Supporting Information

Asymmetric α-selective allylation of amide unit of maleimides and alkenyloxindoles by dual-functional In^{III}/*N*,*N'*-dioxide complex

Wang-Yuren Li, Longqing Yang, Xiaoxue Tang, Wenjun Yan, Zhao Wu, Fei Wang, Shunxi Dong*, Xiaoming Feng*

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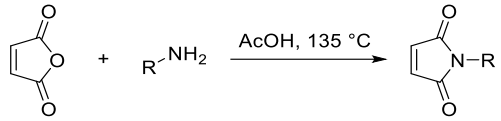
1. General information

^{1}H NMR spectra were recorded at Bruker ASCEND^{TM} 400 M (400 MHz) or 600 M (600 MHz). The chemical shifts were recorded in ppm relative to tetramethylsilane and with the solvent resonance as the internal standard. Data were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, m = multiple), coupling constants (Hz), integration. ^{13}C{^{1}H} NMR data were collected at 100 MHz or 150 MHz with complete proton decoupling. Enantiomeric excesses (ee) were determined by chiral HPLC analysis on Daicel chiralcel IA, chiralcel IE, and chiralcel ID columns. Optical rotations were reported as follows: $[\alpha]^{T}_{\lambda}$ (*c*: g/100 mL, in solvent). High resolution mass spectra (HRMS) analyses were recorded on a Thermo Scientific LTQ Orbitrap XL with positive ion mode and MeOH were used to dissolve the sample; High resolution mass spectra of allylicindium was recorded on a SCIEX X500R QTOF with positive ion mode and DMSO were used to dissolve the sample. IR spectra were recorded on Pierkin Elmer 100 FT/IR spectrometer, and the wave numbers of the absorption peaks are given in cm^{-1}. Unless otherwise indicated, reagents obtained from commercial sources were used without further purification. Metal salts obtained from commercial sources were used without further purification. Chemical reagents were purchased from Alfa, Adamas, Ark, Aladdin, Innochem, TCI, etc. Solvents were dried and distilled prior to use according to the standard methods. The chiral *N,N′*-dioxide ligands were synthesized by the same procedure in the literature.[1] The maleimide were prepared according to literature procedure.[2] The further transformation were followed the literature procedure.[3] Unless otherwise indicated, all reactions below were carried out without the protection of inert gas.

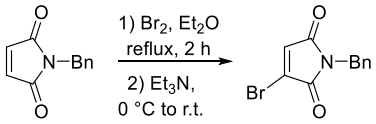
2. General procedures for the synthesis of substrate and catalytic asymmetric reaction

2.1 General procedure for the preparation of the substrates[2]



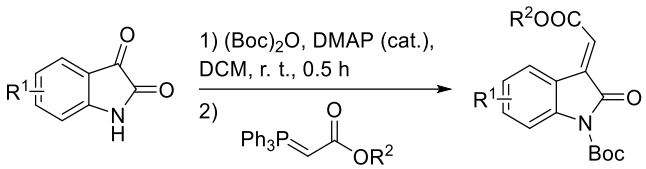
A dry round-bottom was charged with corresponding maleic anhydride (10 mmol, 1.0 equiv.), followed by the addition of AcOH (10 mL) and corresponding primary amine (10 mmol, 1.0 equiv.), The mixture was stirred at 135 ℃ in oil bath for 1-4 h. After completion of the reaction, the reaction mixture was then allowed to cool to ambient temperature, The residue was dissolved in EtOAc (15 mL) and water (15 mL), then $NaHCO_3$ solids are added to the mixture until no gases were emitted. The aqueous mixture was extracted with ethyl acetate (20 mL × 3). The organic layer was further washed with 1(N) HCl (50 mL × 3) and brine solution (30 mL × 1) respectively. The solvent was removed under reduced pressure and the residue was subjected to flash column chromatography on silica gel (eluent: ethyl acetate / petroleum ether = 1/15-1/8, v/v) to afford the corresponding product in good yield (> 80%).

To a solution of maleimide (1.94 g, 20 mmol, 1.0 equiv.) in anhydrous dichloromethane (10 mL) was added di-*t*-butyl dicarbonate (Boc_2O; 6.54 g, 30 mmol, 1.5 equiv.) and a catalytic amount of 4-dimethylaminopyridine (DMAP; ca. 50 mg) at room temperature. After stirring the mixture for 10 min, the solvent was removed under reduced pressure to provide a crude residue. The residue was subjected to flash column chromatography on silica gel (eluent: hexane/AcOEt = 4/1, v/v) to afford the product in good yield (93%).



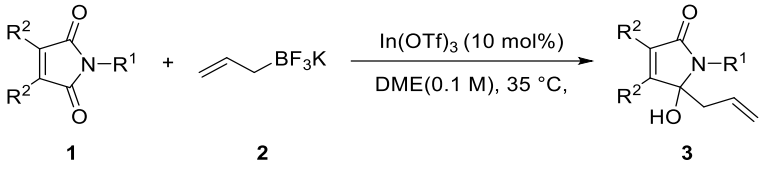
1t

A dry round-bottom was charged with *N*-benzylmaleimide (3.74 g, 20 mmol, 1.0 equiv.), followed by the addition of Et_2O (20 mL). Bromine (3.52 g, 22 mmol, 1.1 equiv.) was added dropwise over 1 h at room temperature. The resulting red clear solution was refluxed for 2 h until the solution color turned to light yellow. The reaction mixture was then allowed to cool to 0 ℃ in ice bath, Et_3N (2.22 g, 22 mmol, 1.1 equiv.) was added dropwise. After stirring the mixture at ambient temperature for 18 h, the solids were removed by filtration through celite, and the filtrate was concentrated in vacuo to give the crude product as an orange oil. The crude product was diluted with 20 mL EtOAc, washed with water (20 mL × 1) and brine (20 mL × 1) and dried over Na_2SO_4. The solvent was removed *in vacuo* and the residue was subjected to by flash column chromatography on silica gel to give the bromomaleimide product in good yield (95%).

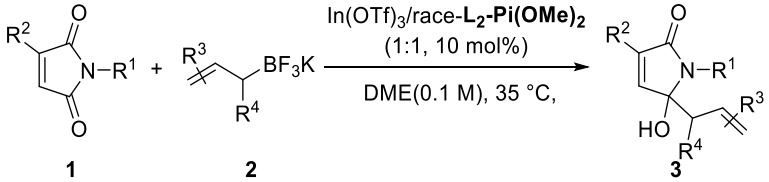


A dry round-bottom was charged with corresponding isatin (10 mmol, 1.0 equiv.), 4-dimethylaminopyridine (DMAP; ca. 50 mg), followed by the addition of DCM (10 mL). Di-*t*-butyl dicarbonate (Boc_2O; 3.76 g, 10 mmol, 1.0 equiv.) was added dropwise. The resulting red mixture was stirred for 0.5 h until the solution color turned to dark yellow. Corresponding Wittig reagent (10 mmol, 1.0 equiv.) was added as one portion and the mixture was stirred at ambient temperature for another 12 h. The solvent was removed under reduced pressure to provide crude residue. The residue was subjected to flash column chromatography on silica gel (eluent: hexane/AcOEt = 20/1, v/v) to give the product in good yield (>90%).

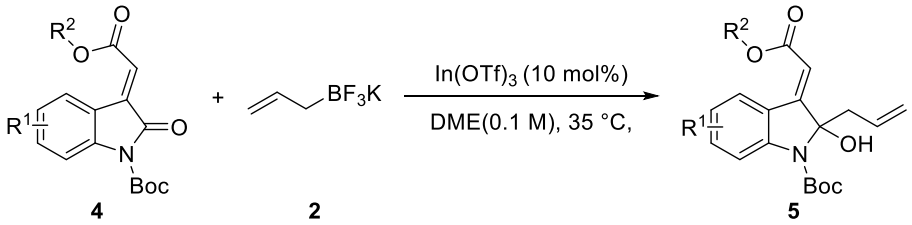
2.2 General procedure for the preparation of the racemic products



Procedure A: Without the protection of inert gas, the reaction was conducted with maleimide **1** (0.10 mmol), potassium allyltrifluoroborates **2** (2 equiv.) and $In(OTf)_3$ (10 mol%) in DME (1.0 mL). The mixture was stirred at 35 ℃ for 4 h. The reaction mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate / petroleum ether, 1:4 – 1:1, v/v) to afford the corresponding product **3**.

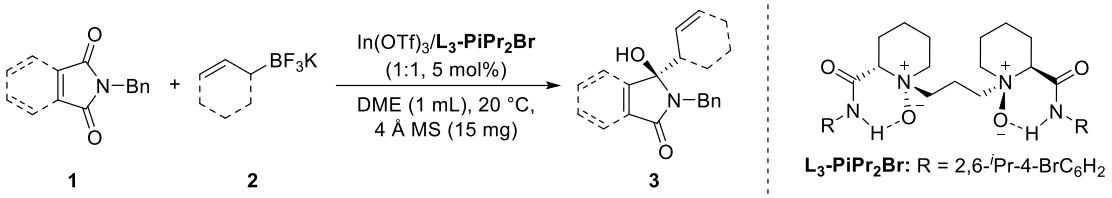


Procedure B: Without the protection of inert gas, the reaction was conducted with maleimide **1** (0.10 mmol), potassium allyltrifluoroborates **2** (2 equiv.) $In(OTf)_3$ (5.6 mg, 10 mol%) and **race-L_2-Pi(OMe)$_2$** (6.0 mg, 10 mol%) in DME (1.0 mL). The mixture was stirred at 35 ℃ for 4 h. The reaction mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate / petroleum ether, 1:4 – 1:1, v/v, 180 mL) to afford the corresponding product **3**.

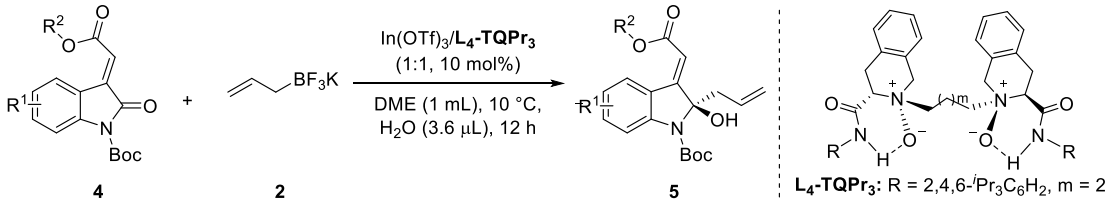


Procedure C: Without the protection of inert gas, the reaction was conducted with alkenyloxindoles **4** (0.10 mmol), potassium allyltrifluoroborates **2** (2 equiv.) and $In(OTf)_3$ (10 mol%) in DME (1.0 mL). The mixture was stirred at 35 ℃ for 6 h. The reaction mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate / petroleum ether, 1:15 – 1:8, v/v, 250 mL) to afford the corresponding product **5**.

2.3 General procedure for the catalytic asymmetric reactions



Procedure D: In glove box, a dry reaction tube was charged with substrate **1** (0.10 mmol), $In(OTf)_3$ (2.8 or 5.6 mg, 5 or 10 mol%), *N,N'*-dioxide ligand **L_3-PiPr$_2$Br** (4.1 or 8.2 mg, 5 or 10 mol%) and 4 Å MS (15 mg) separately, followed by the addition of DME (1.0 mL). After stirring the mixture at 35 ℃ in water bath for 0.5 h, the mixture was allowed to cool to 20 ℃. Then potassium allyltrifluoroborate **2** (0.20 mmol, 2 equiv., 30.0 mg) was added as one portion and resulting the mixture was stirred at 20 ℃ for another 18 h. The reaction mixture was directly subjected to column chromatography on silica gel (eluent: ethyl acetate / petroleum ether, 1:4 – 1:1, v/v) to afford the corresponding product **3**.

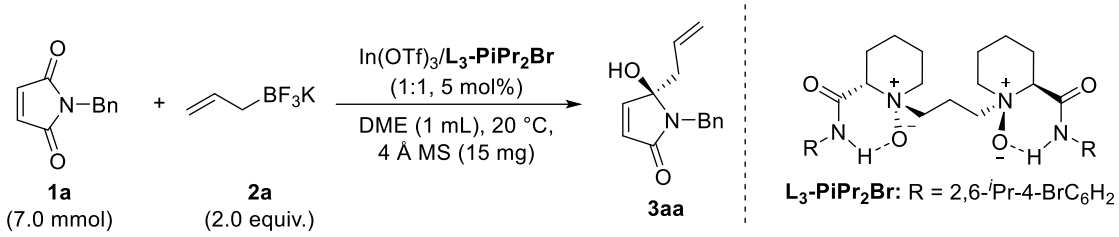


Procedure E: In glove box, a dry reaction tube was charged with substrate **4** (0.10 mmol), $In(OTf)_3$ (5.6 mg, 10 mol%) and **L_4–TQPr$_3$** (8.4 mg, 10 mol%) separately, followed by the addition of DME (1.0 mL). After stirring the mixture at 35 ℃ in water bath for 0.5 h, the mixture was allowed to cool to 10 ℃. Then potassium allyltrifluoroborate **2** (30.0 mg, 0.20 mmol) and H_2O (3.6 μL) was added as one portion and the mixture was stirred at 10 ℃ for another 18 h. The reaction mixture was directly subjected to column chromagraphy on silica gel (eluent: ethyl acetate / petroleum ether, 15:1, v/v) at -20 ℃ (**Fig. 1**) to afford the corresponding product **5**.

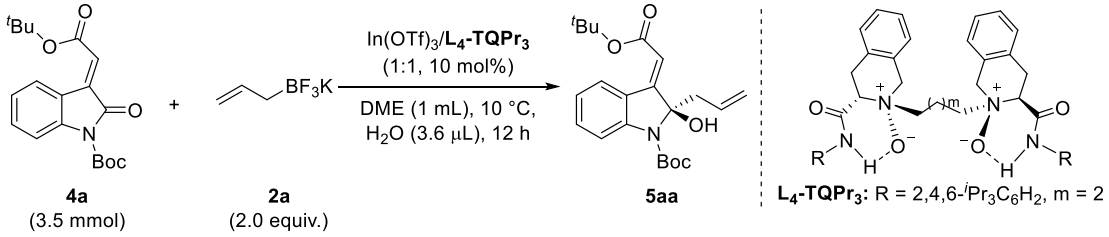
Note： The product **5** slowly racemizes in silica gel. For example, the ee value of **5aa** was reduced from 91% to 70%. To avoid the racemization, all *ee* values and optical rotations of products were determined using column chromatography on silica gel at -20 ℃.

Figure S1 Column chromatography at -20 ℃

2.4 Experimental procedure for the scale-up reaction

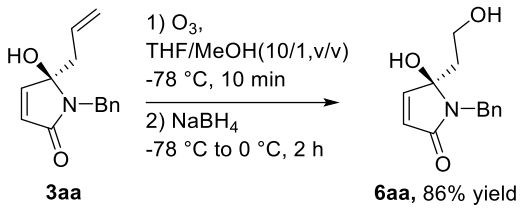


Procedure F: In glove box, a dry round-bottom was charged with substrate **1a** (1.309 g, 7.0 mmol), In(OTf)$_3$/**L-PiPr$_2$Br** (1:1, 5mol%), 4 Å MS (1.05 g), followed by the addition of DME (70 mL). After stirring the mixture at 35 ℃ in water bath for 0.5 h, the mixture was allowed to cool to 20 ℃. Then potassium allyltrifluoroborate **2a** (2.072 g, 0.20 mmol, 2.0 equiv.) was added as one portion and the mixture was stirred at 20 ℃ for another 18 h. The solvent was removed under reduced pressure and the residue was subjected to column chromatography on silica gel (eluent: ethyl acetate/petroleum ether, 1:4 – 1:1, v/v) to afford the corresponding product **3aa** in 93% yield (1.50 g) with 90% ee.



Procedure G: In glove box, a dry reaction tube was charged with substrate **4a** (1.060, 3.5 mmol), In(OTf)$_3$/**L$_4$-TQPr$_3$** (10 mol%, 1:1), followed by the addition of DME (35 mL). After stirring the mixture at 35 ℃ in water bath for 0.5 h, the mixture was allowed to cool to 10 ℃. Then potassium allyltrifluoroborate **2a** (1.036 g, 0.20 mmol, 2.0 equiv.) and H_2O (126 μL) was added as one portion and the mixture was stirred at 10 ℃ for another 18 h. The solvent was removed under reduced pressure and the residue was subjected to column chromatography on silica gel (eluent: ethyl acetate / petroleum ether, 15:1) at –20 ℃ (**Fig. 1**) to afford the corresponding product **5aa**.

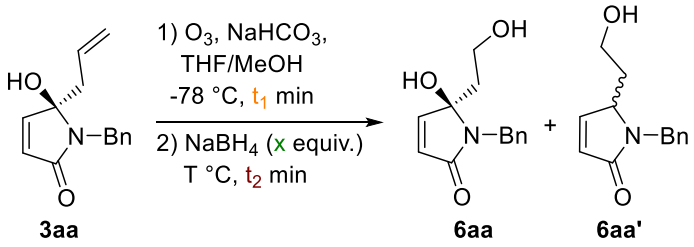
2.5 Experimental procedure for further transformations of the products[3]



3aa **6aa**, 86% yield

Procedure H: To a solution of **3aa** (90.0 mg, 0.4 mmol, 1.0 equiv) in 50 mL of THF and 5 mL of methanol at –78 °C was passed ozone until TLC analysis indicated consumption of the starting material (ca. 10 min). Nitrogen was passed through the solution for an additional 20 min at which time sodium borohydride (7.0 mg, 0.2 mmol, 0.5 equiv) was added in one portion and the solution was stirred at –78 °C for 10 min. The reaction mixture was quenched by slow addition of water. The resulting suspension was concentrated and extracted with ethyl acetate. The combined organic layer was washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated in vacuo. The crude material was subjected to column chromatography on silica gel to provide the diol **6aa** (47 mg, 51%) as a white oil.

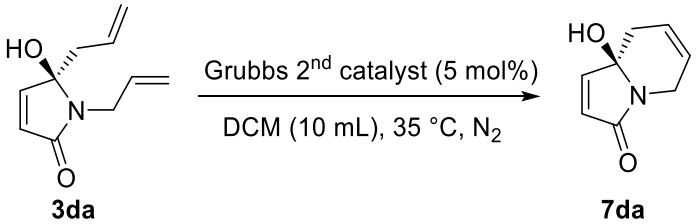
Table S1 Screening of the reaction conditions for ozone oxidation



3aa **6aa** **6aa'**

entry[a]	t_1	t_2	x	T	**6aa**/**6aa'**[b]	yield (%)[c]	ee (%)[d]
1	5	120	2	0	1/1	87	0
2	10	120	2	0	1/1	92	0
3	15	120	2	0	1/1	92	0
4	10	60	2	0	3.4/1	92	0
5	10	10	2	0	9/1	85	0
6	10	5	1	0	Only **6aa**	62	52
7	10	5	0.5	0	Only **6aa**	54	58
8	10	5	0.5	–78	Only **6aa**	51	80

[a] Unless otherwise noted, all reactions were carried out with **3aa** (0.40 mmol), O_3 (1.5 mL/min) in THF (20 mL) at –78 °C for 15 min. [b] determined by ^{1}H NMR. [c] isolated yields; NR = no reaction [c] Determined by HPLC on a chiral stationary phase.



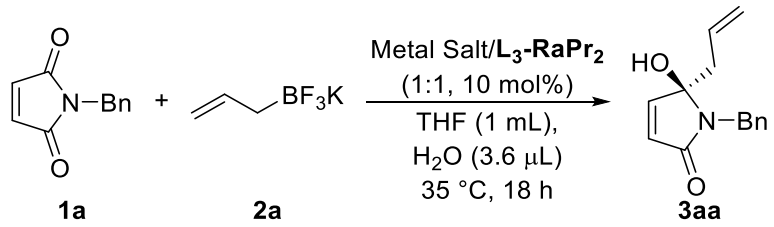
3da **7da**

Procedure I: To a solution of **3da** (17.9 mg, 0.1 mmol, 1.0 equiv.) in 10 mL of DCM at 35 °C under nitrogen atmosphere. Grubbs 2nd catalyst (4.2 mg, 5 mol%) was added slowly to the solution over 10 min. The reaction mixture was allowed to react overnight. The resulting red suspension was concentrated in vacuo. The crude material was subjected to column chromatography on silica gel to provide the product **7da** (12.5 mg, 83%) as a white solid.

3. Optimization of the reaction conditions

3.1 Optimization of the reaction conditions of maleimide 1a with allytrifluoroborate 2a

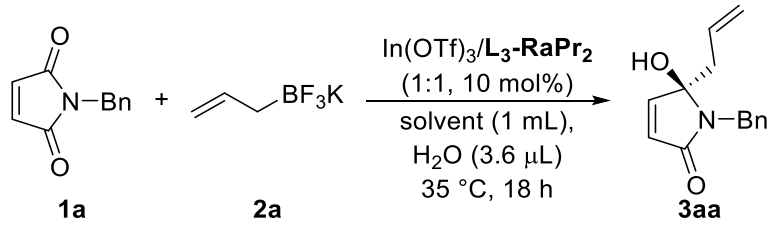
Table S2 Screening of metal salts



entry[a]	metal salt	yield (%)[b]	ee (%)[c]
1	-	0	-
2	$In(OTf)_3$	30	65
3	$Sc(OTf)_3$	0	-
4	$Fe(OTf)_2$	0	-
5	$Co(OTf)_2$	0	-
6	$Ni(OTf)_2$	0	-
7	$Cu(OTf)_2$	42	0
8	$Al(OTf)_3$	0	-
9	$Ga(OTf)_3$	6	0
10	$InCl_3$	13	-

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), and metal salt/**L_3-RaPr$_2$** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 16 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

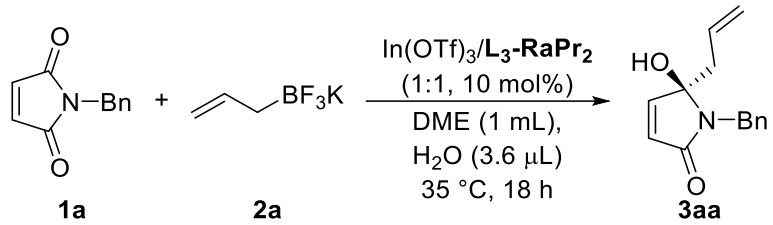
Table S3 Screening of solvent



entry[a]	solvent	yield (%)[b]	ee (%)[c]
1	THF	30	65
2	DMF	ND	0
3	DCM	12	77
4	DME	26	71
5	Toluene	trace	78
6	MeCN	trace	0

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), and $In(OTf)_3$/**L_3-RaPr$_2$** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 16 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

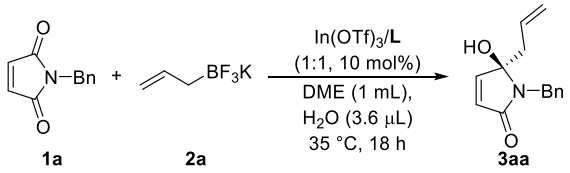
Table S4 Screening of substrate ratio

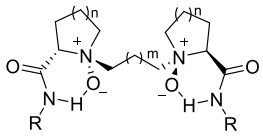


entry[a]	**1a/2a**	yield (%)[b]	ee (%)[c]
1	1/1	trace	-
2	1/1.5	17	77
3	1/2	26	71
4	1.5/1	8	80
5	2/1	trace	-
6[d]	1/2	6	83

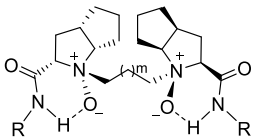
[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), and In(OTf)$_3$/**L$_3$-RaPr$_2$** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 16 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase. [d] At 10 ℃.

Table S5 Screening of ligands

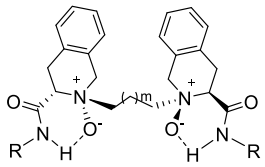




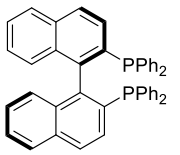
L$_3$-PrPr$_2$: R = 2,6-*i*Pr$_2$C$_6$H$_3$, m = 1, n = 1
L$_3$-PrPr$_3$: R = 2,4,6-*i*Pr$_2$C$_6$H$_2$, m = 1, n = 1
L$_3$-PrPr$_2$^{t}Bu: R = 2,6-*i*Pr$_2$-4-*t*BuC$_6$H$_2$, m = 1, n = 1
L$_3$-Pr-4-OCF$_3$: R = 4-OCF$_3$C$_6$H$_4$, m = 1, n = 1
L$_3$-Pr-4-Br: R = 4-BrC$_6$H$_4$, m = 1, n = 1
L$_3$-PrEt$_2$Me: R = 2,6-*i*Pr$_2$-4-MeC$_6$H$_2$, m = 1, n = 1
L$_3$-PiPr$_2$: R = 2,6-*i*Pr$_2$C$_6$H$_3$, m = 1, n = 2
L$_3$-PiPr$_3$: R = 2,4,6-*i*Pr$_2$C$_6$H$_2$, m = 1, n = 2
L$_2$-PiPr$_2$: R = 2,6-*i*Pr$_2$C$_6$H$_3$, m = 0, n = 2
L$_4$-PiPr$_2$: R = 2,6-*i*Pr$_2$C$_6$H$_3$, m = 2, n = 2
L$_3$-PiPr$_2$Br: R = 2,6-*i*Pr$_2$-4-BrC$_6$H$_2$, m = 1, n = 2
L$_3$-Pi^{t}Bu$_{(2,5)}$: R = 2,5-*t*Bu$_2$C$_6$H$_3$, m = 1, n = 2
L$_3$-Pi(O^{i}Pr)$_2$: R = 2,6-(O*i*Pr)$_2$C$_6$H$_3$, m = 1, n = 2
L$_3$-Pi(O^{t}Bu)$_2$: R = 2,6-(O*t*Bu)$_2$C$_6$H$_3$, m = 1, n = 2
L$_3$-Pi(O^{i}Pr)$_3$: R = 2,4,6-(O*i*Pr)$_2$C$_6$H$_2$, m = 1, n = 2



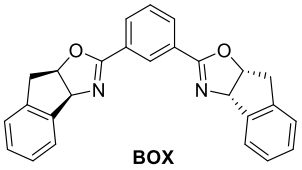
L$_3$-RaMe$_2$: R = 2,6-Me$_2$C$_6$H$_3$, m = 1
L$_3$-RaPr$_3$: R = 2,4,6-*i*Pr$_2$C$_6$H$_3$, m = 1



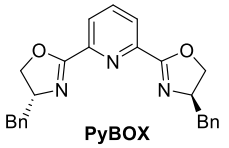
L$_3$-TQPr$_2$: R = 2,6-*i*Pr$_2$C$_6$H$_3$, m = 1
L$_3$-TQ^{t}Bu: R = *t*Bu, m = 1



BINAP



BOX



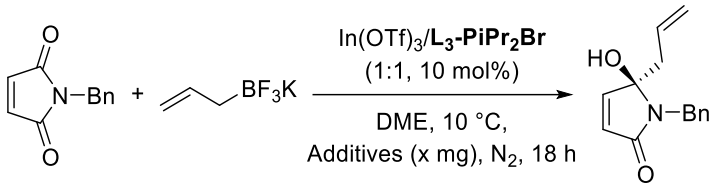
PyBOX

entry[a]	ligand	yield (%)[b]	ee (%)[c]
1	**L$_3$-PrPr$_2$**	ND	83
2	**L$_3$-PrPr$_3$**	18	79
3	**L$_3$-PrPr$_2$^{t}Bu**	ND	67
4	**L$_3$-Pr4-OCF$_3$**	ND	0
5	**L$_3$-Pr4-Br**	ND	5
6	**L$_3$-PrEt$_2$Me**	ND	63
7	**L$_3$-PiPr$_2$**	55	85
8	**L$_3$-PiPr$_3$**	52	81
9	**L$_2$-PiPr$_2$**	37	80
10	**L$_4$-PiPr$_2$**	12	7
11	**L$_3$-PiPr$_2$Br**	55	87
12	**L$_3$-Pi^{t}Bu$_{(2,5)}$**	12	80
13	**L$_3$-Pi(OiPr)$_2$**	79	65

14	**L_3-Pi(OtBu)$_2$**	92	73
15	**L_3-Pi(OiPr)$_3$**	80	83
16	**L_3-RaMe$_2$**	ND	59
17	**L_3-RaPr$_3$**	ND	81
18	**L_3-TQPr$_2$**	ND	3
19	**L_3-TQ^{t}Bu**	ND	11
20	**BINAP**	93	0
21	**BOX**	95	0
22	**PyBOX**	95	0
23[d]	**L_3-PiPr$_2$Br**	43	90

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), and In(OTf)$_3$/**Ligand** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 16 h. [b] Isolated yields; ND = no detected [c] Determined by HPLC on a chiral stationary phase. [d] At 10 ℃.

Table S6 Screening of additives

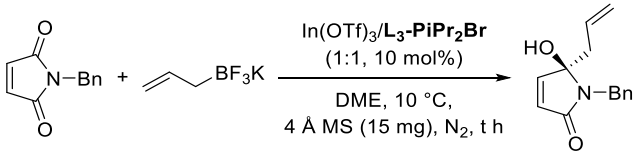


1a **2a** **3aa**

entry[a]	additives	x	yield (%)[b]	ee (%)[c]
1	NH_4Cl	1 equiv., 5.3 mg	trace	87
2	MeOH	1equiv., 4 μL	trace	85
3	EtOH	1equiv., 6 μL	trace	81
4	*i*PrOH	1equiv., 8 μL	trace	81
5	TFE	1equiv., 7 μL	trace	71
6	phenol	1equiv., 9.4 mg	trace	60
7	2-naphthol	1equiv., 14.4 mg	NR	-
8	PhCOOH	1equiv., 12.2 mg	trace	87
9	-	-	60	91
10	3 ÅMS	15 mg	80	93
11	4 ÅMS	15 mg	84	93
12	5 ÅMS	15 mg	70	93
13	4 ÅMS	10 mg	61	92
14	4 ÅMS	15 mg	84	93
15	4 ÅMS	20 mg	70	92

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), additives (x mg) and In(OTf)$_3$/**L_3-PiPr$_2$Br** (1:1, 10 mol%) in DME (1.0 mL) at 10 ℃ for 16 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

Table S7 Screening of reaction time

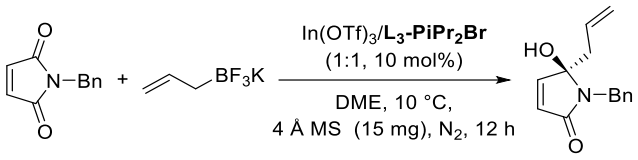


1a **2a** **3aa**

entry[a]	t/h	yield (%)[b]	ee (%)[c]
1	2	49	93
2	3	57	93
3	4	62	93
4	12	86	93
5	18	86	93
6	24	80	87
7	48 h\	43	73

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), 4 Å MS (15mg) and In(OTf)$_3$/**L_3-PiPr$_2$Br** (1:1, 10 mol%) in DME (1.0 mL) at 10 ℃ for t h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

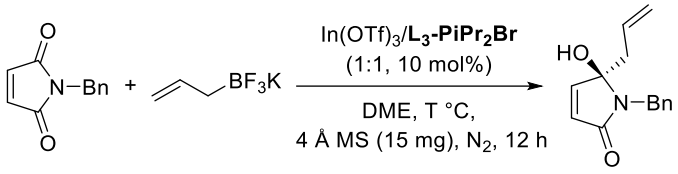
Table S8 Screening of catalyst loading



entry[a]	x	yield (%)[b]	ee (%)[c]
1	1	NR	-
2	2	trace	-
3	5	70	93
4	10	85	93
5	15	85	93

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), 4 Å MS (15mg) and In(OTf)$_3$/**L$_3$-PiPr$_2$Br** (1:1, x mol%) at 10 ℃ for 16 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase. [d] At 10 ℃.

Table S9 Screening of temperature

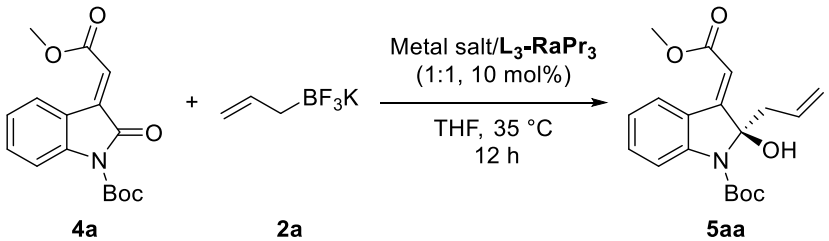


entry[a]	T (℃)	yield (%)[b]	ee (%)[c]
1	0	trace	-
2	10	70	93
3	20	95	93
4	35	99	85
5	40	99	73

[a] Unless otherwise noted, all reactions were carried out with **1a** (0.10 mmol), **2a** (0.20 mmol), 4 Å MS (15mg) and In(OTf)$_3$/**L$_3$-PiPr$_2$Br** (1:1, 10 mol%) in DME (1.0 mL) at T ℃ for 16 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

3.2 Optimization of the reaction conditions of alkenyloxindole 4a with allyltrifluoroborate 2a

Table S10 Screening of metal salts

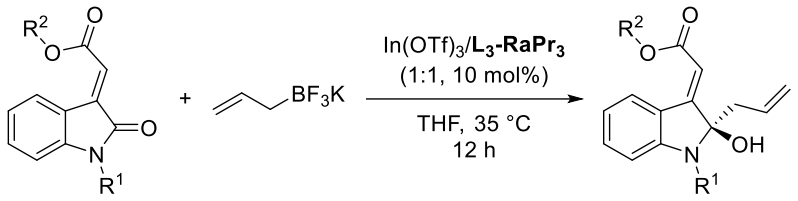


entry[a]	metal salt	yield (%)[b]	ee (%)[c]
1	-	0	-
2	Mg(OTf)$_2$	0	-
3	Ni(OTf)$_2$	0	-
4	Co(OTf)$_2$	0	-
5	Sc(OTf)$_3$	0	-
6	In(OTf)$_3$	32	45
7	Yb(OTf)$_3$	0	-

8	$Ga(OTf)_3$	8	0
9	$La(OTf)_3$	0	-
10	$Al(OTf)_3$	0	-

[a] Unless otherwise noted, all reactions were carried out with **4a** (0.10 mmol), **2a** (0.20 mmol), and metal salt/**L_3-RaPr$_2$** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 18 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

Table S11 Screening of protecting group

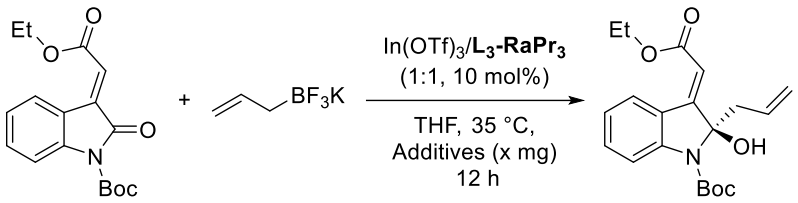


4 **2a** **5a**

Entry[a]	R^1	R^2	Yield (%)[b]	ee (%)[c]
1	Boc	Me	32	45
2	Cbz	Me	35	15
3	Ts	Me	52	3
4	Me	Me	trace	-
5	Bn	Me	trace	-
6	H	Me	trace	-
7	Boc	Et	25	51
8	Boc	*i*Pr	24	35
10	Boc	*t*Bu	21	35

[a] Unless otherwise noted, all reactions were carried out with **4** (0.10 mmol), **2a** (0.20 mmol), and $In(OTf)_3$/**L_3-RaPr$_3$** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 18 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

Table S12 Screening of additives

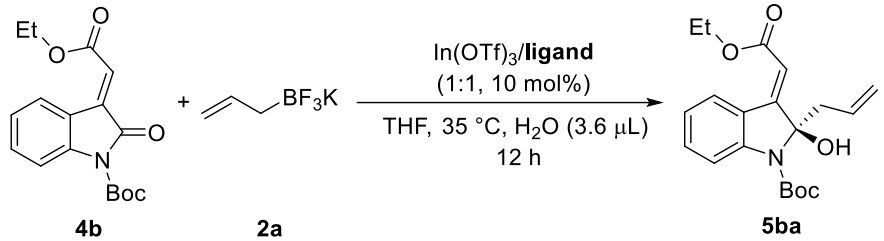


4b **2a** **5ba**

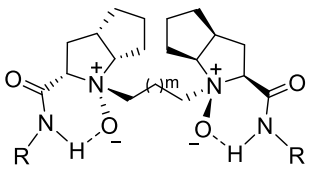
entry[a]	additives	x	yield (%)[b]	ee (%)[c]
1	H_2O	1.8 (1.0 equiv.)	90	20
2	H_2O	3.6 (2.0 equiv.)	86	42
3	H_2O	5.4 (3.0 equiv.)	85	41
4	H_2O	9.0 (5.0 equiv.)	73	38
5	-	-	25	51
6	3 ÅMS	15 mg	82	7
7	4 ÅMS	15 mg	81	25
8	5 ÅMS	15 mg	47	31

[a] Unless otherwise noted, all reactions were carried out with **4b** (0.10 mmol), **2a** (0.20 mmol), H_2O (x μL) and $In(OTf)_3$/**L_3-RaPr$_3$** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 18 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

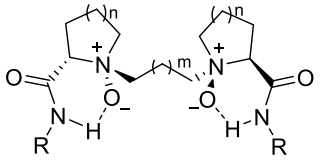
Table S13 Rescreening of ligands



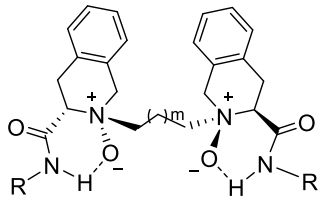
4b **2a** **5ba**



L_2-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 0
L_3-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 1
L_4-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 2
L_5-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 3
L_6-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 4
L_7-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 5
L_8-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 6
L_9-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 7
L_{10}-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 8
L_3-RaPr_3: R = 2,4,6-*i*$Pr_3C_6H_2$, m = 1
L_4-RaMe_2: R = 2,6-$Me_2C_6H_3$, m = 2
L_4-RaEt_2: R = 2,6-$Et_2C_6H_3$, m = 2
L_4-RaPr_2Ad: R = 2,6-*i*Pr_2-4-AdC_6H_3, m = 2
L_4-Ra$(OMe)_2$: R = 2,6-$(OMe)_2C_6H_3$, m = 2



L_3-PrPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 1, n = 1
L_4-PrPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 2, n = 1
L_5-PrPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 3, n = 1
L_6-PrPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 4, n = 1
L_4-PrPr_3: R = 2,4,6-*i*$Pr_3C_6H_2$, m = 2, n = 1
L_3-PiPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 1, n = 2

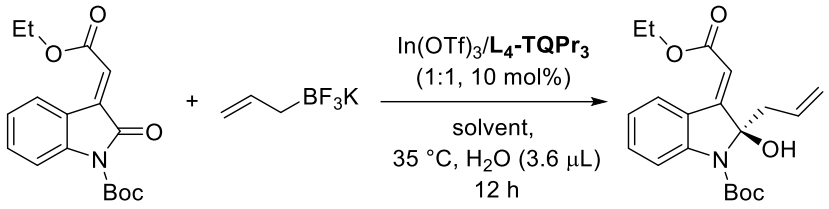


L_4-RaPr_2: R = 2,6-*i*$Pr_2C_6H_3$, m = 2
L_4-RaPr_3: R = 2,4,6-*i*$Pr_3C_6H_2$, m = 2

entry[a]	ligand	yield (%)[b]	ee (%)[c]
1	**L_3-RaPr_2**	45	11
2	**L_3-PrPr_2**	75	15
3	**L_3-PiPr_2**	88	-13
4	**L_2-RaPr_2**	68	5
5	**L_4-RaPr_2**	99	57
6	**L_5-RaPr_2**	79	37
7	**L_6-RaPr_2**	87	31
8	**L_7-RaPr_2**	95	43
9	**L_8-RaPr_2**	96	37
10	**L_9-RaPr_2**	79	40
11	**L_{10}-RaPr_2**	85	43
12	**L_4-PrPr_2**	96	37
13	**L_5-PrPr_2**	96	7
14	**L_6-PrPr_2**	99	0
15	**L_4-PrPr_3**	67	33
16	**L_3-RaPr_3**	74	55
17	**L_4-RaMe_2**	87	26
18	**L_4-RaEt_2**	94	42
19	**L_4-RaPr_2Ad**	88	51
20	**L_4-Ra$(OMe)_2$**	85	29
21	**L_4-TQPr_2**	94	58
22	**L_4-TQPr_3**	74	63

[a] Unless otherwise noted, all reactions were carried out with **4b** (0.10 mmol), **2a** (0.10 mmol), H_2O (3.6 μL) and In$(OTf)_3$/**Ligand** (1:1, 10 mol%) in DME (1.0 mL) at 35 ℃ for 16 h. [b] Isolated yields. [c] Determined by HPLC on a chiral stationary phase.

Table S14 Rescreening of solvent

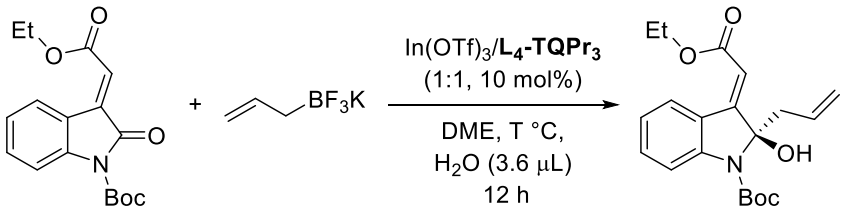


4b **2a** **5ba**

entry[a]	solvent	yield (%)[b]	ee (%)[c]
1	THF	74	63
2	DME	99	75
3	MeCN	19	17
4	EA	89	57
5	DCM	84	77

[a] Unless otherwise noted, all reactions were carried out with **4b** (0.10 mmol), **2a** (0.10 mmol), H_2O (3.6 μL) and $In(OTf)_3$/**L_4-TQPr$_3$** (1:1, 10 mol%) in solvent (1.0 mL) at 35 ℃ for 18 h. [b] NMR yields. [c] Determined by HPLC on a chiral stationary phase.

Table S15 Screening of temperature

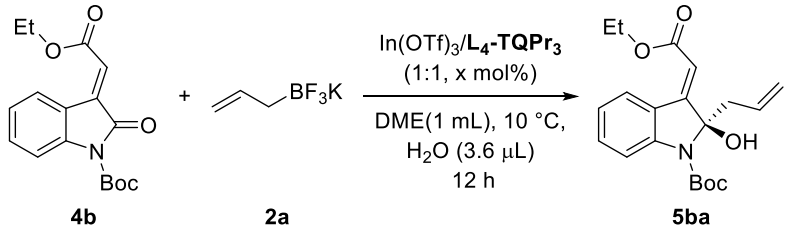


4b **2a** **5ba**

entry[a]	T (℃)	Yield (%)[b]	ee (%)[c]
1	35	99	75
2	20	99	85
3	10	99	93
4	0	87	93
5	-10	30	94

[a] Unless otherwise noted, all reactions were carried out with **4b** (0.10 mmol), **2a** (0.10 mmol), H_2O (3.6 μL) and $In(OTf)_3$/**L_4-RaPr$_2$** (1:1, 10 mol%) in solvent (1.0 mL) at T ℃ for 18 h. [b] NMR yields. [c] Determined by HPLC on a chiral stationary phase.

Table S16 Rescreening of catalyst loading



4b **2a** **5ba**

entry[a]	x	yield (%)[b]	ee (%)[c]
1	10	99	93
2	5	18	88
3	2	2	81
4	1	NR	0

[a] Unless otherwise noted, all reactions were carried out with **4b** (0.10 mmol), **2a** (0.10 mmol), H_2O (3.6 μL) and $In(OTf)_3$/**L_4-RaPr$_2$** (1:1, x mol%) in DME (1.0 mL) at 10 ℃ for 18 h. [b] NMR yields; NR = no reaction [c] Determined by HPLC on a chiral stationary phase.

4. Control experiment and mechanistic studies

4.1 Control experiments to probe the existence of the allylicindium compounds.

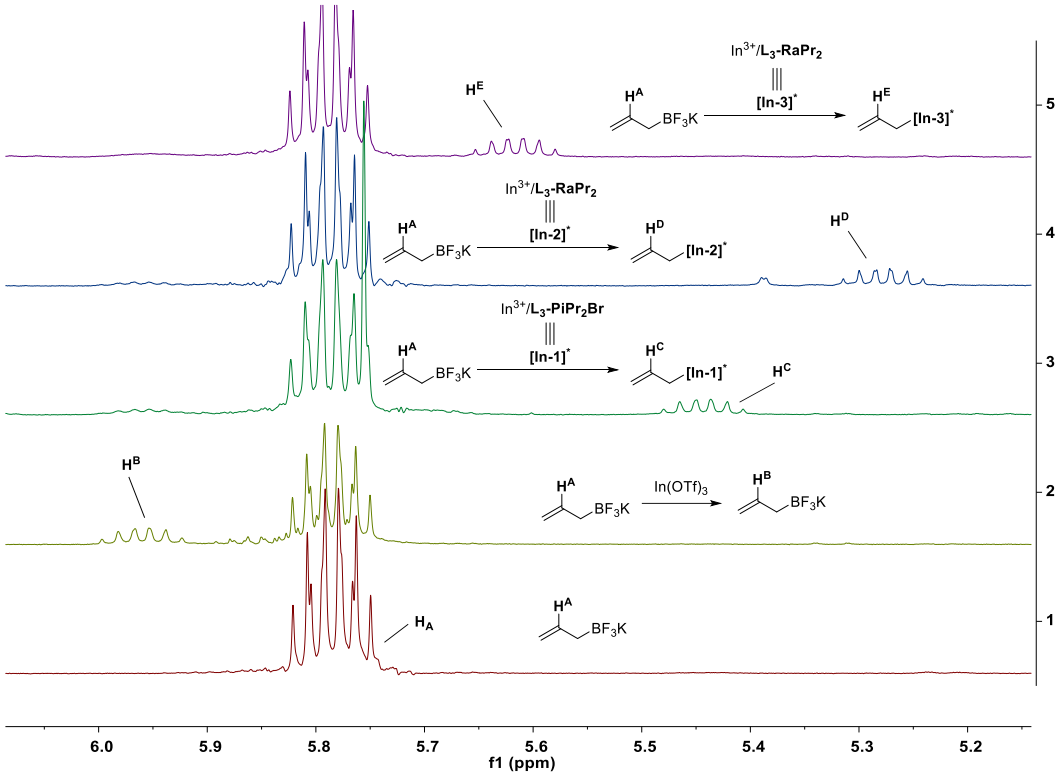


Figure S2 ^{1}H NMR of substrate **2** with different *N,N′*-dioxides

Procedure: In glove box, a dry reaction tube was charged with substrate **2** (7.4 mg, 0.05 mmol), $In(OTf)_3$ (5.6 mg, 0.01 mmol), **L** (0.01 mmol), followed by the addition of DMSO-*d*6 (1.0 mL). After stirring the mixture at 35 ℃ in water bath for 10 min, the mixture was filtrated into NMR tube and performed NMR experiments.

After the addition of $In(OTf)_3$, the C-H signal of H_A was shifted downfield obviously, supporting a allylicindium complex was generated. However, after the addition of $In(OTf)_3$/**L_3-PiPr$_2$Br**, $In(OTf)_3$/**L_3-RaPr$_2$** and $In(OTf)_3$/**L_3-Pi(O^{i}Pr)$_2$**, all of the C-H signal of H_A was shifted upfield obviously, supporting an allylicindium/*N,N′*-dioxide complex was generated respectively.

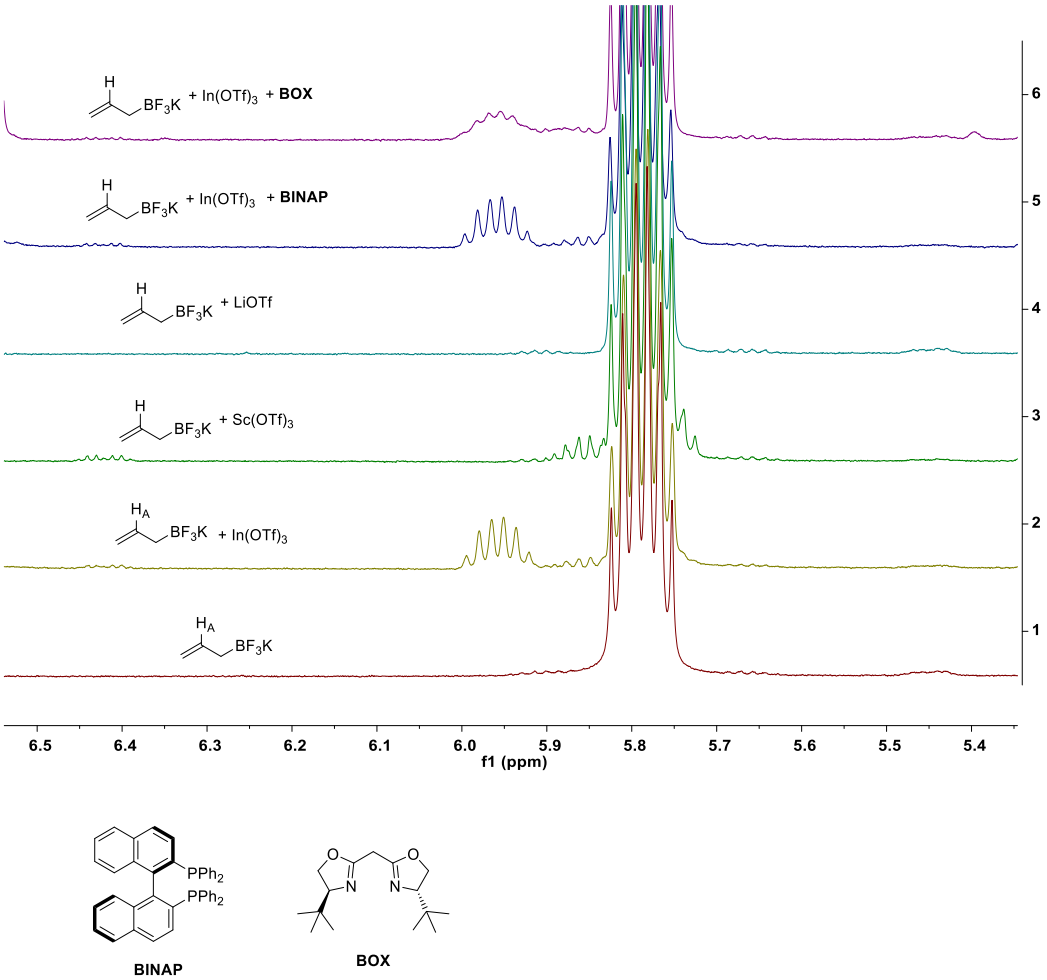


Figure S3 ^{1}H NMR of substrate **2** with different metal salts and ligands

Procedure: In glove box, a dry reaction tube was charged with substrate **2** (7.4 mg, 0.05 mmol), Metal Salt (0.01 mmol), **L** (0.01 mmol), followed by the addition of DMSO-*d*6 (1.0 mL). After stirring the mixture at 35 ℃ in water bath for 10 min, the mixture was filtrated into NMR tube and performed NMR experiments.

After the addition of $In(OTf)_3$, the C-H signal of H_A was shifted downfield obviously, supporting a allylicindium complex was generated. However, after the addition of other metal salt $Sc(OTf)_3$ and LiOTf, no chemical shift changed obviously, showing that no allylicindium complex was generated. Furthermore, after the addition of $In(OTf)_3$/**BINAP**, and $In(OTf)_3$/**BOX**, all of the C-H signal of H_A was shifted downfield obviously.

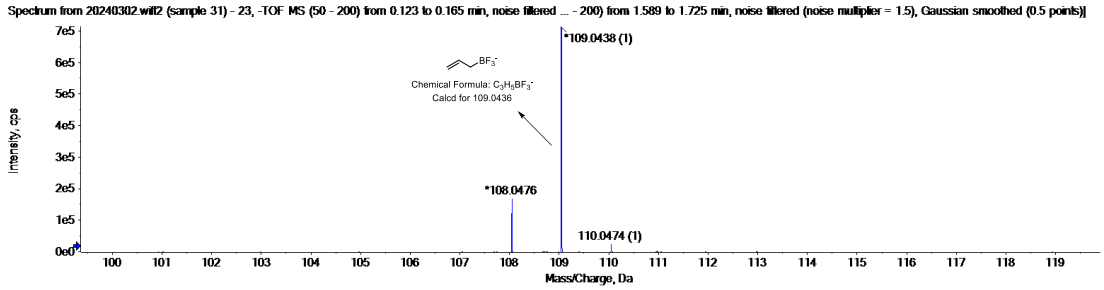


Figure S4 HRMS of substrate **2**

Procedure: In glove box, a dry reaction tube was charged with substrate **2a** (7.4 mg, 0.05 mmol) and DMSO (0.5 mL). After stirring the mixture at 35 ℃ in water bath for 10 min, the mixture was diluted into MS vial and performed MS experiments.

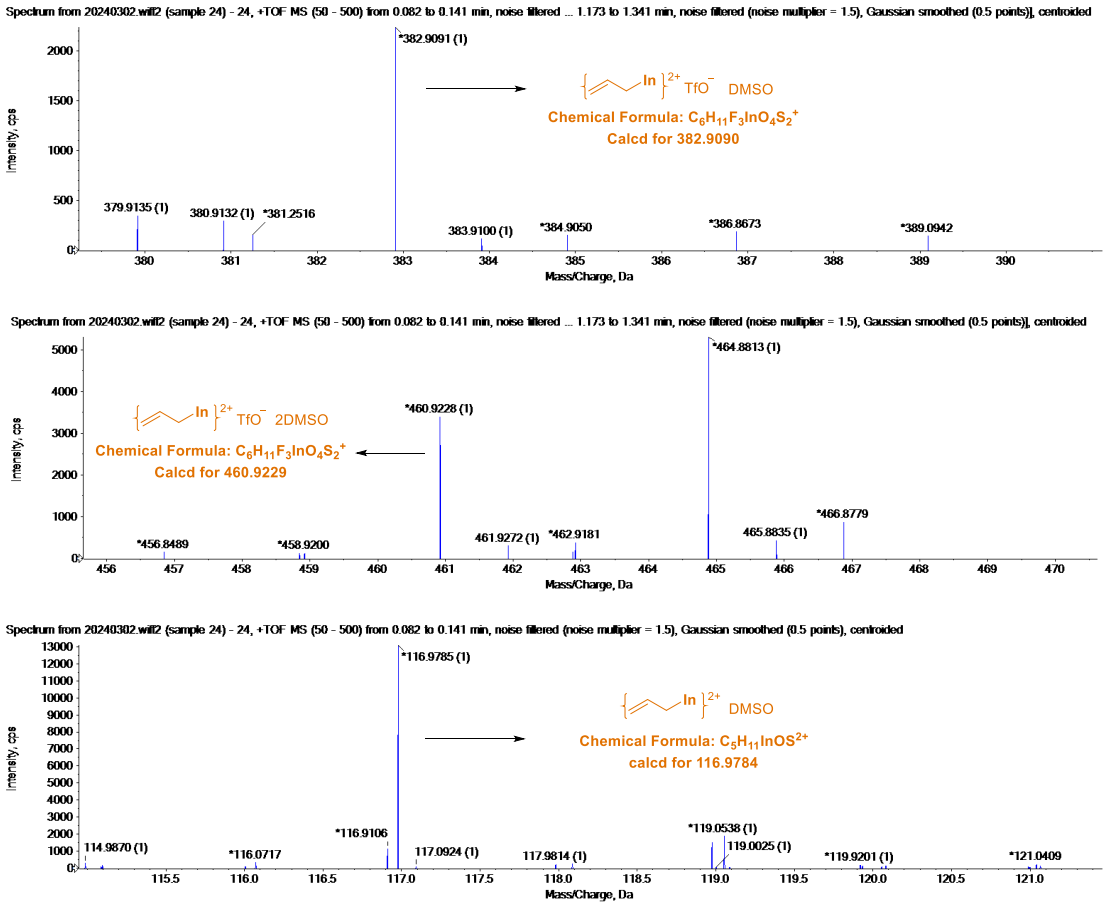


Figure S5 HRMS of substrate **2** with $In(OTf)_3$

Procedure: In glove box, a dry reaction tube was charged with substrate **2** (7.4 mg, 0.05 mmol), $In(OTf)_3$ (5.6 mg, 0.01 mmol), followed by the addition of DMSO (0.5 mL). After stirring the mixture at 35 ℃ in water bath for 10 min, the mixture was diluted into MS vial and performed MS experiments.

After the addition of $In(OTf)_3$, three peaks at *m/z* 382.9091, 460.6228, 116.9785 were observed, which could be assigned to allylicindium complex coordinated with DMSO {$[In(DMSO)(OTf)(C3H5)]^+$, calculated *m/z* 382.9090; $[In(DMSO)_2(OTf)(C3H5)]^+$, calculated *m/z* 460.9229; $[In(DMSO)(C3H5)]^{2+}$, calculated *m/z* 116.9784} based on the data of *m/z* and the isotopic distribution patterns

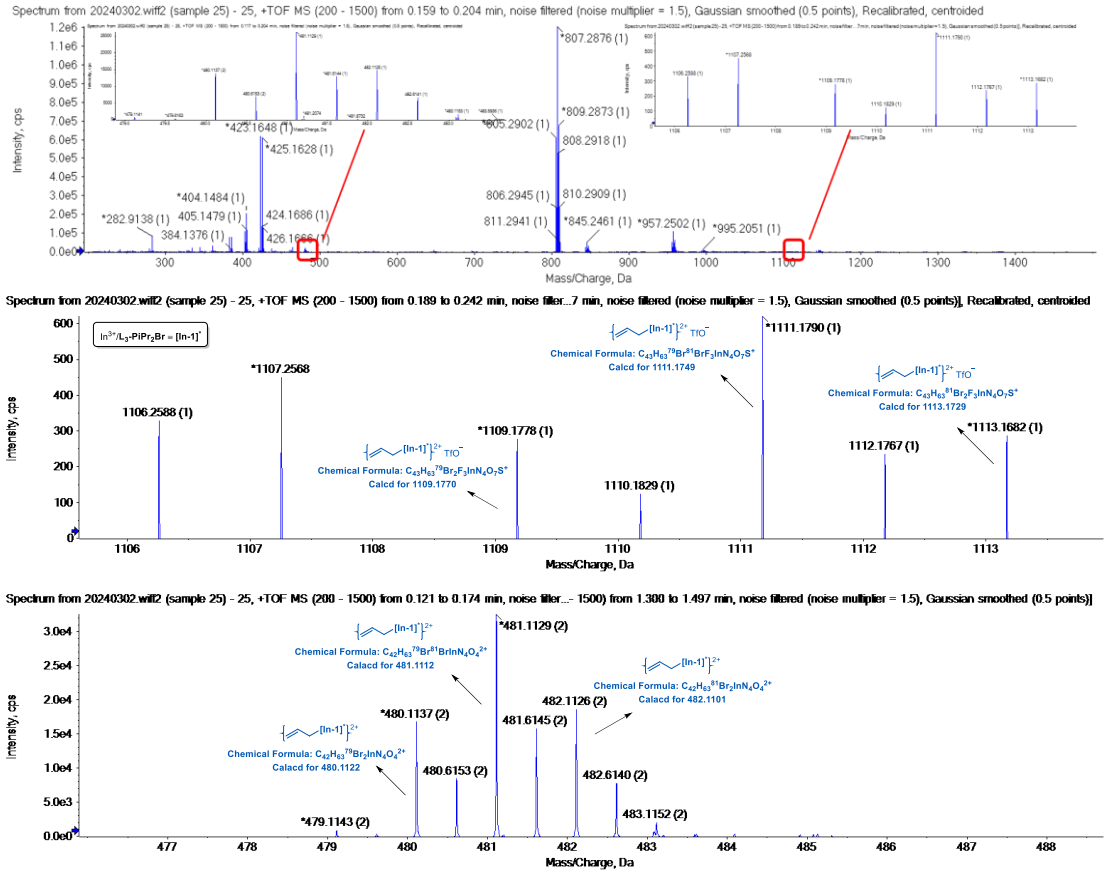
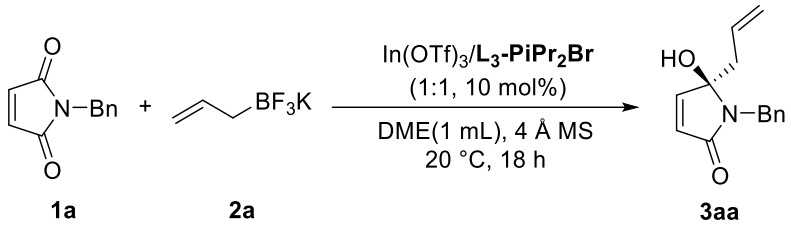


Figure S6 HRMS of substrate **2** with $In(OTf)_3$/**L_3-PiPr$_2$Br**

Procedure: In glove box, a dry reaction tube was charged with substrate **2** (7.4 mg, 0.05 mmol), $In(OTf)_3$ (5.6 mg, 0.01 mmol), **L** (0.01 mmol), followed by the addition of DMSO (0.5 mL). After stirring the mixture at 35 °C in water bath for 10 min, the mixture was diluted into MS vial and performed MS experiments.

After the addition of $In(OTf)_3$/**L_3-PiPr$_2$Br**, six prominent peaks at *m*/*z* 1109.1778, 1111.1790, 1113.1682 and 480.1137, 481.1129, 482.1126 were observed, which could be assigned to allylicindium complex {$[In(OTf)(C_3H_5)$(**L_3-PiPr$_2$Br**)$]^+$, calculated *m*/*z* 1109.1770, 1111.1749, 1111.1729; $[In(C_3H_5)$(**L_3-PiPr$_2$Br**)$]^{2+}$, calculated *m*/*z* 480.1122, 481.1112, 482.1101} based on the data of *m*/*z* and the isotopic distribution patterns

4.2 The relationship of the ee value of product with the optical purity of the chiral ligand.



Combined certain amount of optically pure (D)-**L_3-PiPr$_2$Br** with pure (L)-**L_3-PiPr$_2$Br** led to ligand mixture with specified ee values. Six different control reactions were performed in parallel by using **L-PiPr$_2$Br** with 0% ee, 20% ee, 40% ee, 60% ee, 80% ee and 100% ee. 1-benzyl-1*H*-pyrrole-2,5-dione **1a** (0.1 mmol) and In(OTf)$_3$/**L_3-PiPr$_2$Br** (10 mol%, 1/1) were weighted into a dried test tube.

Procedure: In glove box, a dry reaction tube was charged with substrate **1a** (0.10 mmol), In(OTf)$_3$/**L_3-PiPr$_2$Br** (10 mol%, 1:1), 4 Å MS (15 mg), followed by the addition of DME (1.0 mL). After stirring the mixture at 35 ℃ in water bath for 0.5 h, the mixture was allowed to cool to 20 ℃. Then potassium allyltrifluoroborate **2a** (0.20 mmol, 30.0 mg) was added as one portion and the mixture was stirred at 20 ℃ for another 18 h. The reaction mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate / petroleum ether, 1:4 – 1:1, v/v) to afford the corresponding product **3aa**.

Table S17. Linear relationship between the ee value of products 3aa and the enantiopurity of the chiral ligands

Entry	ee of **L_3-PiPr$_2$Br (%)**	ee of **3aa**
1	0	0
2	20	15
3	40	39
4	60	59
5	80	81
6	100	93

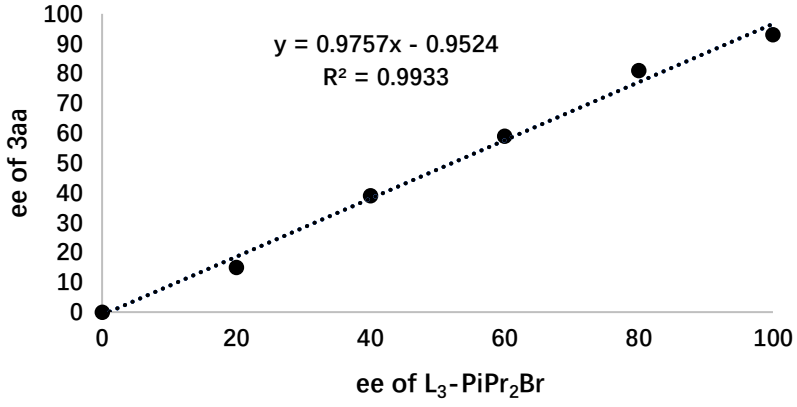
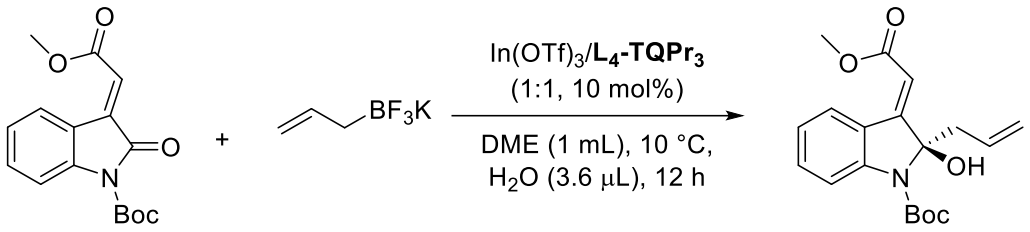


Figure S7 Linear relationship between the ee value of products **3aa** and the enantiopurity of the chiral ligands



4a **2a** **5aa**

Combined certain amount of optically pure (D)-$\mathbf{L_4}$-$\mathbf{TQPr_3}$ with pure (L)- $\mathbf{L_4}$-$\mathbf{TQPr_3}$ led to ligand mixture with specified ee values. Six different control reactions were performed in parallel by using $\mathbf{L_4}$-$\mathbf{TQPr_3}$ with 0% ee, 20% ee, 40% ee, 60% ee, 80% ee and 100% ee. *tert*-Butyl (*E*)-3-(2-methoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **4a** (0.1 mmol) and In(OTf)$_3$/$\mathbf{L_3}$-$\mathbf{PiPr_2Br}$ (10 mol%, 1/1) were weighted into a dried test tube.

Procedure: In glove box, a dry reaction tube was charged with substrate **4a** (0.10 mmol), In(OTf)3/$\mathbf{L_4}$–$\mathbf{TQPr_3}$ (10 mol%, 1:1), followed by the addition of DME (1.0 mL). After stirring the mixture at 35 ℃ in water bath for 0.5 h, the mixture was allowed to cool to 10 ℃. Then potassium allyltrifluoroborate **2a** (30.0 mg, 0.20 mmol) and H_2O (3.6 μL) was added as one portion and the mixture was stirred at 20 ℃ for another 18 h. The reaction mixture was subjected to column chromatography on silica gel (eluent: ethyl acetate / petroleum ether, 15:1, v/v) at -20 ℃ to afford the corresponding product **5aa**.

Table S18. Linear relationship between the ee value of products 3aa and the enantiopurity of the chiral ligands

Entry	ee of $\mathbf{L_4}$-$\mathbf{TQPr_3}$ (%)	ee of **5aa**
1	0	0
2	20	23
3	40	37
4	60	58
5	80	65
6	100	93

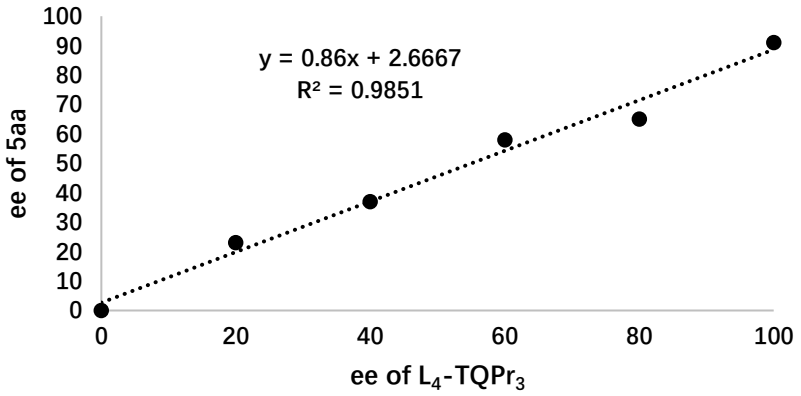


Figure S8 Linear relationship between the ee value of products **5aa** and the enantiopurity of the chiral ligands

5. X-ray crystallography

The colourless crystal in rod-shape, with approximate dimensions of 0.108 × 0.160 × 0.722 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2)K equipped with micro-focus Cu radiation source (Kα = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program packagea. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested. CCDC 2283654 contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

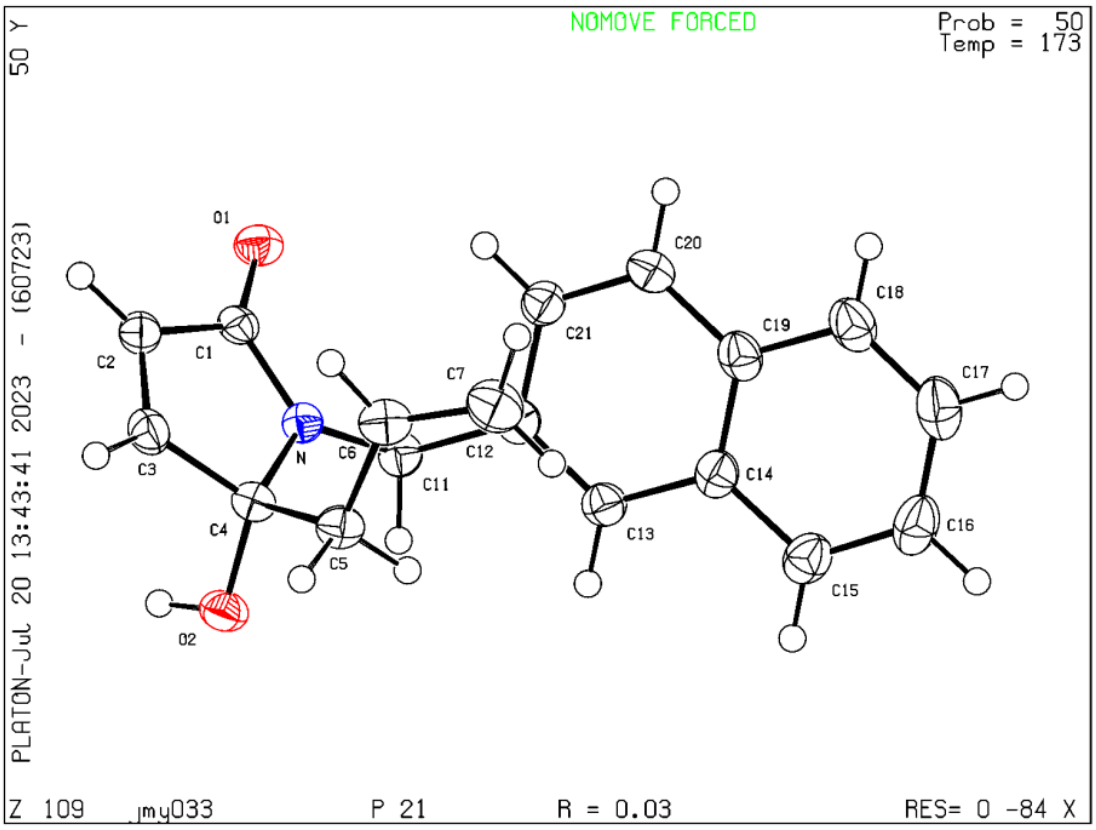


Figure S9 X-ray crystal structure of product **3na**

The crystal of product **3na** was obtained from the solution of ethyl acetate and petroleum ether. CCDC: 2283654.

References:

[a] Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112–122.

[b] Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3–8.

[c] Sheldrick, G. M. *Acta Cryst*. **2015**, *C71*, 3–8.

[d] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J., Howard, J. A. K., Puschmann, H. *J. Appl. Cryst*. **2009**, *42*, 339-341.

[e] Spek, A. L. *J. Appl. Cryst.* **2003**, *36*, 7–13.

Table S19. Crystallographic data for $C_{18}H_{17}NO_2$ (3na)

Formula	$C_{18}H_{17}NO_2$
Formula mass (amu)	279.32
Space group	$P2_12_12_1$
a (Å)	7.0543(2)
b (Å)	7.3349(2)
c (Å)	14.5891(3)
α (deg)	90
β (deg)	103.664
γ (deg)	90
V (Å^3)	733.51(3)
Z	2
λ (Å)	1.54178
T (K)	173
ρ_{calcd} (g cm^{-3})	1.265
μ (mm^{-1})	0.657
Transmission factors	0.695−1.000
θ_{max} (deg)	68.274
No. of unique data, including $F_o^2 < 0$	2688
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	2647
No. of variables	195
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0283
$R_w(F_o^2)$ [b]	0.0783
Goodness of fit	1.080

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

The colourless crystal in flake-shape, with approximate dimensions of 0.110 × 0.155 × 0.500 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2)K equipped with micro-focus Cu radiation source (K_α = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[a, b, c, d]. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[e]. CCDC 2408882 contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

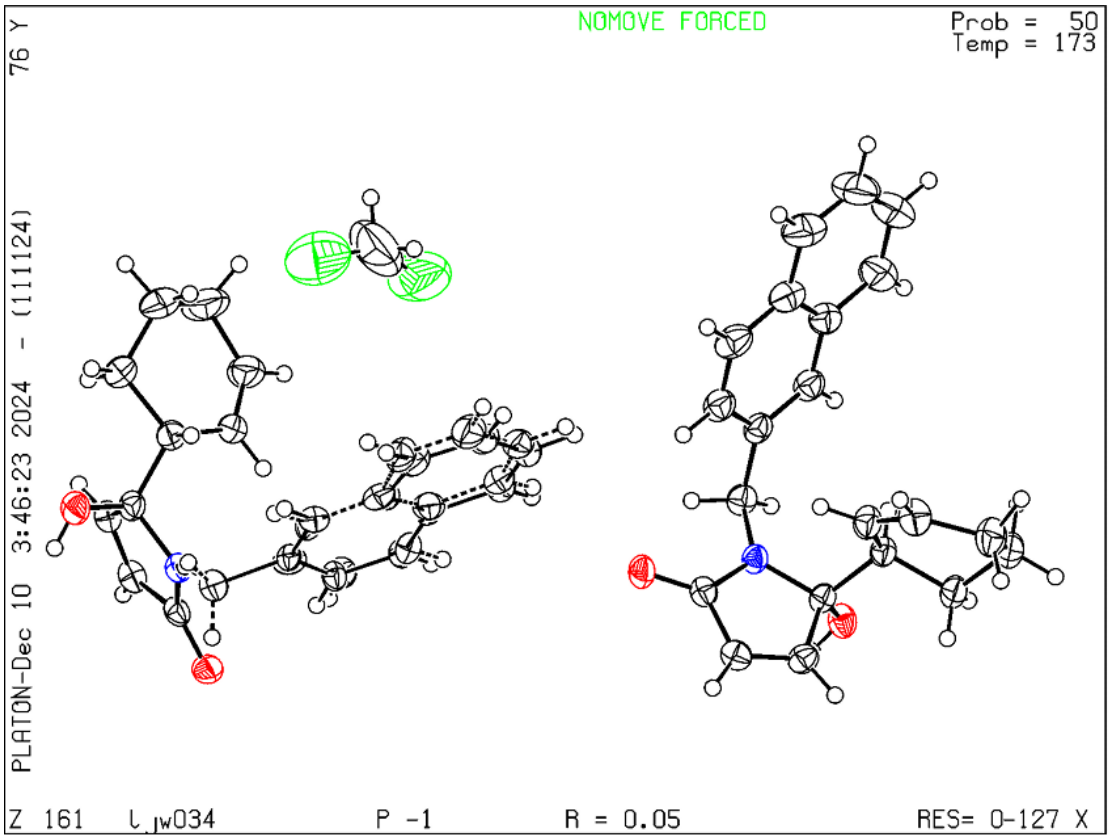


Figure S10 X-ray crystal structure of product **3ne**

The crystal of product **5ua** was obtained from the solution of ethyl acetate and petroleum ether. CCDC: 2283654.

References:

[a] Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112–122.

[b] Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3–8.

[c] Sheldrick, G. M. *Acta Cryst.* **2015**, *C71*, 3–8.

[d] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J., Howard, J. A. K., Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339-341.

[e] Spek, A. L. *J. Appl. Cryst.* **2003**, *36*, 7–13.

Table S20. Crystallographic data for 2($C_{21}H_{21}NO_2$), 0.5(CH_2Cl_2). (3ne)

Formula	2($C_{21}H_{21}NO_2$), 0.5(CH_2Cl_2).
Formula mass (amu)	1362.48
Space group	$P\bar{1}$ (*No*. 2)
a (Å)	5.9509(1)
b (Å)	17.6588(4)
c (Å)	17.8803(4)
α (deg)	71.008(1)
β (deg)	86.669(1)
γ (deg)	88.820(1)
V (Å^3)	2
Z	1.54178
λ (Å)	173(2)
T (K)	173(2)
ρ_{calcd} (g cm^{-3})	1.276
μ (mm^{-1})	1.314
Transmission factors	0.711–1.000
θ_{max} (deg)	68.295
No. of unique data, including $F_o^2 < 0$	6472
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	5706
No. of variables	565
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0467
$R_w(F_o^2)$ [b]	0.1252
Goodness of fit	1.039

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

The colourless crystal in rod-shape, with approximate dimensions of 0.063 × 0.069 × 0.163 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2) K equipped with micro-focus Cu radiation source (K_α = 1.54178 Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[a, b, c, d]. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[e]. CCDC 2393879 contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

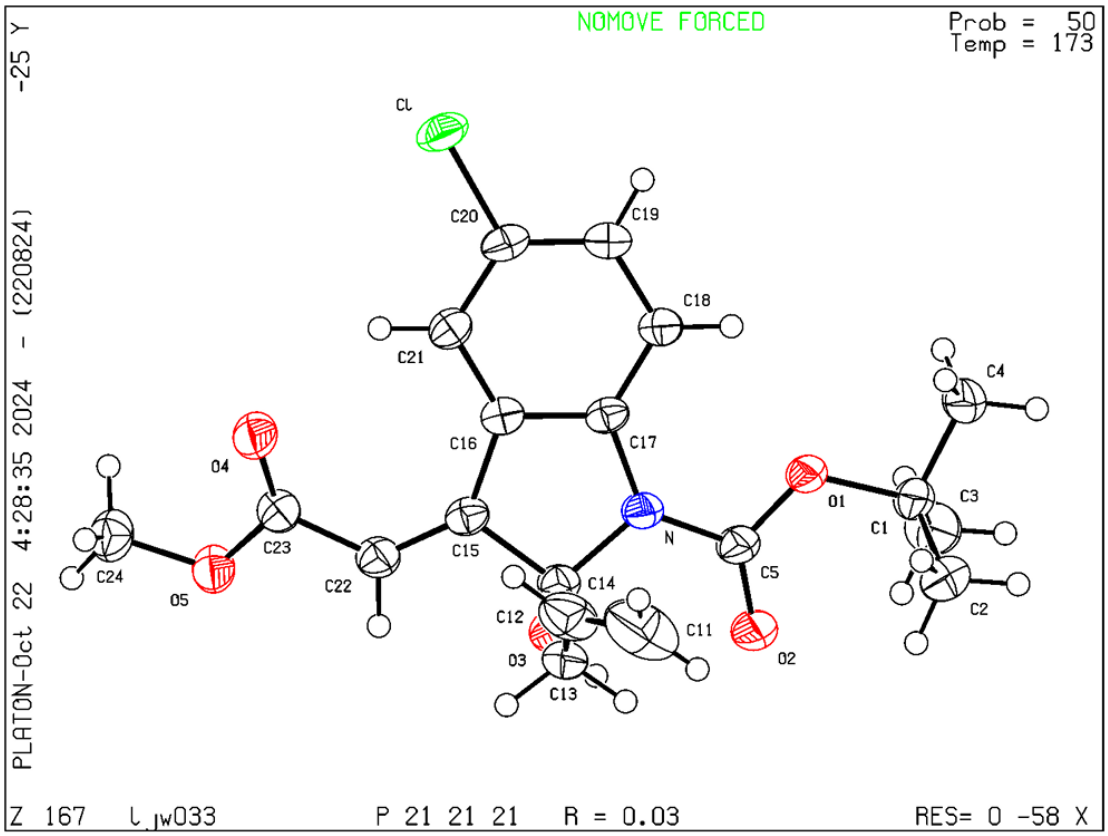


Figure S11 X-ray crystal structure of product **5ua**

The crystal of product **5ua** was obtained from the solution of ethyl acetate and petroleum ether. CCDC: 2283654.

References:

[a] Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112–122.

[b] Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3–8.

[c] Sheldrick, G. M. *Acta Cryst*. **2015**, *C71*, 3–8.

[d] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J., Howard, J. A. K., Puschmann, H. *J. Appl. Cryst*. **2009**, *42*, 339-341.

[e] Spek, A. L. *J. Appl. Cryst.* **2003**, *36*, 7–13.

Table S21. Crystallographic data for $C_{19}H_{22}ClNO_5$ (5ua)

Formula	$C_{19}H_{22}ClNO_5$
Formula mass (amu)	379.12
Space group	$P2_12_12_1$ (*No*. 19)
a (Å)	9.9232(2)
b (Å)	13.3961(3)
c (Å)	14.6378(3)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	1945.83(7)
Z	4
λ (Å)	1.54178
T (K)	173
ρ_{calcd} (g cm^{-3})	1.297
μ (mm^{-1})	1.985
Transmission factors	0.865─1.000
θ_{max} (deg)	68.285
No. of unique data, including $F_o^2 < 0$	3543
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	3358
No. of variables	243
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0267
$R_w(F_o^2)$ [b]	0.0661
Goodness of fit	1.062

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

6. Biological activity study

Cell culture

Hepatocellular carcinoma cell line HCCLM3 (obtained from Procell) were cultured with DMEM (Biological Industries, Shanghai) supplemented with 10% (*v/v*) FBS (Gibco, New York), 1% (*v/v*) penicillin/streptomycin (Beyotime, Shanghai). Lung cancer cell line A549 (obtained from Procell) were cultured with Ham's F-12K (Bosterbio, CA) supplemented with 10% (*v/v*) FBS (Gibco, New York), 1% (*v/v*) penicillin/streptomycin (Beyotime, Shanghai). All cells were cultured in incubator with 5% CO_2 at 37 ℃

Cell Viability Assay

Cells of logarithmic growth stage were inoculated in 96-well plate with density of 1.5×10^4 per well. Overnight all cells which density at 80%, were treated with 1% DMSO (negative control) and other compounds with different concentrations at 37 ℃ for 48 h. No FBS DMEM or F-12K with 10% (*v/v*) CCK-8 (Selleck, Houston) was added to each well and incubated for 1h at 37 ℃. The absorbance was determined at 450 nm to calculated cell viability (%). IC_{50} was detected using Graphpad Prism. Each experiment was repeated three times.

Result

To study the anti-hepatocellular carcinoma (HCCLM3) and lung cancer cell (A549) of synthetic compounds, we measured the HCCLM3 cell and A549 cell viability after exposed to each compound with 25 μM for 48 h. The results indicated that compounds **3nf** had obvious inhibitory effect on the viability of A549 and the IC_{50} value of **3nf** towards A549 was 5.764 μM. And IC_{50} values of **3nf** towards HCCLM3 were 7.035 μM.

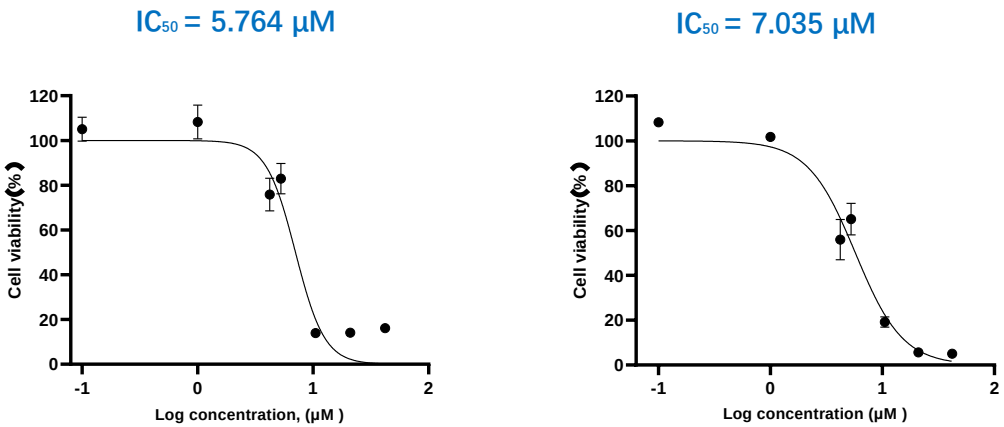
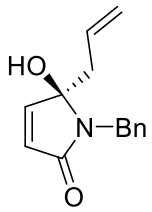


Figure S12 IC_{50} values of **3nf** towards A549 (left) and HCCLM3 (right)

7. Characterization of the products

(*R*)-5-Allyl-1-benzyl-5-hydroxy-1,5-dihydro-2*H*-pyrrol-2-one (3aa)



Viscous colorless oil. R_f = 0.35 (petroleum ether/ethyl acetate = 1/1, v/v), 95% yield, 93% *ee.* $[\alpha]^{25}_D$ = +77.7 (*c* = 0.44, in CH_2Cl_2).

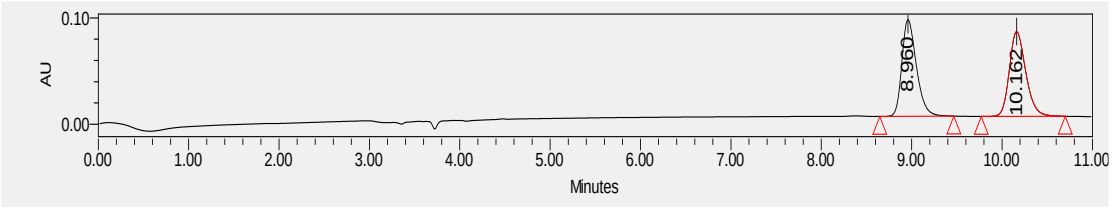
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 10.0 min, t_{minor} = 8.9 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.41 – 7.16 (m, 5H), 6.85 (d, J = 6.0 Hz, 1H), 5.95 (d, J = 6.0 Hz, 1H), 5.46 – 5.29 (m, 1H), 5.02 – 4.79 (m, 2H), 4.69 (s, 1H), 4.62 (d, J = 15.4 Hz, 1H), 4.33 (d, J = 15.4 Hz, 1H), 2.61 – 2.47 (m, 1H), 2.35 – 2.18 (m, 1H).

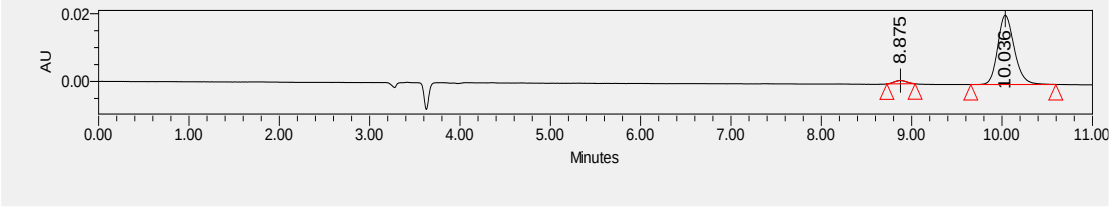
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 170.22, 149.77, 138.14, 131.23, 128.49, 128.34, 127.35, 126.30, 119.37, 92.15, 41.80, 40.77.

IR (neat): *v* (cm^{-1}) 3353, 3008, 2921, 2850, 1681, 1600, 1411, 1081, 751

HRMS (ESI-FT) calcd for $C_{14}H_{15}NO_2Na^+$ ([M]+Na^+) = 252.0995, found 252.0987.

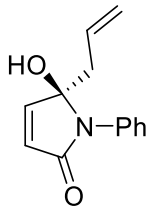


	Retention Time	Area	% Area
1	8.960	1016661	50.26
2	10.162	1006299	49.74



	Retention Time	Area	% Area
1	8.875	9553	3.54
2	10.036	260336	96.46

(*R*)-5-Allyl-5-hydroxy-1-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (3ba)



Viscous colorless oil. R_f = 0.28 (petroleum ether/ethyl acetate = 2/1, v/v), 75% yield, 47% *ee.* $[\alpha]^{25}_D$ = +4.8 (*c* = 0.45, in CH_2Cl_2).

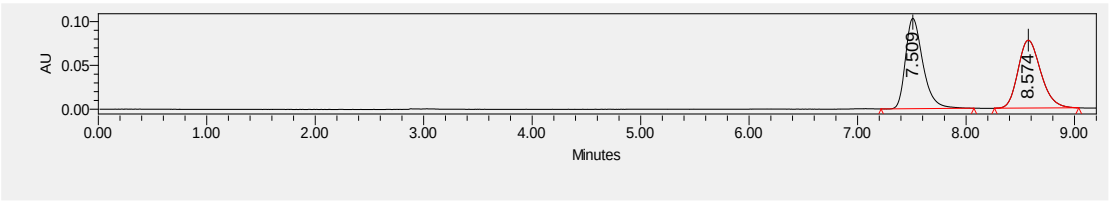
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.4 min, t_{minor} = 7.4 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.54 – 7.46 (m, 2H), 7.41 – 7.32 (m, 2H), 7.31 – 7.22 (m, 2H), 6.91 (d, J = 6.0 Hz, 1H), 6.12 (d, J = 6.0 Hz, 1H), 5.61 – 5.45 (m, 1H), 5.10 – 4.91 (m, 2H), 3.74 (s, 1H), 2.69 – 2.57 (m, 1H), 2.56 – 2.42 (m, 1H).

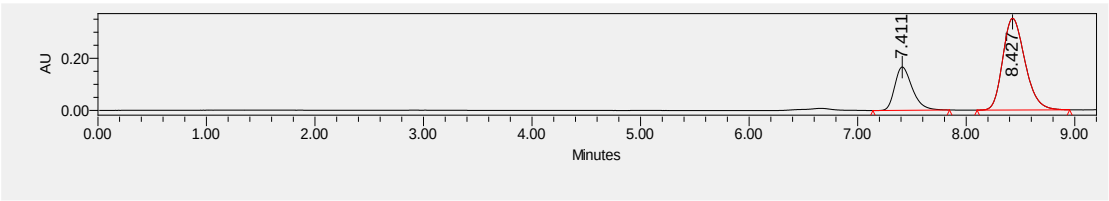
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ 169.13, 149.09, 135.31, 130.79, 128.95, 127.01, 126.78, 126.01, 119.96, 93.36, 39.96.

IR (neat): *v* (cm^{-1}) 3329, 3077, 2923, 2853, 1687, 1598, 1386, 1073, 759

HRMS (ESI-FT) calcd for $C_{13}H_{13}NO_2Na^+$ ([M]+Na^+) = 238.0838, found 238.0832.

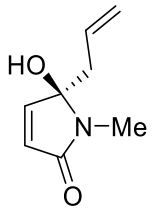


	Retention Time	Area	% Area
1	7.509	1148637	50.46
2	8.574	1127896	49.54



	Retention Time	Area	% Area
1	7.411	1855974	27.09
2	8.427	4995936	72.91

(*R*)-5-Allyl-5-hydroxy-1-methyl-1,5-dihydro-2*H*-pyrrol-2-one (3ca)



Viscous colorless oil. R_f = 0.19 (petroleum ether/ethyl acetate = 2/1, v/v), 60% yield, 80% *ee.* $[\alpha]^{25}_D$ = +13.8 (*c* = 0.16, in CH_2Cl_2).

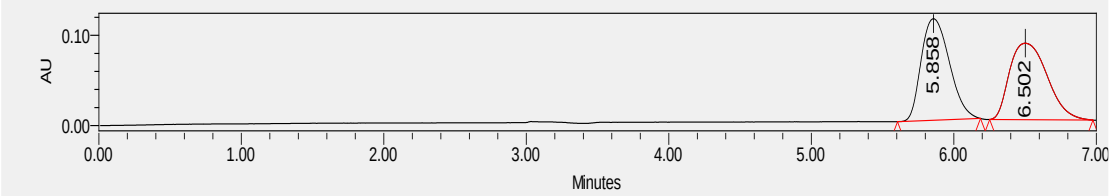
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 6.3 min, t_{minor} = 5.6 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 6.91 (d, J = 6.0 Hz, 1H), 6.03 (d, J = 6.0 Hz, 1H), 5.60 – 5.45 (m, 1H), 5.19 – 5.06 (m, 2H), 3.60 (s, 1H), 2.82 (s, 3H), 2.76 – 2.66 (m, 1H), 2.57 – 2.46 (m, 1H).

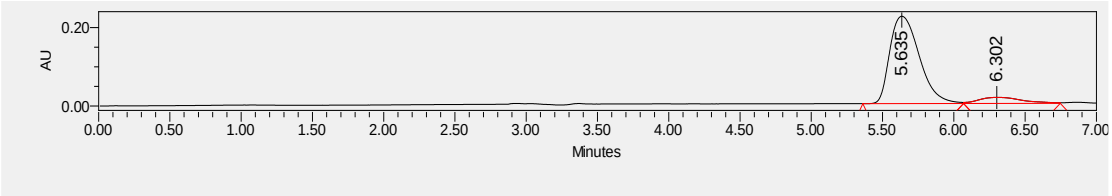
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.31, 148.95, 130.85, 127.18, 119.67, 91.29, 39.35, 23.25.

IR (neat): *v* (cm^{-1}) 3303, 3005, 2926, 2096, 1686, 1597, 1435, 1400, 1082, 811

HRMS (ESI-FT) calcd for $C_8H_{11}NO_2Na^+$ ([M]+Na^+) = 176.0682, found 176.0674.

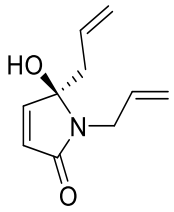


	Retention Time	Area	% Area
1	5.858	1552099	49.86
2	6.502	1560675	50.14



	Retention Time	Area	% Area
1	5.635	3214852	90.62
2	6.302	332600	9.38

(*R*)-1,5-Diallyl-5-hydroxy-1,5-dihydro-2*H*-pyrrol-2-one (3da)



Viscous colorless oil. R_f = 0.29 (petroleum ether/ethyl acetate = 2/1, v/v), 98% yield, 90% *ee.* $[\alpha]^{25}_D$ = +40.5 (*c* = 0.36, in CH_2Cl_2).

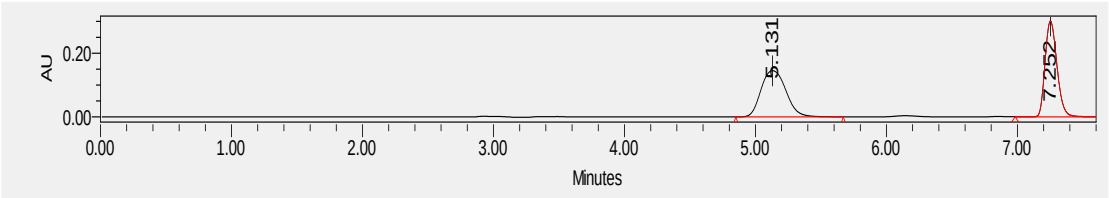
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 5.1 min, t_{minor} = 7.3 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 6.91 (d, J = 6.0 Hz, 1H), 6.06 (d, J = 6.0 Hz, 1H), 5.97 – 5.81 (m, 1H), 5.68 – 5.56 (m, 1H), 5.30 – 5.22 (m, 1H), 5.18 – 5.13 (m, 2H), 5.13 – 5.07 (m, 1H), 4.06 – 3.88 (m, 2H), 3.27 (s, 1H), 2.79 – 2.68 (m, 1H), 2.57 – 2.45 (m, 1H).

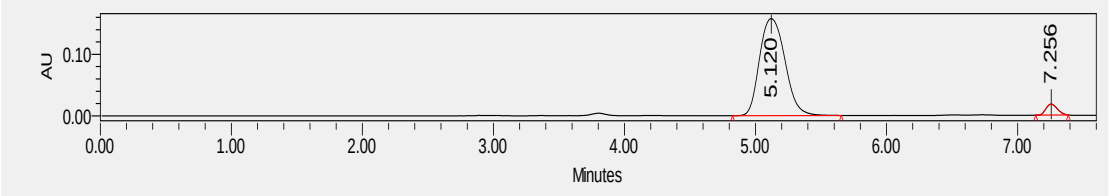
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.37, 149.11, 134.05, 131.21, 126.94, 119.72, 117.25, 91.89, 40.93, 40.40.

IR (neat): *v* (cm^{-1}) 3298, 2919, 2362, 1681, 1600, 1406, 1087, 814.

HRMS (ESI-FT) calcd for $C_{10}H_{13}NO_2Na^+$ ([M]+Na^+) = 202.0838, found 202.0835.

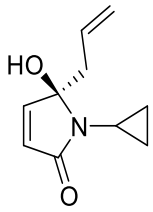


	Retention Time	Area	% Area
1	5.131	1921151	50.24
2	7.252	1902710	49.76



	Retention Time	Area	% Area
1	5.120	2126502	95.15
2	7.256	108348	4.85

(*R*)-5-Allyl-1-cyclopropyl-5-hydroxy-1,5-dihydro-2*H*-pyrrol-2-one (3ea)



Viscous colorless oil. R_f = 0.29 (petroleum ether/ethyl acetate = 2/1, v/v), 41% yield, 80% *ee.* $[\alpha]^{25}_D$ = +7.1 (*c* = 0.14, in CH_2Cl_2).

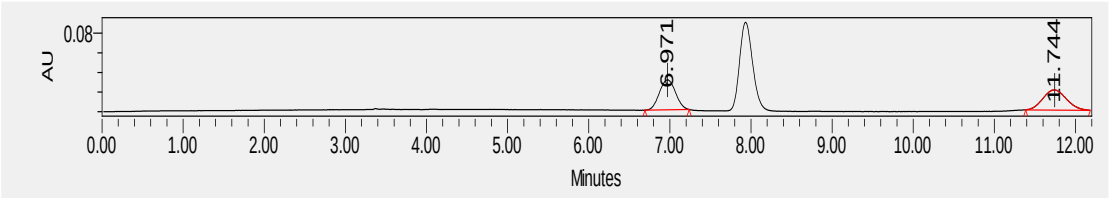
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 5.1 min, t_{minor} = 7.3 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 6.83 (d, J = 6.0 Hz, 1H), 6.06 (d, J = 6.0 Hz, 1H), 5.68 – 5.53 (m, 1H), 5.23 – 5.09 (m, 2H), 2.92 – 2.81 (m, 1H), 2.78 – 2.67 (m, 2H), 2.45 – 2.34 (m, 1H), 1.71 (s, 1H), 1.27 – 1.21 (m, 1H), 0.92 – 0.85 (m, 1H), 0.77 – 0.68 (m, 2H).

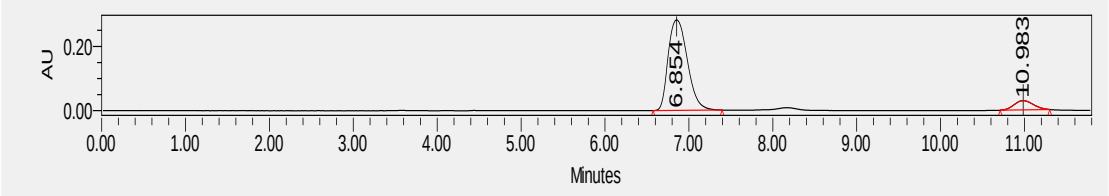
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 170.77, 148.57, 131.27, 127.49, 119.80, 92.66, 40.17, 21.09, 5.61, 3.02.

IR (neat): *v* (cm^{-1}) 3234, 3055, 2923, 2852, 1671, 1602, 1423, 1095, 810, 694.

HRMS (ESI-FT) calcd for $C_{10}H_{14}NO_2^+$ ([M]+H^+) = 180.1019, found 180.1013.

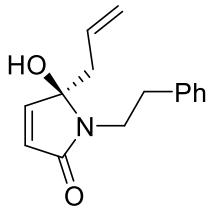


	Retention Time	Area	% Area
1	6.971	423421	50.59
2	11.744	413475	49.41



	Retention Time	Area	% Area
1	6.854	4483591	90.66
2	10.983	461928	9.34

(*R*)-5-Allyl-5-hydroxy-1-phenethyl-1,5-dihydro-2*H*-pyrrol-2-one (3fa)



Viscous colorless oil. R_f = 0.29 (petroleum ether/ethyl acetate = 2/1, v/v), 99% yield, 90% *ee.* $[\alpha]^{25}_D$ = +10.8 (*c* = 0.49, in CH_2Cl_2).

Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 9.1 min, t_{minor} = 8.4 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.33 – 7.26 (m, 2H), 7.25 – 7.18 (m, 3H), 6.83 (d, J = 6.0 Hz, 1H), 6.04 (d, J = 6.0 Hz, 1H), 5.63 – 5.48 (m, 1H), 5.14 – 5.10 (m, 1H), 5.08 (d, J = 1.4 Hz, 1H), 3.68 (ddd, J = 16.0, 12.0, 8.0 Hz, 1H), 3.35 (ddd, J = 16.0, 8.0, 4.0 Hz, 1H), 3.09 (ddd, J = 16.0, 8.0, 4.0 Hz, 1H), 2.90 (ddd, J = 12.0, 8.0, 4.0 Hz, 1H), 2.73 (s, 1H), 2.67 (dd, J = 12.0, 8.0 Hz, 1H), 2.45 (dd, J = 12.0, 8.0 Hz, 1H).

^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.60, 148.95, 139.32, 131.06, 128.96, 128.61, 127.13, 126.54, 119.72, 91.71, 40.60, 40.05, 34.68.

IR (neat): *v* (cm^{-1}) 3273, 2930, 2362, 1676, 1599, 1362, 1082, 753

HRMS (ESI-FT) calcd for $C_{15}H_{17}NO_2Na^+$ ([M]+Na^+) = 266.1152, found 266.1147.

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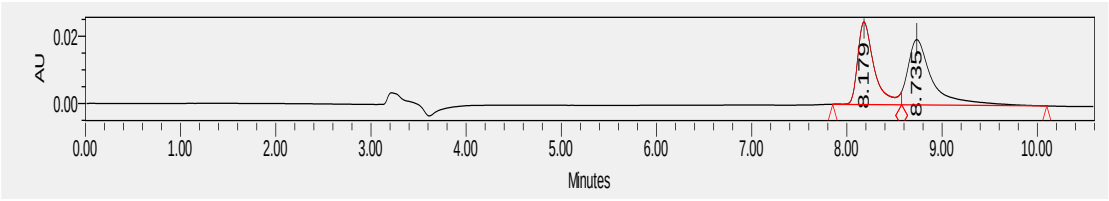
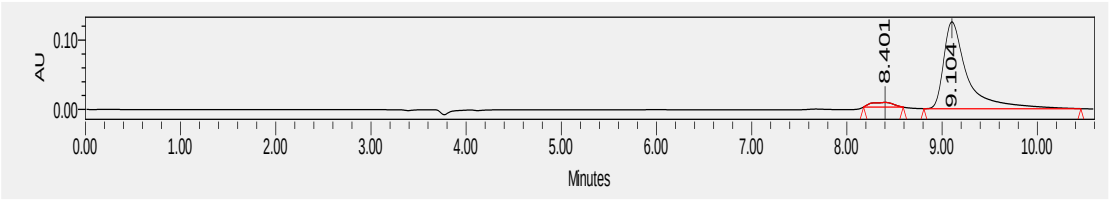
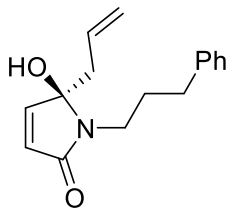


	Retention Time	Area	% Area
1	8.179	299130	46.52
2	8.735	343871	53.48



	Retention Time	Area	% Area
1	8.401	110914	4.87
2	9.104	2166594	95.13

(*R*)-5-Allyl-5-hydroxy-1-(3-phenylpropyl)-1,5-dihydro-2*H*-pyrrol-2-one (3ga)



Viscous colorless oil. R_f = 0.29 (petroleum ether/ethyl acetate = 2/1, v/v), 87% yield, 84% *ee.* $[\alpha]^{25}_D$ = +26.0 (*c* = 0.50, in CH_2Cl_2).

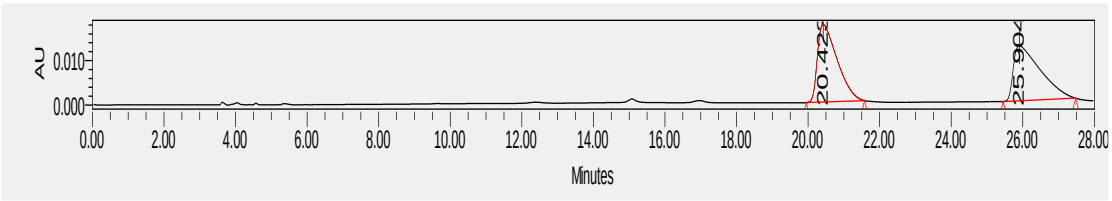
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 20.1 min, t_{minor} = 26.5 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.30 – 7.25 (m, 2H), 7.21 – 7.13 (m, 3H), 6.82 (d, J = 6.0 Hz, 1H), 6.01 (d, J = 6.0 Hz, 1H), 5.65 – 5.48 (m, 1H), 5.14 – 5.07 (m, 2H), 3.52 – 3.41 (m, 1H), 3.26 – 3.14 (m, 1H), 3.04 (s, 1H), 2.73 – 2.62 (m, 3H), 2.53 – 2.44 (m, 1H), 2.07 – 1.86 (m, 2H).

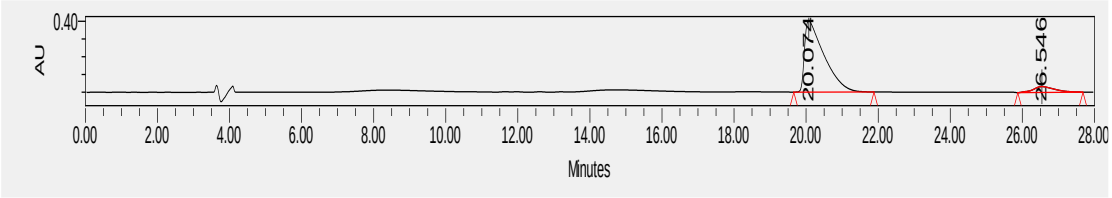
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.60, 148.71, 141.58, 131.11, 128.43, 128.38, 127.16, 125.96, 119.72, 91.86, 40.03, 38.47, 33.64, 30.57.

IR (neat): *v* (cm^{-1}) 3300, 2926, 2361, 1677, 1599, 1417, 1085, 745

HRMS (ESI-FT) calcd for $C_{16}H_{19}NO_2Na^+$ ([M]+Na^+) = 280.1308, found 280.1301.

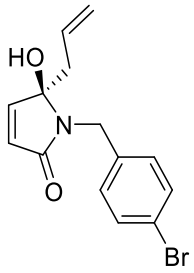


	Retention Time	Area	% Area
1	20.423	667835	50.86
2	25.904	645191	49.14



	Retention Time	Area	% Area
1	20.074	15123887	91.73
2	26.546	1363356	8.27

(*R*)-5-Allyl-1-(4-bromobenzyl)-5-hydroxy-1,5-dihydro-2*H*-pyrrol-2-one (3ha)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 89% yield, 92% *ee.* $[\alpha]^{20}_D$ = +61.3 (*c* = 0.52, in CH_2Cl_2).

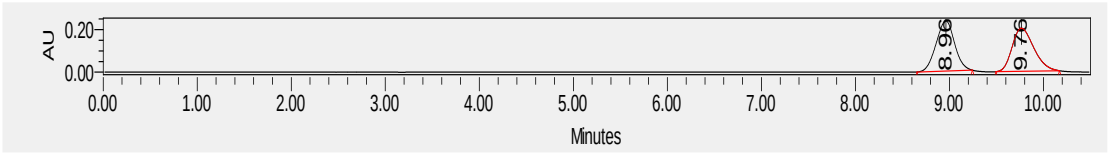
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.8 min, t_{minor} = 9.7 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.41 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 6.90 (d, J = 6.0 Hz, 1H), 6.05 (d, J = 6.0 Hz, 1H), 5.53 – 5.36 (m, 1H), 5.09 – 4.89 (m, 2H), 4.54 – 4.35 (m, 2H), 3.50 (s, 1H), 2.67 – 2.52 (m, 1H), 2.39 – 2.25 (m, 1H).

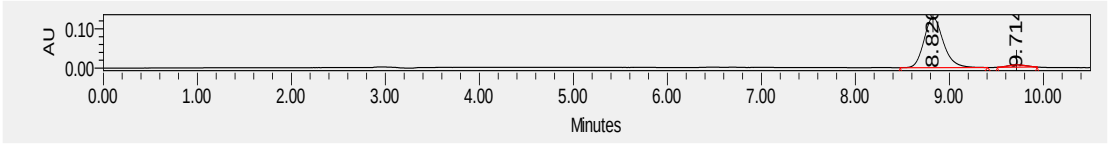
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.89, 149.43, 137.22, 131.61, 130.86, 130.10, 126.70, 121.31, 119.81, 92.01, 41.26, 40.58.

IR (neat): *v* (cm^{-1}) 3300, 2921, 2362, 1678, 1598, 1401, 1153, 1072, 813

HRMS (ESI-FT) calcd for $C_{14}H_{14}^{80.9163}BrNO_2Na^+$ ([M]+Na^+) =332.0080, found 332.0070; $C_{22}H_{28}^{78.7983}BrNO_5Na^+$ ([M]+Na^+) = 330.0100, found 330.0090.

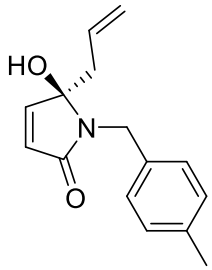


	Retention Time	Area	% Area
1	8.962	3215737	49.77
2	9.765	3245981	50.23



	Retention Time	Area	% Area
1	8.826	1811598	95.90
2	9.714	77460	4.10

(*R*)-5-Allyl-5-hydroxy-1-(4-methylbenzyl)-1,5-dihydro-2*H*-pyrrol-2-one (3ia)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 62% yield, 82% *ee.* $[\alpha]^{20}_D$ = +22.2 (*c* = 0.18, in CH_2Cl_2).

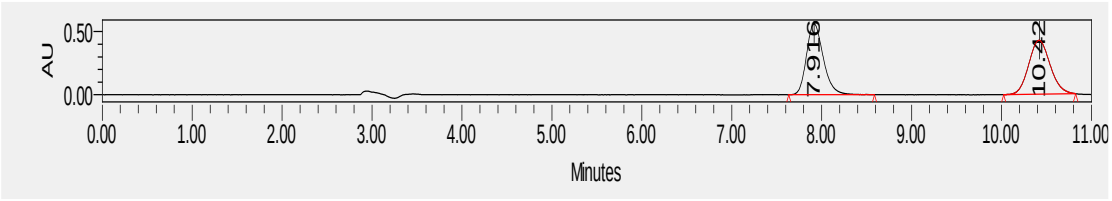
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 10.4 min, t_{minor} = 7.9 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.24 (s, 2H), 7.10 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 4.0 Hz, 1H), 6.12 (d, J = 8.0 Hz, 1H), 5.45 (ddt, J = 17.3, 10.3, 7.2 Hz, 1H), 5.08 – 4.91 (m, 2H), 4.50 (s, 2H), 2.70 – 2.62 (m, 1H), 2.65 – 2.56 (m, 2H), 2.39 (dd, J = 12.0, 8.0 Hz, 1H), 2.31 (s, 3H).

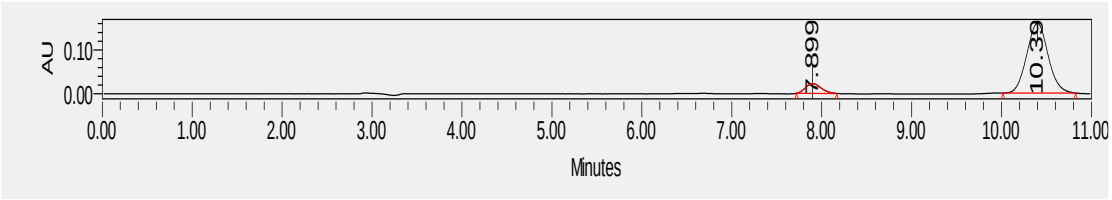
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.62, 148.92, 137.03, 135.19, 131.10, 129.24, 128.27, 127.11, 119.65, 92.02, 41.59, 40.50, 21.12.

IR (neat): *v* (cm^{-1}) 3301, 3008, 2922, 2857, 1678, 1599, 1407, 1089, 812, 694

HRMS (ESI-FT) calcd for $C_{15}H_{17}NO_2Na^+$ ([M]+Na^+) = 266.1152, found 266.1151

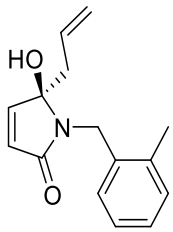


	Retention Time	Area	% Area
1	7.916	7278963	50.83
2	10.421	7042490	49.17



	Retention Time	Area	% Area
1	7.899	268178	9.29
2	10.399	2619841	90.71

(*R*)-5-Allyl-5-hydroxy-1-(2-methylbenzyl)-1,5-dihydro-2*H*-pyrrol-2-one (3ja)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 82% yield, 95% *ee.* $[\alpha]^{20}_D$ = +61.7 (*c* = 0.41, in CH_2Cl_2).

Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IK**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 9.8 min, t_{minor} = 11.7 min.

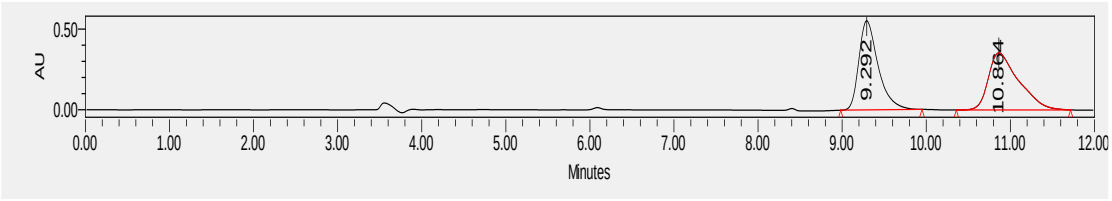
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.24 – 7.21 (m, 1H), 7.17 – 7.10 (m, 3H), 6.91 (d, J = 6.0 Hz, 1H), 6.10 (d, J = 5.9 Hz, 1H), 5.58 – 5.40 (m, 1H), 5.08 – 5.00 (m, 1H), 4.97 – 4.88 (m, 1H), 4.54 (s, 2H), 3.47 – 3.30 (m, 1H), 2.56 – 2.47 (m, 1H), 2.37 (s, 3H), 2.34 – 2.28 (m, 1H).

IR (neat): *v* (cm^{-1}) 3299, 2923, 2361, 1680, 1601, 1410, 1091, 738

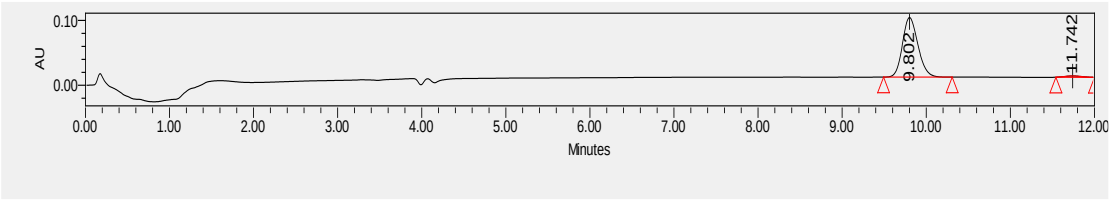
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.90, 149.41, 135.93, 135.45, 131.14, 130.45, 128.36, 127.42, 126.75, 126.10, 119.59, 92.11, 40.68, 39.54, 19.39.

IR (neat): *v* (cm^{-1}) 3299, 2923, 2361, 1680, 1601, 1410, 1091, 738

HRMS (ESI-FT) calcd for $C_{15}H_{17}NO_2Na^+$ ([M]+Na^+) = 266.1152, found 266.1145.

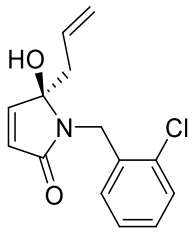


	Retention Time	Area	% Area
1	9.292	6738355	50.28
2	10.864	6664495	49.72



	Retention Time	Area	% Area
1	9.802	1177033	97.76
2	11.742	27007	2.24

(*R*)-5-Allyl-1-(2-chlorobenzyl)-5-hydroxy-1,5-dihydro-2*H*-pyrrol-2-one (3ka)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 85% yield, 98% *ee.* $[\alpha]^{20}_D$ = +81.1 (*c* = 0.28, in CH_2Cl_2).

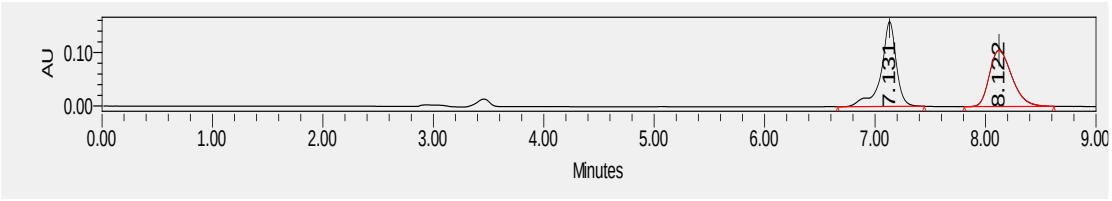
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.0 min, t_{minor} = 7.1 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.42 – 7.13 (m, 4H), 6.95 (d, J = 6.0 Hz, 1H), 6.16 (d, J = 6.0 Hz, 1H), 5.62 – 5.43 (m, 1H), 5.13 – 4.94 (m, 2H), 4.76 (d, J = 16.0 Hz, 1H), 4.60 (d, J = 16.0 Hz, 1H), 3.01 (s, 1H), 2.67 – 2.56 (m, 1H), 2.48 – 2.35 (m, 1H).

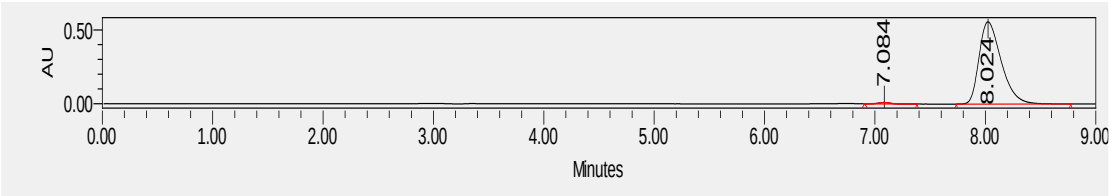
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.98, 149.41, 135.37, 132.77, 130.94, 129.55, 129.48, 128.59, 127.06, 126.86, 119.86, 91.86, 40.45, 38.96.

IR (neat): *v* (cm^{-1}) 3306, 3076, 2923, 1678, 1598, 1472, 1432, 1406, 1087, 814, 691

HRMS (ESI-FT) calcd for $C_{14}H_{14}^{34.9659}ClNO_2Na^+$ ([M]+Na^+) = 286.0605, found 286.0597; $C_{14}H_{14}^{36.9659}ClNO_2Na^+$ ([M]+Na^+) = 288.0576, found 288.0566.

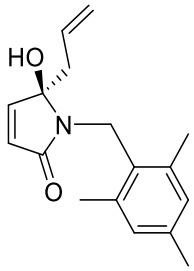


	Retention Time	Area	% Area
1	7.131	1517844	50.48
2	8.122	1489266	49.52



	Retention Time	Area	% Area
1	7.084	88940	1.13
2	8.024	7771106	98.87

(*R*)-5-Allyl-5-hydroxy-1-(2,4,6-trimethylbenzyl)-1,5-dihydro-2*H*-pyrrol-2-one (3la)



Viscous colorless oil. R_f = 0.68 (petroleum ether/ethyl acetate = 2/1, v/v), 74% yield, 70% *ee.* $[\alpha]^{20}_D$ = +20.8 (*c* = 0.27, in CH_2Cl_2).

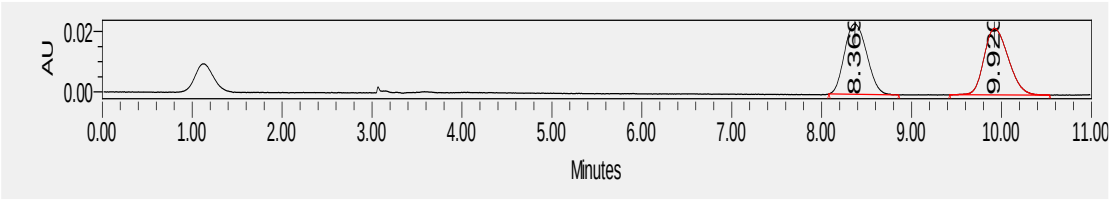
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IB-N5**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.3 min, t_{minor} = 10.0 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 6.85 (d, J = 6.0 Hz, 1H), 6.83 (s, 2H), 6.07 (d, J = 6.0 Hz, 1H), 5.43 – 5.29 (m, 1H), 4.98 – 4.92 (m, 1H), 4.87 – 4.72 (m, 2H), 4.51 (d, J = 16.0 Hz, 1H), 2.91 (s, 1H), 2.39 (s, 6H), 2.35 – 2.29 (m, 1H), 2.25 (s, 3H), 2.07 (dd, J = 16.0, 8.0 Hz, 1H).

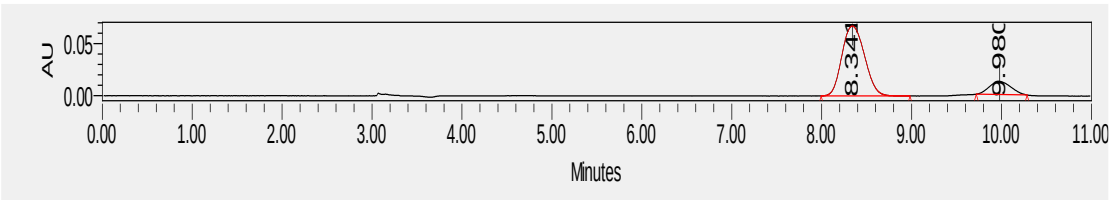
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.48, 149.08, 137.95, 137.26, 131.28, 129.93, 129.45, 126.75, 119.28, 92.58, 40.47, 36.46, 20.90, 20.24.

IR (neat): *v* (cm^{-1}) 3307, 3078, 2921, 2858, 1678, 1604, 1404, 1072, 815, 692

HRMS (ESI-FT) calcd for $C_{17}H_{21}NO_2Na^+$ ([M]+Na^+) = 294.1465, found 294.1456.

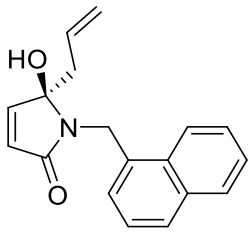


	Retention Time	Area	% Area
1	8.369	402300	49.45
2	9.920	411231	50.55



	Retention Time	Area	% Area
1	8.341	1175461	84.95
2	9.980	208191	15.05

(*R*)-5-Allyl-5-hydroxy-1-(naphthalen-1-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3ma)



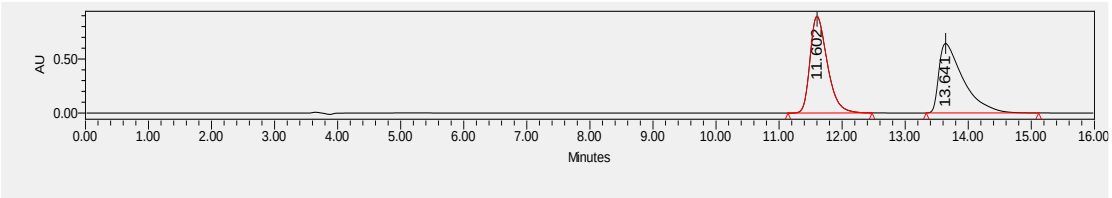
Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 81% yield, 94% *ee.* $[\alpha]^{20}_D$ = +56.7 (*c* = 0.48, in CH_2Cl_2).

Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 11.5 min, t_{minor} = 13.4 min.

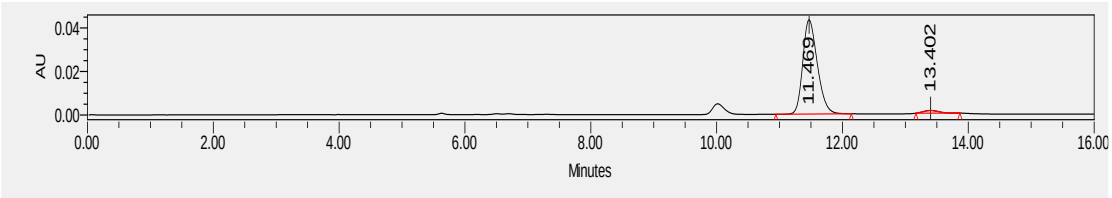
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.26 – 8.16 (m, 1H), 7.89 – 7.73 (m, 2H), 7.59 – 7.37 (m, 4H), 6.87 (d, J = 6.0 Hz, 1H), 6.13 (d, J = 6.0 Hz, 1H), 5.40 – 5.29 (m, 1H), 5.13 – 4.97 (m, 2H), 4.94 – 4.78 (m, 2H), 3.03 (s, 1H), 2.50 (dd, J = 12.0, 4.0 Hz, 1H), 2.32 (dd, J = 12.0, 4.0 Hz, 1H).

^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.81, 149.54, 133.80, 133.01, 131.45, 131.01, 128.76, 128.45, 126.95, 126.77, 126.55, 125.91, 125.26, 123.73, 119.54, 92.33, 40.45, 40.11.

HRMS (ESI-FT) calcd for $C_{18}H_{17}NO_2Na^+$ ([M]+Na^+) = 302.1152, found 302.1148.

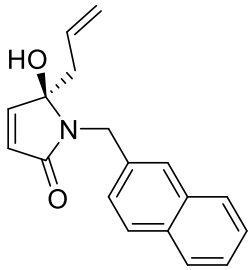


	Retention Time	Area	% Area
1	11.602	16982920	49.67
2	13.641	17210748	50.33



	Retention Time	Area	% Area
1	11.469	696101	97.11
2	13.402	20732	2.89

(*R*)-5-Allyl-5-hydroxy-1-(naphthalen-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3na)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 85% yield, 98% *ee.* $[\alpha]^{20}_D$ = +63.8 (*c* = 0.45, in CH_2Cl_2).

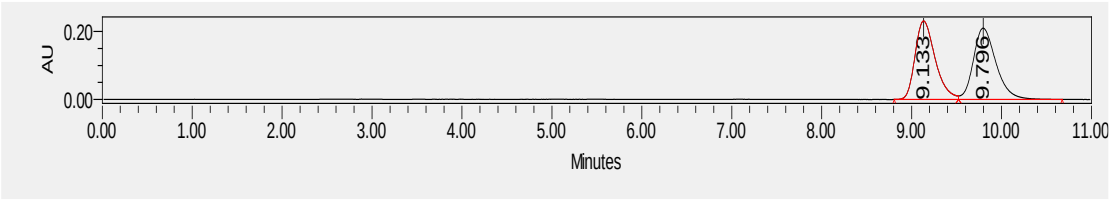
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 9.1 min, t_{minor} = 9.8 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.86 – 7.74 (m, 4H), 7.54 – 7.40 (m, 3H), 6.89 (d, J = 6.0 Hz, 1H), 6.11 (d, J = 6.0 Hz, 1H), 5.53 – 5.35 (m, 1H), 5.03 – 4.86 (m, 2H), 4.69 (q, J = 16.0 Hz, 2H), 3.04 (s, 1H), 2.66 – 2.57 (m, 1H), 2.43 – 2.32 (m, 1H).

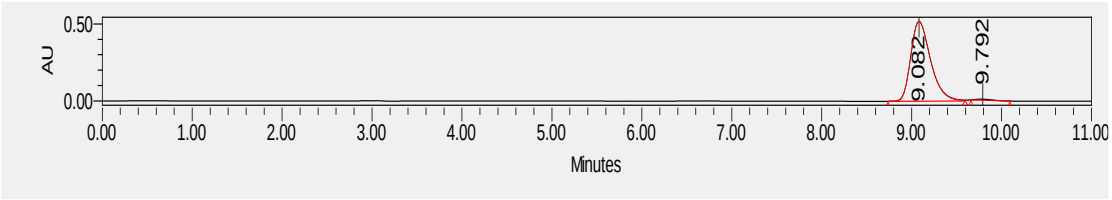
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.87, 149.21, 135.76, 133.30, 132.73, 131.03, 128.38, 127.84, 127.70, 126.92, 126.88, 126.50, 126.19, 125.90, 119.70, 92.10, 42.03, 40.60.

IR (neat): *v* (cm^{-1}) 3212, 2919, 2361, 1678, 1599, 1429, 1082, 753

HRMS (ESI-FT) calcd for $C_{18}H_{17}NO_2Na^+$ ([M]+Na^+) = 302.1152, found 302.1149.

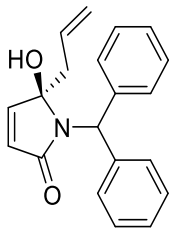


	Retention Time	Area	% Area
1	9.133	3594017	49.38
2	9.796	3684892	50.62



	Retention Time	Area	% Area
1	9.082	7969118	98.99
2	9.792	81441	1.01

(*R*)-5-Allyl-1-benzhydryl-5-hydroxy-1,5-dihydro-2*H*-pyrrol-2-one (3oa)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 50% yield, 75% *ee.* $[\alpha]^{20}_D$ = +31.9 (*c* = 0.43, in CH_2Cl_2).

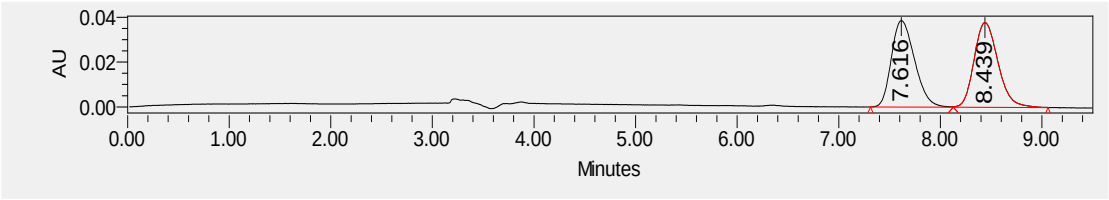
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.7 min, t_{minor} = 7.8 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.50 – 7.36 (m, 2H), 7.38 – 7.17 (m, 9H), 6.87 (d, J = 6.0 Hz, 1H), 6.01 (d, J = 6.0 Hz, 1H), 5.85 (s, 1H), 5.65 – 5.49 (m, 1H), 5.09 – 4.90 (m, 2H), 2.75 – 2.59 (m, 1H), 2.47 – 2.31 (m, 1H).

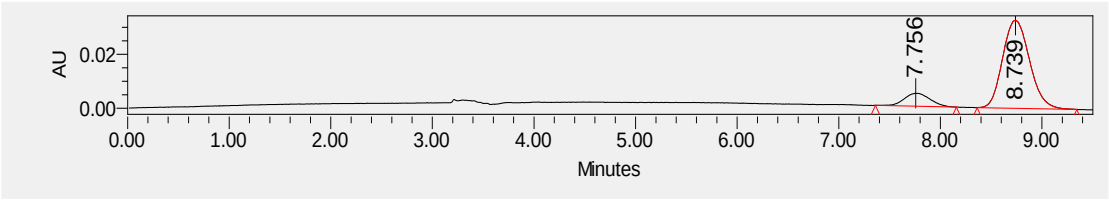
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 168.68, 147.92, 140.26, 140.00, 131.43, 129.00, 128.64, 128.40, 128.30, 128.06, 127.35, 127.27, 119.89, 92.33, 59.06, 41.41.

IR (neat): *v* (cm^{-1}) 3289, 3066, 2371, 1706, 1603, 1494, 1086, 753

HRMS (ESI-FT) calcd for $C_{20}H_{19}NO_2Na^+$ ([M]+Na^+) = 328.1308, found 328.1300

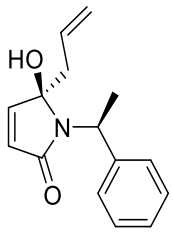


	Retention Time	Area	% Area
1	7.616	600394	50.18
2	8.437	596137	49.82



	Retention Time	Area	% Area
1	7.756	84236	12.32
2	8.739	599279	87.68

(*R*)-5-Allyl-5-hydroxy-1-[(*S*)-1-phenylethyl]-1,5-dihydro-2*H*-pyrrol-2-one (3pa)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 76% yield, 86:14 dr determined by ^{1}H NMR. $[\alpha]^{20}_D$ = +67.5 (*c* = 0.12, in CH_2Cl_2).

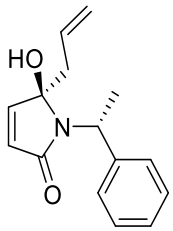
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.53 – 7.47 (m, 2H), 7.34 – 7.24 (m, 4H), 6.85 (d, J = 6.0 Hz, 1H), 6.05 (d, J = 6.0 Hz, 1H), 5.50 – 5.35 (m, 1H), 5.00 – 4.94 (m, 1H), 4.92 – 4.85 (m, 1H), 4.80 (q, J = 8.0 Hz, 1H), 2.65 – 2.58 (m, 1H), 2.37 – 2.28 (m, 1H), 1.84 (d, J = 8.0 Hz, 4H).

^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.46, 147.91, 143.18, 131.46, 128.49, 128.30, 127.77, 127.31, 127.13, 119.60, 92.56, 51.76, 40.89, 20.95.

IR (neat): *v* (cm^{-1}) 3271, 2934, 2360, 1671, 1602, 1425, 1092, 773

HRMS (ESI-FT) calcd for $C_{15}H_{17}NO_2Na^+$ ([M]+Na^+) = 266.1152, found 266.1146.

(*R*)-5-Allyl-5-hydroxy-1-[(*R*)-1-phenylethyl]-1,5-dihydro-2*H*-pyrrol-2-one (3qa)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 76% yield, 90:10 dr determined by ^{1}H NMR. $[\alpha]^{20}_D$ = +1.9 (*c* = 0.06, in CH_2Cl_2).

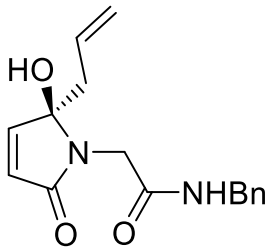
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.61 – 7.51 (m, 2H), 7.37 – 7.23 (m, 3H), 6.79 (d, J = 6.0 Hz, 1H), 5.98 (d, J = 6.0 Hz, 1H), 5.69 – 5.57 (m, 1H), 5.17 – 5.10 (m, 2H), 4.80 (q, J = 8.0 Hz, 1H), 2.77 – 2.65 (m, 1H), 2.53 – 2.48 (m, 1H), 2.47 (s, 1H), 1.84 (d, J = 8.0 Hz, 3H).

^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.10, 148.02, 142.34, 131.55, 128.33, 128.07, 127.73, 127.29, 119.66, 92.77, 50.98, 40.58, 18.73.

IR (neat): *v* (cm^{-1}) 3266, 2926, 2362, 1675, 1600, 1426, 1075, 755

HRMS (ESI-FT) calcd for $C_{15}H_{17}NO_2Na^+$ ([M]+Na^+) = 266.1152, found 266.1145.

(*R*)-2-(2-Allyl-2-hydroxy-5-oxo-2,5-dihydro-1*H*-pyrrol-1-yl)-*N*-benzylacetamide (3ra)



Viscous colorless oil. R_f = 0.27 (petroleum ether/ethyl acetate = 1/1, *v*/*v*), 83% yield, 64% *ee.* $[\alpha]^{20}_D$ = +60.4 (*c* = 0.49, in CH_2Cl_2).

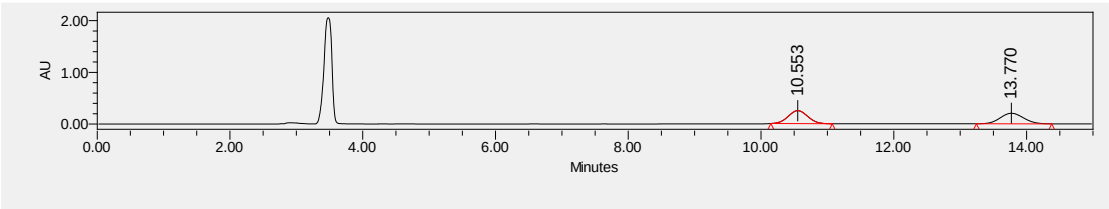
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **AD-H**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 13.8 min, t_{minor} = 10.6 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.36 – 7.24 (m, 6H), 7.04 – 6.97 (m, 1H), 6.61 (s, 1H), 6.06 (d, J = 6.0 Hz, 1H), 5.67 – 5.50 (m, 1H), 5.23 (s, 1H), 5.15 – 5.10 (m, 1H), 4.49 – 4.36 (m, 2H), 4.31 (d, J = 16.0 Hz, 1H), 3.84 (d, J = 16.0 Hz, 1H), 2.85 – 2.62 (m, 1H), 2.60 – 2.44 (m, 1H).

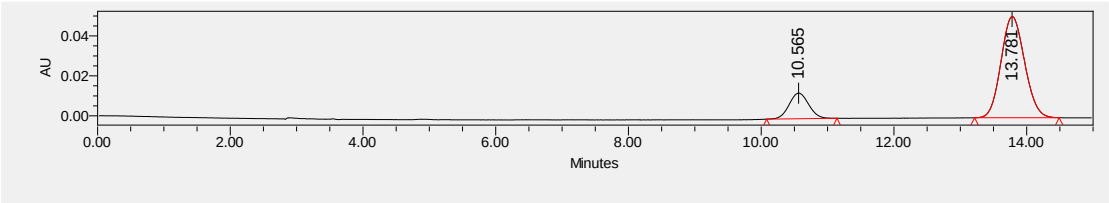
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 170.65, 169.85, 151.21, 137.16, 130.84, 128.81, 127.77 (d, J = 5.8 Hz), 125.63, 119.74, 91.08, 43.99, 42.46, 40.51.

IR (neat): *v* (cm^{-1}) 3306, 2928, 1690, 1546, 1428, 1275, 817, 751

HRMS (ESI-FT) calcd for $C_{16}H_{18}N_2O_3Na^+$ ([M]+Na^+) = 329.1210, found 329.1214.

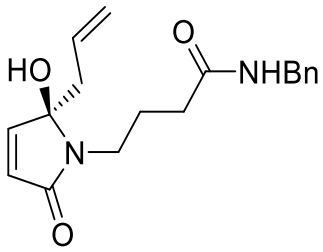


	Retention Time	Area	% Area
1	10.553	5112810	50.65
2	13.770	4982363	49.35



	Retention Time	Area	% Area
1	10.565	263739	17.44
2	13.781	1248421	82.56

(*R*)-4-(2-Allyl-2-hydroxy-5-oxo-2,5-dihydro-1*H*-pyrrol-1-yl)-*N*-benzylbutanamide (3sa)



Viscous colorless oil. R_f = 0.32 (petroleum ether/ethyl acetate = 1/1, *v*/*v*), 78% yield, 95% *ee.* $[\alpha]^{20}_D$ = +125.8 (*c* = 0.50, in CH_2Cl_2).

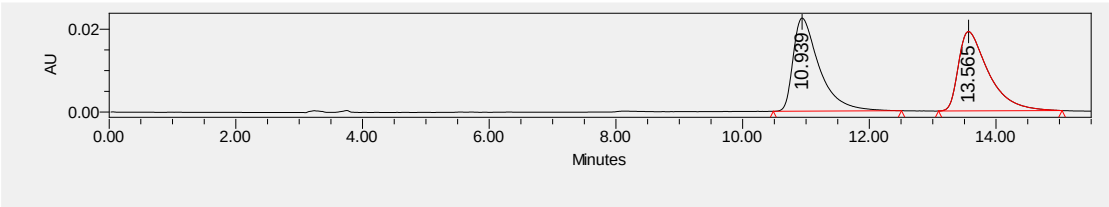
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 10.9 min, t_{minor} = 13.9 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.44 – 7.21 (m, 5H), 6.84 (d, J = 6.0 Hz, 1H), 6.48 (s, 1H), 5.92 (d, J = 6.0 Hz, 1H), 5.75 (s, 1H), 5.58 – 5.36 (m, 1H), 5.21 – 5.02 (m, 2H), 4.44 (dd, J = 16.0, 6.0 Hz, 1H), 4.21 (dd, J = 16.0, 6.0 Hz, 1H), 3.81 – 3.57 (m, 1H), 3.40 – 3.04 (m, 1H), 2.82 – 2.65 (m, 1H), 2.59 – 2.48 (m, 1H), 2.42 – 2.22 (m, 3H), 1.86 – 1.73 (m, 1H).

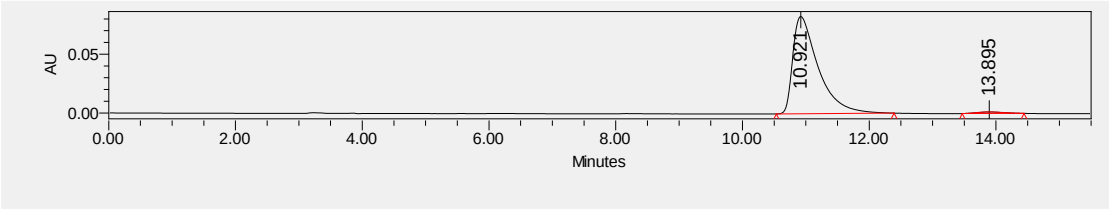
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 174.44, 170.07, 150.30, 137.78, 131.05, 128.73, 127.91, 127.57, 125.83, 119.38, 92.28, 43.85, 39.97, 37.82, 34.03, 24.33.

IR (neat): *v* (cm^{-1}) 3293, 2930, 1680, 1549, 1419, 1240, 1080, 814, 698.

HRMS (ESI-FT) calcd for $C_{18}H_{22}N_2O_3Na^+$ ([M]+Na^+) = 337.1523, found 337.1523.

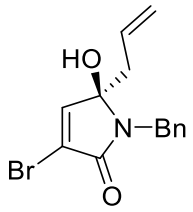


	Retention Time	Area	% Area
1	10.939	645218	50.49
2	13.565	632787	49.51



	Retention Time	Area	% Area
1	10.921	2308871	98.38
2	13.895	37905	1.62

(*R*)-5-Allyl-1-benzyl-3-bromo-5-hydroxy-1,5-dihydro-2*H*-pyrrol-2-one (3ta)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 65% yield, 90% *ee.*, >19:1 rr, $[\alpha]^{20}_D$ = +77.9 (*c* = 0.38, in CH_2Cl_2).

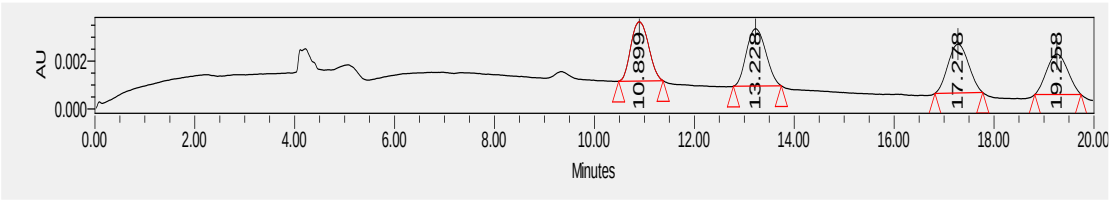
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IK**, hexane/*i*PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 17.1 min, t_{minor} = 13.1 min. (minor isomer) t_{major} = 19.0 min, t_{minor} = 10.9 min. rr > 19:1 determined by ^{1}H NMR and 2D NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.40 – 7.34 (m, 2H), 7.34 – 7.26 (m, 3H), 7.03 (s, 1H), 5.51 – 5.36 (m, 1H), 5.04 (d, J = 8.0 Hz, 1H), 5.00 – 4.91 (m, 1H), 4.64 (d, J = 12.0 Hz, 1H), 4.53 (d, J = 12.0 Hz, 1H), 3.08 (s, 1H), 2.60 (q, J = 8.0 Hz, 1H), 2.34 (q, J = 8.0 Hz, 1H).

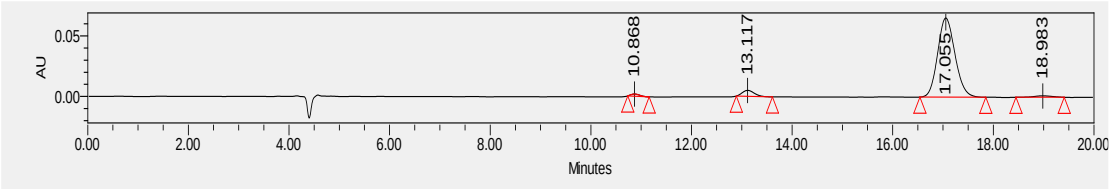
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 164.97, 146.56, 137.59, 130.48, 128.66, 128.46, 127.67, 120.40, 120.23, 91.52, 42.82, 40.67.

IR (neat): *v* (cm^{-1}) 3337, 3085, 2923, 2359, 1690, 1605, 1409, 1054, 757

HRMS (ESI-FT) calcd for $C_{14}H_{14}^{80.9163}BrNO_2Na^+$ ([M]+Na^+) =332.0080, found 332.0070; $C_{22}H_{28}^{78.7983}BrNO_5Na^+$ ([M]+Na^+) = 330.0100, found 330.0091.

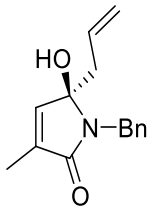


	Retention Time	Area	% Area
1	10.899	61025	26.13
2	13.228	64938	27.80
3	17.278	58416	25.01
4	19.258	49192	21.06



	Retention Time	Area	% Area
1	10.868	21971	1.29
2	13.117	81519	4.79
3	17.055	1568551	92.23
4	18.983	28714	1.69

(*R*)-5-Allyl-1-benzyl-5-hydroxy-3-methyl-1,5-dihydro-2*H*-pyrrol-2-one (3ua)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 75% yield, 91% *ee.* $[\alpha]^{20}_D$ = +17.0 (*c* = 0.12, in CH_2Cl_2).

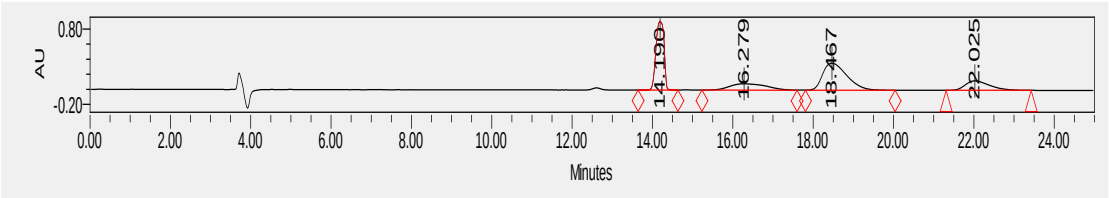
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **ID**, hexane/*i*PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 19.2 min, t_{minor} = 15.3 min. rr > 19:1 determined by ^{1}H NMR and 2D NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.43 – 7.18 (m, 6H), 6.52 (s, 1H), 5.55 – 5.40 (m, 1H), 5.07 – 4.92 (m, 2H), 4.54 (s, 2H), 2.59 (dd, *J* = 16.0, 8.0 Hz, 1H), 2.35 (dd, *J* = 16.0, 8.0 Hz, 1H), 2.22 (s, 1H), 1.91 (d, *J* = 1.7 Hz, 3H).

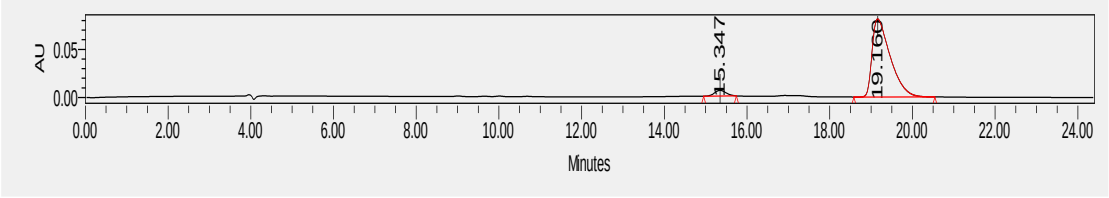
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 170.48, 141.65, 138.45, 135.60, 131.40, 128.53, 128.33, 127.32, 119.42, 90.12, 42.16, 40.66, 10.87.

IR (neat): *v* (cm^{-1}) 3326, 3031, 2923, 2854, 1681, 1653, 1434, 1069, 705

HRMS (ESI-FT) calcd for $C_{15}H_{17}NO_2Na^+$ ([M]+Na^+) = 266.1152, found 266.1144.

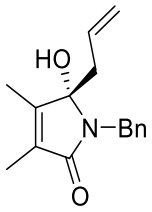


	Retention Time	Area	% Area
1	14.190	12864158	33.31
2	16.279	5411111	14.01
3	18.467	15047223	38.97
4	22.025	5291600	13.70



	Retention Time	Area	% Area
1	15.347	113618	4.41
2	19.160	2463668	95.59

(*S*)-5-Allyl-1-benzyl-5-hydroxy-3,4-dimethyl-1,5-dihydro-2*H*-pyrrol-2-one (3va)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 68% yield, 83% *ee.* $[\alpha]^{20}_D$ = −167 (*c* = 0.34, in CH_2Cl_2).

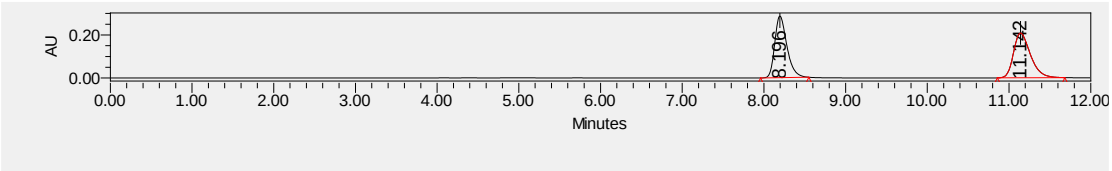
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.2 min, t_{minor} = 11.2 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.44 – 7.35 (m, 2H), 7.33 – 7.18 (m, 3H), 5.10 – 4.95 (m, 1H), 4.89 – 4.78 (m, 2H), 4.53 (dd, J = 24.0, 12.0 Hz, 2H), 2.62 (dd, J = 12.0, 4.0 Hz, 1H), 2.54 (s, 1H), 2.47 (dd, J = 12.0, 8.0 Hz, 1H), 1.85 (s, 3H), 1.78 (s, 3H).

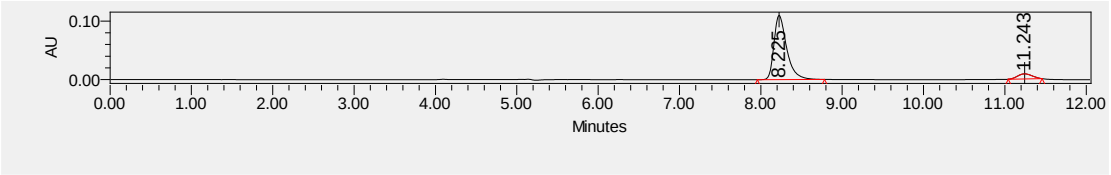
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 171.23, 150.80, 138.70, 130.48, 128.83, 128.61, 128.47, 127.30, 118.82, 91.76, 42.23, 38.18, 9.98, 8.40.

IR (neat): *v* (cm^{-1}) 3304, 2921, 1665, 1494, 1434, 1067, 755, 702.

HRMS (ESI-FT) calcd for $C_{16}H_{19}NO_2Na^+$ ([M]+Na^+) = 280.1308, found 280.1308.

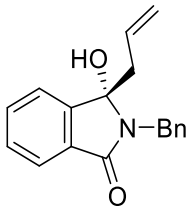


	Retention Time	Area	% Area
1	8.196	2960823	49.80
2	11.142	2984531	50.20



	Retention Time	Area	% Area
1	8.225	1194013	91.66
2	11.243	108613	8.34

(*S*)-3-Allyl-2-benzyl-3-hydroxyisoindolin-1-one (3wa)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 60% yield, 81% *ee.* $[\alpha]^{20}_D$ = –45 (*c* = 0.33, in CH_2Cl_2).

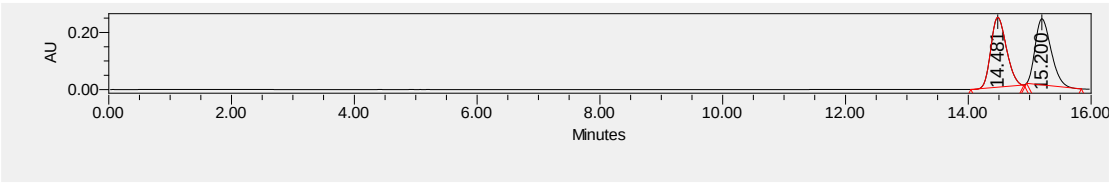
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 14.4 min, t_{minor} = 15.2 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.69 (dd, J = 7.5, 1.1 Hz, 1H), 7.58 – 7.49 (m, 2H), 7.48 – 7.35 (m, 3H), 7.34 – 7.16 (m, 3H), 5.19 – 5.02 (m, 1H), 4.78 (d, J = 8.0 Hz, 1H), 4.68 (d, J = 12.0 Hz, 1H), 4.56 (d, J = 16.0 Hz, 1H), 4.45 (d, J = 16.0 Hz, 1H), 3.41 (s, 1H), 2.82 (dd, J = 16.0, 8.0 Hz, 1H), 2.64 (dd, J = 16.0, 8.0 Hz, 1H).

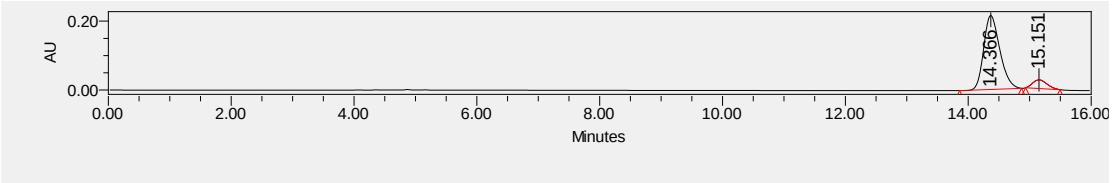
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 167.73, 146.49, 138.33, 132.32, 130.84, 130.59, 129.62, 128.55, 128.48, 127.35, 123.39, 122.34, 119.67, 90.97, 42.07, 41.17.

IR (neat): *v* (cm^{-1}) 3345, 3063, 2922, 2852, 2350, 1678, 1615, 1399, 1069, 707.

HRMS (ESI-FT) calcd for $C_{18}H_{17}NO_2Na^+$ ([M]+Na^+) = 302.1152, found 302.1148.

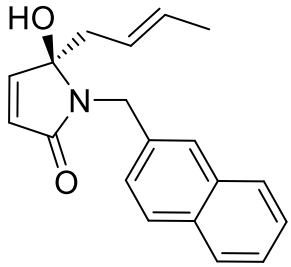


	Retention Time	Area	% Area
1	14.481	4297178	50.95
2	15.200	4137176	49.05



	Retention Time	Area	% Area
1	14.366	3919597	90.58
2	15.151	407524	9.42

(*R*,*E*)-5-(*But*-2-en-1-yl)-5-hydroxy-1-(naphthalen-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3nb)



Viscous colorless oil. R_f = 0.52 (petroleum ether/ethyl acetate = 1/1, v/v), 83% yield, 99%/55% *ee.* 92:8 (*E*/*Z*) determined by ^{1}H NMR, $[\alpha]^{20}_D$ = +4.7 (*c* = 0.472, in CH_2Cl_2).

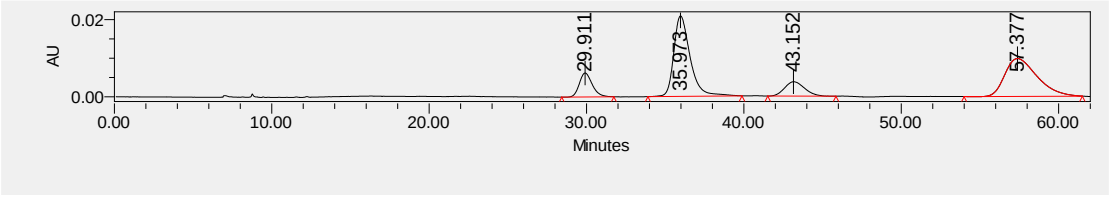
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IH** and **IJ**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 35.4 min, t_{minor} = 57.9 min. (minor isomer) t_{major} = 29.8 min, t_{minor} = 43.0 min. (*Z*/*E*) = 92:8 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.85 – 7.71 (m, 4H), 7.54 – 7.37 (m, 3H), 6.84 (d, J = 6.0 Hz, 1H), 6.08 (d, J = 6.0 Hz, 1H), 5.53 – 5.35 (m, 1H), 5.12 – 4.96 (m, 1H), 4.67 (s, 2H), 3.15 (s, 1H), 2.60 (dd, J = 15.0, 7.1 Hz, 1H), 2.38 (dd, J = 14.9, 7.5 Hz, 1H), 1.43 (d, J = 6.3 Hz, 3H).

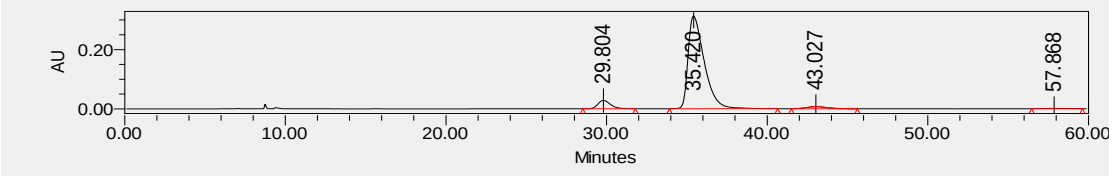
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 169.86, 149.20, 135.63, 133.24, 132.64, 128.25, 128.07, 127.76, 127.61, 126.82, 126.45, 126.07, 125.78, 122.37, 92.55, 41.98, 33.44, 13.00.

IR (neat): *v* (cm^{-1}) 3311, 2921, 1680, 1600, 1427, 1082, 1011, 753.

HRMS (ESI-FT) calcd for $C_{19}H_{19}NO_2Na^+$ ([M]+Na^+) = 316.1308, found 316.1311.

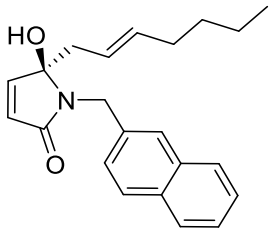


	Retention Time	Area	% Area
1	29.911	354294	9.87
2	35.973	1508034	42.02
3	43.152	329615	9.18
4	57.377	1397027	38.93



	Retention Time	Area	% Area
1	29.804	1555833	6.45
2	35.420	21859598	90.55
3	43.027	635568	2.63
4	57.868	88802	0.37

(*R*,*E*)-5-(Hept-2-en-1-yl)-5-Hydroxy-1-(naphthalen-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3nc)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 67% yield, 99%/18% *ee.* 92.5:7.5 (*E*/*Z*) $[\alpha]^{20}_D$ = +38.9 (*c* = 0.44, in CH_2Cl_2).

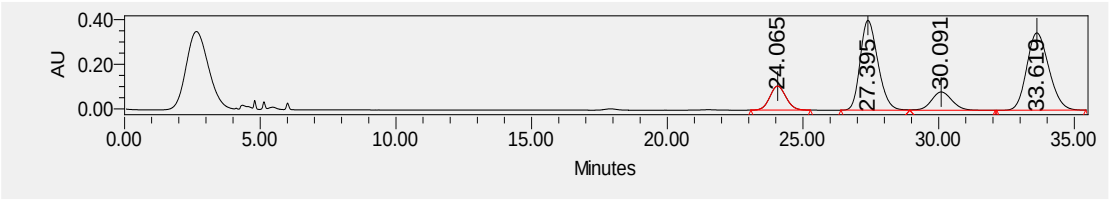
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IG**, hexane/*i*PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 26.9 min, t_{minor} = 33.4 min. (minor isomer) t_{major} = 29.7 min, t_{minor} = 23.6 min. (*E*)/(*Z*) = 92.5:7.5 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.78 (d, J = 8.0 Hz, 3H), 7.54 – 7.47 (m, 1H), 7.51 – 7.37 (m, 2H), 6.87 (d, J = 6.0 Hz, 1H), 6.16 (d, J = 6.0 Hz, 1H), 5.51 – 5.32 (m, 1H), 5.15 – 4.94 (m, 1H), 4.80 – 4.58 (m, 2H), 2.77 – 2.57 (m, 1H), 2.46 – 2.37 (m, 1H), 1.96 – 1.75 (m, 2H), 1.20 (s, 1H), 0.98 – 0.74 (m, 2H).

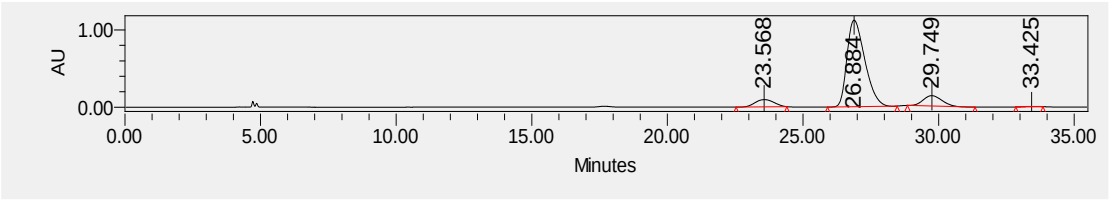
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 149.01, 135.72, 134.31, 133.27, 132.68, 128.33, 127.77, 127.63, 127.08, 126.83, 126.43, 126.12, 125.82, 121.18, 92.45, 42.04, 33.74, 31.35, 27.17, 22.24, 13.87.

IR (neat): *v* (cm^{-1}) 3293, 3055, 2954, 2924, 1677, 1599, 1412, 1077, 813, 729.

HRMS (ESI-FT) calcd for $C_{22}H_{25}NO_2Na^+$ ([M]+Na^+) = 358.1778, found 358.1779

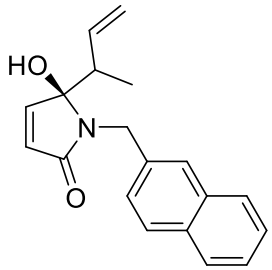


	Retention Time	Area	% Area
1	24.065	4457510	9.55
2	27.395	18252369	39.12
3	30.091	4302022	9.22
4	33.619	19642063	42.10



	Retention Time	Area	% Area
1	23.568	4545247	7.28
2	26.884	51186014	82.03
3	29.749	6498965	10.42
4	33.425	168596	0.27

(5*S*)-5-(*But*-3-en-2-yl)-5-Hydroxy-1-(naphthalen-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3nd)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 62% yield, 82%/82% *ee.* 2:1 dr $[\alpha]^{20}_D$ = 61.7 (*c* = 0.41, in CH_2Cl_2). $[\alpha]^{23}_D$ = +23.1 (c = 0.22, in CH_2Cl_2).

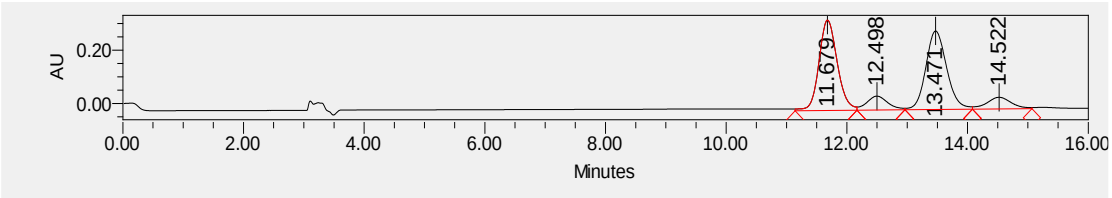
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IK**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 13.3 min, t_{minor} = 11.7 min. (minor) t_{major} = 14.4 min, t_{minor} = 12.5 min. dr = 2:1 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.87 – 7.73 (m, 6H), 7.61 – 7.42 (m, 5H), 6.81 (d, J = 6.0 Hz, 1H), 6.20 (d, J = 6.0 Hz, 1H), 5.97 (ddd, J = 16.0, 12.0, 8.0 Hz, 1H), 5.23 – 5.09 (m, 2H), 4.78 – 4.60 (m, 2H), 2.76 (p, J = 8.0 Hz, 1H), 0.60 (d, J = 6.9 Hz, 3H).

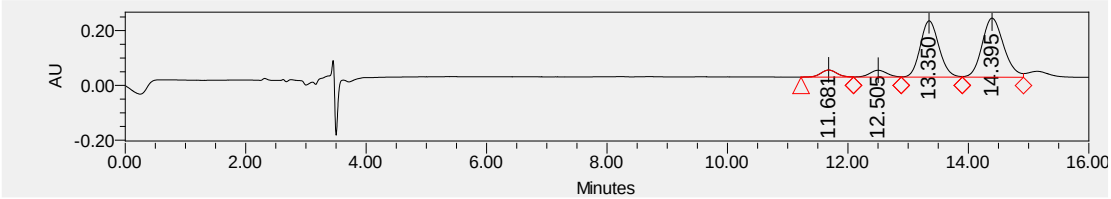
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 146.94, 146.74, 138.08, 136.33, 133.28, 132.73, 128.44, 128.34, 128.30, 127.87, 127.70, 127.21, 127.17, 126.86, 126.17, 126.15, 125.92, 125.88, 117.34, 94.52, 42.64, 42.40, 42.27, 29.74, 15.44, 12.99, 1.05.

IR (neat): *v* (cm^{-1}) 3314, 2982, 2925, 2350, 1681, 1599, 1410, 1061, 814, 751.

HRMS (ESI-FT) calcd for $C_{19}H_{19}NO_2Na^+$ ([M]+Na^+) = 316.1308, found 316.1315.

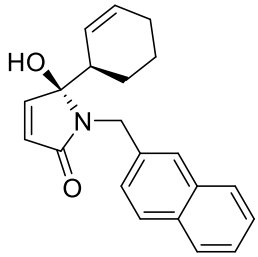


	Retention Time	Area	% Area
1	11.679	7135438	42.71
2	12.498	1269713	7.60
3	13.471	7064292	42.29
4	14.522	1236067	7.40



	Retention Time	Area	% Area
1	11.679	414869	4.19
2	12.509	415762	4.20
3	13.349	4090151	41.30
4	14.394	4982541	50.31

(*S*)-5-[(*R*)-Cyclohex-2-en-1-yl]-5-hydroxy-1-(naphthalen-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3ne)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 63% yield, 81%/25% *ee*. >19:1 dr $[\alpha]^{20}_D$ = +21.1 (c = 0.18, in CH_2Cl_2).

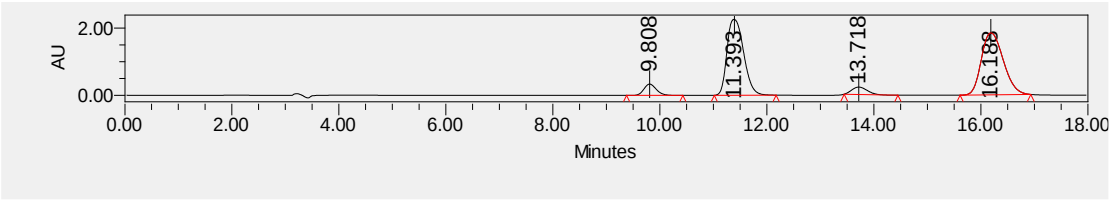
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **OX-H**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 16.5 min, t_{minor} = 11.6 min. (minor) t_{major} = 14.0 min, t_{minor} = 10.0 min. dr > 19:1 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.87 – 7.67 (m, 4H), 7.52 (dd, J = 8.0, 2.0 Hz, 1H), 7.50 – 7.37 (m, 2H), 6.85 (d, J = 6.0 Hz, 1H), 6.13 (d, J = 6.0 Hz, 1H), 5.84 – 5.51 (m, 1H), 5.12 (dt, J = 10.0, 2.0 Hz, 1H), 4.80 (d, J = 16.0 Hz, 1H), 4.57 (d, J = 16.0 Hz, 1H), 2.81 – 2.69 (m, 1H), 2.60 (s, 1H), 2.23 – 1.97 (m, 1H), 1.93 – 1.84 (m, 1H), 1.79 – 1.74 (m, 1H), 1.55 – 1.41 (m, 1H), 1.37 – 1.15 (m, 1H).

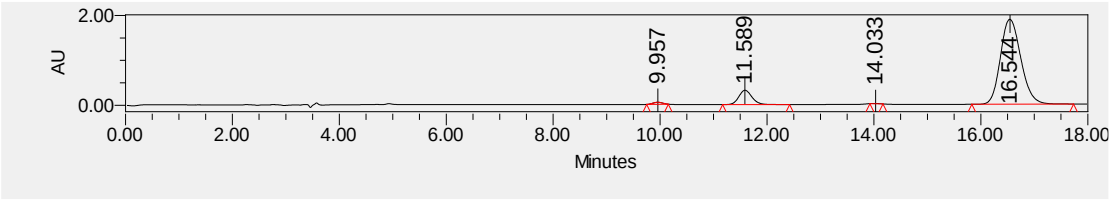
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 170.30, 148.00, 135.76, 133.31, 132.69, 130.49, 128.28, 127.88, 127.69, 127.63, 127.09, 126.69, 126.09, 125.82, 124.08, 94.88, 42.34, 39.99, 24.90, 24.77, 21.77.

IR (neat): *v* (cm^{-1}) 3356, 2922, 2853, 1679, 1463, 1274, 1092, 813, 751

HRMS (ESI-FT) calcd for $C_{20}H_{19}NO_2Na^+$ ([M]+Na^+) = 328.1308, found 328.1300

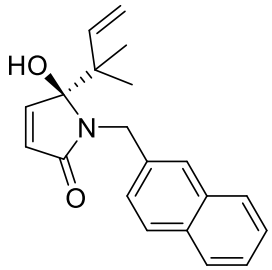


	Retention Time	Area	% Area
1	9.808	5427538	4.88
2	11.393	48879639	43.91
3	13.718	4414243	3.97
4	16.188	52586302	47.24



	Retention Time	Area	% Area
1	9.957	563511	1.00
2	11.589	5419998	9.64
3	14.033	59525	0.11
4	16.544	50152553	89.25

(*S*)-5-Hydroxy-5-(2-methylbut-3-en-2-yl)-1-(naphthalen-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3nf)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 81% yield, 41% *ee.* $[\alpha]^{20}_D$ = +12.5 (*c* = 0.32, in CH_2Cl_2).

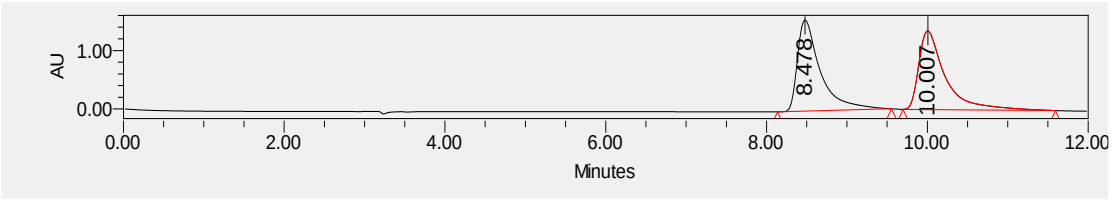
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.5 min, t_{minor} = 10.0 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.88 – 7.68 (m, 1H), 7.59 – 7.38 (m, 1H), 7.01 (dd, J = 6.1, 4.0 Hz, 0H), 6.20 (dd, J = 6.2, 4.3 Hz, 0H), 6.18 – 6.09 (m, 0H), 5.11 (d, J = 8.0 Hz, 0H), 5.06 – 4.96 (m, 0H), 4.79 – 4.67 (m, 0H), 2.60 (d, J = 20.1 Hz, 0H), 1.08 (s, 0H), 1.01 (s, 1H).

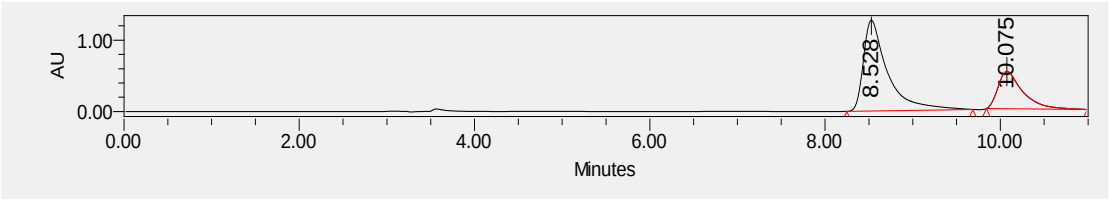
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 171.71, 149.42, 149.38, 143.40, 136.07, 133.34, 132.57, 128.19, 127.86, 127.66, 126.53, 126.20, 126.06, 125.71, 114.20, 96.10, 43.99, 43.61, 24.04, 21.91.

IR (neat): *v* (cm^{-1}) 3306, 3056, 2973, 2931, 1680, 1603, 1404, 1123, 816, 754.

HRMS (ESI-FT) calcd for $C_{20}H_{21}NO_2Na^+$ ([M]+Na^+) = 330.1465, found 330.1468.

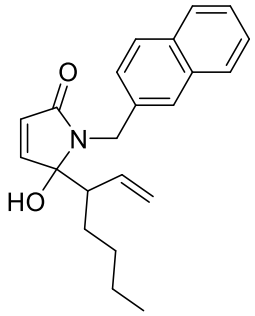


	Retention Time	Area	% Area
1	8.478	30995843	50.00
2	10.007	30996378	50.00



	Retention Time	Area	% Area
1	8.528	24355420	70.46
2	10.075	10212221	29.54

5-(Hept-1-en-3-yl)-5-hydroxy-1-(naphthalen-2-ylmethyl)-1,5-dihydro-2*H*-pyrrol-2-one (3ng)



Viscous colorless oil. R_f = 0.38 (petroleum ether/ethyl acetate = 2/1, v/v), 43% yield, 0% *ee*.

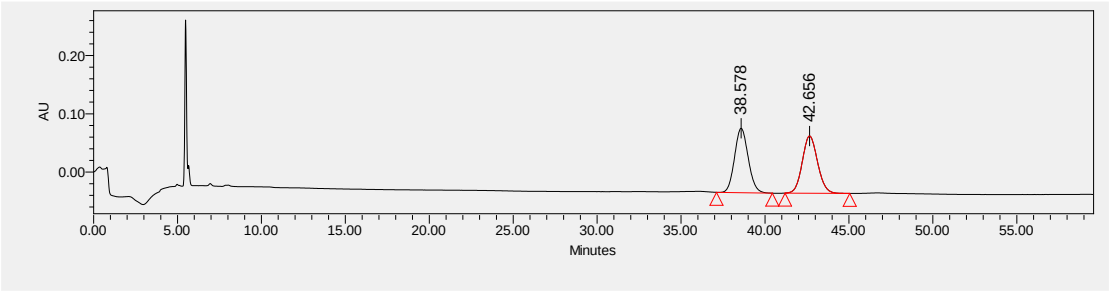
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IK**, hexane/*i*PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 37.7 min, t_{minor} = 441.9 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ = 7.85 – 7.71 (m, 4H), 7.58 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.48 – 7.38 (m, 2H), 6.85 (d, *J* = 6.0 Hz, 1H), 6.19 (d, *J* = 6.0 Hz, 1H), 5.61 (dt, *J* = 16.0, 10.0 Hz, 1H), 5.36 – 5.08 (m, 2H), 4.91 (d, *J* = 8.0 Hz, 1H), 4.48 (d, *J* = 12.0 Hz, 1H), 2.40 – 2.24 (m, 1H), 0.95 – 0.57 (m, 4H), 0.39 (t, *J* = 8.0 Hz, 3H).

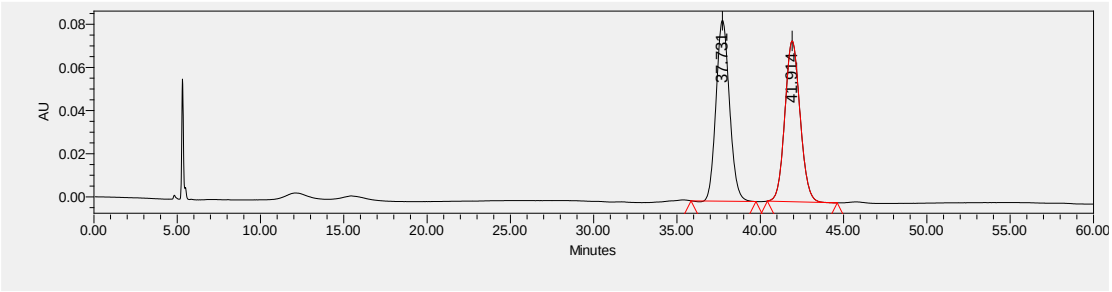
^{13}C{^{1}H} NMR (151 MHz, Chloroform-*d*) δ = 170.37, 147.10, 136.92, 135.66, 133.34, 132.77, 128.37, 127.80, 127.73, 127.62, 127.26, 126.91, 126.18, 125.90, 119.93, 93.85, 50.14, 42.12, 29.18, 27.85, 22.40, 13.65.

IR (neat): *v* (cm^{-1}) 3308, 2955, 2926, 2857, 1681, 1600, 1432, 1119, 1055, 860, 754, 704.

HRMS (ESI-FT) calcd for calcd for $C_{22}H_{25}NO_2Na^+$ ([M]+Na^+) = 358.1778, found 358.1778.

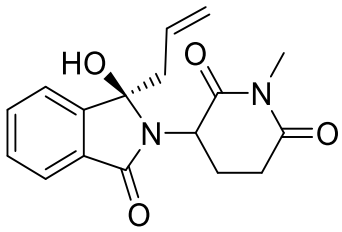


	Retention Time	Area	% Area
1	38.578	6262556	50.20
2	42.656	6213891	49.80



	Retention Time	Area	% Area
1	37.731	4728695	50.06
2	41.914	4717022	49.94

3-[(*R*)-1-Allyl-1-hydroxy-3-oxoisoindolin-2-yl]-1-methylpiperidine-2,6-dione (3xa)



Viscous colorless oil. R_f = 0.27 (petroleum ether/ethyl acetate = 1/1, v/v), 33% yield, 7% *ee.* 92:8 dr $[\alpha]^{20}_D$ = –0.40 (c = 0.26, in CH_2Cl_2).

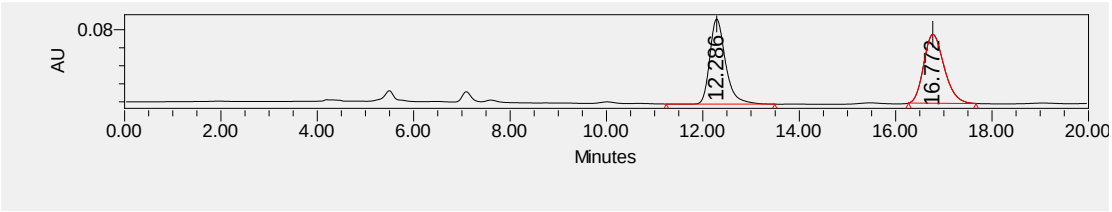
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IK**, hexane/*i*PrOH = 70/30, flow rate = 1.0 mL/min, λ = 254 nm) retention time: (major isomer) t_{major} = 16.5 min, t_{minor} = 11.6 min. dr = 92:8 determined by ^{1}H NMR.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.75 (d, J = 8.0 Hz, 1H), 7.68 – 7.54 (m, 2H), 7.54 – 7.47 (m, 1H), 5.73 – 5.42 (m, 1H), 5.19 – 4.97 (m, 2H), 4.24 (dd, J = 12.0, 6.0 Hz, 1H), 3.67 (s, 1H), 3.19 (s, 3H), 3.17 – 3.04 (m, 1H), 3.03 – 2.95 (m, 1H), 2.94 – 2.85 (m, 1H), 2.84 – 2.75 (m, 1H), 2.73 – 2.59 (m, 1H), 2.20 – 2.06 (m, 1H).

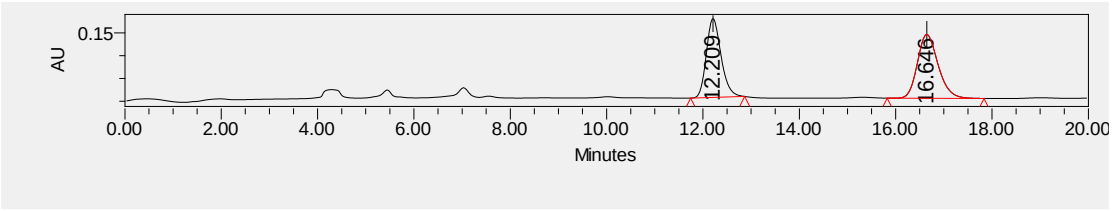
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 172.55, 171.45, 168.68, 147.14, 133.03, 131.24, 130.35, 129.86, 123.67, 122.39, 119.80, 90.21, 52.38, 41.51, 32.15, 27.38, 21.99.

IR (neat): *v* (cm^{-1}) 3343, 2926, 2350, 1674, 1467, 1420, 1278, 1118, 757.

HRMS (ESI-FT) calcd for $C_{17}H_{18}N_2O_4Na^+$ ([M]+Na^+) = 337.1159, found 337.1158.

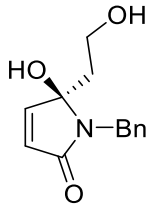


	Retention Time	Area	% Area
1	12.286	2137810	48.81
2	16.772	2242347	51.19



	Retention Time	Area	% Area
1	12.209	3668949	46.79
2	16.646	4172015	53.21

(*R*)-1-Benzyl-5-hydroxy-5-(2-hydroxyethyl)-1,5-dihydro-2H-pyrrol-2-one (6aa)



Viscous colorless oil. R_f = 0.45 (ethyl acetate). 51% yield, 80% *ee*. $[\alpha]^{20}_D$ = +34.2 (c = 0.47, in CH_2Cl_2).

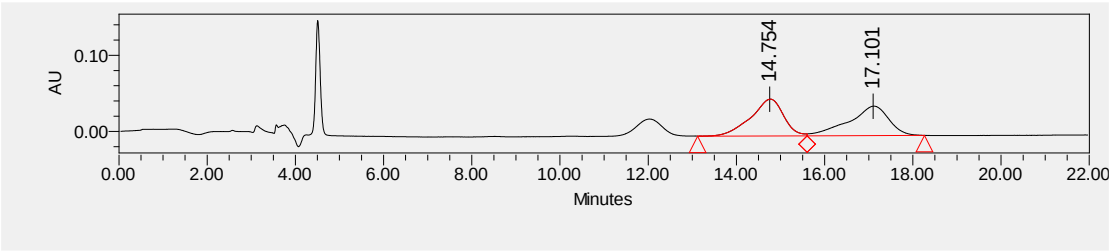
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm)

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.35 – 7.15 (m, 5H), 7.06 (d, J = 6.0 Hz, 1H), 5.99 (d, J = 6.0 Hz, 1H), 5.09 (s, 1H), 4.66 (d, J = 15.6 Hz, 1H), 4.31 (d, J = 15.7 Hz, 1H), 3.61 – 3.37 (m, 2H), 3.12 (s, 1H), 2.15 – 1.86 (m, 1H), 1.69 – 1.41 (m, 1H).

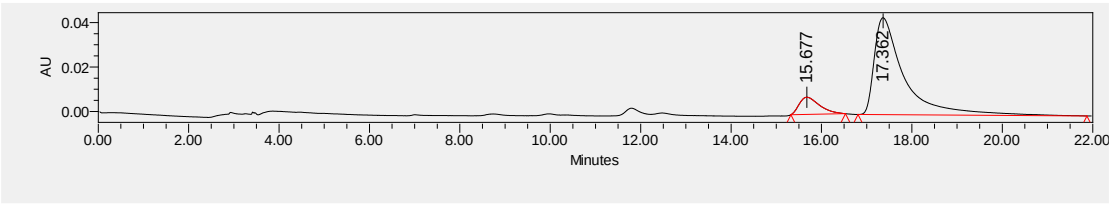
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 170.05, 149.70, 137.99, 128.46, 127.73, 127.24, 125.60, 92.21, 58.25, 41.56, 38.41.

IR (neat): *v* (cm^{-1}) 3339, 2927, 1679, 1600, 1496, 1414, 1082, 751

HRMS (ESI-FT) calcd for $C_{13}H_{15}NO_2Na^+$ ([M]+Na^+) = 256.0944, found 256.0945

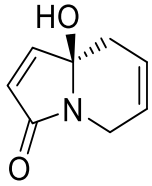


	Retention Time	Area	% Area
1	14.754	2495654	50.76
2	17.101	2420733	49.24



	Retention Time	Area	% Area
1	15.677	242763	10.72
2	17.362	2022710	89.28

(*R*)-8a-Hydroxy-8,8a-dihydroindolizin-3(5*H*)-one (7da)



Viscous colorless oil. R_f = 0.50 (ethyl acetate). 81% yield, 90% *ee*. $[\alpha]^{20}_D$ = –378.9 (c = 0.30, in CH_2Cl_2).

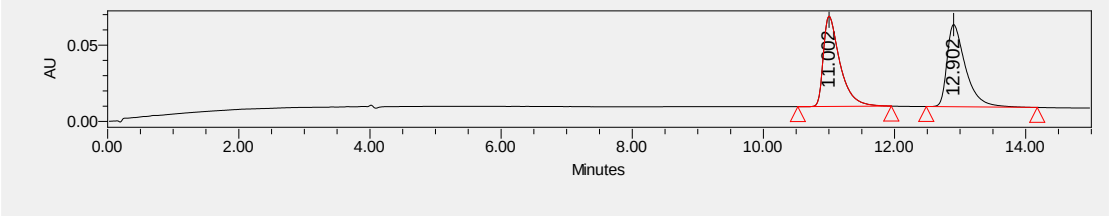
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IA**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm)

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.09 (d, J = 6.0 Hz, 1H), 6.12 (d, J = 6.0 Hz, 1H), 5.96 – 5.62 (m, 2H), 4.41 (d, J = 16.0 Hz, 1H), 3.67 (d, J = 16.0 Hz, 1H), 2.79 (s, 1H), 2.66 – 2.57 (m, 1H), 2.31 (d, J = 16.0 Hz, 1H).

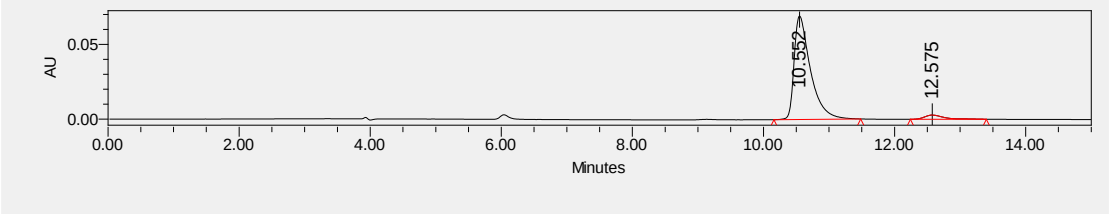
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 149.55, 126.79, 122.88, 120.49, 86.22, 37.19, 33.53.

IR (neat): *v* (cm^{-1}) 3339, 2927, 1679, 1600, 1496, 1414, 1082, 751.

HRMS (ESI-FT) calcd for $C_8H_9NO_2Na^+$ ([M]+Na^+) = 174.0525, found 174.0524

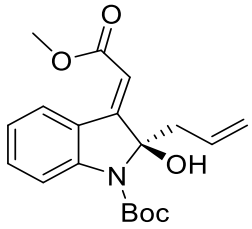


	Retention Time	Area	% Area
1	11.002	1041234	49.59
2	12.902	1058577	50.41



	Retention Time	Area	% Area
1	10.552	1198915	95.39
2	12.575	57945	4.61

***Tert*-butyl (*R, E*)-2-allyl-2-hydroxy-3-(2-methoxy-2-oxoethylidene)indoline-1-carboxylate (5aa)**



Viscous yellow oil; R_f = 0.8 (petroleum ether/ethyl acetate = 4/1, v/v), 99% yield, 91% *ee.* $[\alpha]^{20}_D$ = –80.6 (*c* = 0.06, in CH_2Cl_2).

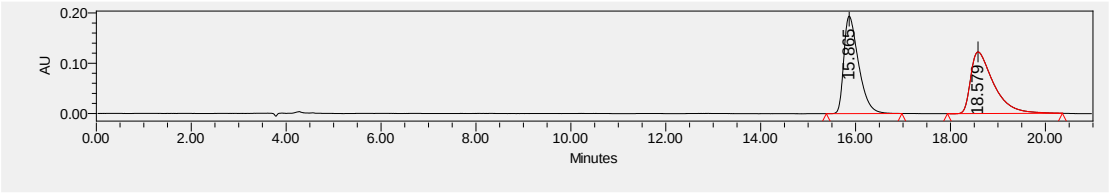
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 15.8 min, t_{minor} = 19.1 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.84 (d, J = 8.0 Hz, 1H), 7.64 (s, 1H), 7.46 – 7.32 (m, 1H), 7.10 – 7.01 (m, 1H), 6.09 (s, 1H), 5.66 – 5.31 (m, 1H), 5.03 (dd, J = 16.0, 2.0 Hz, 1H), 4.92 (dd, J = 12.0, 2.0 Hz, 1H), 3.79 (s, 3H), 3.21 (dd, J = 12.0, 8.0 Hz, 1H), 2.65 (dd, J = 12.0, 4.0 Hz, 1H), 1.63 (s, 9H).

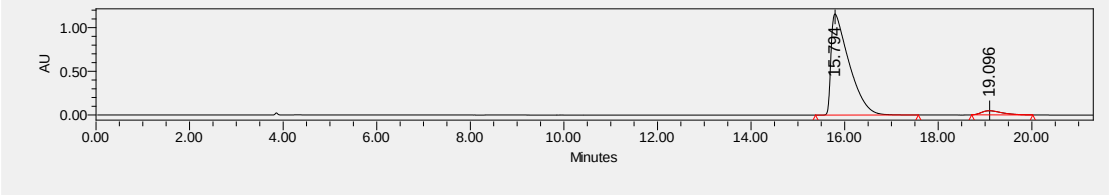
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 166.53, 153.75, 144.63, 132.91, 130.66, 128.83, 123.34, 123.00, 119.61, 114.41, 112.08, 94.70, 83.36, 51.50, 46.19, 28.39.

IR (neat): *v* (cm^{-1}) 3460, 2977, 1682, 1637, 1596, 1466, 1357, 1164, 1101, 1000, 853, 746.

HRMS (ESI-FT) calcd for $C_{19}H_{23}NO_5Na^+$ ([M]+Na^+) = 368.1468, found 368.1462.

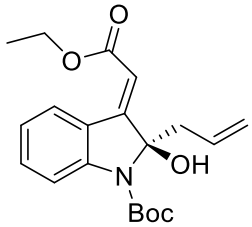


	Retention Time	Area	% Area
1	15.865	4181369	50.39
2	18.579	4116597	49.61



	Retention Time	Area	% Area
1	15.794	31054269	95.50
2	19.096	1463106	4.50

***Tert*-butyl (*R, E*)-2-allyl-3-(2-ethoxy-2-oxoethylidene)-2-hydroxyindoline-1-carboxylate (5ba)**



Viscous yellow oil; R_f = 0.35 (petroleum ether/ethyl acetate = 15/1, v/v), 99% yield, 93% *ee.* $[\alpha]^{20}_D$ = –133.3 (*c* = 0.60, in CH_2Cl_2).

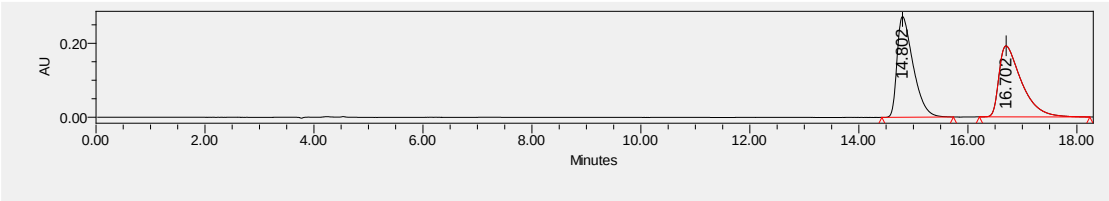
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 15.0 min, t_{minor} = 17.4 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.85 (d, J = 8.0 Hz, 1H), 7.63 (s, 1H), 7.36 (t, J = 8.0 Hz, 1H), 7.06 (t, J = 8.0 Hz, 1H), 6.09 (s, 1H), 5.48 – 5.34 (m, 1H), 5.04 (d, J = 16.0 Hz, 1H), 4.92 (d, J = 12.0 Hz, 1H), 4.30 – 4.22 (m, 2H), 3.22 (dd, J = 12.0, 8.0 Hz, 1H), 2.66 (dd, J = 12.0, 8.0 Hz, 1H), 1.64 (s, 9H), 1.34 (t, J = 8.0 Hz, 3H).

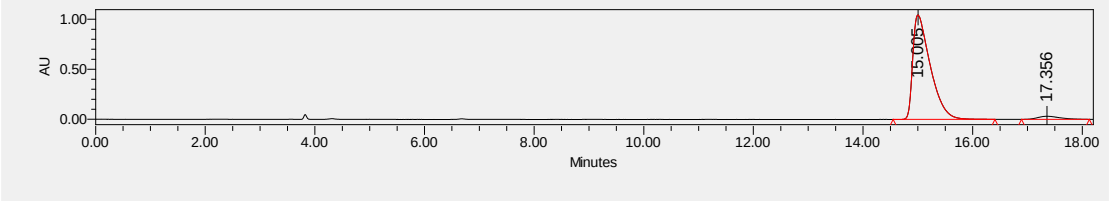
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 166.19, 153.49, 132.88, 130.80, 128.94, 123.48, 123.05, 119.65, 114.45, 112.72, 94.78, 83.42, 60.42, 46.28, 28.47, 14.30.

IR (neat): *v* (cm^{-1}) 3460, 3078, 2979, 2932, 1711, 1682, 1639, 1467, 1367, 1102, 865, 754.

HRMS (ESI-FT) calcd for $C_{20}H_{25}NO_5Na^+$ ([M]+Na^+) = 382.1624, found 382.1627.

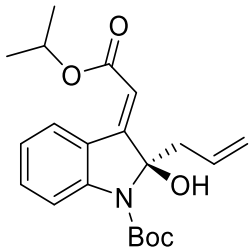


	Retention Time	Area	% Area
1	14.802	5592371	50.36
2	16.702	5511744	49.64



	Retention Time	Area	% Area
1	15.005	23100032	96.45
2	17.356	849028	3.55

***Tert*-butyl (*R, E*)-2-allyl-2-hydroxy-3-(2-isopropoxy-2-oxoethylidene)indoline-1-carboxylate (5ca)**



Viscous yellow oil; R_f = 0.38 (petroleum ether/ethyl acetate = 15/1, v/v), 96% yield, 94% *ee.* $[\alpha]^{20}_D$ = –169.5 (*c* = 0.64, in CH_2Cl_2).

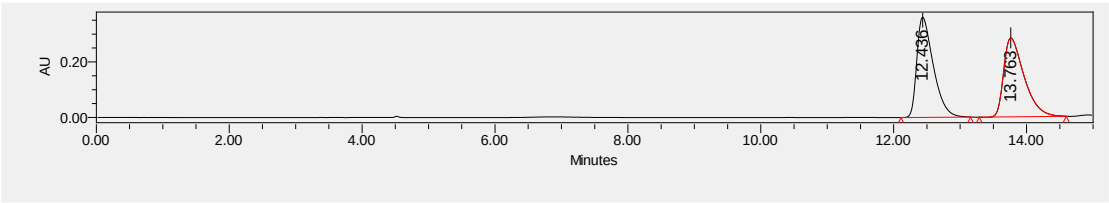
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 12.7 min, t_{minor} = 14.3 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.86 (d, J = 8.0 Hz, 1H), 7.63 (s, 1H), 7.41 – 7.33 (m, 1H), 7.05 (t, J = 8.0 Hz, 1H), 6.06 (s, 1H), 5.49 – 5.35 (m, 1H), 5.11 (p, J = 8.0 Hz, 1H), 5.07 – 5.00 (m, 1H), 4.92 (d, J = 8.0 Hz, 1H), 3.23 (dd, J = 12.0, 8.0 Hz, 1H), 2.65 (q, J = 8.0 Hz, 1H), 1.63 (s, 9H), 1.31 (dd, J = 12.0, 8.0 Hz, 6H).

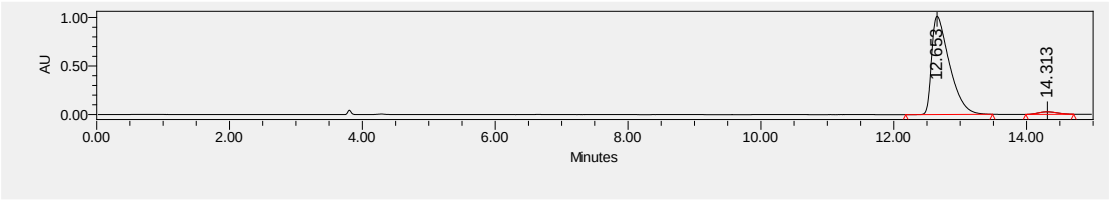
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.72, 153.16, 132.79, 130.86, 128.97, 123.55, 123.03, 119.60, 114.43, 113.33, 94.78, 83.40, 67.79, 46.29, 28.47, 21.97, 21.94.

IR (neat): *v* (cm^{-1}) 3460, 3078, 2979, 2933, 1708, 1680, 1638, 1465, 1355, 1099, 846, 752.

HRMS (ESI-FT) calcd for $C_{21}H_{27}NO_5Na^+$ ([M]+Na^+) = 396.1781, found 396.1784.

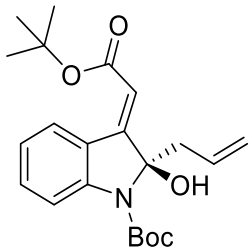


	Retention Time	Area	% Area
1	12.436	6216936	50.69
2	13.763	6047576	49.31



	Retention Time	Area	% Area
1	12.653	8579946	97.33
2	14.317	234939	2.67

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-2-hydroxyindoline-1-carboxylate (5da)**



Viscous yellow oil; R_f = 0.38 (petroleum ether/ethyl acetate = 15/1, v/v), 94% yield, 97% *ee.* $[\alpha]^{20}_D$ = –181.7 (*c* = 0.60, in CH_2Cl_2).

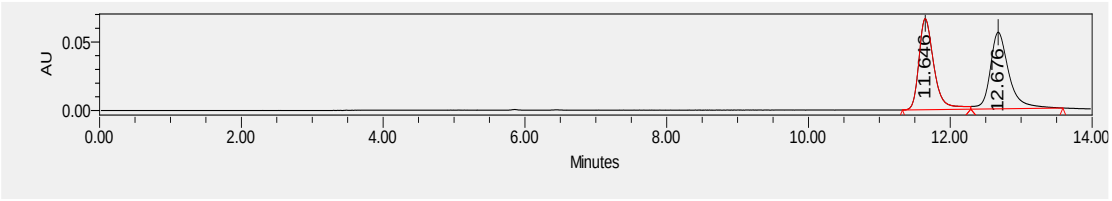
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 11.4 min, t_{minor} = 13.3 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.81 (d, J = 8.0 Hz, 1H), 7.62 (s, 1H), 7.34 (t, J = 8.0 Hz, 1H), 7.05 (t, J = 8.0 Hz, 1H), 6.03 (s, 1H), 5.47 – 5.36 (m, 1H), 5.07 – 5.01 (m, 1H), 4.94 – 4.88 (m, 1H), 3.23 (t, J = 12.0, 8.0 Hz, 1H), 2.64 (dd, J = 12.0, 8.0 Hz, 1H), 1.63 (s, 9H), 1.54 (s, 9H).

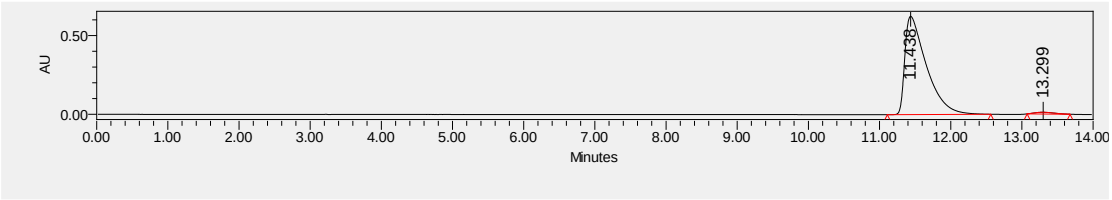
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.53, 152.02, 132.46, 130.91, 128.81, 123.59, 122.93, 119.45, 114.86, 114.33, 94.71, 83.26, 80.53, 46.25, 28.41, 28.17.

IR (neat): *v* (cm^{-1}) 3460, 2978, 1682, 1638, 1597, 1466, 1358, 1298, 1162, 1102, 861, 774.

HRMS (ESI-FT) calcd for $C_{22}H_{29}NO_5Na^+$ ([M]+Na^+) = 410.1938, found 410.1938.

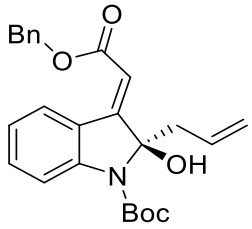


	Retention Time	Area	% Area
1	11.646	981328	49.13
2	12.676	1016056	50.87



	Retention Time	Area	% Area
1	11.438	13089679	98.41
2	13.299	211687	1.59

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(benzyloxy)-2-oxoethylidene)-2-hydroxyindoline-1-carboxylate (5ea)**



Viscous yellow oil; R_f = 0.38 (petroleum ether/ethyl acetate = 15/1, v/v), 98% yield, 96% *ee.* $[\alpha]^{20}_D$ = –165.8 (*c* = 0.62, in CH_2Cl_2).

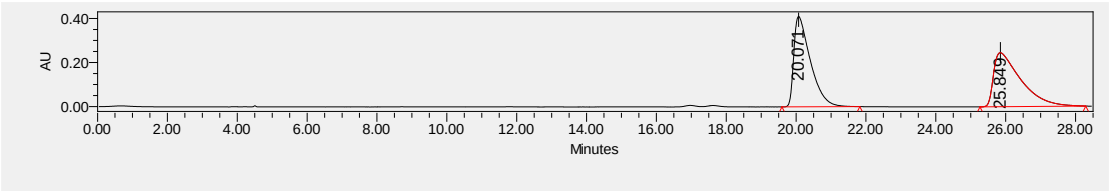
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 20.6 min, t_{minor} = 27.7 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.86 (dd, J = 8.0, 4.0 Hz, 1H), 7.64 (s, 1H), 7.47 – 7.32 (m, 6H), 7.06 (t, J = 4.0 Hz, 1H), 6.15 (s, 1H), 5.46 – 5.35 (m, 1H), 5.24 (d, J = 4.0 Hz, 2H), 5.08 – 5.00 (m, 1H), 4.92 (dd, J = 12.0, 4.0 Hz, 1H), 3.22 (dd, J = 16.0, 8.0 Hz, 1H), 2.70 – 2.61 (m, 1H), 1.64 (s, 9H).

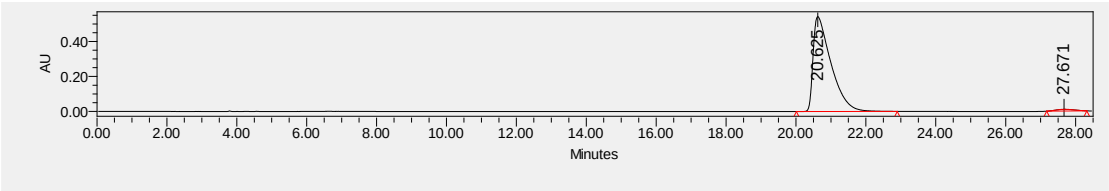
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.92, 154.21, 135.99, 133.06, 130.74, 129.03, 128.62, 128.35, 128.28, 123.42, 123.08, 119.70, 114.48, 112.21, 83.47, 66.29, 46.27, 28.47.

IR (neat): *v* (cm^{-1}) 3462, 2978, 2933, 1711, 1680, 1637, 1467, 1356, 1102, 860, 751.

HRMS (ESI-FT) calcd for $C_{25}H_{27}NO_5Na^+$ ([M]+Na^+) = 444.1781, found 444.1785.

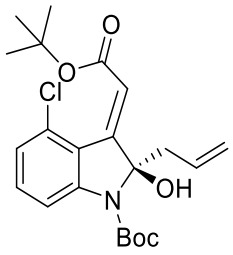


	Retention Time	Area	% Area
1	20.071	13536530	50.57
2	25.849	13233129	49.43



	Retention Time	Area	% Area
1	20.625	19264711	98.12
2	27.671	370079	1.88

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-4-chloro-2-hydroxyindoline-1-carboxylate (5fa)**



Viscous yellow oil; R_f = 0.52 (petroleum ether/ethyl acetate = 15/1, v/v), 48% yield, 71% *ee.* $[\alpha]^{20}_D$ = –1.4 (*c* = 0.74, in CH_2Cl_2).

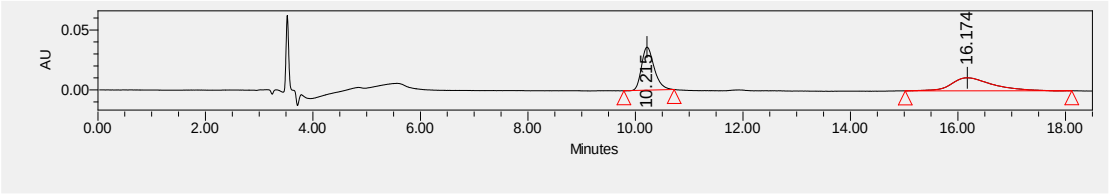
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 15.9 min, t_{minor} = 10.2 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.85 – 7.76 (m, 1H), 7.20 (t, J = 8.0 Hz, 1H), 6.95 (dd, J = 8.0, 2.0 Hz, 1H), 6.61 (s, 1H), 5.47 – 5.32 (m, 1H), 5.03 (dd, J = 16.0, 2.0 Hz, 1H), 4.91 – 4.85 (m, 1H), 3.49 (dd, J = 12.0, 8.0 Hz, 1H), 3.09 – 3.01 (m, 1H), 1.61 (s, 9H), 1.55 (s, 9H).

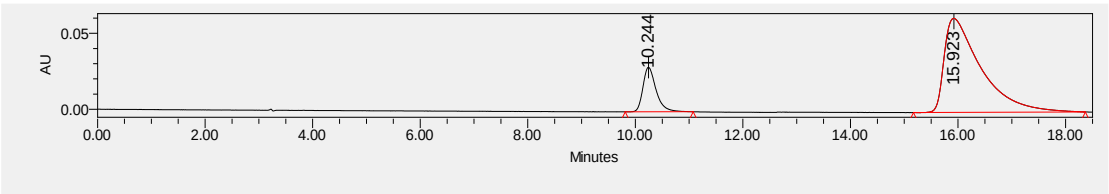
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 168.14, 150.95, 147.51, 132.46, 131.77, 130.46, 124.69, 120.91, 119.20, 115.41, 113.64, 94.42, 82.60, 82.42, 43.16, 28.40, 28.12.

IR (neat): *v* (cm^{-1}) 3337, 2979, 2933, 2357, 1714, 1678, 1618, 1448, 1368, 1149, 865, 781.

HRMS (ESI-FT) calcd for $C_{22}H_{28}{}^{34.9659}ClNO_5Na^+$ ([M]+Na^+) = 444.1548, found 444.1555; $C_{22}H_{28}{}^{36.9659}ClNO_5Na^+$ ([M]+Na^+) = 446.1519, found 446.1524.

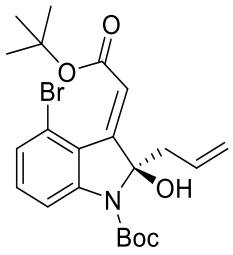


	Retention Time	Area	% Area
1	10.215	589603	50.57
2	16.174	576324	49.43



	Retention Time	Area	% Area
1	10.244	495697	14.45
2	15.923	2935818	85.55

***Tert*-butyl (*R, E*)-2-allyl-4-bromo-3-(2-(tert-butoxy)-2-oxoethylidene)-2-hydroxyindoline-1-carboxylate (5ga)**



Viscous yellow oil; R_f = 0.52 (petroleum ether/ethyl acetate = 15/1, v/v), 45% yield, 70% *ee.* $[\alpha]^{20}_D$ = –7.1 (*c* = 0.56, in CH_2Cl_2).

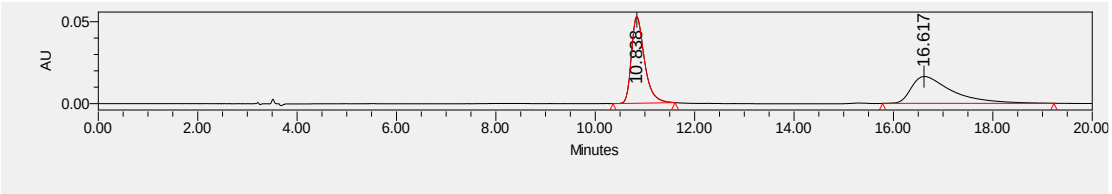
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 16.6 min, t_{minor} = 10.8 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 7.90 – 7.80 (m, 1H), 7.43 (s, 1H), 7.19 – 7.08 (m, 2H), 6.55 (s, 1H), 5.48 – 5.32 (m, 1H), 5.07 – 4.99 (m, 1H), 4.88 (dd, J = 12.0, 2.0 Hz, 1H), 3.47 (dd, J = 12.0, 8.0 Hz, 1H), 3.09 – 3.00 (m, 1H), 1.61 (s, 9H), 1.55 (s, 9H).

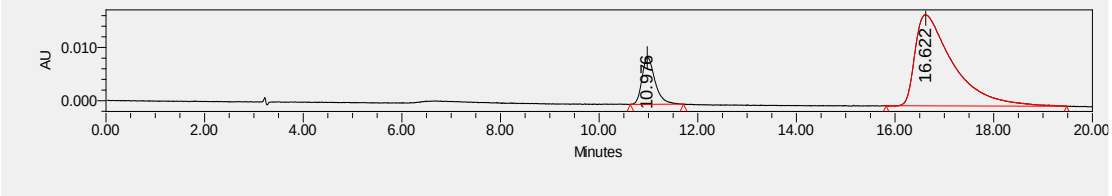
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 167.86, 150.91, 132.55, 131.76, 128.29, 122.09, 119.20, 118.37, 115.02, 114.19, 94.43, 82.66, 82.43, 43.31, 28.40, 28.12.

IR (neat): *v* (cm^{-1}) 3336, 2978, 2932, 1713, 1677, 1618, 1392, 1217, 1147, 993, 856, 779.

HRMS (ESI-FT) calcd for $C_{22}H_{28}{}^{80.9163}BrNO_5Na^+$ ([M]+Na^+) = 488.1043, found 488.1055; $C_{22}H_{28}{}^{78.7983}BrNO_5Na^+$ ([M]+Na^+) = 490.1023, found 490.1032.

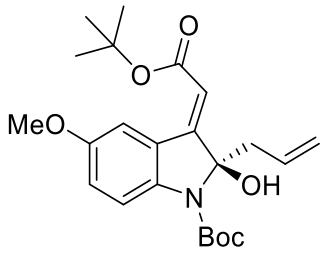


	Retention Time	Area	% Area
1	10.838	965125	50.87
2	16.617	932189	49.13



	Retention Time	Area	% Area
1	10.976	162211	15.05
2	16.622	915599	84.95

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-2-hydroxy-5-methoxyindoline-1-carboxylate (5ha)**



Viscous yellow oil; R_f = 0.60 (petroleum ether/ethyl acetate = 15/1, v/v), 84% yield, 97% *ee.* $[\alpha]^{20}_D$ = –52.5 (*c* = 0.80, in CH_2Cl_2).

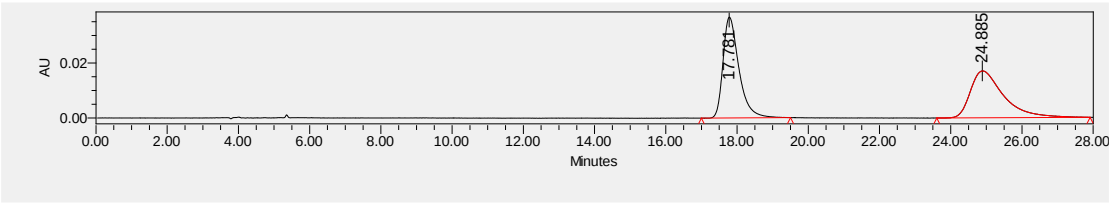
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 15.2 min, t_{minor} = 21.8 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.48 (d, J = 4.0 Hz, 1H), 7.45 (s, 1H), 6.93 (dd, J = 8.0, 2.0 Hz, 1H), 6.01 (s, 1H), 5.47 – 5.35 (m, 1H), 5.04 (dd, J = 16.0, 4.0 Hz, 1H), 4.92 (dd, J = 8.0, 4.0 Hz, 1H), 3.83 (s, 3H), 3.21 (q, J = 8.0 Hz, 1H), 2.62 (dd, J = 12.0, 8.0 Hz, 1H), 1.62 (s, 9H), 1.53 (s, 9H).

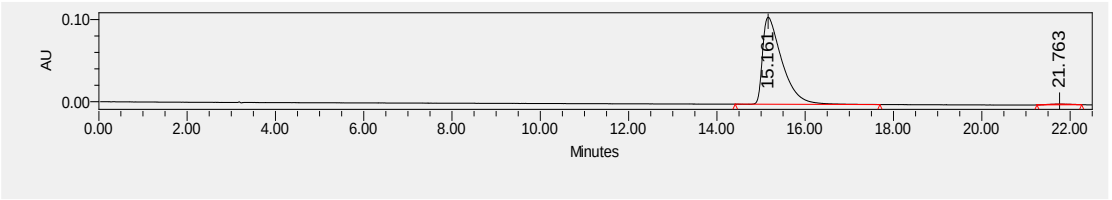
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.48, 155.24, 152.06, 119.61, 119.39, 115.04, 114.98, 112.26, 82.95, 80.50, 55.61, 28.45, 28.14.

IR (neat): *v* (cm^{-1}) 3464, 2978, 2926, 2853, 2349, 1727, 1639, 1613, 1392, 1260, 1152, 914, 847, 805.

HRMS (ESI-FT) calcd for $C_{23}H_{31}NO_6Na^+$ ([M]+Na^+) = 440.2044, found 440.2053.

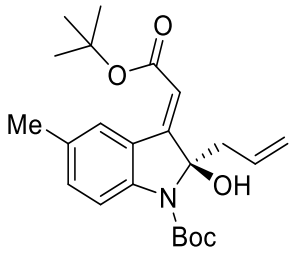


	Retention Time	Area	% Area
1	17.781	1138093	50.88
2	24.885	1098583	49.12



	Retention Time	Area	% Area
1	15.161	3243585	99.12
2	21.763	28654	0.88

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-2-hydroxy-5-methylindoline-1-carboxylate (5ia)**



Viscous yellow oil; R_f = 0.52 (petroleum ether/ethyl acetate = 15/1, v/v), 98% yield, 95% *ee.* $[\alpha]^{20}_D$ = –50.0 (*c* = 0.06, in CH_2Cl_2).

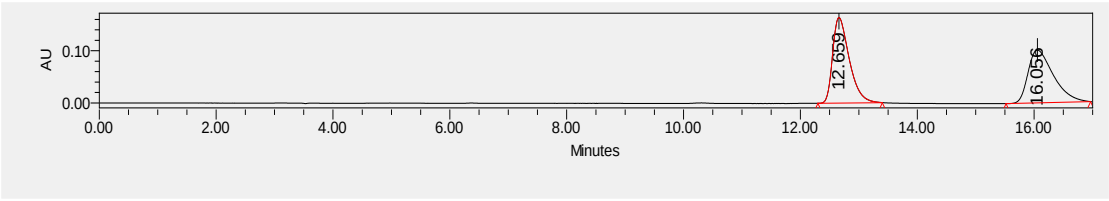
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 12.6 min, t_{minor} = 16.4 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.59 (s, 1H), 7.47 (s, 1H), 7.15 (dd, J = 8.0, 2.0 Hz, 1H), 5.99 (s, 1H), 5.49 – 5.33 (m, 1H), 5.07 – 4.99 (m, 1H), 4.91 (dd, J = 12.0, 4.0 Hz, 1H), 3.21 (q, J = 8.0 Hz, 1H), 2.62 (q, J = 8.0 Hz, 1H), 2.35 (s, 3H), 1.62 (s, 9H), 1.54 (s, 9H).

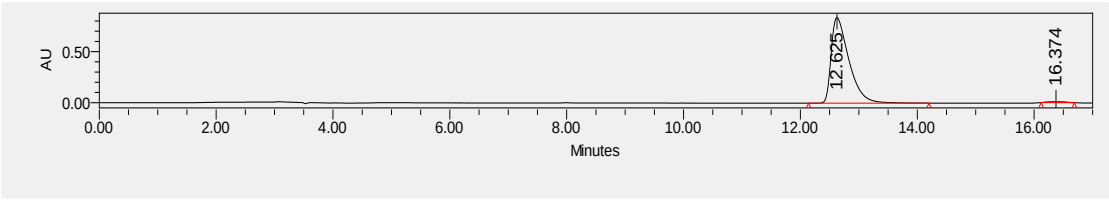
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.56, 151.90, 133.33, 132.35, 130.99, 128.76, 123.61, 119.35, 114.59, 114.07, 94.77, 83.02, 80.45, 46.25, 28.43, 28.19, 21.10.

IR (neat): *v* (cm^{-1}) 3464, 2978, 2927, 1709, 1679, 1638, 1483, 1453, 1367, 1109, 864, 767.

HRMS (ESI-FT) calcd for $C_{23}H_{32}NO_5Na^+$ ([M]+H^+) = 402.2275, found 402.2275.

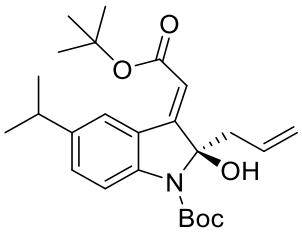


	Retention Time	Area	% Area
1	12.659	3234174	51.56
2	16.056	3038828	48.44



	Retention Time	Area	% Area
1	12.625	17687448	99.00
2	16.374	178130	1.00

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-2-hydroxy-5-isopropylindoline-1-carboxylate (5ja)**



Viscous yellow oil; R_f = 0.50 (petroleum ether/ethyl acetate = 15/1, v/v), 96% yield, 98% *ee.* $[\alpha]^{20}_D$ = –193.0 (*c* = 0.74, in CH_2Cl_2).

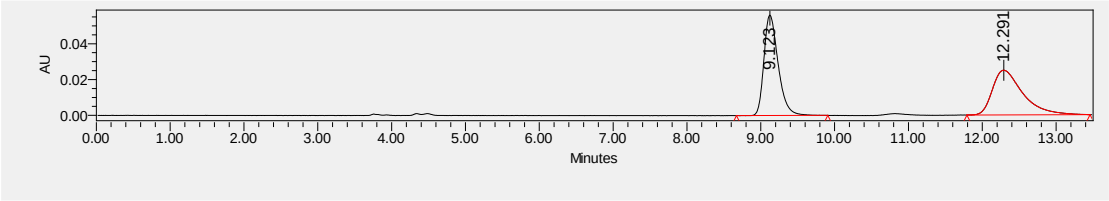
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 9.1 min, t_{minor} = 12.8 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.64 (d, J = 2.0 Hz, 1H), 7.52 (s, 1H), 7.23 (dd, J = 8.6, 2.0 Hz, 2H), 6.00 (s, 1H), 5.43 (dddd, J = 16.3, 10.1, 6.3, 4.3 Hz, 1H), 5.04 (dq, J = 16.9, 1.4 Hz, 1H), 4.93 (dd, J = 10.0, 2.0 Hz, 1H), 3.20 (t, J = 12.0, 8.0 Hz, 1H), 2.93 (p, J = 6.8 Hz, 1H), 2.65 (dd, J = 12.0, 4.0 Hz, 1H), 1.62 (s, 9H), 1.54 (s, 9H), 1.25 (dd, J = 6.8, 2.0 Hz, 7H).

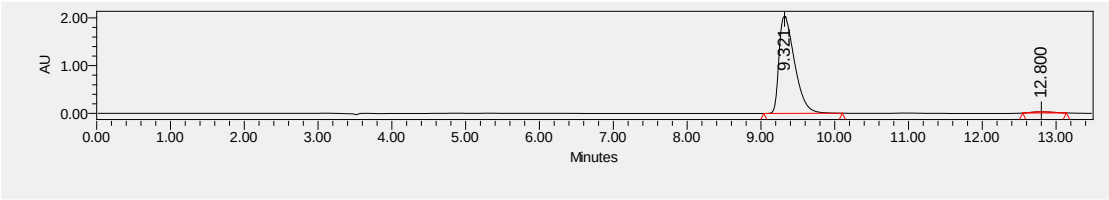
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.59, 151.71, 143.57, 131.08, 130.56, 126.52, 119.35, 114.59, 114.18, 82.99, 80.43, 46.11, 33.75, 28.44, 28.19, 24.11, 24.06.

IR (neat): *v* (cm^{-1}) 3464, 2964, 2928, 1709, 1679, 1639, 1517, 1456, 1367, 1147, 863, 765.

HRMS (ESI-FT) calcd for $C_{25}H_{35}NO_5K^+$ ([M]+K^+) = 468.2147, found 468.2144

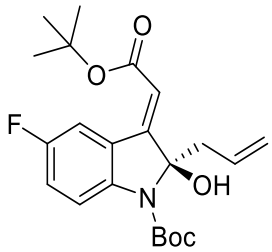


	Retention Time	Area	% Area
1	9.123	752175	51.42
2	12.291	710681	48.58



	Retention Time	Area	% Area
1	9.321	29846987	98.35
2	12.800	501052	1.65

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-5-fluoro-2-hydroxyindoline-1-carboxylate (5ka)**



Viscous yellow oil; R_f = 0.56 (petroleum ether/ethyl acetate = 15/1, v/v), 94% yield, 92% *ee.* $[\alpha]^{20}_D$ = –75.8 (*c* = 0.07, in CH_2Cl_2).

Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 16.8 min, t_{minor} = 18.1 min.

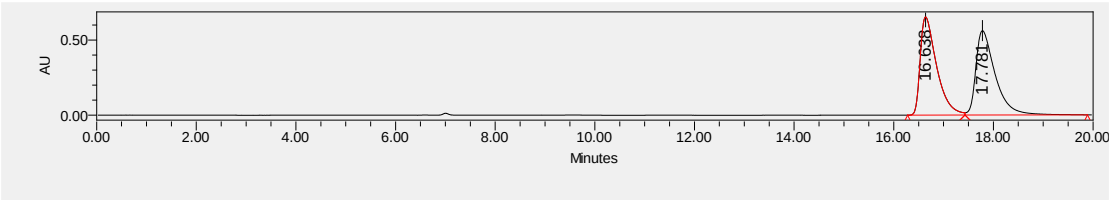
^{1}H NMR (400 MHz, Chloroform-d) δ = 8.61 (dd, J = 12.0, 4.0 Hz, 1H), 7.52 (s, 1H), 7.05 (td, J = 8.0, 2.0 Hz, 1H), 6.05 (s, 1H), 5.47 – 5.32 (m, 1H), 5.09 – 4.99 (m, 1H), 4.93 (dd, J = 10.0, 2.0 Hz, 1H), 3.21 (t, J = 12.0, 8.0 Hz, 1H), 2.62 (dd, J = 12.0, 4.0 Hz, 1H), 1.62 (s, 9H), 1.54 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-d) δ 165.21, 158.24 (d, J = 240.0 Hz), 151.24, 130.67, 119.70, 119.20 (d, J = 23.9 Hz), 116.17, 115.36, 115.07 (d, J = 7.7 Hz), 95.05, 83.44, 80.92, 46.33, 28.42, 28.15.

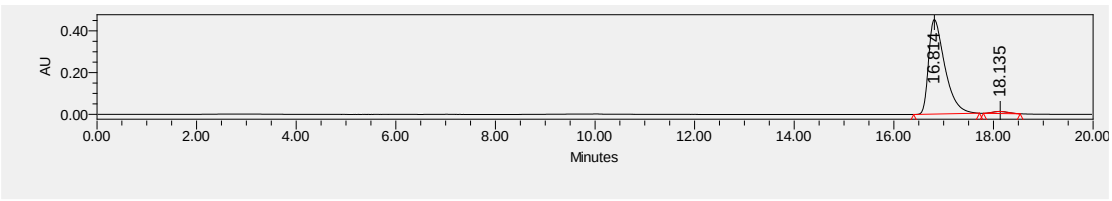
^{19}F NMR (377 MHz, Chloroform-d) δ -119.41.

IR (neat): ν (cm^{-1}) 3463, 3109, 2978, 2931, 1708, 1682, 1640, 1393, 1216, 1145, 1015, 867, 797.

HRMS (ESI-FT) calcd for $C_{25}H_{28}FNO_5Na^+$ ([M]+Na^+) = 428.1844, found 428.1847

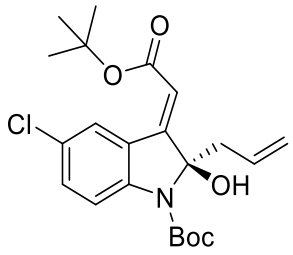


	Retention Time	Area	% Area
1	16.638	14945542	49.69
2	17.781	15129839	50.31



	Retention Time	Area	% Area
1	16.814	10239296	97.96
2	18.135	213657	2.04

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-5-chloro-2-hydroxyindoline-1-carboxylate (5la)**



Viscous yellow oil; R_f = 0.56 (petroleum ether/ethyl acetate = 15/1, v/v), 85% yield, 92% *ee.* $[\alpha]^{20}_D$ = –36.7 (*c* = 0.09, in CH_2Cl_2).

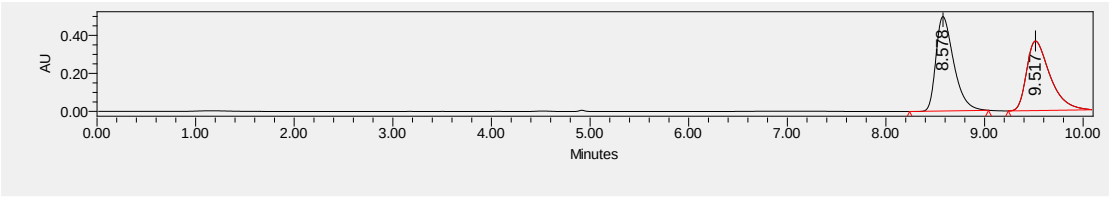
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 8.6 min, t_{minor} = 9.7 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.83 (d, J = 2.0 Hz, 1H), 7.54 (s, 1H), 7.29 (dd, J = 8.0, 2.0 Hz, 1H), 6.05 (s, 1H), 5.38 (dddd, J = 16.0, 10.0, 8.0, 6.0 Hz, 1H), 5.03 (d, J = 16.0 Hz, 1H), 4.93 (d, J = 8.0 Hz, 1H), 3.21 (q, J = 8.0 Hz, 1H), 2.61 (p, J = 8.0 Hz, 1H), 1.62 (s, 9H), 1.54 (s, 9H).

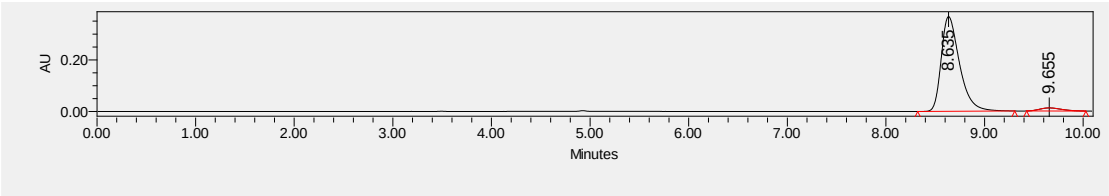
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.14, 150.54, 132.18, 130.60, 128.38, 127.92, 124.93, 119.79, 116.35, 115.30, 95.01, 83.64, 81.00, 46.35, 28.39, 28.15.

IR (neat): *v* (cm^{-1}) 3463, 3108, 2978, 2929, 1708, 1640, 1597, 1392, 1218, 1144, 994, 845, 821.

HRMS (ESI-FT) calcd for $C_{22}H_{28}{}^{34.9659}ClNO_5Na^+$ ([M]+Na^+) = 444.1548, found 444.1526; $C_{22}H_{28}{}^{36.9659}ClNO_5Na^+$ ([M]+Na^+) = 446.1519, found 446.1505.

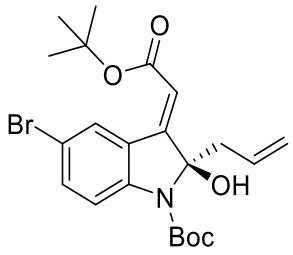


	Retention Time	Area	% Area
1	8.578	6227886	50.87
2	9.517	6014614	49.13



	Retention Time	Area	% Area
1	8.635	4734978	96.14
2	9.655	190211	3.86

***Tert*-butyl (*R, E*)-2-allyl-5-bromo-3-(2-(tert-butoxy)-2-oxoethylidene)-2-hydroxyindoline-1-carboxylate (5ma)**



Viscous yellow oil; R_f = 0.56 (petroleum ether/ethyl acetate = 15/1, v/v), 95% yield, 95% *ee.* $[\alpha]^{20}_D$ = –138.3 (*c* = 0.76, in CH_2Cl_2).

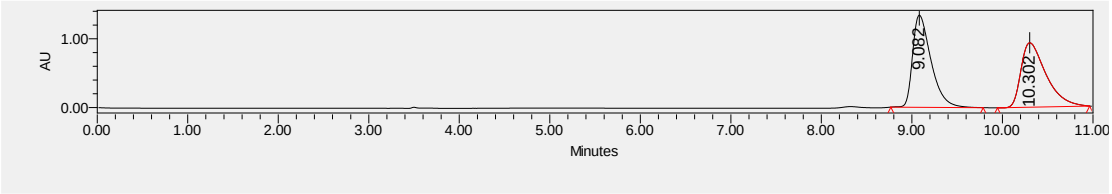
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 9.2 min, t_{minor} = 10.5 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.96 (s, 1H), 7.43 (dd, J = 8.0, 2.0 Hz, 2H), 6.04 (s, 1H), 5.48 – 5.30 (m, 1H), 5.03 (dd, J = 16.0, 2.0 Hz, 1H), 4.93 (dd, J = 12.0, 2.0 Hz, 1H), 3.21 (dd, J = 12.0, 2.0 Hz, 1H), 2.66 – 2.56 (m, 1H), 1.62 (s, 9H), 1.55 (s, 9H).

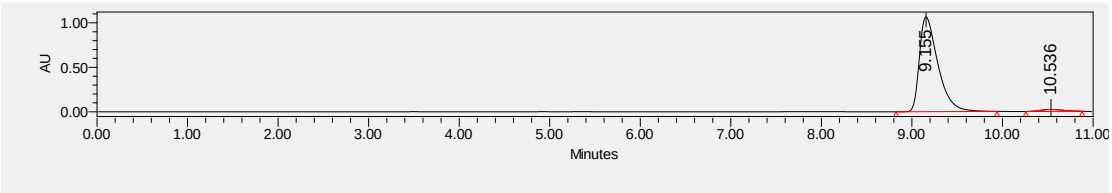
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.12, 150.29, 135.01, 131.24, 130.58, 125.35, 119.81, 116.39, 115.75, 115.42, 94.95, 83.67, 81.04, 46.34, 28.38, 28.15.

IR (neat): *v* (cm^{-1}) 3463, 3107, 2978, 2931, 1708, 1641, 1593, 1392, 1218, 1147, 994, 845, 820.

HRMS (ESI-FT) calcd for $C_{22}H_{28}{}^{80.9163}BrNO_5Na^+$ ([M]+Na^+) = 490.1023, found 490.1006; $C_{22}H_{28}{}^{78.7983}BrNO_5Na^+$ ([M]+Na^+) = 488.1043, found 488.1028.

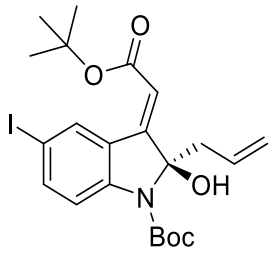


	Retention Time	Area	% Area
1	9.082	18945771	51.26
2	10.302	18012551	48.74



	Retention Time	Area	% Area
1	9.155	15096770	97.48
2	10.536	390753	2.52

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(tert-butoxy)-2-oxoethylidene)-2-hydroxy-5-iodoindoline-1-carboxylate (5na)**



Viscous yellow oil; R_f = 0.56 (petroleum ether/ethyl acetate = 15/1, v/v), 94% yield, 93% *ee.* $[\alpha]^{20}_D$ = –17.6 (*c* = 0.17, in CH_2Cl_2).

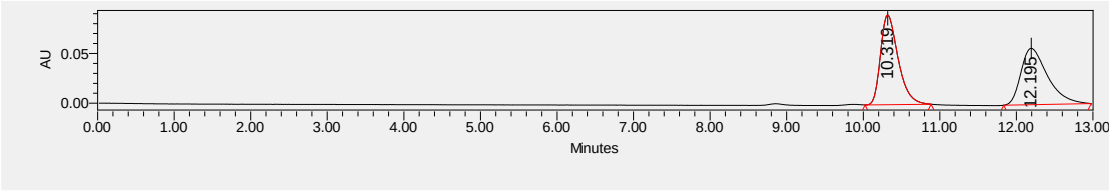
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 9.8 min, t_{minor} = 11.8 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 9.10 (d, J = 2.0 Hz, 1H), 7.62 (dd, J = 8.0, 2.0 Hz, 1H), 7.38 (s, 1H), 6.02 (s, 1H), 5.43 – 5.32 (m, 1H), 5.06 – 4.99 (m, 1H), 4.93 (dd, J = 10.0, 2.0 Hz, 1H), 3.20 (dd, J = 14.0, 8.0 Hz, 1H), 2.65 – 2.57 (m, 1H), 1.62 (s, 9H), 1.55 (s, 9H).

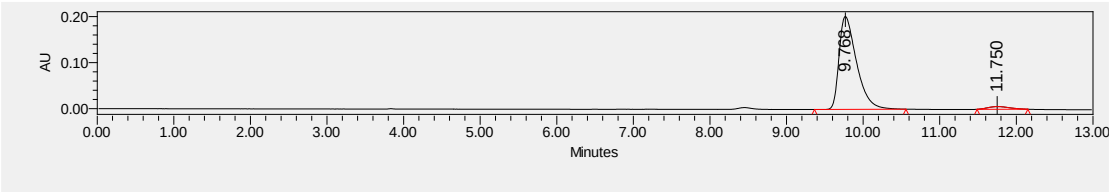
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.15, 149.90, 140.88, 137.02, 130.59, 125.74, 119.82, 116.32, 116.28, 85.76, 83.70, 81.08, 28.39, 28.18.

IR (neat): *v* (cm^{-1}) 3464, 3104, 2978, 2930, 1707, 1685, 1641, 1392, 1219, 1147, 993, 847, 818.

HRMS (ESI-FT) calcd for $C_{22}H_{28}INO_5Na^+$ ([M]+Na^+) = 536.0904, found 536.0859

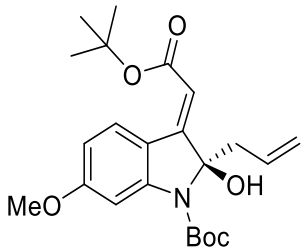


	Retention Time	Area	% Area
1	10.319	1438241	51.25
2	12.195	1368162	48.75



	Retention Time	Area	% Area
1	9.768	3194878	96.55
2	11.750	114008	3.45

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(*tert*-butoxy)-2-oxoethylidene)-2-hydroxy-6-methoxyindoline-1-carboxylate (5oa)**



Viscous yellow oil; R_f = 0.45 (petroleum ether/ethyl acetate = 15/1, v/v), 92% yield, 93% *ee.* $[\alpha]^{20}_D$ = –151.1 (*c* = 0.09, in CH_2Cl_2).

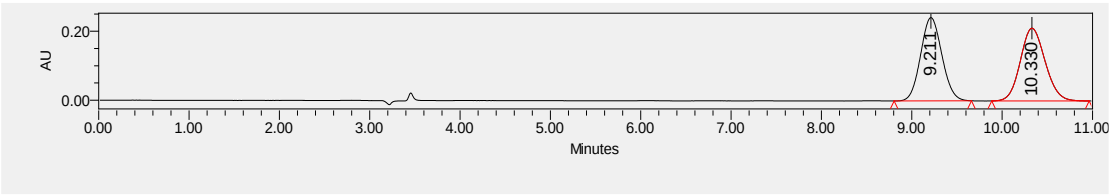
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IG**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 10.2 min, t_{minor} = 9.2 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.82 (d, J = 8.0 Hz, 1H), 7.22 (s, 1H), 6.60 (dd, J = 12.0, 4.0 Hz, 1H), 5.87 (s, 1H), 5.47 – 5.32 (m, 1H), 5.03 (dd, J = 16.0, 4.0 Hz, 1H), 4.91 (dd, J = 12.0, 4.0 Hz, 1H), 3.82 (s, 3H), 3.24 (q, J = 8.0 Hz, 1H), 2.62 (dd, J = 16.0, 4.0 Hz, 1H), 1.63 (s, 9H), 1.52 (s, 9H).

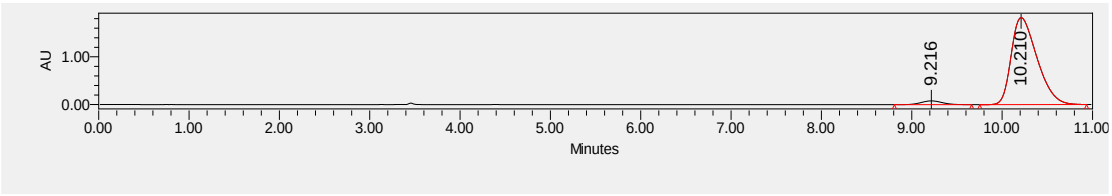
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 166.01, 163.32, 152.12, 131.02, 130.35, 119.31, 116.84, 111.56, 99.62, 95.54, 83.22, 80.09, 55.33, 46.23, 28.39, 28.21.

IR (neat): *v* (cm^{-1}) 3464, 3104, 2978, 2930, 1707, 1685, 1641, 1392, 1219, 1147, 993, 847, 818.

HRMS (ESI-FT) calcd for $C_{23}H_{31}NO_6Na^+$ ([M]+Na^+) = 440.2044, found 440.2044

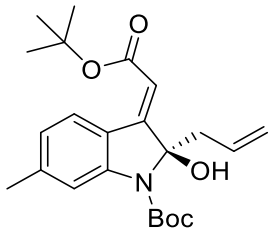


	Retention Time	Area	% Area
1	9.211	3949701	49.57
2	10.330	4018492	50.43



	Retention Time	Area	% Area
1	9.216	1269559	3.40
2	10.210	36079533	96.60

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(*tert*-butoxy)-2-oxoethylidene)-2-hydroxy-6-methylindoline-1-carboxylate (5pa)**



Viscous yellow oil; R_f = 0.45 (petroleum ether/ethyl acetate = 15/1, v/v), 99% yield, 95% *ee.* $[\alpha]^{20}_D$ = –206.4 (*c* = 0.86, in CH_2Cl_2).

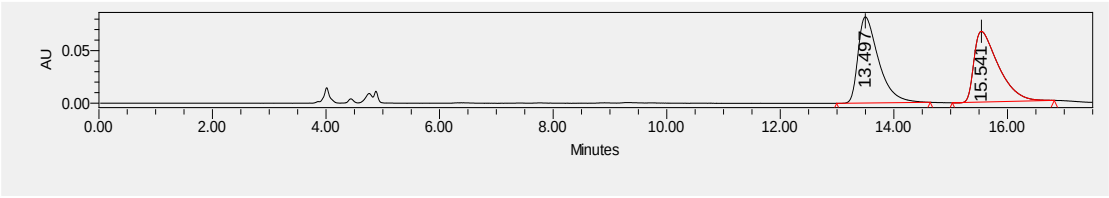
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 15.5 min, t_{minor} = 13.8 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.70 (d, J = 8.0 Hz, 1H), 7.49 (s, 1H), 6.97 – 6.75 (m, 1H), 5.95 (s, 1H), 5.47 – 5.34 (m, 1H), 5.08 – 5.01 (m, 1H), 4.92 (dd, J = 10.0, 2.0 Hz, 1H), 3.22 (dd, J = 14.0, 8.0 Hz, 1H), 2.75 – 2.58 (m, 1H), 2.36 (s, 3H), 1.63 (s, 9H), 1.53 (s, 9H).

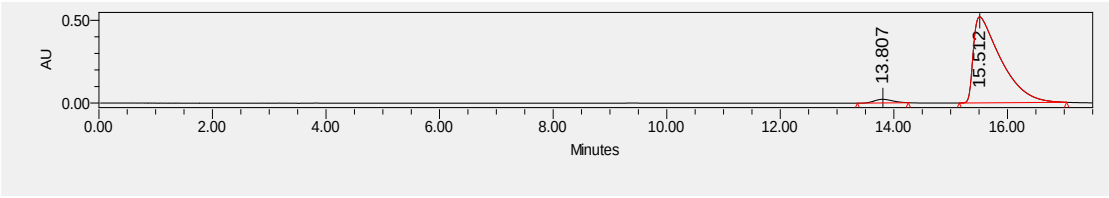
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.72, 152.17, 130.98, 128.60, 124.01, 119.38, 115.00, 113.51, 83.16, 80.34, 28.41, 28.21, 22.42.

IR (neat): *v* (cm^{-1}) 3467, 2977, 2929, 1708, 1680, 1637, 1365, 1217, 1147, 989, 861, 821.

HRMS (ESI-FT) calcd for $C_{23}H_{31}NO_5Na^+$ ([M]+Na^+) = 424.2094, found 424.2098.

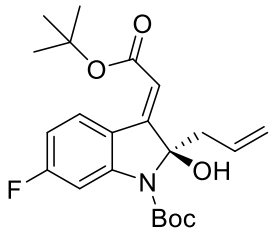


	Retention Time	Area	% Area
1	13.497	2067866	50.73
2	15.541	2008433	49.27



	Retention Time	Area	% Area
1	13.807	488525	2.72
2	15.512	17492113	97.28

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(*tert*-butoxy)-2-oxoethylidene)-6-fluoro-2-hydroxyindoline-1-carboxylate (5qa)**



Viscous yellow oil; R_f = 0.45 (petroleum ether/ethyl acetate = 15/1, v/v), 93% yield, 93% *ee.* $[\alpha]^{20}_D$ = –204.5 (*c* = 0.78, in CH_2Cl_2).

Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 0.5 mL/min, λ = 254 nm) retention time: t_{major} = 7.6 min, t_{minor} = 8.2 min.

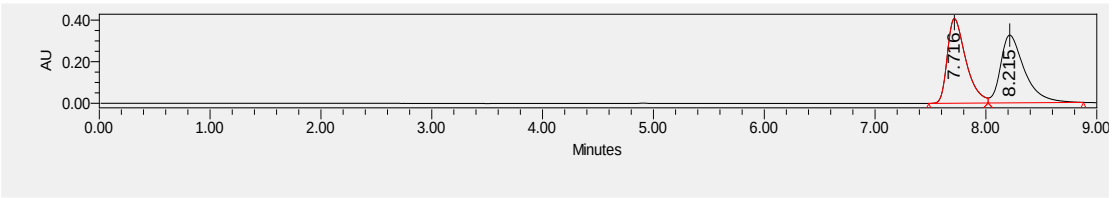
^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.88 (t, J = 8.0, 6.0 Hz, 1H), 7.31 (s, 1H), 6.74 (td, J = 8.0, 2.0 Hz, 1H), 5.98 (s, 1H), 5.39 (dtd, J = 16.0, 10.0, 8.0, 6.0 Hz, 1H), 5.04 (d, J = 16.0 Hz, 0H), 4.93 (d, J = 10.0 Hz, 1H), 3.24 (dd, J = 12.0, 8.0 Hz, 1H), 2.62 (dd, J = 16.0, 8.0 Hz, 1H), 1.63 (s, 9H), 1.53 (s, 9H).

^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.59, 165.40 (d, J = 250.5 Hz), 151.23, 130.74 (d, J = 11.1 Hz), 119.83, 119.68, 114.11 (d, J = 2.9 Hz), 109.98 (d, J = 22.6 Hz), 102.43, 102.13, 95.60, 83.86, 80.59, 46.29, 28.35, 28.17.

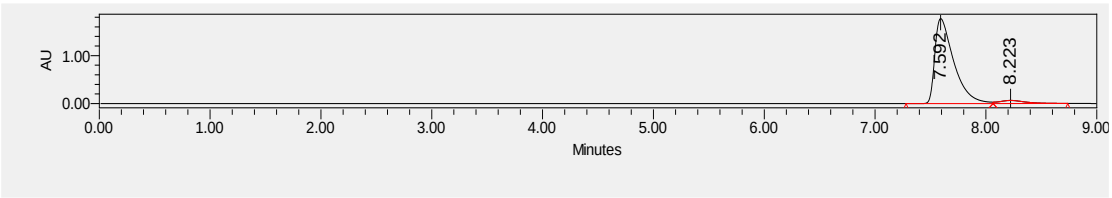
^{19}F NMR (377 MHz, Chloroform-d) δ = -104.82.

IR (neat): *v* (cm^{-1}) 3467, 2978, 2931, 1707, 1639, 1594, 1392, 1219, 1147, 993, 847, 818.

HRMS (ESI-FT) calcd for $C_{23}H_{28}FNO_5Na^+$ ([M]+Na^+) = 440.1844, found 440.1854.

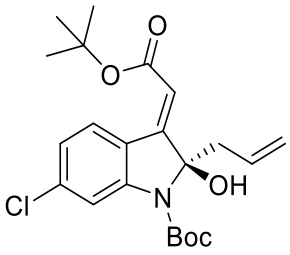


	Retention Time	Area	% Area
1	7.716	4748325	49.28
2	8.215	4887167	50.72



	Retention Time	Area	% Area
1	7.592	21043358	95.37
2	8.223	1021087	4.63

***Tert*-butyl (*R, E*)-2-allyl-3-(2-(*tert*-butoxy)-2-oxoethylidene)-6-chloro-2-hydroxyindoline-1-carboxylate (5ra)**



Viscous yellow oil; R_f = 0.45 (petroleum ether/ethyl acetate = 15/1, v/v), 99% yield, 95% *ee.* $[\alpha]^{20}_D$ = –170.5 (*c* = 0.89, in CH_2Cl_2).

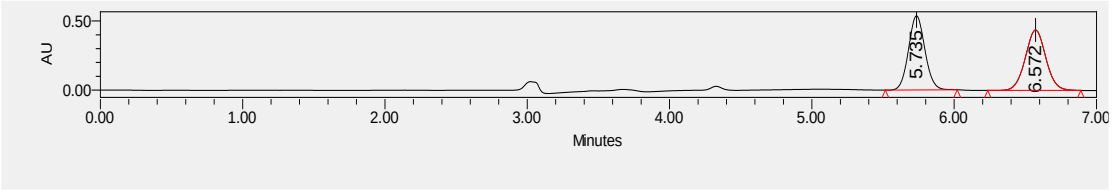
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **AD-H**, hexane/*i*PrOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 5.6 min, t_{minor} = 6.4 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.79 (d, *J* = 8.0 Hz, 1H), 7.64 (s, 1H), 7.01 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.02 (s, 1H), 5.44 – 5.32 (m, 1H), 5.04 (dd, *J* = 17.0, 1.8 Hz, 1H), 4.94 (dd, *J* = 10.0, 2.0 Hz, 1H), 3.22 (t, *J* = 12.0, 8.0 Hz, 1H), 2.62 (dd, *J* = 12.0, 6.0 Hz, 1H), 1.63 (s, 9H), 1.53 (s, 9H).

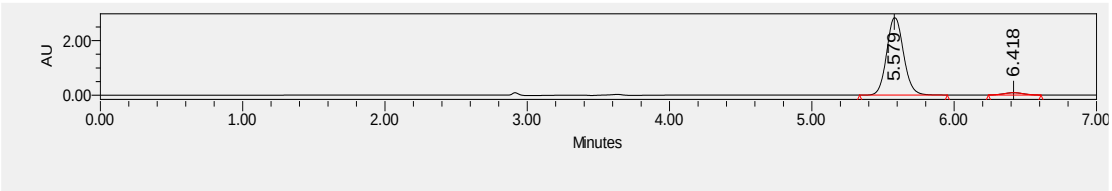
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.49, 151.09, 138.33, 130.65, 129.83, 123.14, 122.19, 119.85, 115.31, 114.84, 95.36, 83.94, 80.81, 46.40, 28.38, 28.21.

IR (neat): *v* (cm^{-1}) 3464, 3104, 2978, 2930, 1707, 1685, 1641, 1392, 1219, 1147, 993, 847, 818.

HRMS (ESI-FT) calcd for $C_{22}H_{28}{}^{34.9659}ClNO_5Na^+$ ([M]+Na^+) = 444.1548, found 444.1557; $C_{22}H_{28}{}^{36.9659}ClNO_5Na^+$ ([M]+Na^+) = 446.1519, found 446.1526.

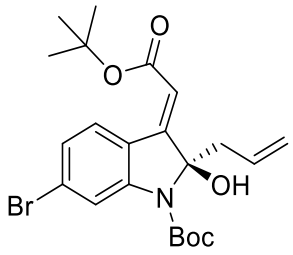


	Retention Time	Area	% Area
1	5.735	4302763	49.55
2	6.572	4380386	50.45



	Retention Time	Area	% Area
1	5.579	23312307	96.67
2	6.418	803654	3.33

***Tert*-butyl (*R, E*)-2-allyl-6-bromo-3-(2-(*tert*-butoxy)-2-oxoethylidene)-2-hydroxyindoline-1-carboxylate (5sa)**



Viscous yellow oil; R_f = 0.45 (petroleum ether/ethyl acetate = 15/1, v/v), 99% yield, 94% *ee.* $[\alpha]^{20}_D$ = –184.8 (*c* = 0.45, in CH_2Cl_2).

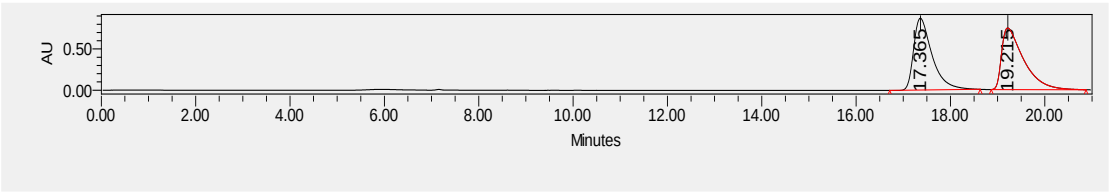
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 99/1, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 16.8 min, t_{minor} = 18.6 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.71 (d, J = 12.0 Hz, 1H), 7.82 (s, 1H), 7.16 (q, J = 4.0 Hz, 1H), 6.04 (s, 1H), 5.45 – 5.32 (m, 1H), 5.06 (dd, J = 8.0, 2.0 Hz, 1H), 4.94 (dd, J = 8.0, 2.0 Hz, 1H), 3.22 (dd, J = 12.0, 8.0 Hz, 1H), 2.66 – 2.58 (m, 1H), 1.63 (s, 9H), 1.53 (s, 9H).

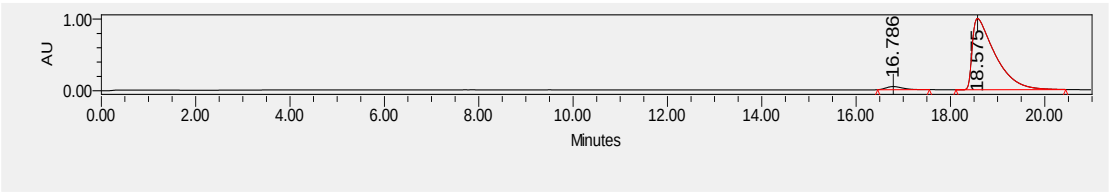
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 165.42, 151.09, 130.57, 129.94, 126.85, 126.01, 122.54, 119.83, 117.73, 115.50, 95.18, 83.90, 80.79, 46.35, 28.32, 28.15.

IR (neat): *v* (cm^{-1}) 3468, 2978, 2930, 1708, 1640, 1590, 1393, 1218, 1149, 992, 850, 820.

HRMS (ESI-FT) calcd for $C_{22}H_{28}{}^{80.9163}BrNO_5Na^+$ ([M]+Na^+) = 488.1043, found 488.1046; $C_{22}H_{28}{}^{78.7983}BrNO_5Na^+$ ([M]+Na^+) = 490.1023, found 490.1024.

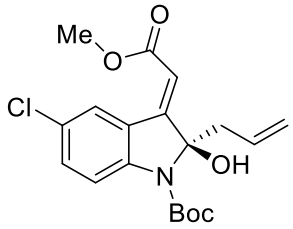


	Retention Time	Area	% Area
1	17.365	23707293	49.54
2	19.215	24151299	50.46



	Retention Time	Area	% Area
1	16.786	1044898	3.03
2	18.575	33489913	96.97

***Tert*-butyl (*R*,*E*)-2-allyl-5-chloro-2-hydroxy-3-(2-methoxy-2-oxoethylidene)indoline-1-carboxylate (5ua)**



Viscous yellow oil; R_f = 0.36 (petroleum ether/ethyl acetate = 8/1, v/v), 90% yield, 92% *ee.* $[\alpha]^{20}_D$ = –184.8 (*c* = 0.45, in CH_2Cl_2).

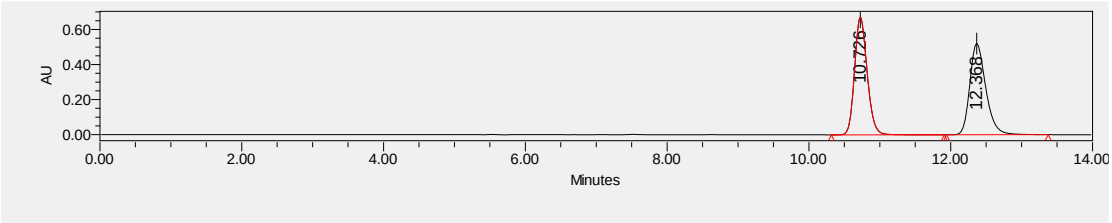
Dissolved in hexane for HPLC; **HPLC** (Chiralcel **IE**, hexane/*i*PrOH = 95/5, flow rate = 1.0 mL/min, λ = 254 nm) retention time: t_{major} = 11.3 min, t_{minor} = 13.1 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ = 8.89 (d, J = 4.0 Hz, 1H), 7.56 (s, 1H), 7.32 (dd, J = 8.0, 2.0 Hz, 1H), 6.12 (s, 1H), 5.37 (dtd, J = 16.0, 10.0, 8.0, 6.0 Hz, 1H), 5.03 (d, J = 16.0 Hz, 1H), 4.94 (d, J = 8.0 Hz, 1H), 3.81 (s, 3H), 3.20 (dd, J = 14.0, 8.0 Hz, 1H), 2.62 (dd, J = 14.0, 6.0 Hz, 1H), 1.63 (s, 9H).

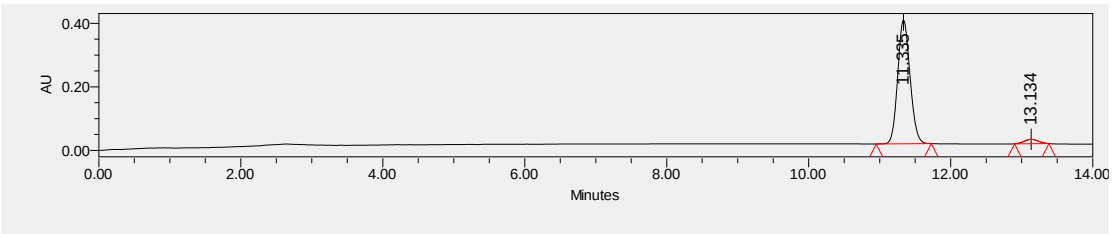
^{13}C{^{1}H} NMR (101 MHz, Chloroform-*d*) δ = 166.27, 152.54, 132.71, 130.39, 128.49, 128.12, 124.69, 120.03, 115.42, 113.56, 83.83, 51.77, 28.43.

IR (neat): *v* (cm^{-1}) 3463, 2924, 2954, 1719, 1640, 1685, 1468, 1394, 1171, 992, 866, 765.

HRMS (ESI-FT) calcd for $C_{19}H_{22}{}^{34.9659}ClNO_5Na^+$ ([M]+Na^+) = 402.1079, found 402.1080; $C_{19}H_{22}{}^{36.9659}ClNO_5Na^+$ ([M]+Na^+) = 404.1049, found 404.1048.



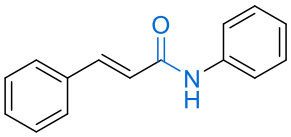
	Retention Time	Area	% Area
1	10.726	14652512	50.61
2	12.368	14298698	49.39



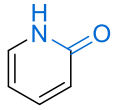
	Retention Time	Area	% Area
1	11.335	4693108	96.06
2	13.134	192325	3.94

8. Scope limitation

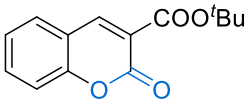
1). ketone compounds



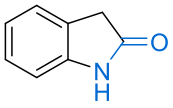
Procedure A, 80 °C
N. R.



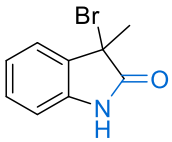
Procedure A, 80 °C
N. R.



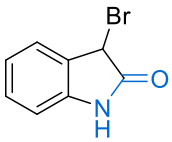
Procedure A, 80 °C
N. R.



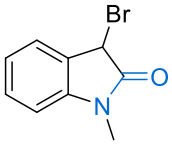
Procedure A, 80 °C
N. R.



Procedure A, 80 °C
N. R.



Procedure A, 80 °C
N. R.



Procedure A, 80 °C
N. R.

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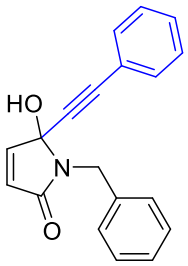
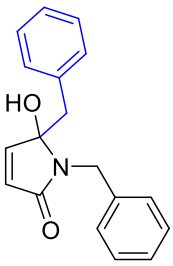
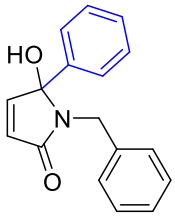
2). potassium borate compounds



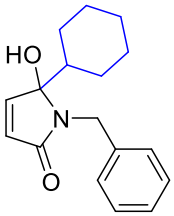
Procedure A, 110 °C
N. R.



Procedure A, 110 °C
N. R.



Procedure A, 80 °C
N. R.



Procedure A, 80 °C
N. R.

9. Computational details

All DFT calculations were performed with the Gaussian 09 software package.[4] The calculations were carried out with the B3LYP[5] and M06L[6] functionals and IEFPCM [7] solvation model. Based on the dielectric properties of the solvent (DME), we employed customized solvation parameters (eps=7.5, epsinf=1.9). The SDD[8] basis set was utilized for Indium atom in the calculations. Geometry optimization was performed using the def2-svp[9] basis set for all elements except indium while the single-point energy calculation was carried out using the def2-tzvp[9] basis set. To account for van der Waals forces, the DFT-D3[10] empirical correction was applied. Frequency calculations were performed at the same theoretical level. The Shermo program has been extensively employed for the computation of thermodynamic data.[11] Raise frequencies lower than a specific threshold to this value. The threshold is controlled by "ravib" parameter, which is 100 by default. The weak interaction analysis was conducted using the independent gradient model based on Hirshfeld partition (IGMH) within the framework of the Multiwfn software.[12] TD-DFT(time-dependent density functional theory) calculations were performed using Gaussian 09 at the B3LYP-D3/6-31G(d,p) level.

Table S22. The thermodynamic parameters set in the Shermo program. (ligand = **L_3-PiPr$_2$Br**)

Temperature	293.150 K
Pressure	1.000 atm
Scale factor of vibrational frequencies for ZPE	0.9610
Scale factor of vibrational frequencies for U(T)-U(0)	1.0003
Scale factor of vibrational frequencies for S(T)	1.0033
Scale factor of vibrational frequencies for CV	1.0000
Low frequencies treatment: Raising low frequencies	

Table S23. The thermodynamic parameters set in the Shermo program. (ligand = Otf)

Temperature	308.150 K
Pressure	1.000 atm
Scale factor of vibrational frequencies for ZPE	0.9610
Scale factor of vibrational frequencies for U(T)-U(0)	1.0003
Scale factor of vibrational frequencies for S(T)	1.0033
Scale factor of vibrational frequencies for CV	1.0000
Low frequencies treatment: Raising low frequencies	

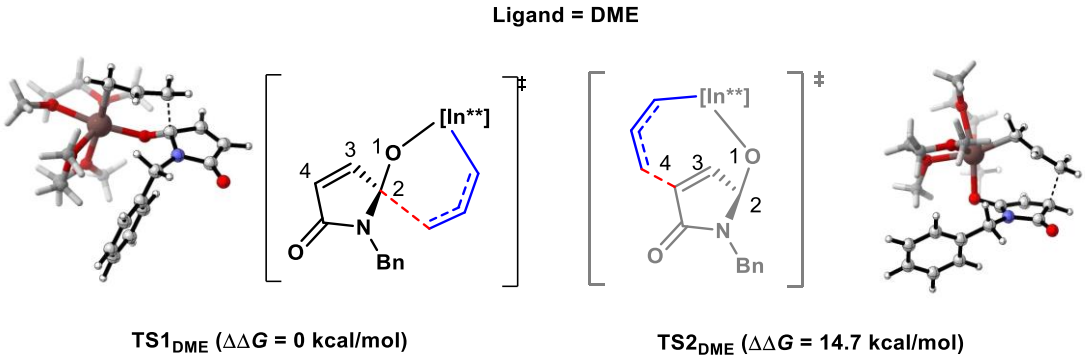


Figure S13 Calculated relative Gibbs free energy of chemical selective allylation of amides of **1a** and **2a** by In(III)/**DME** with B3LYP/def2-tzvp//B3LYP/def2-svp, SDD(In) level of theory. The free energy barriers ($\Delta\Delta G$) are given in kcal/mol.

From **Figure S11**, it can be observed that in the absence of a *N,N'*-dioxide ligand, i.e., when coordinated with DME solvent molecules, the allyl group still attacks the carbonyl carbon of the amide through a 1,2-addition pathway. This is because the eight-membered ring transition state **TS2$_{DME}$** formed by 1,4-addition exhibits a higher energy barrier ($\Delta\Delta G$ = 14.7 kcal/mol) compared to the six-membered ring transition state **TS1$_{DME}$** of the 1,2-addition, which is highly unfavorable kinetically.

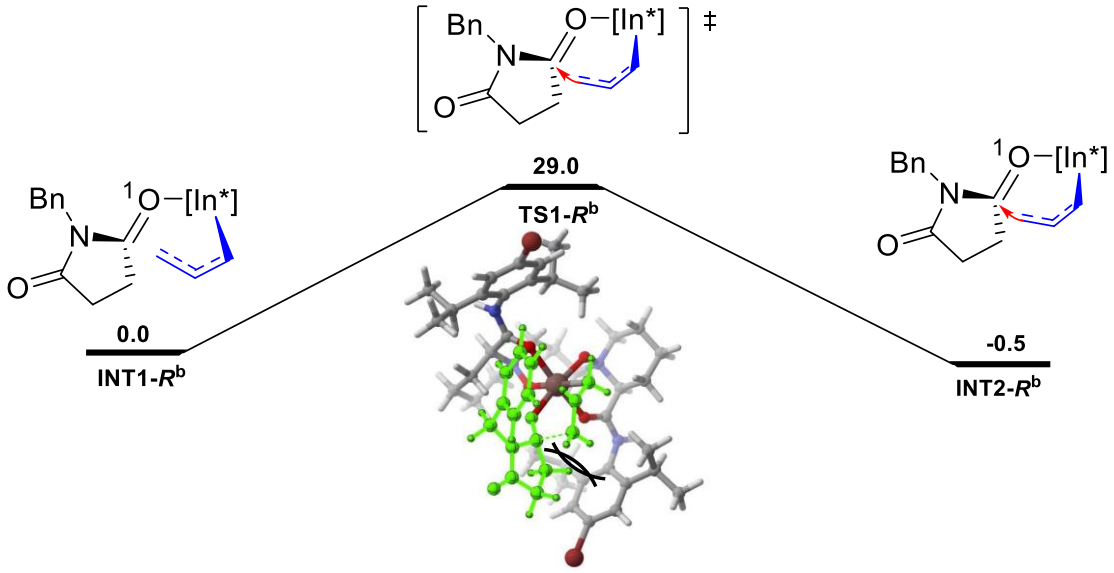


Figure S14 Calculated relative Gibbs free energy amides of *N*-benzylsuccinimide and **2a** by In(III)/ **L_3-PiPr$_2$Br** with B3LYP/def2-tzvp//B3LYP/def2-svp, SDD(In) level of theory. The free energy barriers (ΔG) are given in kcal/mol.

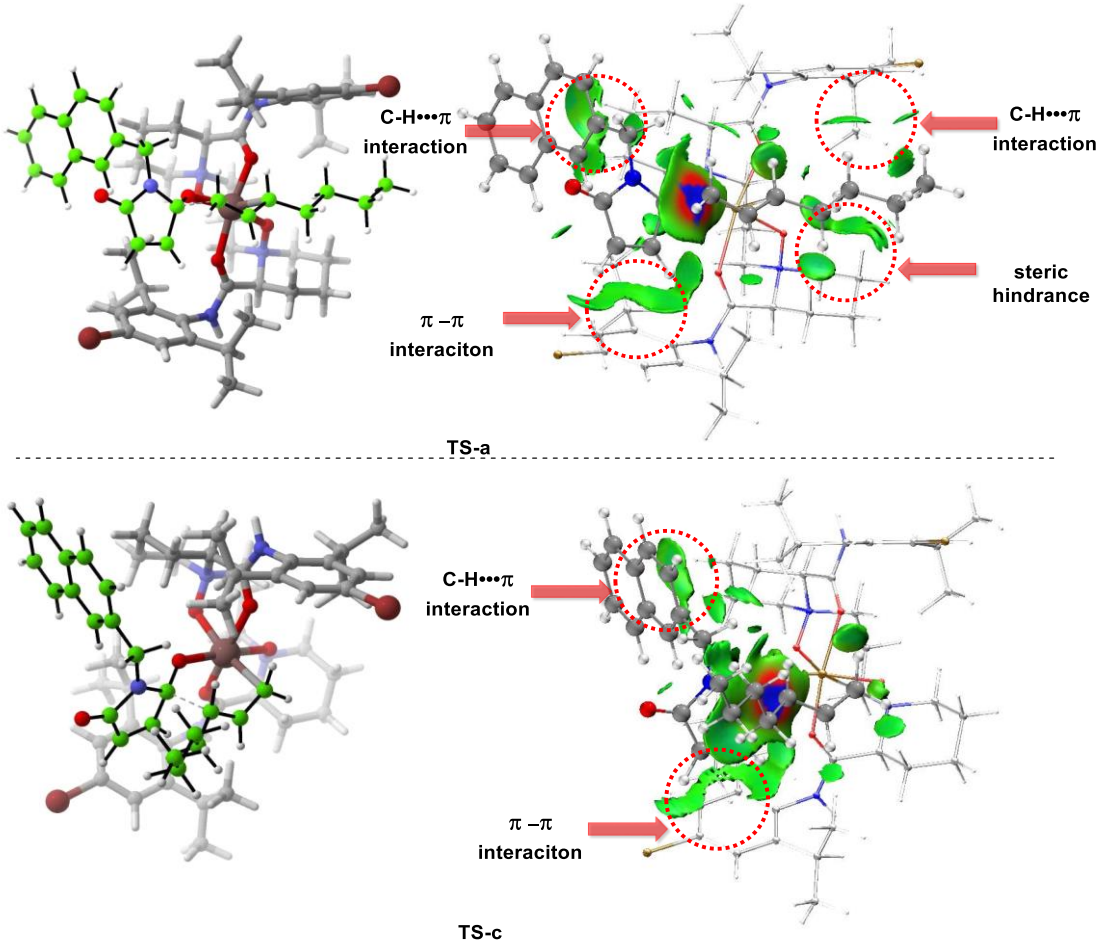


Figure S15 The weak analysis of the transition states **TS3** and **TS4**. (isovalue=0.005)

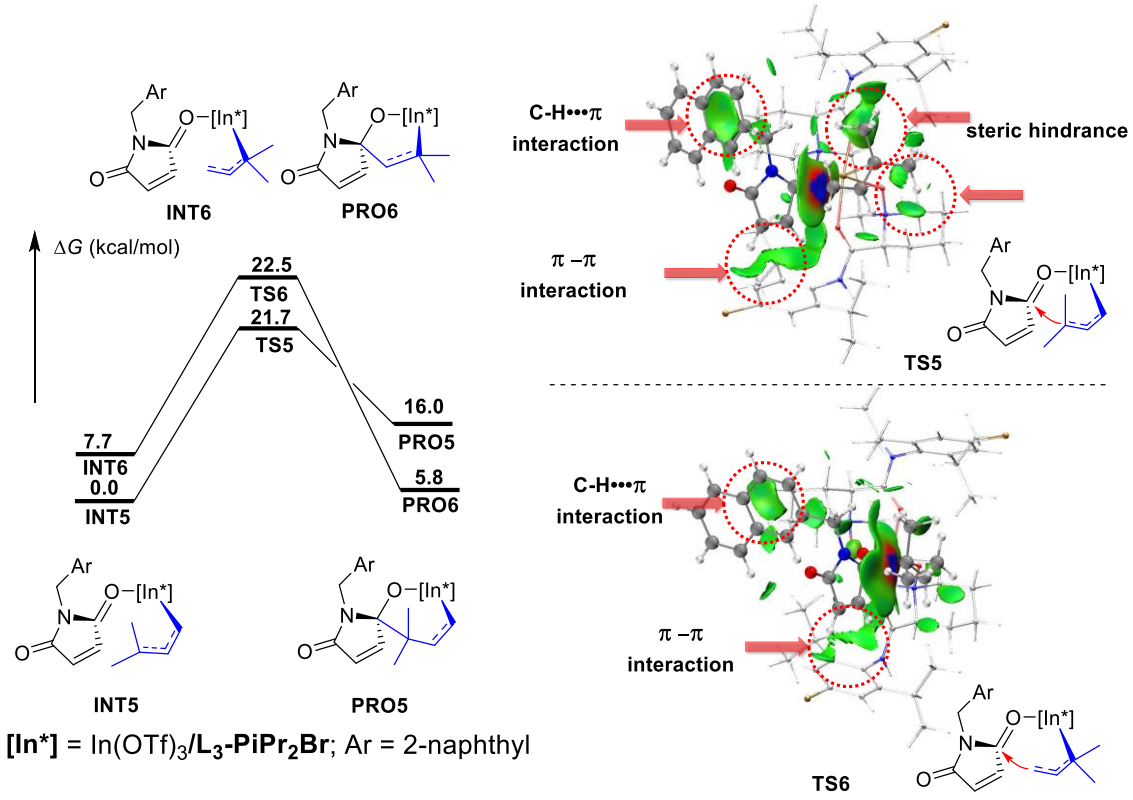


Figure S16 Calculated relative Gibbs free energy of chemical selective allylation of amides of 1n and 1f by In(III)/ L3-PiPr2Br with B3LYP/def2-tzvp//B3LYP/def2-svp, SDD(In) level of theory. The free energy barriers (ΔG) are given in kcal/mol.

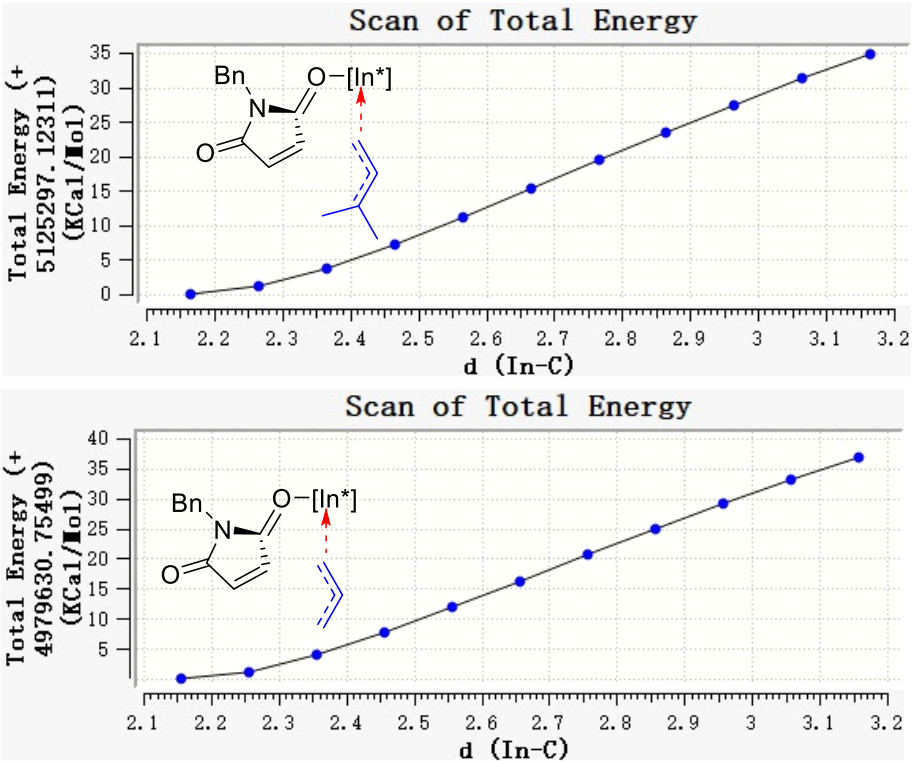


Figure S17 Energy scan diagram of the formation process of allylindium species.

As can be seen from Figure S15, the formation of the allylindium intermediate, which is also the process of the allyl anion gradually approaching the indium ion, is a barrierless process.

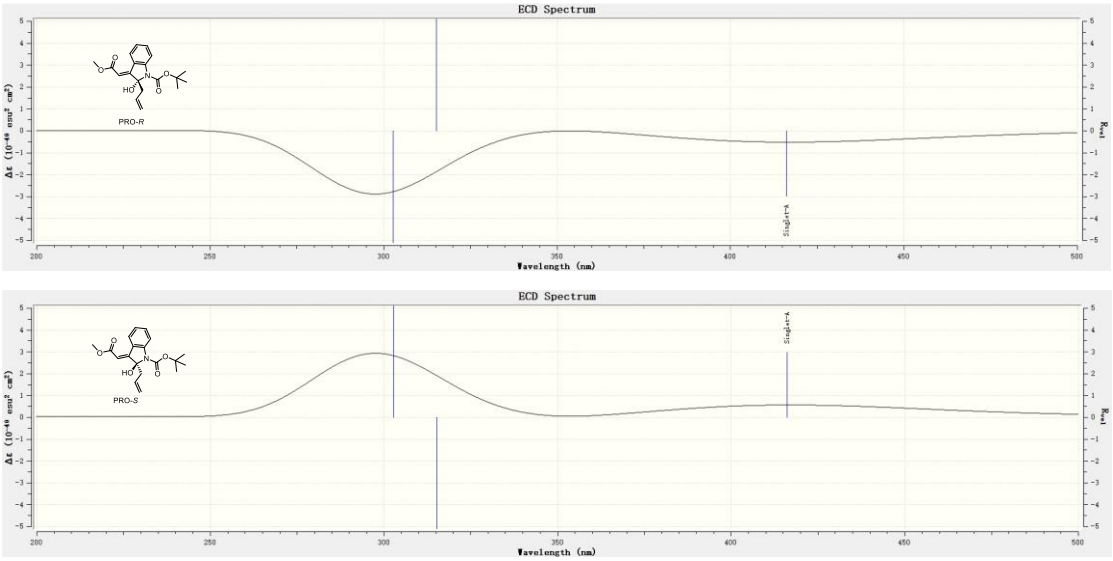


Figure S18 TD-DFT calculated ECD spectra for PRO-*R* (up) and PRO-*S* (down).

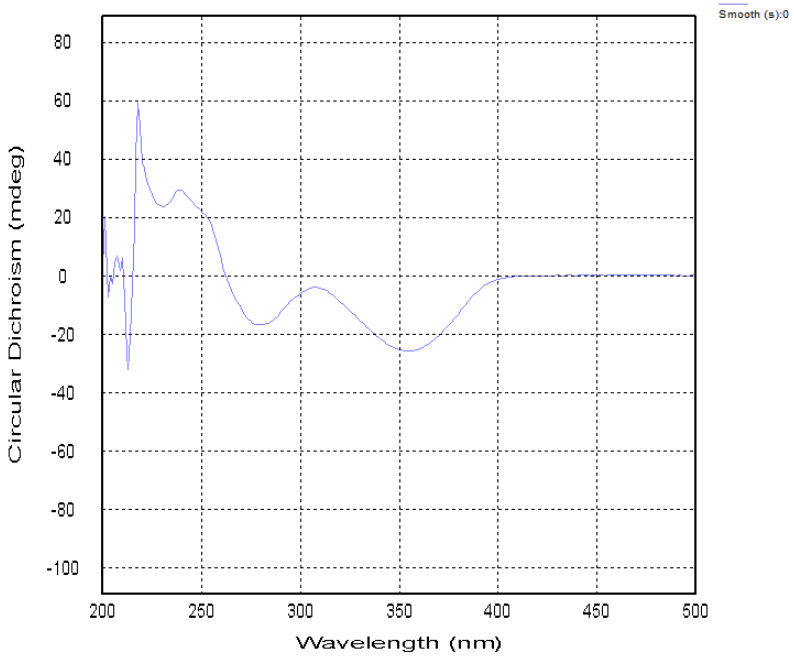


Figure S19 Experimental CD spectra for **5aa**.

Note: Comparison with simulated spectra of both enantiomers and experimental one led to the conclusion that the absolute configuration of **5aa** is *R*.

The Cartesian coordinates of key structures

INT1-R2

O	-2.32775800	-0.18624900	0.50795800
N	-4.11527200	0.94409100	1.24144200
C	-7.12572900	-1.89518200	2.23877000
H	-7.03911800	-2.31522300	3.25277200
H	-7.50015200	-2.70053500	1.58806800
H	-7.88407300	-1.09812600	2.26206300
O	0.02477700	0.08830100	1.93759200
N	-0.88260500	0.42138300	2.91895500
C	-4.72535800	-2.50456200	1.67819000
H	-3.74850900	-2.14801400	1.31845200
H	-5.06691200	-3.27696200	0.97048800
H	-4.59181100	-2.98626000	2.66140100
C	-5.76517300	-1.36639400	1.76695200
H	-5.41042200	-0.65634900	2.53321100
N	0.01306200	-3.37241800	2.23872800
O	-0.82504600	-2.69235400	1.39073400
O	1.67632100	-1.81492800	0.41511500
N	3.43616400	-3.10469000	0.94754700
C	-4.47585800	3.57870000	-0.69543700
H	-3.73258900	4.38638700	-0.78812800
H	-4.71355600	3.46269800	0.37376600
H	-5.39905500	3.90110300	-1.20135400
C	-3.94093600	2.27571500	-1.31886100
H	-2.99294300	2.02403700	-0.81337300
C	-3.59247400	2.48999500	-2.79667300
H	-3.20296300	1.57043400	-3.26060300
H	-2.82701700	3.27470200	-2.89088800
H	-4.46170700	2.82626500	-3.38212200
H	3.76494500	-3.96934300	1.36933900
C	-4.90090500	1.11168800	-1.07816100
H	-4.50024500	1.58656100	1.92935700
C	-5.74876000	0.64208500	-2.08677800
H	-5.74010500	1.09813300	-3.07536100
C	-6.62174500	-0.42205700	-1.84010600
C	-6.65904700	-1.05325300	-0.59625100
H	-7.33809000	-1.89134000	-0.44261400
C	-5.82185800	-0.61862400	0.43893200
C	-4.97472200	0.47463600	0.17922900
C	-2.83022400	0.61056500	1.31962500
C	-2.00361500	1.32768600	2.37631300
H	-2.64022500	1.55075600	3.24687400
C	-1.43595400	2.63915500	1.81601300
H	-0.75805500	2.40945100	0.97928300
H	-2.27424900	3.22293300	1.40707300
C	-0.70421800	3.40367900	2.91688300
H	-0.30324500	4.34374600	2.52388200
H	-1.41158300	3.67050400	3.72275300
C	0.41897800	2.53009800	3.46218400
H	1.15883700	2.34305100	2.67224500
H	0.94649800	3.02514200	4.29201100
C	-0.10821600	1.20188700	3.97974900
H	-0.79143300	1.34202600	4.83221800
H	0.71254400	0.54068400	4.27662300
C	-1.52087300	-0.81148400	3.54717000
H	-2.08330700	-1.31075700	2.75390200
H	-2.22406200	-0.44151600	4.30737900
C	-0.56133000	-1.80239100	4.20666000
H	-1.19967600	-2.55704000	4.69109100
H	-0.02837300	-1.32360200	5.04227800
C	0.51774300	-2.47674200	3.35985500
H	1.13906900	-1.71187100	2.88398400
H	1.14437400	-3.10813500	4.00698500
C	-0.79151500	-4.54168600	2.80261400
H	-0.14338700	-5.06249200	3.52508900
H	-1.63468300	-4.08722800	3.33295100
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H	-0.49522500	-6.61108000	0.02622800
H	0.49966100	-6.68887800	1.48531600
C	0.74617000	-4.86704500	0.34056000
H	1.63881500	-5.24887500	-0.17736200
H	0.18742900	-4.25503100	-0.38180600
C	1.22040000	-3.95410300	1.48161400
H	1.77593300	-4.54596700	2.22538200
C	2.12485700	-2.85554300	0.92938400
C	4.39397700	-2.26033300	0.27291900
C	4.89506900	-2.69753800	-0.97395400
C	5.76641800	-1.84624100	-1.66170600
H	6.17240200	-2.13870200	-2.62931700
C	6.10983300	-0.60464200	-1.12070300
C	5.62819800	-0.20338900	0.12425000
H	5.92869800	0.76391000	0.52815000
C	4.75842900	-1.02853700	0.84996100
C	4.25088600	-0.56055100	2.20757600
H	3.59621900	-1.34756200	2.61430100
C	3.40790700	0.72001200	2.08519000

H	4.00776800	1.55595300	1.69125500
H	3.04197900	1.02445900	3.07825600
H	2.53560100	0.57618000	1.43265400
C	5.41095000	-0.37999400	3.20257600
H	6.00609600	-1.30065400	3.30144500
H	5.02587900	-0.11134800	4.19905300
H	6.09226700	0.42434000	2.88422300
C	4.43919900	-4.01424000	-1.59529400
H	4.22401000	-4.71635200	-0.77096000
C	3.12685100	-3.79656700	-2.37342500
H	3.29725000	-3.12458600	-3.22937500
H	2.34695100	-3.33618900	-1.74951900
H	2.73819400	-4.74958200	-2.76520400
C	5.49858200	-4.68265500	-2.48063300
H	6.45943300	-4.78894200	-1.95509600
H	5.67591500	-4.11458000	-3.40697100
H	5.15929500	-5.68555100	-2.78054000
C	-1.28043500	-5.46491000	1.69780600
H	-1.97983400	-4.90499700	1.05995600
H	-1.84749800	-6.28088400	2.17193100
Br	-7.76384100	-1.02827800	-3.22935600
Br	7.22342500	0.56920400	-2.11618700
In	-0.35322800	-1.00769700	0.12863900
C	2.58353600	2.16563800	-3.19917100
C	3.39841400	0.96976300	-2.80480200
C	2.71506600	0.27860600	-1.88003300
C	1.44544000	1.01093500	-1.59402400
N	1.40452900	2.10593100	-2.39494200
H	4.37445100	0.76107900	-3.24063300
H	2.98319300	-0.63669400	-1.36013300
O	0.59187900	0.75778900	-0.72785900
O	2.80598100	3.01896600	-4.01002400
C	0.34089800	3.08905200	-2.42828500
H	0.42703500	3.60906500	-3.39524200
H	-0.61987700	2.55015800	-2.42536900
C	-0.02094200	-0.53645700	-3.77440000
C	-0.02667800	-1.56116800	-2.90453000
H	0.73543200	-0.45325200	-4.55864200
H	-0.79936800	0.23421500	-3.75013700
H	0.77025000	-2.30919500	-2.99987100
C	-0.99119600	-1.76197300	-1.79456400
H	-1.93878500	-1.22804100	-1.97715400
H	-1.24078400	-2.82804300	-1.65844500
C	0.38375200	4.09313400	-1.29319300
C	1.37662600	4.09468800	-0.33588100
C	-0.64033600	5.08093000	-1.23647500
C	1.39752800	5.05824900	0.71051100
H	2.17935800	3.35461200	-0.36496300
C	-0.64703700	6.03359100	-0.24191200
H	-1.41691500	5.09405400	-2.00625700
C	2.39666000	5.05146900	1.72289900
C	0.36388100	6.05237700	0.76131300
H	-1.43063900	6.79532500	-0.21668600
C	2.37136100	5.98043100	2.74360600
H	3.18902700	4.29890900	1.67856300
C	0.37160200	7.00231700	1.82013100
C	1.35054000	6.96459800	2.79270500
H	3.14672700	5.97066700	3.51347100
H	-0.41069900	7.76502100	1.85275400
H	1.34880000	7.70048300	3.60003500

TS1-R2

O	-2.27492800	-0.12149100	0.51360100
N	-4.12290200	0.93768400	1.18845500
C	-6.94846200	-2.06983500	2.13500400
H	-6.84399800	-2.50502600	3.14099600
H	-7.31063600	-2.87169000	1.47323100
H	-7.72429400	-1.29070900	2.17806900
O	0.01267100	0.21311600	2.07972300
N	-0.95777600	0.52590200	3.00680800
C	-4.53528800	-2.61029800	1.55198600
H	-3.56901200	-2.22400300	1.19498400
H	-4.86066400	-3.38425200	0.83814600
H	-4.38407100	-3.10028800	2.52886600
C	-5.60435900	-1.50140400	1.66072100
H	-5.26296200	-0.79118100	2.43246200
N	-0.02102200	-3.26031200	2.28167300
O	-0.82067500	-2.56628100	1.40157400
O	1.66542000	-1.76031400	0.44557500
N	3.42283700	-3.02489200	1.02032800
C	-4.59287600	3.55430300	-0.70626200
H	-3.89410900	4.40157600	-0.78881900
H	-4.81601500	3.40779400	0.36222900
H	-5.53558400	3.83615800	-1.20023800
C	-3.99192100	2.29590800	-1.36065500
H	-3.02649800	2.08596900	-0.86720100
C	-3.67093200	2.56630500	-2.83532800
H	-3.23431300	1.68335200	-3.32759200

H	-2.95199800	3.39413900	-2.91527400
H	-4.56478600	2.86586800	-3.40347700
H	3.75671100	-3.87494900	1.46751600
C	-4.87952900	1.07102400	-1.14330200
H	-4.55592200	1.57166700	1.85562500
C	-5.67492100	0.55012000	-2.16964100
H	-5.68543200	1.01654300	-3.15328900
C	-6.46874300	-0.58001700	-1.94847000
C	-6.47629300	-1.22705000	-0.71238600
H	-7.09092500	-2.11686100	-0.57833500
C	-5.69224000	-0.74097400	0.34157400
C	-4.92772000	0.41683900	0.10685500
C	-2.83096400	0.65960300	1.31135100
C	-2.06810500	1.40301700	2.39639600
H	-2.75161100	1.62046900	3.23209400
C	-1.49680400	2.72035600	1.85137600
H	-0.77192800	2.49992400	1.05167000
H	-2.32416200	3.28354500	1.39363100
C	-0.84113600	3.50865500	2.98358700
H	-0.43406100	4.45090600	2.60239700
H	-1.59798800	3.77228600	3.74458800
C	0.26432200	2.66301000	3.60427200
H	1.05168400	2.48068300	2.86078600
H	0.73386400	3.17849600	4.45608600
C	-0.26657300	1.33177500	4.10716500
H	-1.00621800	1.46503900	4.91226700
H	0.54640600	0.68999700	4.46255200
C	-1.58935600	-0.72566500	3.60043900
H	-2.12800700	-1.22358000	2.78930300
H	-2.31518300	-0.38079400	4.35094500
C	-0.62182700	-1.70780600	4.26215500
H	-1.25278300	-2.46751500	4.74807900
H	-0.09365800	-1.22312300	5.09723600
C	0.46639600	-2.37551400	3.42060900
H	1.10225300	-1.60978000	2.96552600
H	1.07859000	-3.01761800	4.07069000
C	-0.87253500	-4.40573000	2.82475000
H	-0.26450800	-4.92830500	3.57992900
H	-1.72673700	-3.92625300	3.31336400
C	-0.15235900	-5.92321000	0.95029000
H	-0.50206500	-6.53535200	0.10577600
H	0.42910000	-6.59452100	1.60663400
C	0.75134400	-4.80331300	0.43333200
H	1.65607300	-5.20994200	-0.04241400
H	0.23118700	-4.19927800	-0.32300900
C	1.19990900	-3.86650500	1.56562800
H	1.73688700	-4.44177900	2.33530000
C	2.11412900	-2.78432200	0.99635400
C	4.37829100	-2.20737100	0.30543800
C	4.92167100	-2.73197200	-0.88921700
C	5.81090800	-1.92909500	-1.60985900
H	6.25017900	-2.28914400	-2.53922100
C	6.12921800	-0.64702700	-1.15397200
C	5.59066700	-0.15247300	0.03228300
H	5.86208200	0.84987600	0.36440600
C	4.69915600	-0.92468900	0.78882300
C	4.12783000	-0.34229000	2.07497700
H	3.41903100	-1.07185500	2.49715400
C	3.34824500	0.95637300	1.80806200
H	4.01289000	1.74399500	1.42041200
H	2.91073500	1.33081900	2.74563800
H	2.53352900	0.81154500	1.08514200
C	5.23369700	-0.13018100	3.12428200
H	5.77690900	-1.06425400	3.33515100
H	4.80419000	0.23914900	4.06920900
H	5.97096800	0.61317700	2.78329400
C	4.48158000	-4.08782400	-1.43370400
H	4.24930200	-4.73985000	-0.57314600
C	3.18471700	-3.91897000	-2.25046600
H	3.37402300	-3.29881000	-3.14090700
H	2.39605200	-3.42088400	-1.66657400
H	2.80165500	-4.89394800	-2.59088000
C	5.55643600	-4.81018100	-2.25547800
H	6.50640200	-4.88285100	-1.70522100
H	5.75292300	-4.29989600	-3.21095700
H	5.22253300	-5.83002000	-2.49927600
C	-1.33624200	-5.33716700	1.71717700
H	-1.99781100	-4.77498100	1.04176600
H	-1.94032200	-6.13163600	2.18191500
Br	-7.53864500	-1.25558000	-3.36255400
Br	7.28388600	0.44997400	-2.18632600
In	-0.27768800	-0.83675000	0.25344300
C	2.51677700	2.22671800	-3.14083400
C	3.34971700	1.04734000	-2.74775200
C	2.60385600	0.21904000	-2.00445900
C	1.20710700	0.77575100	-1.88363800
N	1.25987500	2.01370900	-2.55182000
H	4.39426700	0.94993500	-3.04116200

H	2.89074800	-0.71774700	-1.53169900
O	0.53144300	0.72451800	-0.76605800
O	2.81375700	3.19082500	-3.80248900
C	0.20810400	3.00011200	-2.55549800
H	0.28768100	3.55706500	-3.50325700
H	-0.76296000	2.47944500	-2.56223300
C	0.22421900	-0.31633500	-3.20811900
C	-0.01013800	-1.56647600	-2.60471700
H	0.91525000	-0.28314800	-4.05264000
H	-0.64345900	0.34597200	-3.29675700
H	0.75687300	-2.33917900	-2.74273700
C	-1.04513600	-1.82686200	-1.69084100
H	-1.96055600	-1.22510100	-1.77269300
H	-1.22737100	-2.86617900	-1.39453700
C	0.25476200	3.98445300	-1.40097000
C	1.21693000	3.92303500	-0.41490600
C	-0.71159300	5.02952700	-1.36530000
C	1.27110000	4.88830800	0.62826200
H	1.96255300	3.12652200	-0.42728700
C	-0.69308000	5.97849700	-0.36687500
H	-1.46025400	5.09505400	-2.15994600
C	2.25623400	4.83734700	1.65375400
C	0.29667900	5.94199600	0.65632000
H	-1.43075600	6.78529700	-0.36037800
C	2.27358000	5.77747100	2.66436500
H	3.00506900	4.04163200	1.62446600
C	0.34632500	6.90105100	1.70631600
C	1.30989000	6.81867800	2.69171900
H	3.04023400	5.73320000	3.44186400
H	-0.39020700	7.70870900	1.72024400
H	1.34166900	7.56349100	3.49025700

INT2-R2

O	-2.19252500	-0.02850900	0.54889000
N	-4.09678200	0.98634600	1.12077900
C	-6.85797700	-2.04227600	2.13952500
H	-6.77615100	-2.42144700	3.17002200
H	-7.18678800	-2.88428300	1.51111900
H	-7.64784700	-1.27657200	2.11849800
O	0.02633400	0.41844600	2.25305500
N	-1.01637800	0.72192300	3.10292700
C	-4.41777100	-2.56400900	1.65738900
H	-3.44790000	-2.17642000	1.31154900
H	-4.70563700	-3.38110400	0.97612000
H	-4.29019500	-3.00002400	2.66305000
C	-5.51052900	-1.47397700	1.67424900
H	-5.20599800	-0.71657000	2.41578300
N	-0.08256500	-3.08437600	2.35020900
O	-0.82823200	-2.35523600	1.44417400
O	1.67969000	-1.66650700	0.55900000
N	3.38896600	-2.99470500	1.11919500
C	-4.56731000	3.47958900	-0.87859400
H	-3.89182500	4.34169300	-0.99228400
H	-4.78117400	3.36414000	0.19526200
H	-5.51936600	3.71960400	-1.37670100
C	-3.93256000	2.21998800	-1.49900100
H	-2.95541100	2.05347100	-1.01020500
C	-3.63952200	2.46206200	-2.98421600
H	-3.16931300	1.58720200	-3.45933800
H	-2.95844300	3.31684600	-3.09438200
H	-4.55280700	2.70678500	-3.54779000
H	3.69617000	-3.86045800	1.55568100
C	-4.77749800	0.97232300	-1.24150800
H	-4.57788600	1.62564000	1.74896100
C	-5.51086300	0.35986900	-2.26409100
H	-5.50518600	0.77145800	-3.27168400
C	-6.26369100	-0.79137500	-2.00993700
C	-6.29389100	-1.36806500	-0.74007800
H	-6.87739000	-2.27401800	-0.57749700
C	-5.57222500	-0.79044600	0.31221500
C	-4.84439700	0.38297600	0.04010500
C	-2.80349900	0.75987000	1.30239700
C	-2.10717000	1.55520700	2.39690400
H	-2.83724300	1.78947100	3.18733800
C	-1.52246500	2.86068500	1.83544300
H	-0.75755500	2.62647800	1.07792100
H	-2.33172200	3.39632700	1.31597300
C	-0.93509300	3.69978900	2.96924800
H	-0.50482500	4.62351600	2.56758300
H	-1.73819000	3.99820800	3.66746800
C	0.13062700	2.89336600	3.70344700
H	0.97438900	2.69147400	3.02948100
H	0.52981500	3.45072300	4.56476400
C	-0.42290900	1.57789500	4.22379800
H	-1.22696900	1.73233600	4.96018000
H	0.36477200	0.96072300	4.66912900
C	-1.63822200	-0.54167400	3.67979500
H	-2.16658600	-1.03998900	2.86206400

H	-2.37475100	-0.21105100	4.42603000
C	-0.66396800	-1.52003300	4.34064700
H	-1.29308400	-2.26556100	4.85052500
H	-0.11788500	-1.02449500	5.15780200
C	0.41086300	-2.21854800	3.50312500
H	1.08380600	-1.47453200	3.06645800
H	0.99131200	-2.88415600	4.15853300
C	-1.00475800	-4.18381500	2.87160500
H	-0.44332900	-4.72907000	3.64635200
H	-1.84839900	-3.66103700	3.33307000
C	-0.30601400	-5.74535300	1.02555300
H	-0.66079400	-6.34509000	0.17429800
H	0.22511600	-6.43975600	1.70002900
C	0.66282000	-4.67210300	0.52905100
H	1.55844800	-5.12334300	0.07758200
H	0.19282300	-4.04556800	-0.24202100
C	1.12829700	-3.75040600	1.66696800
H	1.62230600	-4.34169000	2.45290700
C	2.09237500	-2.71020200	1.10501700
C	4.36539500	-2.21565100	0.38635400
C	4.92565700	-2.80347400	-0.77051800
C	5.83327900	-2.04403900	-1.51402400
H	6.28456200	-2.45236400	-2.41727200
C	6.15062600	-0.74141000	-1.11980600
C	5.59193300	-0.18361500	0.02850300
H	5.86019300	0.83459300	0.31105500
C	4.68246100	-0.91021400	0.80789400
C	4.08722600	-0.25068000	2.04536700
H	3.35255800	-0.94269200	2.48555600
C	3.34341200	1.04682800	1.68311800
H	4.04862800	1.82170700	1.34494500
H	2.81732400	1.44281800	2.56457100
H	2.60770300	0.89653700	0.88055500
C	5.16438500	-0.00272600	3.11601600
H	5.67381900	-0.93568800	3.40286300
H	4.71539000	0.43743900	4.02080900
H	5.93273700	0.69779100	2.75390100
C	4.47663300	-4.17633400	-1.26326400
H	4.21470200	-4.78859600	-0.38162100
C	3.20208200	-4.02297800	-2.11781300
H	3.42111400	-3.44374500	-3.02833000
H	2.40803800	-3.48731800	-1.57476800
H	2.81015300	-5.00551100	-2.42496200
C	5.55770500	-4.95123800	-2.02716000
H	6.49354100	-5.01355000	-1.45203600
H	5.78401000	-4.48655900	-2.99902200
H	5.21282800	-5.97564700	-2.23380100
C	-1.48115000	-5.10033000	1.75727700
H	-2.10027100	-4.51403000	1.06262300
H	-2.13337900	-5.86233100	2.21111700
Br	-7.24483900	-1.59145000	-3.42261400
Br	7.32422200	0.29680900	-2.18830000
In	-0.16379400	-0.60657400	0.43874900
C	2.50314900	2.06853600	-3.15045000
C	3.26729300	0.84428700	-2.74569400
C	2.43849000	-0.00122800	-2.12791200
C	1.01756900	0.56517800	-2.08243000
N	1.19366100	1.84668300	-2.74121000
H	4.33611800	0.74226800	-2.93063500
H	2.68824700	-0.96006000	-1.67617000
O	0.53142600	0.74277700	-0.79028200
O	2.90722000	3.06521600	-3.70363400
C	0.19119200	2.88026300	-2.79719500
H	0.35210400	3.44307900	-3.73191800
H	-0.80297400	2.41438600	-2.87520500
C	0.01647200	-0.31892200	-2.91257100
C	-0.26369900	-1.64162800	-2.27550200
H	0.44193100	-0.46849000	-3.91692500
H	-0.91975200	0.25184900	-3.01105600
H	0.55262900	-2.37550000	-2.29496600
C	-1.42575700	-1.98182900	-1.67683000
H	-2.29026300	-1.30891800	-1.67795100
H	-1.58431200	-2.97530000	-1.24830900
C	0.19891300	3.87259000	-1.64531400
C	1.12050200	3.81857000	-0.62085800
C	-0.75073600	4.93381300	-1.66560400
C	1.15677900	4.81252700	0.39598700
H	1.84254700	3.00288200	-0.58571600
C	-0.75686400	5.90509800	-0.68825700
H	-1.46539500	4.99646400	-2.49139200
C	2.12046200	4.78618800	1.44340400
C	0.20024800	5.88274700	0.36564600
H	-1.48127700	6.72302900	-0.72815700
C	2.13956400	5.76770800	2.41413000
H	2.85724900	3.97933300	1.45715400
C	0.24714800	6.88129600	1.37878300
C	1.19406900	6.82553000	2.38250300
H	2.89421600	5.74351100	3.20425800

H	-0.47454200	7.70184300	1.34591200
H	1.22691600	7.60365800	3.14862500

INT1-S2

O	-1.10095200	1.71619400	-0.19442000
N	-2.69055100	3.30967500	-0.20950300
C	-5.52881600	2.33228500	2.78161200
H	-5.26465000	2.67607700	3.79377300
H	-6.06721100	1.37872100	2.89531000
H	-6.22303900	3.06387000	2.34174000
O	1.45792400	2.60566100	0.68628900
N	0.66538200	3.59822200	1.20336800
C	-3.32765800	1.10456900	2.53340700
H	-2.42379200	0.94515200	1.92705600
H	-3.85276700	0.14072400	2.60393500
H	-3.02501800	1.39463000	3.55408500
C	-4.26180500	2.17104400	1.92998900
H	-3.72541300	3.13436300	1.96421600
N	0.95987600	0.10406600	3.00677900
O	0.17533200	0.26612000	1.88800400
O	2.66161000	-0.20119900	0.70514300
N	4.21328800	-1.21423900	1.97261100
C	-4.00131000	3.36411400	-4.19945000
H	-3.35065900	3.89750300	-4.90938400
H	-4.76502800	4.06845000	-3.83642600
H	-4.51454900	2.57144300	-4.76544500
C	-3.16618100	2.79071200	-3.04441500
H	-2.60810500	3.63281500	-2.60373300
C	-2.12682100	1.77726300	-3.56289800
H	-1.50097600	1.38015100	-2.75055600
H	-1.46680000	2.24994700	-4.30726200
H	-2.62415800	0.92677300	-4.05579700
H	4.42836900	-1.67944200	2.85080500
C	-4.02468900	2.18405200	-1.93824000
H	-2.90285200	4.29595300	-0.07917500
C	-5.09189400	1.33474900	-2.25741800
H	-5.32986400	1.12187400	-3.29975600
C	-5.86539900	0.75915100	-1.24784400
C	-5.60336700	1.01798200	0.09981700
H	-6.22650500	0.55290400	0.86276000
C	-4.55613000	1.87120700	0.46257700
C	-3.77570900	2.42846000	-0.57291400
C	-1.42842100	2.91067700	-0.06178200
C	-0.41476100	4.02646100	0.19523200
H	-0.93161800	4.87634000	0.66741900
C	0.23041300	4.48390200	-1.12098000
H	0.75606100	3.62972600	-1.56931100
H	-0.57966600	4.76847400	-1.81006400
C	1.19254900	5.65058000	-0.88965600
H	1.68518600	5.91769400	-1.83624400
H	0.62469500	6.54116800	-0.56666700
C	2.23125400	5.27878200	0.16780100
H	2.89138300	4.48237400	-0.20397200
H	2.86643000	6.14195500	0.42029000
C	1.57400600	4.80000300	1.45275700
H	0.95607600	5.58287200	1.91995200
H	2.32420600	4.45339400	2.17144200
C	-0.00699200	3.15953200	2.49534600
H	-0.72628600	2.38281200	2.22322300
H	-0.55016500	4.03585100	2.87861100
C	0.92605000	2.63130800	3.58575800
H	0.29588900	2.50639200	4.47978500
H	1.65675600	3.40212400	3.87579000
C	1.74835900	1.36664500	3.33058800
H	2.42315500	1.53331300	2.48690400
H	2.33957400	1.13891100	4.22973500
C	0.01212400	-0.23898700	4.15081800
H	0.62218900	-0.30836600	5.06502300
H	-0.67068300	0.61278100	4.23328900
C	0.17140000	-2.70444700	3.61829600
H	-0.41452800	-3.58943800	3.32877400
H	0.70944600	-2.96859500	4.54594000
C	1.17638500	-2.36474700	2.51593700
H	1.91861700	-3.16809400	2.39130000
H	0.67052800	-2.23134900	1.54935400
C	1.94091000	-1.07410900	2.84388900
H	2.44227600	-1.17267100	3.81910900
C	2.97290300	-0.77519400	1.76316100
C	5.23721300	-1.14010600	0.95598600
C	5.54737800	-2.31919700	0.24485900
C	6.49339700	-2.23261700	-0.78071300
H	6.76573300	-3.11581200	-1.35710300
C	7.09164300	-1.00649900	-1.08604100
C	6.78342300	0.14364900	-0.35945300
H	7.28078800	1.08193600	-0.60768700
C	5.85168700	0.09703100	0.68605300
C	5.55967100	1.36172700	1.48510300
H	4.84664300	1.09906200	2.28318900

C	4.89746500	2.44184700	0.61348100
H	5.56916600	2.76526100	-0.19703800
H	4.66363300	3.33130400	1.22128100
H	3.96252600	2.07965400	0.16562700
C	6.82772100	1.89331900	2.17589800
H	7.29558400	1.12381100	2.80883400
H	6.58643600	2.76069500	2.81085200
H	7.57866200	2.22209600	1.44099200
C	4.82202900	-3.62915200	0.53732800
H	4.56788500	-3.63834700	1.61168000
C	3.49793500	-3.68250900	-0.24955200
H	3.70940500	-3.72572700	-1.32981300
H	2.87655800	-2.79063200	-0.07928800
H	2.91554600	-4.57748200	0.02246900
C	5.66757500	-4.88099800	0.27252100
H	6.63900800	-4.83046300	0.78671400
H	5.85811100	-5.02581600	-0.80220800
H	5.13738300	-5.77727100	0.62884900
C	-0.75735900	-1.51808500	3.86937900
H	-1.39583500	-1.34579900	2.99307300
H	-1.41862800	-1.70609400	4.72895200
Br	-7.31585300	-0.36993000	-1.71691300
Br	8.34451700	-0.90820200	-2.50708600
In	0.83888000	0.68734200	-0.09587300
C	-0.39504800	-1.96075600	-1.49661000
C	0.41330200	-3.00644100	-2.19344400
C	-0.32656800	-3.51493200	-3.19133500
C	-1.65391600	-2.81783000	-3.18933500
N	-1.59877600	-1.88208300	-2.10787500
H	1.43084800	-3.24243800	-1.89697000
H	-0.07253700	-4.28401800	-3.91960100
O	-2.60210900	-2.95362000	-3.90990400
O	-0.04617700	-1.27012600	-0.52205100
C	-2.76726400	-1.13328200	-1.63370100
H	-2.39789500	-0.24863200	-1.10156300
H	-3.30664900	-0.79654000	-2.52616900
C	3.17657000	-0.92902100	-2.66503500
C	2.03587100	-0.23324200	-2.80384700
H	3.37123300	-1.82478200	-3.26030000
H	3.96164700	-0.61504300	-1.96917900
H	1.29121200	-0.60472700	-3.52020500
C	1.66704700	1.00424900	-2.06173100
H	2.55795000	1.61760600	-1.84288300
H	0.97349200	1.62554200	-2.65093700
C	-3.66348700	-1.97445100	-0.75313600
C	-3.49974500	-1.97285000	0.61982900
C	-4.66686300	-2.79086900	-1.34321500
C	-4.34016100	-2.75031300	1.46359700
H	-2.71965400	-1.35141600	1.06567700
C	-5.48804500	-3.56541400	-0.55458600
H	-4.78391400	-2.79245100	-2.42857300
C	-4.22307200	-2.74440300	2.88288000
C	-5.35941800	-3.56425900	0.86163700
H	-6.26451000	-4.18243800	-1.01339400
C	-5.06632900	-3.50312200	3.66791700
H	-3.45579000	-2.12318800	3.34767800
C	-6.21086100	-4.33778400	1.69958000
C	-6.06928200	-4.30933400	3.07102300
H	-4.96714400	-3.48604900	4.75609800
H	-6.98429600	-4.95618200	1.23702400
H	-6.73043700	-4.90618700	3.70334100

TS1-S2

O	-1.13409500	1.49319100	-0.17888400
N	-2.75230400	3.06429300	-0.02644300
C	-5.36223400	1.76489400	3.09941500
H	-5.01267100	2.02217600	4.11130700
H	-5.83126800	0.77094500	3.16415900
H	-6.13657500	2.49101200	2.80997700
O	1.41855500	2.36447600	0.60242100
N	0.65952700	3.34964900	1.19338300
C	-3.14391300	0.70552700	2.52719300
H	-2.31276100	0.62353000	1.81531000
H	-3.61749500	-0.28371500	2.58201600
H	-2.73587700	0.93766600	3.52596800
C	-4.18197000	1.76686500	2.11843800
H	-3.69489200	2.75484600	2.20337700
N	1.16774800	-0.11506100	3.00237600
O	0.28528100	0.03973100	1.96075400
O	2.74685900	-0.23787400	0.57324100
N	4.42921400	-1.15166800	1.76240200
C	-4.41586000	3.46257100	-3.96054300
H	-3.84411300	4.13042200	-4.62264800
H	-5.28977700	4.01645200	-3.58646200
H	-4.78055200	2.62972200	-4.58158000
C	-3.52305400	2.96806100	-2.81422200
H	-3.09706800	3.86676700	-2.33351300
C	-2.34375000	2.14541700	-3.36857900

H	-1.65677600	1.81690000	-2.57644400
H	-1.77270600	2.73726000	-4.10167200
H	-2.71450400	1.24398900	-3.88033800
H	4.69630600	-1.62547700	2.62199500
C	-4.28905000	2.20759300	-1.73145700
H	-2.94532200	4.04431200	0.17009000
C	-5.44932800	1.48762400	-2.03716000
H	-5.81812900	1.44513000	-3.06090500
C	-6.17586700	0.85554500	-1.02553500
C	-5.75765800	0.89976900	0.30566200
H	-6.35183100	0.39801800	1.06766400
C	-4.60830100	1.61625400	0.65906800
C	-3.88731700	2.24130500	-0.37955500
C	-1.48506500	2.67421100	0.02883300
C	-0.47881400	3.79958600	0.26918300
H	-0.97789800	4.62098100	0.80563400
C	0.06701200	4.32243700	-1.06557800
H	0.56298200	3.49168100	-1.58343800
H	-0.79263300	4.62325400	-1.68366600
C	1.03584900	5.48613600	-0.85371200
H	1.45648600	5.80081700	-1.82019900
H	0.48785200	6.35586800	-0.45019700
C	2.14958100	5.07271000	0.10719300
H	2.78086500	4.29663000	-0.34736700
H	2.80287700	5.92526200	0.34907700
C	1.58979600	4.53904500	1.41610000
H	1.01050500	5.30218400	1.95898200
H	2.38993600	4.16344000	2.06206100
C	0.05169000	2.89762400	2.51688600
H	-0.66382200	2.10631300	2.27900500
H	-0.49475200	3.76609400	2.91235600
C	1.02836100	2.40282000	3.58368900
H	0.41768500	2.23714200	4.48471100
H	1.72489500	3.20545500	3.87170400
C	1.90449900	1.18343500	3.29786700
H	2.53483200	1.38641500	2.42774000
H	2.54499800	0.98638800	4.16990400
C	0.33505500	-0.55590900	4.20291500
H	1.02166900	-0.63745500	5.05988600
H	-0.37691600	0.25669000	4.38252000
C	0.57217400	-2.98165300	3.53091800
H	0.00961200	-3.87984400	3.23603100
H	1.18560700	-3.26381000	4.40505100
C	1.48065100	-2.54369500	2.37915100
H	2.25664900	-3.29852900	2.17670400
H	0.90769000	-2.40556700	1.45007500
C	2.19660500	-1.22844700	2.71795500
H	2.76134100	-1.34008600	3.65637000
C	3.15039800	-0.81651500	1.60123200
C	5.45034600	-0.93159100	0.76376400
C	5.86731500	-2.03320900	-0.01471600
C	6.83858400	-1.80896200	-0.99498500
H	7.19280600	-2.62866000	-1.61864400
C	7.36571800	-0.52826100	-1.18665900
C	6.95849800	0.54131300	-0.38955700
H	7.40560000	1.52386200	-0.54478600
C	5.99685100	0.35676100	0.61264200
C	5.60346900	1.53431500	1.49599200
H	4.91996600	1.15786700	2.27426400
C	4.84459700	2.60338600	0.69301300
H	5.47538300	3.01641800	-0.10974300
H	4.56176000	3.44293100	1.34937700
H	3.92955000	2.19449300	0.24236600
C	6.82098900	2.13125600	2.22265400
H	7.36407300	1.36505800	2.79657800
H	6.50340800	2.92231400	2.92058100
H	7.53233500	2.58431900	1.51515100
C	5.24323100	-3.41145900	0.17506500
H	4.99452900	-3.51875200	1.24573400
C	3.92386600	-3.50897000	-0.61345800
H	4.12025200	-3.44098900	-1.69567900
H	3.22207700	-2.70155800	-0.35551000
H	3.43245600	-4.47580800	-0.41934100
C	6.17903100	-4.57322400	-0.18112900
H	7.14716500	-4.48779700	0.33461500
H	6.37218200	-4.62557700	-1.26385800
H	5.71972800	-5.53001100	0.11009900
C	-0.39230000	-1.85780300	3.90981900
H	-1.10129500	-1.67099600	3.09220400
H	-0.98071300	-2.12215800	4.80177600
Br	-7.81193600	0.00124900	-1.46571400
Br	8.66497900	-0.24596900	-2.53926500
In	0.75938100	0.43231800	-0.05161100
C	-0.04048900	-2.15313200	-1.62666500
C	0.45201600	-3.57928400	-1.70630600
C	-0.44354000	-4.32963000	-2.35898300
C	-1.62222100	-3.47704000	-2.70090100
N	-1.33900200	-2.20358300	-2.18753200

H	1.42235200	-3.86851400	-1.31222200
H	-0.39021900	-5.38564100	-2.62039600
O	-2.64312700	-3.77621100	-3.27292400
O	0.16072200	-1.45943900	-0.53080400
C	-2.40654000	-1.23624300	-1.97563000
H	-1.96352000	-0.32865500	-1.55040600
H	-2.84714500	-0.97371400	-2.94860800
C	1.12960900	-1.46524000	-3.01417600
C	0.91338600	-0.07265700	-2.99610800
H	0.74319400	-2.01593400	-3.87357100
H	2.11286300	-1.79874800	-2.66315700
H	0.04339700	0.30591700	-3.54844000
C	1.60327800	0.82338000	-2.16551100
H	2.63209800	0.55727800	-1.88237800
H	1.45317900	1.89319500	-2.34171200
C	-3.47854300	-1.78296000	-1.05098600
C	-3.19559400	-2.02554300	0.28174000
C	-4.75137700	-2.13154800	-1.57123000
C	-4.16749100	-2.59801300	1.14693500
H	-2.20114500	-1.78945400	0.67216300
C	-5.71792000	-2.67907900	-0.75771000
H	-4.95537600	-1.97574500	-2.63220400
C	-3.90873600	-2.87455700	2.52013300
C	-5.46598700	-2.91212400	0.62037200
H	-6.69456300	-2.94142100	-1.16825600
C	-4.88570800	-3.40302700	3.33780700
H	-2.91518700	-2.66470100	2.92026500
C	-6.45376000	-3.45621700	1.48971800
C	-6.17507700	-3.69093100	2.81952200
H	-4.66973700	-3.61099700	4.38881700
H	-7.44071000	-3.68969600	1.08213000
H	-6.94112400	-4.10969000	3.47609400

INT2-S2

O	-1.11879500	1.49829100	-0.18908400
N	-2.75230400	3.05919300	-0.02644300
C	-5.36223400	1.76489400	3.09941500
H	-5.01267100	2.02217600	4.11130700
H	-5.83126800	0.77094500	3.16415900
H	-6.13657500	2.49101200	2.80997700
O	1.41855500	2.35427600	0.58202100
N	0.65952700	3.33944900	1.18318300
C	-3.14391300	0.70552700	2.52719300
H	-2.31276100	0.61843000	1.81021000
H	-3.61749500	-0.28371500	2.58201600
H	-2.73587700	0.93766600	3.52596800
C	-4.18197000	1.76686500	2.11843800
H	-3.69489200	2.75484600	2.20337700
N	1.16774800	-0.11506100	3.00747600
O	0.28528100	0.04993100	1.97095400
O	2.74685900	-0.22257400	0.56304100
N	4.42411400	-1.15166800	1.75730200
C	-4.41586000	3.46257100	-3.96054300
H	-3.84411300	4.13042200	-4.62264800
H	-5.28977700	4.01645200	-3.58646200
H	-4.78055200	2.62972200	-4.58158000
C	-3.52305400	2.96806100	-2.81422200
H	-3.09706800	3.86676700	-2.33351300
C	-2.34375000	2.14541700	-3.36857900
H	-1.66187600	1.81690000	-2.57644400
H	-1.77270600	2.73726000	-4.10167200
H	-2.71450400	1.24398900	-3.88033800
H	4.68610600	-1.63057700	2.61179500
C	-4.28905000	2.20759300	-1.73145700
H	-2.94532200	4.03921200	0.18029000
C	-5.44932800	1.48762400	-2.03716000
H	-5.81812900	1.44513000	-3.06090500
C	-6.17586700	0.85554500	-1.02553500
C	-5.75765800	0.89976900	0.30566200
H	-6.35183100	0.39801800	1.06766400
C	-4.60830100	1.61625400	0.65906800
C	-3.88731700	2.24130500	-0.37955500
C	-1.48506500	2.67421100	0.02373300
C	-0.47881400	3.79958600	0.26918300
H	-0.97279800	4.62098100	0.80563400
C	0.06701200	4.32753700	-1.06557800
H	0.55788200	3.49678100	-1.58853800
H	-0.79263300	4.62835400	-1.68366600
C	1.03584900	5.48613600	-0.85371200
H	1.45648600	5.80591700	-1.82019900
H	0.48785200	6.35586800	-0.45019700
C	2.14958100	5.07271000	0.10719300
H	2.78596500	4.30173000	-0.35246700
H	2.80287700	5.92526200	0.35417700
C	1.59489600	4.52884500	1.41100000
H	1.01050500	5.28688400	1.95898200
H	2.39503600	4.15324000	2.05696100
C	0.05169000	2.89252400	2.51178600

H	-0.66382200	2.10121300	2.27900500
H	-0.48965200	3.76609400	2.90215600
C	1.02836100	2.40282000	3.58368900
H	0.41258500	2.23714200	4.47961100
H	1.72489500	3.20545500	3.87170400
C	1.90449900	1.18343500	3.30296700
H	2.53993200	1.38641500	2.43284000
H	2.54499800	0.98638800	4.17500400
C	0.33505500	-0.55590900	4.20801500
H	1.02166900	-0.64255500	5.05988600
H	-0.37691600	0.25669000	4.38762000
C	0.57217400	-2.98165300	3.53091800
H	0.00961200	-3.87984400	3.23093100
H	1.18560700	-3.26381000	4.39995100
C	1.47555100	-2.54369500	2.37405100
H	2.25154900	-3.29852900	2.17160400
H	0.90259000	-2.40556700	1.43987500
C	2.19660500	-1.22844700	2.71285500
H	2.76644100	-1.34008600	3.64617000
C	3.14529800	-0.81141500	1.59613200
C	5.45034600	-0.93159100	0.76376400
C	5.86731500	-2.03320900	-0.01471600
C	6.83858400	-1.80896200	-0.99498500
H	7.19280600	-2.62866000	-1.61864400
C	7.36571800	-0.52826100	-1.18665900
C	6.95849800	0.54131300	-0.38955700
H	7.40560000	1.52386200	-0.54478600
C	5.99685100	0.35676100	0.61264200
C	5.60346900	1.53431500	1.49599200
H	4.91996600	1.15786700	2.27426400
C	4.84459700	2.60338600	0.69301300
H	5.47538300	3.01641800	-0.10974300
H	4.56176000	3.44293100	1.34937700
H	3.92955000	2.19449300	0.24746600
C	6.82098900	2.13125600	2.22265400
H	7.36407300	1.36505800	2.79657800
H	6.50340800	2.92231400	2.92058100
H	7.53233500	2.58431900	1.51515100
C	5.24323100	-3.41145900	0.17506500
H	4.99452900	-3.51875200	1.24573400
C	3.92386600	-3.50897000	-0.61345800
H	4.12025200	-3.44098900	-1.69567900
H	3.21697700	-2.70665800	-0.35041000
H	3.43245600	-4.47580800	-0.41934100
C	6.17903100	-4.57322400	-0.18112900
H	7.14716500	-4.48779700	0.33461500
H	6.37218200	-4.62557700	-1.26385800
H	5.71972800	-5.53001100	0.11009900
C	-0.39230000	-1.85780300	3.90981900
H	-1.10129500	-1.67099600	3.09220400
H	-0.98071300	-2.12215800	4.80177600
Br	-7.81193600	0.00124900	-1.46571400
Br	8.66497900	-0.24596900	-2.53926500
In	0.74918100	0.41701800	-0.04141100
C	0.12781100	-2.05113200	-1.82046500
C	0.45711600	-3.58438400	-1.70630600
C	-0.45374000	-4.32453000	-2.33348300
C	-1.62222100	-3.45664000	-2.69580100
N	-1.32370200	-2.19338300	-2.23343200
H	1.42745200	-3.89911400	-1.32242200
H	-0.43101900	-5.39584100	-2.54899600
O	-2.64822700	-3.78131100	-3.25762400
O	0.19132200	-1.43393900	-0.54610400
C	-2.39124000	-1.24134300	-1.98583000
H	-1.95332000	-0.33885500	-1.54020600
H	-2.86244500	-0.94821400	-2.94350800
C	0.94600900	-1.54684000	-2.76937600
C	0.88278600	-0.03185700	-2.94510800
H	0.73809400	-1.98533400	-3.79197100
H	2.02106300	-1.78344800	-2.57135700
H	0.03319700	0.35691700	-3.52294000
C	1.64917800	0.84378000	-2.27261100
H	2.60149800	0.49607800	-1.78547800
H	1.49907900	1.92379500	-2.35701200
C	-3.46834300	-1.78806000	-1.05608600
C	-3.19049400	-2.03064300	0.27664000
C	-4.74627700	-2.13154800	-1.57123000
C	-4.16749100	-2.59801300	1.14693500
H	-2.18584500	-1.80985400	0.66196300
C	-5.71282000	-2.67907900	-0.75771000
H	-4.94517600	-1.98084500	-2.63220400
C	-3.90873600	-2.87455700	2.52013300
C	-5.46598700	-2.91212400	0.62037200
H	-6.68946300	-2.94142100	-1.16825600
C	-4.88570800	-3.40302700	3.33780700
H	-2.91518700	-2.66470100	2.92026500
C	-6.45376000	-3.45621700	1.48971800
C	-6.17507700	-3.69093100	2.81952200

H	-4.66973700	-3.61099700	4.38881700
H	-7.44071000	-3.68969600	1.08213000
H	-6.94112400	-4.10969000	3.47609400

TS1-R4

O	-0.97607800	1.85893700	-0.32947400
N	-2.72465300	3.24996300	-0.53692700
C	-5.67274800	2.41165400	2.44479200
H	-5.54087500	2.97442900	3.38174300
H	-6.03075700	1.40744800	2.71955900
H	-6.46159200	2.90493900	1.85738000
O	1.45436700	3.07477200	0.35697400
N	0.62481300	4.12479600	0.66853800
C	-3.27408300	1.59678200	2.48365000
H	-2.31152500	1.53536700	1.95598900
H	-3.59912600	0.56220200	2.67148900
H	-3.11212800	2.08564000	3.45906600
C	-4.34679000	2.35065800	1.67490100
H	-3.99759400	3.39070200	1.55277500
N	1.03968400	1.18520600	3.28112600
O	0.23030800	1.09504200	2.17103500
O	2.73817400	0.49778900	1.12621800
N	4.02334100	-0.88010400	2.32256400
C	-3.37188300	3.53464500	-3.74159500
H	-2.68571800	3.93924100	-4.50249500
H	-3.46944200	4.28352500	-2.93930400
H	-4.36376900	3.42625800	-4.20660700
C	-2.86981500	2.17495900	-3.21930000
H	-1.86761600	2.32854900	-2.78247300
C	-2.68480000	1.18955400	-4.38095500
H	-2.34384100	0.19804800	-4.04708300
H	-1.93730200	1.58393000	-5.08681800
H	-3.61598400	1.05142600	-4.95158300
H	4.18845900	-1.35896100	3.20340000
C	-3.76325800	1.65817700	-2.09353800
H	-3.05069500	4.21357300	-0.54734600
C	-4.68478800	0.62814200	-2.30612200
H	-4.78600000	0.17272300	-3.29006700
C	-5.46343700	0.14585700	-1.24991000
C	-5.37279500	0.69936800	0.02782700
H	-5.99354500	0.29841200	0.82786700
C	-4.48297900	1.75073800	0.27863900
C	-3.68584100	2.19914500	-0.79172100
C	-1.42801500	3.02327000	-0.35880600
C	-0.52507800	4.25650900	-0.34544000
H	-1.10481200	5.13142300	-0.01344500
C	0.00299000	4.50241600	-1.76808900
H	0.53327300	3.60118800	-2.10434700
H	-0.87106600	4.62209200	-2.42633300
C	0.91750600	5.72569500	-1.83687400
H	1.33045000	5.82040400	-2.85210500
H	0.32713600	6.64003700	-1.65018200
C	2.03825900	5.60821700	-0.80550700
H	2.71068300	4.77272700	-1.05077800
H	2.64986200	6.52325700	-0.77935600
C	1.47811900	5.38981800	0.58960800
H	0.84137400	6.22852300	0.91198300
H	2.28053200	5.24109500	1.31944800
C	0.02731900	3.98738300	2.06351000
H	-0.67552900	3.15045700	2.02104200
H	-0.52914500	4.91731000	2.24985200
C	1.02416100	3.76905600	3.20427500
H	0.44053300	3.89599200	4.12893900
H	1.75893400	4.58805300	3.23653900
C	1.84587400	2.47849000	3.26635300
H	2.51084600	2.42093800	2.40179800
H	2.44833200	2.48363000	4.18675600
C	0.11300300	1.16646900	4.49581500
H	0.74860400	1.30657600	5.38436500
H	-0.53998600	2.03665900	4.37745000
C	0.19812900	-1.34011400	4.63856900
H	-0.40313900	-2.26101200	4.60979200
H	0.75667700	-1.35158300	5.59148900
C	1.16871300	-1.33612600	3.45931300
H	1.88093900	-2.16987800	3.53914600
H	0.63074200	-1.45871900	2.50878000
C	1.98529800	-0.03113000	3.38434900
H	2.55719900	0.11459200	4.31515600
C	2.95183300	-0.09777000	2.20101900
C	4.75824900	-1.29555900	1.14800400
C	4.64864100	-2.64827900	0.75715500
C	5.15524100	-3.00414500	-0.49852600
H	5.07265100	-4.03187100	-0.85159600
C	5.74401600	-2.04025900	-1.31951000
C	5.92234800	-0.72940900	-0.87536900
H	6.44428600	-0.01424100	-1.51216000
C	5.44004100	-0.33110600	0.37779200
C	5.73082100	1.08193400	0.87549000

H	5.22943400	1.21057300	1.84722700
C	5.20048100	2.17658200	-0.06527700
H	5.66995100	2.11760200	-1.05965700
H	5.43625500	3.17185900	0.34455100
H	4.11159900	2.10999700	-0.19141400
C	7.24234000	1.24837300	1.12422800
H	7.62373600	0.48136900	1.81544400
H	7.45534600	2.23827100	1.55768000
H	7.81261300	1.16505400	0.18580900
C	3.96146100	-3.69818900	1.62860100
H	3.94684900	-3.32233600	2.66691300
C	2.49929900	-3.90897000	1.19640600
H	2.45519100	-4.34418500	0.18644800
H	1.93251900	-2.96746900	1.16981600
H	1.98853400	-4.60172800	1.88360100
C	4.72701800	-5.02963200	1.66796000
H	5.78242800	-4.88369500	1.94317800
H	4.69665100	-5.54629800	0.69646000
H	4.26848300	-5.70556700	2.40578300
C	-0.70363300	-0.11153800	4.57375200
H	-1.36073000	-0.16317700	3.69474800
H	-1.34821700	-0.03863600	5.46349400
Br	-6.64721000	-1.30436700	-1.55458300
Br	6.30729300	-2.52012300	-3.06985800
In	0.92538100	0.99076000	0.14547900
C	-0.39799400	-2.02077100	-2.94884500
C	1.11573900	-2.15972800	-2.92540800
C	1.50515100	-2.05981700	-1.57123400
C	0.39501800	-1.55985100	-0.86393200
N	-0.73466500	-1.57492200	-1.66080100
H	1.58462600	-2.81218100	-3.66444600
H	2.50706800	-2.13776400	-1.15951300
O	0.33904500	-1.01891900	0.30625600
O	-1.16933500	-2.17356300	-3.86074100
C	-2.08499800	-1.17273700	-1.26011700
H	-2.67832900	-1.22632500	-2.17948900
H	-2.05213400	-0.12357000	-0.94357800
C	1.53534600	-0.47520600	-3.90619800
C	1.14310800	0.61714800	-3.11205700
H	0.99293200	-0.64896400	-4.83969600
H	2.60807400	-0.68875300	-3.94458100
H	0.19496300	1.11424700	-3.35619400
C	1.85629800	1.05530000	-1.95338300
H	2.87178700	0.64825300	-1.85743900
H	1.86789900	2.15167500	-1.84737200
C	-2.72683900	-2.01555700	-0.18168100
C	-3.56905400	-3.05836700	-0.51583000
C	-2.52030200	-1.70060400	1.19191500
C	-4.24023200	-3.82033500	0.47985800
H	-3.75037200	-3.29833700	-1.56734300
C	-3.15346300	-2.41966900	2.18116000
H	-1.84924000	-0.88054300	1.44563600
C	-5.12702300	-4.88140700	0.14713100
C	-4.03134700	-3.49516600	1.86248200
H	-2.99692400	-2.16648900	3.23454900
C	-5.77489600	-5.59242600	1.13576400
H	-5.28879100	-5.12440400	-0.90624500
C	-4.71312800	-4.24827200	2.85718900
C	-5.56534100	-5.27374700	2.50206400
H	-6.45408700	-6.40580700	0.87013900
H	-4.55473400	-4.00192500	3.91078500
H	-6.08535000	-5.84567400	3.27419800

INT0

C	1.78838600	2.70911100	2.48891700
C	0.57598900	2.27970500	2.11401700
H	-0.14021000	1.97640100	2.89041700
C	0.08828900	2.14690200	0.70241700
H	0.79068700	2.64450600	0.01061700
H	2.07238600	2.75801300	3.54321700
H	2.54078500	3.01511500	1.75491700
C	-1.34151300	2.66709400	0.47661700
H	-1.35411900	3.75259400	0.68761700
H	-2.02051100	2.20879100	1.21781700
C	-1.89051200	2.41549200	-0.92948300
H	-1.21851400	2.87009500	-1.68038300
H	-1.87720600	1.32789200	-1.13938300
C	-3.32001500	2.92078400	-1.13938300
H	-3.95621300	2.54268100	-0.32018300
H	-3.33312100	4.02198400	-1.05338300
C	-3.91151200	2.48888100	-2.48138300
H	-3.96880700	1.38918100	-2.54738300
H	-4.92891500	2.88607500	-2.62308300
H	-3.29381400	2.83978400	-3.32488300
In	0.25810000	0.07450300	0.15881700
C	4.14870000	0.09892400	-0.30088300
F	3.67279400	1.22342100	0.23581700
F	4.94160300	-0.50657200	0.56631700
F	4.81839900	0.38442700	-1.40548300

S	2.70140600	-1.01898400	-0.72348300
O	1.76490100	-0.12418900	-1.51578300
O	1.96590700	-1.16528800	0.61771700
O	3.23291300	-2.21428100	-1.33568300
C	-3.52509300	-1.17521700	0.32781700
F	-3.46740000	0.14488300	0.51141700
F	-4.09079200	-1.43032000	-0.84118300
F	-4.22629000	-1.72692100	1.30271700
S	-1.78038900	-1.87470800	0.34541700
O	-1.08969300	-1.16030400	1.49321700
O	-1.12449300	-1.23380400	-0.88678300
O	-1.90038200	-3.31400800	0.37391700

INT1

C	4.75546700	0.08435400	-2.02401600
C	4.66696300	-1.31938000	-1.50570400
C	3.42083500	-1.52660500	-1.06133900
C	2.63655900	-0.26608600	-1.27287400
N	3.46055200	0.65160900	-1.85196800
H	5.52111200	-1.99450800	-1.50952500
H	2.97866700	-2.39602800	-0.58099900
O	1.46296700	-0.05226800	-0.96612700
O	5.69723300	0.67106200	-2.48495400
C	3.14183900	2.03653700	-2.23918800
H	4.10056600	2.57594800	-2.19283000
H	2.81645800	2.04190900	-3.29139600
C	1.33165800	-3.00936900	-2.94136500
C	0.25549900	-2.24746000	-2.69057200
H	0.05824900	-1.39383900	-3.35541700
C	-0.72762300	-2.43454900	-1.58210000
H	-0.52748000	-3.39961100	-1.08192300
C	2.09248400	2.66753300	-1.35673600
C	0.87782700	3.05238500	-1.88532700
C	2.32033600	2.79196100	0.04179300
C	-0.16667900	3.54393700	-1.05821900
H	0.68657400	2.93998700	-2.95685000
C	1.32593300	3.25482500	0.87238000
H	3.27829700	2.47407500	0.46140000
C	-1.44482000	3.88378800	-1.57828500
C	0.05499400	3.63167400	0.35531000
H	1.49275100	3.31220400	1.95083700
C	-2.46497300	4.27341000	-0.73596300
H	-1.61319500	3.81101500	-2.65638900
C	-1.01350400	4.04427700	1.19435300
C	-2.24848500	4.34908000	0.66268000
H	-3.45071700	4.51183100	-1.14296000
H	-0.85461700	4.07722900	2.27441600
H	-3.07170500	4.63062100	1.32292400
H	1.99969100	-2.79936900	-3.78108700
H	1.57041400	-3.88001200	-2.32108500
C	-2.18610900	-2.41370600	-2.09049100
H	-2.24144000	-3.04982000	-2.99441300
H	-2.46031900	-1.39773100	-2.42693400
C	-3.22103400	-2.91733800	-1.08199600
H	-2.94814000	-3.94086600	-0.76401900
H	-3.18324600	-2.30540300	-0.16784700
C	-4.65192000	-2.92049900	-1.62688500
H	-4.89410400	-1.91269600	-2.00682500
H	-4.71186500	-3.59710600	-2.49885800
C	-5.68649500	-3.32705700	-0.57673100
H	-5.68108800	-2.62068400	0.26958900
H	-6.70600800	-3.34394800	-0.99431400
H	-5.47344600	-4.33070000	-0.17185700
In	-0.23942100	-0.99568800	-0.02354400
C	3.18251500	-0.87884600	2.39553200
F	3.44526700	0.02570500	1.44483500
F	3.45636700	-0.35350800	3.57584800
F	3.94556900	-1.94731400	2.18892700
S	1.36629100	-1.37984700	2.34023100
O	1.24359900	-2.30988600	1.14070100
O	0.64807400	-0.13139200	1.87684200
O	1.07670300	-1.91931100	3.65185500
C	-4.00362900	0.64304400	0.21510700
F	-3.88194000	0.18209700	-1.02848000
F	-4.87905500	-0.10589100	0.87555400
F	-4.43149300	1.89695100	0.17787100
S	-2.33802000	0.57312700	1.08843400
O	-1.34276800	0.90817800	-0.01790500
O	-2.08791500	-0.89925000	1.34990300
O	-2.44892300	1.46594500	2.22318200

TS1

C	-0.44696500	3.70692800	-2.12514700
C	-0.41280700	4.33215400	-0.75380300
C	-0.12925000	3.37457300	0.13958700
C	0.05124300	2.09502000	-0.61206700
N	-0.11379500	2.34200400	-1.93503400
H	-0.61237200	5.39097600	-0.59509500

H	-0.04914700	3.41938300	1.22440000
O	0.29106600	0.97314400	-0.16317900
O	-0.71626000	4.21104300	-3.18137700
C	-0.19863600	1.28856600	-2.96502300
H	-0.26063700	1.81924300	-3.92486200
H	0.72989000	0.70411200	-2.92432700
C	2.69562900	1.02603700	2.26184400
C	2.67609100	-0.24386000	2.91247900
H	2.15397200	1.83862200	2.77485600
H	3.39783200	-0.97706600	2.51940900
C	1.65121800	-0.75633000	3.73878200
H	1.03932700	-0.06821000	4.33637400
H	1.72694300	-1.78241800	4.10358100
C	-1.40798600	0.41847200	-2.70202300
C	-1.26428500	-0.78117400	-2.03243300
C	-2.71092700	0.90138400	-3.01000800
C	-2.39664900	-1.52367900	-1.60486000
H	-0.26858700	-1.14809400	-1.78716500
C	-3.82884500	0.19239600	-2.62807800
H	-2.81746700	1.84876600	-3.54695100
C	-2.26042100	-2.72119700	-0.84891800
C	-3.70924400	-1.02684700	-1.90222000
H	-4.82773300	0.56713900	-2.86840100
C	-3.37637800	-3.39961400	-0.40701600
H	-1.25566100	-3.07895300	-0.61387800
C	-4.83874400	-1.75754600	-1.44068900
C	-4.67572400	-2.91502000	-0.70780500
H	-3.26366900	-4.31241000	0.18301200
H	-5.84025100	-1.38119300	-1.66699500
H	-5.55129900	-3.46332700	-0.35075200
C	3.83964200	1.44793200	1.35753300
H	4.49663500	2.16333200	1.88823000
H	4.45800300	0.56622000	1.12401300
C	3.37962800	2.07029200	0.03414900
H	2.69000300	2.91278800	0.24000800
H	2.79620500	1.31860400	-0.52068900
C	4.50946300	2.55344600	-0.87395600
H	5.09714400	3.33498800	-0.35886200
H	5.20353200	1.71302700	-1.05207600
C	3.98948400	3.08060400	-2.21251400
H	3.43892100	2.29291400	-2.75390700
H	3.29888500	3.92970300	-2.06644800
H	4.80695800	3.42686100	-2.86447000
In	0.79172100	-0.15580500	1.57962100
C	-3.13606500	0.97459200	1.39997600
F	-2.57311000	1.33015500	0.24629800
F	-4.07931900	0.07881300	1.17655000
F	-3.65666600	2.04929900	1.97855600
S	-1.84238800	0.23696500	2.54501300
O	-1.26006900	-0.92917000	1.75949600
O	-0.69648800	1.24608100	2.55277700
O	-2.51532200	-0.03988000	3.79617500
C	2.32839300	-3.41406200	-1.34466100
F	3.22246000	-3.63508400	-2.30075100
F	2.53042000	-4.26293800	-0.34456800
F	1.10388200	-3.59925500	-1.83791300
S	2.50679500	-1.65195700	-0.74034600
O	3.80628800	-1.55094200	-0.07606300
O	2.23745200	-0.80027600	-1.90307800
O	1.33934300	-1.65275400	0.27372400

TS2

C	-3.55218100	3.79778600	0.27192300
C	-4.60415000	2.74570300	0.37896800
C	-4.01081800	1.54805400	0.44633500
C	-2.51720400	1.72331600	0.37850600
N	-2.32541300	3.12189500	0.21765000
H	-5.66618000	2.98583500	0.39659300
H	-4.46304800	0.56224300	0.52048400
O	-1.80408300	0.89649200	-0.31311500
O	-3.68363600	5.00198600	0.24502000
C	-1.07806500	3.86430900	0.29367800
H	-1.31022200	4.85730300	-0.12480700
H	-0.81185300	4.04394400	1.35114700
C	-2.17379600	1.33856600	2.34808500
C	-0.77290500	1.30598800	2.42242700
H	-0.26407500	2.27293400	2.51195300
C	0.06635500	0.18301000	2.24436900
H	-0.37604600	-0.76180000	2.60802000
C	0.10206300	3.26255800	-0.43271500
C	1.33681900	3.21255700	0.18368200
C	-0.01934000	2.81961000	-1.78110700
C	2.49627100	2.74966600	-0.50040500
H	1.44822400	3.55490300	1.21714200
C	1.07617000	2.34736800	-2.46427300
H	-1.00147100	2.83671300	-2.25742600
C	3.77824200	2.71870000	0.11401700
C	2.36285500	2.30137600	-1.85452400

H	0.96874500	1.98739200	-3.49026600
C	4.88073400	2.26308100	-0.57948600
H	3.87776400	3.06286300	1.14728000
C	3.51405500	1.82287400	-2.53559100
C	4.74655100	1.80691400	-1.91447000
H	5.86143000	2.24492200	-0.09753500
H	3.40660600	1.46299900	-3.56215700
H	5.62348000	1.43380500	-2.44890200
H	-2.68235500	2.20823000	2.76884800
H	-2.70428200	0.38507500	2.44736900
C	1.57048400	0.34272800	2.50703500
H	1.70696600	1.10295800	3.29767100
H	2.08042000	0.75368400	1.62108000
C	2.26486800	-0.94923700	2.94357400
H	1.74345000	-1.36512700	3.82544800
H	2.16097000	-1.70635000	2.15122100
C	3.74620600	-0.74983400	3.27648200
H	4.24035900	-0.23861700	2.43275300
H	3.83765700	-0.06691000	4.14098500
C	4.47080600	-2.06385300	3.56952600
H	4.44572800	-2.72705500	2.68940900
H	5.52691300	-1.89524200	3.83370000
H	3.99824200	-2.60485700	4.40638600
In	-0.49218600	-0.57909700	0.13655200
C	-4.16529100	-2.11893300	-0.67977800
F	-4.12543400	-0.98115800	-1.36284900
F	-4.72200600	-3.06291200	-1.41748300
F	-4.88680200	-1.93113700	0.42657400
S	-2.41823700	-2.64839100	-0.19774200
O	-2.11130400	-1.84370400	1.06190000
O	-1.52887400	-1.99817300	-1.24211200
O	-2.44375700	-4.09112700	-0.09515000
C	3.45871700	-1.52120900	-0.66669200
F	3.51843700	-0.43111000	0.09009500
F	3.94685400	-2.55353900	0.01144700
F	4.16267700	-1.33929200	-1.77143500
S	1.67216500	-1.88170300	-1.12228700
O	1.05664500	-0.50211500	-1.38232600
O	1.01142300	-2.29043900	0.18327300
O	1.72565000	-2.82293800	-2.21812400

INT2

C	-3.08376500	-2.52186900	-1.57185100
C	-3.62408100	-3.08985700	-0.29345100
C	-2.90271800	-2.59464900	0.72433700
C	-1.86612800	-1.68483700	0.16132400
N	-2.02326400	-1.65487900	-1.19340900
H	-4.46301200	-3.78350300	-0.27652700
H	-2.98661100	-2.77614900	1.79421800
O	-0.96416900	-1.12915000	0.79884600
O	-3.42586900	-2.73560000	-2.70490100
C	-1.15311500	-0.97047300	-2.14705900
H	-1.56740500	-1.21761100	-3.13723200
H	-1.24719400	0.11567800	-2.00432800
C	-4.07816500	0.34052000	0.90587400
C	-3.11043400	1.27902800	0.98273500
H	-4.22616800	-0.33208400	1.76163800
H	-3.00667600	1.97429600	0.13760200
C	-2.11564800	1.42806100	2.06626900
H	-2.35958000	0.83657400	2.96296800
H	-1.96228300	2.48198400	2.35215700
C	0.30289800	-1.38627500	-2.04248700
C	1.29459600	-0.48644400	-2.37786700
C	0.66592800	-2.69087500	-1.61055500
C	2.66946000	-0.83498100	-2.29271700
H	1.02914200	0.52787600	-2.68132000
C	1.98901500	-3.05361700	-1.49664800
H	-0.11216100	-3.41184400	-1.34757100
C	3.70403000	0.08113600	-2.63075600
C	3.02853900	-2.14157400	-1.82508400
H	2.25547400	-4.05167100	-1.13913500
C	5.02990100	-0.27337800	-2.49911500
H	3.42897300	1.07609300	-2.98484900
C	4.40481500	-2.47534500	-1.69537700
C	5.38447400	-1.56190200	-2.02286000
H	5.81531000	0.44170500	-2.75635700
H	4.67367500	-3.46851400	-1.32562000
H	6.43932000	-1.82691300	-1.91576100
C	-5.03510200	0.18397400	-0.23577800
H	-4.79083800	0.90698600	-1.03308800
H	-4.90904300	-0.82034300	-0.68997200
C	-6.51093000	0.32796500	0.16665400
H	-6.67033400	1.33205300	0.59842900
H	-6.73858500	-0.38882500	0.97791600
C	-7.48075900	0.10471600	-0.99637200
H	-7.24524300	0.81956800	-1.80556400
H	-7.30758500	-0.89957600	-1.42517700
C	-8.94884200	0.24780300	-0.59427400

H	-9.22051000	-0.47874200	0.19011400
H	-9.15603100	1.25493100	-0.19538000
H	-9.62222600	0.08258300	-1.45028700
In	-0.18452600	0.81287400	1.31943400
C	2.41420100	-2.14627800	2.16413800
F	1.26374100	-2.68619800	1.77838800
F	3.39015800	-2.56283300	1.36902600
F	2.67488600	-2.50823700	3.41376800
S	2.30596000	-0.27455000	2.08421600
O	1.77653700	0.02475200	0.69030100
O	1.10974100	0.07299300	2.96765100
O	3.61010100	0.22866700	2.45574400
C	1.98171200	3.23335200	-1.20322300
F	2.45290500	4.46564400	-1.08767300
F	2.84722300	2.37081100	-0.70186900
F	1.77706500	2.95823100	-2.49426100
S	0.34198500	3.11893300	-0.29002300
O	0.72427300	2.90039600	1.15882500
O	-0.40649700	4.31038300	-0.63943100
O	-0.25236600	1.78089200	-0.71752200

INT3

C	-0.57723400	4.94477800	0.98763500
C	-2.04442800	4.81235200	0.72680900
C	-2.36699500	3.51819700	0.72415800
C	-1.14000100	2.64308000	0.95409300
N	-0.08576800	3.65127400	1.08676900
H	-2.68247400	5.67955900	0.56136900
H	-3.33589400	3.05697100	0.53103500
O	-0.94888700	1.83301600	-0.15970700
O	0.07185400	5.96350300	1.11170900
C	1.27834000	3.39585600	1.47980900
H	1.72622900	4.39556900	1.61304000
H	1.31978400	2.90847500	2.47186500
C	-1.30207300	1.80050100	2.25963600
C	-0.43066500	0.56751800	2.32599800
H	0.65561700	0.69030000	2.20563700
C	-0.91753700	-0.64389200	2.69442200
H	-2.00227400	-0.72453100	2.84722100
C	2.12372400	2.61740300	0.48867500
C	3.19775700	1.87212700	0.93696400
C	1.89139000	2.72796800	-0.91057200
C	4.10452700	1.25182800	0.03289200
H	3.38841400	1.77872500	2.01160900
C	2.73176000	2.11537600	-1.81102600
H	1.01909000	3.28437700	-1.25483300
C	5.24467100	0.52558900	0.47621800
C	3.86497900	1.37250300	-1.37574800
H	2.53411800	2.19204300	-2.88333600
C	6.11221000	-0.04946900	-0.42909500
H	5.42640700	0.43505100	1.55098700
C	4.76887700	0.75363200	-2.28252100
C	5.87090700	0.06278600	-1.82207400
H	6.98839100	-0.59890500	-0.07524300
H	4.57837200	0.84074500	-3.35570100
H	6.56120200	-0.40300400	-2.52981500
H	-1.09633600	2.45398000	3.12339200
H	-2.35467600	1.48532900	2.33918600
C	-0.13641200	-1.89228200	2.96237600
H	0.11793300	-1.89855400	4.04038300
H	0.82428600	-1.85624600	2.42771100
C	-0.91385300	-3.17329500	2.61968900
H	-1.73274300	-3.30332400	3.35056500
H	-1.39629700	-3.05901600	1.63718200
C	-0.02770600	-4.41861100	2.60045200
H	0.77387900	-4.26753500	1.85718200
H	0.47666200	-4.52861000	3.57836100
C	-0.80109100	-5.69352800	2.26522700
H	-1.28160500	-5.61298200	1.27614700
H	-0.14034300	-6.57457500	2.24630300
H	-1.59611000	-5.88657100	3.00498400
In	-0.82976000	-0.11436500	-0.22223000
C	-4.64198300	0.12673400	-1.37579300
F	-4.15698400	1.33537800	-1.10419000
F	-5.01339900	0.06787700	-2.64273000
F	-5.67724800	-0.12267800	-0.58746100
S	-3.31060900	-1.15705100	-1.05494900
O	-2.84657300	-0.85551600	0.36919200
O	-2.12391600	-0.68623200	-1.89233300
O	-3.88303800	-2.45476900	-1.33197800
C	2.65078900	-2.19265700	-0.11842800
F	2.63430600	-1.34861600	0.91309700
F	2.68132400	-3.43906500	0.33905700
F	3.70237900	-1.96697500	-0.87717300
S	1.08950800	-1.96053000	-1.12949100
O	0.99780600	-0.46451500	-1.39914400
O	-0.02964200	-2.15438200	-0.10001400
O	1.16883200	-2.87626400	-2.24353800

PRO2

C	-3.49464600	-1.84138900	-0.42537300
C	-4.66361400	-1.49147000	0.43677500
C	-4.48713000	-0.27086800	0.95408500
C	-3.13016400	0.35486800	0.59257900
N	-2.60706500	-0.80737900	-0.32313800
H	-5.48535300	-2.19488100	0.58754000
H	-5.13948800	0.26192600	1.65049300
O	-2.40632300	0.61929400	1.64549600
O	-3.36632300	-2.85678200	-1.10864800
C	-1.41009600	-0.79633800	-1.11932500
H	-1.52253300	-1.58968100	-1.87798800
H	-1.33239100	0.16406500	-1.65808000
C	-3.38641200	1.62096000	-0.34234100
C	-2.13234300	2.32134400	-0.79222000
H	-1.98124500	2.43206300	-1.87685500
C	-1.16825200	2.76419000	0.03060400
H	-1.31194900	2.59597500	1.10334100
C	-0.08772400	-1.00315200	-0.39465400
C	1.04276500	-1.31186100	-1.13167000
C	0.02733600	-0.81345000	1.01249400
C	2.32423400	-1.42037400	-0.52783700
H	0.96319600	-1.46117500	-2.21430800
C	1.25732400	-0.92637700	1.62669700
H	-0.87935300	-0.50472600	1.55885300
C	3.50400400	-1.70047100	-1.27448500
C	2.43777100	-1.22153100	0.89065700
H	1.34175000	-0.76207300	2.70590100
C	4.73801500	-1.77547400	-0.65967700
H	3.41556000	-1.84963800	-2.35511600
C	3.72354300	-1.30979200	1.49326500
C	4.84965600	-1.57803500	0.74104200
H	5.63420900	-1.98444300	-1.25109400
H	3.80494900	-1.15167300	2.57312900
H	5.83108500	-1.63528100	1.22057100
H	-4.01012600	1.34125000	-1.20857300
H	-3.98810900	2.29679500	0.29030700
C	0.14619700	3.33917400	-0.41832300
H	0.29809100	4.34306900	0.02887900
H	0.14211600	3.48777700	-1.51504300
C	1.34187700	2.45273100	-0.03019200
H	1.32988500	2.28494600	1.06154100
H	1.20838900	1.45297300	-0.47430800
C	2.70092200	3.01960900	-0.44631700
H	2.70817800	3.17666300	-1.54185000
H	2.83279700	4.02450200	-0.00069700
C	3.87334200	2.11939200	-0.05132700
H	3.78286800	1.12029700	-0.50586800
H	4.84259200	2.54681100	-0.36041700
H	3.90586900	1.96591400	1.04009400

TS3

C	3.03583200	-2.59077900	1.70812700
C	3.45798400	-3.35445500	0.49265300
C	2.96668900	-2.74352800	-0.59286700
C	2.24090600	-1.49193400	-0.18471700
N	2.29352600	-1.50418300	1.23856500
H	4.04572500	-4.26903400	0.55739700
H	3.04270800	-3.03240700	-1.64067500
O	1.10589600	-1.22869900	-0.77480600
O	3.24817700	-2.84701000	2.87288200
C	1.47688500	-0.68883900	2.11291000
H	1.88903300	-0.84048800	3.12361900
H	1.60950000	0.37675400	1.86516100
C	3.62225400	-0.19156700	-0.77385500
C	2.92061900	1.02686500	-0.99926900
H	3.89188400	-0.69833500	-1.70986600
H	2.92471200	1.76613000	-0.18589600
C	2.09793900	1.29576600	-2.09170200
H	2.19626500	0.67932600	-2.99481000
H	1.75737900	2.32487000	-2.25399300
C	-0.00550700	-1.04463400	2.10108300
C	-0.94358900	-0.11439400	2.50785300
C	-0.44499500	-2.33457400	1.69567500
C	-2.33297800	-0.41343300	2.51556000
H	-0.62446100	0.88810000	2.80234900
C	-1.78374500	-2.65368500	1.68353600
H	0.28662400	-3.07251800	1.36400300
C	-3.31085400	0.53849500	2.91752900
C	-2.76745600	-1.70811200	2.07954000
H	-2.10703700	-3.64170800	1.34626100
C	-4.65448500	0.23122700	2.87447000
H	-2.97928900	1.52555300	3.24763000
C	-4.15991100	-1.99293600	2.04112300
C	-5.08409500	-1.04477400	2.42729700
H	-5.39597800	0.97370500	3.18037900
H	-4.48667000	-2.97678900	1.69381900
H	-6.15232000	-1.27295800	2.39046300

C	4.73106400	-0.16809600	0.25824700
H	4.35445500	0.29571800	1.18582000
H	5.01184400	-1.19915100	0.52514200
C	5.98854400	0.57301900	-0.21750400
H	5.72755100	1.61771700	-0.46899300
H	6.34538800	0.11862500	-1.16040000
C	7.11893400	0.56313700	0.81462700
H	6.75187900	1.01052300	1.75604800
H	7.37475600	-0.48344700	1.06061000
C	8.37069600	1.30427400	0.34431700
H	8.77785300	0.85495500	-0.57709800
H	8.14902000	2.36220600	0.12475500
H	9.16542800	1.28103500	1.10654600
In	0.10805900	0.48051500	-1.17785700
C	-2.44038000	-2.45524200	-1.96155700
F	-1.28850500	-2.95646800	-1.54104000
F	-3.40999400	-2.78799500	-1.12013700
F	-2.71841000	-2.92301600	-3.17041200
S	-2.32396800	-0.58285900	-2.04757200
O	-1.89674000	-0.16612900	-0.64445400
O	-1.05674000	-0.31385500	-2.86303700
O	-3.58765100	-0.10289300	-2.55879500
C	-1.98181700	3.39579800	0.74929100
F	-2.48982100	4.55247300	0.35484400
F	-2.82590300	2.41556500	0.49098100
F	-1.72643800	3.44111700	2.05510500
S	-0.36476600	3.09848600	-0.16365700
O	-0.76333800	2.55340200	-1.52202700
O	0.39685400	4.33053900	-0.11064100
O	0.24534100	1.88026400	0.53189700

INT4

C	2.97327300	-2.81375000	1.56998000
C	3.40132100	-3.44789600	0.28413900
C	3.09083300	-2.63165200	-0.72472600
C	2.48538500	-1.32910000	-0.21509300
N	2.44077900	-1.57704800	1.23277700
H	3.85304400	-4.43853300	0.24984800
H	3.22954700	-2.78796700	-1.79506100
O	1.24066900	-1.14729800	-0.77797500
O	3.03565300	-3.27734100	2.69019300
C	1.61693100	-0.85054200	2.17286100
H	1.98302600	-1.13539900	3.17295500
H	1.78001400	0.23463100	2.07083500
C	3.48272600	-0.14956700	-0.60906100
C	2.83244900	1.20137200	-0.56489300
H	3.73121800	-0.35013800	-1.66507900
H	2.73223400	1.67661100	0.41931700
C	2.39137500	1.87615800	-1.64602000
H	2.50448500	1.46646400	-2.65659600
H	1.98921200	2.88875600	-1.56417900
C	0.12215300	-1.15671800	2.09017400
C	-0.80131300	-0.22937500	2.54023600
C	-0.34655800	-2.41132800	1.60462400
C	-2.19938800	-0.48323300	2.49644400
H	-0.46183700	0.74023300	2.91102900
C	-1.69270200	-2.69355500	1.56386500
H	0.36896400	-3.14485700	1.23416500
C	-3.15620100	0.48812400	2.89971300
C	-2.65933600	-1.74253100	1.99098000
H	-2.03654800	-3.65305700	1.16969900
C	-4.50731900	0.22979400	2.79809800
H	-2.80305900	1.45218300	3.27446600
C	-4.05736200	-1.97934300	1.89934300
C	-4.96218800	-1.01449900	2.29161800
H	-5.23434200	0.98686200	3.10288000
H	-4.40480000	-2.93606100	1.50055800
H	-6.03542800	-1.20452200	2.21083700
C	4.77401700	-0.16101500	0.22412600
H	4.53091100	0.11805400	1.26349300
H	5.15589800	-1.19323800	0.27293700
C	5.87000500	0.75867500	-0.31962700
H	5.49976300	1.79917700	-0.36572500
H	6.09804200	0.47752500	-1.36489000
C	7.15593900	0.71744900	0.50991500
H	6.92093200	0.99383000	1.55379800
H	7.52629300	-0.32293800	0.55217000
C	8.25294900	1.63425400	-0.03175800
H	8.53125800	1.35724600	-1.06254900
H	7.91990800	2.68561800	-0.05212500
H	9.16429700	1.58461300	0.58485700
In	0.03220400	0.38756600	-0.84698500
C	-2.40856500	-2.45173000	-2.07833000
F	-1.27821700	-2.97344200	-1.62615000
F	-3.41612400	-2.81591800	-1.29569300
F	-2.63210000	-2.86433300	-3.31689000
S	-2.27983700	-0.57731300	-2.07399800
O	-2.00279100	-0.23820400	-0.60509500

O	-0.93973300	-0.27561000	-2.73276300
O	-3.49016000	-0.06211000	-2.67218700
C	-2.16729800	3.42910900	0.57395200
F	-2.64184300	4.51499500	-0.01256000
F	-2.95384700	2.39769500	0.33522100
F	-2.06487800	3.62986900	1.88273200
S	-0.44690600	3.07529100	-0.10354500
O	-0.66485000	2.41624800	-1.45885100
O	0.30939100	4.31044300	-0.05458600
O	0.05653700	1.90531000	0.74533700

PRO1

C	-0.50088500	-1.29669300	1.24579500
C	-1.23179200	-0.87621800	2.48488100
C	-1.76728600	0.33607800	2.29671000
C	-1.46362600	0.91830400	0.90455300
N	-0.67006000	-0.28970800	0.34068300
H	-1.23343100	-1.50022100	3.38118400
H	-2.33106700	0.93668200	3.01517800
O	-0.81912900	2.04578400	0.91207300
O	0.14936400	-2.32558100	1.07995700
C	0.16799500	-0.17384000	-0.82572300
H	0.04817300	-1.05751700	-1.47718700
H	-0.18010700	0.71310200	-1.37534700
C	-2.86768400	1.00530700	0.08002300
C	-2.63537400	1.57433600	-1.28813800
H	-3.42608700	1.74792000	0.67791200
H	-2.70643400	0.86662500	-2.12725500
C	-2.26679200	2.83762000	-1.53985100
H	-2.12370500	3.54103200	-0.71676500
H	-2.03814200	3.17533900	-2.55702600
C	1.63935700	0.02031200	-0.49859600
C	2.61976000	-0.79525500	-1.02451700
C	2.00470700	1.08788500	0.37598300
C	3.99715000	-0.58394400	-0.73463200
H	2.34118400	-1.63535700	-1.66835500
C	3.32938200	1.31691000	0.67456600
H	1.17895000	1.68684500	0.79204100
C	5.02629100	-1.40919100	-1.26804500
C	4.36462200	0.50159400	0.13176900
H	3.60703200	2.13780900	1.34399800
C	6.35547700	-1.17809200	-0.97170300
H	4.74276600	-2.23911000	-1.92274800
C	5.74179900	0.71238600	0.41784600
C	6.71806800	-0.10415700	-0.11944100
H	7.13223900	-1.82375700	-1.39203600
H	6.01671600	1.54050300	1.07880300
H	7.77246800	0.07338400	0.11223200
C	-3.67381500	-0.29820900	0.02096000
H	-3.14135200	-1.01568700	-0.62949800
H	-3.69647500	-0.76716000	1.01814600
C	-5.11241600	-0.12600200	-0.47701100
H	-5.10848100	0.35521800	-1.47255000
H	-5.64585300	0.57973900	0.18866700
C	-5.89897300	-1.43739600	-0.55470200
H	-5.36437200	-2.13976700	-1.22041900
H	-5.90317800	-1.91811300	0.44105100
C	-7.33719900	-1.26025300	-1.04511800
H	-7.90512300	-0.58923100	-0.37758600
H	-7.36050800	-0.81097900	-2.05300900
H	-7.87926800	-2.21985600	-1.09411700

INT-a

O	2.09256100	0.18145500	0.82566700
N	3.76964200	-0.63466200	2.05768600
C	6.49726000	2.39289600	1.32561300
H	6.37335100	3.34145800	1.87134800
H	7.04300200	2.61915400	0.39657200
H	7.13030000	1.72805800	1.93260300
O	-0.40503500	0.39117000	2.02150800
N	0.44726800	0.71696000	3.05661100
C	4.24236900	2.69064800	0.18726900
H	3.25282600	2.25037600	-0.00500100
H	4.71471200	2.89606100	-0.78655100
H	4.10657200	3.65899700	0.69781300
C	5.12723700	1.75733400	1.03754600
H	4.62560300	1.62119700	2.00982400
N	-0.44788300	3.41574400	0.20735500
O	0.48011400	2.42916300	-0.05928600
O	-1.93764900	1.05106300	-0.32964800
N	-3.73983700	2.20754400	-0.97791000
C	4.69835200	-3.80613600	2.05746900
H	4.12909900	-4.63112400	2.51383200
H	4.88770200	-3.05277100	2.84028700
H	5.67907800	-4.20102700	1.75046900
C	3.94751100	-3.22802800	0.84229700
H	2.96770800	-2.85729600	1.19525300
C	3.65236000	-4.33019100	-0.18211700

H	3.14134800	-3.93415600	-1.07262800
H	3.00530200	-5.09755900	0.26921300
H	4.57184500	-4.83817800	-0.51139600
H	-4.14572900	3.10086700	-1.24689000
C	4.68765700	-2.02453200	0.26452200
H	4.09900000	-0.96855300	2.96016400
C	5.44152800	-2.12257100	-0.90837100
H	5.52201300	-3.07117500	-1.43674100
C	6.08081700	-0.99410500	-1.43207200
C	5.99693700	0.24342300	-0.79539500
H	6.50166800	1.10585700	-1.23187700
C	5.25611300	0.38474700	0.38587000
C	4.62241900	-0.76238700	0.89583300
C	2.51727600	-0.20925300	1.92821800
C	1.61187100	-0.29004900	3.15551800
H	2.17967400	0.00317600	4.05243000
C	1.06951600	-1.71921800	3.32487900
H	0.51338500	-1.99319200	2.41565800
H	1.93386700	-2.39714300	3.39115200
C	0.18053000	-1.84196200	4.56328000
H	-0.24204800	-2.85625100	4.61546700
H	0.79397100	-1.70744000	5.47157000
C	-0.93534700	-0.79924000	4.52512400
H	-1.63986300	-1.01634000	3.70956100
H	-1.51169300	-0.80199300	5.46318600
C	-0.38313600	0.60474200	4.33360900
H	0.26861400	0.91252200	5.16604900
H	-1.19437500	1.33100500	4.21865600
C	1.00275700	2.13165500	2.90424300
H	1.65338400	2.12156500	2.02642400
H	1.61645200	2.31272200	3.79878000
C	-0.02121800	3.26363000	2.77605900
H	0.57335800	4.19027200	2.79127500
H	-0.63912900	3.32551500	3.68536100
C	-1.02158700	3.28897600	1.61698700
H	-1.62180400	2.37586500	1.63122100
H	-1.68774700	4.15428900	1.74675600
C	0.29725500	4.73969000	0.04869000
H	-0.41257500	5.53870000	0.31371100
H	1.10467100	4.70986400	0.78810300
C	-0.25135900	4.81869400	-2.41335200
H	0.17980000	4.85607000	-3.42457400
H	-0.92688600	5.68797600	-2.32608700
C	-1.05783100	3.52921100	-2.24395100
H	-1.91487500	3.50097400	-2.93421500
H	-0.43853400	2.64707600	-2.46596500
C	-1.60672700	3.39967000	-0.81517600
H	-2.22054900	4.28036500	-0.57099500
C	-2.44811800	2.13492700	-0.67094400
C	-4.56472600	1.01758700	-0.95985200
C	-4.77033200	0.33012200	-2.17402900
C	-5.46442200	-0.88382000	-2.12213600
H	-5.64483200	-1.45442800	-3.03251400
C	-5.91962100	-1.38407300	-0.89941500
C	-5.72948700	-0.67361300	0.28590400
H	-6.11170600	-1.08120900	1.22227700
C	-5.04423500	0.54731600	0.27761600
C	-4.82606100	1.29454400	1.58844600
H	-4.34723900	2.25900000	1.35154200
C	-3.86769800	0.52043200	2.51126500
H	-4.31091100	-0.43865100	2.82226900
H	-3.66598900	1.10027300	3.42802900
H	-2.91217800	0.30361600	2.01360000
C	-6.15436100	1.61467200	2.29395800
H	-6.83565900	2.17481300	1.63576900
H	-5.97505100	2.21917400	3.19711900
H	-6.67437900	0.69728300	2.61028000
C	-4.20178600	0.84960900	-3.49150600
H	-4.12844000	1.94820200	-3.41031600
C	-2.77605400	0.30622400	-3.71353800
H	-2.79364400	-0.79158500	-3.80329800
H	-2.10461900	0.55281800	-2.87812700
H	-2.34244000	0.71469000	-4.63992100
C	-5.09543700	0.55165300	-4.70315000
H	-6.13065900	0.88448100	-4.53515500
H	-5.11698600	-0.52313400	-4.94101400
H	-4.70857800	1.06965800	-5.59377400
C	0.85149300	4.90469300	-1.35814300
H	1.61329100	4.12998800	-1.52849100
H	1.36184100	5.87937400	-1.39975700
Br	7.05079200	-1.14704500	-3.05652100
Br	-6.79753400	-3.06643200	-0.84642700
In	0.10059900	0.37470300	-0.02637400
C	0.27565400	-1.25132700	-1.41461500
C	1.67077800	-1.29065800	-1.96200400
H	2.45465100	-1.58906800	-1.25545100
C	2.03698600	-0.97089500	-3.21020400
H	1.30411400	-0.66796200	-3.96635700

H	3.08431400	-1.01224700	-3.52134000
C	-0.15938800	-2.54100000	-0.68529200
H	-0.19618100	-3.36718300	-1.41776000
H	0.61897600	-2.83717000	0.04536000
H	-0.44134100	-1.03958800	-2.22621100
C	-1.51274100	-2.42458100	0.02430200
H	-1.46888300	-1.60998800	0.77856600
H	-2.28434000	-2.10308100	-0.69846000
C	-1.97215000	-3.69521000	0.74100200
H	-1.18378300	-4.01723500	1.44738400
H	-2.06718500	-4.51359300	0.00679600
C	-3.29425700	-3.50968300	1.48643700
H	-3.60172300	-4.43134400	2.00305800
H	-3.21448000	-2.70989700	2.24366200
H	-4.10566900	-3.22982100	0.79561100

INT-b

O	-2.28833800	0.46539000	0.62252400
N	-3.64337600	2.23307900	0.83701700
C	-7.55265400	1.22231500	2.31138000
H	-7.67028400	1.36572600	3.39627000
H	-8.07115500	0.28605400	2.05271800
H	-8.06616900	2.04980700	1.79922700
O	0.19413500	0.58406900	1.82305300
N	-0.57621700	1.28365200	2.72446100
C	-5.38031100	-0.04079300	2.61713400
H	-4.31671200	-0.11790200	2.34520800
H	-5.85830800	-0.97540700	2.29024000
H	-5.46663200	0.02235300	3.71383700
C	-6.06396200	1.16738800	1.94615700
H	-5.60160600	2.08128000	2.35819600
N	-0.48395800	-2.68297700	2.77241500
O	-1.21168000	-2.01540700	1.81952800
O	1.34378800	-1.87320500	0.64519200
N	2.84118300	-3.37095300	1.39886200
C	-3.11492500	3.85369700	-1.92411500
H	-2.15910500	4.31392600	-2.22273800
H	-3.35289200	4.20476000	-0.90879600
H	-3.89885300	4.23620800	-2.59570900
C	-3.02916700	2.31708600	-2.01096200
H	-2.19269800	1.98582500	-1.37244600
C	-2.67454800	1.89392900	-3.44192900
H	-2.61881900	0.80087400	-3.55063900
H	-1.69535000	2.31068600	-3.72454100
H	-3.40530600	2.27281200	-4.17273800
H	3.01098900	-4.18702300	1.98119000
C	-4.30066700	1.66472800	-1.46643200
H	-3.83698200	3.11618200	1.30193100
C	-5.21377300	1.02929500	-2.31481200
H	-5.02341700	0.96076700	-3.38414400
C	-6.38546100	0.46521700	-1.80148100
C	-6.69321500	0.54478600	-0.44383700
H	-7.62369700	0.11155000	-0.07986300
C	-5.79845700	1.15522200	0.44339800
C	-4.61209400	1.69394200	-0.08854100
C	-2.52260300	1.57451800	1.12934900
C	-1.51287300	2.28631000	2.01722700
H	-2.04172000	2.81474600	2.82645400
C	-0.70356000	3.29028900	1.18397400
H	-0.14530800	2.73462400	0.41584100
H	-1.41302600	3.95044800	0.66359700
C	0.24989700	4.08377600	2.07011900
H	0.82975300	4.78361000	1.45828700
H	-0.32400600	4.68886900	2.79483300
C	1.17549600	3.11559200	2.79712200
H	1.81263600	2.59856700	2.06803100
H	1.84400600	3.64419700	3.49374000
C	0.39353800	2.08370400	3.59402500
H	-0.20600300	2.55022000	4.39163700
H	1.06430300	1.33822100	4.03357400
C	-1.40675900	0.34666800	3.59263000
H	-2.09569400	-0.16739900	2.91889100
H	-1.98042900	0.98488600	4.28042800
C	-0.62339600	-0.68290600	4.41013500
H	-1.36996800	-1.18421300	5.04508800
H	0.04481000	-0.18040600	5.12624100
C	0.24781100	-1.71640800	3.69327600
H	0.98685100	-1.20164400	3.07167300
H	0.76553500	-2.33306400	4.44289600
C	-1.47864500	-3.53306200	3.55941500
H	-0.91203700	-4.03768500	4.35800000
H	-2.18053700	-2.82186900	4.00699000
C	-1.22681100	-5.44085900	1.93135300
H	-1.76288400	-6.08540600	1.21893100
H	-0.72996200	-6.11204800	2.65420300
C	-0.17337200	-4.61992500	1.18577000
H	0.59391100	-5.26846200	0.73660400
H	-0.63522700	-4.04776800	0.36902200

C	0.53698700	-3.63160500	2.12284000
H	1.00582900	-4.17639900	2.95676100
C	1.60740300	-2.86540100	1.34985100
C	3.92176100	-2.87871600	0.57757800
C	4.25763900	-3.61136300	-0.58301700
C	5.26818800	-3.10210100	-1.40549300
H	5.55794800	-3.62977600	-2.31330200
C	5.90768800	-1.90453500	-1.07481100
C	5.57968500	-1.20959300	0.08786400
H	6.10727500	-0.28544200	0.32597900
C	4.57729000	-1.68763700	0.94252500
C	4.24041100	-0.90419900	2.20457400
H	3.47446200	-1.46853200	2.76014000
C	3.64279600	0.47077300	1.86286800
H	4.35751200	1.07721800	1.28478000
H	3.41693000	1.02712300	2.78603900
H	2.71280500	0.38251100	1.28480800
C	5.46320600	-0.77401300	3.12924900
H	5.89079600	-1.75784500	3.37561400
H	5.18210600	-0.27628700	4.07082000
H	6.25901300	-0.17188200	2.66387800
C	3.49675900	-4.87578500	-0.97003300
H	3.18078200	-5.37283600	-0.03614900
C	2.22160600	-4.50047700	-1.74944100
H	2.48493300	-4.02339500	-2.70673000
H	1.59213500	-3.78910000	-1.19623000
H	1.61883400	-5.39468400	-1.97290600
C	4.33863500	-5.89263800	-1.75091300
H	5.28143600	-6.12398800	-1.23287000
H	4.58299400	-5.53135700	-2.76189900
H	3.77625900	-6.83046400	-1.87368200
C	-2.20552000	-4.51902900	2.65776100
H	-2.81272200	-3.95522100	1.93480700
H	-2.89881400	-5.09711000	3.28802100
Br	-7.56702000	-0.45192400	-2.97089400
Br	7.22652500	-1.19763800	-2.24607700
In	-0.49417500	-0.72357500	0.26167300
C	3.14481500	1.53870100	-3.21034000
C	3.62215500	0.18695100	-2.77691700
C	2.75860700	-0.29744800	-1.87060100
C	1.69766400	0.72886800	-1.63985000
N	1.95088400	1.78162000	-2.45896800
H	4.52614300	-0.26677700	-3.18036100
H	2.77447300	-1.24161800	-1.33321700
O	0.77375000	0.71083600	-0.81191400
O	3.60483200	2.30685300	-4.00598700
C	1.23661300	3.04257400	-2.47016500
H	1.31893400	3.44876500	-3.49000600
H	0.17311600	2.82584100	-2.28142400
C	0.17316600	-0.99406500	-3.56962100
C	-0.31623400	-1.78830900	-2.60163000
H	-0.20682400	0.02104800	-3.72038000
H	0.08139500	-2.80937500	-2.53309500
C	-1.36333900	-1.44121700	-1.60428000
H	-1.87963600	-0.52097000	-1.92782900
C	1.75867500	4.06120100	-1.47234100
C	2.74832400	3.77172600	-0.55491500
C	1.21006900	5.37462600	-1.51445900
C	3.23797500	4.75920100	0.34658300
H	3.19014100	2.77376400	-0.50809300
C	1.66557000	6.35612600	-0.66220400
H	0.43531500	5.60961700	-2.25020700
C	4.24441300	4.47337400	1.30990700
C	2.68851900	6.08373200	0.29142400
H	1.24778800	7.36479800	-0.71427500
C	4.68528900	5.44988600	2.18003300
H	4.67043100	3.46753800	1.34725000
C	3.16770100	7.06930300	1.19795900
C	4.14290300	6.75936000	2.12378300
H	5.46488100	5.22137800	2.91079300
H	2.75341500	8.07956600	1.14851000
H	4.50750500	7.52489400	2.81246500
H	0.94157900	-1.34404100	-4.26267200
C	-2.41322600	-2.56295200	-1.46384000
H	-1.92335000	-3.49611600	-1.12466300
H	-2.79431700	-2.80016200	-2.47461200
C	-3.61168300	-2.26540200	-0.55945000
H	-3.27186800	-2.09491300	0.47679500
H	-4.08504600	-1.31959800	-0.87502300
C	-4.64783000	-3.39330400	-0.57986900
H	-5.02420500	-3.51949700	-1.60996000
H	-4.15024400	-4.34894600	-0.32650700
C	-5.82476100	-3.16536800	0.36689500
H	-6.56182800	-3.98021300	0.30200500
H	-5.48741500	-3.10413000	1.41595300
H	-6.34494800	-2.22419200	0.12771700

TS-a

O	-2.19313600	0.58121900	0.52100500
N	-3.66388300	2.23373200	0.82166200
C	-7.41195100	0.87460700	2.37882800
H	-7.49191500	0.94241400	3.47451100
H	-7.90117200	-0.06480000	2.07810100
H	-7.97977900	1.70984200	1.94225100
O	0.21964800	0.73267900	1.90852600
N	-0.60123200	1.44998500	2.74548600
C	-5.17156100	-0.30182100	2.52149500
H	-4.13011500	-0.33397900	2.16695300
H	-5.64523700	-1.23598300	2.18723300
H	-5.18041500	-0.29017900	3.62357000
C	-5.93850300	0.91070500	1.95468200
H	-5.49995500	1.81871500	2.40244400
N	-0.59484300	-2.51354400	2.75428500
O	-1.24919100	-1.82925400	1.75314000
O	1.28732400	-1.86538400	0.63710300
N	2.72009400	-3.38084900	1.45820400
C	-3.31552600	3.96862800	-1.90045500
H	-2.40368400	4.50100700	-2.21463200
H	-3.54277400	4.27394400	-0.86790500
H	-4.14606600	4.31298600	-2.53572100
C	-3.12590400	2.44493300	-2.03440400
H	-2.25357400	2.15785400	-1.42244100
C	-2.77403000	2.08630800	-3.48342200
H	-2.64688400	1.00216500	-3.62385900
H	-1.83371000	2.57954500	-3.77319700
H	-3.54561500	2.43037900	-4.18904000
H	2.86457300	-4.17685800	2.07463700
C	-4.33488100	1.68710400	-1.48357600
H	-3.90900300	3.09304200	1.30683700
C	-5.22302300	1.01408300	-2.33019900
H	-5.06055800	0.99979000	-3.40633200
C	-6.33369900	0.34424200	-1.80724000
C	-6.60366000	0.34765900	-0.43916000
H	-7.48523600	-0.17139500	-0.06545500
C	-5.73144300	0.99327600	0.44544200
C	-4.60995100	1.64648200	-0.09850500
C	-2.49251700	1.65709000	1.07372000
C	-1.51738900	2.41172800	1.96033000
H	-2.07676200	2.97249400	2.72580700
C	-0.68098100	3.38141700	1.11151400
H	-0.08135900	2.79966000	0.39433400
H	-1.37442200	4.01064900	0.53322400
C	0.22531200	4.22217400	2.00512900
H	0.82754300	4.89808200	1.38826500
H	-0.38536500	4.85440700	2.67481600
C	1.12488400	3.29751600	2.81850000
H	1.79669200	2.74860800	2.14526400
H	1.75848200	3.86592200	3.51608900
C	0.31358500	2.30010700	3.62931100
H	-0.33283200	2.79746500	4.36959800
H	0.96544500	1.58313100	4.13951900
C	-1.45161600	0.52244200	3.59833100
H	-2.13996400	0.01675200	2.91658500
H	-2.02849900	1.16087200	4.28320400
C	-0.67976500	-0.51755800	4.41237800
H	-1.42409400	-0.99784200	5.06574800
H	0.01285600	-0.02353400	5.11092900
C	0.15805400	-1.57548500	3.69117500
H	0.92658400	-1.08587600	3.08570800
H	0.64090000	-2.21774600	4.44223400
C	-1.66668300	-3.28002900	3.52486500
H	-1.16180300	-3.76761100	4.37377900
H	-2.35454600	-2.51625400	3.90187900
C	-1.43272800	-5.27589900	2.00422100
H	-1.96843000	-5.93502300	1.30487400
H	-0.98944600	-5.92797200	2.77741300
C	-0.32407600	-4.53223400	1.25962800
H	0.42893700	-5.22861300	0.86091900
H	-0.73710300	-3.97597100	0.40781000
C	0.39893900	-3.53063900	2.17079500
H	0.82845700	-4.05505900	3.03803400
C	1.50854500	-2.83779500	1.38584700
C	3.82009200	-2.95152900	0.62454500
C	4.13386900	-3.73893400	-0.50571300
C	5.18401300	-3.31240600	-1.32449000
H	5.46269300	-3.88492400	-2.20816000
C	5.87883600	-2.13764000	-1.02284500
C	5.55220800	-1.37536900	0.09713600
H	6.11028100	-0.46154500	0.30291100
C	4.50908600	-1.76740600	0.94661200
C	4.16272700	-0.89644300	2.14772900
H	3.33841600	-1.38146000	2.69495600
C	3.67043400	0.49232700	1.70410900
H	4.45718900	1.02612100	1.14921400
H	3.41717700	1.10371100	2.58419600
H	2.78116400	0.43619500	1.06154400

C	5.34742700	-0.78905900	3.12372900
H	5.69526300	-1.78112900	3.45037700
H	5.05891600	-0.21392100	4.01783300
H	6.20275300	-0.27183500	2.66197500
C	3.30306100	-4.96546400	-0.87265200
H	2.94362200	-5.42032300	0.06713900
C	2.06248300	-4.53518600	-1.68267500
H	2.37174100	-4.09396100	-2.64369200
H	1.46283200	-3.77984300	-1.15326400
H	1.41635800	-5.40030300	-1.90021400
C	4.09091300	-6.05062300	-1.61717700
H	5.01057700	-6.32523800	-1.07925700
H	4.37178200	-5.72874300	-2.63189200
H	3.47478000	-6.95581700	-1.72682900
C	-2.39771300	-4.27951600	2.64382900
H	-2.95152600	-3.73045300	1.87017000
H	-3.14035200	-4.79446200	3.27253000
Br	-7.47773900	-0.61768600	-2.97772800
Br	7.26750700	-1.55348200	-2.17820700
In	-0.37454900	-0.52806100	0.28962900
C	3.25019100	1.54470300	-3.09805600
C	3.72064200	0.19921200	-2.64505000
C	2.76542400	-0.36273700	-1.89131500
C	1.56989000	0.55452500	-1.83598600
N	1.97417400	1.70666400	-2.53469100
H	4.69940500	-0.19427900	-2.91548600
H	2.77157300	-1.32590100	-1.38570500
O	0.85444500	0.72556700	-0.75934900
O	3.81024300	2.36764400	-3.77994800
C	1.25628200	2.95786500	-2.56003600
H	1.33464300	3.37541400	-3.57700200
H	0.19178500	2.74226200	-2.37039900
C	0.38405000	-0.30841500	-3.15540700
C	-0.25033900	-1.39874200	-2.53225700
H	-0.23986500	0.57301600	-3.32722200
H	0.21918600	-2.38732200	-2.63150700
C	-1.38026400	-1.30407100	-1.69216000
H	-1.95608400	-0.37525000	-1.82580600
C	1.75995000	3.99324000	-1.56736000
C	2.69469600	3.69722600	-0.59630600
C	1.26841000	5.32492800	-1.67629500
C	3.19206200	4.69846800	0.28472300
H	3.07825800	2.67998400	-0.49893300
C	1.72599100	6.31886300	-0.83911200
H	0.53874800	5.56499500	-2.45564400
C	4.15078100	4.41029300	1.29563500
C	2.70073100	6.04156000	0.16199300
H	1.35260100	7.34091300	-0.94354700
C	4.59915400	5.39947300	2.14725300
H	4.53331500	3.39069800	1.38354300
C	3.18625900	7.03993300	1.05146400
C	4.11272600	6.72653400	2.02488300
H	5.34272100	5.16744300	2.91374800
H	2.81610100	8.06347000	0.94993900
H	4.48287800	7.50221100	2.69920700
H	1.09223300	-0.53052400	-3.95571500
C	-2.28011400	-2.52949000	-1.51504900
H	-1.69536500	-3.39186000	-1.14859900
H	-2.62379000	-2.83046000	-2.52112300
C	-3.51727000	-2.31813300	-0.63961600
H	-3.21283100	-2.07805700	0.39212000
H	-4.07082400	-1.43368300	-0.99981100
C	-4.44142900	-3.53982000	-0.65022200
H	-4.76839400	-3.73297100	-1.68669000
H	-3.86591000	-4.43647300	-0.35053300
C	-5.66827900	-3.39547300	0.24834800
H	-6.32964600	-4.27167800	0.17260600
H	-5.37989800	-3.28830700	1.30768100
H	-6.25698000	-2.50696900	-0.02981500

TS-b

O	-2.16899500	0.04950900	0.20011700
N	-4.12297000	0.50935100	1.20581100
C	-6.34000200	-2.64257200	2.57757600
H	-6.09537100	-3.05388200	3.56977800
H	-6.84474300	-3.43842900	2.00859200
H	-7.06089300	-1.82213800	2.71433100
O	0.03184100	0.03700100	1.86052900
N	-0.91077000	0.32186800	2.82108500
C	-4.05267100	-3.30368300	1.67703100
H	-3.12959500	-2.95928900	1.18631200
H	-4.47926100	-4.10546000	1.05384200
H	-3.79440500	-3.74947900	2.65296200
C	-5.06602600	-2.15972700	1.86621000
H	-4.59172400	-1.41367700	2.52420700
N	0.20793700	-3.37426000	2.04218100
O	-0.61093300	-2.70373600	1.15554700
O	1.86116700	-1.63402300	0.38963600

N	3.65399400	-2.80995200	1.13406700
C	-5.80302800	2.71840500	-1.86421900
H	-5.43208500	3.73784800	-2.05430800
H	-6.59823000	2.77708900	-1.10536700
H	-6.25843800	2.36196800	-2.80077000
C	-4.65265300	1.80554300	-1.40620200
H	-4.21616700	2.26278600	-0.50362800
C	-3.54049400	1.72512300	-2.46869600
H	-2.64413400	1.23819500	-2.05860600
H	-3.26296100	2.73153600	-2.81793300
H	-3.87128000	1.15668700	-3.35133100
H	3.96092300	-3.67353600	1.57429600
C	-5.14978900	0.41220400	-1.03722900
H	-4.59562300	0.93003500	2.00116700
C	-5.86509500	-0.32822700	-1.98733700
H	-6.06827000	0.09703800	-2.97065600
C	-6.32295400	-1.61260800	-1.69280500
C	-6.08237600	-2.18745100	-0.44376700
H	-6.45013900	-3.19315000	-0.23763600
C	-5.36519000	-1.48567900	0.53118400
C	-4.90997100	-0.18795000	0.21455600
C	-2.78884400	0.53061000	1.16209200
C	-2.04645400	1.22822900	2.28909500
H	-2.71140600	1.38706100	3.15179100
C	-1.50674900	2.56382700	1.78627800
H	-0.87502300	2.37251800	0.90961100
H	-2.36637900	3.15313200	1.43933500
C	-0.73797100	3.31619500	2.86831700
H	-0.31194200	4.23362500	2.43803300
H	-1.42830200	3.63230000	3.67014800
C	0.35964600	2.41957700	3.43501200
H	1.11890900	2.22067900	2.66662000
H	0.87213800	2.89678300	4.28495000
C	-0.19418500	1.09009200	3.92644500
H	-0.91962000	1.22675500	4.74387700
H	0.61206500	0.43137300	4.26401000
C	-1.53740600	-0.95066000	3.36777600
H	-2.03692400	-1.43156200	2.52186000
H	-2.29632200	-0.64005000	4.10042600
C	-0.58337400	-1.93875900	4.03767800
H	-1.21862800	-2.74704800	4.43094000
H	-0.13416300	-1.48633900	4.93516400
C	0.58356700	-2.51302800	3.23594600
H	1.19371300	-1.69455500	2.84326900
H	1.19810000	-3.14450100	3.89466200
C	-0.56651100	-4.61111400	2.48703400
H	0.05807000	-5.13200100	3.22997400
H	-1.47060200	-4.23205100	2.97306500
C	0.32467600	-5.93755800	0.53435800
H	0.04173800	-6.51000600	-0.36137300
H	0.94014000	-6.61021200	1.15779200
C	1.15337300	-4.71827100	0.12564000
H	2.10489900	-5.01859200	-0.33858100
H	0.61348100	-4.10791800	-0.61103600
C	1.48444000	-3.84144000	1.34031900
H	2.02782300	-4.44013700	2.08767000
C	2.34248300	-2.65000400	0.92870900
C	4.65893500	-1.88238500	0.68071800
C	5.32411300	-2.16424000	-0.53279800
C	6.19367200	-1.19024600	-1.03413000
H	6.71158100	-1.34703700	-1.97942000
C	6.40743000	-0.00694200	-0.32137000
C	5.82791700	0.19957200	0.93060900
H	6.06765900	1.10279000	1.49294700
C	4.94376400	-0.74832700	1.46375100
C	4.36427000	-0.54957200	2.86039800
H	3.82644900	-1.47352800	3.12906600
C	3.34640300	0.60008300	2.90869400
H	3.80350600	1.55019600	2.58983900
H	2.98619400	0.74319400	3.94056800
H	2.47591500	0.40557600	2.26656000
C	5.47947800	-0.35664500	3.90268700
H	6.21620400	-1.17314900	3.86222900
H	5.05372300	-0.32838600	4.91802900
H	6.01979300	0.59009700	3.74768300
C	5.11581600	-3.49504400	-1.25164000
H	4.88233100	-4.24331900	-0.47381900
C	3.91802700	-3.44193600	-2.21330400
H	4.15197300	-2.79696000	-3.07155600
H	3.01619800	-3.02934800	-1.73865300
H	3.68562000	-4.44629600	-2.60077600
C	6.37380400	-3.99323200	-1.97614600
H	7.25017000	-4.00658700	-1.31085500
H	6.61569400	-3.36752200	-2.84929600
H	6.21131500	-5.01553200	-2.34978000
C	-0.92075400	-5.50196600	1.30645100
H	-1.60993300	-4.95189500	0.65004700
H	-1.46673600	-6.37321000	1.70007600

Br	-7.27935700	-2.59254300	-3.00631600
Br	7.51686200	1.34445100	-1.06825400
In	-0.24630800	-0.97128000	-0.05381000
C	2.85809700	3.35700000	-1.56498400
C	3.68896500	2.29303300	-0.91680900
C	2.87014000	1.30960500	-0.51771200
C	1.47148900	1.68475900	-0.87761600
N	1.50685700	2.89858900	-1.49006600
H	4.77298100	2.36579500	-0.84618200
H	3.10643500	0.36337300	-0.04195600
O	0.43805600	1.02828400	-0.68063900
O	3.19220700	4.39721600	-2.05935700
C	0.37422800	3.65030900	-2.03270600
H	0.77534200	4.22099400	-2.88457000
H	-0.35406200	2.92319200	-2.41710000
C	0.36643000	-1.43877100	-2.52085600
C	-1.01183800	-1.42058000	-2.23588100
H	-1.53719900	-0.50084700	-2.53625900
C	-1.76447100	-2.31855400	-1.44683700
H	-1.43007100	-3.35582600	-1.34234900
H	-2.83257100	-2.13767800	-1.31797000
C	0.98151100	-0.42792000	-3.46317200
H	0.66540200	-0.62538600	-4.50612700
H	0.58472600	0.57762200	-3.23340500
C	-0.27229600	4.58617700	-1.03120300
C	-1.63719900	4.55829600	-0.83002900
C	0.51801200	5.53301700	-0.31586400
C	-2.27398200	5.43363300	0.09293000
H	-2.25132600	3.83816200	-1.37221500
C	-0.06649100	6.39174200	0.58930900
H	1.59072500	5.59667100	-0.50812000
C	-3.67690900	5.39507200	0.33003800
C	-1.47021500	6.36392500	0.83167300
H	0.54672500	7.11981300	1.12681900
C	-4.25751000	6.23617800	1.25803300
H	-4.29252900	4.69892300	-0.24490000
C	-2.10001800	7.22159700	1.77570700
C	-3.46242100	7.15755900	1.98692000
H	-5.33710500	6.20708000	1.42438300
H	-1.48823600	7.93852900	2.32945000
H	-3.93639000	7.82530200	2.71001600
H	0.88476200	-2.40643200	-2.44351600
C	2.51146900	-0.40810500	-3.42427100
H	2.85662000	-0.43714600	-2.37524700
H	2.88381500	-1.34361300	-3.87289900
C	3.15533600	0.77491100	-4.14558500
H	2.77734000	1.71936000	-3.71277300
H	2.82219000	0.78718000	-5.19798900
C	4.68280300	0.75320400	-4.08208600
H	5.12588800	1.62349700	-4.58939000
H	5.04106000	0.75706800	-3.03933100
H	5.08610800	-0.15301800	-4.56381400

INT-c

O	-2.02685100	0.42531900	0.48106600
N	-3.67565500	1.89974400	0.84359300
C	-7.42948200	0.43841200	2.32053200
H	-7.54381700	0.53367300	3.41098100
H	-7.83978600	-0.54355200	2.03843100
H	-8.04427500	1.21606800	1.84343300
O	0.27917400	0.72543100	2.11858500
N	-0.69629100	1.27075200	2.92292900
C	-5.12005700	-0.56596700	2.56291300
H	-4.06912900	-0.53483100	2.23925200
H	-5.51751200	-1.54140500	2.25110400
H	-5.15974100	-0.51699600	3.66312000
C	-5.95124800	0.56927400	1.93337400
H	-5.59640700	1.52052700	2.36788800
N	-0.33540300	-2.68695000	2.56076200
O	-0.98140000	-1.96261300	1.57394300
O	1.59147800	-1.73160700	0.63941900
N	3.10577800	-3.20223400	1.38343300
C	-3.37523000	3.72838000	-1.76279700
H	-2.48284600	4.30148500	-2.05763000
H	-3.57100900	3.94643900	-0.70281500
H	-4.23314200	4.10446100	-2.34119500
C	-3.15842000	2.22458500	-2.03065300
H	-2.24557400	1.91167400	-1.49374400
C	-2.89352400	2.00830700	-3.52596700
H	-2.72172000	0.95056000	-3.77618200
H	-2.00323000	2.57443400	-3.83501400
H	-3.73095700	2.36937800	-4.14239100
H	3.28965800	-4.04368900	1.92451200
C	-4.32015800	1.39033800	-1.48622300
H	-4.00797400	2.68420000	1.39899000
C	-5.19043800	0.70515400	-2.34364600
H	-5.03249700	0.71995800	-3.42009800
C	-6.28223800	-0.00500500	-1.83558100

C	-6.56325200	-0.01955000	-0.46952500
H	-7.44136100	-0.55327900	-0.10925000
C	-5.70931900	0.63244700	0.42702200
C	-4.58745700	1.30221000	-0.10180500
C	-2.46380700	1.42091600	1.09970700
C	-1.63765200	2.19386400	2.12103700
H	-2.32059800	2.62057000	2.87272500
C	-0.84555600	3.32597700	1.44707000
H	-0.12172200	2.89497200	0.73628000
H	-1.55303000	3.92871600	0.85760900
C	-0.14250700	4.17101900	2.50842200
H	0.42756700	4.97527700	2.03148100
H	-0.89361800	4.65355700	3.16015600
C	0.78105100	3.28235900	3.33339100
H	1.58146500	2.88507300	2.69473000
H	1.26397300	3.85009000	4.14334200
C	0.02509700	2.12706000	3.96582700
H	-0.74433500	2.47516100	4.67269600
H	0.70569500	1.43949900	4.47900600
C	-1.50044000	0.17780500	3.60819200
H	-2.08190200	-0.32072700	2.82890400
H	-2.19101000	0.68036500	4.30035600
C	-0.67994000	-0.86057700	4.37680900
H	-1.41046800	-1.45589900	4.94531500
H	-0.06833200	-0.37382400	5.15158400
C	0.28234000	-1.78157200	3.62160900
H	1.04774400	-1.18552100	3.11601900
H	0.77040400	-2.45130400	4.34445400
C	-1.39021000	-3.58840200	3.19800400
H	-0.89909900	-4.09818200	4.04170400
H	-2.15857200	-2.90982400	3.58229700
C	-0.91215000	-5.43482000	1.54705600
H	-1.35615100	-6.07195100	0.76766600
H	-0.45917100	-6.11455000	2.29004100
C	0.17218600	-4.55041700	0.93212000
H	0.99646200	-5.15296300	0.52292200
H	-0.23455300	-3.95093700	0.10576000
C	0.76615900	-3.58287500	1.96528800
H	1.17885200	-4.14657000	2.81573000
C	1.86019700	-2.75087600	1.30722500
C	4.19211200	-2.63616100	0.61227900
C	4.65699100	-3.37960300	-0.49579900
C	5.69028800	-2.83131300	-1.26056400
H	6.07881500	-3.36430100	-2.12723100
C	6.22040500	-1.58011400	-0.93324100
C	5.74398000	-0.86233200	0.16197400
H	6.17378000	0.11385800	0.38766600
C	4.71260100	-1.37535900	0.95925000
C	4.20877500	-0.54693300	2.13413500
H	3.37257900	-1.08869700	2.60380700
C	3.67189400	0.81739700	1.66718600
H	4.48316000	1.43817700	1.25655600
H	3.23852200	1.36409700	2.51824200
H	2.89991400	0.72240200	0.89078000
C	5.29774500	-0.38660100	3.20956100
H	5.66270300	-1.36207400	3.56675300
H	4.90712600	0.17335600	4.07431700
H	6.16417900	0.16997100	2.81999900
C	3.98592300	-4.68544800	-0.91254000
H	3.63369400	-5.19461700	0.00255600
C	2.74723800	-4.37591600	-1.77849800
H	3.05185200	-3.88848800	-2.71775800
H	2.04887400	-3.69318000	-1.27037900
H	2.20436900	-5.29951300	-2.03473600
C	4.92060800	-5.66785200	-1.62908900
H	5.83762200	-5.85057700	-1.04927500
H	5.21327700	-5.30080300	-2.62479900
H	4.41172200	-6.63200800	-1.77912800
C	-1.98581900	-4.57093100	2.20476100
H	-2.54290400	-4.00743500	1.44648200
H	-2.71573000	-5.18953900	2.74930700
Br	-7.39298000	-0.98330600	-3.02339000
Br	7.57594300	-0.82724900	-2.02575800
In	-0.08248700	-0.42632700	0.40169300
C	3.15680900	1.67757300	-3.10908700
C	3.69088300	0.36470800	-2.62424100
C	2.71411400	-0.30026300	-2.00137600
C	1.40393700	0.48907300	-2.04423700
N	1.81922100	1.69715700	-2.73791300
H	4.73040100	0.07512200	-2.77164000
H	2.78316300	-1.26936600	-1.51079500
O	0.88218700	0.79830000	-0.78838700
O	3.73734400	2.56472800	-3.69221500
C	1.00478300	2.87531400	-2.88456600
H	1.23386400	3.32364000	-3.86611600
H	-0.05424400	2.57543100	-2.90798600
C	0.32061400	-0.24877400	-2.89034200
C	-0.30879500	-1.44329300	-2.23118800

H	-0.46354600	0.48643900	-3.12064300
H	0.30272300	-2.35242200	-2.14224900
C	-1.62431800	-1.50924600	-1.91121000
H	-2.23208800	-0.60716200	-2.05660200
C	1.19695800	3.94446600	-1.82290500
C	2.07938200	3.80106900	-0.77348000
C	0.46409400	5.15805900	-1.95388200
C	2.28707000	4.84883400	0.16547700
H	2.63235400	2.86891000	-0.65511600
C	0.62919600	6.18941300	-1.05554900
H	-0.21980400	5.28033500	-2.79964100
C	3.20055000	4.72152900	1.24944500
C	1.54726500	6.07159600	0.02640900
H	0.06929600	7.12075500	-1.17524200
C	3.36704800	5.74584000	2.15976500
H	3.77531300	3.79707800	1.34467200
C	1.74663100	7.11206300	0.97662500
C	2.63206500	6.95206800	2.02391900
H	4.07880600	5.63881200	2.98221300
H	1.18892000	8.04546200	0.86296100
H	2.78106600	7.76022300	2.74380600
H	0.77308000	-0.56125300	-3.84521700
C	-2.40294500	-2.74434900	-1.57714800
H	-1.73307500	-3.55139900	-1.23443400
H	-2.81162200	-3.10083900	-2.54302200
C	-3.57562000	-2.55454900	-0.60985400
H	-3.18500200	-2.30016200	0.38997100
H	-4.17366000	-1.68348000	-0.92474500
C	-4.47069400	-3.79755100	-0.56004600
H	-4.90239400	-3.95932100	-1.56297900
H	-3.85030700	-4.69168200	-0.36121000
C	-5.59627500	-3.71887100	0.46830000
H	-6.23891000	-4.61122200	0.43026600
H	-5.19867600	-3.64037000	1.49442700
H	-6.23500200	-2.84012300	0.28647700

INT-d

O	2.42199500	-0.05344600	-0.76478100
N	4.24665000	1.15363800	-1.23835000
C	7.28674200	-1.52893900	-2.53014700
H	7.24399100	-1.78670800	-3.59966700
H	7.62993800	-2.42849900	-1.99609100
H	8.04745100	-0.74499500	-2.39715300
O	0.13733800	0.46177400	-2.24311700
N	1.09389600	0.92071100	-3.12125900
C	4.86221700	-2.19469100	-2.17539200
H	3.87129400	-1.88886800	-1.80743000
H	5.17019300	-3.07025900	-1.58155800
H	4.77127300	-2.51750500	-3.22617500
C	5.90801500	-1.06639200	-2.04174100
H	5.58967900	-0.24330800	-2.70371900
N	0.14922000	-2.92309000	-3.03252900
O	0.94655700	-2.37879100	-2.05684900
O	-1.59652000	-1.62613900	-1.08908200
N	-3.33355400	-2.80565400	-1.88879500
C	4.53114000	3.45199100	1.10179600
H	3.78787400	4.24408400	1.28481500
H	4.81870700	3.50066900	0.03967700
H	5.43078600	3.68048300	1.69397200
C	3.96099100	2.07431300	1.48828500
H	3.03652600	1.91677500	0.90708200
C	3.54455500	2.05847900	2.96395400
H	3.12731900	1.08294400	3.25866100
H	2.78056100	2.82902200	3.14515400
H	4.38727100	2.28667600	3.63419800
H	-3.64256600	-3.59806900	-2.44567900
C	4.92564700	0.95078700	1.11221700
H	4.66644500	1.88738300	-1.80360500
C	5.72415100	0.32038700	2.07230600
H	5.67197700	0.61749300	3.11840800
C	6.60273200	-0.70252300	1.70235500
C	6.69453500	-1.13328400	0.37843800
H	7.37604700	-1.94522400	0.12664800
C	5.90754500	-0.53352500	-0.61273300
C	5.05436700	0.51606500	-0.22440800
C	2.96496200	0.84990900	-1.42406100
C	2.19233100	1.72458200	-2.39997500
H	2.87060500	2.06511400	-3.19806800
C	1.60457400	2.94643500	-1.68030400
H	0.88592400	2.60505700	-0.91893800
H	2.42520900	3.45375400	-1.15111600
C	0.93086700	3.87246800	-2.69069100
H	0.51496600	4.74940800	-2.18372900
H	1.67819000	4.24654600	-3.41363800
C	-0.16800000	3.10144100	-3.41178900
H	-0.94625200	2.80935100	-2.69403500
H	-0.65194000	3.71900900	-4.18405100
C	0.37720500	1.85686100	-4.09294800

H	1.10234100	2.11127600	-4.88200800
H	-0.43148400	1.25622400	-4.52230900
C	1.75419200	-0.21742800	-3.88970800
H	2.27579700	-0.83159700	-3.15117800
H	2.49445500	0.24883200	-4.55598100
C	0.82216100	-1.09337300	-4.72751200
H	1.47953000	-1.77678600	-5.28649800
H	0.32996700	-0.49393600	-5.50852900
C	-0.29769200	-1.87166800	-4.03699700
H	-0.93876000	-1.17610300	-3.48674400
H	-0.89460400	-2.39806500	-4.79643700
C	0.97712800	-4.00821700	-3.71710100
H	0.36368300	-4.41611300	-4.53599700
H	1.84614000	-3.49137400	-4.13722500
C	0.20913000	-5.72961500	-2.04236900
H	0.54357200	-6.44308900	-1.27470900
H	-0.38080400	-6.30808100	-2.77539400
C	-0.67864400	-4.66174100	-1.40056000
H	-1.59604800	-5.10465500	-0.98456200
H	-0.15466600	-4.16114700	-0.57358700
C	-1.09533000	-3.59516800	-2.42453700
H	-1.61395700	-4.07285500	-3.27007900
C	-2.02361800	-2.57697100	-1.76810800
C	-4.32297900	-2.05543300	-1.15116200
C	-4.89949200	-2.66395200	-0.01343400
C	-5.79923700	-1.90846000	0.74560300
H	-6.26170600	-2.33390600	1.63536100
C	-6.09851700	-0.59391500	0.37913200
C	-5.54464800	-0.02180000	-0.76474800
H	-5.81240800	0.99995900	-1.03560800
C	-4.64383800	-0.74576900	-1.55736800
C	-4.06019900	-0.09152600	-2.80264300
H	-3.38521800	-0.81765900	-3.28269300
C	-3.22410000	1.15030900	-2.45111200
H	-3.84371900	1.92611400	-1.97375100
H	-2.80419800	1.59118300	-3.36868200
H	-2.38931200	0.90655800	-1.77957600
C	-5.16364500	0.24100300	-3.82267500
H	-5.75320600	-0.65051100	-4.08586600
H	-4.72436000	0.64764300	-4.74742700
H	-5.86077200	0.99660800	-3.42823700
C	-4.49368400	-4.06631900	0.42901200
H	-4.23861000	-4.64303700	-0.47720600
C	-3.22590700	-3.98809700	1.30078300
H	-3.43602400	-3.44449600	2.23546400
H	-2.40974400	-3.45307800	0.79449800
H	-2.86724800	-4.99440300	1.56839100
C	-5.60804700	-4.83886300	1.14598100
H	-6.53879200	-4.84865100	0.55917400
H	-5.83157600	-4.41078500	2.13545100
H	-5.29620600	-5.88112300	1.31139600
C	1.41003400	-5.08218300	-2.73126200
H	2.07997300	-4.62374600	-1.98931600
H	1.99652200	-5.82913100	-3.28828800
Br	7.67640500	-1.53097500	3.03039900
Br	-7.25183600	0.43969500	1.47900100
In	0.41936400	-0.88317400	-0.59402700
C	-2.66052100	1.74200000	3.04144800
C	-3.45334100	0.63131700	2.42255700
C	-2.72556900	0.08962900	1.43095900
C	-1.44186600	0.83515100	1.33573500
N	-1.43081500	1.77806500	2.31529600
H	-4.45244300	0.36873300	2.76641200
H	-2.97217500	-0.72561400	0.75788700
O	-0.55010800	0.73270600	0.47265400
O	-2.93262000	2.48021300	3.94668400
C	-0.37088300	2.73590100	2.55264100
H	-0.51284900	3.10893900	3.57908800
H	0.58899300	2.19600600	2.52475500
C	-0.26451200	-1.11724400	3.30064200
C	-0.10121600	-1.96769700	2.26497200
H	0.47118400	-0.31050500	3.43085100
H	-0.82872000	-2.78318400	2.16906900
C	0.96263000	-1.89932700	1.23672600
H	1.84044100	-1.33356800	1.59061400
H	1.31788800	-2.90258000	0.94541600
C	-0.34555900	3.89731200	1.57829200
C	-1.28721600	4.05648200	0.58329100
C	0.68876400	4.86574900	1.71934800
C	-1.24478500	5.16369100	-0.30870300
H	-2.09690900	3.33369300	0.46223200
C	0.75616400	5.95423400	0.87821900
H	1.42413400	4.75293700	2.52076100
C	-2.19131300	5.32354500	-1.35850900
C	-0.20114300	6.13738700	-0.16029400
H	1.54672300	6.69839400	1.00547500
C	-2.10625500	6.39319200	-2.22685300
H	-2.99146500	4.58567300	-1.46530200

C	-0.14693700	7.23407000	-1.06477600
C	-1.07568100	7.35715400	-2.07869200
H	-2.84173800	6.51041300	-3.02642400
H	0.64254900	7.98049300	-0.94492900
H	-1.02676800	8.20486200	-2.76595300
C	-1.31851500	-1.22110600	4.35660700
H	-2.01336100	-2.04532000	4.11770000
H	-1.93512800	-0.30012900	4.35998200
C	-0.75540700	-1.40399300	5.77591200
H	-0.04266700	-0.58668900	5.99170100
H	-0.16607200	-2.33712900	5.81268900
C	-1.84145200	-1.43042000	6.85461700
H	-2.42340600	-0.49185400	6.80394900
H	-2.55677400	-2.24204500	6.62734100
C	-1.28273700	-1.61620600	8.26528000
H	-2.08594800	-1.63104500	9.01789800
H	-0.72535000	-2.56349900	8.35258000
H	-0.59157300	-0.79931000	8.53132100

TS-c

O	2.28669700	-0.39893600	-0.81538900
N	4.10074400	0.59398300	-1.65420900
C	6.96768200	-2.48255100	-1.90281600
H	6.88665400	-3.13440600	-2.78654300
H	7.36703400	-3.09903100	-1.08274900
H	7.70500400	-1.69616800	-2.12386500
O	-0.01075100	-0.40302000	-2.40436200
N	0.96240200	-0.29784300	-3.37383700
C	4.57835900	-2.99363500	-1.20274500
H	3.59189800	-2.58238800	-0.94144600
H	4.93146400	-3.57658800	-0.33677700
H	4.45961100	-3.69257600	-2.04802600
C	5.59631400	-1.88730800	-1.55423900
H	5.22653000	-1.37605700	-2.45858200
N	0.03396500	-3.83013000	-1.81271400
O	0.83503100	-2.95814600	-1.10938000
O	-1.64640100	-1.94745700	-0.37334500
N	-3.40141000	-3.32021900	-0.57103100
C	4.53009500	3.55584200	-0.38823400
H	3.82830800	4.39633400	-0.50578400
H	4.76225500	3.17301600	-1.39424100
H	5.46808200	3.94719200	0.03507400
C	3.92788200	2.47760400	0.53283600
H	2.96453800	2.15693900	0.09618400
C	3.60445000	3.08030800	1.90539900
H	3.15036300	2.34126000	2.58360100
H	2.89943300	3.91594500	1.79054900
H	4.50126500	3.48830000	2.39599500
H	-3.74247600	-4.25126700	-0.79660900
C	4.81701800	1.23631700	0.60480100
H	4.52723200	1.10424100	-2.42367600
C	5.58524600	0.94938500	1.73814200
H	5.57637800	1.61774100	2.59730200
C	6.37417100	-0.20460200	1.78774500
C	6.40522400	-1.10442200	0.72261600
H	7.01471600	-2.00464700	0.79984800
C	5.65011100	-0.85678700	-0.43122200
C	4.88913600	0.32593700	-0.47262800
C	2.82575000	0.23582700	-1.74352200
C	2.06039500	0.70642400	-2.97070000
H	2.74739200	0.74039900	-3.83094400
C	1.46801900	2.10419600	-2.73409200
H	0.74353500	2.05516000	-1.90562300
H	2.28503300	2.76740800	-2.41190100
C	0.80622200	2.61291900	-4.01334800
H	0.38295200	3.60923600	-3.84867800
H	1.56295000	2.71465200	-4.81243000
C	-0.28318300	1.63454800	-4.43547100
H	-1.07299300	1.60802200	-3.67273100
H	-0.75421900	1.94221400	-5.38160600
C	0.27101700	0.23407300	-4.62973100
H	1.01636600	0.19751400	-5.43979500
H	-0.52983400	-0.48250400	-4.83971200
C	1.60282300	-1.64726800	-3.66807100
H	2.14293900	-1.94537800	-2.76517700
H	2.32746500	-1.47776200	-4.47760100
C	0.64001400	-2.75888500	-4.08959700
H	1.27526900	-3.60668300	-4.38786500
H	0.11343300	-2.48000200	-5.01486700
C	-0.45064100	-3.22287300	-3.12249000
H	-1.09026700	-2.37671400	-2.85302000
H	-1.05858500	-3.99629500	-3.61432300
C	0.88463400	-5.06859300	-2.08709900
H	0.27698200	-5.74438200	-2.70932600
H	1.73999400	-4.70937500	-2.66806800
C	0.15797800	-6.13833100	0.07025800
H	0.50325400	-6.55352600	1.02872500
H	-0.42361800	-6.93451700	-0.42714100

C	-0.74224400	-4.93028200	0.32884400
H	-1.64831400	-5.22006600	0.88121900
H	-0.21994300	-4.17814200	0.93574900
C	-1.18795000	-4.25894300	-0.98004100
H	-1.73149100	-4.98390700	-1.60521300
C	-2.09627000	-3.07565900	-0.65249900
C	-4.33724900	-2.36043700	-0.02678700
C	-4.82174800	-2.59082100	1.28062800
C	-5.69712200	-1.64822500	1.82809500
H	-6.09286100	-1.78154600	2.83404800
C	-6.05591800	-0.51306400	1.09639900
C	-5.56794100	-0.30522100	-0.19209400
H	-5.86541700	0.59085900	-0.73730500
C	-4.69272500	-1.22701600	-0.78189100
C	-4.16712100	-0.95105300	-2.18463500
H	-3.47399200	-1.76220600	-2.45792600
C	-3.37714600	0.36805500	-2.23519700
H	-4.03013300	1.22609600	-2.01248500
H	-2.96585900	0.52289600	-3.24415500
H	-2.54328000	0.38187000	-1.51979800
C	-5.30677900	-0.96538600	-3.21868400
H	-5.85932600	-1.91740600	-3.19968200
H	-4.90776800	-0.81921200	-4.23509400
H	-6.03006600	-0.15728700	-3.02840900
C	-4.32801900	-3.76935900	2.11475900
H	-4.11167300	-4.60581400	1.42697600
C	-3.00616800	-3.38744700	2.81186500
H	-3.17921900	-2.57242900	3.53241100
H	-2.25024900	-3.03360300	2.09469800
H	-2.58749300	-4.24479100	3.36230100
C	-5.35244000	-4.28917700	3.13100200
H	-6.32024500	-4.50703900	2.65520600
H	-5.52602000	-3.56663000	3.94323800
H	-4.98394800	-5.21484600	3.59834700
C	1.34525600	-5.73419200	-0.80120000
H	2.00401100	-5.03708700	-0.26259200
H	1.95104900	-6.61057100	-1.07876200
Br	7.40299400	-0.56066400	3.34227900
Br	-7.19197200	0.78542800	1.88770300
In	0.28791700	-1.01238900	-0.38994000
C	-2.44714600	2.73615600	2.23165900
C	-3.23622800	1.46554400	2.16297800
C	-2.46241500	0.50336600	1.64074900
C	-1.08592000	1.04945300	1.37762900
N	-1.18822700	2.42246600	1.70383200
H	-4.27653500	1.41074100	2.48107600
H	-2.72489600	-0.52906700	1.42084100
O	-0.43943800	0.75489600	0.26768300
O	-2.77864700	3.82661000	2.63142400
C	-0.18143300	3.41763000	1.43569700
H	-0.26834100	4.18771400	2.21954300
H	0.80961500	2.95269600	1.54574600
C	0.00623300	0.39297400	2.85176800
C	0.13262300	-0.99973300	2.60311000
H	0.89295300	0.95588600	2.52913200
H	-0.62691500	-1.64999700	3.05741300
C	1.05863600	-1.58049700	1.72984000
H	2.01029100	-1.05424800	1.57511800
H	1.14837600	-2.67197000	1.71704500
C	-0.28649200	4.09066200	0.08031300
C	-1.26449800	3.76706400	-0.83624400
C	0.64224900	5.12493800	-0.22822900
C	-1.37176000	4.45462800	-2.07704200
H	-1.97871400	2.97245000	-0.61426200
C	0.57092000	5.80922200	-1.42149100
H	1.40491100	5.39695200	0.50734700
C	-2.36985600	4.12933100	-3.03751600
C	-0.43648300	5.50096500	-2.37955700
H	1.28027200	6.61191100	-1.63974100
C	-2.43595100	4.79823700	-4.24319600
H	-3.08904000	3.34113600	-2.80174900
C	-0.53684100	6.17864300	-3.62665500
C	-1.51107500	5.83211600	-4.54142000
H	-3.21206300	4.54440000	-4.96948100
H	0.17025100	6.98175000	-3.85039100
H	-1.58142100	6.36209100	-5.49410900
C	-0.56440300	0.86160900	4.18651500
H	-0.62605800	0.01322600	4.88894000
H	-1.60409400	1.20803700	4.06909000
C	0.26099600	1.98538500	4.82365500
H	0.38056400	2.80546100	4.09467600
H	1.28116200	1.61748500	5.03898200
C	-0.37004300	2.54532100	6.10033500
H	-1.38040300	2.92263500	5.86043200
H	-0.51362100	1.72464400	6.82612100
C	0.45888400	3.66077600	6.73656000
H	-0.02212400	4.04959200	7.64686600
H	1.46391100	3.30356800	7.01662700

H	0.58702800	4.50727200	6.04128400

INT-e

O	2.20830700	-0.16949800	-0.86373500
N	4.10179300	0.81846200	-1.50578700
C	6.87102300	-2.29297100	-2.12941900
H	6.80645000	-2.79307500	-3.10828800
H	7.20918900	-3.04774900	-1.40282900
H	7.64639500	-1.51488000	-2.19323100
O	-0.00737700	0.08653300	-2.60269500
N	1.03796000	0.28834600	-3.47891900
C	4.43419500	-2.80006800	-1.61270500
H	3.45369200	-2.39167200	-1.32607300
H	4.72637900	-3.52778400	-0.83828300
H	4.32690700	-3.35196100	-2.56224000
C	5.50861000	-1.69976600	-1.74473200
H	5.19966200	-1.03774200	-2.57064800
N	0.09329800	-3.40772500	-2.29313100
O	0.83975300	-2.58198600	-1.47536300
O	-1.66594600	-1.78568100	-0.68490700
N	-3.37496300	-3.17802300	-1.05200400
C	4.55582400	3.52269200	0.19239500
H	3.88519500	4.39595400	0.19538100
H	4.78044300	3.28064600	-0.85781800
H	5.50406800	3.81466400	0.66959000
C	3.90579200	2.34930100	0.95087400
H	2.93276100	2.13050600	0.47376800
C	3.60091700	2.77037600	2.39337900
H	3.11373800	1.96567400	2.96523800
H	2.93022900	3.64036700	2.39342700
H	4.51220200	3.07032100	2.93297200
H	-3.68540700	-4.09075700	-1.37585000
C	4.74394300	1.07440000	0.85381700
H	4.58693200	1.39642800	-2.18780900
C	5.44837900	0.57579800	1.95542900
H	5.42679900	1.09966100	2.90915900
C	6.19005800	-0.60563800	1.85177000
C	6.23891300	-1.32432600	0.65749100
H	6.81254400	-2.24995700	0.61256900
C	5.54716100	-0.86327600	-0.47002600
C	4.82972300	0.34158800	-0.35069900
C	2.81669800	0.54688800	-1.68673000
C	2.12550800	1.20219300	-2.87326700
H	2.85942700	1.34125400	-3.68249300
C	1.53558500	2.56426700	-2.47439700
H	0.76804100	2.41880900	-1.69751000
H	2.34143200	3.15992800	-2.01895400
C	0.95160600	3.26156600	-3.70195700
H	0.51806900	4.22565100	-3.41474900
H	1.75699000	3.47602600	-4.42784500
C	-0.10982200	2.37099400	-4.33851700
H	-0.95577700	2.24913100	-3.64819600
H	-0.50686200	2.82061900	-5.26156400
C	0.44844100	1.00434300	-4.69588500
H	1.25569900	1.07175600	-5.44184200
H	-0.33654800	0.33760600	-5.06839400
C	1.66025100	-1.03492300	-3.90022600
H	2.18392500	-1.43457900	-3.02725500
H	2.40047500	-0.79577800	-4.67716600
C	0.68585300	-2.08197400	-4.44627300
H	1.31516600	-2.88260000	-4.86393800
H	0.14422600	-1.68393200	-5.31782100
C	-0.39469700	-2.67783300	-3.53883700
H	-1.06813200	-1.88789900	-3.19272200
H	-0.97385500	-3.41292800	-4.11656100
C	1.01365300	-4.56106300	-2.68533300
H	0.45214800	-5.18973100	-3.39404000
H	1.85894400	-4.09559700	-3.20184300
C	0.31008400	-5.90516300	-0.67847300
H	0.66175200	-6.40738400	0.23493000
H	-0.22080100	-6.66900400	-1.27341800
C	-0.65740300	-4.78156200	-0.30614300
H	-1.55502200	-5.17831600	0.19031200
H	-0.18730500	-4.07583300	0.39301400
C	-1.11940600	-3.98881900	-1.53940000
H	-1.61725300	-4.66120700	-2.25461600
C	-2.07962700	-2.88952900	-1.09347200
C	-4.34281400	-2.31814000	-0.40287300
C	-4.88192600	-2.76262800	0.82575300
C	-5.78400900	-1.92267200	1.48458700
H	-6.21970200	-2.21984300	2.43751600
C	-6.11559600	-0.67953100	0.93914100
C	-5.57539500	-0.26220400	-0.27559400
H	-5.85249900	0.71359100	-0.67511900
C	-4.67217800	-1.07409200	-0.97403300
C	-4.09281300	-0.56378500	-2.28732100
H	-3.36618600	-1.30487000	-2.65492600
C	-3.34021300	0.76334900	-2.08429500

H	-4.03962600	1.57536900	-1.83192400
H	-2.82022400	1.05220400	-3.01005700
H	-2.59824600	0.70352800	-1.27568700
C	-5.18293900	-0.43466100	-3.36557400
H	-5.69884600	-1.39192900	-3.53790400
H	-4.74398000	-0.10268300	-4.32006300
H	-5.94442100	0.30623900	-3.07675800
C	-4.41500100	-4.06159300	1.47694100
H	-4.16388900	-4.77740200	0.67360700
C	-3.12716500	-3.79676500	2.28304700
H	-3.33422500	-3.10852000	3.11732600
H	-2.34545600	-3.33079300	1.66356800
H	-2.72386300	-4.73117700	2.70436100
C	-5.47707200	-4.74098000	2.35047000
H	-6.42234600	-4.87876500	1.80466500
H	-5.68970700	-4.16031600	3.26113300
H	-5.12138300	-5.73010100	2.67635000
C	1.48744700	-5.34641800	-1.47431300
H	2.10476300	-4.68570800	-0.84817100
H	2.14070700	-6.15444400	-1.83816500
Br	7.12842400	-1.25030200	3.36952000
Br	-7.28188300	0.47505700	1.89025400
In	0.18013300	-0.72620500	-0.68129600
C	-2.47211200	2.37580400	2.53869200
C	-3.22293200	1.09874900	2.31111100
C	-2.38171400	0.18372000	1.82274100
C	-0.96853900	0.75522200	1.69297400
N	-1.16743000	2.11913100	2.14521500
H	-4.29116400	1.01252900	2.50656300
H	-2.62253400	-0.83186500	1.51280200
O	-0.50564400	0.76287600	0.37579500
O	-2.88119000	3.43071200	2.96892900
C	-0.17198000	3.15616200	2.06840500
H	-0.31865600	3.82342800	2.93444300
H	0.82292800	2.70339700	2.18636700
C	0.07839200	0.00045500	2.60608700
C	0.30582800	-1.39406500	2.09421500
H	1.02202400	0.55770500	2.47837800
H	-0.53285700	-2.09223200	2.22114200
C	1.45619400	-1.85454700	1.55748600
H	2.34159600	-1.21602000	1.46708800
H	1.58000900	-2.90246400	1.27029200
C	-0.20205000	4.00576300	0.80931500
C	-1.12174600	3.81042100	-0.19954400
C	0.72740000	5.07941800	0.70038600
C	-1.17555500	4.67322800	-1.32912600
H	-1.82602200	2.98111900	-0.13375600
C	0.71661300	5.92468400	-0.38767700
H	1.44082100	5.25370000	1.51123800
C	-2.13523300	4.50044600	-2.36619400
C	-0.23821700	5.75604300	-1.43036600
H	1.42619100	6.75419600	-0.44893800
C	-2.16686600	5.35237800	-3.45212700
H	-2.85762200	3.68512600	-2.28076200
C	-0.29832700	6.61953400	-2.56013800
C	-1.23936500	6.42181200	-3.55133600
H	-2.91758800	5.21638400	-4.23465000
H	0.40928500	7.45006300	-2.62879400
H	-1.28175200	7.09693800	-4.40919600
C	-0.26935300	-0.06908700	4.11327600
H	0.33079600	-0.88132900	4.55892400
H	-1.32345300	-0.37275100	4.23112600
C	-0.00062100	1.20704600	4.92053800
H	-0.67001400	2.01587800	4.59489100
H	1.02863700	1.55701300	4.71604900
C	-0.17470100	0.99909200	6.42798700
H	-1.19548600	0.62376400	6.62325700
H	0.51135500	0.20338800	6.77134400
C	0.06613500	2.27582700	7.23347900
H	-0.06607400	2.10245700	8.31232300
H	1.08963900	2.65730200	7.08022700
H	-0.63416400	3.07307100	6.93443800

PRO-a

C	0.62863600	-2.28935600	1.35744500
C	-0.50209100	-1.77047500	2.19261700
C	-1.37241700	-1.11314000	1.41625700
C	-0.96275900	-1.11423400	-0.07356200
N	0.33415400	-1.95350100	0.07044700
H	-0.51425500	-1.90891500	3.27627800
H	-2.28367300	-0.59762800	1.72676900
O	-0.77620200	0.05679200	-0.63182700
O	1.63786800	-2.87329400	1.74679600
C	1.33103100	-1.95283100	-0.96594700
H	1.72172700	-2.97274300	-1.13138100
H	0.82134000	-1.61831500	-1.88432600
C	-1.96952400	-2.03740400	-0.86937200
C	-3.37572200	-1.49896600	-0.98042600

H	-1.53391600	-2.13627600	-1.88174300
H	-4.18582500	-2.24580600	-0.96453300
C	-3.71109400	-0.20645600	-1.10238500
H	-2.88483000	0.51700500	-1.09971400
C	2.49023300	-1.00145800	-0.69949300
C	2.22694700	0.32920000	-0.41725900
C	3.83483700	-1.45385500	-0.73357800
C	3.28729900	1.24393600	-0.18280900
H	1.16948700	0.63747800	-0.37306300
C	4.88747200	-0.58842700	-0.51217700
H	4.03035000	-2.51347600	-0.92391200
C	3.04223200	2.61861400	0.10400300
C	4.64957700	0.78499600	-0.23457000
H	5.91962700	-0.95273500	-0.53391800
C	4.08208500	3.49771300	0.32629000
H	2.00361300	2.95831300	0.14440100
C	5.69968000	1.71757700	0.00089100
C	5.42660100	3.04243600	0.27393800
H	3.87518400	4.54926500	0.54617800
H	6.73485300	1.36288400	-0.03744700
H	6.24495600	3.74635100	0.45306400
H	-1.98953500	-3.05141400	-0.43262300
C	-5.12096500	0.30888800	-1.17383300
H	-5.83756600	-0.53267200	-1.22987800
H	-5.26049500	0.89625000	-2.10404700
C	-5.49005300	1.21010400	0.01573200
H	-5.38477200	0.62851900	0.94976900
H	-4.75178600	2.02958500	0.09031100
C	-6.90033200	1.79987600	-0.06584900
H	-6.99761900	2.38056800	-1.00215100
H	-7.63487700	0.97688200	-0.14749200
C	-7.25788200	2.68842200	1.12692700
H	-8.27741100	3.10116200	1.04347700
H	-7.20130000	2.12392600	2.07327200
H	-6.55844100	3.53736700	1.21279100

PRO-b

C	-0.77350000	-0.52940000	1.61280000
C	-1.15390000	0.66280000	2.43620000
C	-1.41880000	1.69940000	1.63020000
C	-1.30410000	1.33760000	0.13790000
N	-0.90580000	-0.15000000	0.30900000
H	-1.13750000	0.62540000	3.52780000
H	-1.69300000	2.71600000	1.91910000
O	-0.46650000	2.02670000	-0.58230000
O	-0.38150000	-1.62160000	2.01660000
C	-0.22680000	-0.84480000	-0.75410000
H	-0.62100000	-1.87080000	-0.86410000
H	-0.44830000	-0.28040000	-1.67400000
C	-2.79810000	1.34630000	-0.50710000
C	-3.35110000	2.75040000	-0.47460000
H	-2.57160000	1.09060000	-1.55670000
H	-4.24910000	2.90240000	0.14310000
C	-2.81340000	3.80980000	-1.09270000
H	-1.88460000	3.69180000	-1.65640000
H	-3.25130000	4.80960000	-0.99270000
C	1.28430000	-0.90030000	-0.58090000
C	1.99970000	0.27830000	-0.44390000
C	1.97270000	-2.14090000	-0.54610000
C	3.41140000	0.25690000	-0.29290000
H	1.42710000	1.21900000	-0.44000000
C	3.34460000	-2.19460000	-0.40390000
H	1.39430000	-3.06670000	-0.61760000
C	4.16960000	1.45610000	-0.15570000
C	4.10710000	-1.00180000	-0.27760000
H	3.86180000	-3.15890000	-0.37180000
C	5.54160000	1.42060000	-0.01370000
H	3.63250000	2.40860000	-0.16480000
C	5.52320000	-1.00380000	-0.12840000
C	6.22670000	0.17650000	-0.00030000
H	6.10730000	2.35100000	0.09150000
H	6.04810000	-1.96460000	-0.11530000
H	7.31470000	0.15770000	0.11420000
C	-3.79250000	0.31520000	0.06600000
H	-4.81480000	0.74040000	0.07260000
H	-3.54770000	0.12000000	1.12480000
C	-3.84400000	-1.01690000	-0.68530000
H	-2.82830000	-1.43340000	-0.75530000
H	-4.17730000	-0.83830000	-1.72610000
C	-4.75850000	-2.05480000	-0.03070000
H	-4.40780000	-2.23640000	1.00140000
H	-5.78020000	-1.64020000	0.06480000
C	-4.81120000	-3.38110000	-0.79120000
H	-5.46700000	-4.11690000	-0.29550000
H	-5.18660000	-3.23700000	-1.81940000
H	-3.80590000	-3.82850000	-0.87040000

INT5

O	-2.32810600	-0.39554800	0.94265100
N	-4.02284800	0.97851800	1.42612300
C	-6.63105000	-2.08008200	2.13663500
H	-6.51511600	-2.68721000	3.04833900
H	-7.21715800	-2.67420100	1.41842000
H	-7.22156300	-1.18681800	2.39171600
O	0.08957400	0.07675200	2.18993400
N	-0.78285300	0.43922500	3.19091900
C	-4.42330800	-2.95266400	1.22447900
H	-3.42590800	-2.68497000	0.84866300
H	-4.92548100	-3.56557300	0.45951100
H	-4.29803200	-3.58251400	2.12054600
C	-5.25385600	-1.70128500	1.56460500
H	-4.71770800	-1.15367300	2.35603300
N	0.28756000	-3.35280400	2.67570200
O	-0.64623200	-2.79142100	1.83933400
O	1.71336000	-1.78921300	0.67152500
N	3.57269800	-2.99410200	0.99392400
C	-5.07249800	3.74432800	0.05462800
H	-4.54724700	4.71068000	0.11224500
H	-5.23587800	3.39257700	1.08688800
H	-6.06843500	3.92319500	-0.37900700
C	-4.28152700	2.74383000	-0.81133900
H	-3.28055900	2.61978000	-0.35948600
C	-4.06393700	3.32720300	-2.21223300
H	-3.52225700	2.62923700	-2.86624800
H	-3.48046800	4.25779100	-2.14474200
H	-5.01627200	3.58311600	-2.70115900
H	4.00204900	-3.81966200	1.40335400
C	-4.93523300	1.36352600	-0.80757300
H	-4.36388700	1.76294200	1.97516000
C	-5.65982500	0.89382300	-1.90623700
H	-5.77924600	1.50875800	-2.79668900
C	-6.22641200	-0.38484800	-1.88279900
C	-6.09556700	-1.20980200	-0.76723800
H	-6.54839100	-2.20182700	-0.77865800
C	-5.38600600	-0.77433000	0.36106500
C	-4.82041400	0.51285500	0.31618400
C	-2.78127800	0.53942800	1.62502600
C	-1.94305100	1.29744300	2.64829700
H	-2.56531300	1.53761800	3.52497600
C	-1.41707300	2.59620600	2.01535000
H	-0.78848200	2.33479100	1.15085500
H	-2.28125800	3.16042300	1.63543600
C	-0.63138400	3.42214000	3.02846600
H	-0.25459500	4.33409800	2.55169600
H	-1.29610600	3.73960700	3.85207600
C	0.51975400	2.58365200	3.56799200
H	1.22294100	2.35113600	2.75720000
H	1.08344500	3.12431100	4.34374700
C	0.01696000	1.28754600	4.18001200
H	-0.64120900	1.47298200	5.04367200
H	0.85223100	0.65188600	4.49027700
C	-1.34913700	-0.78266300	3.90306300
H	-1.92196900	-1.33936900	3.15651600
H	-2.03377000	-0.40477600	4.67653200
C	-0.31790300	-1.70051200	4.56488500
H	-0.90215300	-2.46645700	5.09695000
H	0.21166300	-1.16435900	5.36684700
C	0.77505200	-2.35409000	3.71519200
H	1.32769000	-1.58366400	3.16847500
H	1.46406600	-2.90237000	4.37451000
C	-0.39422600	-4.53654700	3.36106400
H	0.33039400	-4.95732000	4.07601100
H	-1.23774700	-4.10697900	3.91038100
C	0.28760300	-6.10063800	1.51546900
H	-0.07762900	-6.79250400	0.74203200
H	0.98467000	-6.67543800	2.15082400
C	1.03089100	-4.94010200	0.85449300
H	1.92110300	-5.29463600	0.31435500
H	0.38636900	-4.43454100	0.12219200
C	1.49259100	-3.89499800	1.88476600
H	2.14683900	-4.36999900	2.63241700
C	2.26481500	-2.78921600	1.16492900
C	4.36440200	-2.16222700	0.11675800
C	4.67732200	-2.66680800	-1.16530200
C	5.37688800	-1.83199600	-2.04341300
H	5.63528600	-2.17783500	-3.04361700
C	5.73405500	-0.53986600	-1.65061800
C	5.43529100	-0.06747100	-0.37392300
H	5.73999000	0.94082000	-0.09184600
C	4.74257100	-0.87385400	0.53936600
C	4.42534300	-0.32327300	1.92362500
H	3.89914300	-1.10761400	2.49049500
C	3.48770400	0.89236800	1.83770200
H	3.95918200	1.71168000	1.27310000
H	3.27015900	1.27629000	2.84662200
H	2.53339200	0.64168400	1.35453300

C	5.71127800	0.01006400	2.70030100
H	6.37977300	-0.86167800	2.76899900
H	5.46889000	0.33825100	3.72343600
H	6.27395400	0.82410300	2.21722500
C	4.19218400	-4.03955200	-1.62064600
H	4.12084700	-4.68424600	-0.72767900
C	2.77754400	-3.91598200	-2.21988100
H	2.80848300	-3.31445100	-3.14206500
H	2.07624600	-3.42189000	-1.53132000
H	2.36888800	-4.90571500	-2.47717200
C	5.14396400	-4.74276000	-2.59690000
H	6.17089100	-4.78396600	-2.20394800
H	5.17254200	-4.23952800	-3.57572900
H	4.80400600	-5.77378200	-2.77706900
C	-0.87208000	-5.57050500	2.35556400
H	-1.63565400	-5.10730900	1.71338900
H	-1.35998600	-6.38188700	2.91748000
Br	-7.17054300	-1.01037800	-3.40655300
Br	6.61079400	0.60263800	-2.89012100
In	-0.35756100	-1.14602100	0.47535800
C	1.93015900	2.15762800	-3.17703300
C	2.74614000	0.91853200	-2.98165600
C	2.20045300	0.20240900	-1.98313200
C	1.01480700	0.94348000	-1.47250400
N	0.87457300	2.07378800	-2.21268500
H	3.63369400	0.70719100	-3.57578200
H	2.53306400	-0.73497300	-1.54441100
O	0.30298300	0.67829800	-0.48550200
O	2.06960600	3.07004500	-3.94246500
C	-0.09909100	3.12480600	-1.99129000
H	-0.20723100	3.65672500	-2.94911600
H	-1.06667000	2.65107000	-1.76704000
C	-0.71770100	-0.65006800	-3.38333600
C	-0.33152500	-1.68427400	-2.59456500
H	0.55149100	-2.24844300	-2.91272700
C	-0.99589400	-2.13470800	-1.34710300
H	-2.08477500	-1.96431200	-1.36679300
H	-0.84613300	-3.21526400	-1.18975900
C	0.26759700	4.11109400	-0.89850200
C	1.40052100	3.99004500	-0.12069200
C	-0.60723700	5.21515400	-0.68753800
C	1.71429800	4.94607900	0.88727400
H	2.09034100	3.15605000	-0.26775400
C	-0.32962600	6.16337700	0.27137200
H	-1.49703300	5.32015700	-1.31442600
C	2.86379000	4.82405300	1.71574000
C	0.83336700	6.06123300	1.08743100
H	-1.00022500	7.01503600	0.41217500
C	3.12752100	5.75605500	2.69922100
H	3.54136900	3.98159000	1.55861200
C	1.13618600	7.00858500	2.10406300
C	2.25674700	6.85828500	2.89557000
H	4.01774600	5.65534200	3.32479400
H	0.46784200	7.86138700	2.24845800
H	2.48255100	7.59388000	3.67094000
C	-1.93501600	0.18005300	-3.05584400
H	-1.91480700	1.14153400	-3.59006200
H	-2.86439400	-0.33588900	-3.35691800
H	-2.02947100	0.38402900	-1.97688600
C	-0.00608800	-0.32690200	-4.66459700
H	-0.69229000	-0.40741300	-5.52601800
H	0.35820200	0.71721300	-4.67422200
H	0.85026600	-0.99118900	-4.84958100

TS5

O	-2.29586700	-0.36420000	0.90096500
N	-4.05736600	0.94307800	1.31746300
C	-6.58193800	-2.19120800	2.06092100
H	-6.47689600	-2.74703100	3.00601800
H	-7.10396400	-2.84911800	1.34898500
H	-7.22791300	-1.31942300	2.24551700
O	0.07092800	0.22173700	2.28444900
N	-0.87885500	0.56569900	3.22029400
C	-4.29724600	-2.98862800	1.28033600
H	-3.28742400	-2.68793300	0.96820700
H	-4.72165400	-3.64236800	0.50203900
H	-4.20710900	-3.58980500	2.20036600
C	-5.20132000	-1.76698200	1.53037900
H	-4.72697300	-1.16191400	2.31974200
N	0.20095800	-3.23014900	2.66504200
O	-0.67872200	-2.63990800	1.78373400
O	1.69603800	-1.75601300	0.65776300
N	3.53214400	-2.96411000	1.06862300
C	-5.17480900	3.61446000	-0.16292400
H	-4.68992300	4.60250700	-0.12892000
H	-5.34086100	3.29022500	0.87805200
H	-6.16973300	3.73815700	-0.61755000
C	-4.32798700	2.62205500	-0.98477100

H	-3.33114200	2.55266200	-0.51242700
C	-4.11060200	3.17379000	-2.39830800
H	-3.53706900	2.47803500	-3.02660700
H	-3.55645700	4.12268500	-2.34757800
H	-5.06480700	3.38456500	-2.90497000
H	3.94274700	-3.78105100	1.51377800
C	-4.92548900	1.21693100	-0.95018400
H	-4.44590200	1.72508800	1.83838200
C	-5.60190800	0.67950100	-2.04890600
H	-5.72211300	1.25843700	-2.96312700
C	-6.11916000	-0.61913200	-1.99330300
C	-5.98765900	-1.39840700	-0.84471200
H	-6.40562400	-2.40563800	-0.83051200
C	-5.32682300	-0.89521800	0.28485400
C	-4.80810800	0.41010200	0.20495200
C	-2.80551500	0.56666100	1.55648100
C	-2.03008500	1.37524700	2.58921400
H	-2.69986400	1.62682600	3.42680400
C	-1.49742600	2.66548600	1.94201800
H	-0.81273500	2.39569200	1.12268500
H	-2.35111500	3.19430700	1.49304700
C	-0.79767600	3.54220700	2.97699400
H	-0.40840100	4.44573100	2.49375200
H	-1.52327100	3.87150600	3.74272400
C	0.33347300	2.75248600	3.62355900
H	1.09893800	2.51523600	2.87249000
H	0.82616200	3.33364800	4.41797900
C	-0.17655400	1.46236400	4.24212800
H	-0.90308600	1.65178200	5.04799500
H	0.64943400	0.85893500	4.63216900
C	-1.43614700	-0.67163800	3.90955300
H	-1.99084500	-1.23159900	3.15111000
H	-2.13810100	-0.31419200	4.67695500
C	-0.39583700	-1.57921600	4.57193700
H	-0.97161500	-2.33682300	5.12482600
H	0.14573800	-1.03060500	5.35731200
C	0.68948000	-2.24865900	3.72376500
H	1.27288200	-1.48701700	3.19723300
H	1.35478600	-2.82075100	4.38684300
C	-0.56162100	-4.37547100	3.32927800
H	0.10779800	-4.80741100	4.08978500
H	-1.41644100	-3.90331600	3.82334800
C	0.15994100	-6.00151100	1.55686500
H	-0.18546600	-6.70316800	0.78316900
H	0.80496100	-6.57933300	2.24215900
C	0.97130800	-4.88183800	0.90673700
H	1.87522000	-5.27601000	0.41959300
H	0.38016400	-4.37809700	0.13038500
C	1.41635800	-3.82003400	1.92655700
H	2.03663100	-4.28825600	2.70631600
C	2.22655100	-2.74586400	1.19993800
C	4.36354300	-2.16219500	0.19752100
C	4.76795500	-2.73298700	-1.03029000
C	5.52306400	-1.94104700	-1.90069400
H	5.85323100	-2.33629200	-2.86046700
C	5.84615700	-0.62617100	-1.55445700
C	5.44851000	-0.08687700	-0.33263800
H	5.72174700	0.93995200	-0.08836600
C	4.69472400	-0.84667400	0.57184800
C	4.27113900	-0.21653500	1.89214100
H	3.66897200	-0.95199700	2.44865200
C	3.39214500	1.02295700	1.66043500
H	3.95509300	1.80541700	1.12977700
H	3.07058700	1.44585200	2.62422000
H	2.49472600	0.79568400	1.06928100
C	5.49376800	0.11642300	2.76569600
H	6.11556800	-0.77339900	2.94872500
H	5.17345900	0.51886800	3.73984200
H	6.13213700	0.87590900	2.28813500
C	4.32060300	-4.13245500	-1.44249400
H	4.22013600	-4.74011900	-0.52575200
C	2.92991000	-4.05750200	-2.10338800
H	2.98744000	-3.48683900	-3.04395600
H	2.19674400	-3.55305600	-1.45621600
H	2.54842700	-5.06322900	-2.34011700
C	5.31852500	-4.86567600	-2.34769500
H	6.32921100	-4.87368800	-1.91309700
H	5.37964600	-4.40599600	-3.34614100
H	4.99957800	-5.90876300	-2.49365600
C	-1.02339200	-5.41289300	2.32080200
H	-1.73684600	-4.93853600	1.63077500
H	-1.56932400	-6.19342000	2.87288500
Br	-7.00243900	-1.33379500	-3.51372000
Br	6.81459300	0.45125900	-2.78105800
In	-0.27966700	-0.94258600	0.54735400
C	1.94055700	2.32627900	-2.99465500
C	2.84417500	1.16719800	-2.71863900
C	2.18062300	0.27214100	-1.97610000

C	0.75618300	0.72918700	-1.77039600
N	0.71951500	2.01450600	-2.37594600
H	3.87546700	1.13607600	-3.06847500
H	2.55065900	-0.66565500	-1.56337200
O	0.20737000	0.65907200	-0.56611300
O	2.17252000	3.35677400	-3.57914300
C	-0.27035300	3.03739900	-2.11319500
H	-0.47849700	3.56256400	-3.05915200
H	-1.20000900	2.54466100	-1.80340900
C	-0.28361600	-0.39414800	-2.96087400
C	-0.16134000	-1.66583500	-2.30395300
H	0.75424400	-2.22946500	-2.51950100
C	-1.01268500	-2.17316500	-1.32799100
H	-2.04887900	-1.81670700	-1.27711400
H	-0.87273700	-3.20851100	-1.00235100
C	0.11050400	4.06176300	-1.05880600
C	1.18640200	3.90883600	-0.20907400
C	-0.70452800	5.22399800	-0.94574300
C	1.50247000	4.89454700	0.76898600
H	1.81450100	3.01870500	-0.27732800
C	-0.43360100	6.19355100	-0.00628900
H	-1.54421500	5.35624000	-1.63433700
C	2.60161000	4.75388200	1.66139300
C	0.67414000	6.06212000	0.87828300
H	-1.06056800	7.08656000	0.06083300
C	2.86317400	5.71070300	2.62126500
H	3.24295400	3.87551500	1.57099500
C	0.97322600	7.03399300	1.87323800
C	2.04090200	6.86132500	2.73040900
H	3.71598800	5.59257900	3.29439100
H	0.34411400	7.92496500	1.94698600
H	2.26396200	7.61631200	3.48779900
C	-1.67925600	0.21675900	-2.93803800
H	-1.70109600	1.14183200	-3.52724100
H	-2.40722800	-0.47818200	-3.38817400
H	-2.02510300	0.44285500	-1.91906700
C	0.36946500	-0.32598400	-4.33423200
H	-0.29711400	-0.77544800	-5.08795100
H	0.54022800	0.71911600	-4.63208800
H	1.33183300	-0.85532300	-4.37311300

PRO5

O	-2.22218200	-0.30386400	0.91196100
N	-4.04236200	0.93960500	1.26810100
C	-6.48738400	-2.24557300	2.09232000
H	-6.39337900	-2.74559900	3.06922700
H	-6.95190200	-2.96352200	1.39885400
H	-7.17831300	-1.39660800	2.20652300
O	0.08670200	0.37932400	2.39321600
N	-0.92562100	0.66713200	3.28508200
C	-4.14109900	-2.97355400	1.43502600
H	-3.13565900	-2.64091600	1.14315900
H	-4.50661600	-3.68503100	0.67746200
H	-4.05951000	-3.52402800	2.38738300
C	-5.10832200	-1.78519000	1.58904300
H	-4.69134700	-1.12007900	2.36257300
N	0.22856300	-3.12010800	2.64800900
O	-0.62183300	-2.50503000	1.75063500
O	1.76651300	-1.62550000	0.71522000
N	3.59321400	-2.84995300	1.12201800
C	-5.22237200	3.49772200	-0.32699200
H	-4.77725200	4.50466700	-0.33406500
H	-5.37078900	3.20960100	0.72711800
H	-6.22311900	3.56333600	-0.78092300
C	-4.33704800	2.51112100	-1.11520600
H	-3.33510100	2.50260300	-0.64677900
C	-4.15625200	3.01913600	-2.55000800
H	-3.55306300	2.33089400	-3.15841600
H	-3.64997100	3.99464900	-2.53811800
H	-5.12391400	3.16312800	-3.05464200
H	3.99231400	-3.68181500	1.55009900
C	-4.87499500	1.08433400	-1.02765700
H	-4.47609900	1.71136200	1.76863900
C	-5.49800500	0.46604100	-2.11584000
H	-5.61769100	0.99536400	-3.05946000
C	-5.95769200	-0.85098400	-2.01340000
C	-5.83001600	-1.56837500	-0.82447300
H	-6.20881800	-2.58973000	-0.77193000
C	-5.22454300	-0.98345000	0.29628300
C	-4.75251800	0.33584700	0.16495400
C	-2.78569400	0.61413700	1.54508000
C	-2.07497000	1.44520600	2.60784500
H	-2.78556100	1.66584000	3.42013500
C	-1.55817700	2.76054100	1.99783100
H	-0.83511300	2.52998000	1.19921000
H	-2.41073000	3.26502500	1.51849800
C	-0.93330700	3.64623300	3.07442800
H	-0.54390300	4.56525600	2.62075100

H	-1.70646100	3.94870000	3.80390800
C	0.18523900	2.88566900	3.77652000
H	1.00028400	2.68358900	3.06862200
H	0.61189900	3.47500400	4.60255600
C	-0.31294200	1.57345700	4.35535600
H	-1.09143800	1.72780000	5.11883900
H	0.50913100	0.99316800	4.78700700
C	-1.45966300	-0.60695300	3.92611000
H	-1.98863200	-1.16033800	3.14491600
H	-2.18412500	-0.29022600	4.69018800
C	-0.40680100	-1.50641800	4.58208100
H	-0.97474000	-2.27537600	5.12750000
H	0.12624100	-0.95753300	5.37310200
C	0.69286000	-2.16005200	3.73803600
H	1.29252600	-1.39044100	3.24239600
H	1.34362300	-2.74678300	4.40262600
C	-0.56805700	-4.26657000	3.26857900
H	0.07307400	-4.71651400	4.04273400
H	-1.43324100	-3.79246900	3.74243300
C	0.18918600	-5.87175300	1.48993300
H	-0.14164900	-6.55582400	0.69445400
H	0.80803700	-6.46906500	2.18240200
C	1.03218700	-4.75091300	0.88351300
H	1.94646000	-5.14821100	0.41898400
H	0.47437900	-4.22642700	0.09602800
C	1.45848300	-3.71067100	1.93270100
H	2.05357100	-4.19522400	2.72188500
C	2.28900700	-2.62998700	1.24175000
C	4.44374500	-2.03523300	0.28046500
C	4.90901700	-2.60587700	-0.92566200
C	5.67833700	-1.80260300	-1.77232000
H	6.05213500	-2.19593300	-2.71668800
C	5.95590600	-0.47735600	-1.42601100
C	5.50171600	0.05993000	-0.22299400
H	5.74166400	1.09457100	0.02324300
C	4.73292200	-0.71080600	0.65868500
C	4.24998500	-0.08111700	1.95847100
H	3.62803600	-0.81788700	2.49056600
C	3.37670100	1.15370200	1.68444600
H	3.97595000	1.96065400	1.23652500
H	2.95285700	1.53927700	2.62380300
H	2.54916300	0.93541100	0.99546800
C	5.43071200	0.25902100	2.88498300
H	6.04132200	-0.62988800	3.10636000
H	5.06599100	0.67292000	3.83861900
H	6.09215700	1.01193900	2.42910500
C	4.50682700	-4.01623000	-1.34740400
H	4.38797200	-4.62490100	-0.43287300
C	3.13909700	-3.97212200	-2.05652600
H	3.21146300	-3.39377100	-2.99093900
H	2.37323400	-3.48886300	-1.43131700
H	2.78936000	-4.98547000	-2.30932300
C	5.55095700	-4.73044600	-2.21490200
H	6.54621800	-4.71403300	-1.74631700
H	5.63524500	-4.27302500	-3.21260100
H	5.26028300	-5.78089000	-2.36691400
C	-1.00900600	-5.28424500	2.23108200
H	-1.70219700	-4.79515100	1.53110700
H	-1.57580600	-6.06831200	2.75646400
Br	-6.75634100	-1.67743600	-3.52366000
Br	6.93366900	0.61661400	-2.62809700
In	-0.17200000	-0.75107900	0.65014900
C	1.93006600	2.19025100	-3.06538600
C	2.83125200	1.05038700	-2.70889000
C	2.12061900	0.12760300	-2.05674900
C	0.64629200	0.53235000	-1.96034600
N	0.66211300	1.83914700	-2.60585500
H	3.89619800	1.05800800	-2.93874700
H	2.49328300	-0.79980900	-1.62297800
O	0.20344800	0.65849400	-0.65001400
O	2.21173400	3.23857000	-3.59831200
C	-0.34567400	2.86414300	-2.42821300
H	-0.48813700	3.37628400	-3.39395600
H	-1.29584900	2.38135100	-2.17864700
C	-0.28642900	-0.51678500	-2.76845200
C	-0.26213600	-1.82255300	-2.00908900
H	0.68832400	-2.36851000	-2.05207300
C	-1.27933000	-2.38076400	-1.31469100
H	-2.27626200	-1.93299300	-1.27010200
H	-1.17646900	-3.36552800	-0.85250500
C	-0.06704900	3.91506400	-1.36715100
C	0.93639200	3.80460700	-0.42784800
C	-0.91487200	5.05940900	-1.34337900
C	1.14317200	4.81487200	0.55392000
H	1.58129200	2.92502500	-0.42532000
C	-0.75872800	6.04523500	-0.39509200
H	-1.68911800	5.16410800	-2.10865300
C	2.17877500	4.72723400	1.52586200

C	0.27171800	5.95555400	0.58246600
H	-1.41328400	6.92088800	-0.39575900
C	2.33459100	5.70304300	2.48982900
H	2.85710000	3.87350000	1.49205600
C	0.46049600	6.94817900	1.58438000
C	1.46474200	6.82306500	2.52339500
H	3.14050300	5.62469600	3.22393400
H	-0.20149800	7.81811800	1.59665500
H	1.60337900	7.59436000	3.28455500
C	-1.72072500	0.01617500	-2.90022500
H	-1.74528600	0.86425800	-3.59482600
H	-2.38307300	-0.75840100	-3.31486500
H	-2.13689100	0.33835800	-1.93528000
C	0.28790100	-0.77147100	-4.17683800
H	-0.40198300	-1.39341800	-4.76693600
H	0.41889100	0.18742000	-4.69941800
H	1.26498100	-1.27492200	-4.14801900

INT6

O	-2.35661100	-0.14205000	0.65508000
N	-4.09320100	1.11012500	1.31092000
C	-7.06472900	-1.71449400	2.35734200
H	-6.98192700	-2.12517600	3.37558400
H	-7.48313100	-2.51032500	1.72191900
H	-7.78759200	-0.88507300	2.38016700
O	0.04796400	0.21652200	1.95193800
N	-0.82944000	0.58102100	2.95111100
C	-4.69783600	-2.43058500	1.78042800
H	-3.70066200	-2.11235900	1.44299800
H	-5.05902500	-3.18786000	1.06613800
H	-4.60119700	-2.91935700	2.76436300
C	-5.68868400	-1.25033400	1.85919400
H	-5.29586100	-0.54115100	2.60687700
N	0.06645800	-3.23766600	2.39158200
O	-0.78957300	-2.59639000	1.52986800
O	1.67661800	-1.75719800	0.45898100
N	3.46634100	-2.98104900	1.07238400
C	-4.55439300	3.73657300	-0.55745800
H	-3.83744900	4.56666800	-0.65977400
H	-4.75185700	3.59633900	0.51687300
H	-5.50313000	4.04433200	-1.02350300
C	-4.00745300	2.46402100	-1.23183300
H	-3.03584100	2.22376600	-0.76438600
C	-3.71912100	2.73513400	-2.71325000
H	-3.33419600	1.84183100	-3.22621400
H	-2.96833400	3.53408300	-2.80625500
H	-4.61672900	3.07911200	-3.24955300
H	3.79794900	-3.81804300	1.54451800
C	-4.92132800	1.26296000	-0.99120300
H	-4.44812600	1.81901700	1.94754400
C	-5.74342100	0.75320100	-2.00094800
H	-5.75928000	1.21200400	-2.98805600
C	-6.54930800	-0.36423500	-1.76048500
C	-6.55360600	-0.99874700	-0.51827000
H	-7.18480300	-1.87422800	-0.36731100
C	-5.74779200	-0.51812800	0.52235300
C	-4.95667000	0.61584700	0.26376900
C	-2.82165000	0.72956700	1.40789400
C	-1.96231400	1.47603400	2.41594000
H	-2.57257500	1.72824800	3.29744400
C	-1.40721700	2.76809300	1.80042700
H	-0.74990400	2.50954100	0.95541200
H	-2.25424100	3.34071700	1.39427600
C	-0.64798300	3.56478000	2.85859700
H	-0.25533300	4.49185000	2.42750300
H	-1.33500200	3.85666700	3.67333500
C	0.48751200	2.70483800	3.39882000
H	1.20434900	2.49824200	2.59378500
H	1.03831500	3.22150800	4.19975900
C	-0.02275300	1.39004000	3.96554600
H	-0.67903400	1.55153200	4.83527200
H	0.80822300	0.73773400	4.25367100
C	-1.45364200	-0.62992600	3.63543500
H	-2.03120200	-1.15657300	2.87172500
H	-2.14173600	-0.23306900	4.39585400
C	-0.48134200	-1.59652300	4.31090400
H	-1.10946200	-2.33618200	4.83052800
H	0.06501400	-1.08973200	5.12097300
C	0.58413500	-2.29542900	3.46778000
H	1.19000800	-1.54513400	2.95016700
H	1.22908400	-2.89679500	4.12524200
C	-0.72392000	-4.38783900	3.01076600
H	-0.06448100	-4.87523200	3.74630100
H	-1.56434200	-3.91737000	3.53152600
C	-0.06142500	-5.93356000	1.13234300
H	-0.44293100	-6.56592600	0.31696600
H	0.56503700	-6.58284000	1.76935400
C	0.79331900	-4.80647300	0.55073200

H	1.68447900	-5.20186200	0.04024400
H	0.22412700	-4.22986700	-0.19060700
C	1.26840600	-3.84030100	1.64379500
H	1.83943600	-4.39139400	2.40678100
C	2.15026200	-2.75548900	1.03039000
C	4.43034100	-2.17244900	0.36465200
C	4.97803300	-2.69141800	-0.83037000
C	5.85090500	-1.87483100	-1.55711500
H	6.28713200	-2.22940100	-2.49028200
C	6.15842900	-0.59106600	-1.09993200
C	5.64487300	-0.11436800	0.10497500
H	5.92498200	0.88166200	0.44922100
C	4.77047800	-0.90136400	0.86628300
C	4.24300900	-0.35714900	2.18677500
H	3.58337200	-1.12019300	2.62943300
C	3.40321500	0.91352000	1.98224300
H	4.00140600	1.71755000	1.52501900
H	3.04890200	1.28792500	2.95478000
H	2.52387700	0.72665000	1.35062400
C	5.39148600	-0.12014000	3.18377800
H	5.98698900	-1.03269500	3.33941700
H	4.99475000	0.20183000	4.15974400
H	6.07519500	0.66685300	2.82928600
C	4.57734300	-4.06468600	-1.35896800
H	4.31901200	-4.69535600	-0.49054400
C	3.31392300	-3.93608700	-2.22936900
H	3.53644300	-3.35886700	-3.14046900
H	2.50581900	-3.40836300	-1.70355500
H	2.94376000	-4.92600100	-2.53916900
C	5.69927500	-4.78997000	-2.11304800
H	6.62479500	-4.83660700	-1.51967700
H	5.93157200	-4.30050200	-3.07148600
H	5.38951500	-5.81969400	-2.34702400
C	-1.21817600	-5.35697400	1.94828400
H	-1.92494000	-4.82550700	1.29449400
H	-1.77798300	-6.15518800	2.45965100
Br	-7.64281300	-1.03868000	-3.15761800
Br	7.27210300	0.53196700	-2.15225600
In	-0.37716500	-0.95807700	0.20470500
C	2.58375800	2.09580800	-3.25471700
C	3.42142200	0.93487400	-2.81929700
C	2.74587700	0.25234500	-1.88033300
C	1.46078200	0.96535300	-1.61876100
N	1.38617800	2.02071600	-2.46874900
H	4.40456600	0.73446600	-3.24267600
H	3.02706800	-0.64226900	-1.33375700
O	0.61158500	0.72647400	-0.74456800
O	2.79618900	2.94468600	-4.07266400
C	0.34231900	3.02756400	-2.49217900
H	0.41393300	3.52488700	-3.47200200
H	-0.63300400	2.51745400	-2.45218100
C	0.69039000	-1.47986300	-3.47337600
C	0.04018500	-2.13459200	-2.49312800
H	0.43609700	-3.11793100	-2.20584000
C	-1.15574700	-1.68735200	-1.72750800
C	0.44064600	4.05758300	-1.38327700
C	1.44546800	4.04833200	-0.43830500
C	-0.54427500	5.08544600	-1.34198000
C	1.51742200	5.04093500	0.57859300
H	2.22044200	3.27898100	-0.45404800
C	-0.50067200	6.06661900	-0.37669000
H	-1.32965800	5.10681200	-2.10240800
C	2.53042700	5.02692300	1.57688400
C	0.52473600	6.07658500	0.61171600
H	-1.25353700	6.85906300	-0.36508800
C	2.55725800	5.98819900	2.56713300
H	3.29161900	4.24249300	1.54632100
C	0.58592500	7.05907100	1.63861400
C	1.57718300	7.01359000	2.59828700
H	3.34332500	5.97202600	3.32596400
H	-0.16496800	7.85316400	1.65684700
H	1.61696100	7.77468900	3.38087400
H	0.34412100	-0.52062000	-3.86537100
H	1.57670700	-1.90887500	-3.94485900
C	-2.13118700	-2.85561700	-1.47569500
H	-1.64356300	-3.72784000	-1.01187600
H	-2.96438400	-2.55347600	-0.82282700
H	-2.56890800	-3.19801600	-2.43070000
C	-1.91291400	-0.53684600	-2.40876700
H	-2.23590000	-0.84284800	-3.42043000
H	-2.81145200	-0.26525000	-1.83863800
H	-1.30358200	0.37173000	-2.52545400

TS6

O	-2.24650900	-0.10193200	0.58383200
N	-4.05649600	0.99380200	1.32472100
C	-6.81540200	-2.03748800	2.37234000
H	-6.67008700	-2.47472600	3.37237400

H	-7.20744700	-2.83686700	1.72473100
H	-7.58639700	-1.25623400	2.44909000
O	0.09651700	0.22637100	2.03557600
N	-0.83381300	0.54299900	3.00136100
C	-4.43280800	-2.58424400	1.68713600
H	-3.46868000	-2.19327400	1.33199200
H	-4.77245300	-3.33738900	0.95792100
H	-4.27166000	-3.10130700	2.64828600
C	-5.49004700	-1.47174700	1.84284700
H	-5.11317500	-0.76642700	2.60242300
N	0.06251000	-3.23339100	2.22504700
O	-0.74469400	-2.53644600	1.35111900
O	1.72761900	-1.73305600	0.38606000
N	3.50136300	-2.96422000	1.01799500
C	-4.72282400	3.66242000	-0.42374000
H	-4.05218600	4.52899900	-0.53388100
H	-4.85398900	3.47738500	0.65410300
H	-5.70884000	3.93753400	-0.82882900
C	-4.14985500	2.44271000	-1.17030800
H	-3.14614300	2.23624200	-0.75759100
C	-3.94993800	2.77784300	-2.65306500
H	-3.55809500	1.92006800	-3.21943800
H	-3.23552700	3.60724200	-2.75301900
H	-4.88730600	3.10285100	-3.12995300
H	3.82614500	-3.80809100	1.48339400
C	-4.99111300	1.18949200	-0.93426000
H	-4.43996900	1.64842900	2.00211000
C	-5.83675400	0.67691000	-1.92359300
H	-5.92913500	1.17686900	-2.88618700
C	-6.56468800	-0.49525200	-1.69641300
C	-6.47008900	-1.18170700	-0.48515900
H	-7.04536800	-2.09630600	-0.34303000
C	-5.64342500	-0.69762900	0.53693400
C	-4.92678100	0.48809700	0.28931400
C	-2.76306200	0.69777300	1.38856300
C	-1.95341400	1.43662100	2.44012500
H	-2.60256100	1.65614700	3.30223000
C	-1.39325500	2.75291200	1.88476600
H	-0.69344200	2.53480400	1.06222700
H	-2.23098600	3.32433800	1.45705200
C	-0.70201100	3.52512100	3.00651300
H	-0.30622000	4.47315300	2.62896200
H	-1.43467400	3.77724200	3.79467600
C	0.42130300	2.66808400	3.57720400
H	1.17977900	2.49546200	2.80247000
H	0.92289800	3.17040100	4.41868300
C	-0.09256200	1.32982500	4.08197300
H	-0.79560200	1.45372900	4.92075600
H	0.73291600	0.67993700	4.39159400
C	-1.46812000	-0.70292900	3.60501000
H	-2.02949900	-1.18959700	2.80326100
H	-2.17393500	-0.35235900	4.37171600
C	-0.50283100	-1.70186700	4.23899300
H	-1.13257400	-2.46505800	4.72127300
H	0.04255500	-1.23453200	5.07309900
C	0.56499400	-2.35909400	3.36739300
H	1.19170100	-1.58755100	2.90967600
H	1.18936800	-3.00925800	3.99710800
C	-0.78952100	-4.37976800	2.76201700
H	-0.18516000	-4.90246800	3.52013600
H	-1.64763400	-3.90177600	3.24566900
C	-0.05344300	-5.89636900	0.89019900
H	-0.39854400	-6.50526400	0.04135400
H	0.52034900	-6.57129300	1.54946100
C	0.85801600	-4.77832000	0.38260200
H	1.77105300	-5.18420800	-0.07835900
H	0.34988000	-4.17810400	-0.38267600
C	1.28615900	-3.83537000	1.51304700
H	1.82179700	-4.40332200	2.28883600
C	2.19019800	-2.74175800	0.95243600
C	4.48308400	-2.13721900	0.35335600
C	5.05708100	-2.63140300	-0.83998600
C	5.97593000	-1.81654800	-1.50772600
H	6.43765000	-2.15137200	-2.43563200
C	6.29681700	-0.55444900	-1.00032600
C	5.73326300	-0.09326300	0.18780300
H	6.00859300	0.89312700	0.56192000
C	4.81068200	-0.87853200	0.89164700
C	4.20940000	-0.33472800	2.18046100
H	3.50064500	-1.08308900	2.56938600
C	3.42011500	0.96135600	1.93107600
H	4.07637700	1.75883100	1.54919700
H	2.98671500	1.32068700	2.87640200
H	2.60093100	0.81786300	1.21286400
C	5.29135300	-0.13799400	3.25721600
H	5.84559800	-1.06947900	3.44991100
H	4.83778600	0.19487200	4.20446600
H	6.02282500	0.62743600	2.95491300

C	4.62340000	-3.96760900	-1.43506200
H	4.36073400	-4.63943800	-0.59872700
C	3.35319000	-3.76638700	-2.28477700
H	3.57307300	-3.12725500	-3.15437500
H	2.55479000	-3.27113000	-1.71292500
H	2.97051600	-4.72906400	-2.65892800
C	5.71794900	-4.67565900	-2.24306900
H	6.65029500	-4.77126100	-1.66670600
H	5.94693000	-4.14096700	-3.17775600
H	5.38409100	-5.68560500	-2.52514200
C	-1.24333200	-5.30954900	1.64854000
H	-1.89710300	-4.74566900	0.96777300
H	-1.85192100	-6.10455500	2.10626100
Br	-7.68791900	-1.17257700	-3.06758000
Br	7.49214100	0.56127300	-1.96348800
In	-0.24791400	-0.80819200	0.20226700
C	2.66479600	2.24869600	-3.10194200
C	3.54752400	1.15713000	-2.59209300
C	2.81334700	0.32443500	-1.83845100
C	1.38551500	0.78842900	-1.83151100
N	1.38636100	1.97481000	-2.57876800
H	4.60887800	1.10606800	-2.83076700
H	3.12295600	-0.57220400	-1.31031400
O	0.61763100	0.73863100	-0.77955100
O	2.93379200	3.19872900	-3.79565000
C	0.29951700	2.92109700	-2.63685100
H	0.40125000	3.46974100	-3.58720600
H	-0.65450200	2.37003600	-2.67834700
C	0.65367100	-0.58072300	-3.19615200
C	0.04952000	-1.64489800	-2.49730800
H	0.64242600	-2.55683400	-2.34924300
C	-1.22310500	-1.60601300	-1.88990700
C	0.27568100	3.92100000	-1.49347200
C	1.23694800	3.93210200	-0.50420000
C	-0.74605800	4.91204000	-1.47723500
C	1.23849400	4.91988000	0.51847100
H	2.02802400	3.18089300	-0.49915100
C	-0.78380700	5.87742000	-0.49482700
H	-1.49223300	4.92385100	-2.27630800
C	2.23207800	4.94924600	1.53696500
C	0.20618600	5.91701700	0.52815900
H	-1.56461900	6.64267100	-0.50468300
C	2.20471700	5.91536600	2.52253400
H	3.02497100	4.19649700	1.52020000
C	0.20821000	6.90258800	1.55464300
C	1.18339400	6.90074500	2.53221200
H	2.97889300	5.93509200	3.29350800
H	-0.57244800	7.66784200	1.55502100
H	1.17935100	7.66674900	3.31108200
H	-0.01195400	0.13655800	-3.67947700
H	1.55440700	-0.80972400	-3.76753100
C	-1.92924800	-2.92023700	-1.57425100
H	-1.23113200	-3.74484500	-1.37603900
H	-2.61689900	-2.83166700	-0.72166700
H	-2.53632900	-3.21308100	-2.44903500
C	-2.18856200	-0.50465100	-2.31599600
H	-2.44552200	-0.63980600	-3.38185100
H	-3.11680400	-0.54880600	-1.73659900
H	-1.77155000	0.50457300	-2.20038800

PRO6

O	-2.14844600	-0.09707300	0.62631800
N	-3.99998200	1.00179400	1.25998200
C	-6.73523700	-2.06030800	2.26993900
H	-6.60301900	-2.49249700	3.27394100
H	-7.10851900	-2.86570200	1.61871300
H	-7.51482500	-1.28625700	2.33059300
O	0.13820100	0.36018400	2.23979900
N	-0.86706800	0.67189200	3.12778000
C	-4.33560800	-2.58646000	1.62740600
H	-3.36771500	-2.18780600	1.29089200
H	-4.65686600	-3.34536600	0.89557000
H	-4.18822600	-3.09981200	2.59269400
C	-5.40661900	-1.48353100	1.76106100
H	-5.04948100	-0.77160800	2.52393000
N	0.11962000	-3.11182400	2.38699700
O	-0.67034900	-2.43799400	1.46970100
O	1.79268900	-1.65483200	0.55655500
N	3.56786800	-2.90815700	1.09354400
C	-4.60242000	3.64472100	-0.53689600
H	-3.91856300	4.50163900	-0.63924800
H	-4.76301100	3.47343000	0.53926500
H	-5.57494800	3.92586900	-0.96943600
C	-4.02419800	2.41148700	-1.25707600
H	-3.02855200	2.20410900	-0.82406600
C	-3.79562100	2.72895900	-2.73964700
H	-3.38545500	1.86770600	-3.28865800
H	-3.08455400	3.56081700	-2.83493500

H	-4.72492200	3.04070100	-3.24044200
H	3.91679900	-3.75130200	1.54268500
C	-4.87553500	1.16437600	-1.02328000
H	-4.41204800	1.67449300	1.90223000
C	-5.69798900	0.63851600	-2.02494700
H	-5.77181000	1.12879400	-2.99409000
C	-6.41929600	-0.53898900	-1.80491700
C	-6.34424500	-1.21641600	-0.58696200
H	-6.91200400	-2.13668400	-0.45124100
C	-5.54478000	-0.71654100	0.44932000
C	-4.83395100	0.47379600	0.20699100
C	-2.70931000	0.72161600	1.38767600
C	-1.96801800	1.51084200	2.45806200
H	-2.67332300	1.74923300	3.26963900
C	-1.39637400	2.81599500	1.88253100
H	-0.65243100	2.58109800	1.10450800
H	-2.21852900	3.35557700	1.38838000
C	-0.77970800	3.64890700	3.00524200
H	-0.36401000	4.57753700	2.60012000
H	-1.56312400	3.93860000	3.72921100
C	0.30817600	2.83749000	3.69934200
H	1.12721500	2.63707000	2.99543500
H	0.73778200	3.38909500	4.54964800
C	-0.22953300	1.51972900	4.23043200
H	-1.00463200	1.67106600	4.99803600
H	0.57345800	0.89871800	4.64140500
C	-1.48210800	-0.58650600	3.72099100
H	-2.01481500	-1.09247300	2.91045300
H	-2.21315600	-0.25439200	4.47209300
C	-0.49454600	-1.55310300	4.37416300
H	-1.10762600	-2.31834100	4.87390900
H	0.04019700	-1.05641100	5.19799600
C	0.59289900	-2.21041000	3.52337700
H	1.22592900	-1.44296500	3.06863100
H	1.21025400	-2.84672500	4.17351200
C	-0.74700200	-4.23680700	2.94685800
H	-0.16427400	-4.71548400	3.74946400
H	-1.62153400	-3.73963700	3.37850700
C	0.04932900	-5.84196100	1.17836700
H	-0.26873500	-6.49820600	0.35459300
H	0.61582500	-6.47449300	1.88422600
C	0.95639300	-4.73878200	0.63460600
H	1.87866900	-5.15611400	0.20456200
H	0.45294700	-4.17820800	-0.16260000
C	1.36109100	-3.73725300	1.72295900
H	1.89165700	-4.25910700	2.53384900
C	2.26155800	-2.66889200	1.10952400
C	4.50039700	-2.10840800	0.32807400
C	5.03098000	-2.68056900	-0.85026700
C	5.90749600	-1.90502600	-1.61408100
H	6.33676100	-2.30068100	-2.53349500
C	6.22303900	-0.60258200	-1.21737700
C	5.68909100	-0.05829100	-0.05113900
H	5.95199900	0.96166600	0.23019300
C	4.81089900	-0.80156900	0.74827400
C	4.23802900	-0.15910800	2.00487900
H	3.53785000	-0.87194300	2.46827500
C	3.44522600	1.11528300	1.66723600
H	4.11088900	1.89686100	1.26961600
H	2.97264800	1.51771100	2.57576000
H	2.65976900	0.93485500	0.92015800
C	5.34231100	0.12077900	3.03945800
H	5.89233500	-0.79557100	3.30413100
H	4.91015300	0.54195100	3.96131900
H	6.07402300	0.84836900	2.65546400
C	4.58319500	-4.05595300	-1.33704800
H	4.36964900	-4.67905600	-0.44991200
C	3.27108200	-3.91758800	-2.13578400
H	3.44088200	-3.32459800	-3.04787400
H	2.48949500	-3.40321700	-1.55588500
H	2.88596600	-4.90449600	-2.43762000
C	5.64303500	-4.80608600	-2.15346100
H	6.60366400	-4.85787900	-1.61961600
H	5.81978900	-4.32910600	-3.12966400
H	5.30639200	-5.83428600	-2.35490200
C	-1.16329400	-5.23127500	1.87742400
H	-1.81034000	-4.71821700	1.15303900
H	-1.77231800	-6.00691800	2.36682100
Br	-7.49372200	-1.24480500	-3.20017100
Br	7.36014700	0.45451700	-2.30721500
In	-0.10460700	-0.66992100	0.42417900
C	2.49271400	2.17274500	-3.08662500
C	3.30007800	0.97283200	-2.69491200
C	2.50688700	0.09896000	-2.06921900
C	1.06584700	0.61092200	-2.01687900
N	1.19574800	1.90459100	-2.66862200
H	4.36839700	0.90502500	-2.89650000
H	2.79196100	-0.85608300	-1.63096000

O	0.57297600	0.76748200	-0.72027700
O	2.85846500	3.18685100	-3.63608700
C	0.16648500	2.91241700	-2.68734900
H	0.25758800	3.46614700	-3.63685000
H	-0.81960200	2.42007800	-2.69880300
C	0.10427600	-0.29757800	-2.84556100
C	-0.27692500	-1.59413500	-2.18209100
H	0.52891900	-2.33222100	-2.06931700
C	-1.55099900	-2.01490100	-1.93225900
C	0.21494800	3.92025100	-1.54950000
C	1.16357600	3.86790400	-0.54995800
C	-0.72819700	4.98712000	-1.55142100
C	1.22928000	4.86484600	0.46206900
H	1.88230000	3.04886700	-0.52883200
C	-0.70923100	5.95912300	-0.57486800
H	-1.45927200	5.05282700	-2.36232300
C	2.21821900	4.83714600	1.48556600
C	0.27098700	5.93384700	0.45745800
H	-1.43168300	6.77945700	-0.59872300
C	2.25505500	5.81215800	2.46217700
H	2.95738700	4.03267000	1.47812100
C	0.33669100	6.92584600	1.47583800
C	1.30431100	6.86574000	2.45922100
H	3.02729000	5.78591700	3.23507100
H	-0.38801000	7.74431900	1.46402700
H	1.35024500	7.63803200	3.23057300
H	-0.79333900	0.29584100	-3.06177100
H	0.58191200	-0.51975600	-3.81382000
C	-1.86150100	-3.42728900	-1.51847400
H	-0.96993700	-4.06576000	-1.47396800
H	-2.37448300	-3.44538600	-0.54490300
H	-2.55691000	-3.87057600	-2.25088400
C	-2.76984100	-1.17120200	-2.18523400
H	-3.17255700	-1.40671800	-3.18581200
H	-3.56078000	-1.39759400	-1.45911300
H	-2.56875500	-0.09626600	-2.14278600

INT-R^b

O	-2.06190300	-0.47976800	0.58599700
N	-3.91752700	-0.68668200	1.86240200
C	-5.35625900	-3.66619600	-0.34266500
H	-4.84075400	-4.63925000	-0.38322300
H	-6.07056200	-3.63026100	-1.18052000
H	-5.93241300	-3.62021700	0.59460300
O	0.33205100	-1.18995700	1.88306300
N	-0.56834400	-1.73609000	2.76780300
C	-3.50328900	-2.60340900	-1.71623900
H	-2.74704900	-1.80893800	-1.75198900
H	-4.13671600	-2.52247900	-2.61338500
H	-2.98189600	-3.57037000	-1.76251100
C	-4.33432500	-2.51787100	-0.42962900
H	-3.64509300	-2.64316900	0.41615100
N	0.73078500	-3.76860300	-0.36331600
O	-0.20984800	-2.77717400	-0.54250100
O	2.15977900	-1.22519100	-0.35500600
N	4.06527700	-2.30915000	-0.85572000
C	-6.34566700	1.06020900	3.43113800
H	-6.20412100	1.61813100	4.36983600
H	-6.10078800	0.00340200	3.62654400
H	-7.41349200	1.10141100	3.16439800
C	-5.49030400	1.67152600	2.30310000
H	-4.43509500	1.61815400	2.61586100
C	-5.82700800	3.15651500	2.12252000
H	-5.26289000	3.60319600	1.29092400
H	-5.57505600	3.70730600	3.04153000
H	-6.90117600	3.31183300	1.93579200
H	4.49849900	-3.17890400	-1.15719900
C	-5.62673900	0.84124000	1.03037700
H	-4.27311400	-0.84955600	2.80094900
C	-6.53055400	1.20722100	0.02756000
H	-7.12296200	2.11556500	0.12506500
C	-6.66191800	0.41701900	-1.11562500
C	-5.93741900	-0.76107300	-1.27139500
H	-6.08216000	-1.37108500	-2.16336000
C	-5.03443100	-1.17302500	-0.27967300
C	-4.87325000	-0.34187500	0.84490600
C	-2.59158100	-0.67033200	1.69742400
C	-1.77192900	-0.80671300	2.97375400
H	-2.37931700	-1.28267500	3.75560900
C	-1.30270400	0.57592000	3.44672000
H	-0.65915900	1.00638000	2.66695900
H	-2.19020200	1.21790600	3.54679500
C	-0.55042700	0.47058700	4.77267900
H	-0.17756900	1.46306300	5.06667700
H	-1.24290900	0.13902900	5.56542600
C	0.60908700	-0.51382600	4.63491900
H	1.36737900	-0.10732100	3.95281500
H	1.09933600	-0.69131700	5.60437300

C	0.15059000	-1.86458300	4.10713200
H	-0.54670800	-2.36406100	4.79623500
H	1.00547000	-2.52175300	3.92218500
C	-1.06438000	-3.09356200	2.29246100
H	-1.58738200	-2.91182500	1.34949000
H	-1.78693700	-3.44222800	3.04304100
C	0.00614800	-4.16321400	2.08962500
H	-0.54075000	-5.08270500	1.83255900
H	0.49739100	-4.39936900	3.04524800
C	1.13998900	-3.91439300	1.09669700
H	1.67169900	-2.99681500	1.36222800
H	1.84102600	-4.75912100	1.13496800
C	0.10429500	-5.06633400	-0.86567300
H	0.82862900	-5.87022500	-0.66418400
H	-0.78619100	-5.21981700	-0.24850100
C	0.95950900	-4.65988900	-3.20162100
H	0.66395500	-4.52415200	-4.25258000
H	1.67595200	-5.49890100	-3.17351200
C	1.63999500	-3.38922000	-2.69348200
H	2.57429400	-3.19393500	-3.24115300
H	0.98392400	-2.51914300	-2.83308600
C	1.98956600	-3.50664700	-1.20263000
H	2.63121300	-4.38401600	-1.04291800
C	2.73543800	-2.25923400	-0.74179600
C	4.90468300	-1.16782500	-0.59612600
C	5.35821800	-0.40664200	-1.69414100
C	6.09714000	0.75232800	-1.42729200
H	6.45275600	1.37921300	-2.24389100
C	6.36539400	1.11938600	-0.10827300
C	5.95043600	0.33552800	0.96590400
H	6.19101100	0.63983400	1.98493200
C	5.21124100	-0.83462100	0.73687600
C	4.75351800	-1.67654800	1.91994900
H	4.29748000	-2.59560700	1.52241300
C	3.67728000	-0.94215900	2.73584200
H	4.07764700	-0.01381000	3.17482900
H	3.33411800	-1.57858400	3.56671000
H	2.80402000	-0.68780800	2.11981200
C	5.93561200	-2.11005400	2.80229700
H	6.70134400	-2.64089000	2.21571800
H	5.58444700	-2.78380700	3.59974300
H	6.41826800	-1.24748400	3.28818400
C	5.00892200	-0.79716600	-3.12610100
H	4.88100500	-1.89102900	-3.14701400
C	3.66796100	-0.16708500	-3.54313300
H	3.75119700	0.93129800	-3.55528200
H	2.85371600	-0.43383800	-2.85503900
H	3.37774800	-0.49812200	-4.55226000
C	6.11044900	-0.45554800	-4.13780500
H	7.08766400	-0.85124300	-3.82137800
H	6.21087300	0.63168500	-4.28210400
H	5.86359300	-0.88980000	-5.11857400
C	-0.25881800	-4.98166400	-2.33906400
H	-1.02906900	-4.20869200	-2.46748200
H	-0.70556900	-5.94616800	-2.62468500
Br	-7.86540600	0.96565900	-2.49288400
Br	7.30421400	2.74763300	0.23166200
In	0.02570200	-0.67485300	-0.15394400
C	2.35918700	4.24125200	-0.05293400
C	3.37203600	3.30759500	-0.68882000
C	2.88116100	1.89845700	-0.34725900
C	1.53935900	2.11478400	0.29524600
N	1.33462700	3.43909100	0.50543800
H	4.37860200	3.53861000	-0.31200600
H	2.77752100	1.22864900	-1.20643900
O	0.72525300	1.25071800	0.64963500
O	2.35225300	5.44452000	-0.01348800
C	0.13760500	3.99126300	1.14829300
H	-0.05960500	3.39440200	2.04846700
H	0.40465200	5.01193700	1.45275900
C	-1.06099100	3.99109900	0.22337200
C	-2.08845000	3.05323200	0.38230000
C	-1.12538300	4.90224200	-0.84250100
C	-3.16354500	3.01767300	-0.51095600
H	-2.03211600	2.32701100	1.19271800
C	-2.20120500	4.87180900	-1.73372400
H	-0.32227800	5.63224100	-0.97453400
C	-3.22294700	3.92826400	-1.56997400
H	-3.94183800	2.26356900	-0.39189600
H	-2.24116800	5.58442700	-2.56100300
H	-4.06051700	3.89706900	-2.27093500
C	0.68942500	2.24324700	-2.92256700
C	-0.28697300	1.53735900	-2.32858800
H	0.64235400	3.33464500	-2.97340600
H	1.55045500	1.75692600	-3.39134800
H	-1.12113100	2.09869400	-1.89768600
C	-0.35185800	0.06156300	-2.15844200
H	0.35776200	-0.44862400	-2.83145300

H	-1.36061100	-0.31031100	-2.40549400
H	3.37457600	3.50126100	-1.77259500
H	3.52140600	1.38035900	0.38246000

TS1-*R*[b]

O	-1.98437900	-0.56357500	0.63187600
N	-3.86843100	-0.77657900	1.85351300
C	-5.42513300	-3.65185900	-0.44377300
H	-4.95698800	-4.64841800	-0.48040100
H	-6.09815600	-3.56737400	-1.31156100
H	-6.04053300	-3.59297200	0.46737200
O	0.37293700	-1.38415800	1.98720900
N	-0.57434600	-1.96737500	2.79415000
C	-3.45990700	-2.65921200	-1.71336600
H	-2.63833200	-1.93169700	-1.67928200
H	-4.03975200	-2.49558100	-2.63507300
H	-3.01878700	-3.66516900	-1.76983100
C	-4.34470500	-2.55503900	-0.46231000
H	-3.70059700	-2.73385800	0.40960200
N	0.70855800	-3.72373300	-0.48713800
O	-0.19120800	-2.67860200	-0.58189100
O	2.17836600	-1.22230400	-0.37736600
N	4.06312500	-2.26825100	-0.99387000
C	-6.12703000	1.15431600	3.42141300
H	-5.92839400	1.71071400	4.35063100
H	-5.95538100	0.08485900	3.62648000
H	-7.19379900	1.26988200	3.17287300
C	-5.25057700	1.69179500	2.27260200
H	-4.19553000	1.56753600	2.56826500
C	-5.48385100	3.19483000	2.07773400
H	-4.90693900	3.58694000	1.22757400
H	-5.17332800	3.73784800	2.98342800
H	-6.54798000	3.42442700	1.91116900
H	4.49802000	-3.11728100	-1.34841300
C	-5.46017400	0.86303300	1.00916800
H	-4.25697600	-0.97044600	2.77315800
C	-6.34812700	1.27752300	0.01112900
H	-6.88557500	2.21931000	0.10881000
C	-6.52197400	0.49882600	-1.13442500
C	-5.85626600	-0.71314400	-1.29918200
H	-6.02836600	-1.30755700	-2.19694500
C	-4.98008700	-1.17879100	-0.30746500
C	-4.78277300	-0.36359100	0.82289800
C	-2.54228600	-0.79584700	1.72533000
C	-1.76223900	-1.02246100	3.01314600
H	-2.40704900	-1.52633900	3.74684200
C	-1.27519300	0.32261700	3.57384800
H	-0.59856400	0.78259000	2.83835700
H	-2.15136100	0.98047000	3.67874900
C	-0.56720500	0.12585300	4.91423600
H	-0.17476400	1.09061700	5.26849000
H	-1.29253500	-0.22349100	5.66927200
C	0.56826700	-0.88481800	4.76248300
H	1.36071100	-0.46790500	4.12710500
H	1.01898900	-1.12630900	5.73715900
C	0.09342100	-2.19300200	4.14823600
H	-0.63917500	-2.71218100	4.78327800
H	0.93903500	-2.85907600	3.94973400
C	-1.07050000	-3.28532200	2.21167200
H	-1.59533100	-3.04660900	1.27873700
H	-1.79195100	-3.69221300	2.93380800
C	0.01244000	-4.32541900	1.93514100
H	-0.52025900	-5.23669900	1.62554800
H	0.51696400	-4.61171000	2.86971100
C	1.13325100	-3.99790400	0.95098400
H	1.67957000	-3.11281600	1.28726900
H	1.82385600	-4.85075800	0.90216000
C	-0.00506400	-4.94675100	-1.05727700
H	0.64970300	-5.81272200	-0.88067200
H	-0.91442700	-5.04962900	-0.45662900
C	0.90794200	-4.51533000	-3.36220600
H	0.64217900	-4.34077500	-4.41521500
H	1.57869200	-5.39103100	-3.33840300
C	1.63540700	-3.29216500	-2.80917900
H	2.57790900	-3.11168500	-3.34641700
H	1.00963900	-2.39729700	-2.92799900
C	1.97353600	-3.46334700	-1.32007600
H	2.59938700	-4.35628400	-1.18285600
C	2.73997200	-2.23871000	-0.82806000
C	4.88619100	-1.11200700	-0.73657400
C	5.32219600	-0.34587500	-1.83937500
C	6.03691000	0.82930800	-1.57902000
H	6.37759100	1.45969900	-2.39931200
C	6.29808100	1.20851200	-0.26154700
C	5.89952500	0.42149800	0.81527900
H	6.13275800	0.73663700	1.83264600
C	5.18324400	-0.76337400	0.59441200
C	4.75575500	-1.61097500	1.78486400

H	4.27160900	-2.51875700	1.39534500
C	3.72871700	-0.87623400	2.66194800
H	4.16857600	0.02537600	3.11800800
H	3.39623100	-1.53351200	3.48076500
H	2.84276400	-0.57588000	2.08704800
C	5.97133600	-2.07341200	2.60642400
H	6.69885600	-2.61146900	1.97906400
H	5.64878600	-2.74764000	3.41569300
H	6.49149200	-1.22152700	3.07243200
C	4.97416600	-0.74693300	-3.26888400
H	4.87117400	-1.84371200	-3.28914700
C	3.61551700	-0.14817400	-3.67425700
H	3.67632300	0.95091200	-3.71253500
H	2.82775500	-0.41174300	-2.95504800
H	3.30706700	-0.51032500	-4.66710100
C	6.05921000	-0.38475000	-4.29095600
H	7.04578100	-0.76513100	-3.98510900
H	6.14046400	0.70417000	-4.43387200
H	5.80969200	-0.82130300	-5.27016900
C	-0.34146700	-4.78248500	-2.52937700
H	-1.05306300	-3.95299800	-2.64048200
H	-0.85216600	-5.70193300	-2.85333000
Br	-7.68843200	1.12001200	-2.51189000
Br	7.20017800	2.85793100	0.07187600
In	0.10603300	-0.66805200	0.02626500
C	1.97112200	4.38160600	0.58183300
C	3.24099900	3.68012200	0.11194000
C	2.92582000	2.19577600	0.29572500
C	1.39524500	2.13999100	0.21431900
N	0.97291400	3.42997000	0.65739600
H	4.11162300	4.03795300	0.67771800
H	3.42423000	1.51544800	-0.40174700
O	0.75795500	1.13224900	0.73009000
O	1.82759900	5.56067400	0.84479300
C	-0.37167600	3.71380000	1.13339800
H	-0.64621800	2.94407000	1.86787300
H	-0.30949400	4.68319200	1.64838500
C	-1.39788200	3.77222000	0.02076700
C	-2.43759300	2.83724100	-0.05922600
C	-1.27941000	4.74597800	-0.98465100
C	-3.33938400	2.86258300	-1.12979000
H	-2.52568600	2.05920500	0.69989400
C	-2.17651800	4.77354800	-2.05480100
H	-0.46974700	5.47852500	-0.92512400
C	-3.20846900	3.82815300	-2.13153200
H	-4.13260100	2.11681000	-1.18718800
H	-2.07174000	5.53364400	-2.83286600
H	-3.90790800	3.84410100	-2.97081300
C	1.15380600	2.17233400	-1.76329500
C	-0.06373000	1.51557100	-2.02567600
H	1.17444000	3.24628900	-1.95985700
H	2.05936400	1.63795400	-2.05963600
H	-0.97408300	2.11913100	-2.01503900
C	-0.22202900	0.12143900	-2.10759700
H	0.63552100	-0.43888200	-2.49992100
H	-1.19657700	-0.26363200	-2.42839700
H	3.41084800	3.94464100	-0.94488500
H	3.17792700	1.86615800	1.31597500

INT2-*R*[b]

O	-1.73614700	-0.83655500	0.64960500
N	-3.63193600	-0.94551600	1.87321700
C	-5.23546600	-3.87895900	-0.45338700
H	-4.76646200	-4.87591000	-0.46656400
H	-5.84955000	-3.79284700	-1.36294100
H	-5.91383200	-3.82975500	0.41195900
O	0.64073800	-1.56005300	2.09562000
N	-0.33006000	-2.18305000	2.83916500
C	-3.21142600	-2.85275700	-1.59752300
H	-2.38947800	-2.12946900	-1.50546200
H	-3.74899500	-2.65746700	-2.53845900
H	-2.77319700	-3.86094300	-1.67208800
C	-4.16145400	-2.77828100	-0.39090800
H	-3.56198300	-2.97039800	0.51316300
N	1.07551100	-3.68510100	-0.57102200
O	0.13119100	-2.67515900	-0.63094400
O	2.40314300	-1.15346600	-0.30312500
N	4.34166600	-1.98074900	-1.04759300
C	-5.65385500	1.10826600	3.44650100
H	-5.38555000	1.71139000	4.32768800
H	-5.45653900	0.04985900	3.69423700
H	-6.74029600	1.19661700	3.29276100
C	-4.89366900	1.59702800	2.19690300
H	-3.81059100	1.50327500	2.39402800
C	-5.16983800	3.08592400	1.95439600
H	-4.68167000	3.44493300	1.03724000
H	-4.78976500	3.67971900	2.79935200
H	-6.24870400	3.29136600	1.87611400

H	4.83271500	-2.74887600	-1.49802800
C	-5.19315200	0.70759500	0.99379300
H	-4.01854900	-1.05939900	2.80746800
C	-6.09213600	1.10241800	0.00123600
H	-6.59226300	2.06721800	0.06227800
C	-6.31937200	0.28463300	-1.10840200
C	-5.68362800	-0.94927600	-1.23752500
H	-5.89225300	-1.56986100	-2.10975300
C	-4.79287700	-1.39769300	-0.25247000
C	-4.55499700	-0.54447400	0.84056000
C	-2.31215700	-1.01834100	1.74716100
C	-1.54959700	-1.26651000	3.04550100
H	-2.20303500	-1.81494200	3.74126200
C	-1.11390100	0.06657200	3.67754100
H	-0.42633900	0.58132700	2.98745500
H	-2.01282000	0.69420800	3.77806900
C	-0.45536200	-0.17265000	5.03720800
H	-0.09867200	0.78307100	5.44865200
H	-1.20110100	-0.56616300	5.75085800
C	0.70619800	-1.15467300	4.89291300
H	1.50987900	-0.70301500	4.29584700
H	1.12919700	-1.41953400	5.87439300
C	0.27666900	-2.44813300	4.21643100
H	-0.48056300	-2.99537100	4.79931300
H	1.13708500	-3.10191500	4.03827200
C	-0.74993800	-3.48047600	2.16748700
H	-1.27591100	-3.19909400	1.24969500
H	-1.45572800	-3.97975100	2.84742000
C	0.39458500	-4.43919800	1.82895900
H	-0.08708000	-5.36366700	1.47569700
H	0.92051700	-4.74485500	2.74662400
C	1.50076700	-4.00834000	0.85999000
H	2.00752400	-3.11917300	1.24435800
H	2.22727700	-4.82934000	0.77569400
C	0.41689700	-4.91401800	-1.19610100
H	1.11439100	-5.75449800	-1.05511900
H	-0.48582900	-5.08641200	-0.60126500
C	1.31407600	-4.35978700	-3.47592800
H	1.04816400	-4.15918400	-4.52428700
H	2.01768000	-5.21088600	-3.48459700
C	1.99123800	-3.12985400	-2.87386400
H	2.92540300	-2.88707300	-3.40148800
H	1.33199600	-2.25678000	-2.96522000
C	2.33474300	-3.33259400	-1.38854900
H	3.00227700	-4.20180800	-1.28351300
C	3.03136500	-2.08423500	-0.84353400
C	5.06159700	-0.74941600	-0.80221200
C	5.51224600	-0.01967500	-1.92499700
C	6.14011600	1.20863500	-1.69598400
H	6.50041400	1.80761200	-2.53140900
C	6.29486400	1.68913900	-0.39284300
C	5.86354700	0.94180300	0.70240300
H	6.01937600	1.33073300	1.70904700
C	5.24040600	-0.29968800	0.52016700
C	4.82030500	-1.10025700	1.74614400
H	4.30085000	-2.00884700	1.40346100
C	3.83896900	-0.31595000	2.63226400
H	4.32103400	0.57248400	3.06920100
H	3.50990000	-0.94954100	3.47043400
H	2.95177100	0.01640900	2.07538600
C	6.05349800	-1.56377300	2.54292200
H	6.74356100	-2.15006500	1.91665800
H	5.74909100	-2.18871400	3.39766300
H	6.61539800	-0.70560500	2.94312000
C	5.24847400	-0.50094900	-3.34900800
H	5.22455600	-1.60544300	-3.33679400
C	3.86359900	-0.01185800	-3.81415000
H	3.84736600	1.08751900	-3.87540400
H	3.06811000	-0.30906800	-3.11428800
H	3.61451400	-0.41164100	-4.80975400
C	6.33762100	-0.10065800	-4.35280900
H	7.33867100	-0.39318800	-4.00235300
H	6.34415500	0.98441400	-4.53809900
H	6.15593900	-0.59029500	-5.32150800
C	0.07213300	-4.70657800	-2.66030700
H	-0.67530500	-3.90399000	-2.73642600
H	-0.40123600	-5.63204800	-3.02308500
Br	-7.47586600	0.88701500	-2.48644100
Br	7.09371100	3.38683100	-0.11055400
In	0.36117100	-0.72185300	0.18780700
C	0.19484100	4.44996500	1.12482400
C	1.71463800	4.52137900	1.06615900
C	2.13670800	3.05244500	1.04797100
C	0.94856100	2.29979200	0.39089100
N	-0.18435100	3.19758900	0.68564800
H	2.09942200	5.10354000	1.91409200
H	3.09099600	2.85140200	0.54092000
O	0.76269000	1.06069500	0.93959600

O	-0.57376400	5.31784900	1.48332000
C	-1.57809100	2.77897900	0.76710900
H	-1.59288600	1.70688300	0.99961900
H	-2.01037700	3.31755000	1.62627900
C	-2.43072500	3.05853400	-0.45769300
C	-3.03130000	2.01227400	-1.17449000
C	-2.64207100	4.38204200	-0.88090700
C	-3.81815400	2.27671100	-2.30095000
H	-2.88365000	0.97958900	-0.84933800
C	-3.43199000	4.64556400	-2.00288200
H	-2.19307100	5.19909800	-0.31164300
C	-4.02125600	3.59459200	-2.71699100
H	-4.28643000	1.45397900	-2.84509400
H	-3.59497000	5.67880500	-2.31888700
H	-4.64332900	3.80353900	-3.59040300
C	1.22709400	2.19201500	-1.17887800
C	0.13236700	1.47469500	-1.85899000
H	1.31783800	3.21783000	-1.56467100
H	2.18902600	1.66833100	-1.29308600
H	-0.80788400	2.01916500	-1.98386300
C	0.15515300	0.15399900	-2.18904000
H	1.11841200	-0.35834800	-2.26042000
H	-0.70318200	-0.32337700	-2.67250100
H	2.00266500	5.05870300	0.14642200
H	2.21010600	2.65981300	2.07275400

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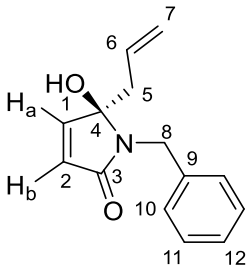
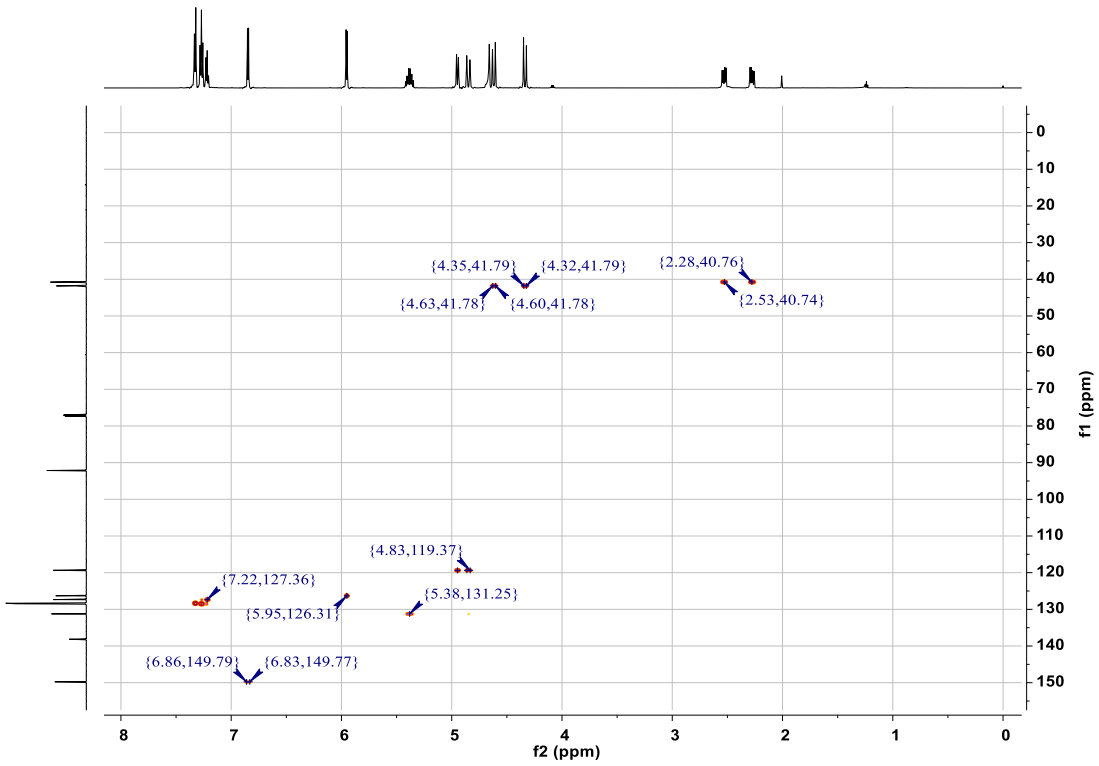
11. Copies of 2D NMR

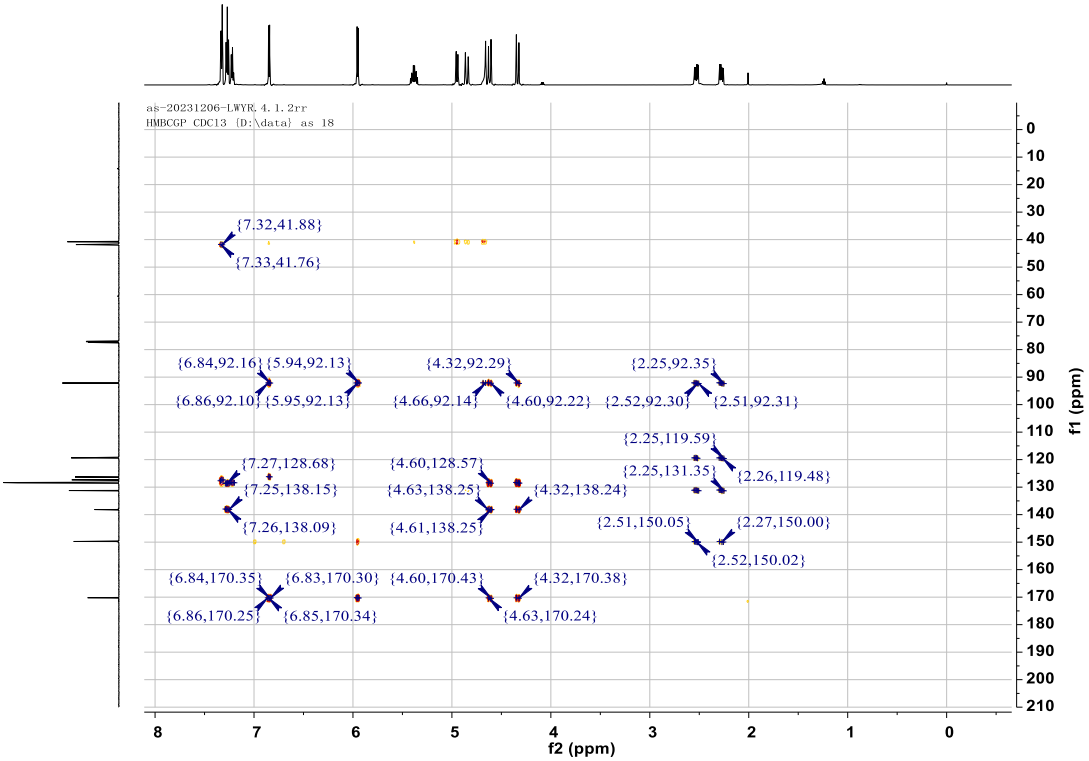


Number of C atom	C	H
1	149.8	$\mathbf{H_b}$ 5.95 (d, J = 6.0 Hz, 1H)
2	126.3	$\mathbf{H_a}$ 6.85 (d, J = 6.0 Hz, 1H)
3	170.0	-
4	92.1	-
5	40.8	2.53 (dd, J = 12.0, 4.0 Hz, 1H) 2.28 (dd, J = 12.0, 4.0 Hz, 1H)
6	131.2	5.44 – 5.32 (m, 1H)
7	119.4	4.95 (d, J = 8.0 Hz, 1H) 4.85 (d, J = 8.0 Hz, 1H)
8	41.8	4.62 (d, J = 12.0 Hz, 1H) 4.34 (d, J = 12.0 Hz, 1H)
9	138.2	-
10	128.4	7.34 – 7.31 (m, 2H)
11	128.5	7.29 – 7.25 (m, 2H)
12	127.4	7.24 – 7.19 (m, 1H)

HSQC:



HMBC: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HMBCGP CDC13 (D:\data) as 18
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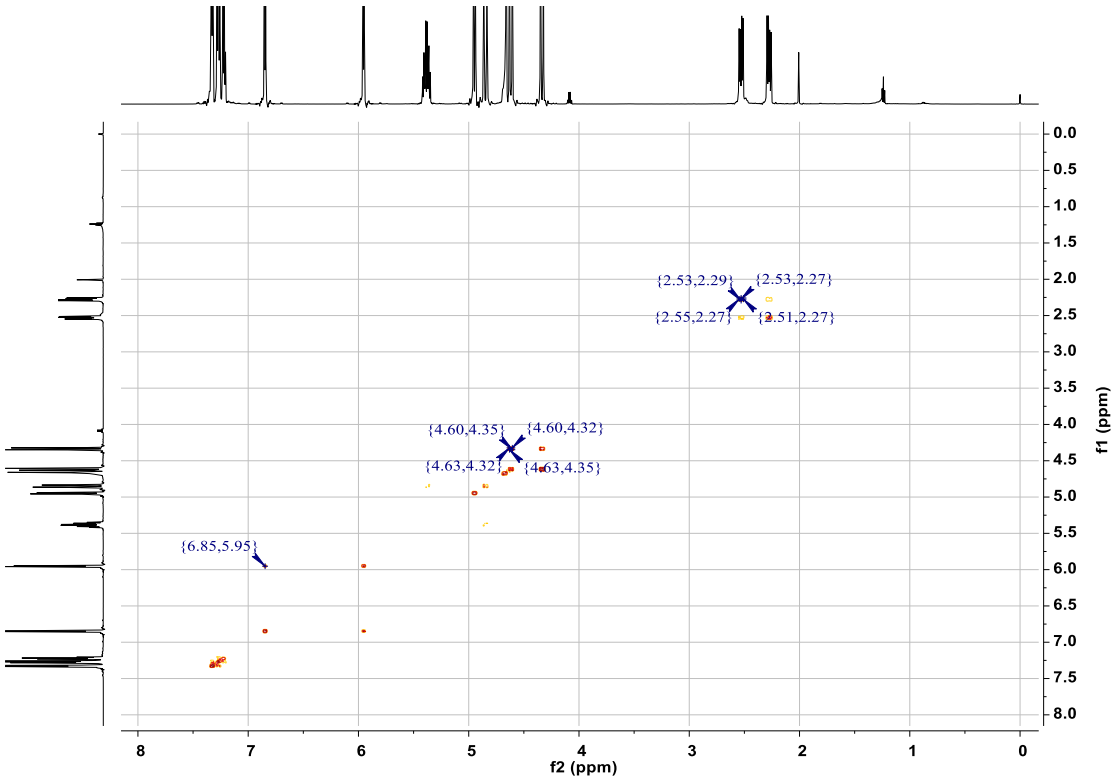
{7.33,41.76}
{6.84,92.16}
{5.94,92.13}
{6.86,92.10}
{5.95,92.13}
{4.32,92.29}
{4.66,92.14}
{4.60,92.22}
{2.25,92.35}
{2.52,92.30}
{2.51,92.31}
{2.25,119.59}
{2.25,131.35}
{2.26,119.48}
{7.27,128.68}
{7.25,138.15}
{7.26,138.09}
{4.60,128.57}
{4.63,138.25}
{4.32,138.24}
{4.61,138.25}
{2.51,150.05}
{2.27,150.00}
{2.52,150.02}
{6.84,170.35}
{6.83,170.30}
{6.86,170.25}
{6.85,170.34}
{4.60,170.43}
{4.32,170.38}
{4.63,170.24}
f2 (ppm)
f1 (ppm)

COSY:


{2.53,2.29}
{2.53,2.27}
{2.55,2.27}
{2.51,2.27}
{4.60,4.35}
{4.60,4.32}
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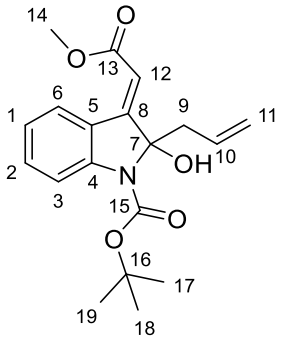
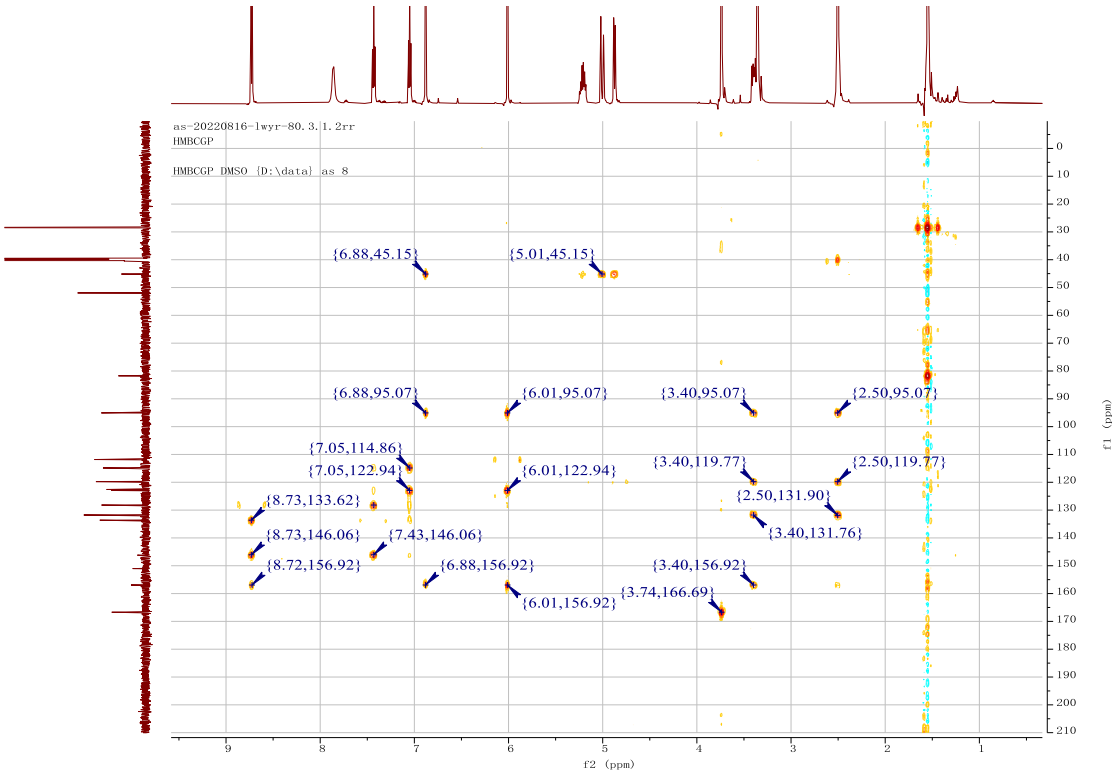
{6.85,5.95}
f2 (ppm)
f1 (ppm)

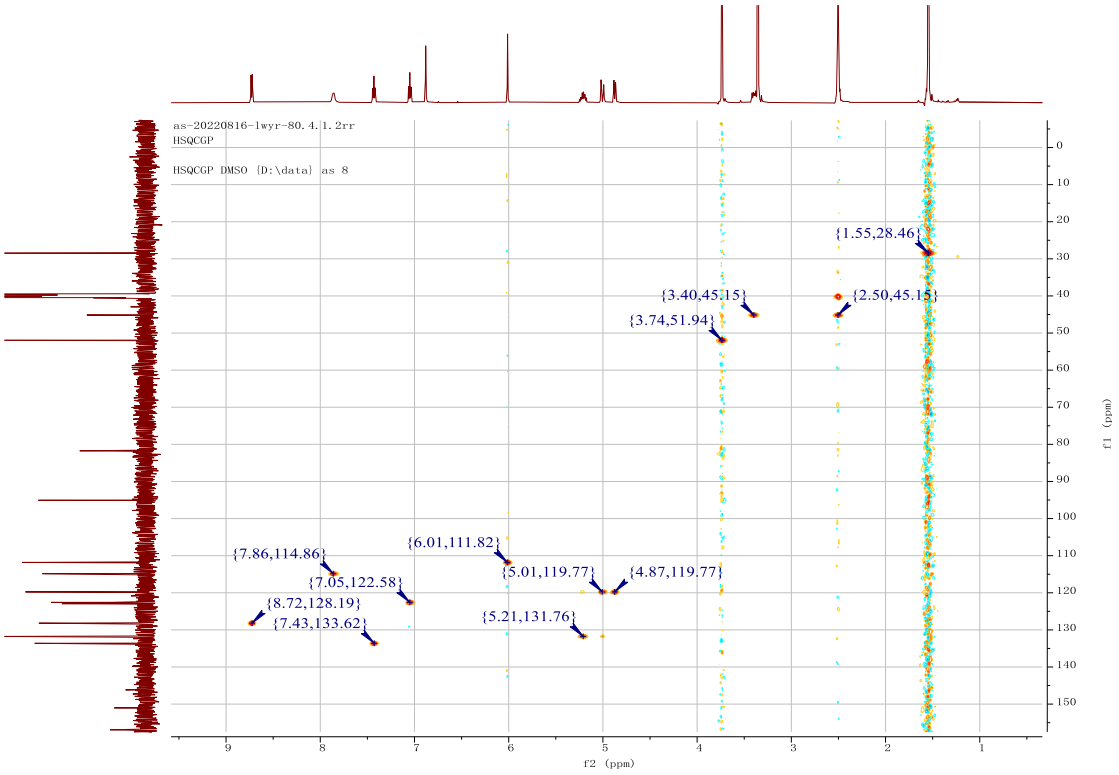


Number of C atom	C	H
1	122.6	7.05 (t, J = 4.0 Hz, 1H)
2	133.6	7.43 (t, J = 4.0 Hz, 1H)
3	114.9	7.86 (d, J = 4.0 Hz, 1H)
4	146.2	-
5	122.9	-
6	128.2	8.73 (d, J = 4.0 Hz, 1H)
7	95.1	-
8	156.9	-
9	45.2	3.46 – 3.38 (m, 1H) 2.52 – 2.48 (m, 1H)
10	131.8	5.33 – 5.15 (m, 1H)
11	119.8	5.01 (dd, J = 12.0, 2.0 Hz, 1H) 4.87 (dd, J = 12.0, 2.0 Hz, 1H)
12	111.8	6.01 (s, 1H)
13	166.7	-
14	51.9	3.74 (s, 3H)
15	151.0	-
16	81.8	-
17 18 19	28.5	1.55 (s, 9H)

HMBC:



HSQC: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HSQCGP
HSQCGP DMSO {D:\data} as 8
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{3.40,45.15}
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{7.86,114.86}
{5.01,119.77}
{4.87,119.77}
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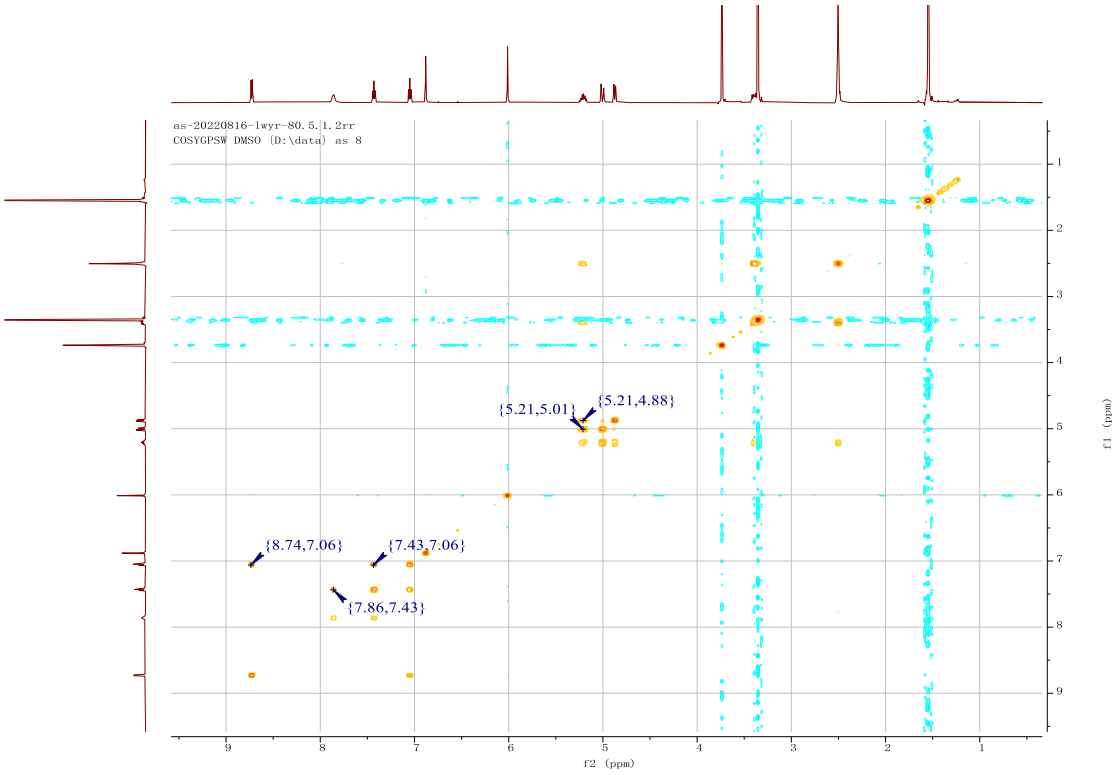
{8.72,128.19}
{5.21,131.76}
{7.43,133.62}
f2 (ppm)
f1 (ppm)

COSY: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{5.21,4.88}
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{7.43,7.06}
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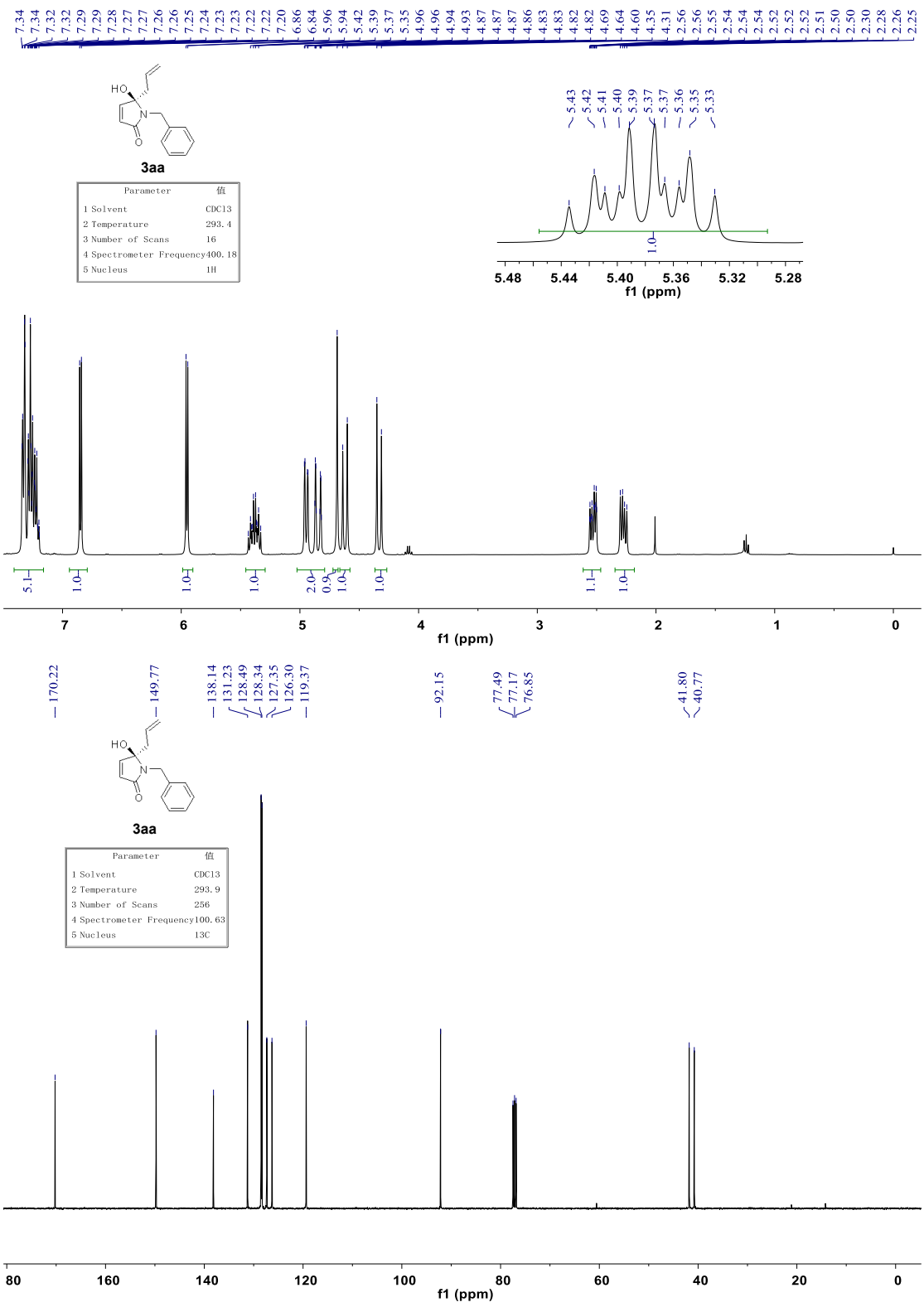
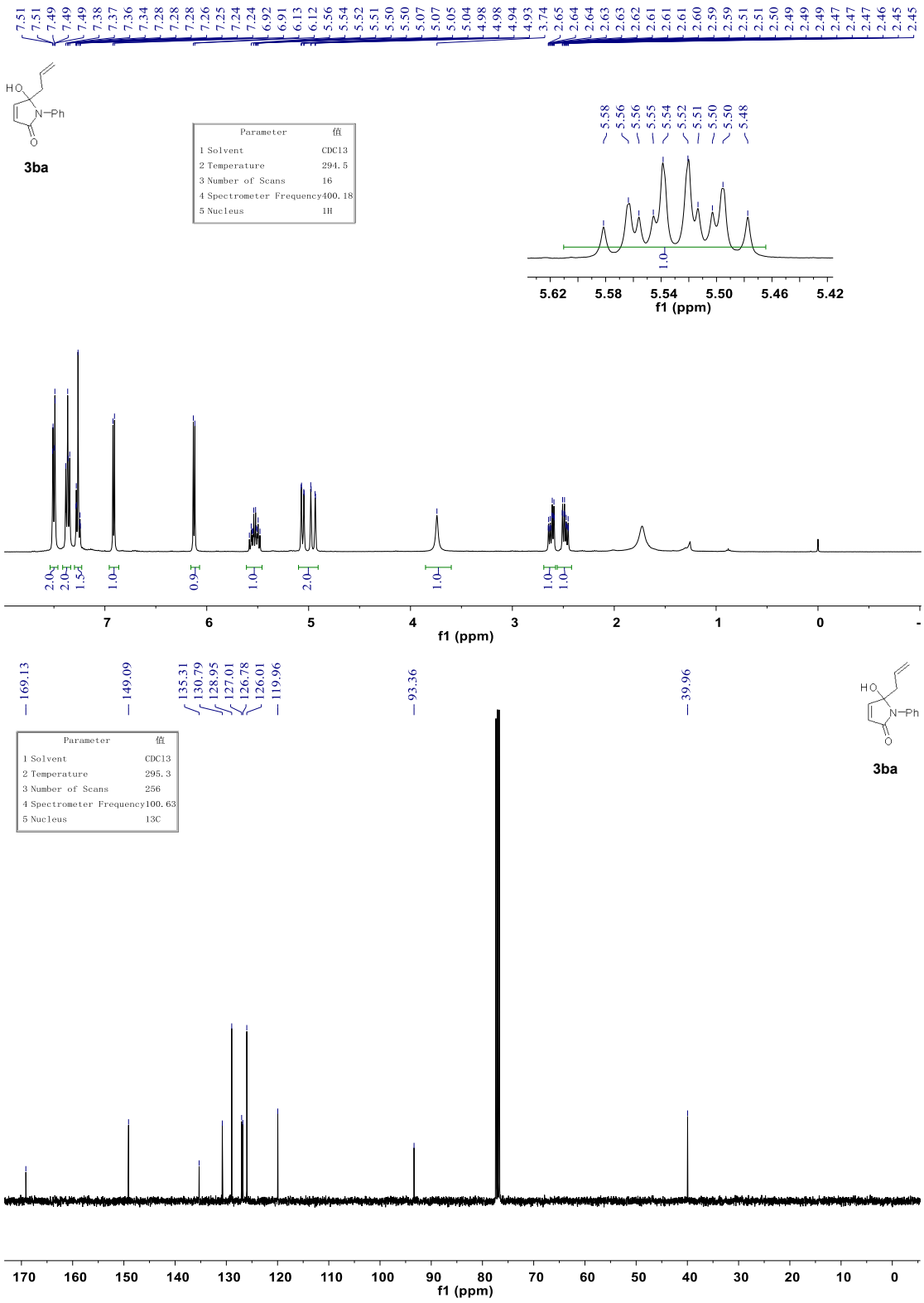
f2 (ppm)
f1 (ppm)

12. Copies of NMR spectra




7.51 7.51 7.49 7.49 7.49 7.38 7.37 7.36 7.34 7.28 7.28 7.28 7.26 7.25 7.24 7.24 6.92 6.91 6.13 6.12 5.56 5.54 5.52 5.51 5.50 5.50 5.07 5.05 5.04 4.98 4.98 4.94 4.93 3.74 2.65 2.64 2.64 2.63 2.63 2.62 2.61 2.61 2.61 2.60 2.59 2.59 2.51 2.51 2.50 2.49 2.49 2.49 2.47 2.47 2.47 2.46 2.45 2.45
HO
N–Ph
O
3ba
Parameter 值
1 Solvent CDCl3
2 Temperature 294.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.58 5.56 5.56 5.55 5.54 5.52 5.51 5.50 5.50 5.48
1.0
5.62 5.58 5.54 5.50 5.46 5.42
f1 (ppm)
2.0 2.0 1.5 1.0 0.9 1.0 2.0 1.0 1.0 1.0
7 6 5 4 3 2 1 0
f1 (ppm)
169.13 149.09 135.31 130.79 128.95 127.01 126.78 126.01 119.96 93.36 39.96
HO
N–Ph
O
3ba
Parameter 值
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3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
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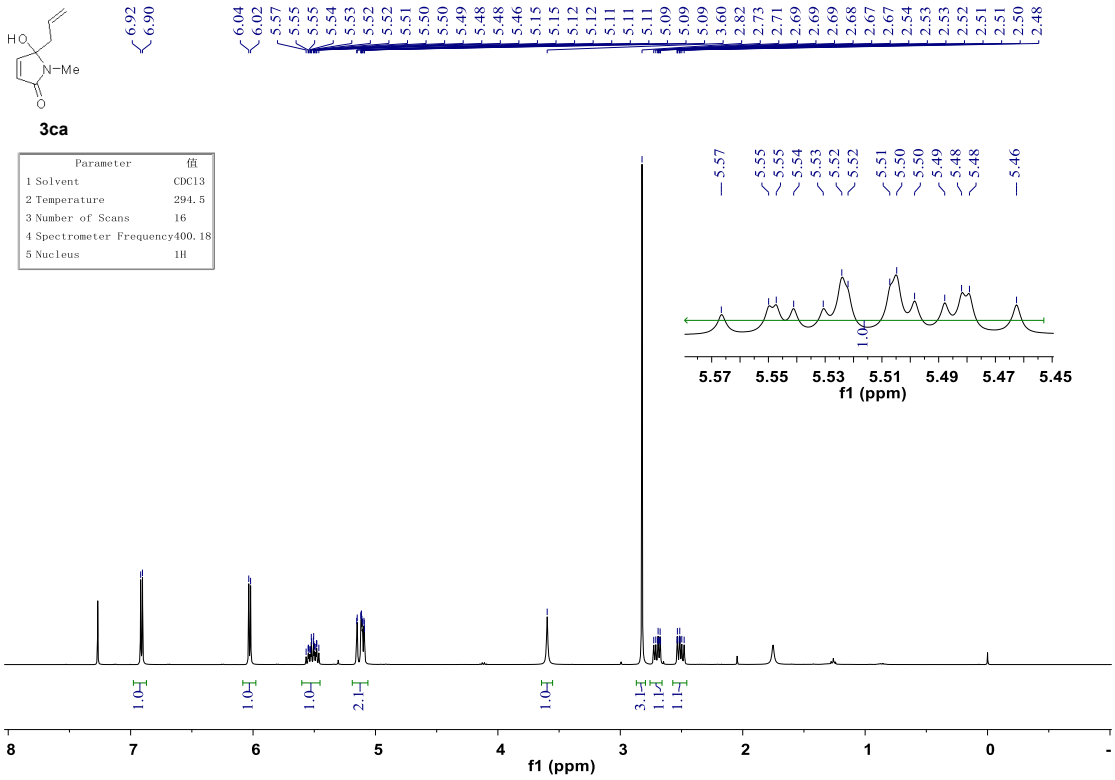
f1 (ppm)


HO
N-Me
O
3ca
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6.90
6.04
6.02
5.57
5.55
5.55
5.54
5.53
5.52
5.52
5.51
5.50
5.50
5.49
5.48
5.48
5.46
5.15
5.12
5.12
5.11
5.11
5.11
5.09
5.09
5.09
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2.69
2.68
2.67
2.67
2.54
2.53
2.53
2.52
2.51
2.51
2.50
2.48
Parameter 值
1 Solvent CDCl3
2 Temperature 294.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.57
5.55
5.55
5.54
5.53
5.52
5.52
5.51
5.50
5.50
5.49
5.48
5.48
5.46
1.0
5.57 5.55 5.53 5.51 5.49 5.47 5.45
f1 (ppm)
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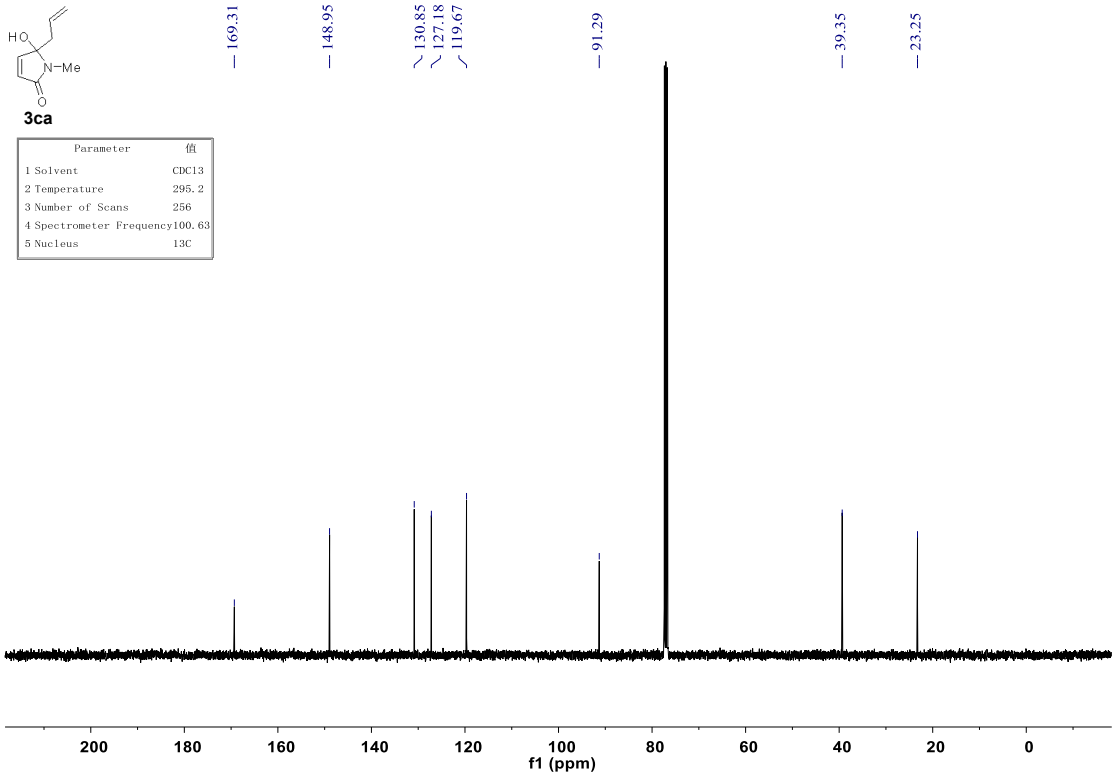
1.0
1.0
2.1
1.0
3.1
1.1
1.1
8 7 6 5 4 3 2 1 0
f1 (ppm)


HO
N-Me
O
3ca
169.31
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130.85
127.18
119.67
91.29
39.35
23.25
Parameter 值
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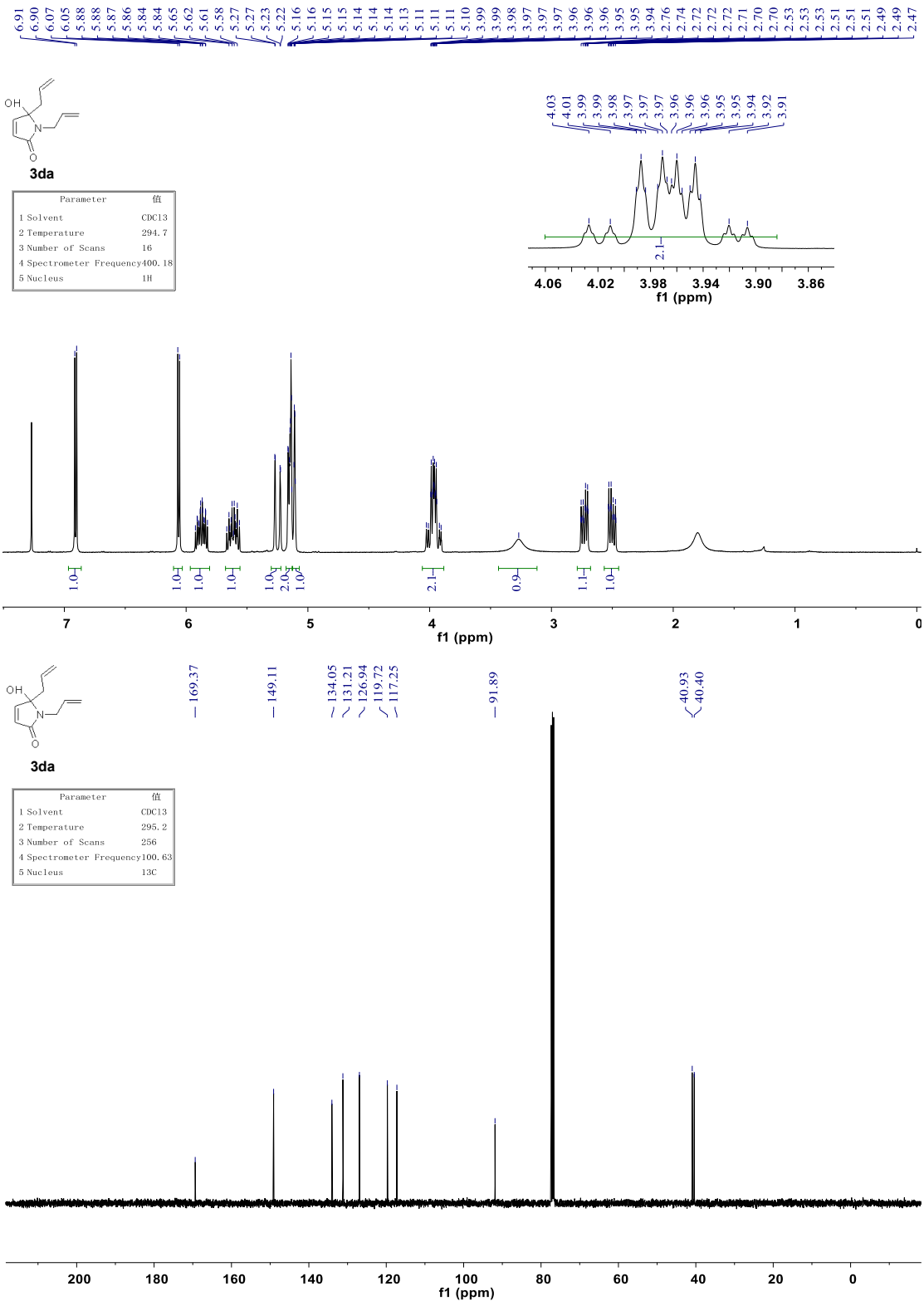
2 Temperature 295.2
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)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OH
N
O
3da
Parameter 值
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2 Temperature 294.7
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
4.03 4.01 3.99 3.99 3.98 3.97 3.97 3.97 3.96 3.96 3.96 3.95 3.95 3.94 3.92 3.91
2.1
4.06 4.02 3.98 3.94 3.90 3.86
f1 (ppm)
1.0 1.0 1.0 1.0 1.0 2.0 1.0 2.1 0.9 1.1 1.0
7 6 5 4 3 2 1 0
f1 (ppm)
OH
N
O
3da
Parameter 值
1 Solvent CDCl3
2 Temperature 295.2
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
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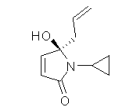
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)



3ea

Parameter	值
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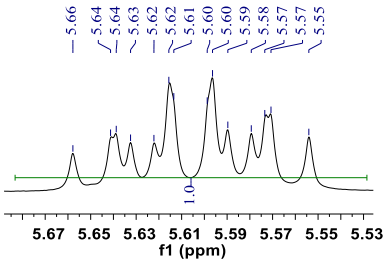
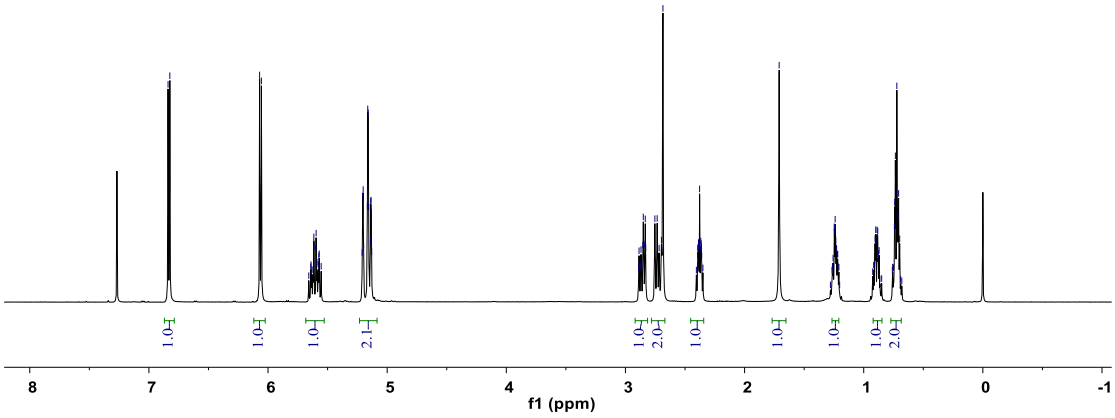
3 Number of Scans	16
4 Spectrometer Frequency	400.18
5 Nucleus	1H





3ea

Parameter	值
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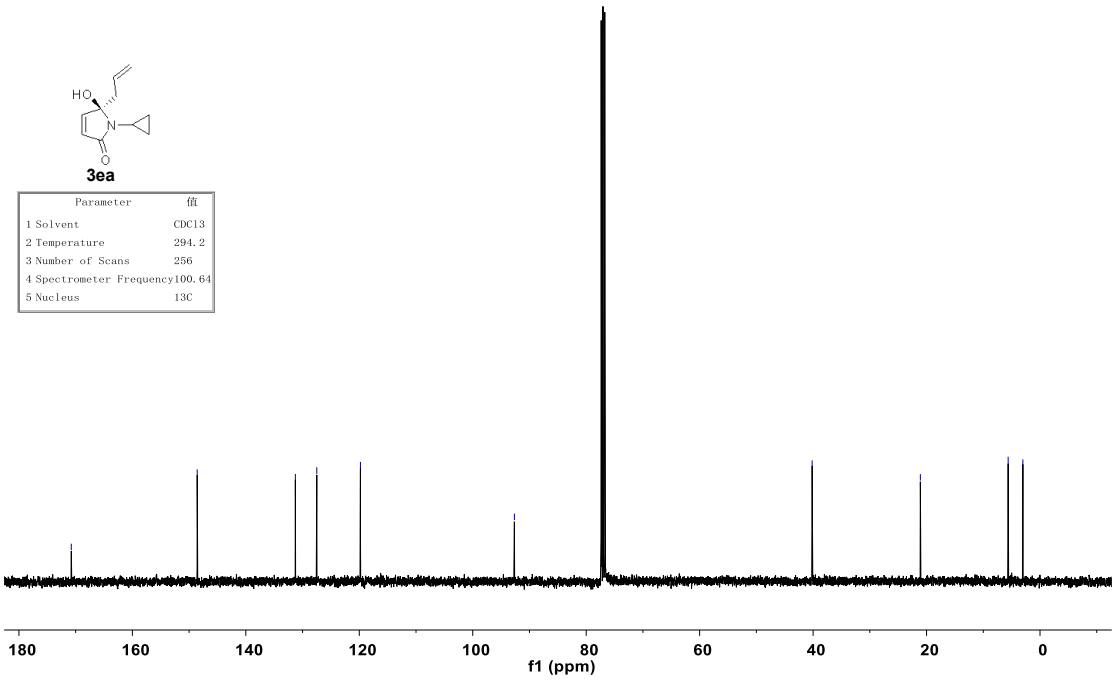
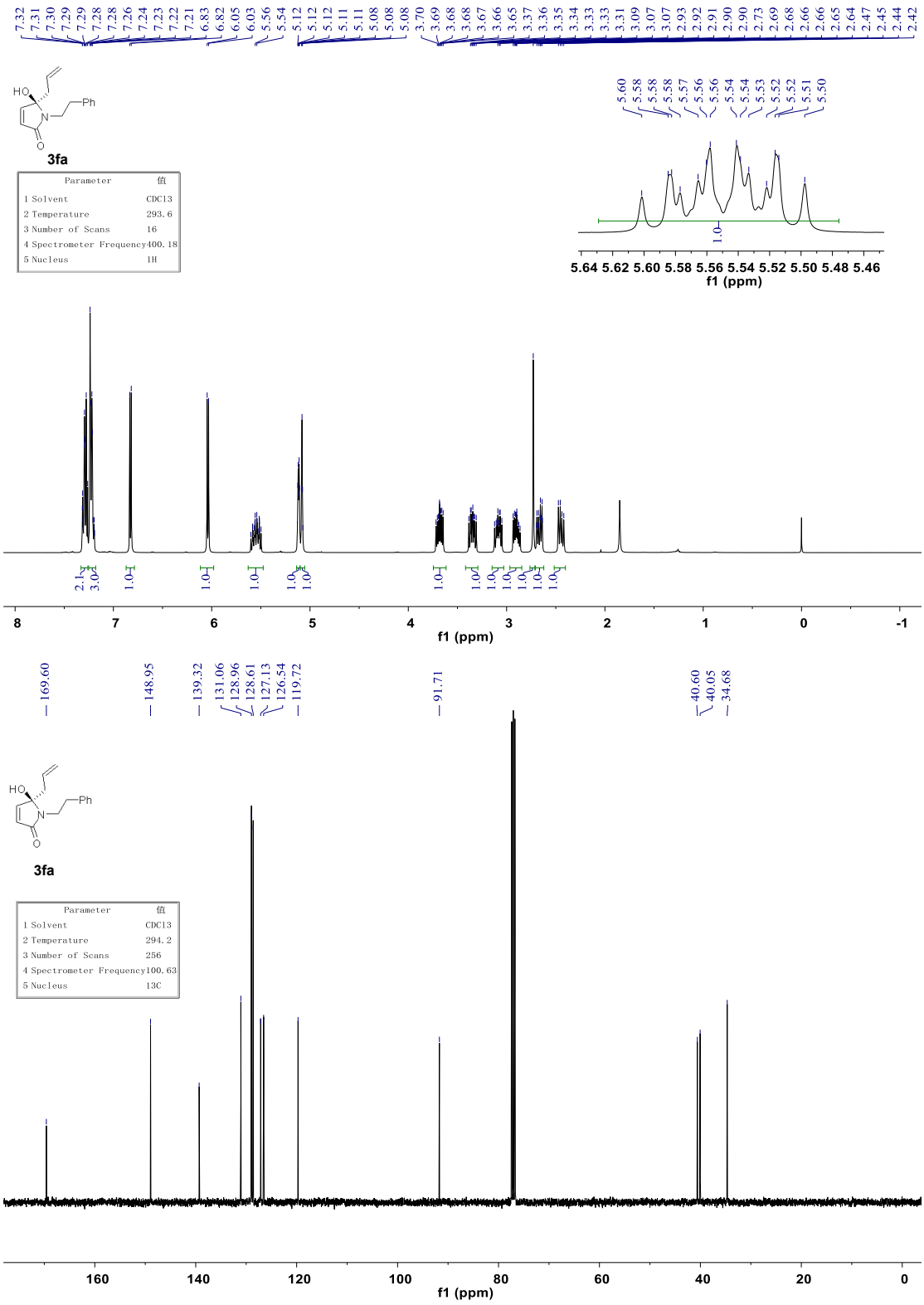
5 Nucleus	13C

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HO
Ph
N
O
3fa
Parameter 值
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2 Temperature 293.6
3 Number of Scans 16
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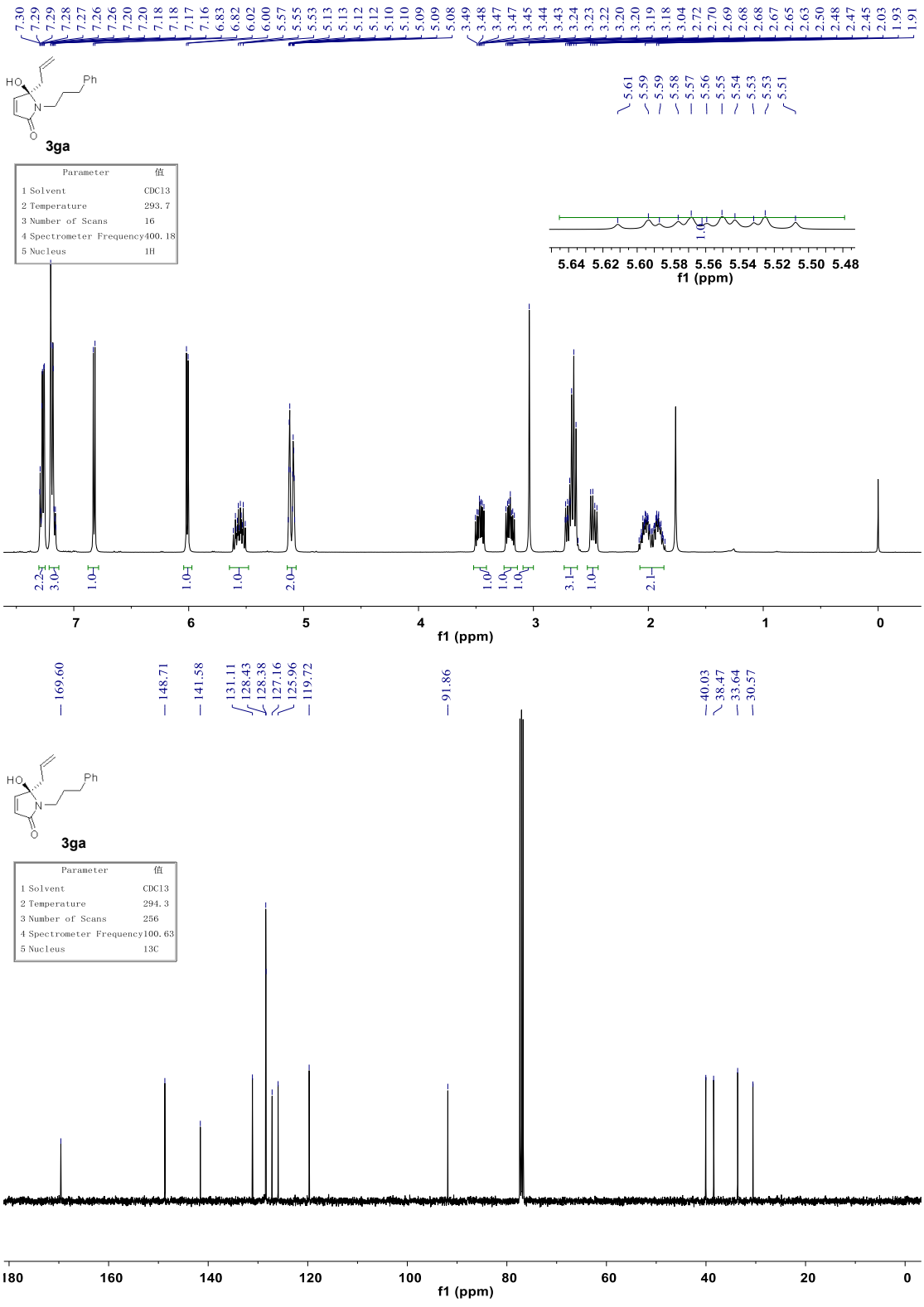
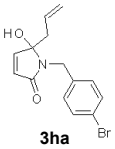
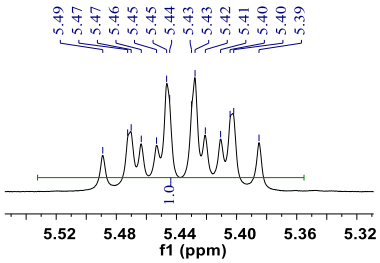
5 Nucleus 1H
5.60 5.58 5.58 5.58 5.57 5.56 5.56 5.54 5.54 5.53 5.52 5.52 5.51 5.50
1.0
5.64 5.62 5.60 5.58 5.56 5.54 5.52 5.50 5.48 5.46
f1 (ppm)
2.1 3.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
169.60 148.95 139.32 131.06 128.96 128.61 127.13 126.54 119.72 91.71 40.60 40.05 34.68
HO
Ph
N
O
3fa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.2
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
160 140 120 100 80 60 40 20 0
f1 (ppm)

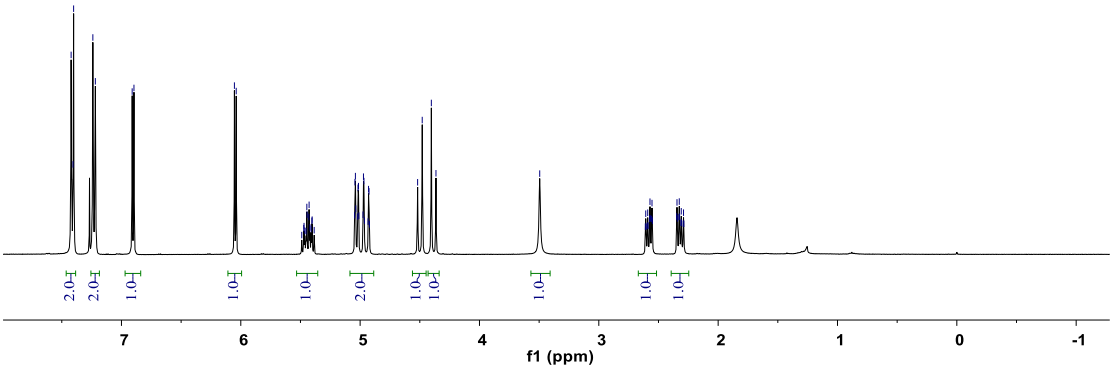

7.30 7.29 7.29 7.28 7.27 7.26 7.26 7.20 7.20 7.18 7.18 7.17 7.16 6.83 6.82 6.02 6.00 5.57 5.55 5.53 5.13 5.13 5.12 5.12 5.10 5.10 5.09 5.09 5.08 3.49 3.48 3.47 3.47 3.45 3.44 3.43 3.24 3.23 3.22 3.20 3.20 3.19 3.18 3.04 2.72 2.70 2.69 2.68 2.68 2.67 2.65 2.63 2.50 2.48 2.47 2.45 2.03 1.93 1.91
HO
Ph
N
O
3ga
5.61 5.59 5.59 5.58 5.57 5.56 5.55 5.54 5.53 5.53 5.51
Parameter 值
1 Solvent CDCl3
2 Temperature 293.7
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.00
5.64 5.62 5.60 5.58 5.56 5.54 5.52 5.50 5.48
f1 (ppm)
2.2 3.0 1.0 1.0 1.0 2.0 1.0 1.0 1.0 3.1 1.0 2.1
7 6 5 4 3 2 1 0
f1 (ppm)
169.60 148.71 141.58 131.11 128.43 128.38 127.16 125.96 119.72 91.86 40.03 38.47 33.64 30.57
HO
Ph
N
O
3ga
Parameter 值
1 Solvent CDCl3
2 Temperature 294.3
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
180 160 140 120 100 80 60 40 20 0
f1 (ppm)



3ha

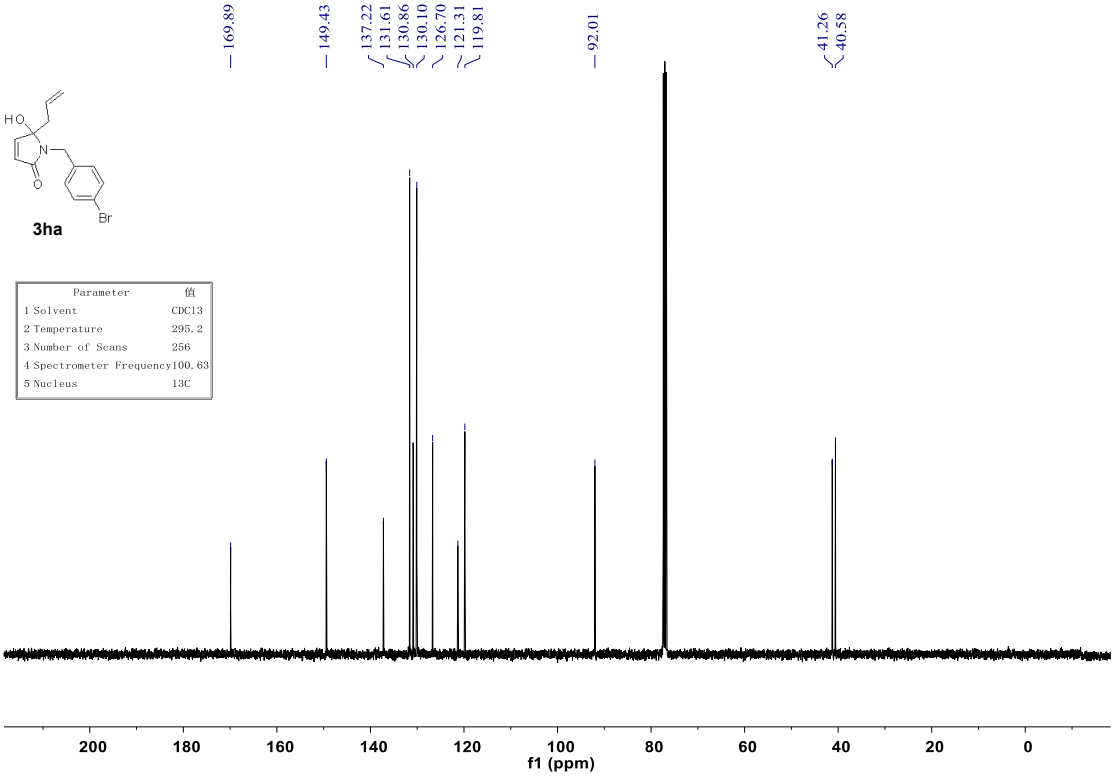
Parameter	值
1 Solvent	CDCl3
2 Temperature	294.6
3 Number of Scans	16
4 Spectrometer Frequency	400.18
5 Nucleus	1H

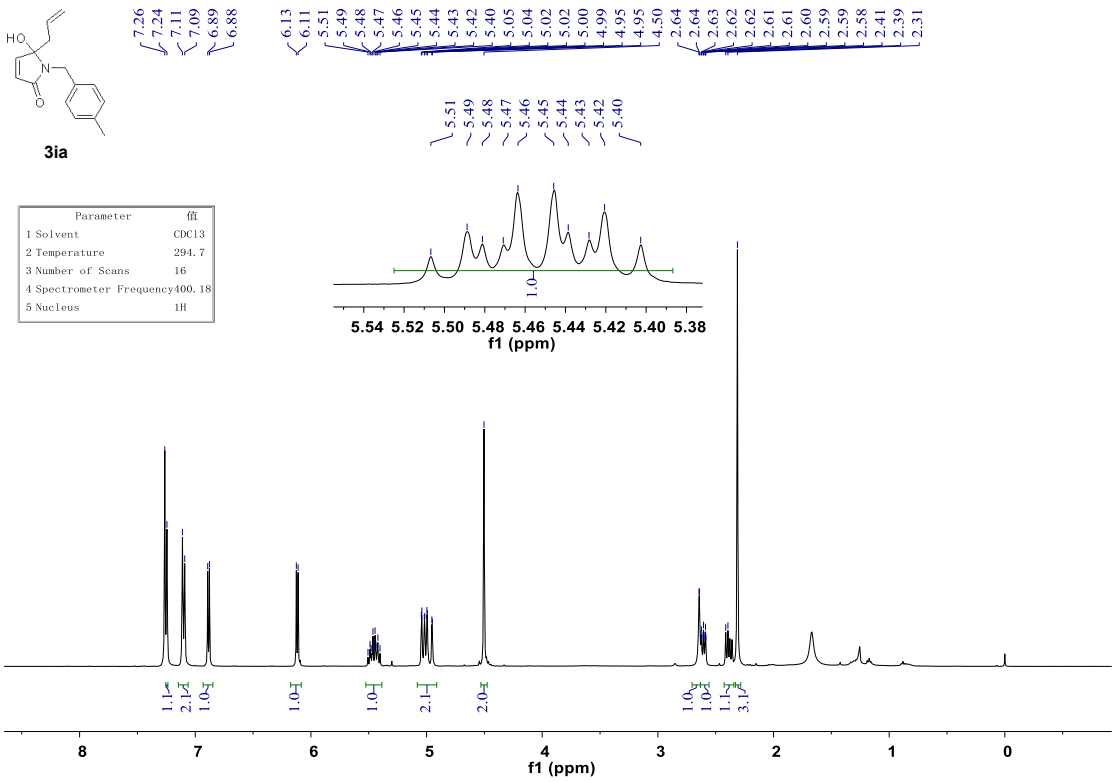


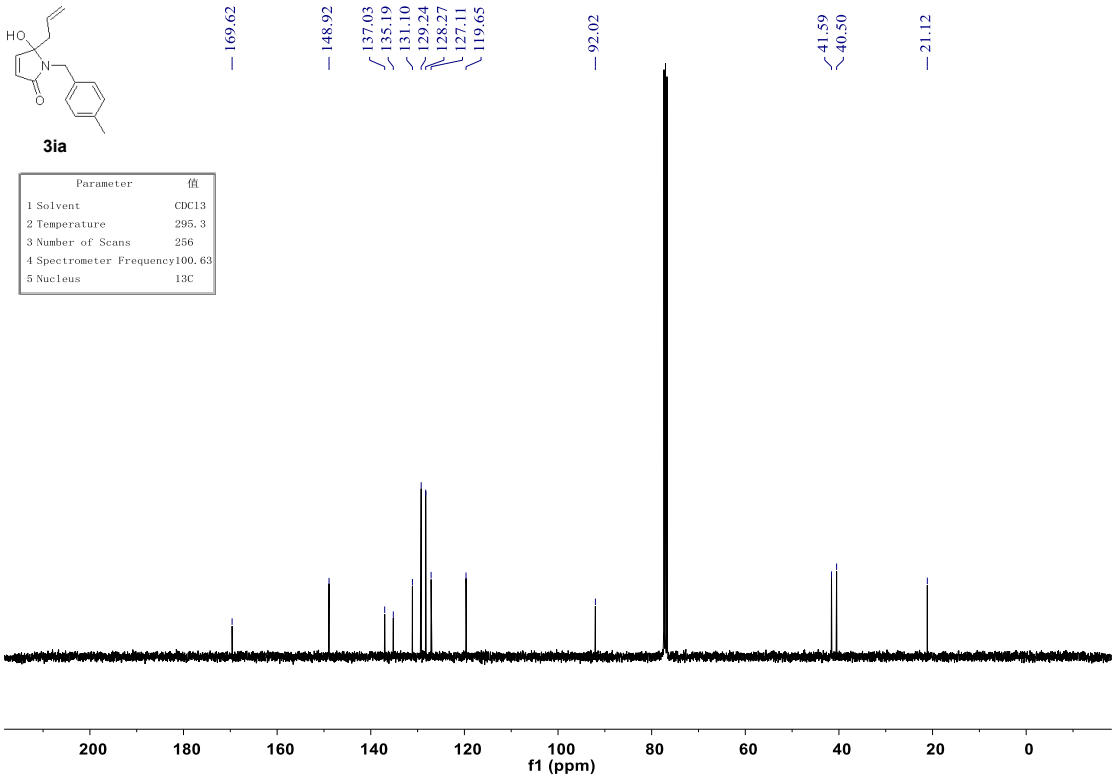


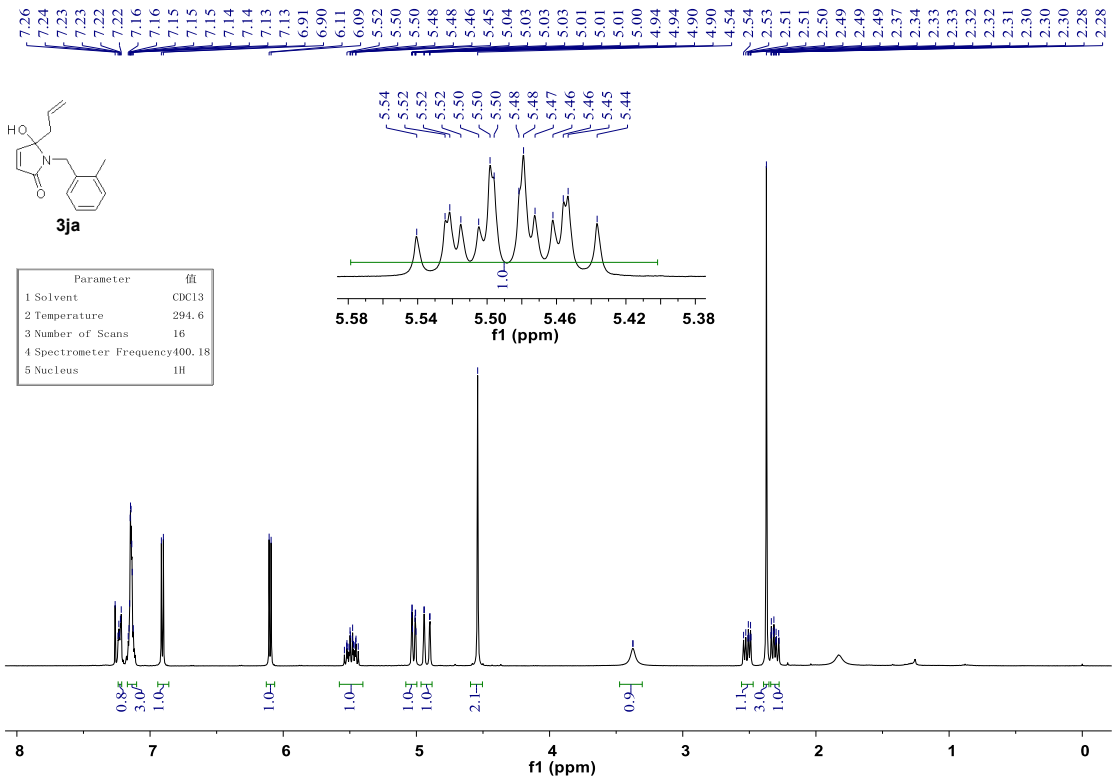
3ha

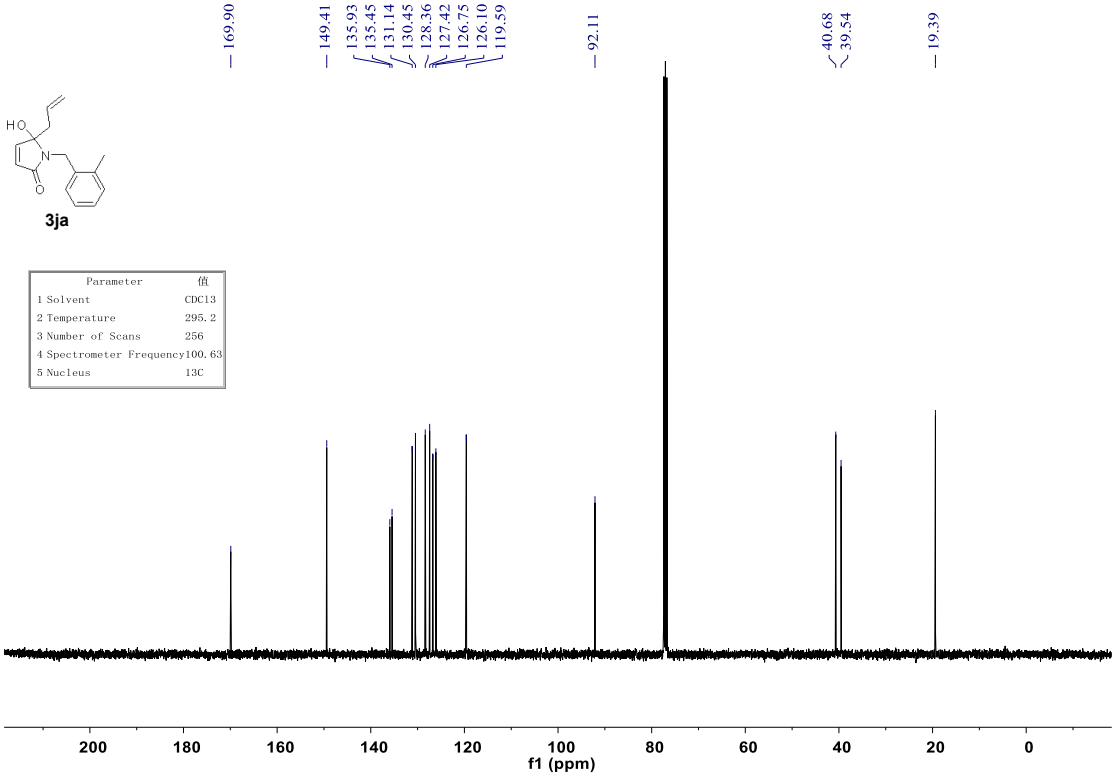
Parameter	值
1 Solvent	CDCl3
2 Temperature	295.2
3 Number of Scans	256
4 Spectrometer Frequency	100.63
5 Nucleus	13C

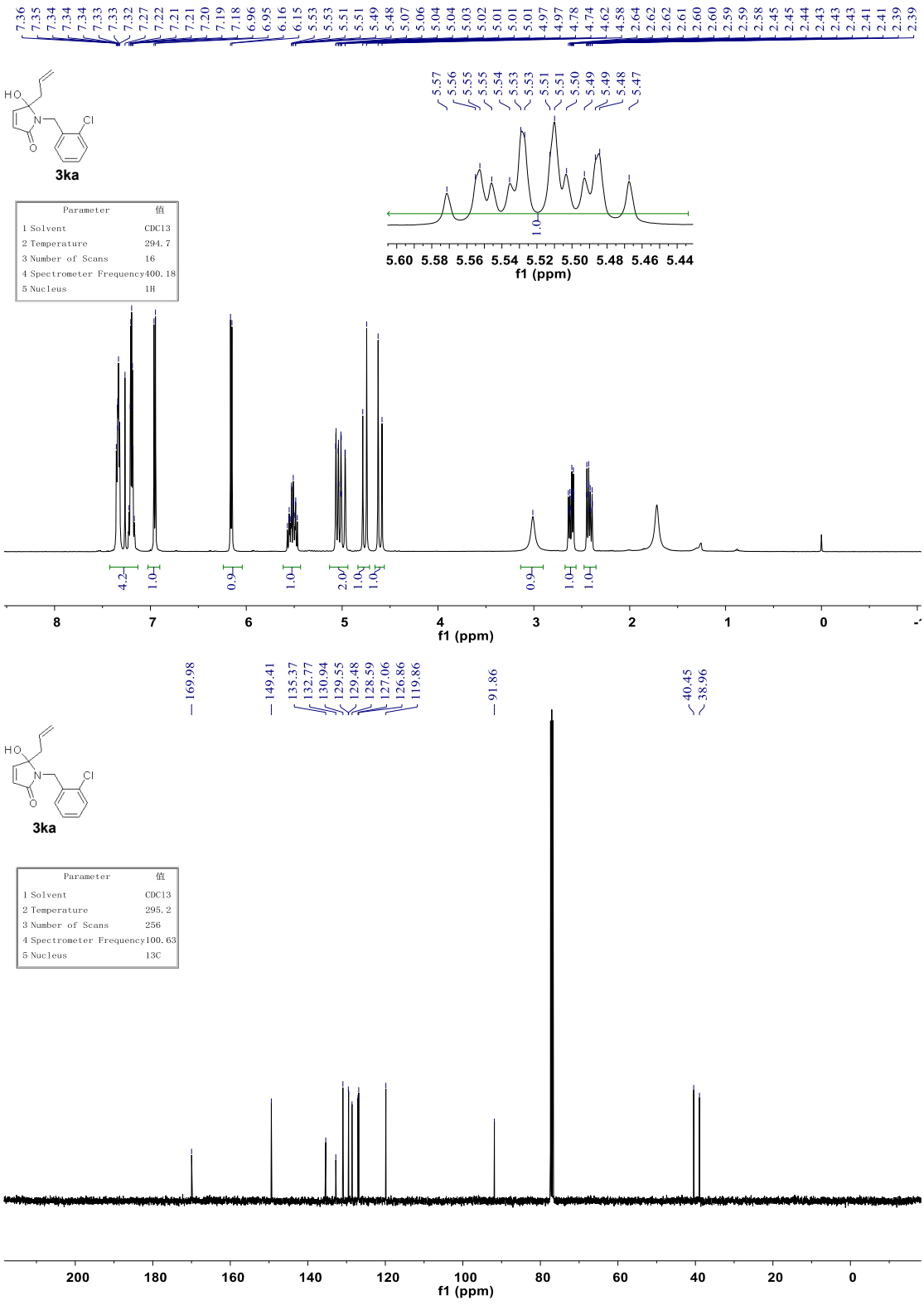


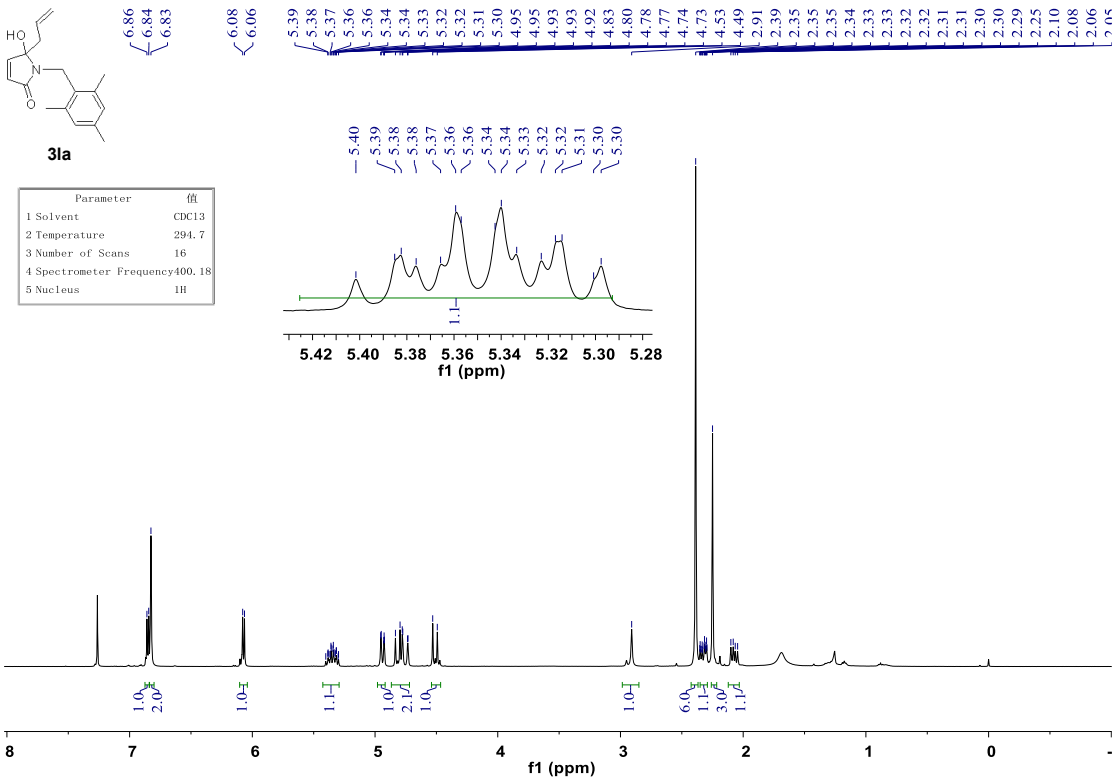

3ia
Parameter 值
1 Solvent CDCl3
2 Temperature 294.7
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

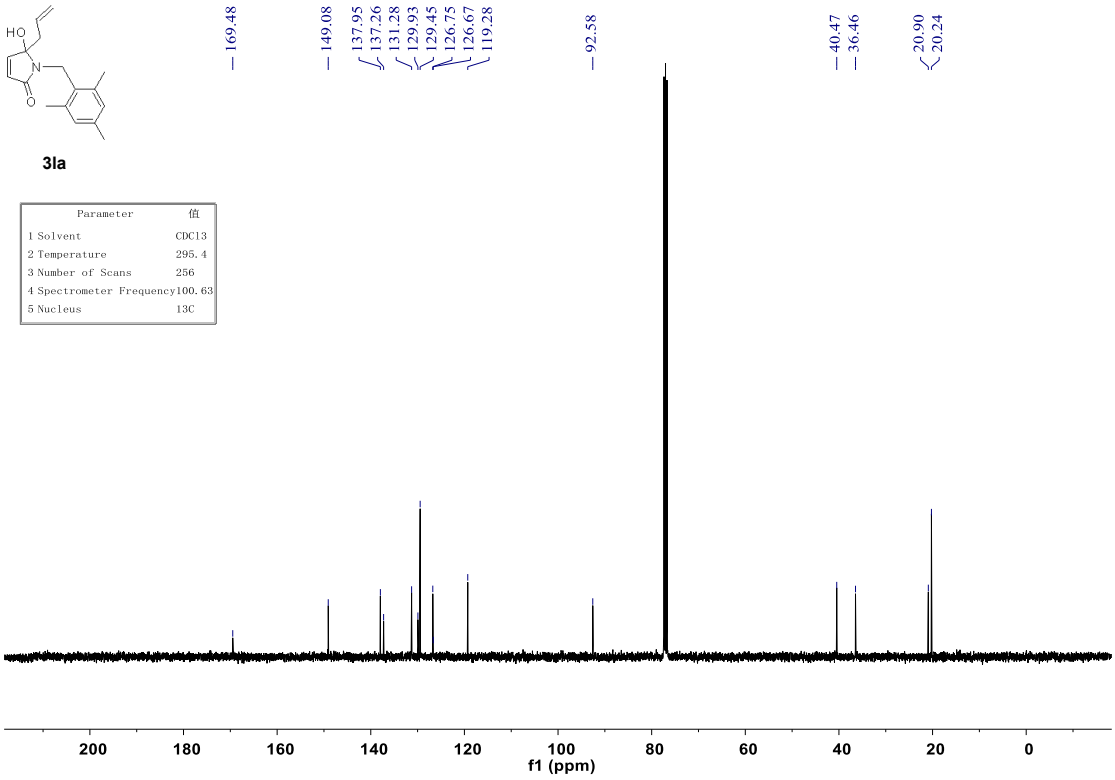

3ia
Parameter 值
1 Solvent CDCl3
2 Temperature 295.3
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

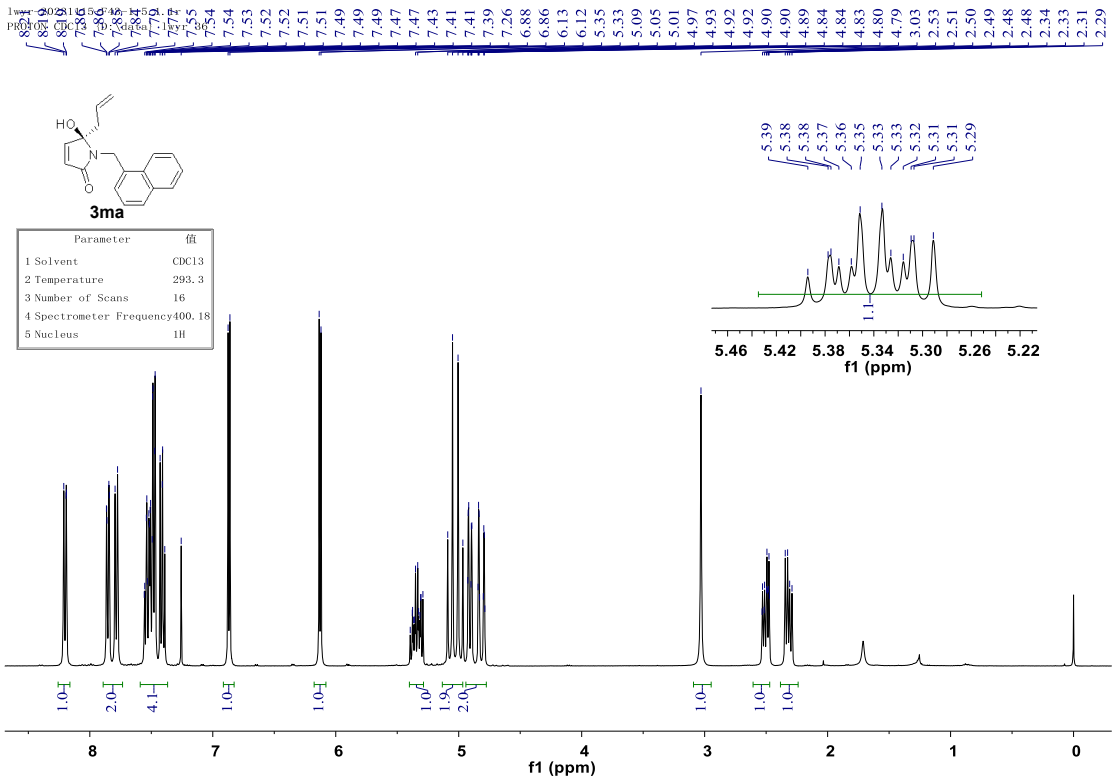

3ja
Parameter ffi
1 Solvent CDCl3
2 Temperature 294.6
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

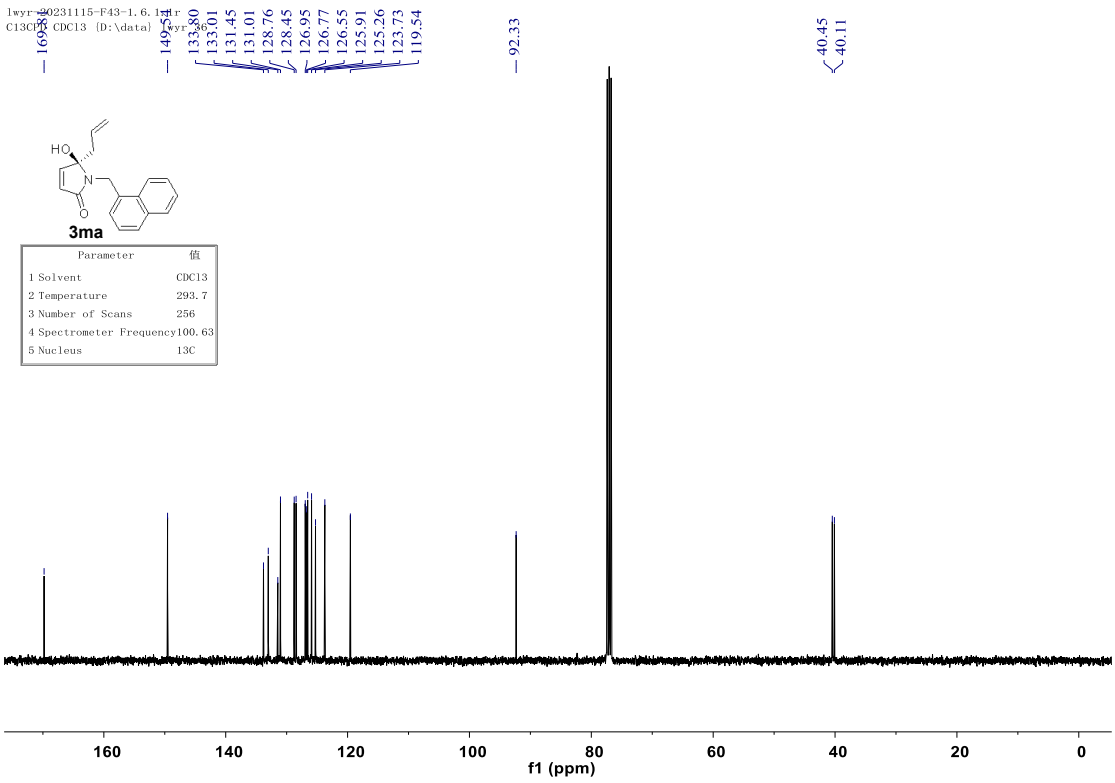

3ja
Parameter ffi
1 Solvent CDCl3
2 Temperature 295.2
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

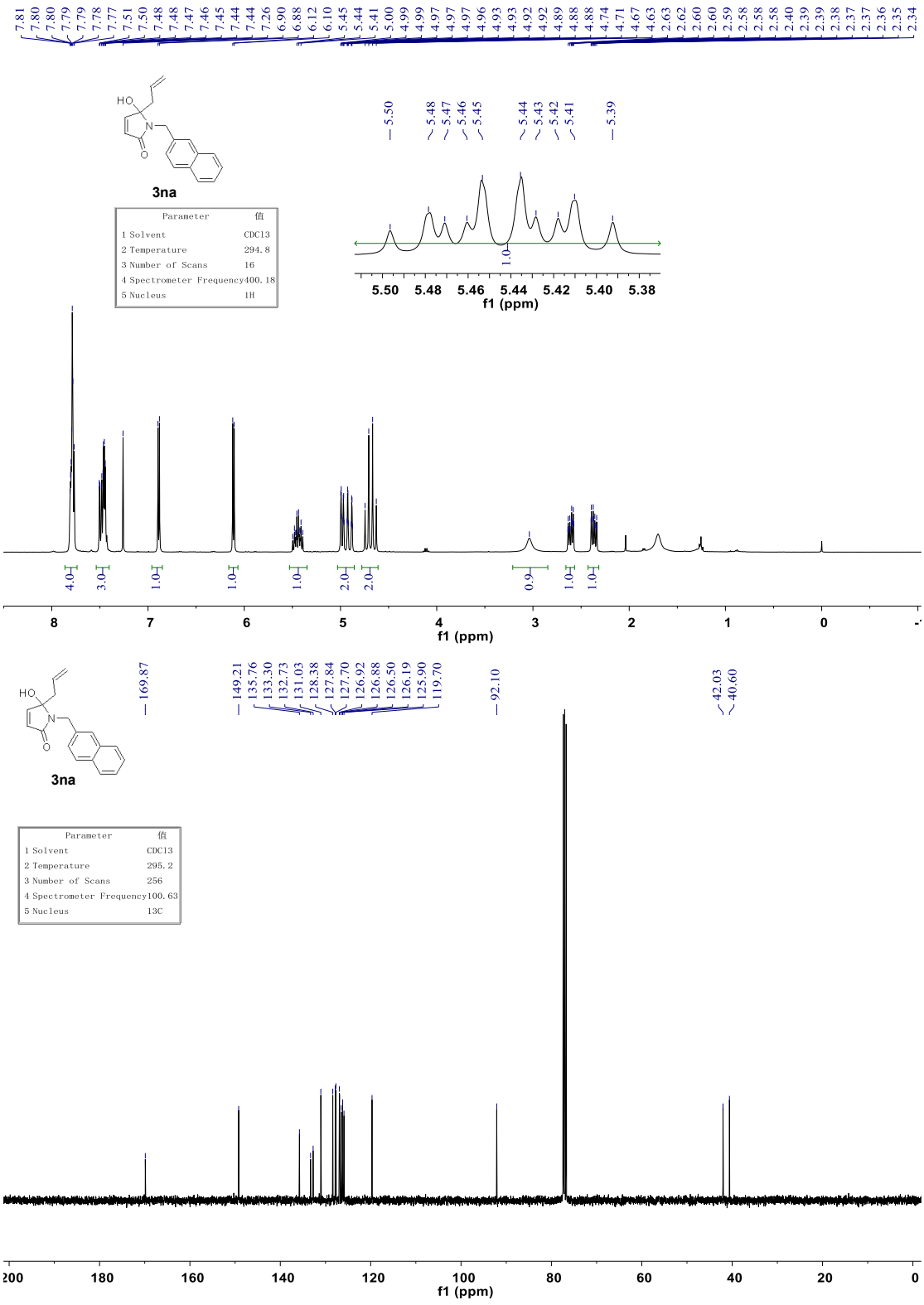

7.36 7.35 7.34 7.34 7.34 7.33 7.33 7.32 7.27 7.22 7.21 7.21 7.20 7.19 7.18 6.96 6.95 6.16 6.15 5.53 5.53 5.51 5.51 5.49 5.48 5.07 5.06 5.04 5.04 5.03 5.02 5.01 5.01 5.01 4.97 4.97 4.78 4.74 4.62 4.58 2.64 2.62 2.62 2.61 2.60 2.60 2.59 2.59 2.58 2.45 2.45 2.44 2.43 2.43 2.43 2.41 2.41 2.39 2.39
HO
N
O
Cl
3ka
Parameter 值
1 Solvent CDCl3
2 Temperature 294.7
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.57 5.56 5.55 5.55 5.54 5.53 5.53 5.51 5.51 5.50 5.49 5.49 5.48 5.47
1.0
5.60 5.58 5.56 5.54 5.52 5.50 5.48 5.46 5.44
f1 (ppm)
4.2 1.0 0.9 1.0 2.0 1.0 1.0 0.9 1.0 1.0
8 7 6 5 4 3 2 1 0
f1 (ppm)
169.98 149.41 135.37 132.77 130.94 129.55 129.48 128.59 127.06 126.86 119.86 91.86 40.45 38.96
HO
N
O
Cl
3ka
Parameter 值
1 Solvent CDCl3
2 Temperature 295.2
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

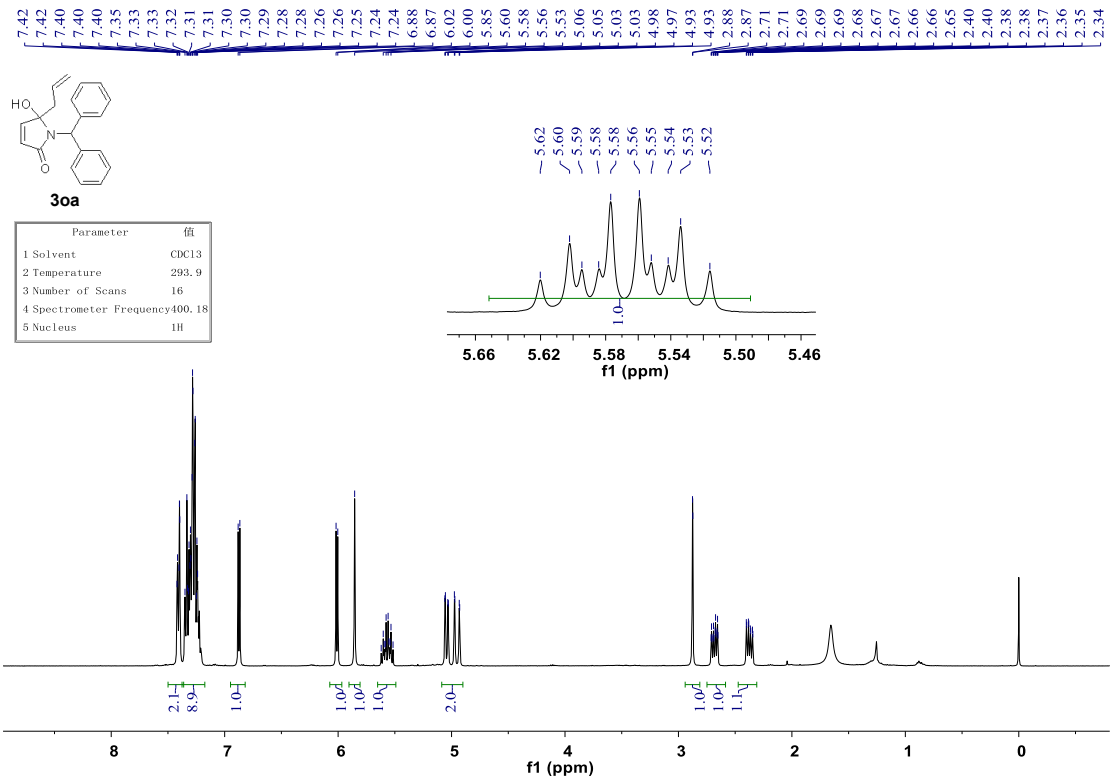

3la
Parameter 值
1 Solvent CDCl3
2 Temperature 294.7
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

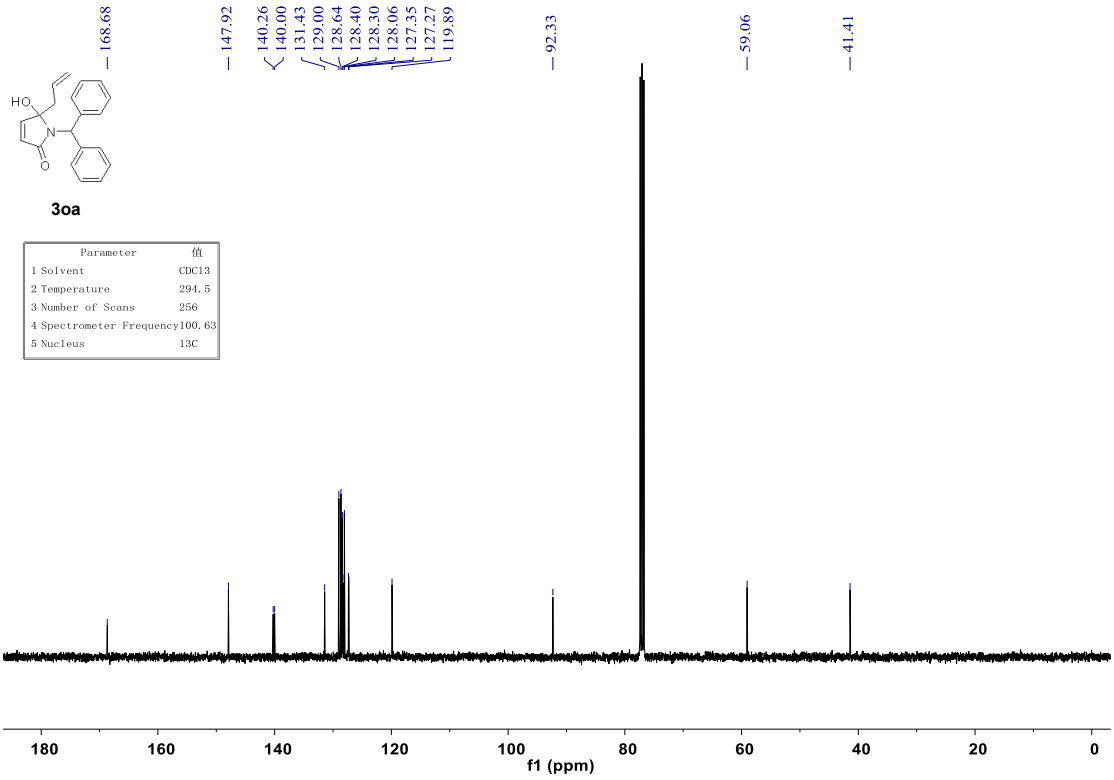

3la
Parameter 值
1 Solvent CDCl3
2 Temperature 295.4
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

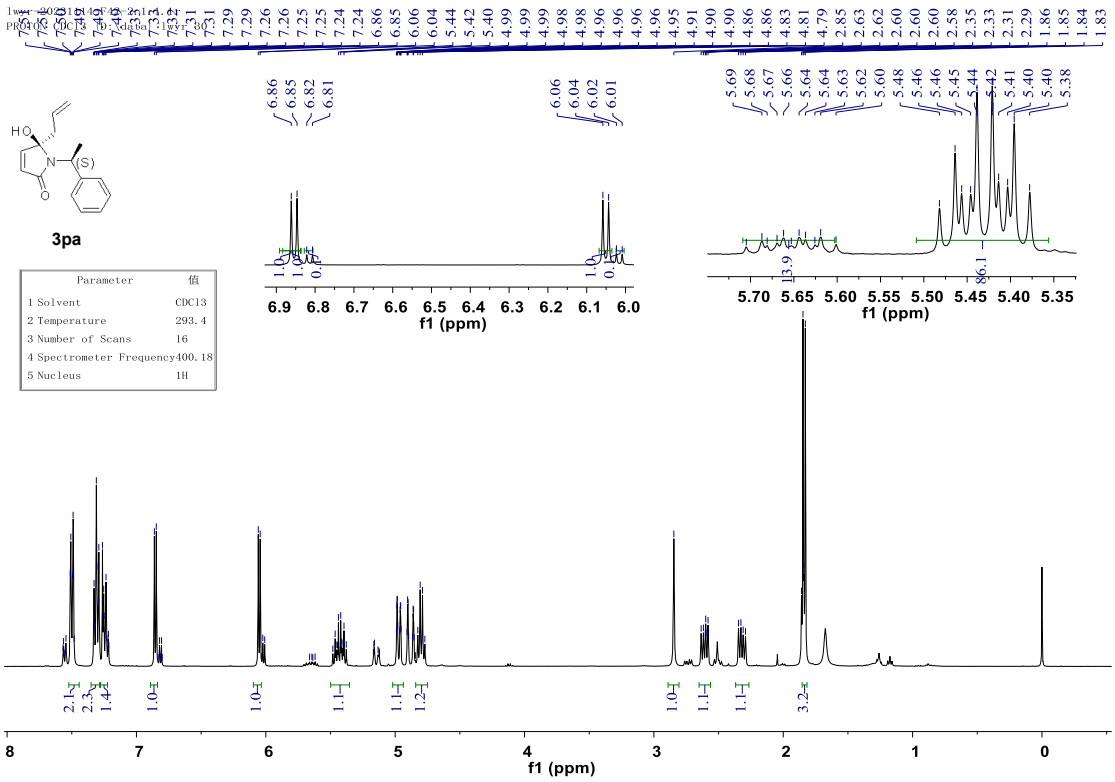

3ma
Parameter 值
1 Solvent CDCl3
2 Temperature 293.3
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

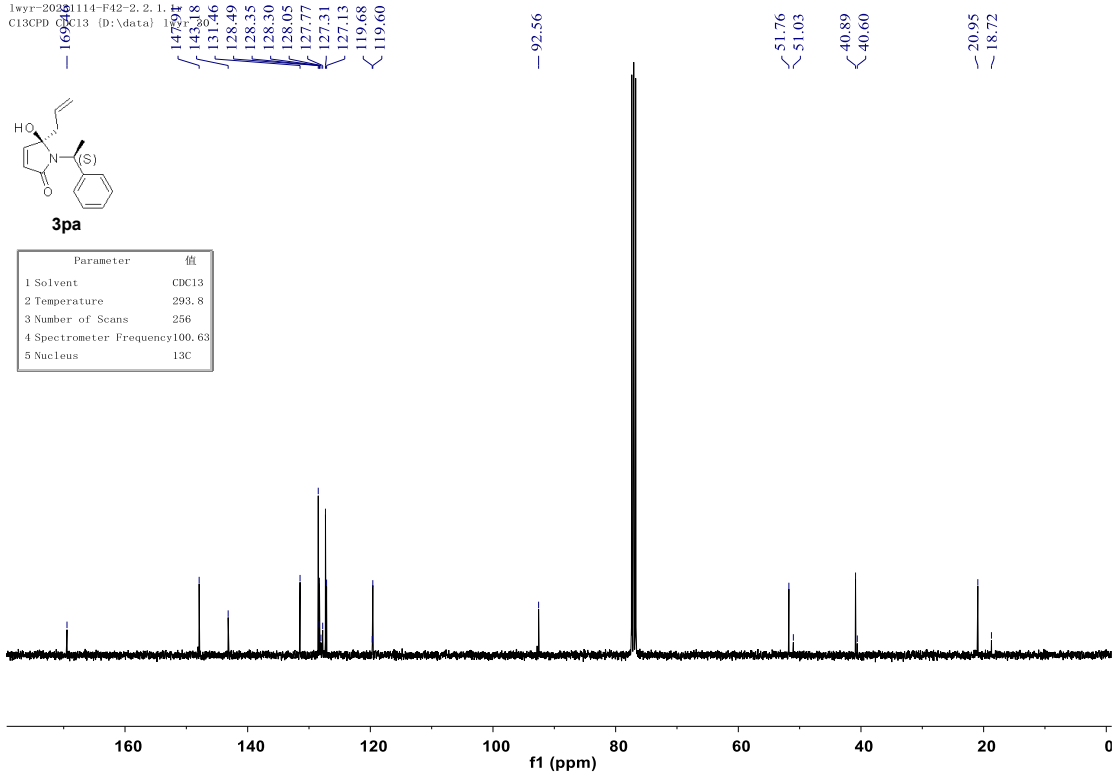

3ma
Parameter 值
1 Solvent CDCl3
2 Temperature 293.7
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

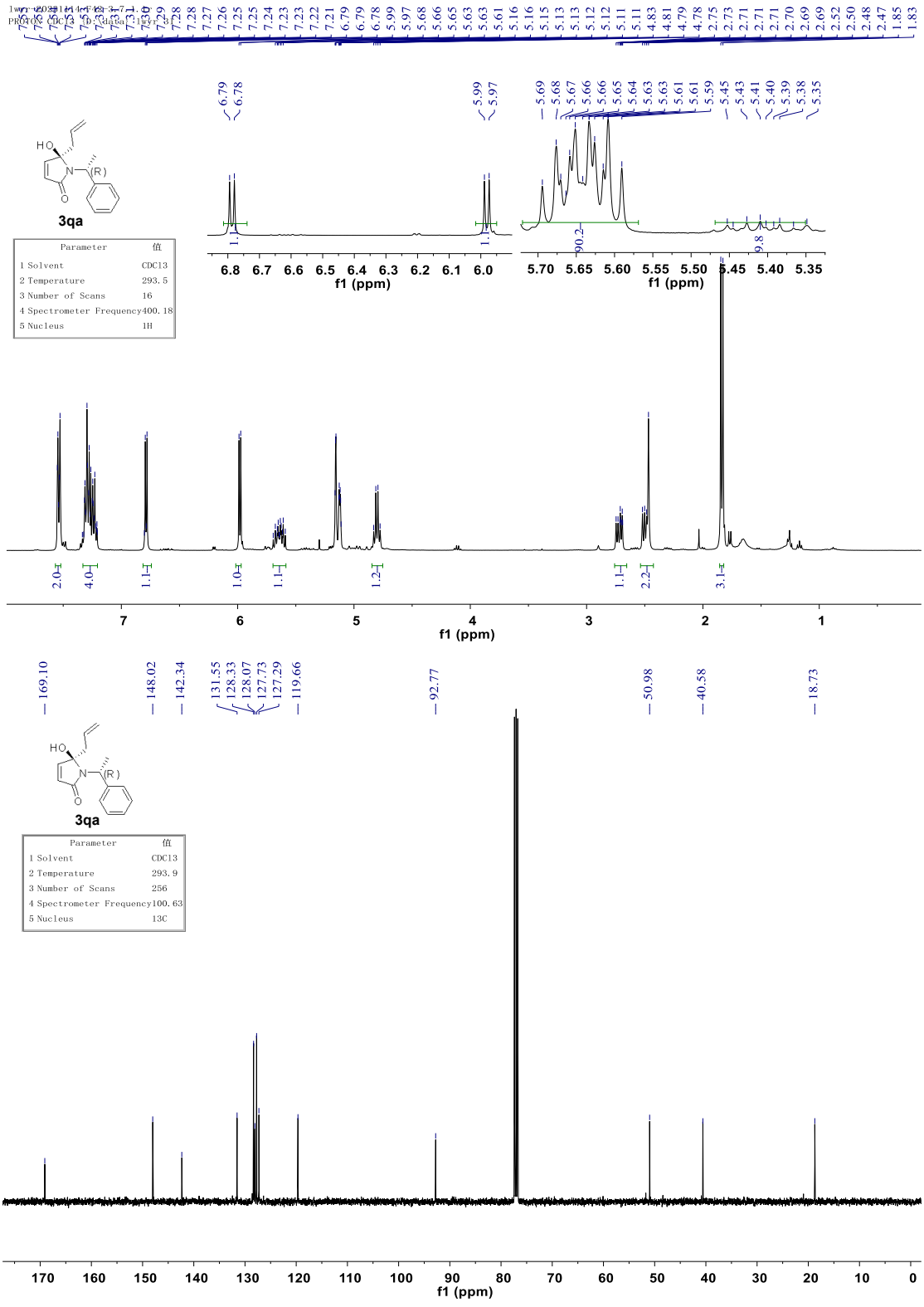

3na
Parameter 值
1 Solvent CDCl3
2 Temperature 294.8
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)
3na
Parameter 值
1 Solvent CDCl3
2 Temperature 295.2
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

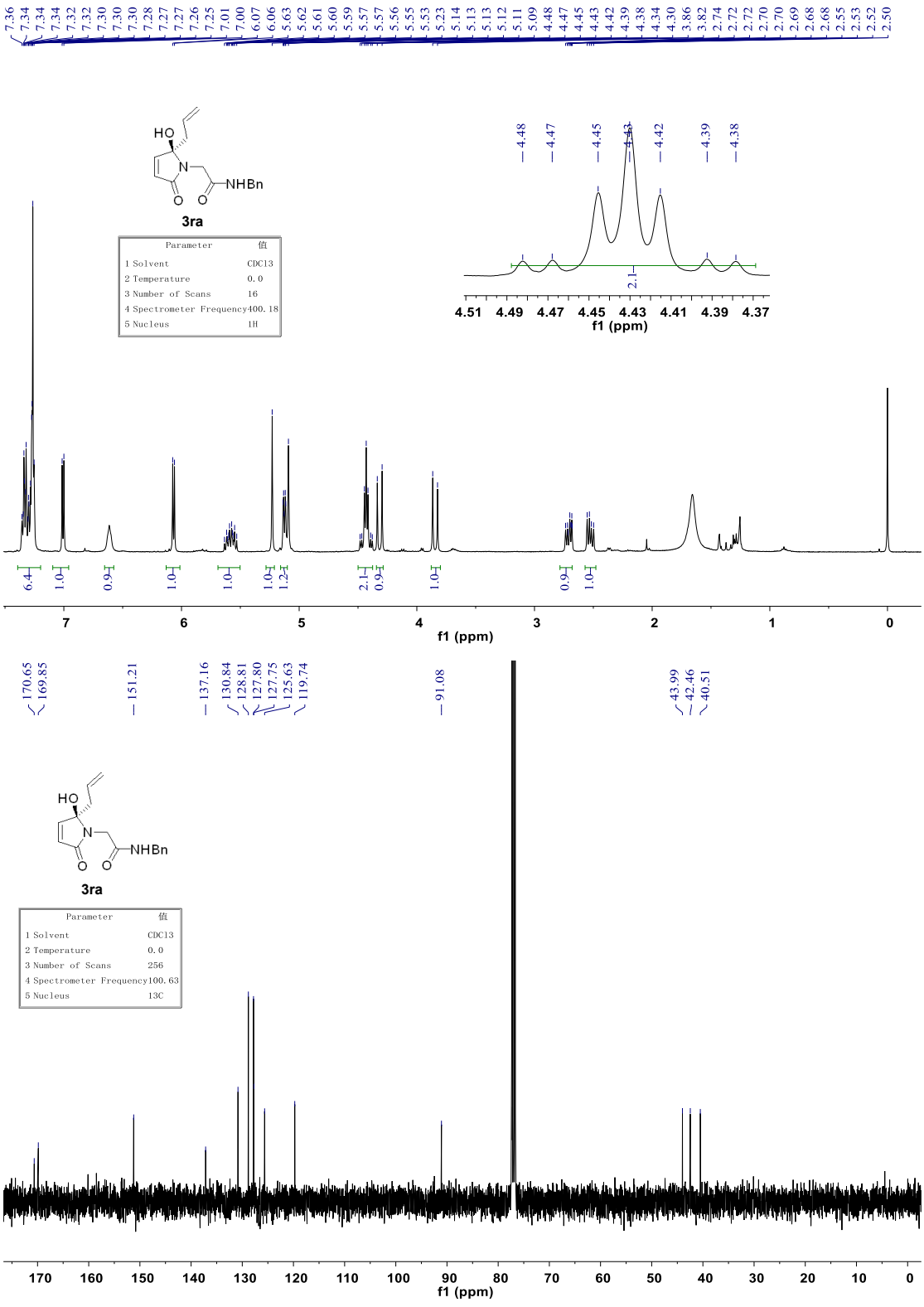

7.42 7.42 7.40 7.40 7.40 7.35 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.29 7.28 7.28 7.26 7.26 7.25 7.24 7.24 6.88 6.87 6.02 6.00 5.85 5.60 5.58 5.56 5.53 5.06 5.05 5.03 5.03 4.98 4.97 4.93 4.93 2.88 2.87 2.71 2.71 2.69 2.69 2.69 2.68 2.67 2.67 2.66 2.66 2.65 2.40 2.40 2.38 2.37 2.36 2.35 2.34
HO
N
O
3oa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.9
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.62 5.60 5.59 5.58 5.58 5.56 5.55 5.54 5.53 5.52
1.0
5.66 5.62 5.58 5.54 5.50 5.46
f1 (ppm)
2.1 8.9 1.0 1.0 1.0 1.0 2.0 1.0 1.0 1.1
8 7 6 5 4 3 2 1 0
f1 (ppm)

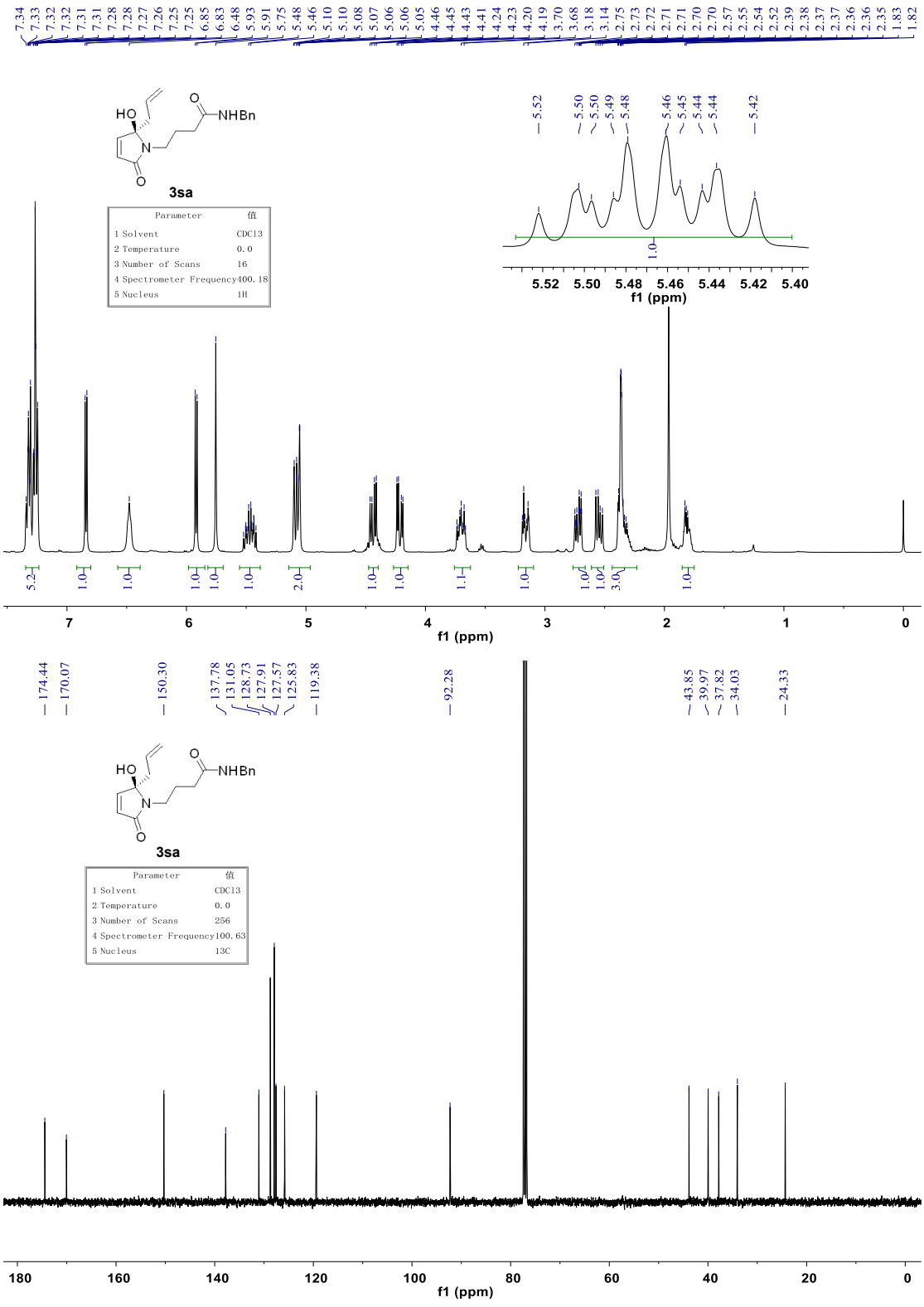

168.68 147.92 140.26 140.00 131.43 129.00 128.64 128.40 128.30 128.06 127.35 127.27 119.89 92.33 59.06 41.41
HO
N
O
3oa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.5
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
180 160 140 120 100 80 60 40 20 0
f1 (ppm)

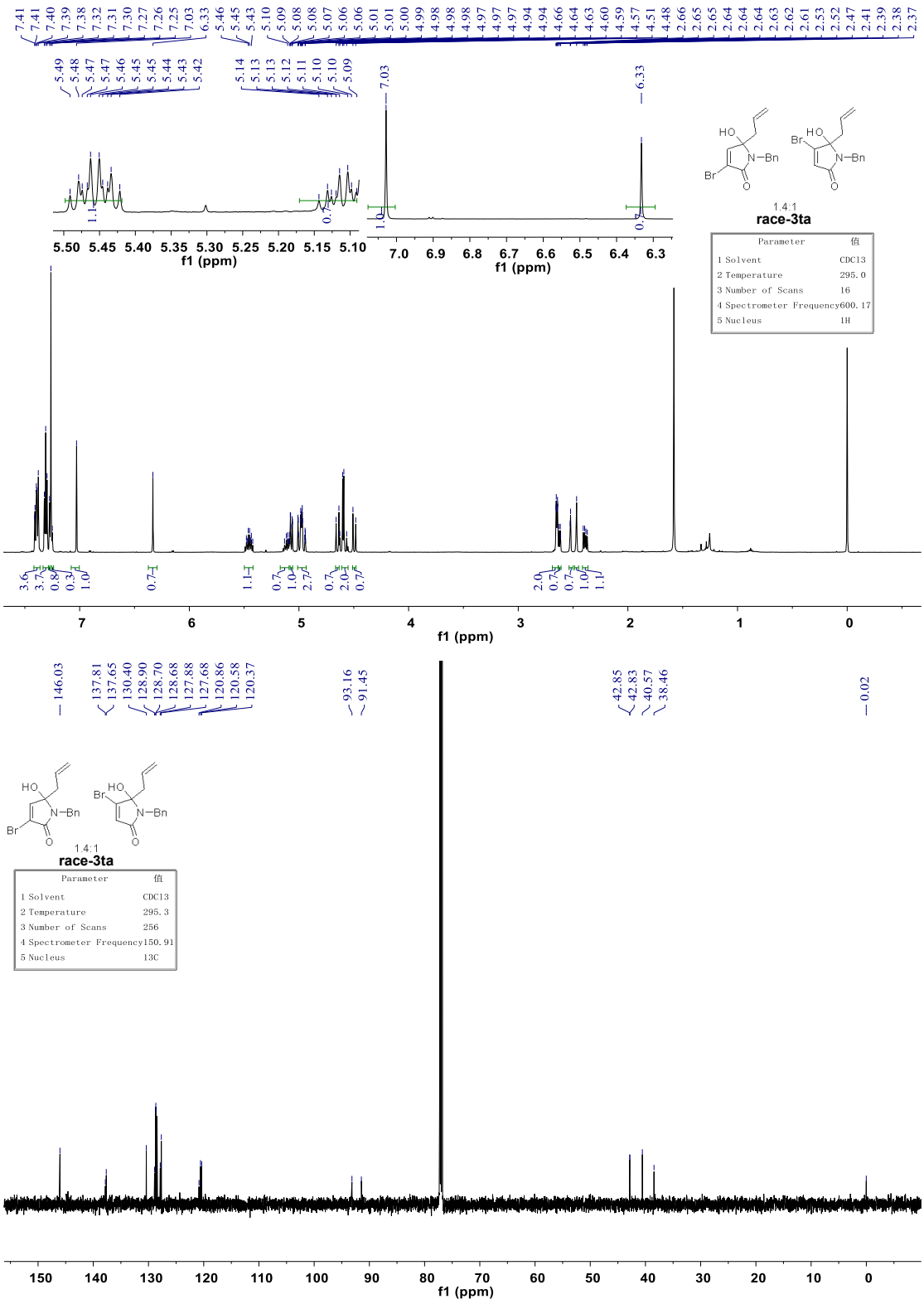

3pa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.4
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

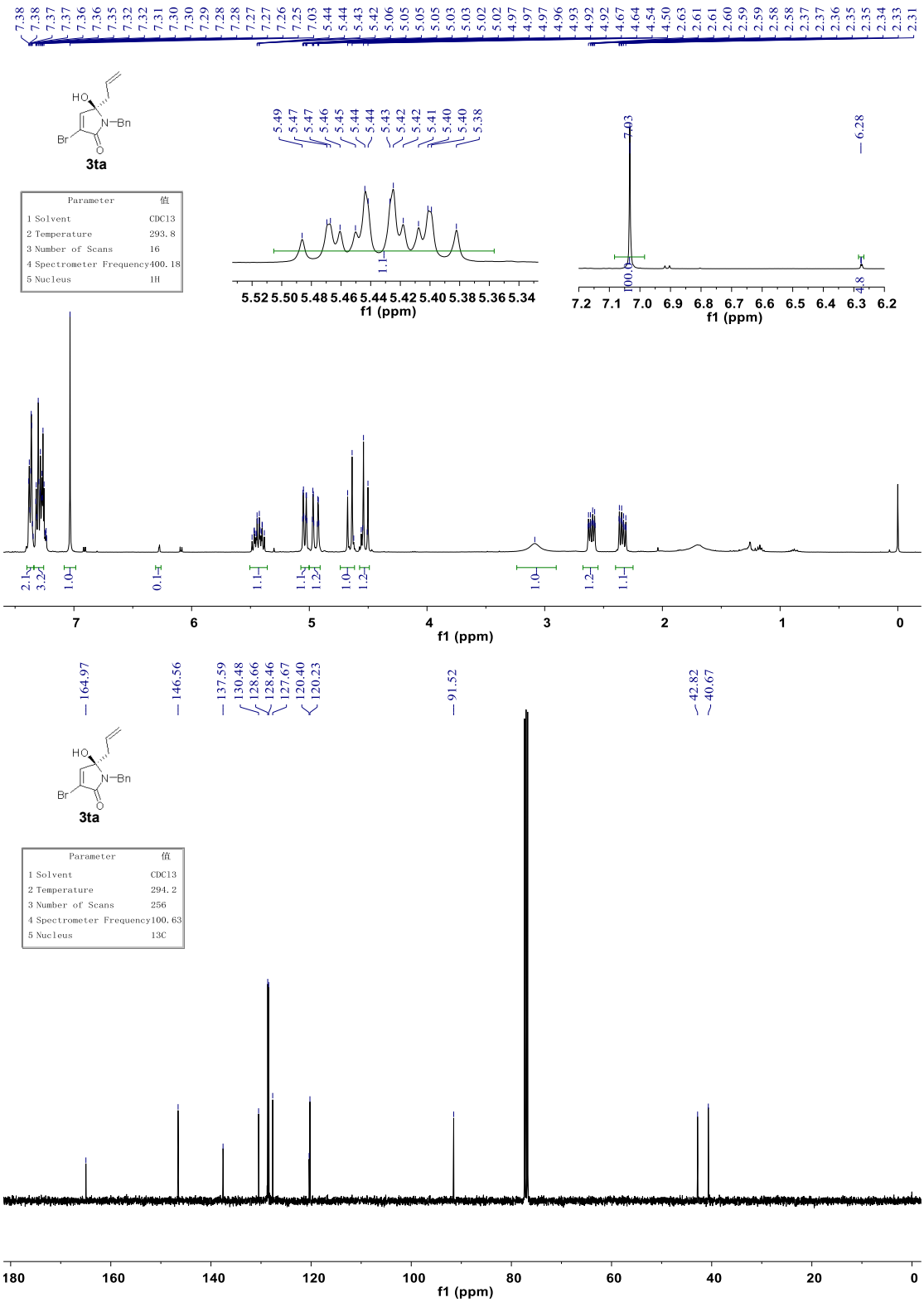

3pa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.8
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

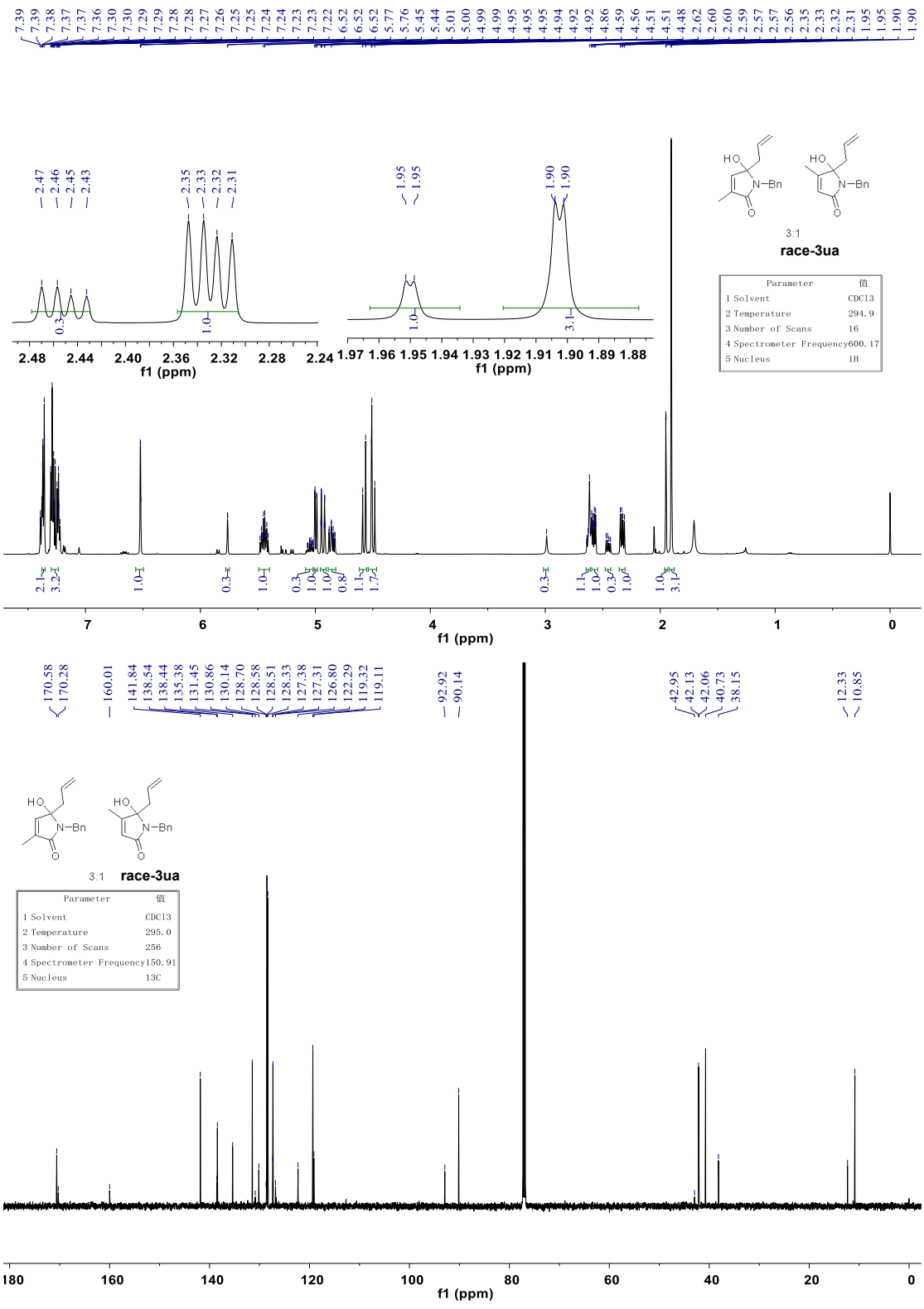

3qa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)
3qa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.9
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

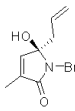

7.36 7.34 7.34 7.34 7.32 7.32 7.30 7.30 7.30 7.28 7.27 7.27 7.26 7.25 7.01 7.00 6.07 6.06 5.63 5.62 5.61 5.60 5.59 5.57 5.57 5.56 5.55 5.53 5.23 5.14 5.13 5.13 5.12 5.11 5.09 4.48 4.47 4.45 4.43 4.42 4.39 4.38 4.34 4.30 3.86 3.82 2.74 2.72 2.72 2.70 2.70 2.69 2.68 2.68 2.55 2.53 2.52 2.50
HO
N
O
O
NHBn
3ra
Parameter 值
1 Solvent CDCl3
2 Temperature 0.0
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
4.48 4.47 4.45 4.43 4.42 4.39 4.38
2.1
4.51 4.49 4.47 4.45 4.43 4.41 4.39 4.37
f1 (ppm)
6.4 1.0 0.9 1.0 1.0 1.0 1.2 2.1 0.9 1.0 0.9 1.0
7 6 5 4 3 2 1 0
f1 (ppm)
170.65 169.85 151.21 137.16 130.84 128.81 127.80 127.75 125.63 119.74 91.08 43.99 42.46 40.51
HO
N
O
O
NHBn
3ra
Parameter 值
1 Solvent CDCl3
2 Temperature 0.0
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.34 7.33 7.32 7.32 7.31 7.31 7.28 7.28 7.27 7.26 7.25 7.25 6.85 6.83 6.48 5.93 5.91 5.75 5.48 5.46 5.10 5.10 5.08 5.07 5.06 5.06 5.05 4.46 4.45 4.43 4.41 4.24 4.23 4.20 4.19 3.70 3.68 3.18 3.14 2.75 2.73 2.72 2.71 2.71 2.70 2.70 2.57 2.55 2.54 2.52 2.39 2.38 2.37 2.37 2.36 2.36 2.35 1.83 1.82
HO
O
NHBn
N
O
3sa
Parameter 值
1 Solvent CDCl3
2 Temperature 0.0
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.52 5.50 5.50 5.49 5.48 5.46 5.45 5.44 5.44 5.42
1.0
5.52 5.50 5.48 5.46 5.44 5.42 5.40
f1 (ppm)
5.2 1.0 1.0 1.0 1.0 1.0 2.0 1.0 1.0 1.1 1.0 1.0 1.0 3.0 1.0
7 6 5 4 3 2 1 0
f1 (ppm)
174.44 170.07 150.30 137.78 131.05 128.73 127.91 127.57 125.83 119.38 92.28 43.85 39.97 37.82 34.03 24.33
HO
O
NHBn
N
O
3sa
Parameter 值
1 Solvent CDCl3
2 Temperature 0.0
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
180 160 140 120 100 80 60 40 20 0
f1 (ppm)


1.4:1
race-3ta
Parameter 值
1 Solvent CDCl3
2 Temperature 295.0
3 Number of Scans 16
4 Spectrometer Frequency 600.17
5 Nucleus 1H
f1 (ppm)
1.4:1
race-3ta
Parameter 值
1 Solvent CDCl3
2 Temperature 295.3
3 Number of Scans 256
4 Spectrometer Frequency 150.91
5 Nucleus 13C
f1 (ppm)

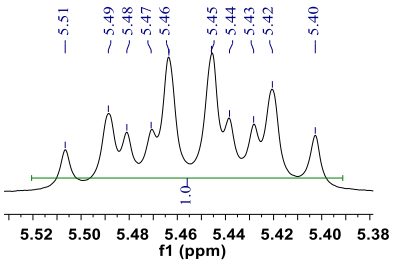

3ta
Parameter 值
1 Solvent CDCl3
2 Temperature 293.8
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)
3ta
Parameter 值
1 Solvent CDCl3
2 Temperature 294.2
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

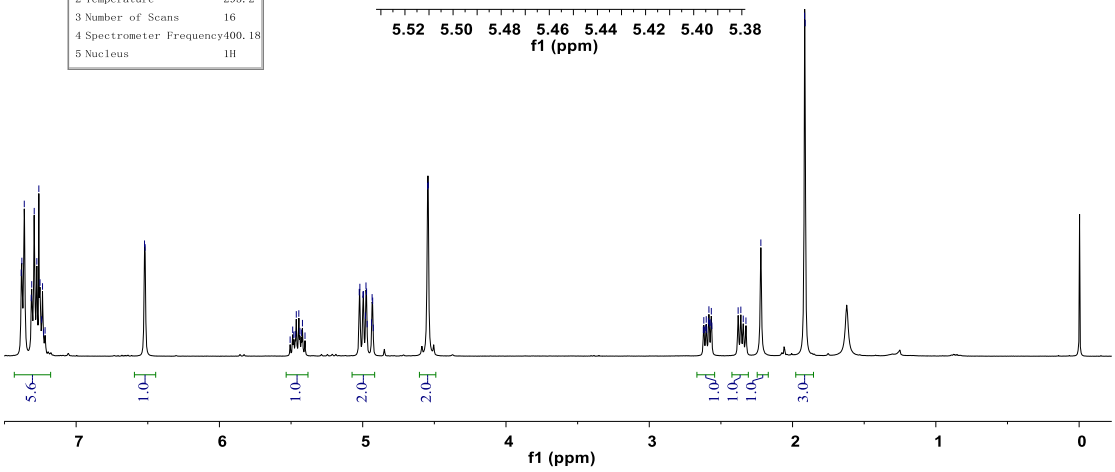

3:1
race-3ua
Parameter 值
1 Solvent CDCl3
2 Temperature 294.9
3 Number of Scans 16
4 Spectrometer Frequency 600.17
5 Nucleus 1H
f1 (ppm)
3:1
race-3ua
Parameter 值
1 Solvent CDCl3
2 Temperature 295.0
3 Number of Scans 256
4 Spectrometer Frequency 150.91
5 Nucleus 13C
f1 (ppm)

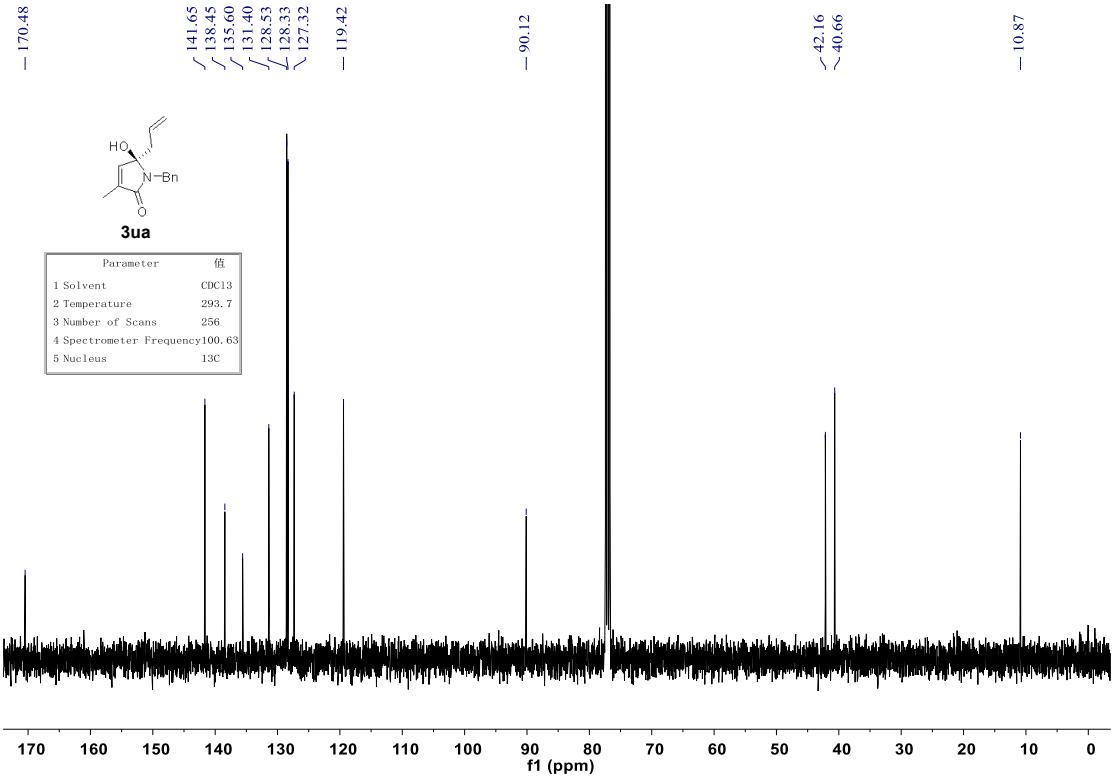


3ua

Parameter	值
1 Solvent	CDCl3
2 Temperature	293.2
3 Number of Scans	16
4 Spectrometer Frequency	400.18
5 Nucleus	1H



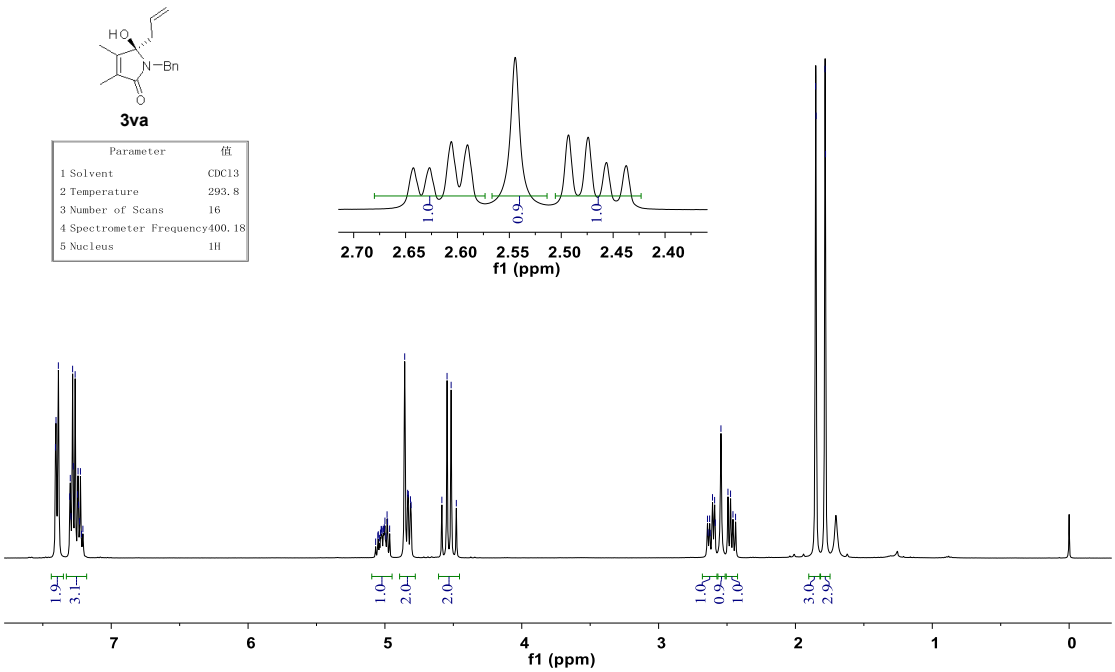


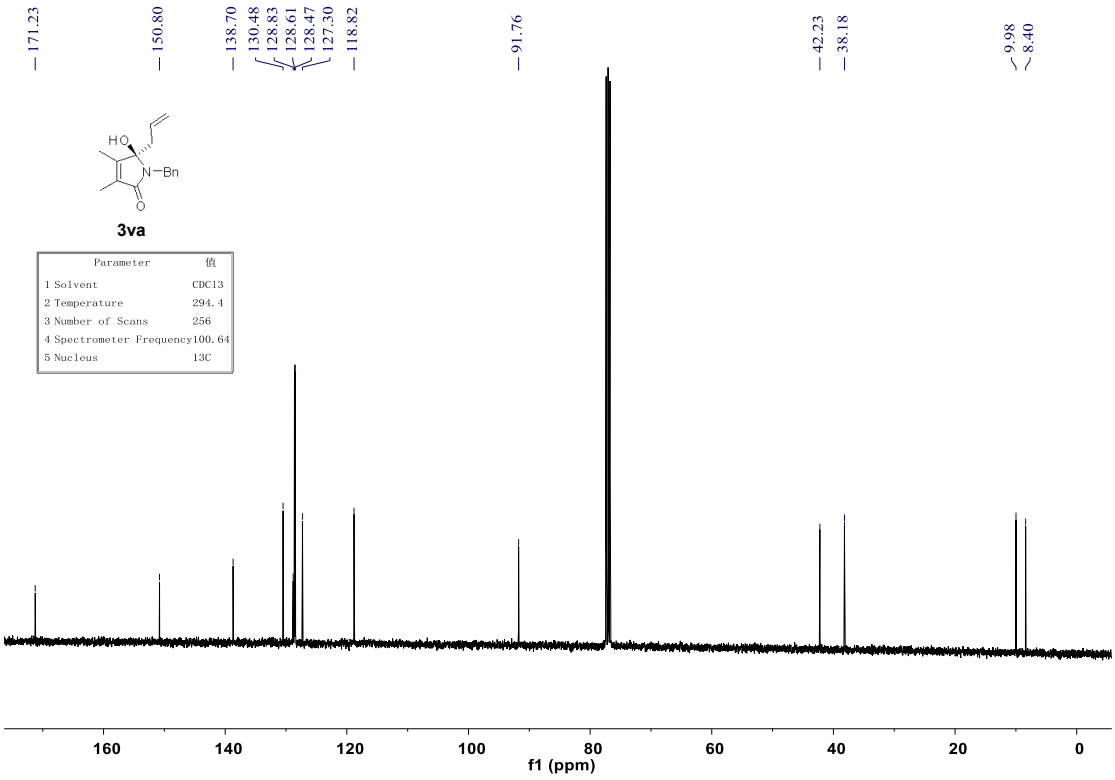


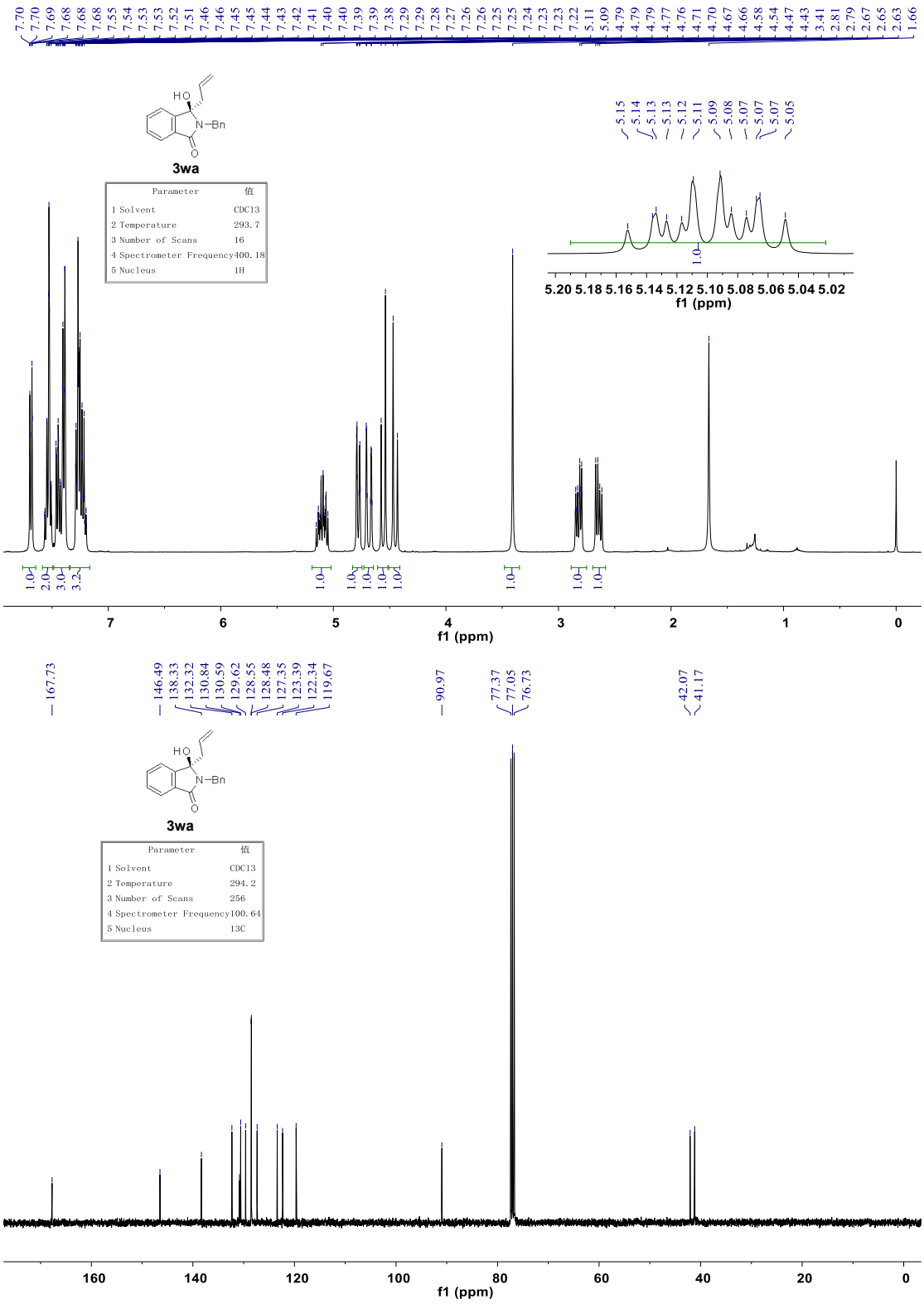
3ua

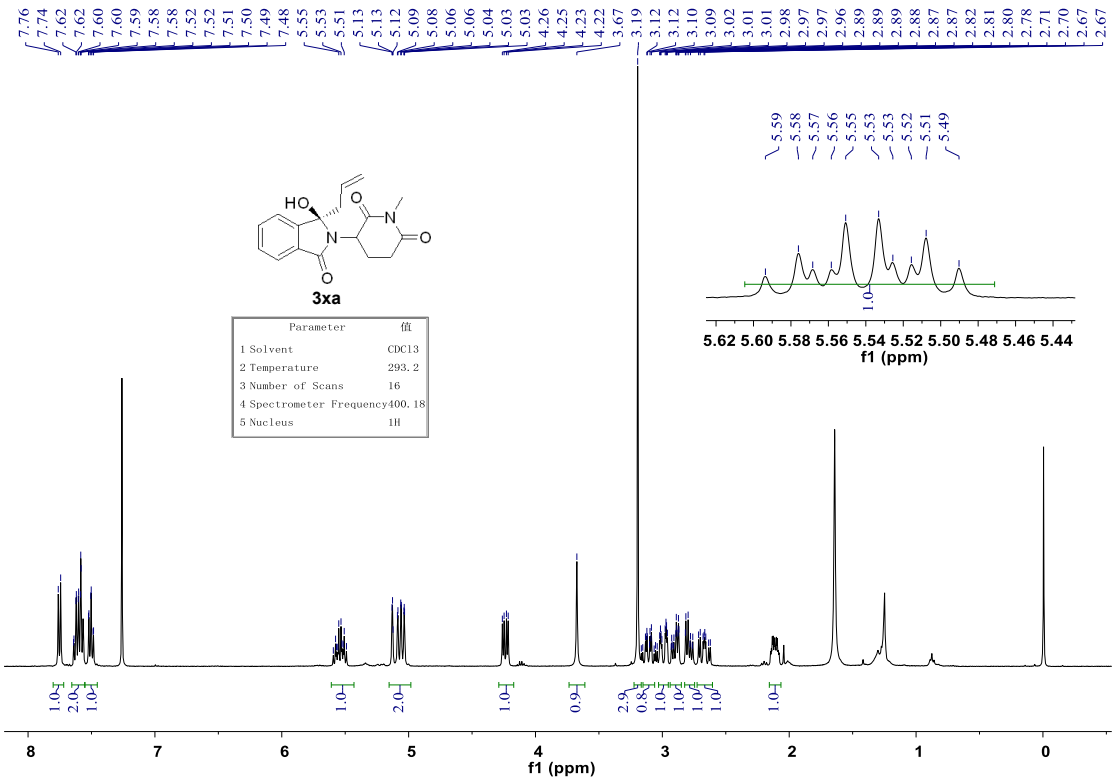
Parameter	值
1 Solvent	CDCl3
2 Temperature	293.7
3 Number of Scans	256
4 Spectrometer Frequency	100.63
5 Nucleus	13C

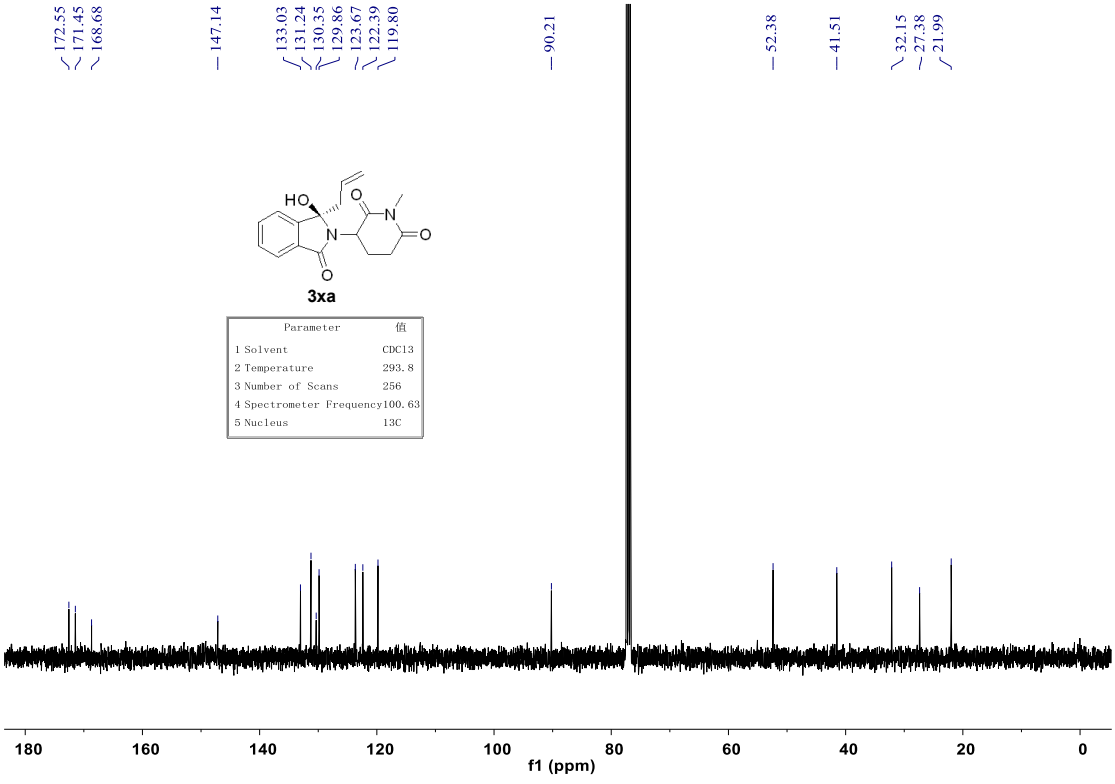

7.41 7.40 7.39 7.30 7.30 7.29 7.28 7.28 7.26 7.25 7.24 7.24 7.23 7.22 7.22 7.21
5.07 5.05 5.05 5.04 5.03 5.03 5.02 5.02 5.01 5.01 5.00 5.00 4.99 4.98 4.98 4.97 4.86 4.83 4.83 4.81 4.81 4.58 4.55 4.52 4.48 2.64 2.64 2.63 2.62 2.61 2.59 2.59 2.54 2.49 2.47 2.46 2.44 1.85 1.85 1.78 1.78

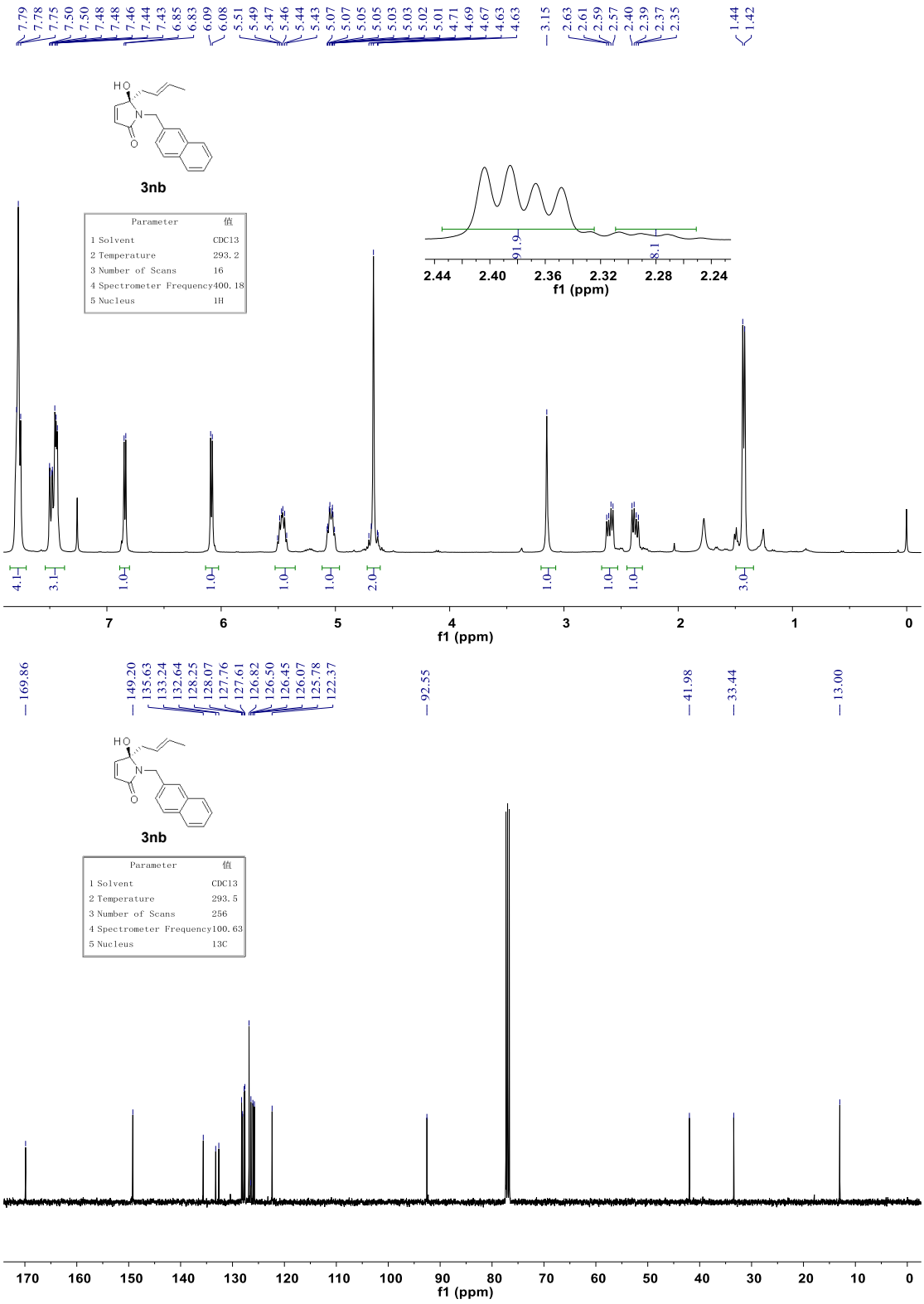

HO
N—Bn
O
3va
Parameter 值
1 Solvent CDCl3
2 Temperature 293.8
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0 0.9 1.0
2.70 2.65 2.60 2.55 2.50 2.45 2.40
f1 (ppm)
1.9 3.1 1.0 2.0 2.0 1.0 0.9 1.0 3.0 2.9
7 6 5 4 3 2 1 0
f1 (ppm)

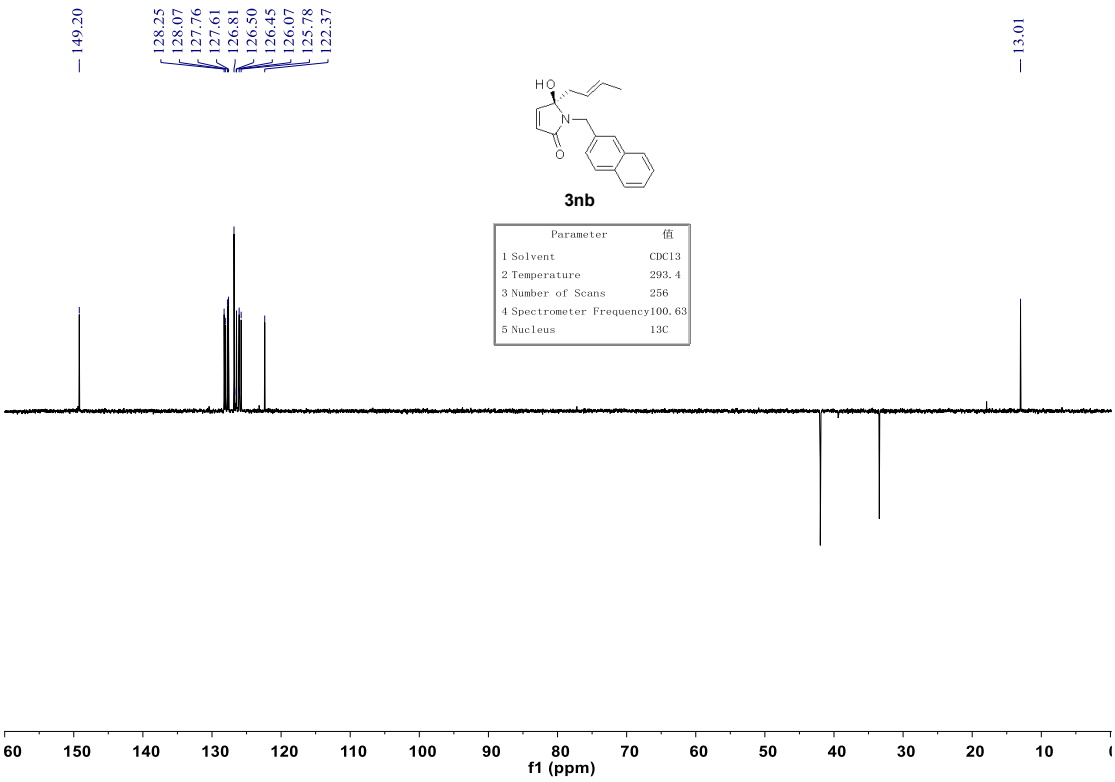

171.23 150.80 138.70 130.48 128.83 128.61 128.47 127.30 118.82 91.76 42.23 38.18 9.98 8.40
HO
N—Bn
O
3va
Parameter 值
1 Solvent CDCl3
2 Temperature 294.4
3 Number of Scans 256
4 Spectrometer Frequency 100.64
5 Nucleus 13C
160 140 120 100 80 60 40 20 0
f1 (ppm)

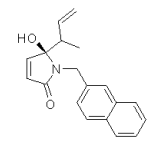

7.70 7.70 7.69 7.68 7.68 7.68 7.55 7.54 7.53 7.53 7.52 7.51 7.46 7.46 7.45 7.45 7.44 7.43 7.42 7.41 7.40 7.40 7.39 7.39 7.38 7.29 7.29 7.28 7.27 7.26 7.26 7.25 7.25 7.24 7.23 7.23 7.22 5.11 5.09 4.79 4.79 4.79 4.77 4.76 4.71 4.70 4.67 4.66 4.58 4.54 4.47 4.43 3.41 2.81 2.79 2.67 2.65 2.63 1.66
HO
N–Bn
O
3wa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.7
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.15 5.14 5.13 5.13 5.12 5.11 5.09 5.08 5.07 5.07 5.07 5.05
1.0
5.20 5.18 5.16 5.14 5.12 5.10 5.08 5.06 5.04 5.02
f1 (ppm)
1.0 2.0 3.0 3.2 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
7 6 5 4 3 2 1 0
f1 (ppm)
167.73 146.49 138.33 132.32 130.84 130.59 129.62 128.55 128.48 127.35 123.39 122.34 119.67 90.97 77.37 77.05 76.73 42.07 41.17
HO
N–Bn
O
3wa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.2
3 Number of Scans 256
4 Spectrometer Frequency 100.64
5 Nucleus 13C
160 140 120 100 80 60 40 20 0
f1 (ppm)


7.76 7.74 7.62 7.62 7.60 7.60 7.59 7.58 7.58 7.52 7.52 7.51 7.50 7.49 7.48 5.55 5.53 5.51 5.13 5.13 5.12 5.09 5.08 5.06 5.06 5.04 5.03 5.03 4.26 4.25 4.23 4.22 3.67 3.19 3.12 3.12 3.10 3.09 3.02 3.01 3.01 2.98 2.97 2.97 2.96 2.89 2.89 2.89 2.88 2.87 2.87 2.82 2.81 2.80 2.78 2.71 2.70 2.67 2.67
HO
O
N
N
O
O
3xa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.2
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.59 5.58 5.57 5.56 5.55 5.53 5.53 5.52 5.51 5.49
1.0
5.62 5.60 5.58 5.56 5.54 5.52 5.50 5.48 5.46 5.44
f1 (ppm)
1.0 2.0 1.0 1.0 2.0 1.0 0.9 2.9 0.8 1.0 1.0 1.0 1.0 1.0
8 7 6 5 4 3 2 1 0
f1 (ppm)


172.55 171.45 168.68 147.14 133.03 131.24 130.35 129.86 123.67 122.39 119.80 90.21 52.38 41.51 32.15 27.38 21.99
HO
O
N
N
O
O
3xa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.8
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
180 160 140 120 100 80 60 40 20 0
f1 (ppm)

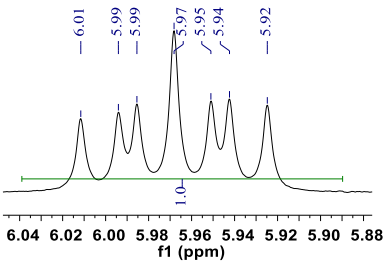

7.79 7.78 7.75 7.50 7.50 7.48 7.48 7.46 7.44 7.43 6.85 6.83 6.09 6.08 5.51 5.49 5.47 5.46 5.44 5.43 5.07 5.07 5.05 5.05 5.03 5.03 5.02 5.01 4.71 4.69 4.67 4.63 4.63 3.15 2.63 2.61 2.59 2.57 2.40 2.39 2.37 2.35 1.44 1.42
3nb
Parameter 值
1 Solvent CDCl3
2 Temperature 293.2
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
91.9
8.1
f1 (ppm)
4.1 3.1 1.0 1.0 1.0 1.0 2.0 1.0 1.0 1.0 3.0
f1 (ppm)
169.86 149.20 135.63 133.24 132.64 128.25 128.07 127.76 127.61 126.82 126.50 126.45 126.07 125.78 122.37 92.55 41.98 33.44 13.00
3nb
Parameter 值
1 Solvent CDCl3
2 Temperature 293.5
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

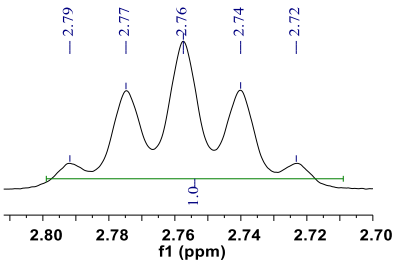

149.20
128.25
128.07
127.76
127.61
126.81
126.50
126.45
126.07
125.78
122.37
13.01
HO
N
O
3nb
Parameter 值
1 Solvent CDCl3
2 Temperature 293.4
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
60 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

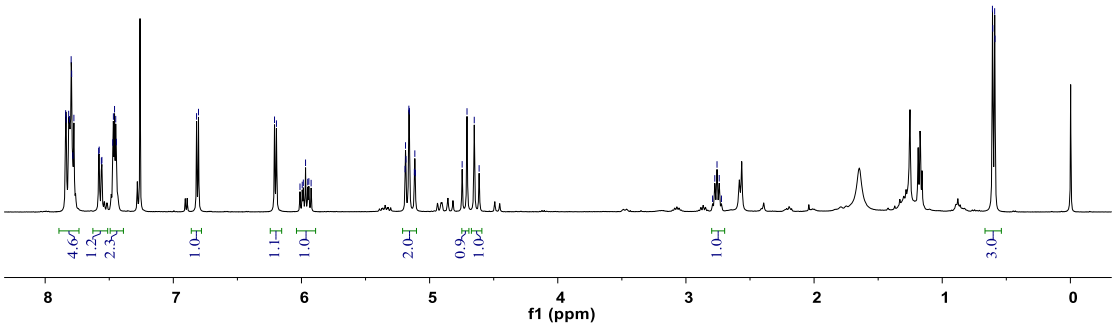


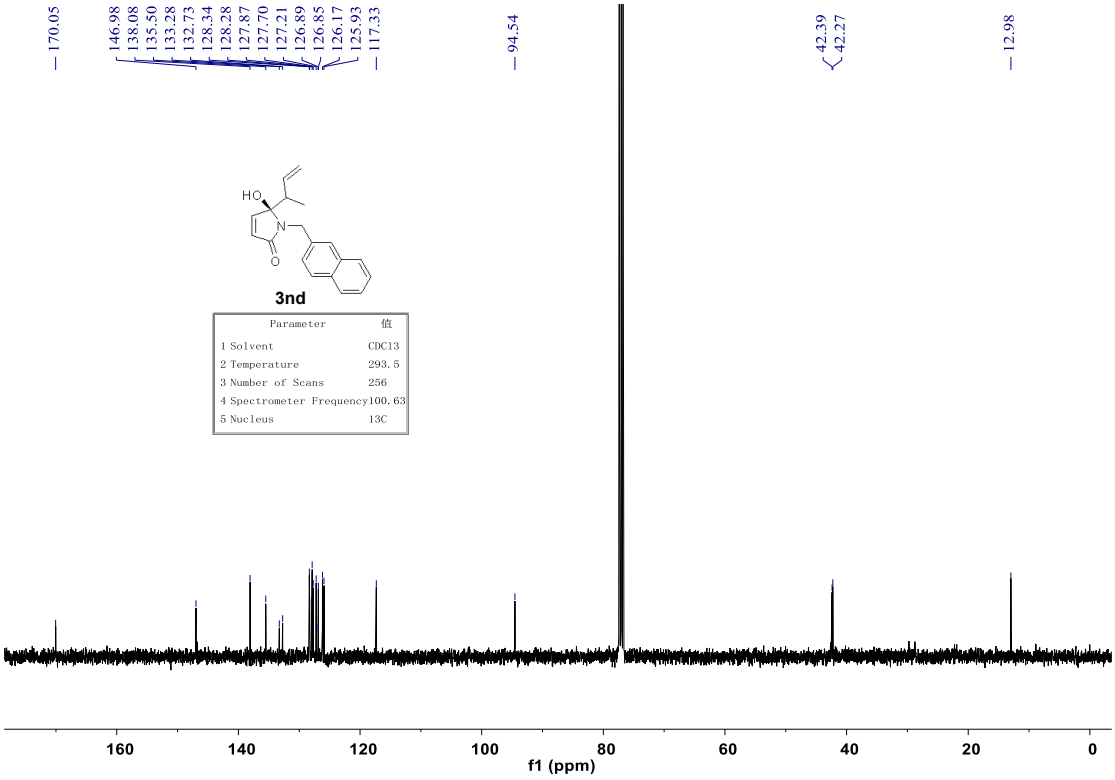
3nd

Parameter	值
1 Solvent	CDCl3
2 Temperature	293.2
3 Number of Scans	16
4 Spectrometer Frequency	400.18
5 Nucleus	1H



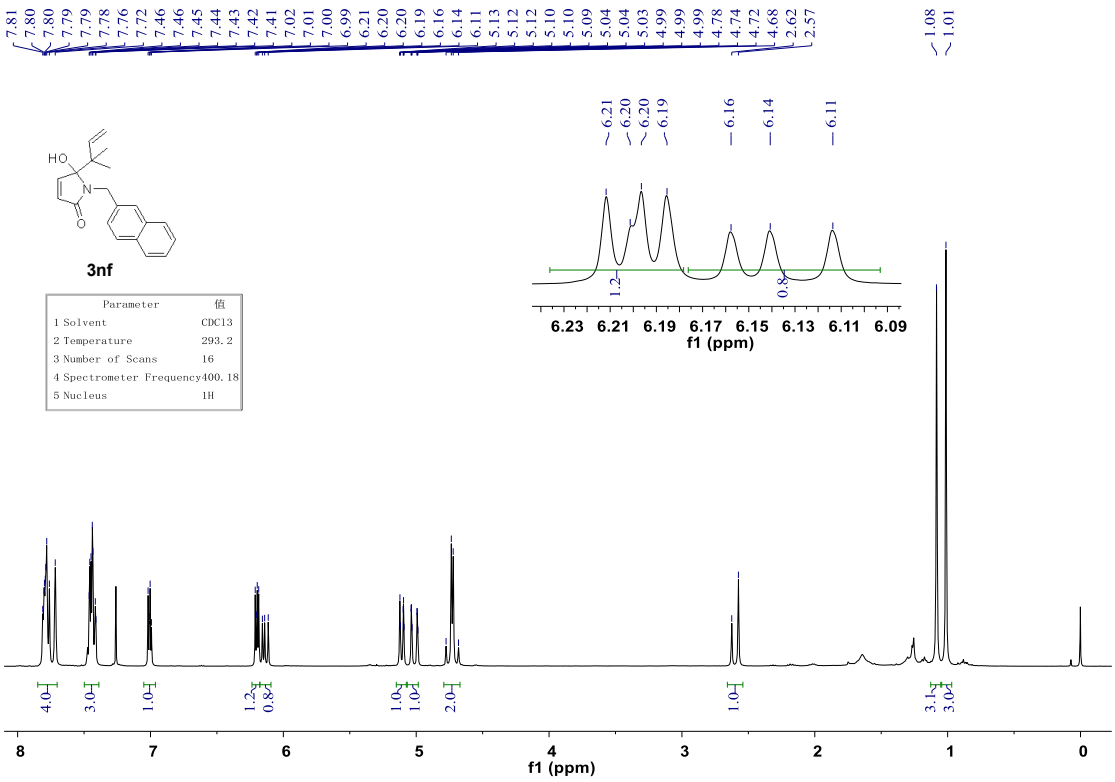


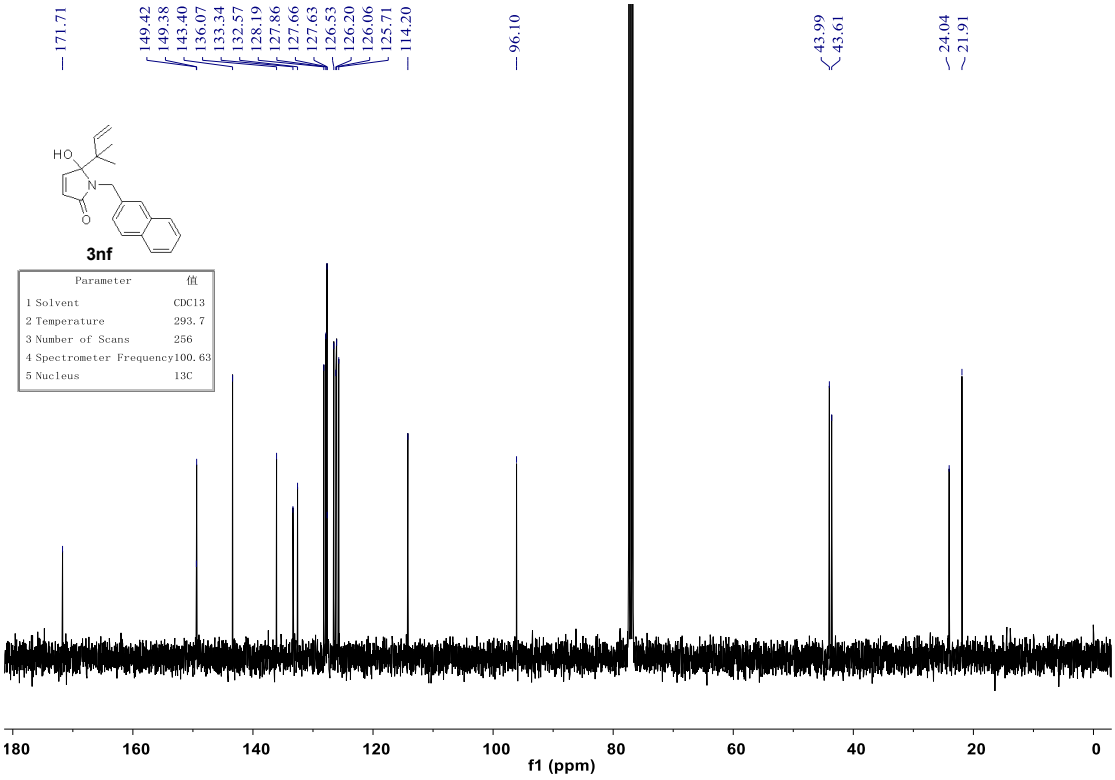


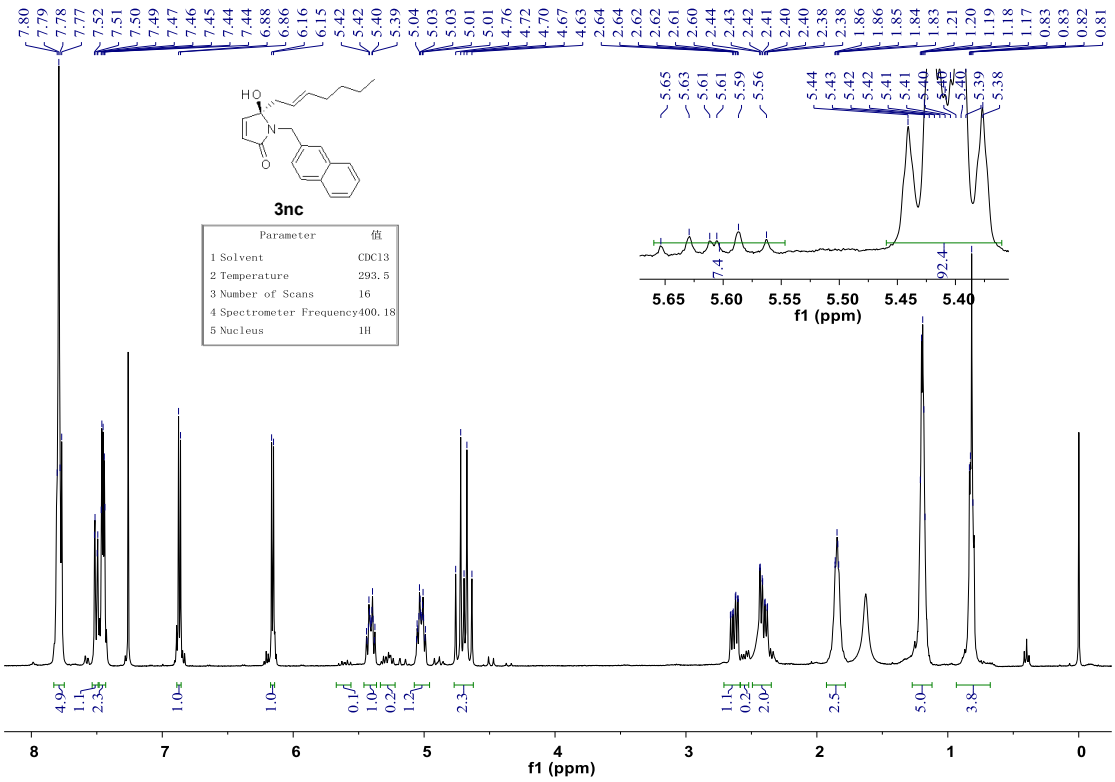


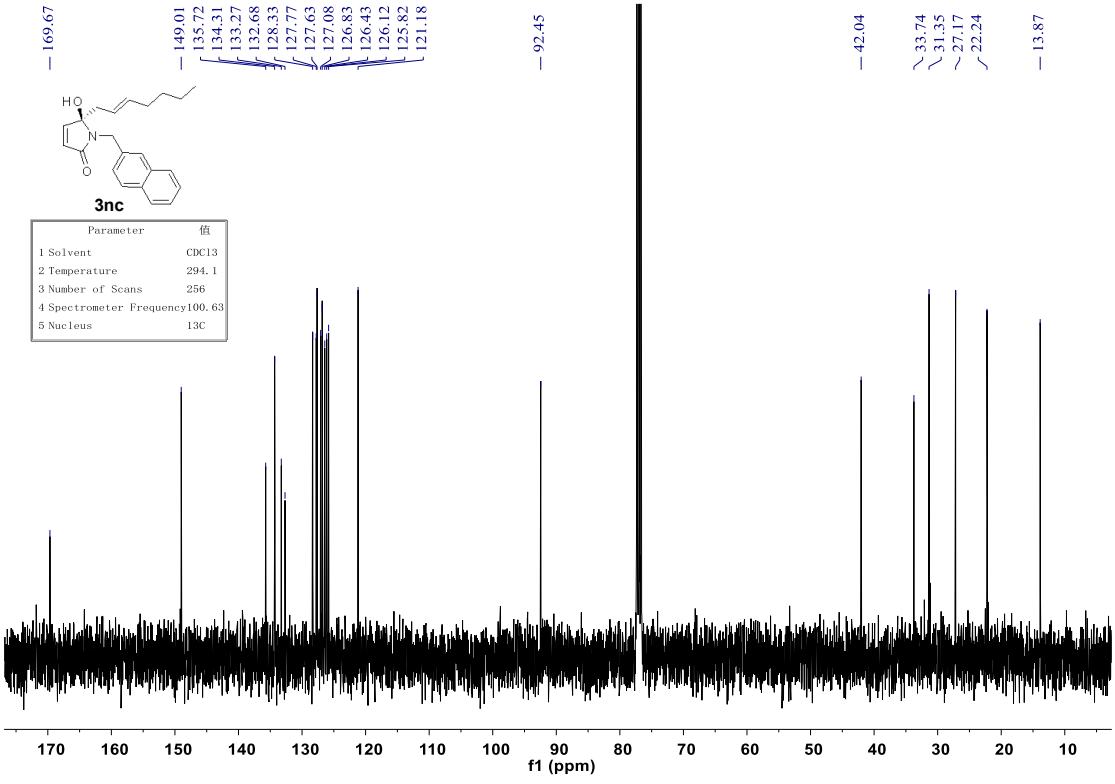
3nd

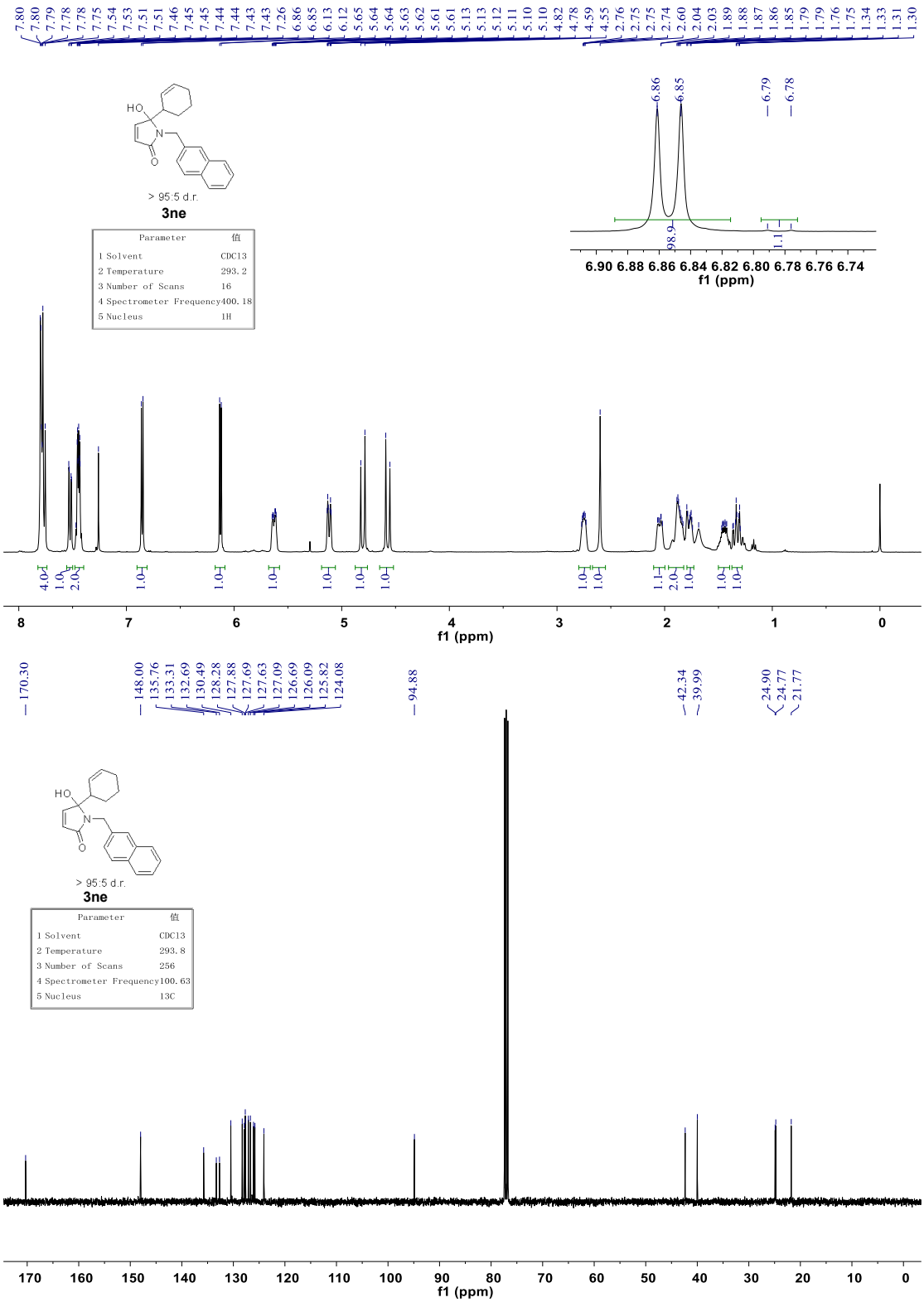
Parameter	值
1 Solvent	CDCl3
2 Temperature	293.5
3 Number of Scans	256
4 Spectrometer Frequency	100.63
5 Nucleus	13C

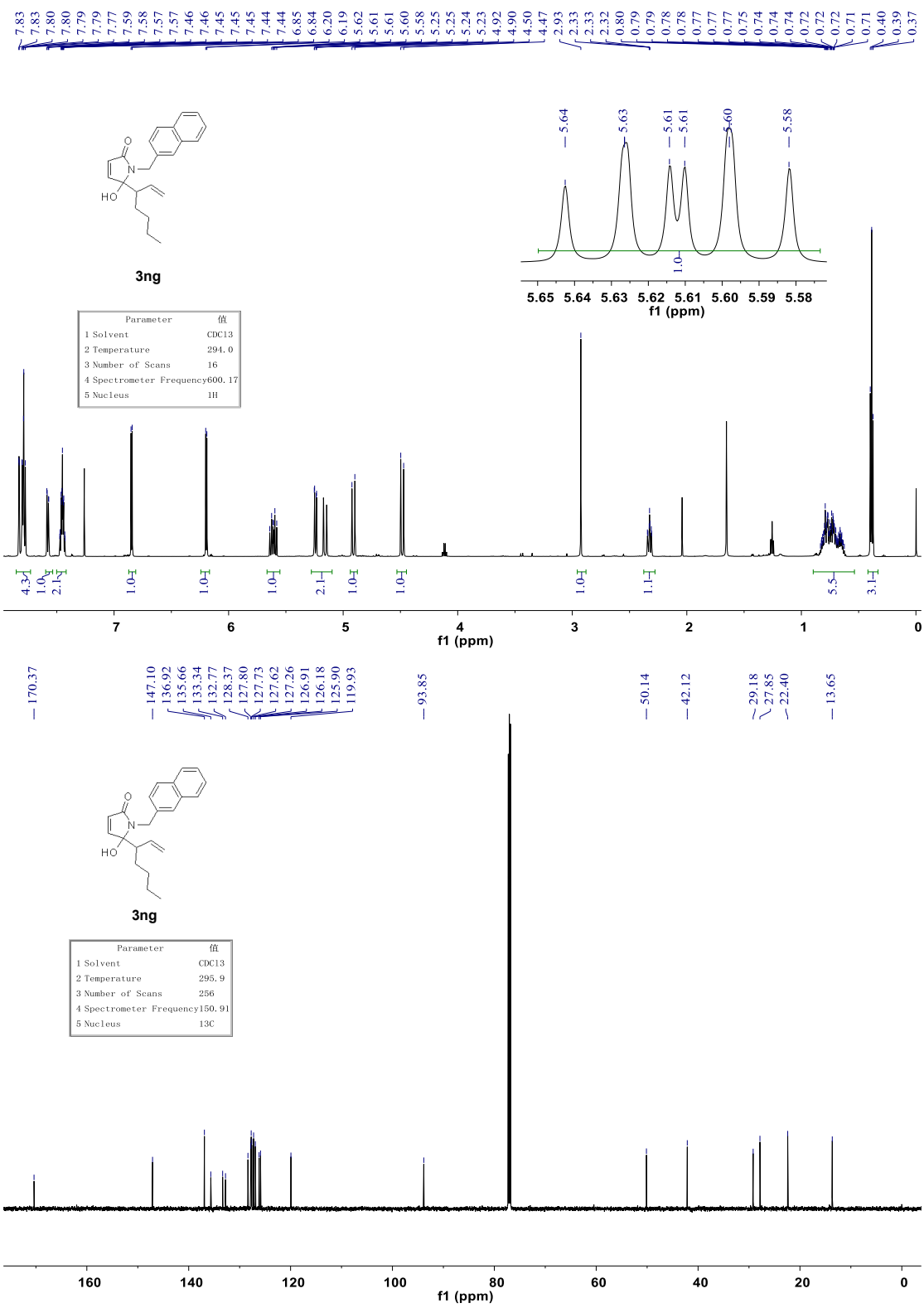

7.81 7.80 7.80 7.79 7.79 7.78 7.76 7.72 7.46 7.46 7.45 7.44 7.43 7.42 7.41 7.02 7.01 7.00 6.99 6.21 6.20 6.20 6.19 6.16 6.14 6.11 5.13 5.12 5.12 5.10 5.10 5.09 5.04 5.04 5.03 4.99 4.99 4.99 4.78 4.74 4.72 4.68 2.62 2.57
1.08 1.01
6.21 6.20 6.20 6.19 6.16 6.14 6.11
1.2 0.8
6.23 6.21 6.19 6.17 6.15 6.13 6.11 6.09
f1 (ppm)
HO
N
O
3nf
Parameter 值
1 Solvent CDCl3
2 Temperature 293.2
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
4.0 3.0 1.0 1.2 0.8 1.0 1.0 2.0 1.0 3.1 3.0
8 7 6 5 4 3 2 1 0
f1 (ppm)

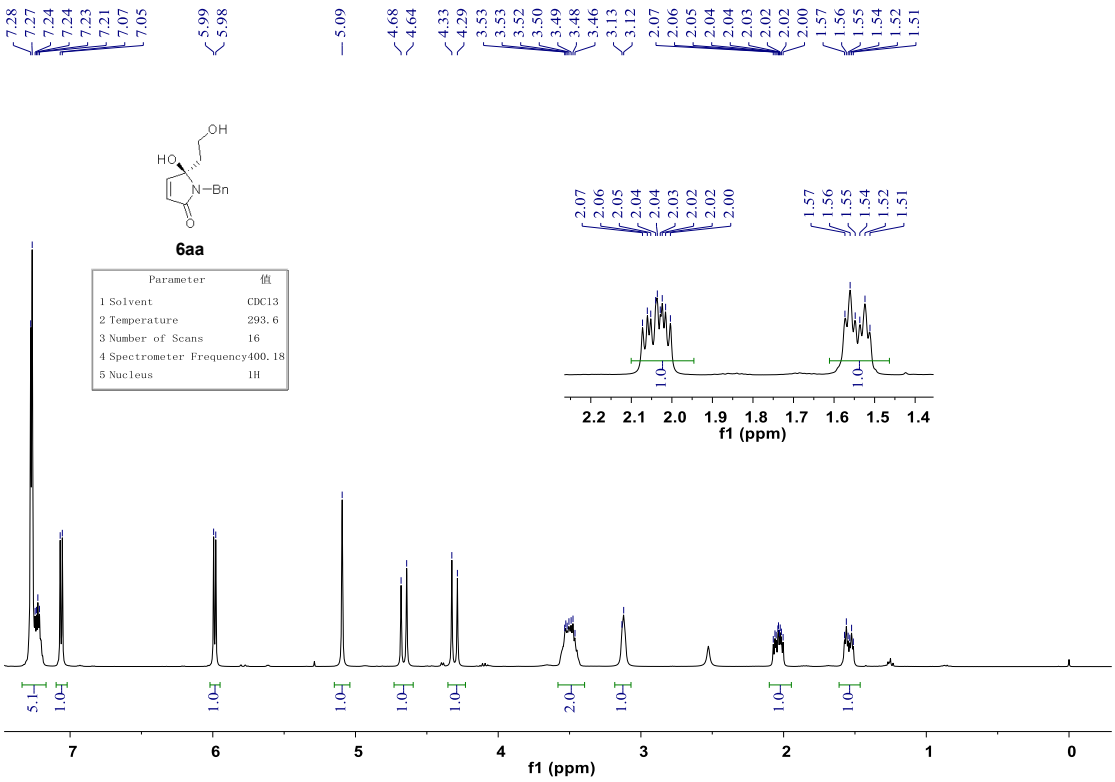

171.71
149.42 149.38 143.40 136.07 133.34 132.57 128.19 127.86 127.66 127.63 126.53 126.20 126.06 125.71 114.20
96.10
43.99 43.61
24.04 21.91
HO
N
O
3nf
Parameter 值
1 Solvent CDCl3
2 Temperature 293.7
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
180 160 140 120 100 80 60 40 20 0
f1 (ppm)

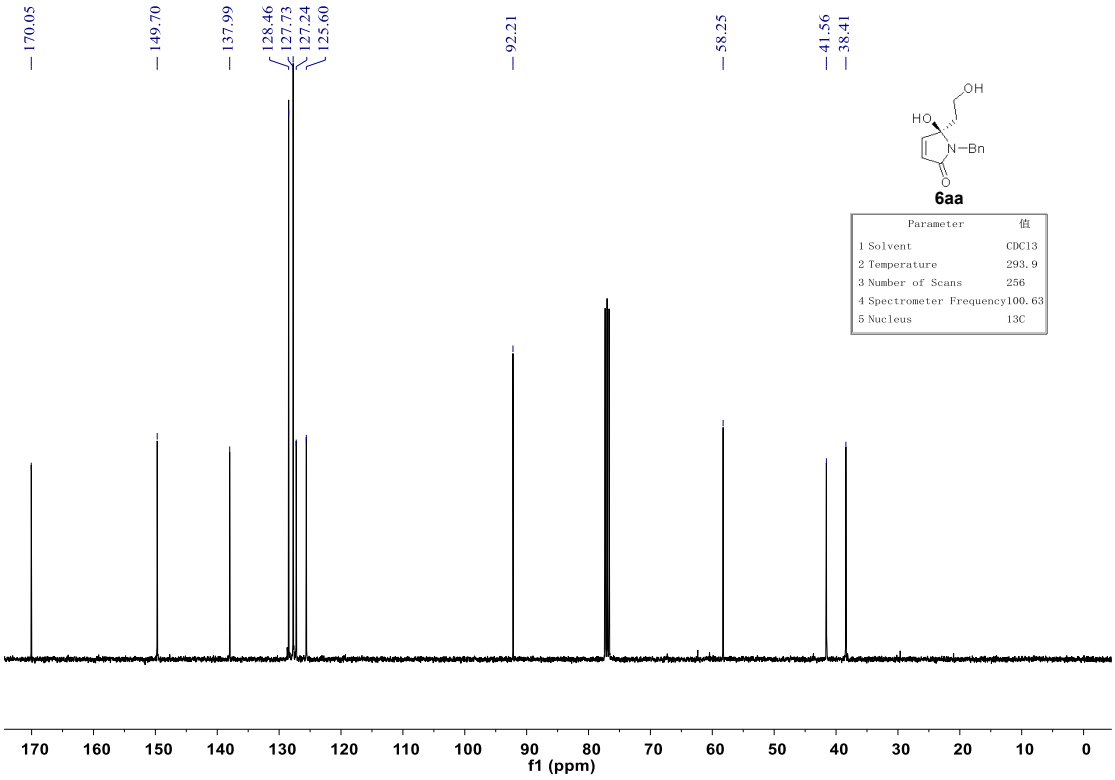

3nc
Parameter 值
1 Solvent CDCl3
2 Temperature 293.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

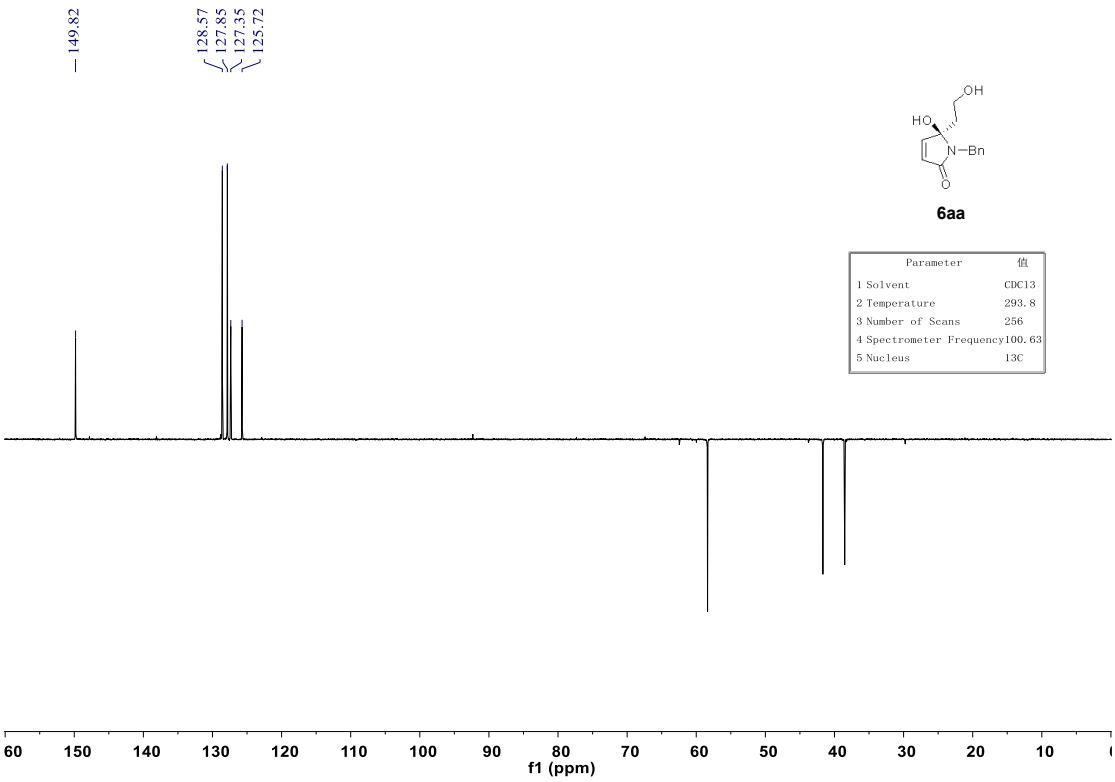

3nc
Parameter 值
1 Solvent CDCl3
2 Temperature 294.1
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

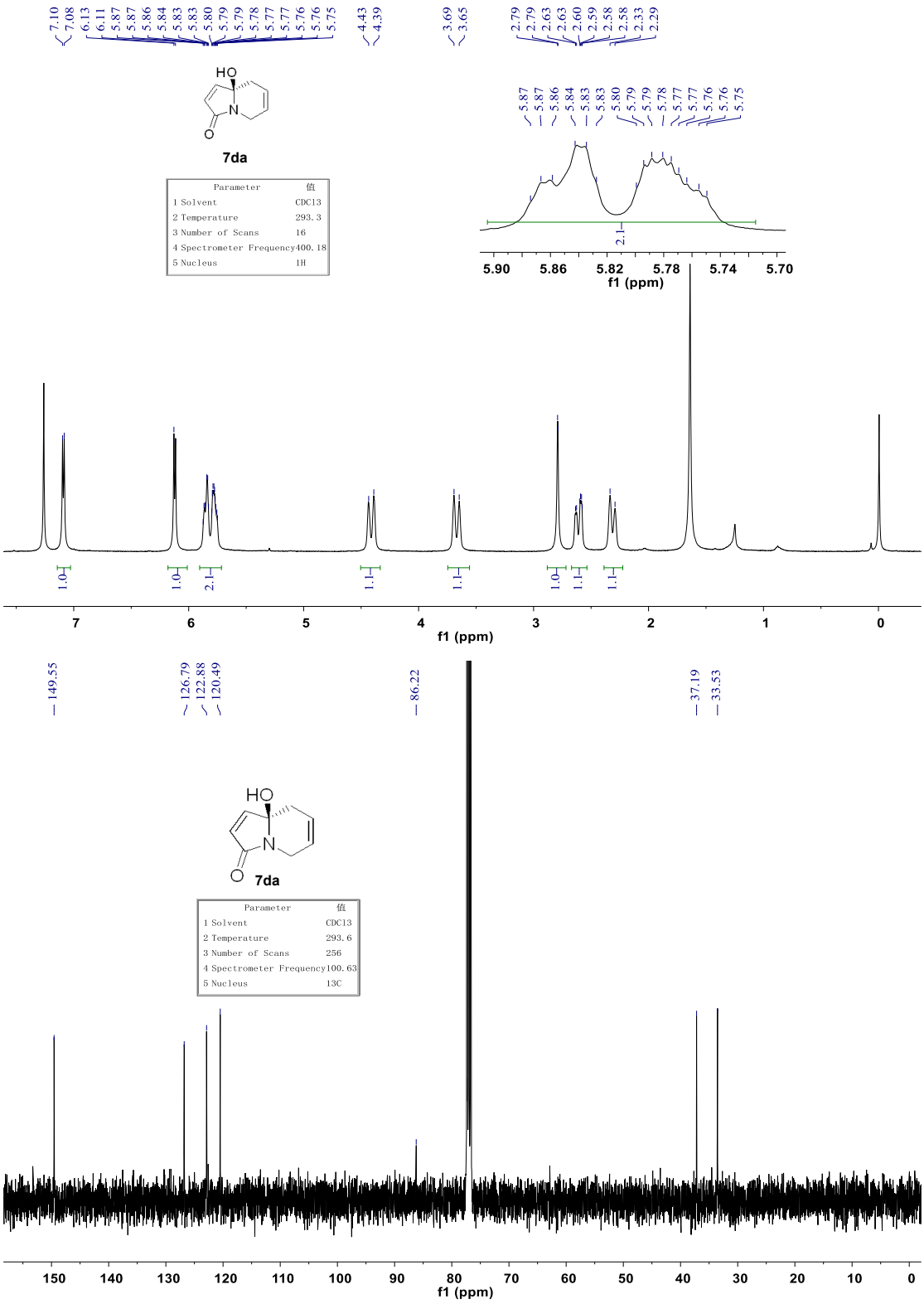

> 95:5 d.r.
3ne
Parameter 值
1 Solvent CDCl3
2 Temperature 293.2
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)
> 95:5 d.r.
3ne
Parameter 值
1 Solvent CDCl3
2 Temperature 293.8
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

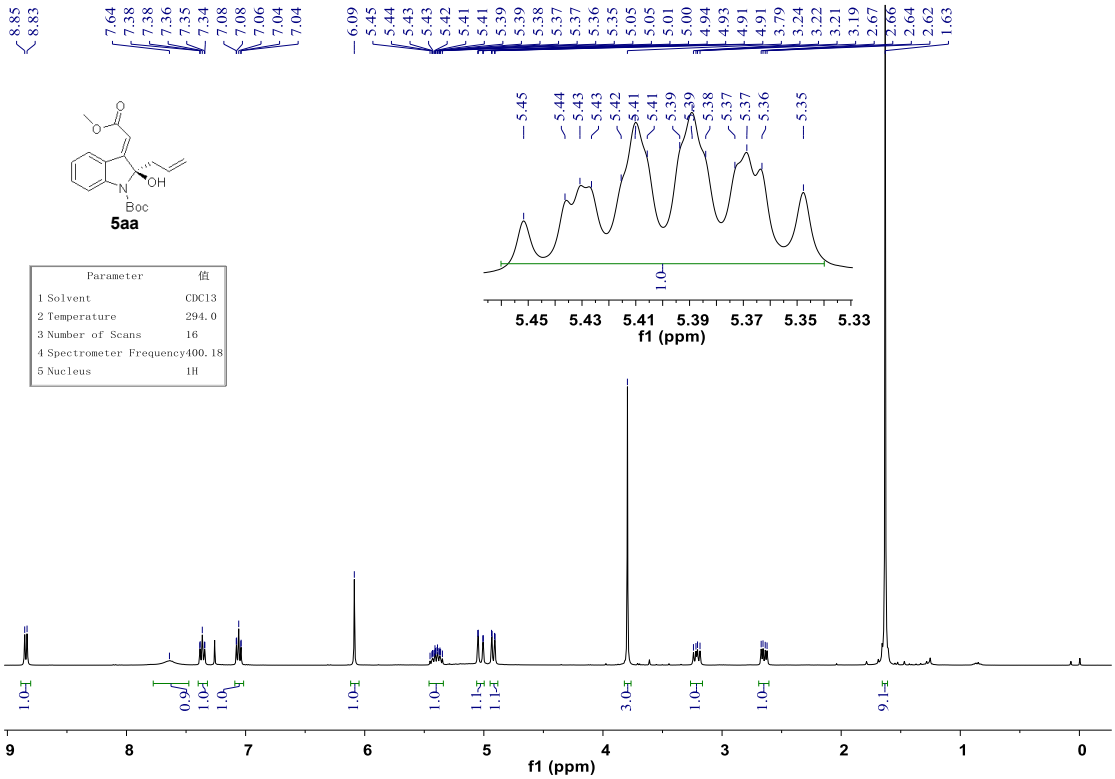

3ng
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 16
4 Spectrometer Frequency 600.17
5 Nucleus 1H
f1 (ppm)
3ng
Parameter 值
1 Solvent CDCl3
2 Temperature 295.9
3 Number of Scans 256
4 Spectrometer Frequency 150.91
5 Nucleus 13C
f1 (ppm)

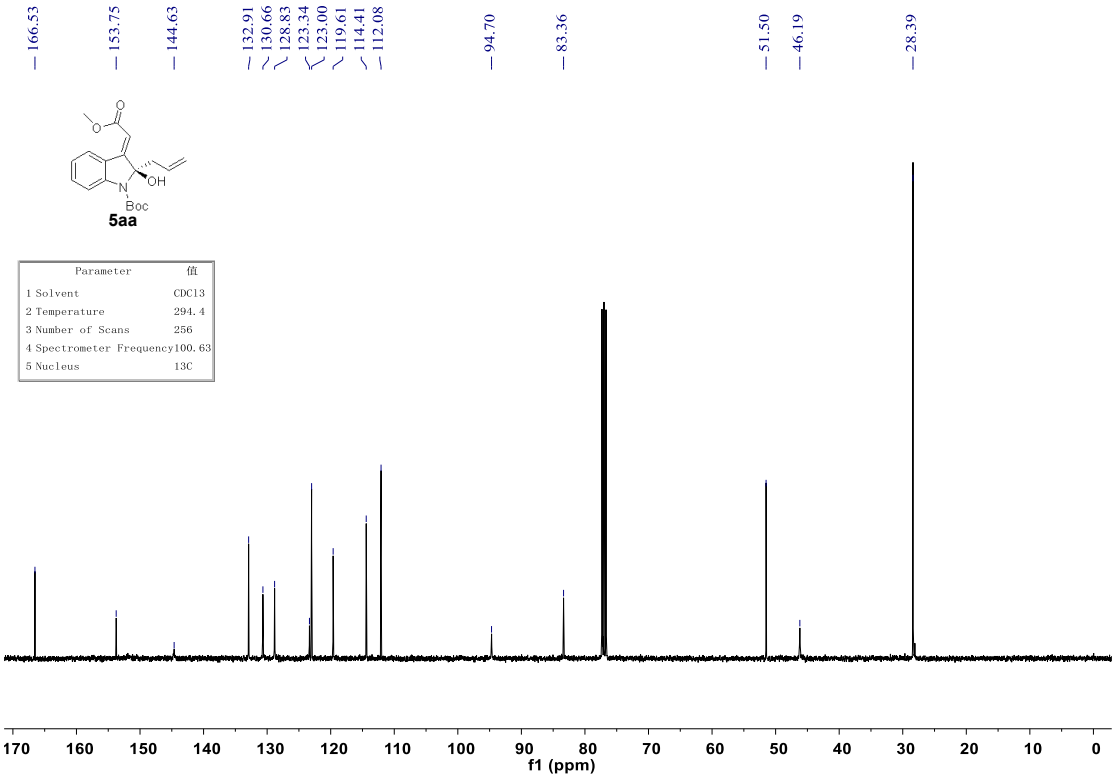

7.28
7.27
7.24
7.24
7.23
7.21
7.07
7.05
5.99
5.98
5.09
4.68
4.64
4.33
4.29
3.53
3.52
3.50
3.49
3.48
3.46
3.13
3.12
2.07
2.06
2.05
2.04
2.04
2.03
2.02
2.02
2.00
1.57
1.56
1.55
1.54
1.52
1.51
OH
HO
N–Bn
O
6aa
Parameter 值
1 Solvent CDC13
2 Temperature 293.6
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0
1.0
2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4
f1 (ppm)
5.1
1.0
1.0
1.0
1.0
1.0
2.0
1.0
1.0
1.0
7 6 5 4 3 2 1 0
f1 (ppm)

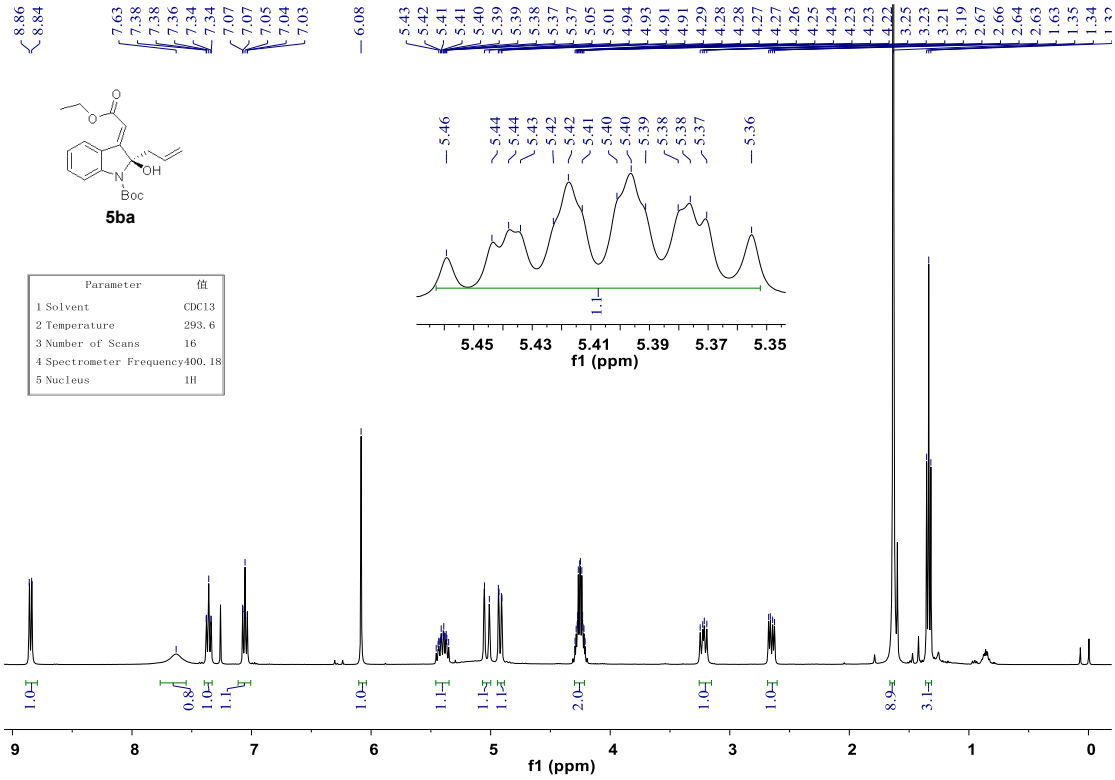

170.05
149.70
137.99
128.46
127.73
127.24
125.60
92.21
58.25
41.56
38.41
OH
HO
N–Bn
O
6aa
Parameter 值
1 Solvent CDC13
2 Temperature 293.9
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

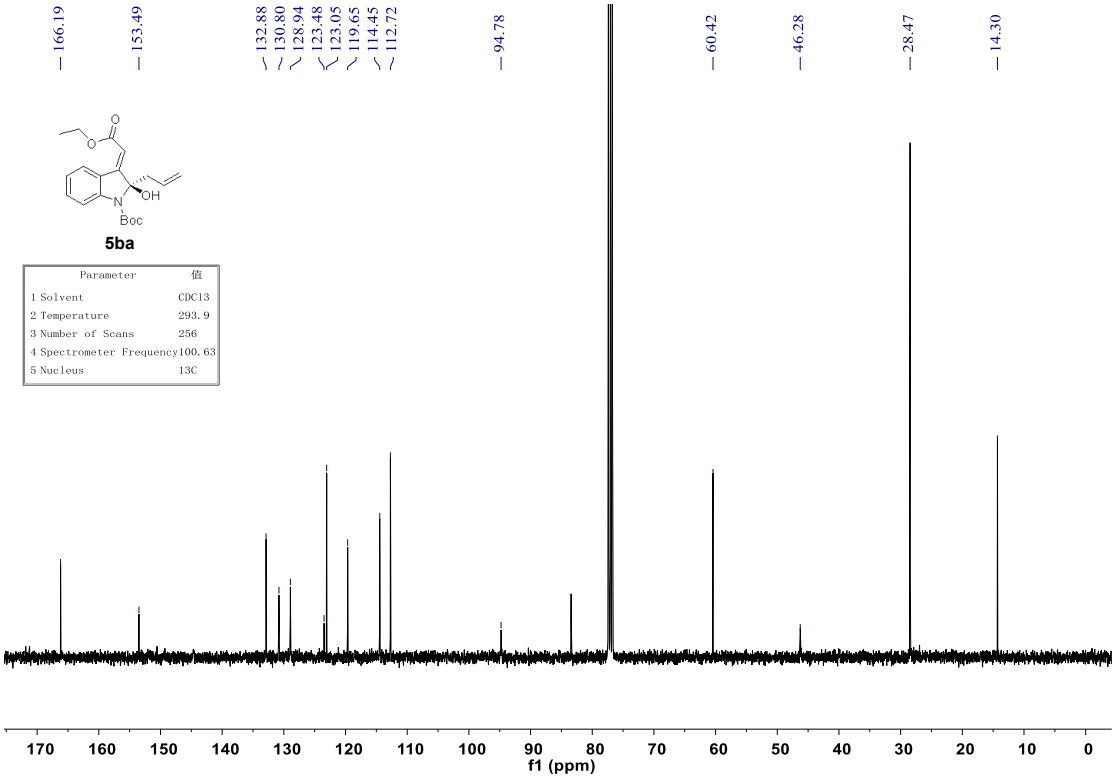

149.82
128.57
127.85
127.35
125.72
OH
HO
N—Bn
O
6aa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.8
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
60 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

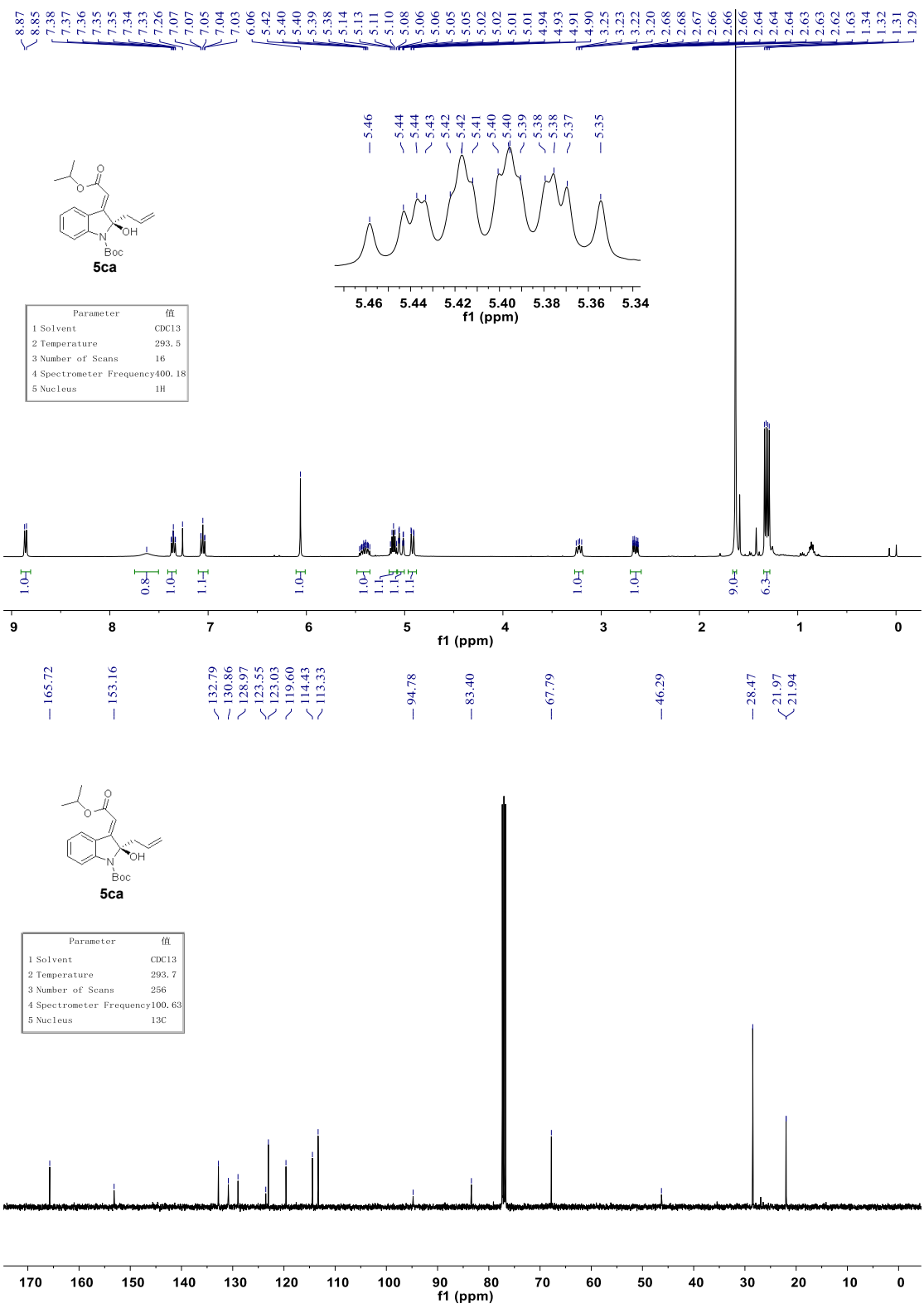

7.10
7.08
6.13
6.11
5.87
5.87
5.86
5.84
5.83
5.83
5.80
5.79
5.79
5.78
5.77
5.77
5.76
5.76
5.75
4.43
4.39
3.69
3.65
2.79
2.79
2.63
2.63
2.60
2.59
2.58
2.58
2.33
2.29
HO
N
O
7da
Parameter 值
1 Solvent CDCl3
2 Temperature 293.3
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.87
5.87
5.86
5.84
5.83
5.83
5.80
5.79
5.79
5.78
5.77
5.77
5.76
5.76
5.75
2.1
5.90
5.86
5.82
5.78
5.74
5.70
f1 (ppm)
1.0
1.0
2.1
1.1
1.1
1.0
1.1
1.1
7
6
5
4
3
2
1
0
f1 (ppm)
149.55
126.79
122.88
120.49
86.22
37.19
33.53
HO
N
O
7da
Parameter 值
1 Solvent CDCl3
2 Temperature 293.6
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

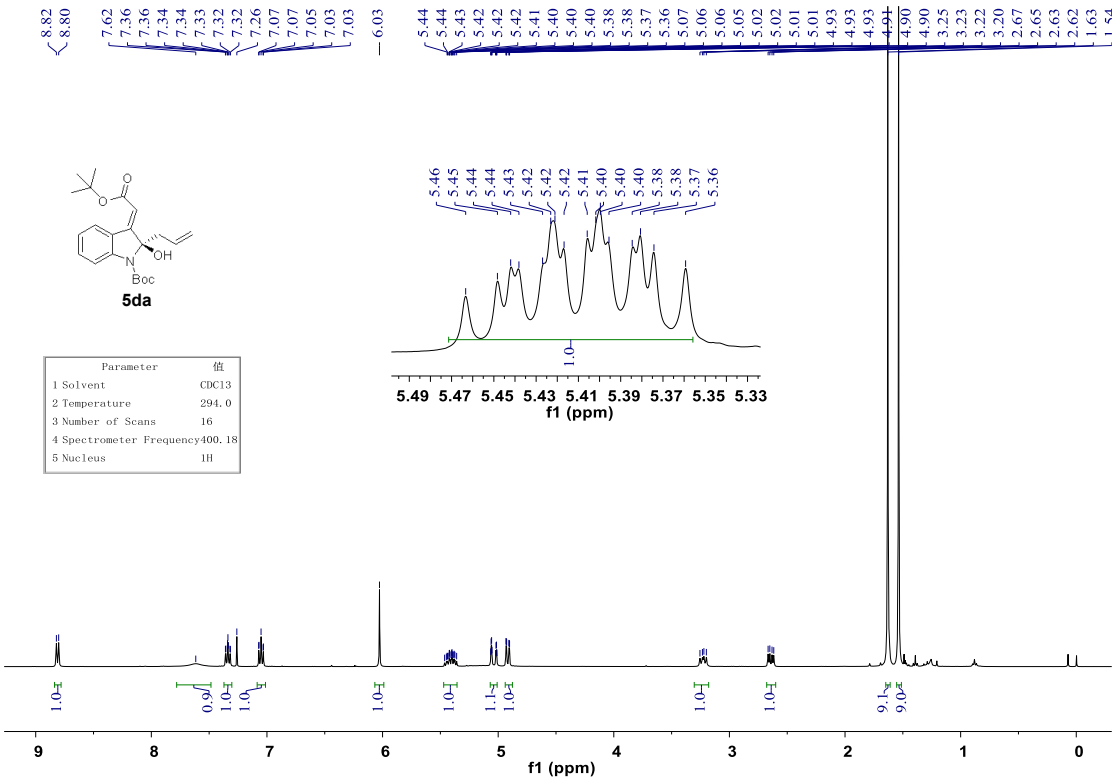

5aa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

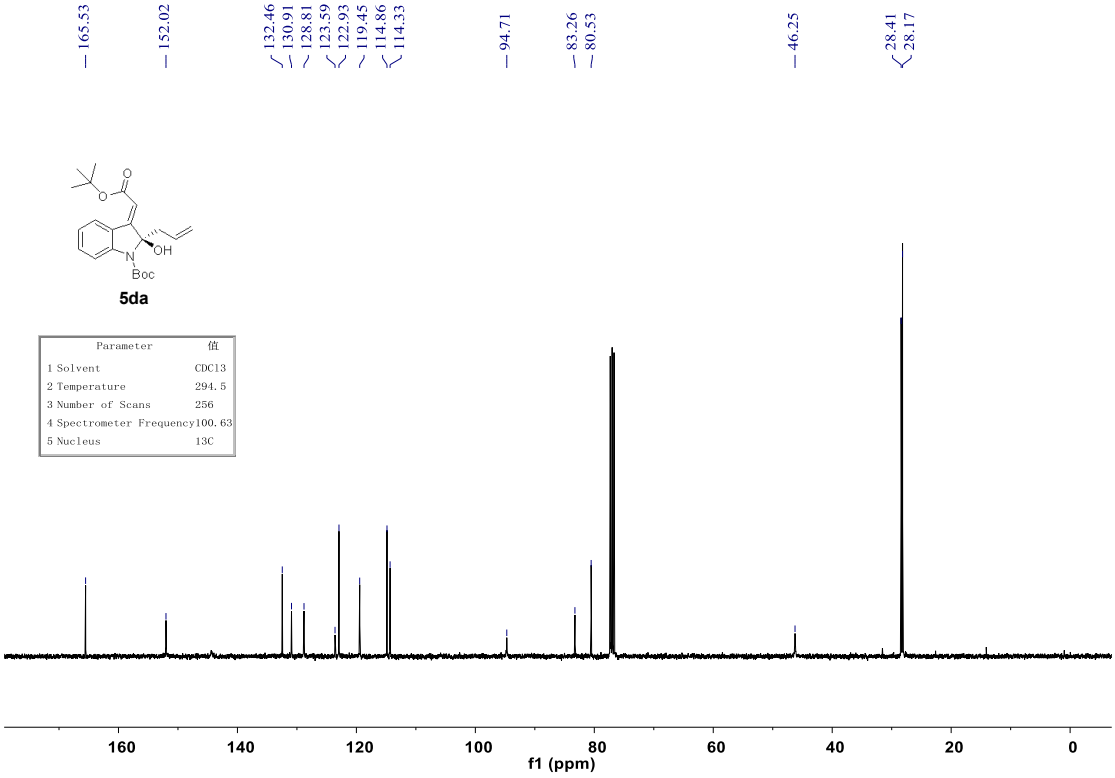

5aa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.4
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

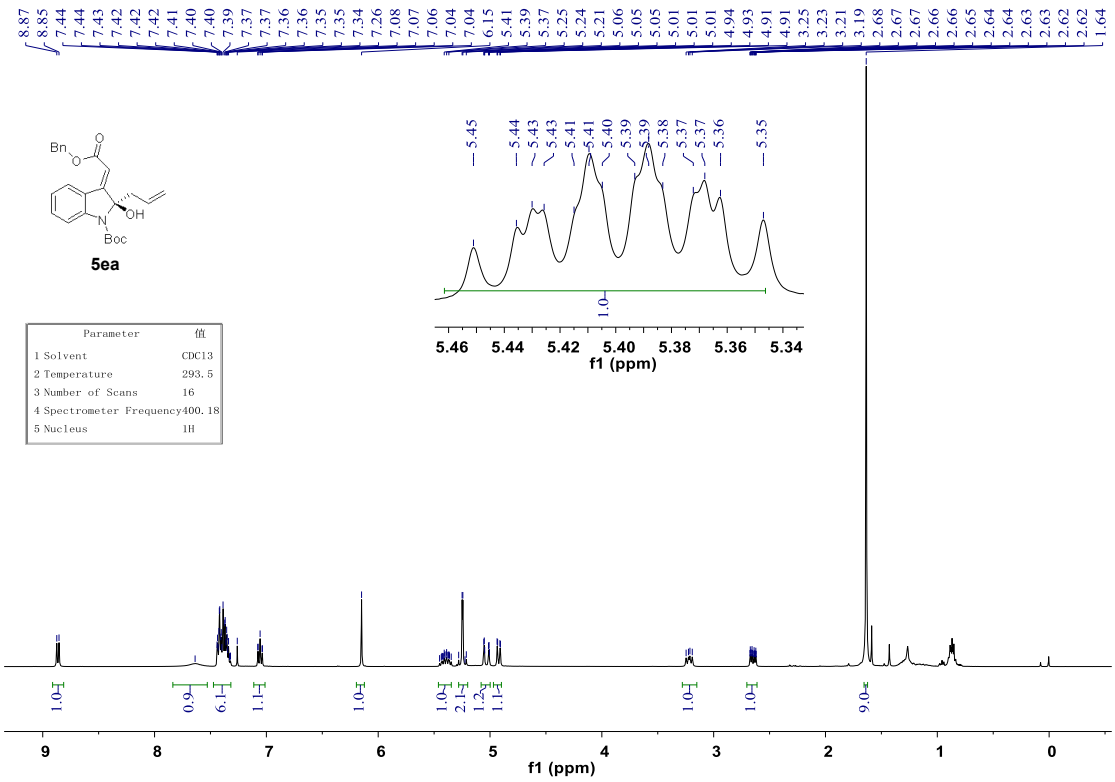

5ba
Parameter 值
1 Solvent CDCl3
2 Temperature 293.6
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

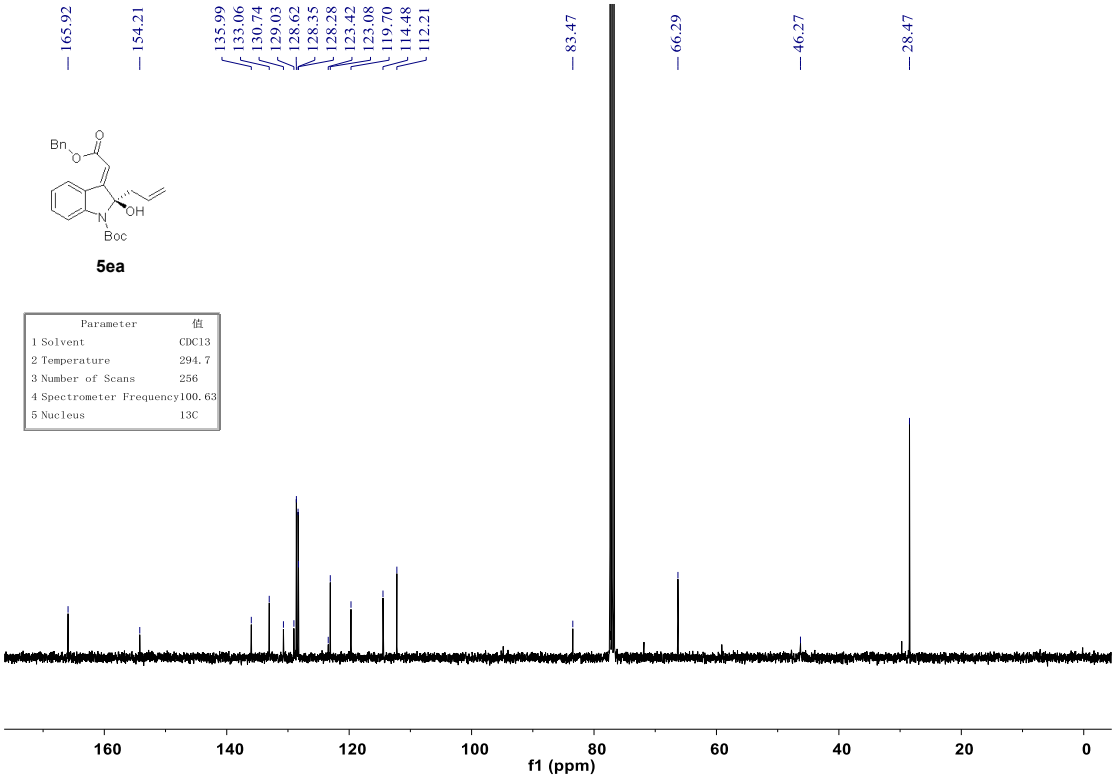

5ba
Parameter 值
1 Solvent CDCl3
2 Temperature 293.9
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

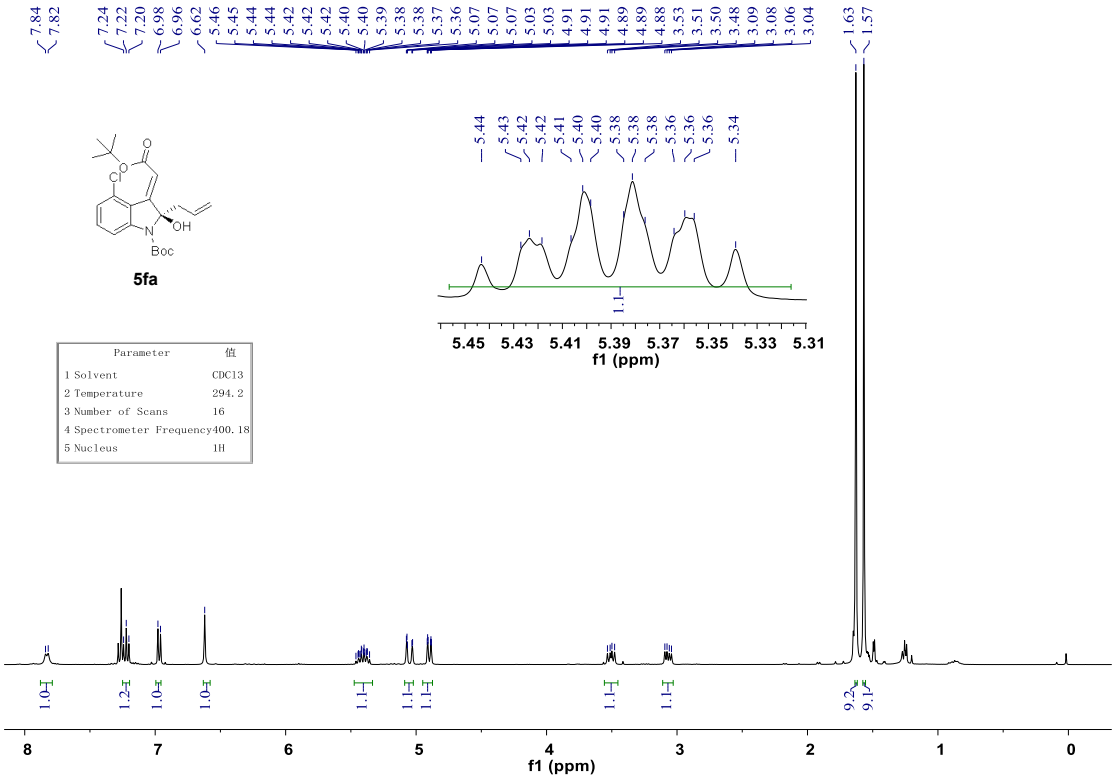

8.87 8.85 7.38 7.37 7.36 7.35 7.35 7.34 7.33 7.26 7.07 7.07 7.05 7.04 7.03 6.06 5.42 5.40 5.40 5.39 5.38 5.14 5.13 5.11 5.10 5.08 5.06 5.06 5.05 5.05 5.02 5.02 5.01 5.01 4.94 4.93 4.91 4.90 3.25 3.23 3.22 3.20 2.68 2.68 2.67 2.66 2.66 2.66 2.64 2.64 2.64 2.63 2.63 2.62 1.63 1.34 1.32 1.31 1.29
5.46 5.44 5.44 5.43 5.42 5.42 5.41 5.40 5.40 5.39 5.38 5.38 5.37 5.35
5.46 5.44 5.42 5.40 5.38 5.36 5.34
f1 (ppm)
O
O
OH
N
Boc
5ca
Parameter 值
1 Solvent CDCl3
2 Temperature 293.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0 0.8 1.0 1.1 1.0 1.0 1.1 1.1 1.0 1.0 9.0 6.3
9 8 7 6 5 4 3 2 1 0
f1 (ppm)
165.72 153.16 132.79 130.86 128.97 123.55 123.03 119.60 114.43 113.33 94.78 83.40 67.79 46.29 28.47 21.97 21.94
O
O
OH
N
Boc
5ca
Parameter 值
1 Solvent CDCl3
2 Temperature 293.7
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

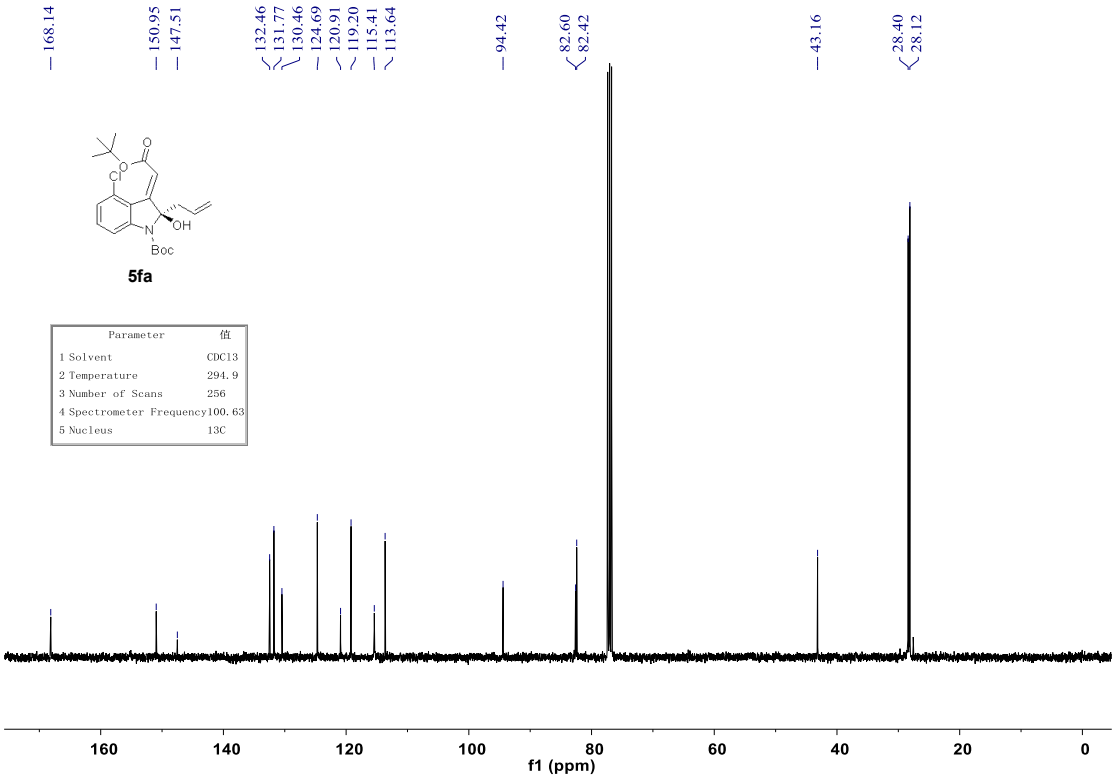

5da
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

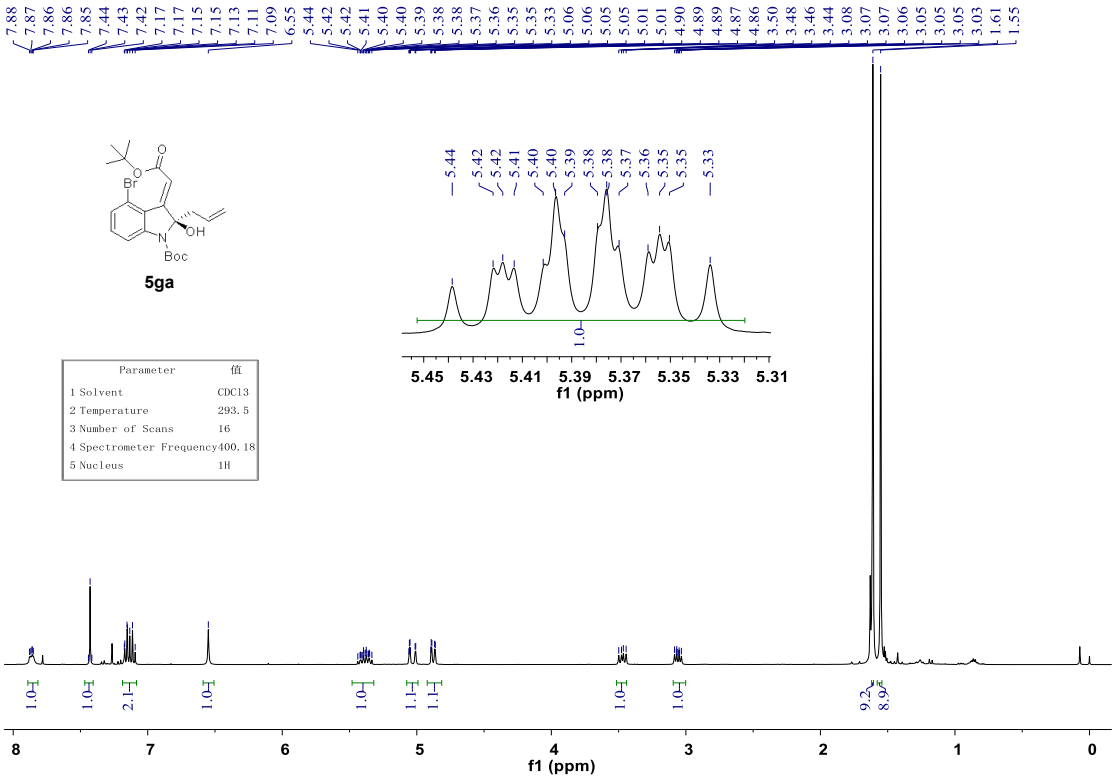

5da
Parameter 值
1 Solvent CDCl3
2 Temperature 294.5
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)

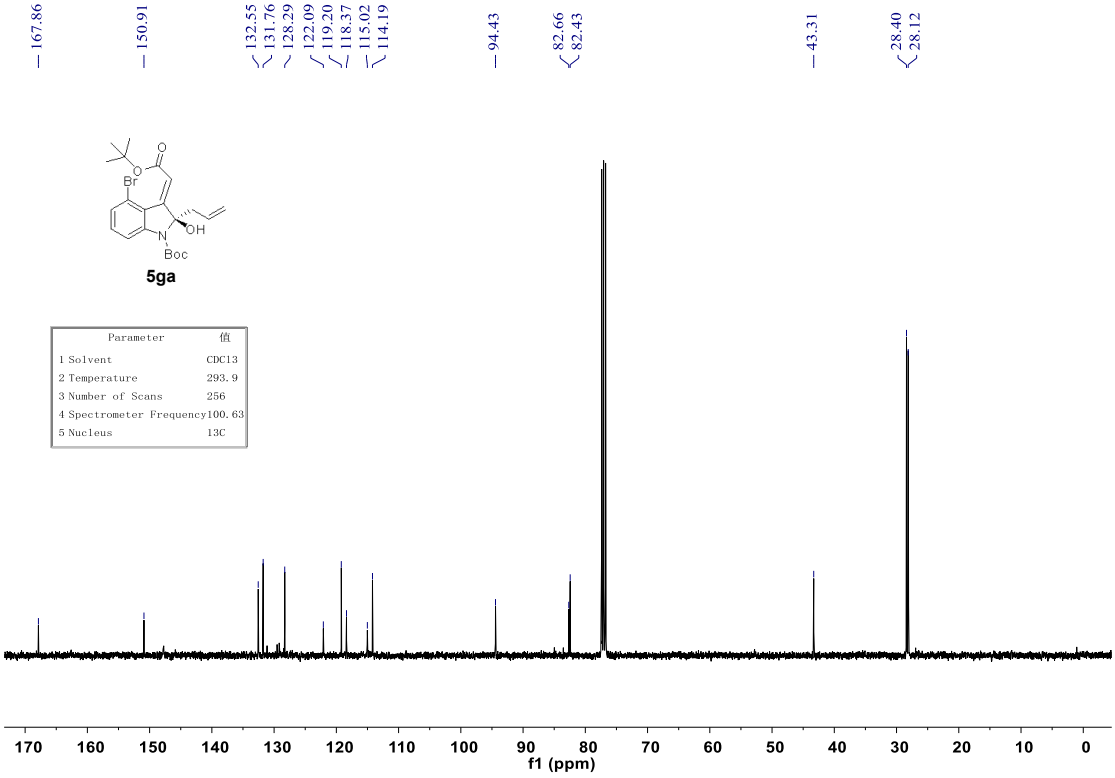

8.87 8.85 7.44 7.44 7.43 7.42 7.42 7.42 7.41 7.40 7.40 7.39 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.26 7.08 7.07 7.06 7.04 7.04 6.15 5.41 5.39 5.37 5.25 5.24 5.21 5.06 5.05 5.05 5.01 5.01 5.01 4.94 4.93 4.91 4.91 3.25 3.23 3.21 3.19 2.68 2.67 2.67 2.66 2.66 2.65 2.64 2.64 2.63 2.63 2.62 2.62 1.64
5.45 5.44 5.43 5.43 5.41 5.41 5.40 5.39 5.39 5.38 5.37 5.37 5.36 5.35
1.0
5.46 5.44 5.42 5.40 5.38 5.36 5.34
f1 (ppm)
Bn
O
OH
N
Boc
5ea
Parameter 值
1 Solvent CDCl3
2 Temperature 293.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0 0.9 6.1 1.1 1.0 1.0 2.1 1.2 1.1 1.0 1.0 9.0
9 8 7 6 5 4 3 2 1 0
f1 (ppm)

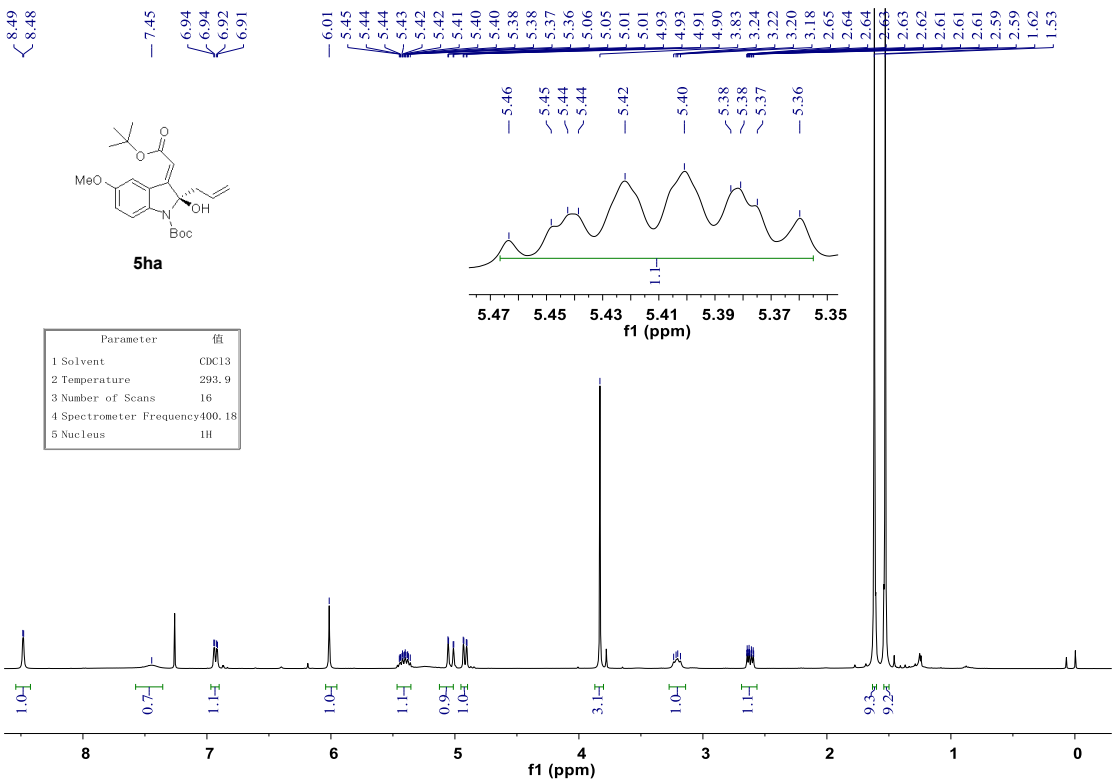

165.92 154.21 135.99 133.06 130.74 129.03 128.62 128.35 128.28 123.42 123.08 119.70 114.48 112.21 83.47 66.29 46.27 28.47
Bn
O
OH
N
Boc
5ea
Parameter 值
1 Solvent CDCl3
2 Temperature 294.7
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
160 140 120 100 80 60 40 20 0
f1 (ppm)


7.84
7.82
7.24
7.22
7.20
6.98
6.96
6.62
5.46
5.45
5.44
5.44
5.42
5.42
5.42
5.40
5.40
5.39
5.38
5.38
5.37
5.36
5.07
5.07
5.03
5.03
4.91
4.91
4.91
4.89
4.89
4.88
3.53
3.51
3.50
3.48
3.09
3.08
3.06
3.04
1.63
1.57
5.44
5.43
5.42
5.42
5.41
5.40
5.40
5.38
5.38
5.38
5.36
5.36
5.36
5.34
1.1
5.45 5.43 5.41 5.39 5.37 5.35 5.33 5.31
f1 (ppm)
Cl
O
O
OH
N
Boc
5fa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.2
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0
1.2
1.0
1.0
1.1
1.1
1.1
1.1
1.1
9.2
9.1
8 7 6 5 4 3 2 1 0
f1 (ppm)


168.14
150.95
147.51
132.46
131.77
130.46
124.69
120.91
119.20
115.41
113.64
94.42
82.60
82.42
43.16
28.40
28.12
Cl
O
O
OH
N
Boc
5fa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.9
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
160 140 120 100 80 60 40 20 0
f1 (ppm)


7.88 7.87 7.86 7.86 7.85 7.44 7.43 7.42 7.17 7.17 7.15 7.15 7.13 7.11 7.09 6.55
5.44 5.42 5.42 5.41 5.40 5.40 5.39 5.38 5.38 5.37 5.36 5.35 5.33 5.06 5.06 5.05 5.05 5.01 5.01 4.90 4.89 4.89 4.87 4.86 3.50 3.48 3.46 3.44 3.08 3.07 3.07 3.06 3.05 3.05 3.05 3.03 1.61 1.55
Br
O
OH
N
Boc
5ga
5.44 5.42 5.42 5.41 5.40 5.40 5.39 5.38 5.38 5.37 5.36 5.35 5.35 5.33
1.0
5.45 5.43 5.41 5.39 5.37 5.35 5.33 5.31
f1 (ppm)
Parameter 值
1 Solvent CDCl3
2 Temperature 293.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0 1.0 2.1 1.0 1.0 1.1 1.1 1.0 1.0 9.2 8.9
8 7 6 5 4 3 2 1 0
f1 (ppm)


167.86 150.91 132.55 131.76 128.29 122.09 119.20 118.37 115.02 114.19 94.43 82.66 82.43 43.31 28.40 28.12
Br
O
OH
N
Boc
5ga
Parameter 值
1 Solvent CDCl3
2 Temperature 293.9
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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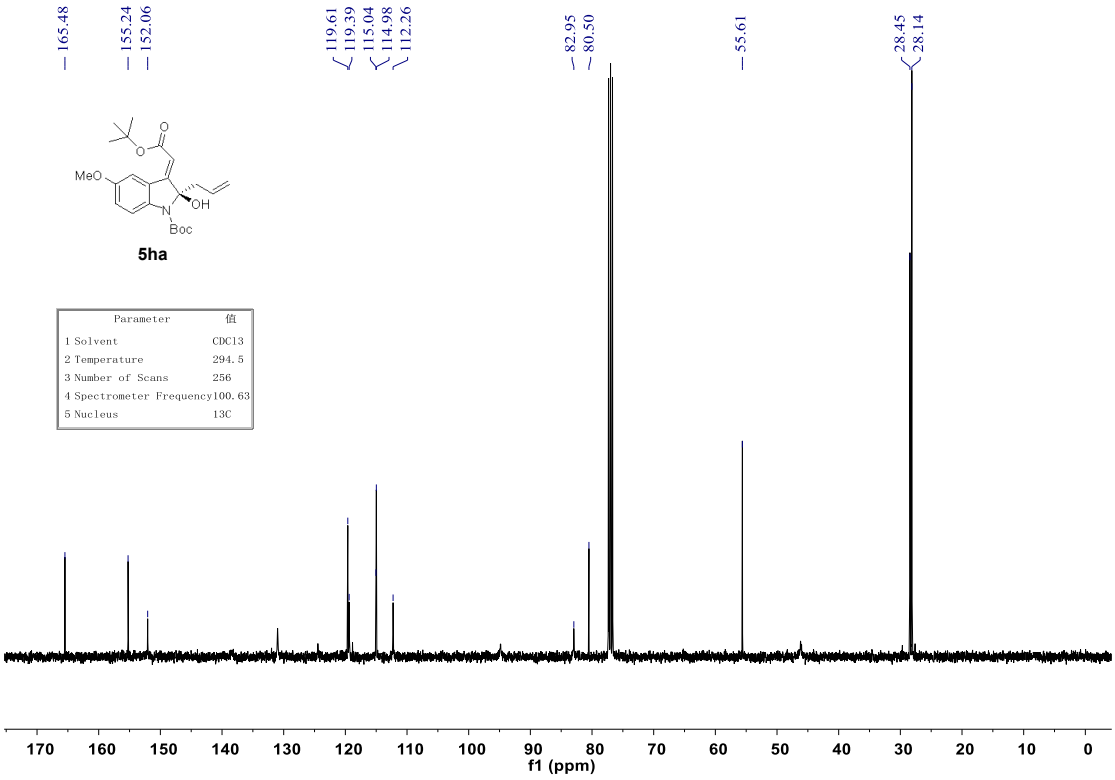
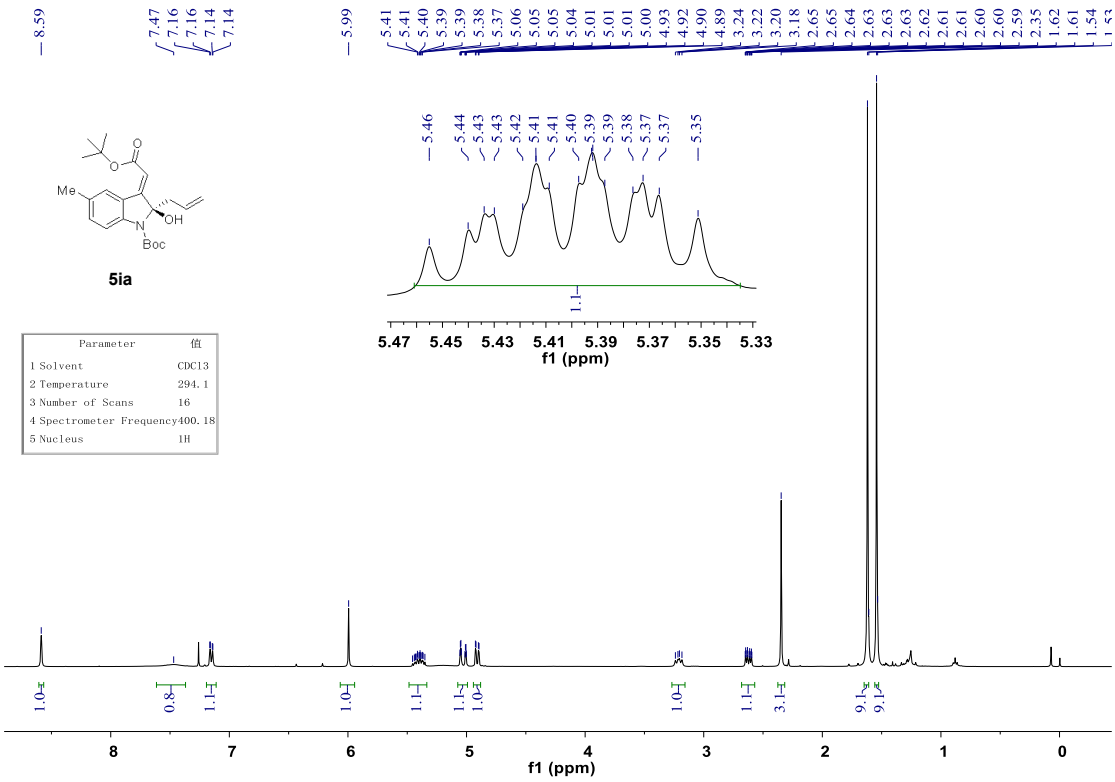
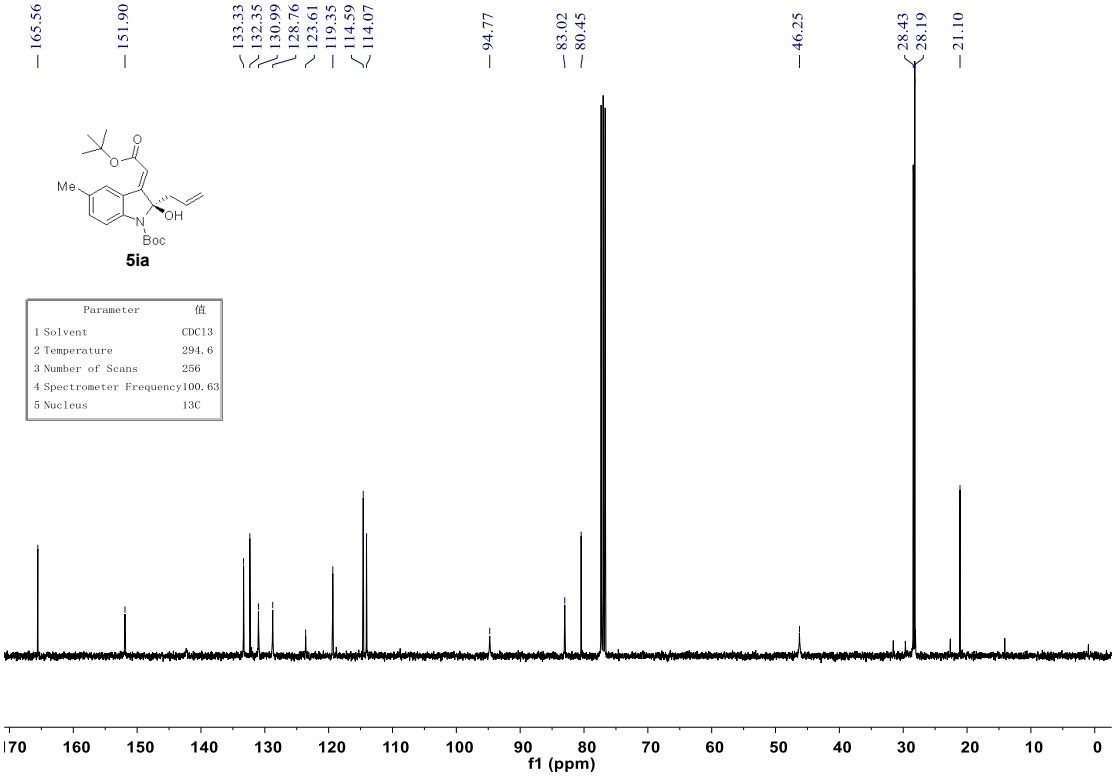
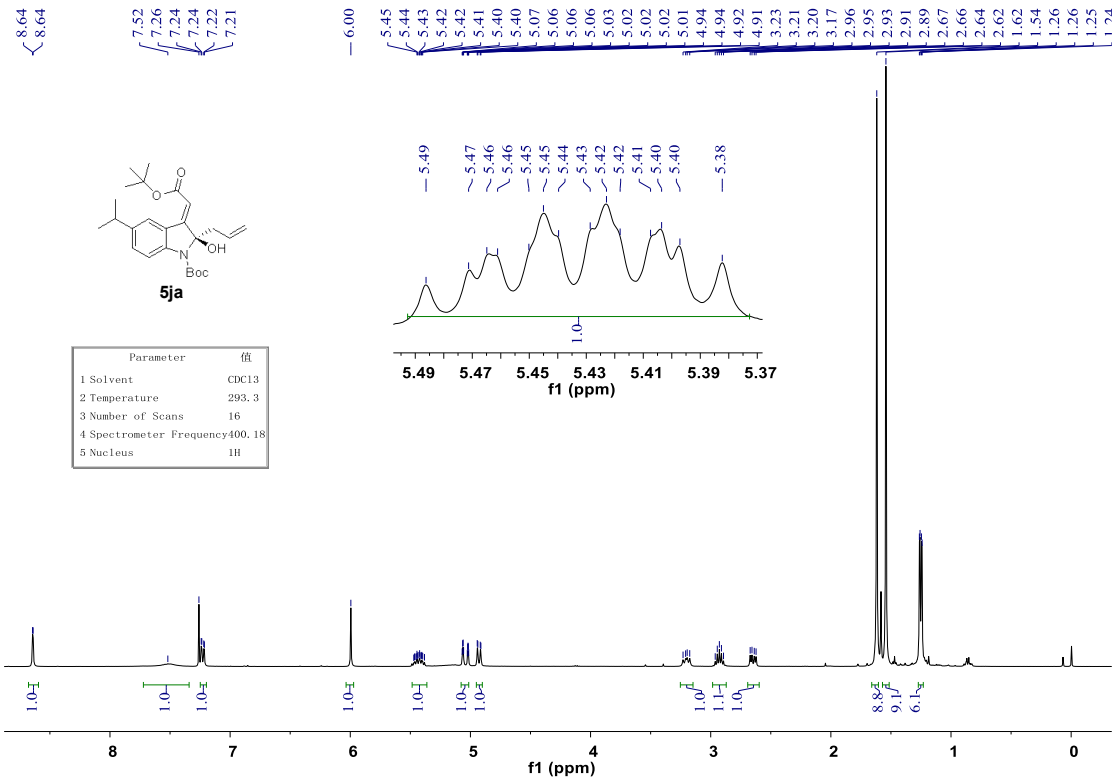
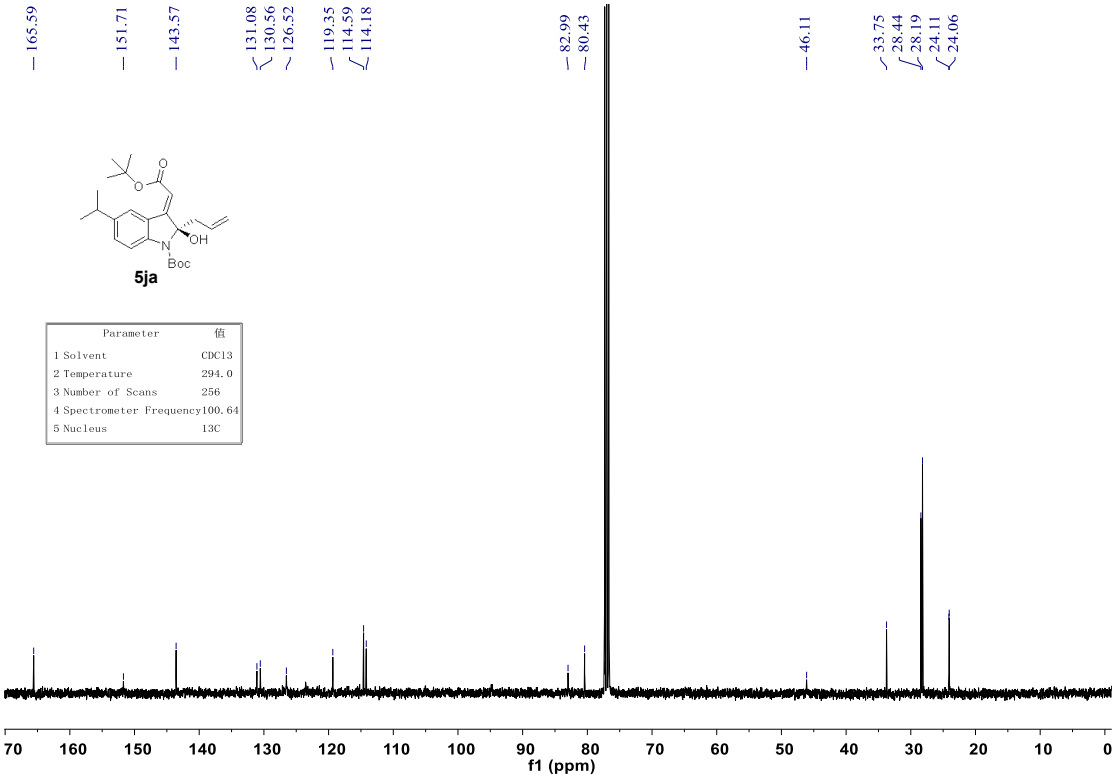
8.48
7.45
6.94
6.94
6.92
6.91
6.01
5.45
5.44
5.44
5.43
5.42
5.42
5.41
5.40
5.40
5.38
5.38
5.37
5.36
5.06
5.05
5.01
5.01
4.93
4.93
4.91
4.90
3.83
3.24
3.22
3.20
3.18
2.65
2.64
2.64
2.63
2.63
2.62
2.61
2.61
2.61
2.59
2.59
1.62
1.53
5.46
5.45
5.44
5.44
5.42
5.40
5.38
5.38
5.37
5.36
1.1
5.47 5.45 5.43 5.41 5.39 5.37 5.35
f1 (ppm)
MeO
OH
Boc
5ha
Parameter 值
1 Solvent CDCl3
2 Temperature 293.9
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0
0.7
1.1
1.0
1.1
0.9
1.0
3.1
1.0
1.1
9.3
9.2
8 7 6 5 4 3 2 1 0
f1 (ppm)

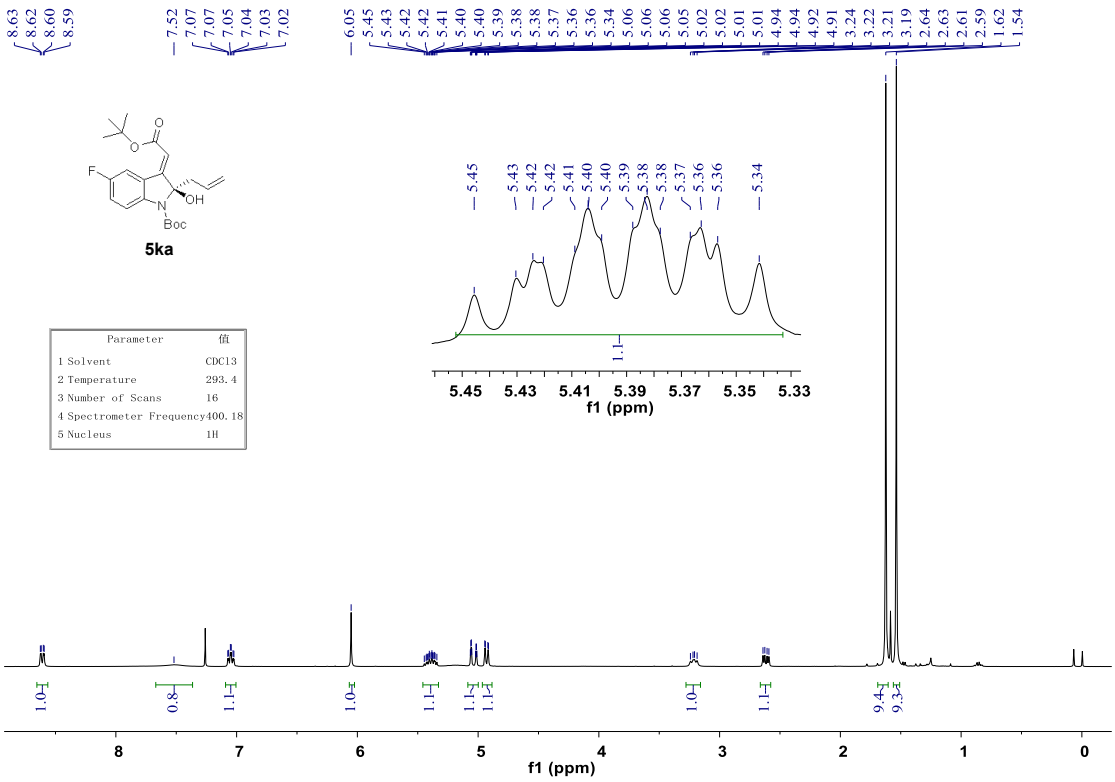

165.48
155.24
152.06
119.61
119.39
115.04
114.98
112.26
82.95
80.50
55.61
28.45
28.14
MeO
OH
Boc
5ha
Parameter 值
1 Solvent CDCl3
2 Temperature 294.5
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

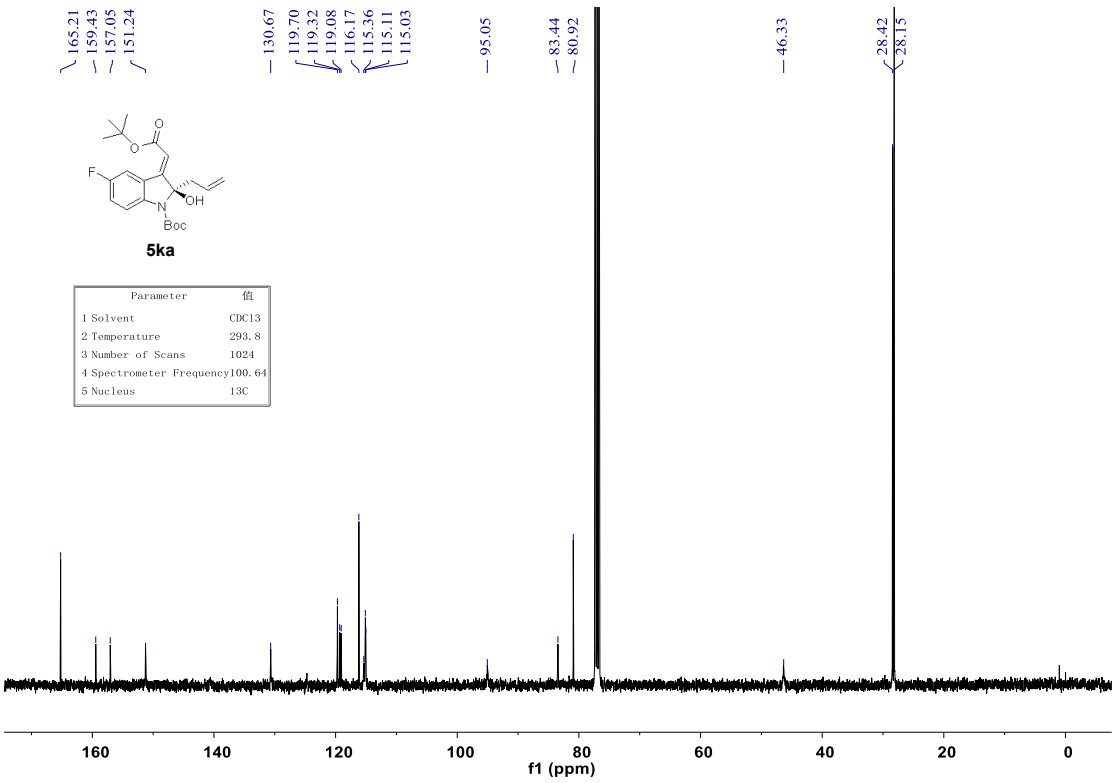

5ia
Parameter 值
1 Solvent CDCl3
2 Temperature 294.1
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)


5ia
Parameter 值
1 Solvent CDCl3
2 Temperature 294.6
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)


8.64
8.64
7.52
7.26
7.24
7.24
7.22
7.21
6.00
5.45
5.44
5.43
5.42
5.42
5.41
5.40
5.40
5.07
5.06
5.06
5.03
5.02
5.02
5.02
5.01
4.94
4.94
4.92
4.91
3.23
3.21
3.20
3.17
2.96
2.95
2.93
2.91
2.89
2.67
2.66
2.64
2.62
1.62
1.54
1.26
1.26
1.25
5.49
5.47
5.46
5.46
5.45
5.45
5.44
5.43
5.42
5.42
5.41
5.40
5.40
5.38
1.0
5.49 5.47 5.45 5.43 5.41 5.39 5.37
f1 (ppm)
O
O
OH
N
Boc
5ja
Parameter 值
1 Solvent CDCl3
2 Temperature 293.3
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0
1.0
1.0
1.0
1.0
1.0
1.0
1.0
1.1
1.0
8.8
9.1
6.1
8 7 6 5 4 3 2 1 0
f1 (ppm)

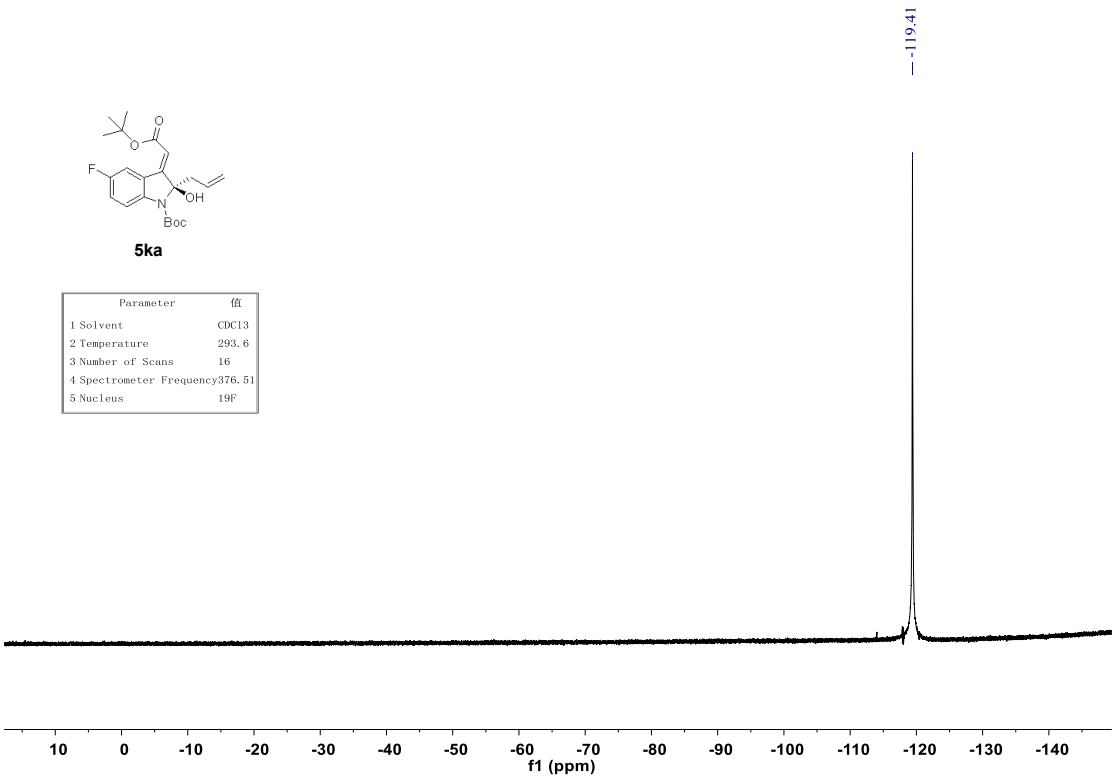

165.59
151.71
143.57
131.08
130.56
126.52
119.35
114.59
114.18
82.99
80.43
46.11
33.75
28.44
28.19
24.11
24.06
O
O
OH
N
Boc
5ja
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 256
4 Spectrometer Frequency 100.64
5 Nucleus 13C
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

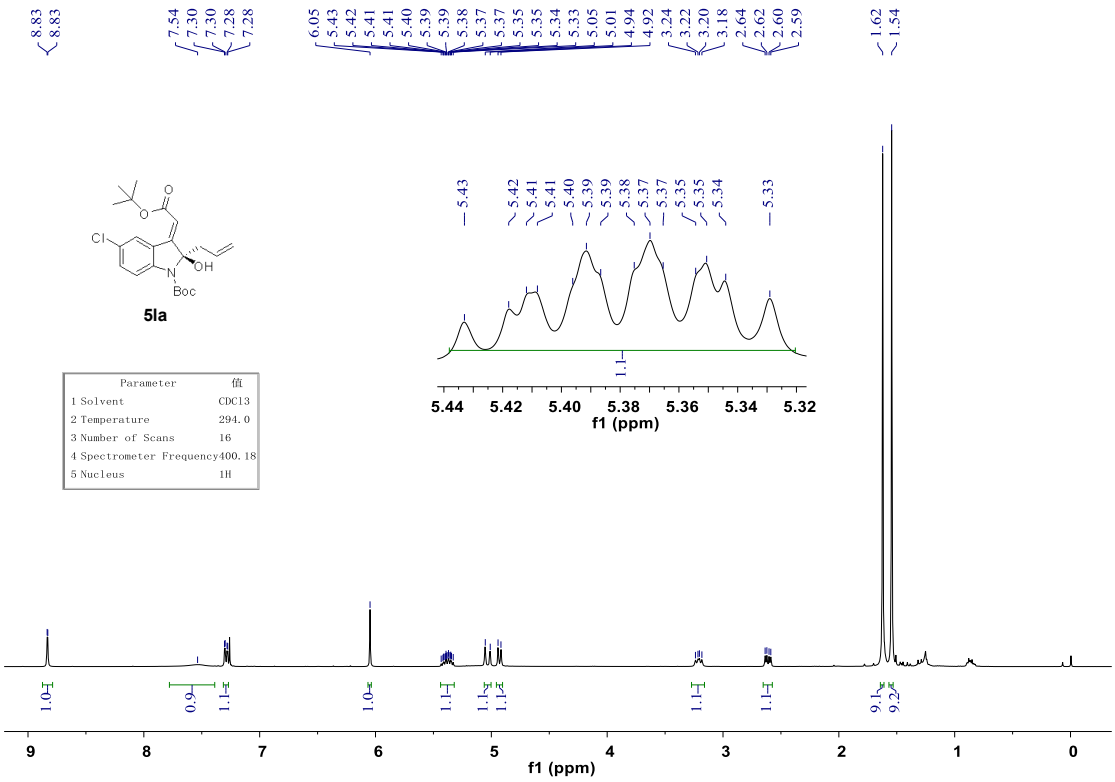

8.63
8.62
8.60
8.59
7.52
7.07
7.07
7.05
7.04
7.03
7.02
6.05
5.45
5.43
5.42
5.42
5.41
5.40
5.40
5.39
5.38
5.38
5.37
5.36
5.36
5.34
5.06
5.06
5.05
5.02
5.02
5.01
5.01
4.94
4.94
4.92
4.91
3.24
3.22
3.21
3.19
2.64
2.63
2.61
2.59
1.62
1.54
F
O
OH
N
Boc
5ka
5.45
5.43
5.42
5.42
5.41
5.40
5.40
5.39
5.38
5.38
5.37
5.36
5.36
5.34
1.1
5.45 5.43 5.41 5.39 5.37 5.35 5.33
f1 (ppm)
Parameter 值
1 Solvent CDCl3
2 Temperature 293.4
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0
0.8
1.1
1.0
1.1
1.1
1.1
1.0
1.1
9.4
9.3
8 7 6 5 4 3 2 1 0
f1 (ppm)


165.21
159.43
157.05
151.24
130.67
119.70
119.32
119.08
116.17
115.36
115.11
115.03
95.05
83.44
80.92
46.33
28.42
28.15
F
O
OH
N
Boc
5ka
Parameter 值
1 Solvent CDCl3
2 Temperature 293.8
3 Number of Scans 1024
4 Spectrometer Frequency 100.64
5 Nucleus 13C
160 140 120 100 80 60 40 20 0
f1 (ppm)

5ka

Parameter	值
1 Solvent	CDCl3
2 Temperature	293.6
3 Number of Scans	16
4 Spectrometer Frequency	376.51
5 Nucleus	19F




8.83
8.83
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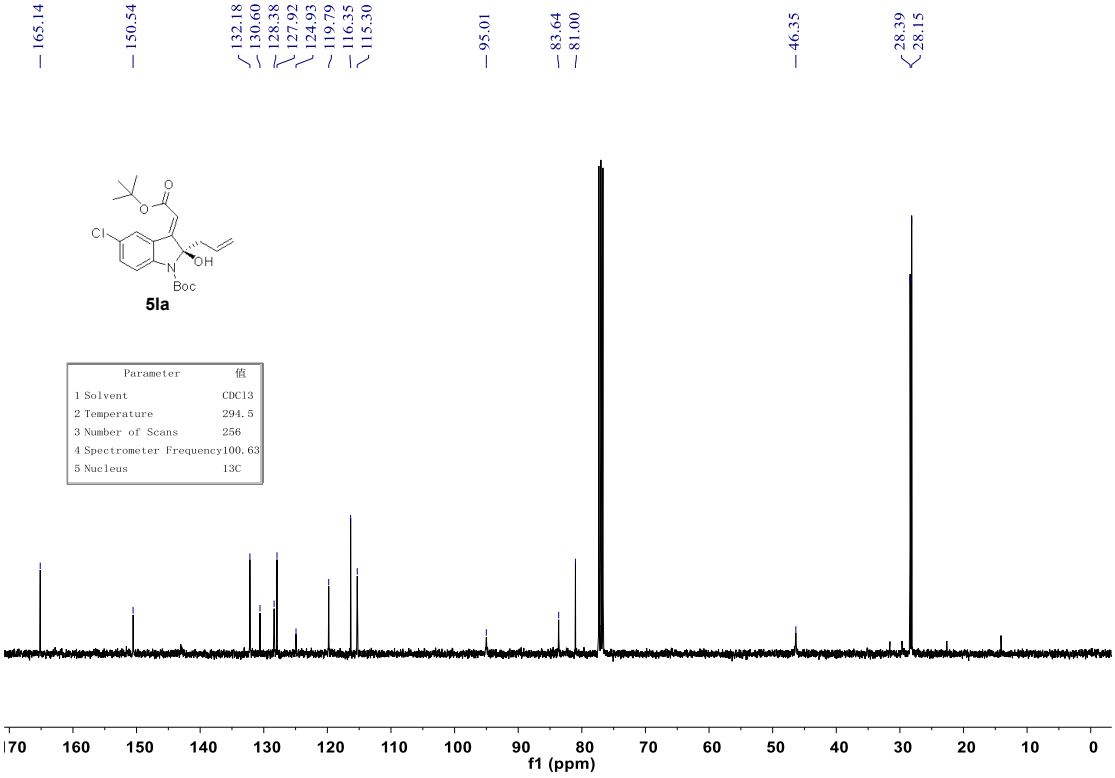
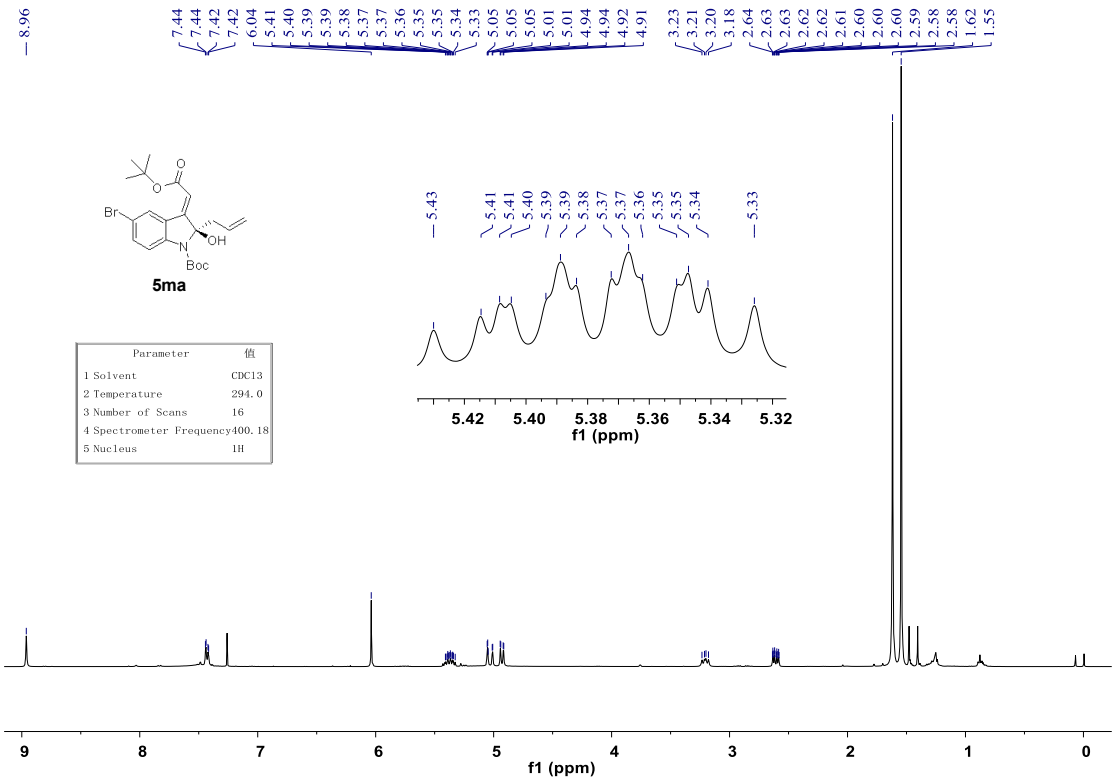
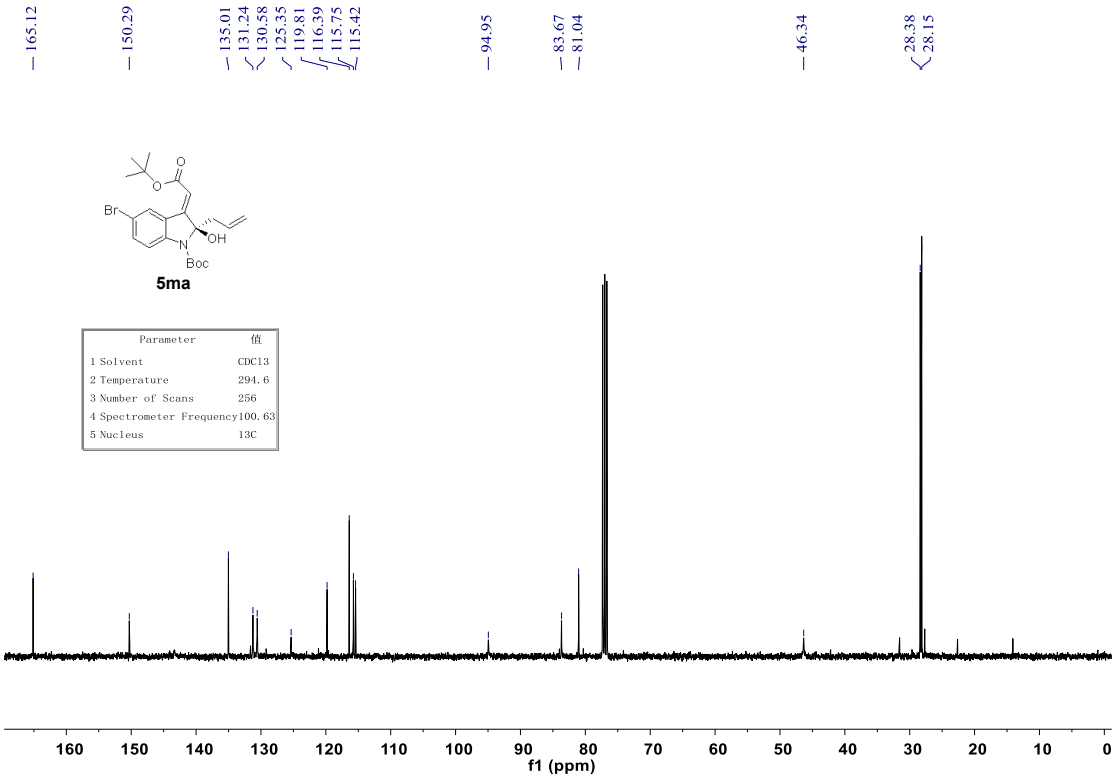
7.30
7.30
7.28
7.28
6.05
5.43
5.42
5.41
5.41
5.40
5.39
5.39
5.38
5.37
5.37
5.35
5.35
5.34
5.33
5.05
5.01
4.94
4.92
3.24
3.22
3.20
3.18
2.64
2.62
2.60
2.59
1.62
1.54
5.43
5.42
5.41
5.41
5.40
5.39
5.39
5.38
5.37
5.37
5.35
5.35
5.34
5.33
1.1
5.44
5.42
5.40
5.38
5.36
5.34
5.32
f1 (ppm)
Cl
O
OH
N
Boc
5la
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0
0.9
1.1
1.0
1.1
1.1
1.1
1.1
1.1
9.1
9.2
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


165.14
150.54
132.18
130.60
128.38
127.92
124.93
119.79
116.35
115.30
95.01
83.64
81.00
46.35
28.39
28.15
Cl
O
OH
N
Boc
5la
Parameter 值
1 Solvent CDCl3
2 Temperature 294.5
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.96
7.44
7.44
7.42
7.42
6.04
5.41
5.40
5.39
5.39
5.38
5.37
5.37
5.36
5.35
5.35
5.34
5.33
5.05
5.05
5.01
5.01
4.94
4.94
4.92
4.91
3.23
3.21
3.20
3.18
2.64
2.63
2.63
2.62
2.62
2.61
2.60
2.60
2.60
2.59
2.58
2.58
1.62
1.55
Br
OH
N
Boc
5ma
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.43
5.41
5.41
5.40
5.39
5.39
5.38
5.37
5.37
5.36
5.35
5.35
5.34
5.33
5.42 5.40 5.38 5.36 5.34 5.32
f1 (ppm)
9 8 7 6 5 4 3 2 1 0
f1 (ppm)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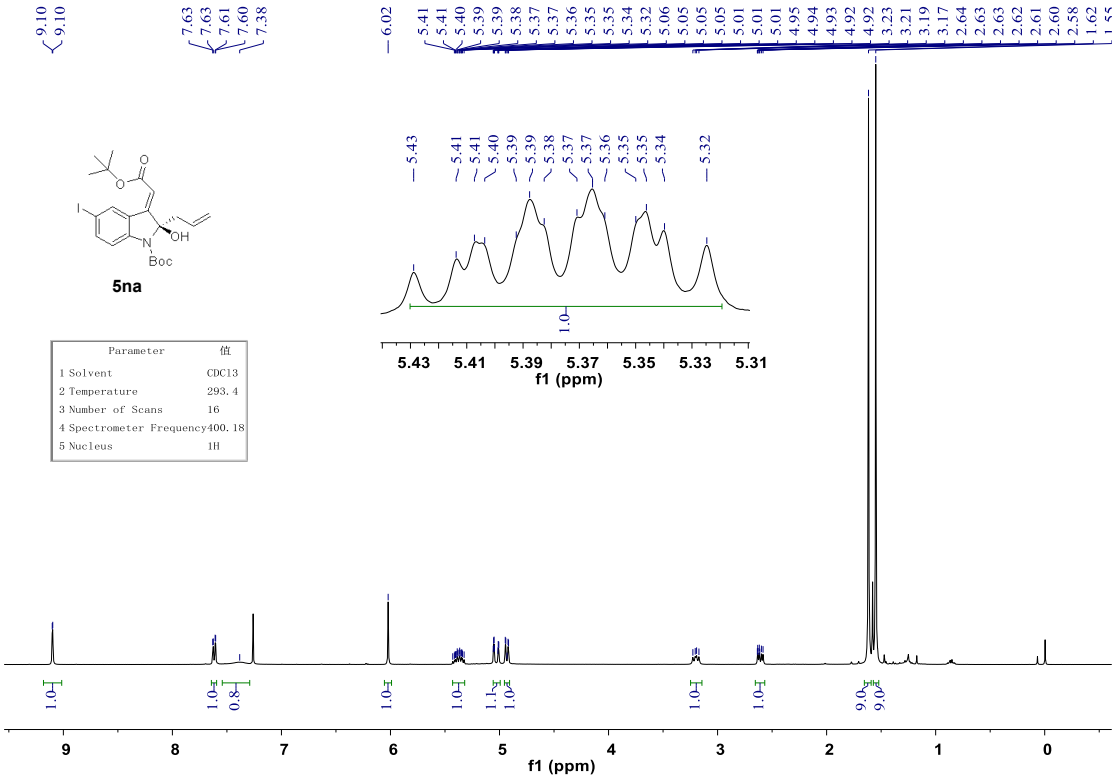
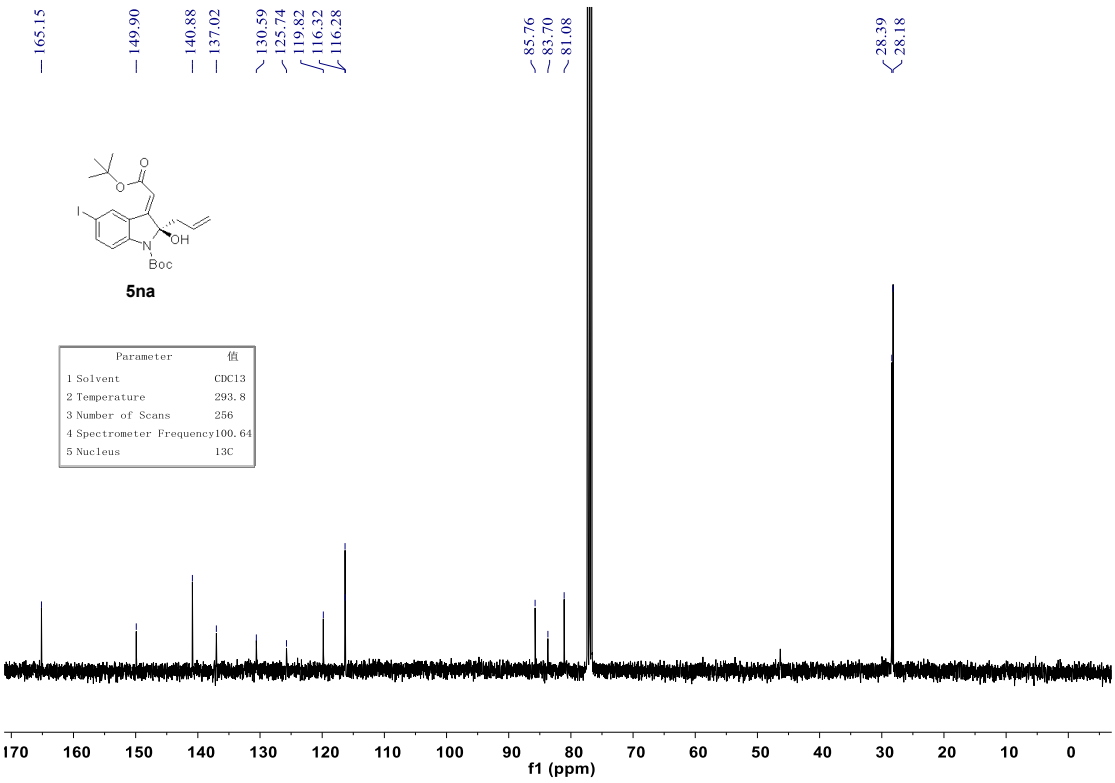
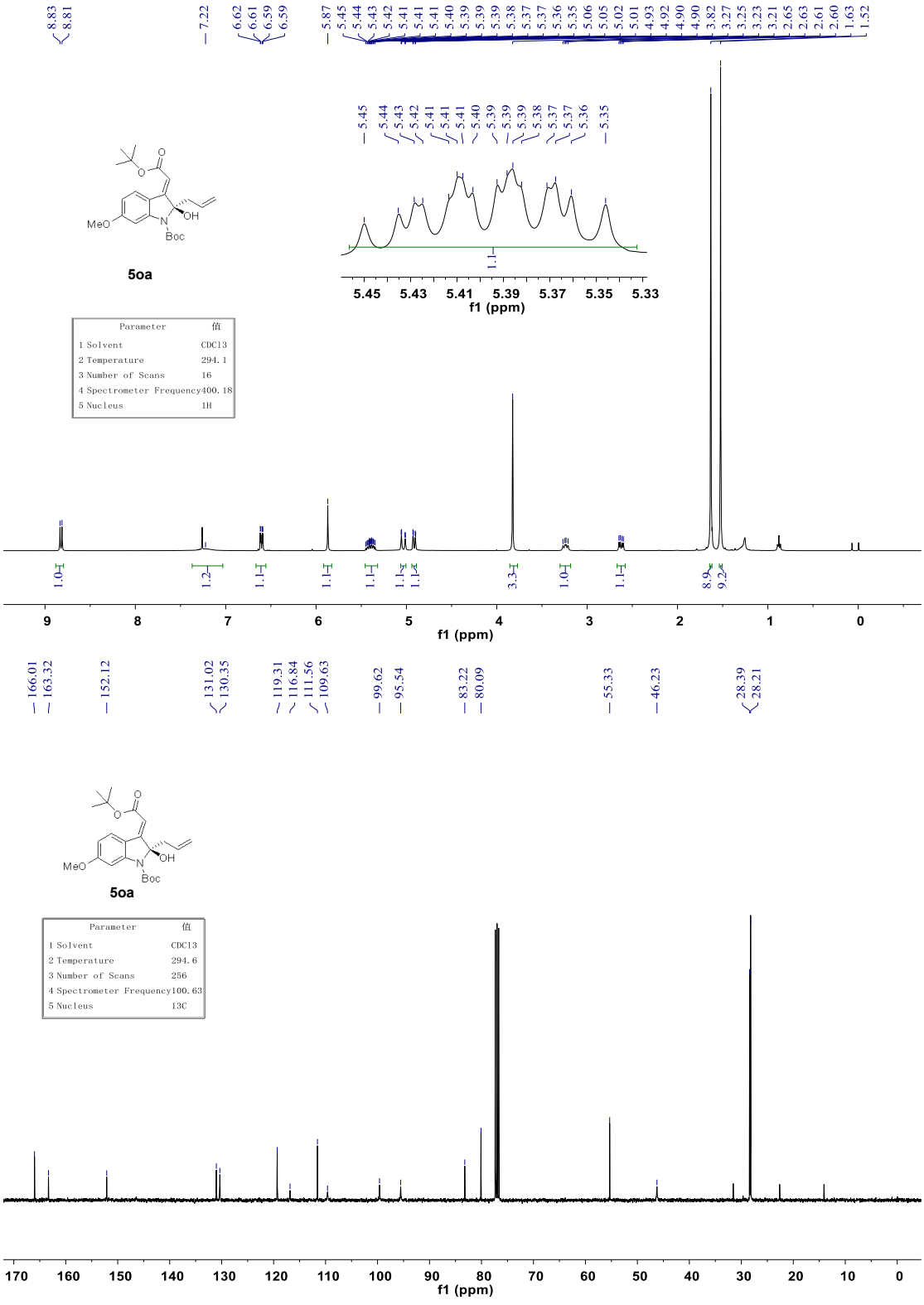
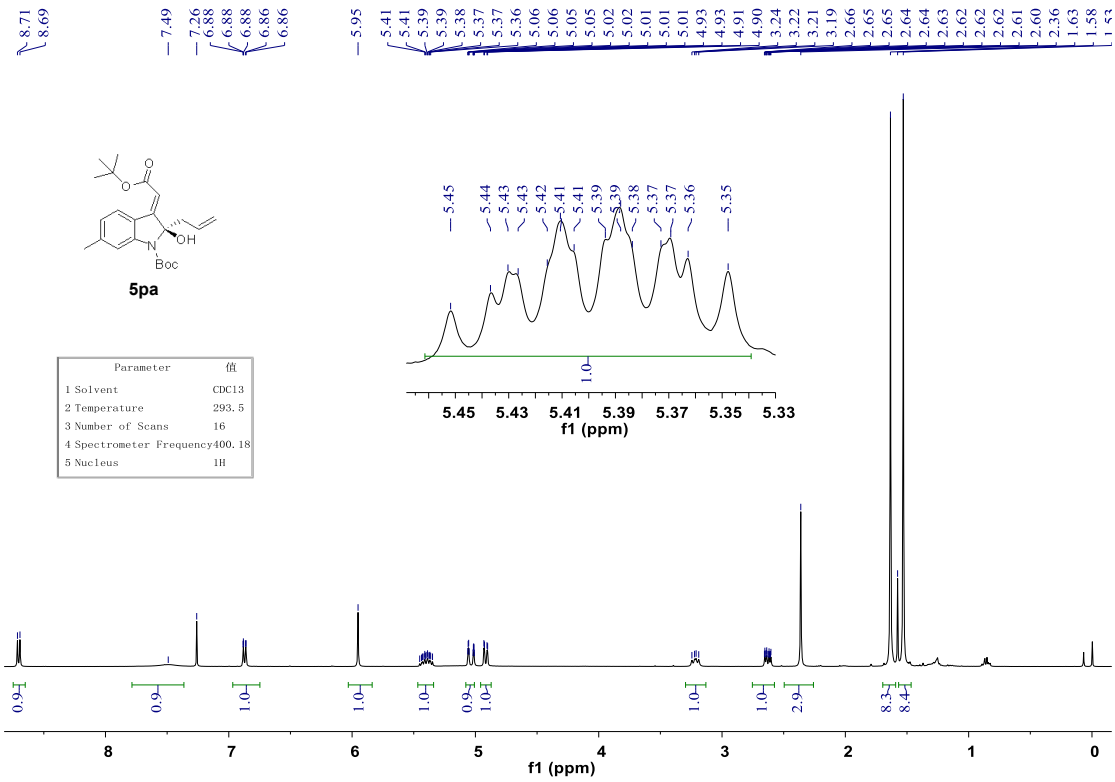
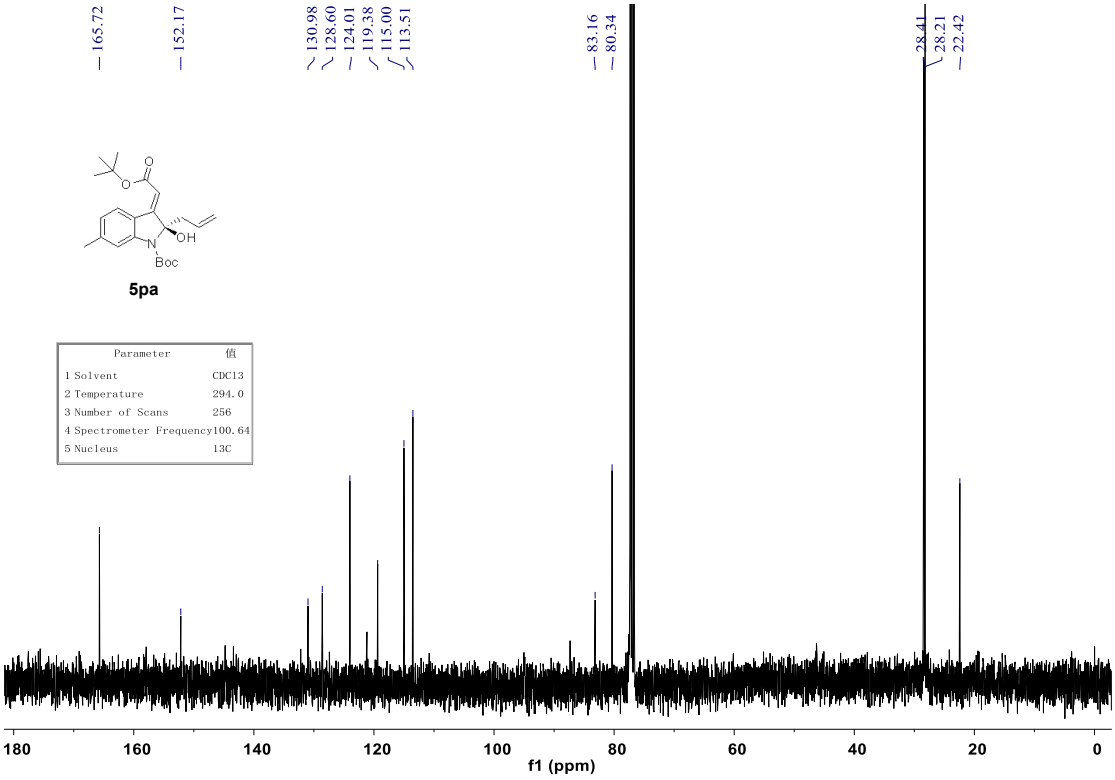
150.29
135.01
131.24
130.58
125.35
119.81
116.39
115.75
115.42
94.95
83.67
81.04
46.34
28.38
28.15
Br
OH
N
Boc
5ma
Parameter 值
1 Solvent CDCl3
2 Temperature 294.6
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

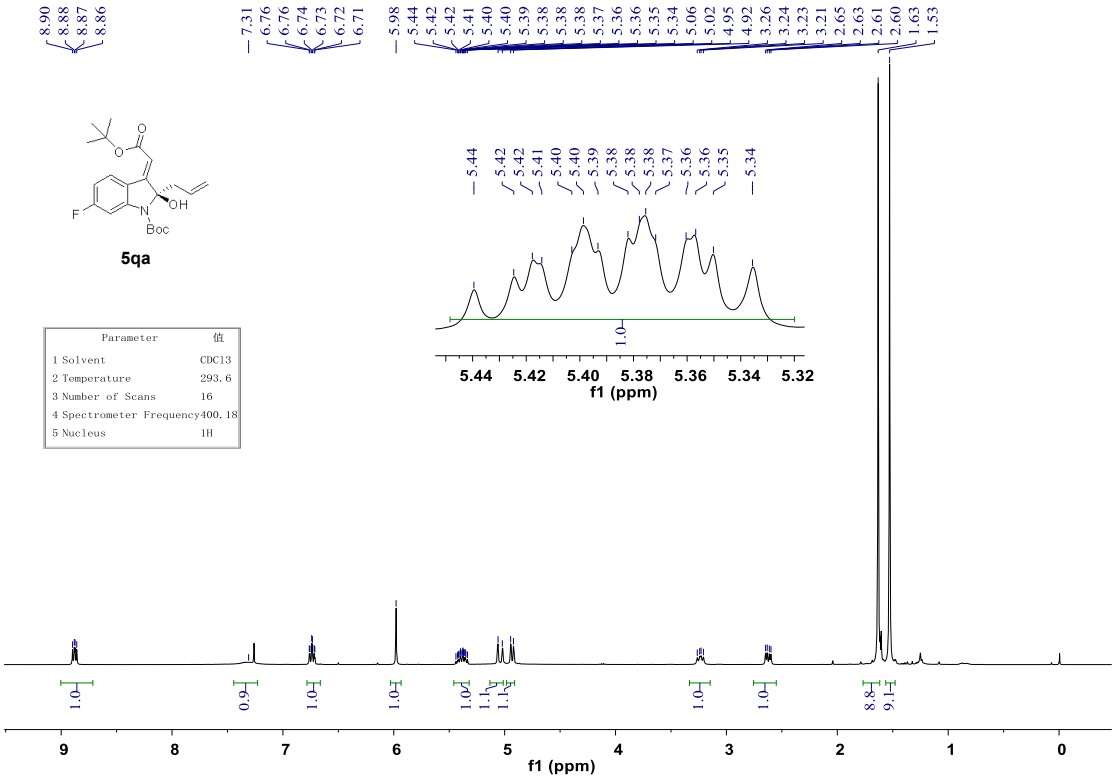

5na
Parameter 值
1 Solvent CDC13
2 Temperature 293.4
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)

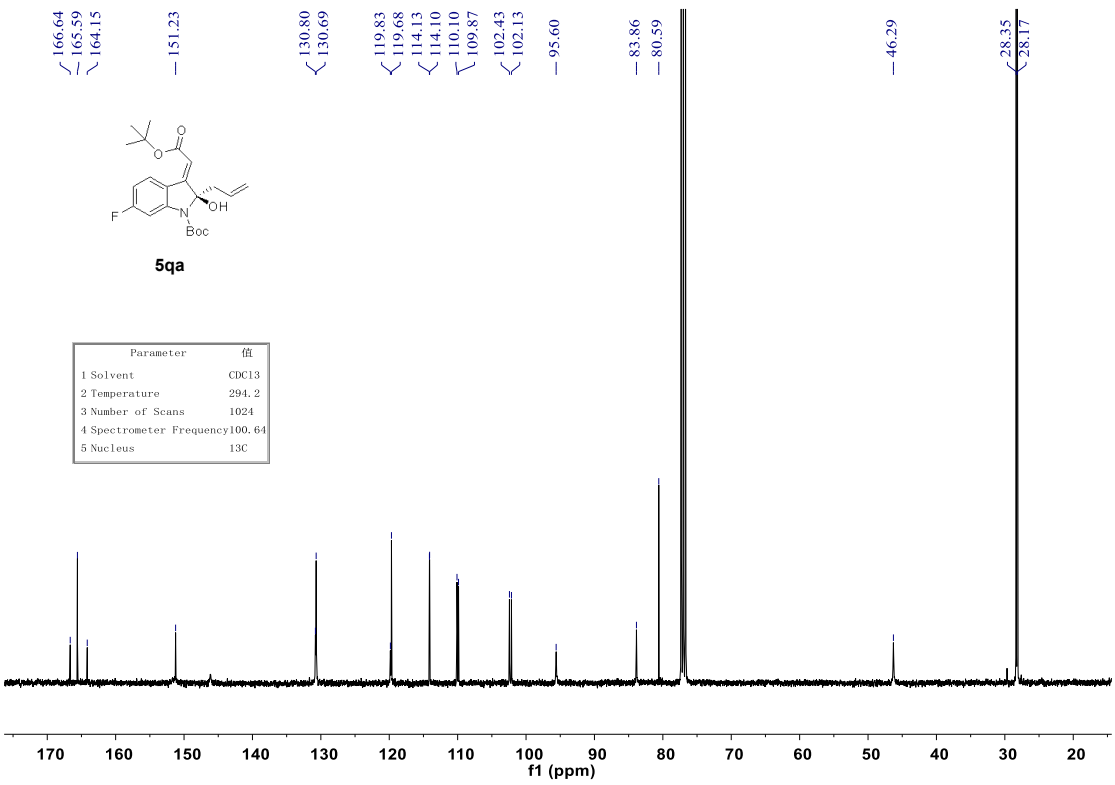

5na
Parameter 值
1 Solvent CDC13
2 Temperature 293.8
3 Number of Scans 256
4 Spectrometer Frequency 100.64
5 Nucleus 13C
f1 (ppm)

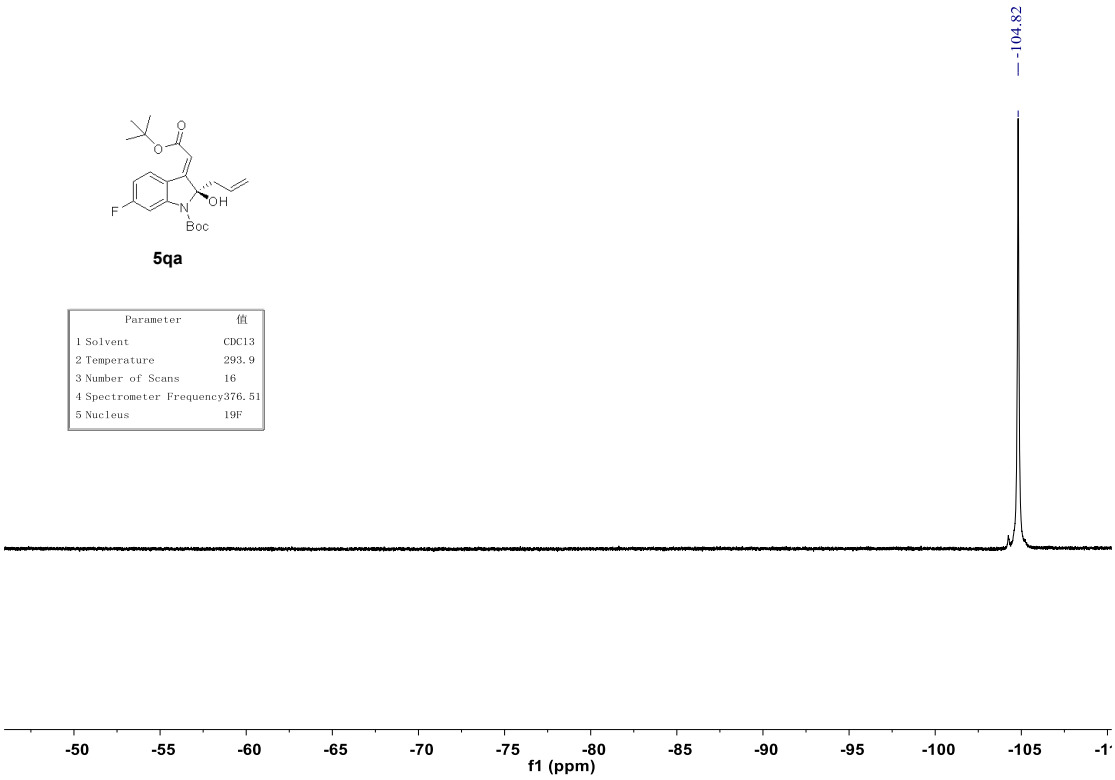

8.83
8.81
7.22
6.62
6.61
6.59
6.59
5.87
5.45
5.44
5.43
5.42
5.41
5.41
5.41
5.40
5.39
5.39
5.38
5.37
5.37
5.36
5.35
5.06
5.05
5.02
5.01
4.93
4.92
4.90
4.90
3.82
3.27
3.25
3.23
3.21
2.65
2.63
2.61
2.60
1.63
1.52
MeO
OH
N
Boc
O
5oa
5.45 5.44 5.43 5.42 5.41 5.41 5.41 5.40 5.39 5.39 5.39 5.38 5.37 5.37 5.36 5.35
1.1
5.45 5.43 5.41 5.39 5.37 5.35 5.33
f1 (ppm)
Parameter 值
1 Solvent CDCl3
2 Temperature 294.1
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
1.0 1.2 1.1 1.1 1.1 1.1 1.1 3.3 1.0 1.1 8.9 9.2
9 8 7 6 5 4 3 2 1 0
f1 (ppm)
166.01
163.32
152.12
131.02
130.35
119.31
116.84
111.56
109.63
99.62
95.54
83.22
80.09
55.33
46.23
28.39
28.21
MeO
OH
N
Boc
O
5oa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.6
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.71
8.69
7.49
7.26
6.88
6.88
6.86
6.86
5.95
5.41
5.41
5.39
5.39
5.38
5.37
5.37
5.36
5.06
5.05
5.05
5.02
5.02
5.01
5.01
5.01
4.93
4.93
4.91
4.90
3.24
3.22
3.21
3.19
2.66
2.65
2.65
2.64
2.64
2.63
2.62
2.62
2.62
2.61
2.60
2.36
1.63
1.58
OH
Boc
5pa
5.45
5.44
5.43
5.43
5.42
5.41
5.41
5.39
5.39
5.38
5.37
5.37
5.36
5.35
1.0
5.45 5.43 5.41 5.39 5.37 5.35 5.33
f1 (ppm)
Parameter 值
1 Solvent CDCl3
2 Temperature 293.5
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
0.9
0.9
1.0
1.0
1.0
0.9
1.0
1.0
1.0
2.9
8.3
8.4
8 7 6 5 4 3 2 1 0
f1 (ppm)


165.72
152.17
130.98
128.60
124.01
119.38
115.00
113.51
83.16
80.34
28.41
28.21
22.42
OH
Boc
5pa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 256
4 Spectrometer Frequency 100.64
5 Nucleus 13C
180 160 140 120 100 80 60 40 20 0
f1 (ppm)

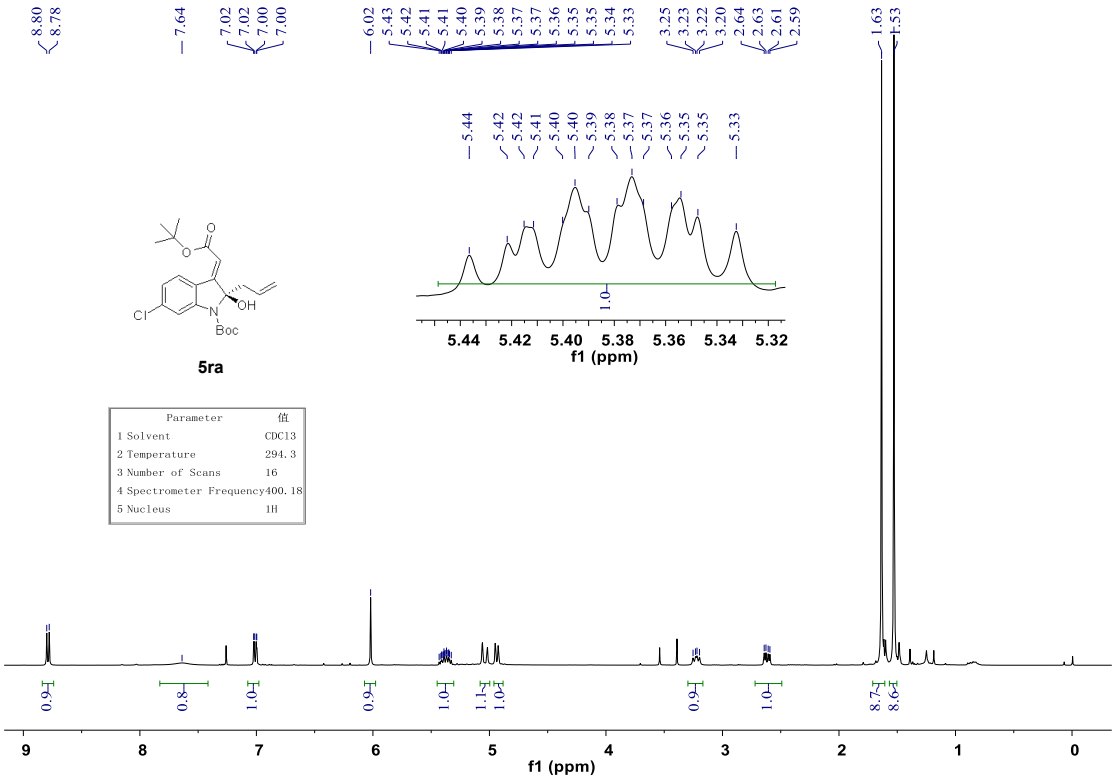

8.90
8.88
8.87
8.86
7.31
6.76
6.76
6.74
6.73
6.72
6.71
5.98
5.44
5.42
5.42
5.41
5.40
5.40
5.39
5.38
5.38
5.37
5.36
5.36
5.35
5.34
5.06
5.02
4.95
4.92
3.26
3.24
3.23
3.21
2.65
2.63
2.61
2.60
1.63
1.53
F
OH
N
Boc
5qa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.6
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.44 5.42 5.42 5.41 5.40 5.40 5.39 5.38 5.38 5.38 5.37 5.36 5.36 5.35 5.34
1.0
5.44 5.42 5.40 5.38 5.36 5.34 5.32
f1 (ppm)
1.0 0.9 1.0 1.0 1.0 1.1 1.1 1.0 1.0 8.8 9.1
9 8 7 6 5 4 3 2 1 0
f1 (ppm)

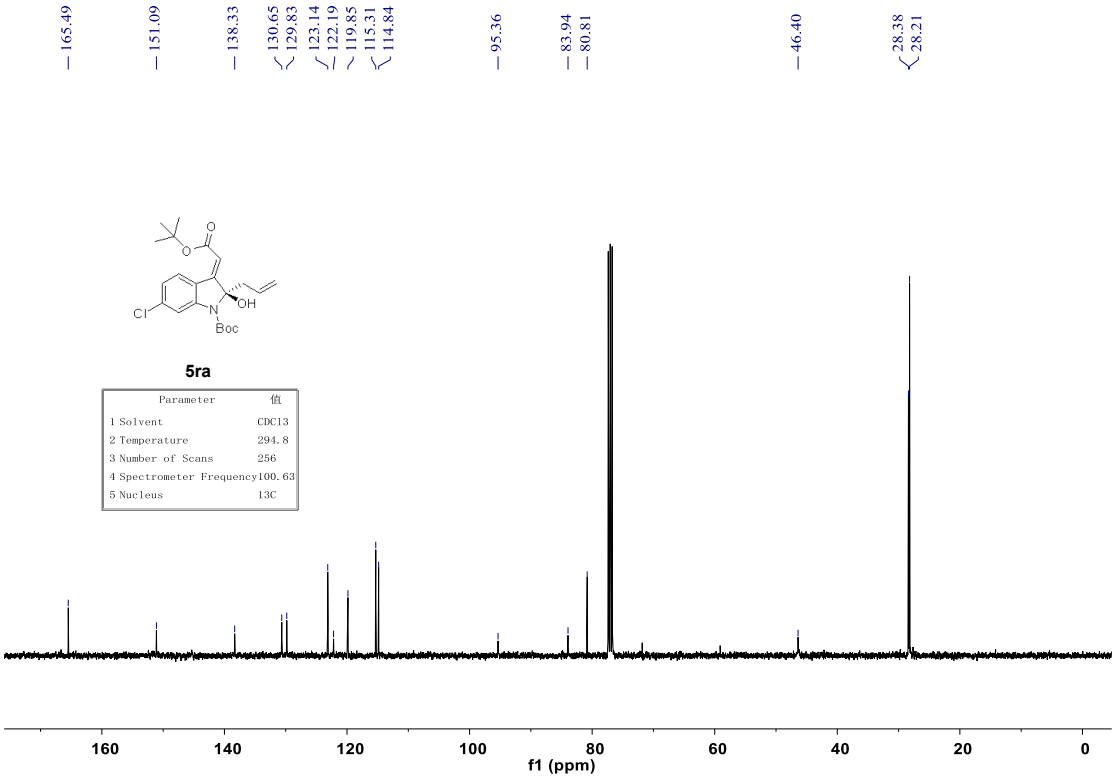

166.64
165.59
164.15
151.23
130.80
130.69
119.83
119.68
114.13
114.10
110.10
109.87
102.43
102.13
95.60
83.86
80.59
46.29
28.35
28.17
F
OH
N
Boc
5qa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.2
3 Number of Scans 1024
4 Spectrometer Frequency 100.64
5 Nucleus 13C
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)

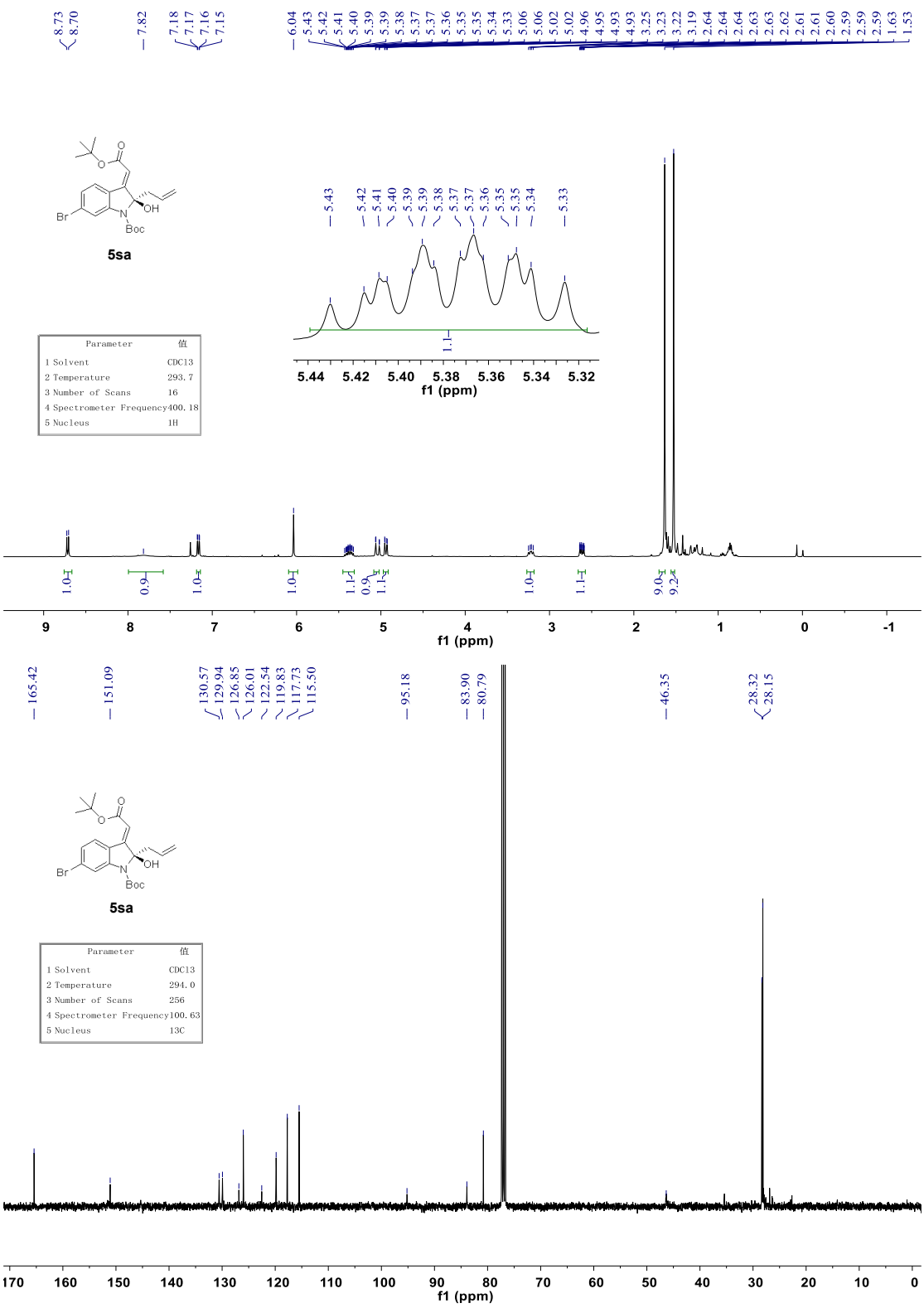


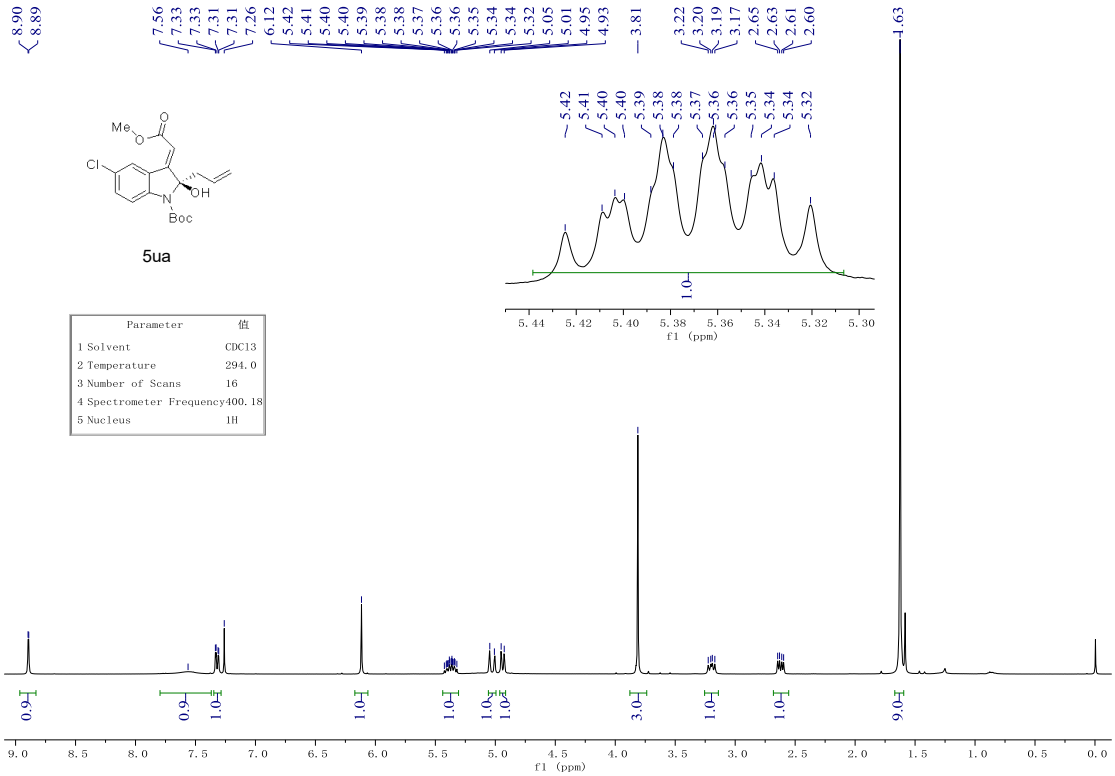
5qa

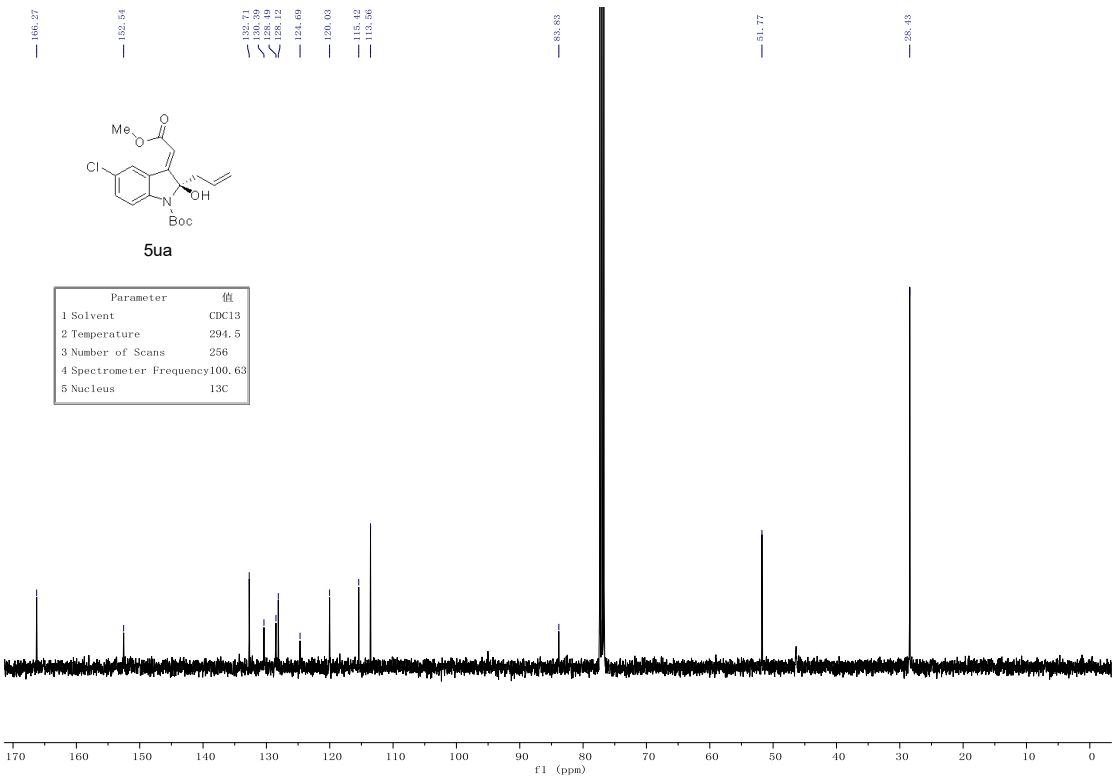
Parameter	值
1 Solvent	CDCl3
2 Temperature	293.9
3 Number of Scans	16
4 Spectrometer Frequency	376.51
5 Nucleus	19F


8.80
8.78
7.64
7.02
7.02
7.00
7.00
6.02
5.43
5.42
5.41
5.41
5.40
5.39
5.38
5.37
5.37
5.36
5.35
5.35
5.34
5.33
3.25
3.23
3.22
3.20
2.64
2.63
2.61
2.59
1.63
1.53
5.44
5.42
5.42
5.41
5.40
5.40
5.39
5.38
5.37
5.37
5.36
5.35
5.35
5.33
1.0
5.44 5.42 5.40 5.38 5.36 5.34 5.32
f1 (ppm)
Cl
OH
N
Boc
O
5ra
Parameter 值
1 Solvent CDCl3
2 Temperature 294.3
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
0.9
0.8
1.0
0.9
1.0
1.1
1.0
0.9
1.0
8.7
8.6
9 8 7 6 5 4 3 2 1 0
f1 (ppm)


165.49
151.09
138.33
130.65
129.83
123.14
122.19
119.85
115.31
114.84
95.36
83.94
80.81
46.40
28.38
28.21
Cl
OH
N
Boc
O
5ra
Parameter 值
1 Solvent CDCl3
2 Temperature 294.8
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
160 140 120 100 80 60 40 20 0
f1 (ppm)


8.73
8.70
7.82
7.18
7.17
7.16
7.15
6.04
5.43
5.42
5.41
5.40
5.39
5.39
5.38
5.37
5.37
5.36
5.35
5.35
5.34
5.33
5.06
5.06
5.02
5.02
4.96
4.95
4.93
4.93
3.25
3.23
3.22
3.19
2.64
2.64
2.64
2.63
2.63
2.62
2.61
2.61
2.60
2.59
2.59
2.59
1.63
1.53
Br
OH
N
Boc
O
5sa
Parameter 值
1 Solvent CDCl3
2 Temperature 293.7
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
5.43
5.42
5.41
5.40
5.39
5.39
5.38
5.37
5.37
5.36
5.35
5.35
5.34
5.33
1.1
5.44
5.42
5.40
5.38
5.36
5.34
5.32
f1 (ppm)
1.0
0.9
1.0
1.0
1.1
0.9
1.1
1.0
1.1
9.0
9.2
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)
165.42
151.09
130.57
129.94
126.85
126.01
122.54
119.83
117.73
115.50
95.18
83.90
80.79
46.35
28.32
28.15
Br
OH
N
Boc
O
5sa
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.90
8.89
7.56
7.33
7.33
7.31
7.31
7.26
6.12
5.42
5.41
5.40
5.40
5.39
5.38
5.38
5.37
5.36
5.36
5.35
5.34
5.34
5.32
5.05
5.01
4.95
4.93
3.81
3.22
3.20
3.19
3.17
2.65
2.63
2.61
2.60
1.63
Me
O
Cl
OH
N
Boc
5ua
Parameter 值
1 Solvent CDCl3
2 Temperature 294.0
3 Number of Scans 16
4 Spectrometer Frequency 400.18
5 Nucleus 1H
f1 (ppm)


166.27
152.54
132.71
130.39
128.49
128.12
124.69
120.03
115.42
113.56
83.83
51.77
28.43
Me
O
Cl
OH
N
Boc
5ua
Parameter 值
1 Solvent CDCl3
2 Temperature 294.5
3 Number of Scans 256
4 Spectrometer Frequency 100.63
5 Nucleus 13C
f1 (ppm)