

Tunable CTPhos and Chloride Enabled Direct Asymmetric Reductive Amination for the Synthesis of Chiral Hydroxylamines

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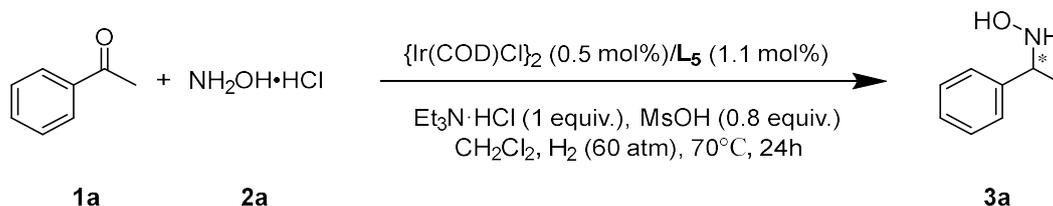
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1. General remarks

All reactions were performed in the nitrogen-filled glovebox or under nitrogen using standard Schlenk techniques unless otherwise noted. Unless otherwise noted, all reagents and solvents were purchased from commercial suppliers without further purification. Column chromatography was performed using silica gel 60 (200 – 300 mesh). ¹H NMR and ¹³C NMR spectral data were obtained from Bruker 400 MHz spectrometers. Chemical shifts are reported in *ppm*. Enantiomeric excess values were determined by chiral HPLC on an Agilent 1220 Series instrument or by an Agilent 7890 Series GC to determine the enantiomeric excesses. Key new products were further characterized by HRMS. A positive ion mass spectrometers of sample was acquired on a Thermo Scientific LTQ Orbitrap XL mass spectrometer with an electrospray ionization source. Ligands **L5** were synthesized according to literature.¹

2. Optimization of reaction conditions

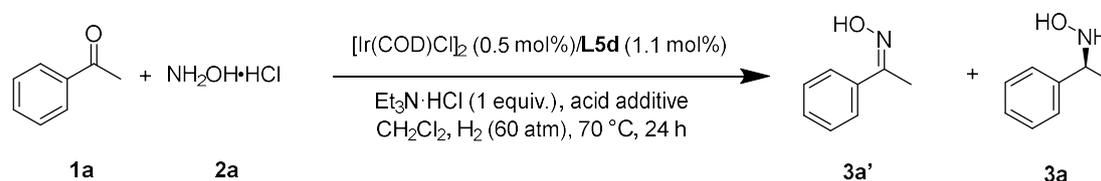
Table S1 Exploring the additive effect



Entry	Additive ^b	Solvent	Yield (%)	<i>ee</i> (%)
1	--	EtOAc	<3	--
2	PhCOOH	EtOAc	<3	--
3	PhB(OH) ₂	EtOAc	<3	--
4	PPA	EtOAc	<3	--
5	TsOH	EtOAc	2	17
6	(<i>L</i>)-CAS	EtOAc	3	19
7	MsOH	EtOAc	3	23
8	$\text{Et}_3\text{N}\cdot\text{HCl}$	EtOAc	17	29
9	DIPEA·HCl	EtOAc	16	29

^a Reaction conditions: **1a** (0.3 mmol), **2a** (0.6 mmol), [Ir(COD)Cl]₂ (0.5 mol%), L (1.1 mol%), EtOAc (1 mL), H₂ (60 atm), 70 °C, 24 h. Enantiomeric excesses (*ee*) and yields were determined by chiral HPLC analysis using a chiral stationary phase. ^b Additive (1.0 equiv.), PPA: Phenylphosphonic acid, MsOH: MeSO₃H.

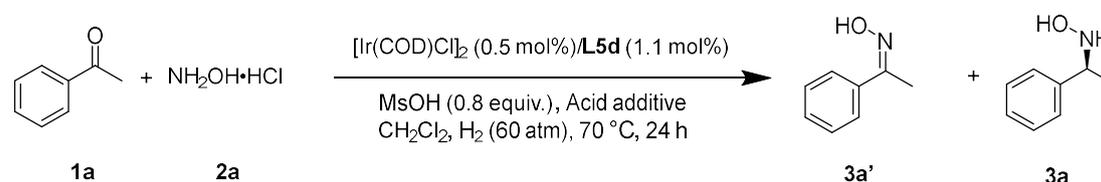
Table S2 Exploring the acid additive2 effects^a



Entry	Acid additive ^b	1a (%)	3a' (%)	3a	
				Yield (%)	<i>ee</i> (%)
1	PhB(OH) ₂	18	17	61	91
2	PhCOOH	4	16	78	91
3	PPA	3	66	31	92
4	AcOH	13	32	55	95
5 ^c	I ₂	4	77	19	91
6	TsOH	2	19	79	95
7	(<i>L</i>)-CAS	4	20	76	96
8	MsOH	2	-	97	98
9 ^d	MsOH	2	-	97	98

^a Reaction conditions: **1a** (0.3 mmol), **2a** (0.6 mmol), Et₃N·HCl (1.0 equiv.), [Ir(COD)Cl]₂ (0.5 mol%), L5d (1.1 mol%), CH₂Cl₂ (1 mL), H₂ (60 atm), 70 °C, 24 h. Enantiomeric excesses (*ee*) and yields were determined by chiral HPLC analysis using a chiral stationary phase. ^b Acid addition (1.0 equiv.). ^c I₂ (0.1 equiv.). ^d MsOH (0.8 equiv.).

Table S3 Exploring the additive1 effects^a

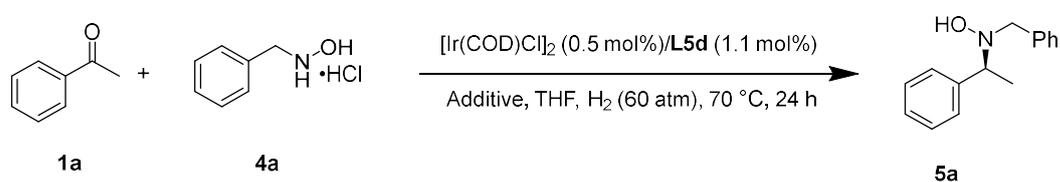


Entry	Acid additive ^b	1a (%)	3a' (%)	3a	
				Yield (%)	<i>ee</i> (%)
1	Et ₃ N·HCl	1	1	97	98

2	DIPEA·HCl	3	7	90	96
3	Me ₃ N·HCl	5	10	85	87
4	DBU·HCl	3	10	87	87
5	DABCO·HCl	10	64	26	90
6	Et ₃ N·HBr	12	30	59	91

^a Reaction conditions: **1a** (0.3 mmol), **2a** (0.6 mmol), MsOH (0.8 equiv.), [Ir(COD)Cl]₂ (0.5 mol%), **L5d** (1.1 mol%), CH₂Cl₂ (1 mL), H₂ (60 atm), 70 °C, 24 h. Enantiomeric excesses (*ee*) and yields were determined by chiral HPLC analysis using a chiral stationary phase. ^b Additive (1.0 equiv.).

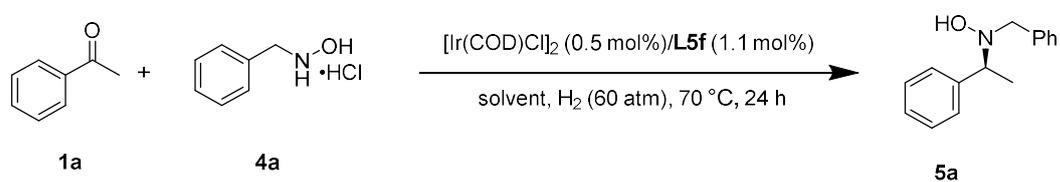
Table S4 Exploring the additive effects^a



Entry	Additive ^b	Ligand	Solvent	Yield (%)	<i>ee</i> (%)
1	--	L5d	THF	84	83
2	Et ₃ N·HCl	L5d	THF	70	80
3	TsOH	L5d	THF	44	83
4	MsOH	L5d	THF	51	78
5	PPA	L5d	THF	57	82
5	AcOH	L5d	THF	50	80
6	Et ₃ N	L5d	THF	--	
7 ^c	I ₂	L5d	THF	--	

^a Reaction conditions: **1a** (0.3 mmol), **2a** (0.6 mmol), [Ir(COD)Cl]₂ (0.5 mol%), **L5d** (1.1 mol%), THF (1 mL), H₂ (60 atm), 70 °C, 24 h. Enantiomeric excesses (*ee*) were determined by chiral HPLC analysis using a chiral stationary phase. ^b Additive (1.0 equiv.). ^c I₂ (0.1 equiv.).

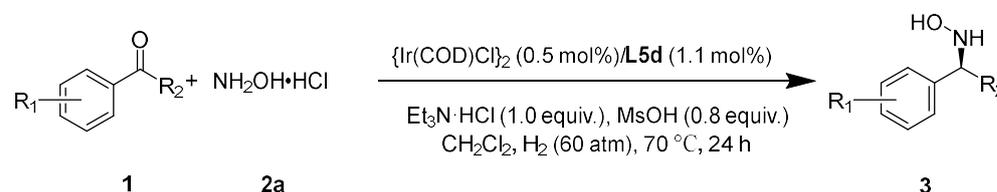
Table S5 Exploring the solvent effects^a



Entry	Solvent	Yield (%)	ee (%)
1	CH ₂ Cl ₂	29	75
2	EtOAc	34	80
3	<i>n</i> -hexane	40	71
4	C ₂ H ₄ Cl ₂	83	42
5	THF	93	93
6	PhMe	25	77
7	CH ₃ CN	22	70
8	MeOH	19	34

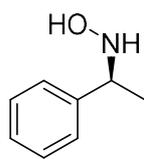
^a Reaction conditions: **1a** (0.3 mmol), **2a** (0.6 mmol), [Ir(COD)Cl]₂ (0.5 mol%), **L5d** (1.1 mol%), solvent (1 mL), H₂ (60 atm), 70 °C, 24 h. Enantiomeric excesses (*ee*) were determined by chiral HPLC analysis using a chiral stationary phase.

3. General procedure for the asymmetric reductive amination



In the nitrogen-filled glovebox, [Ir(COD)Cl]₂ (6.0 mg, 0.009 mmol) and (*R*)-**L5d** (17.3 mg, 0.0020 mmol) were dissolved in anhydrous CH₂Cl₂ (0.9 mL) in a 5 mL vial equipped with a stir bar. The above solution was stirred at room temperature for 30 minutes to *in situ* generate the Ir-**L5** complex. Into a 5 mL vial were added **1** (0.3 mmol), **2** (0.6 mmol), Et₃N·HCl (41.3 mg, 1.0 equiv.), MsOH (15.6 μL, 0.8 equiv.) and the stock solution containing the iridium catalyst (150 μL). The total amount of solvent was made to 1 mL. The vials were transferred to an autoclave, which was purged with H₂ 3 times and then charged with 60 atm of H₂, and stirred at 70 °C for 24 h. After the reaction was complete, the hydrogen gas was released slowly and saturated NaHCO₃ (2 mL) was added into the reaction mixture, which was then extracted with CH₂Cl₂ (1 mL*3). The organic layers were combined, dried over anhydrous Na₂SO₄ and concentrated to give the crude product, which was purified by column chromatography.

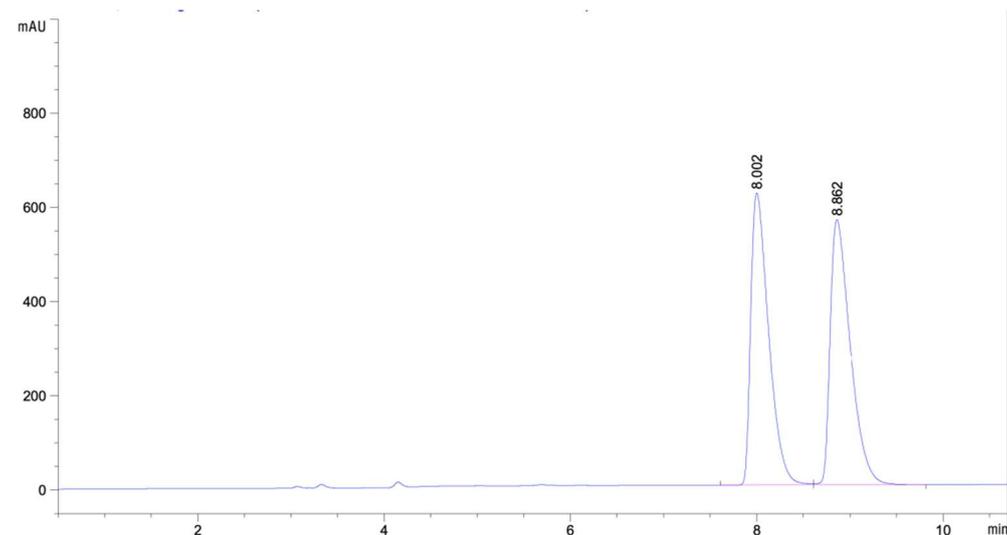
(S)-N-(1-phenylethyl)hydroxylamine (3a)



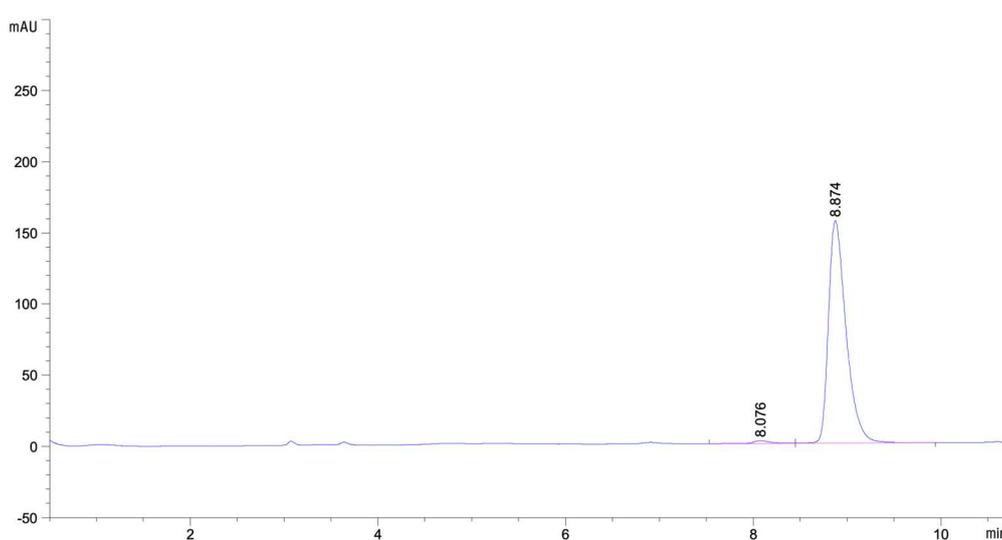
3a

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH_2Cl_2 :MeOH = 10:1), 39.9 mg, 97% yield, 98% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.39–7.22 (m, 5H), 4.12 (q, J = 6.6 Hz, 1H), 1.38 (d, J = 6.7 Hz, 3H).

Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 80/20; 1.0 mL/min; 220 nm): t_R (minor) = 8.0 min, t_R (major) = 8.8 min. The analytical data are in accordance with the literature².

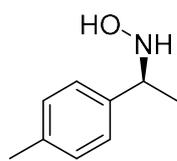


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.002	WV	0.2056 8277.90820	620.52911	49.5061
2	8.862	VB	0.2289 8443.08301	563.05975	50.4939



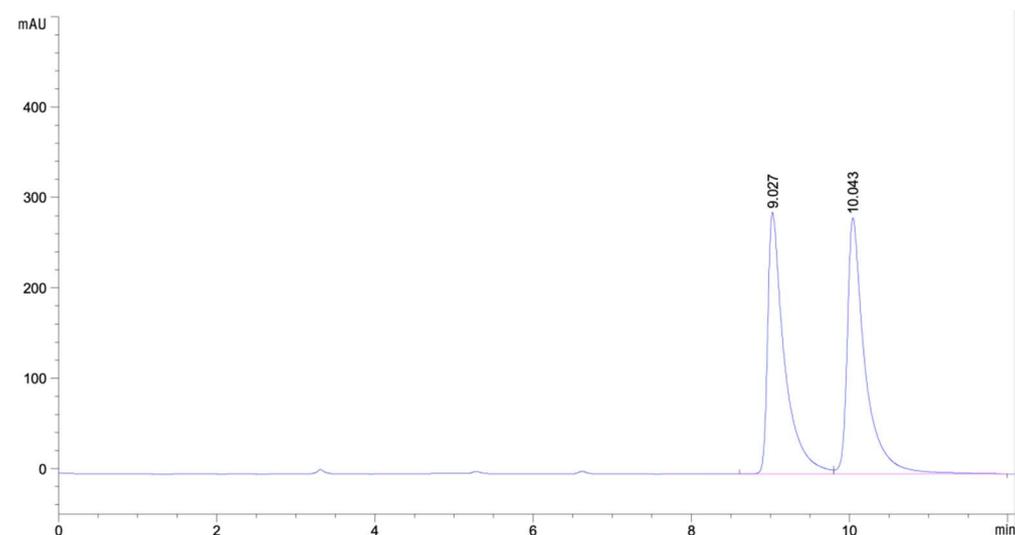
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1	8.076	BV	0.1958 24.99712	1.87208	1.2106
2	8.874	VB	0.1983 2039.91370	156.28922	98.7894

(S)-N-(1-(p-tolyl)propyl)hydroxylamine (3b)

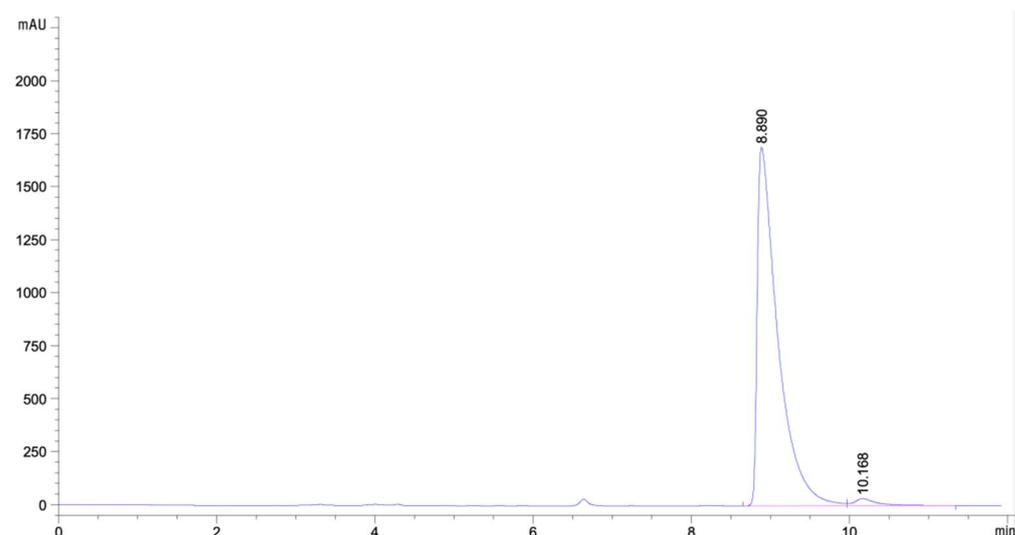


White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 43.6 mg, 96% yield, 96% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.24 (m, $J = 8.0$ Hz, 4H), 4.11 (q, $J = 6.7$ Hz, 1H), 2.36 (s, 3H), 1.42 (d, $J = 6.7$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC

3b (Chiralpak IB-3, *n*-hexane/isopropanol = 90/10, 1.0 mL/min; 220 nm): t_R (major) = 9.0 min, t_R (minor) = 10.0 min. The analytical data are in accordance with the literature².

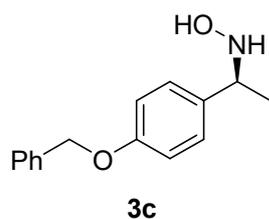


#	[min]	[min]	[mAU*s]	[mAU]	%
1	9.027 BV	0.2091	4240.93994	289.20676	48.9316
2	10.043 VV	0.2225	4426.14014	283.02518	51.0684

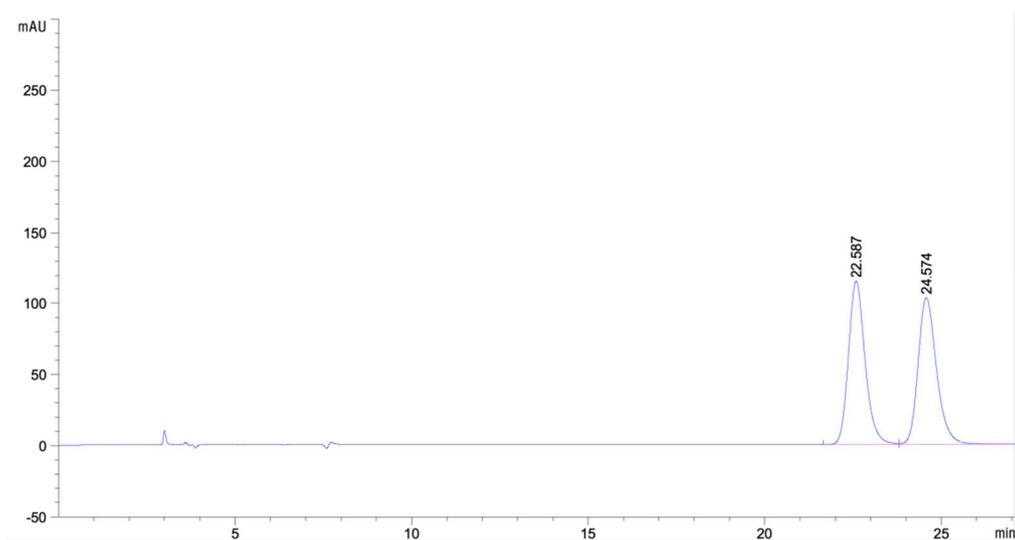


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.890 BV	0.2611	3.04381e4	1690.54871	97.8035
2	10.168 VB	0.2815	683.58795	33.86364	2.1965

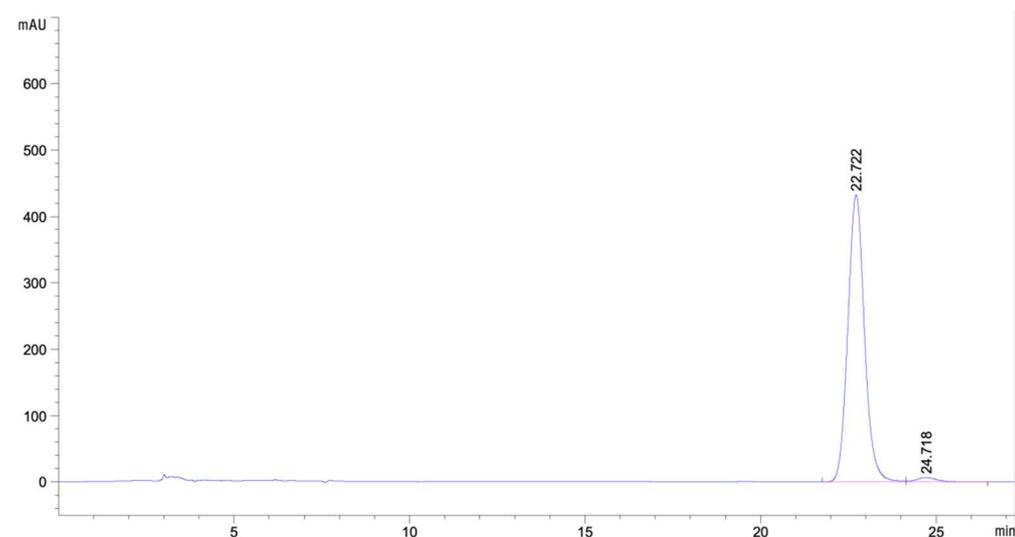
(S)-N-(1-(4-methoxyphenyl)ethyl)hydroxylamine (3c)



White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 70.1 mg, 96% yield, 96% *ee*. $^1\text{H NMR}$ (400 MHz, CHCl_3-d) δ 7.49–7.32 (m, 5H), 7.31–7.24 (m, 2H), 7.02–6.93 (m, 2H), 5.08 (s, 2H), 4.09 (q, $J = 6.6$ Hz, 1H), 1.42 (d, $J = 6.6$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 22.7 min, t_R (minor) = 24.7 min. The analytical data are in accordance with the literature².

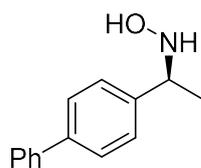


#	[min]	[min]	[mAU*s]	[mAU]	%
1	22.587 BV	0.5008	3750.70020	114.60824	50.1157
2	24.574 VBA	0.5534	3733.38477	102.88155	49.8843



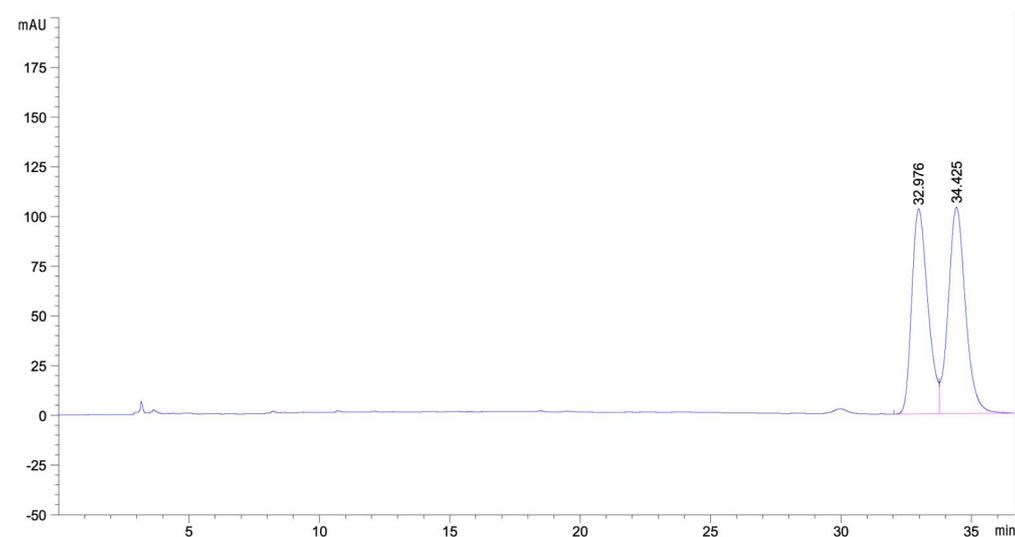
#	[min]	[min]	[mAU*s]	[mAU]	%
1	22.722 BV	0.5056	1.42242e4	432.61984	98.2035
2	24.718 VB	0.5858	260.21198	6.60178	1.7965

(S)-N-(1-([1,1'-biphenyl]-4-yl)ethyl)hydroxylamine (3d)

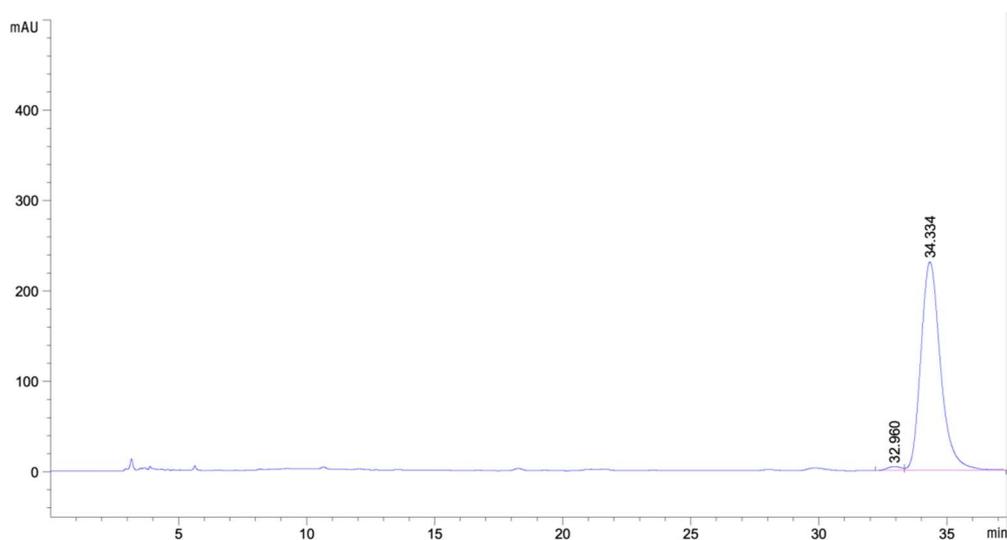


3d

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ (CH_2Cl_2 :MeOH = 10:1), 61.4 mg, 96% yield, 98% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.57 (dt, $J = 8.2, 1.8$ Hz, 4H), 7.47–7.38 (m, 5H), 4.17 (q, $J = 6.7$ Hz, 1H), 1.42 (d, $J = 6.6$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 32.9 min, t_R (major) = 34.3 min. The analytical data are in accordance with the literature³.

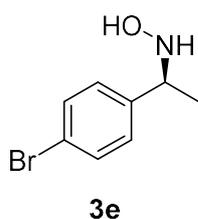


#	[min]	[min]	[min]	[mAU*s]	[mAU]	%
1	32.976	BV	0.6607	4421.46338	103.03030	48.0470
2	34.425	VBA	0.7009	4780.91357	103.88699	51.9530



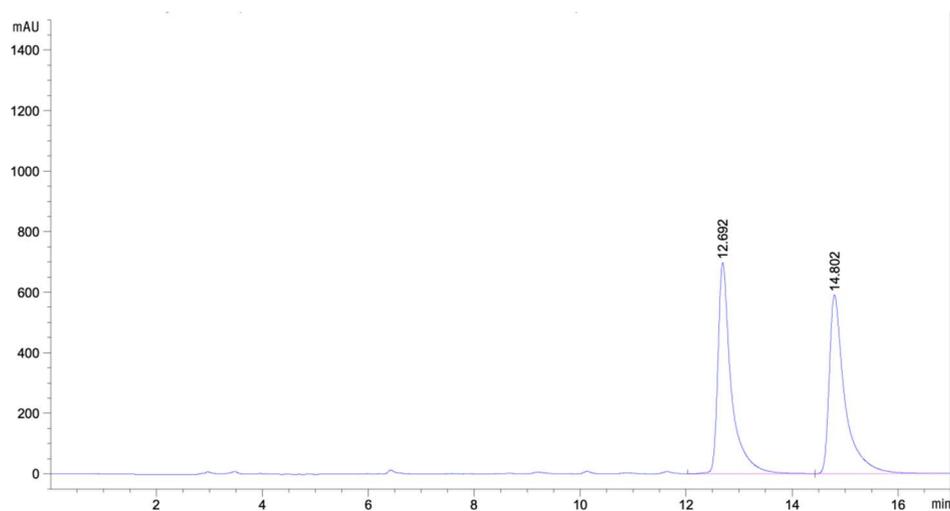
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1	32.960	BV	0.5792	155.33290	4.20279	1.2501
2	34.334	VB	0.8169	1.22703e4	230.55666	98.7499

(S)-N-(1-(4-bromophenyl)ethyl)hydroxylamine (3e)

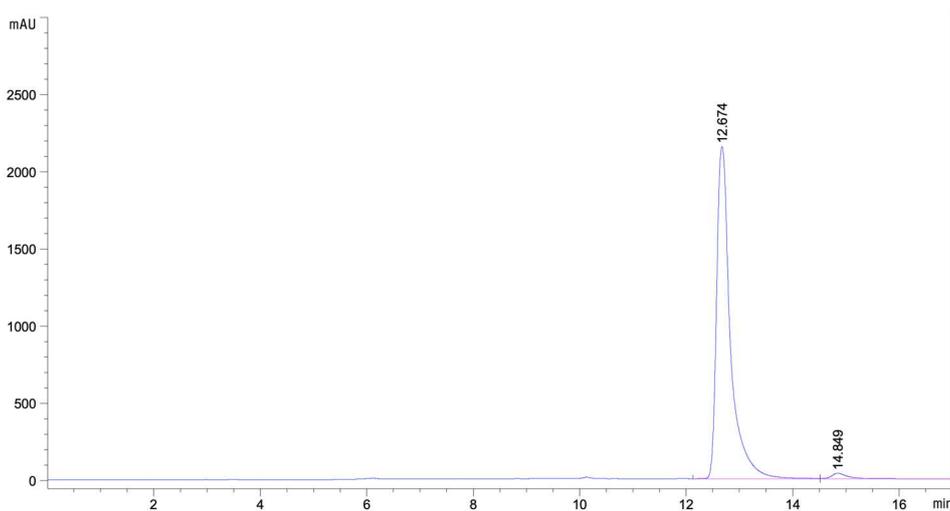


White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 62.2 mg, 96% yield, 97% *ee*. $^1\text{H NMR}$ (400 MHz, $\text{CHloroform-}d$) δ 7.51–7.43 (m, 2H), 7.27–7.18 (m, 2H), 4.08 (q, $J = 6.7$ Hz, 1H), 1.34 (s, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak IA-3, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 12.6 min, t_R (minor) = 14.8 min. The analytical data are in accordance with the

literature².

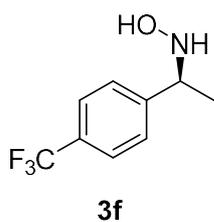


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	12.692	VB	0.2519	1.22068e4	698.43658	50.2885
2	14.802	BBA	0.2963	1.20668e4	590.88330	49.7115



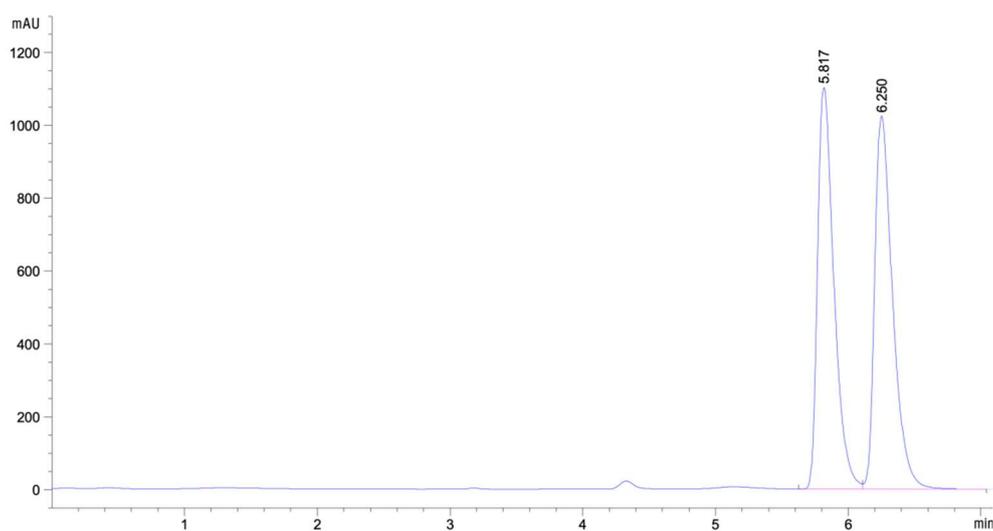
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1	12.674	VV	0.2690	3.88914e4	2150.11841	97.8443
2	14.849	VBA	0.3309	856.86780	36.90482	2.1557

(S)-N-(1-(4-(trifluoromethyl)phenyl)ethyl)hydroxylamine (3f)

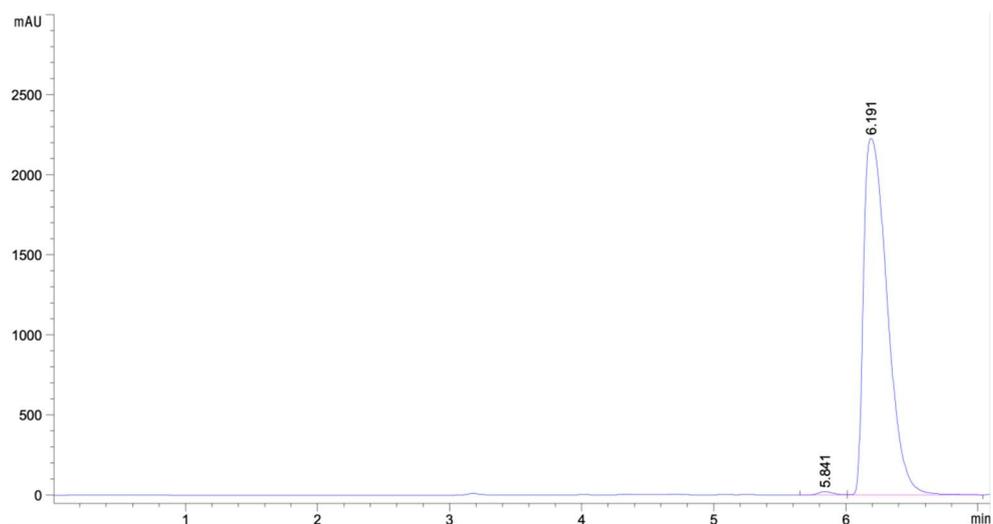


White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 59.7 mg, 97% yield, 99% *ee*. ¹H NMR (600 MHz, Chloroform-*d*) δ 7.68–7.54 (m, 2H), 7.54–7.39 (m, 2H), 4.19 (q, *J* = 6.2 Hz, 1H), 1.36 (d, *J* = 6.6 Hz, 3H). ¹⁹F NMR (600 MHz, Chloroform-*d*) δ -62.51. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 80/20; 1.0 mL/min; 220 nm): t_R (minor)

= 5.8 min, t_R (major) = 6.1 min. The analytical data are in accordance with the literature².

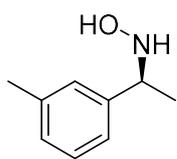


#	[min]	[min]	[mAU*s]	[mAU]	%
1	5.817 BV	0.1319	9438.65723	1102.09338	49.4200
2	6.250 WV	0.1441	9660.20801	1023.87280	50.5800



#	[min]	[min]	[mAU*s]	[mAU]	%
1	5.841 BV	0.1233	169.52158	20.75478	0.6089
2	6.191 WV	0.1971	2.76725e4	2224.63306	99.3911

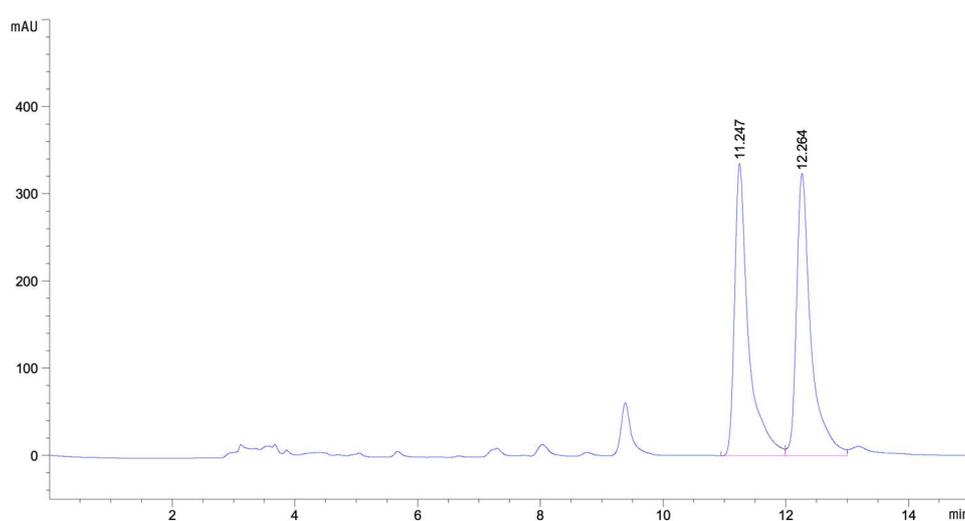
(S)-N-(1-(m-Tolyl)ethyl)hydroxylamine (3g)



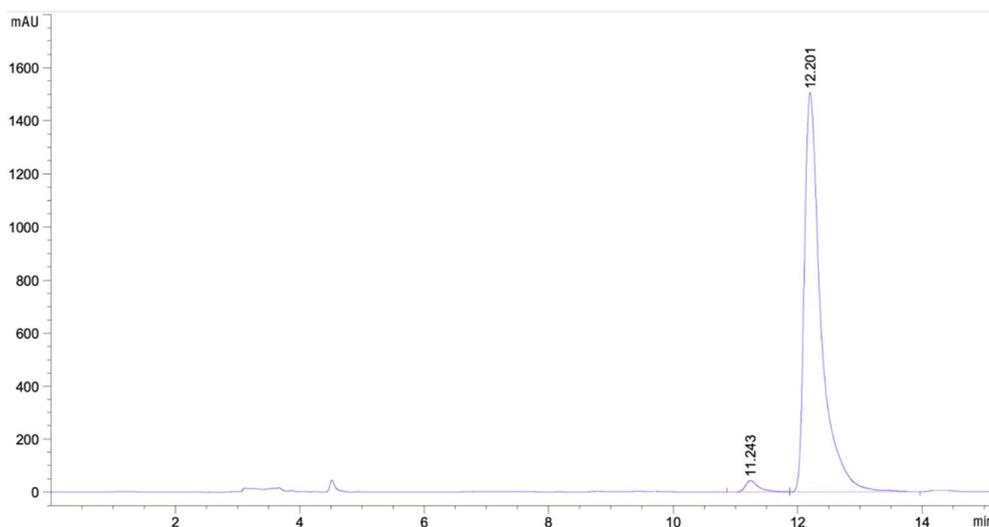
3g

with the literature².

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 40.8 mg, 90% yield, 97% *ee*. $^1\text{H NMR}$ (400 MHz, $\text{Chloroform-}d$) δ 7.29–7.23 (m, 1H), 7.17–7.10 (m, 3H), 4.11 (q, $J = 6.6$ Hz, 1H), 2.37 (s, 3H), 1.41 (d, $J = 6.6$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak IA-3, *n*-hexane/isopropanol = 80/20; 1.0 mL/min; 220 nm): t_R (minor) = 11.2 min, t_R (major) = 12.2 min. The analytical data are in accordance

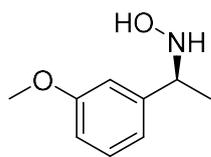


#	[min]	[min]	[mAU*s]	[mAU]	%
1	11.247 BV	0.2278	5281.85400	335.28027	49.9818
2	12.264 VV	0.2387	5285.69189	323.41650	50.0182



#	[min]	[min]	[mAU*s]	[mAU]	%
1	11.243 BV	0.2198	643.68665	42.72289	2.2543
2	12.201 VV	0.2745	2.79102e4	1504.22693	97.7457

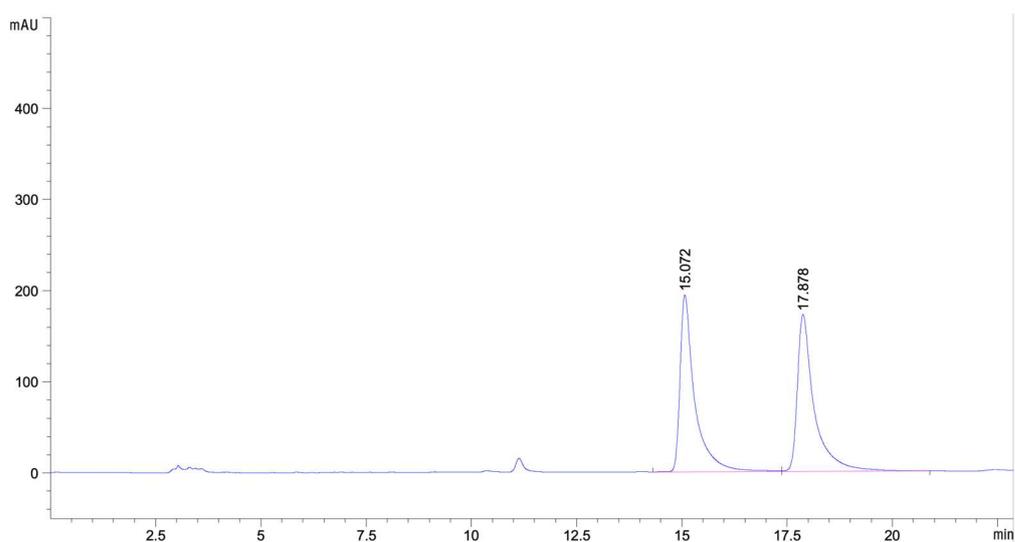
(S)-N-(1-(3-methoxyphenyl)ethyl)hydroxylamine (3h)



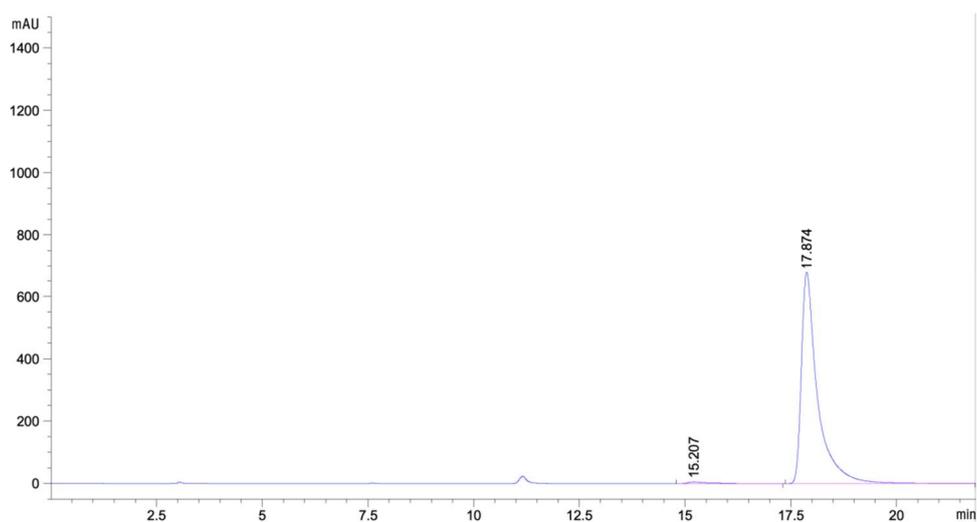
White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 48.2 mg, 96% yield, 98% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform- d) δ 7.27 (t, $J = 7.9$ Hz, 1H), 6.95–6.87 (m, 2H), 6.84 (dd, $J = 8.3, 2.6$ Hz, 1H), 4.09 (q, $J = 6.6$ Hz, 1H), 3.82 (s, 3H), 1.41 (d, $J = 6.6$ Hz, 3H).

3h

Enantiomeric excess was determined by chiral HPLC (Chiralpak IA-3, n-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 15.2 min, t_R (major) = 17.8 min. The analytical data are in accordance with the literature².

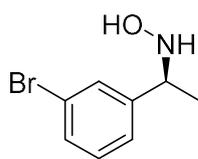


#	[min]	[min]	[mAU*s]	[mAU]	%
1	15.072 W	0.3457	4725.97852	194.35704	49.6051
2	17.878 VB	0.3987	4801.22559	172.52159	50.3949



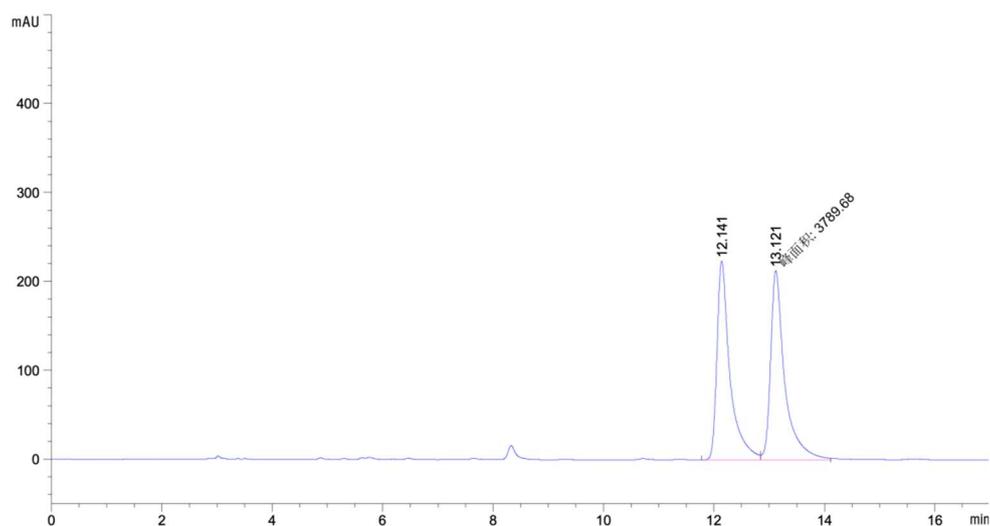
#	[min]	[min]	[mAU*s]	[mAU]	%
1	15.207 VB	0.4812	201.15262	5.70751	1.1071
2	17.874 BBA	0.3791	1.79679e4	678.09546	98.8929

(S)-N-(1-(3-bromophenyl)ethyl)hydroxylamine (3i)

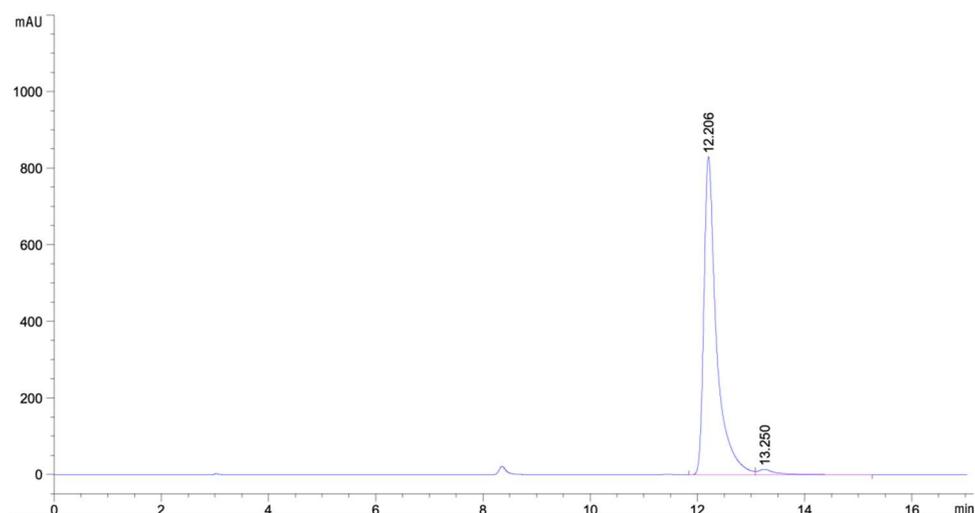


3h

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 61.6mg, 95% yield, 95% *ee*.
¹H NMR (400 MHz, Chloroform-*d*) δ 7.47 (t, *J* = 1.8 Hz, 1H), 7.39 (dt, *J* = 7.3, 1.9 Hz, 1H), 7.24–7.16 (m, 2H), 4.01 (q, *J* = 6.7 Hz, 1H), 1.31 (d, *J* = 6.7 Hz, 3H).
Enantiomeric excess was determined by chiral HPLC (Chiralpak IA-3, *n*-hexane/isopropanol = 80/20; 1.0 mL/min; 220 nm): t_R (major) = 12.2 min, t_R (minor) = 13.2 min. The analytical data are in accordance with the literature².

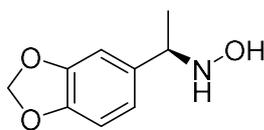


#	[min]	[min]	[mAU*s]	[mAU]	%
1	12.141	BV	0.2369 3660.73511	223.66646	49.1346
2	13.121	MF	0.2965 3789.68384	212.99869	50.8654



#	[min]	[min]	[mAU*s]	[mAU]	%
1	12.206	BV	0.2365 1.35538e4	830.10254	97.5815
2	13.250	VB	0.3277 335.92831	14.11292	2.4185

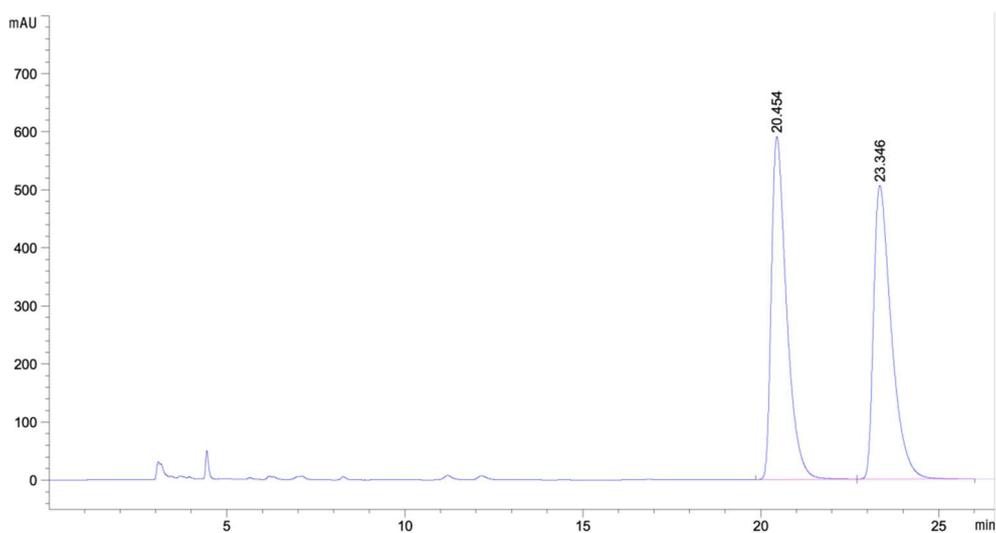
(S)-N-(1-(benzo[1,3]dioxol-5-yl)ethyl)hydroxylamine (3j)



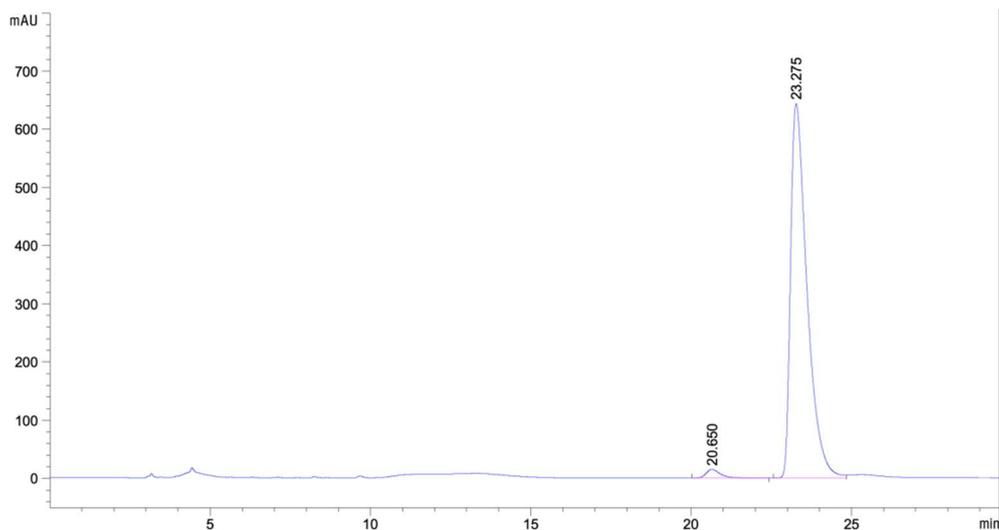
3j

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 52.2 mg, 96% yield, 96% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 6.82 (s, 1H) 6.79–6.74 (m, 2H), 5.95–5.90 (m, 2H), 4.02 (q, J = 6.6 Hz, 1H), 1.35 (d, J = 6.7 Hz, 3H).

Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 20.6 min, t_R (major) = 23.2 min. The analytical data are in accordance with the literature².

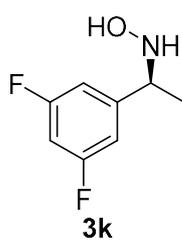


#	[min]	[min]	[mAU*s]	[mAU]	%
1	20.454 VB	0.4485	1.75381e4	590.52844	50.0352
2	23.346 BB	0.5244	1.75135e4	505.22034	49.9648

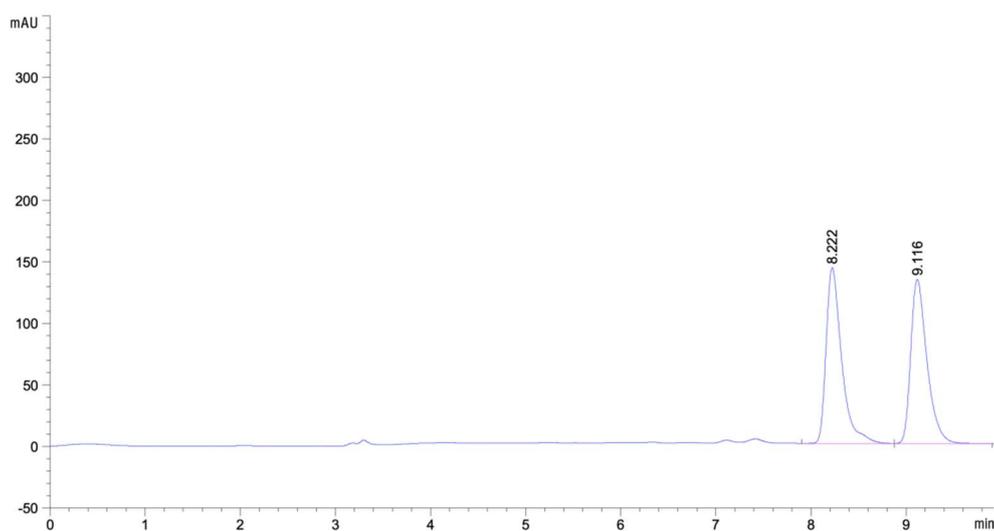


#	[min]	[min]	[mAU*s]	[mAU]	%
1	20.650 BB	0.4447	427.81024	14.56332	1.8397
2	23.275 BV	0.5341	2.28260e4	643.07507	98.1603

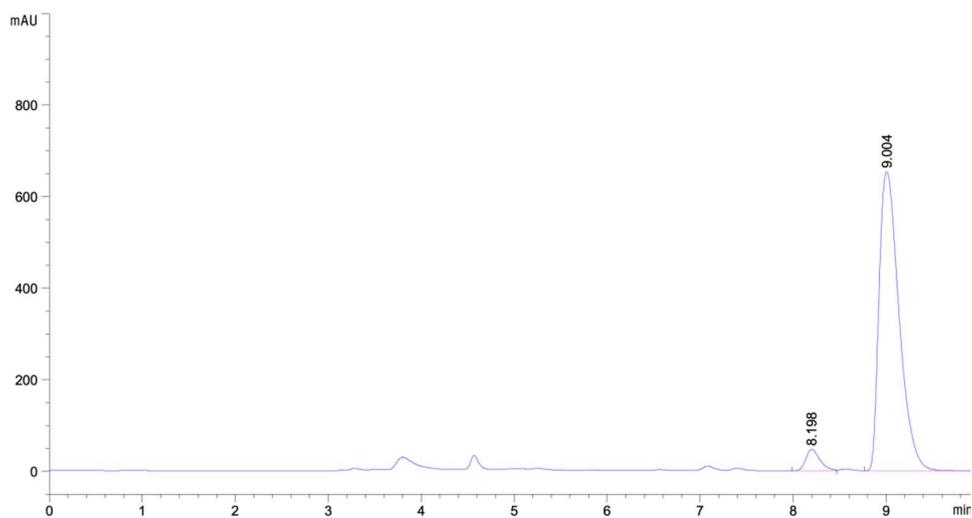
(S)-N-(1-(3,5-Difluorophenyl)ethyl)hydroxylamine (3k)



White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 47.8 mg, 92% yield, 90% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 6.93–6.82 (m, 2H), 6.71 (tt, J = 8.9, 2.4 Hz, 1H), 4.09 (q, J = 6.7 Hz, 1H), 1.32 (d, J = 6.7 Hz, 3H). ¹⁹F NMR (600 MHz, Chloroform-*d*) δ -109.67. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-Hexane/*i*-PrOH = 95/5; 1.0 mL/min; 220 nm): t_R (minor) = 8.2 min, t_R (major) = 9.0 min. The analytical data are in accordance with the literature².

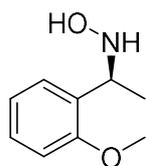


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.222 BB	0.1706	1622.08228	142.73537	50.6478
2	9.116 BBA	0.1803	1580.58899	133.35802	49.3522



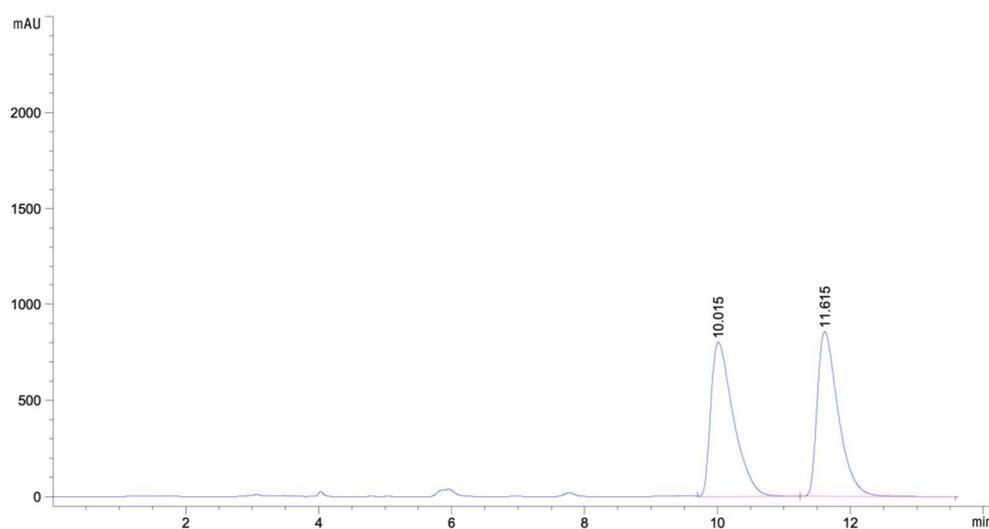
#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.198 BV	0.1595	495.42343	46.80427	4.8485
2	9.004 BBA	0.2315	9722.60156	653.85236	95.1515

(S)-N-(1-(2-methoxyphenyl)ethyl)hydroxylamine (3l)

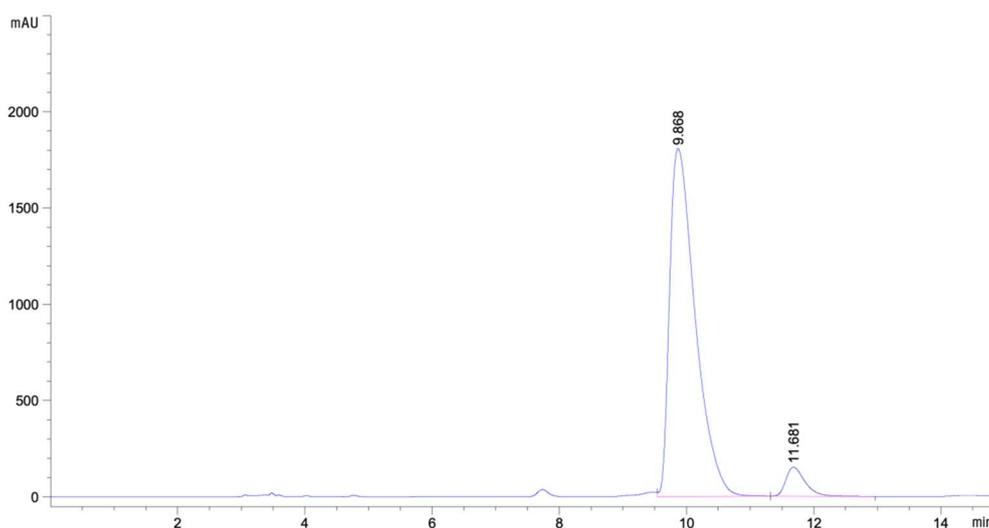


Colorless oil, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ (CH_2Cl_2 :MeOH = 10:1), 37.6 mg, 75% yield, 88% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.33–7.20 (m, 2H), 6.98–6.84 (m, 2H), 4.46 (q, $J = 6.8$ Hz, 1H), 3.83 (s, 3H), 1.43 (d, $J = 6.8$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC

3l (Chiralpak AS-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 9.8 min, t_R (minor) = 11.6 min. The analytical data are in accordance with the literature².

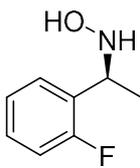


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	10.015	VB	0.3553	1.89085e4	801.28339	50.1998
2	11.615	BBA	0.3338	1.87580e4	855.52765	49.8002

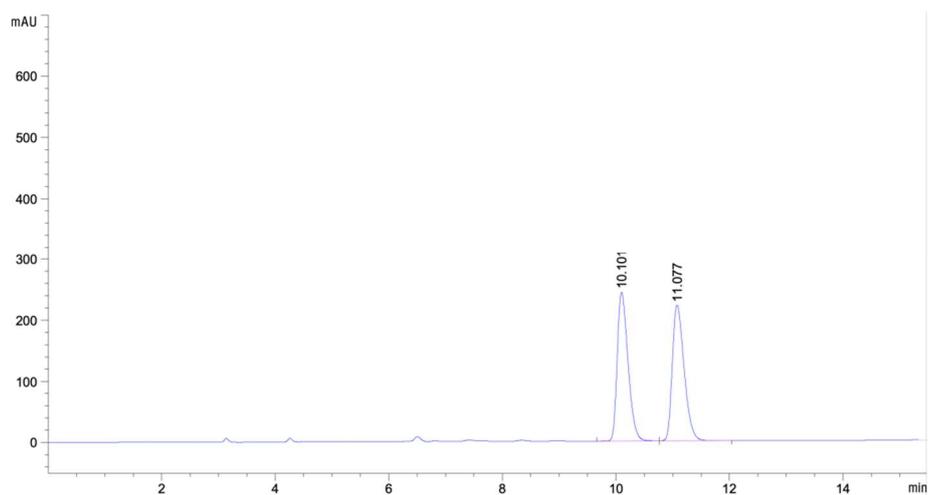


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	9.868	VB	0.4228	5.02848e4	1806.06152	94.1482
2	11.681	BB	0.3165	3125.47925	150.38127	5.8518

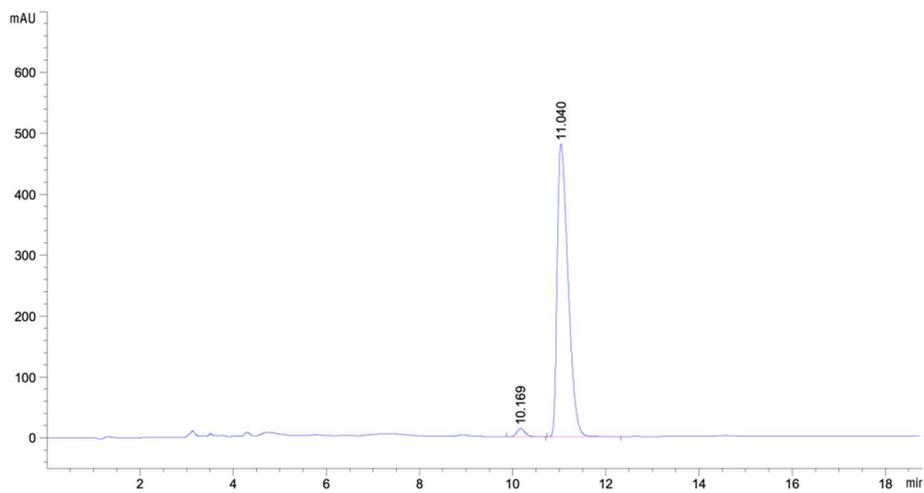
(S)-N-(1-(2-fluorophenyl)ethyl)hydroxylamine (3m)



Colorless oil, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 19.6 mg, 42% yield, 96% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.33 (td, $J = 7.5, 1.8$ Hz, 1H), 7.22 (tdd, $J = 7.5, 5.3, 1.8$ Hz, 1H), 7.10 (td, $J = 7.5, 1.3$ Hz, 1H), 7.02 (ddd, $J = 10.7, 8.2, 1.2$ Hz, 1H), 4.42 (q, $J = 6.7$ Hz, 1H), 1.38 (d, $J = 6.8$ Hz, 3H). $^{19}\text{F NMR}$ (600 MHz, Chloroform-*d*) δ -119.19. Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 95/5; 1.0 mL/min, 220 nm): t_R (minor) = 10.1 min, t_R (major) = 11.0 min. The analytical data are in accordance with the literature².

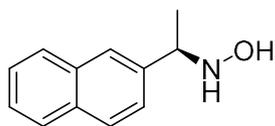


#	[min]	[min]	[mAU*s]	[mAU]	%
1	10.101 BB	0.2029	3187.30078	243.18936	49.8270
2	11.077 BV	0.2248	3209.43066	221.80412	50.1730



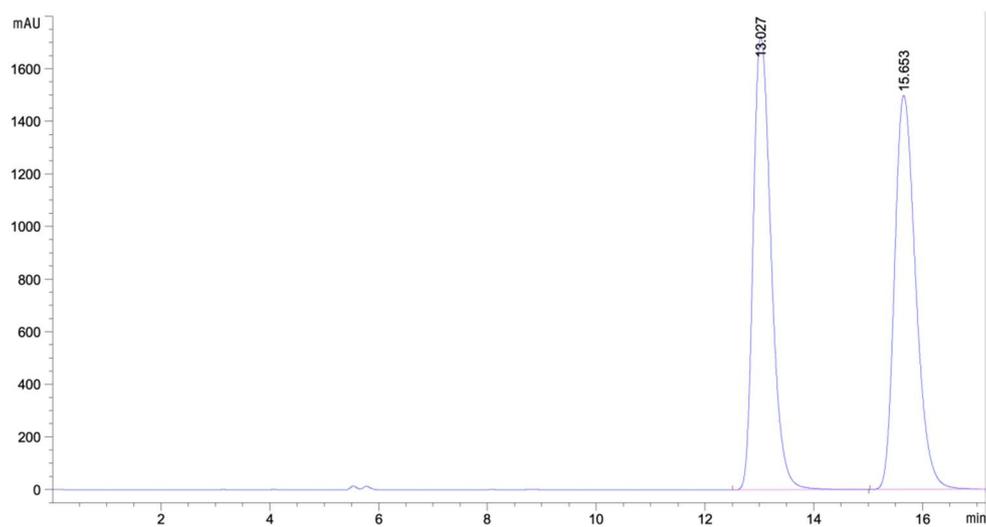
#	[min]	[min]	[mAU*s]	[mAU]	%
1	10.169 BB	0.1905	165.90979	13.39186	2.0902
2	11.040 BB	0.2527	7771.71631	480.45847	97.9098

(S)-N-(1-(naphthalen-2-yl)ethyl)hydroxylamine (3n)

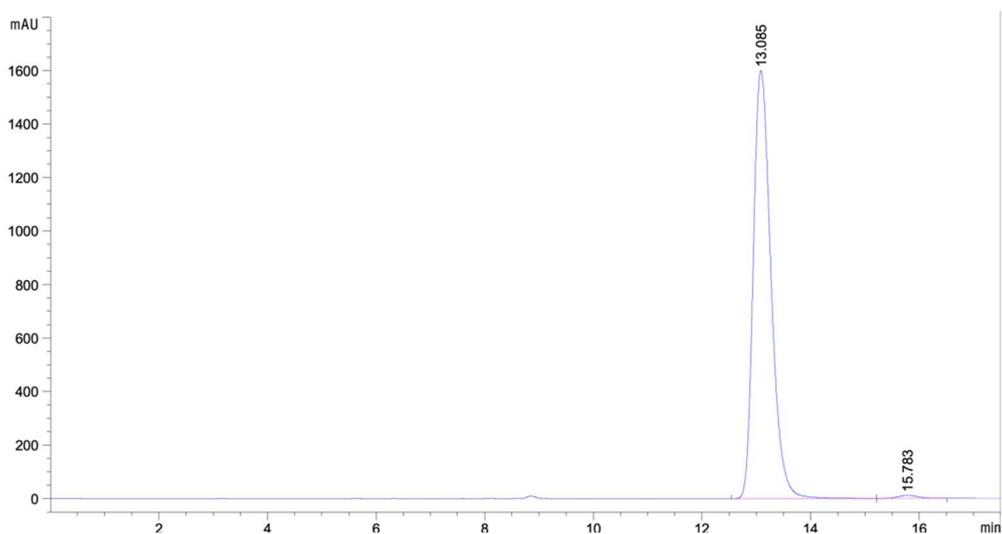


3n

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 53.3 mg, 95% yield, 99% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.78 (dd, *J* = 8.3, 4.9 Hz, 3H), 7.72 (s, 1H), 7.49–7.37 (m, 3H), 4.23 (q, *J* = 6.7 Hz, 1H), 1.44 (d, *J* = 6.6 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AS-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 13.0 min, t_R (minor) = 15.7 min. The analytical data are in accordance with the literature².

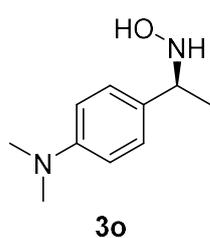


#	[min]	[min]	[mAU*s]	[mAU]	%
1	13.027 BB	0.3549	3.94315e4	1723.55542	49.4035
2	15.653 BBA	0.4185	4.03836e4	1497.91406	50.5965

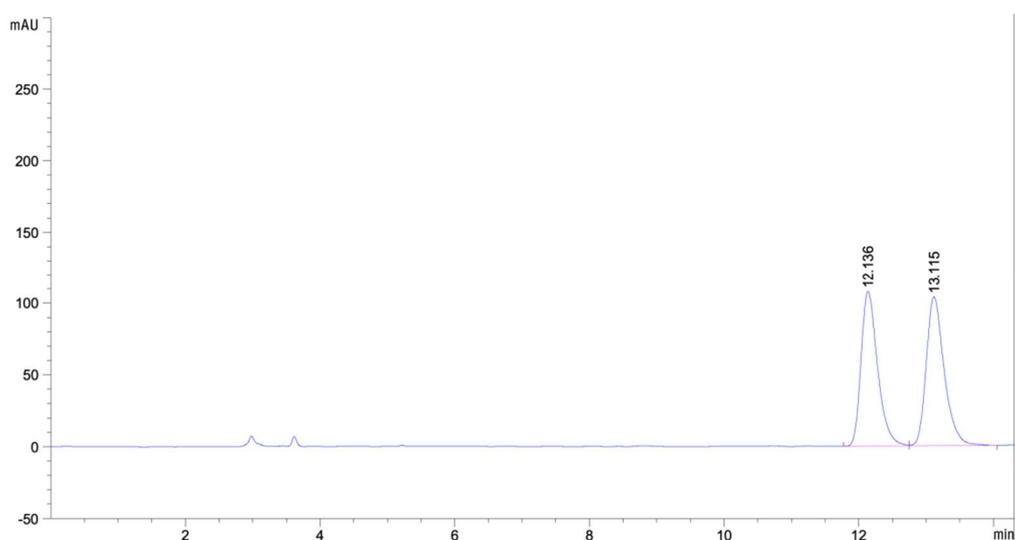


#	[min]	[min]	[mAU*s]	[mAU]	%
1	13.085 BV	0.3517	3.61628e4	1599.94641	99.2394
2	15.783 VB	0.3961	277.16754	10.77641	0.7606

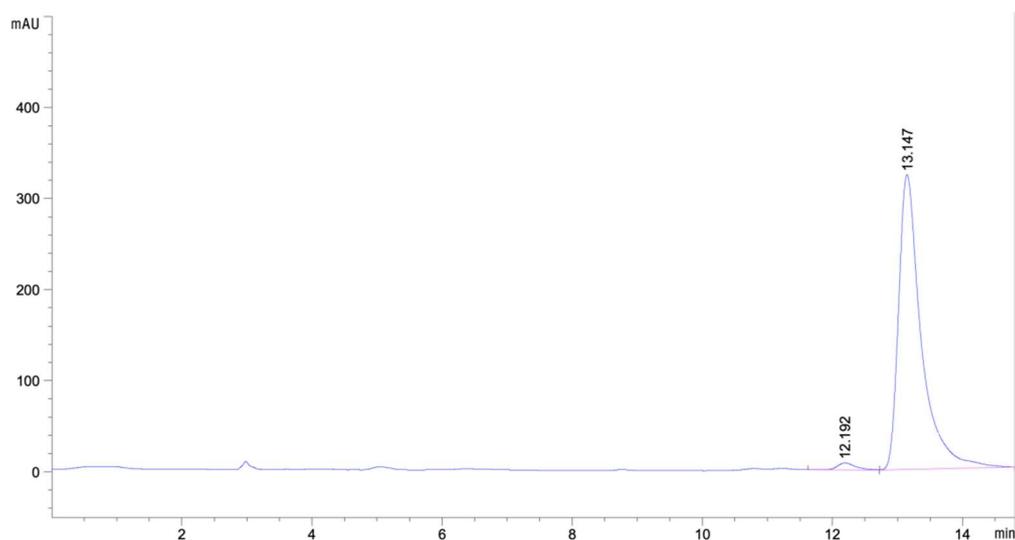
(S)-4-(1-(hydroxyamino)ethyl)-N,N-dimethylaniline (3o)



White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ (CH_2Cl_2 :MeOH = 10:1), 51.9 mg, 96% yield, 96% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.24 – 7.15 (m, 2H), 6.75 – 6.65 (m, 2H), 4.03 (q, $J = 6.6$ Hz, 1H), 2.93 (s, 6H), 1.40 (d, $J = 6.6$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 12.1 min, t_R (major) = 13.1 min. The analytical data are in accordance with the literature³.

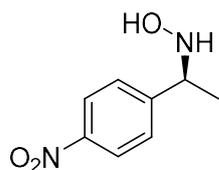


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	12.136	BV	0.2613	1841.94409	107.82986	48.8166
2	13.115	VB	0.2811	1931.24536	103.78660	51.1834



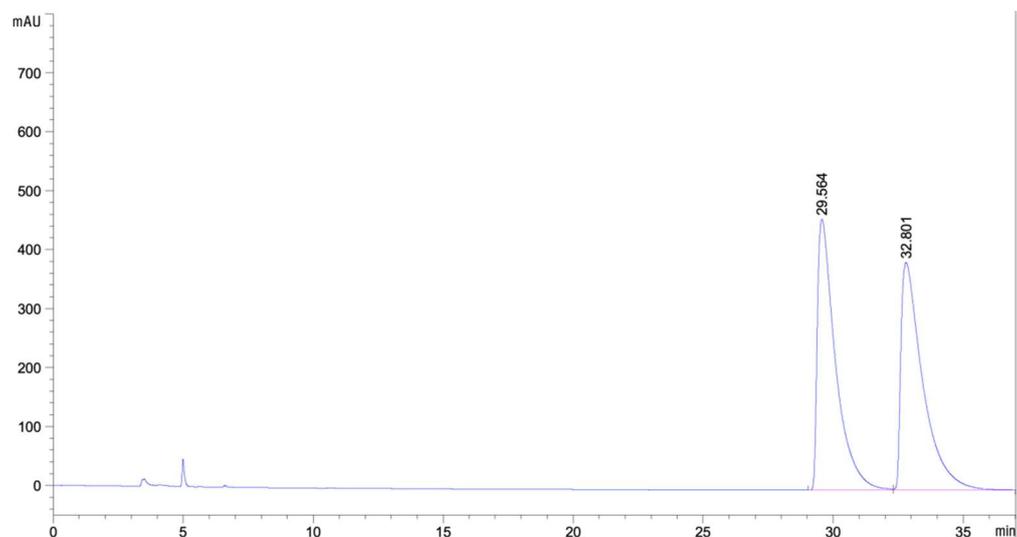
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	12.192	BB	0.2874	146.49655	7.64972	1.8346
2	13.147	BBA	0.3567	7838.55664	323.46164	98.1654

(S)-N-(1-(4-nitrophenyl)ethyl)hydroxylamine (3p)

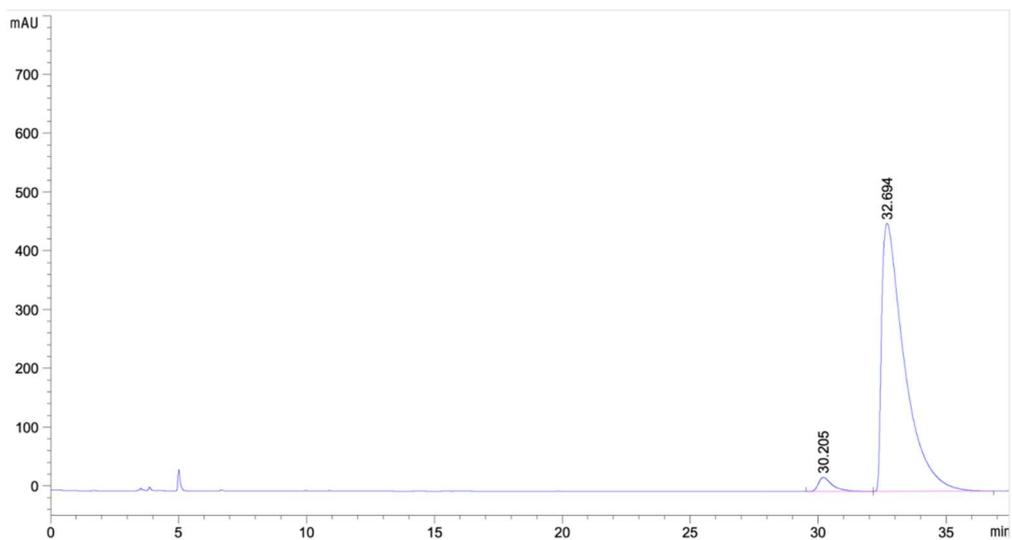


3p

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 53.6 mg, 98% yield, 94% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform- d) δ 8.24–8.16 (m, 2H), 7.55–7.47 (m, 2H), 4.24 (q, $J = 6.7$ Hz, 1H), 1.36 (d, $J = 6.8$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-3, n-Hexane/*i*-PrOH = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 30.2 min, t_R (minor) = 32.7 min. The analytical data are in accordance with the literature².

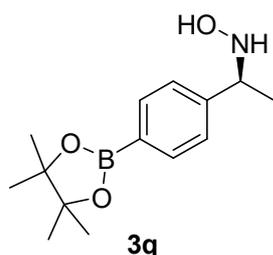


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	29.564	BV	0.7069	2.22630e4	459.76089	49.7981
2	32.801	VBA	0.8404	2.24436e4	385.98511	50.2019



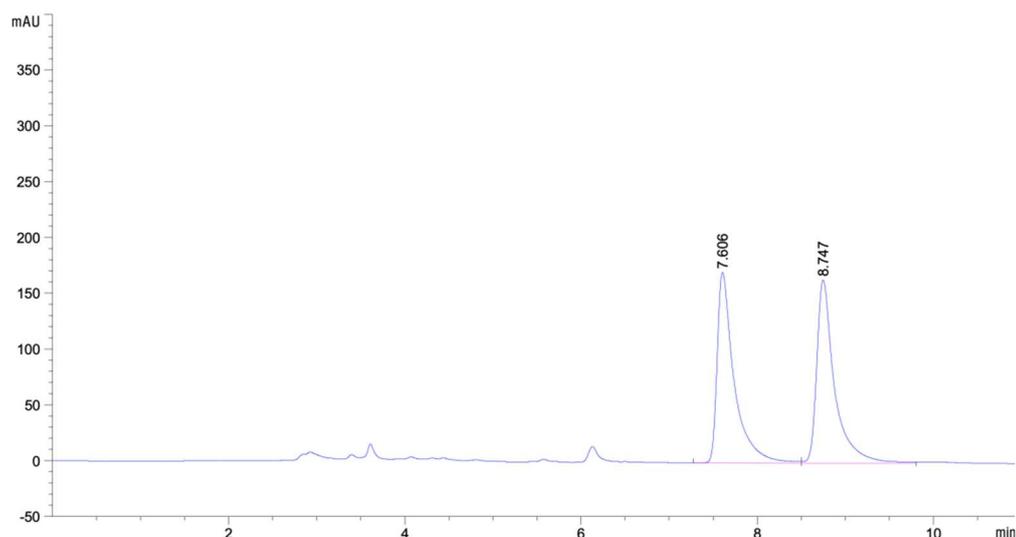
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	30.205	BB	0.5658	921.42584	24.00825	3.1732
2	32.694	BB	0.8976	2.81160e4	455.86551	96.8268

(S)-N-(1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)ethyl)hydroxylamine (3q)

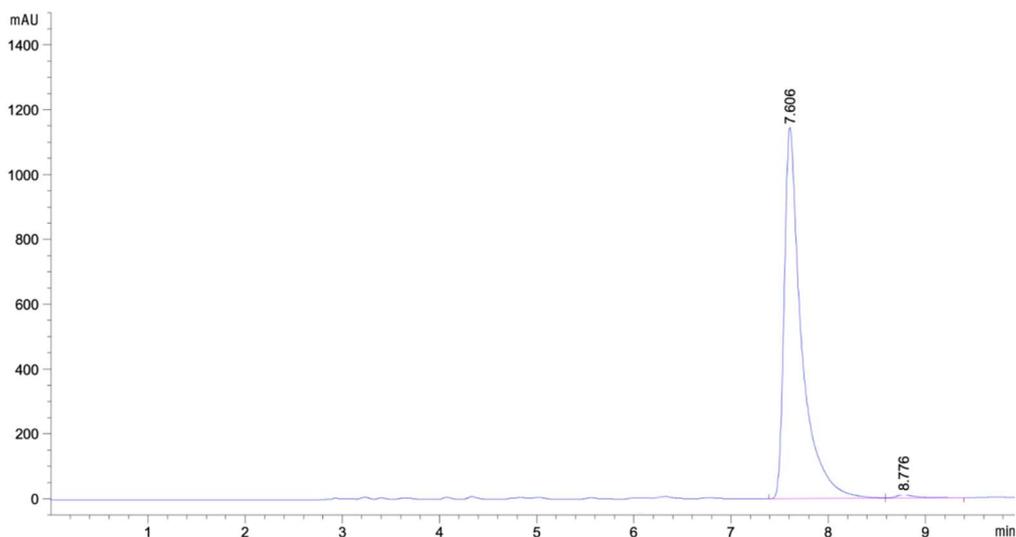


White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 77.4 mg, 98% yield, 98% *ee*. $^1\text{H NMR}$ (400 MHz, CHCl_3-d) δ 7.83–7.76 (m, 1H), 7.39–7.23 (m, 3H), 4.13 (qd, $J = 6.7, 4.9$ Hz, 1H), 1.34 (s, 3H), 1.16 (s, 12H). Enantiomeric excess was determined by chiral HPLC (Chiralpak IA-3, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 7.6 min, t_R

(minor) = 8.7 min. The analytical data are in accordance with the literature³.

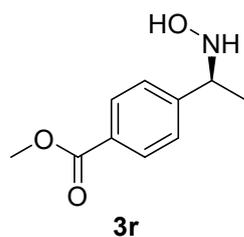


#	[min]	[min]	[mAU*s]	[mAU]	%
1	7.606 BV	0.1925	2290.65283	170.74698	49.7975
2	8.747 VW	0.2022	2309.28638	164.12569	50.2025



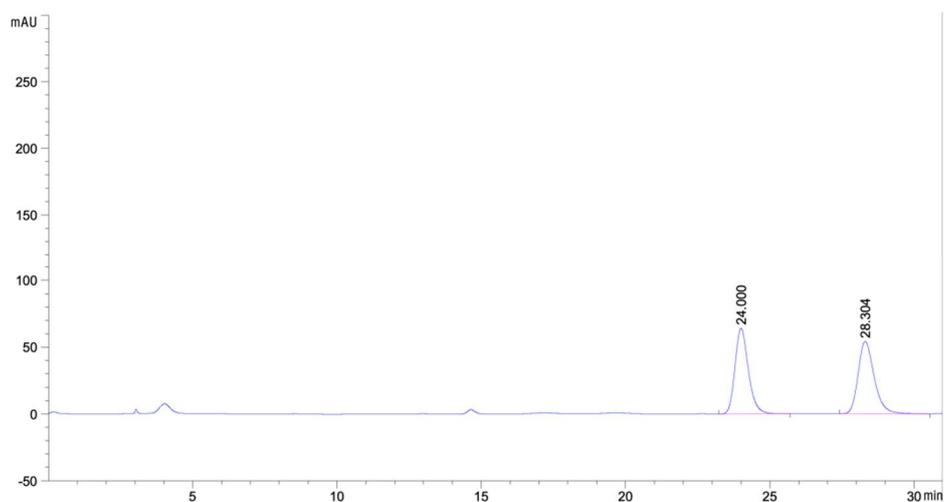
#	[min]	[min]	[mAU*s]	[mAU]	%
1	7.606 BV	0.1768	1.42037e4	1144.63977	98.8394
2	8.776 VB	0.2281	166.77763	10.45711	1.1606

(S)-4-(1-(hydroxyamino)ethyl)benzoate (3r)

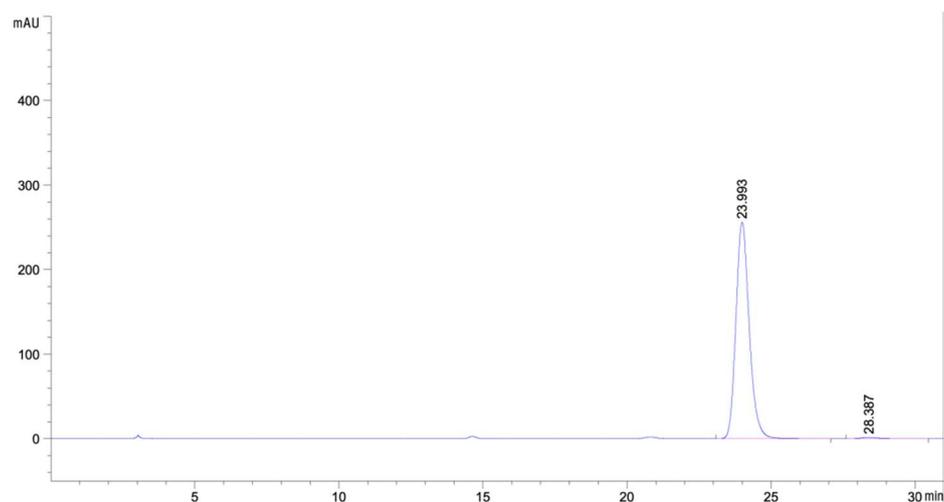


White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 56.2 mg, 96% yield, 98% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, J = 7.9 Hz, 2H), 7.38 (dd, J = 8.2, 1.7 Hz, 2H), 4.16 (q, J = 6.7 Hz, 1H), 3.90 (s, 3H), 1.37 (d, J = 6.7 Hz, 3H). ¹³C NMR (400 MHz, Chloroform-*d*) δ 166.92, 147.69, 129.88, 129.40, 127.15, 61.55, 52.14, 19.39. Enantiomeric excess was determined by chiral

HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 24.0 min, t_R (minor) = 28.3 min.

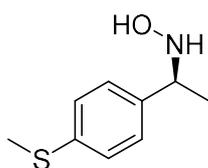


#	[min]	[min]	[mAU*s]	[mAU]	%
1	24.000	BB	0.4939 2069.90063	64.23728	49.6135
2	28.304	VB	0.5903 2102.15210	54.21752	50.3865



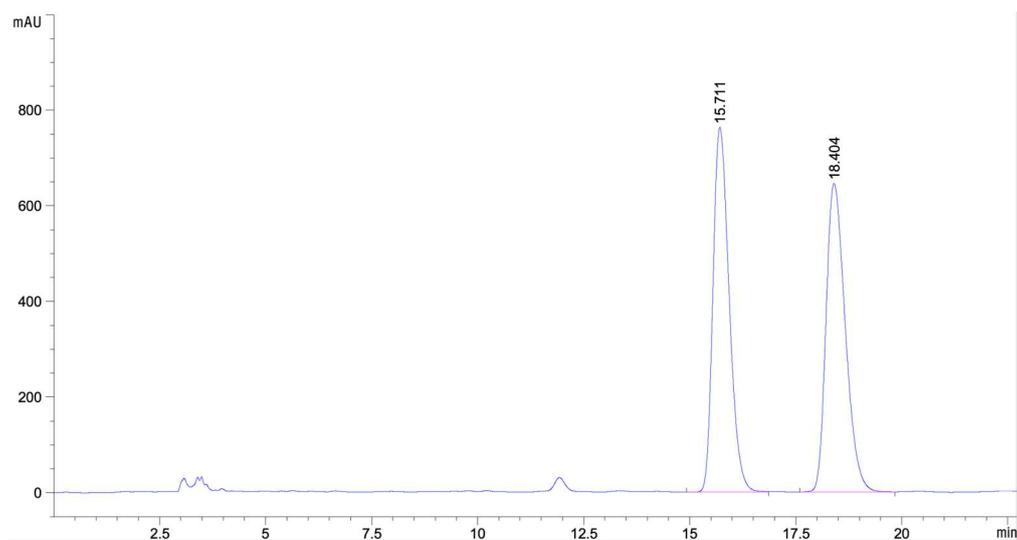
#	[min]	[min]	[mAU*s]	[mAU]	%
1	23.993	BB	0.4934 8244.56152	256.25293	99.1964
2	28.387	BB	0.6260 66.78609	1.58366	0.8036

(S)-N-(1-(4-(methylthio)phenyl)ethyl)hydroxylamine (3s)

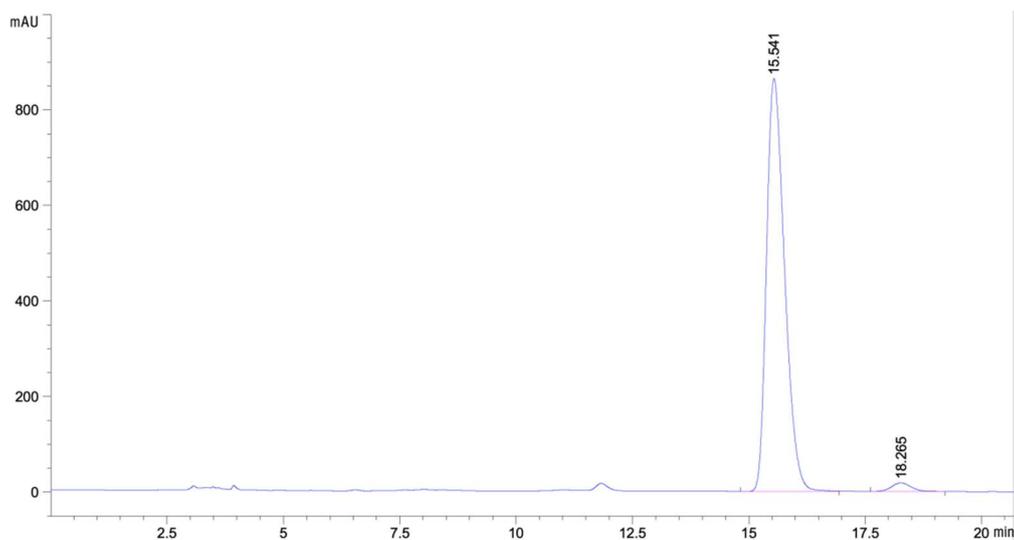


3s

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH_2Cl_2 :MeOH = 10:1), 53.8 mg, 98% yield, 95% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.22 (s, 4H), 4.05 (qd, J = 6.6, 1.5 Hz, 1H), 2.46 (s, 3H), 1.36 (d, J = 6.6 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AS-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 15.5 min, t_R (minor) = 18.2 min. The analytical data are in accordance with the literature⁴.

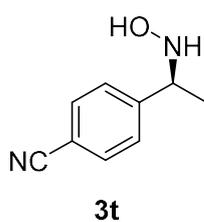


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	15.711	BV	0.4134	2.02405e4	763.16504	49.8196
2	18.404	BV	0.4924	2.03870e4	645.68481	50.1804



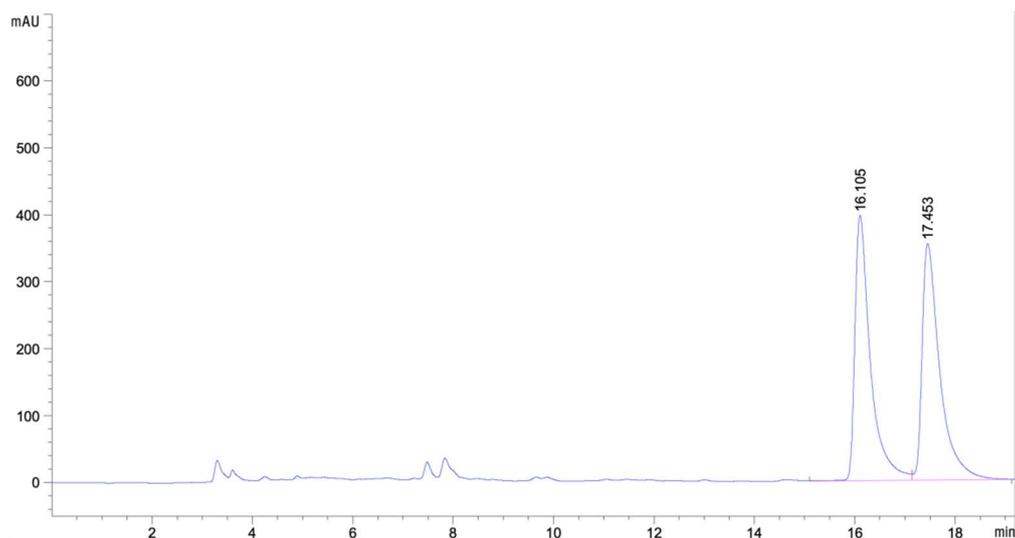
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	15.541	BV	0.4194	2.33675e4	864.40759	97.6547
2	18.265	BB	0.4634	561.19666	18.42245	2.3453

(S)-4-(1-(hydroxyamino)ethyl)benzonitrile (3t)

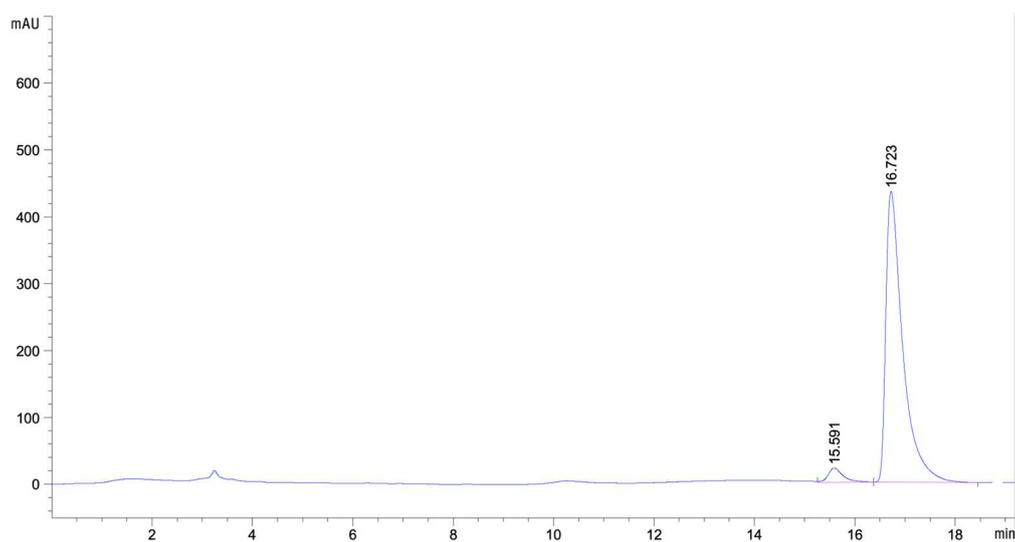


White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH_2Cl_2 :MeOH = 10:1), 47.6 mg, 98% yield, 92% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.77–7.53 (m, 4H), 4.13 (q, J = 6.6 Hz, 1H), 1.30 (d, J = 6.7 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-3, *n*-hexane/isopropanol = 80/20; 1.0 mL/min; 220 nm): t_R (minor)

= 15.5 min, t_R (major) = 16.7 min. The analytical data are in accordance with the literature⁴.

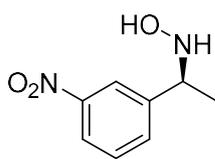


#	[min]	[min]	[mAU*s]	[mAU]	%
1	16.105	W	0.3179 8554.02832	396.18588	49.7120
2	17.453	VB	0.3618 8653.13281	353.26364	50.2880



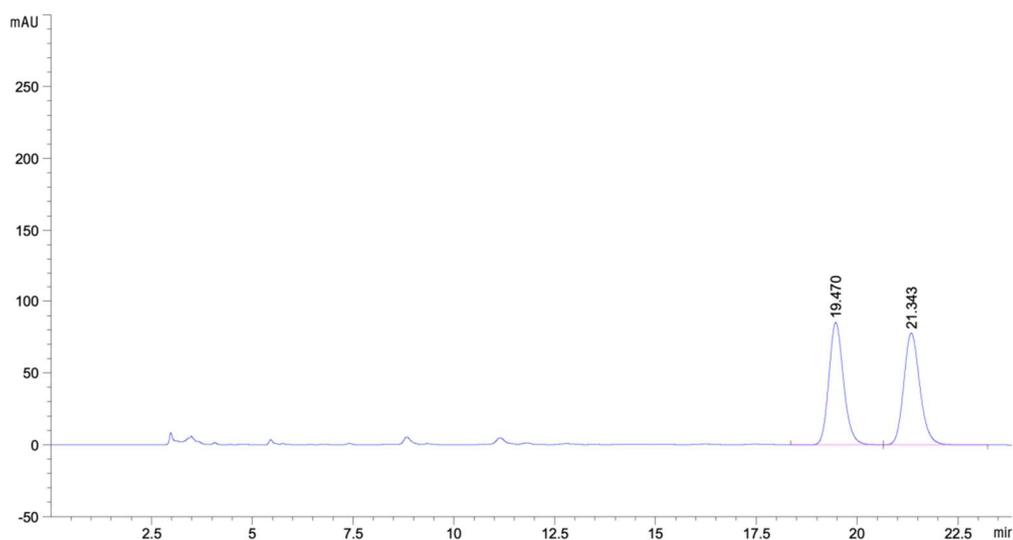
#	[min]	[min]	[mAU*s]	[mAU]	%
1	15.591	VB	0.3013 431.83768	21.23057	4.0544
2	16.723	BB	0.3483 1.02192e4	434.60959	95.9456

(S)-N-(1-(3-nitrophenyl)ethyl)hydroxylamine (3u)

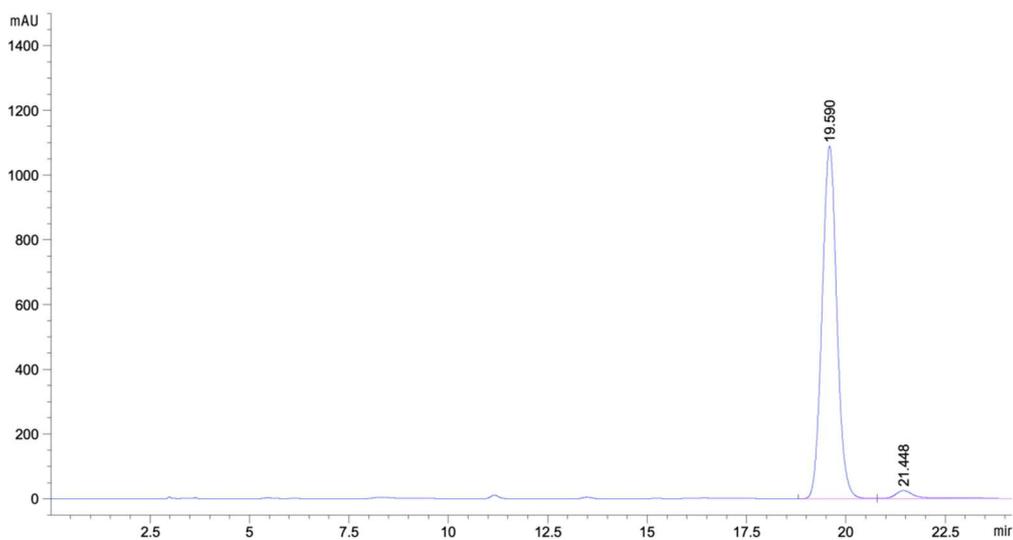


3u

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 50.3 mg, 92% yield, 94% *ee*.
¹H NMR (400 MHz, Chloroform-*d*) δ 8.23 (t, J = 2.1 Hz, 1H), 8.12 (ddt, J = 8.1, 2.1, 0.9 Hz, 1H), 7.66 (dt, J = 7.6, 1.4 Hz, 1H), 7.51 (t, J = 7.9 Hz, 1H), 4.23 (q, J = 6.7 Hz, 1H), 1.38 (d, J = 6.8 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 19.5 min, t_R (major) = 21.4 min. The analytical data are in accordance with the literature⁴.

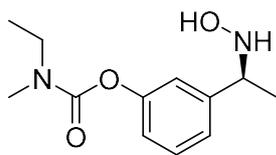


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	19.470	BB	0.3885	2151.48633	85.22868	49.9242
2	21.343	BB	0.4251	2158.01782	77.92476	50.0758



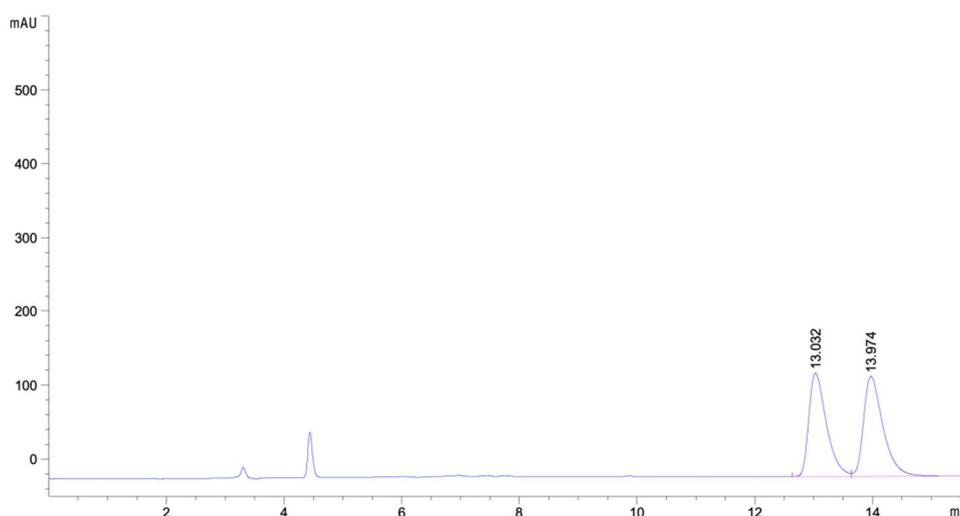
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	19.590	BV	0.3980	2.80101e4	1089.45166	96.9594
2	21.447	MF	0.5966	878.38928	24.53870	3.0406

(S)-3-(1-(hydroxyamino)ethyl)phenyl ethyl(methyl)carbamate (3v)

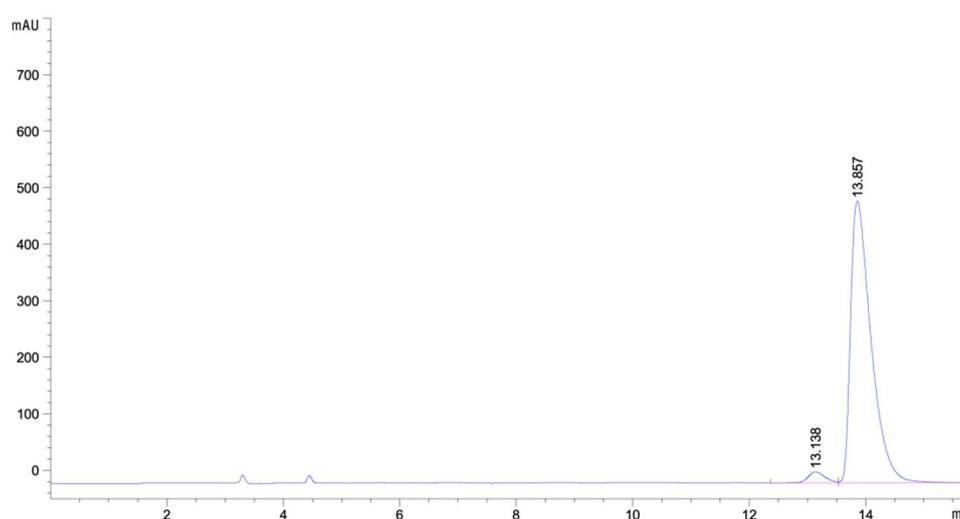


3v

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH_2Cl_2 :MeOH = 10:1), 69.2 mg, 95% yield, 94% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.27 (t, J = 7.9 Hz, 1H), 7.12 (d, J = 7.4 Hz, 2H), 7.00 (dt, J = 7.2, 3.0 Hz, 1H), 4.03 (q, J = 7.1 Hz, 1H), 3.40 (dq, J = 24.7, 7.1 Hz, 2H), 2.99 (d, J = 30.6 Hz, 3H), 1.33–1.12 (m, 6H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 13.1 min, t_R (major) = 13.8 min. The analytical data are in accordance with the literature³.

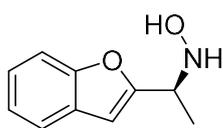


#	[min]	[min]	[mAU*s]	[mAU]	%
1	13.032 BV	0.3161	2890.63745	139.27625	48.2495
2	13.974 VB	0.3483	3100.37817	134.81433	51.7505



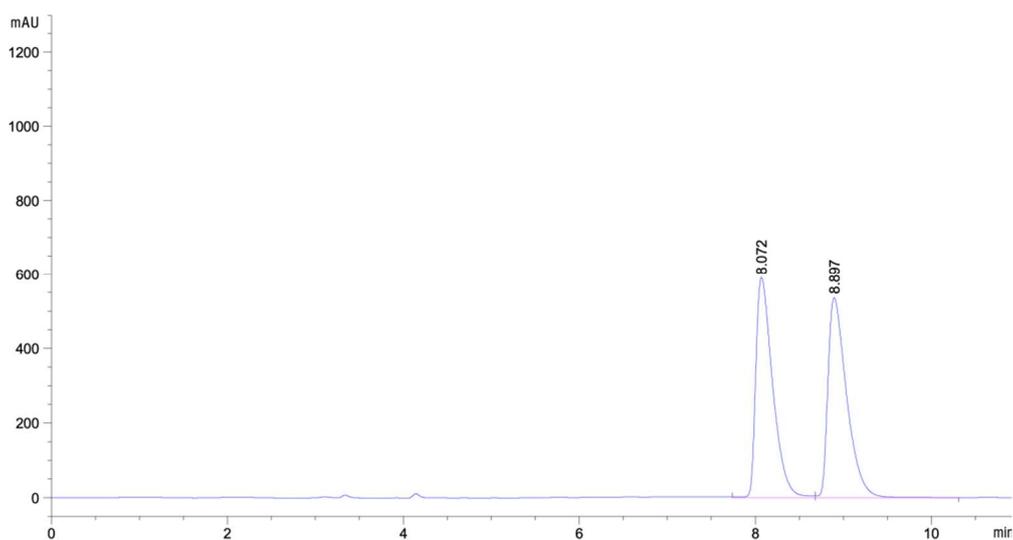
#	[min]	[min]	[mAU*s]	[mAU]	%
1	13.138 BV	0.3117	400.00958	19.47212	3.1824
2	13.857 VBA	0.3685	1.21694e4	498.99323	96.8176

(S)-N-(1-(benzofuran-2-yl)ethyl)hydroxylamine (3w)

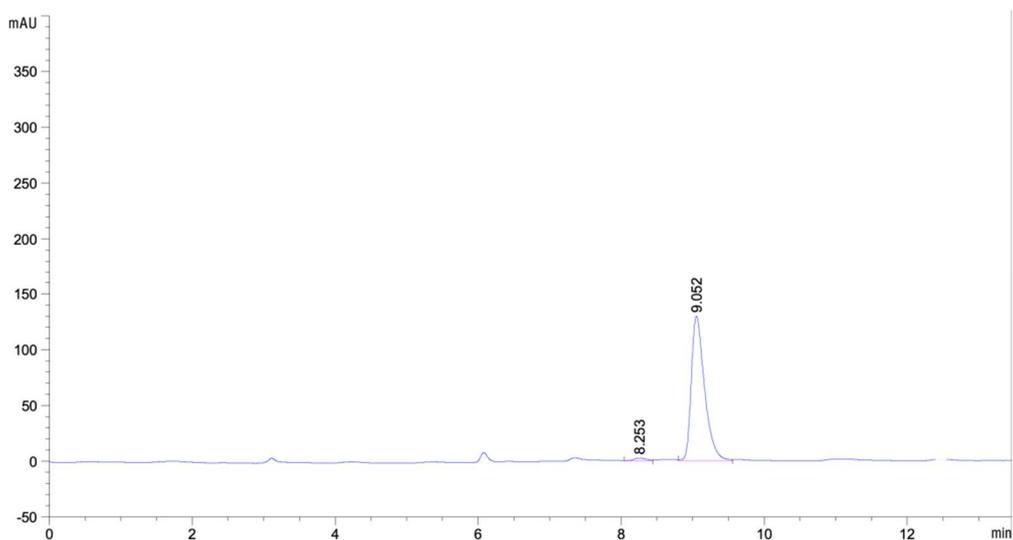


3w

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 51.5 mg, 97% yield, 97% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.52–7.45 (m, 2H), 7.32–7.13 (m, 2H), 6.56 (s, 1H), 4.23 (q, *J* = 6.8 Hz, 1H), 1.46 (d, *J* = 6.8 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak IA-3, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 8.2 min, t_R (major) = 9.0 min. The analytical data are in accordance with the literature³.

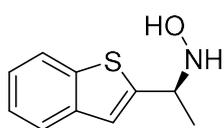


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.072 W	0.2012	7848.08691	589.99786	49.8102
2	8.897 VB	0.2263	7907.90186	535.56482	50.1898



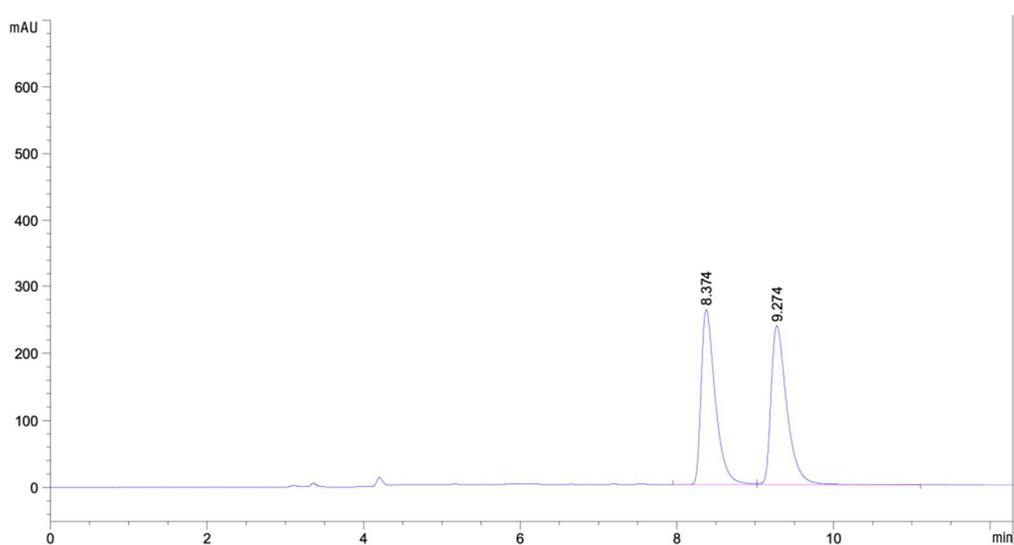
#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.253 BV	0.1690	26.13568	2.32773	1.5417
2	9.052 W	0.1943	1669.13672	129.54652	98.4583

(S)-N-(1-(benzothiophen-2-yl)-ethyl)hydroxylamine (3x)

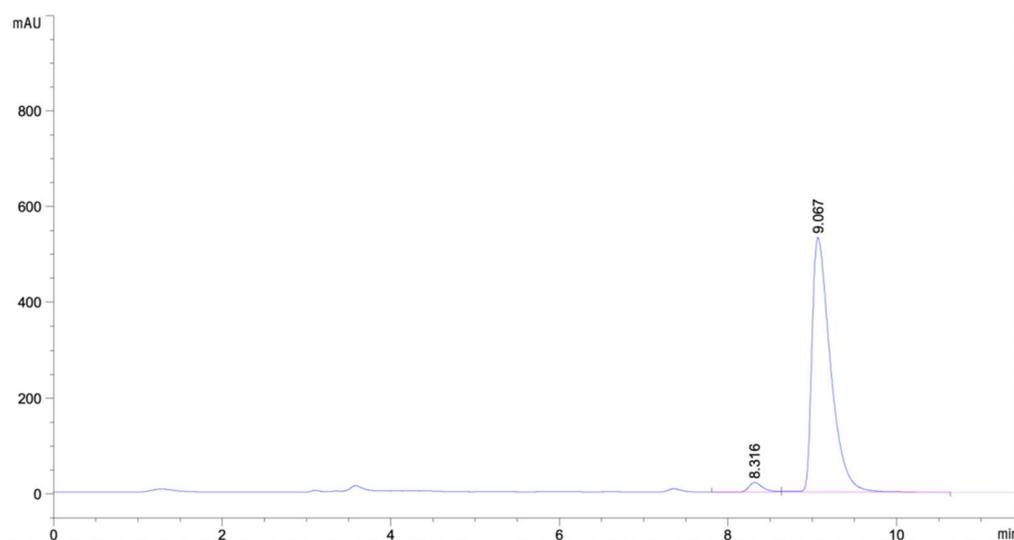


3x

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 56.8 mg, 93% yield, 94% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.77 (dd, J = 7.5, 1.4 Hz, 1H), 7.69 (dd, J = 6.9, 1.4 Hz, 1H), 7.36–7.22 (m, 2H), 7.18 (s, 1H), 4.44 (q, J = 6.6 Hz, 1H), 1.51 (d, J = 6.7 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-3, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 8.3 min, t_R (major) = 9.2 min. The analytical data are in accordance with the literature⁵.

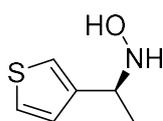


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.374 BV	0.1900	3265.45532	260.99594	49.5612
2	9.274 VW	0.2118	3323.28369	236.69943	50.4388



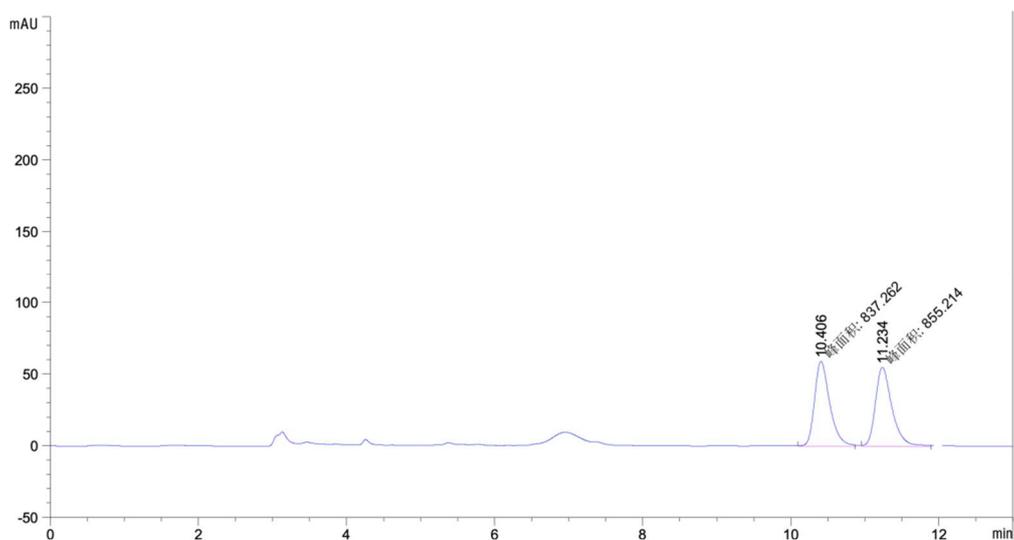
#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.316 BV	0.1769	233.24622	19.87270	2.8008
2	9.067 VW	0.2318	8094.69238	531.03845	97.1992

(S)-N-(1-(thiophen-3-yl)ethyl)hydroxylamine (3y)

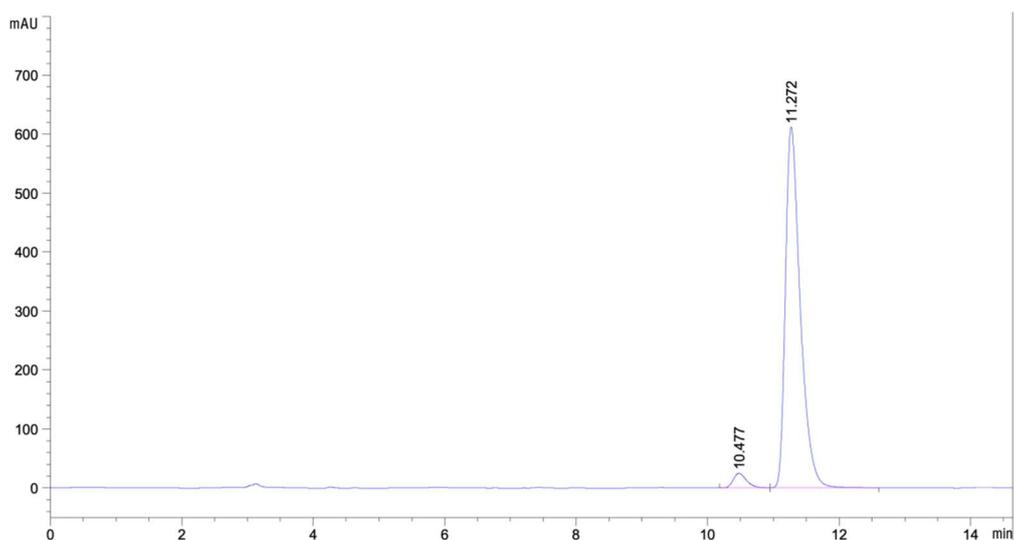


3y

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 39.5 mg, 92% yield, 93% *ee*. $^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 7.28 (dd, $J = 5.0, 3.0$ Hz, 1H), 7.18 (dd, $J = 3.0, 1.3$ Hz, 1H), 7.07 (dd, $J = 5.0, 1.3$ Hz, 1H), 4.20 (q, $J = 6.6$ Hz, 1H), 1.41 (d, $J = 6.7$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 10.4 min, t_R (major) = 11.2 min. The analytical data are in accordance with the literature³.

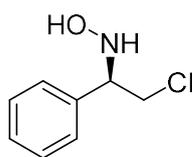


#	[min]	[min]	[mAU*s]	[mAU]	%
1	10.406 MM	0.2362	837.26215	59.06762	49.4697
2	11.234 MM	0.2590	855.21387	55.03428	50.5303

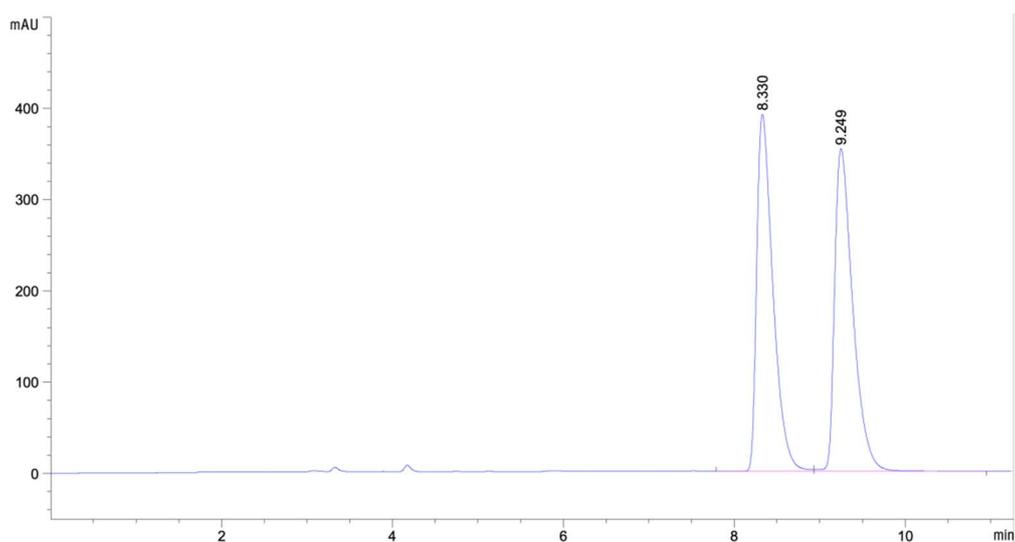


#	[min]	[min]	[mAU*s]	[mAU]	%
1	10.477 W	0.2123	351.01947	24.91993	3.5157
2	11.272 VB	0.2376	9633.23145	612.13867	96.4843

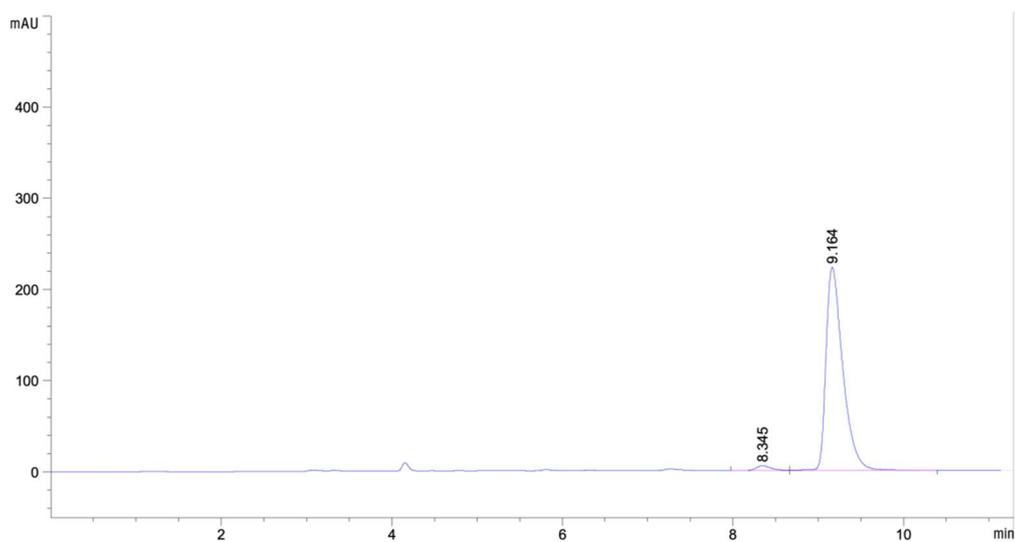
(R)-N-(2-chloro-1-phenylethyl)hydroxylamine (3z)



3z White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 48.4 mg, 94% yield, 96% *ee*. $^1\text{H NMR}$ (400 MHz, CHCl_3-d) δ 7.44–7.33 (m, 5H), 4.24 (ddt, $J = 7.4, 5.2, 1.2$ Hz, 1H), 3.84 (dd, $J = 11.2, 8.0$ Hz, 1H), 3.76 (dd, $J = 11.2, 5.0$ Hz, 1H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 80/20; 1.0 mL/min; 220 nm): t_R (minor) = 8.3 min, t_R (major) = 9.1 min. The analytical data are in accordance with the literature³.

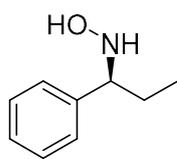


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.330 BV	0.1996	5151.87500	391.35016	49.7350
2	9.249 VB	0.2239	5206.76709	353.41760	50.2650



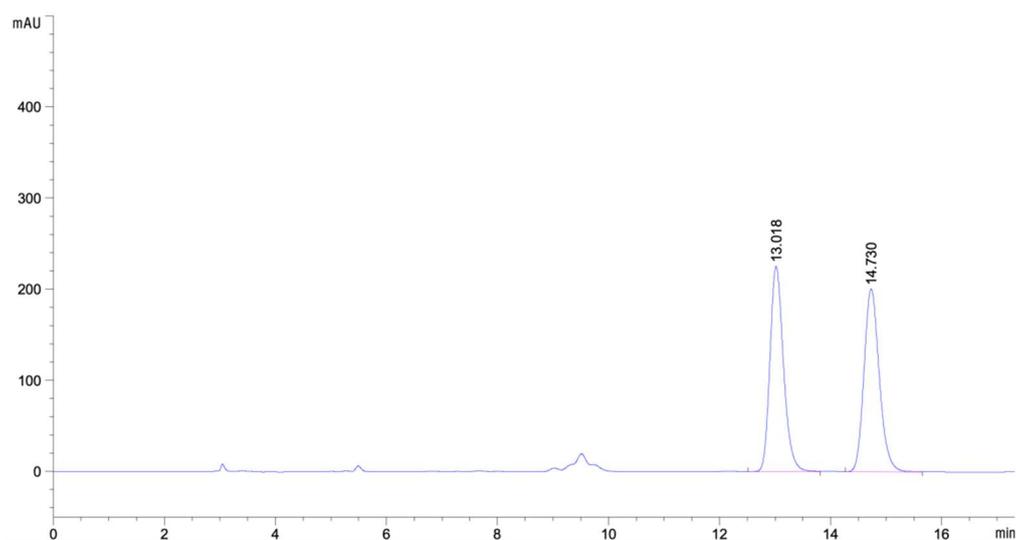
#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.345 BV	0.1802	63.61958	5.29579	2.0517
2	9.164 VB	0.2072	3037.23779	222.58987	97.9483

(S)-N-(1-Phenylpropyl)hydroxylamine (3aa)

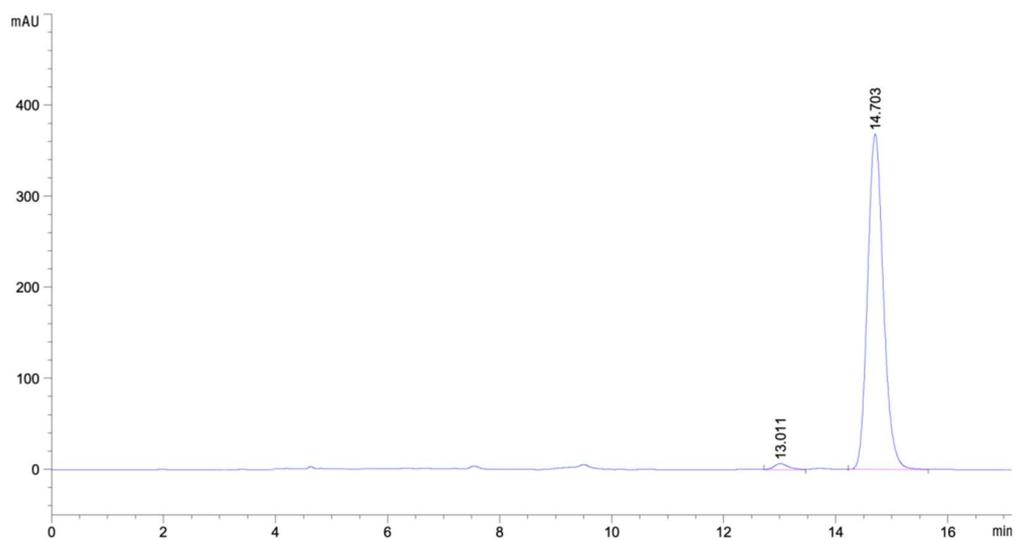


3aa

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 43.5 mg, 94% yield, 97% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.34–7.18 (m, 5H), 3.75 (dd, $J = 9.1, 5.2$ Hz, 1H), 1.84 (ddd, $J = 13.3, 7.6, 5.5$ Hz, 1H), 1.63–1.49 (m, 1H), 0.76 (t, $J = 7.5$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 13.0 min, t_R (major) = 14.7 min. The analytical data are in accordance with the literature².

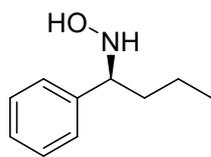


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	13.018	VV	0.2623	3831.59302	225.45975	49.9030
2	14.730	BV	0.2957	3846.48755	200.58537	50.0970



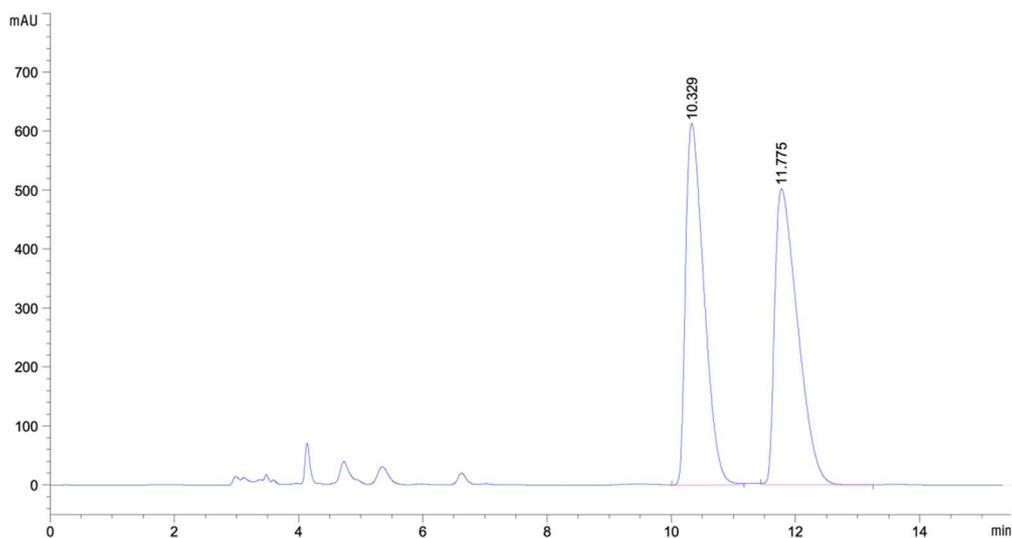
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	13.011	VV	0.2661	112.87811	6.38862	1.5427
2	14.703	BV	0.3021	7203.99756	368.40048	98.4573

(S)-N-(1-Phenylbutyl)hydroxylamine (3ab)

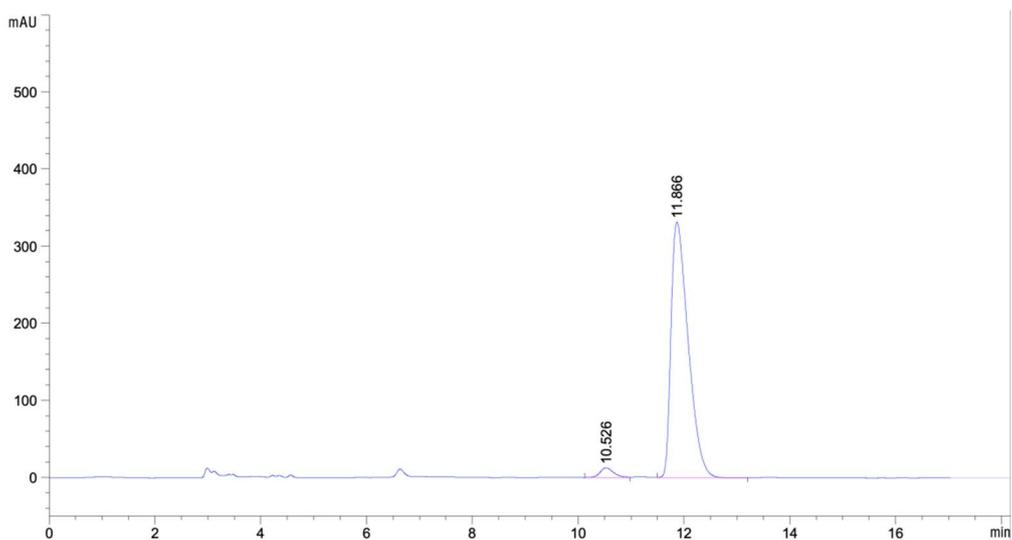


3ab

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH_2Cl_2 :MeOH = 10:1), 47.1 mg, 95% yield, 94% *ee*. ^1H NMR (400 MHz, Chloroform- d) δ 7.37–7.19 (m, 5H), 3.90 (dd, J = 8.9, 5.4 Hz, 1H), 1.90–1.76 (m, 1H), 1.66–1.53 (m, 1H), 1.33–1.08 (m, 2H), 0.88 (t, J = 7.4 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AS-H, *n*-Hexane/*i*-PrOH = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 10.5 min, t_R (major) = 11.8 min. The analytical data are in accordance with the literature².

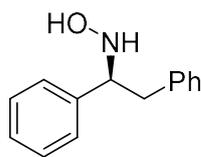


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	10.329	BV	0.3189	1.25518e4	612.84796	49.3297
2	11.775	VB	0.3994	1.28929e4	502.45236	50.6703



#	[min]	[min]	[mAU*s]	[mAU]	%	
1	10.526	BV	0.2696	228.44868	12.83742	2.9728
2	11.866	VB	0.3442	7456.06006	331.76471	97.0272

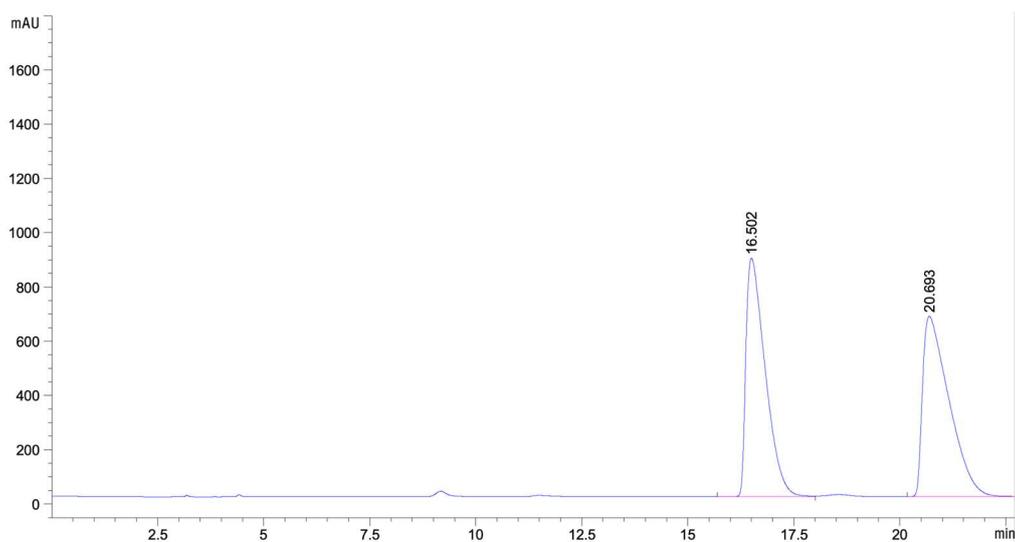
(S)-N-(1,2-Diphenylethyl)hydroxylamine (3ac)



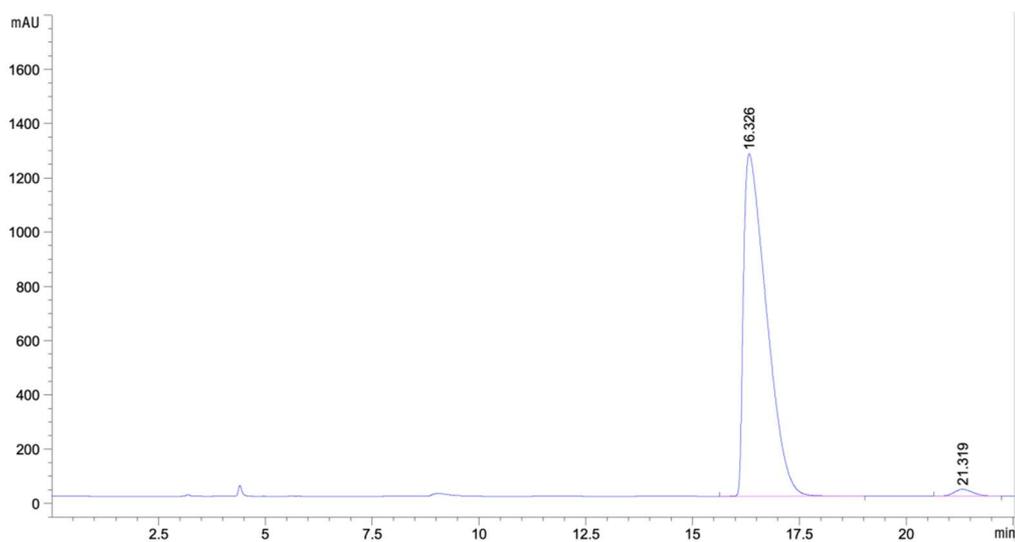
White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 59.5 mg, 93% yield, 97% *ee*.

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.33–7.13 (m, 8H), 7.10–7.02 (m, 2H), 4.11 (dd, $J = 7.9, 6.6$ Hz, 1H), 3.04 (dd, $J = 13.6, 7.9$ Hz, 1H), 2.88 (dd, $J = 13.6, 6.6$ Hz, 1H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-Hexane/*i*-PrOH = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 16.3 min, t_R (minor) = 21.3 min. The analytical data are in accordance with the literature².

3ac

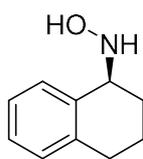


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	16.502	VV	0.4855	2.78482e4	879.20557	49.2402
2	20.693	BBA	0.6537	2.87076e4	664.91669	50.7598

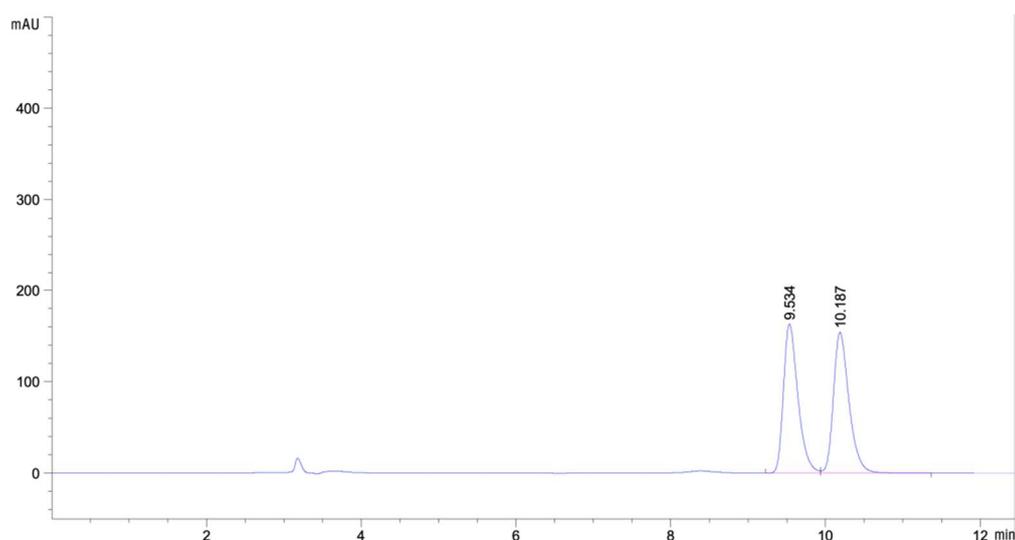


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	16.326	VB	0.5821	4.69798e4	1262.68188	98.3654
2	21.319	VV	0.4703	780.69006	25.41786	1.6346

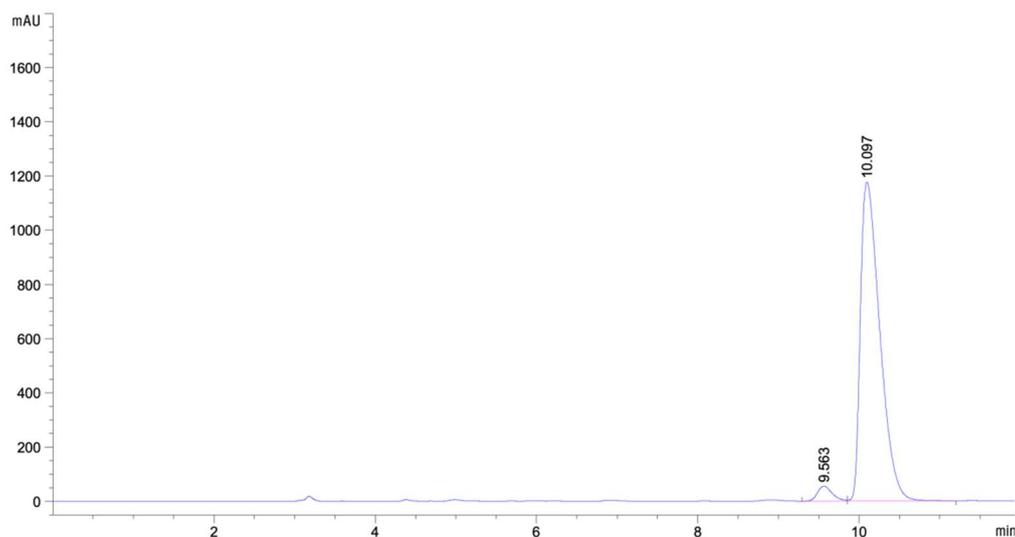
(S)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)hydroxylamine (3ad)



White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 47.0 mg, 96% yield, 93% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.34 (dd, $J = 6.7, 2.3$ Hz, 1H), 7.22–7.09 (m, 3H), 4.11 (t, $J = 4.2$ Hz, 1H), 2.87–2.67 (m, 2H), 2.28–2.17 (m, 1H), 2.04–1.67 (m, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, n-hexane/isopropanol = 80/20; 1.0 mL/min; 220 nm): t_R (minor) = 9.5 min, t_R (major) = 10.0 min. The analytical data are in accordance with the literature³.

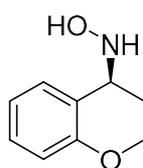


#	[min]	[min]	[mAU*s]	[mAU]	%
1	9.534 BV	0.1976	2119.39600	163.12781	49.5898
2	10.187 VB	0.2132	2154.45508	154.02229	50.4102



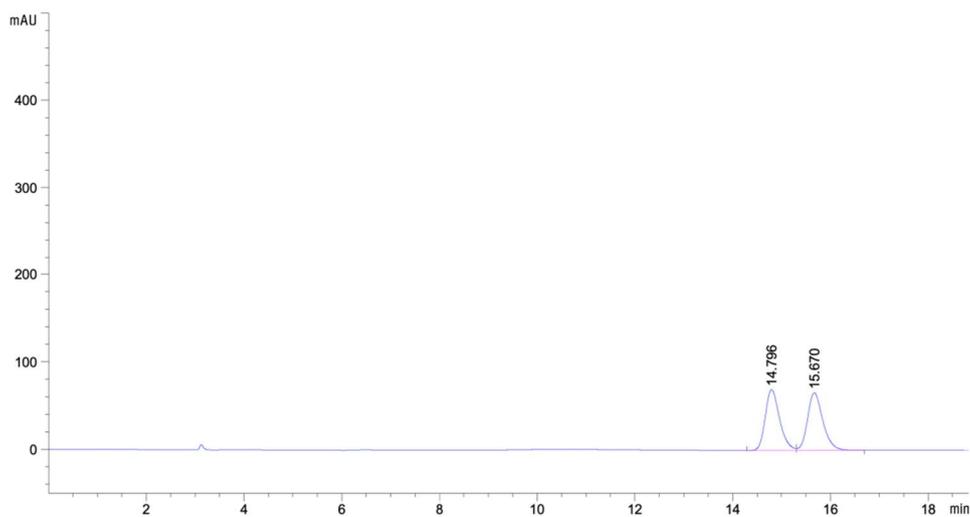
#	[min]	[min]	[mAU*s]	[mAU]	%
1	9.563 BV	0.1908	695.05554	55.24979	3.4116
2	10.097 W	0.2592	1.96785e4	1176.24353	96.5884

(S)-N-(4-chroman-4-yl)hydroxylamine (3ae)

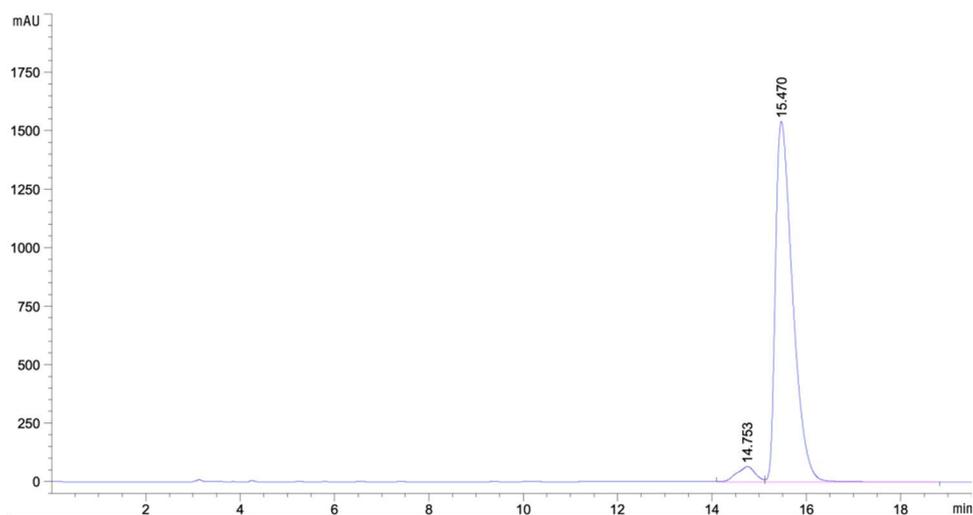


3ae

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), $R_f = 0.6$ ($\text{CH}_2\text{Cl}_2:\text{MeOH} = 10:1$), 45.6 mg, 92% yield, 91% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.28–7.14 (m, 2H), 6.94–6.81 (m, 2H), 4.28–4.14 (m, 2H), 4.07 (t, $J = 3.7$ Hz, 1H), 2.22 (dq, $J = 14.4, 3.0$ Hz, 1H), 2.09–1.96 (m, 1H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, n-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 14.7 min, t_R (major) = 15.6 min. The analytical data are in accordance with the literature⁶.

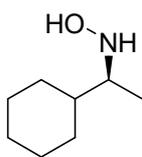


#	[min]	[min]	[mAU*s]	[mAU]	%
1	14.796 BV	0.3098	1411.62793	69.55006	49.7382
2	15.670 VB	0.3311	1426.48975	65.74846	50.2618

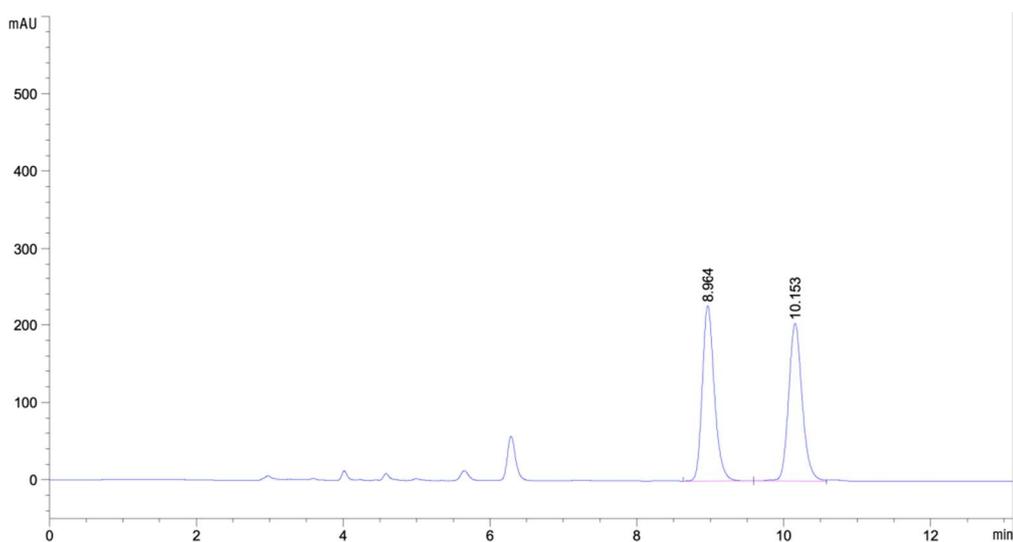


#	[min]	[min]	[mAU*s]	[mAU]	%
1	14.753 VV	0.3819	1744.41577	64.84198	4.2848
2	15.470 VB	0.3891	3.89672e4	1540.61536	95.7152

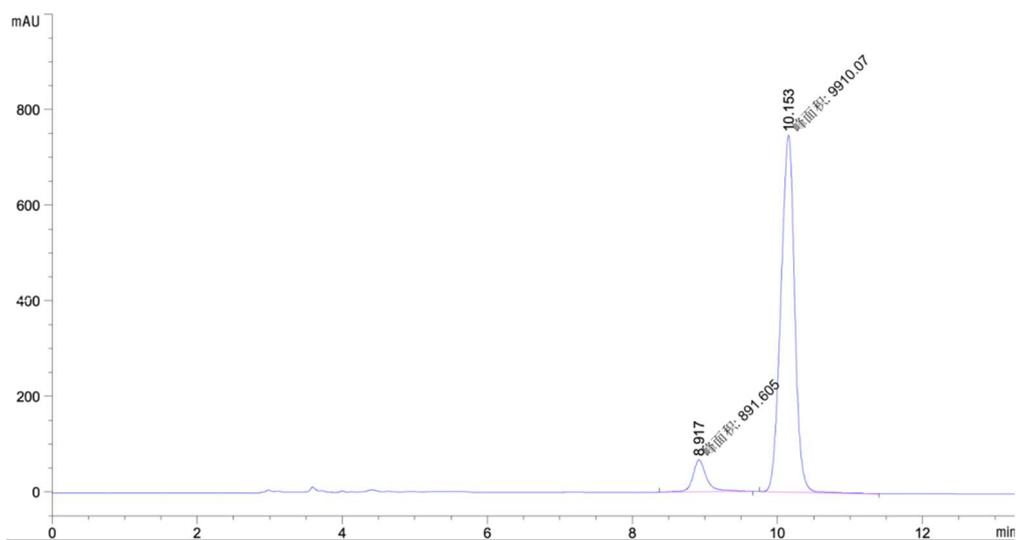
(S)-N-(1-cyclohexylethyl)hydroxylamine (3af)



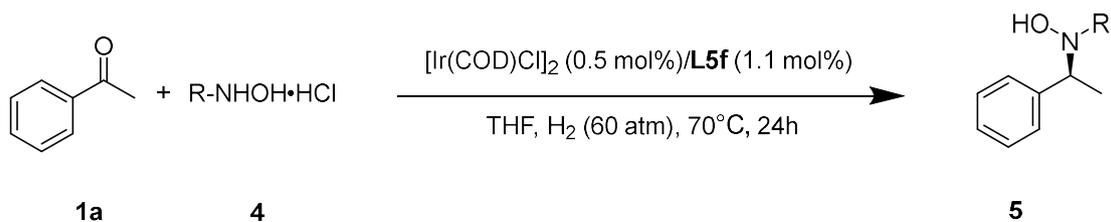
White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), R_f = 0.6 (CH₂Cl₂:MeOH = 10:1), 41.2 mg, 96% yield, 83% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 2.87–2.76 (m, 1H), 1.70 (ddt, *J* = 33.1, 12.1, 3.6 Hz, 5H), 1.48 (dddd, *J* = 11.9, 8.5, 5.2, 2.6 Hz, 1H), 1.23–1.11 (m, 3H), 1.06 (d, *J* = 6.6 Hz, 3H), 1.03–0.92 (m, 2H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 98/2; 1.0 mL/min; 210 nm): t_R (minor) = 8.9 min, t_R (major) = 10.1 min. The analytical data are in accordance with the literature³.



#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.964 BB	0.1753	2589.51709	226.70837	49.7809
2	10.153 BV	0.1974	2612.31592	203.99933	50.2191

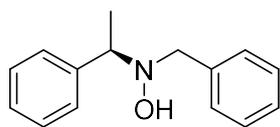


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.917 MM	0.2223	891.60455	66.83925	8.2543
2	10.153 MM	0.2211	9910.07129	747.06482	91.7457



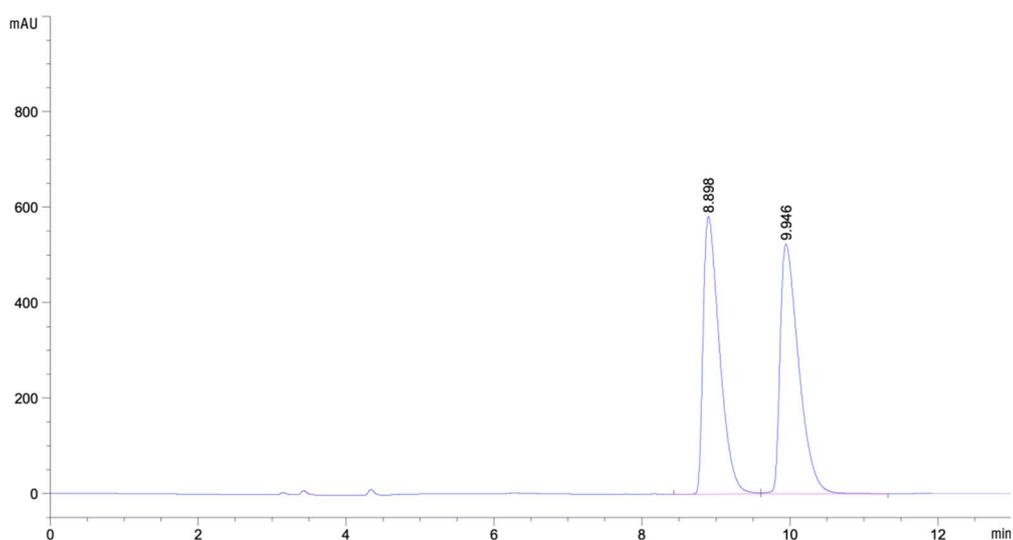
In the nitrogen-filled glovebox, $[\text{Ir}(\text{COD})\text{Cl}]_2$ (1 mg, 0.0015 mmol) and (*R*)-**L5f** (3.6 mg, 0.0033 mmol) were dissolved in 0.2 mL anhydrous THF in a 3 mL vial equipped with a stir bar. The above solution was stirred at room temperature for 30 minutes to in situ generate the Ir-**L5f** complex. A specified amount of the resulting solution (0.2 mL) was transferred to a vial charged with **1** (0.3 mmol), **4** (0.6 mmol). Then, 1 mL THF was added into the vial by syringe. The vials were transferred to an autoclave, which was purged with H_2 3 times and then charged with 60 atm of H_2 , and stirred at 70 °C for 24 h. After the reaction was complete, the hydrogen gas was released slowly and saturated NaHCO_3 (2 mL) was added into the reaction mixture, which was then extracted with CH_2Cl_2 (1 mL*3). The organic layers were combined, dried over anhydrous Na_2SO_4 and concentrated to give the crude product, which was purified by column chromatography. The product was analyzed by NMR spectroscopy for conversion and chiral HPLC for *ee* values.

(S)-N-Benzyl-N-hydroxy-1-phenylethanamine (5a)

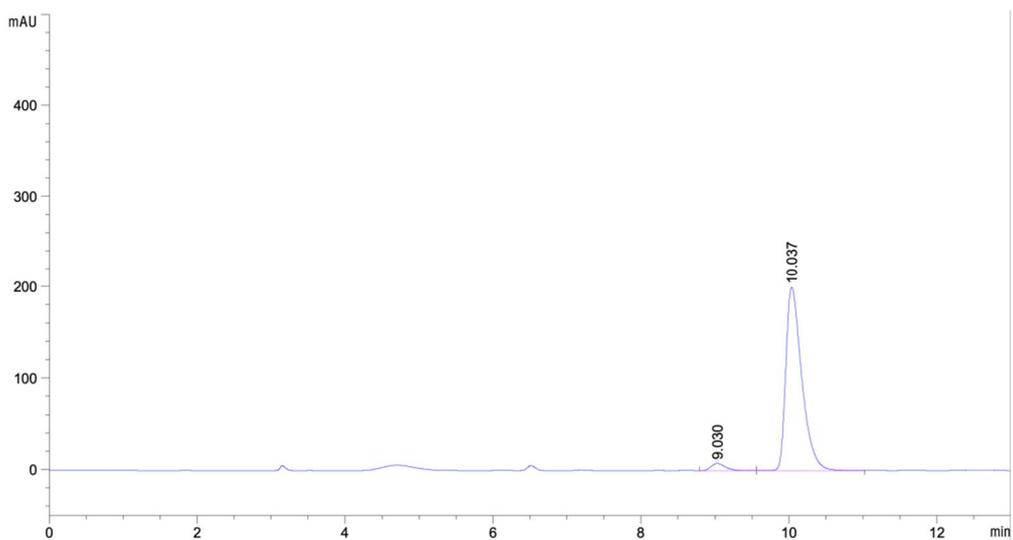


5a

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), $R_f = 0.5$ (petroleum ether/EtOAc = 10/1), 63.4 mg, 93% yield, 93% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.38–7.18 (m, 10H), 3.75 (q, $J = 6.6$ Hz, 1H), 3.67 (d, $J = 13.2$ Hz, 1H), 3.53 (d, $J = 13.4$ Hz, 1H), 1.42 (d, $J = 6.6$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 9.0 min, t_R (major) = 10.0 min. The analytical data are in accordance with the literature⁷.

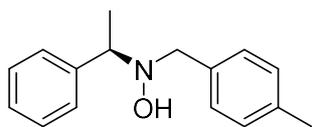


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.898 BV	0.2354	8939.16797	581.44598	49.4371
2	9.946 VB	0.2657	9142.73438	523.64368	50.5629



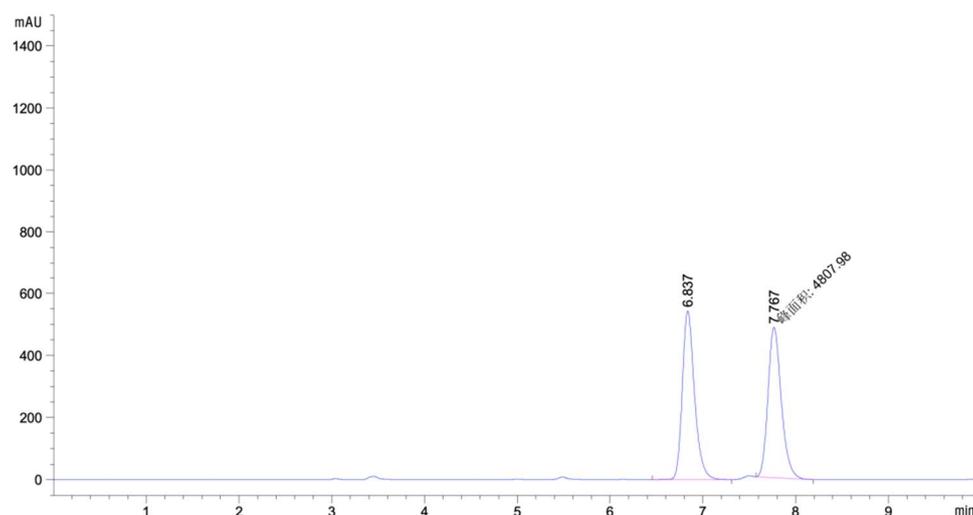
#	[min]	[min]	[mAU*s]	[mAU]	%
1	9.030 BV	0.2176	112.04968	7.89234	3.5883
2	10.037 W	0.2274	3010.56836	200.21324	96.4117

(S)-N-(4-methylbenzyl)-N-(1-phenylethyl)hydroxylamine (5b)

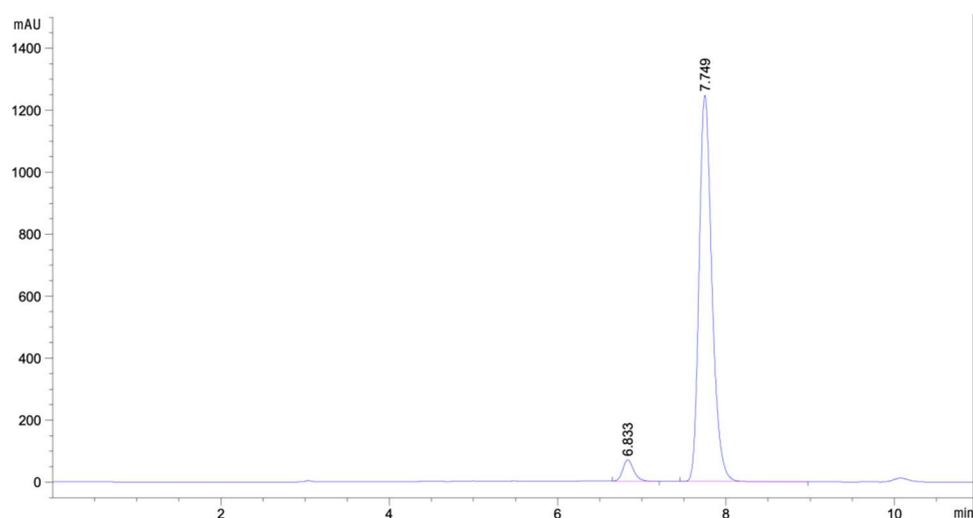


5b

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), $R_f = 0.5$ (petroleum ether/EtOAc = 10/1), 66.6 mg, 92% yield, 91% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.38–7.18 (m, 5H), 7.18–7.05 (m, 4H), 3.73 (q, $J = 6.6$ Hz, 1H), 2.29 (s, 3H), 1.40 (d, $J = 6.7$ Hz, 3H). ^{13}C NMR (400 MHz, Chloroform-*d*) δ 142.70, 136.84, 134.93, 129.69, 128.95, 128.49, 128.09, 127.37, 66.40, 60.69, 21.20, 19.34. Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 6.8 min, t_R (major) = 7.7 min.

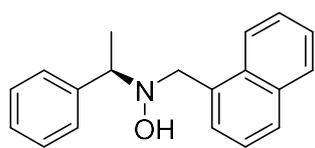


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	8.898	BV	0.2354	8939.16797	581.44598	49.4371
2	9.946	VB	0.2657	9142.73438	523.64368	50.5629



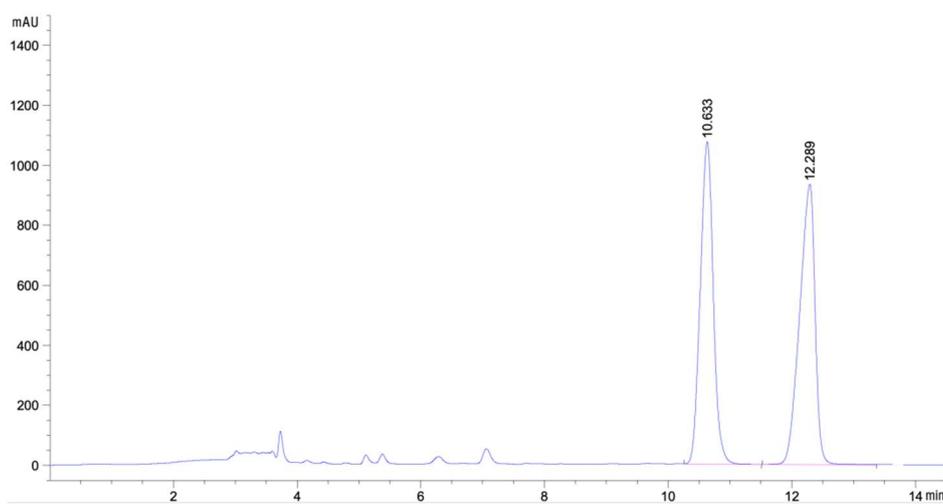
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	6.833	VB	0.1376	629.36835	69.54355	4.5411
2	7.749	VB	0.1628	1.32301e4	1246.31677	95.4589

(S)-N-(naphthalen-1-ylmethyl)-N-(1-phenylethyl)hydroxylamine (5c)

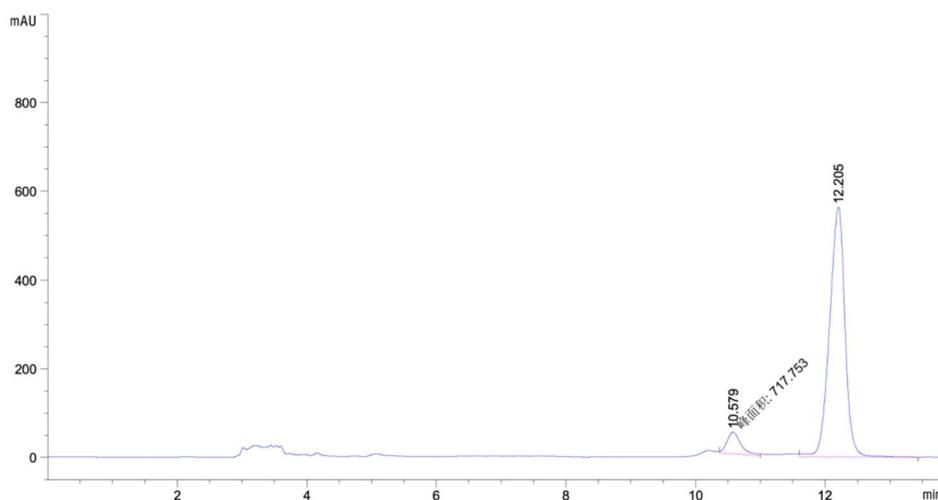


5c

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), $R_f = 0.5$ (petroleum ether/EtOAc = 10/1), 71.4 mg, 86% yield, 89% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.78 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.70 (t, $J = 8.6$ Hz, 2H), 7.47–7.24 (m, 10H), 3.98 (d, $J = 42.3$ Hz, 2H), 3.52 (q, $J = 6.8$ Hz, 1H), 1.19 (d, $J = 6.7$ Hz, 3H). ^{13}C NMR (400 MHz, Chloroform-*d*) δ 142.41, 133.86, 132.43, 128.80, 128.50, 128.49, 128.46, 128.22, 128.15, 127.60, 125.79, 125.52, 125.24, 124.36, 67.69, 58.48, 18.25. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 10.5 min, t_R (major) = 12.2 min.

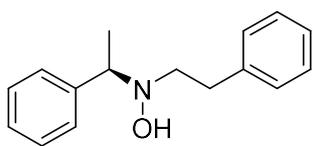


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	10.633	VB	0.2283	1.56878e4	1074.93262	49.3096
2	12.289	BV	0.2674	1.61271e4	934.16687	50.6904



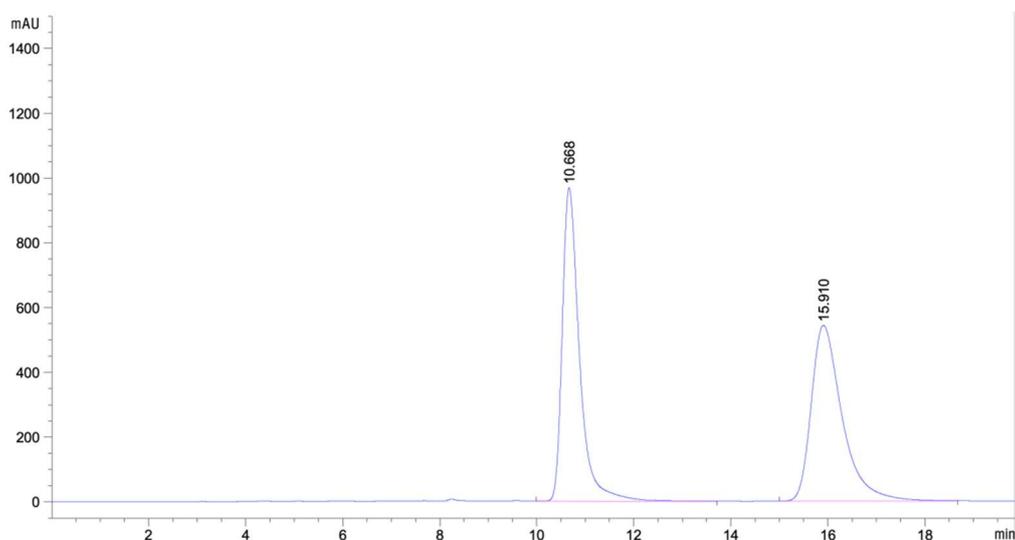
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	10.577	MM	0.2060	552.69513	44.71469	5.5897
2	12.205	VB	0.2554	9335.06934	563.04486	94.4103

(S)-N-phenethyl-N-(1-phenylethyl)hydroxylamine (5d)

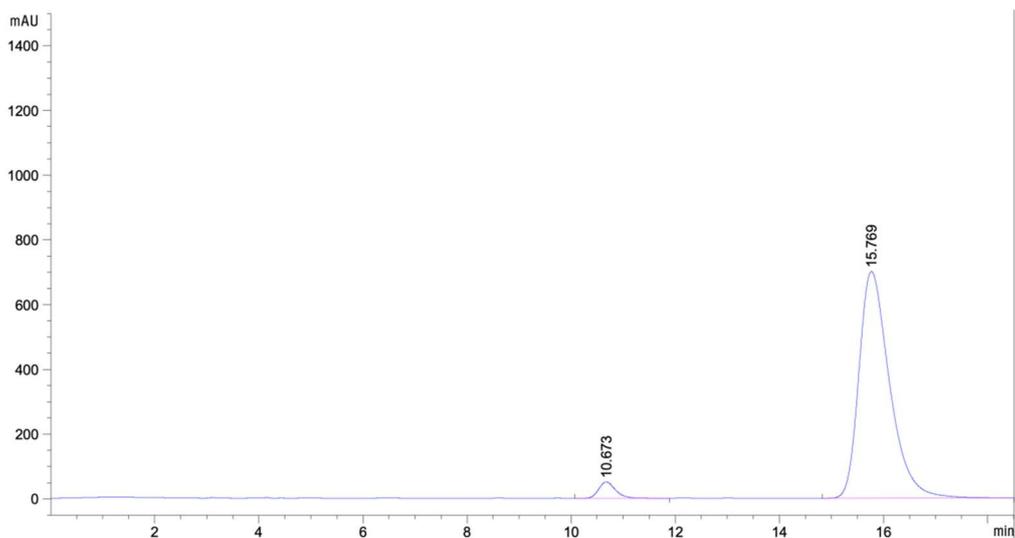


5d

Colourless oil, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 57.8 mg, 80% yield, 92% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.35–7.09 (m, 10H), 3.81 (q, J = 6.6 Hz, 1H), 3.00–2.79 (m, 4H), 1.46 (d, J = 6.7 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 10.6 min, t_R (major) = 15.7 min. The analytical data are in accordance with the literature⁸.

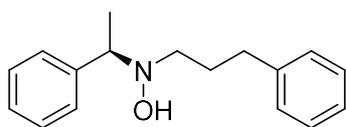


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	10.668	WV	0.3724	2.39352e4	968.20844	49.8798
2	15.910	WV	0.6688	2.40506e4	542.91864	50.1202



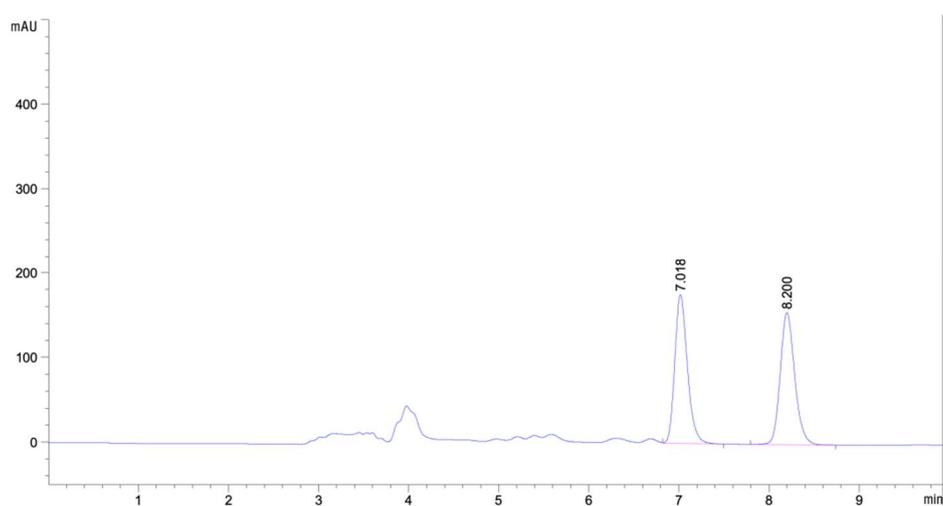
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	10.673	WV	0.3474	1156.62341	50.64510	3.8866
2	15.769	BBA	0.6223	2.86030e4	700.54419	96.1134

(S)-N-(1-phenylethyl)-N-(3-phenylpropyl)hydroxylamine (5e)

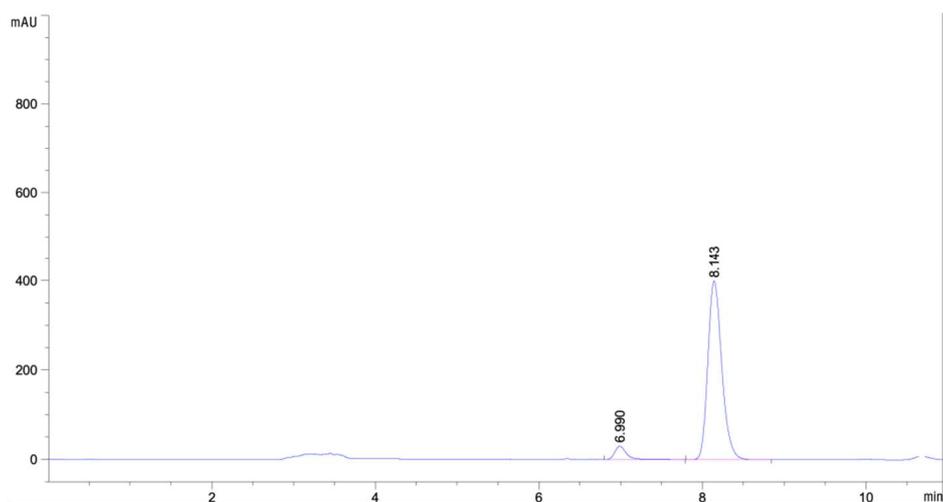


5e

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 65.6 mg, 86% yield, 88% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.24 (d, J = 4.4 Hz, 4H), 7.22–7.11 (m, 3H), 7.11–7.00 (m, 3H), 3.68 (q, J = 6.6 Hz, 1H), 2.52 (ddd, J = 15.1, 11.5, 6.5 Hz, 4H), 1.83 (p, J = 7.5 Hz, 2H), 1.36 (d, J = 6.6 Hz, 3H). ^{13}C NMR (400 MHz, Chloroform-*d*) δ 142.66, 142.25, 128.44, 128.42, 128.29, 127.91, 127.34, 125.71, 67.54, 56.36, 33.39, 28.76, 19.53. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 7.0 min, t_R (major) = 8.1 min.

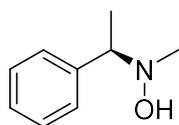


#	[min]	[min]	[mAU*s]	[mAU]	%
1	7.018 VB	0.1497	1715.10144	175.97180	49.5723
2	8.200 BB	0.1706	1744.69751	155.91571	50.4277



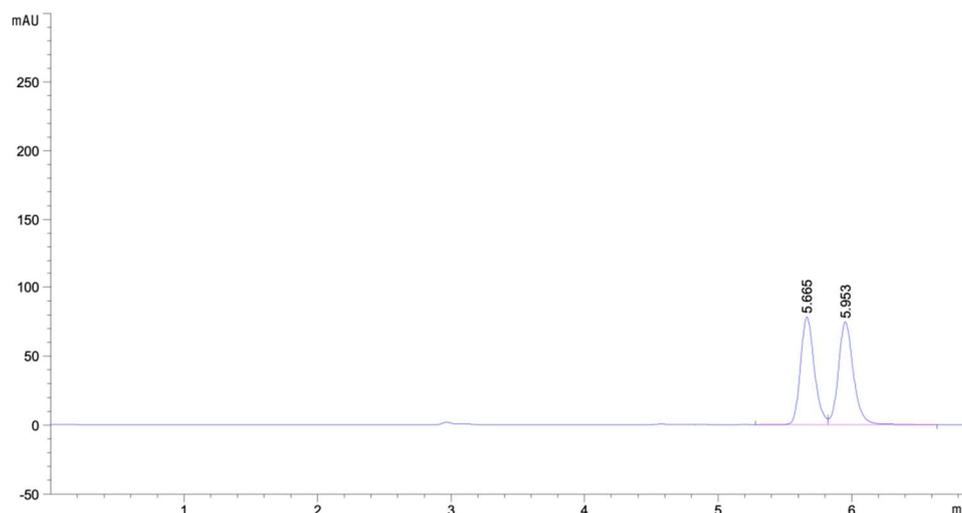
#	[min]	[min]	[mAU*s]	[mAU]	%
1	6.990 BB	0.1572	314.60223	29.79292	6.2248
2	8.143 BB	0.1822	4739.42725	399.96155	93.7752

(S)-N-methyl-N-(1-phenylethyl)hydroxylamine (5f)

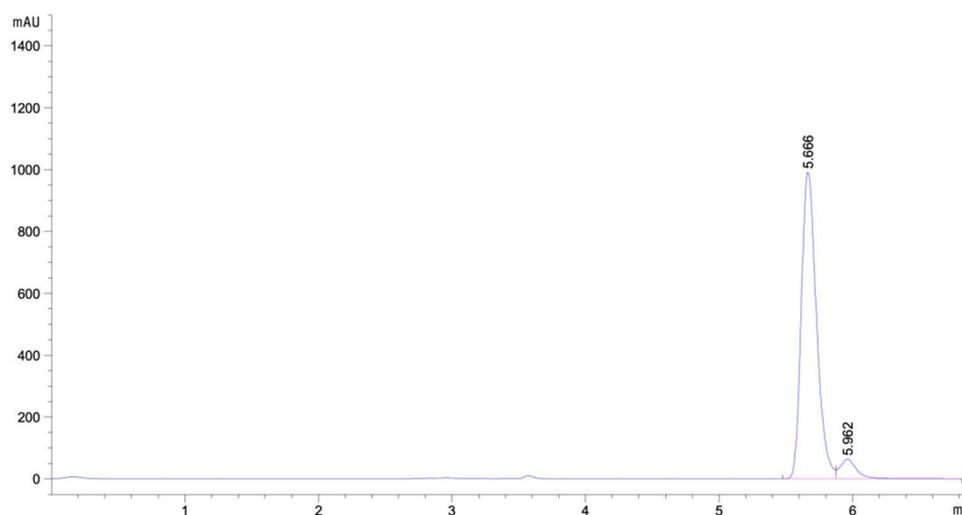


5f

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 39.0 mg, 86% yield, 86% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.27–7.12 (m, 5H), 3.56 (q, J = 6.8 Hz, 1H), 2.40 (s, 3H), 1.41 (d, J = 6.8 Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 95/5; 1.0 mL/min; 220 nm): t_R (major) = 5.6 min, t_R (minor) = 5.9 min. The analytical data are in accordance with the literature⁹.

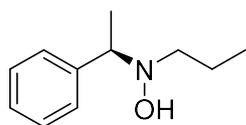


#	[min]	[min]	[mAU*s]	[mAU]	%
1	5.665 BV	0.1111	562.79358	78.11491	49.1415
2	5.953 VW	0.1192	582.45697	74.53342	50.8585



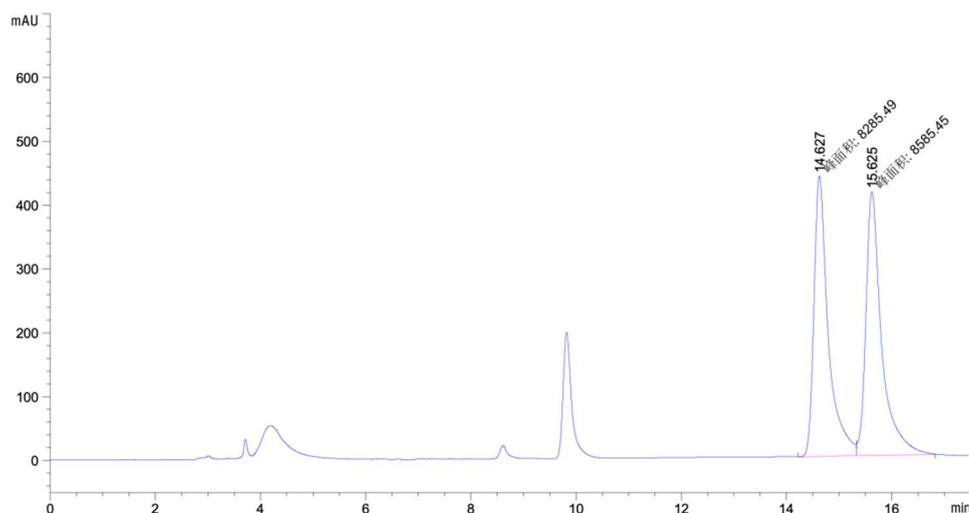
#	[min]	[min]	[mAU*s]	[mAU]	%
1	5.666 W	0.1220	7821.87500	991.40186	93.2142
2	5.962 W	0.1309	569.41803	63.34264	6.7858

(S)-N-(1-phenylethyl)-N-propylhydroxylamine (5g)

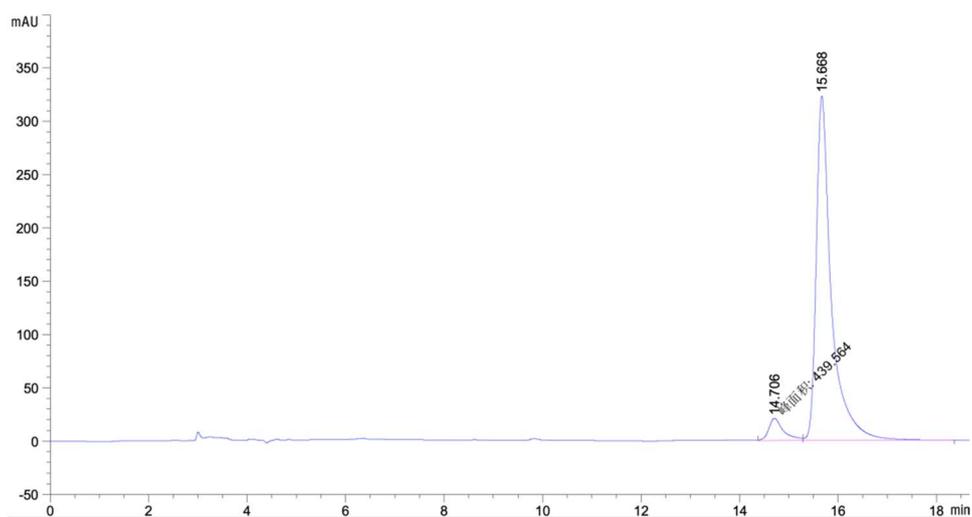


5g

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), $R_f = 0.5$ (petroleum ether/EtOAc = 10/1), 42.9 mg, 80% yield, 88% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.38–7.21 (m, 5H), 3.75 (q, $J = 6.6$ Hz, 1H), 2.57–2.41 (m, $J = 6.9$ Hz, 2H), 1.66–1.53 (m, 2H), 1.45 (d, $J = 6.6$ Hz, 3H), 0.86 (t, $J = 7.4$ Hz, 3H). $^{13}\text{C NMR}$ (400 MHz, Chloroform-*d*) δ 138.43, 128.99, 128.73, 127.32, 73.30, 61.21, 20.16, 19.17, 11.05. Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 14.7 min, t_R (major) = 15.6 min.

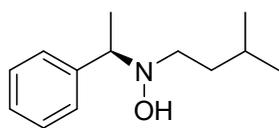


#	[min]	[min]	[mAU*s]	[mAU]	%
1	14.627 MM	0.3143	8285.48828	439.38916	49.1110
2	15.625 MM	0.3464	8585.44824	413.08389	50.8890



#	[min]	[min]	[mAU*s]	[mAU]	%
1	14.706 FM	0.3490	439.56357	20.98910	5.9682
2	15.668 VB	0.3100	6925.56055	323.15994	94.0318

(S)-N-isopentyl-N-(1-phenylethyl)hydroxylamine (5h)

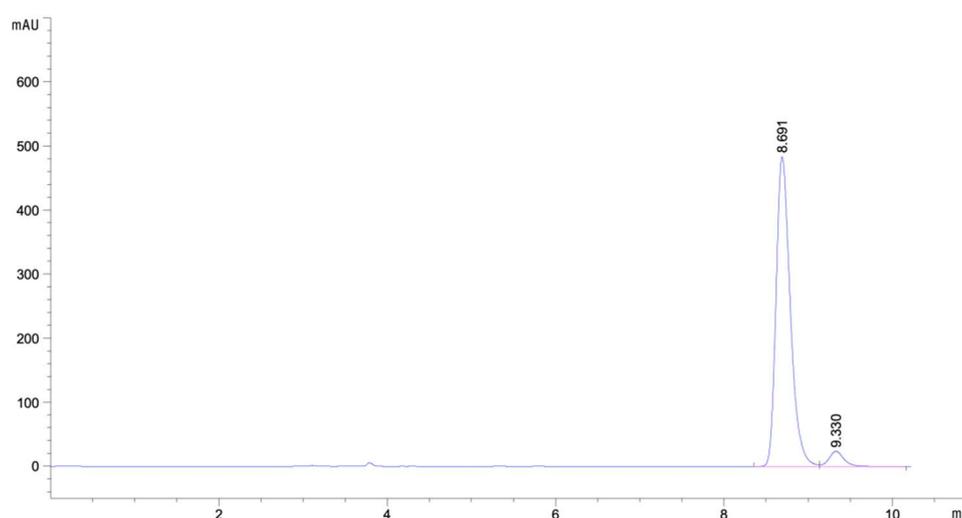


5h

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 50.9 mg, 82% yield, 90% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.41–7.21 (m, 5H), 3.76 (q, J = 6.7 Hz, 1H), 2.59 (t, J = 7.3 Hz, 2H), 1.63–1.48 (m, 3H), 1.46 (d, J = 6.6 Hz, 3H), 0.83 (dd, J = 10.1, 6.5 Hz, 6H). ^{13}C NMR (400 MHz, Chloroform-*d*) δ 142.78, 128.39, 127.87, 127.27, 67.58, 55.40, 36.08, 26.19, 22.86, 19.73. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 8.6 min, t_R (major) = 9.2 min.

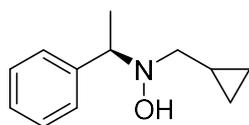


#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.670 BV	0.1792	3934.87183	334.58328	50.3783
2	9.293 W	0.1915	3875.78003	310.84750	49.6217



#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.691 BV	0.1786	5664.03662	483.72876	95.1308
2	9.330 W	0.1877	289.90964	23.53891	4.8692

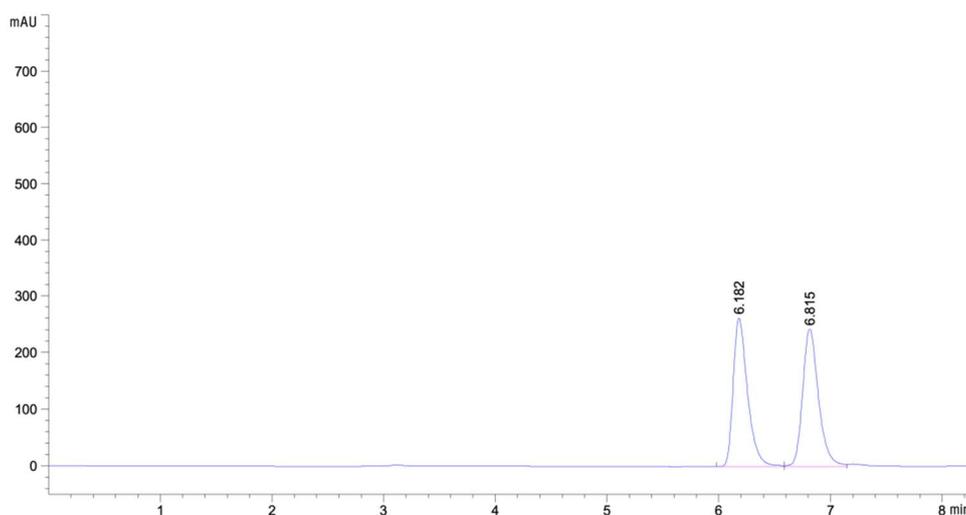
(S)-N-(cyclopropylmethyl)-N-(1-phenylethyl)hydroxylamine (5i)



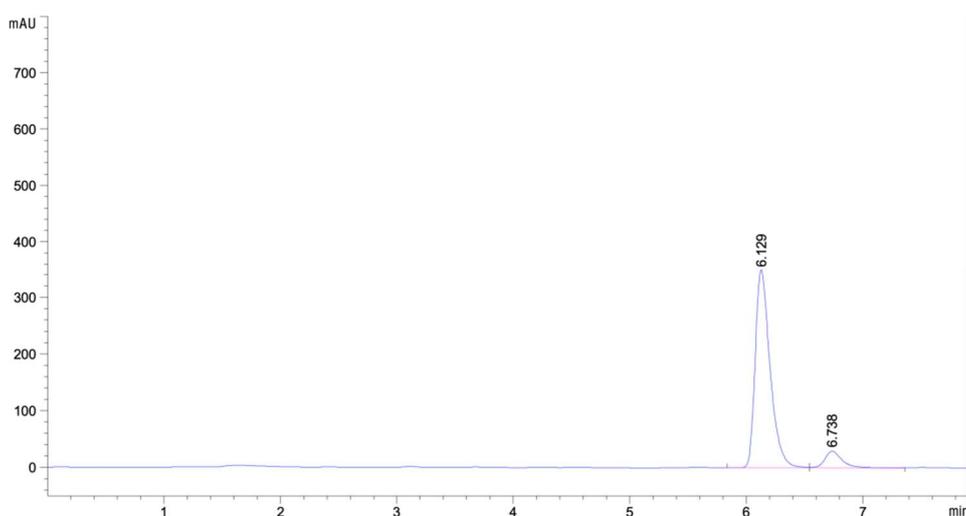
5i

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 43.0 mg, 75% yield, 82% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.31–7.11 (m, 5H), 3.77 (q, J = 6.7 Hz, 1H), 2.35 (qd, J = 13.2, 6.8 Hz, 2H), 1.40 (d, J = 6.7 Hz, 3H), 1.02 – 0.88 (m, 1H), 0.38 (dd, J = 8.2, 1.5 Hz, 2H), 0.01 (q, J = 3.9 Hz, 2H).

^{13}C NMR (400 MHz, Chloroform-*d*) δ 142.68, 128.39, 127.92, 127.25, 66.82, 61.82, 19.49, 8.84, 3.90, 3.67. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 6.1 min, t_R (major) = 6.7 min.

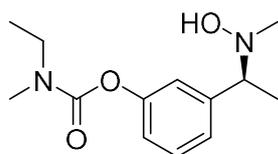


#	[min]	[min]	[mAU*s]	[mAU]	%
1	6.182 BV	0.1353	2339.88208	261.64301	49.4076
2	6.815 VV	0.1501	2395.99243	242.80923	50.5924



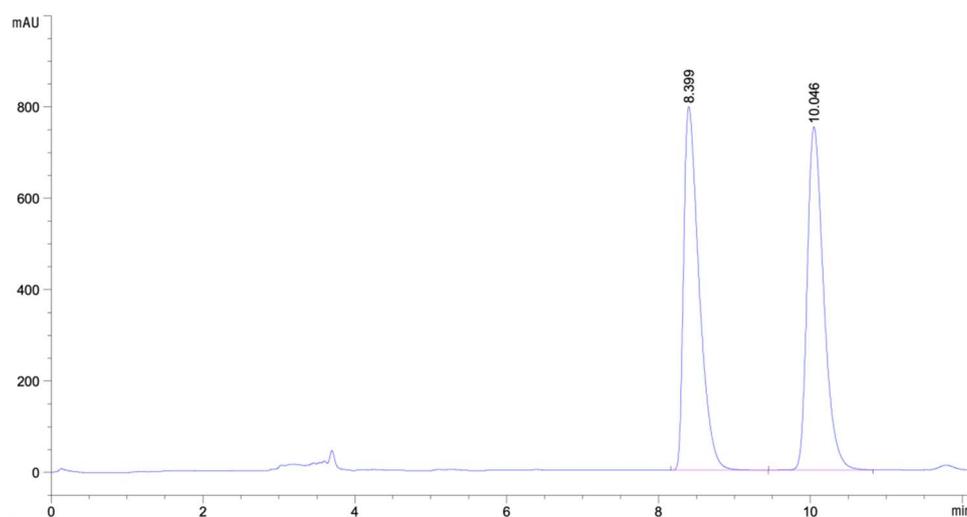
#	[min]	[min]	[mAU*s]	[mAU]	%
1	6.129 BV	0.1354	3095.47192	349.21396	91.0768
2	6.738 VV	0.1517	303.27798	29.54862	8.9232

(S)-3-(1-(hydroxy(methyl)amino)ethyl)phenyl ethyl(methyl)carbamate (5j)

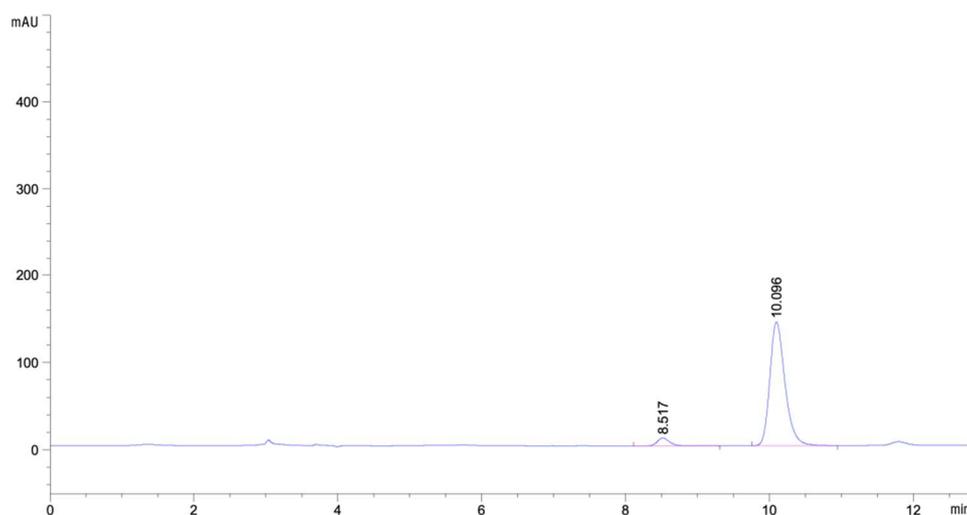


5j

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 68.8 mg, 92% yield, 91% *ee*. $^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.30 (t, J = 7.8 Hz, 1H), 7.10–6.98 (m, 3H), 3.63 (q, J = 6.6 Hz, 1H), 3.43 (dq, J = 25.6, 7.1 Hz, 2H), 3.02 (d, J = 30.7 Hz, 3H), 2.52 (s, 3H), 1.45 (d, J = 6.7 Hz, 3H), 1.28–1.10 (m, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak AD-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (minor) = 8.5 min, t_R (major) = 10.0 min.

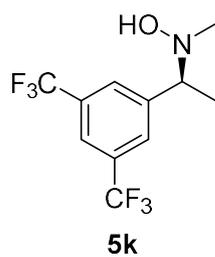


#	[min]	[min]	[mAU*s]	[mAU]	%	
1	8.399	BB	0.2149	1.12416e4	795.43195	49.7241
2	10.046	BV	0.2326	1.13664e4	751.06140	50.2759



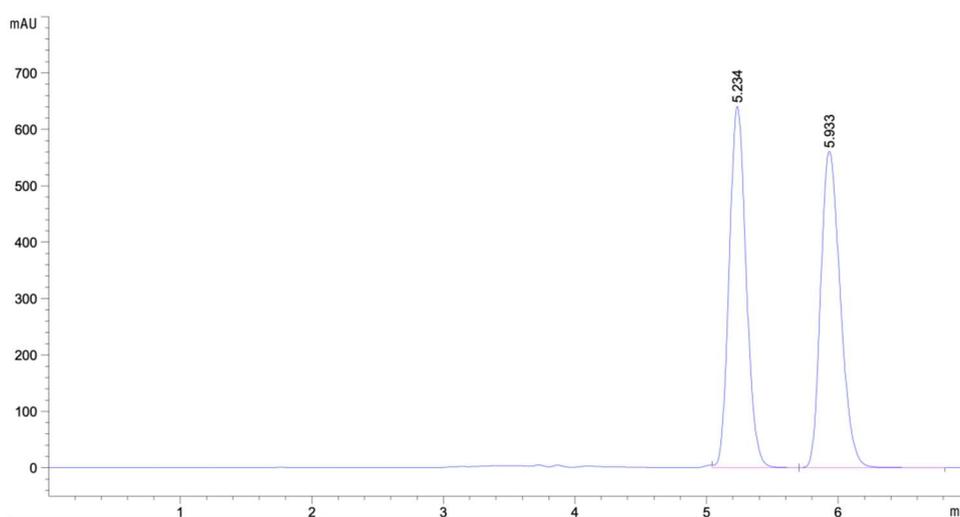
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	8.517	BB	0.1937	118.35079	9.22481	5.4005
2	10.096	VB	0.2231	2073.11646	141.34628	94.5995

(S)-N-(1-(3,5-bis(trifluoromethyl)phenyl)ethyl)-N-methylhydroxylamine (5k)

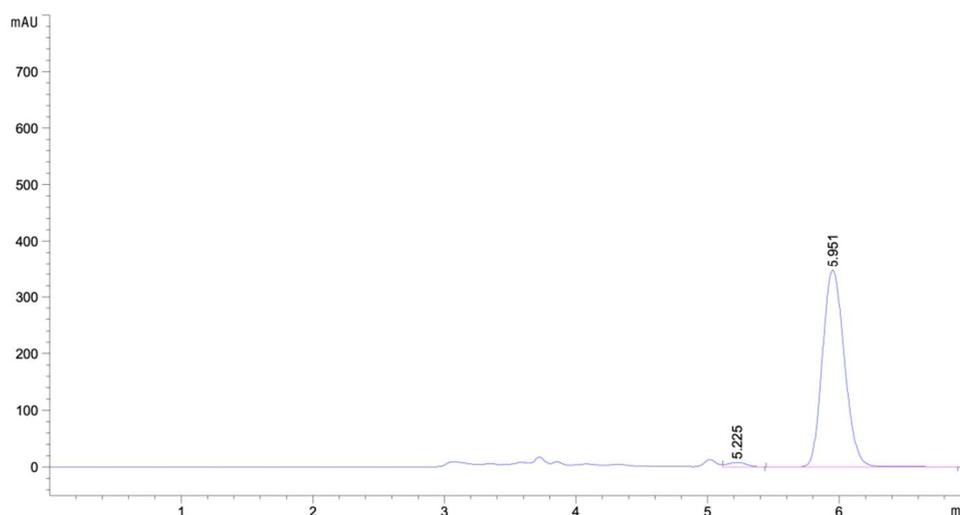


White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 68.9 mg, 80% yield, 96% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, J = 6.0 Hz, 3H), 3.79 (q, J = 6.7 Hz, 1H), 2.50 (s, 3H), 1.44 (d, J = 6.9 Hz, 3H). ^{19}F NMR (600 MHz, Chloroform-*d*) δ -62.76. Enantiomeric excess was determined by chiral HPLC (Chiralpak AS-H, *n*-hexane/isopropanol = 95/5; 1.0 mL/min; 220 nm): t_R (minor)

= 5.2 min, t_R (major) = 5.9 min.



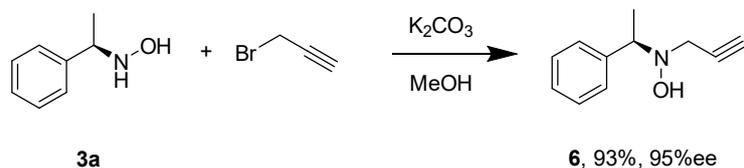
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	5.234	VB	0.1385	5732.71094	640.31665	49.6008
2	5.933	BV	0.1632	5824.98926	560.54193	50.3992



#	[min]	[min]	[mAU*s]	[mAU]	%	
1	5.225	VB	0.1580	76.85748	7.66669	1.8666
2	5.951	BV	0.1838	4040.64038	347.13876	98.1334

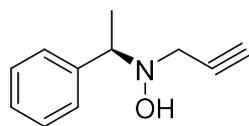
4. Applications

(1)



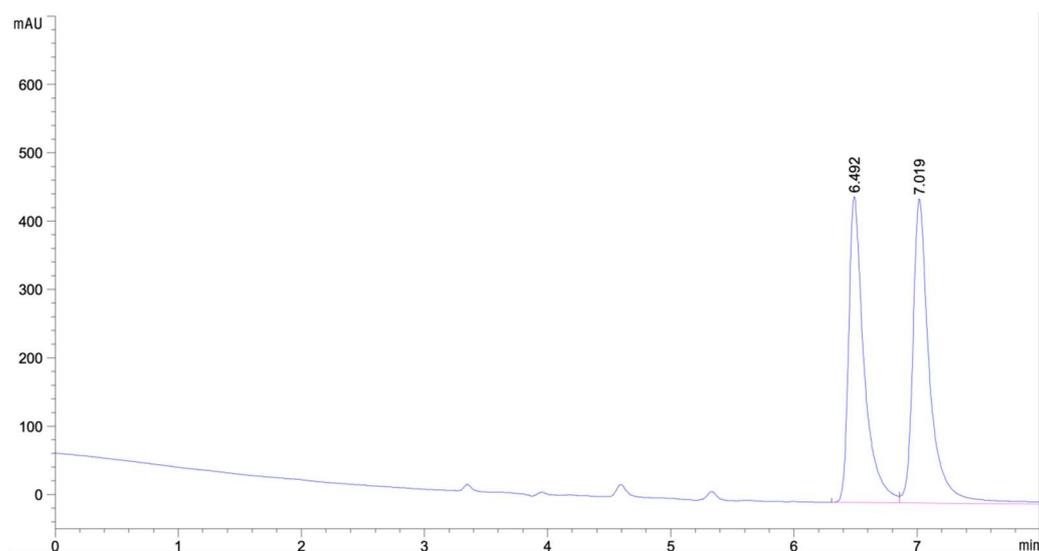
To a solution of (*S*)-**3a** (0.3 mmol, 1.0 equiv.) in MeOH (1.0 mL) was added 3-bromopropyne (0.36 mmol, 1.2 equiv.) and K₂CO₃ (0.45 mmol, 1.5 equiv.). The mixture was stirred under nitrogen atmosphere at 80 °C for 1 h. The insoluble solid was filtered off and washed with MeOH. The combined filtrate was evaporated under reduced pressure. The crude residue was purified by column chromatography to afford (*S*)-**6**.

(*S*)-*N*-(1-phenylethyl)-*N*-(prop-2-yn-1-yl)hydroxylamine (**6**)

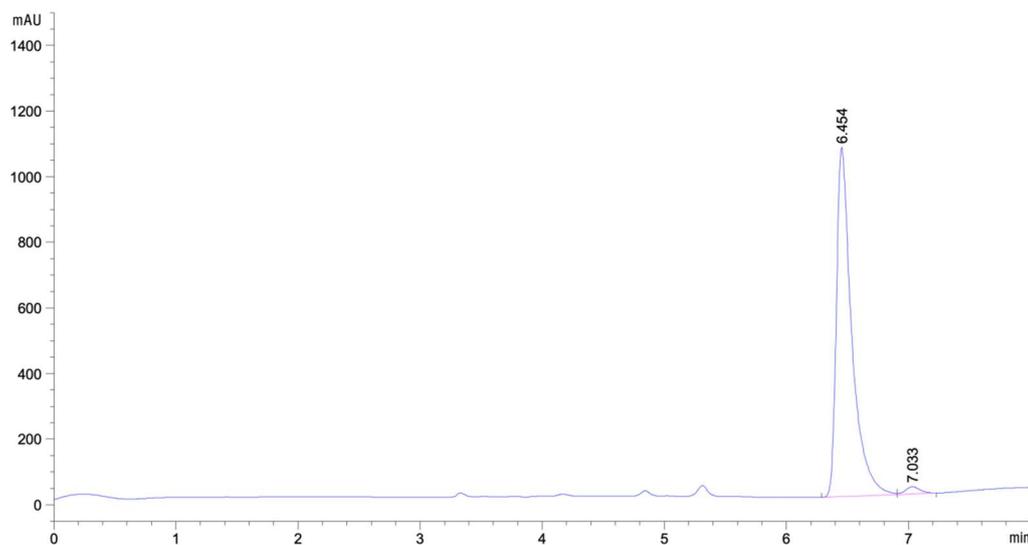


6

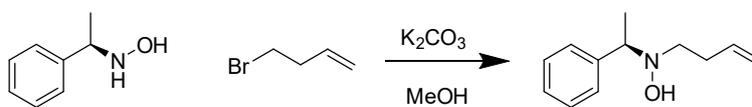
White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 48.8 mg, 93% yield, 95% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.39–7.21 (m, 5H), 4.06 (q, *J* = 6.6 Hz, 1H), 3.60 (dd, *J* = 17.0, 2.5 Hz, 1H), 3.43–3.24 (m, 1H), 2.31 (t, *J* = 2.4 Hz, 1H), 1.50 (d, *J* = 6.7 Hz, 3H). ¹³C NMR (400 MHz, Chloroform-*d*) δ 141.82, 128.65, 127.90, 127.79, 78.33, 73.78, 65.30, 46.79, 20.32. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-3, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 6.4 min, t_R (minor) = 7.0 min.



#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.492	BV	0.1260	3874.22168	447.58414	47.3441
2	7.019	VBA	0.1399	4308.90039	445.38702	52.6559



#	[min]		[min]	[mAU*s]	[mAU]	%
1	6.454	BV	0.1278	9291.51953	1064.43823	98.0758
2	7.033	VB	0.1251	182.29106	22.12202	1.9242

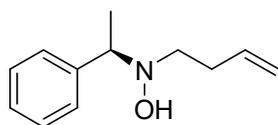


3a

7, 92%, 95%ee

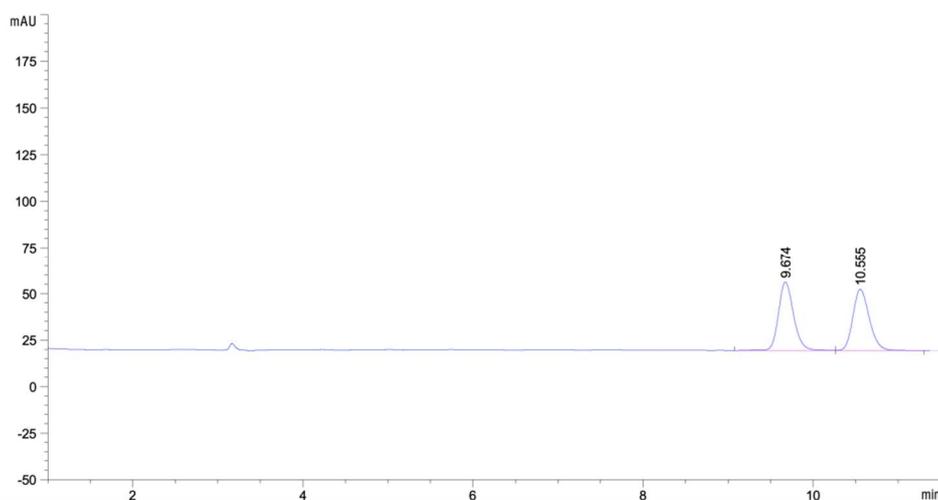
To a solution of (*S*)-**3a** (0.3 mmol, 1.0 equiv.) in MeOH (1.0 mL) was added 4-bromobut-1-ene (0.36 mmol, 1.2 equiv.) and K₂CO₃ (0.45 mmol, 1.5 equiv.). The mixture was stirred under nitrogen atmosphere at 80°C for 1 h. The insoluble solid was filtered off and washed with MeOH. The combined filtrate was evaporated under reduced pressure. The crude residue was purified by column chromatography to afford (*S*)-**7**.

(S)-N-(but-3-en-1-yl)-N-(1-phenylethyl)hydroxylamine (7)

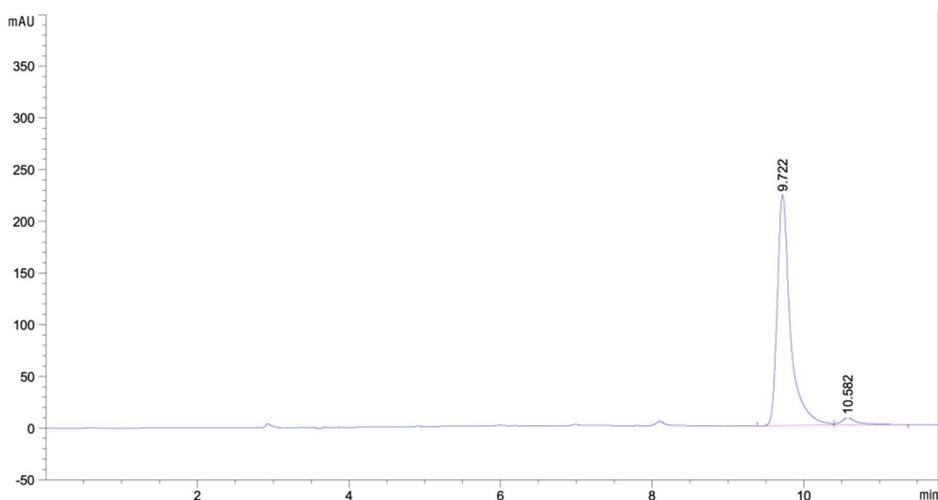


7

White solid, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), R_f = 0.5 (petroleum ether/EtOAc = 10/1), 52.7mg, 92% yield, 94% *ee*. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.29 (dd, J = 24.9, 4.0 Hz, 5H), 5.78 (ddt, J = 17.0, 10.2, 6.7 Hz, 1H), 5.03–4.93 (m, 2H), 3.76 (q, J = 6.7 Hz, 1H), 2.64 (dd, J = 8.6, 5.5 Hz, 2H), 2.35 (q, J = 7.1 Hz, 2H), 1.45 (d, J = 6.6 Hz, 3H). ^{13}C NMR (400 MHz, Chloroform-*d*) δ 142.78, 136.74, 128.41, 127.83, 127.29, 115.54, 67.58, 56.39, 31.88, 19.75. Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 9.7 min, t_R (minor) = 10.5 min.

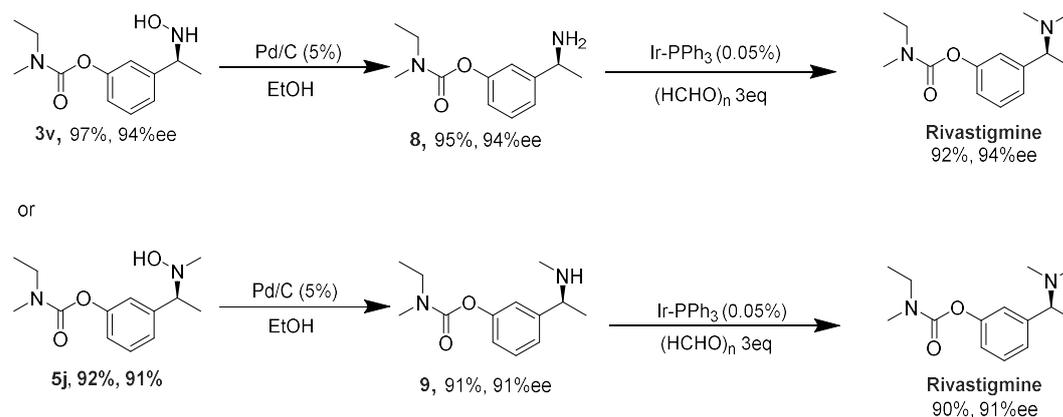


#	[min]	[min]	[mAU*s]	[mAU]	%
1	9.674 BV	0.1902	459.35745	36.91425	50.9289
2	10.555 WV	0.2068	442.60098	32.93695	49.0711



#	[min]	[min]	[mAU*s]	[mAU]	%
1	9.722 BV	0.1754	2668.11230	223.25244	96.1395
2	10.582 VB	0.2164	107.13945	7.00615	3.8605

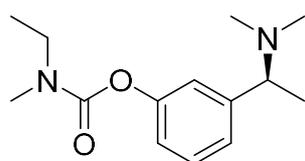
(2) Synthesis of rivastigmine.



Pd on carbon (5%) was added to the solution of (*S*)-**3u** or (*S*)-**5j** (0.1 mmol) in EtOH (1 mL). The resulting mixture was transferred to an autoclave, which was charged with 40 atm of H₂, and stirred at 30 °C for 24 h. The hydrogen gas was released slowly and the solution was filter and quenched with aqueous sodium bicarbonate solution. The organic phase was concentrated and passed through a short column of silica gel to remove the metal complex to give the crude product, which was purified with column chromatography to afford (*S*)-**8** (95% yield, 94% *ee*) or (*S*)-**9** (91% yield, 91% *ee*).

In a nitrogen-filled glovebox, [Ir(cod)Cl]₂ (2.0 mg, 3 μmol) and PPh₃ (3.5 mg, 13.2 μmol) were dissolved in anhydrous trifluoroethanol (0.2 mL) in a 10 mL vial equipped with a stir bar. The above solution was stirred at room temperature for 20 minutes to in situ generate the Ir-PPh₃ complex. To a 5 mL vial equipped with a stir bar were added (*S*)-**8** or (*S*)-**9** (0.3 mmol) and paraformaldehyde (0.9 mmol) substrates, followed by the addition of anhydrous trifluoroethanol (1.0 mL) and the Ir-PPh₃ complex solution (100 μL, 0.05 mol%). The resulting vial was transferred to an autoclave, which was purged with H₂ 3 times and then charged with H₂ (30 atm), and stirred at room temperature for 24 h. The hydrogen gas was released slowly and the solution was concentrated to give the crude products, which were purified by column chromatography to afford the final product Rivastigmine.^{10,11}

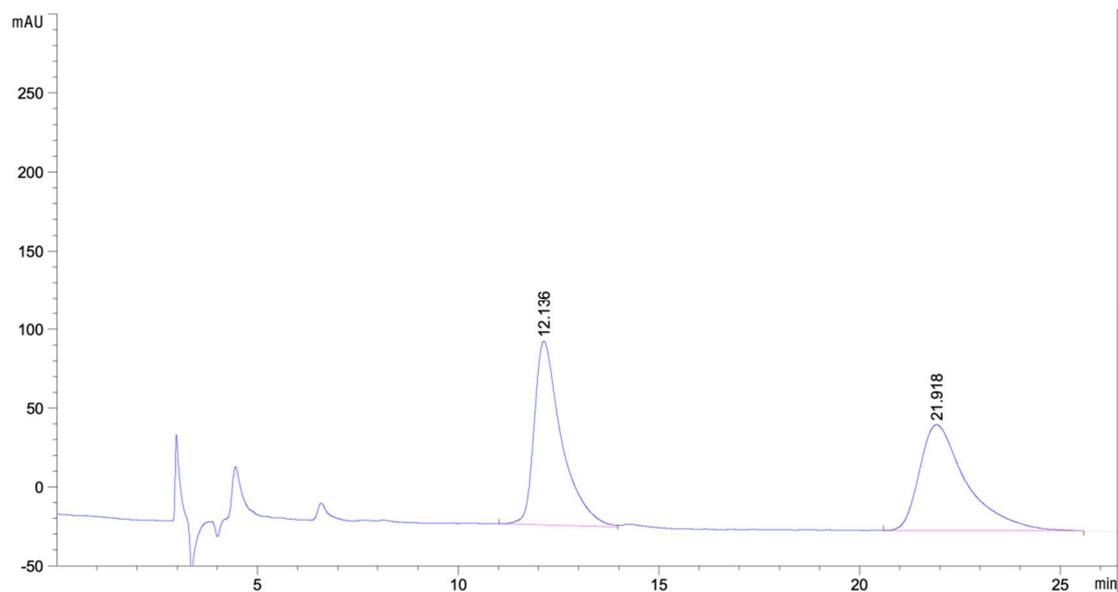
(*S*)-3-[1-(Dimethylamino)ethyl]phenyl ethyl-(methyl)carbamate (Rivastigmine)



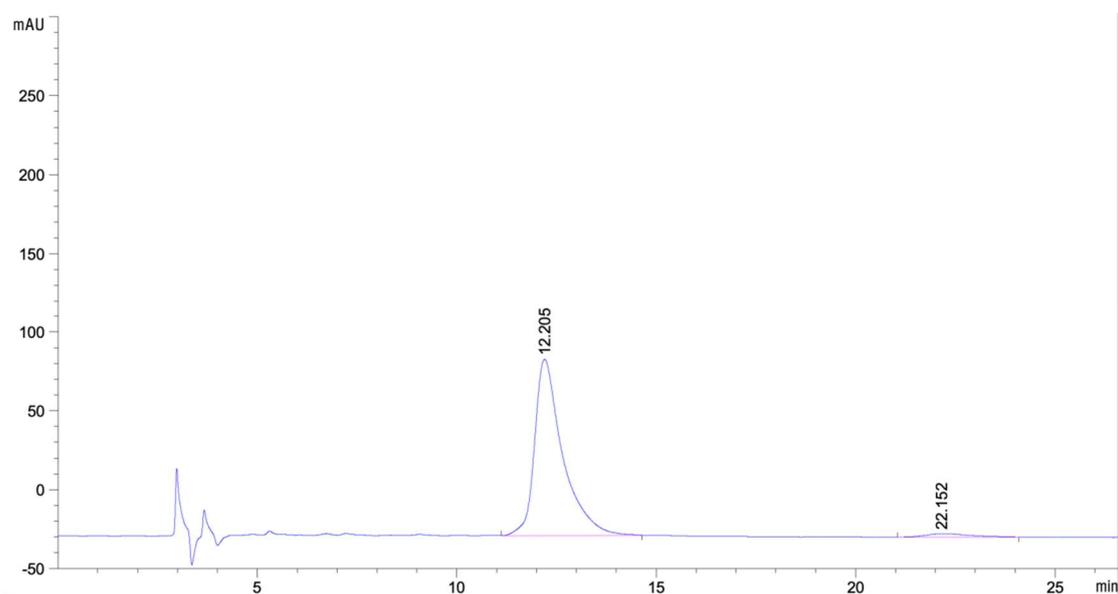
Brown oil, purified by column chromatography (silica gel, petroleum ether/EtOAc = 5/1), *R_f* = 0.6 (CH₂Cl₂:MeOH = 10:1), 69.0 mg, 92% yield, 94% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.34–7.26 (m, 1H), 7.17–6.94 (m, 3H), 3.56–3.36 (m, 2H), 3.27 (d, *J* = 6.7 Hz, 1H), 3.03 (d, *J* = 29.9 Hz, 3H), 2.21 (s, 6H), 1.37 (d, *J* = 6.7 Hz, 3H), 1.26–1.27 (m, 3H).

Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, Hex/IPA/TFA/DEA =

85/15/0.2/0.1; 1.0 mL/min; 220 nm): t_R (major) = 12.2 min, t_R (minor) = 22.1 min. The analytical data are in accordance with the literature¹⁰.

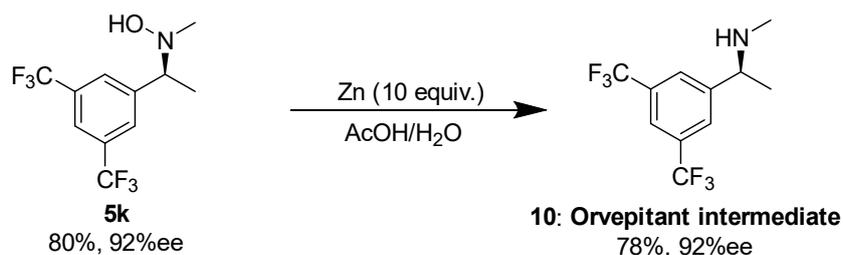


#	[min]	[min]	[mAU*s]	[mAU]	%
1	12.136 BV	0.6903	5515.58887	116.51347	50.1898
2	21.918 VB	1.1883	5473.88379	67.20217	49.8102



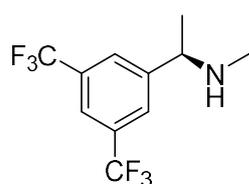
#	[min]	[min]	[mAU*s]	[mAU]	%
1	12.205 W	0.7093	5472.95361	111.76668	96.8384
2	22.152 W	0.9511	178.68025	2.22451	3.1616

(3) Synthesis of orvepitant intermediate.

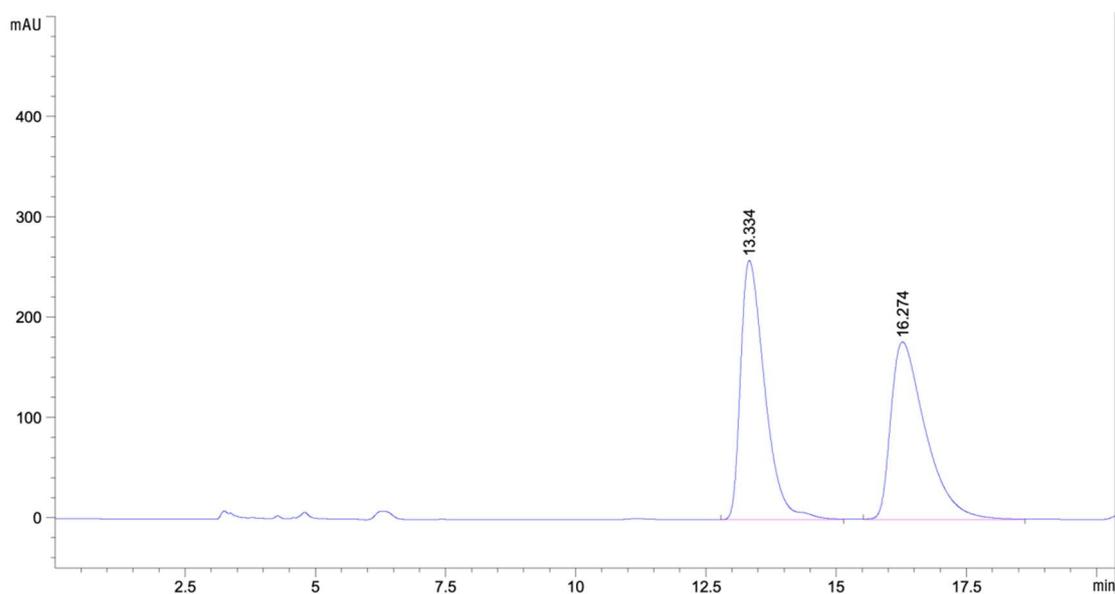


To a solution of **5k** (0.3 mmol) in AcOH-H₂O (5 mL, v/v=1:1), zinc powder (3 mmol, 10 equiv.) was slowly added. The mixture was then stirred at room temperature overnight. The residue was filtered over a celite pad, then diluted with water (2 mL), basified to pH 9-10 with 1M NaOH aqueous solution and extracted with CH₂Cl₂ (5 × 2 mL). The combined organic extracts were dried with anhydrous Na₂SO₄ and concentrated under reduced pressure to give crude reaction mixture. The crude reaction mixture was purified by flash column chromatography to afford product **10**.

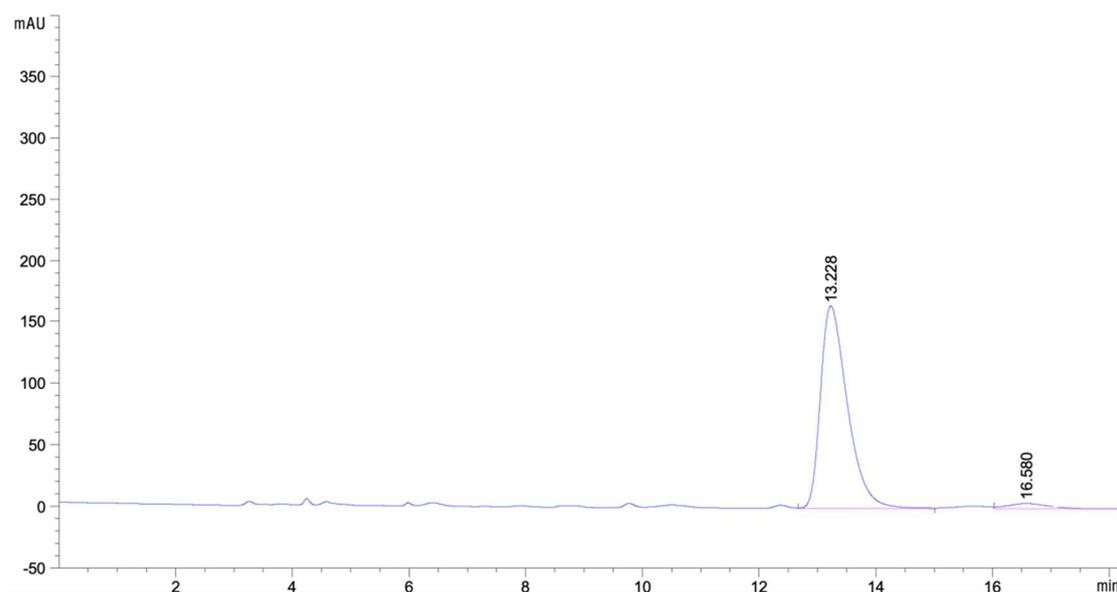
(S)-1-(3,5-bis(trifluoromethyl)phenyl)-N-methylethan-1-amine (10)



Brown oil, purified by column chromatography (silica gel, petroleum ether/EtOAc = 15/1), $R_f = 0.5$ (petroleum ether/EtOAc = 10/1), 63.4 mg, 80% yield of c steps, 92% *ee*. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.81 (s, 2H), 7.77 (s, 1H), 3.80 (q, $J = 6.6$ Hz, 1H), 2.32 (s, 3H), 1.38 (d, $J = 6.6$ Hz, 3H). Enantiomeric excess was determined by chiral HPLC (Chiralpak OJ-H, *n*-hexane/isopropanol = 90/10; 1.0 mL/min; 220 nm): t_R (major) = 13.2 min, t_R (minor) = 16.5 min. The analytical data are in accordance with the literature¹².



#	[min]	[min]	[min]	[mAU*s]	[mAU]	%
1	13.334 BV	0.4970	8347.40625	258.34402	50.4296	
2	16.274 W	0.6924	8205.18848	177.13063	49.5704	



#	[min]	[min]	[min]	[mAU*s]	[mAU]	%
1	13.228 W	0.4907	5272.32520	164.13937	96.2434	
2	16.580 VBA	0.7154	205.79109	4.23154	3.7566	

5. Characterization of the phosphoramidite ligands

N-(2-(diphenylphosphanyl)benzyl)-*N*-methyl-2,6-di(naphthalen-1-yl)dinaphtho[2,1-*d*:1',2'-

f][1,3,2]dioxaphosphepin-4-amine (**L5d**): White solid, 66% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.14 (s, 1H), 8.08 (s, 2H), 8.02 (d, *J* = 14.3 Hz, 4H), 7.92–7.82 (m, 3H), 7.76 (dd, *J* = 21.3, 7.4 Hz, 7H), 7.38 (ddp, *J* = 37.6, 14.2, 7.4 Hz, 18H), 7.21 (d, *J* = 8.5 Hz, 2H), 7.13 (d, *J* = 7.6 Hz, 3H), 7.02 (d, *J* = 7.4 Hz, 2H), 6.88 (dt, *J* = 32.5, 7.8 Hz, 5H), 6.73 (t, *J* = 7.7 Hz, 1H), 6.58–6.51 (m, 1H), 6.20 (s, 1H), 3.73 (d, *J* = 40.8 Hz, 1H), 1.90 (d, *J* = 10.8 Hz, 3H). ³¹P NMR (162 MHz, Chloroform-*d*) δ -14.89 (minor), 143.72 (major).

2,6-di([1,1':3',1''-terphenyl]-5'-yl)-*N*-(2-(diphenylphosphanyl)benzyl)-*N*-methylidinaphtho[2,1-

d:1',2'-*f*][1,3,2]dioxaphosphepin-4-amine (**L5f**): White solid, 57% yield. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 7.99–7.87 (m, 5H), 7.85–7.58 (m, 6H), 7.58–7.43 (m, 7H), 7.43–7.36 (m, 5H), 7.35–7.25 (m, 7H), 7.23–7.13 (m, 5H), 7.13–7.01 (m, 2H), 3.71–3.51 (m, 2H), 1.60 (d, *J* = 9.9 Hz, 3H). ³¹P NMR (162 MHz, Chloroform-*d*) δ -18.11 (major), 143.92 (minor).

6. DFT calculations

All calculations were performed using Gaussian 16 software¹³ with the density functional theory (DFT). Optimizations of intermediates and transition states were carried out at the B3LYP-D3(BJ) level of theory with the 6-31G(d,p) basis set for C, P, N, O, Cl, H and LANL2DZ for Ir in the gas phase. The vibrational frequencies were also computed at the same level so as to confirm each stationary point as a transition state (one and only one imaginary frequency) or a minimum (zero imaginary frequency). Single point energy calculations were performed on optimized geometries in dichloromethane solvent using the IEFPCM model at the B3LYP-D3(BJ) level of theory. For all nonmetallic atoms, the 6-311++G(d,p) basis set was adopted. For iridium, the LANL2DZ was employed, which was augmented with one f-polarization function (0.938). The Gibbs Free Energy of the optimized structure was obtained from the thermal correction to Gibbs Free Energy in frequency analysis and the single point energy.

7. Cartesian coordinates of optimized structures

Complex I

E(RB3LYP) = -6918.03887125

Thermal correction to Gibbs Free Energy= 1.407928

G = -6916.630943

C	-4.94747300	0.19044800	-0.08586700
C	-4.38211600	1.10920700	-0.95857100
C	-4.33036600	0.91537100	-2.36889800
C	-4.90012300	-0.23636500	-2.87445000
C	-5.00322300	0.50118400	1.36873000
C	-3.83624100	0.87329500	2.01495000
C	-3.78084700	1.24471600	3.39171100
C	-4.95259200	1.13849700	4.11871900
C	-6.18039500	0.76660300	3.51871300

C	-6.22706000	0.48314800	2.11440800
H	-4.90265000	-0.40024100	-3.94765700
H	-4.94411800	1.36407900	5.18092300
C	-5.84557700	-2.12825500	0.21168200
C	-5.97975900	-2.43820300	-2.56660200
C	-6.41793400	-3.44659000	-1.73992600
C	-6.32050500	-3.29833300	-0.33614400
H	-5.76909900	-2.02693900	1.28562000
H	-6.01178100	-2.55308600	-3.64596900
H	-6.81791700	-4.36472200	-2.16034800
H	-6.62038200	-4.11300700	0.31575600
C	-7.37961000	0.71122900	4.27884100
C	-7.49252200	0.22257300	1.52286800
C	-8.63835600	0.19272100	2.28527200
C	-8.58377300	0.42488200	3.68008700
H	-7.32616900	0.91493500	5.34497400
H	-7.54703200	0.04801900	0.45587600
H	-9.59436300	-0.00705800	1.81081800
H	-9.49443400	0.39060100	4.27026600
C	-5.42516900	-1.05202400	-0.61451200
C	-5.44279000	-1.23705300	-2.03347500
O	-2.66771500	0.87412700	1.29351200
O	-3.82334700	2.26605700	-0.44561100
P	-2.31281000	2.17630700	0.28310900
N	-2.48072700	3.54596800	1.21987600

C	-3.74418400	4.19130300	1.56272500
H	-3.78883600	5.19965700	1.13322900
H	-4.57920300	3.61341000	1.17741500
H	-3.83482900	4.26620100	2.65307800
C	-1.28400600	4.21407200	1.74399300
H	-1.51012000	4.56666900	2.75462900
H	-0.48058800	3.48558900	1.84848900
C	-2.54649500	1.79835400	4.00491500
C	-2.66202700	2.86345400	4.91594700
C	-1.25738500	1.32863300	3.69649400
C	-1.53466600	3.44039000	5.49913200
H	-3.64635500	3.25923900	5.14562700
C	-0.13205400	1.90689800	4.28060600
H	-1.13480400	0.52987300	2.97856800
C	-0.26224400	2.96586700	5.17973900
H	-1.65235700	4.26859800	6.19194900
H	0.85252300	1.53483500	4.02439300
H	0.62103100	3.42007900	5.61803300
C	-3.63273100	1.87327900	-3.26076000
C	-2.78383300	1.38029000	-4.26438900
C	-3.79162700	3.26258900	-3.13860500
C	-2.12862100	2.25009600	-5.13404300
H	-2.60991800	0.31208400	-4.33117900
C	-3.12925400	4.13130100	-4.00321600
H	-4.43384600	3.65960500	-2.36234800

C	-2.30013600	3.62945300	-5.00844900
H	-1.46924500	1.84842000	-5.89795600
H	-3.26389300	5.20329100	-3.89339400
H	-1.78229500	4.30960400	-5.67820900
C	-0.89589600	5.35989800	0.84164100
C	-0.13303100	5.12788800	-0.32151000
C	-1.38225500	6.64372800	1.09611600
C	0.08929000	6.18189400	-1.21517900
C	-1.15112200	7.69235400	0.20377500
H	-1.94944400	6.82004600	2.00618500
C	-0.42394900	7.45582700	-0.95954900
H	0.67648400	6.01365800	-2.10957600
H	-1.53852400	8.68403100	0.41765300
H	-0.24087800	8.26019300	-1.66562700
P	0.66105400	3.48124100	-0.57983700
C	1.94454800	3.52182100	0.73918500
C	2.23592300	2.34451700	1.44084400
C	2.58628200	4.71748100	1.09682000
C	3.14674000	2.37289200	2.49884400
H	1.74423700	1.42092600	1.15661100
C	3.51016900	4.73557000	2.14041800
H	2.35053800	5.63617800	0.56921800
C	3.78276800	3.56405000	2.84982100
H	3.36327200	1.46378300	3.04758800
H	4.00284600	5.66528900	2.40982100

H	4.48972200	3.57881900	3.67447700
C	1.54390000	3.72855700	-2.16769300
C	0.79569600	3.50828000	-3.33591600
C	2.87750200	4.13459800	-2.26445800
C	1.37183800	3.71782500	-4.58508500
H	-0.22874900	3.16028600	-3.25441700
C	3.44652100	4.35099900	-3.52162600
H	3.47931800	4.26714100	-1.37265700
C	2.69854700	4.14668800	-4.68035900
H	0.78449400	3.54145600	-5.48092100
H	4.48073200	4.66905500	-3.58880700
H	3.14918800	4.31352100	-5.65467200
Ir	-0.52560800	1.59749500	-0.77043600
Cl	1.52457300	0.51352100	-1.60638600
Cl	-1.52399900	-0.51418900	-1.60689700
C	4.94747800	-0.19029900	-0.08586900
C	4.38235300	-1.10960200	-0.95814200
C	4.33061800	-0.91651100	-2.36856700
C	4.90033900	0.23497500	-2.87471500
C	5.00301700	-0.50020300	1.36890500
C	3.83600600	-0.87216800	2.01516300
C	3.78046900	-1.24265400	3.39216300
C	4.95204500	-1.13566300	4.11933000
C	6.17987600	-0.76392200	3.51928900
C	6.22672300	-0.48143500	2.11479700

H	4.90285000	0.39830800	-3.94800600
H	4.94340600	-1.36050100	5.18168900
C	5.84512100	2.12874600	0.21046700
C	5.97987700	2.43701400	-2.56797300
C	6.41778900	3.44594900	-1.74182100
C	6.32003600	3.29854300	-0.33797100
H	5.76838400	2.02810100	1.28445100
H	6.01213500	2.55121800	-3.64740700
H	6.81780000	4.36385100	-2.16271500
H	6.61968100	4.11364500	0.31350200
C	7.37894400	-0.70777100	4.27959400
C	7.49224700	-0.22105600	1.52329700
C	8.63794200	-0.19045100	2.28588000
C	8.58315700	-0.42161400	3.68085300
H	7.32534800	-0.91073100	5.34586200
H	7.54692500	-0.04727100	0.45619000
H	9.59399600	0.00914600	1.81144500
H	9.49370400	-0.38673000	4.27117100
C	5.42504500	1.05195000	-0.61516100
C	5.44288200	1.23615000	-2.03422700
O	2.66754300	-0.87368300	1.29362900
O	3.82368100	-2.26623800	-0.44460500
P	2.31300500	-2.17635100	0.28373100
N	2.48084100	-3.54565500	1.22099900
C	3.74431200	-4.19046600	1.56479800

H	3.78895300	-5.19937300	1.13661000
H	4.57931200	-3.61307300	1.17868900
H	3.83497800	-4.26394000	2.65524600
C	1.28408700	-4.21344300	1.74544800
H	1.51014000	-4.56548900	2.75629000
H	0.48065900	-3.48490600	1.84949200
C	2.54612600	-1.79612800	4.00552700
C	2.66174500	-2.86058600	4.91730600
C	1.25696900	-1.32691300	3.69655400
C	1.53442300	-3.43736300	5.50071400
H	3.64612500	-3.25599300	5.14741400
C	0.13167400	-1.90501600	4.28090300
H	1.13431700	-0.52869300	2.97803300
C	0.26194900	-2.96332200	5.18079900
H	1.65218600	-4.26506700	6.19412000
H	-0.85294400	-1.53335600	4.02427200
H	-0.62129600	-3.41740100	5.61928800
C	3.63283500	-1.87483300	-3.25987700
C	2.78354000	-1.38225500	-4.26337200
C	3.79186200	-3.26408200	-3.13724400
C	2.12801000	-2.25243100	-5.13242000
H	2.60956700	-0.31407900	-4.33047500
C	3.12917400	-4.13315700	-4.00125000
H	4.43438900	-3.66075300	-2.36106600
C	2.29961700	-3.63173000	-5.00633200

H	1.46830300	-1.85109100	-5.89622500
H	3.26389100	-5.20509900	-3.89106900
H	1.78150600	-4.31216600	-5.67559500
C	0.89604300	-5.35972700	0.84365900
C	0.13323600	-5.12828400	-0.31965000
C	1.38241600	-6.64341900	1.09877800
C	-0.08896500	-6.18270700	-1.21284600
C	1.15138100	-7.69247400	0.20690900
H	1.94953900	-6.81929400	2.00897300
C	0.42430400	-7.45650700	-0.95658500
H	-0.67610300	-6.01491800	-2.10736300
H	1.53877700	-8.68404400	0.42129100
H	0.24132400	-8.26120200	-1.66231200
P	-0.66087000	-3.48175100	-0.57875700
C	-1.94409200	-3.52161600	0.74054600
C	-2.23582700	-2.34388200	1.44130500
C	-2.58540000	-4.71722900	1.09914400
C	-3.14657500	-2.37176600	2.49937600
H	-1.74453000	-1.42031800	1.15632300
C	-3.50923100	-4.73483500	2.14279900
H	-2.34935000	-5.63625900	0.57226300
C	-3.78218600	-3.56286100	2.85131300
H	-3.36339000	-1.46231700	3.04743900
H	-4.00159000	-5.66451300	2.41292600
H	-4.48909300	-3.57721700	3.67601700

C	-1.54412800	-3.73000800	-2.16626600
C	-0.79628100	-3.51000900	-3.33477600
C	-2.87758300	-4.13663400	-2.26256000
C	-1.37260200	-3.72041300	-4.58371900
H	0.22806500	-3.16163400	-3.25366400
C	-3.44679300	-4.35388800	-3.51948900
H	-3.47917100	-4.26891600	-1.37056800
C	-2.69915600	-4.14986600	-4.67849300
H	-0.78552000	-3.54424900	-5.47977000
H	-4.48089900	-4.67239200	-3.58629000
H	-3.14995300	-4.31736700	-5.65261900
Ir	0.52586500	-1.59818100	-0.77040500

Complex II

E(RB3LYP) = -7379.40453914

Thermal correction to Gibbs Free Energy= 1.431582

G = -7377.972957

C	2.90099200	1.22655000	2.79161300
C	1.65865400	1.70286300	3.17842200
C	0.88517700	1.15569400	4.23775000
C	1.42808400	0.09595500	4.93425100
C	3.66962300	1.91762500	1.71457900
C	3.05758000	2.19886200	0.50336400
C	3.66811600	2.94612900	-0.54780800
C	4.99451700	3.29184500	-0.36978400

C	5.68976800	3.02907000	0.83461800
C	5.01216700	2.38570800	1.92186700
H	0.87768700	-0.33339700	5.76617100
H	5.51697900	3.81576400	-1.16403300
C	4.57840500	-0.61795100	3.03775000
C	3.18944000	-1.60379200	5.26046000
C	4.34772200	-2.21680100	4.84631000
C	5.03584700	-1.72609200	3.71342200
H	5.10470900	-0.26517700	2.16011700
H	2.62965600	-1.99452400	6.10487000
H	4.71981300	-3.09213100	5.36831200
H	5.92857700	-2.23477800	3.36381300
C	7.03454000	3.45514300	1.00609200
C	5.69160700	2.27893600	3.16521200
C	6.98754800	2.72211500	3.30452000
C	7.67591800	3.29929800	2.21169200
H	7.53983900	3.92480200	0.16687200
H	5.17832000	1.84548300	4.01334500
H	7.48500400	2.63154900	4.26501000
H	8.70103900	3.63397200	2.33418200
C	3.40469200	0.06021700	3.46080500
C	2.67556900	-0.47205700	4.57368100
O	1.74429700	1.77384400	0.32680300
O	1.10551700	2.79798600	2.52370300
P	0.55576300	2.70157100	0.98300500
N	0.79287900	4.28741200	0.58736800
C	1.76789200	5.16572200	1.24162300

H	2.42410000	5.59834700	0.47970400
H	1.25274900	5.97011700	1.77727200
H	2.37109700	4.60707900	1.95040600
C	-0.00128100	4.92401300	-0.46713200
H	0.65576900	5.60058700	-1.01849800
H	-0.31412000	4.17148500	-1.18852700
C	2.89503600	3.44814300	-1.71242600
C	3.14363200	4.74601200	-2.19452400
C	1.87905300	2.70052000	-2.32435600
C	2.39057400	5.28027400	-3.24052900
H	3.91548000	5.35071700	-1.72846900
C	1.10924500	3.24369900	-3.35061300
H	1.68939900	1.69107500	-1.99916600
C	1.35685000	4.53641700	-3.81297600
H	2.60070400	6.28580700	-3.59302900
H	0.31713600	2.64540200	-3.78879200
H	0.75021800	4.95834500	-4.60815600
C	-0.48480900	1.66587300	4.49960100
C	-1.54751100	0.75611100	4.58121200
C	-0.76687000	3.03774900	4.59833600
C	-2.85943800	1.20222500	4.73482100
H	-1.33823000	-0.30029800	4.47064500
C	-2.07768800	3.48457400	4.75034300
H	0.04254100	3.75551000	4.54444000
C	-3.13086300	2.56895000	4.81349800
H	-3.67573800	0.48669000	4.77494900
H	-2.27726700	4.54944900	4.82041000

H	-4.15251800	2.91914800	4.92648500
C	-1.16467800	5.66395500	0.14506800
C	-2.38275100	5.00290800	0.40270100
C	-1.01414200	6.99382700	0.54484200
C	-3.40339900	5.67543500	1.08609500
C	-2.03289300	7.65847400	1.22940700
H	-0.08819900	7.51240900	0.31386100
C	-3.22331500	6.99264800	1.51093900
H	-4.34540100	5.17774600	1.27835800
H	-1.89649300	8.69060100	1.53627400
H	-4.02240900	7.49894400	2.04269200
P	-2.66072600	3.31289700	-0.24815100
C	-2.66998400	3.51806400	-2.07003300
C	-2.85977400	2.38269800	-2.87497900
C	-2.53054100	4.77552700	-2.67365300
C	-2.90401300	2.51832100	-4.26159100
H	-2.97020000	1.40584000	-2.41979000
C	-2.54986000	4.89777200	-4.06295700
H	-2.40712600	5.66264400	-2.06486200
C	-2.73632600	3.76937200	-4.85947200
H	-3.06832700	1.64620400	-4.88358100
H	-2.43176800	5.87652200	-4.51709300
H	-2.76212400	3.86255900	-5.94072600
C	-4.40406400	2.96894300	0.18480500
C	-4.71618600	2.51526800	1.47606000
C	-5.43330600	3.19376900	-0.73727400
C	-6.04235300	2.29075400	1.83433500

H	-3.92548700	2.32954500	2.19316500
C	-6.75993000	2.95855600	-0.37390000
H	-5.20295100	3.54711400	-1.73548400
C	-7.06670400	2.50689100	0.90944100
H	-6.27437800	1.93695300	2.83416400
H	-7.55202500	3.12914700	-1.09618800
H	-8.09954900	2.32312600	1.18859400
Ir	-1.34510600	1.60766100	0.55422400
Cl	-0.44659500	0.46107400	-1.58712500
Cl	-0.44654500	-0.46159000	1.58708300
C	2.90226600	-1.22463200	-2.79147400
C	1.66021900	-1.70161300	-3.17843200
C	0.88656900	-1.15479700	-4.23780500
C	1.42898700	-0.09470400	-4.93416300
C	3.67117100	-1.91533300	-1.71442400
C	3.05921000	-2.19696000	-0.50326300
C	3.67018500	-2.94373900	0.54798700
C	4.99684200	-3.28856000	0.37010600
C	5.69199000	-3.02542700	-0.83427200
C	5.01402300	-2.38257900	-1.92160400
H	0.87844000	0.33440400	-5.76611000
H	5.51958400	-3.81205800	1.16444900
C	4.57864700	0.62087100	-3.03720400
C	3.18936600	1.60613000	-5.25998200
C	4.34721700	2.21979300	-4.84560900
C	5.03550500	1.72935600	-3.71269700
H	5.10503900	0.26832100	-2.15953600

H	2.62945200	1.99662900	-6.10441300
H	4.71883800	3.09541400	-5.36745500
H	5.92787900	2.23854700	-3.36291600
C	7.03705200	-3.45063200	-1.00564100
C	5.69347000	-2.27545700	-3.16491300
C	6.98970900	-2.71779600	-3.30411700
C	7.67840000	-3.29445000	-2.21121000
H	7.54259400	-3.91990900	-0.16635300
H	5.17996200	-1.84240600	-4.01311900
H	7.48714800	-2.62697500	-4.26459100
H	8.70374800	-3.62845500	-2.33362200
C	3.40538300	-0.05794500	-3.46048400
C	2.67609400	0.47399900	-4.57340100
O	1.74562200	-1.77282600	-0.32675300
O	1.10772600	-2.79716000	-2.52385400
P	0.55774300	-2.70126600	-0.98321000
N	0.79577700	-4.28698800	-0.58771500
C	1.77144100	-5.16471100	-1.24179000
H	1.25686300	-5.96977900	-1.77696200
H	2.37397800	-4.60581400	-1.95094100
H	2.42822100	-5.59644600	-0.47985100
C	0.00237500	-4.92385300	0.46720400
H	0.66008600	-5.59964900	1.01873800
H	-0.31100500	-4.17130400	1.18833900
C	2.89735500	-3.44625100	1.71254600
C	3.14692700	-4.74389300	2.19474900
C	1.88072200	-2.69937400	2.32432400

C	2.39421100	-5.27867600	3.24073100
H	3.91928800	-5.34801800	1.72879100
C	1.11125800	-3.24309600	3.35054600
H	1.69031800	-1.69009100	1.99906100
C	1.35985300	-4.53558500	3.81302100
H	2.60512000	-6.28400300	3.59334900
H	0.31860000	-2.64542700	3.78858100
H	0.75350100	-4.95791900	4.60819500
C	-0.48314900	-1.66558000	-4.49981200
C	-1.54622300	-0.75626700	-4.58151100
C	-0.76463700	-3.03756800	-4.59861200
C	-2.85795800	-1.20290100	-4.73522600
H	-1.33737400	0.30022300	-4.47091400
C	-2.07526200	-3.48492400	-4.75074000
H	0.04507100	-3.75499700	-4.54469000
C	-3.12881600	-2.56973700	-4.81393900
H	-3.67451000	-0.48765900	-4.77543400
H	-2.27438300	-4.54987900	-4.82087800
H	-4.15032000	-2.92035100	-4.92699900
C	-1.16053200	-5.66496700	-0.14448900
C	-2.37914000	-5.00492300	-0.40221500
C	-1.00906700	-6.99490100	-0.54367200
C	-3.39938100	-5.67853400	-1.08514600
C	-2.02744300	-7.66063600	-1.22774500
H	-0.08269000	-7.51267400	-0.31260900
C	-3.21839400	-6.99581900	-1.50939400
H	-4.34178500	-5.18164900	-1.27751200

H	-1.89033100	-8.69280900	-1.53413800
H	-4.01718800	-7.50294200	-2.04081100
P	-2.65840300	-3.31483200	0.24795400
C	-2.66779400	-3.51933100	2.06991500
C	-2.85905000	-2.38387900	2.87439200
C	-2.52705800	-4.77640500	2.67404600
C	-2.90349900	-2.51905300	4.26103600
H	-2.97042900	-1.40730300	2.41880600
C	-2.54654200	-4.89815700	4.06338900
H	-2.40256600	-5.66363700	2.06565100
C	-2.73451800	-3.76968100	4.85943700
H	-3.06900300	-1.64690900	4.88266100
H	-2.42740500	-5.87660600	4.51790100
H	-2.76048900	-3.86247500	5.94072000
C	-4.40189500	-2.97227000	-0.18543300
C	-4.71409500	-2.51892000	-1.47678200
C	-5.43115400	-3.19784900	0.73645200
C	-6.04037000	-2.29546600	-1.83534000
H	-3.92338500	-2.33261900	-2.19373000
C	-6.75788500	-2.96371200	0.37278400
H	-5.20073000	-3.55095900	1.73473000
C	-7.06473900	-2.51235400	-0.91064900
H	-6.27246600	-1.94189600	-2.83523400
H	-7.54999500	-3.13489600	1.09491500
H	-8.09766600	-2.32941300	-1.19003700
Ir	-1.34391500	-1.60874700	-0.55445200
Cl	-3.21395000	-0.00115400	-0.00035000

H	-1.86591100	-2.06647000	-1.95075300
H	-1.86750300	2.06506800	1.95047200

Complex III

E(RB3LYP) = -3591.24916997

Thermal correction to Gibbs Free Energy= 0.738282

G = -3590.510888 hartree

C	3.55643600	-0.94597100	0.13611900
C	2.41619500	-1.43480100	0.75755300
C	2.05155300	-2.81154900	0.78241100
C	2.91492000	-3.70121700	0.16827700
C	3.80301500	0.52546000	0.10229500
C	2.81706400	1.35017000	-0.40739500
C	2.89734500	2.76916700	-0.45455300
C	4.08298200	3.33278300	-0.01882300
C	5.13757900	2.55311000	0.51748300
C	4.99564500	1.12924700	0.61721300
H	2.67710300	-4.76004900	0.17866100
H	4.20909100	4.41000600	-0.06729000
C	5.54049700	-1.46878400	-1.30399900
C	4.93330100	-4.20468600	-1.15865100
C	6.03393500	-3.77864200	-1.86301000
C	6.32967900	-2.39719100	-1.94439900
H	5.77575600	-0.41498300	-1.38073200
H	4.68320800	-5.25999100	-1.10625300

H	6.67062500	-4.49692500	-2.36889900
H	7.18643000	-2.06588900	-2.52230200
C	6.32506900	3.16473800	1.00189100
C	6.02499200	0.38636400	1.25313100
C	7.15559800	1.01389300	1.72552200
C	7.31554300	2.41330000	1.58884600
H	6.42984700	4.24168800	0.90882900
H	5.91194100	-0.68482600	1.36666600
H	7.93164400	0.43043700	2.21040400
H	8.21671500	2.89108600	1.95897200
C	4.41252900	-1.87639900	-0.54248000
C	4.08947800	-3.27309900	-0.49646000
O	1.62549400	0.74595000	-0.82922700
O	1.52533800	-0.52774600	1.34271600
P	0.53883600	0.34551500	0.36069600
N	0.26093900	1.61957400	1.35523500
C	1.14899700	2.03234800	2.44864600
H	0.62876900	1.93804300	3.40675300
H	2.03860200	1.40942400	2.47031500
H	1.44541300	3.07399900	2.29420000
C	-0.95847600	2.42656100	1.18664700
H	-0.69249500	3.46769300	1.38075900
H	-1.27167200	2.39568400	0.14405300
C	1.72435400	3.59788300	-0.83272300
C	1.43048300	4.75123800	-0.08537500

C	0.85294300	3.24709600	-1.87918600
C	0.29473600	5.51482200	-0.35680800
H	2.08676300	5.03747800	0.73068500
C	-0.28924000	4.00157300	-2.14026500
H	1.07126300	2.37965800	-2.48874800
C	-0.57912100	5.13332700	-1.37543900
H	0.08856400	6.40005600	0.23704800
H	-0.95668000	3.70558100	-2.94235400
H	-1.47544100	5.71077800	-1.57652600
C	0.75604600	-3.26300500	1.34801100
C	-0.03701200	-4.15998100	0.61023500
C	0.28475600	-2.80947200	2.59189300
C	-1.25899800	-4.60662600	1.11247000
H	0.29072500	-4.47016600	-0.37603100
C	-0.94072900	-3.25096800	3.08620600
H	0.88364100	-2.11684700	3.17075900
C	-1.71291200	-4.15562900	2.35294000
H	-1.85934000	-5.29555000	0.52684200
H	-1.28827400	-2.89705400	4.05166700
H	-2.66430300	-4.50136300	2.74516200
C	-2.03165300	1.94994900	2.13432300
C	-2.89316600	0.88376900	1.79619100
C	-2.12071100	2.51605300	3.40796400
C	-3.78984300	0.39150600	2.75345400
C	-3.01566700	2.02036700	4.35782000

H	-1.48151000	3.35855800	3.65581200
C	-3.84147300	0.94787400	4.03234900
H	-4.45998000	-0.41983400	2.49886400
H	-3.06709800	2.47321700	5.34268500
H	-4.54071500	0.55221100	4.76157700
P	-2.93325000	0.20731400	0.09300100
C	-3.41968900	1.62371600	-0.96306000
C	-3.25953100	1.51793200	-2.35458900
C	-3.94324800	2.80512100	-0.41699800
C	-3.60889200	2.58499300	-3.18178400
H	-2.89120000	0.59678500	-2.79169800
C	-4.28466600	3.86992800	-1.25016500
H	-4.07961600	2.89706300	0.65431900
C	-4.11488200	3.76411200	-2.63193500
H	-3.48940800	2.49074000	-4.25646100
H	-4.68969500	4.77973500	-0.81863500
H	-4.38424500	4.59382600	-3.27776700
C	-4.34245600	-0.93827500	0.10089800
C	-4.13786700	-2.26396400	0.50669900
C	-5.62815700	-0.49601000	-0.23208100
C	-5.21810900	-3.13771900	0.58856800
H	-3.14047900	-2.61310900	0.74430700
C	-6.70442200	-1.38051300	-0.15727200
H	-5.78871600	0.52765100	-0.55211800
C	-6.50166200	-2.69828700	0.25439600

H	-5.05663300	-4.16510900	0.89947700
H	-7.69961200	-1.03970600	-0.42380900
H	-7.34120400	-3.38393300	0.30918900
Ir	-1.02287700	-0.75241800	-0.81574700
N	0.64451700	-1.68146800	-1.91815800
H	0.99524100	-1.02812800	-2.62354600
H	1.43042400	-1.87382300	-1.29730900
O	0.40631900	-2.92312800	-2.56274900
H	-0.56758100	-2.91988000	-2.69842800
Cl	-2.41503200	-1.93391300	-2.39538300
H	-0.98651500	-1.75496400	0.34599200

Complex IV

E(RB3LYP) = -3592.42895438

Thermal correction to Gibbs Free Energy= 0.756077

G = -3591.672877 hartree

C	3.43761500	-0.99548100	0.01808000
C	2.28585500	-1.48821900	0.61513100
C	1.91379000	-2.86437600	0.59780400
C	2.74299600	-3.72479900	-0.10477400
C	3.78135000	0.44821300	0.15732900
C	2.85526900	1.39314900	-0.23760400
C	3.02102300	2.79684100	-0.08559700
C	4.23729200	3.21451500	0.42592100
C	5.23868100	2.30521700	0.84580900

C	5.00770800	0.89349400	0.74846300
H	2.52137900	-4.78711700	-0.10640400
H	4.43054600	4.27797600	0.52579400
C	5.36031500	-1.44884000	-1.52058600
C	4.68057900	-4.17247100	-1.57153900
C	5.76660000	-3.71749300	-2.28101600
C	6.09968400	-2.34197300	-2.26246900
H	5.62187500	-0.39815400	-1.51696600
H	4.40778700	-5.22344500	-1.58956000
H	6.36562600	-4.40854800	-2.86485400
H	6.94579500	-1.98785800	-2.84231200
C	6.46003800	2.76898900	1.40458500
C	5.98654300	0.00668500	1.26948600
C	7.15263800	0.49125000	1.81777600
C	7.39994000	1.88339500	1.87600100
H	6.63153600	3.83987100	1.46109300
H	5.80812700	-1.06090900	1.23524600
H	7.88950900	-0.20103800	2.21222500
H	8.32796900	2.24818000	2.30391500
C	4.24449800	-1.88921900	-0.75989800
C	3.88536400	-3.27502100	-0.80961300
O	1.65101000	0.90995500	-0.77351900
O	1.42099500	-0.58169700	1.24899900
P	0.50904700	0.39576100	0.29527000
N	0.11936100	1.56947400	1.35908500

C	0.92473000	1.91374900	2.53742600
H	0.35911100	1.70447000	3.45015000
H	1.84169600	1.33032400	2.54976700
H	1.17667600	2.97663500	2.49502800
C	-1.11767200	2.34888700	1.16612700
H	-0.88247700	3.39807000	1.36192100
H	-1.41763000	2.29895100	0.11768100
C	1.91903400	3.75427500	-0.35170700
C	1.70705300	4.81689700	0.54499900
C	1.04563800	3.61549700	-1.44220300
C	0.64979000	5.70758800	0.36281800
H	2.36578300	4.93294300	1.40036900
C	-0.01784400	4.49950400	-1.61616100
H	1.17822300	2.80828100	-2.14881900
C	-0.22204300	5.54706900	-0.71629800
H	0.50515200	6.52166100	1.06660800
H	-0.68694900	4.35859000	-2.45849800
H	-1.05080900	6.23425000	-0.85552400
C	0.71272600	-3.38603600	1.29672000
C	-0.02918800	-4.43088300	0.71904000
C	0.31130900	-2.89736000	2.55135900
C	-1.12143800	-4.98664700	1.38189000
H	0.24776400	-4.80760600	-0.26078500
C	-0.78995000	-3.44449100	3.20676300
H	0.87099000	-2.09788500	3.01953900

C	-1.50577200	-4.49602000	2.63114700
H	-1.67245300	-5.79970500	0.91950000
H	-1.07929200	-3.05847700	4.17910200
H	-2.35579900	-4.92651900	3.15088100
C	-2.17309600	1.82665600	2.11026100
C	-2.95162800	0.69592500	1.78305400
C	-2.31013700	2.40194300	3.37528800
C	-3.81909800	0.15416200	2.73965700
C	-3.17788500	1.85840500	4.32459800
H	-1.72963800	3.28775100	3.61647600
C	-3.92196000	0.72474400	4.00933700
H	-4.42888000	-0.70562500	2.49194500
H	-3.26977300	2.32024400	5.30229800
H	-4.59725300	0.29094800	4.73944700
P	-2.98582600	0.05272300	0.06876000
C	-3.88741200	1.33372500	-0.87037700
C	-4.12693000	1.11688100	-2.23645800
C	-4.38912400	2.49029600	-0.25916800
C	-4.85409900	2.04301200	-2.97688100
H	-3.73947300	0.23140500	-2.72509200
C	-5.10619900	3.42315700	-1.00970300
H	-4.23181900	2.66521100	0.79795100
C	-5.33942500	3.20189900	-2.36615600
H	-5.03029300	1.86647100	-4.03274000
H	-5.48749000	4.31804200	-0.52845800

H	-5.89922900	3.92765800	-2.94737900
C	-4.13847600	-1.36451700	0.13607100
C	-3.67538500	-2.60133000	0.61166100
C	-5.48393600	-1.22341500	-0.23143900
C	-4.54753400	-3.68262700	0.70874400
H	-2.64275600	-2.72050000	0.91447300
C	-6.34980800	-2.31387700	-0.13868000
H	-5.85394000	-0.27026600	-0.58976800
C	-5.88443500	-3.54329600	0.32853200
H	-4.17867200	-4.63319600	1.07921300
H	-7.38837100	-2.19959400	-0.43196100
H	-6.56075200	-4.38935200	0.39759400
Ir	-1.00513900	-0.66365200	-0.98765300
N	0.65908100	-1.45425000	-2.12849700
H	1.47594600	-0.84130600	-2.04755900
H	0.94603200	-2.38609600	-1.83004900
O	0.35054900	-1.58890600	-3.51105500
H	-0.05495800	-0.71281200	-3.71228700
Cl	-0.95838200	1.07979800	-2.81707500
H	-0.91436600	-1.79888800	0.10148900
H	-2.05334400	-1.45079100	-2.28424500
H	-2.02625900	-2.00204600	-1.68814500

Complex V

E(RB3LYP) = -4032.83429777

Thermal correction to Gibbs Free Energy= 0.901213

G = -4031.933085 hartree

C	-3.33977400	0.87652200	0.73605300
C	-2.20384100	0.74230000	1.52740600
C	-1.55990000	1.84370600	2.17001300
C	-2.08572000	3.10165800	1.92803700
C	-4.00986200	-0.34543900	0.20592400
C	-3.26748100	-1.25413400	-0.52463300
C	-3.77285600	-2.49695100	-1.00055900
C	-5.11201300	-2.74975300	-0.76583100
C	-5.93496300	-1.85975900	-0.03248900
C	-5.37914600	-0.65055700	0.50041700
H	-1.65715400	3.96085400	2.43304900
H	-5.55064500	-3.66919600	-1.14119300
C	-4.84732200	2.43915400	-0.51350300
C	-3.61775200	4.63061700	0.73444100
C	-4.63483700	4.83195800	-0.16930200
C	-5.24529800	3.72411200	-0.80586200
H	-5.31927700	1.59724000	-1.00478200
H	-3.14265500	5.47263300	1.23068300
H	-4.97350500	5.83781300	-0.39679900
H	-6.03639400	3.89064700	-1.52980600
C	-7.29832500	-2.16674200	0.22286500
C	-6.20150300	0.16957900	1.31744000
C	-7.51576400	-0.16494400	1.55595500

C	-8.07614900	-1.33648800	0.99499700
H	-7.71142200	-3.07953900	-0.19651600
H	-5.78475400	1.06539500	1.76084500
H	-8.12742000	0.47432600	2.18473400
H	-9.11546000	-1.58279500	1.18675400
C	-3.80825300	2.19621700	0.42486200
C	-3.16553700	3.31818500	1.04031800
O	-1.94238200	-0.93173300	-0.79360100
O	-1.64214300	-0.52440400	1.66482100
P	-0.75520700	-1.07240600	0.35995100
N	-0.56638300	-2.64477000	0.80172800
C	-1.53411000	-3.39410300	1.60554400
H	-1.15276900	-3.55334000	2.61980800
H	-2.46857400	-2.84078600	1.67415900
H	-1.73064200	-4.35735100	1.12702500
C	0.73800600	-3.28516000	0.55719600
H	0.55118200	-4.34775200	0.37748700
H	1.16061100	-2.88765600	-0.36615300
C	-2.88182200	-3.51458500	-1.61101900
C	-3.03251500	-4.86166600	-1.23857700
C	-1.85234800	-3.18034300	-2.50572300
C	-2.17269200	-5.84179000	-1.73157200
H	-3.81076100	-5.13447700	-0.53240900
C	-0.98748700	-4.15909400	-2.99016400
H	-1.71170100	-2.15318200	-2.81144200

C	-1.13991700	-5.49189800	-2.60332900
H	-2.30396400	-6.87554800	-1.42640100
H	-0.19053200	-3.87078900	-3.66787100
H	-0.46284300	-6.25213000	-2.98066800
C	-0.37146500	1.67826200	3.04287900
C	0.59934800	2.69462500	3.08991800
C	-0.17754500	0.54055400	3.84398700
C	1.72143700	2.58025200	3.90570600
H	0.48694300	3.56670000	2.45505000
C	0.95650900	0.41904300	4.64408800
H	-0.91433800	-0.25078600	3.84004700
C	1.91235900	1.43456900	4.67877000
H	2.45838200	3.37706100	3.92469900
H	1.09119300	-0.47564600	5.24278700
H	2.79572800	1.33659300	5.30168300
C	1.64838700	-3.08883000	1.75267600
C	2.50684400	-1.97177900	1.87548300
C	1.55891800	-3.99089000	2.81786200
C	3.19587300	-1.76506600	3.07722500
C	2.25598300	-3.78181700	4.00821700
H	0.93303600	-4.87172100	2.70851500
C	3.06359400	-2.65578800	4.14252000
H	3.84281200	-0.90403200	3.18460500
H	2.16726700	-4.49522000	4.82131100
H	3.60568400	-2.47480200	5.06518900

P	2.78048800	-0.82439900	0.46745100
C	3.70664200	-1.81258300	-0.76849900
C	4.18539900	-1.13941900	-1.90298700
C	3.97825600	-3.17575100	-0.61684700
C	4.91141100	-1.82018800	-2.87336600
H	3.98755400	-0.08008400	-2.02235100
C	4.70082500	-3.86026500	-1.59763400
H	3.63999200	-3.70626600	0.26557400
C	5.16536900	-3.18696900	-2.72548100
H	5.27514800	-1.28822500	-3.74689900
H	4.90422400	-4.91902800	-1.47193300
H	5.72777800	-3.72059400	-3.48503900
C	4.08045500	0.32695400	1.05856400
C	3.76621900	1.63705900	1.43819600
C	5.41094000	-0.11329400	1.14483100
C	4.76718600	2.49417800	1.89601800
H	2.74220000	1.97790000	1.37729800
C	6.40778500	0.74620400	1.60238900
H	5.66683700	-1.12483000	0.84835400
C	6.08827300	2.05328500	1.97703200
H	4.51391400	3.50804500	2.19215700
H	7.43381000	0.39730100	1.66143500
H	6.86650100	2.72318500	2.32913600
Ir	0.96459500	0.26871800	-0.40933300
N	-0.59382000	1.58022700	-1.20601900

H	-1.50325000	1.38364000	-0.78726000
H	-0.36840400	2.54889400	-0.98810500
O	-0.81135200	1.56126200	-2.61747000
H	-0.46885600	0.67376200	-2.87079700
Cl	0.97266800	-0.90352100	-2.74223900
H	0.91396200	1.07754100	0.92318400
H	2.15694900	1.69598500	-2.22155400
H	2.08894600	1.36358000	-0.84223400
C	1.61153300	3.18848700	-3.51639500
N	2.15615100	2.05648400	-3.21001800
O	2.60043400	1.18186200	-4.15598200
H	2.20456400	0.31139400	-3.84455700
C	1.40511600	3.55434000	-4.94465000
H	1.09338400	2.67955100	-5.51912200
H	0.68023400	4.36153500	-5.03803400
H	2.35503700	3.90195600	-5.36728900
C	1.20427500	4.02586700	-2.37799700
C	1.99206900	4.09298400	-1.21568600
C	-0.06234800	4.63750700	-2.39878800
C	1.50778200	4.74511800	-0.08462200
H	2.97887800	3.64387100	-1.19762500
C	-0.55019900	5.26299100	-1.25451900
H	-0.69009300	4.55860000	-3.27861500
C	0.23360100	5.31611700	-0.09732300
H	2.12400500	4.79839700	0.80628000

H	-1.54867300	5.68583300	-1.25620200
H	-0.14901400	5.80852000	0.79066800

TS-R

E(RB3LYP) = -4032.81473934

Thermal correction to Gibbs Free Energy= 0.907974

G = -4031.906765 hartree

Imaginary frequency: -531.0394 cm⁻¹

C	3.93529600	-1.10949600	0.12287700
C	2.82999100	-1.36972000	0.92186300
C	2.41579200	-2.68711600	1.28733000
C	3.17603100	-3.74288500	0.81287200
C	4.32259500	0.30031600	-0.16813900
C	3.37993200	1.16307400	-0.69635300
C	3.60761500	2.54819200	-0.93438300
C	4.88596500	3.01470800	-0.69059100
C	5.90358000	2.18941900	-0.15268400
C	5.62047900	0.81831700	0.15626300
H	2.91310400	-4.75589500	1.10122600
H	5.11625200	4.05660600	-0.89093000
C	5.70575100	-2.05726600	-1.37278100
C	5.00451900	-4.65402100	-0.57343200
C	6.03392400	-4.46024600	-1.46332800
C	6.37531100	-3.14990400	-1.87498800
H	5.97278700	-1.06042900	-1.69977500
H	4.72002800	-5.65559800	-0.26455100

H	6.57866300	-5.30964600	-1.86229500
H	7.17176200	-3.00589400	-2.59790600
C	7.19216200	2.71389400	0.13583600
C	6.62414000	0.05096600	0.80533500
C	7.85684500	0.59583800	1.08625200
C	8.15208900	1.93461100	0.73670700
H	7.39902600	3.74955700	-0.11749400
H	6.41201700	-0.97330700	1.08451600
H	8.60953100	-0.00695900	1.58431900
H	9.13178800	2.34613600	0.95659200
C	4.65536800	-2.21952500	-0.43064800
C	4.28050300	-3.54918000	-0.05020400
O	2.09958000	0.65276000	-0.93357800
O	2.06031600	-0.30783200	1.38904800
P	1.08251300	0.55121700	0.36281800
N	1.06971300	1.97027600	1.19668600
C	2.13815000	2.38728700	2.11328400
H	1.80628400	2.30089300	3.15291200
H	3.02165300	1.77080200	1.97732600
H	2.39550300	3.42773000	1.89694000
C	-0.14461900	2.80084400	1.22666000
H	0.17339000	3.84420600	1.28854400
H	-0.66722600	2.70589800	0.27650200
C	2.49837800	3.46848500	-1.28886000
C	2.40603600	4.70992700	-0.63555100

C	1.49476400	3.12113200	-2.20604000
C	1.33149800	5.56646100	-0.87259800
H	3.16966500	4.99172400	0.08304600
C	0.41709100	3.97408300	-2.43503400
H	1.53988400	2.17592500	-2.72813500
C	0.32441500	5.19522300	-1.76549400
H	1.27708900	6.51798700	-0.35230900
H	-0.35008000	3.67377800	-3.14076200
H	-0.52335600	5.85092400	-1.93763100
C	1.17475600	-2.93193300	2.06547000
C	0.32244700	-3.98253800	1.68462500
C	0.80603400	-2.13790400	3.16422600
C	-0.85802900	-4.23786400	2.38112400
H	0.58766500	-4.60333400	0.83329500
C	-0.37860500	-2.38633200	3.85310700
H	1.44919300	-1.32573200	3.47676900
C	-1.21290800	-3.43868800	3.46879300
H	-1.49768700	-5.05961900	2.07375400
H	-0.64834800	-1.75766400	4.69567300
H	-2.13126900	-3.63283300	4.01402900
C	-0.99004500	2.40652100	2.41561600
C	-1.91091900	1.33896500	2.34064000
C	-0.76432600	3.02344900	3.64833100
C	-2.53915100	0.89088800	3.50814800
C	-1.39676300	2.57425500	4.80874900

H	-0.08253900	3.86753500	3.69731900
C	-2.27204600	1.49426300	4.73916900
H	-3.25668500	0.08213000	3.46229800
H	-1.20637100	3.06715000	5.75667900
H	-2.76985500	1.13245300	5.63315500
P	-2.40031700	0.68670300	0.68470100
C	-3.11774000	2.21265100	-0.04217800
C	-2.82441600	2.61647300	-1.34815800
C	-3.94196100	3.02204900	0.76017800
C	-3.37210700	3.79494100	-1.85853900
H	-2.14822400	2.02940300	-1.95366500
C	-4.49478400	4.19056200	0.24273400
H	-4.14555600	2.74248500	1.78827200
C	-4.21407500	4.57809200	-1.07051400
H	-3.13117800	4.09969100	-2.87227900
H	-5.13573500	4.80429100	0.86765300
H	-4.64065100	5.49323400	-1.46909600
C	-3.82882100	-0.38908500	1.08961500
C	-3.57276600	-1.64504700	1.66266200
C	-5.15317000	0.03493800	0.93925500
C	-4.62395100	-2.45150300	2.09255800
H	-2.55256500	-1.98440200	1.78828600
C	-6.20271700	-0.77974200	1.36547000
H	-5.37397700	0.98674900	0.47530800
C	-5.94425400	-2.01939800	1.94748700

H	-4.40910400	-3.41577400	2.54339600
H	-7.22544800	-0.44267100	1.23249600
H	-6.76412900	-2.64679300	2.28261600
Ir	-0.77034000	-0.53402000	-0.42346400
N	0.59703800	-2.04384300	-1.24888400
H	1.42140600	-2.19343900	-0.66603000
H	0.08992500	-2.92790600	-1.27479300
O	1.09777600	-1.87237500	-2.57624700
H	0.85075100	-0.93438000	-2.78487700
H	-0.77968000	-1.36289500	0.90529300
H	-2.05016900	-1.52973100	-1.07120600
Cl	-0.67538600	0.43416100	-2.80051400
C	-2.82663900	-2.38303200	-1.93080600
N	-2.23988600	-2.45041600	-3.15500100
H	-2.28238300	-1.64317900	-3.76933400
O	-1.10999200	-3.23730900	-3.32795300
H	-0.32523800	-2.63616400	-3.32059500
C	-2.75107600	-3.64954300	-1.10552600
H	-3.16438700	-3.46806800	-0.11602700
H	-3.32283300	-4.43600600	-1.60759400
H	-1.72598500	-4.00301400	-1.01154900
C	-4.12742500	-1.63089000	-1.97862000
C	-4.15421600	-0.30600000	-2.43157700
C	-5.32686600	-2.27057600	-1.64797900
C	-5.36393700	0.37144900	-2.55358400

H	-3.22306000	0.19481200	-2.66535500
C	-6.53800400	-1.59482300	-1.78949000
H	-5.32577000	-3.29126700	-1.28539100
C	-6.56114100	-0.27567800	-2.24222400
H	-5.36582100	1.40562800	-2.88190600
H	-7.46404700	-2.10088400	-1.53697200
H	-7.50654200	0.24770400	-2.34440800

TS-S

E(RB3LYP) = -4032.82252355

Thermal correction to Gibbs Free Energy= 0.907953

G = -4031.914571 hartree

Imaginary frequency: -296.0472 cm⁻¹

C	-3.29009800	1.03948600	0.49509700
C	-2.15961000	0.98254800	1.30265300
C	-1.50982900	2.13660100	1.83852300
C	-2.01204800	3.36333500	1.43351100
C	-4.00554900	-0.21986500	0.13908900
C	-3.31085900	-1.24564000	-0.47124900
C	-3.86240000	-2.52344000	-0.76603500
C	-5.20422500	-2.69446200	-0.47798200
C	-5.98340100	-1.68435100	0.13791400
C	-5.37890000	-0.43354800	0.49204000
H	-1.59264500	4.27389000	1.84496800
H	-5.67906000	-3.64088300	-0.71741100
C	-4.75895600	2.46466900	-0.94918000

C	-3.47988700	4.76576100	0.02539400
C	-4.48597000	4.87587000	-0.90512900
C	-5.12278100	3.71295200	-1.40172000
H	-5.24985900	1.57954600	-1.33490300
H	-2.98087100	5.65044100	0.41015500
H	-4.79301000	5.85246300	-1.26526200
H	-5.90540200	3.80747600	-2.14746300
C	-7.35102700	-1.90635800	0.45180800
C	-6.15880400	0.51906700	1.19946400
C	-7.47852100	0.26569500	1.49967100
C	-8.08682700	-0.95153200	1.11298000
H	-7.80127900	-2.85283100	0.16719800
H	-5.70622600	1.45286900	1.50863900
H	-8.05771800	1.00607400	2.04224500
H	-9.12997800	-1.13271100	1.35071100
C	-3.72942700	2.31817400	0.01837400
C	-3.06523500	3.49166600	0.49860600
O	-1.97623500	-1.00460200	-0.80167900
O	-1.61957200	-0.27424400	1.58138100
P	-0.79099700	-1.01477200	0.35002300
N	-0.62614600	-2.52086300	0.98006400
C	-1.61124200	-3.11838900	1.88855700
H	-1.23968000	-3.11342600	2.91860200
H	-2.54219000	-2.55668000	1.85526200
H	-1.81033800	-4.14403100	1.56788200
C	0.66908300	-3.21267700	0.86770700
H	0.46306900	-4.28619500	0.84403500

H	1.12271100	-2.96543200	-0.09303700
C	-3.01892000	-3.64571700	-1.24559000
C	-3.19780600	-4.92039700	-0.68048700
C	-2.00975200	-3.47559100	-2.20610100
C	-2.38318500	-5.98844000	-1.05242000
H	-3.96228700	-5.06423700	0.07698700
C	-1.19037300	-4.54150800	-2.57090700
H	-1.85116500	-2.50763400	-2.66031500
C	-1.36960100	-5.80006400	-1.99403000
H	-2.53523400	-6.96403100	-0.60070900
H	-0.40868300	-4.38000300	-3.30590800
H	-0.72854300	-6.62858000	-2.27900700
C	-0.38006300	2.06597400	2.80364100
C	0.50259200	3.15618900	2.92342500
C	-0.18124200	0.97146200	3.66504900
C	1.52084500	3.16632600	3.87252600
H	0.39447100	4.00531600	2.26151900
C	0.85941100	0.96899800	4.59244500
H	-0.84789500	0.12285000	3.62108100
C	1.71433000	2.06463200	4.70695300
H	2.16900700	4.03364800	3.95372700
H	0.99234000	0.10491100	5.23476000
H	2.51653700	2.06363100	5.43782200
C	1.54739200	-2.85176900	2.04624200
C	2.39628500	-1.72252900	2.02302500
C	1.44822200	-3.59902800	3.22309400
C	3.09327700	-1.36093500	3.18167400

C	2.14222600	-3.22920400	4.37649600
H	0.82347000	-4.48735800	3.23178200
C	2.95778800	-2.10112700	4.35695000
H	3.75341800	-0.50320400	3.16910400
H	2.04941900	-3.82444900	5.27919900
H	3.50552400	-1.80356000	5.24528800
P	2.70453800	-0.82691100	0.45065200
C	3.67082200	-2.02967300	-0.53457200
C	4.03321600	-1.68658800	-1.84504600
C	4.12606700	-3.23938200	0.00710100
C	4.82943300	-2.53915000	-2.60382700
H	3.69153400	-0.75521800	-2.27297100
C	4.91462300	-4.09769400	-0.76088400
H	3.87505300	-3.51410000	1.02419100
C	5.26667800	-3.75131900	-2.06491700
H	5.10037100	-2.25992600	-3.61698700
H	5.25730800	-5.03483000	-0.33390900
H	5.88127400	-4.42043800	-2.65864400
C	3.93324200	0.45660200	0.89015200
C	3.49949200	1.60258200	1.57346500
C	5.28674900	0.32534100	0.55549600
C	4.40465600	2.61047700	1.89658700
H	2.45982100	1.70342100	1.85771500
C	6.18768600	1.34467100	0.87033200
H	5.63761100	-0.56095000	0.04112500
C	5.74933500	2.49022300	1.53420600
H	4.05757500	3.48841600	2.43100400

H	7.23249400	1.23956600	0.59613300
H	6.45148900	3.28180900	1.77591000
Ir	0.90021300	0.15956000	-0.61934700
N	-0.63331600	1.34304000	-1.61964600
H	-1.56226400	1.20513800	-1.21878600
H	-0.40532800	2.33438700	-1.53654100
O	-0.77798800	1.12637700	-3.02746100
H	-0.52411500	0.17493900	-3.11860700
H	0.85986900	1.17408400	0.57194300
H	2.01898900	1.24411800	-1.37074500
Cl	0.86100900	-1.36182300	-2.69212800
C	2.40874900	2.22895100	-2.40350100
N	2.07563300	1.68883500	-3.60381700
H	1.07781500	1.58588900	-3.79016700
O	2.82622900	0.61182500	-4.06418000
H	2.31825300	-0.17907000	-3.75828500
C	3.87988000	2.28067100	-2.06169500
H	4.33915900	3.03800100	-2.70638000
H	4.02270300	2.57098600	-1.02302500
H	4.36490900	1.32534800	-2.24597700
C	1.57998100	3.42520700	-2.02877700
C	0.80129700	4.09203300	-2.98819300
C	1.57852400	3.88906400	-0.70356000
C	0.00943800	5.18082000	-2.62047400
H	0.82669200	3.77474000	-4.02360500
C	0.80374400	4.98928800	-0.34982700
H	2.16166000	3.37053500	0.04785900

C	0.00693900	5.63122600	-1.30173600
H	-0.59370400	5.68034500	-3.37106100
H	0.82382600	5.35358000	0.67146200
H	-0.60300400	6.48242700	-1.01797500

Complex II+P-R

E(RB3LYP) = -4032.81957030

Thermal correction to Gibbs Free Energy= 0.910859

G = -4031.908711 hartree

C	3.91913100	-1.11927700	0.09693000
C	2.82149100	-1.39867700	0.89505000
C	2.41384600	-2.71769500	1.25200500
C	3.16780200	-3.76429700	0.74840200
C	4.30281200	0.29722300	-0.16915100
C	3.36452800	1.17309000	-0.68224400
C	3.58564300	2.56208200	-0.89486100
C	4.86373000	3.02457200	-0.64036200
C	5.88104400	2.18923900	-0.11765000
C	5.59988500	0.81172400	0.16485700
H	2.91086800	-4.78244800	1.02368500
H	5.09433600	4.06962500	-0.82241800
C	5.68365900	-2.03831600	-1.42272500
C	4.97959900	-4.64904700	-0.67473300
C	6.00362100	-4.43950100	-1.56762500
C	6.34682800	-3.12209700	-1.95271600
H	5.95227400	-1.03578100	-1.73081300
H	4.69398500	-5.65618700	-0.38584300

H	6.54232300	-5.28186700	-1.98893700
H	7.13902300	-2.96488700	-2.67752800
C	7.16908700	2.70932200	0.18130900
C	6.60416500	0.03225500	0.79807400
C	7.83603300	0.57309200	1.08974400
C	8.12942100	1.91903000	0.76681900
H	7.37529800	3.74976400	-0.05187400
H	6.39327900	-0.99794800	1.05509200
H	8.58977400	-0.03851500	1.57517800
H	9.10871100	2.32710200	0.99469200
C	4.63826000	-2.21807000	-0.47955200
C	4.26236100	-3.55390700	-0.12396000
O	2.07822500	0.66675400	-0.93305900
O	2.04422300	-0.34205300	1.37632800
P	1.07287800	0.52089100	0.37310500
N	1.04173400	1.93144200	1.21038000
C	2.09644700	2.33060300	2.15429900
H	1.73560300	2.25112800	3.18428100
H	2.97408400	1.70207500	2.03910700
H	2.37229500	3.36674600	1.94119900
C	-0.14923700	2.79754400	1.20750400
H	0.19892000	3.83169800	1.25292400
H	-0.66457300	2.69895900	0.25329100
C	2.47599000	3.48644000	-1.23823100
C	2.38824200	4.72220700	-0.57314900
C	1.47054900	3.15148700	-2.15867000
C	1.31825800	5.58624500	-0.80410900

H	3.15282700	4.99486300	0.14798900
C	0.39653700	4.01130000	-2.37998000
H	1.50982000	2.21306300	-2.69345400
C	0.30978200	5.22742100	-1.70056100
H	1.26862500	6.53383700	-0.27630000
H	-0.37148700	3.72056800	-3.08867000
H	-0.53407300	5.88915000	-1.86856100
C	1.19273700	-2.97231800	2.06030300
C	0.33101500	-4.02085000	1.69488100
C	0.85354600	-2.18806100	3.17591900
C	-0.82968100	-4.28278700	2.42196400
H	0.56954600	-4.63390900	0.83031000
C	-0.31058800	-2.44409600	3.89606400
H	1.50554000	-1.37951900	3.48007900
C	-1.15463600	-3.49395300	3.52612700
H	-1.47711500	-5.10177200	2.12407400
H	-0.55587500	-1.82504300	4.75320100
H	-2.05715500	-3.69366800	4.09509000
C	-1.01096700	2.44269900	2.39502700
C	-1.91794000	1.36425600	2.33053600
C	-0.81112500	3.09301000	3.61398600
C	-2.56243500	0.93581000	3.49594800
C	-1.46249400	2.66632900	4.77310700
H	-0.13546300	3.94254600	3.65447500
C	-2.32415100	1.57463700	4.71538200
H	-3.26905000	0.11694900	3.45632900
H	-1.29499600	3.18437700	5.71185700

H	-2.83295000	1.22966500	5.60975600
P	-2.38508900	0.69330900	0.67837500
C	-3.14663300	2.19258600	-0.05384700
C	-2.86268100	2.59392000	-1.36315900
C	-3.99624300	2.98175500	0.74206600
C	-3.44676500	3.75049300	-1.88323200
H	-2.17278000	2.01763600	-1.96536200
C	-4.58403200	4.12822600	0.21428000
H	-4.19293300	2.70384200	1.77193300
C	-4.31349100	4.51328000	-1.10193600
H	-3.21661700	4.05312800	-2.90006200
H	-5.24518600	4.72661900	0.83294900
H	-4.76867300	5.41085400	-1.50871900
C	-3.76539700	-0.43907200	1.08956800
C	-3.46189700	-1.68523700	1.66070100
C	-5.10499700	-0.05896900	0.94834400
C	-4.48317600	-2.52927800	2.09110000
H	-2.43135000	-1.99070100	1.78695000
C	-6.12253800	-0.91029300	1.37680700
H	-5.36039900	0.88531000	0.48740000
C	-5.81742200	-2.14315900	1.95226600
H	-4.23224100	-3.48699500	2.53651200
H	-7.15675900	-0.60927600	1.24864500
H	-6.61360100	-2.80092700	2.28616300
Ir	-0.73023300	-0.51848600	-0.44819500
N	0.58540600	-2.05817600	-1.26521500
H	1.08679800	-2.55282000	-0.52752300

H	-0.02913900	-2.71500700	-1.75547500
O	1.55400900	-1.73888900	-2.26134900
H	1.67852500	-0.77559300	-2.16890900
H	-0.74325300	-1.35464300	0.88038000
H	-2.13982300	-1.51397400	-1.27225600
Cl	-0.67545700	0.43644900	-2.79622100
C	-2.81158000	-2.26654600	-1.92868400
N	-2.36115100	-2.30129300	-3.27521300
H	-2.55074000	-1.43892300	-3.77985700
O	-0.99531000	-2.63494700	-3.43917800
H	-0.52678600	-1.77252500	-3.48850500
C	-2.65620300	-3.60853400	-1.22745100
H	-2.99430000	-3.53345600	-0.19435600
H	-3.24168900	-4.36462800	-1.75551500
H	-1.61665500	-3.93830900	-1.23392200
C	-4.19456800	-1.65238200	-1.93220700
C	-4.32474300	-0.31448600	-2.32740700
C	-5.34097500	-2.39235600	-1.63519300
C	-5.58014200	0.27818500	-2.42525200
H	-3.43378100	0.26319700	-2.54590300
C	-6.60050500	-1.80223300	-1.74644000
H	-5.26207500	-3.42619200	-1.32132500
C	-6.72455100	-0.47022200	-2.14200800
H	-5.65976300	1.32094400	-2.71576100
H	-7.48652200	-2.38706900	-1.52093300
H	-7.70740400	-0.01702700	-2.22538700

Complex II+P-R

E(RB3LYP) = -4032.82573348

Thermal correction to Gibbs Free Energy= 0.910156

G = -4031.915577 hartree

C	-3.28729100	1.01522700	0.47656500
C	-2.15659800	0.98114100	1.28448500
C	-1.53398800	2.14341100	1.83238300
C	-2.06502500	3.36049300	1.43487100
C	-3.98349300	-0.25578200	0.12369800
C	-3.27796300	-1.27455700	-0.48508400
C	-3.80870400	-2.56253900	-0.77053200
C	-5.14667900	-2.75239700	-0.47635800
C	-5.93885500	-1.75088700	0.13679300
C	-5.35237500	-0.48923300	0.48318400
H	-1.66961700	4.27771100	1.85447700
H	-5.60718200	-3.70771500	-0.70816800
C	-4.78278800	2.41598900	-0.96379000
C	-3.55535600	4.73875700	0.02764100
C	-4.56030000	4.83216800	-0.90584700
C	-5.17132900	3.65891300	-1.41041100
H	-5.25327900	1.52286500	-1.35651500
H	-3.07438400	5.63156600	0.41617000
H	-4.88518700	5.80380600	-1.26346800
H	-5.95282800	3.74116000	-2.15872600
C	-7.30169100	-1.99282300	0.45681000
C	-6.14394400	0.45382800	1.19042300
C	-7.45831200	0.18105400	1.49686400
C	-8.04941500	-1.04675400	1.11703600

H	-7.73836300	-2.94717700	0.17760500
H	-5.70525400	1.39585200	1.49418700
H	-8.04668500	0.91447400	2.03893600
H	-9.08877500	-1.24282900	1.35936500
C	-3.75295000	2.28670200	0.00557400
C	-3.11609900	3.47116600	0.49563200
O	-1.94450400	-1.01440900	-0.82162700
O	-1.58678900	-0.26700000	1.55857400
P	-0.77300600	-1.00964700	0.33228300
N	-0.58536100	-2.50896900	0.96283600
C	-1.56144000	-3.09504500	1.89188800
H	-1.18012400	-3.07014700	2.91769600
H	-2.49723100	-2.54218200	1.85548000
H	-1.75379400	-4.12677400	1.58809500
C	0.70273800	-3.21272000	0.84355000
H	0.48508300	-4.28345300	0.80864200
H	1.16008900	-2.96034000	-0.11402400
C	-2.94892900	-3.67512700	-1.24333600
C	-3.09888000	-4.94486000	-0.65895200
C	-1.95245300	-3.49896100	-2.21544900
C	-2.26684600	-6.00211400	-1.02315200
H	-3.85508000	-5.09279700	0.10605800
C	-1.11588300	-4.55403000	-2.57298000
H	-1.81806000	-2.53471300	-2.68529200
C	-1.26542100	-5.80733500	-1.97656300
H	-2.39652900	-6.97428600	-0.55735500
H	-0.34439700	-4.38854300	-3.31768500

H	-0.61132400	-6.62734500	-2.25632900
C	-0.40682700	2.09158900	2.80239000
C	0.44288800	3.20560300	2.94299600
C	-0.18008200	0.99185500	3.65079700
C	1.45321900	3.23338000	3.90013400
H	0.31458800	4.06217900	2.29457500
C	0.85476600	1.00720400	4.58467800
H	-0.82214600	0.12531400	3.59468600
C	1.67498400	2.12659700	4.72059200
H	2.07250600	4.11967600	3.99851900
H	1.00874200	0.13875700	5.21645800
H	2.47162300	2.14002100	5.45734200
C	1.57496100	-2.86654000	2.02977000
C	2.40083200	-1.72120200	2.02499300
C	1.48673100	-3.63279800	3.19465800
C	3.08810600	-1.35996900	3.18916600
C	2.17220900	-3.26523300	4.35423500
H	0.87732400	-4.53179000	3.18996400
C	2.96440700	-2.12024200	4.35310500
H	3.73056300	-0.48872000	3.18927500
H	2.08967700	-3.87457000	5.24844200
H	3.50367200	-1.82482400	5.24726300
P	2.70288500	-0.81405500	0.46122500
C	3.69811200	-1.98750600	-0.52755200
C	4.09407900	-1.60515800	-1.81752500
C	4.13650400	-3.21382000	-0.00993400
C	4.90597100	-2.43826700	-2.58111100

H	3.77189100	-0.65898200	-2.22927200
C	4.94110500	-4.05154300	-0.78389600
H	3.86148400	-3.51786100	0.99237200
C	5.32557700	-3.66787300	-2.06817800
H	5.20247900	-2.12815600	-3.57788900
H	5.27122000	-5.00173300	-0.37637100
H	5.95261300	-4.32136800	-2.66627100
C	3.88570800	0.50443300	0.91171000
C	3.41665400	1.62848200	1.60844500
C	5.24501100	0.41144500	0.58538400
C	4.29387100	2.65411400	1.95149300
H	2.37335800	1.69838000	1.88919400
C	6.11696900	1.44739600	0.92319100
H	5.62163800	-0.45771500	0.06050400
C	5.64362300	2.57201000	1.59897500
H	3.92023600	3.51634100	2.49252700
H	7.16608900	1.37287400	0.65594900
H	6.32318200	3.37815600	1.85643200
Ir	0.87965700	0.14890900	-0.63385000
N	-0.64610000	1.31666700	-1.65886800
H	-1.57297800	1.20908900	-1.24437300
H	-0.39366900	2.30588900	-1.60245500
O	-0.80128500	1.06443500	-3.05576000
H	-0.51562500	0.12330500	-3.13840300
H	0.81268600	1.16971000	0.55382400
H	2.03989500	1.34347600	-1.48651200
Cl	0.89325400	-1.39202800	-2.65904100

C	2.37535400	2.19818200	-2.29860900
N	2.14945000	1.73549800	-3.61050300
H	1.16452400	1.55401800	-3.80003500
O	2.92350800	0.61567800	-3.97024300
H	2.39383300	-0.16123700	-3.68536100
C	3.85200800	2.39668800	-1.97642100
H	4.23353600	3.18364000	-2.63288400
H	3.97941900	2.70484100	-0.93985100
H	4.41898000	1.48555000	-2.15744300
C	1.52230200	3.41553900	-1.99501300
C	0.86247100	4.10936400	-3.01932500
C	1.39169500	3.86670600	-0.67233100
C	0.06050900	5.21335700	-2.72195500
H	0.98748900	3.79411500	-4.04773300
C	0.60686200	4.98069600	-0.38537200
H	1.89478200	3.33681200	0.12831200
C	-0.07180100	5.65113500	-1.40596000
H	-0.45137400	5.73295400	-3.52522800
H	0.52931000	5.33614500	0.63637700
H	-0.69015000	6.51269200	-1.17621300

Complex II'

E(RB3LYP) = -3460.16984156

Thermal correction to Gibbs Free Energy= 0.701673

G = -3459.468169

C	3.58160500	-1.04261200	-0.00357400
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C	2.41543200	-1.53970900	0.56070900
C	2.04064300	-2.91291700	0.50954200
C	2.91375800	-3.78572700	-0.11096900
C	3.84111800	0.42518400	0.04849000
C	2.85543800	1.27886500	-0.42100500
C	2.95786700	2.70183700	-0.38979900
C	4.14347100	3.23336100	0.08223800
C	5.18589400	2.41823500	0.58906400
C	5.02979100	0.99303900	0.60989700
H	2.67245900	-4.84396100	-0.14317000
H	4.28117100	4.31058100	0.08874800
C	5.60172500	-1.52336200	-1.40945300
C	4.97097100	-4.25246100	-1.39513500
C	6.09829900	-3.81053100	-2.04639700
C	6.40605300	-2.42969800	-2.06268600
H	5.84235300	-0.46813700	-1.43884300
H	4.70977200	-5.30709400	-1.39435900
H	6.74473500	-4.51473500	-2.56097500
H	7.28175700	-2.08051400	-2.60127400
C	6.37282900	2.99167400	1.11928700
C	6.04610000	0.21084500	1.22116600
C	7.17665500	0.80053400	1.74018500
C	7.35097300	2.20347400	1.67876200
H	6.48589500	4.07185900	1.08457100
H	5.91912600	-0.86338000	1.27664600
H	7.94035500	0.18394100	2.20431400
H	8.25112200	2.65441800	2.08495100

C	4.44675100	-1.94945200	-0.69939700
C	4.11086000	-3.34255900	-0.72386100
O	1.69272300	0.72087500	-0.90483700
O	1.54527700	-0.65718200	1.17807200
P	0.51706500	0.22851100	0.19625800
N	0.27556800	1.48113100	1.26286100
C	1.15231100	1.82714000	2.37889500
H	0.63639800	1.67349400	3.33404000
H	2.04417700	1.20764600	2.36370800
H	1.44771500	2.87950800	2.29857000
C	-0.93057500	2.30526000	1.13595900
H	-0.65506200	3.34190900	1.34821000
H	-1.26805000	2.29088600	0.10083200
C	1.79931200	3.56459900	-0.73961300
C	1.53753600	4.70756300	0.03603000
C	0.90717600	3.25538500	-1.78257800
C	0.41668800	5.50218000	-0.20544200
H	2.20253200	4.95506900	0.85774900
C	-0.22144000	4.04007100	-2.01146600
H	1.08181400	2.38252500	-2.39621200
C	-0.47684600	5.16279600	-1.22200700
H	0.23272200	6.37379900	0.41610200
H	-0.91378600	3.76222600	-2.79937600
H	-1.36837800	5.75792300	-1.39381900
C	0.74226400	-3.38368300	1.05225200
C	-0.03338100	-4.28146200	0.30273000
C	0.25981300	-2.96134000	2.30160400

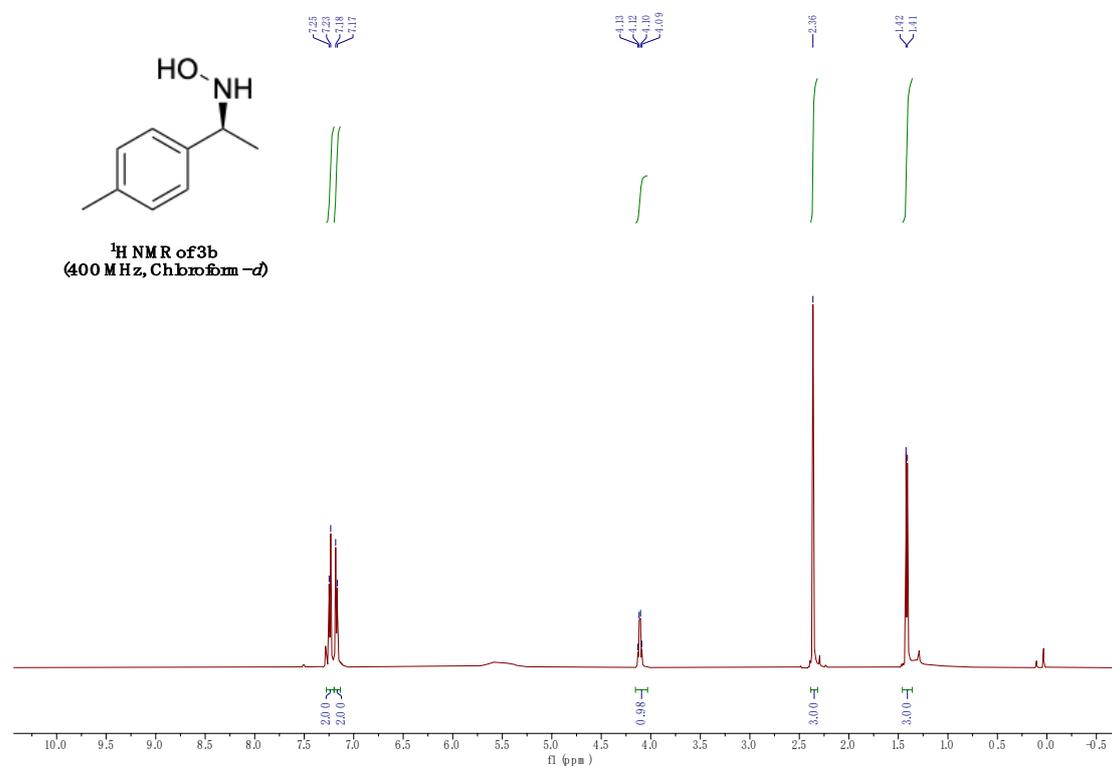
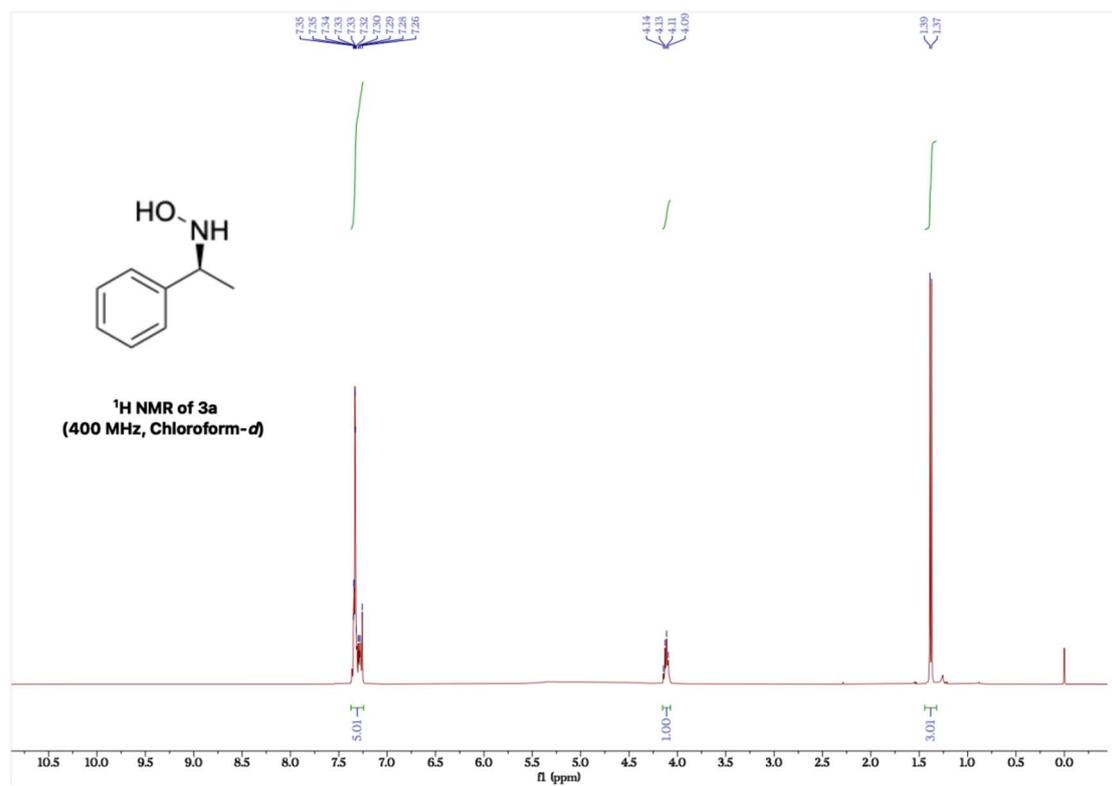
C	-1.24681100	-4.76002400	0.79313000
H	0.30490700	-4.58160100	-0.68353100
C	-0.95627900	-3.43419700	2.78806700
H	0.84073900	-2.26054100	2.88806900
C	-1.71116000	-4.34026400	2.04016000
H	-1.83678500	-5.44312300	0.19001700
H	-1.31430600	-3.09604200	3.75593600
H	-2.66109400	-4.70364000	2.42086800
C	-1.99143300	1.82023100	2.09551300
C	-2.86128700	0.76336700	1.75142800
C	-2.05025500	2.35874700	3.38329300
C	-3.72892900	0.24790200	2.72209800
C	-2.92141400	1.84298700	4.34411000
H	-1.40112400	3.19369300	3.63243900
C	-3.75137400	0.77508400	4.01462100
H	-4.39914300	-0.56340400	2.46752800
H	-2.94847500	2.27348500	5.34055700
H	-4.42980200	0.35819600	4.75253800
P	-2.91329800	0.12312800	0.02360800
C	-3.49163800	1.57834500	-0.94058500
C	-3.29764700	1.57946300	-2.33074100
C	-4.08920700	2.68758900	-0.32624900
C	-3.68826800	2.68359100	-3.08734800
H	-2.84442800	0.71615600	-2.80542700
C	-4.46915700	3.79302000	-1.08851400
H	-4.24308600	2.69712400	0.74699100
C	-4.26519700	3.79510600	-2.46889200

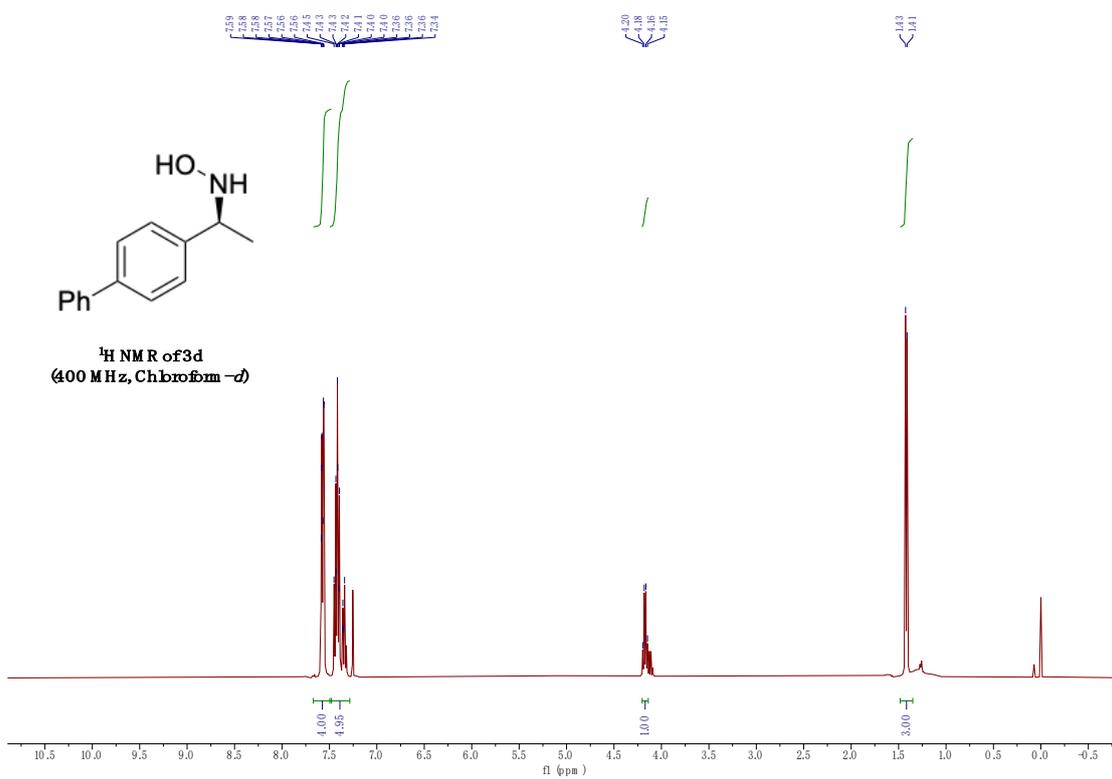
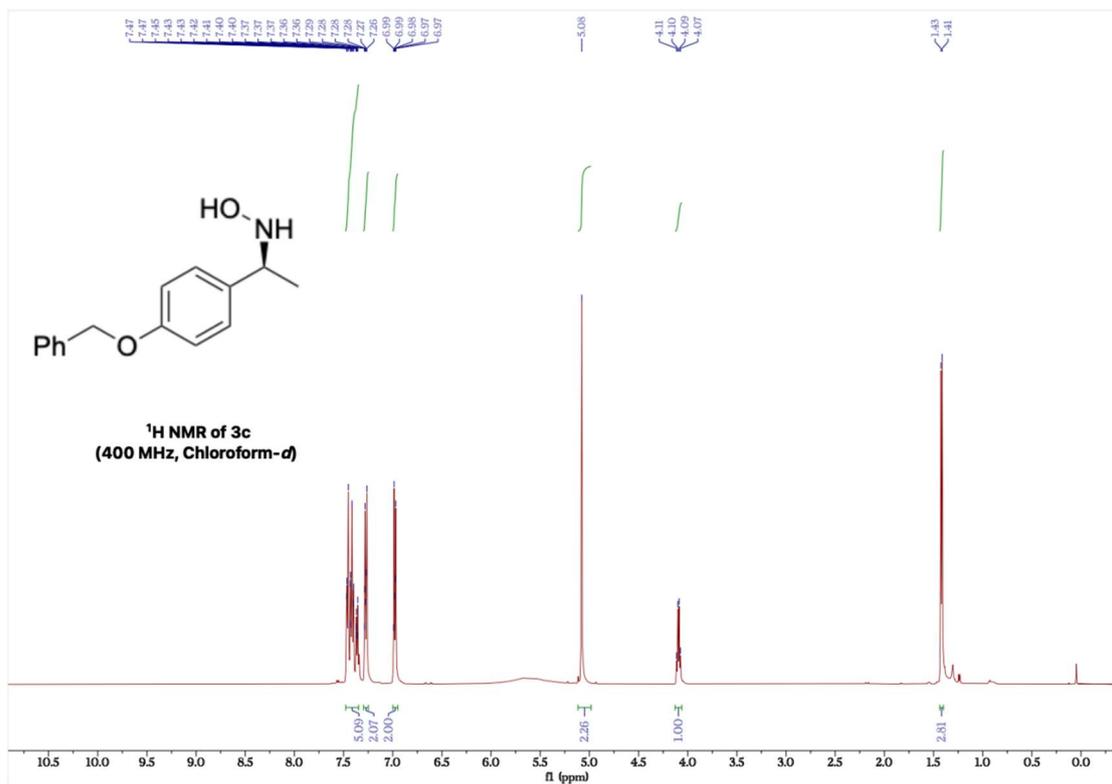
H	-3.53573300	2.67537100	-4.16241000
H	-4.92369700	4.65087700	-0.60193700
H	-4.55826800	4.65722000	-3.06081400
C	-4.32621000	-1.02856400	0.07485900
C	-4.06610600	-2.37607500	0.35303000
C	-5.64447100	-0.58848100	-0.08345100
C	-5.12243300	-3.27280300	0.49043300
H	-3.04139900	-2.71517100	0.44501400
C	-6.69866500	-1.49388500	0.04281300
H	-5.84641500	0.45344100	-0.30854400
C	-6.43934000	-2.83415600	0.33375900
H	-4.91524600	-4.31742900	0.70257400
H	-7.72098100	-1.15256000	-0.08924900
H	-7.26172900	-3.53686800	0.43029300
Ir	-1.01943900	-0.76329700	-0.99241000
Cl	-2.46626100	-1.93475500	-2.53802100
H	0.22908800	-1.74481600	-1.64545800
H	0.18102600	-1.03675900	-2.17761100

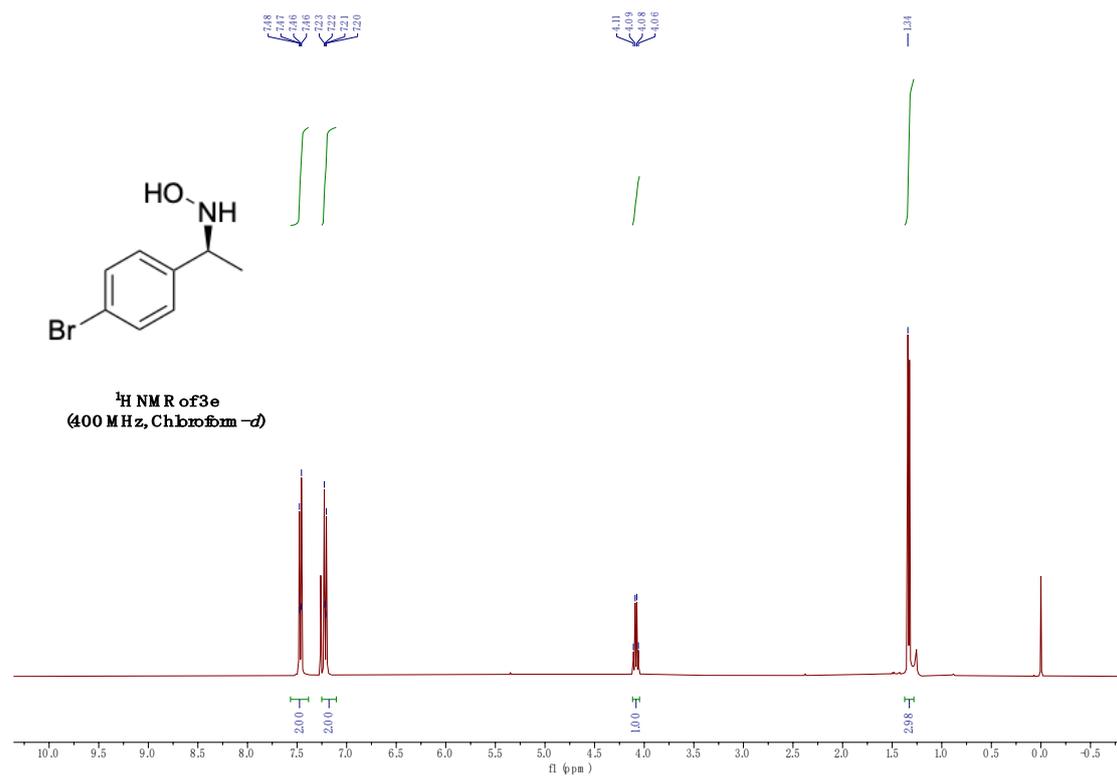
8. References

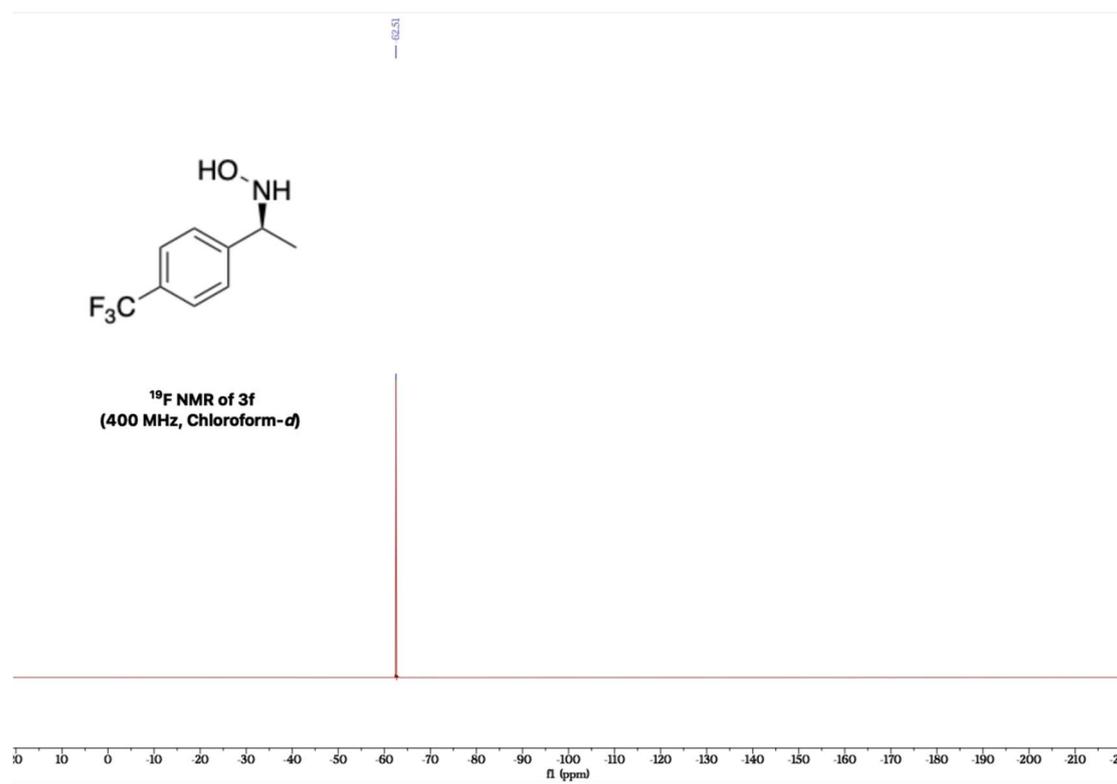
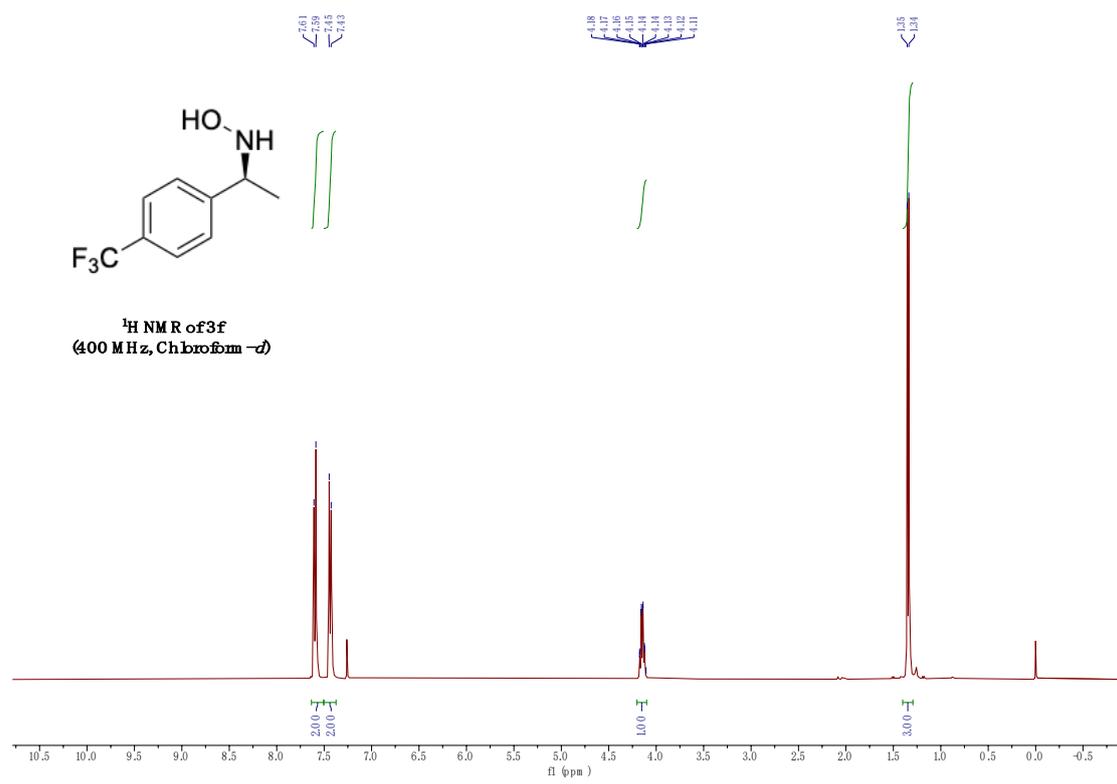
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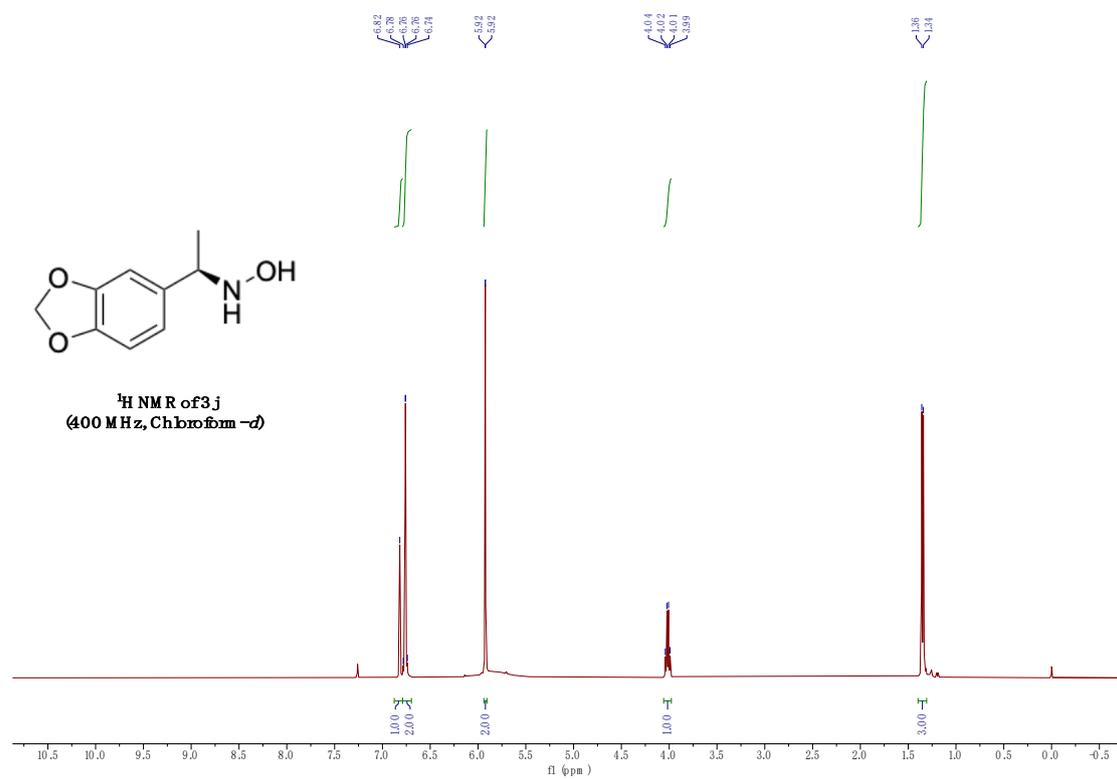
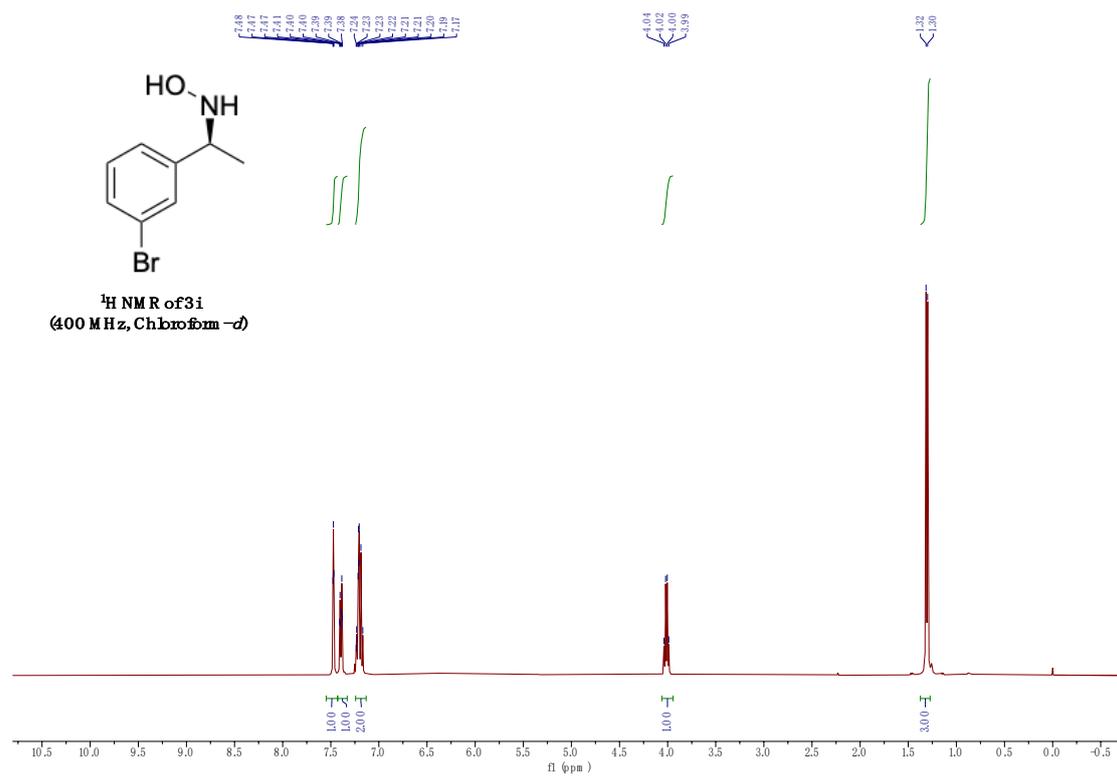
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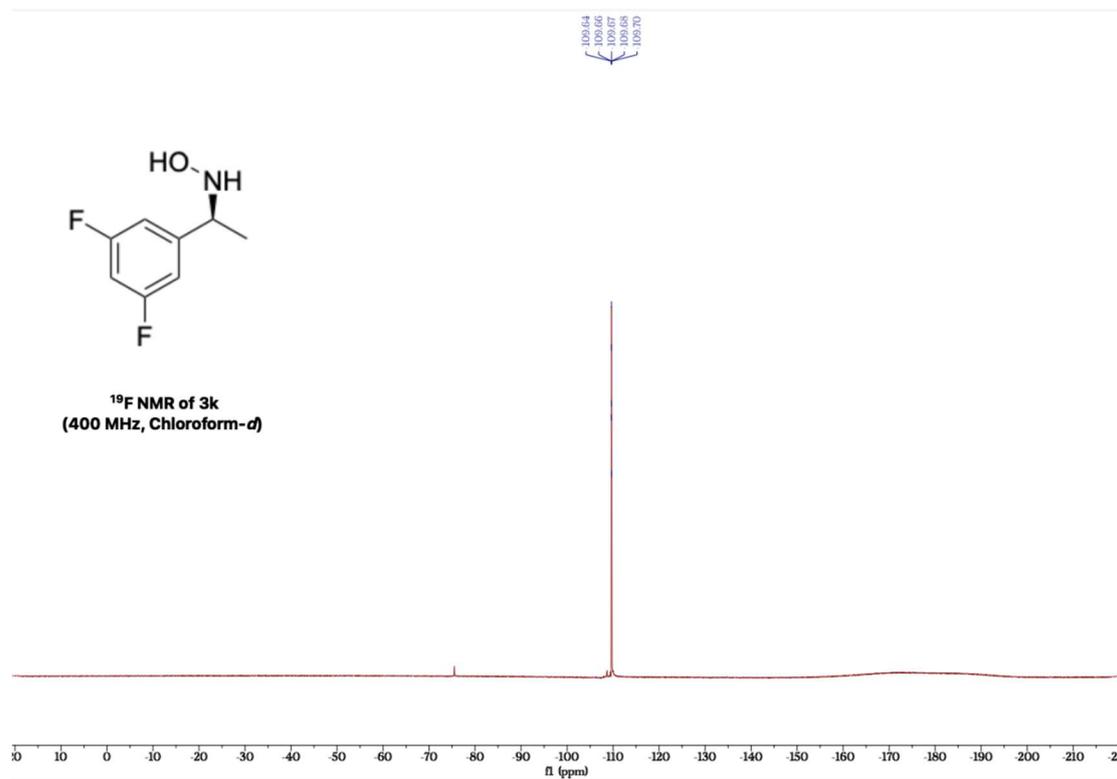
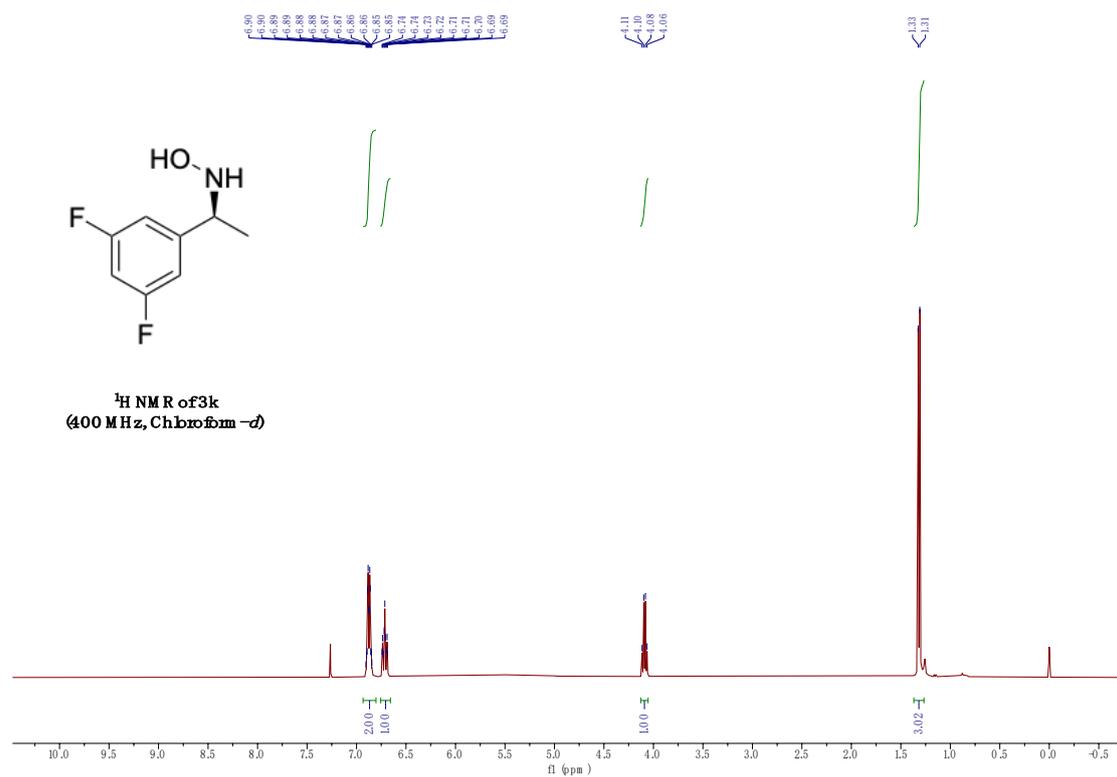


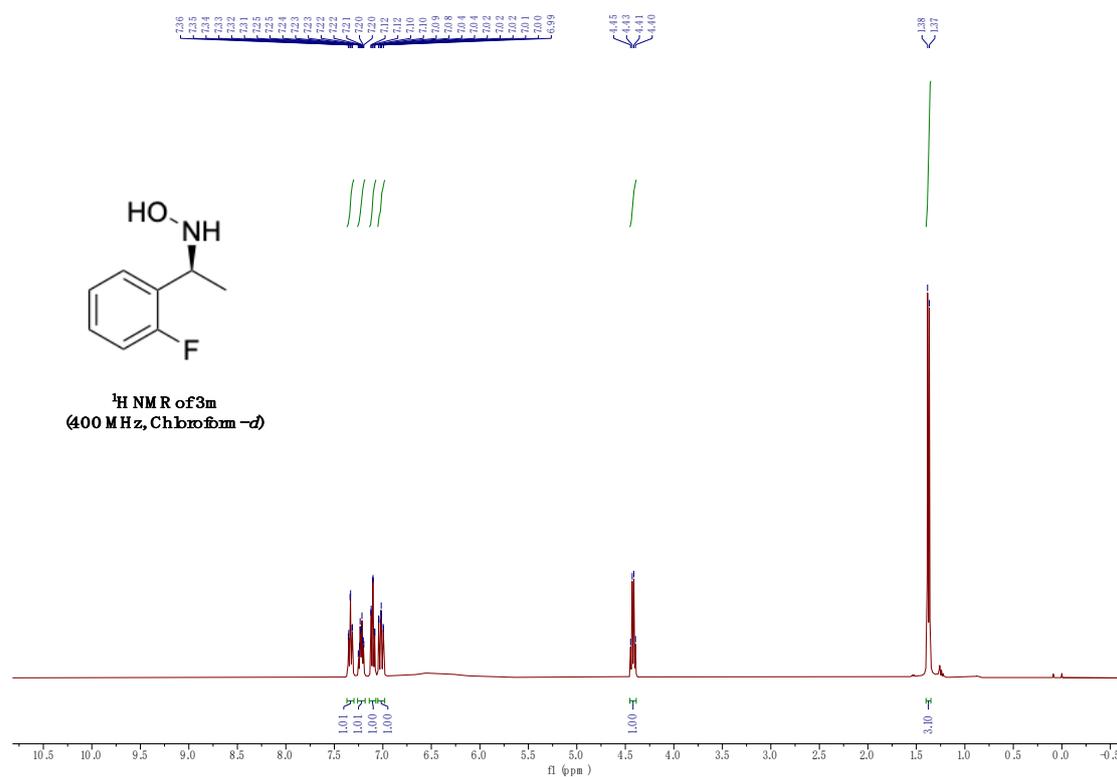
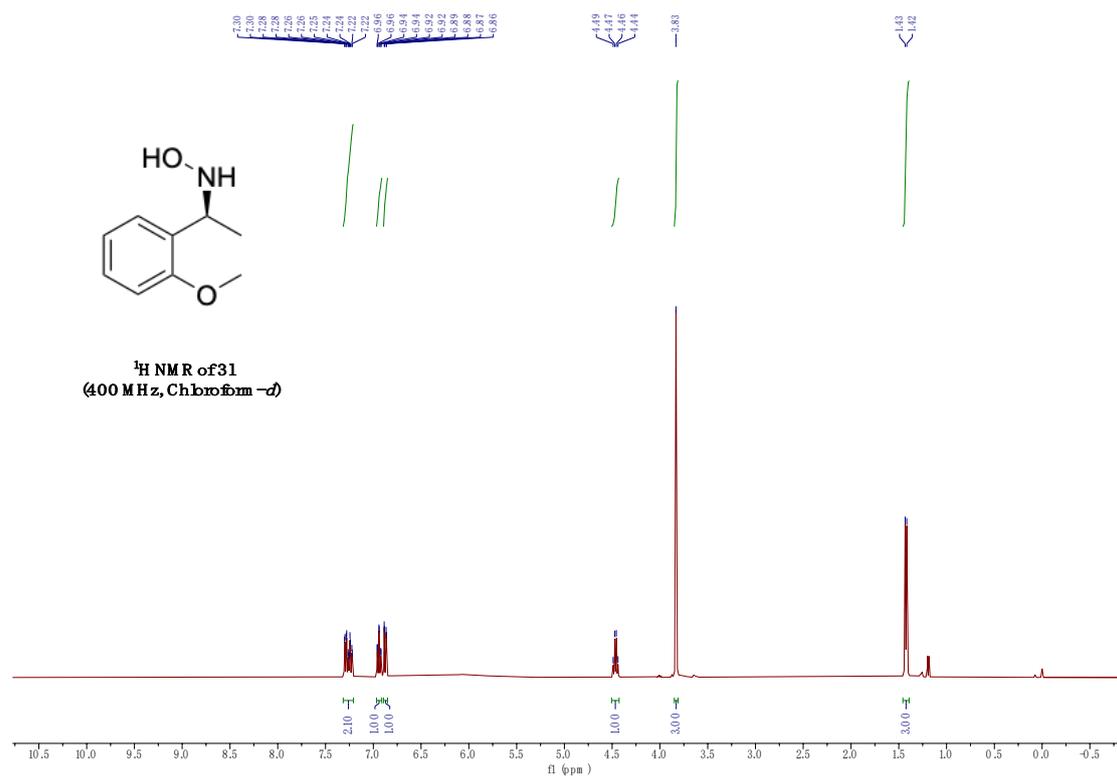


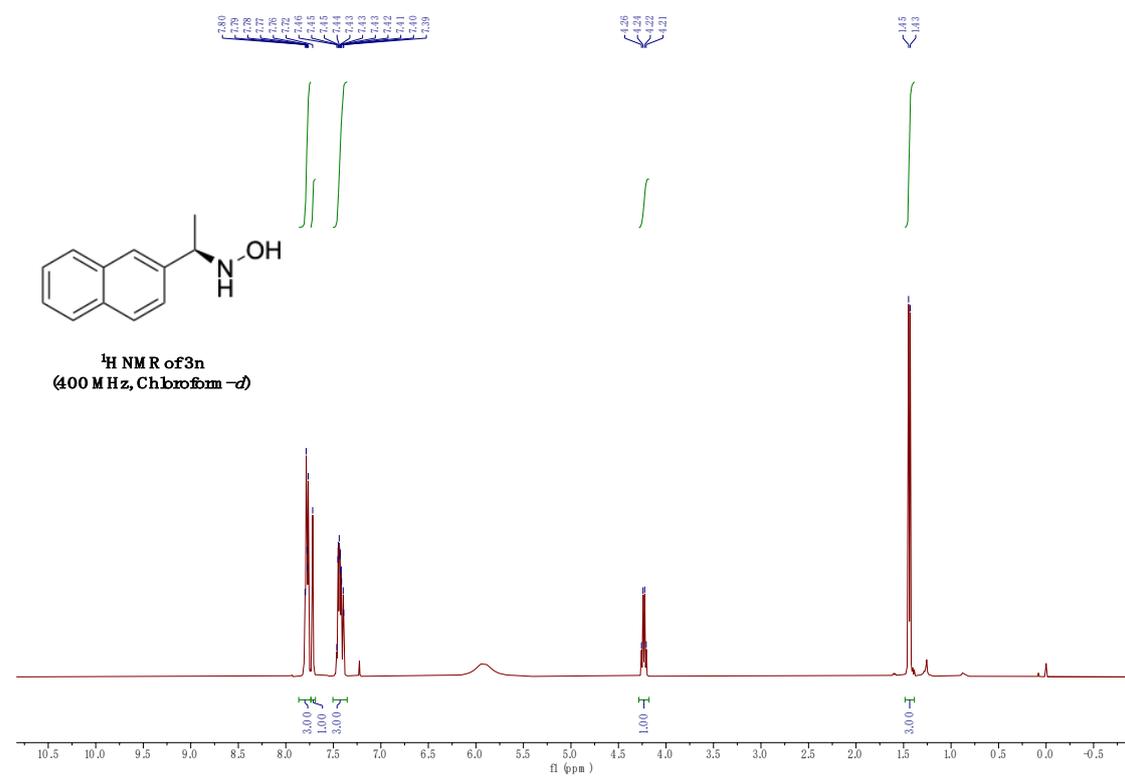
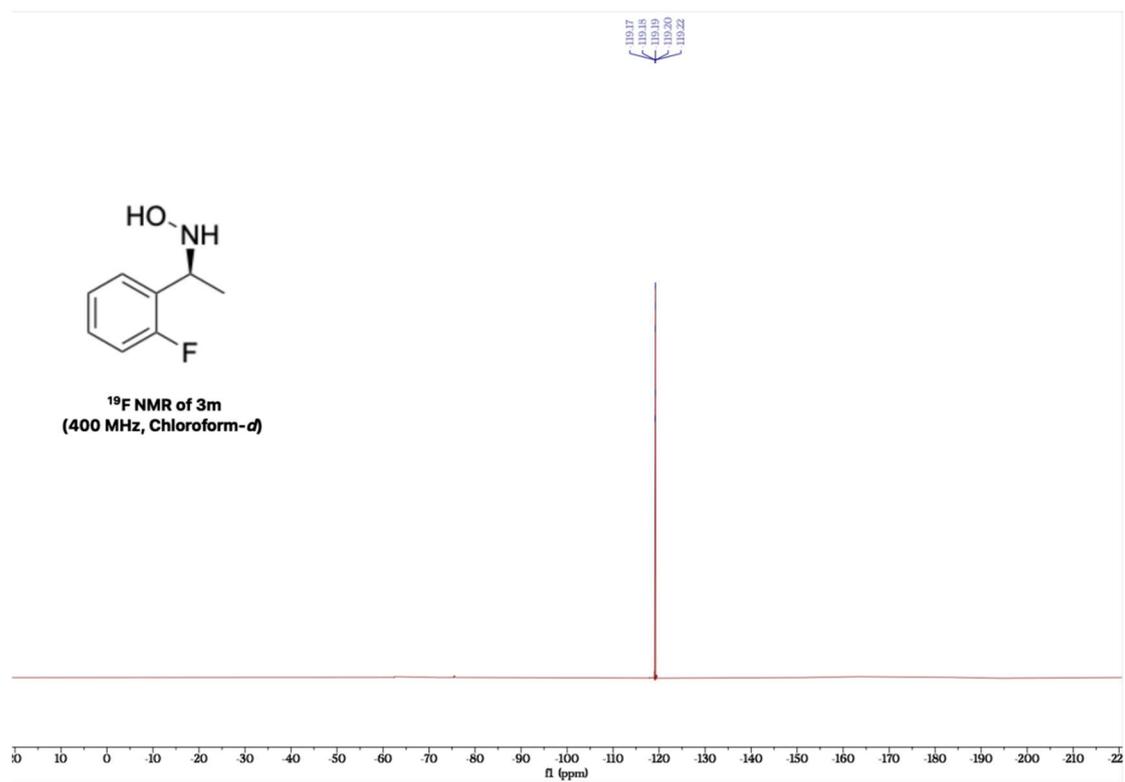


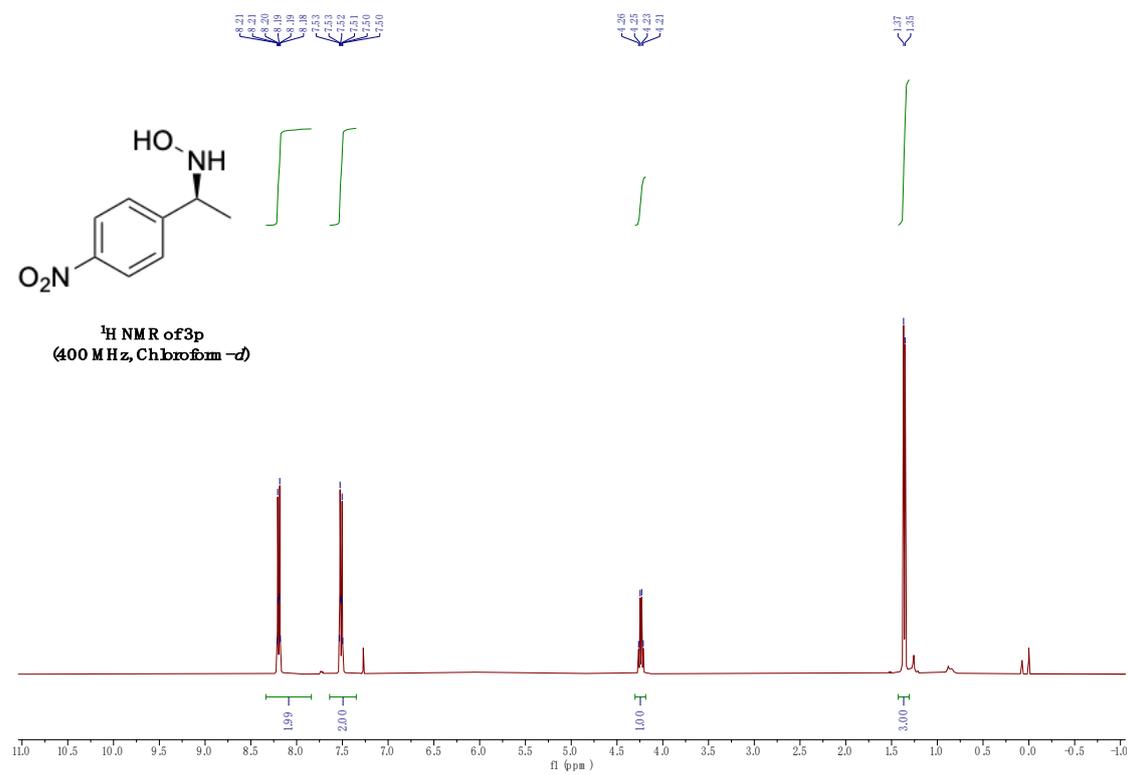
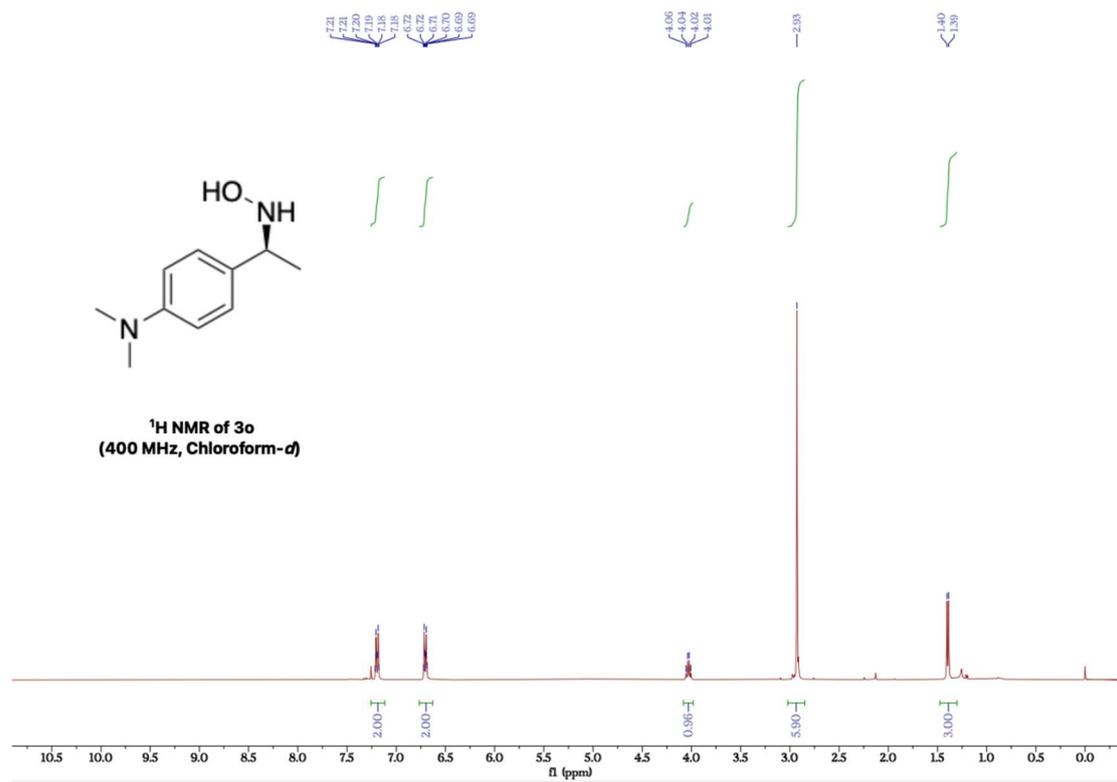


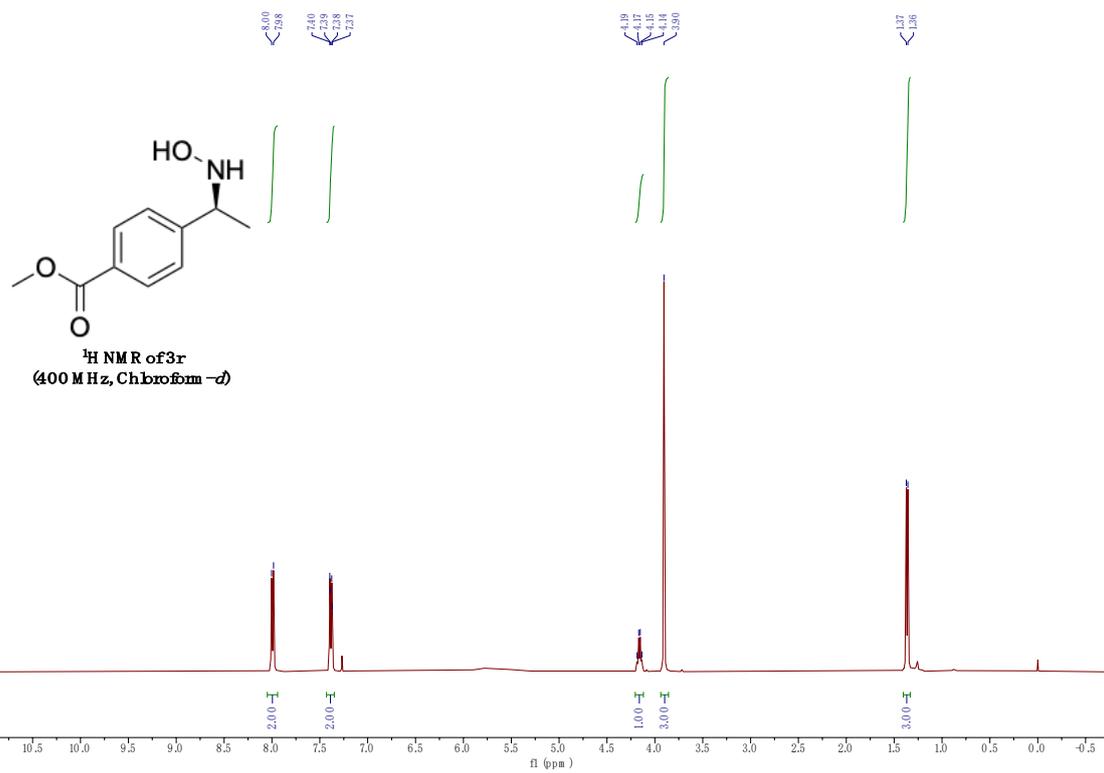
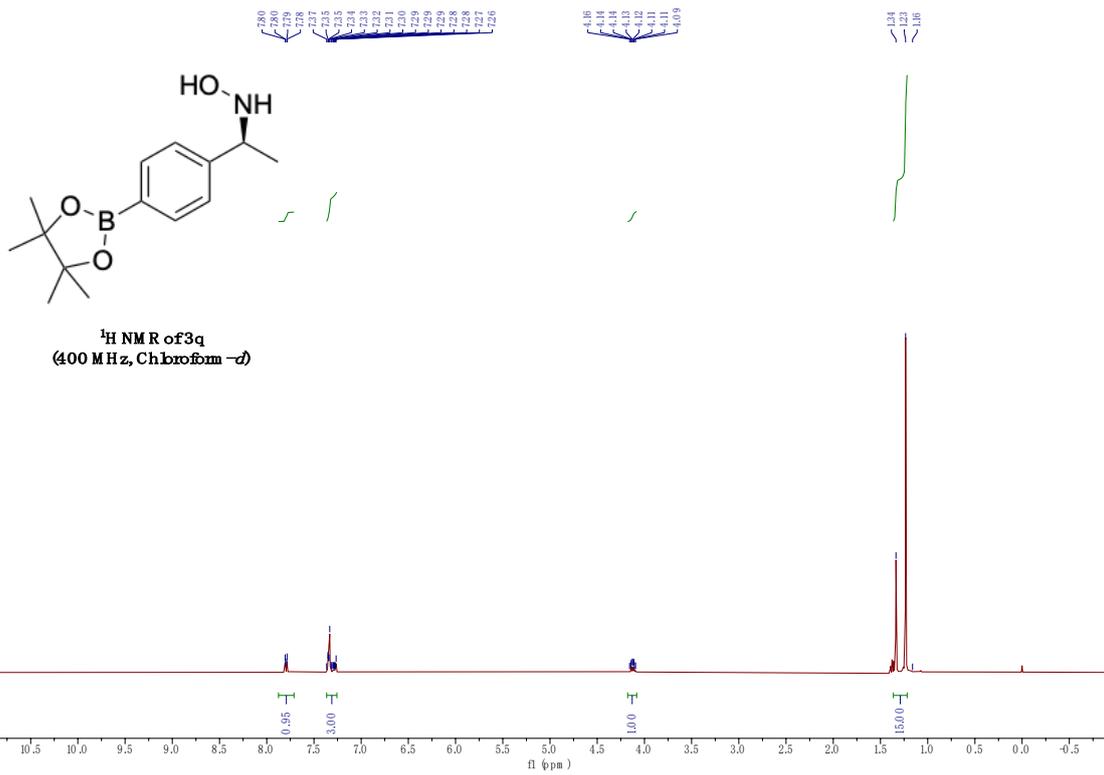


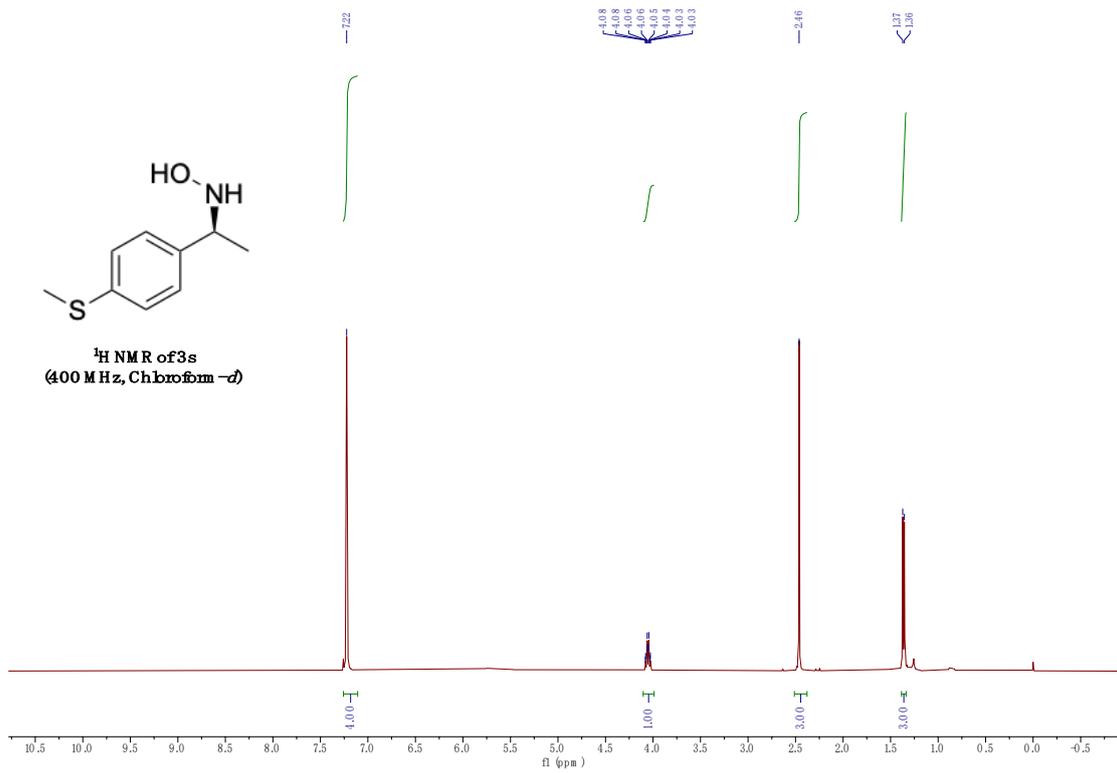
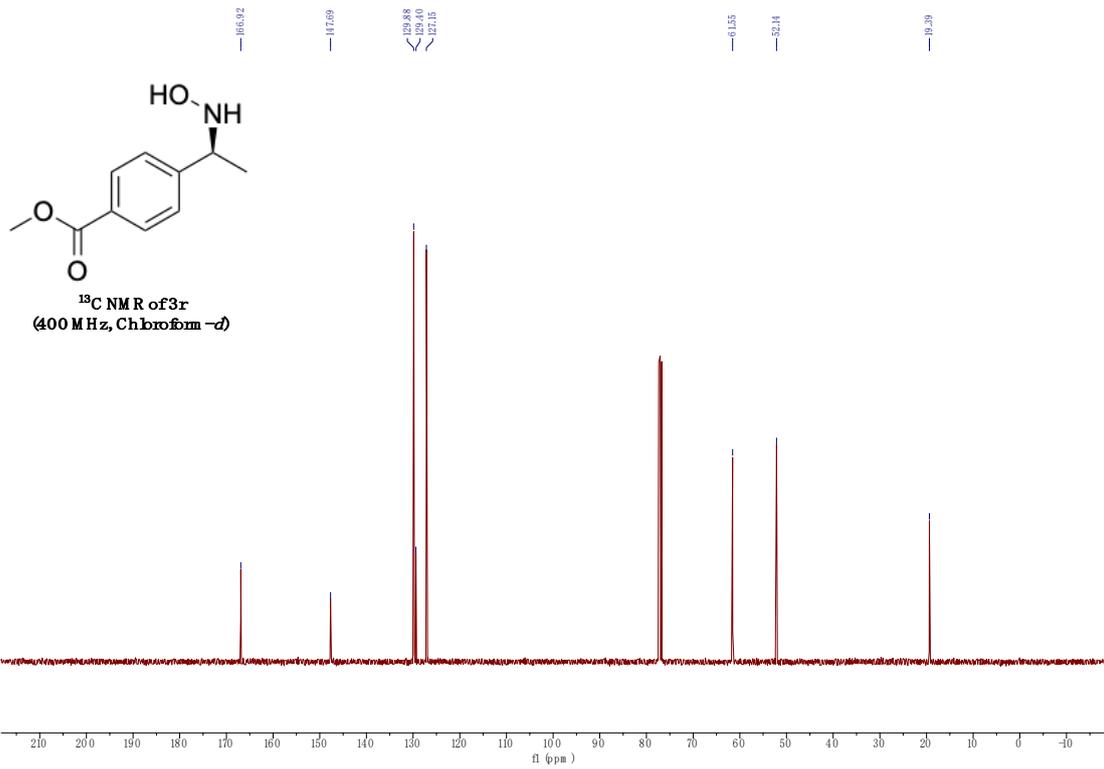


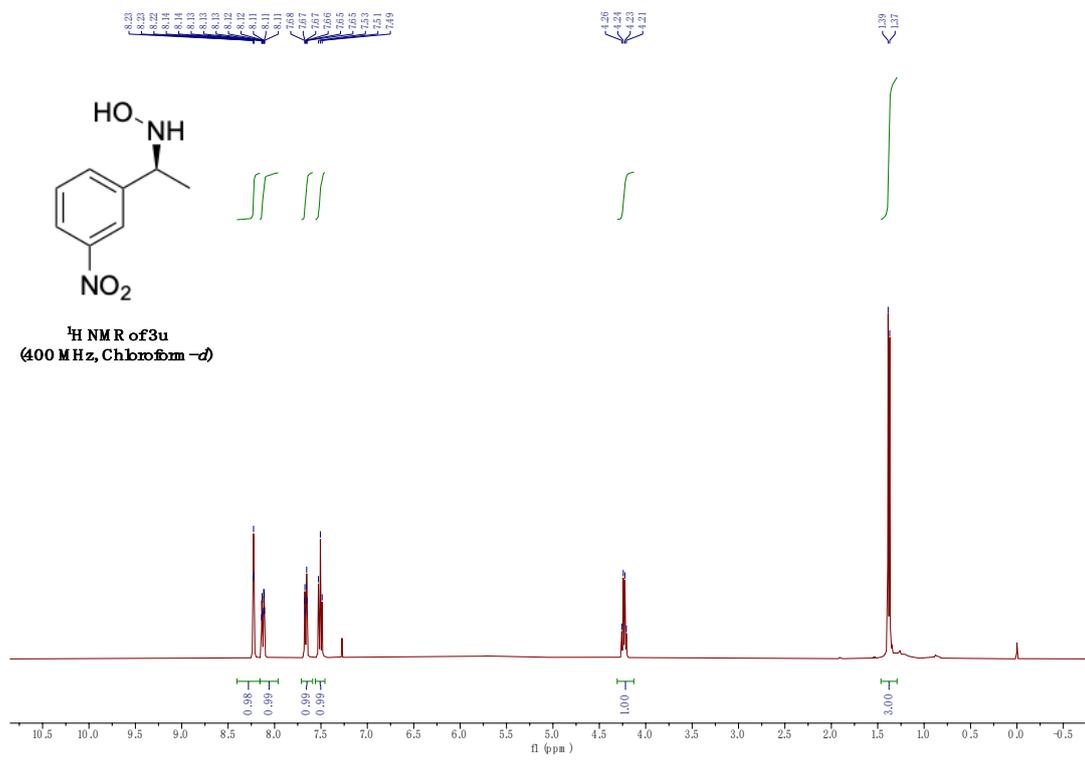
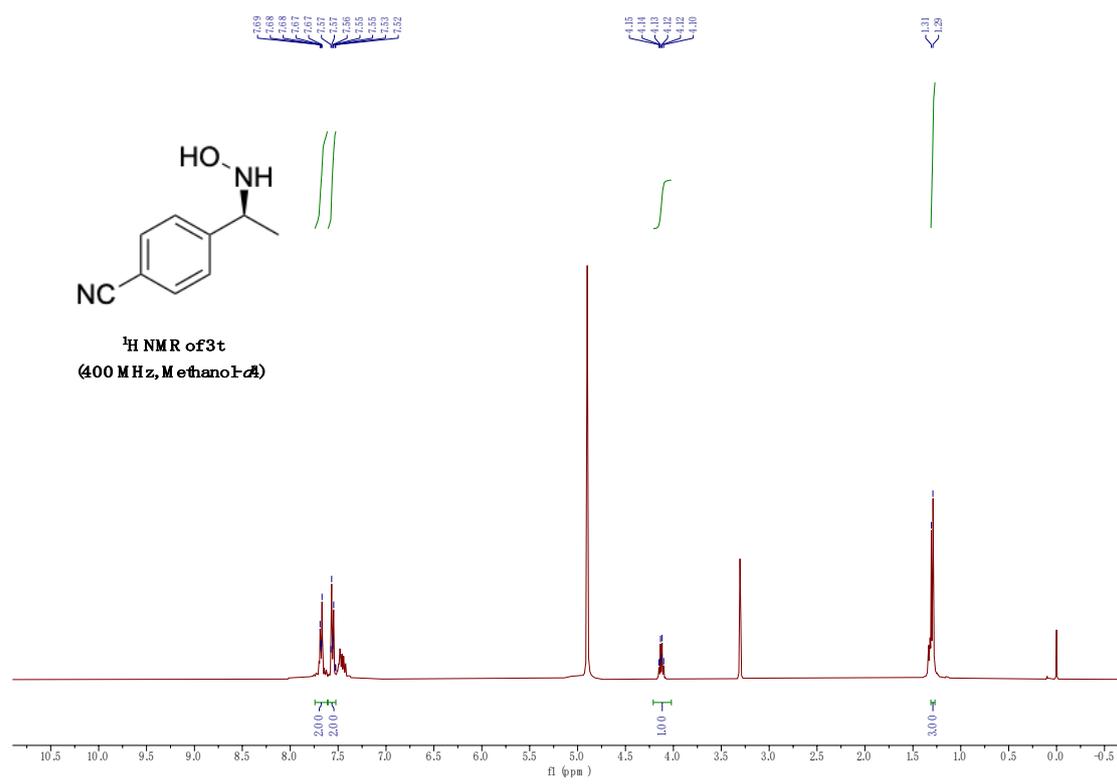


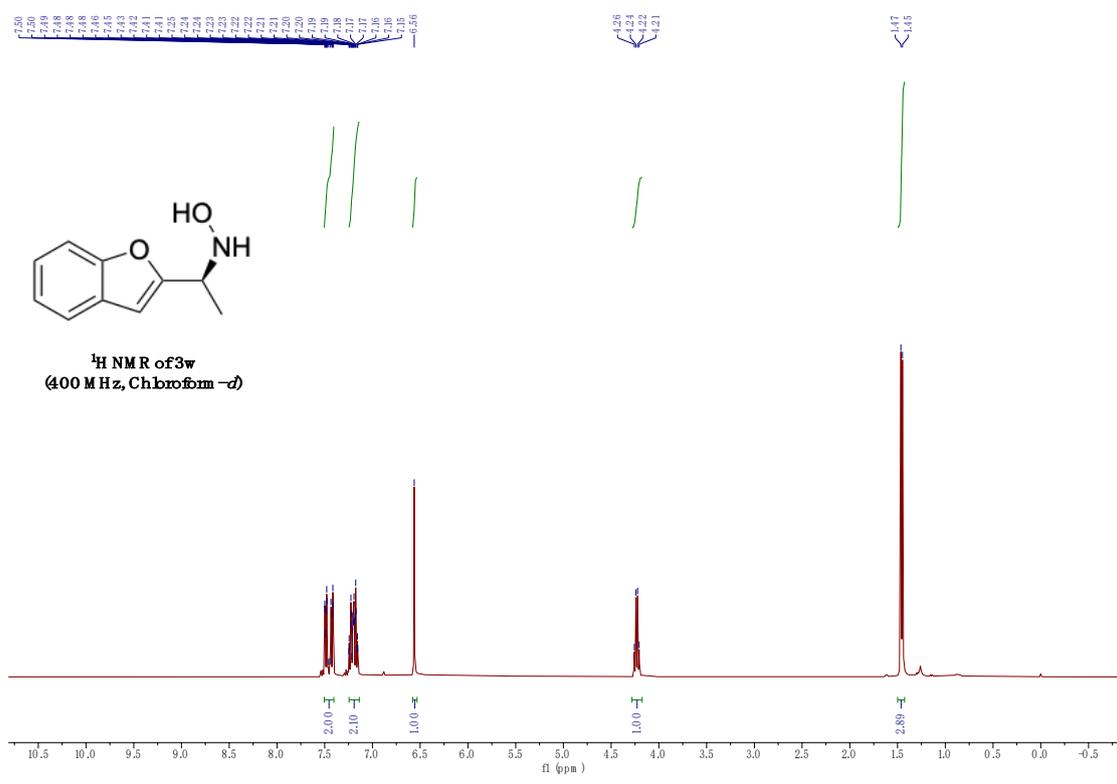
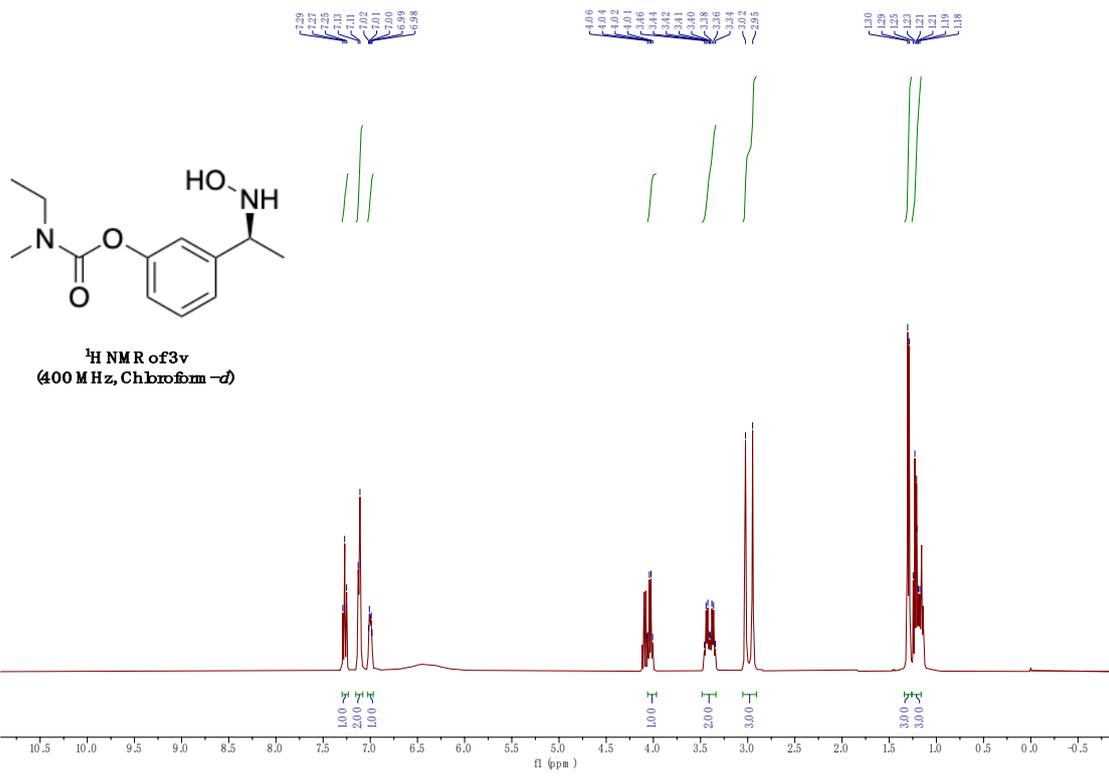


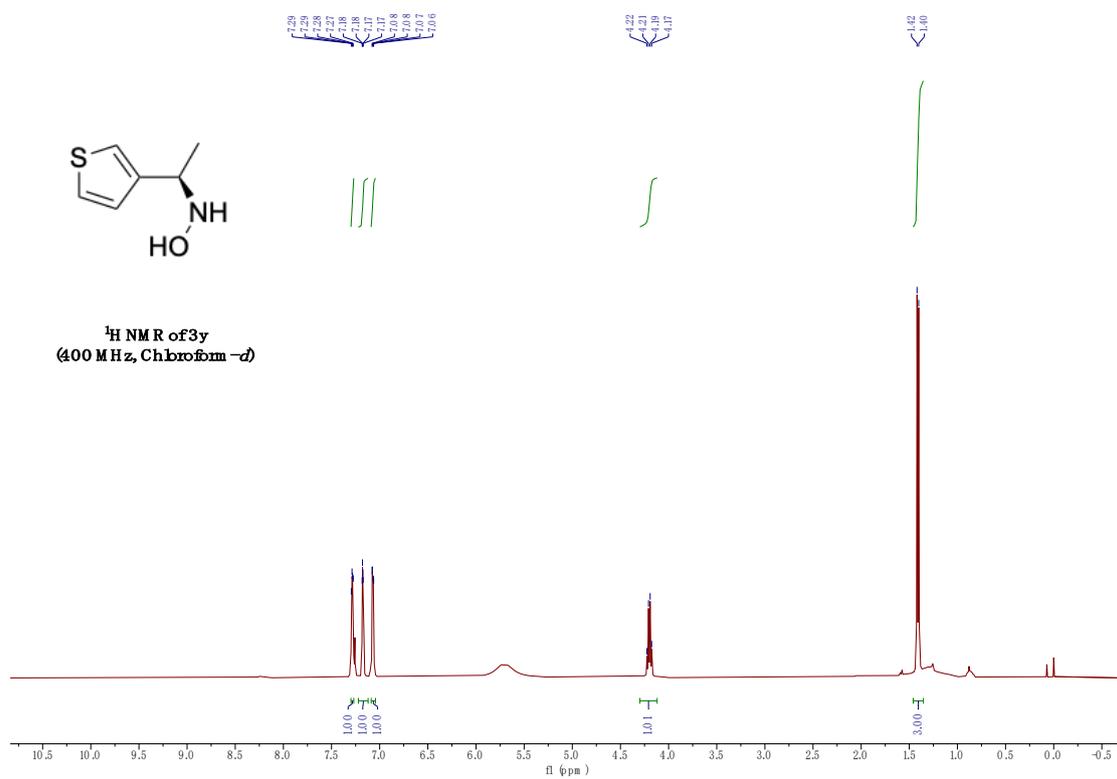
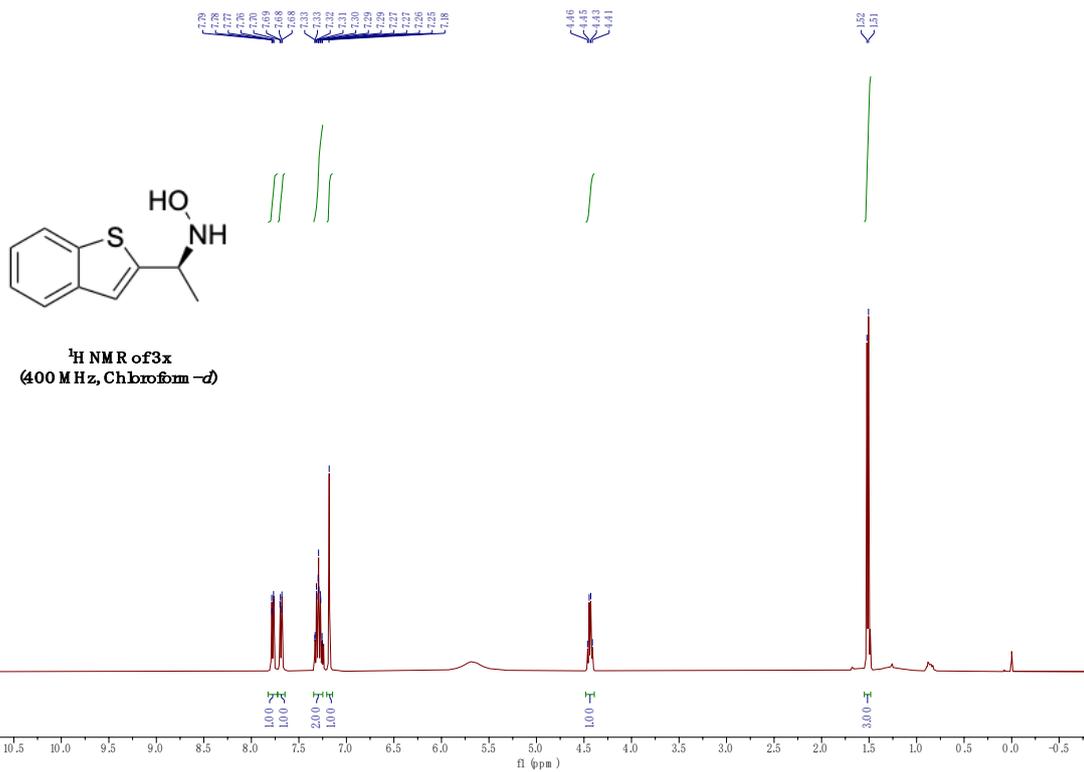


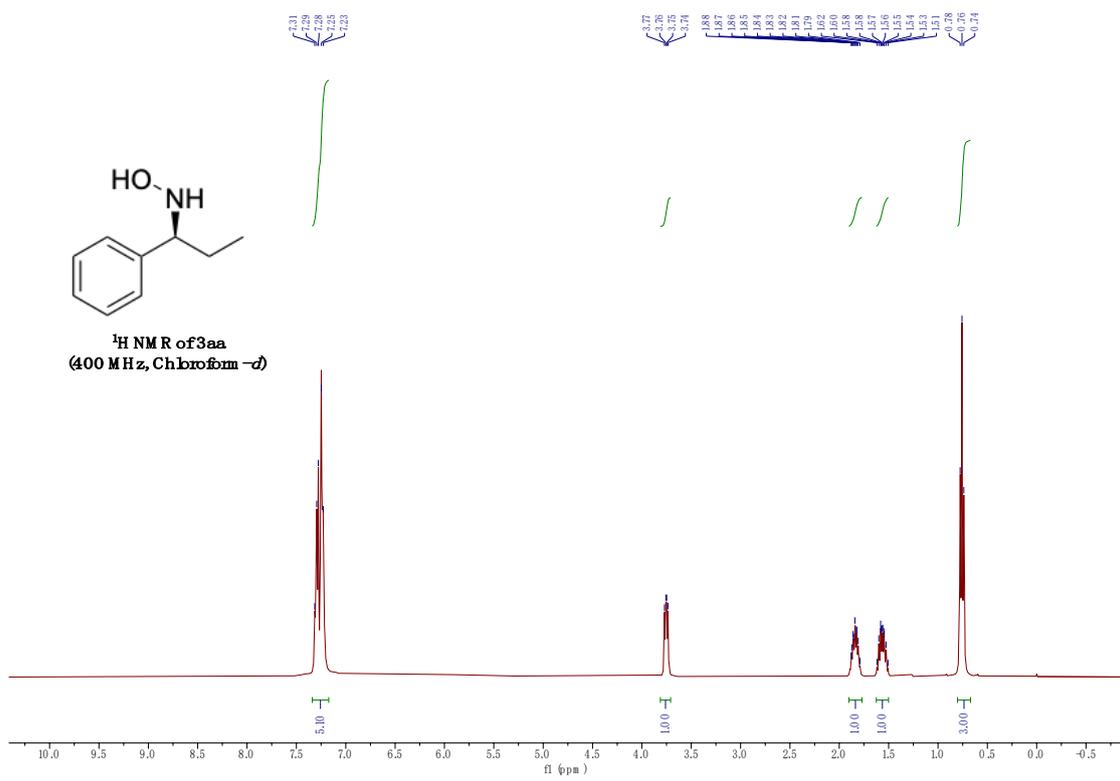
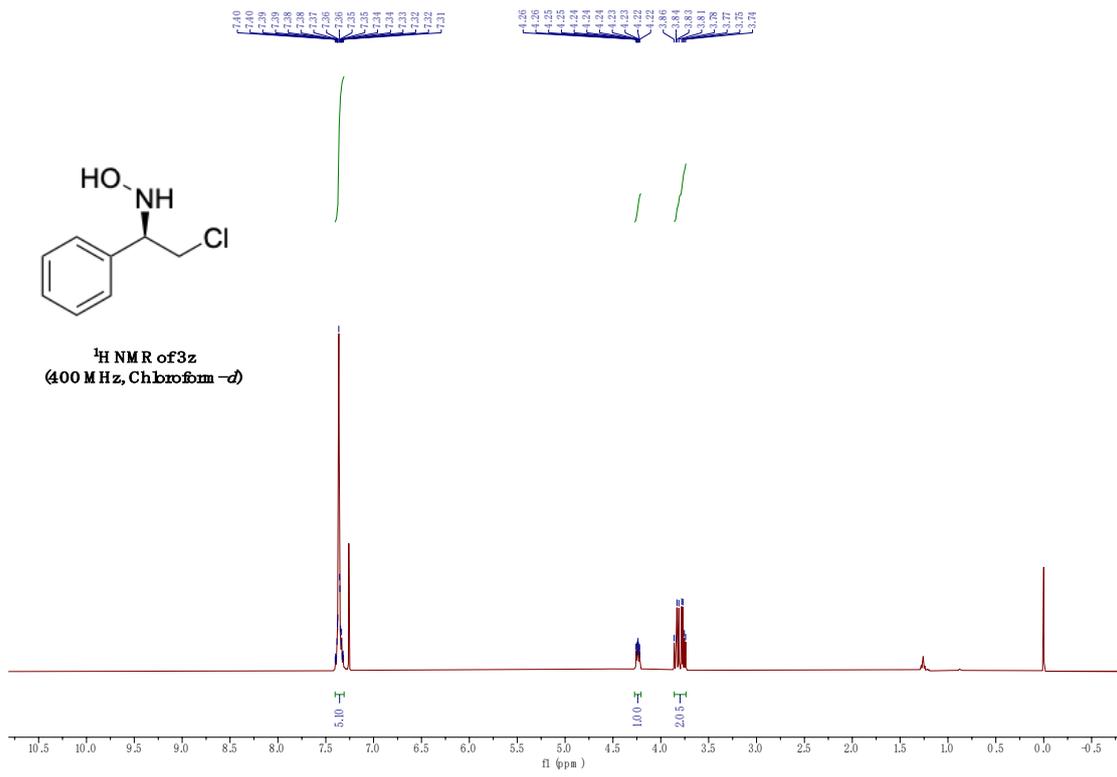


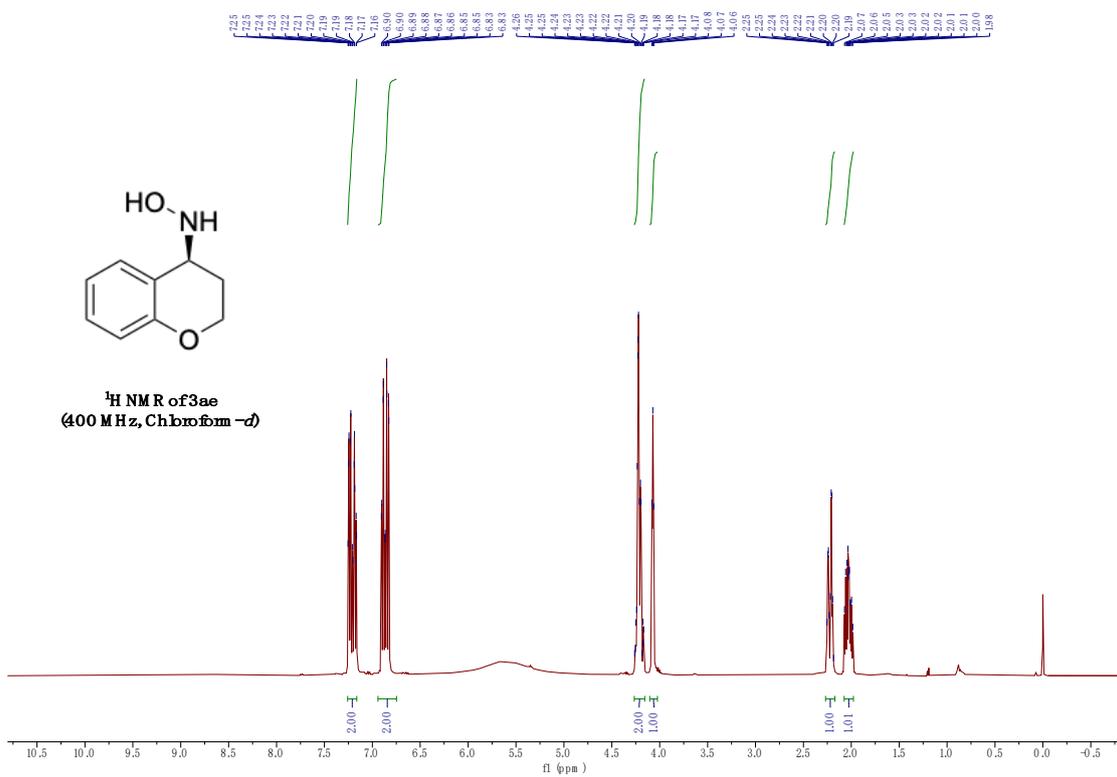
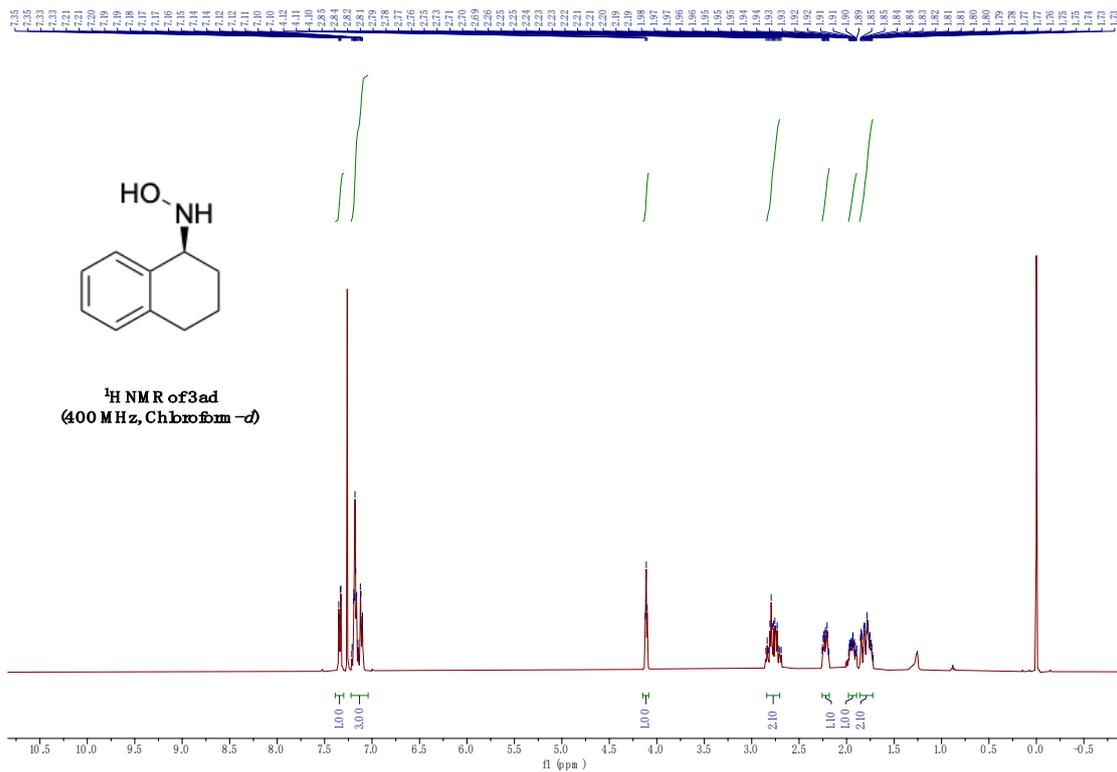


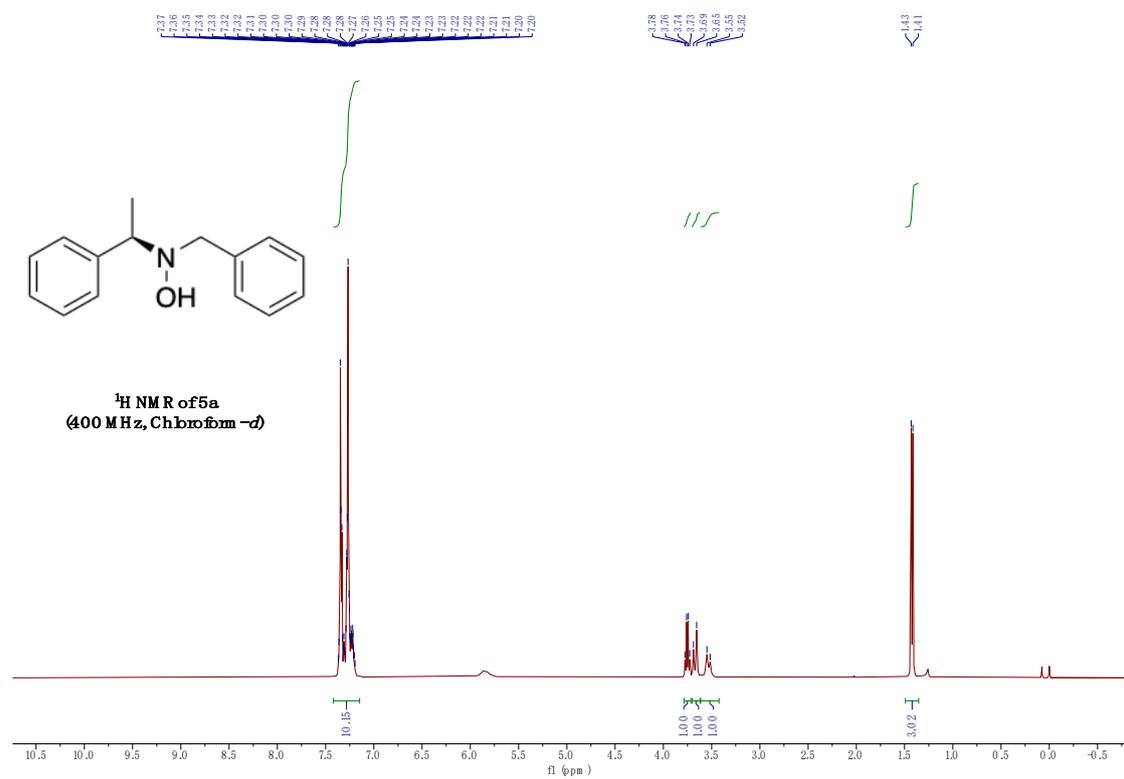
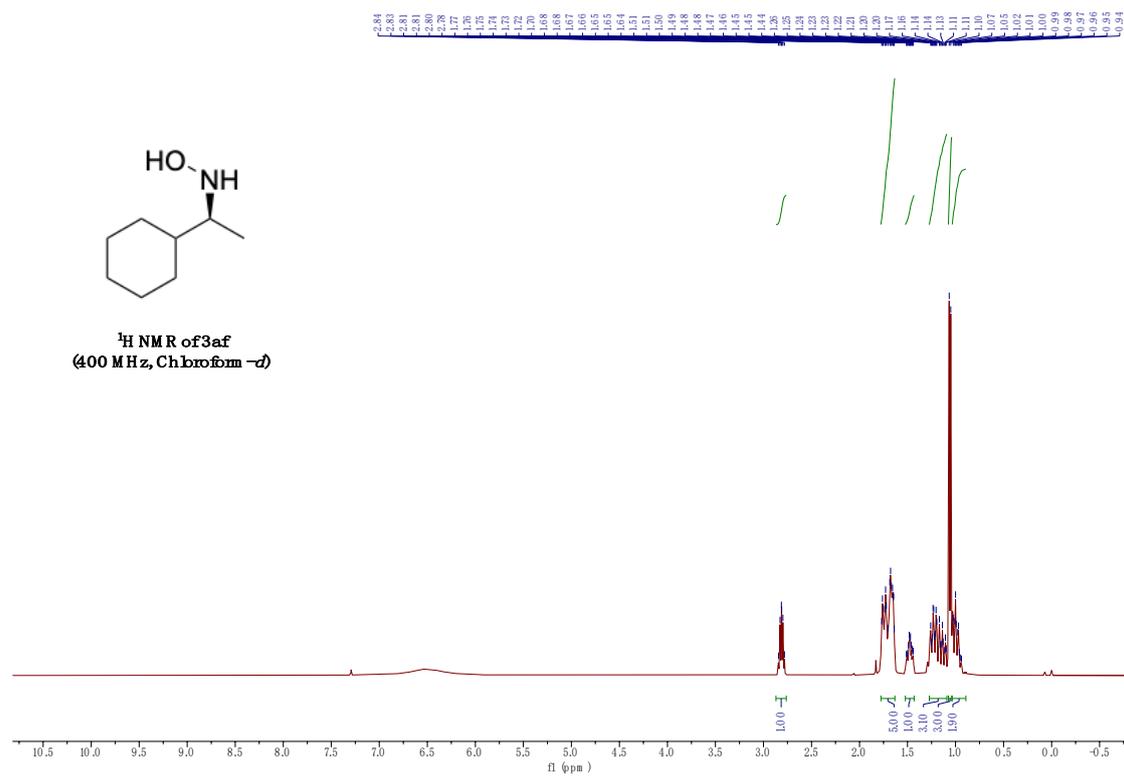


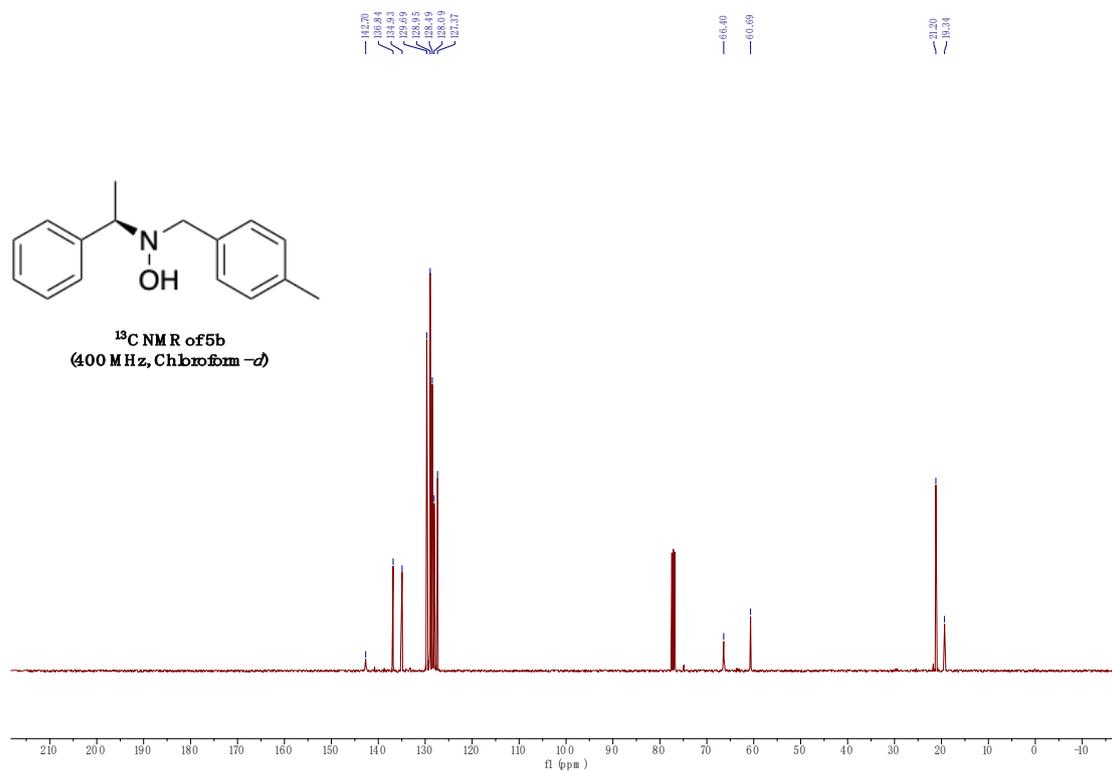
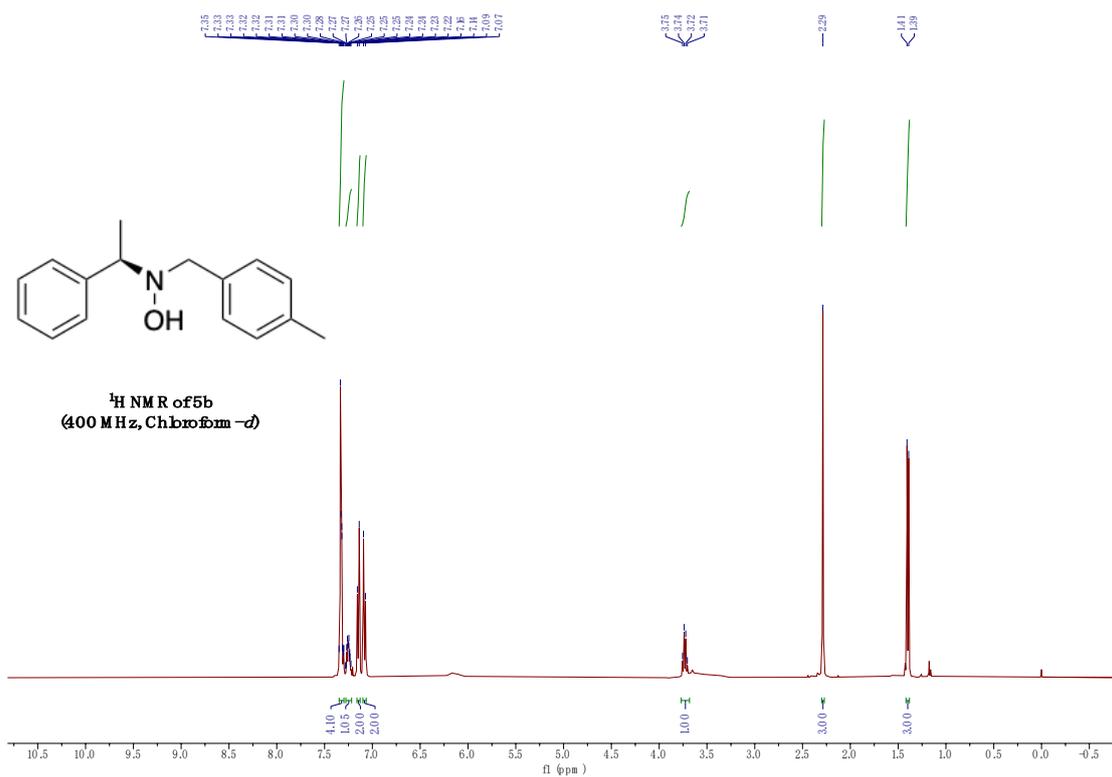


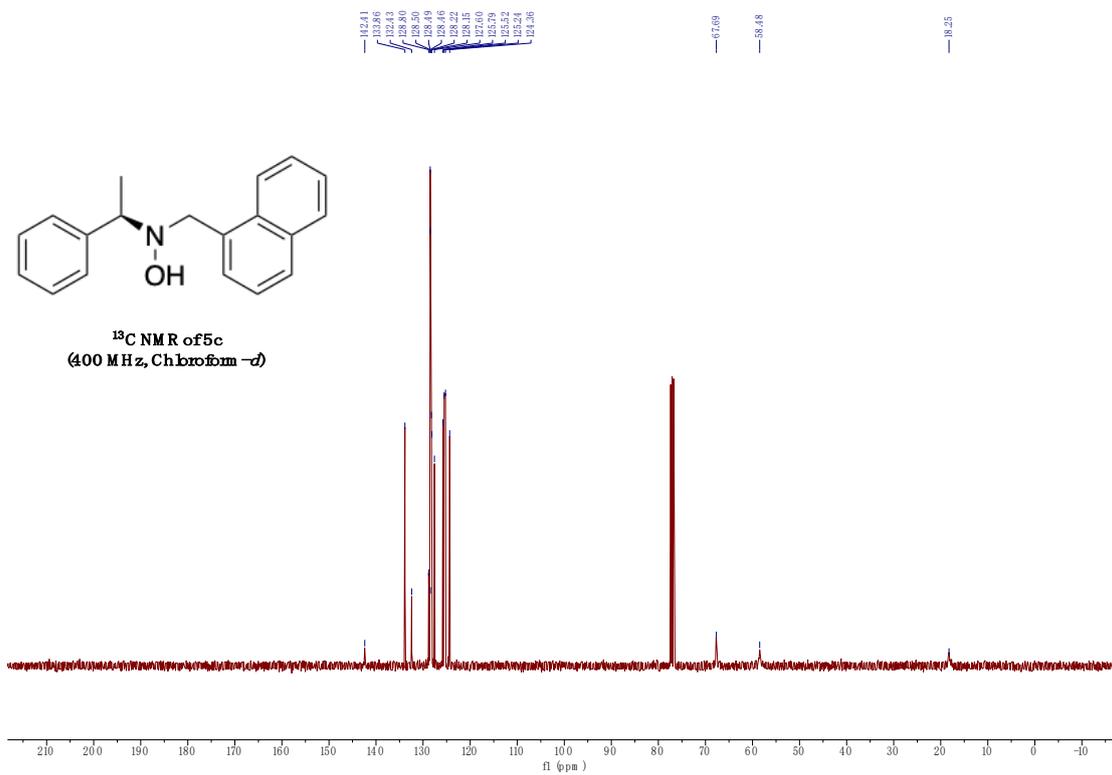
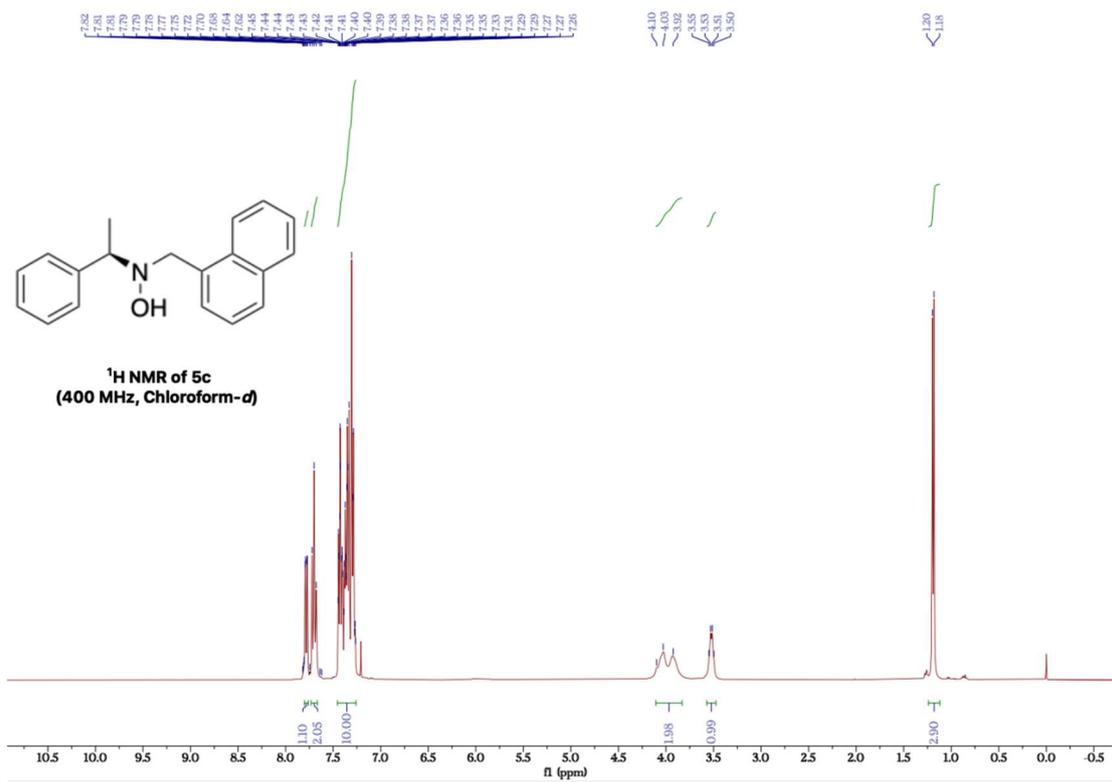


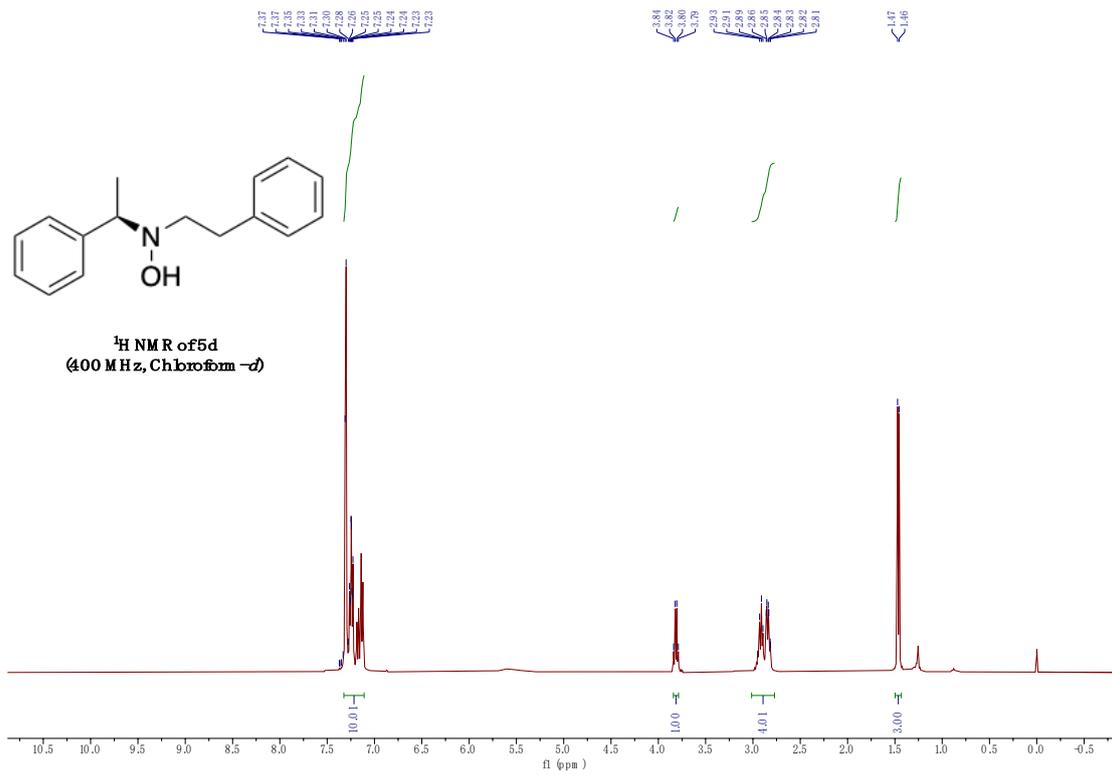


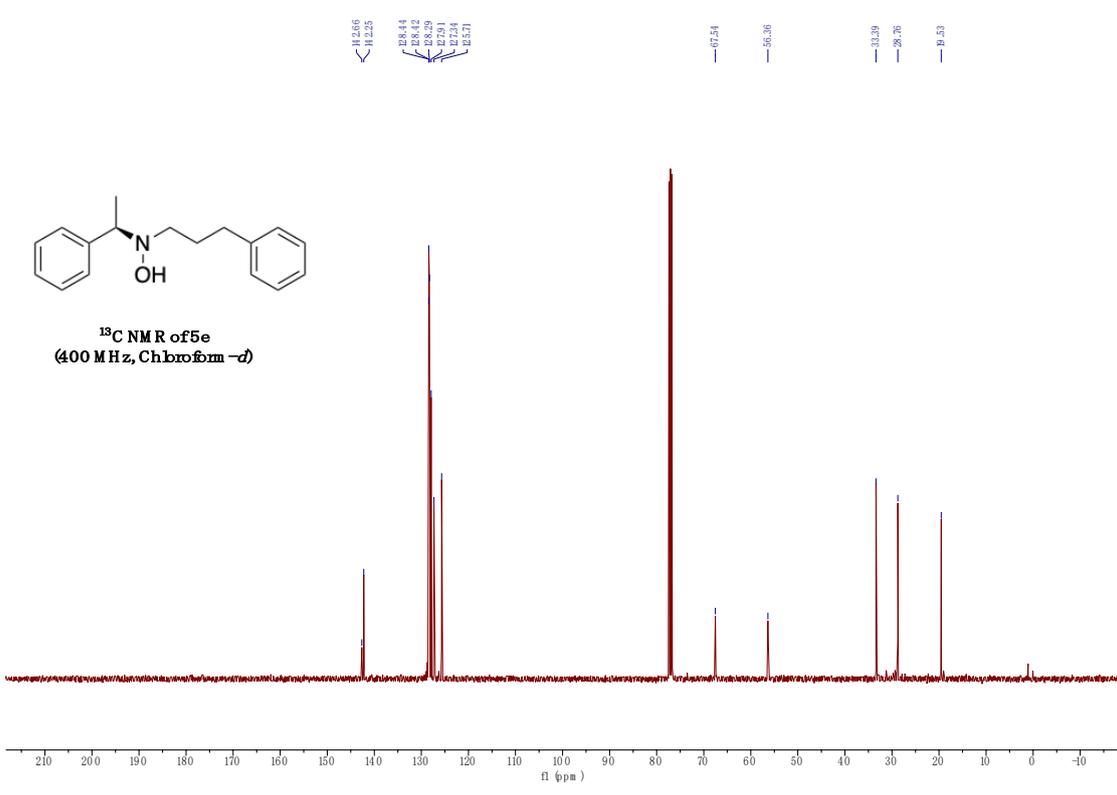
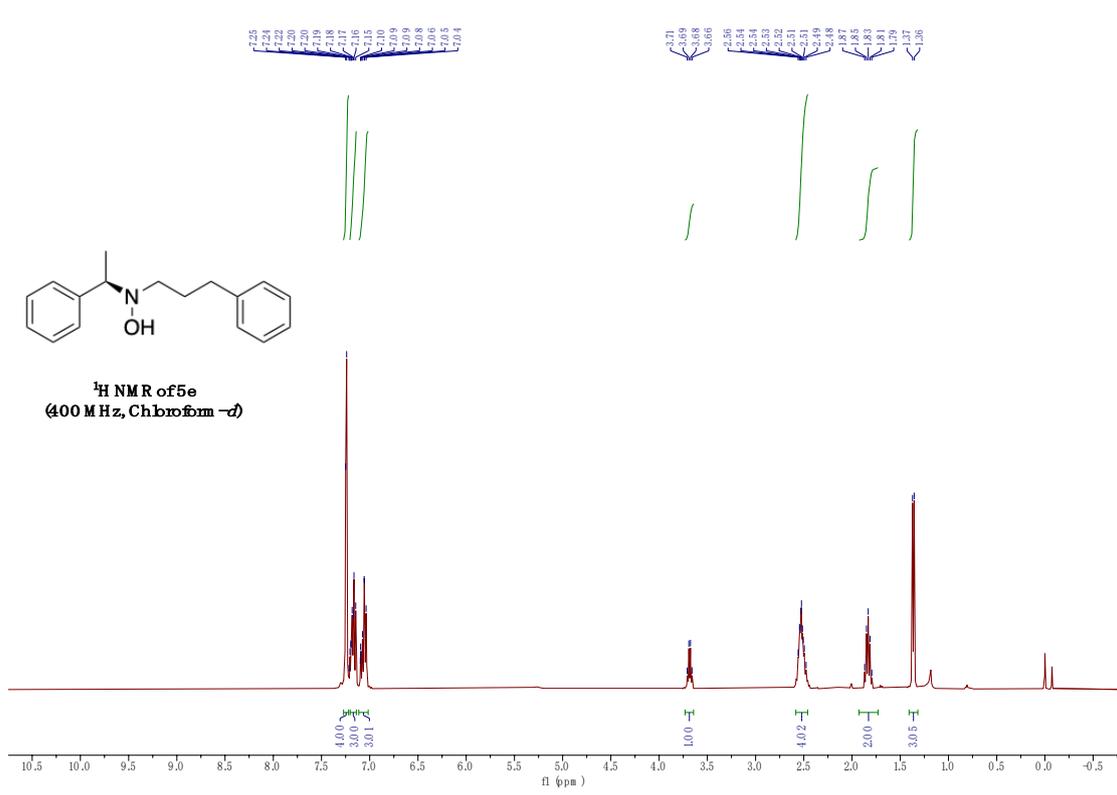


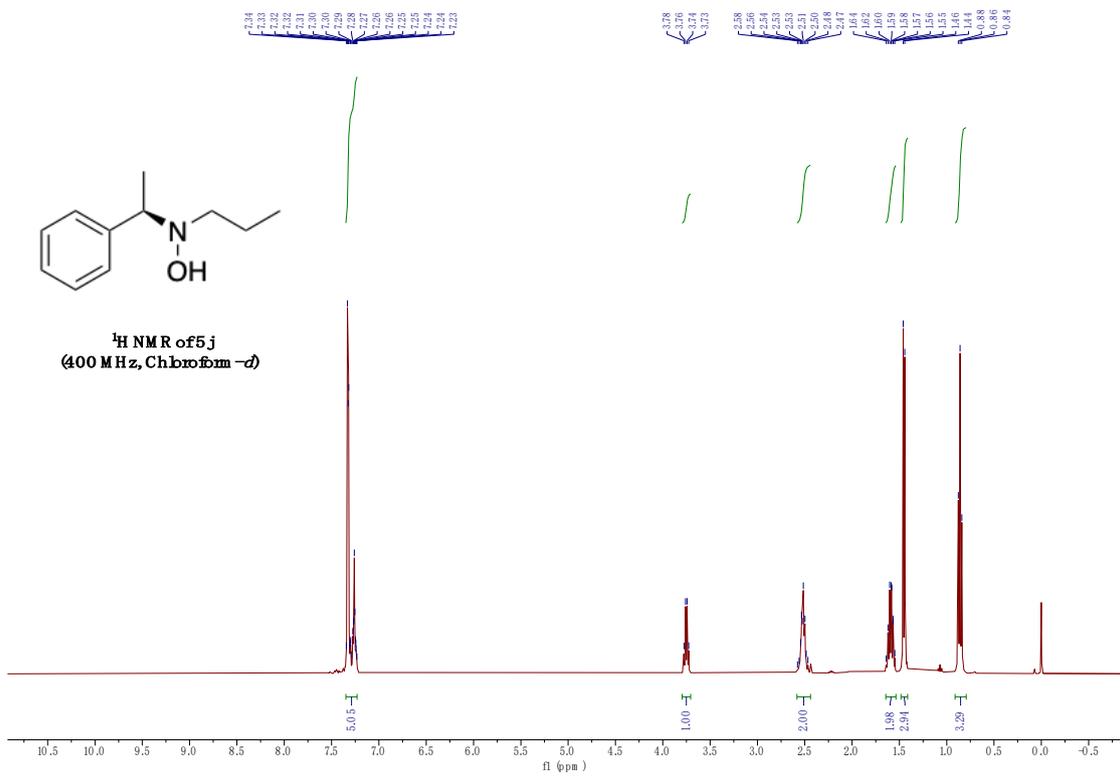
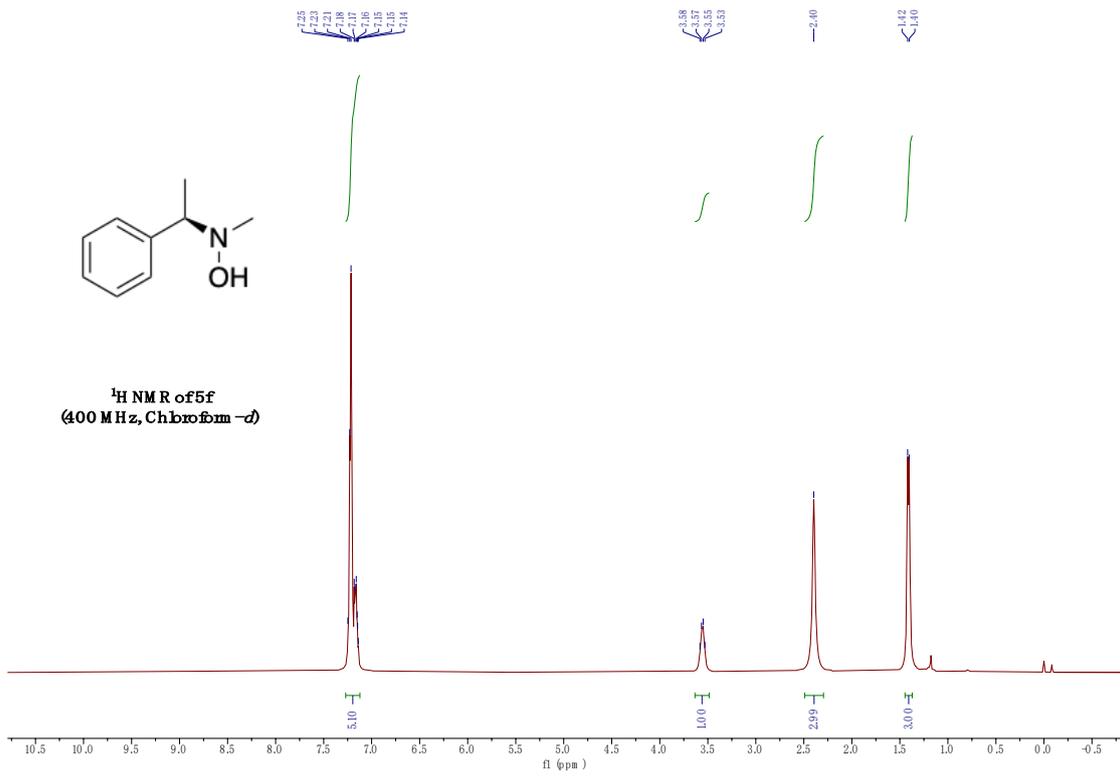


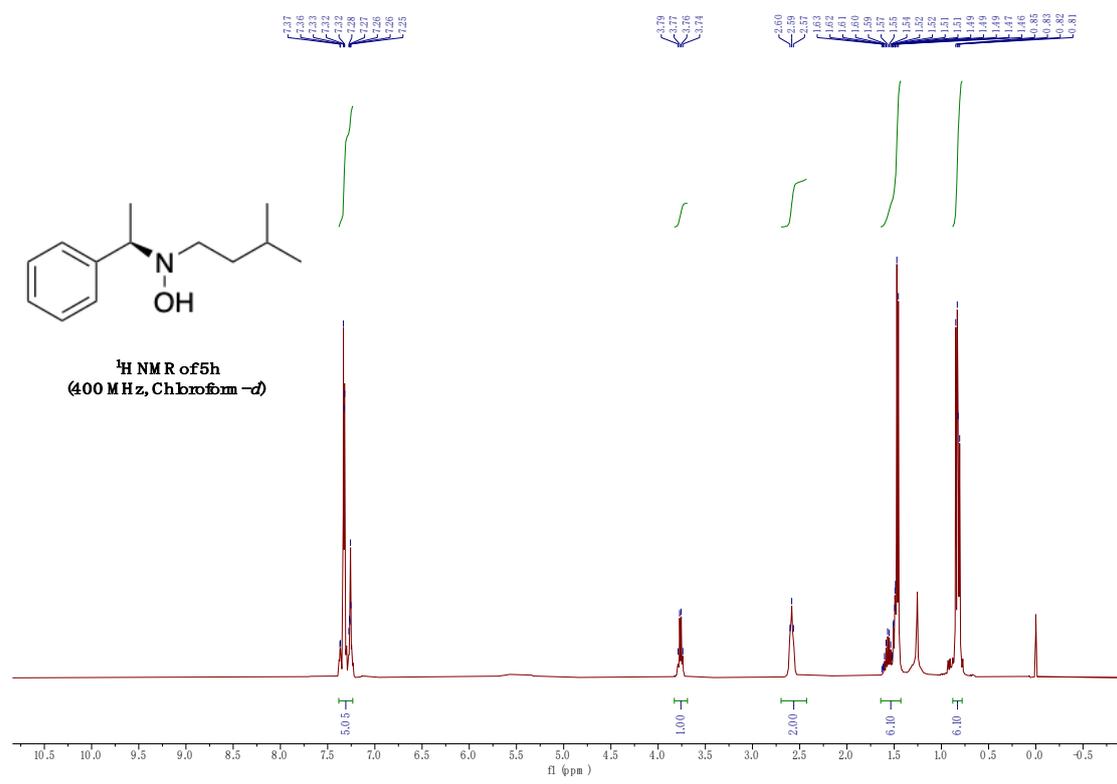
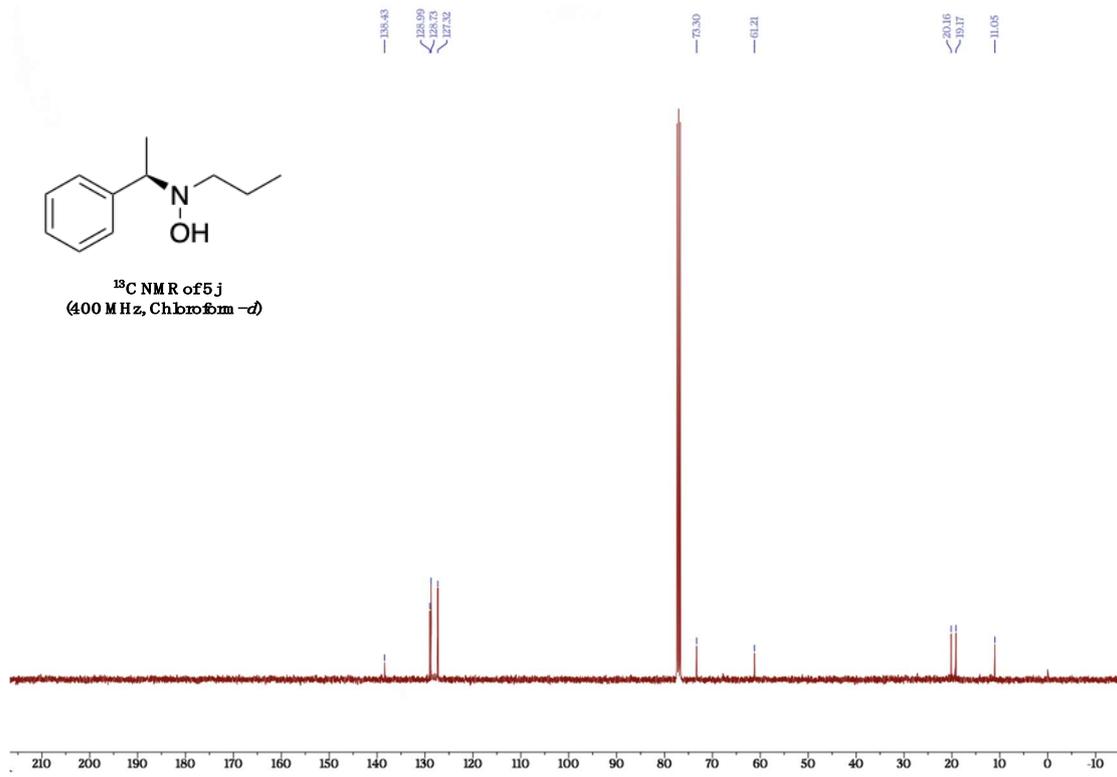


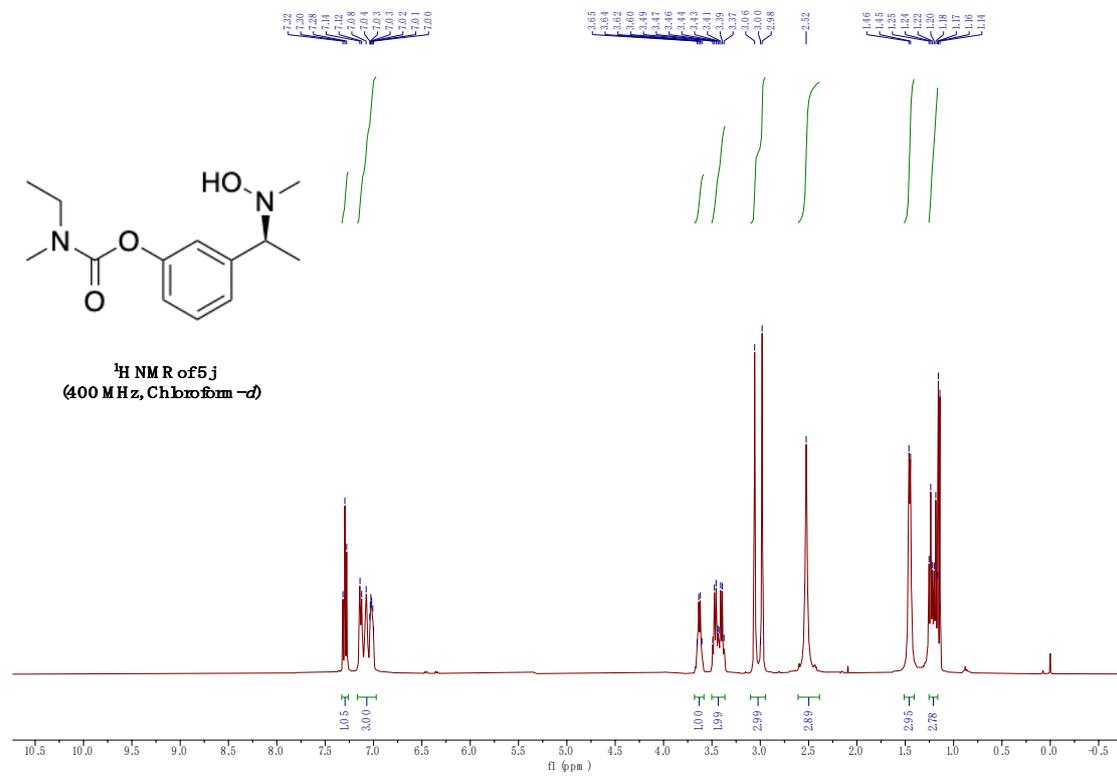
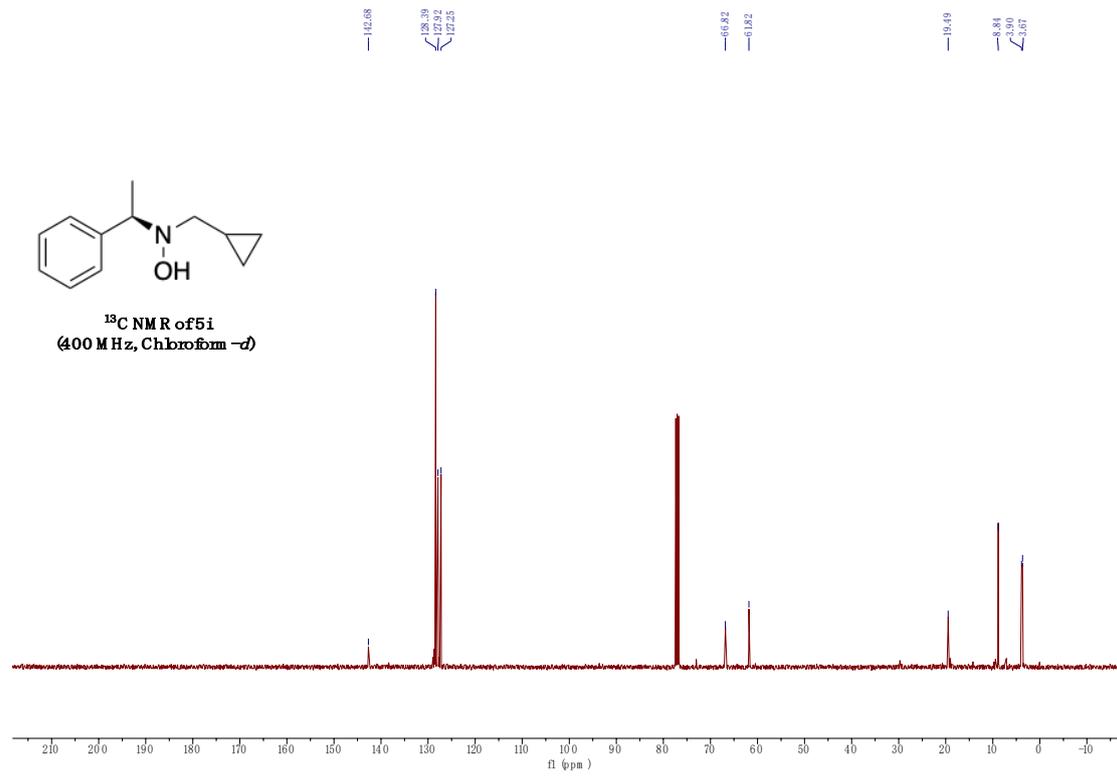


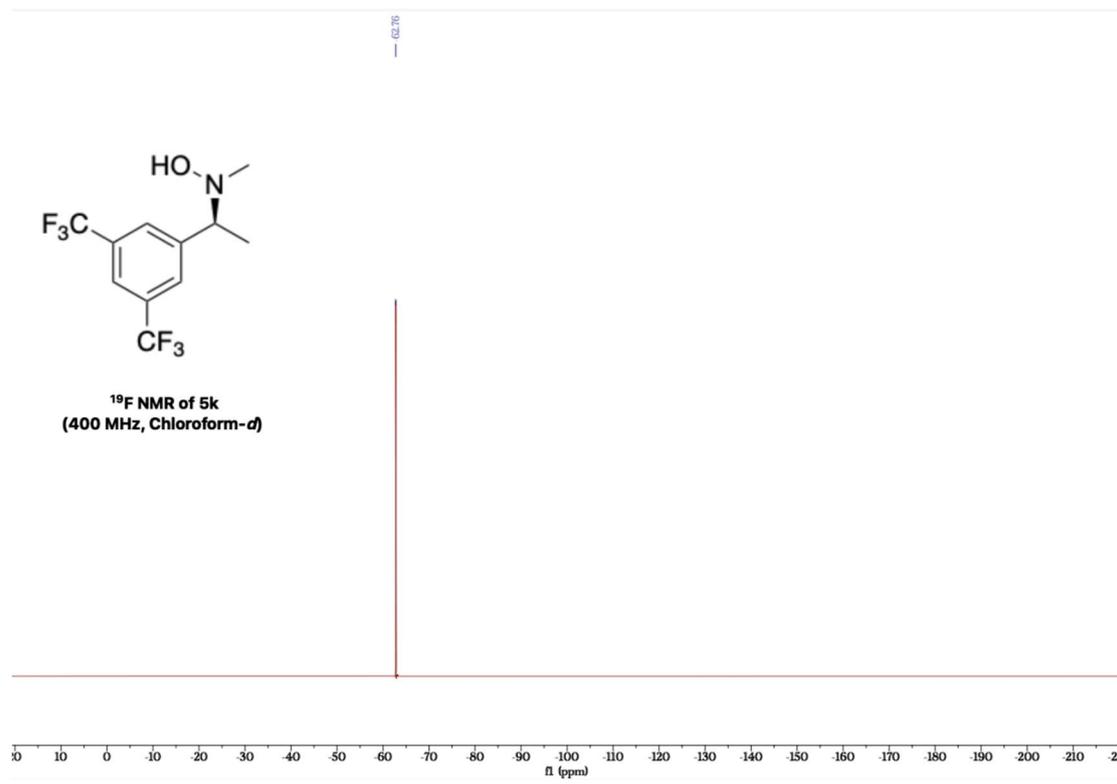
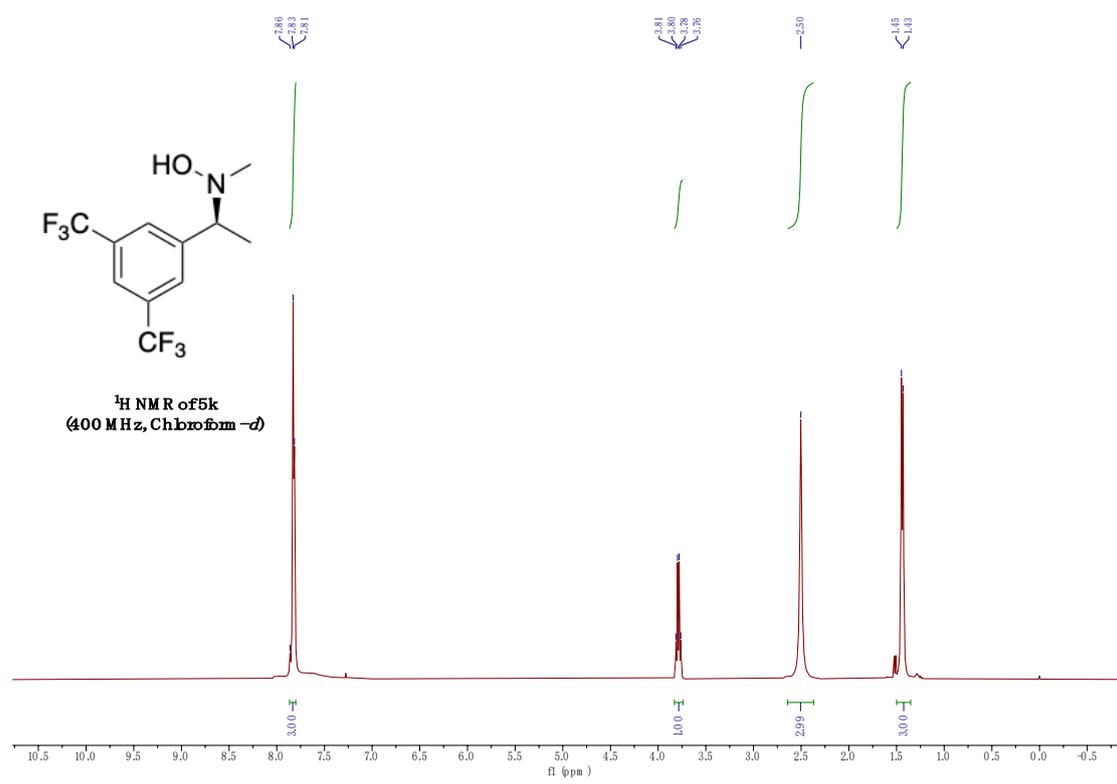


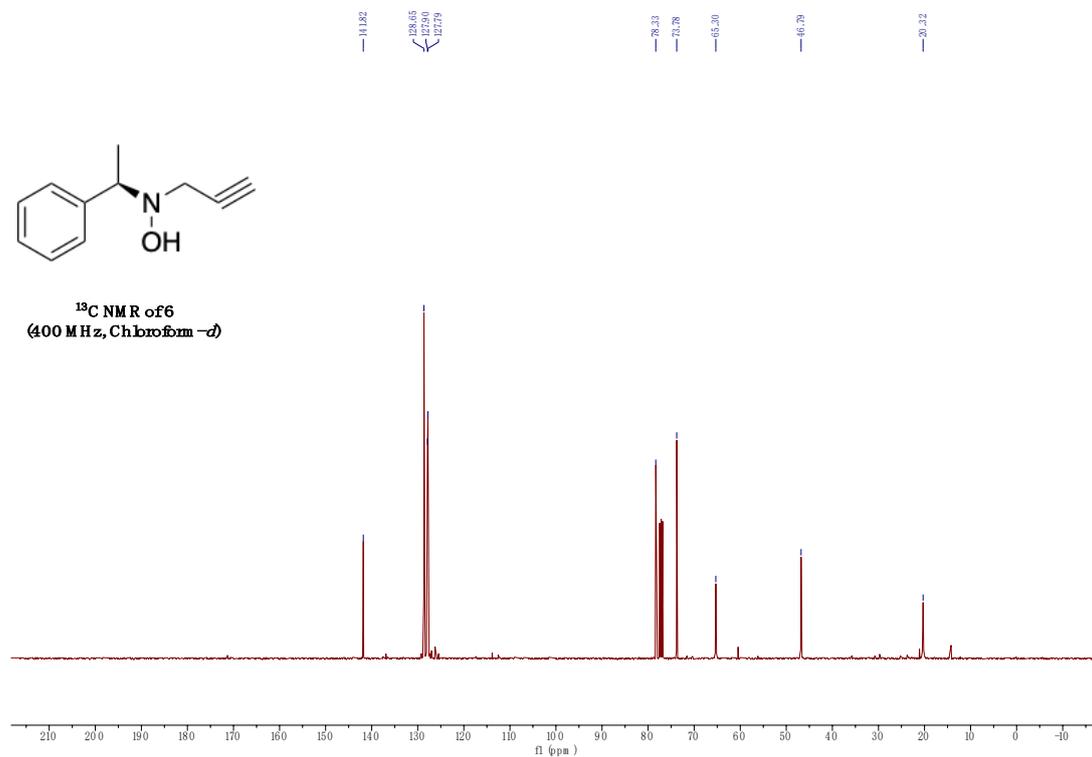
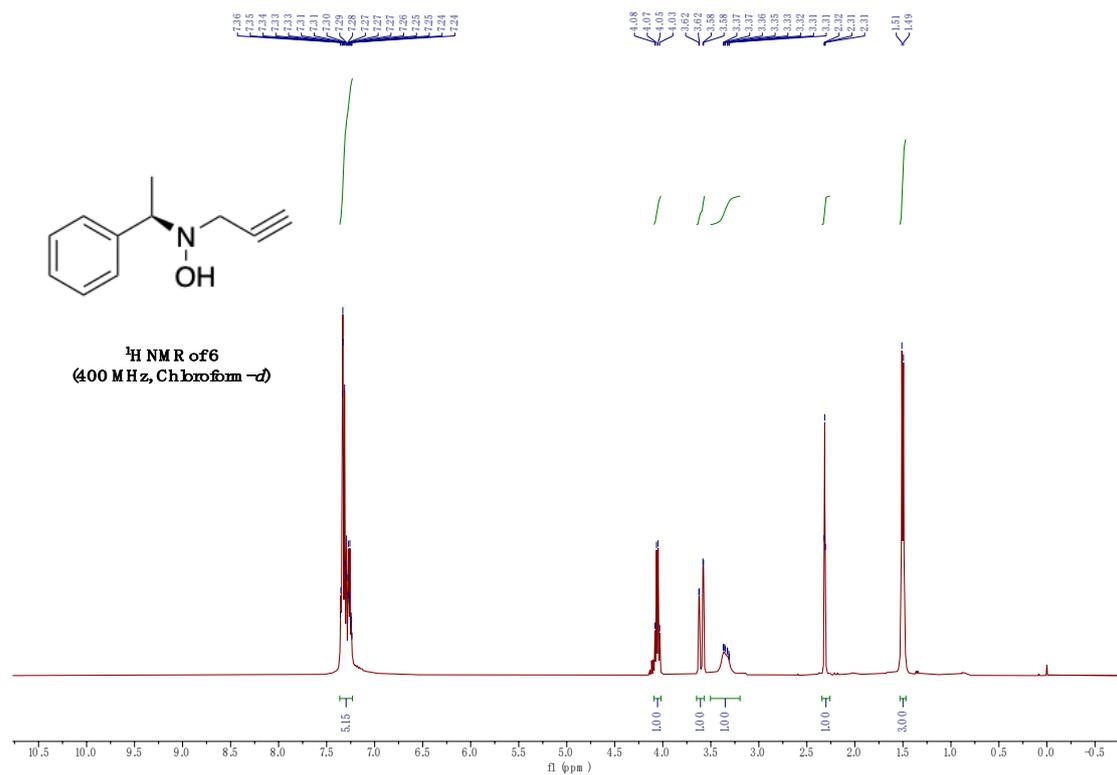


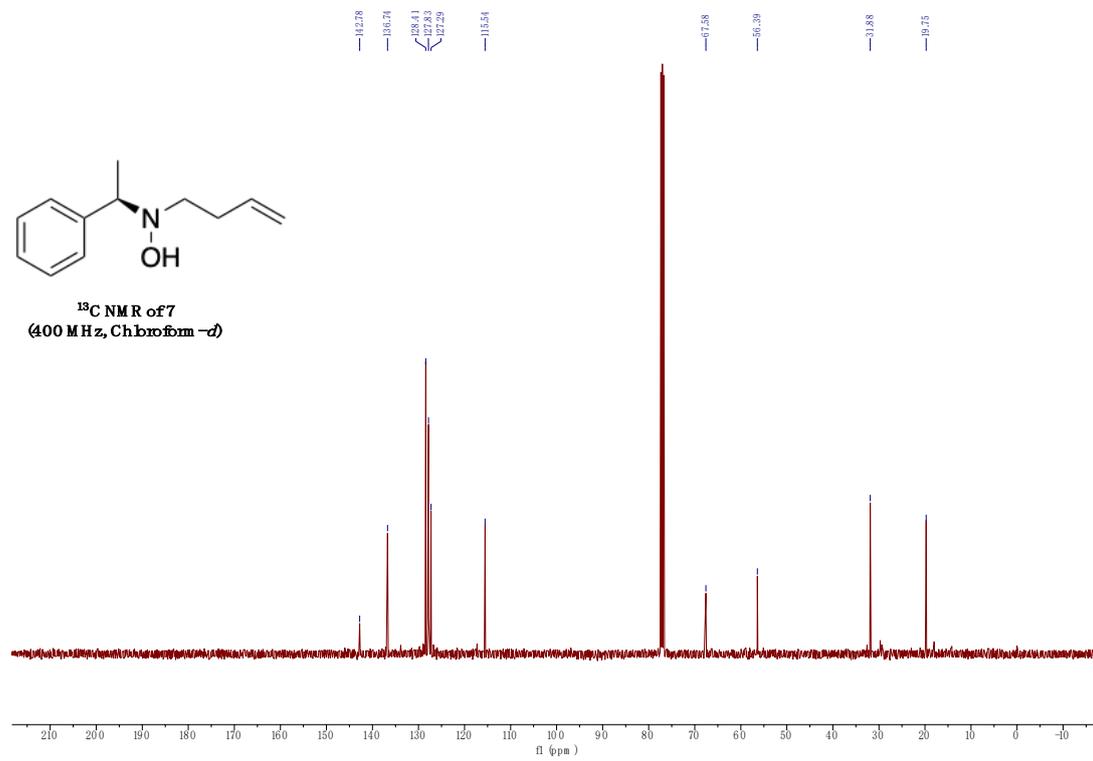
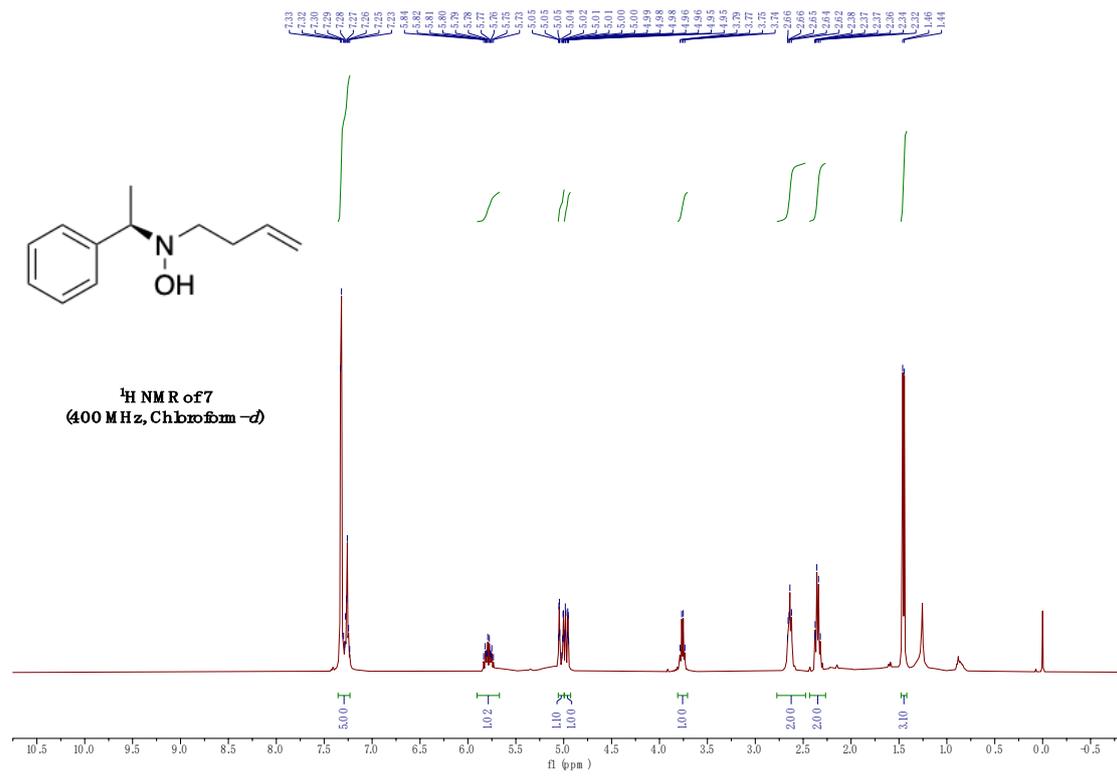


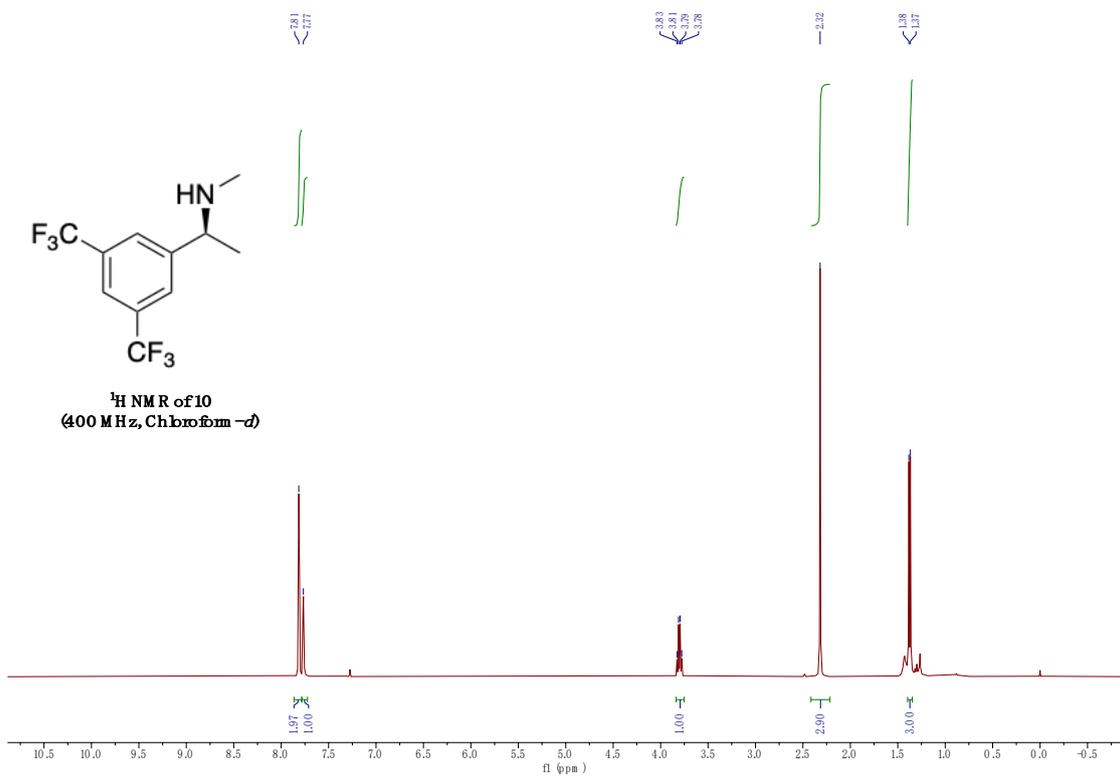
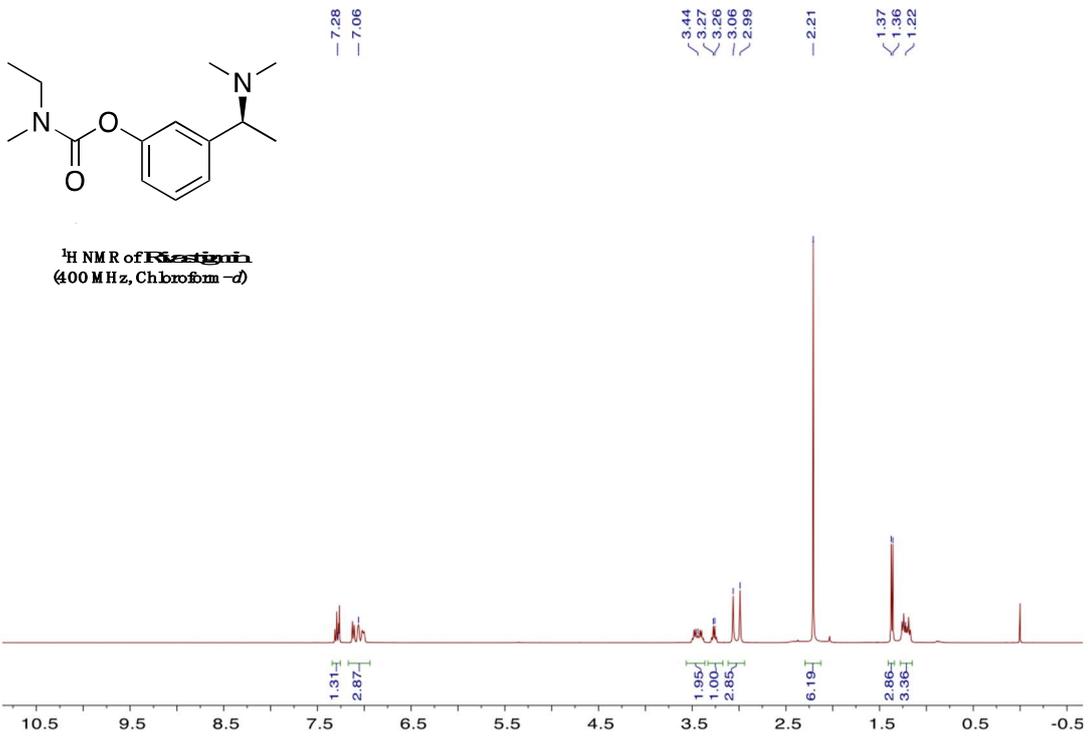


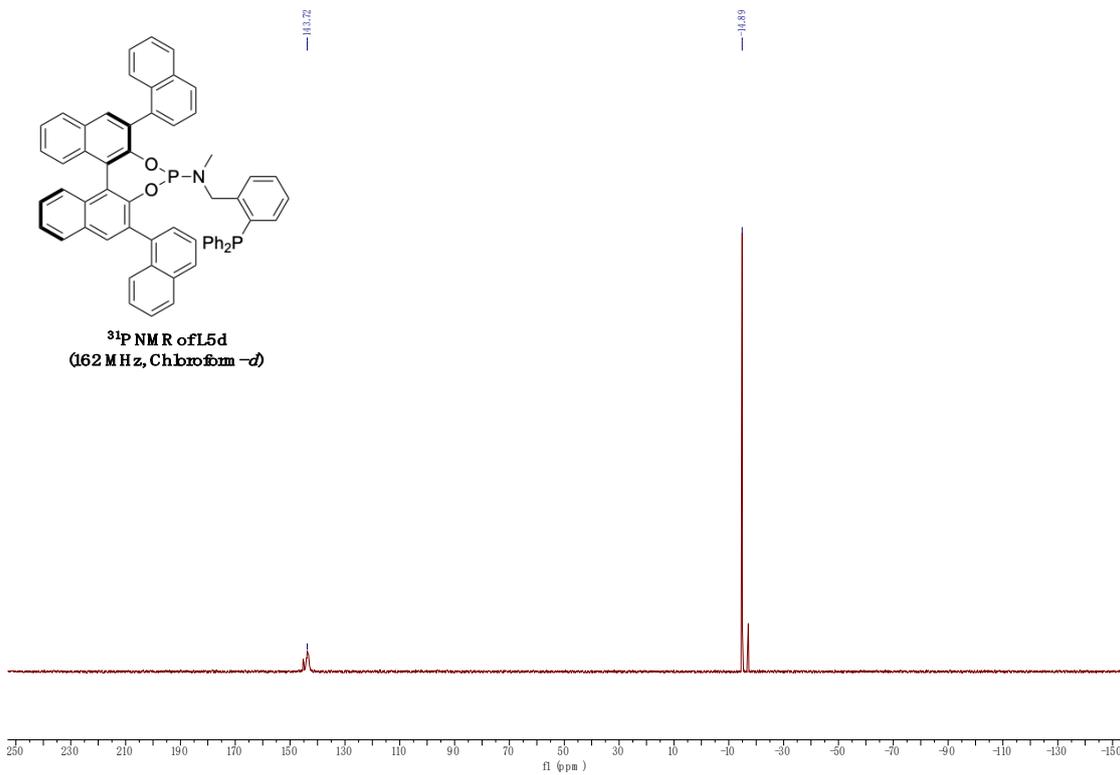
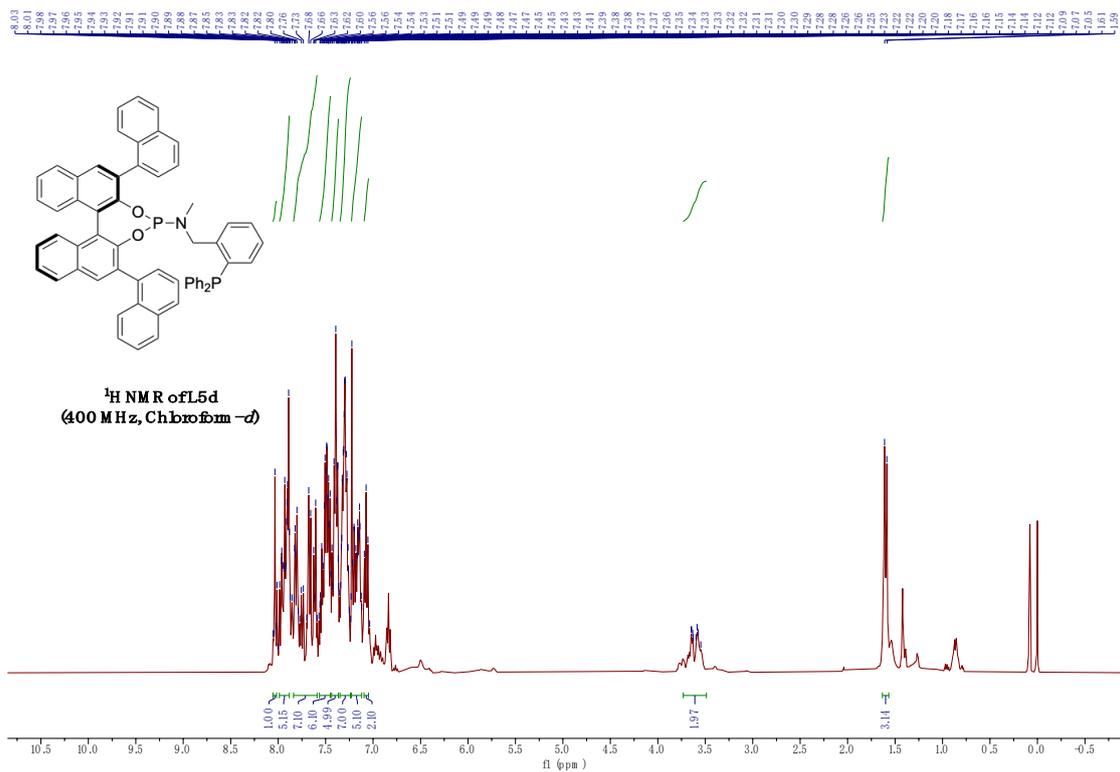


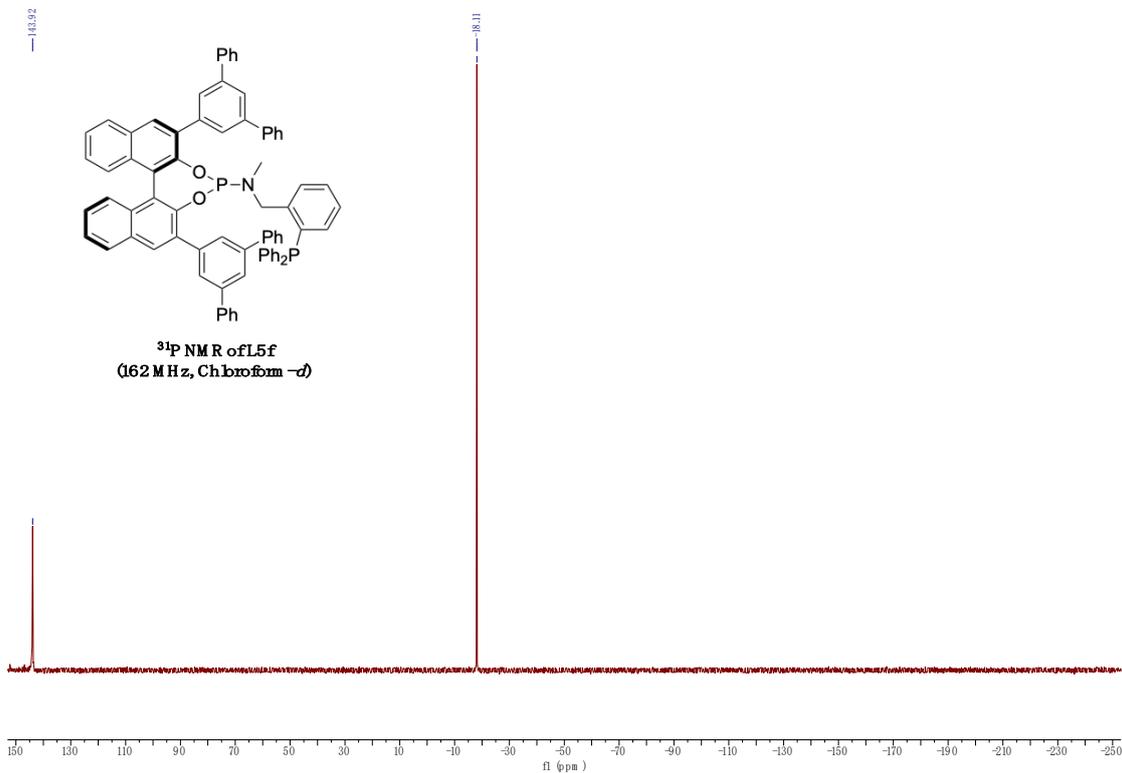
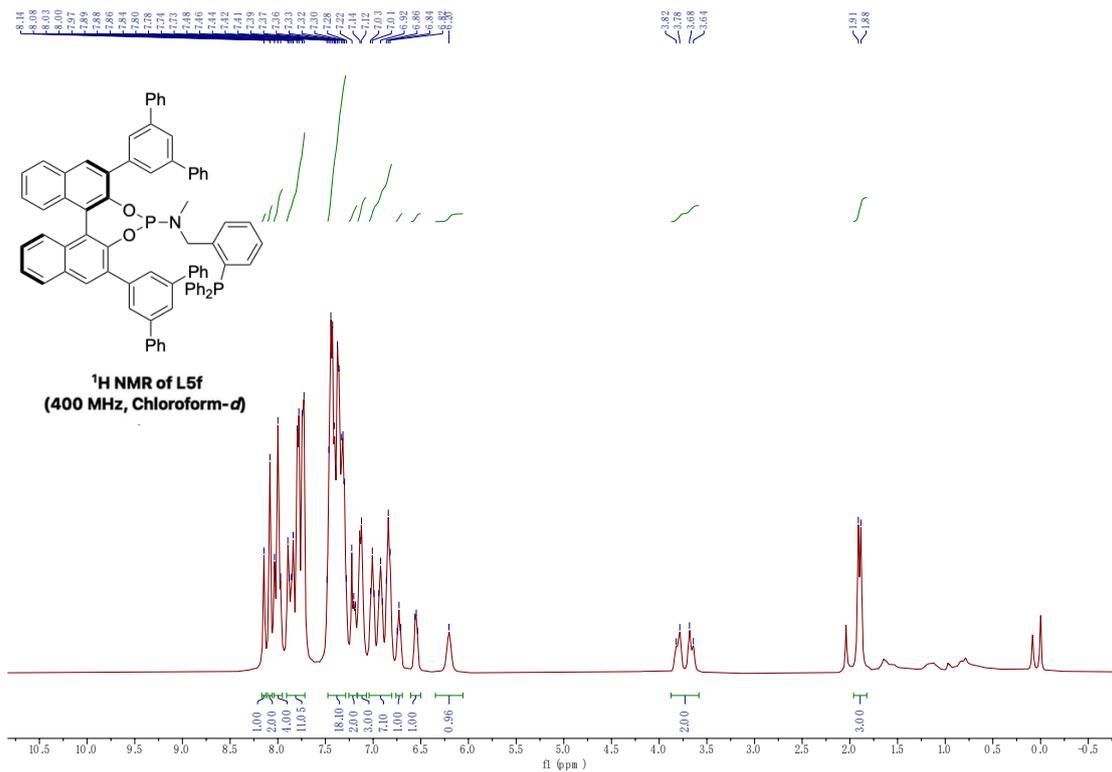




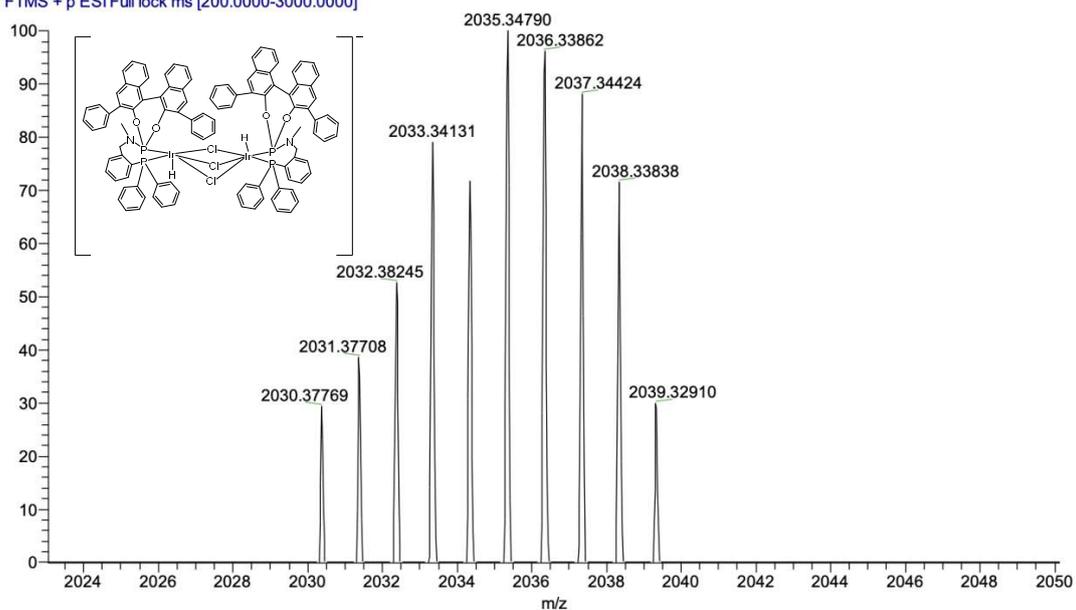








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