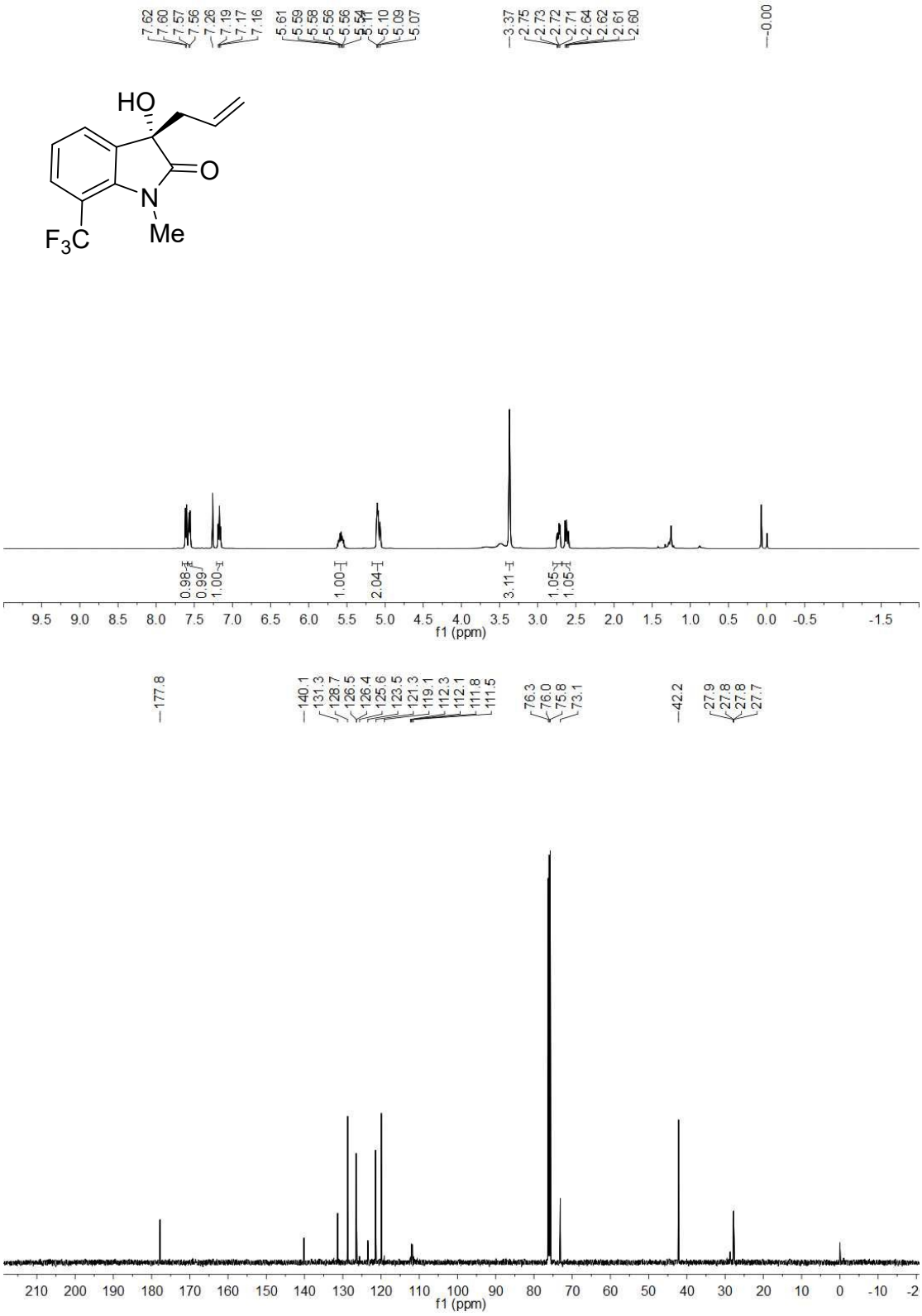
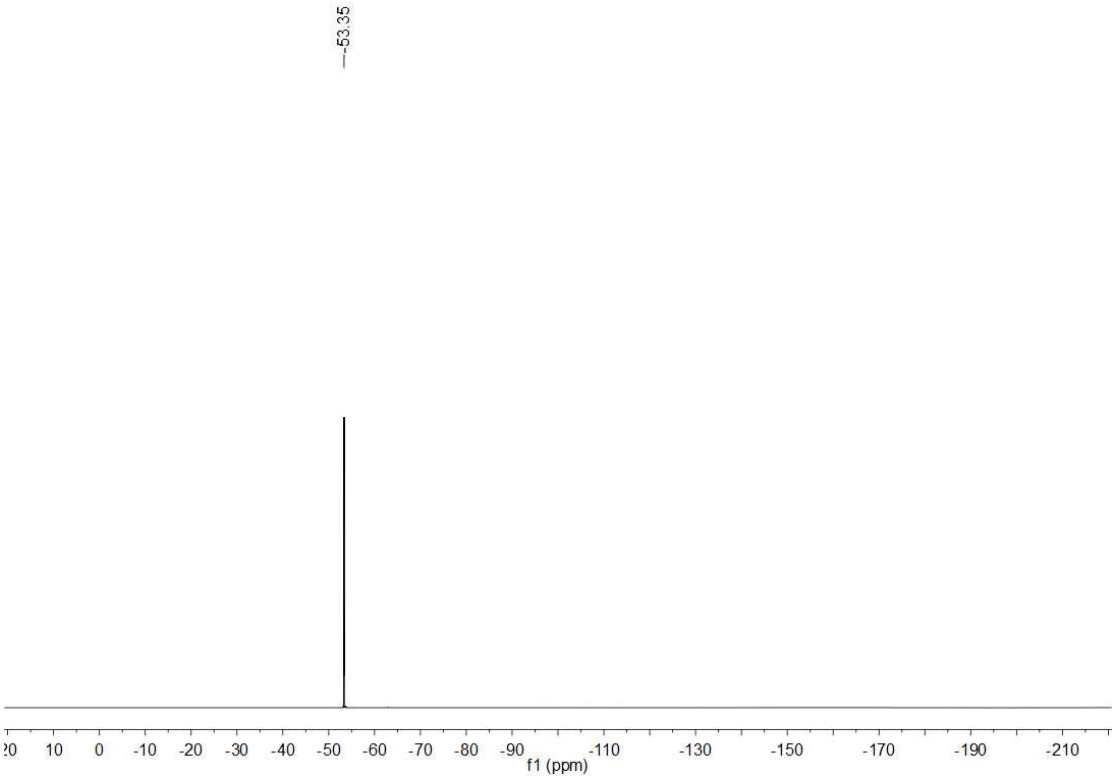
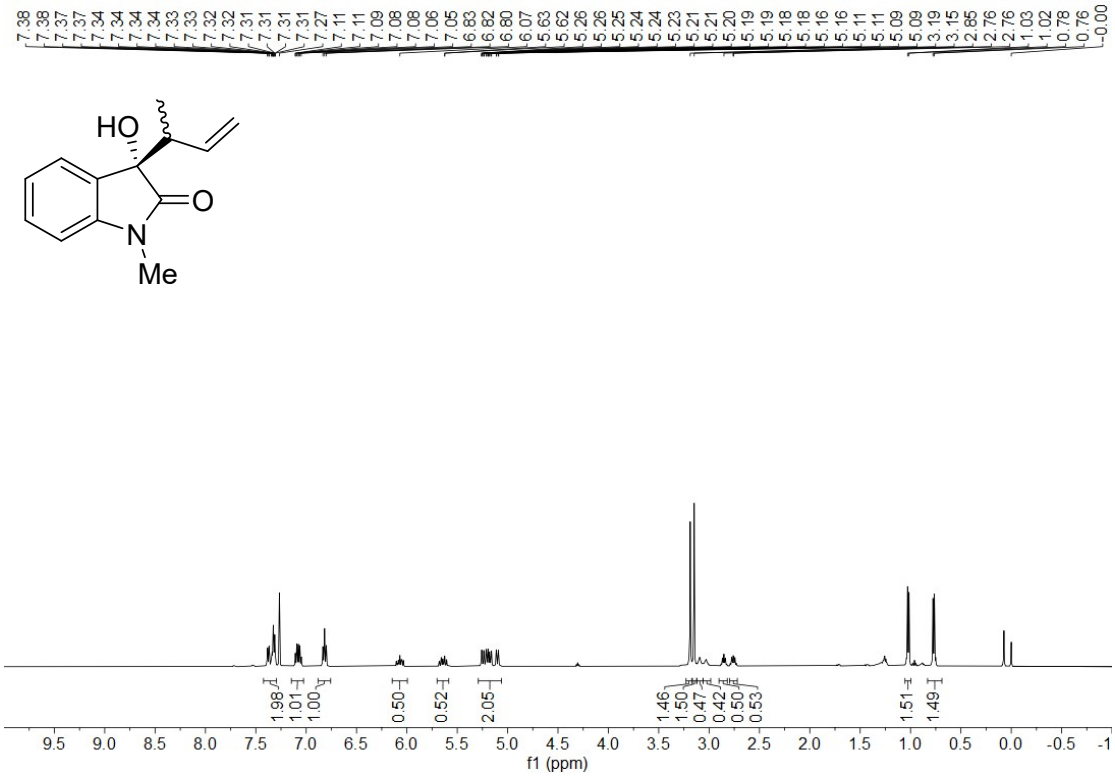


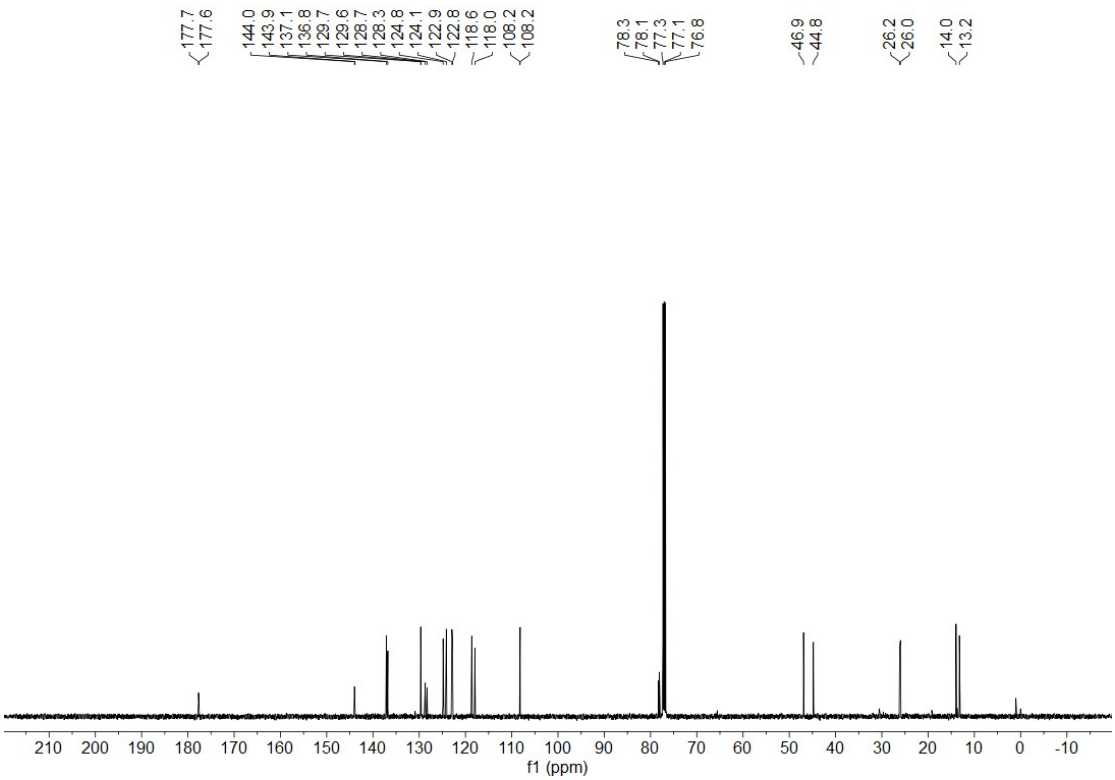
^{1}H NMR, ^{13}C NMR and ^{19}F NMR of **3at**



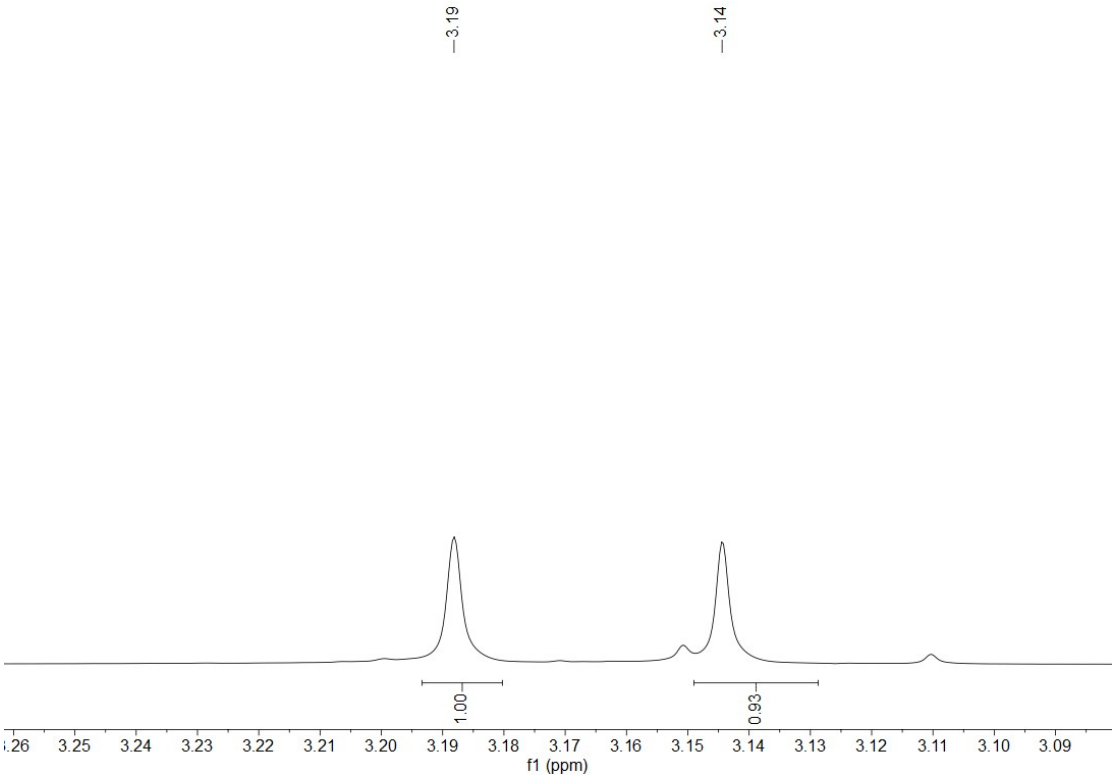


^{1}H NMR and ^{13}C NMR of **3au**



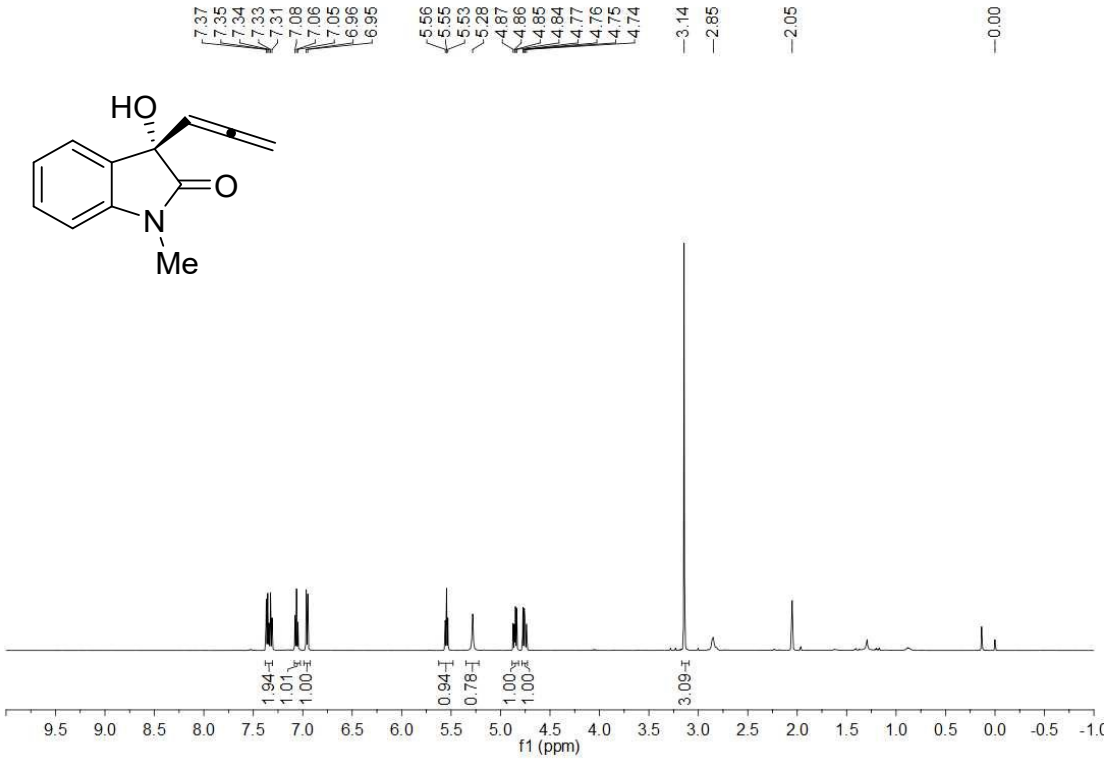


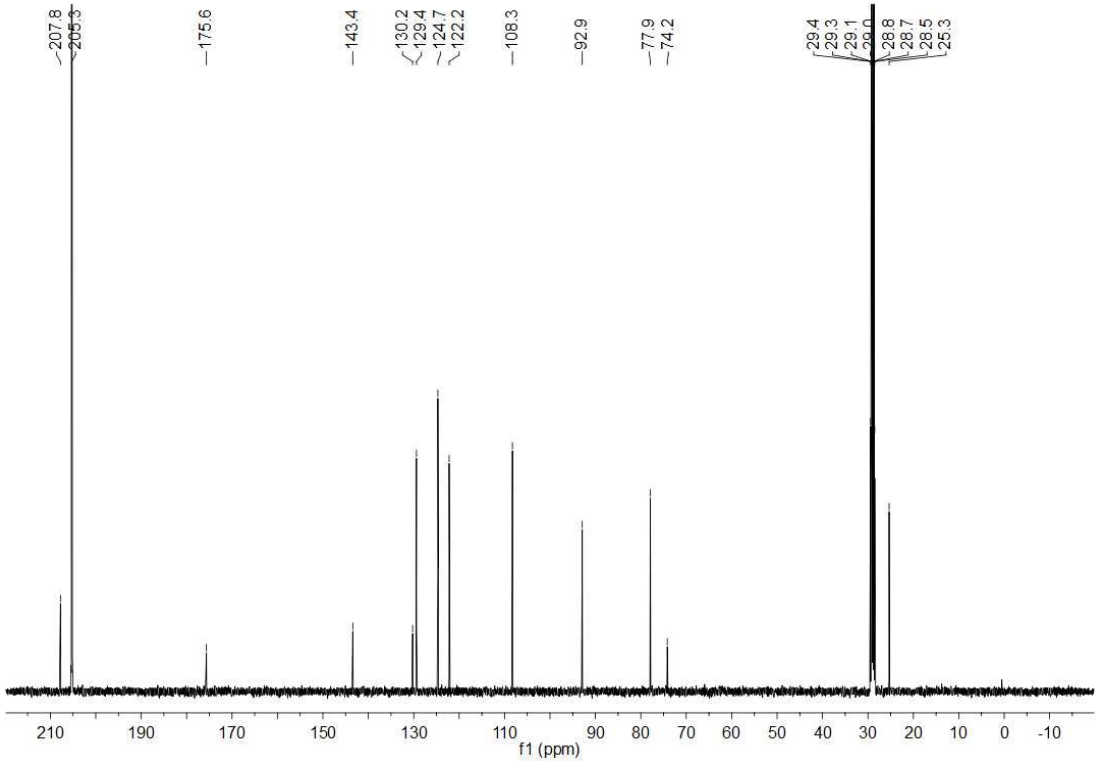
^{1}H NMR of the crude product **3au**



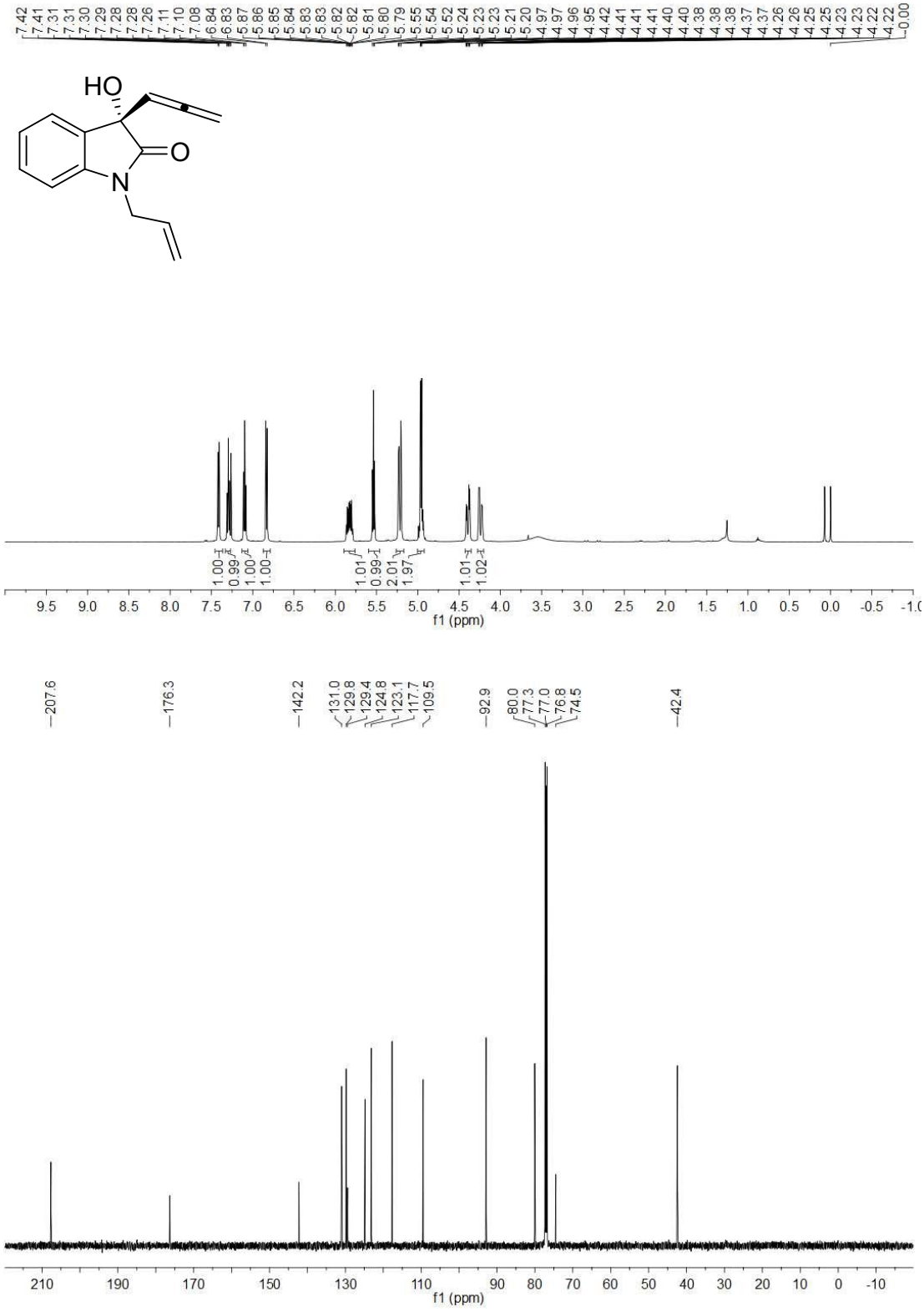
^{1}H NMR and ^{13}C NMR of **3av**

^{1}H NMR and ^{13}C NMR of **3ba**

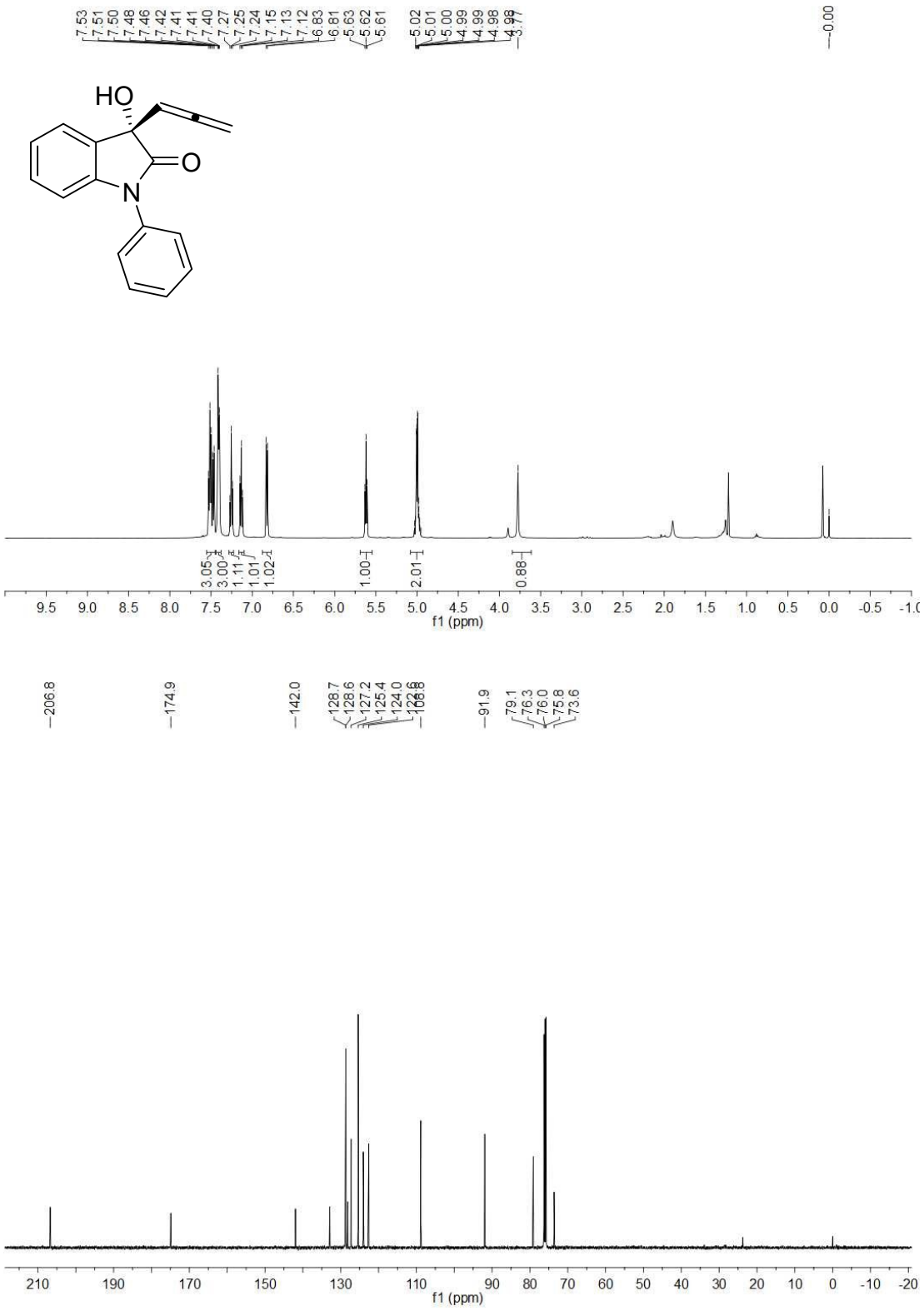




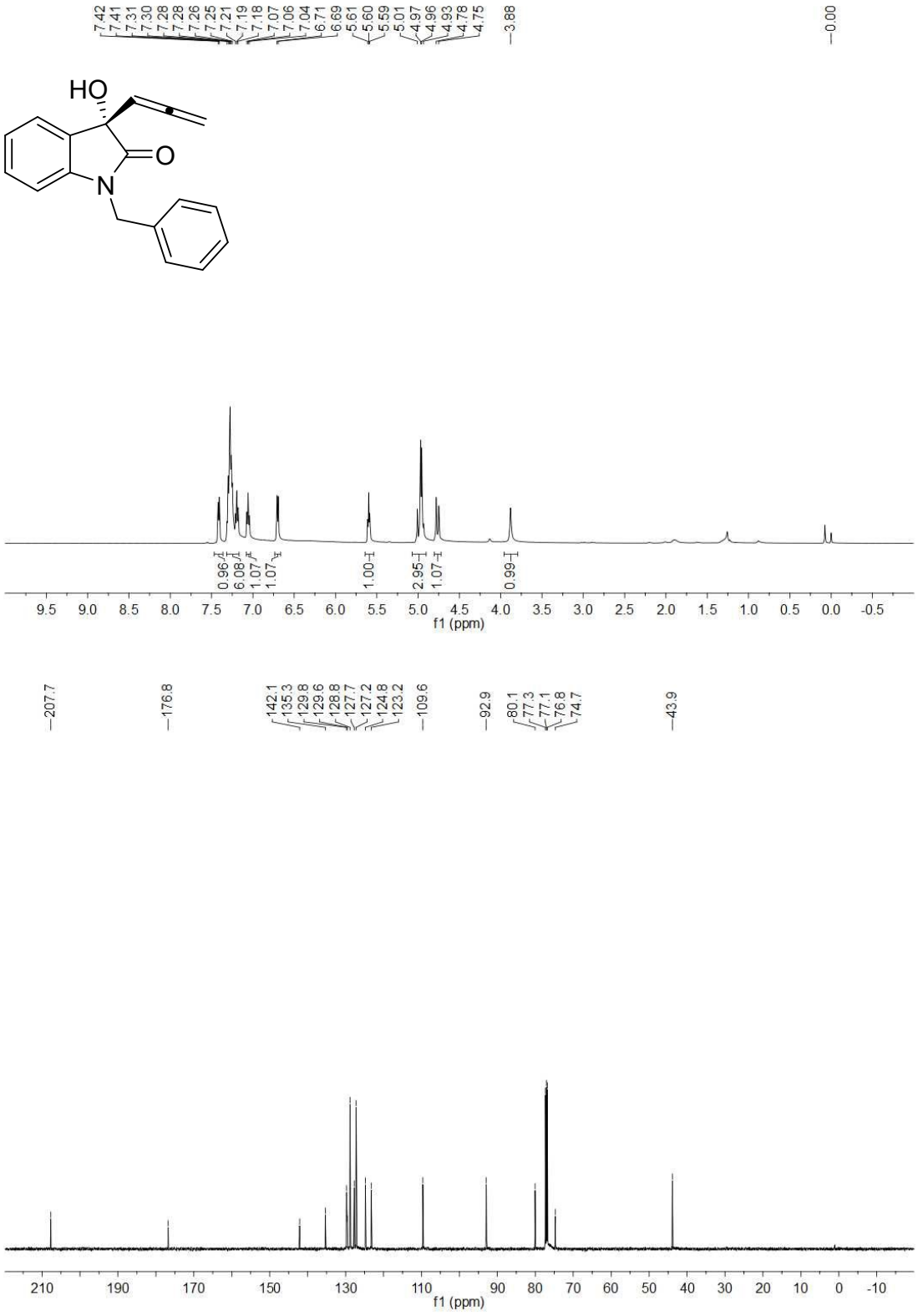
^{1}H NMR and ^{13}C NMR of **3bb**



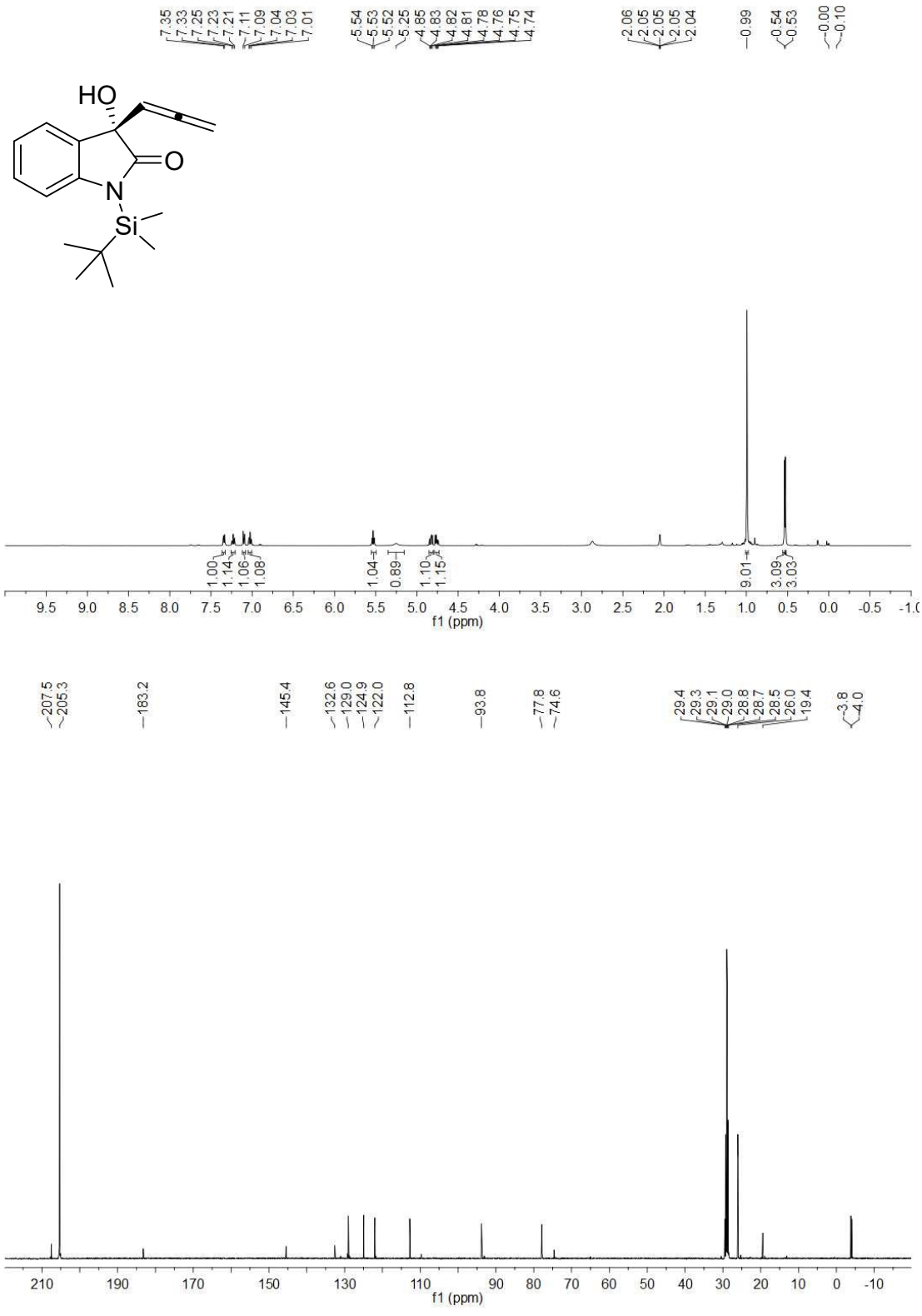
^{1}H NMR and ^{13}C NMR of **3bc**



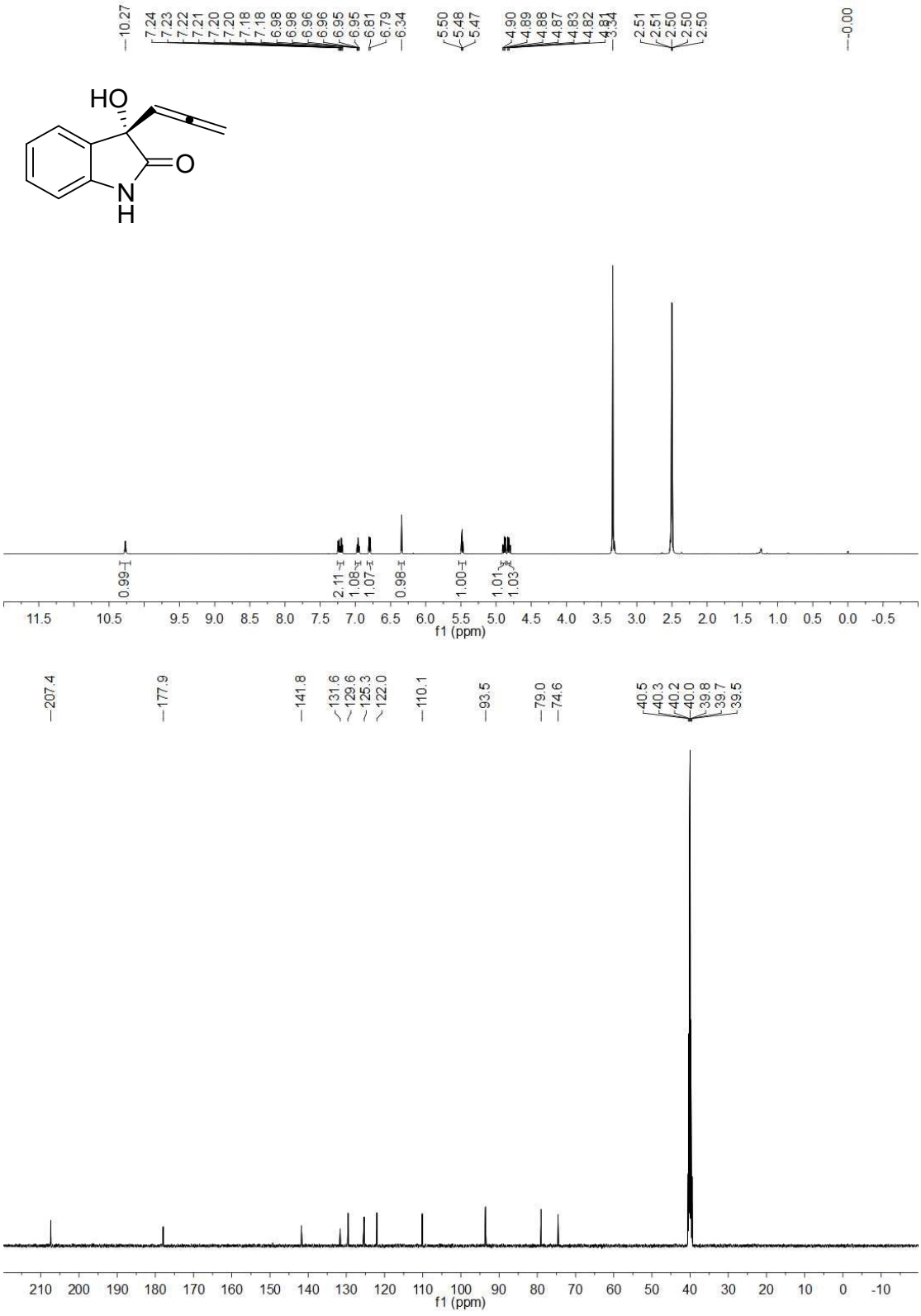
^{1}H NMR and ^{13}C NMR of **3bd**



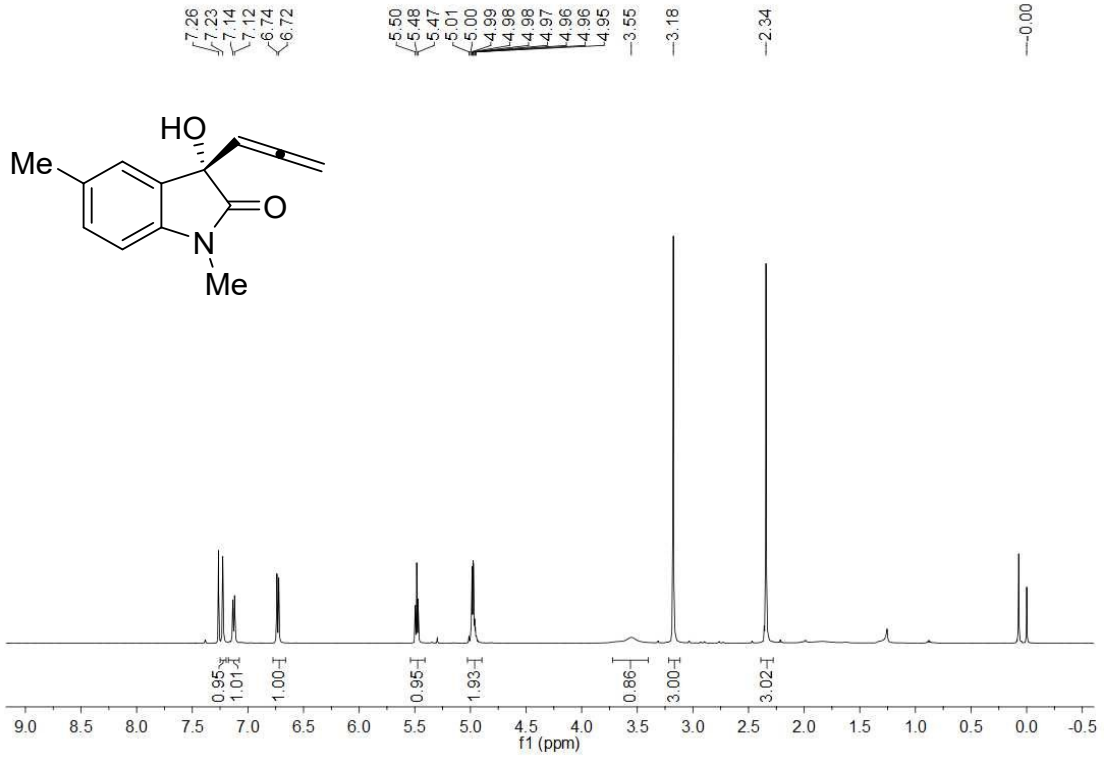
^{1}H NMR and ^{13}C NMR of **3be**

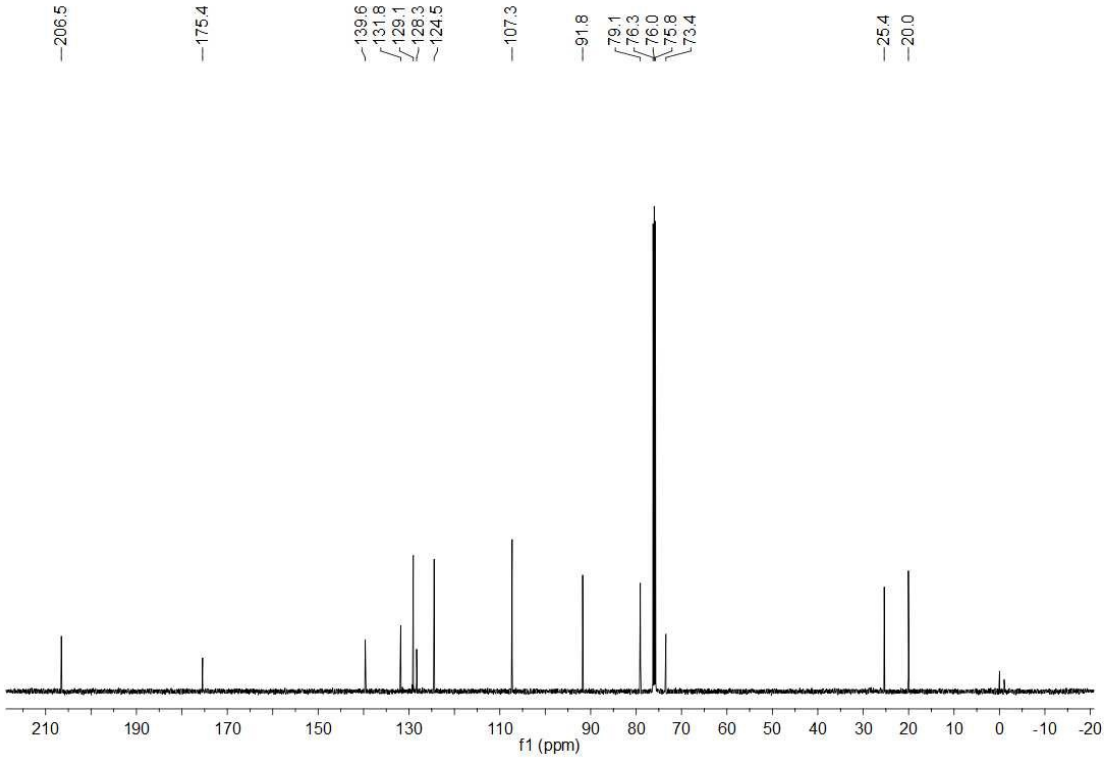


^{1}H NMR and ^{13}C NMR of **3bf**

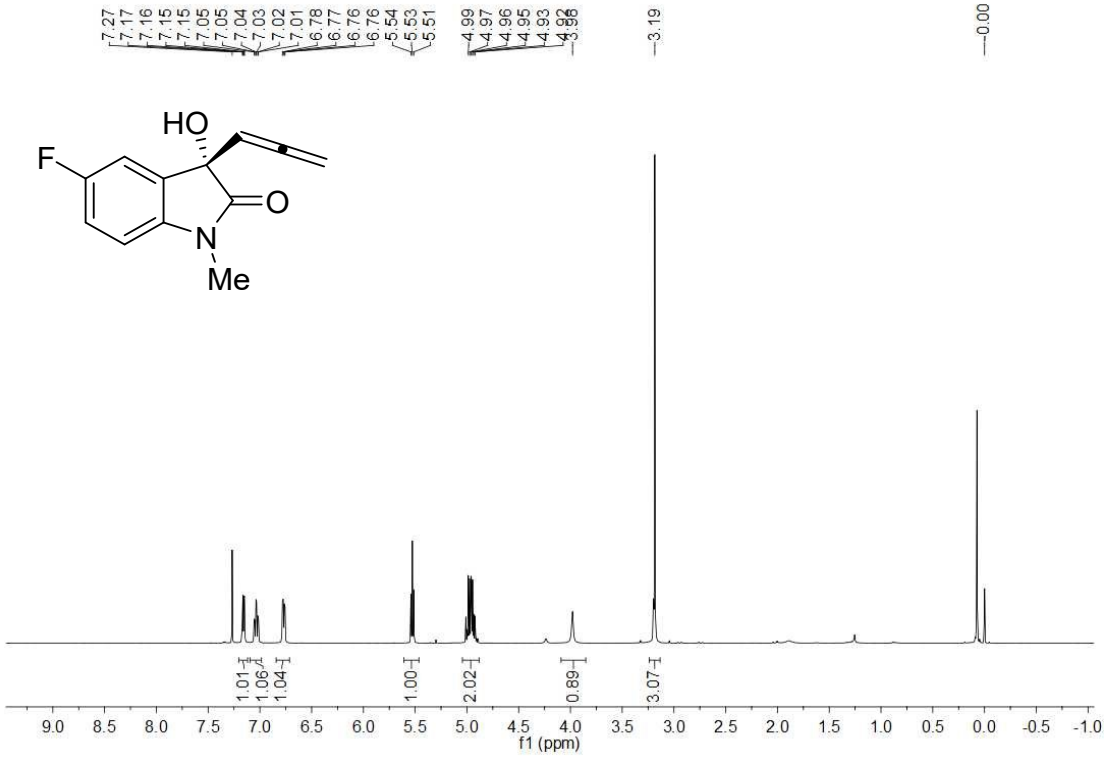


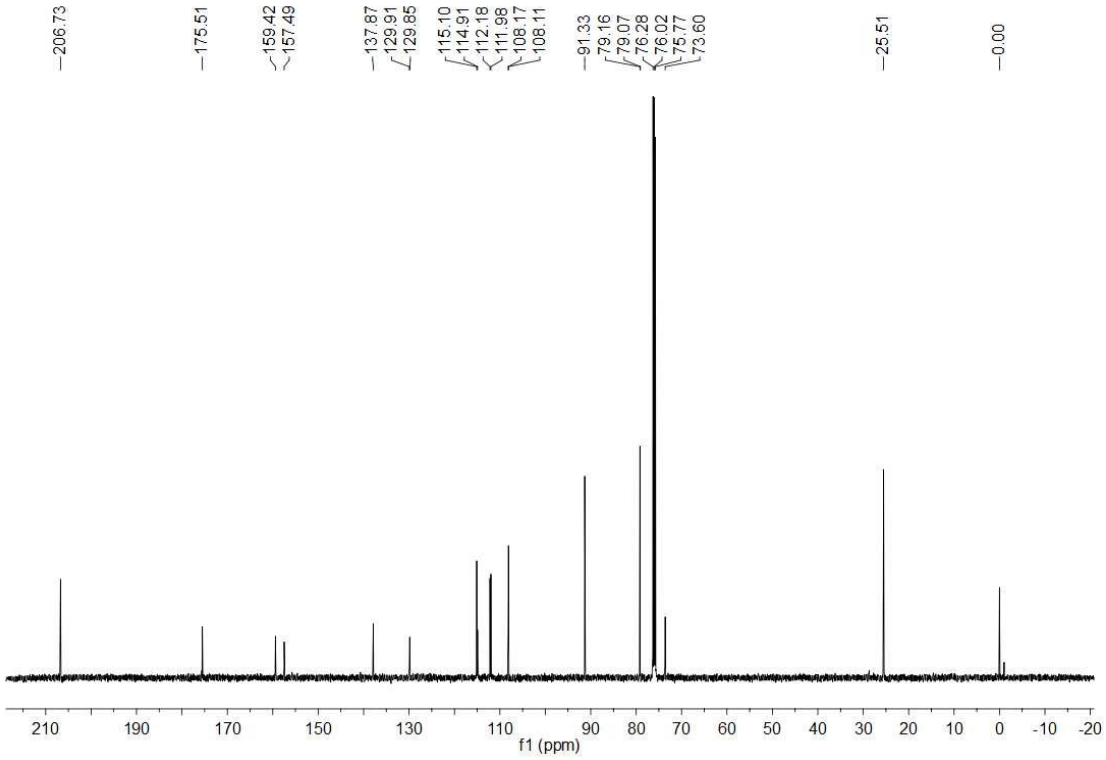
^{1}H NMR and ^{13}C NMR of **3bg**

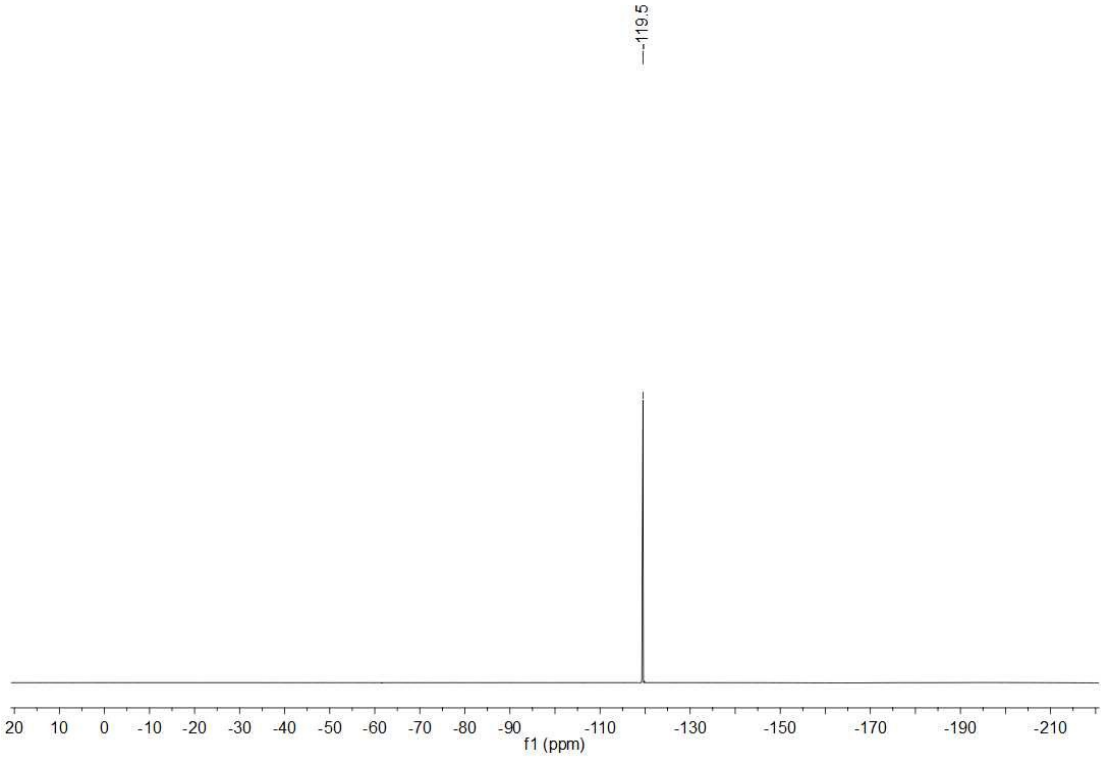




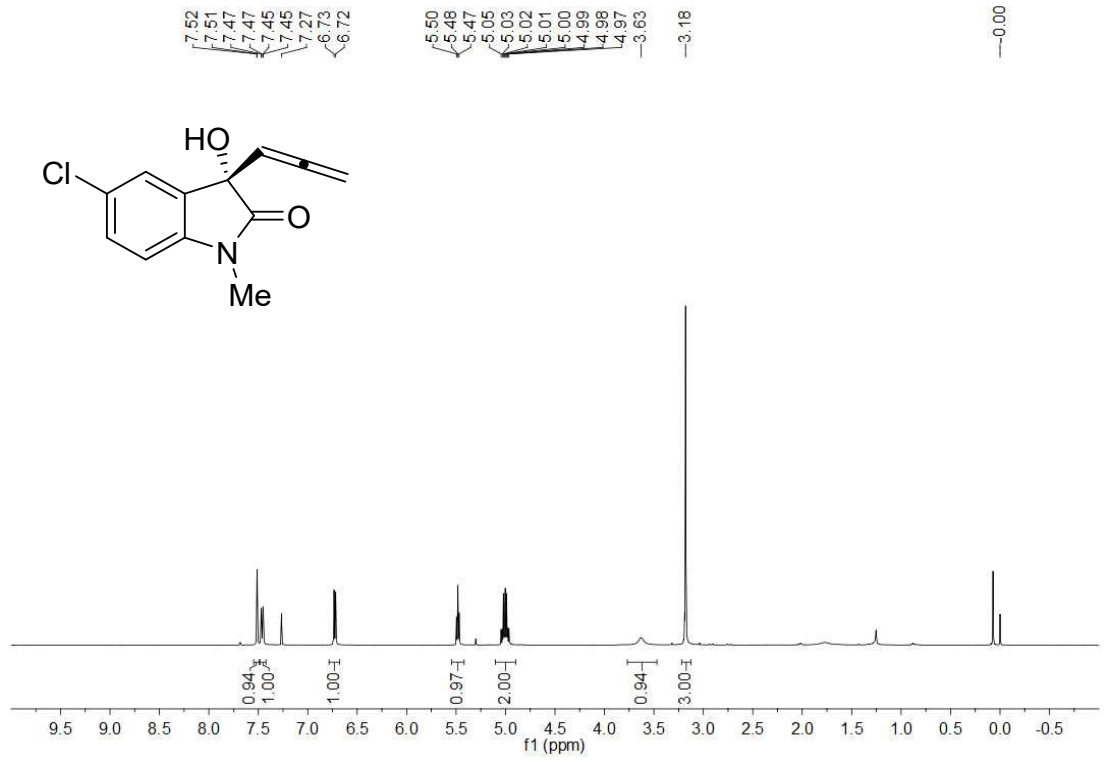
^{1}H NMR and ^{13}C NMR of **3bh**

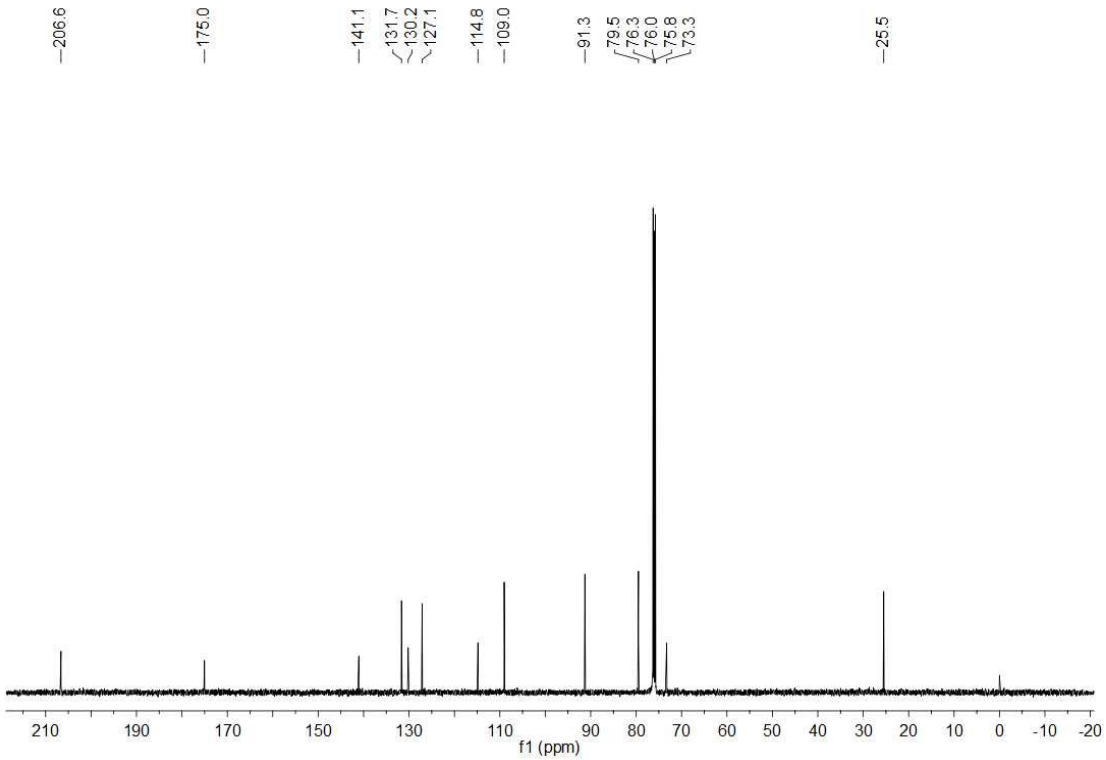




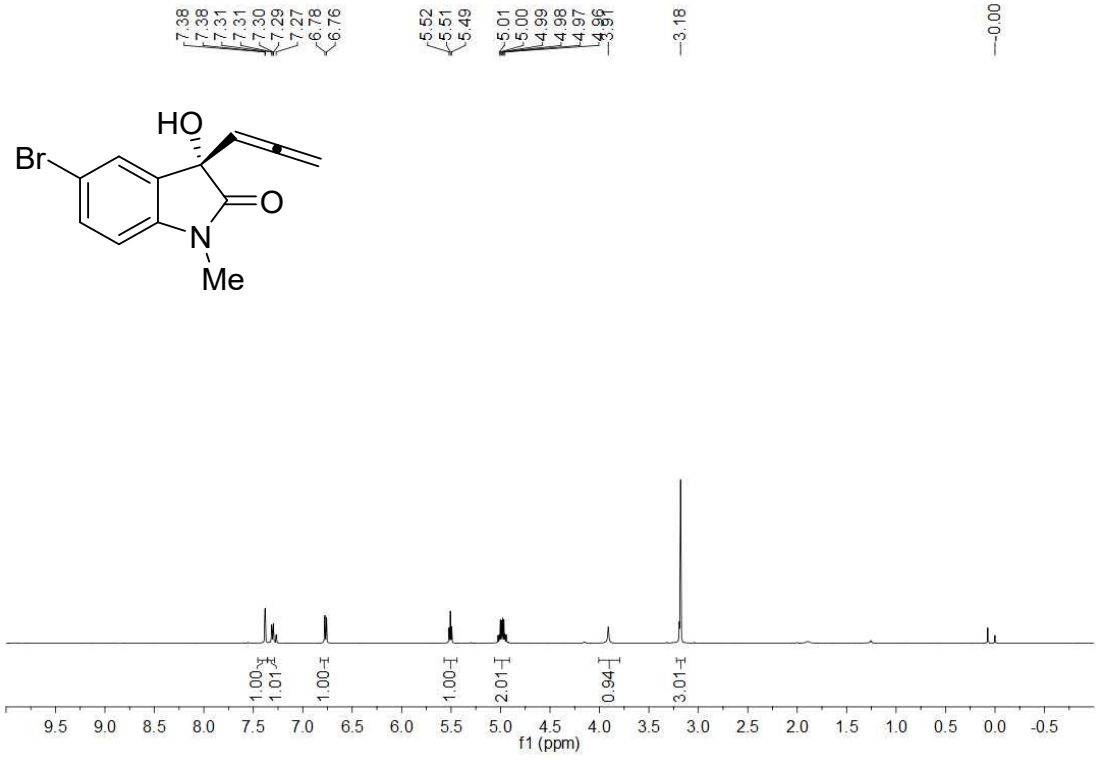


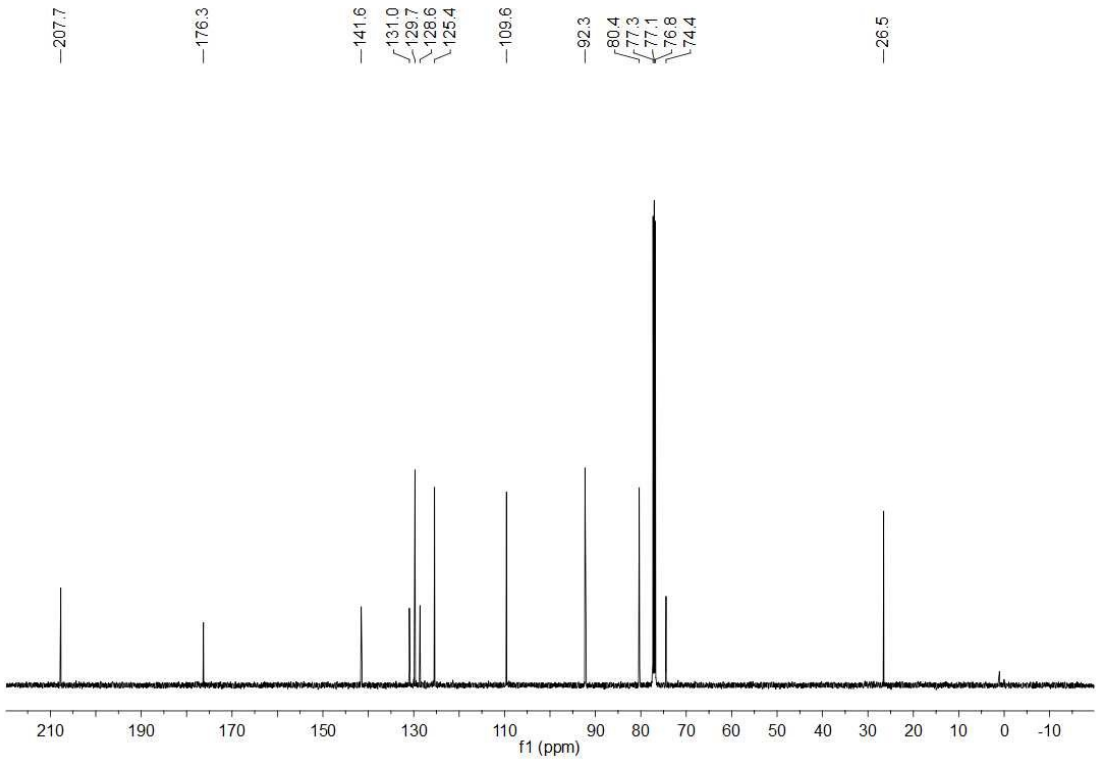
^{1}H NMR and ^{13}C NMR of **3bi**



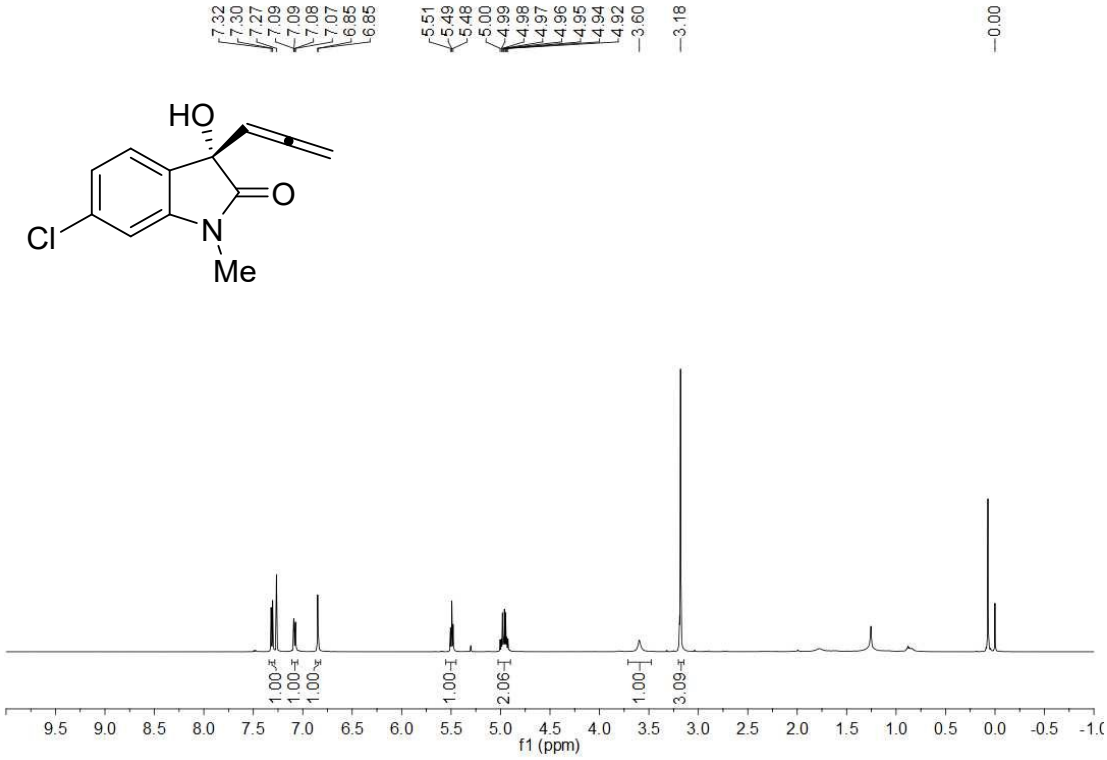


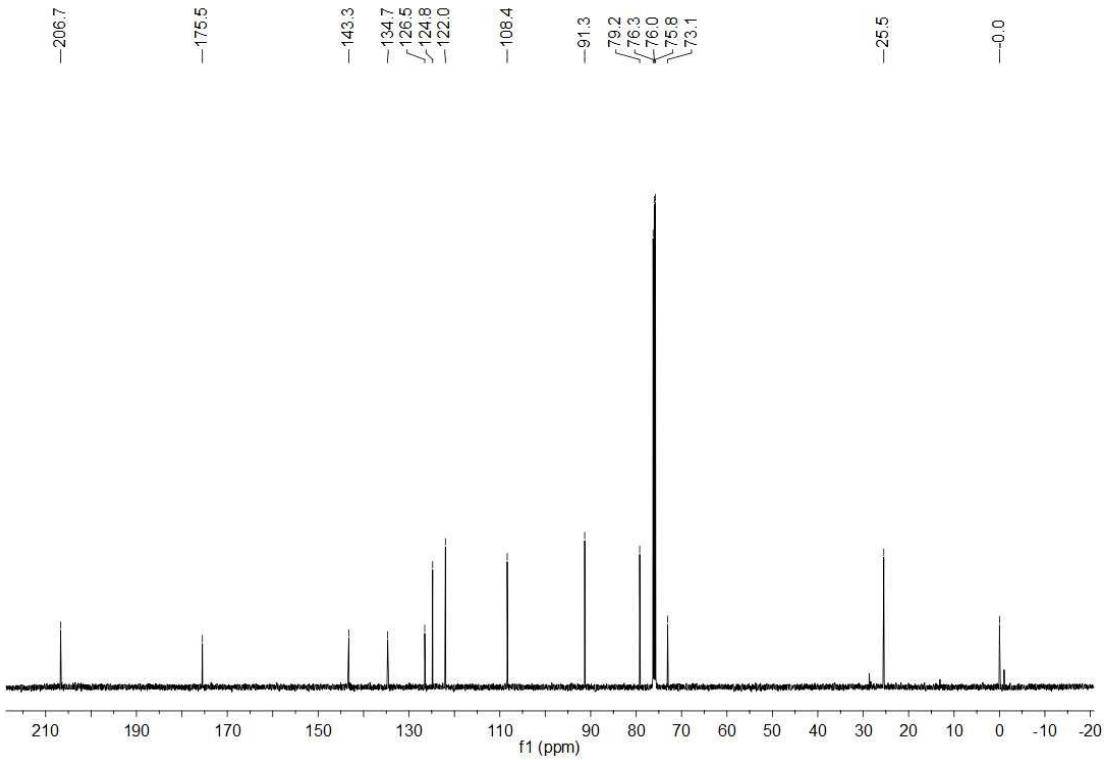
^{1}H NMR and ^{13}C NMR of **3bj**



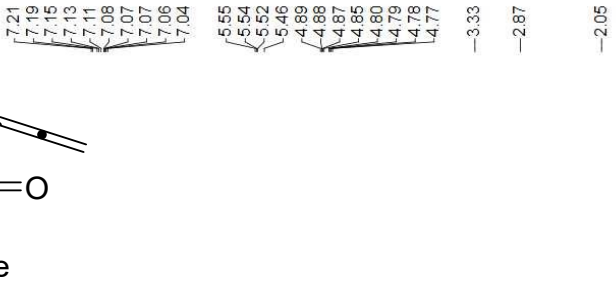


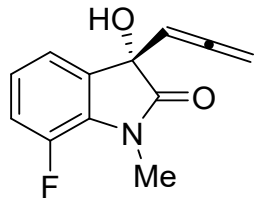
^{1}H NMR and ^{13}C NMR of **3bk**

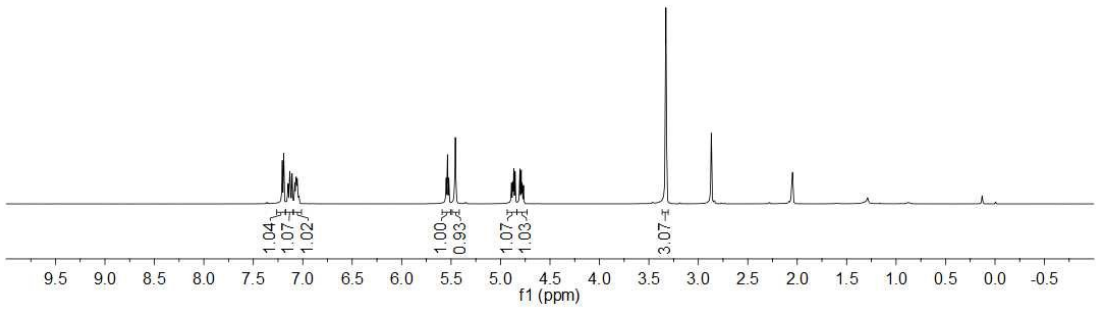


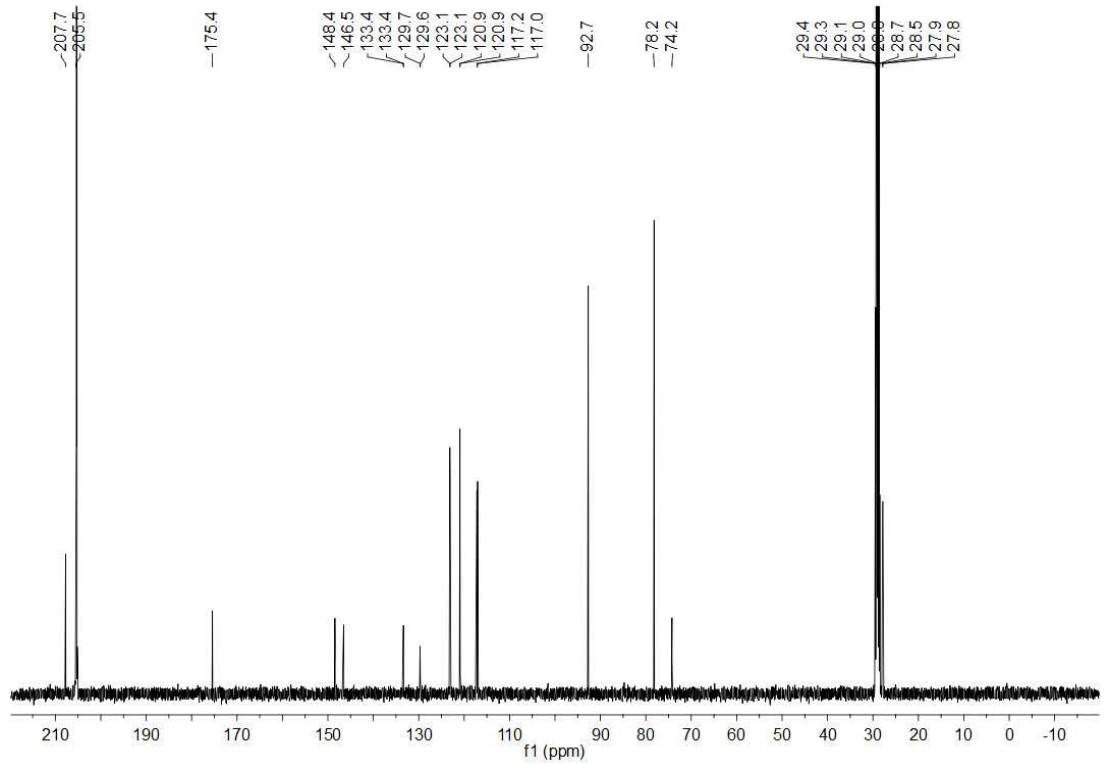


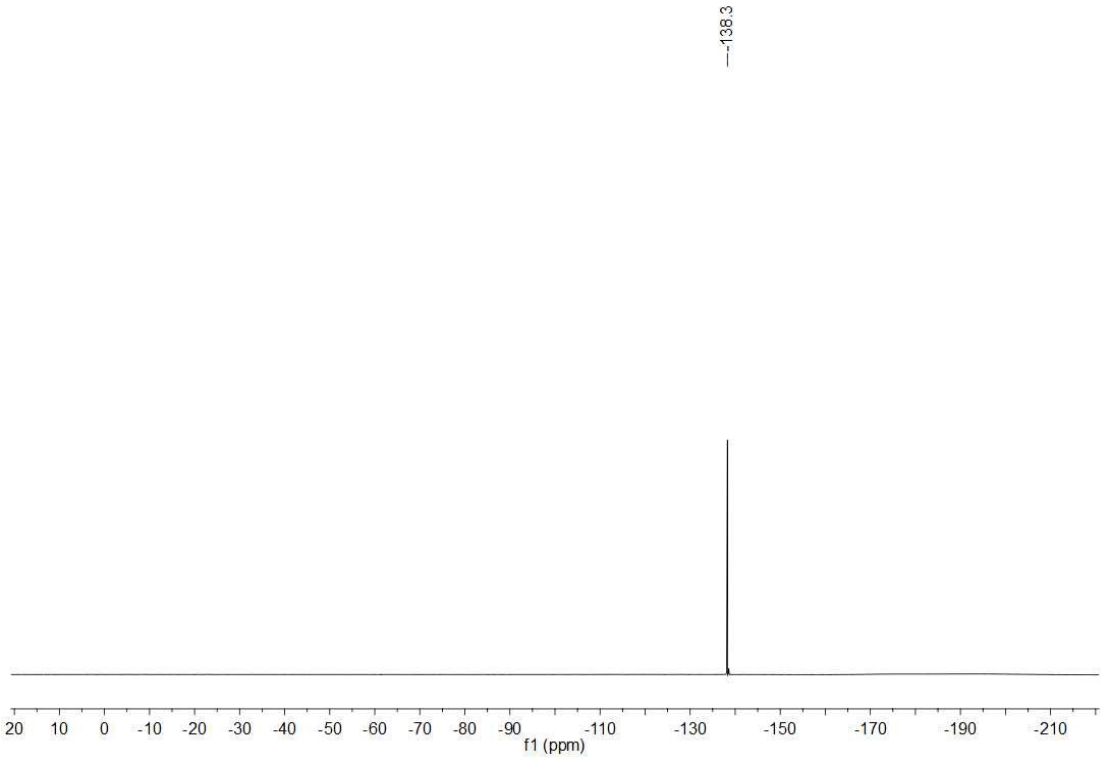
^{1}H NMR and ^{13}C NMR of **3bl**



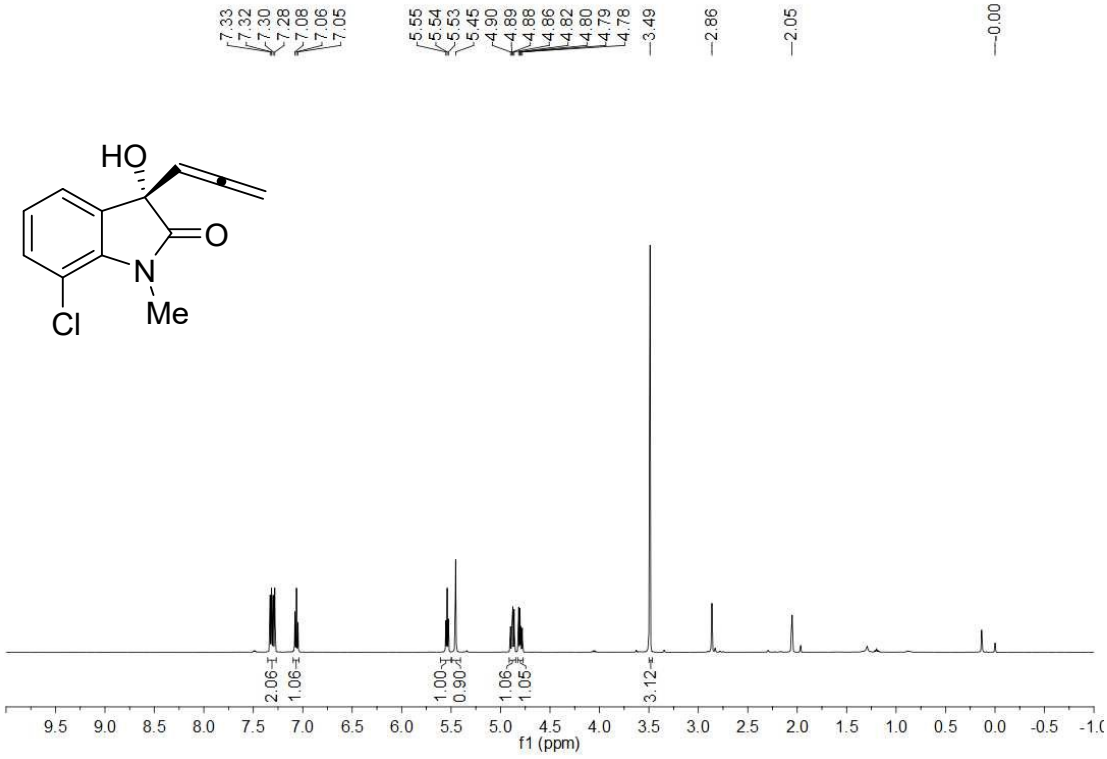


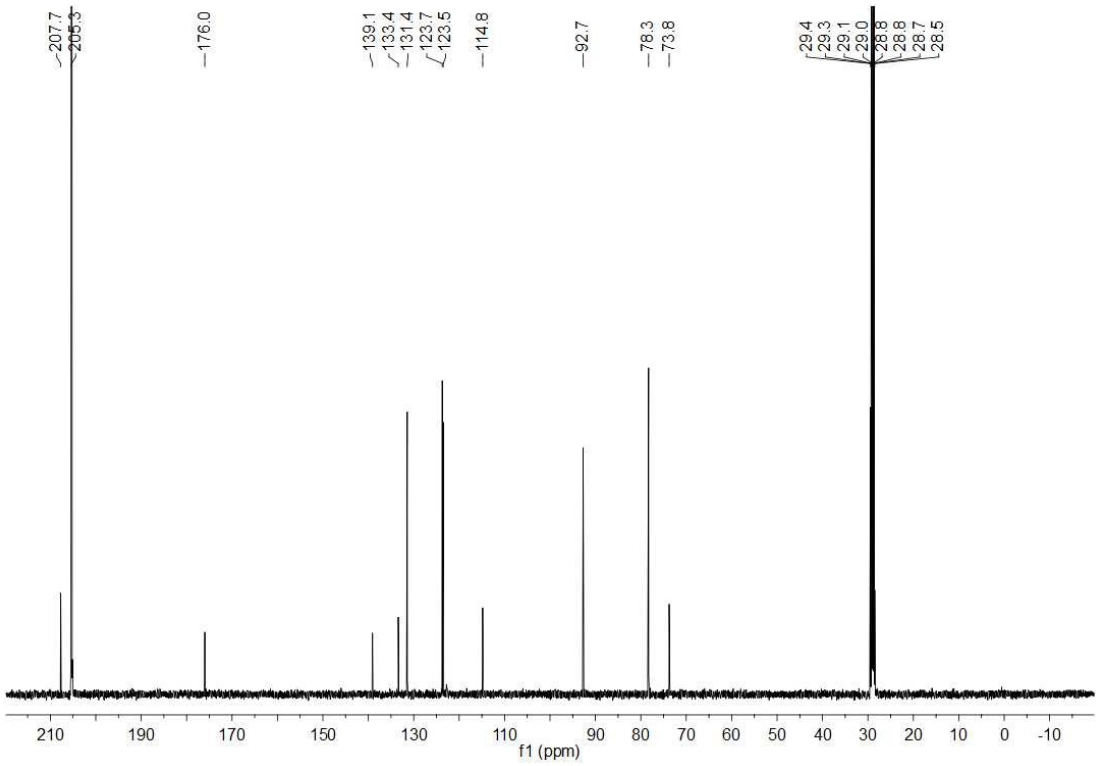



207.7
205.5
175.4
148.4
146.5
133.4
133.4
129.7
129.6
123.1
123.1
120.9
120.9
117.2
117.0
92.7
78.2
74.2
29.4
29.3
29.1
29.0
28.7
28.5
27.9
27.8
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

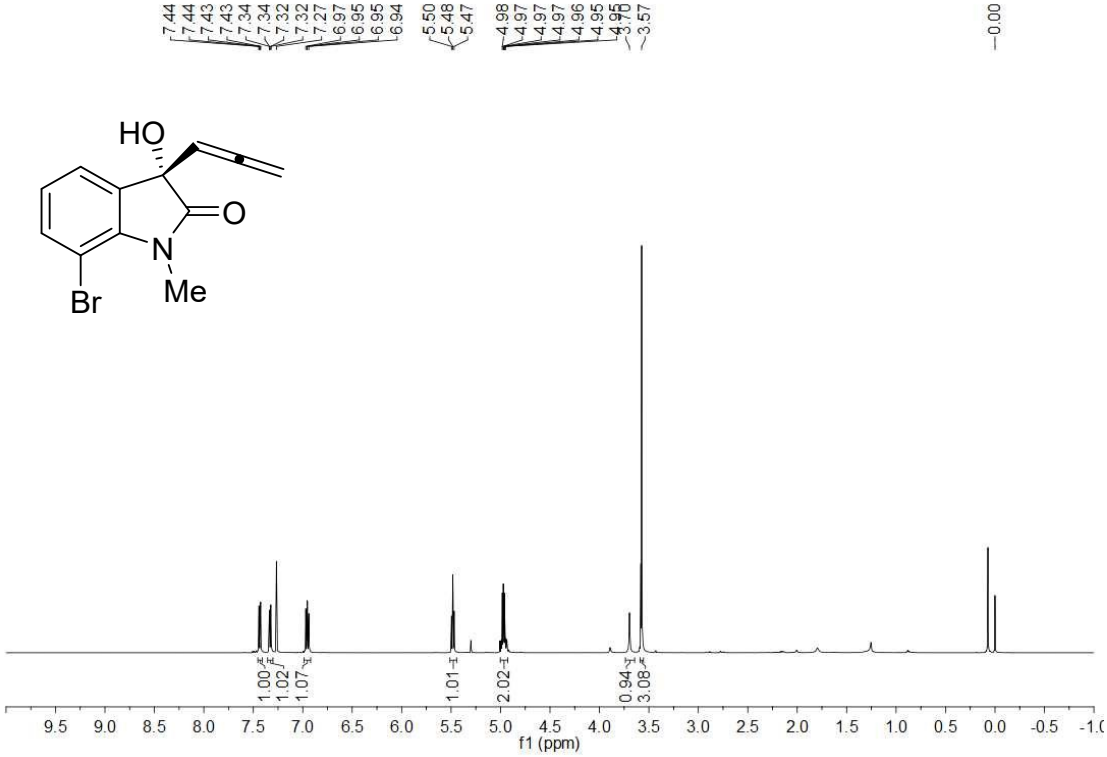

138.3
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

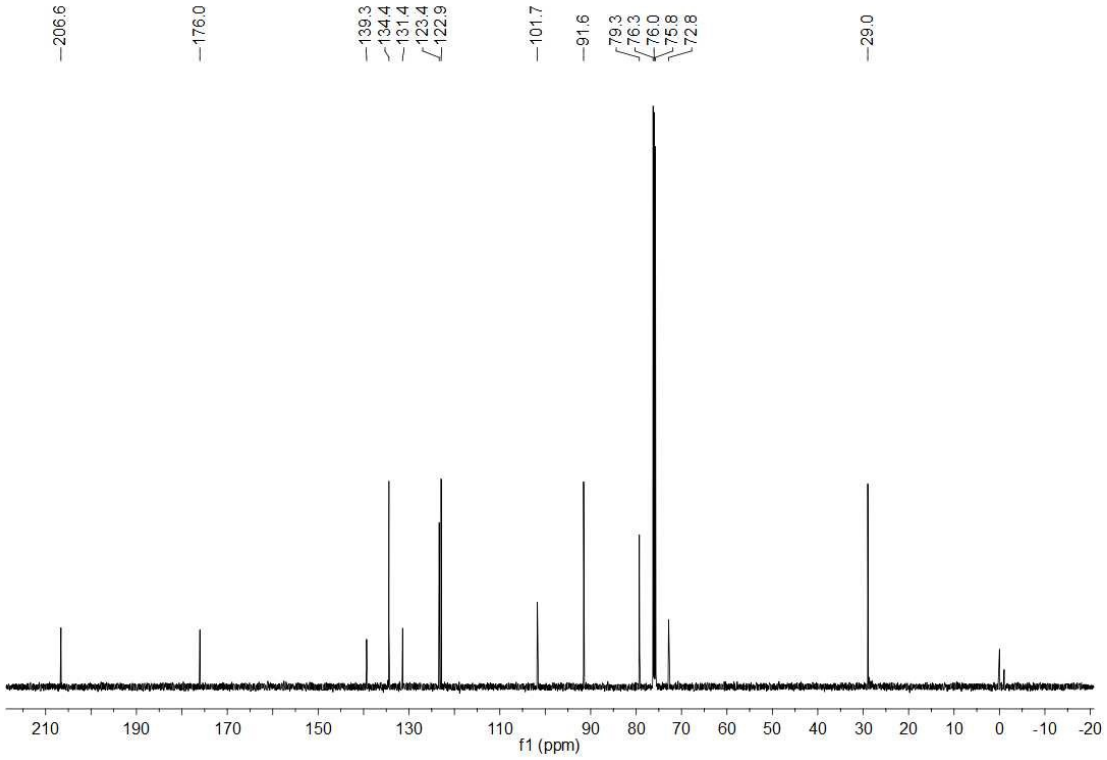
^{1}H NMR and ^{13}C NMR of **3bm**



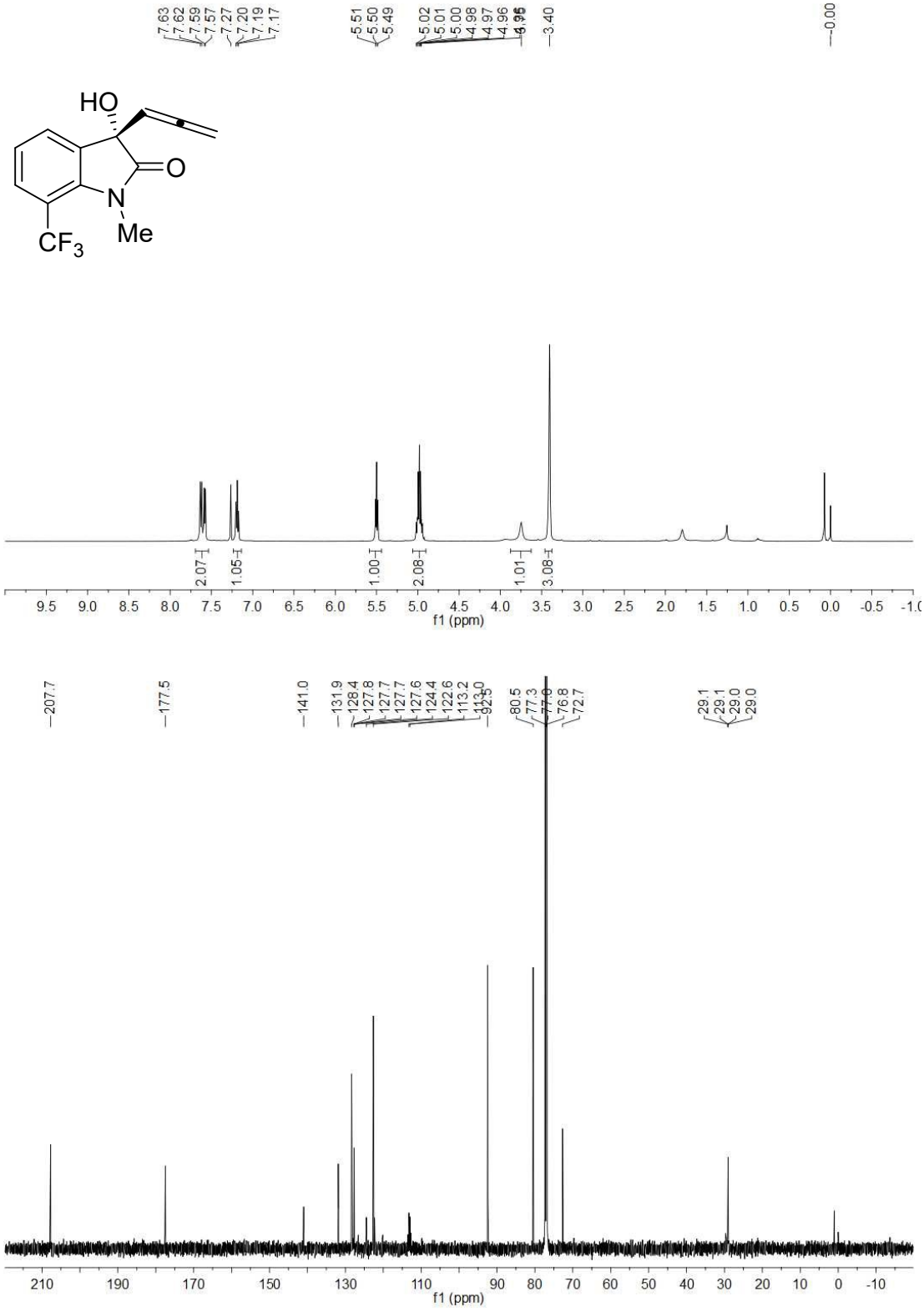


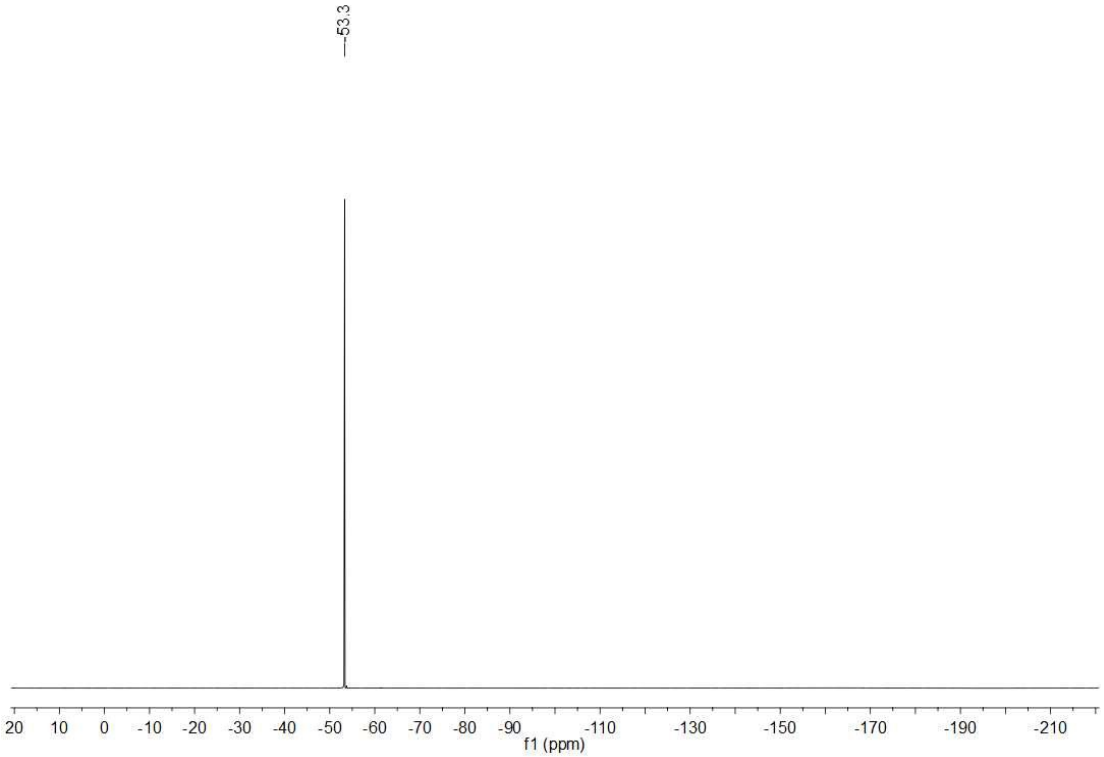
^{1}H NMR and ^{13}C NMR of **3bn**



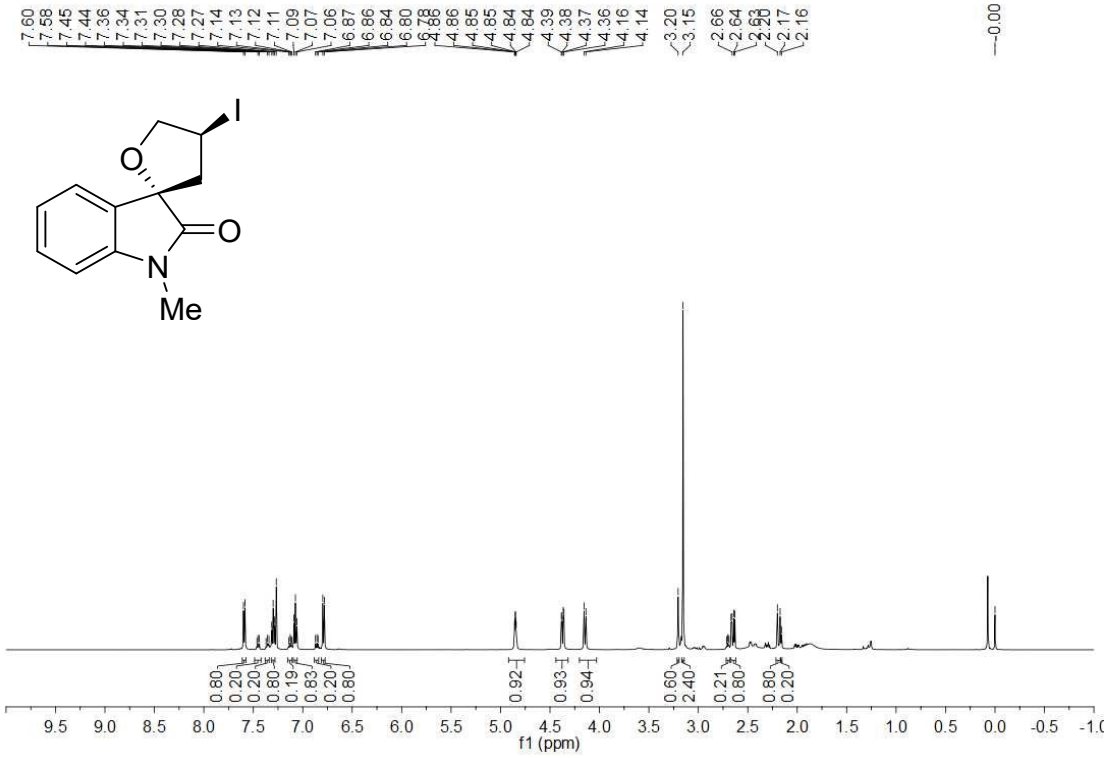


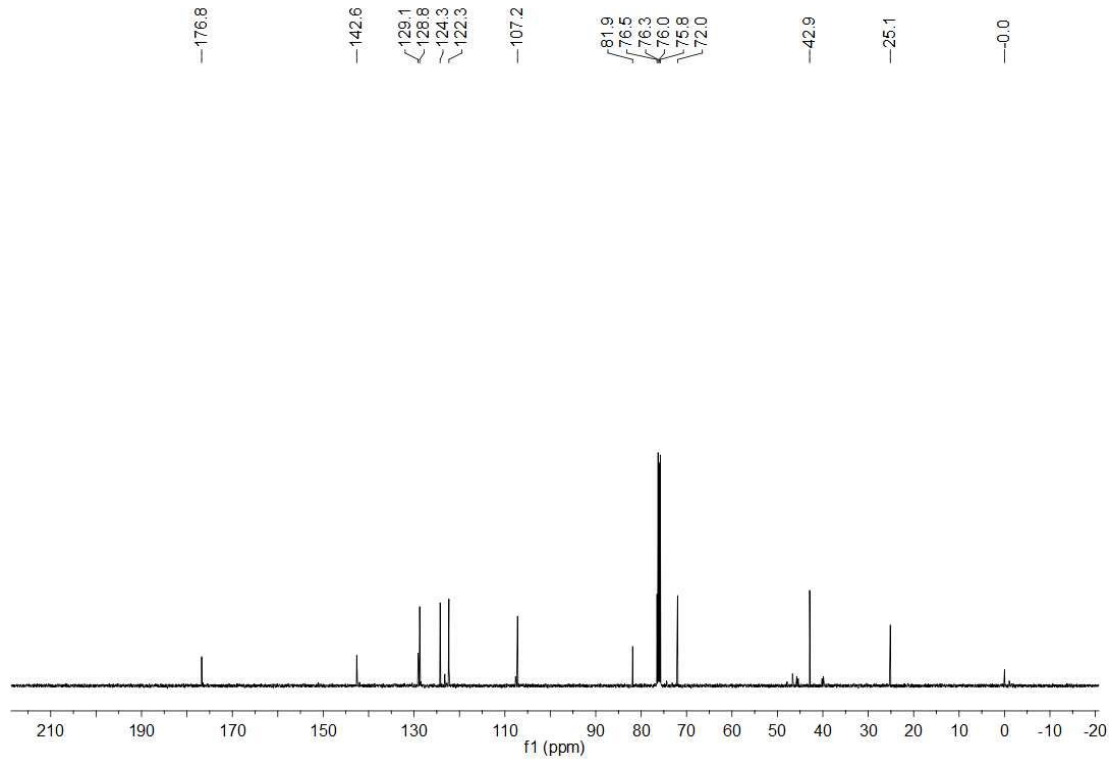
^{1}H NMR and ^{13}C NMR of **3bo**



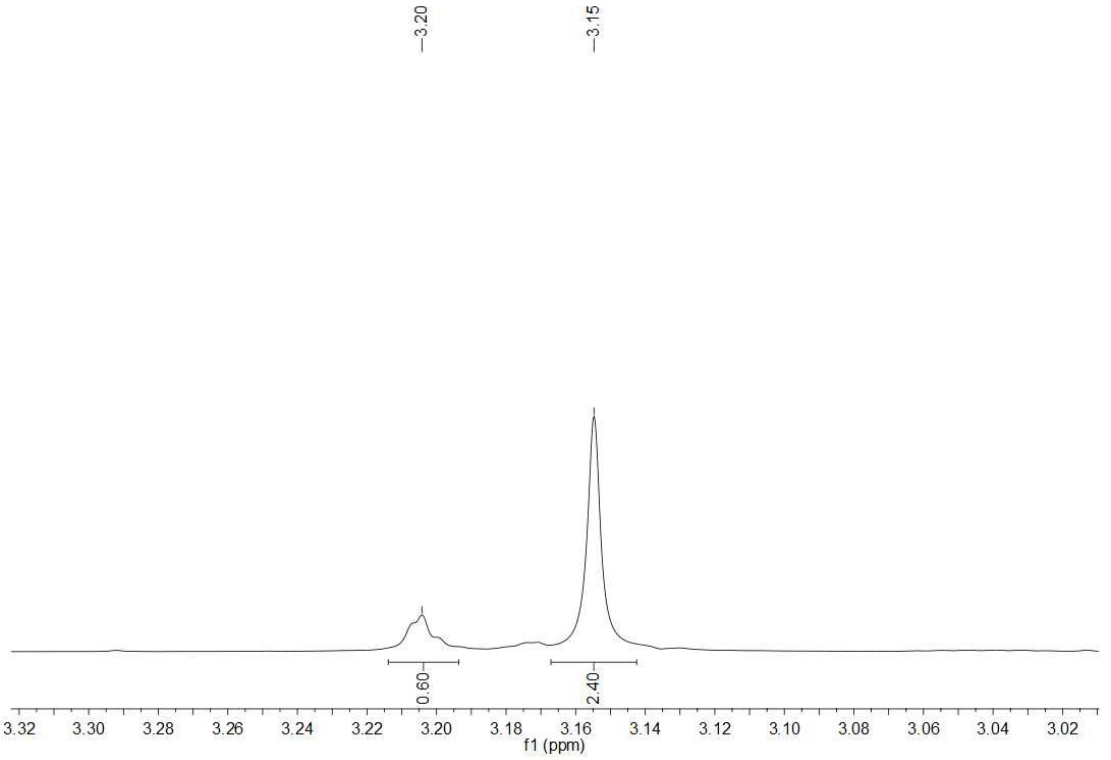


^{1}H NMR and ^{13}C NMR of **4a**

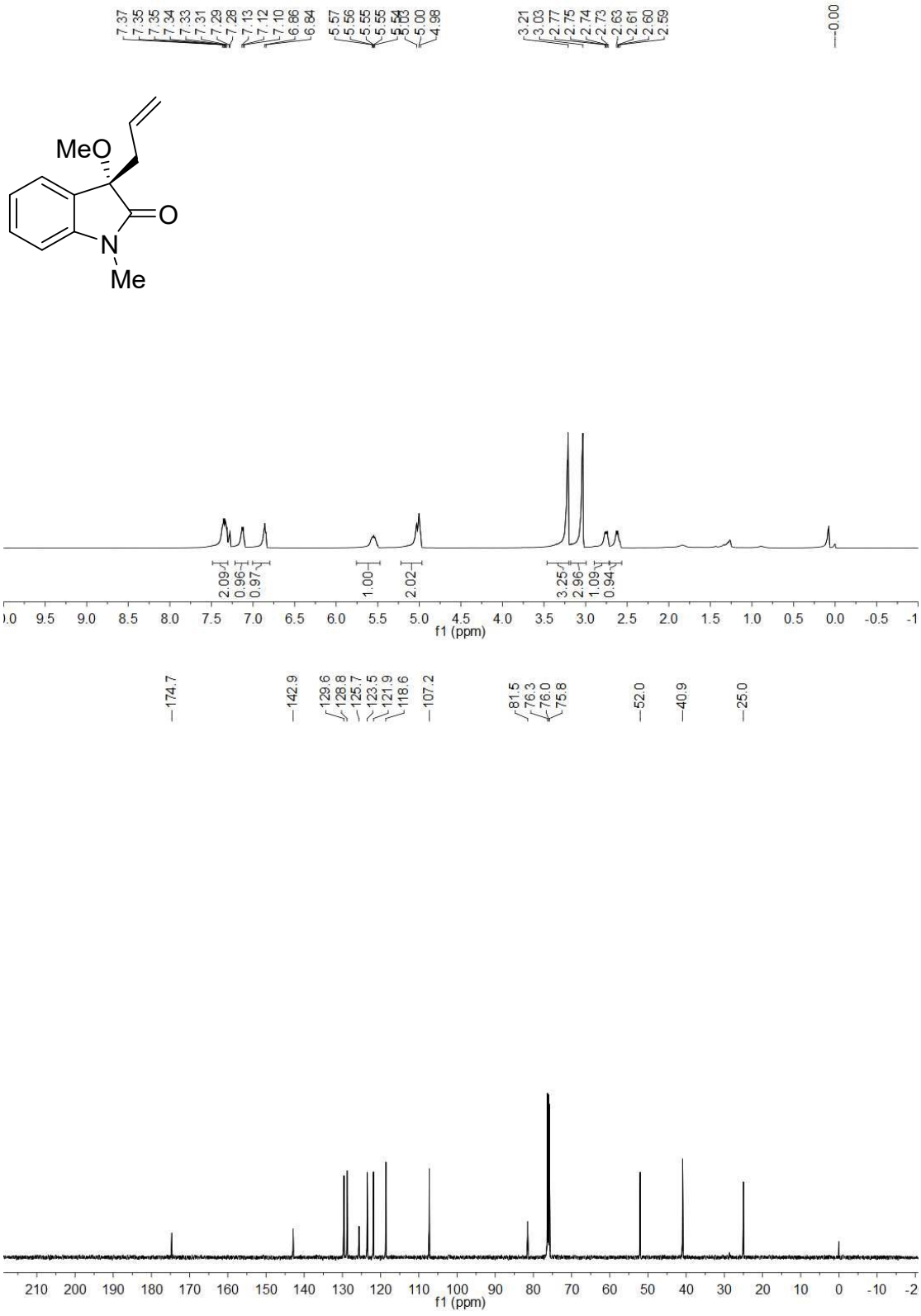




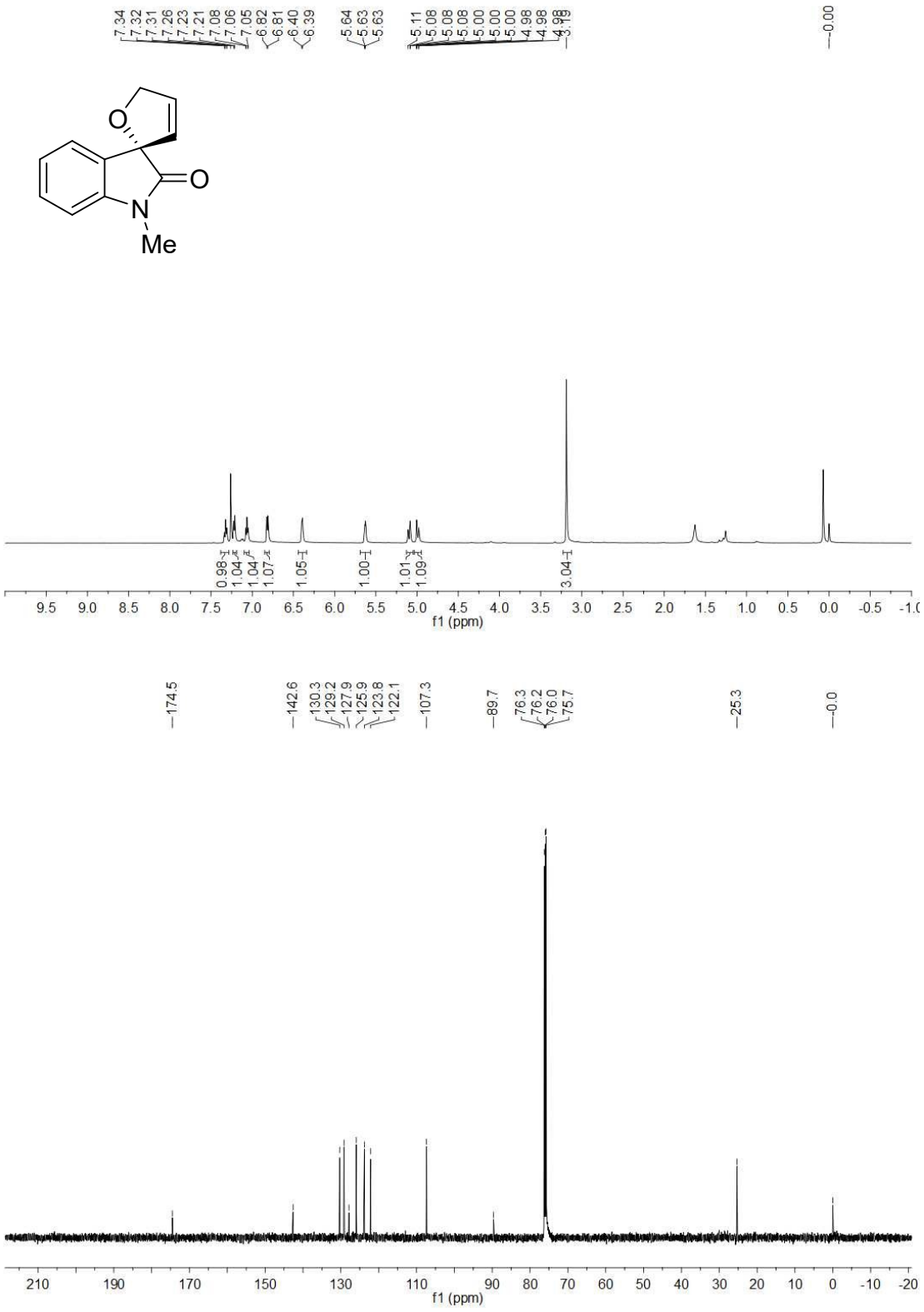
^{1}H NMR of the crude product **4a**



^{1}H NMR and ^{13}C NMR of **4b**

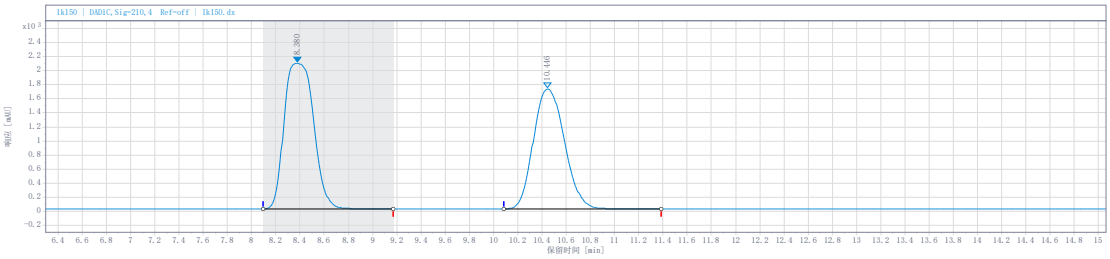


^{1}H NMR and ^{13}C NMR of **4c**



Part III HPLC Spectra

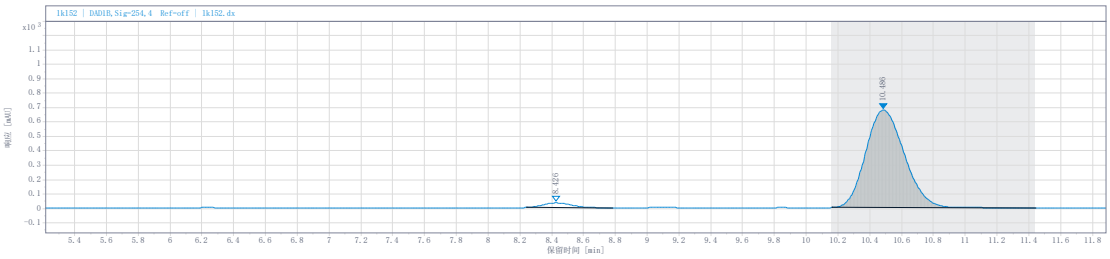
3aa racemic mixture



Signal: DAD1C, Sig=210, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.38	1.08	35074.72	2067.48	53.48
10.4	1.30	30513.54	1707.63	46.52

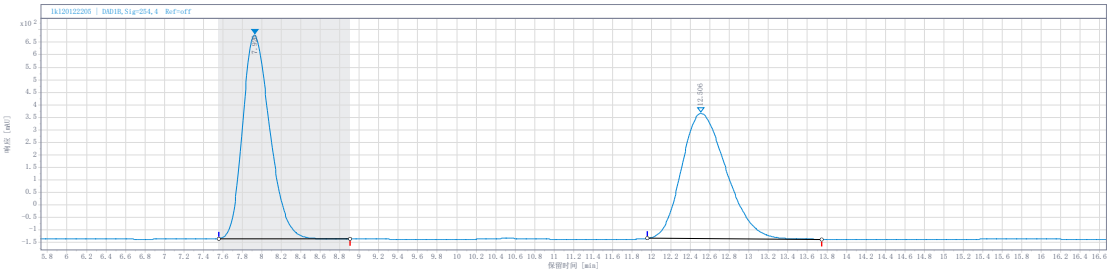
3aa



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.43	0.54	410.60	32.83	3.47
10.5	1.28	11427.23	677.23	96.53

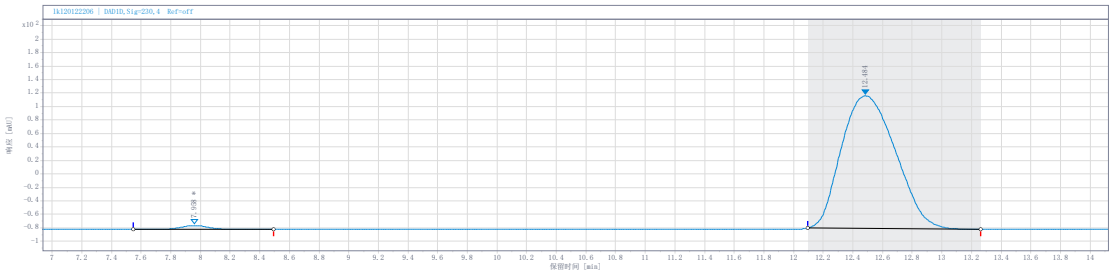
3ab racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.93	1.35	15822.07	816.01	49.73
12.5	1.79	15996.56	501.17	50.27

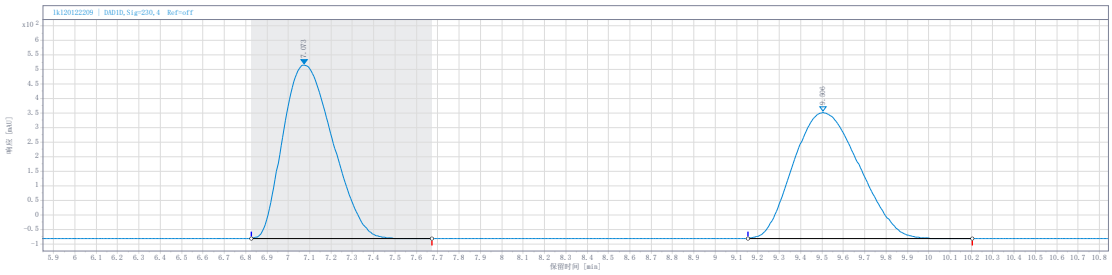
3ab



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.96	0.95	79.74	6.04	1.57
12.5	1.17	5002.99	196.93	98.43

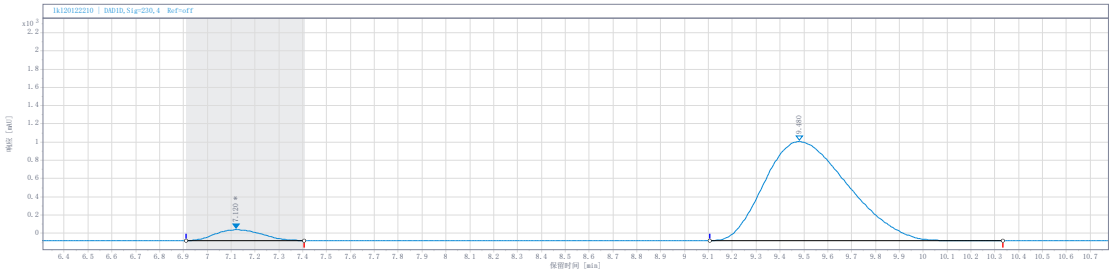
3ac racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.07	0.85	9659.63	596.80	50.98
9.51	1.05	9287.80	432.69	49.02

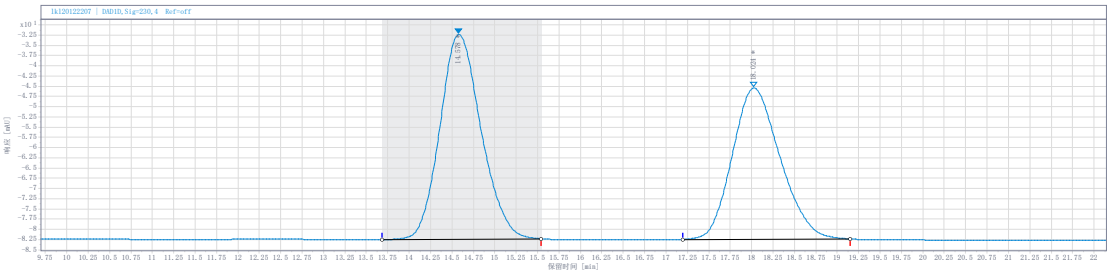
3ac



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.12	0.42	1468.22	113.50	5.27
9.48	1.23	26385.43	1085.86	94.73

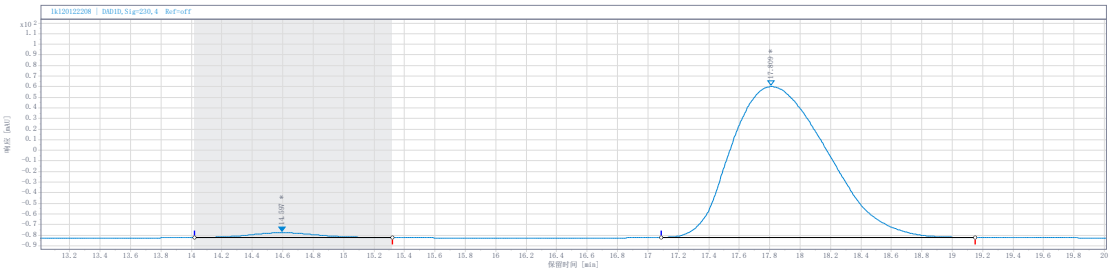
3ad racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
14.6	1.86	1675.21	50.06	53.84
18.0	1.96	1436.35	36.99	46.16

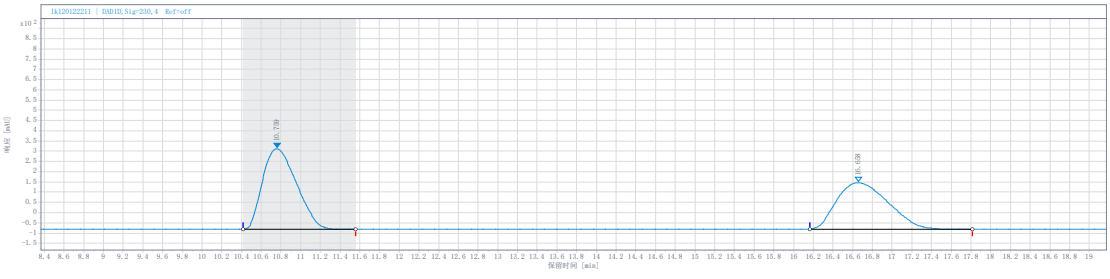
3ad



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
14.6	1.30	145.69	4.63	2.29
17.8	2.06	6211.40	142.31	97.71

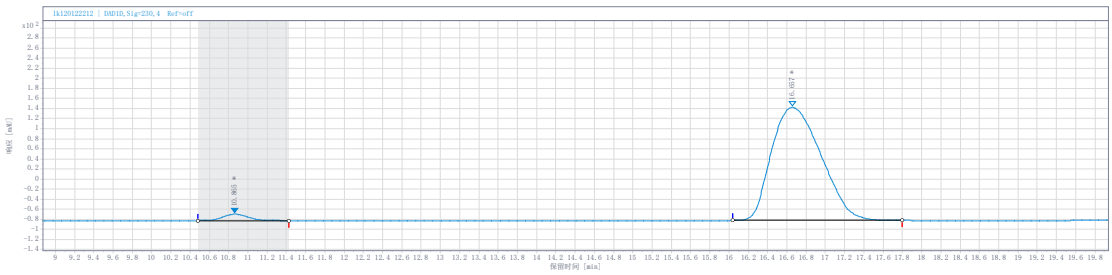
3ae racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

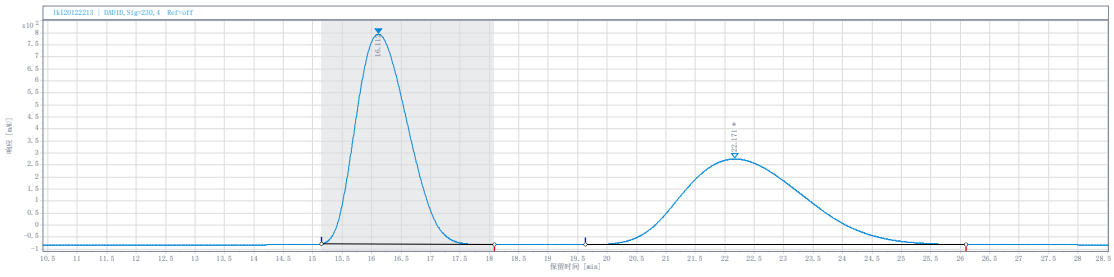
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
10.8	1.14	9390.87	393.04	53.32
16.7	1.65	8222.77	226.55	46.68

3ae



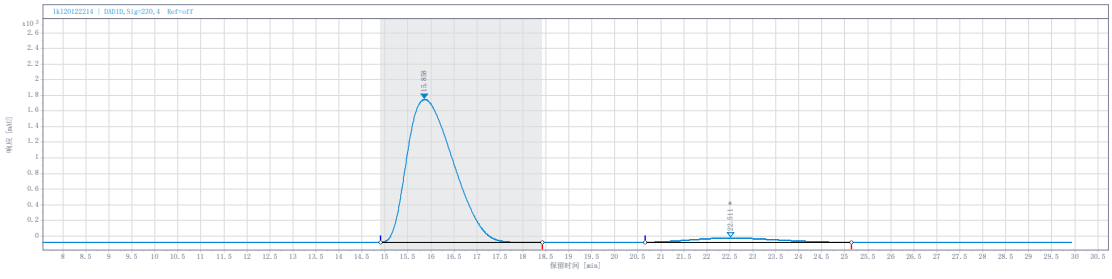
Signal:	DAD1D, Sig=230, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
10.9	0.95	227.60	12.67	2.75
16.7	1.76	8041.29	224.48	97.25

3af racemic mixture



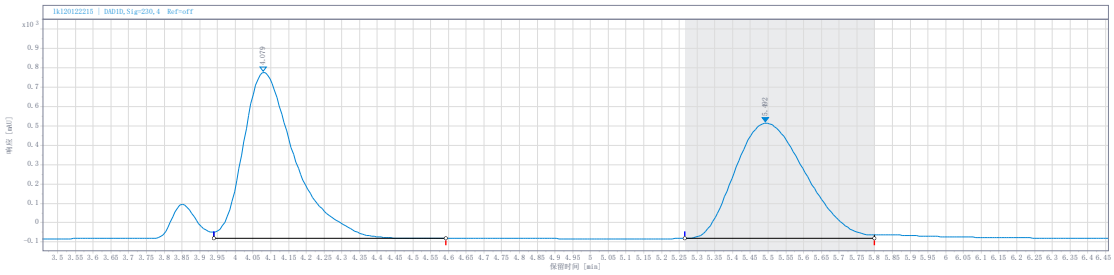
Signal:	DAD1D, Sig=230, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
16.1	2.93	53267.95	874.58	51.07
22.2	6.47	51032.58	356.51	48.93

3af



Signal:	DAD1D, Sig=230, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
15.9	3.51	126752.24	1827.41	94.76
22.5	4.48	7011.24	54.75	5.24

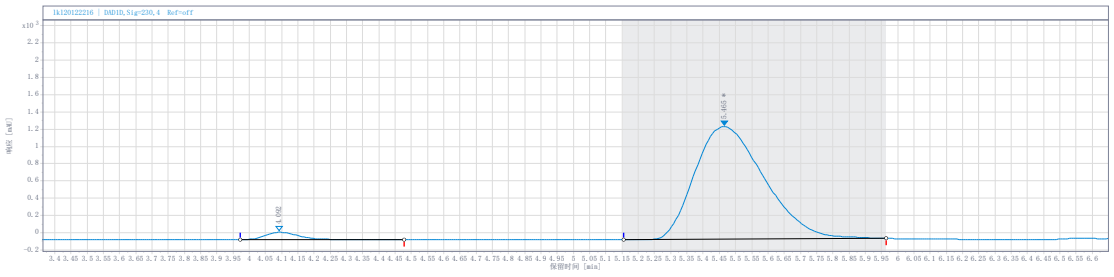
3ag racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
4.08	0.65	8653.65	854.98	51.18
5.49	0.53	8254.23	594.02	48.82

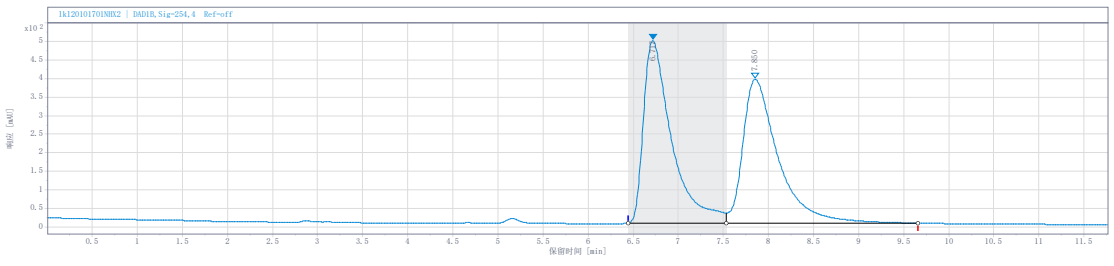
3ag



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
4.09	0.51	630.60	86.05	3.14
5.46	0.81	19464.99	1305.15	96.86

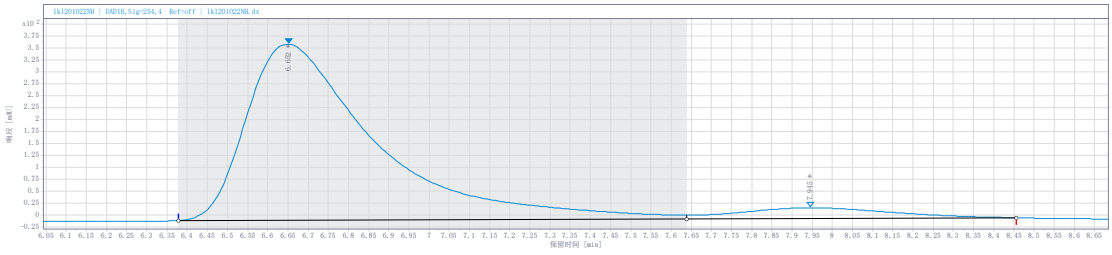
3ah racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.72	1.09	10703.85	491.45	50.39
7.85	2.13	10539.46	387.90	49.61

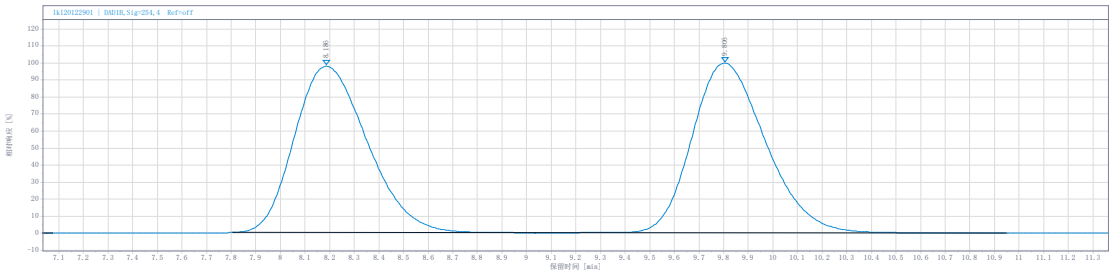
3ah



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.65	1.26	8206.20	368.25	93.33
7.94	0.82	586.09	22.31	6.67

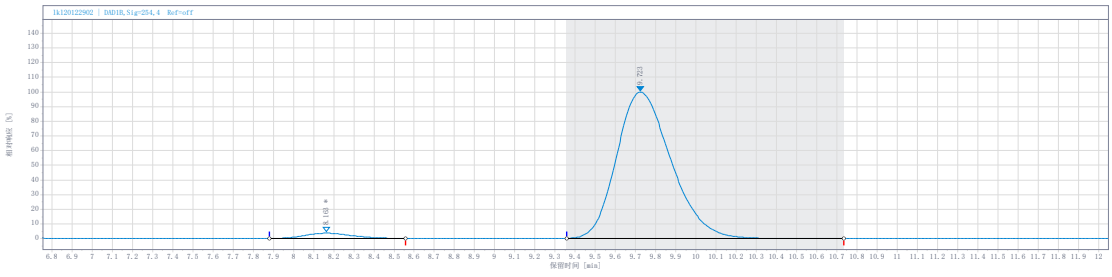
3ai racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.19	1.23	22931.90	1111.46	49.29
9.81	1.91	23590.12	1133.93	50.71

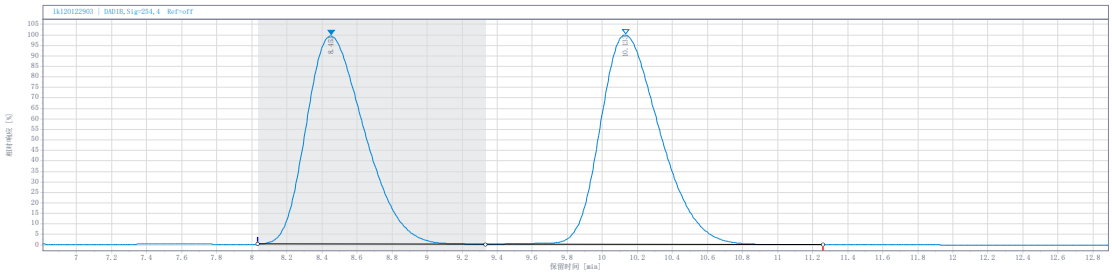
3ai



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.16	0.68	682.22	41.76	3.05
9.72	1.38	21662.24	1153.22	96.95

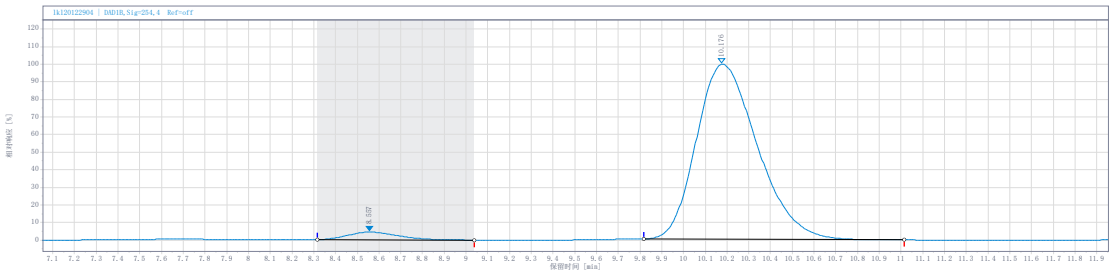
3aj racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.45	1.30	38565.89	1668.28	49.17
10.1	1.93	39863.53	1680.20	50.83

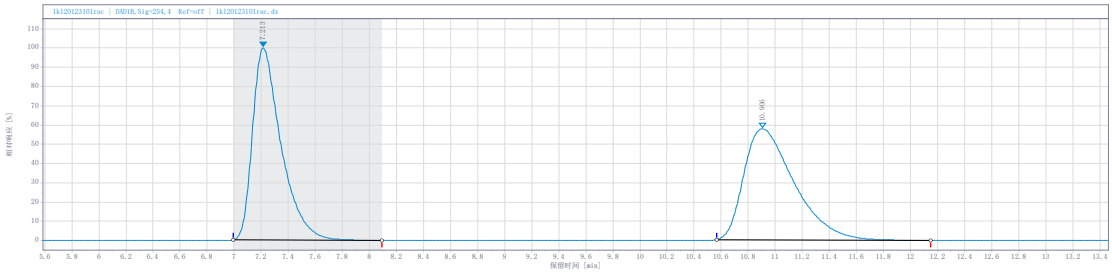
3aj



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.56	0.72	909.10	57.00	3.45
10.2	1.20	25413.98	1299.50	96.55

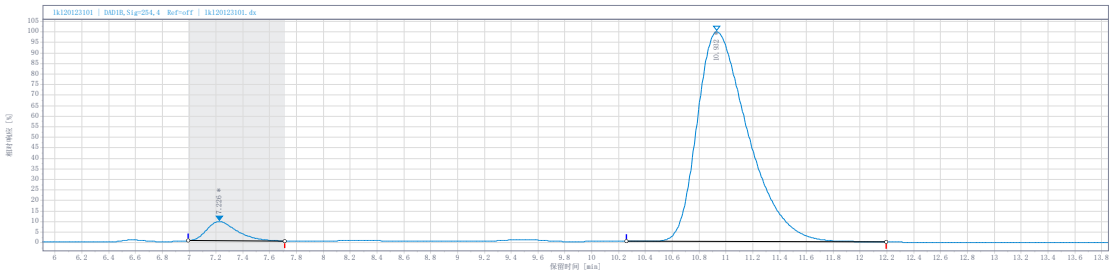
3ak racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

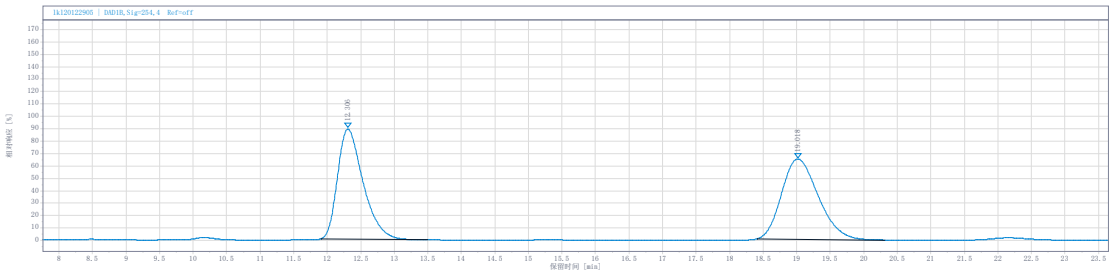
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.21	1.10	5247.31	357.93	49.56
10.9	1.58	5339.42	206.87	50.44

3ak



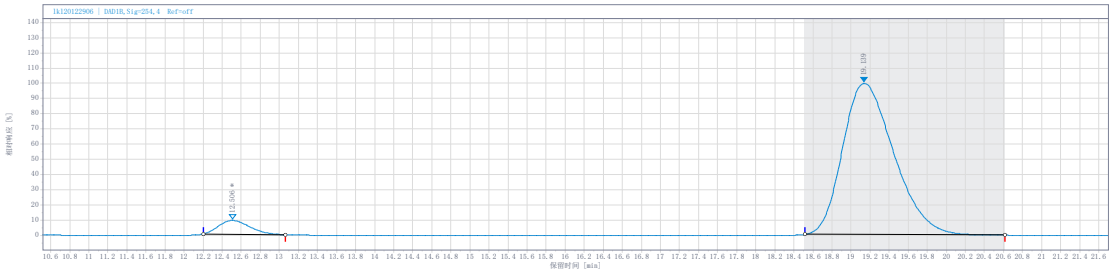
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.23	0.72	168.02	10.71	5.23
10.9	1.94	3047.23	115.69	94.77

3al racemic mixture



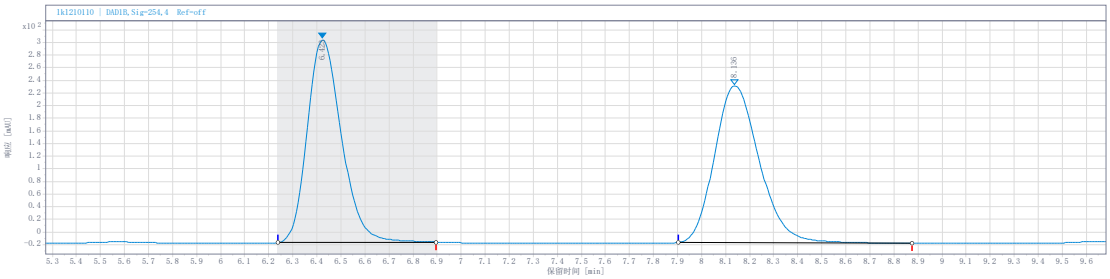
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.3	1.58	7627.59	287.84	49.00
19.0	1.89	7939.00	209.67	51.00

3al



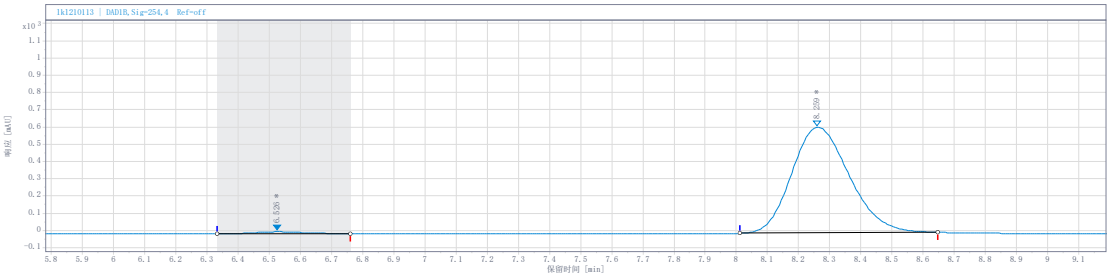
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.5	0.86	1111.51	49.20	5.22
19.1	2.10	20195.48	540.23	94.78

3am racemic mixture



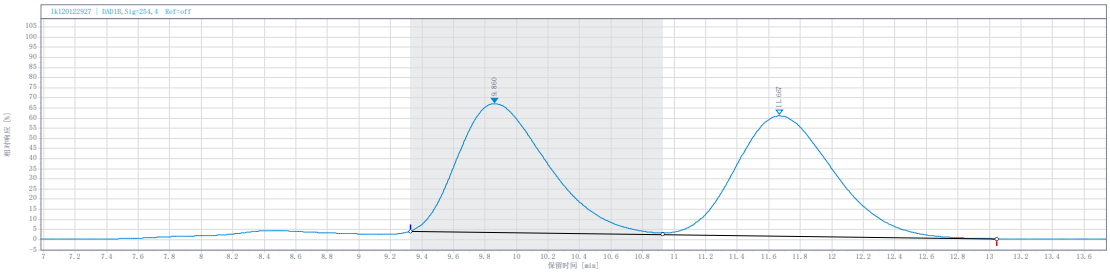
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.42	0.66	3169.88	320.75	49.70
8.14	0.97	3208.48	247.80	50.30

3am



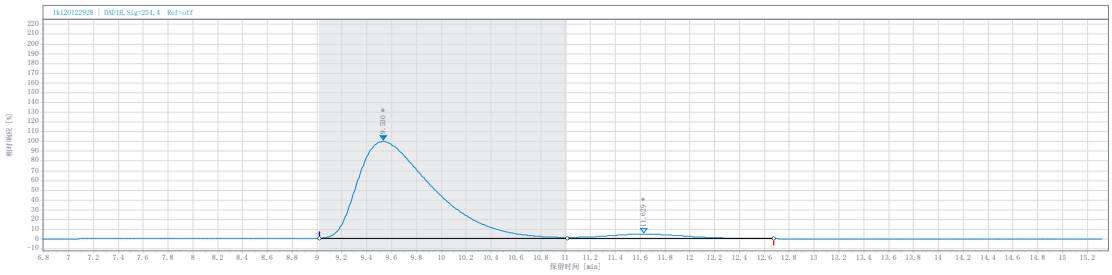
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.53	0.43	100.50	10.52	1.26
8.26	0.63	7873.40	612.77	98.74

3an racemic mixture



Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
9.86	1.60	5119.65	129.61	49.49
11.7	2.12	5225.39	120.95	50.51

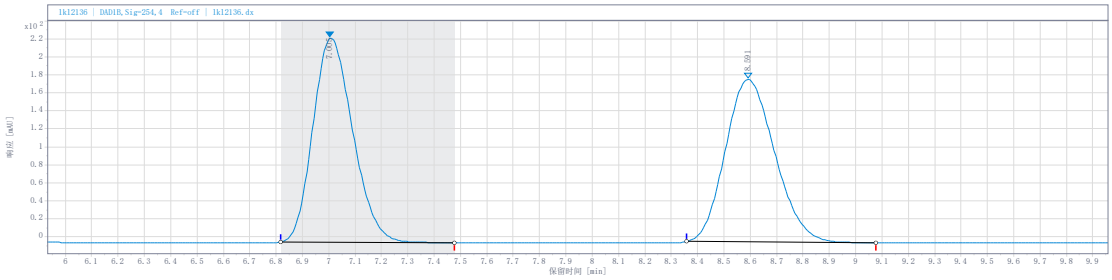
3an



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
9.53	2.00	36808.10	868.71	95.26
11.6	1.66	1832.96	39.94	4.74

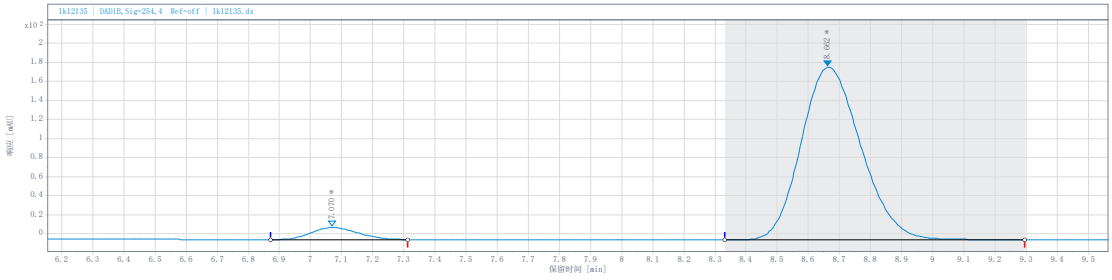
3ao racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.00	0.66	2381.33	226.59	50.24
8.59	0.72	2358.41	180.71	49.76

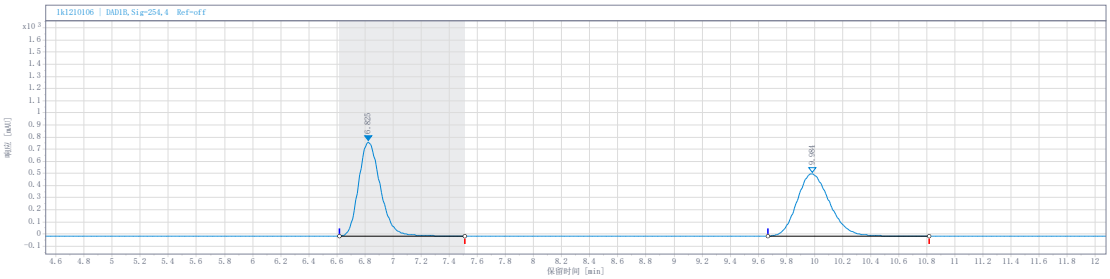
3ao



Signal: DAD1B, Sig=254, 4 Ref=off

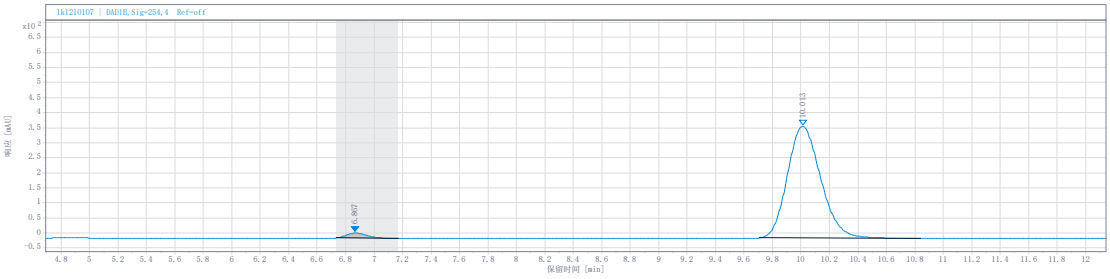
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.07	0.44	132.02	12.61	5.14
8.66	0.96	2434.82	181.28	94.86

3ap racemic mixture



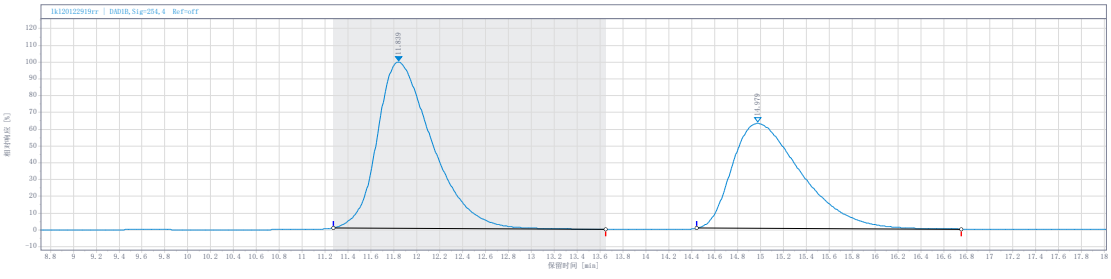
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.83	0.89	8312.70	773.24	50.01
9.98	1.15	8310.37	513.60	49.99

3ap



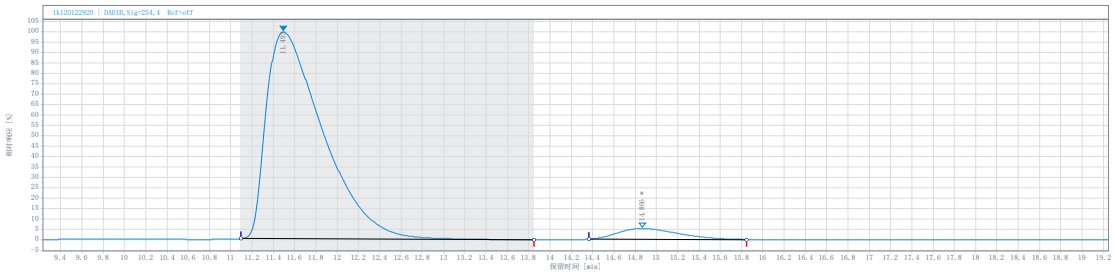
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.87	0.43	166.48	16.69	2.68
10.0	1.13	6052.96	371.32	97.32

3aq racemic mixture



Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
11.8	2.37	12847.20	384.24	55.69
15.0	2.31	10222.45	242.52	44.31

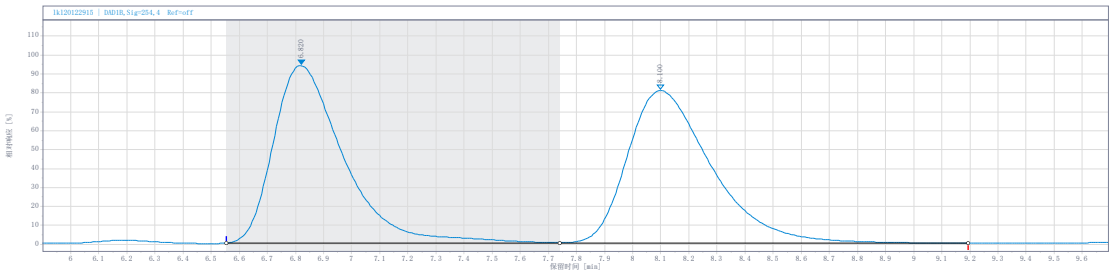
3aq



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
11.5	2.76	50759.17	1371.15	94.77
14.9	1.48	2803.46	71.15	5.23

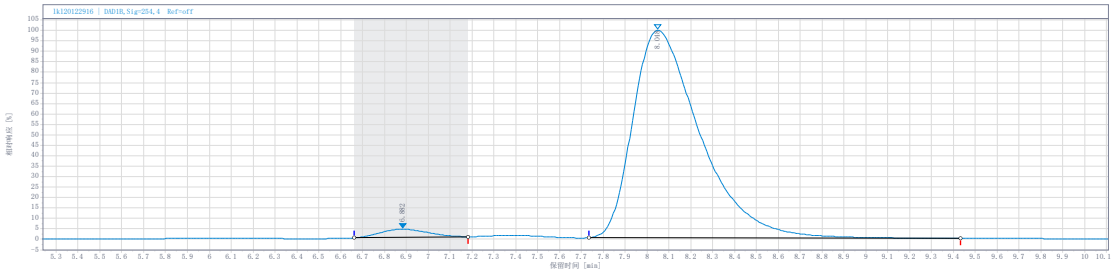
3ar racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.82	1.19	7417.50	426.88	49.35
8.10	1.45	7613.89	366.64	50.65

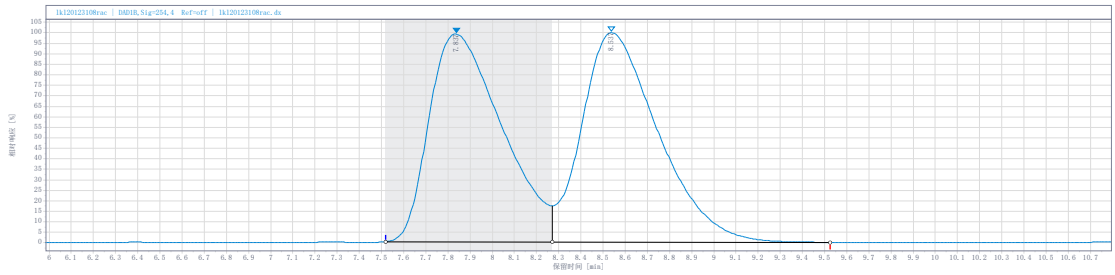
3ar



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.88	0.52	374.11	25.18	2.65
8.05	1.70	13725.56	641.04	97.35

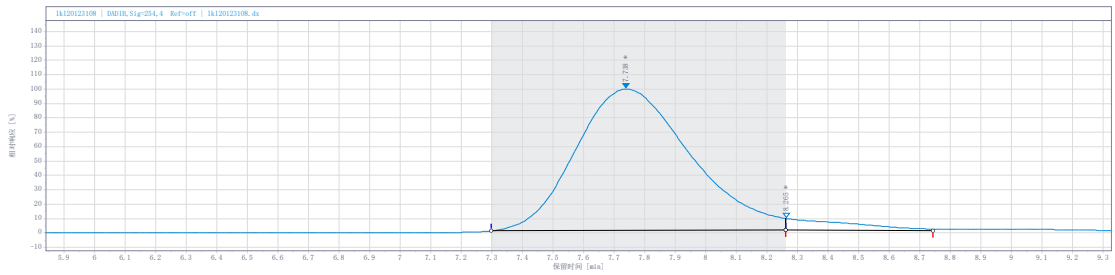
3as racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.84	0.75	11518.47	504.81	48.59
8.54	1.25	12185.36	508.26	51.41

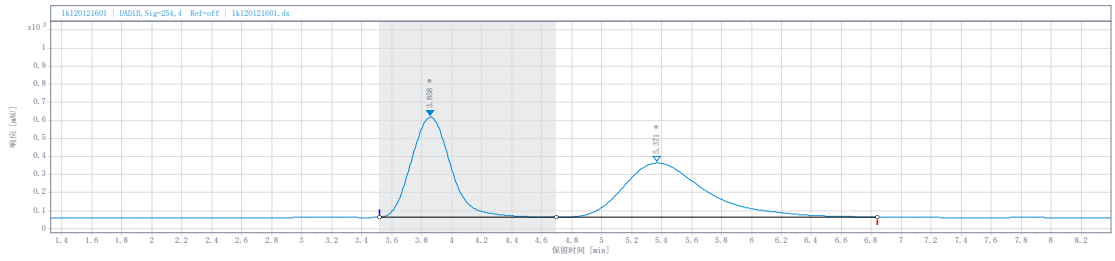
3as



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.74	0.96	6447.74	246.40	95.67
8.26	0.48	292.13	19.92	4.33

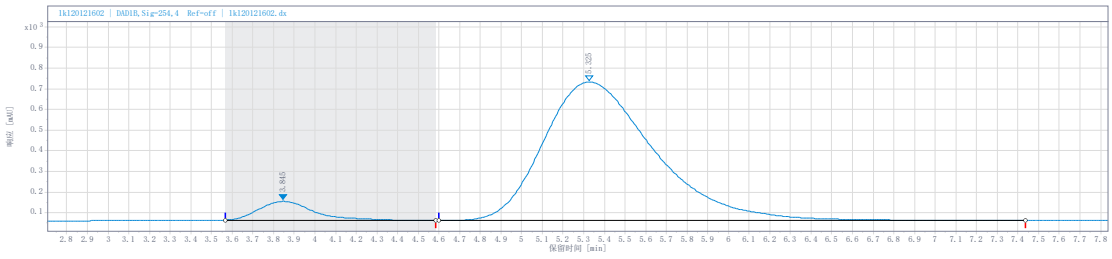
3at racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
3.86	1.18	10044.41	554.77	46.75
5.37	2.14	11441.20	299.93	53.25

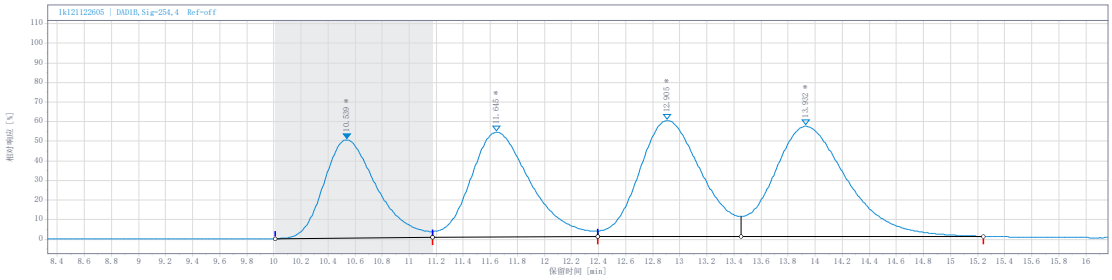
3at



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
3.85	1.02	1697.16	91.79	6.34
5.32	2.84	25077.18	670.67	93.66

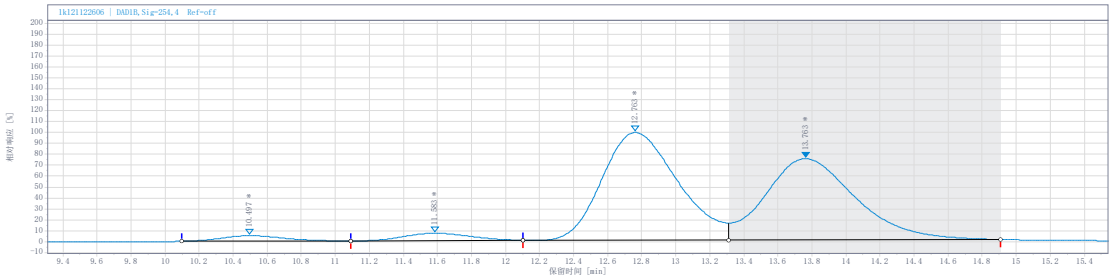
3au racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
10.5	1.17	1138.43	41.96	19.33
11.6	1.22	1385.19	44.77	23.52
12.9	1.06	1587.49	49.48	26.95
13.9	1.79	1778.96	46.96	30.20

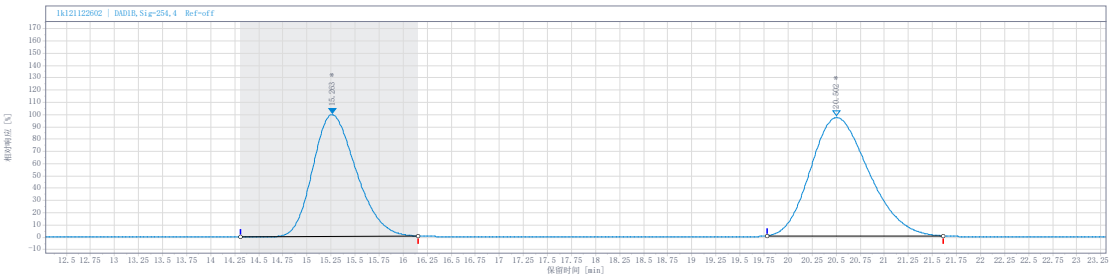
3au



Signal: DAD1B, Sig=254, 4 Ref=off

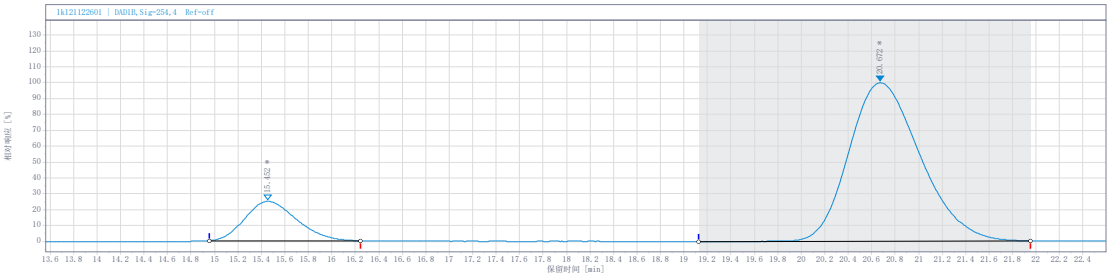
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
10.5	0.99	103.72	4.13	2.08
11.6	1.01	150.04	5.59	3.01
12.8	1.21	2496.18	80.74	50.07
13.8	1.60	2235.66	60.93	44.84

3av racemic mixture



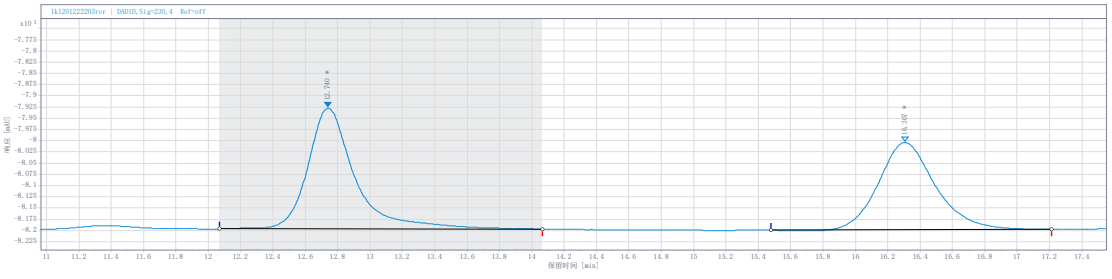
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
15.3	1.84	2073.35	66.27	43.47
20.5	1.83	2696.13	64.32	56.53

3av



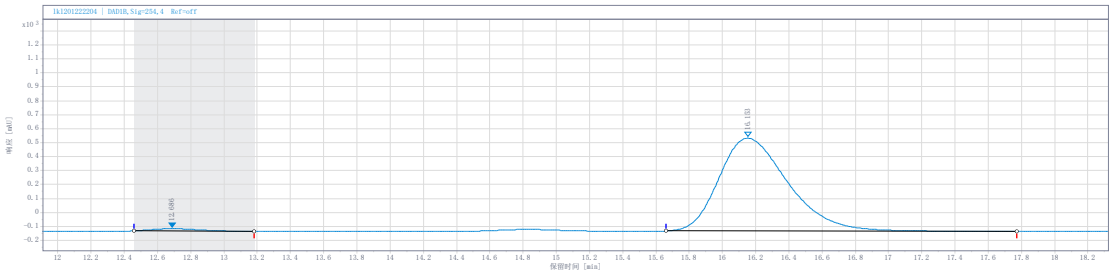
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
15.5	1.29	1115.74	36.54	15.24
20.7	2.83	6205.35	146.81	84.76

3ba racemic mixture



Signal:	DAD1D, Sig=230, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.7	2.00	54.65	2.69	53.76
16.3	1.74	47.01	1.94	46.24

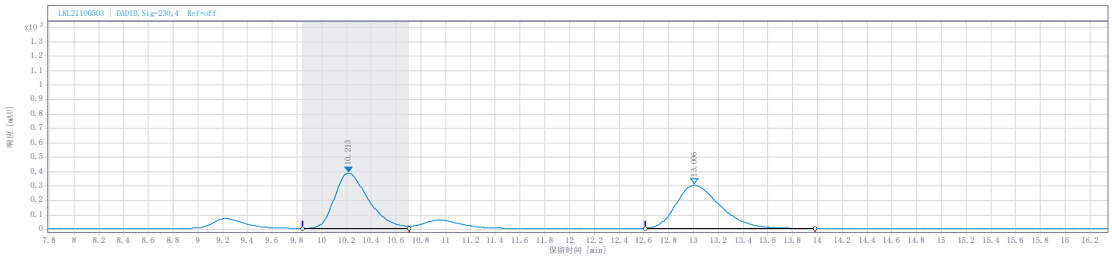
3ba



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.7	0.72	302.76	16.46	1.55
16.2	2.11	19246.19	666.03	98.45

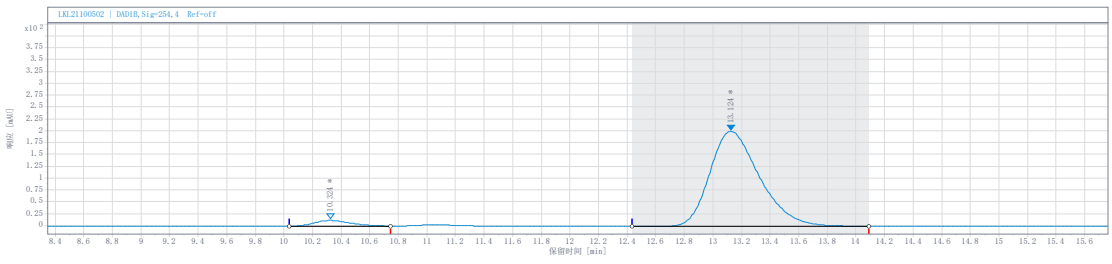
3bb racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
10.2	0.86	7278.34	382.08	49.82
13.0	1.37	7331.95	297.66	50.18

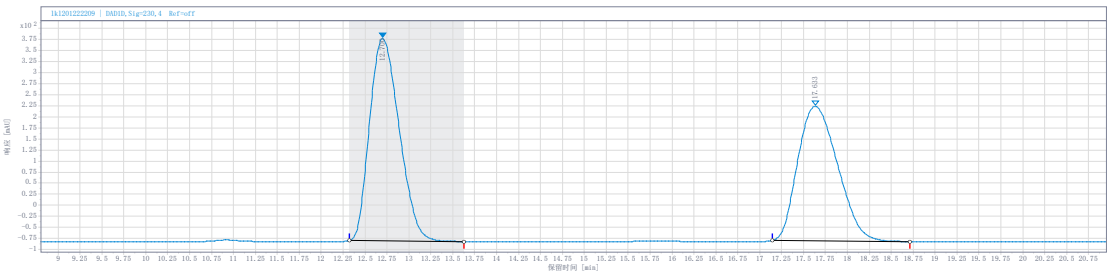
3bb



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
10.3	0.71	212.67	12.11	4.21
13.1	1.66	4841.22	200.41	95.79

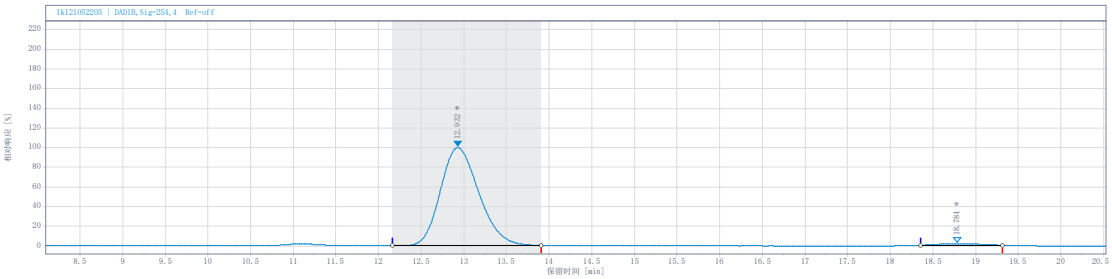
3bc racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.7	1.31	10732.60	456.90	52.85
17.6	1.57	9576.20	303.49	47.15

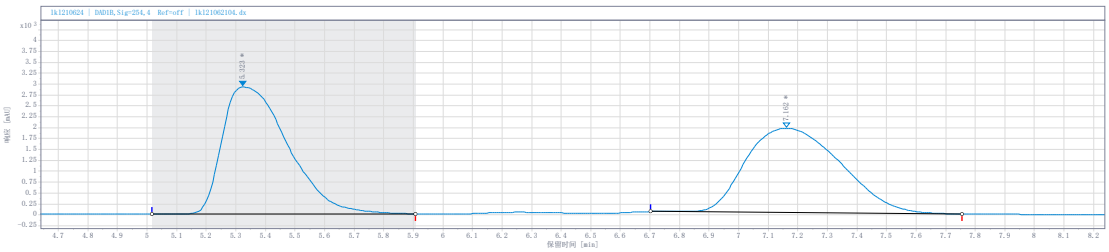
3bc



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.9	1.75	3314.68	105.88	98.37
18.8	0.96	55.04	1.64	1.63

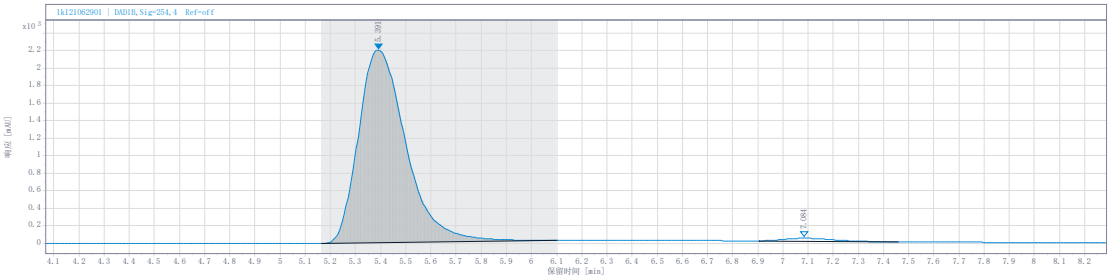
3bd racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
5.32	0.89	45008.95	2912.86	51.02
7.16	1.05	43203.53	1935.68	48.98

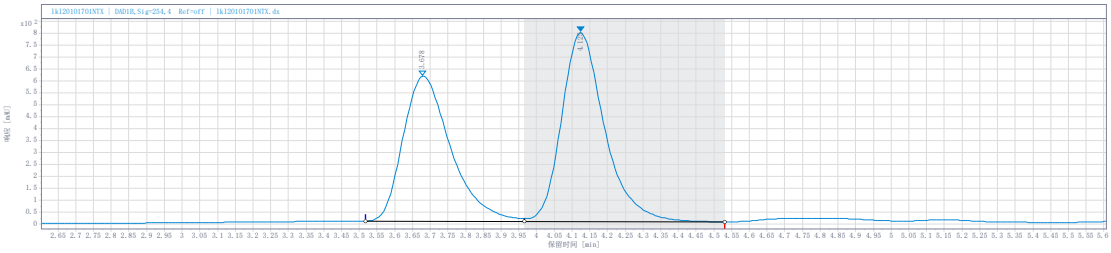
3bd



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
5.39	0.93	28856.16	2194.57	98.42
7.08	0.55	462.69	34.09	1.58

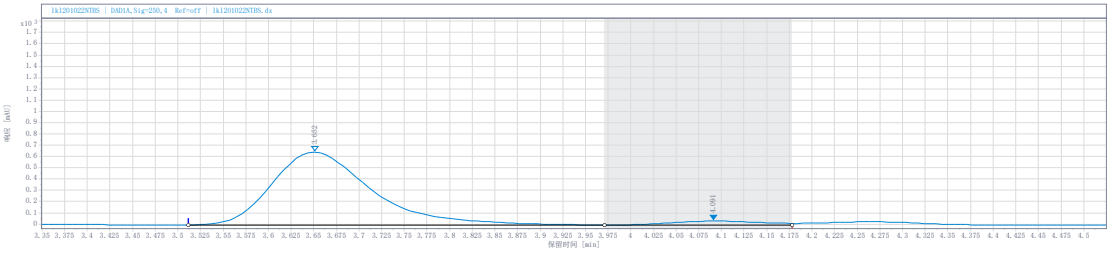
3be racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
3.68	0.45	5701.43	606.13	46.05
4.12	0.57	6678.81	790.78	53.95

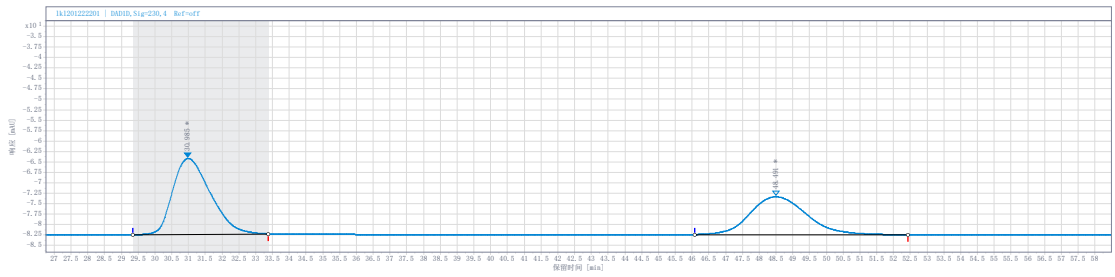
3be



Signal: DAD1A, Sig=250, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
3.65	0.46	4938.90	644.33	94.88
4.09	0.21	266.59	37.48	5.12

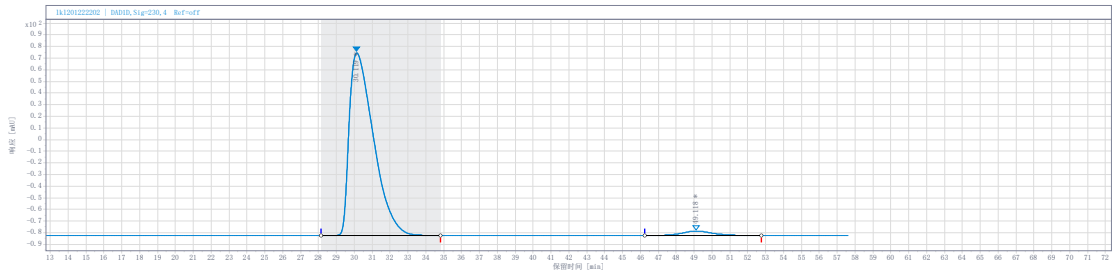
3bf racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
31.0	4.03	1410.77	18.18	57.13
48.5	6.36	1058.84	9.06	42.87

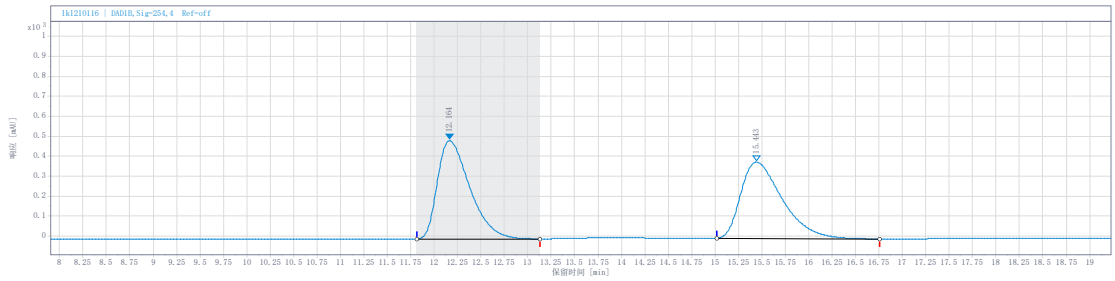
3bf



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
30.1	6.69	14789.58	156.88	97.01
49.1	6.54	455.72	3.83	2.99

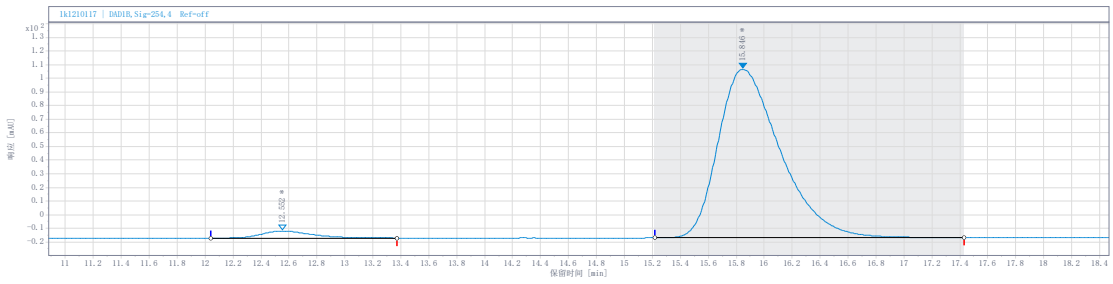
3bg racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.2	1.31	11843.44	493.20	50.06
15.4	1.74	11817.40	382.76	49.94

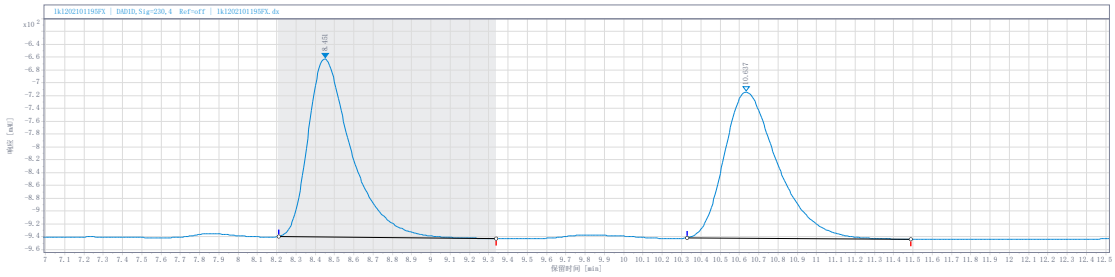
3bg



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.6	1.33	124.89	5.12	3.16
15.8	2.21	3825.73	123.54	96.84

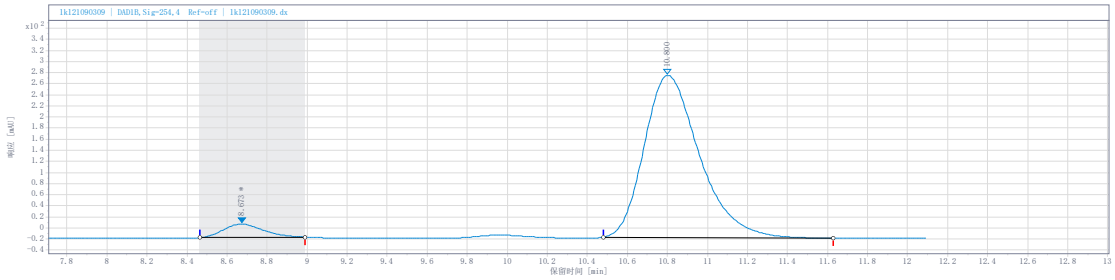
3bh racemic mixture



Signal: DAD1D, Sig=230, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.45	1.13	4357.24	277.79	49.82
10.6	1.16	4388.90	227.56	50.18

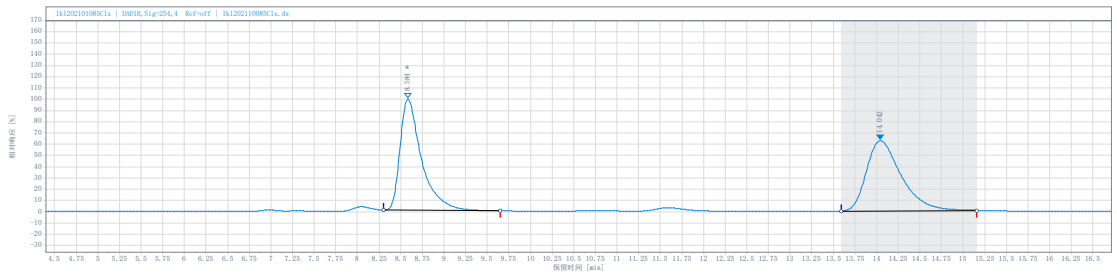
3bh



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.67	0.43	276.63	22.10	4.71
10.8	1.15	5596.22	292.22	95.29

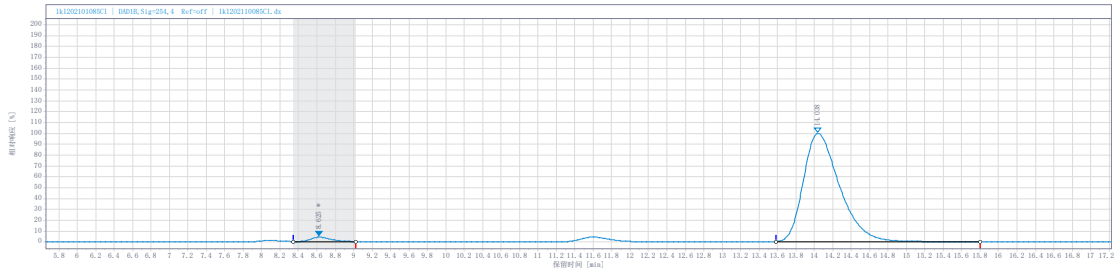
3bi racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.58	1.35	17150.17	993.93	49.57
14.0	1.57	17447.65	627.26	50.43

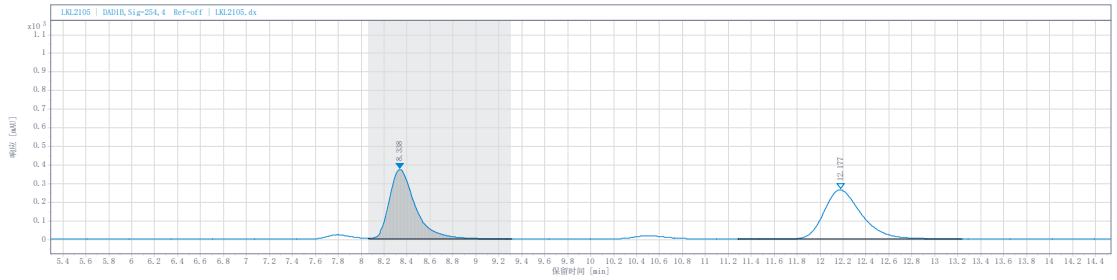
3bi



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.63	0.67	399.41	26.53	2.20
14.0	2.21	17746.90	648.40	97.80

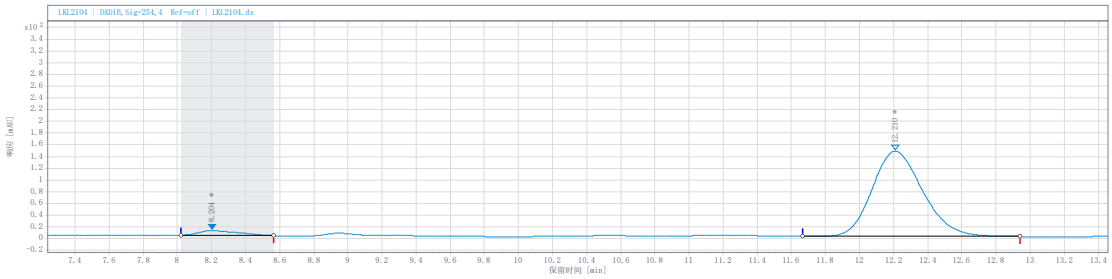
3bj racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.34	1.24	5768.02	372.36	49.25
12.2	1.95	5944.10	263.84	50.75

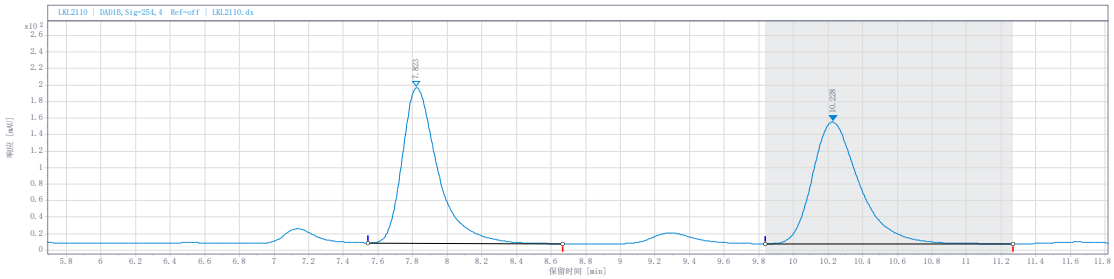
3bj



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.20	0.55	107.37	7.66	3.48
12.2	1.28	2979.55	144.81	96.52

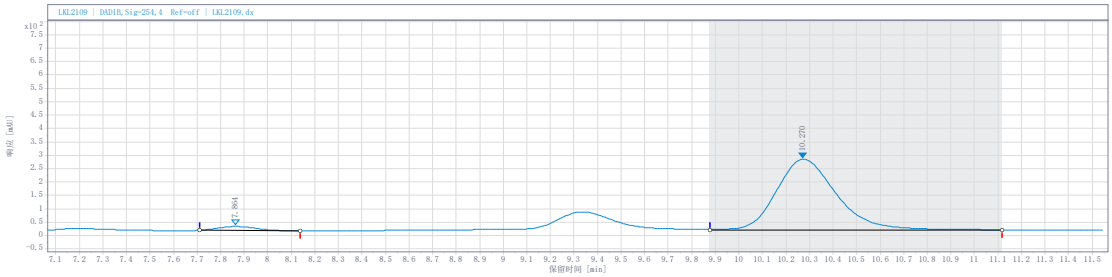
3bk racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.82	1.13	2687.03	188.46	49.22
10.2	1.43	2772.28	147.42	50.78

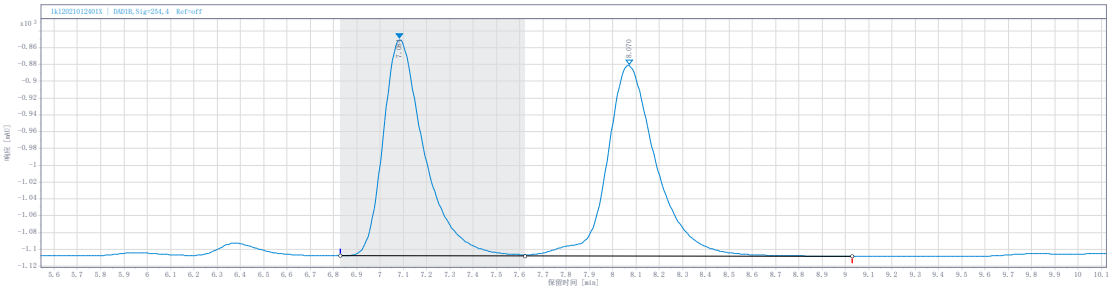
3bk



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.86	0.43	166.88	15.03	3.43
10.3	1.24	4698.77	264.67	96.57

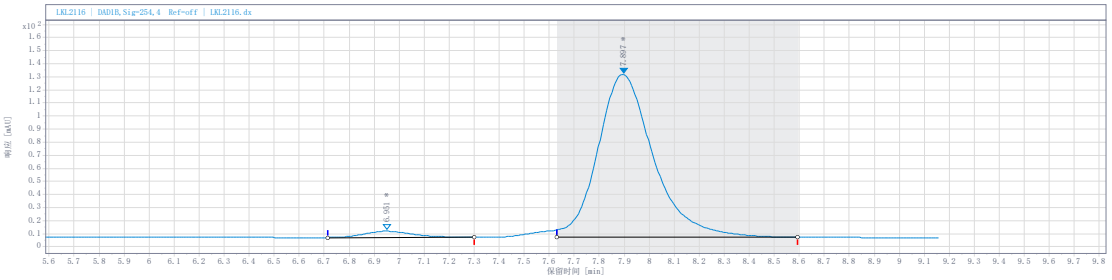
3bl racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.08	0.79	3171.54	257.10	48.63
8.07	1.41	3350.15	226.69	51.37

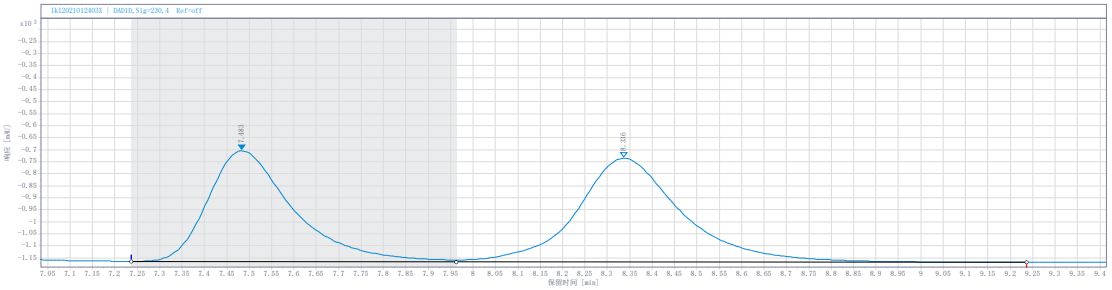
3bl



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
6.95	0.59	63.51	4.75	3.18
7.90	0.96	1932.46	124.55	96.82

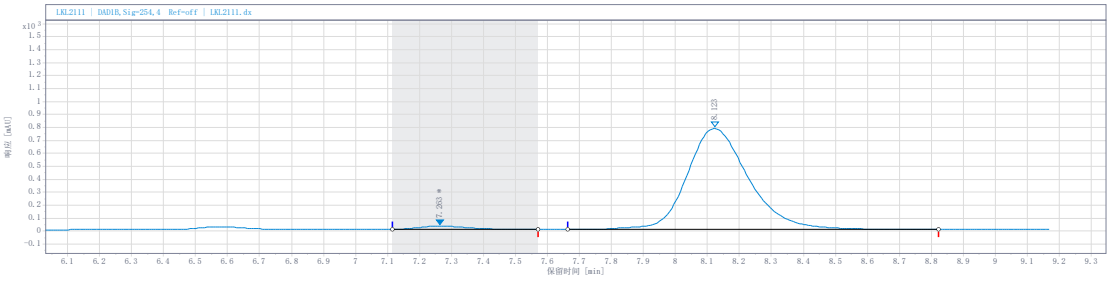
3bm racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.48	0.68	2584.49	195.45	43.99
8.34	1.31	3290.78	189.98	56.01

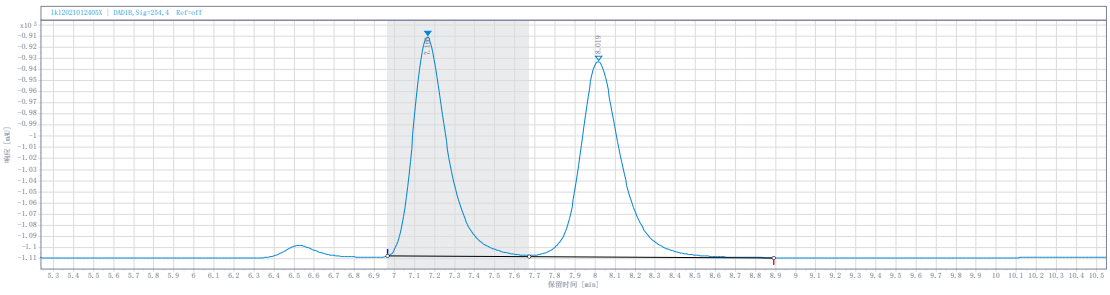
3bm



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.26	0.46	277.24	25.75	2.58
8.12	1.16	10466.02	779.08	97.42

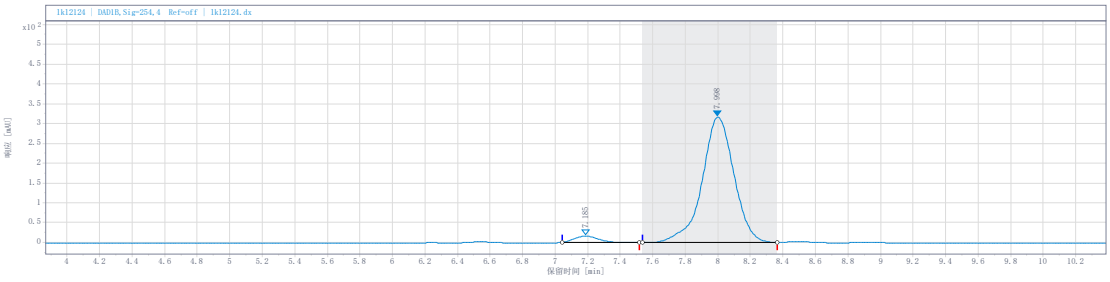
3bn racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.17	0.71	2382.27	196.80	48.60
8.02	1.22	2519.90	175.33	51.40

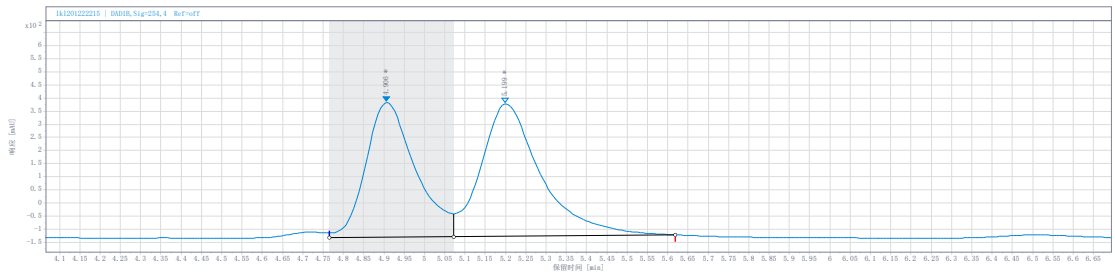
3bn



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
7.19	0.47	160.25	15.84	3.59
8.00	0.83	4305.52	316.36	96.41

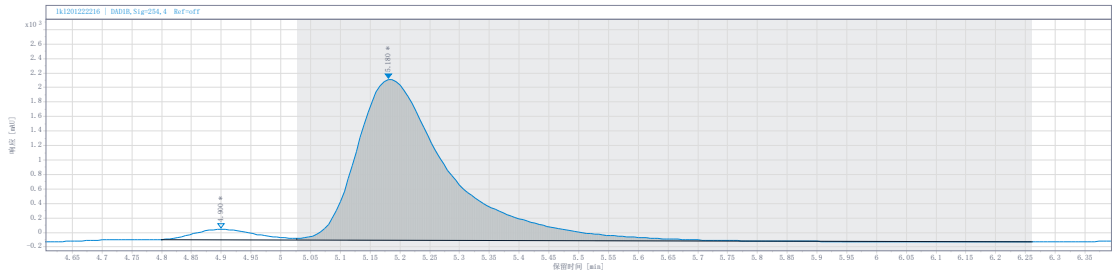
3bo racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
4.91	0.31	4360.41	513.13	45.74
5.20	0.54	5172.09	503.91	54.26

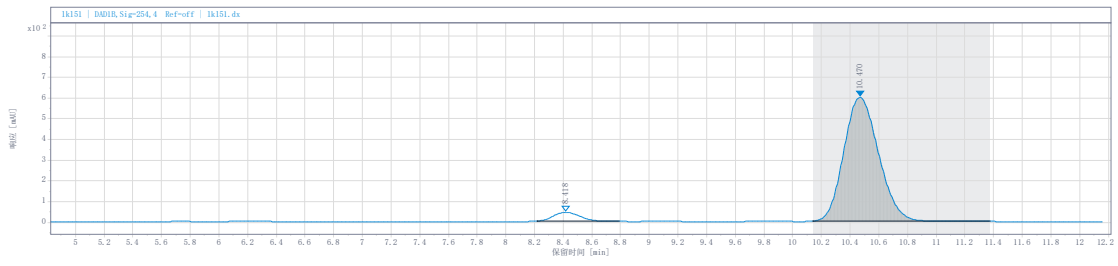
3bo



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
4.90	0.23	1043.71	144.67	4.17
5.18	1.23	23963.36	2219.31	95.83

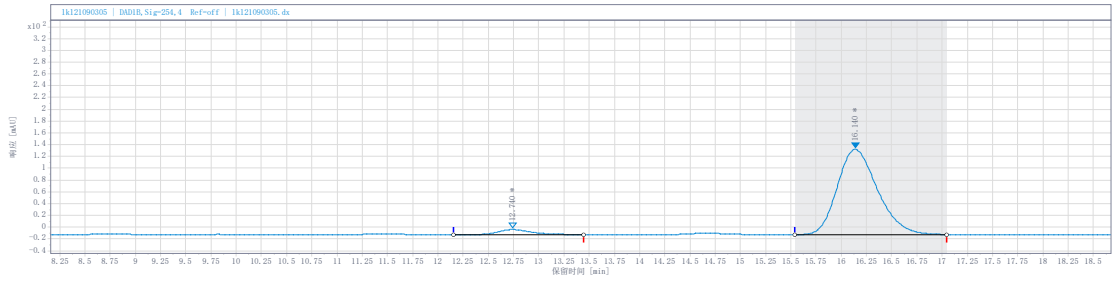
3aa(Gram scale)



Signal: DAD1B, Sig=254, 4 Ref=off

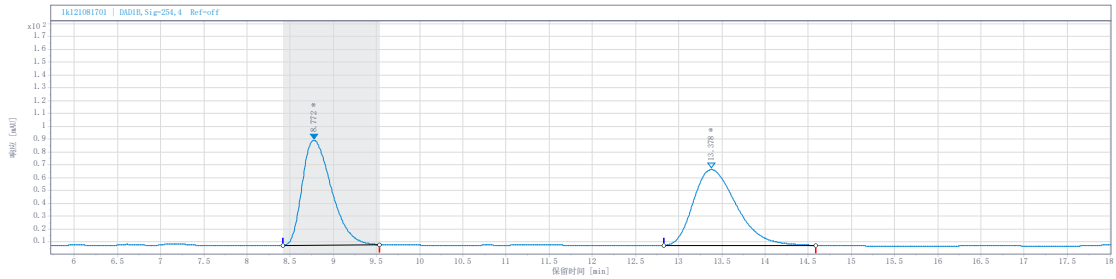
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.42	0.57	554.92	43.45	5.22
10.5	1.23	10070.06	598.07	94.78

3ba(Gram scale)



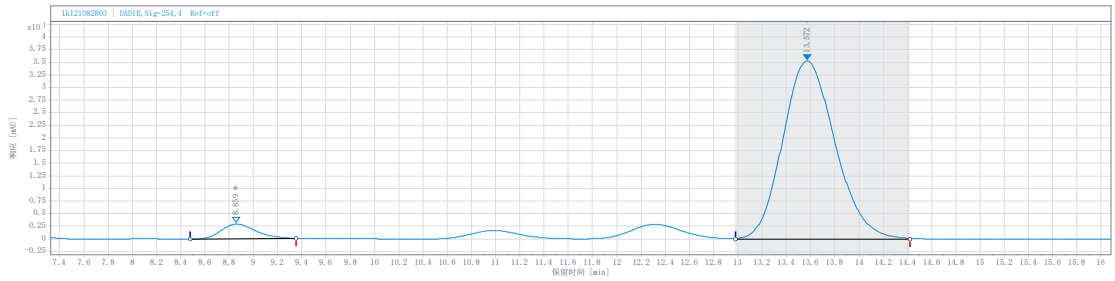
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.7	1.29	186.93	8.46	4.46
16.1	1.51	3999.89	144.35	95.54

4a racemic mixture



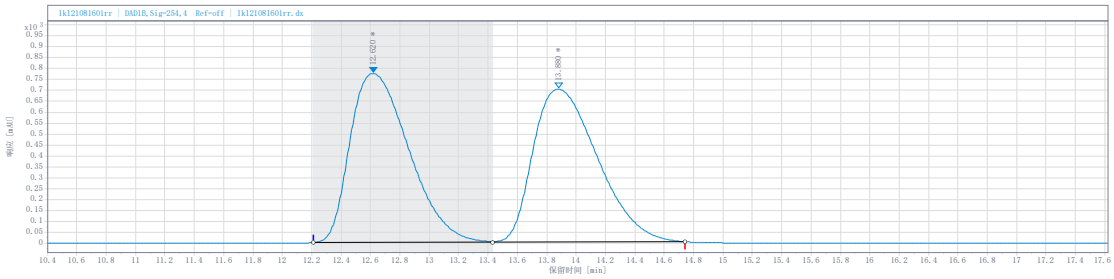
Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.77	1.13	1919.82	81.73	48.40
13.4	1.75	2046.73	59.13	51.60

4a



Signal:	DAD1B, Sig=254, 4	Ref=off		
RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.86	0.87	57.21	2.92	5.12
13.6	1.44	1061.22	35.29	94.88

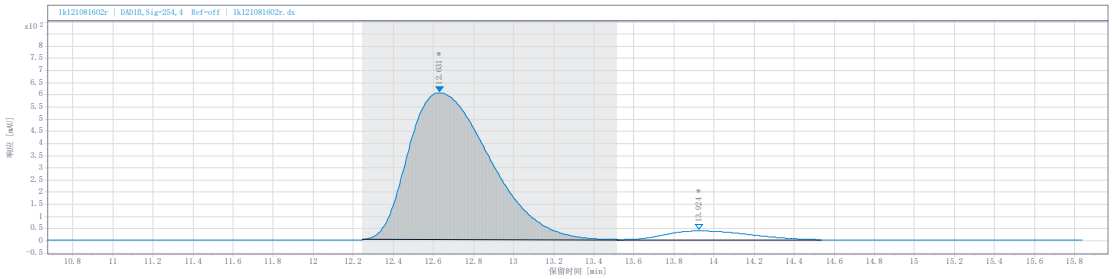
4b racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.6	1.22	21507.29	773.21	50.20
13.9	1.31	21338.33	699.83	49.80

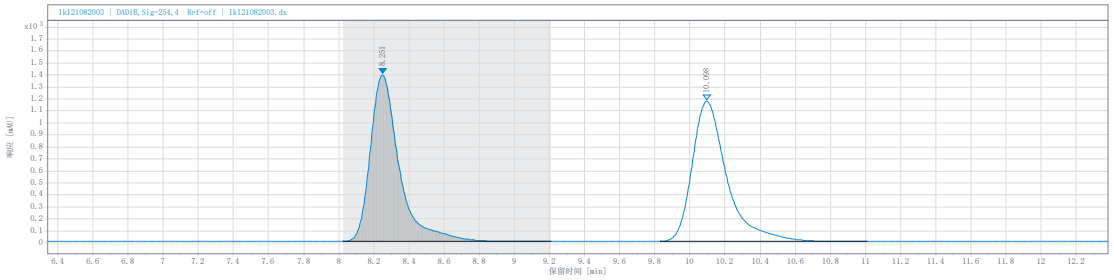
4b



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
12.6	1.27	17034.34	603.47	94.82
13.9	1.02	931.03	34.69	5.18

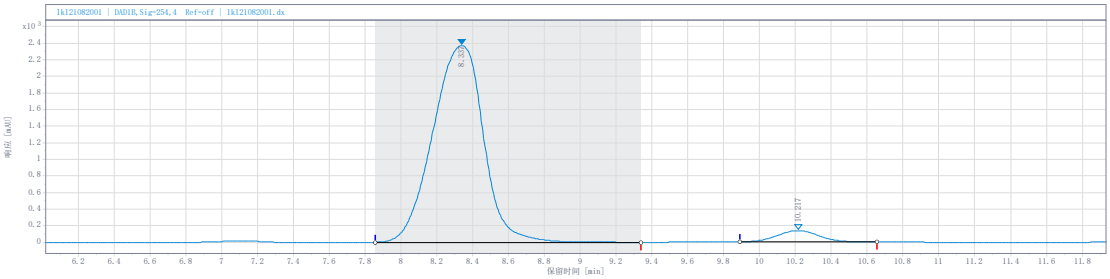
4c racemic mixture



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.25	1.18	15800.84	1387.88	49.64
10.1	1.17	16030.98	1167.69	50.36

4c



Signal: DAD1B, Sig=254, 4 Ref=off

RetTime [min]	width [min]	Arer [mAU*s]	Height [mAU]	Area%
8.34	1.48	46465.59	2368.52	95.44
10.2	0.77	2220.15	137.11	4.56