Supporting Information

Electroreductive Hydroxymethylation of Imines with Ketones To Access β-Amino Alcohols

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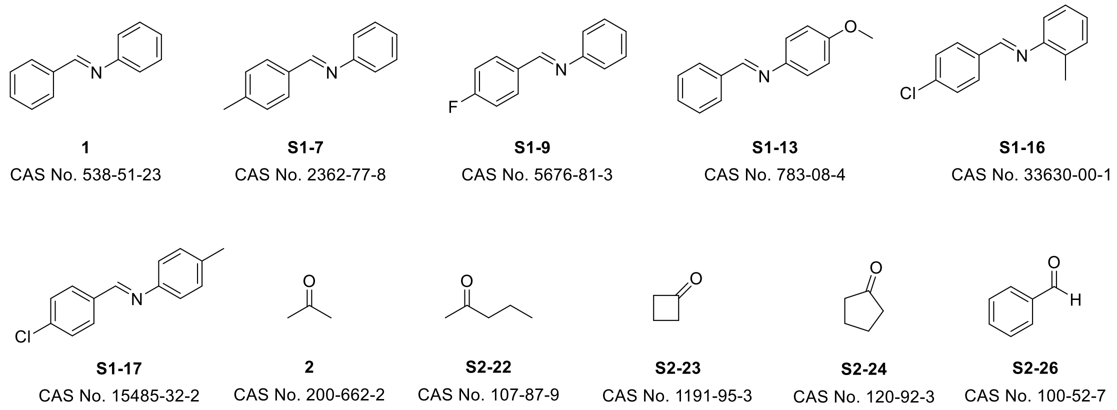
Contents

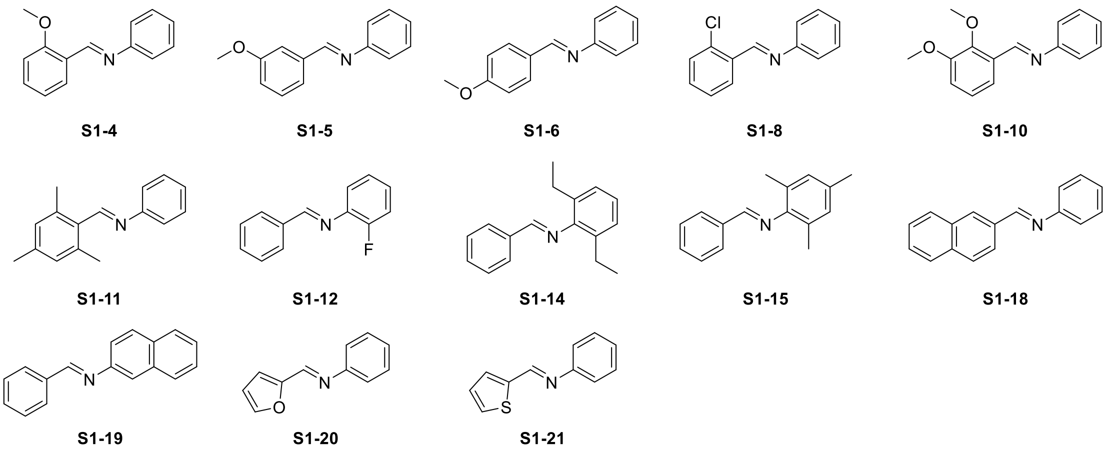
A. Preparation and characterization of substrates

The following substrates were purchased from commercial sources (Scheme S1).



Scheme S1. Substrates purchased from commercial sources.

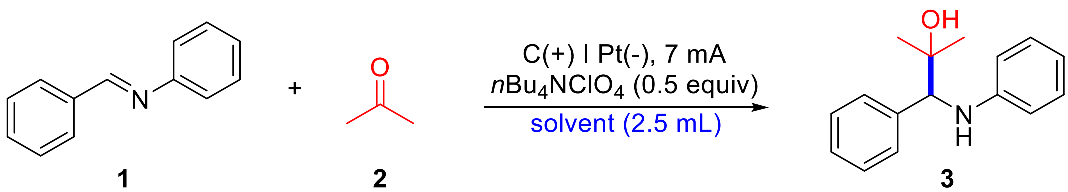
The following imines were synthesized according to literature (Scheme S2).



Scheme S2. Imines synthesized according to literature.

B. Optimization of reaction conditions

Table S1. Solvent screening[a]

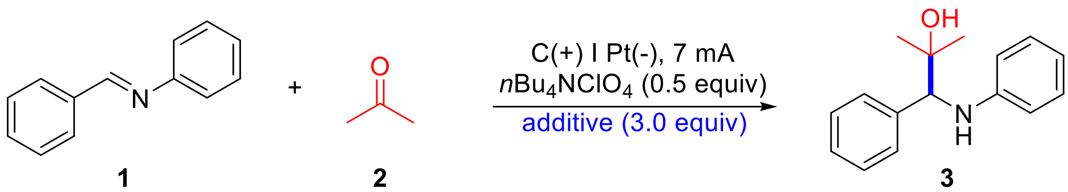


Entry	Solvent	Yield (%)[b]
1	CH_3CN	32
2	DMF	34

3	DCE	46
4	CH_3OH	N.D.[c]
5	——	54

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (2.5 mL), *n*Bu_4NClO_4 (0.15 mmol, 0.5 equiv), solvent (2.5 mL), graphite rod (*Φ* = 6 mm) anode and Pt sheet (10 mm × 10 mm × 0.2 mm) cathode, constant current = 7 mA, 2.17 F/mol, room temperature. [b]Yield of the isolated product after chromatography on silica gel. [c]N.D. = Not Detected.

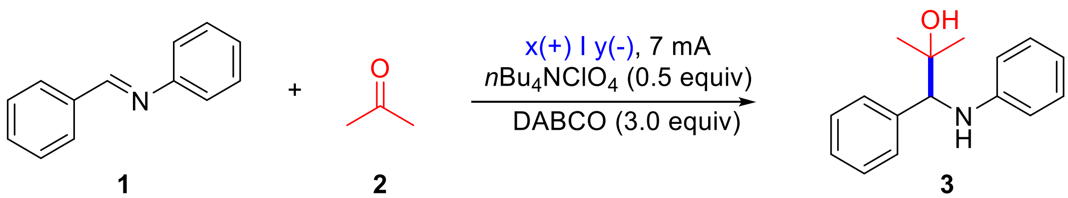
Table S2. Additive screening[a]



Entry	Additive	Yield (%)[b]
1	TEA	55
2	DIPEA	45
3	TEOA	N.R.[c]
4	DABCO	78
5	——	54

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (5 mL), *n*Bu_4NClO_4 (0.15 mmol, 0.5 equiv), additive (3.0 equiv), graphite rod (*Φ* = 6 mm) anode and Pt sheet (10 mm × 10 mm × 0.2 mm) cathode, constant current = 7 mA, 2.17 F/mol, room temperature. [b]Yield of the isolated product after chromatography on silica gel. [c]N.R. = No Reaction.

Table S3. Electrode screening[a]

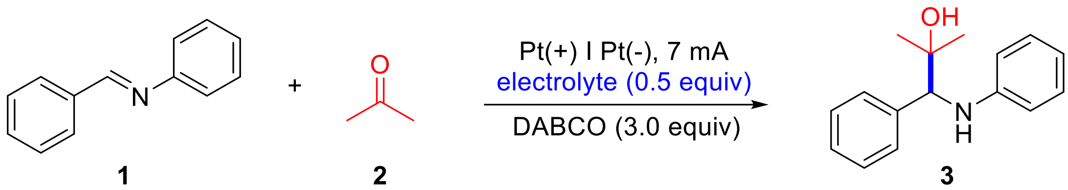


Entry	Anode	Cathode	Yield (%)[b]
1	graphite rod	graphite rod	63
2	graphite rod	Pt sheet	78

3	Pt sheet	graphite rod	55
4	Pt sheet	Pt sheet	87
5	Zn sheet	graphite rod	55

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (5 mL), *n*Bu_4NClO_4 (0.15 mmol, 0.5 equiv), DABCO (0.9 mmol, 3.0 equiv), x anode and y cathode (graphite rod (Φ = 6 mm) and Pt sheet (10 mm × 10 mm × 0.2 mm)), constant current = 7 mA, 2.17 F/mol, room temperature. [b]Yield of the isolated product after chromatography on silica gel.

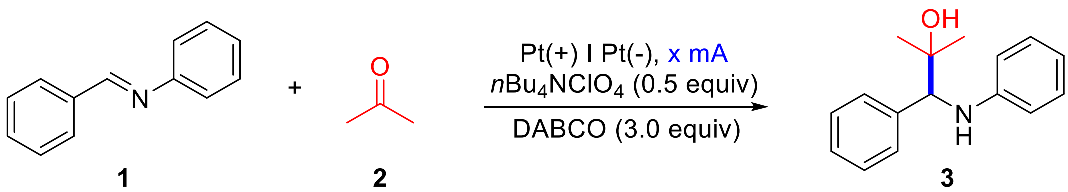
Table S4. Electrolyte screening[a]



Entry	Electrolyte	Yield (%)[b]
1	*n*Bu_4NClO_4	87
2	Na_2SO_4	34
3	*n*Bu_4NBF_4	45
4	Et_4NCl	32
5	NaI	81
6	$KClO_4$	trace

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (5 mL), electrolyte (0.15 mmol, 0.5 equiv), DABCO (0.9 mmol, 3.0 equiv), Pt sheet (10 mm × 10 mm × 0.2 mm) anode and cathode, constant current = 7 mA, 2.17 F/mol, room temperature. [b]Yield of the isolated product after chromatography on silica gel. [c]N.R. = No Reaction.

Table S5. Optimization of the current[a]

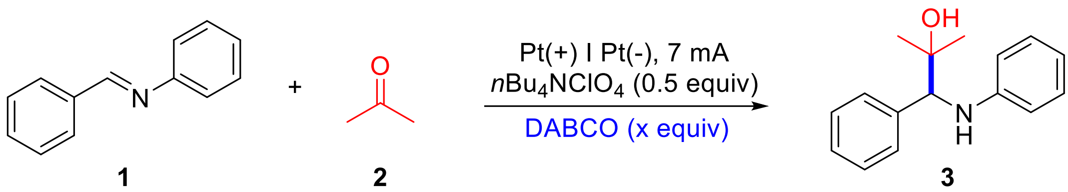


Entry	Current	Yield (%)[b]
1	5	65
2	7	87

3	9	72

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (5 mL), *n*Bu_4NClO_4 (0.15 mmol, 0.5 equiv), DABCO (0.9 mmol, 3.0 equiv), Pt sheet (10 mm × 10 mm × 0.2 mm) anode and cathode, constant current = x mA, 2.17 F/mol, room temperature. [b]Yield of the isolated product after chromatography on silica gel.

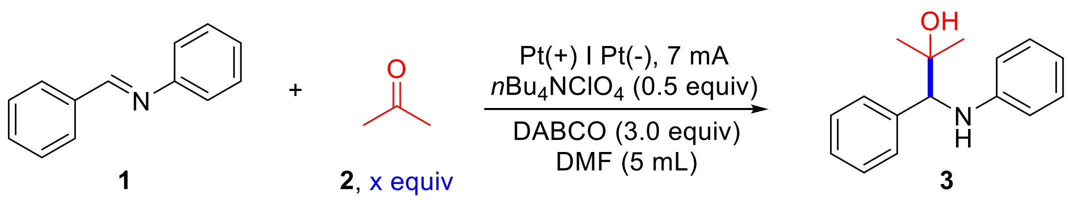
Table S6. Optimization of the amount of DABCO[a]



Entry	Equivalent of DABCO	Yield (%)[b]
1	1.0	42
2	2.0	59
3	3.0	87
4	4.0	81

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (5 mL), *n*Bu_4NClO_4 (0.15 mmol, 0.5 equiv), DABCO (x equiv), Pt sheet (10 mm × 10 mm × 0.2 mm) anode and cathode, constant current = 7 mA, 2.17 F/mol, room temperature. [b]Yield of the isolated product after chromatography on silica gel.

Table S7. Optimization of the amount of acetone[a]



Entry	Equivalent of acetone	Yield (%)[b]
1	5	21
2	10	27
3	15	31
4	30	45
5	50	64
6	225 (5 mL)[c]	87

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (x equiv), $n\mathrm{Bu_4NClO_4}$ (0.15 mmol, 0.5 equiv), DABCO (3.0 equiv), DMF (5 mL), Pt sheet (10 mm × 10 mm × 0.2 mm) anode and cathode, constant current = 7 mA, 2.17 F/mol, room temperature. [b]Yield of the isolated product after chromatography on silica gel. [c]Acetone (5 mL) instead of DMF (5 mL).

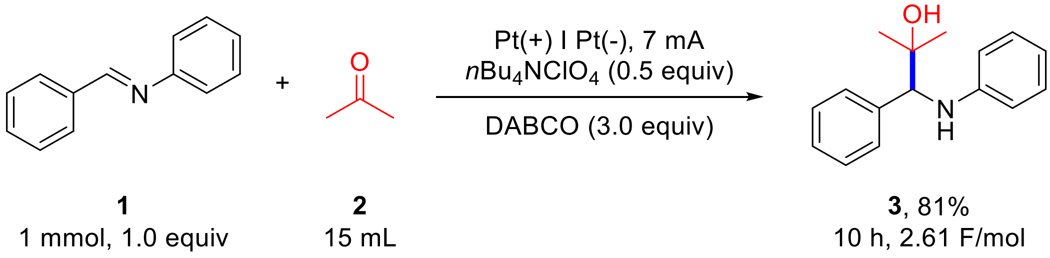
C. General procedures for the electrolysis

C1. The materials used to make the electrolytic cell

All the materials used to make the electrolytic cell were commercially available (Figure S1). The anode and cathode used were all Pt sheet (10 mm × 10 mm × 0.2 mm).

Figure S1. The materials used to make the electrolytic cell for the synthesis of β-amino alcohols.

C2. 1 mmol-scale electrosynthesis of β-amino alcohols



An undivided test tube-type electrolysis cell (10 mL) was charged with a stir bar, imine **1** (1 mmol, 1.0 equiv), acetone **2** (15 mL), $n\mathrm{Bu_4NClO_4}$ (0.5 mmol, 0.5 equiv) and DABCO (3.0 mmol, 3.0 equiv), and the resulting suspension was stirred until the solids were dissolved. Then the prepared electrodes were placed into the reaction mixture. Both anode and cathode were Pt sheet (10 mm × 10 mm × 0.2 mm). The mixture was electrolyzed at a constant current of 7 mA for 10 h at room temperature until the imine was consumed entirely (monitored by TLC). The electrodes were taken out, washed twice with ethyl acetate (20 mL) ultrasonically, and the ethyl acetate was combined with the reaction mixture. The combined mixture was washed with H_2O (10 mL × 3), brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography with petroleum ether and ethyl acetate as eluents (7:1 v/v) to afford the desired product **3** in 81% yield (195 mg).

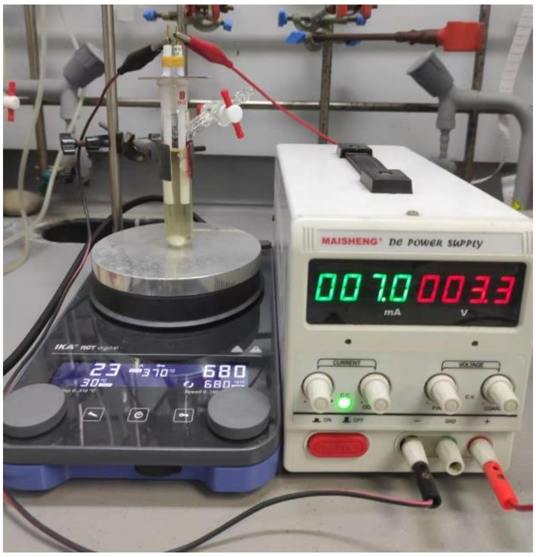
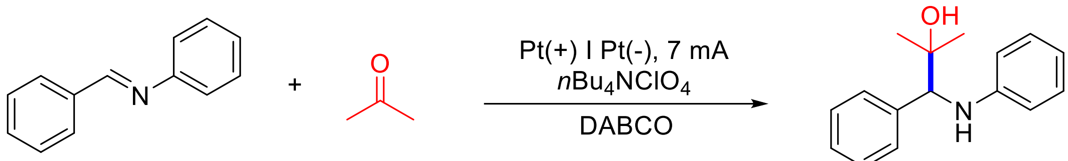


Figure S2. 1 mmol-scale experimental setup.

D. Control experiments

To gain insight into this electrosynthesis, several control experiments were performed (Table S8). The results revealed that electricity and electrolyte play an indispensable role in the reaction, because without any of them, no product was detected (Table S8, entries 2 and 3). Besides, when there was no DABCO as an additive, the yield of **3** significantly decreased (Table S8, entry 4), indicating that the addition of a sacrificial reducing agent is conducive to the reaction.

Table S8. Control experiments[a]

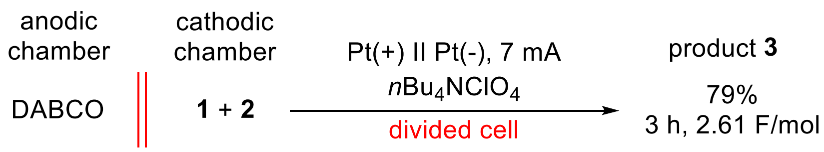


1 2 3

Entry	Variation from standard conditions	Charge (F/mol)	Yield (%)[b]
1	None	2.17	87
2	No electricity	0	0
3	No electrolyte (nBu$_4$NClO$_4$)	0	0
4	No DABCO	2.17	54

[a]Reaction conditions: **1** (0.3 mmol, 1.0 equiv), **2** (5 mL), nBu$_4$NClO$_4$ (0.15 mmol, 0. 5 equiv), DABCO (0.6 mmol, 2.0 equiv), Pt sheet (10 mm × 10 mm × 0.2 mm) anode and cathode, constant current = 7 mA, room temperature. [b]Yield of the isolated product after chromatography on silica gel.

E. Divided-cell electrolysis experiment



The divided-cell electrolysis was conducted in a H-type divided cell. Both anode and cathode were Pt sheet (10 mm × 10 mm × 0.2 mm), which were separated by a cation exchange membrane. Imine **1** (0.3 mmol, 1.0 equiv), acetone **2** (5 mL) and nBu$_4$NClO$_4$ (0.5 mmol, 0.5 equiv) were only added into the cathode, while acetone **2** (5 mL), nBu$_4$NClO$_4$ (0.5 mmol, 0.5 equiv) and DABCO (3.0 mmol, 3.0 equiv) were only added into the anode. The reaction system was electrolyzed at a constant current of 7 mA at room temperature until the imine was consumed entirely (monitored by TLC). The electrodes were taken out, washed twice with ethyl acetate (20 mL) ultrasonically, and the ethyl acetate was combined with the reaction mixture. The combined mixture was washed with H_2O (10 mL × 3), brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography with petroleum ether and ethyl acetate as eluents (7:1 v/v) to afford the desired product **3** in 79% yield (57 mg).

Figure S3. Reaction setup for divided-cell electrolysis.

F. Cyclic voltammetry experiments

The cyclic voltammetry experiments were carried out with a computer-controlled electrochemical analyzer for electrochemical measurements. The solution of interest was sparged with argon for 5 minutes before data collection with the CHI 700E potentiostat (CH Instruments, Inc.). The experiment was performed in a three-electrode cell with DMF (15 mL) as the solvent, $n\mathrm{Bu_4NClO_4}$ (0.05 M) as the supporting electrolyte, and the concentration of the tested compound was 2.0 mM. The scan speed was 100 mV/s. The potential ranges investigated were -3.2 V to +1.2 V *vs.* SCE (saturated aqueous KCl). CV plotting convention is IUPAC.

Working electrode: The working electrode is a 3 mm diameter glassy carbon working electrode. Polished with 0.05 μm aluminum oxide and then sonicated in distilled water and ethanol before measurements.

Reference electrode: The reference electrode is SCE (saturated aqueous KCl) that was washed with water and ethanol before measurements.

Counter electrode: The counter electrode is a platinum wire that was polished with 0.05 μm aluminum oxide and then sonicated in distilled water and ethanol before measurements.

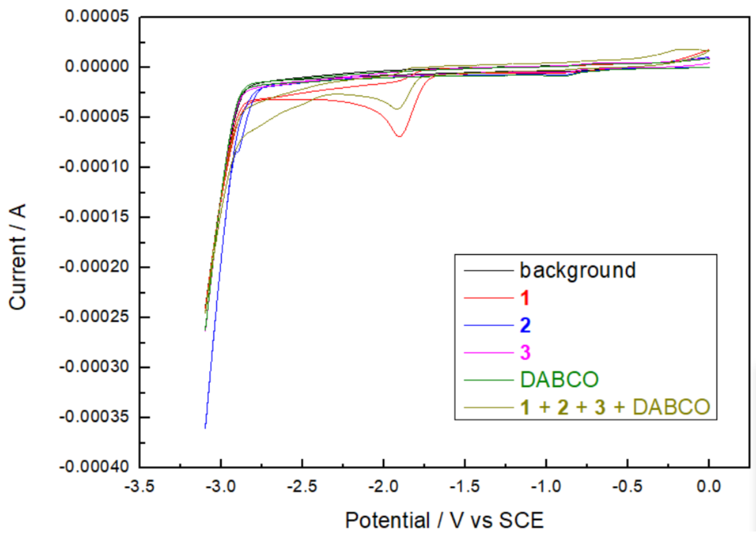


Figure S4. Cyclic voltammogram of background, **1**, **2**, **3**, DABCO and the mixture of **1** + **2** + **3** + DABCO in an electrolyte of *n*Bu_4NClO_4 (0.05 M) in DMF from 0 to -3.2 V. The onset potential for the reduction of **1** is around -1.68 V and the E_{red} is approximately -1.91 V. The onset potential for the reduction of **2** is around -2.74 V and the E_{red} is approximately -2.90 V. The onset potential for the reduction of the mixture of **1** + **2** + **3** + DABCO is around -1.76 V and the E_{red} is approximately -1.93 V. **3** and DABCO are not likely to be reduced in this reaction.

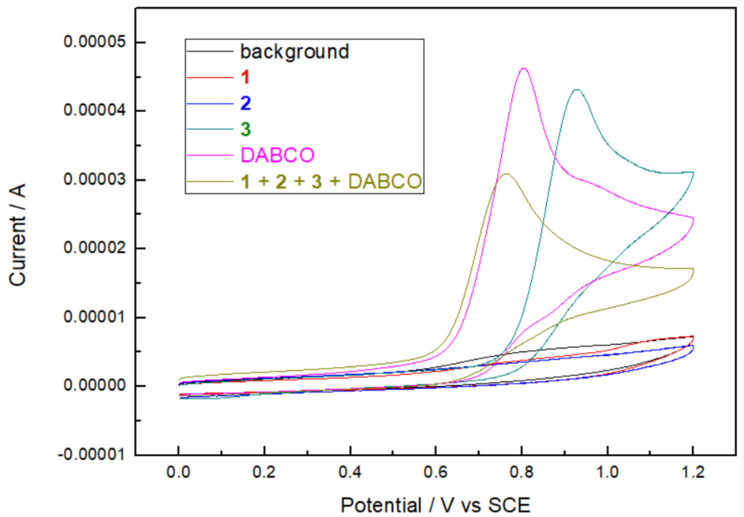


Figure S5. Cyclic voltammogram of background, **1**, **2**, **3**, DABCO and the mixture of **1** + **2** + **3** + DABCO in an electrolyte of *n*Bu_4NClO_4 (0.05 M) in DMF from 0 to +1.2 V. The onset potential for the oxidation of **3** is around +0.72 V and the E_{ox} is approximately +0.93 V. The onset potential for the oxidation of DABCO is around +0.44 V and the E_{ox} is approximately +0.80 V. The onset potential for the oxidation of the mixture of **1** + **2** + **3** + DABCO is around +0.41 V and the E_{ox} is approximately +0.77 V. **1** and **2** are not likely to be oxidized in this reaction.

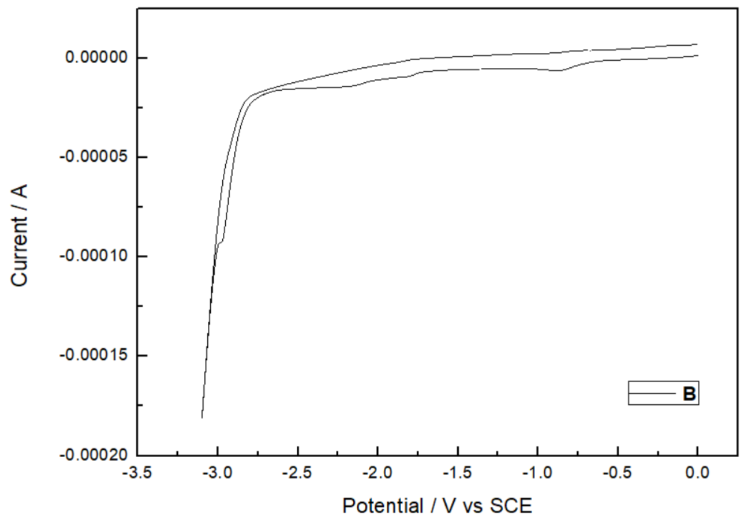


Figure S6. Cyclic voltammogram of **B** in an electrolyte of *n*Bu_4NClO_4 (0.05 M) in DMF from 0 to -3.1 V. The onset potential for the reduction of **B** is around -2.47 V and the E_{red} is approximately -2.97 V.

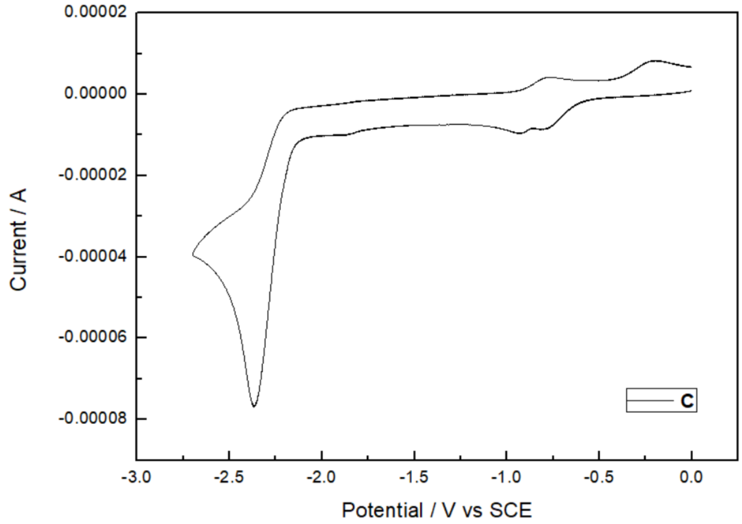
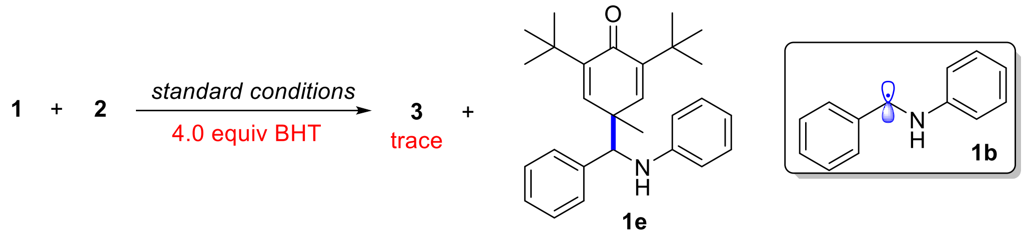


Figure S7. Cyclic voltammogram of **C** in an electrolyte of *n*Bu_4NClO_4 (0.05 M) in DMF from 0 to -2.7 V. The onset potential for the reduction of **C** is around -2.08 V and the E_{red} is approximately -2.36 V.

G. Radical trapping experiment

In order to confirm if the reaction undergoes a radical mechanism, radical trapping experiment was taken.



HRMS $[M+H]^+$, Cal. 402.2791,Found: 402.2798

Scheme S3. The radical trapping experiment.

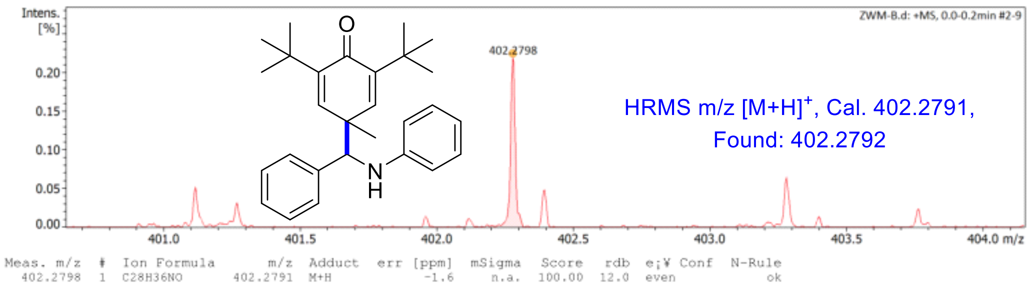


Figure S8. Mass spectrometry (HRMS) data of **1e**.

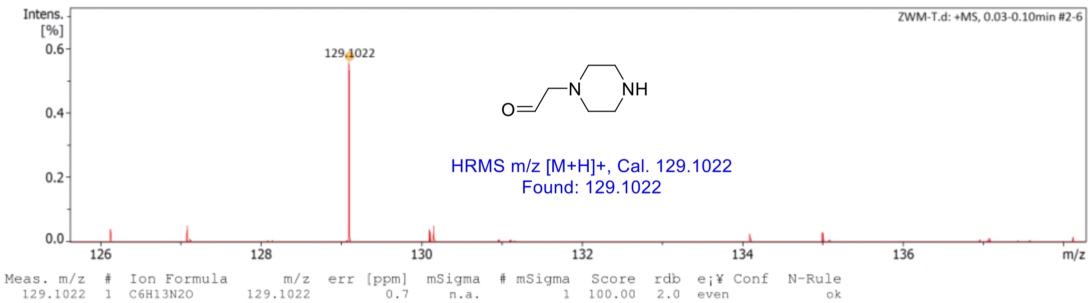


Figure S9. Mass spectrometry (HRMS) data of **III**

H. Electron paramagnetic resonance (EPR) experiment of 1

An undivided test tube-type electrolysis cell (10 mL) was charged with a stir bar, **1** (0.3 mmol, 1.0 equiv), $n\mathrm{Bu_4NClO_4}$ (0.15 mmol, 0.5 equiv), DMPO (70 μL)) and DMF (5 mL). The resulting suspension was stirred until the solids were dissolved. Then the prepared Mg anode and Pt cathode were placed into the solution. The mixture was electrolyzed at a constant current of 7 mA. After 10 min, a capillary reaction solution was taken out and analyzed by EPR at room temperature.

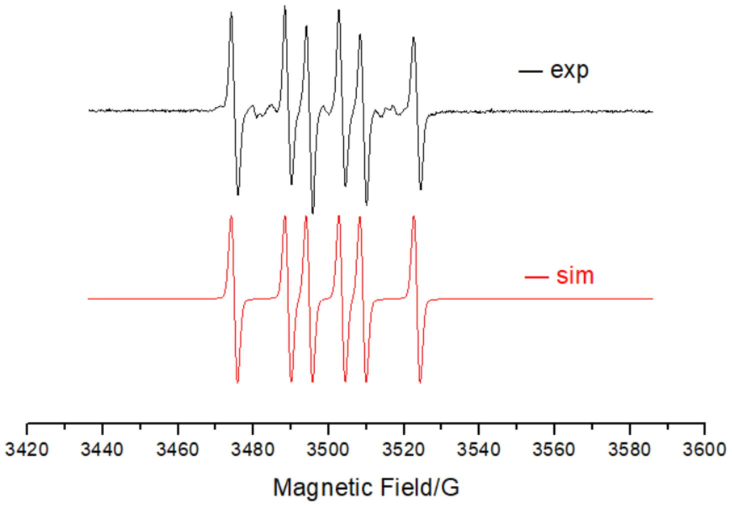
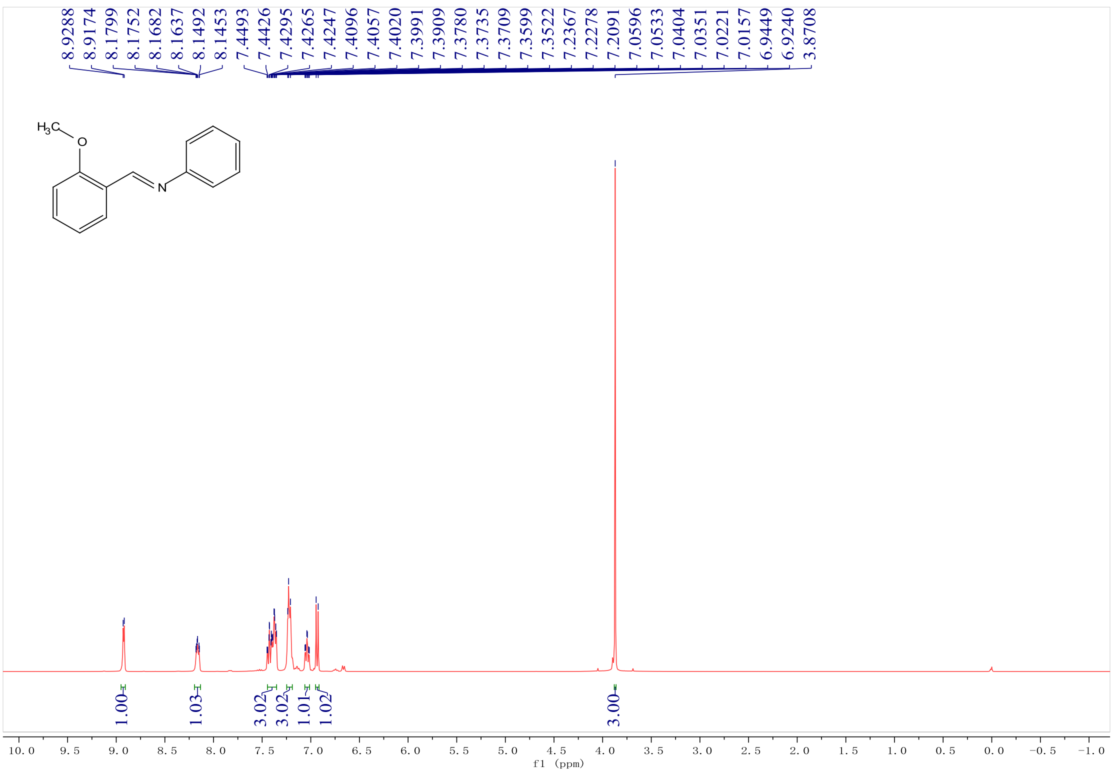


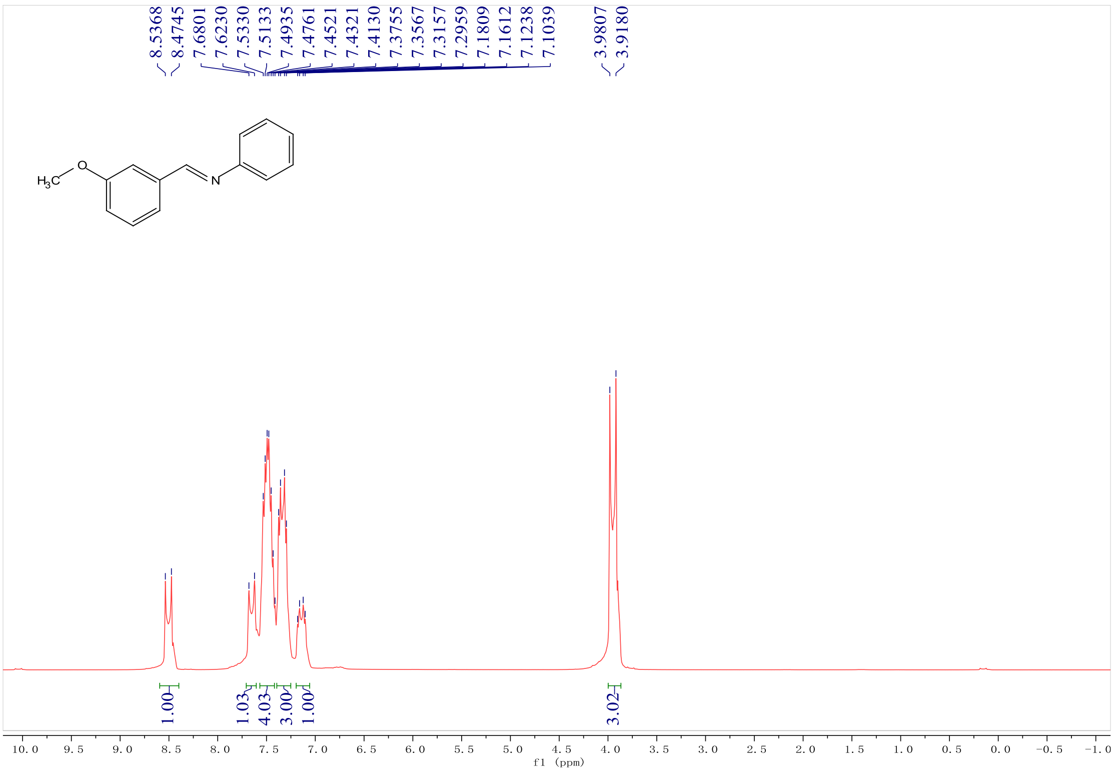
Figure S10. EPR experiment of **1** (g-factor = 2.0059, α_N(G) = 14.3, α_H(G) = 19.90).

I. NMR spectra of substrate imines and products

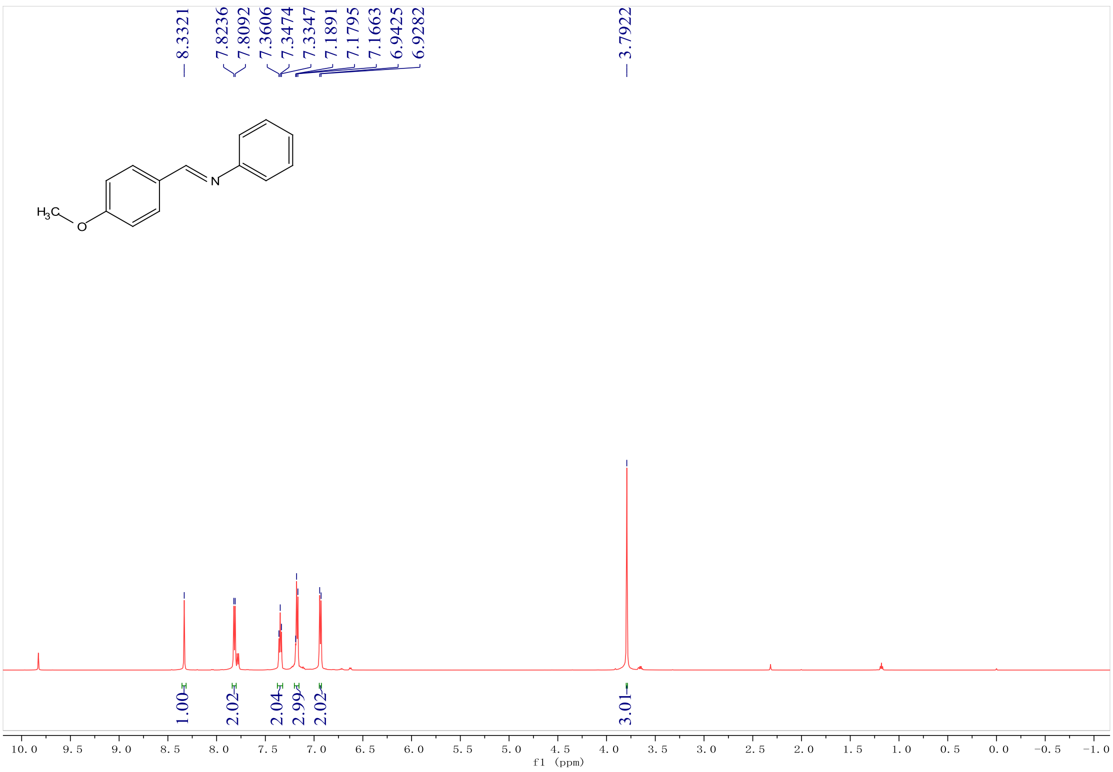
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-4**



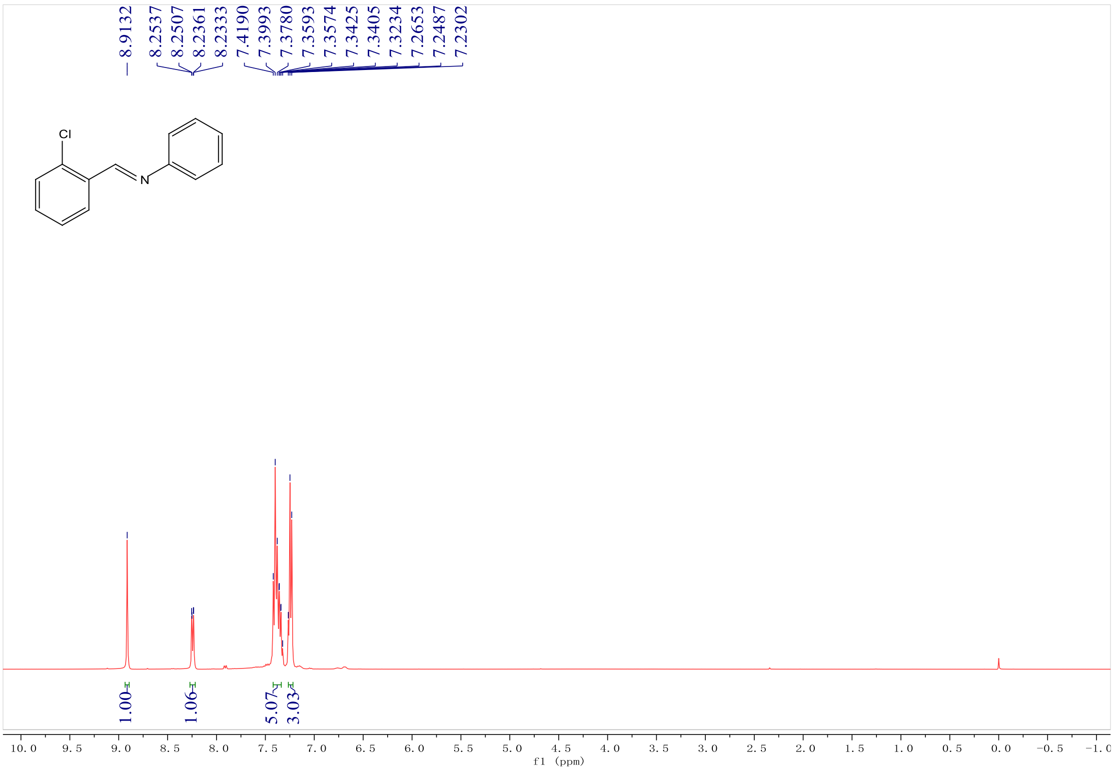
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-5**



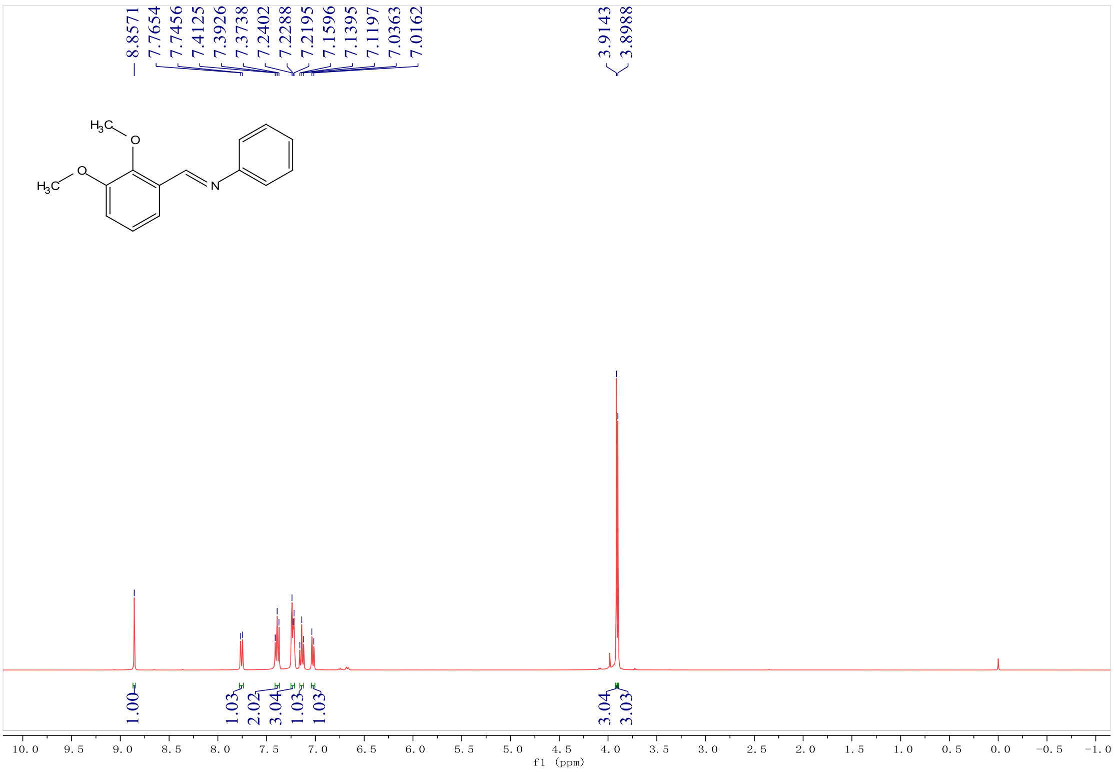
[1]H-NMR Spectrum (600 MHz, $CDCl_3$) of **S1-6**



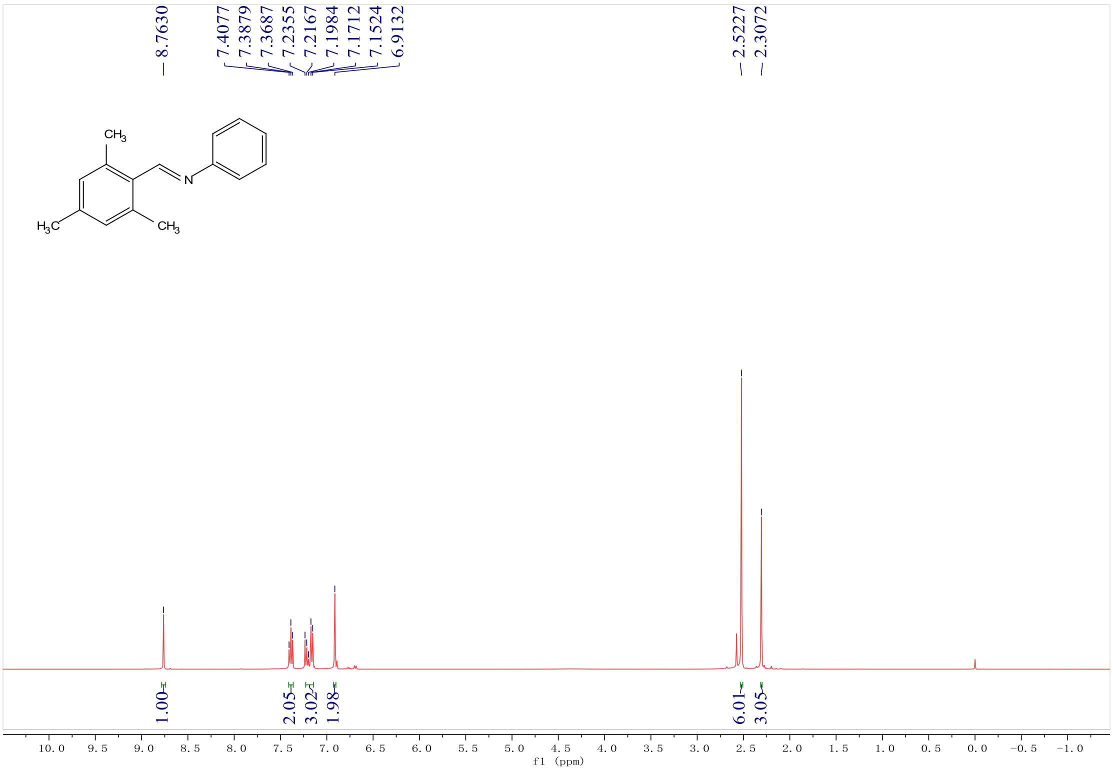
[1]H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-8**



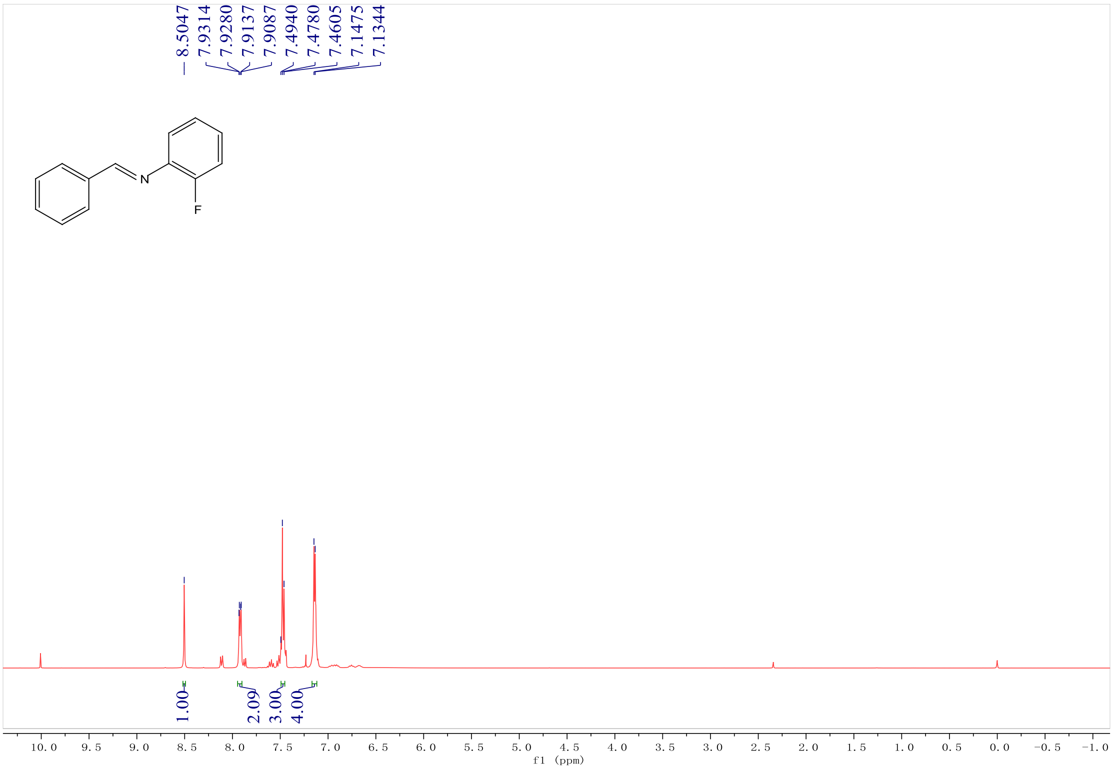
[1]H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-10**



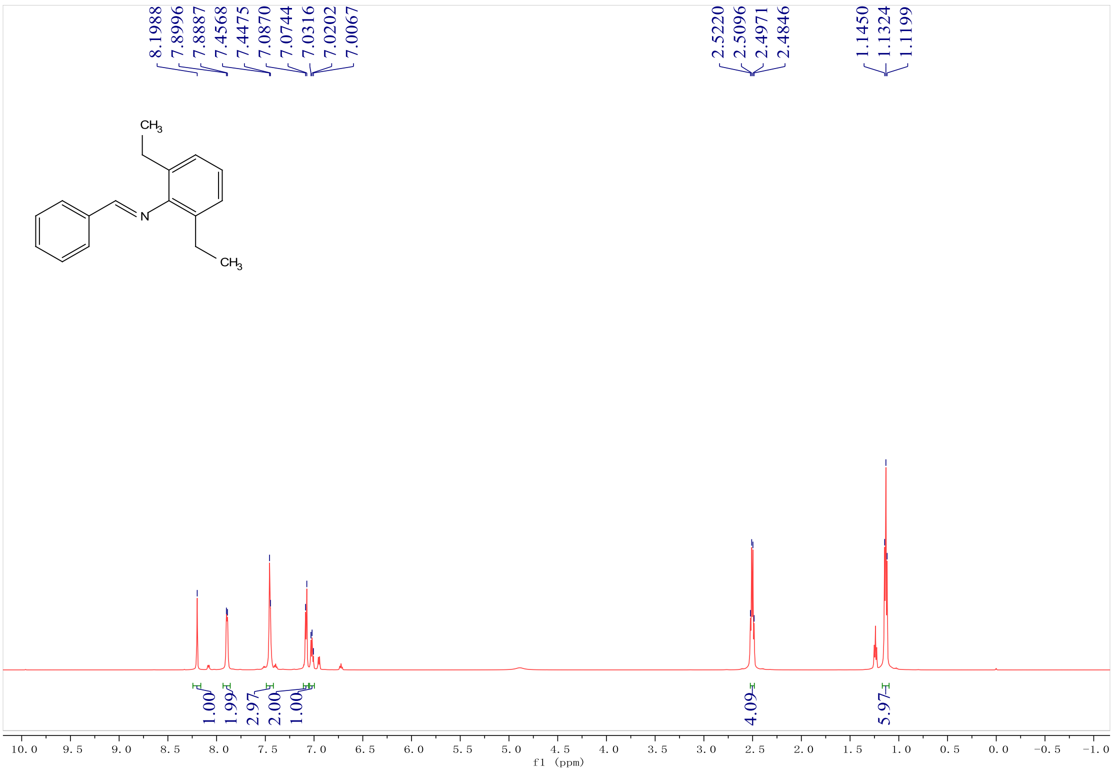
[1]H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-11**



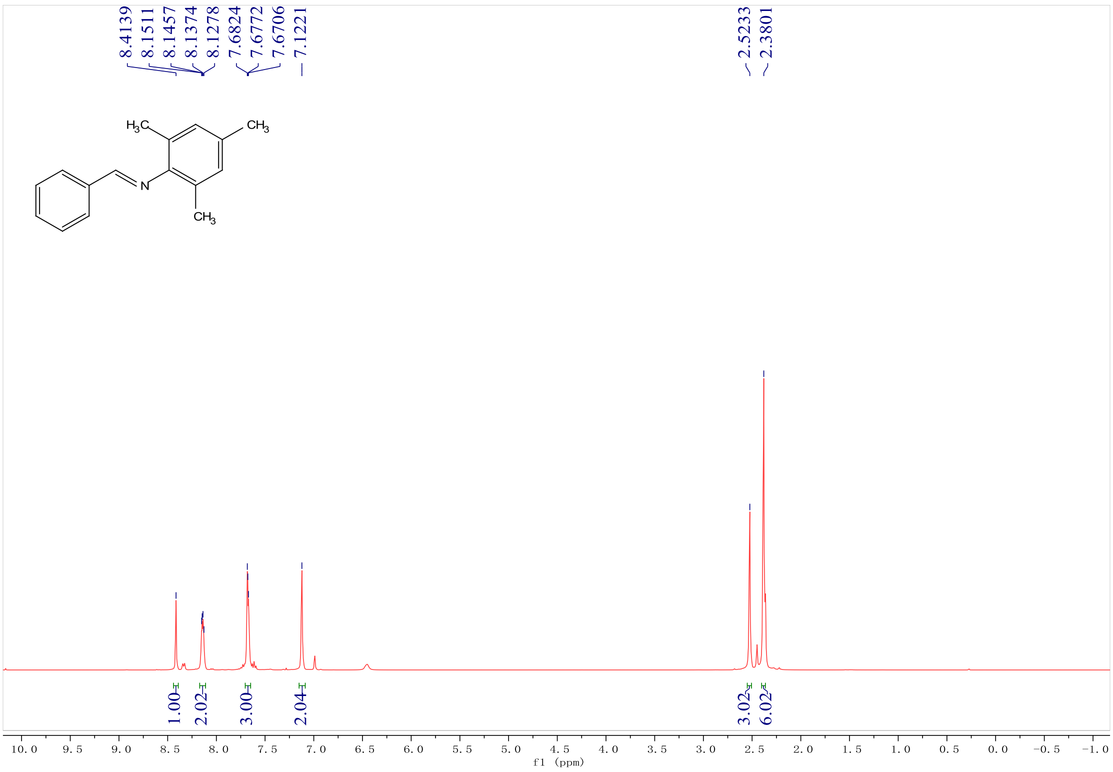
[1]H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-12**



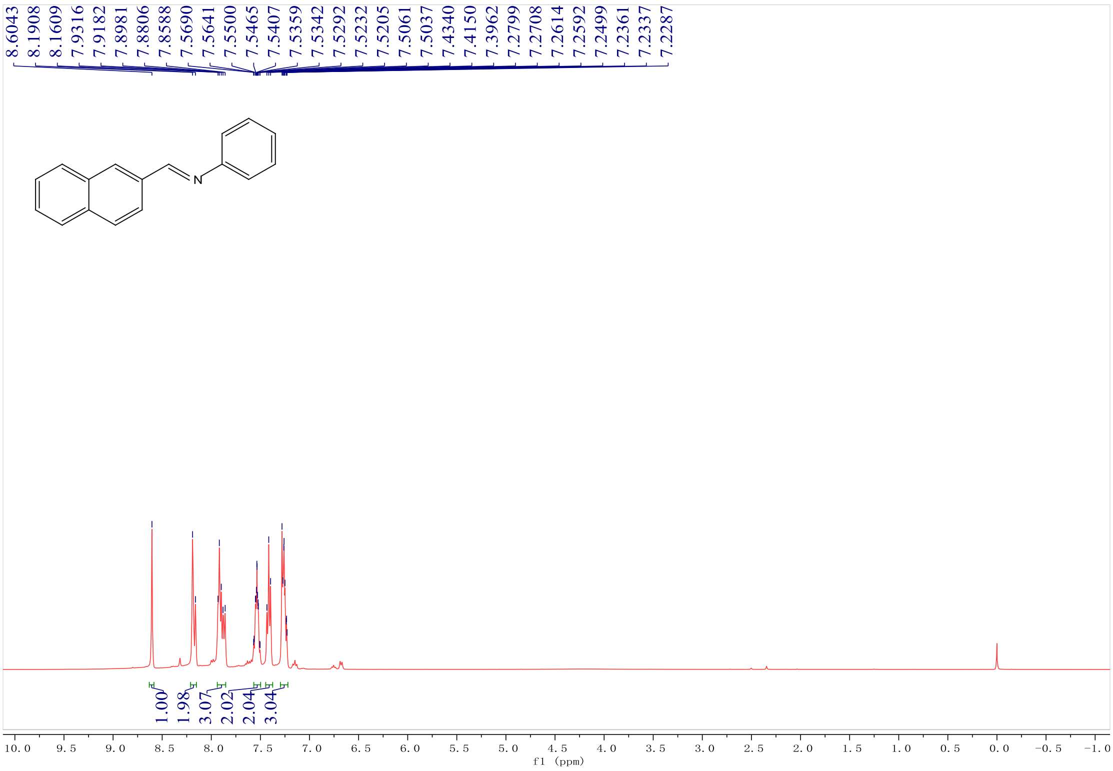
[1]H-NMR Spectrum (600 MHz, $CDCl_3$) of **S1-14**



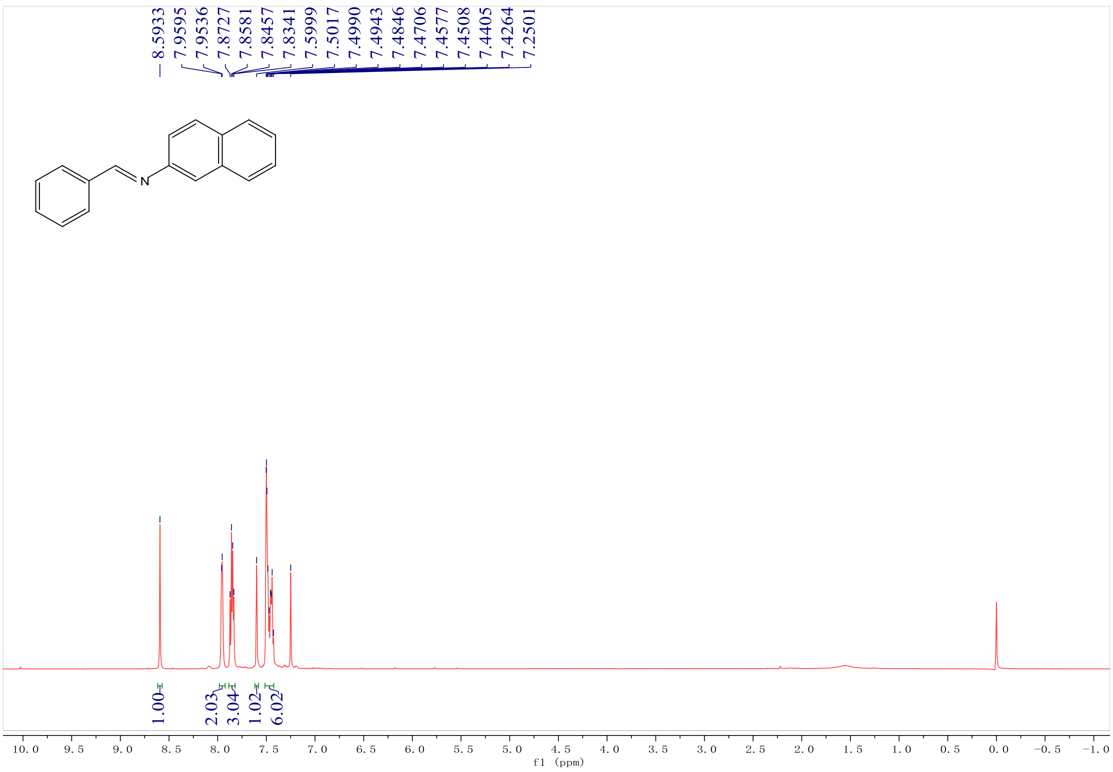
[1]H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-15**



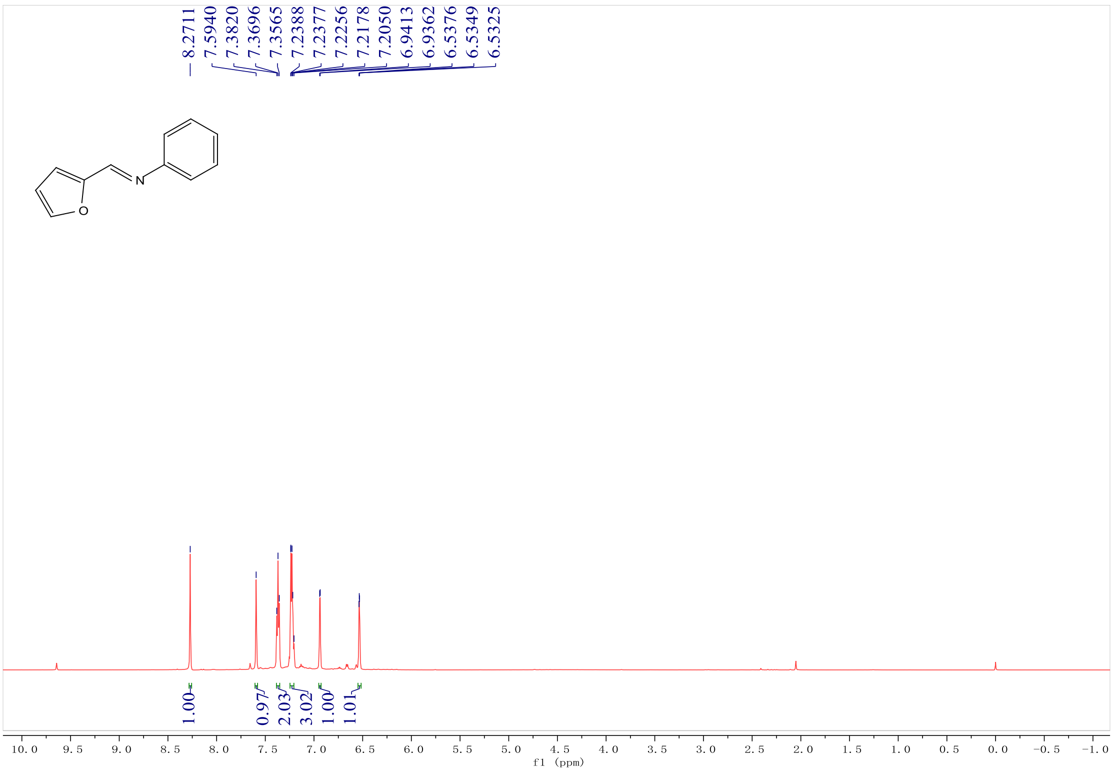
[1]H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-18**



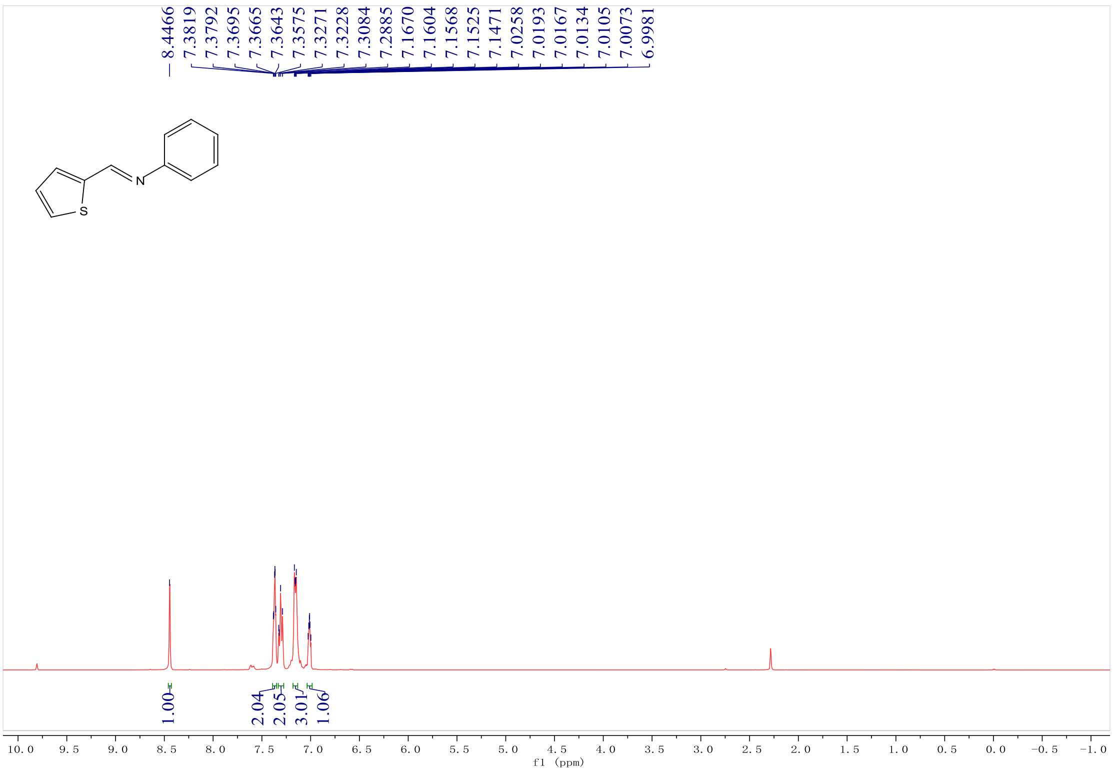
[1]H-NMR Spectrum (600 MHz, $CDCl_3$) of **S1-19**



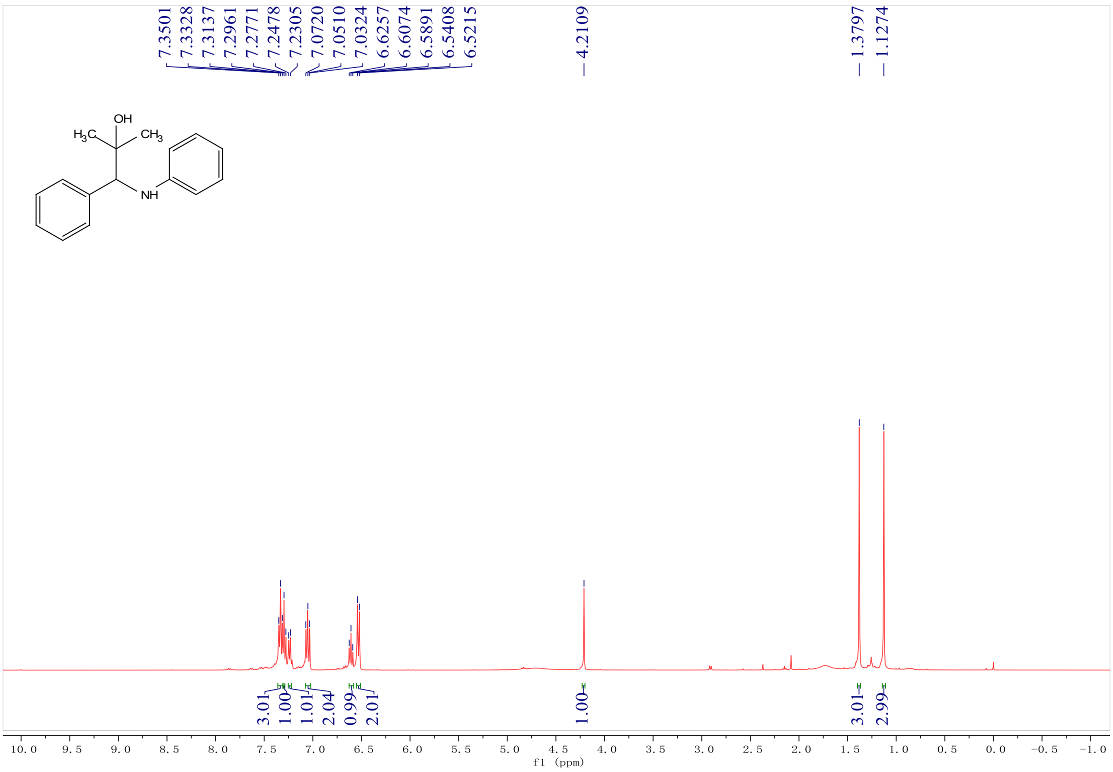
[1]H-NMR Spectrum (600 MHz, $CDCl_3$) of **S1-20**



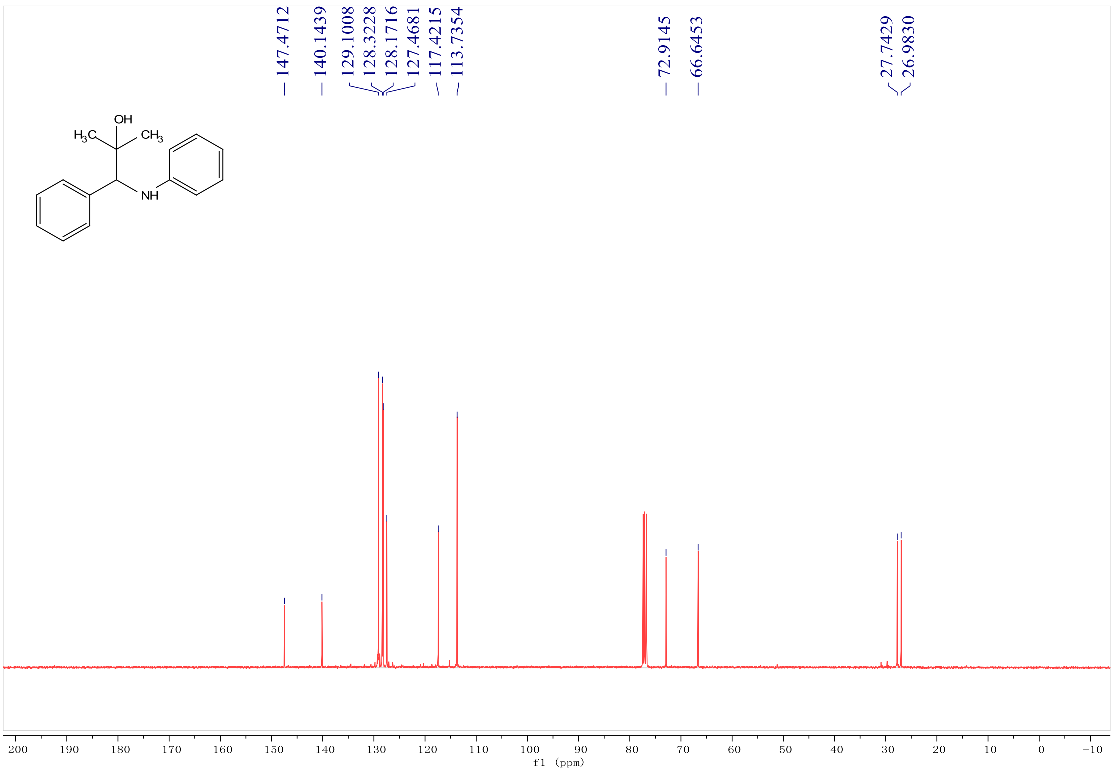
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **S1-21**



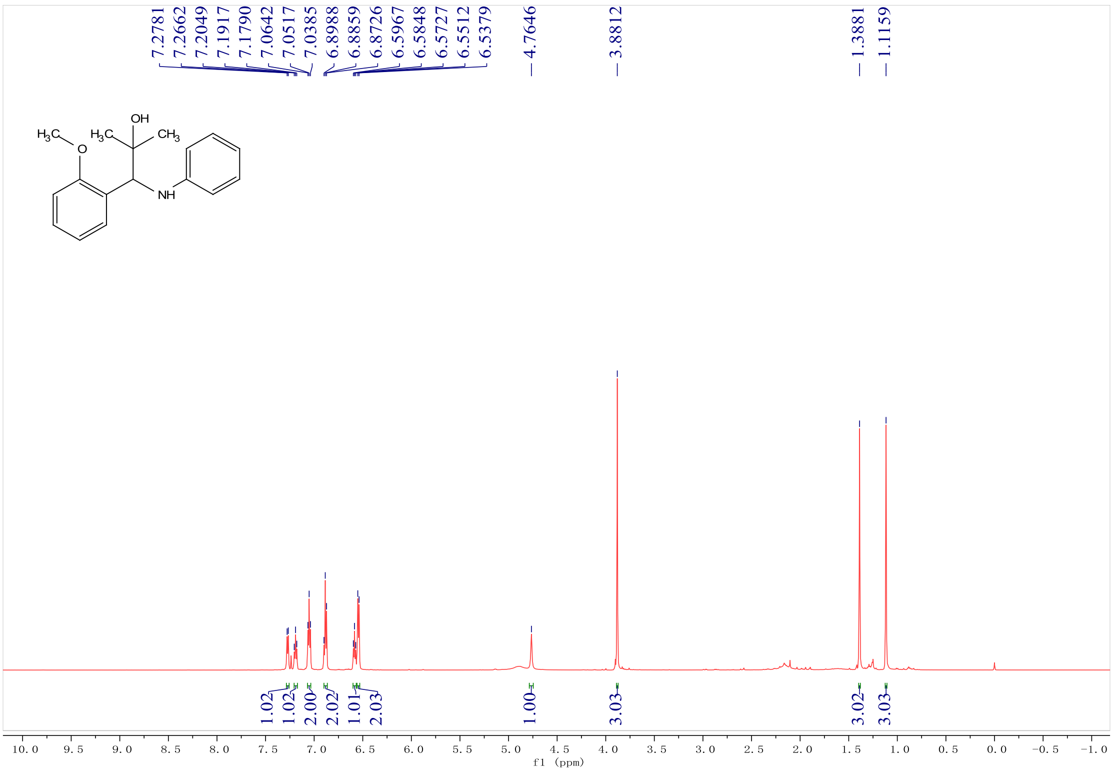
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **3**



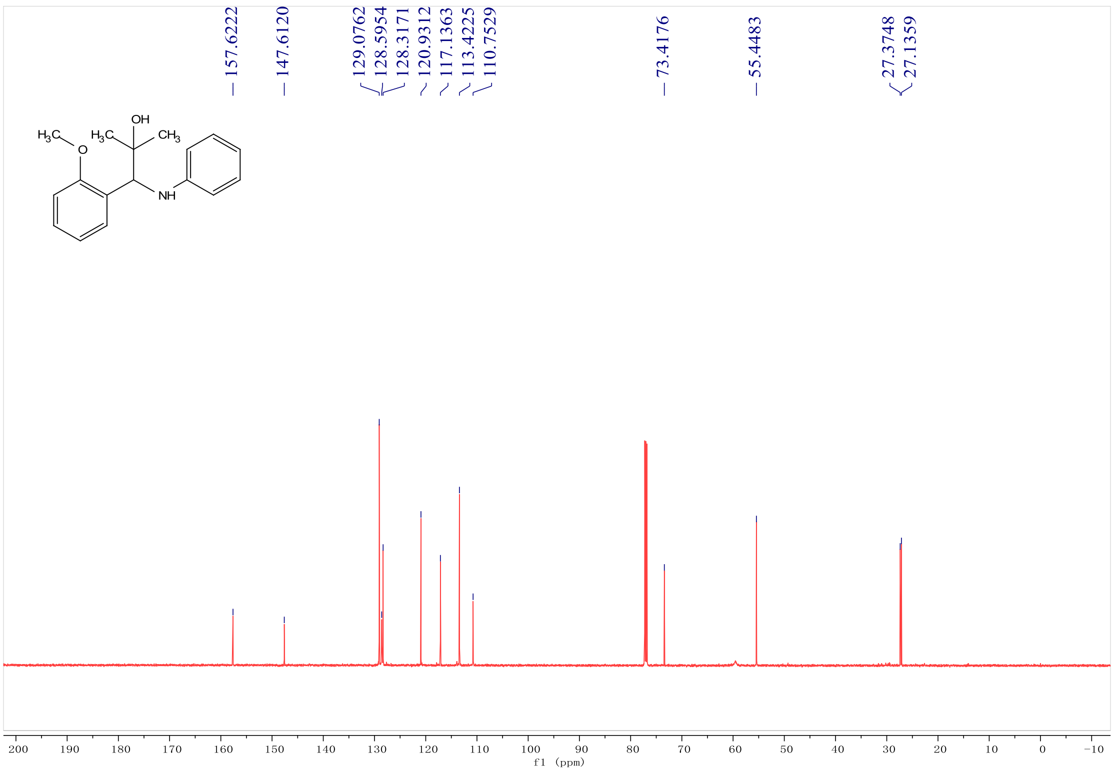
$^{13}C\{^{1}H\}$-NMR Spectrum (101 MHz, $CDCl_3$) of **3**



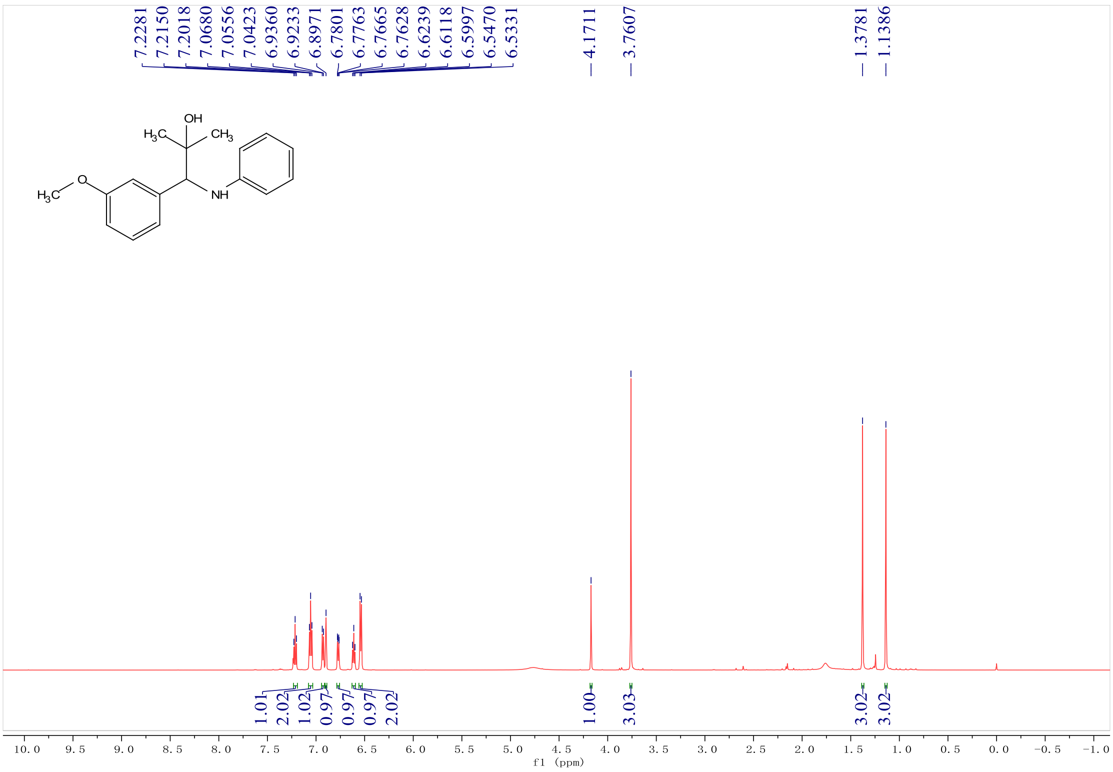
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **4**



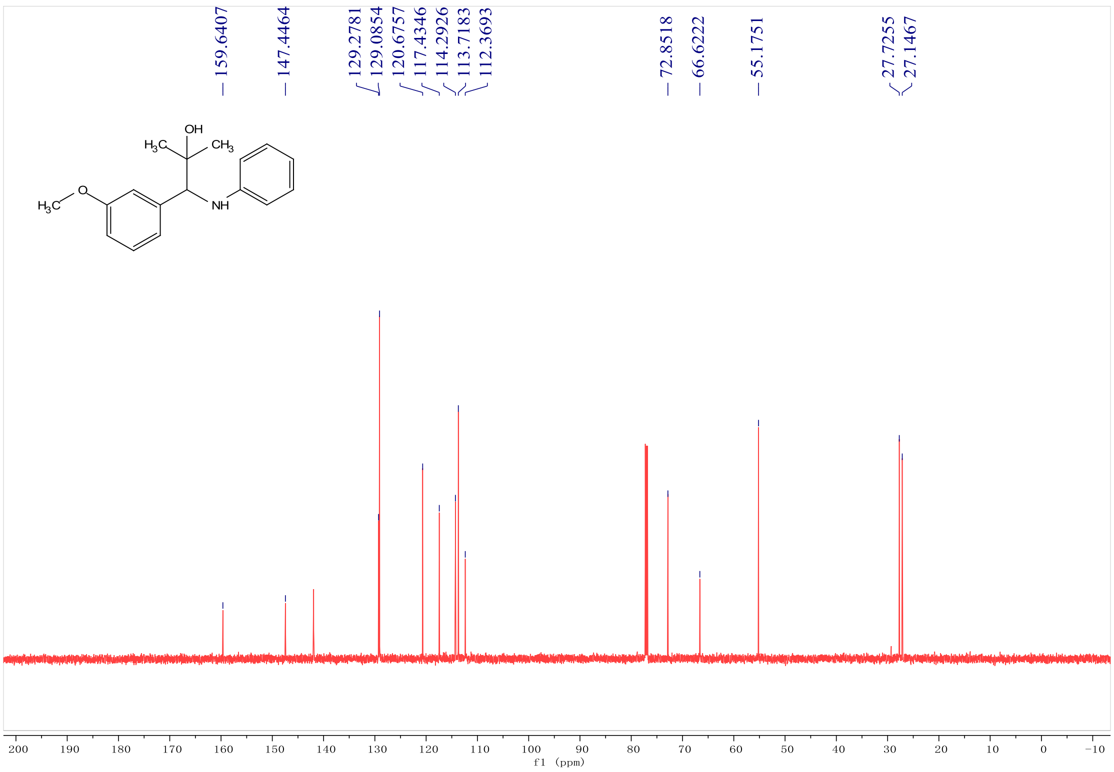
$^{13}C\{^1H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **4**



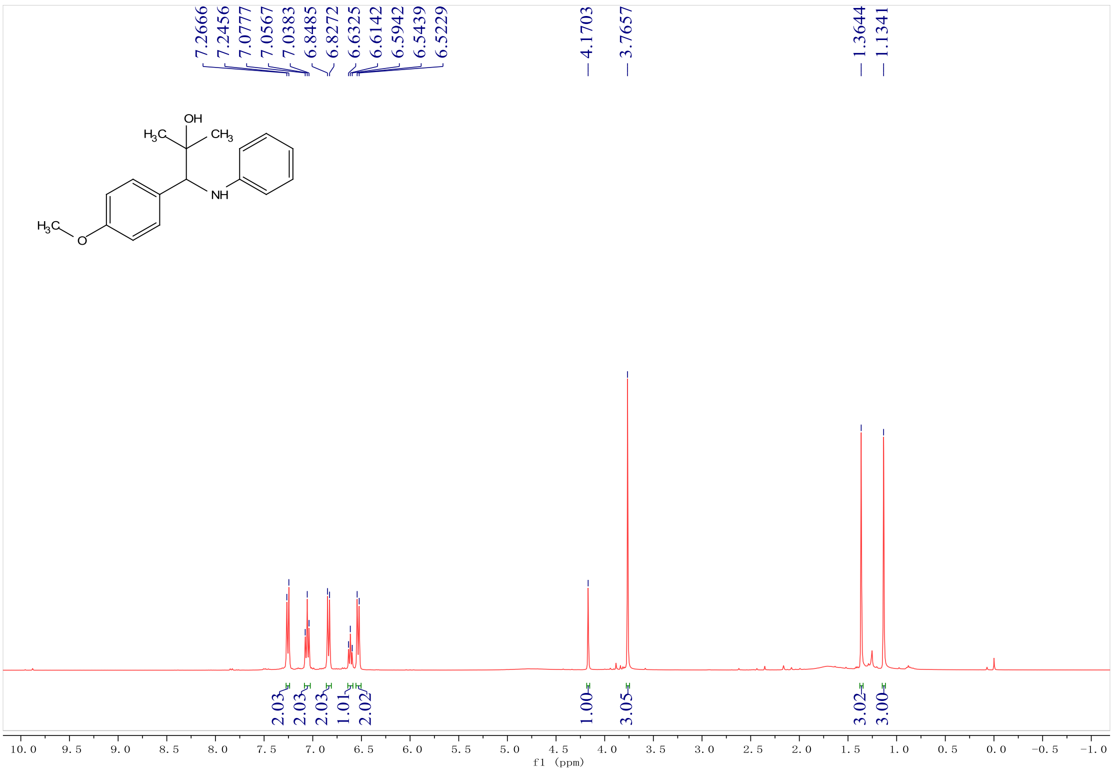
^1H-NMR Spectrum (600 MHz, $CDCl_3$) of **5**



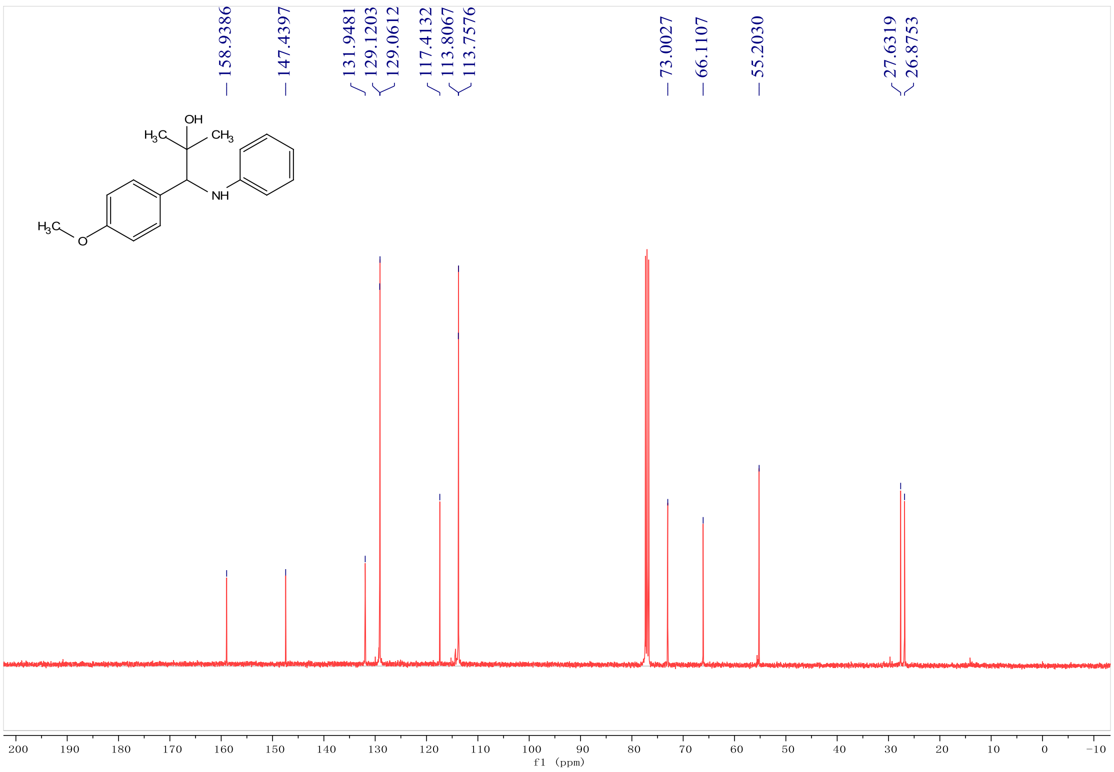
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **5**



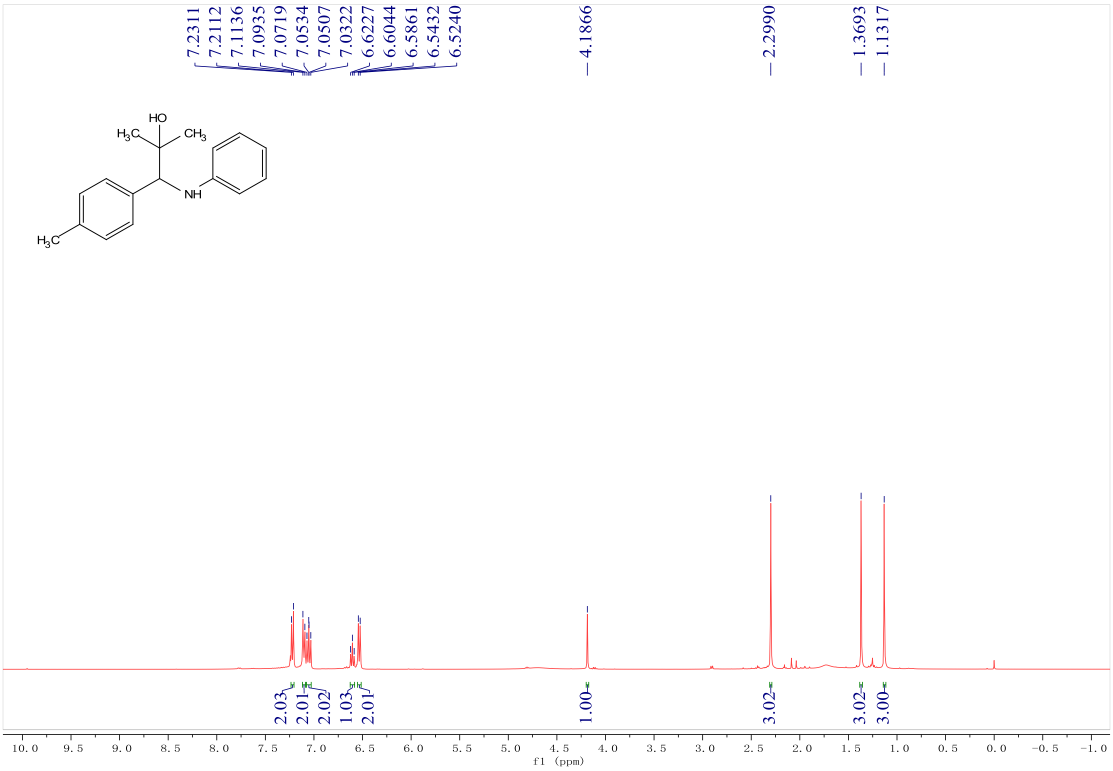
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **6**



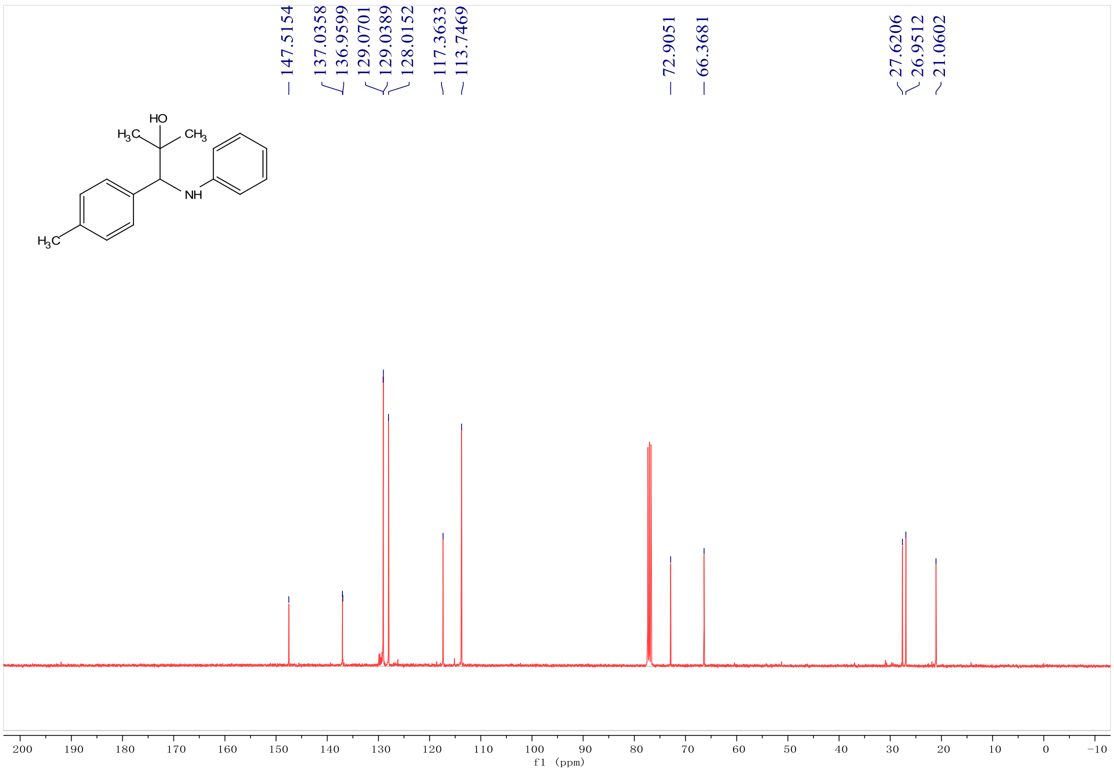
$^{13}C\{^{1}H\}$-NMR Spectrum (101 MHz, $CDCl_3$) of **6**



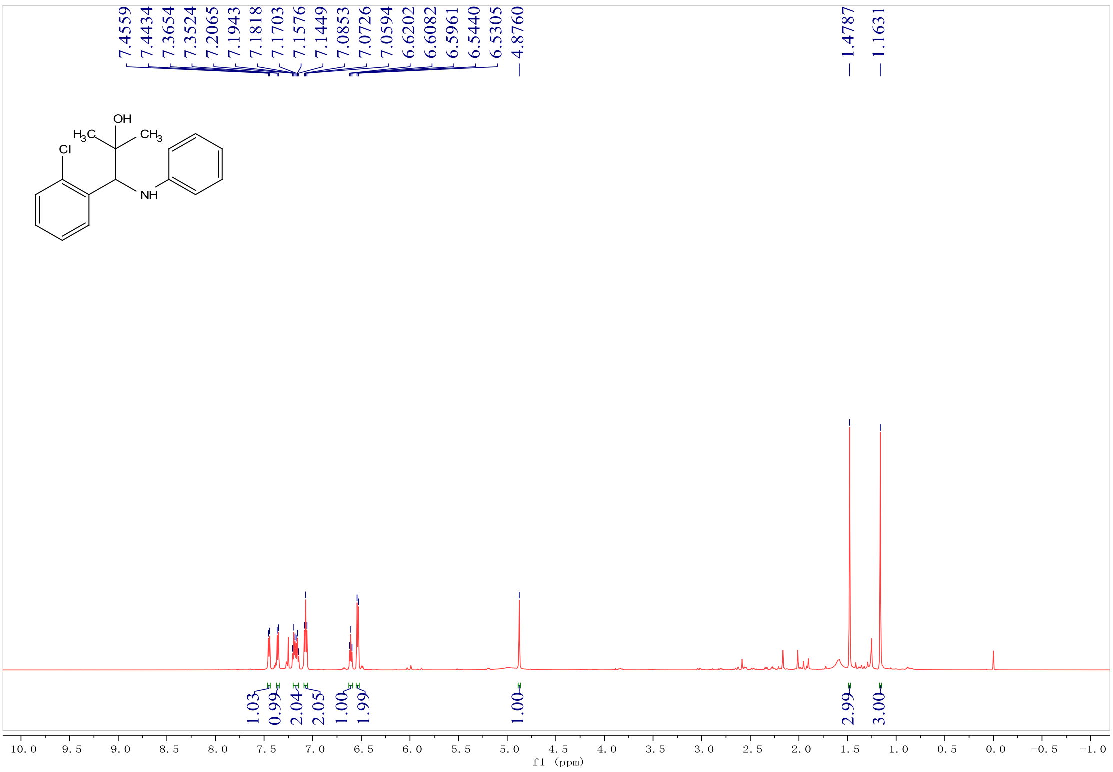
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **7**



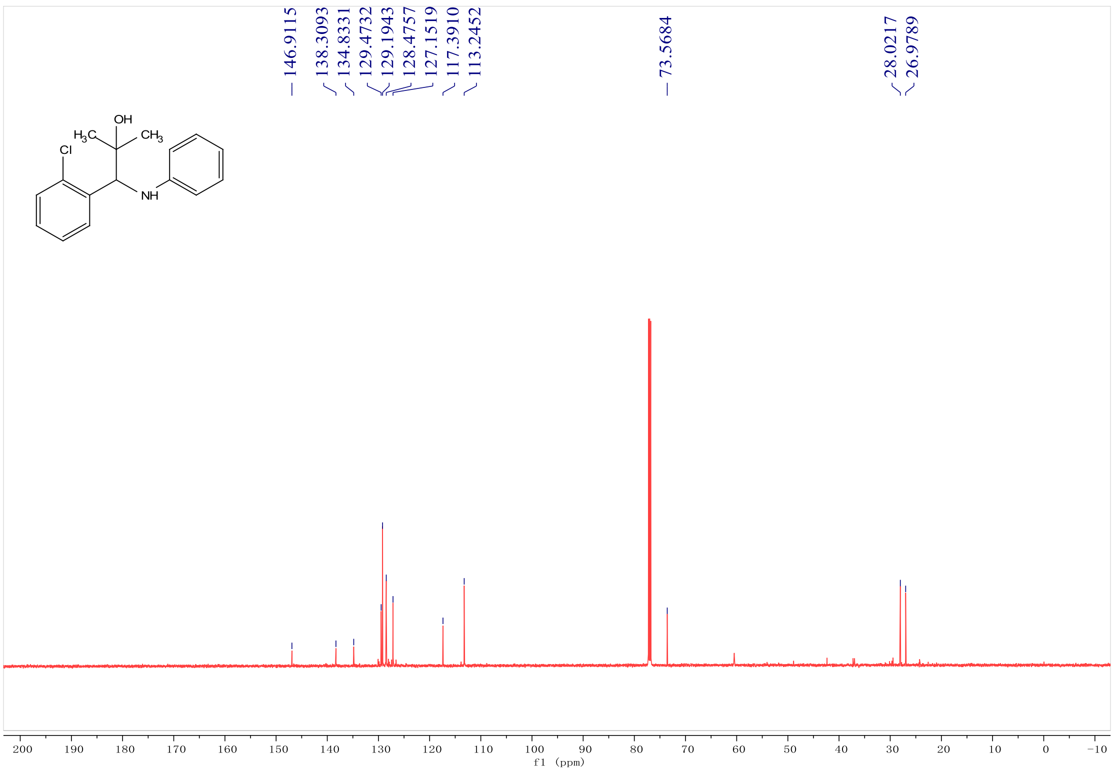
$^{13}C\{^{1}H\}$-NMR Spectrum (101 MHz, $CDCl_3$) of **7**



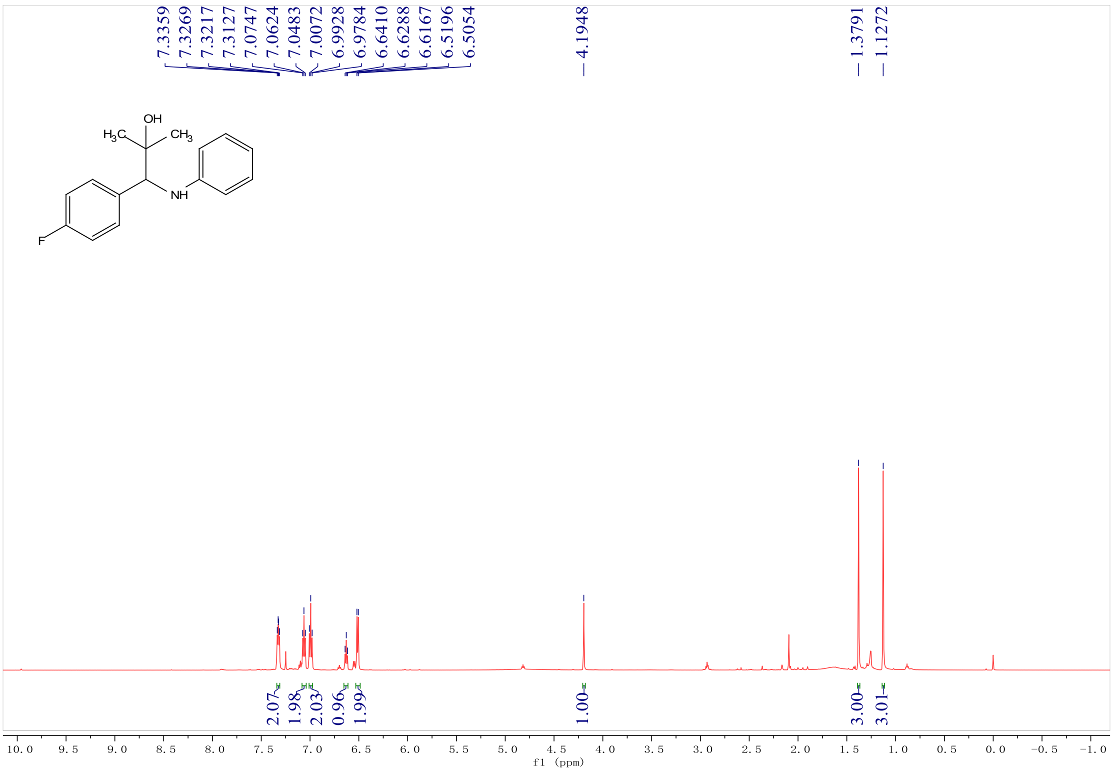
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **8**



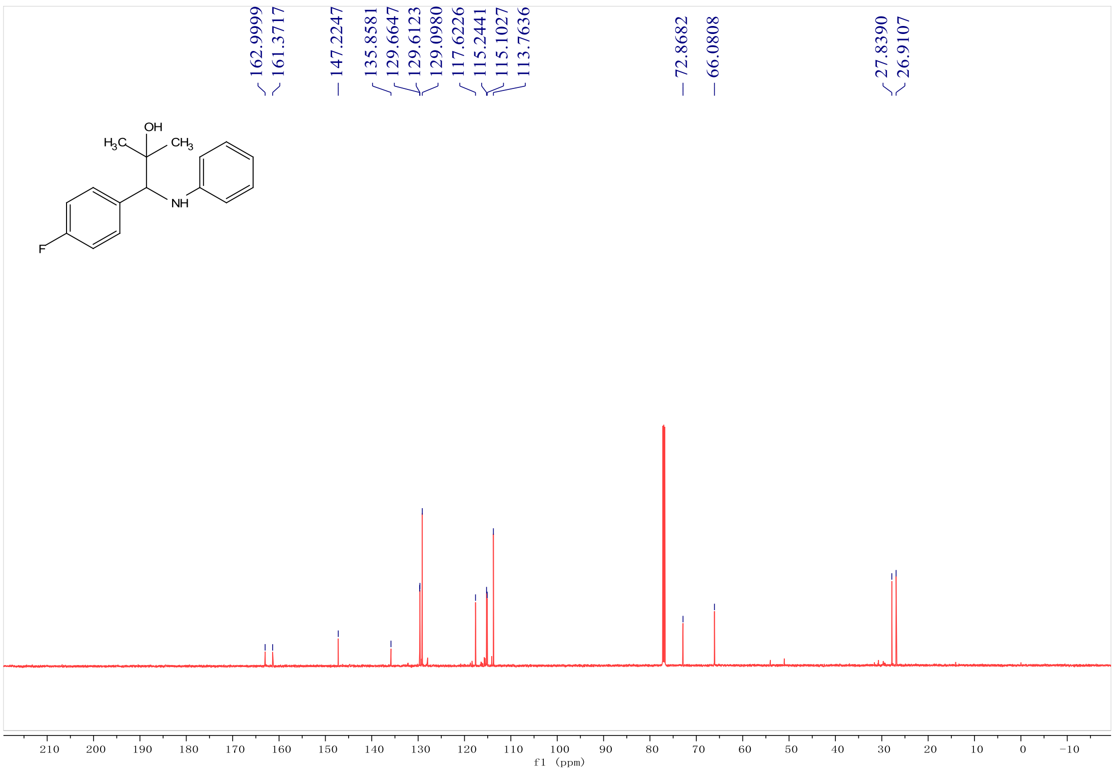
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **8**



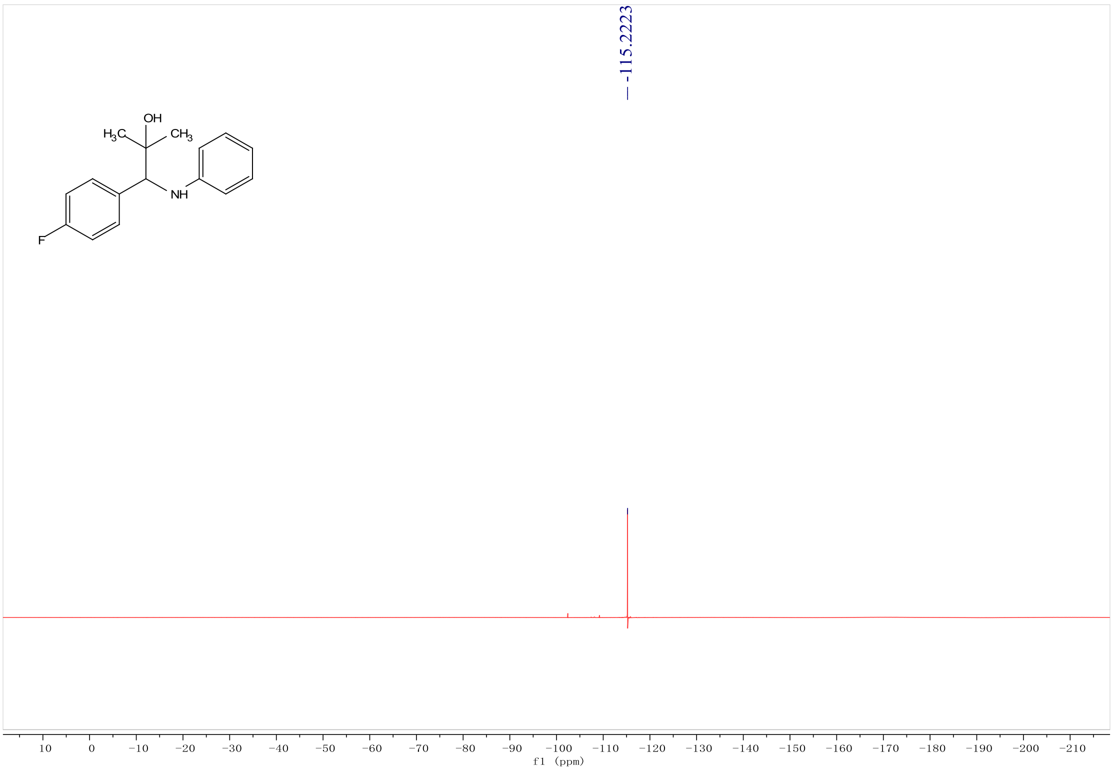
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **9**



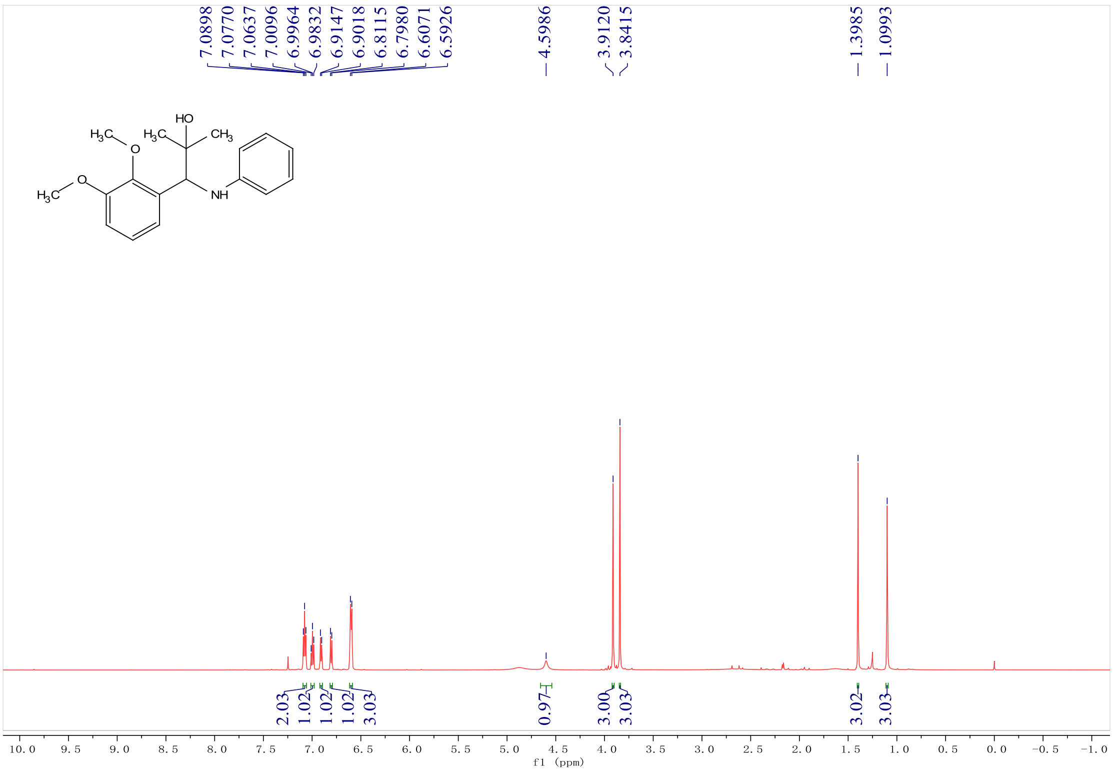
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **9**



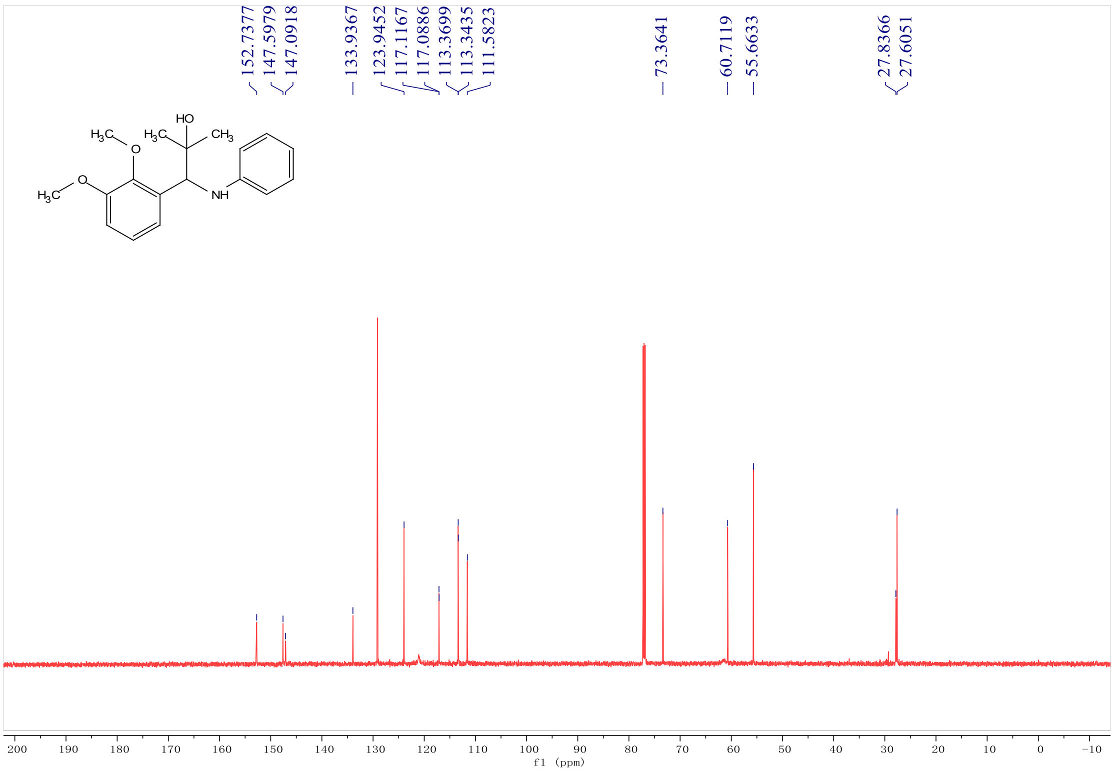
^{19}F-NMR Spectrum (376 MHz, $CDCl_3$) of **9**



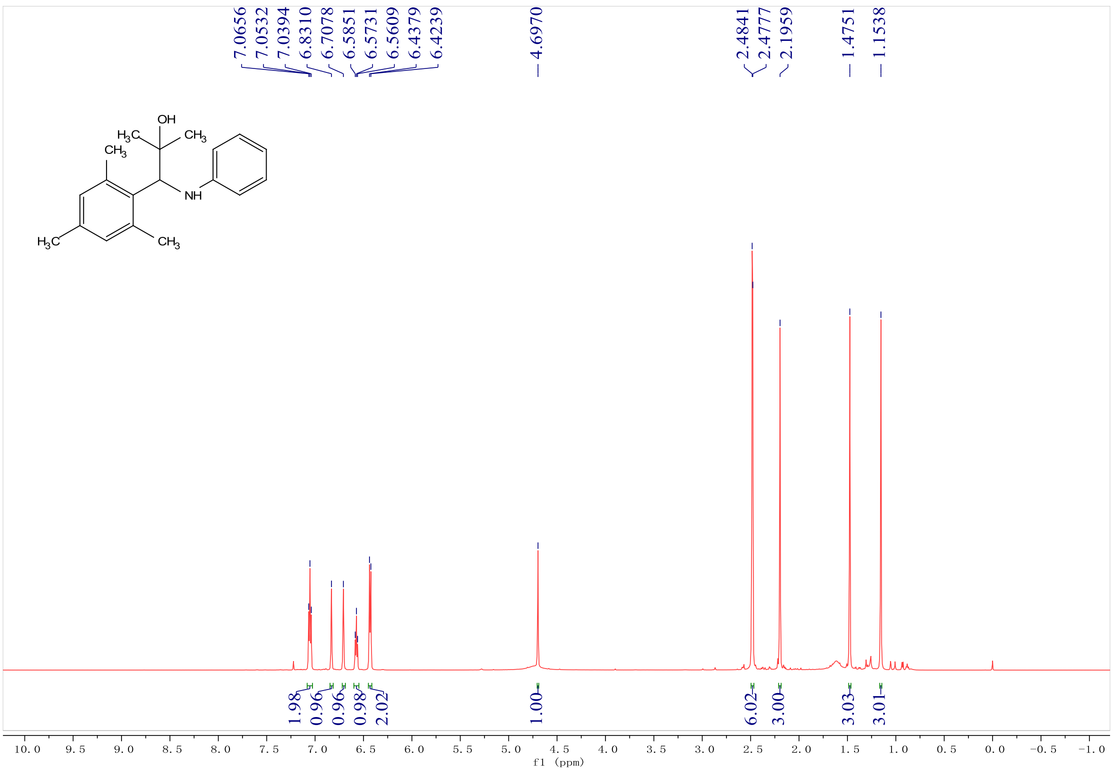
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **10**



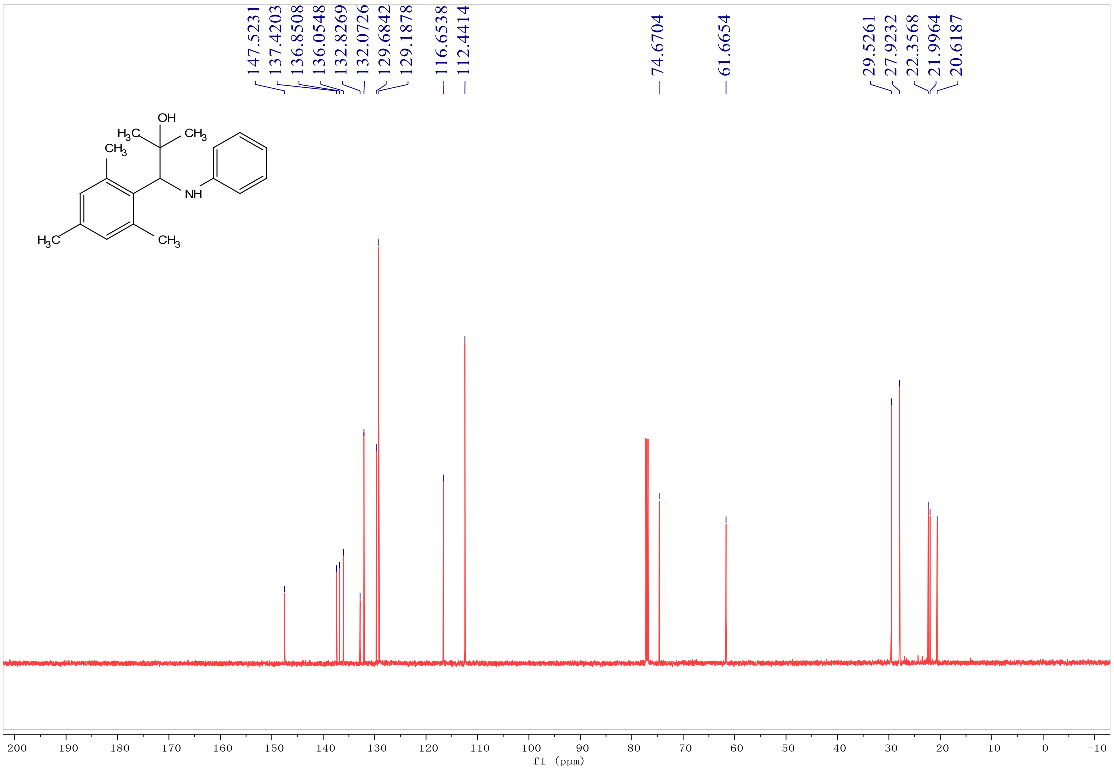
^{13}C{^{1}H}-NMR Spectrum (151 MHz, $CDCl_3$) of **10**



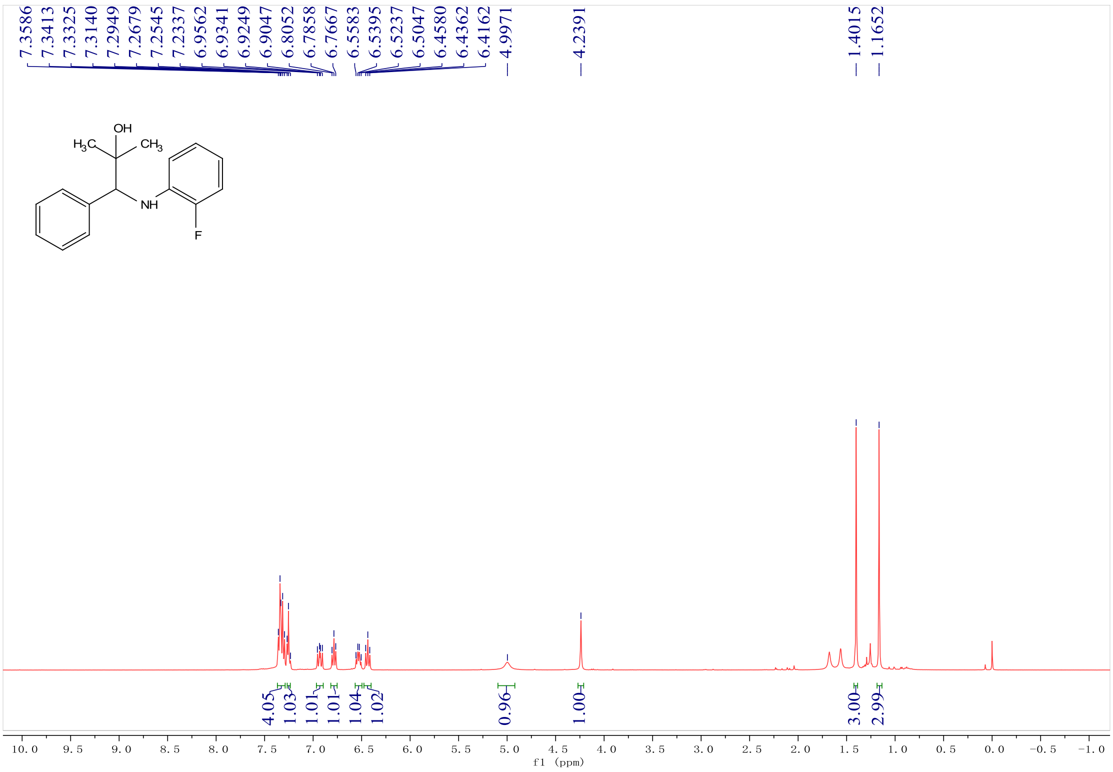
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **11**



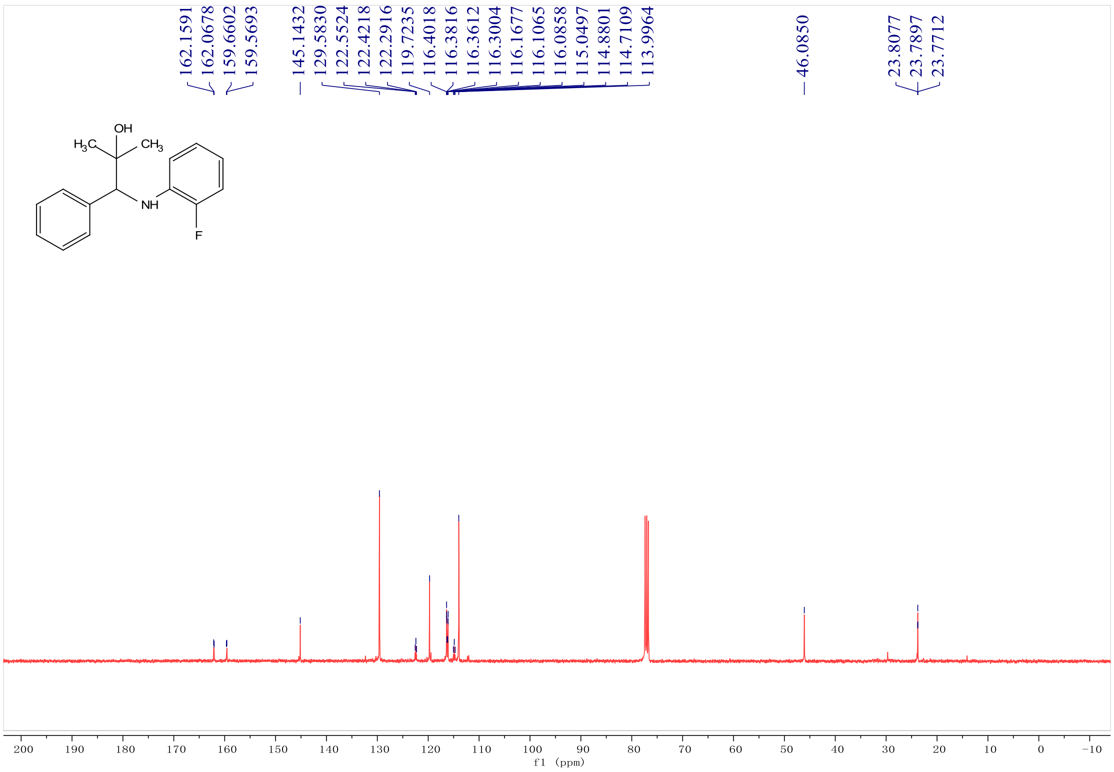
^{13}C{^{1}H}-NMR Spectrum (151 MHz, $CDCl_3$) of **11**



^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **12**

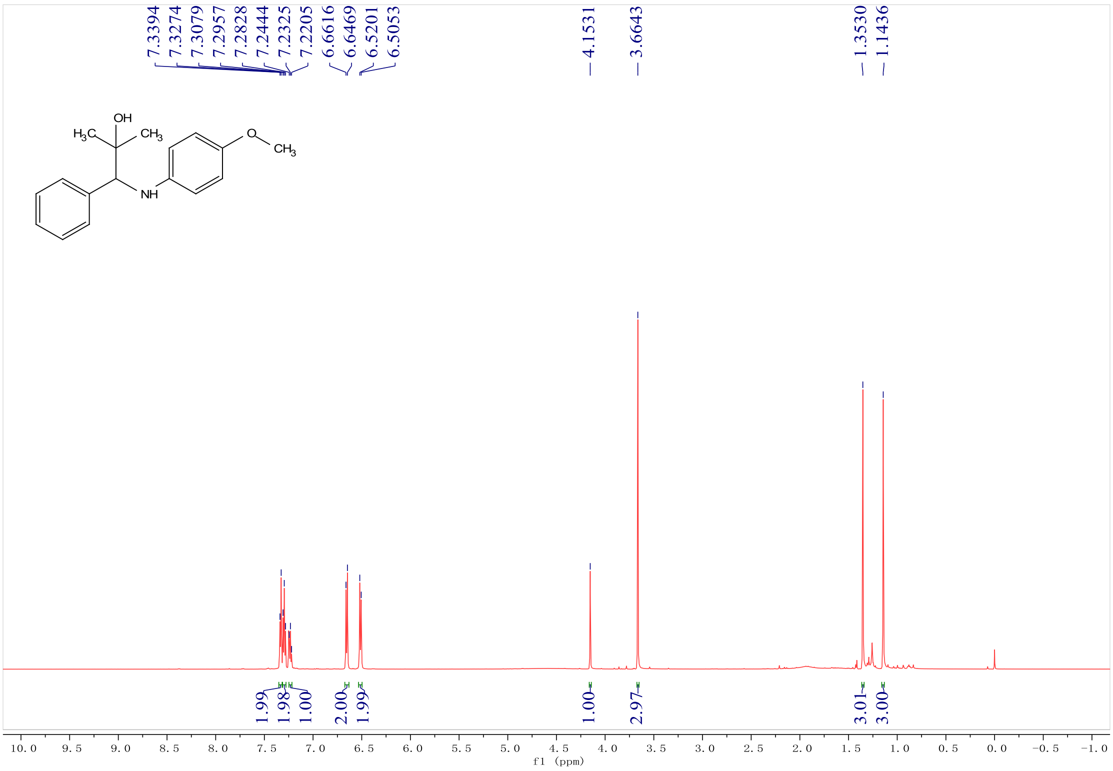


^{13}C{^{1}H}-NMR Spectrum (101 MHz, $CDCl_3$) of **12**

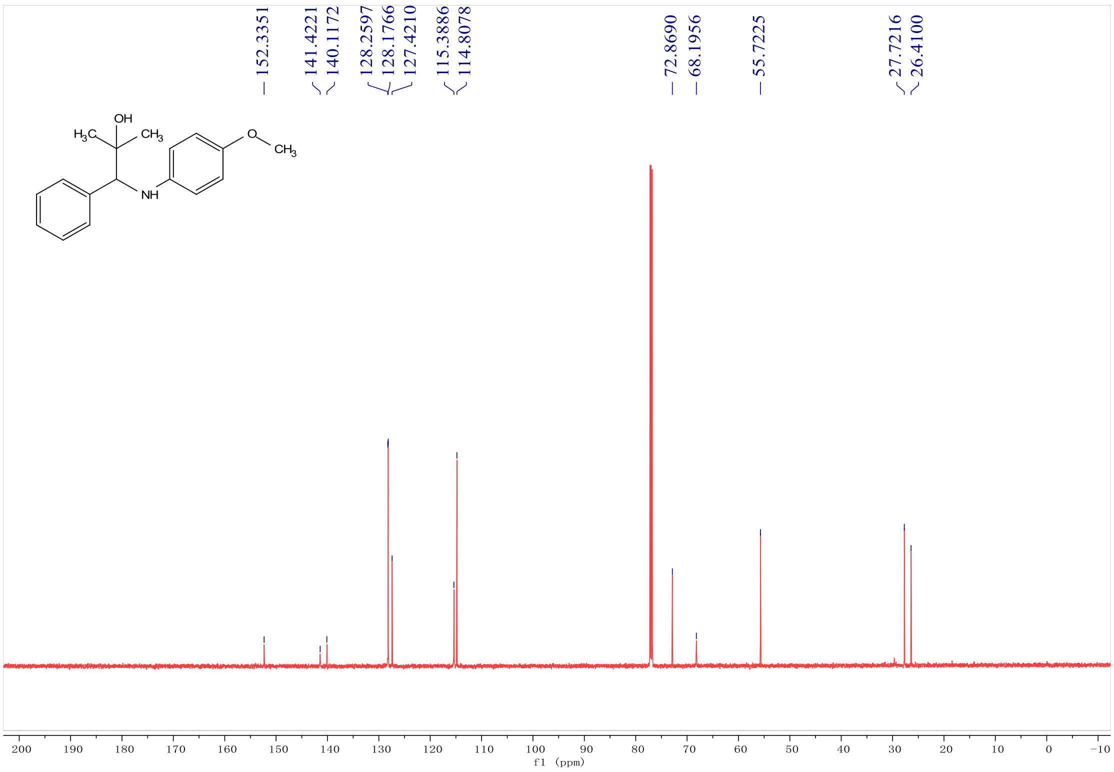


^{19}F-NMR Spectrum (376 MHz, $CDCl_3$) of **12**

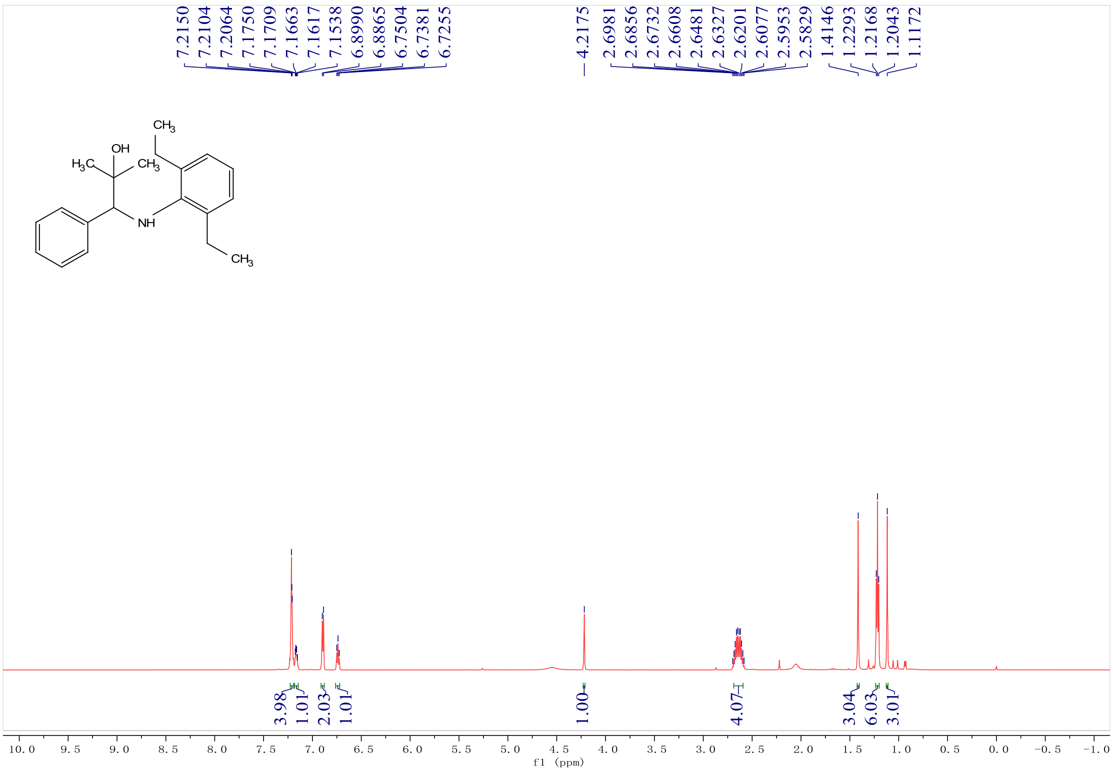
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **13**



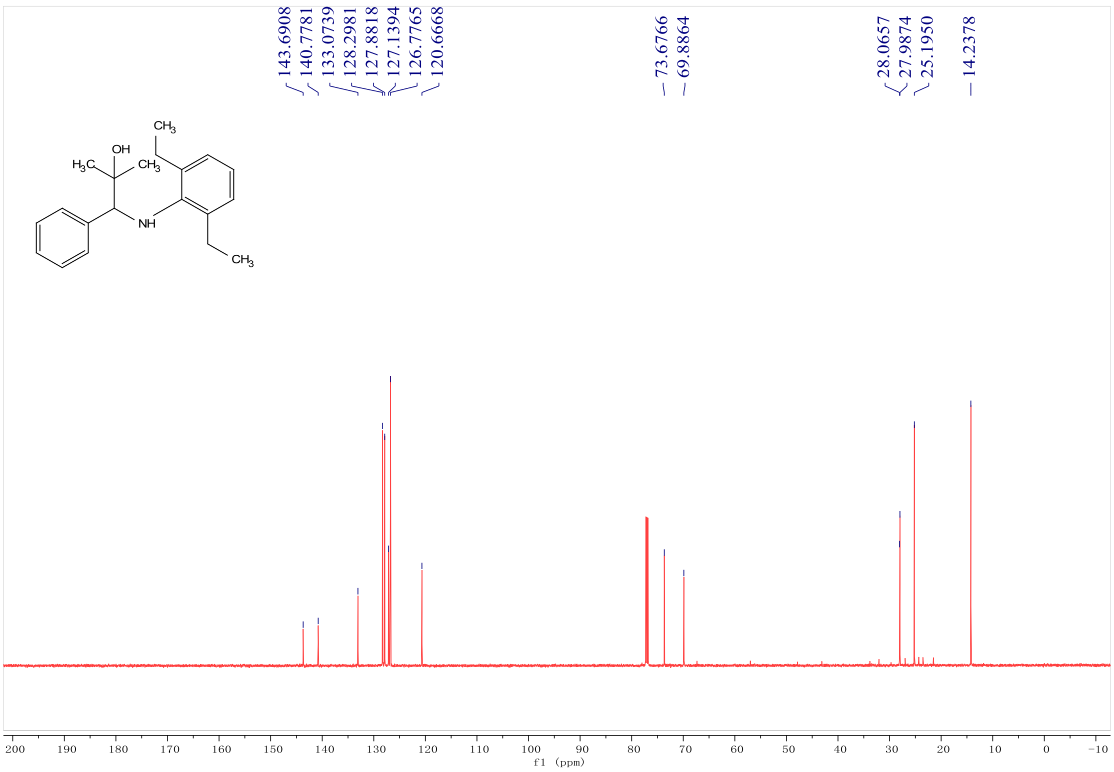
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **13**



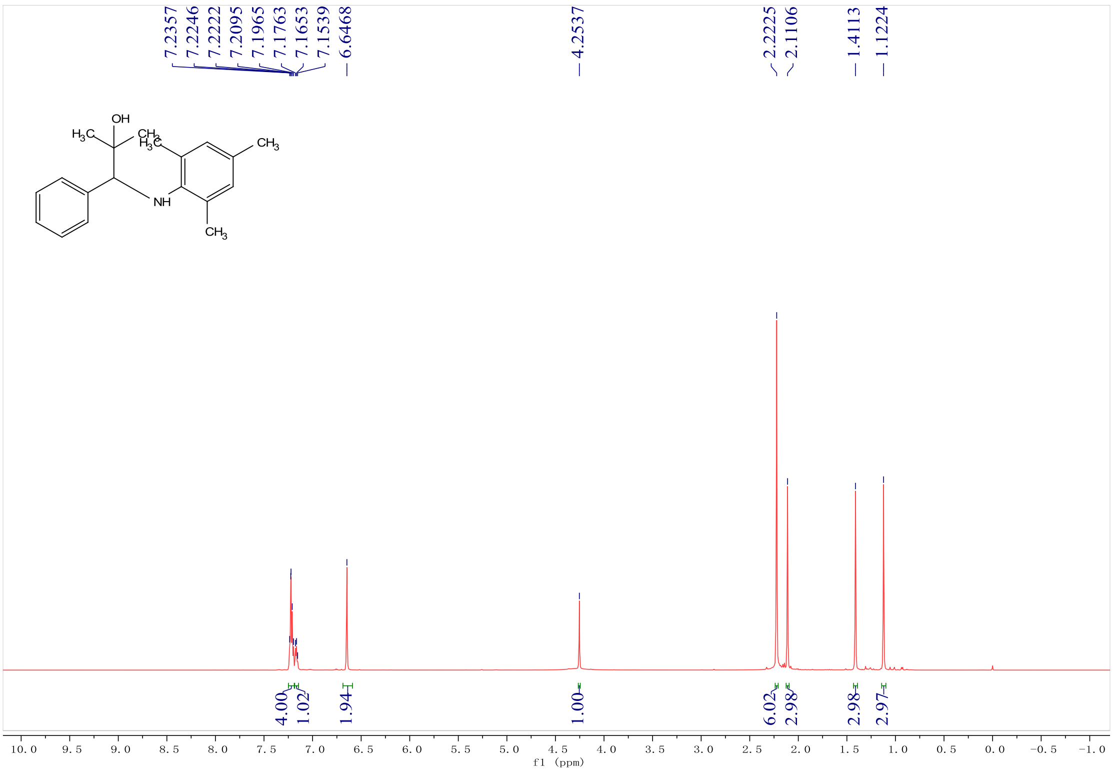
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **14**



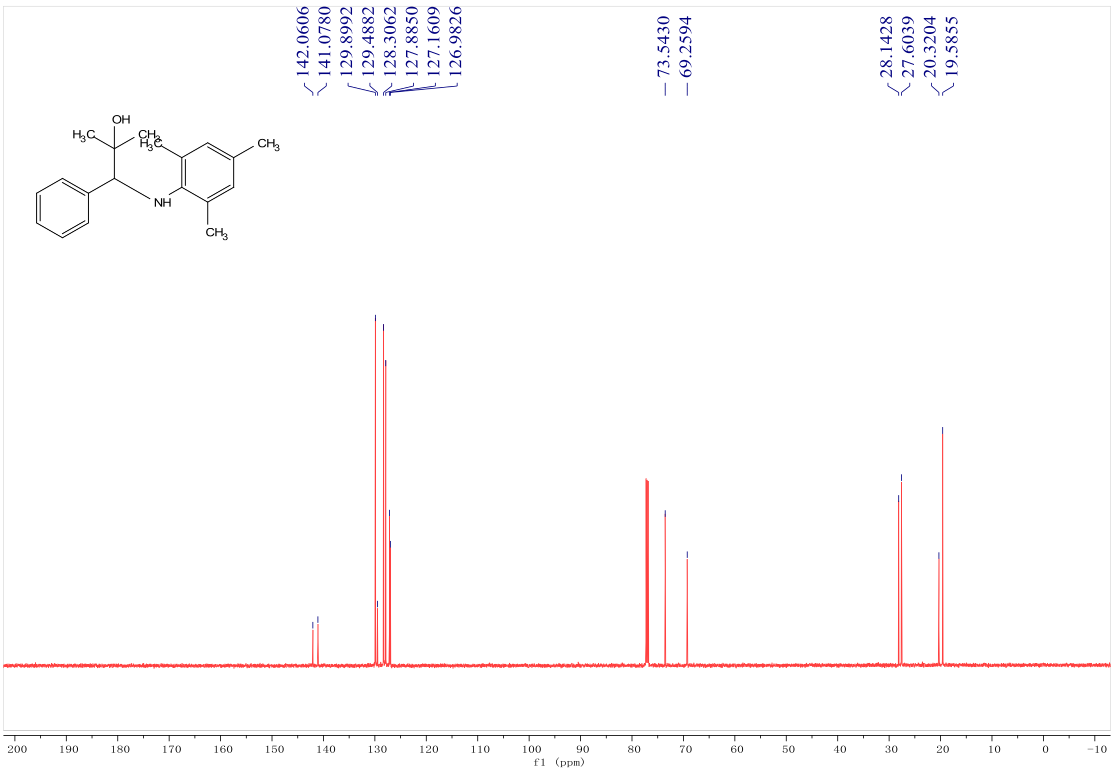
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **14**



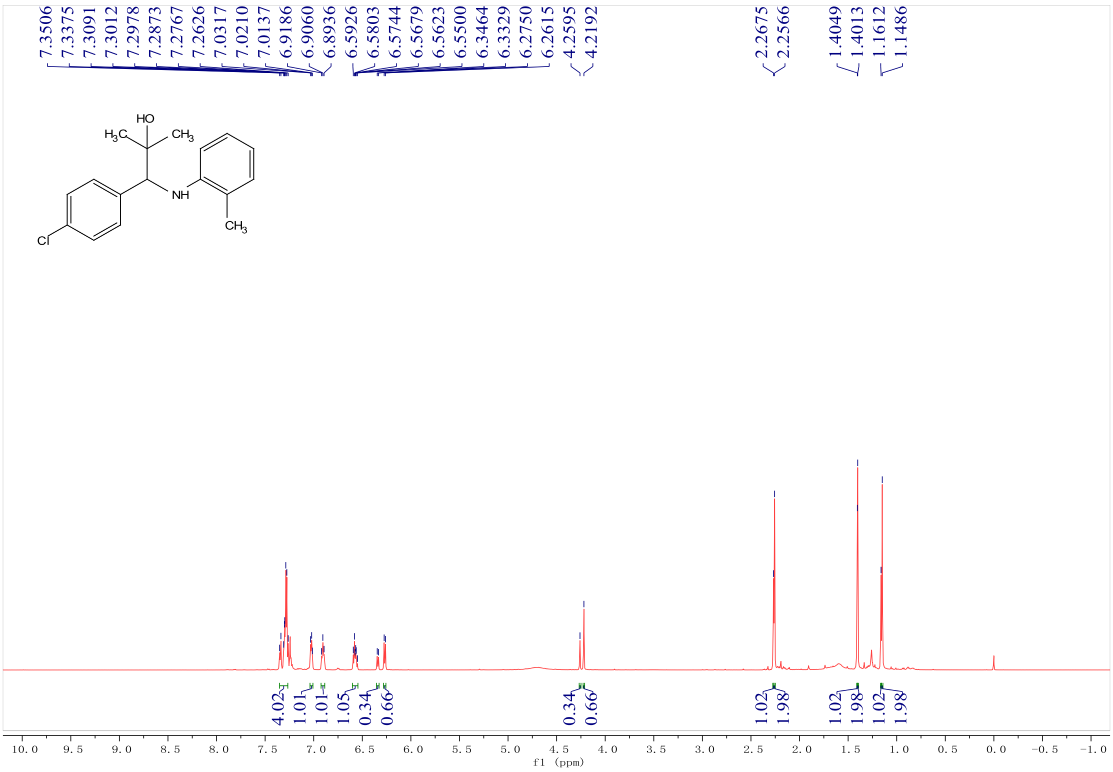
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **15**



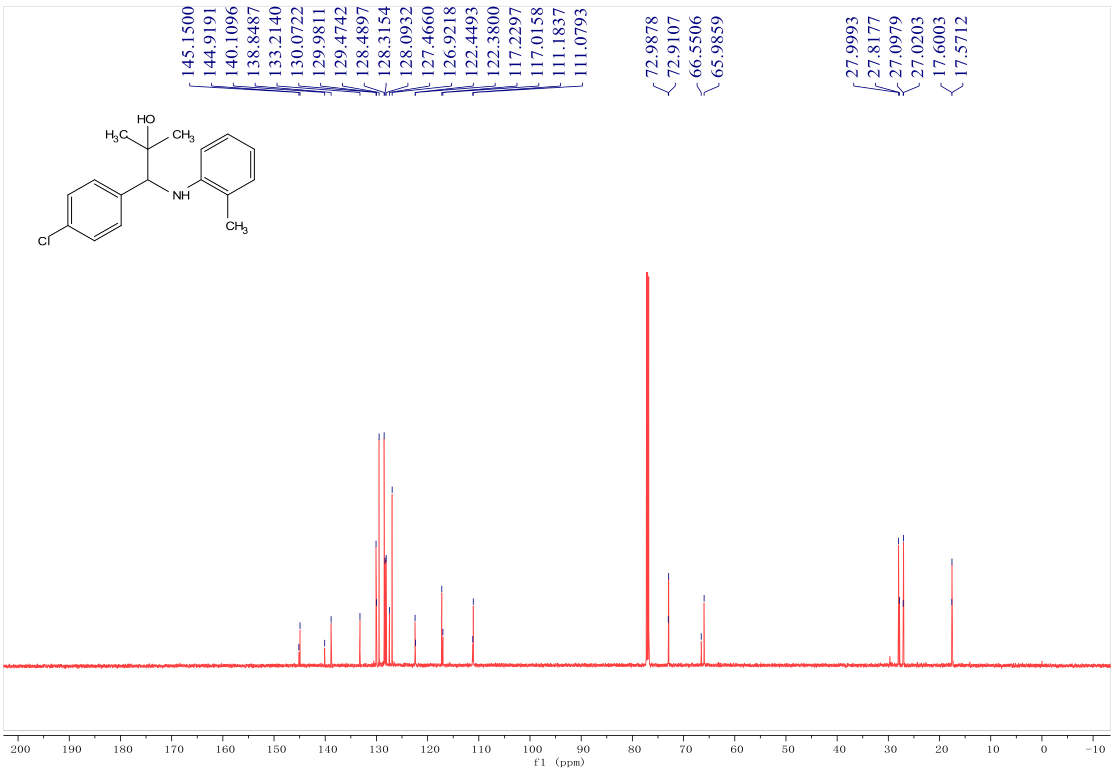
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **15**



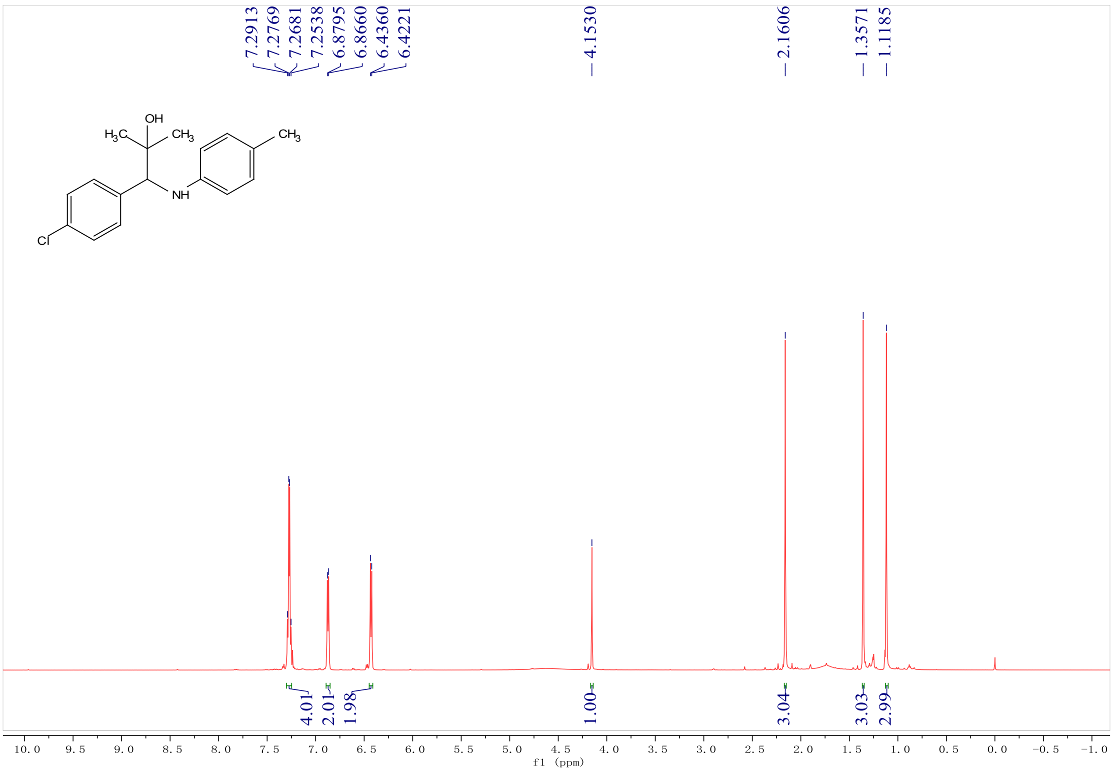
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **16**



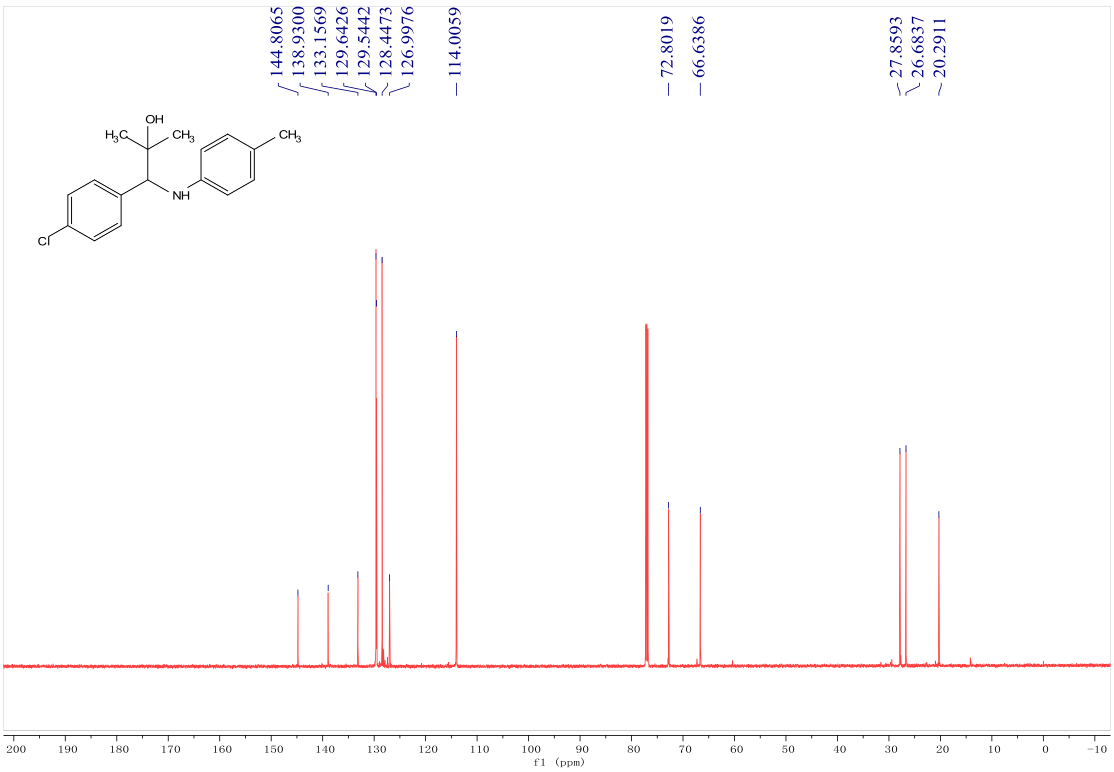
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **16**



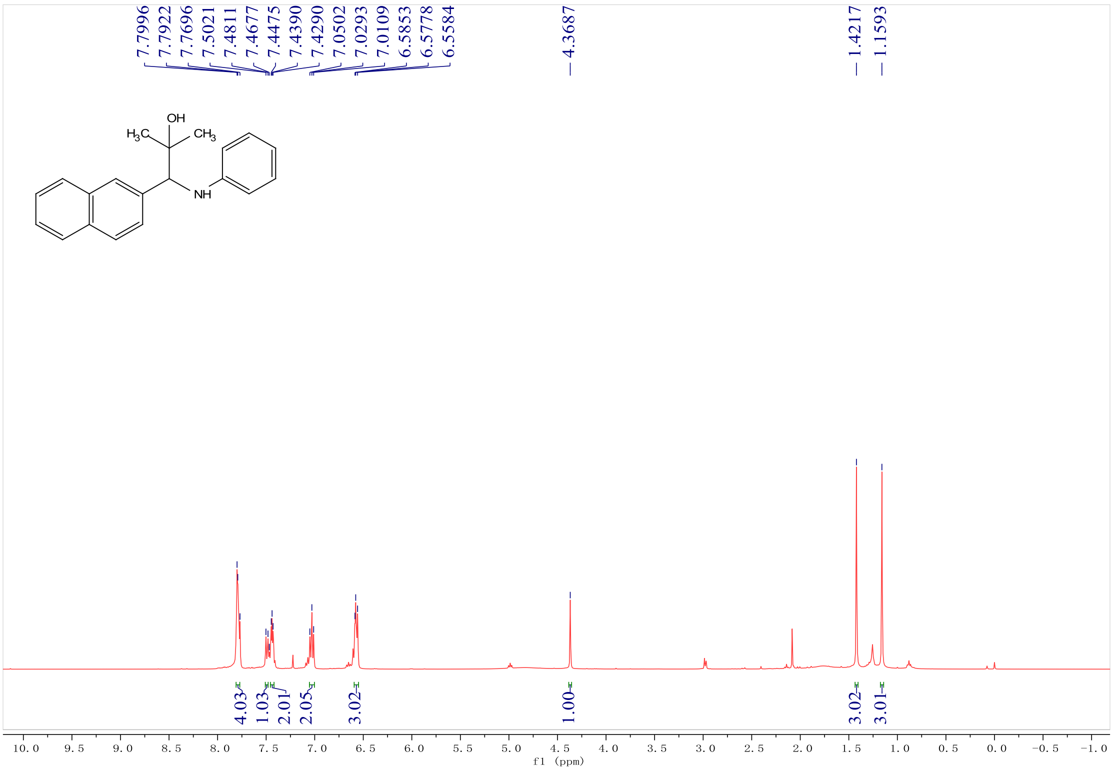
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **17**



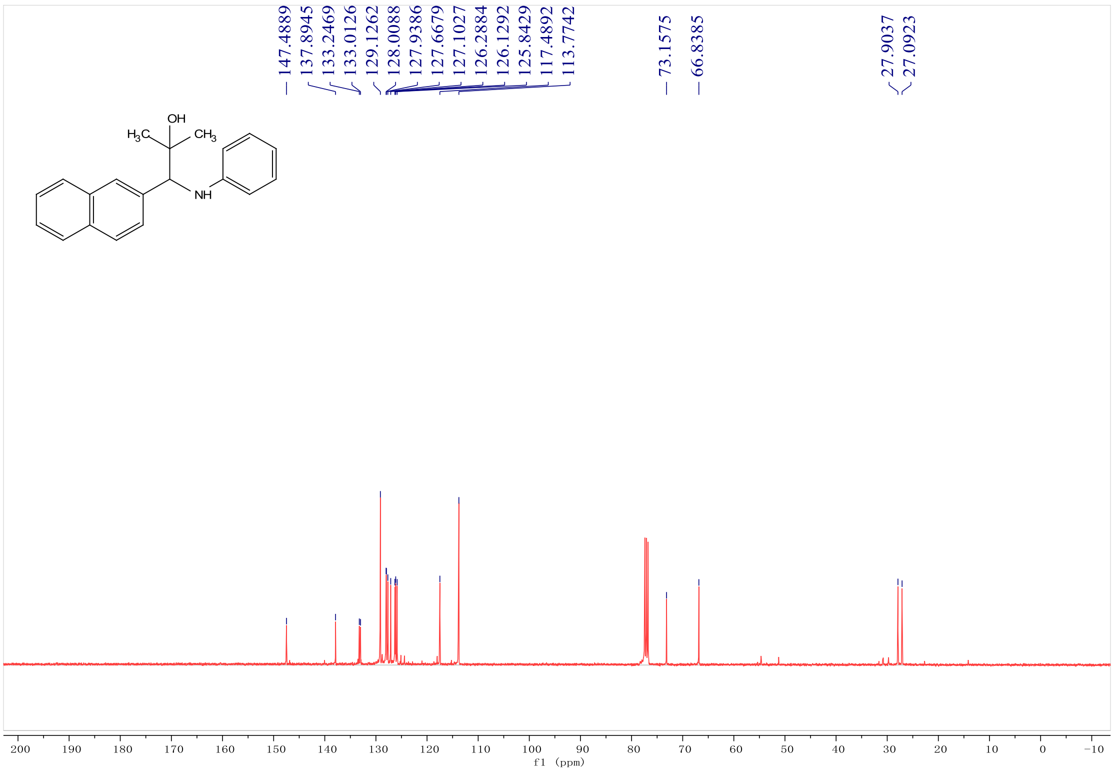
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **17**



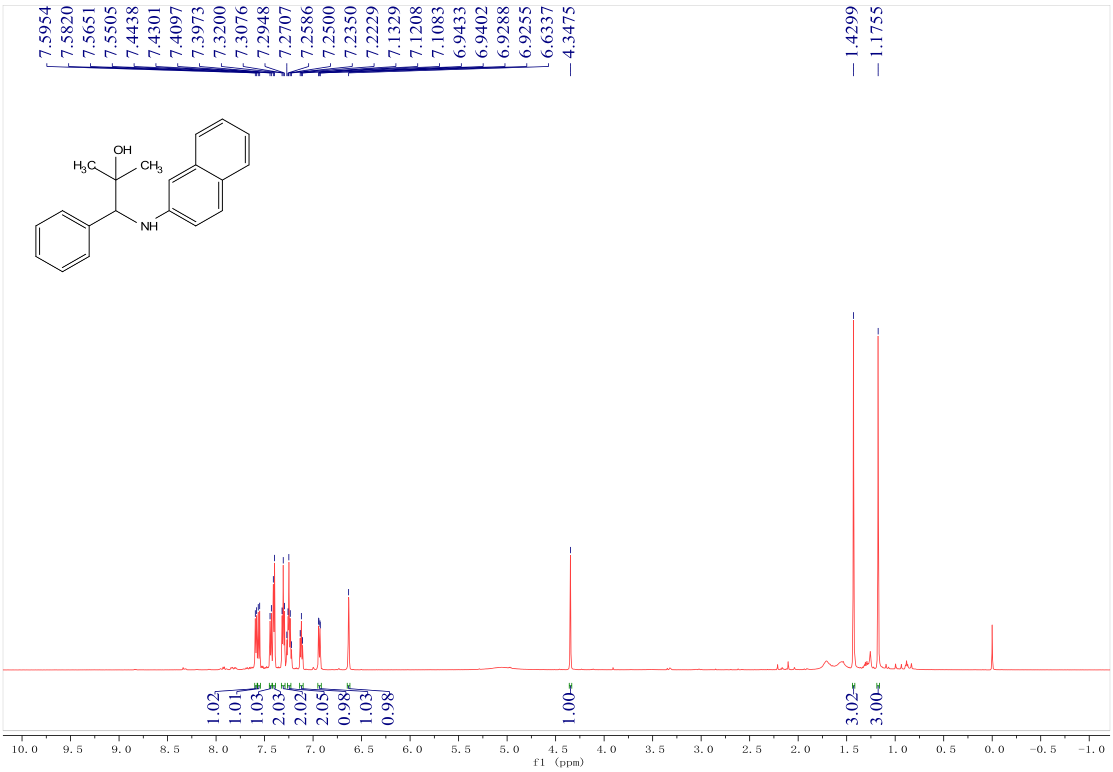
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **18**



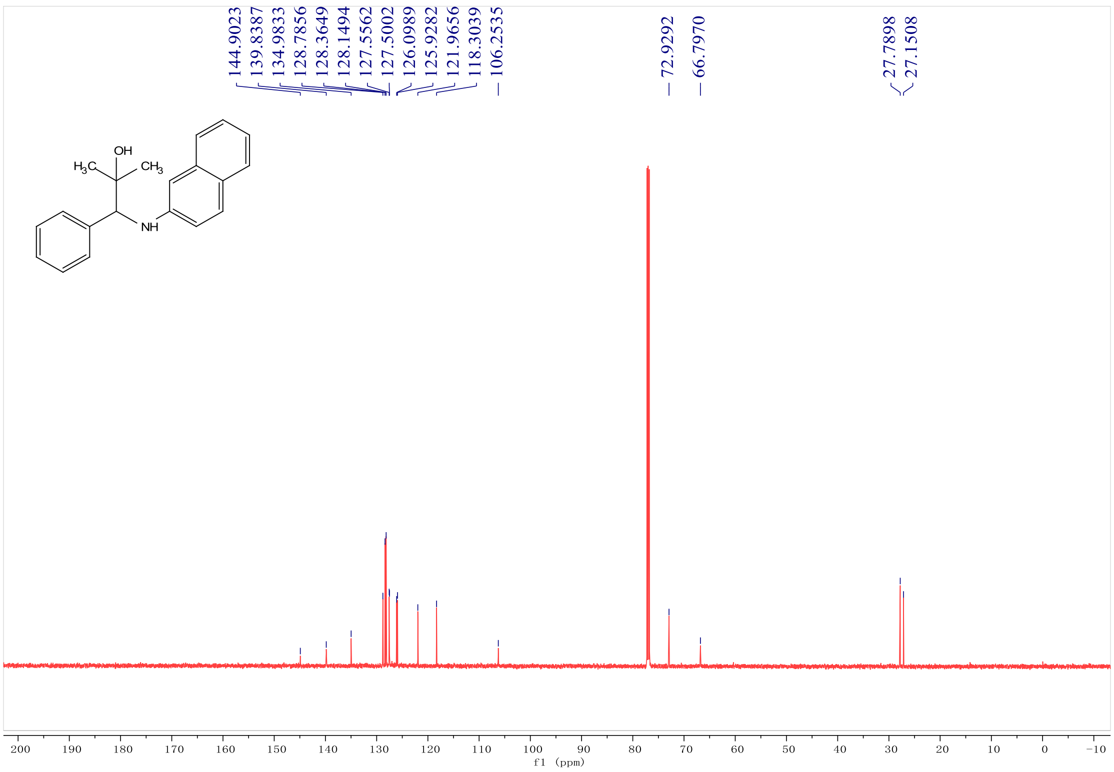
$^{13}C\{^{1}H\}$-NMR Spectrum (101 MHz, $CDCl_3$) of **18**



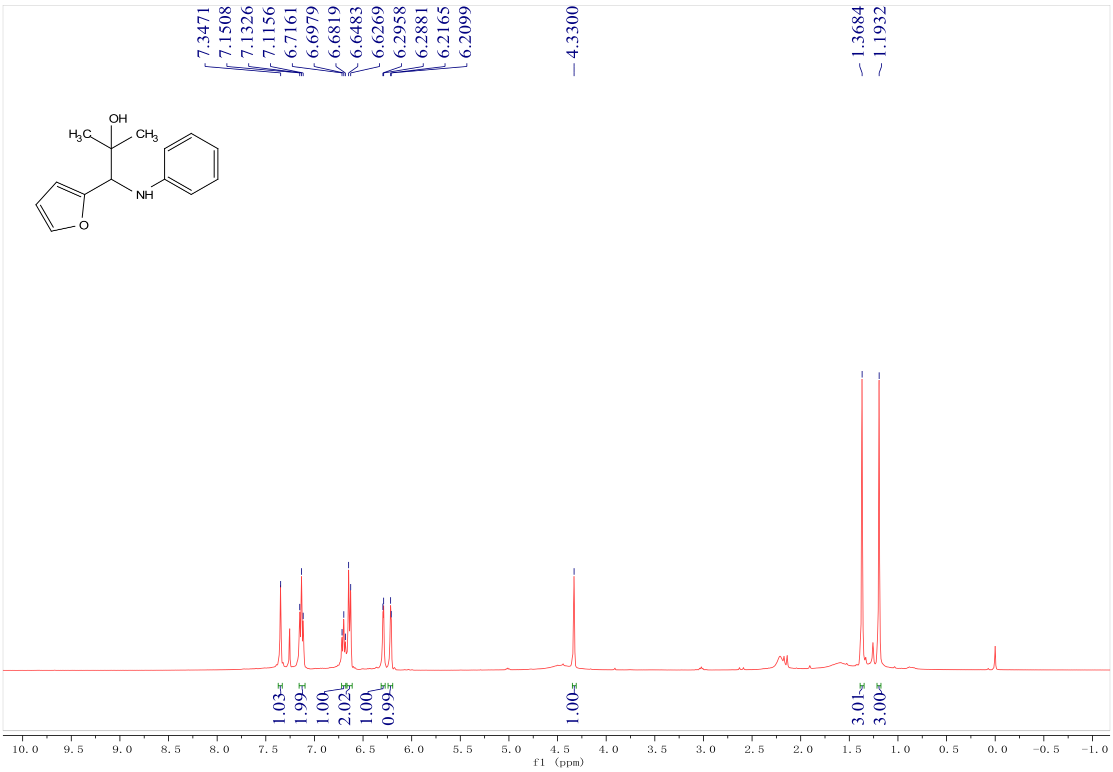
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **19**



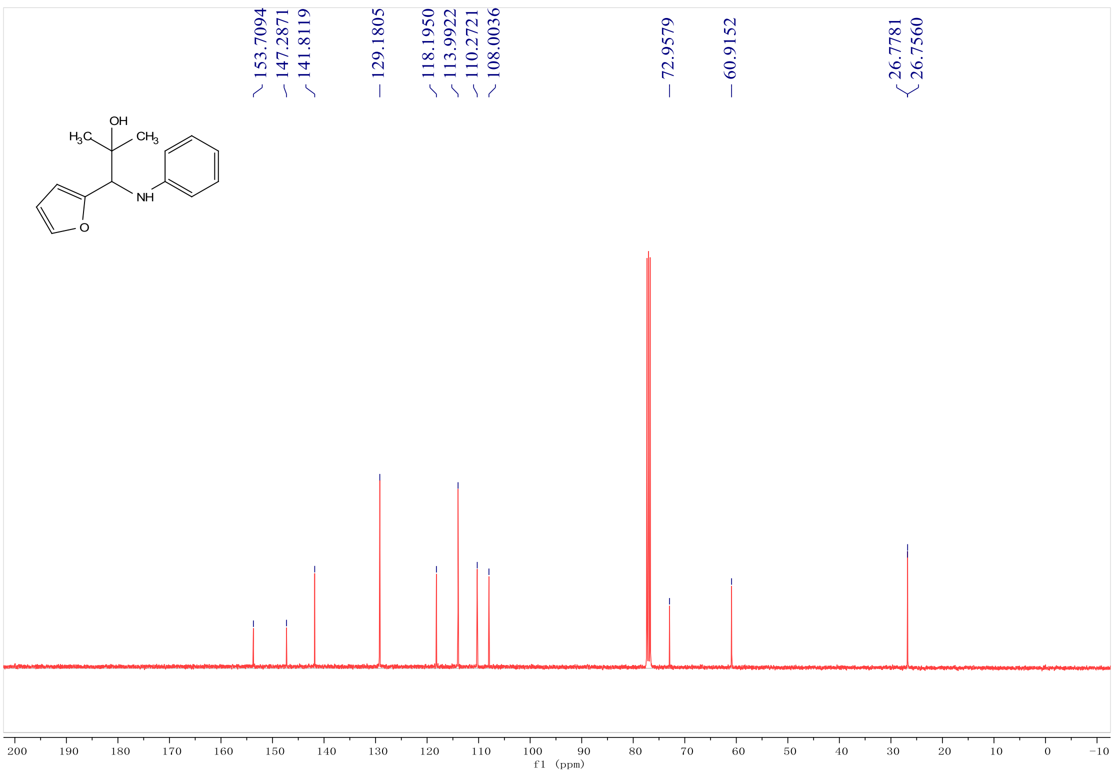
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **19**



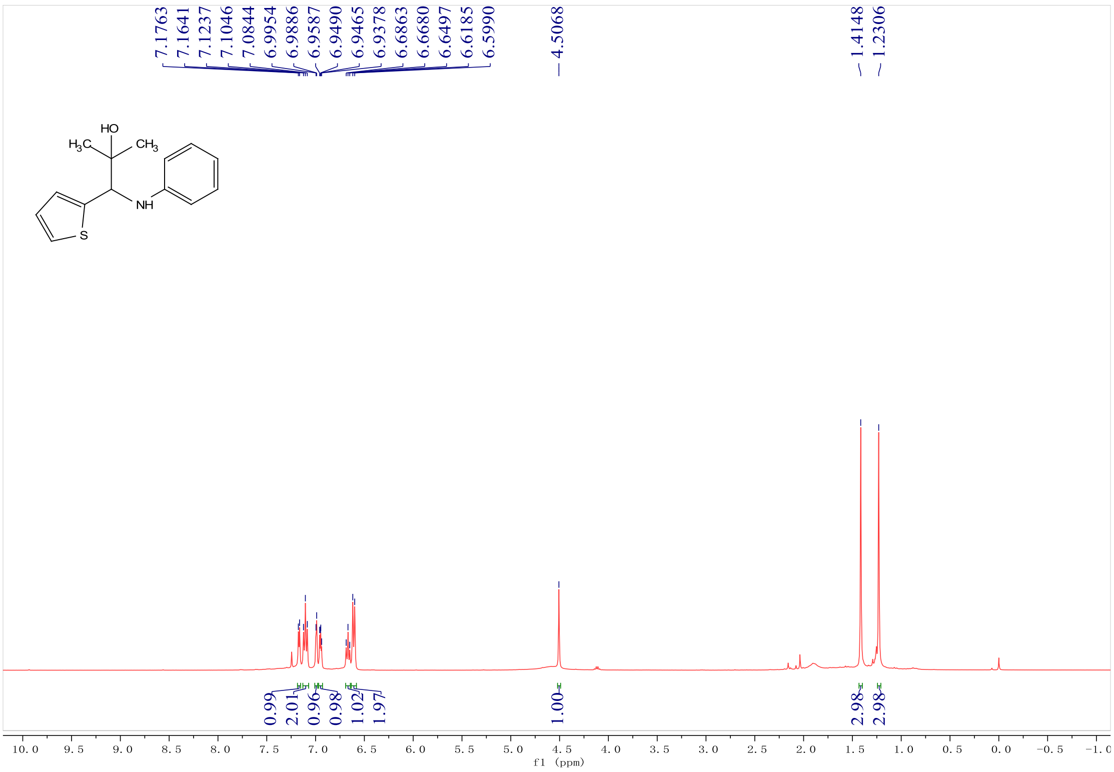
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **20**



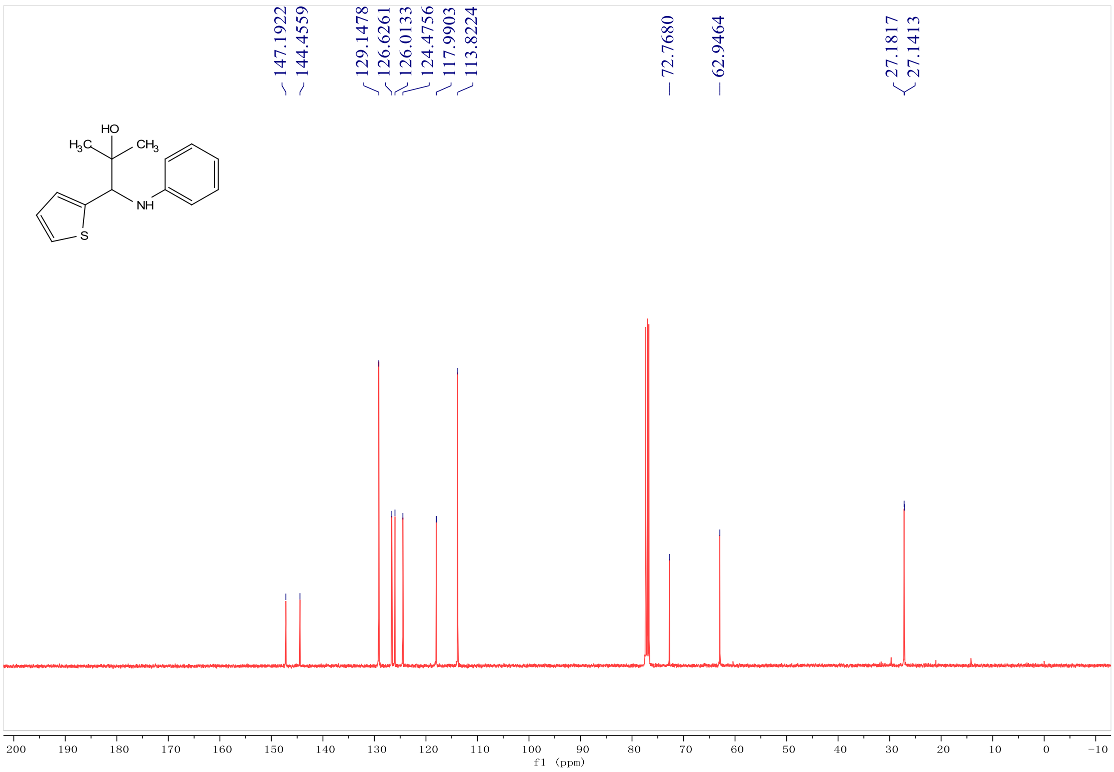
$^{13}C\{^{1}H\}$-NMR Spectrum (101 MHz, $CDCl_3$) of **20**



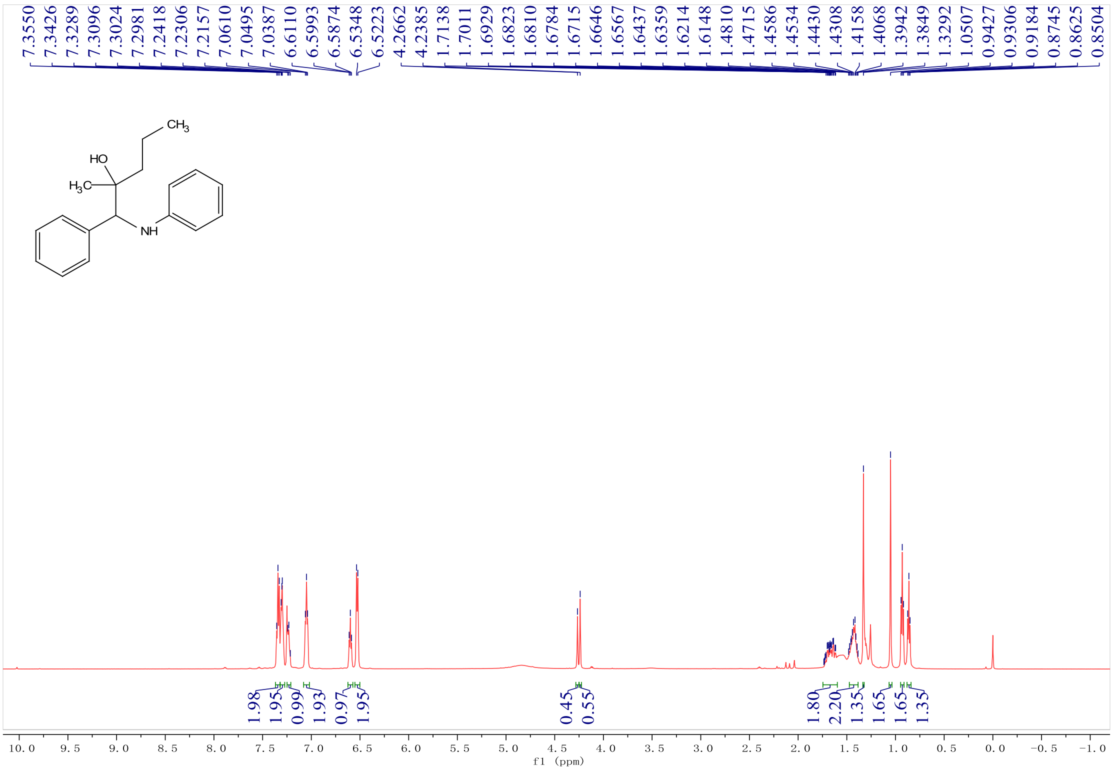
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **21**



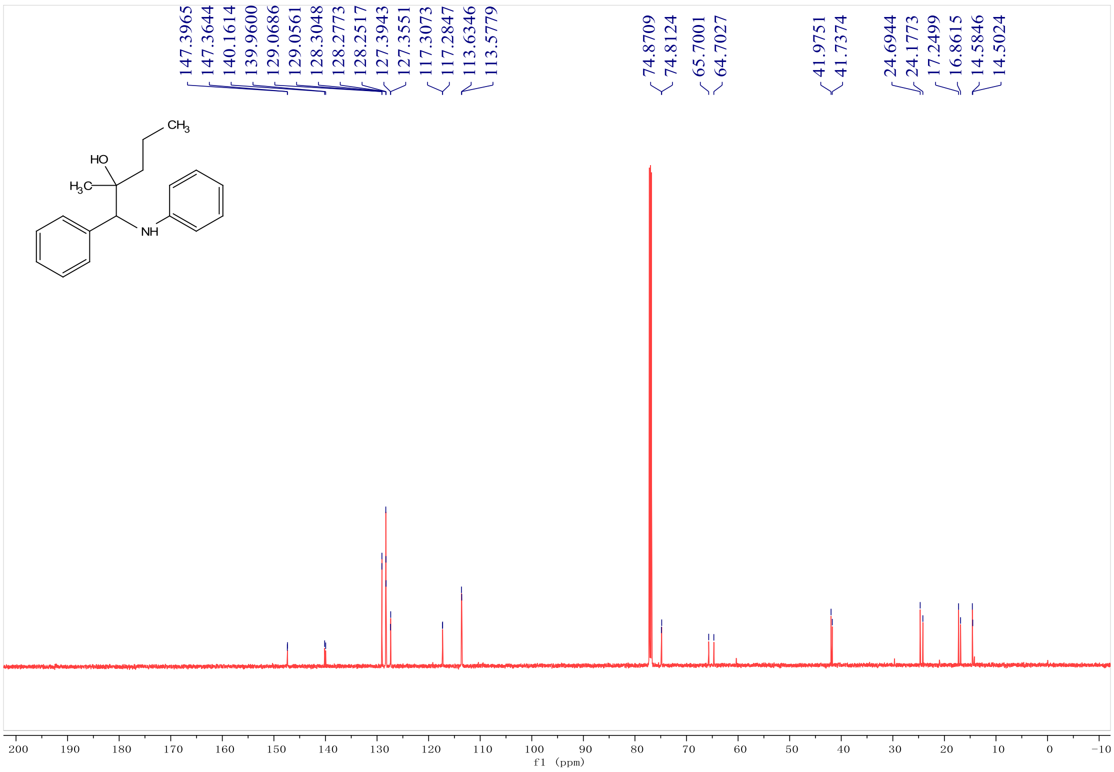
$^{13}C\{^{1}H\}$-NMR Spectrum (101 MHz, $CDCl_3$) of **21**



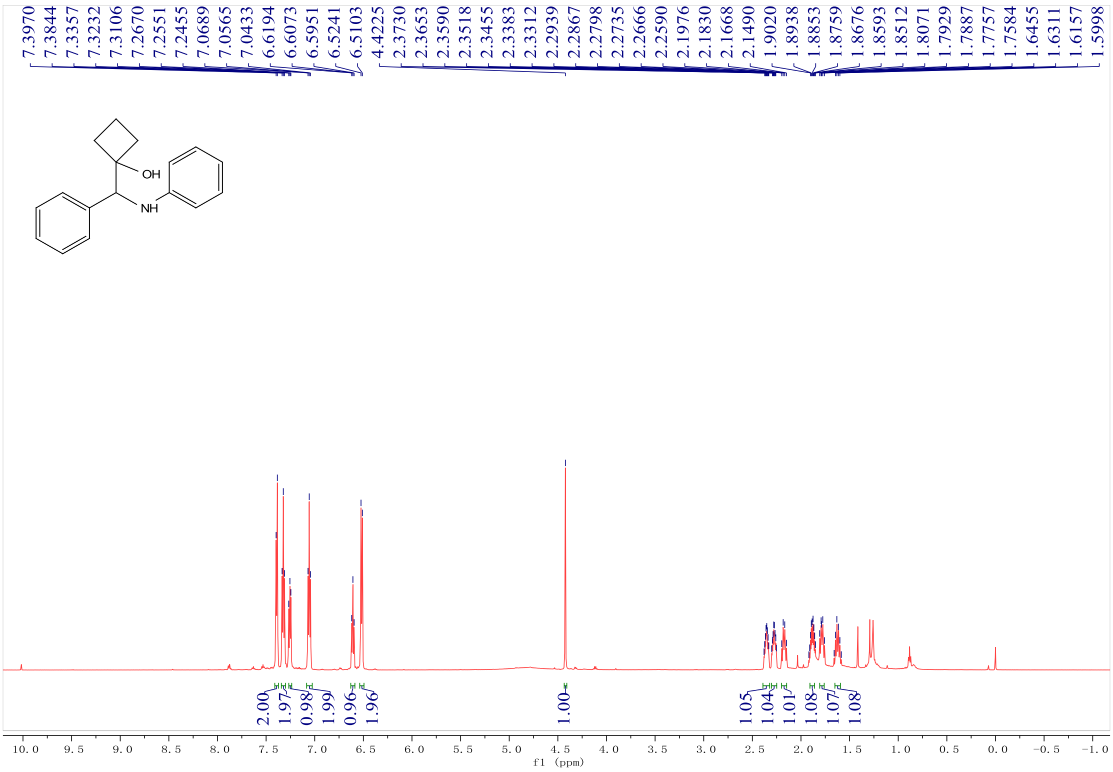
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **22**



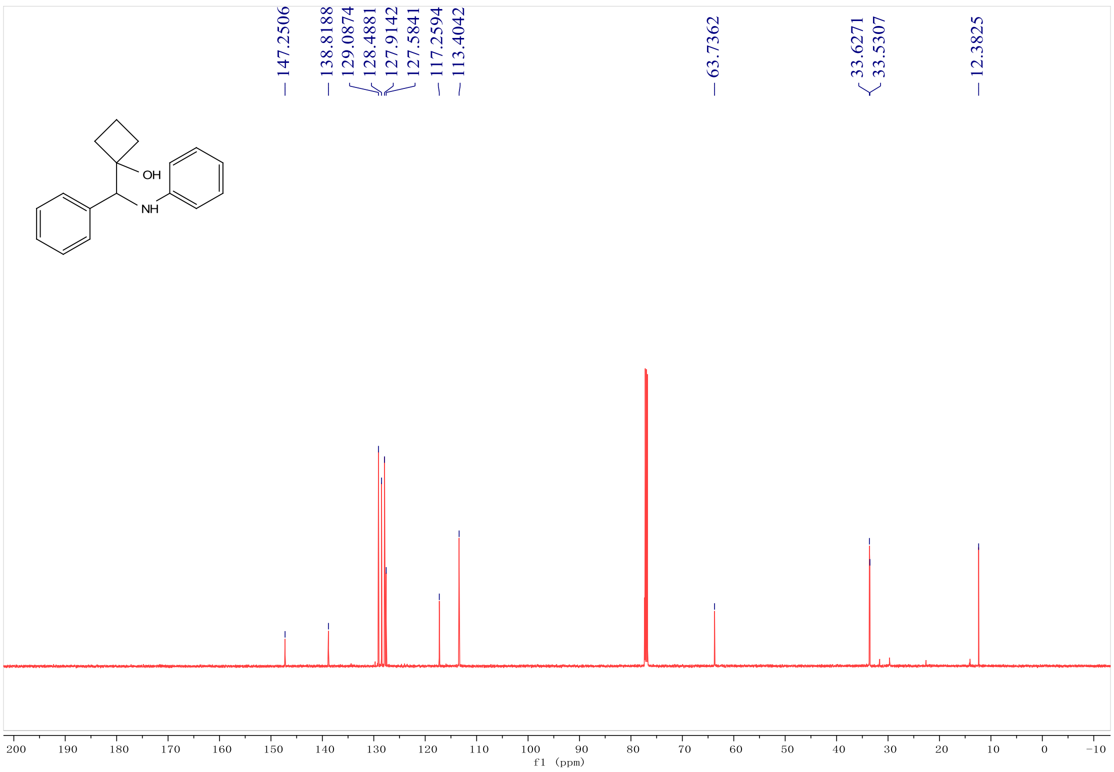
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **22**



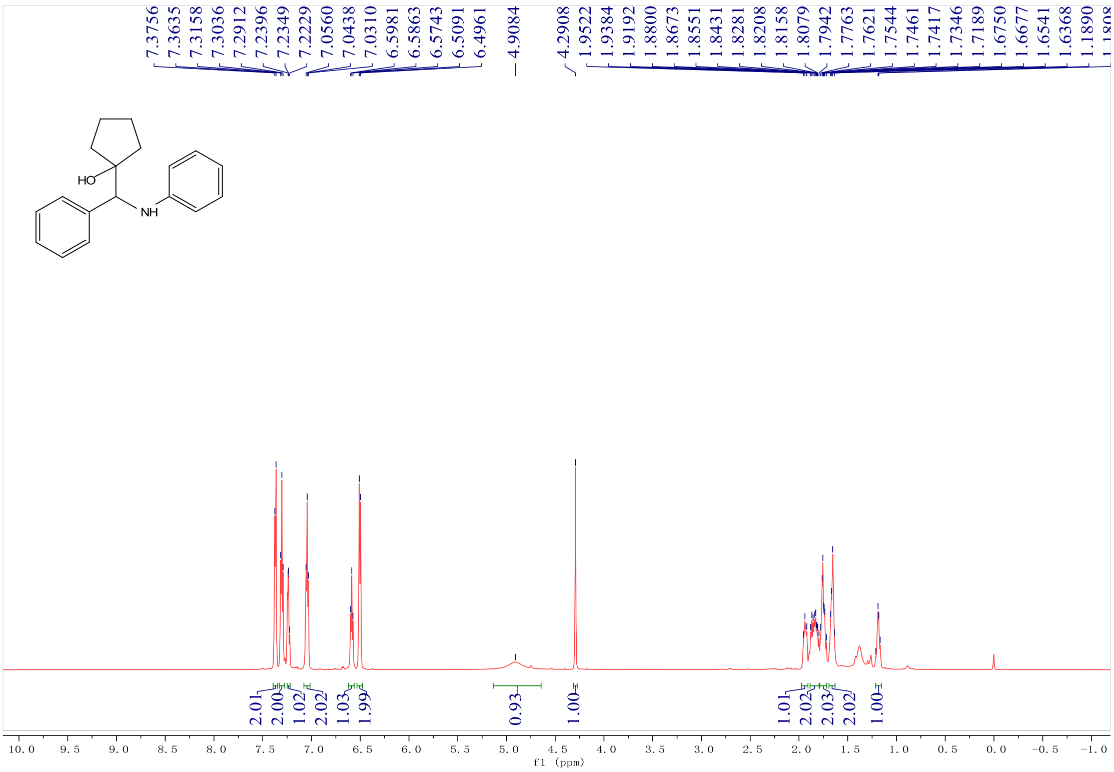
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **23**



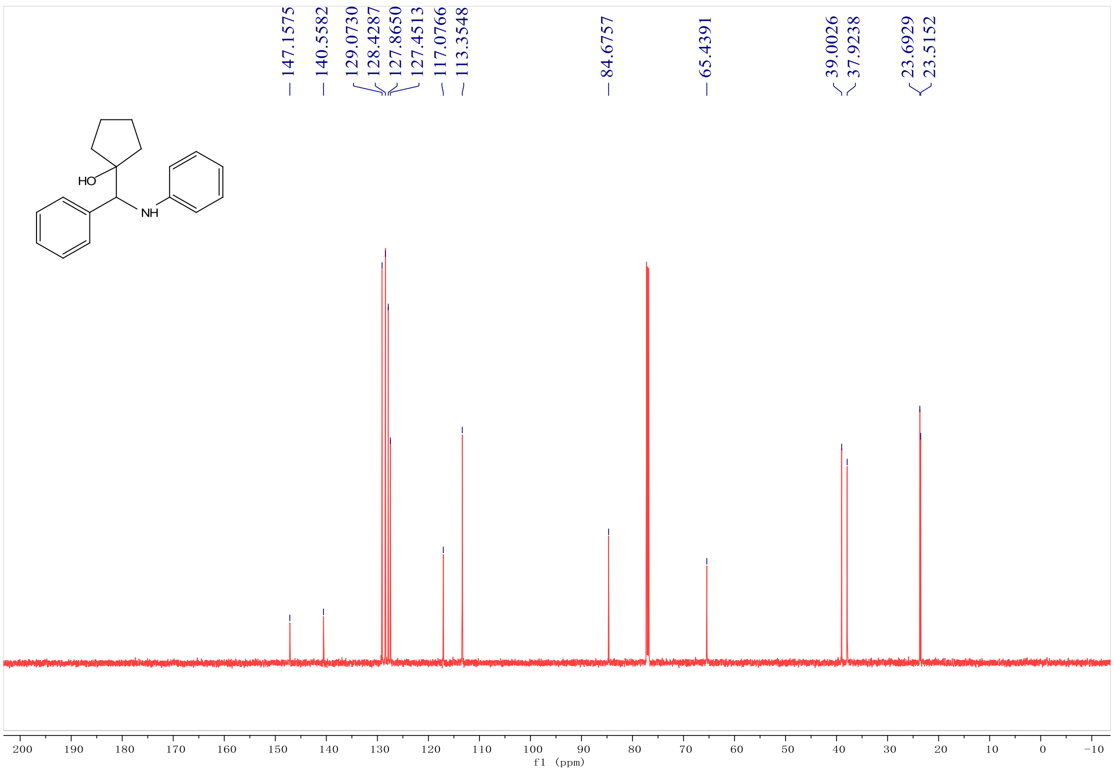
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **23**



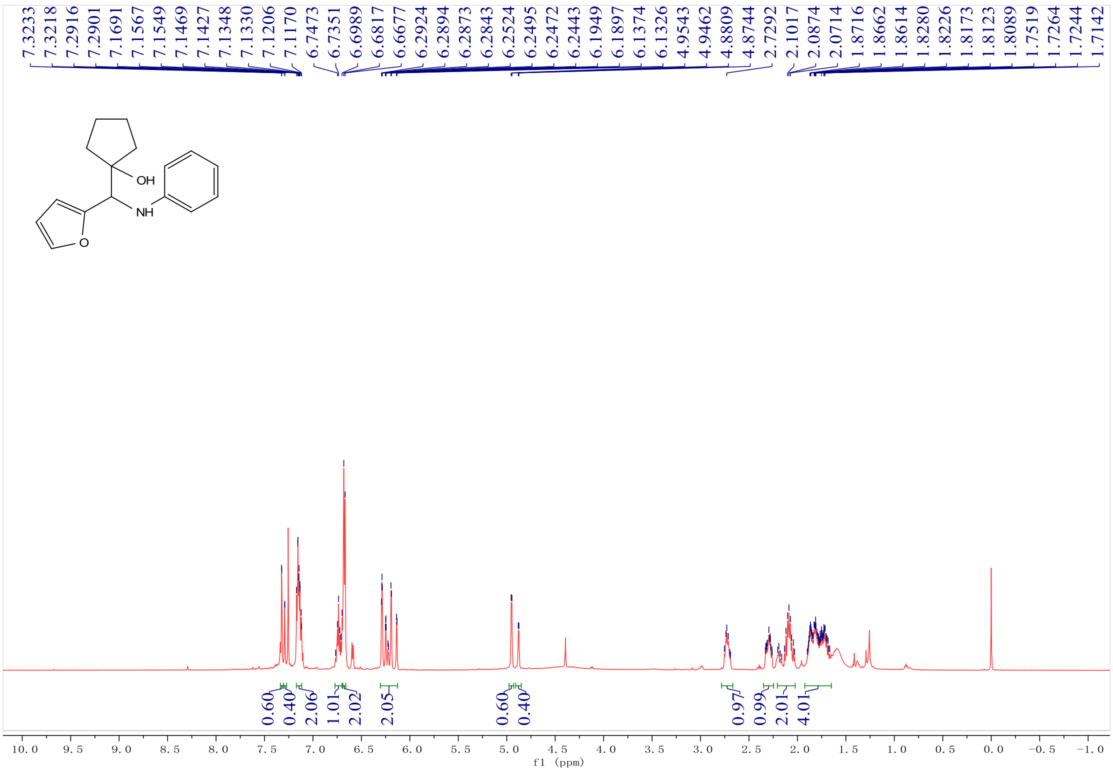
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **24**



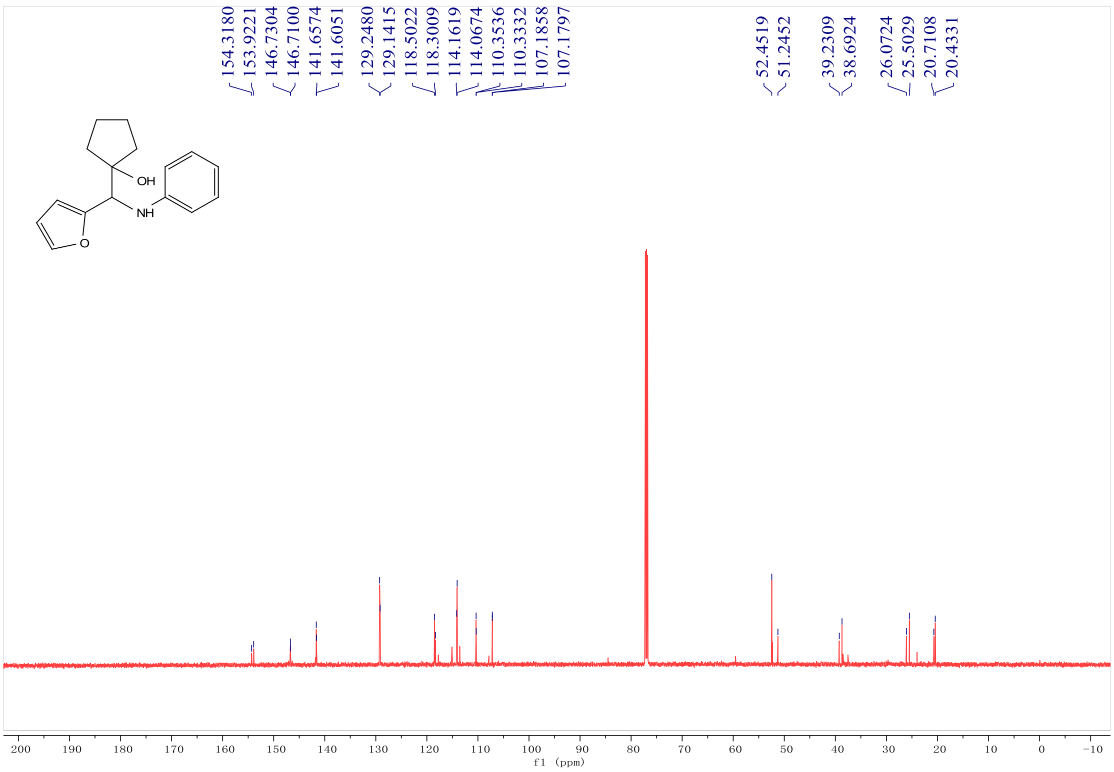
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **24**



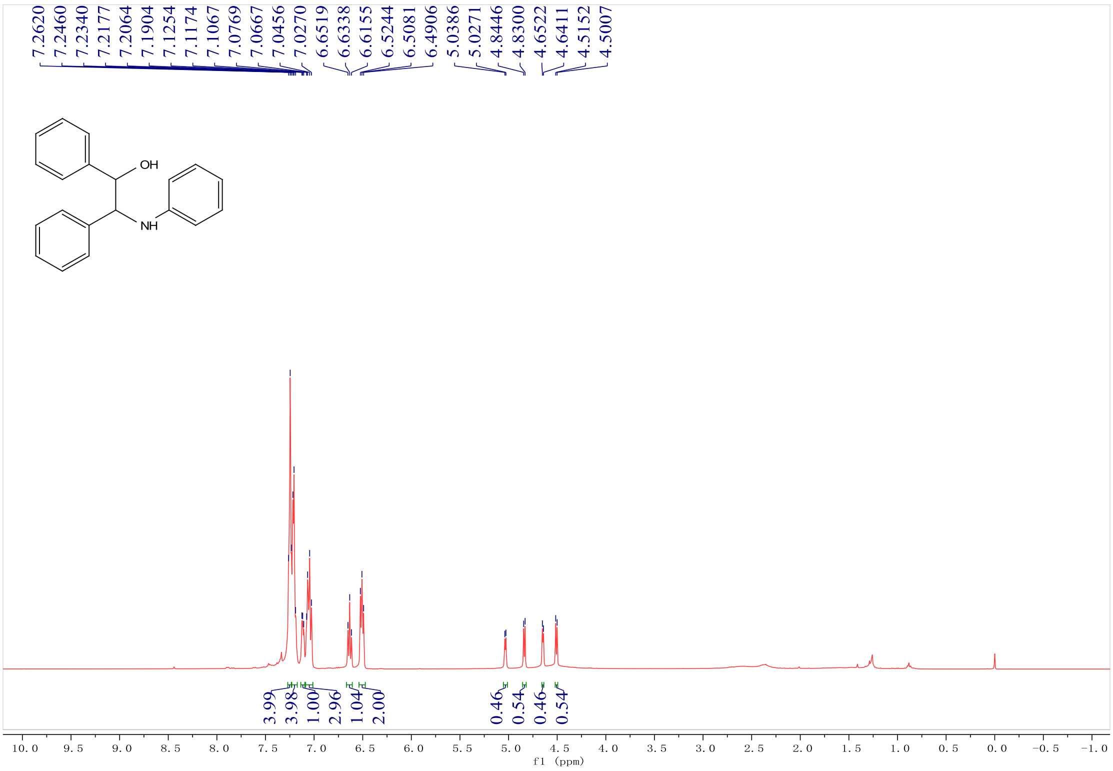
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **25**



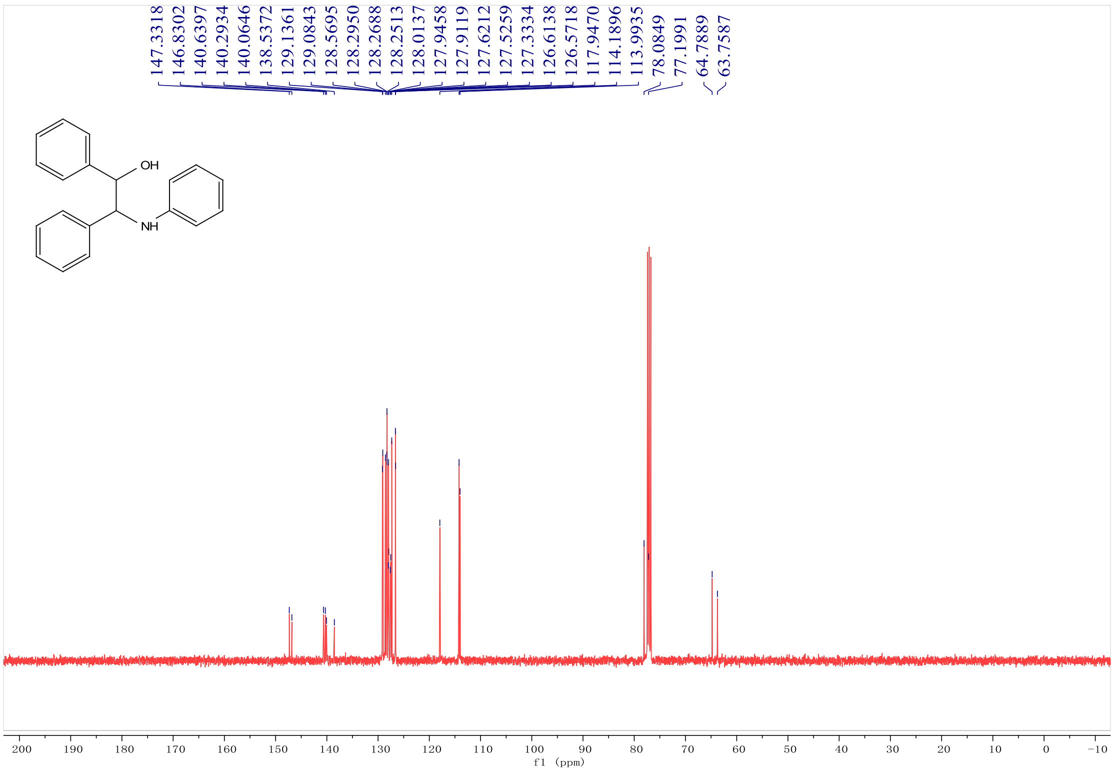
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **25**



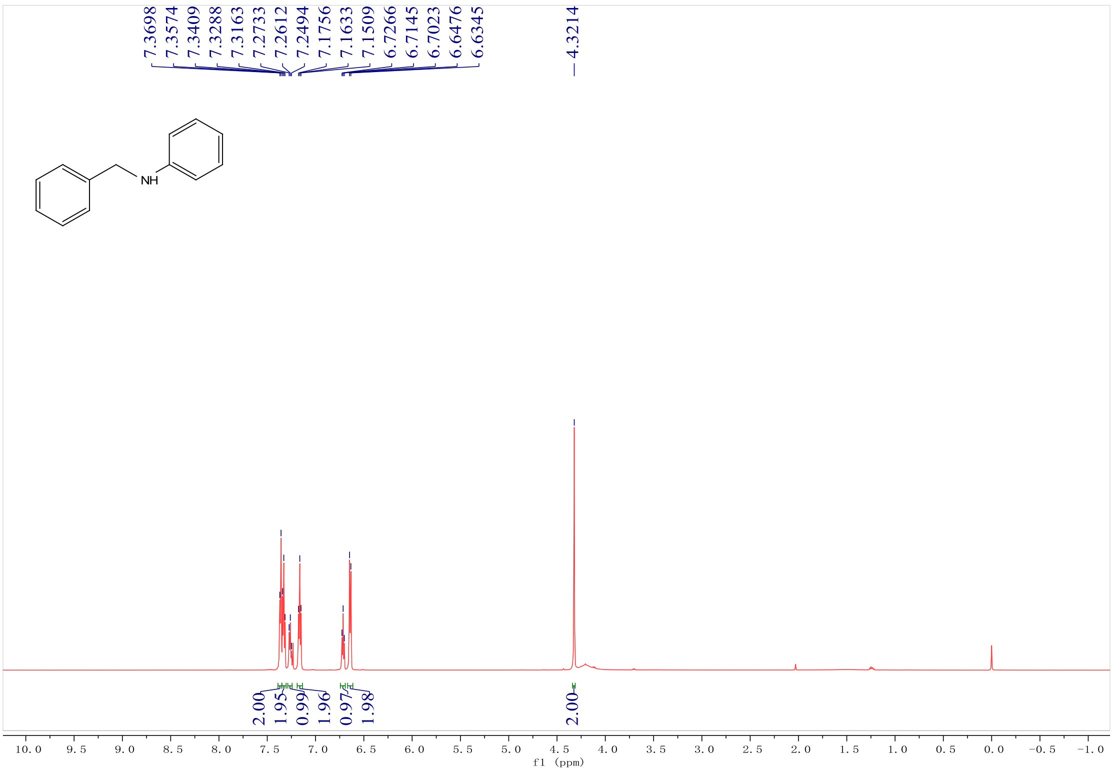
^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **26**



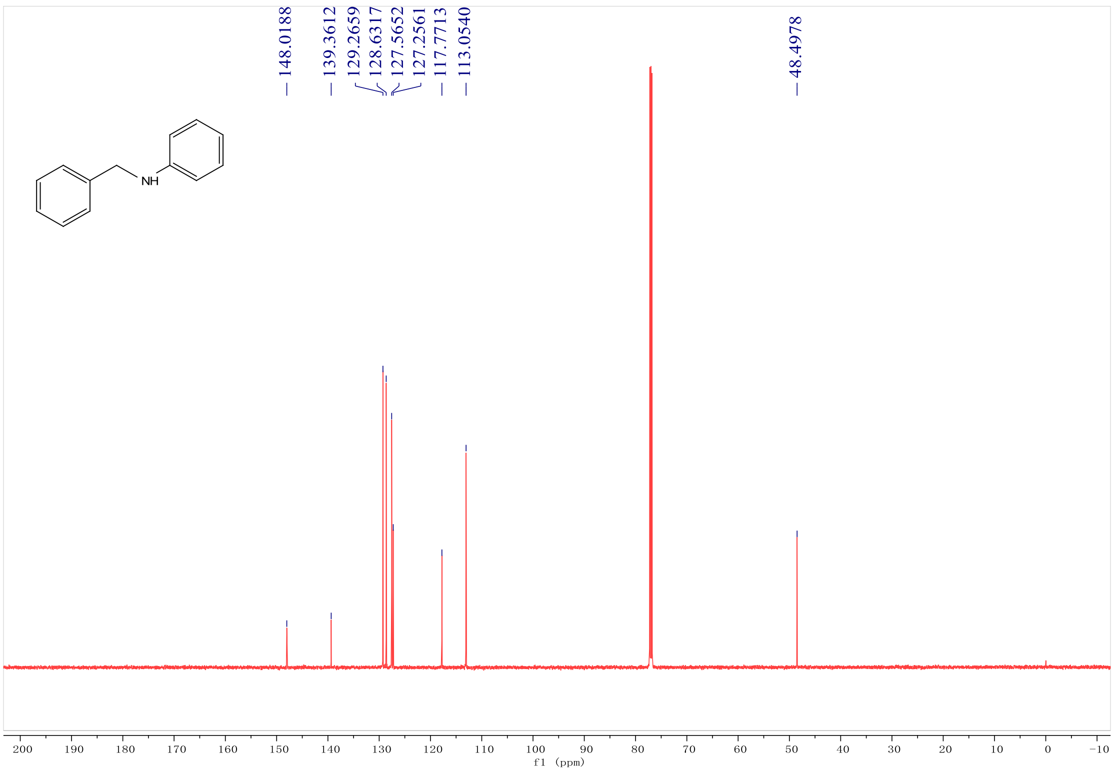
$^{13}C\{^{1}H\}$-NMR Spectrum (101 MHz, $CDCl_3$) of **26**



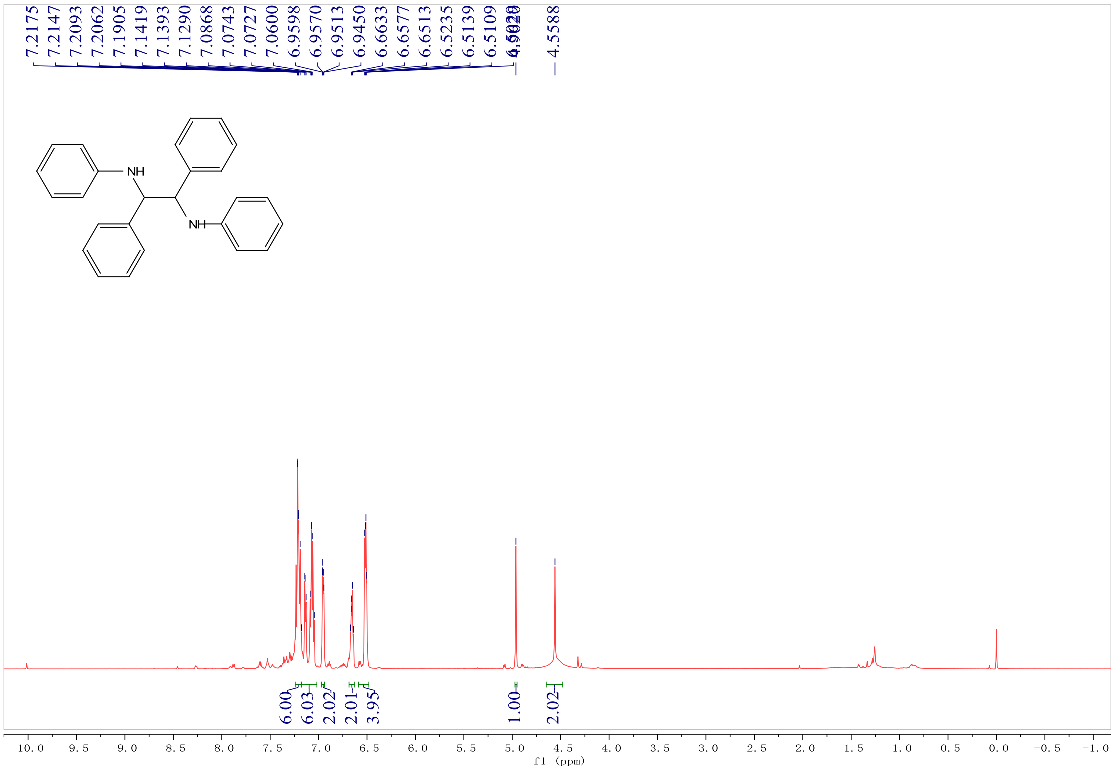
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **1c**



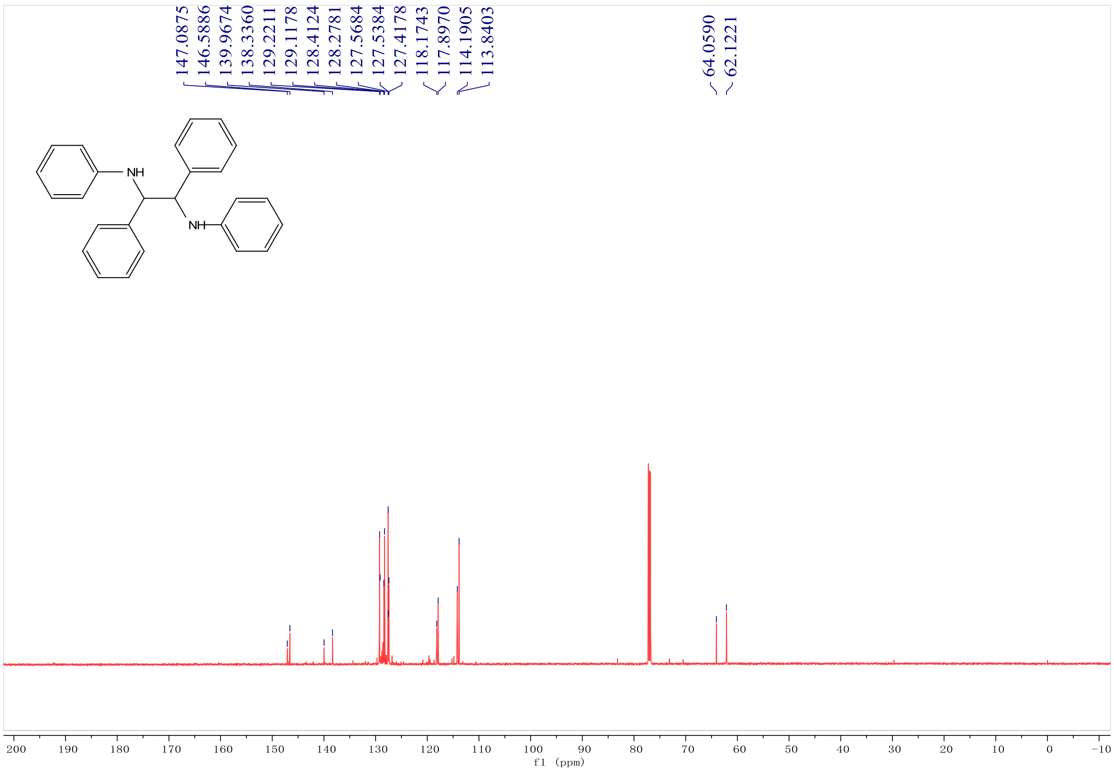
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **1c**



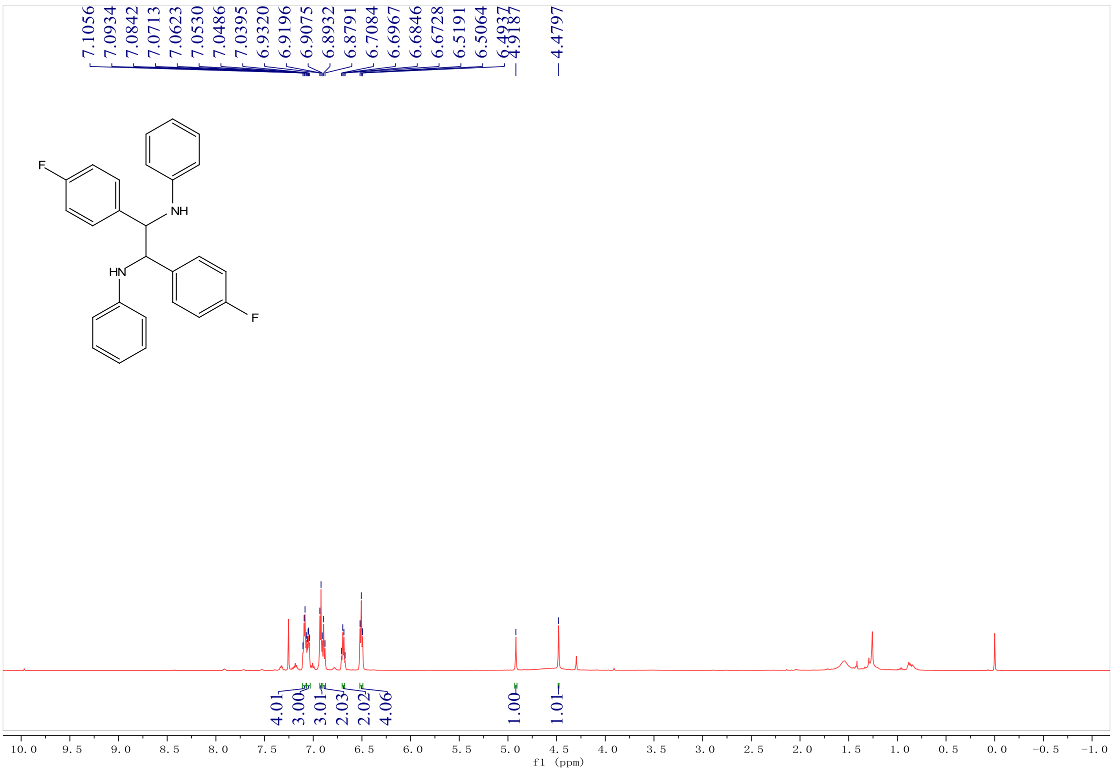
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **1d**



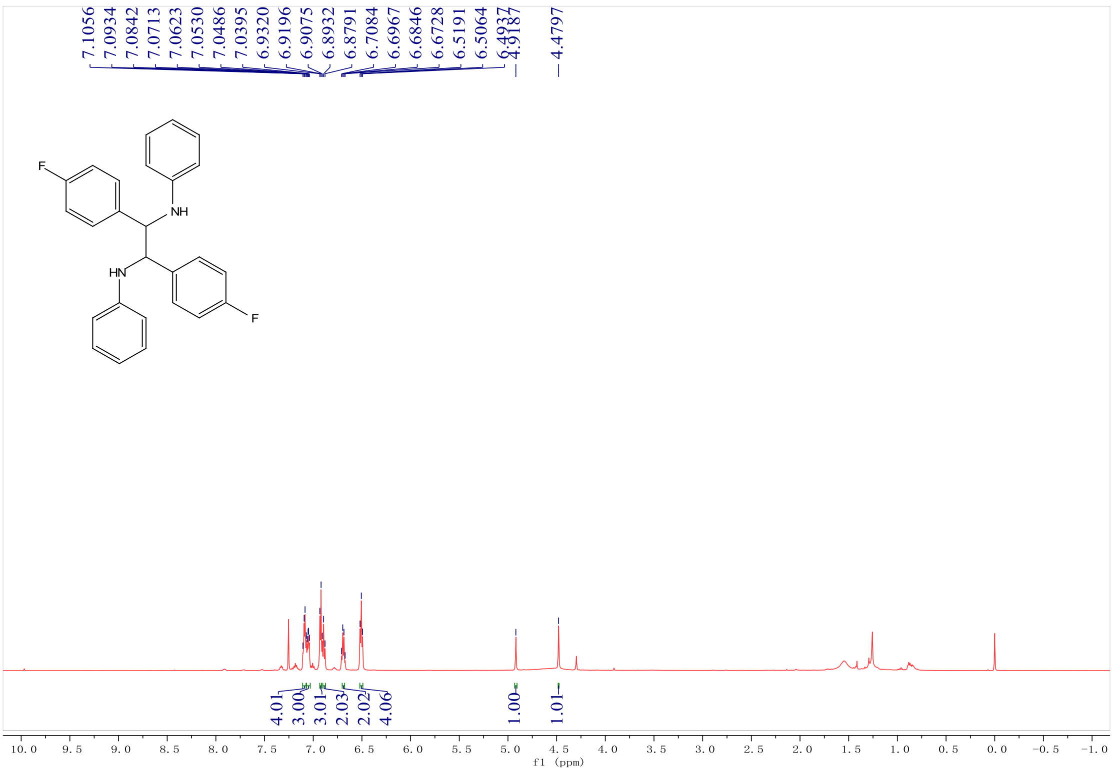
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **1d**



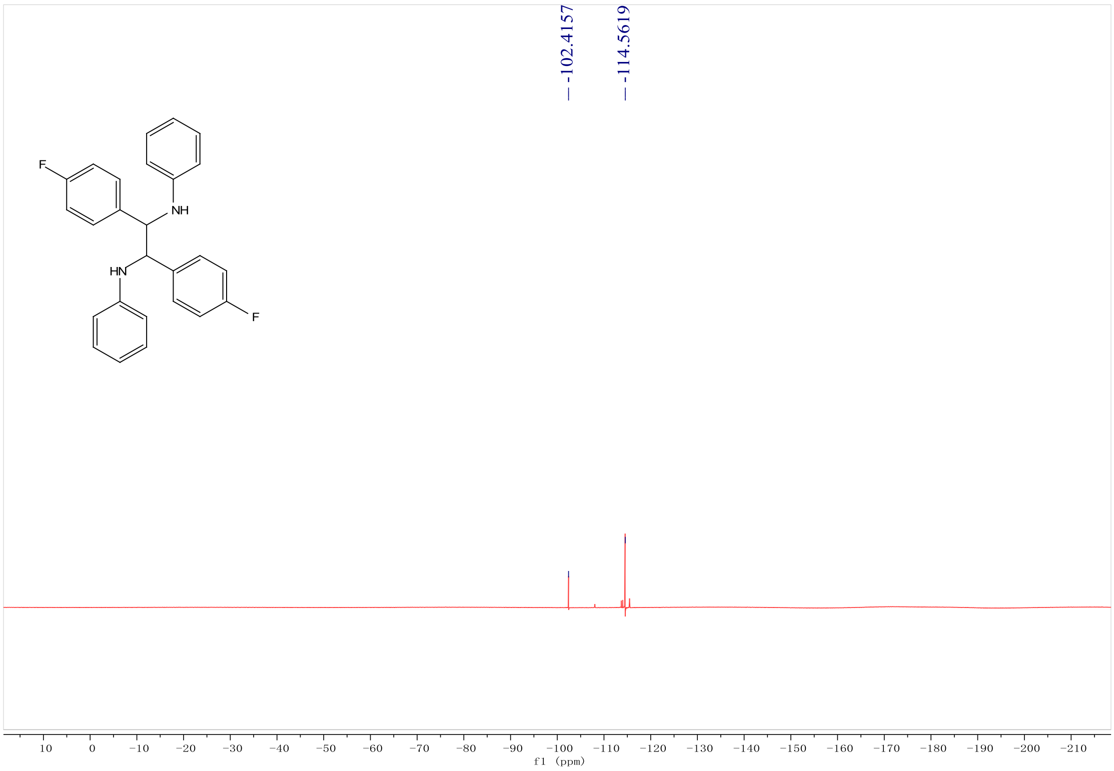
^{1}H-NMR Spectrum (600 MHz, $CDCl_3$) of **9’**



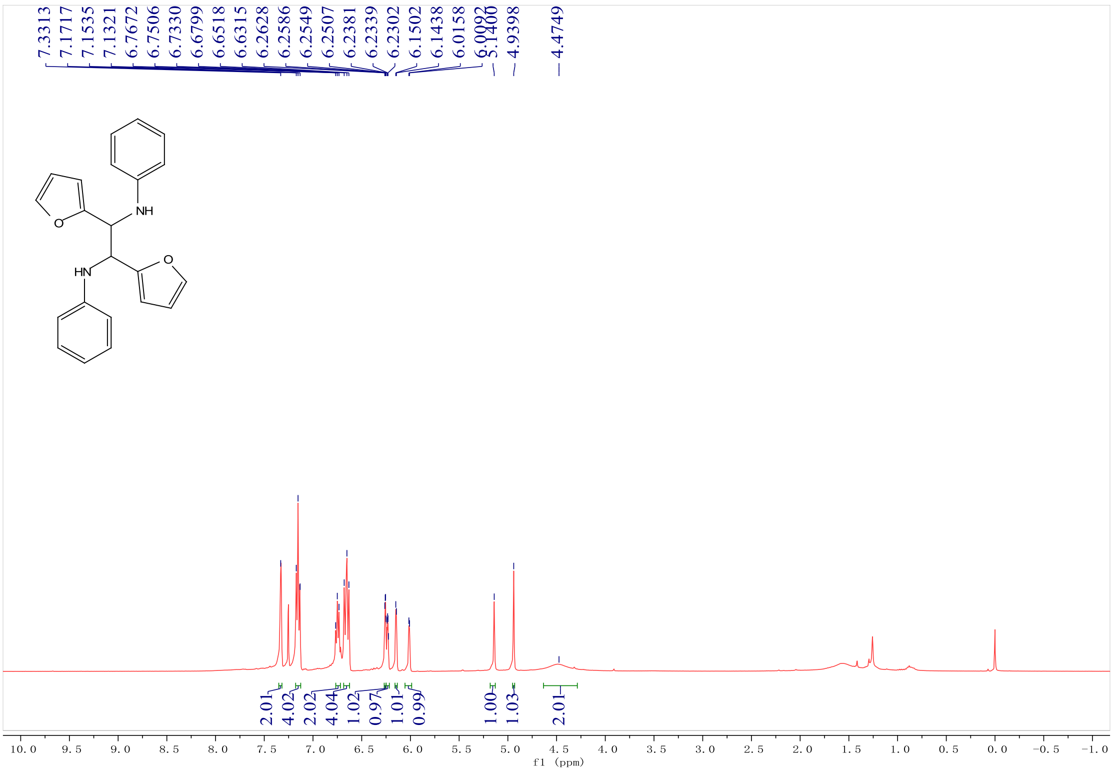
$^{13}C\{^{1}H\}$-NMR Spectrum (151 MHz, $CDCl_3$) of **9’**



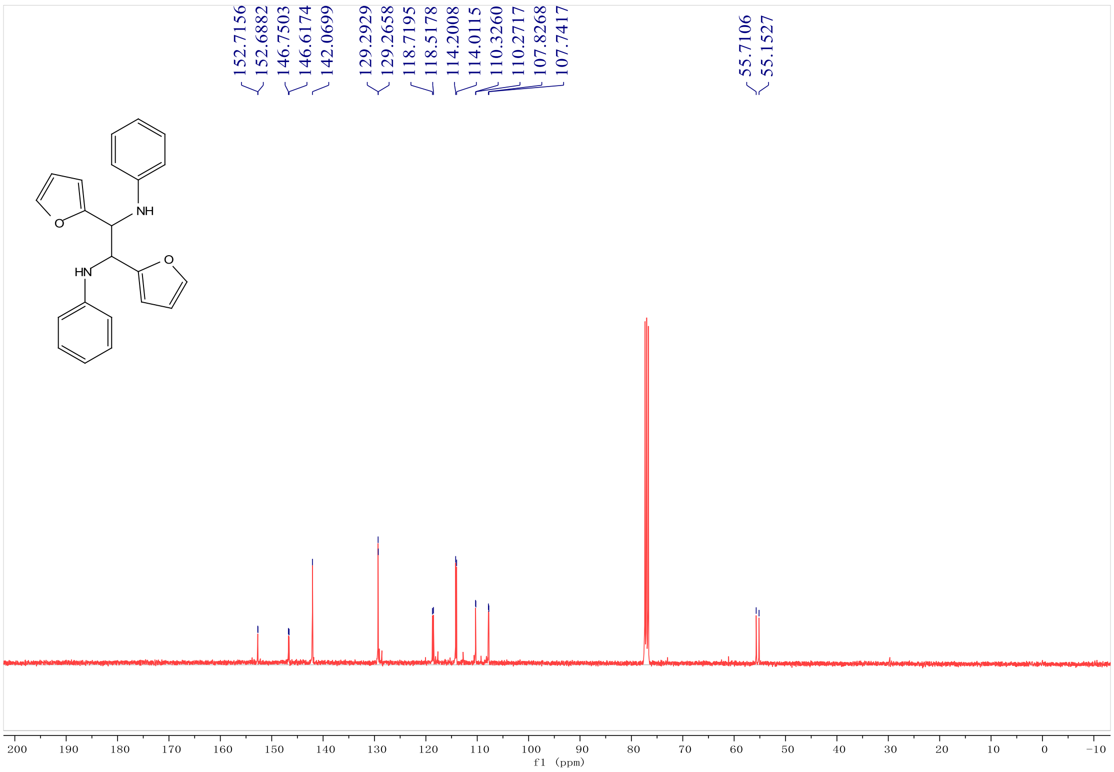
^{19}C-NMR Spectrum (376 MHz, $CDCl_3$) of **9’**



^{1}H-NMR Spectrum (400 MHz, $CDCl_3$) of **20’**

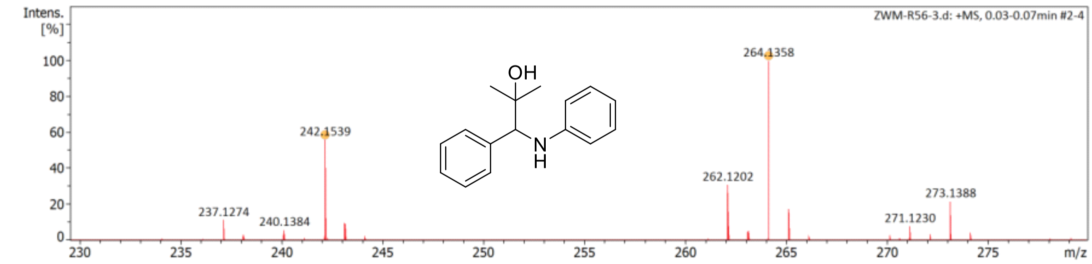


^{13}C{^{1}H}-NMR Spectrum (101 MHz, $CDCl_3$) of **20’**



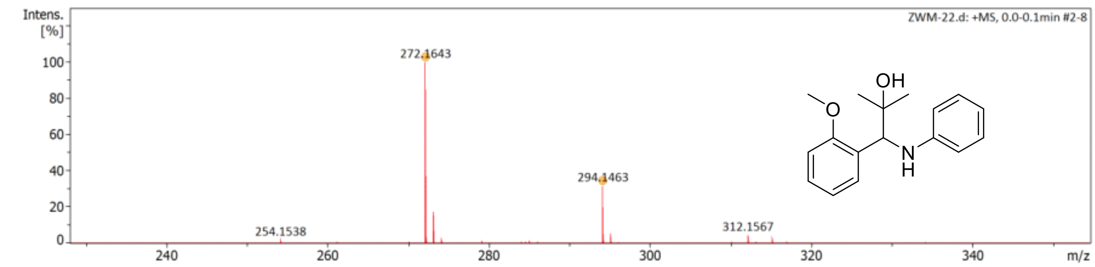
J. HRMS spectra of products

HRMS (ESI) Spectrum of **3**



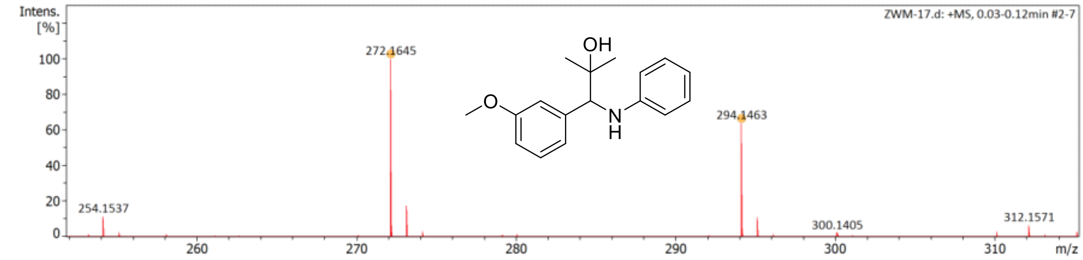
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	e¡¥ Conf	rdb	N-Rule
242.1539	1	C16H20NO	242.1539	M+H	0.2	8.8	100.00	even	8.0	ok
264.1358	1	C16H19NNaO	264.1359	M+Na	0.3	2.5	100.00	even	8.0	ok

HRMS (ESI) Spectrum of **4**



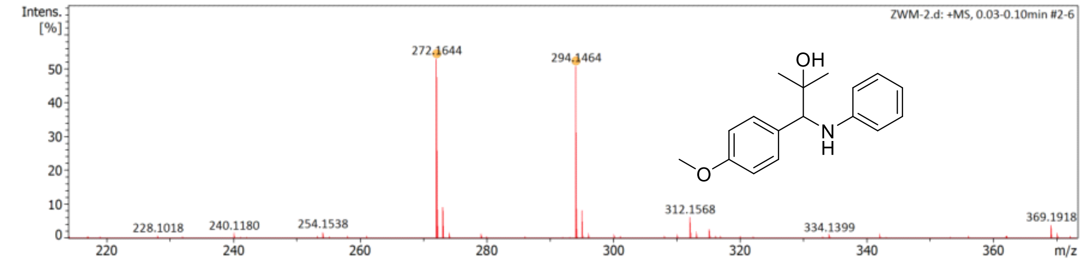
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
272.1643	1	C17H22NO2	272.1645	M+H	0.7	9.6	100.00	8.0	ok
294.1463	1	C17H21NNaO2	294.1464	M+Na	0.6	6.1	100.00	8.0	ok

HRMS (ESI) Spectrum of **5**



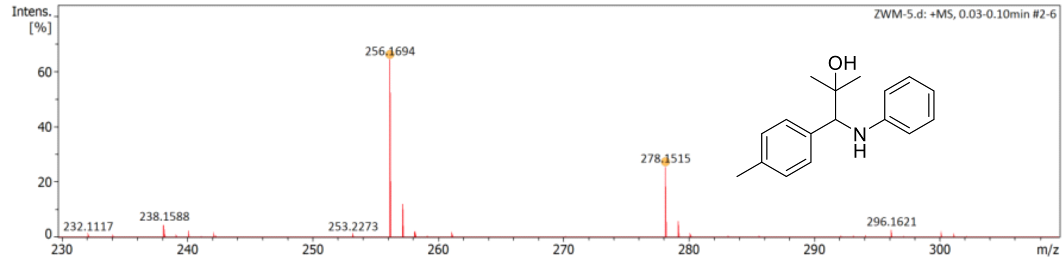
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
272.1645	1	C17H22NO2	272.1645	M+H	0.2	8.3	100.00	8.0	ok
294.1463	1	C17H21NNaO2	294.1464	M+Na	0.5	12.2	100.00	8.0	ok

HRMS (ESI) Spectrum of **6**



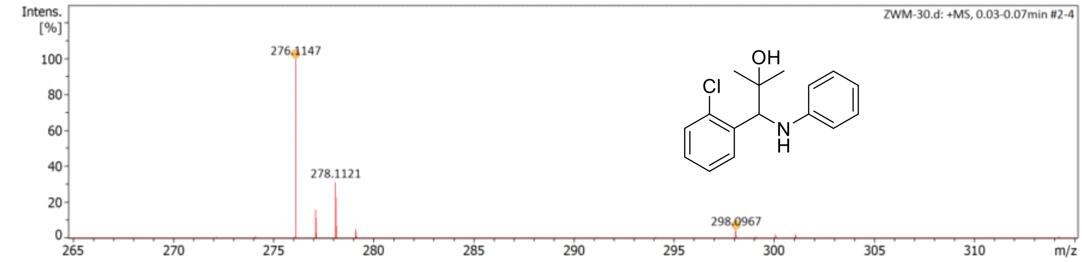
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
272.1644	1	C17H22NO2	272.1645	M+H	0.6	7.9	100.00	8.0	ok
294.1464	1	C17H21NNaO2	294.1464	M+Na	0.3	14.2	100.00	8.0	ok

HRMS (ESI) Spectrum of **7**



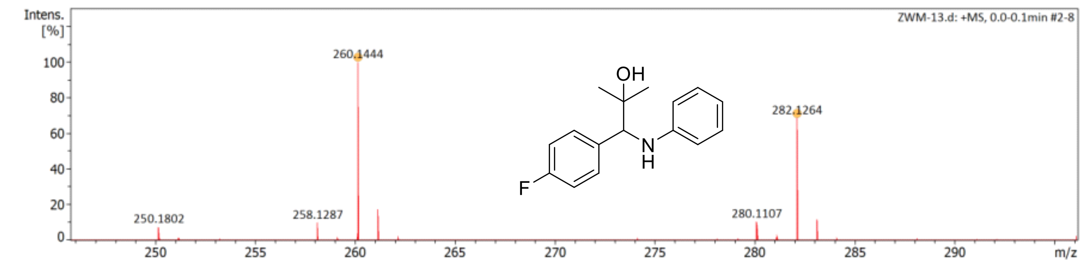
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
256.1694	1	C17H22NO	256.1696	M+H	0.7	0.6	100.00	8.0	ok
278.1515	1	C17H21NNaO	278.1515	M+Na	0.3	23.2	100.00	8.0	ok

HRMS (ESI) Spectrum of **8**



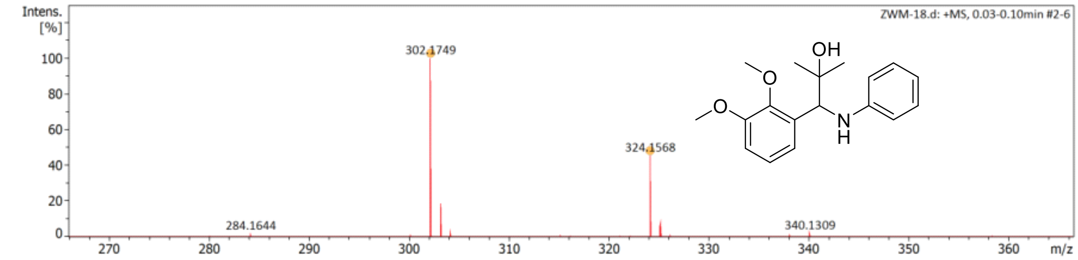
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
276.1147	1	C16H19ClNO	276.1150	M+H	0.8	14.8	100.00	11.0	ok
298.0967	1	C16H18ClNNaO	298.0969	M+Na	0.6	122.8	100.00	11.0	ok

HRMS (ESI) Spectrum of **9**



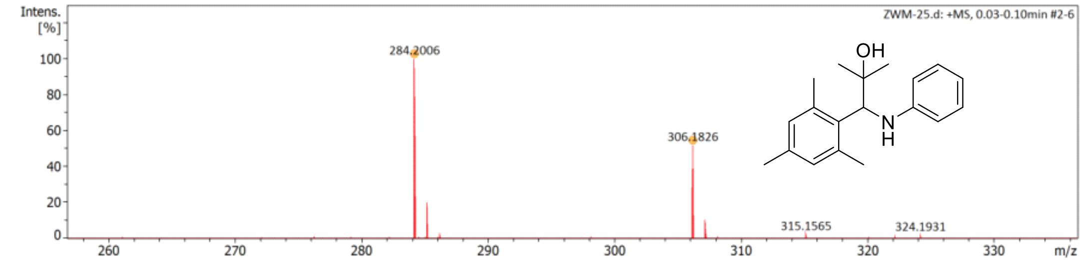
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
260.1444	1	C16H19FNO	260.1445	M+H	0.5	1.3	100.00	8.0	ok
282.1264	1	C16H18FNNaO	282.1265	M+Na	0.4	5.2	100.00	8.0	ok

HRMS (ESI) Spectrum of **10**



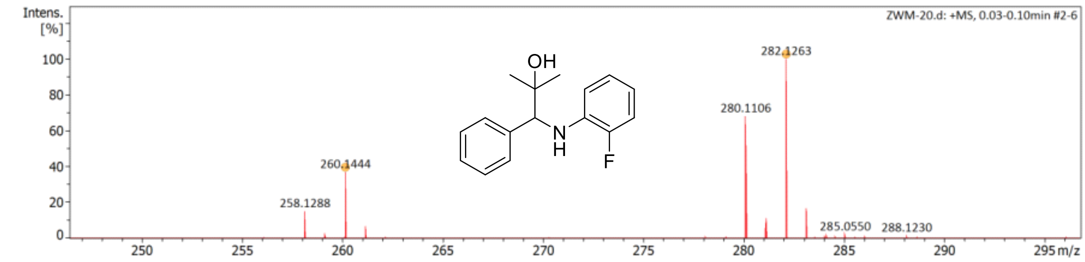
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
302.1749	1	C18H24NO3	302.1751	M+H	0.6	8.3	100.00	8.0	ok
324.1568	1	C18H23NNaO3	324.1570	M+Na	0.7	15.3	100.00	8.0	ok

HRMS (ESI) Spectrum of **11**



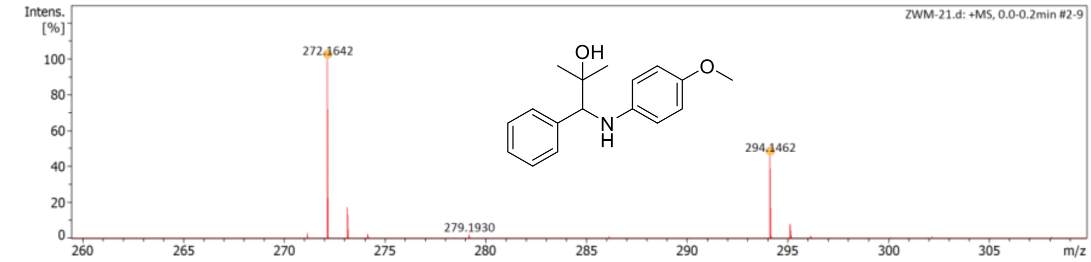
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	e¡¥ Conf	N-Rule
284.2006	1	C19H26NO	284.2009	M+H	0.9	7.0	100.00	even	ok
306.1826	1	C19H25NNaO	306.1828	M+Na	0.7	6.6	100.00	even	ok

HRMS (ESI) Spectrum of **12**



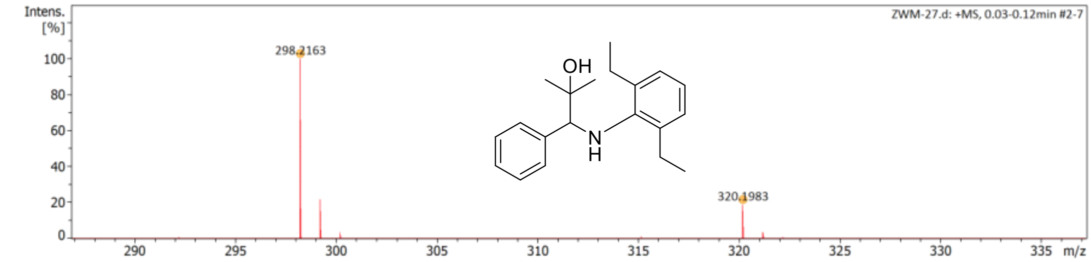
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
260.1444	1	C16H19FNO	260.1445	M+H	0.6	4.3	100.00	8.0	ok
282.1263	1	C16H18FNNaO	282.1265	M+Na	0.7	4.7	100.00	8.0	ok

HRMS (ESI) Spectrum of **13**



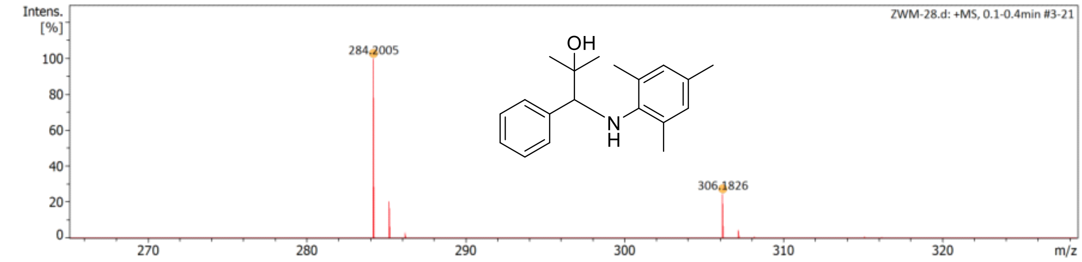
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	Score	rdb	e¡¥ Conf	N-Rule
272.1642	1	C17H22NO2	272.1645	M+H	1.1	100.00	8.0	even	ok
294.1462	1	C17H21NNaO2	294.1464	M+Na	0.8	100.00	8.0	even	ok

HRMS (ESI) Spectrum of **14**



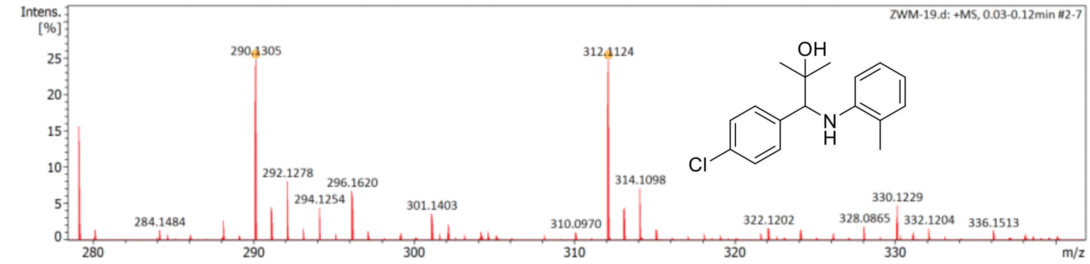
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
298.2163	1	C20H28NO	298.2165	M+H	0.7	3.1	100.00	8.0	ok
320.1983	1	C20H27NNaO	320.1985	M+Na	0.5	10.6	100.00	8.0	ok

HRMS (ESI) Spectrum of **15**



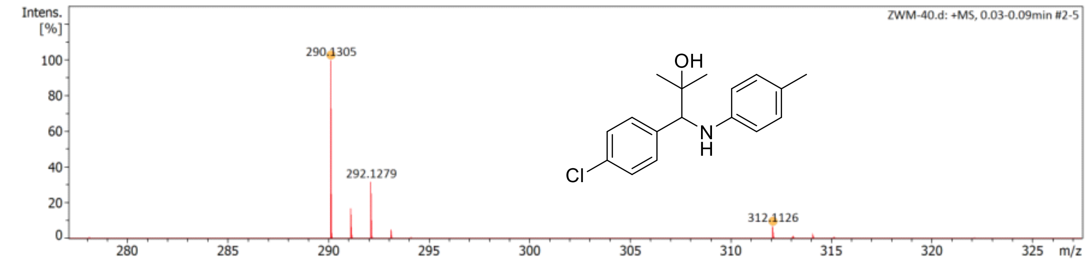
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
284.2005	1	C19H26NO	284.2009	1.3	2.9	1	100.00	8.0	even	ok
306.1826	1	C19H25NNaO	306.1828	0.9	10.0	1	100.00	8.0	even	ok

HRMS (ESI) Spectrum of **16**



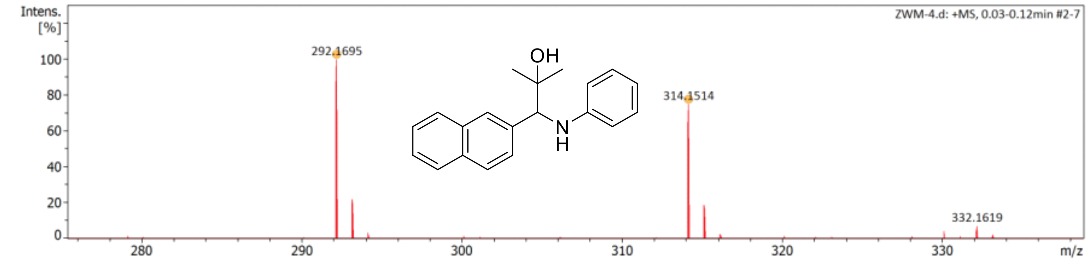
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
290.1305	1	C17H21ClNO	290.1306	0.5	7.7	1	100.00	11.0	even	ok
312.1124	1	C17H20ClNNaO	312.1126	0.5	26.2	1	100.00	11.0	even	ok

HRMS (ESI) Spectrum of **17**



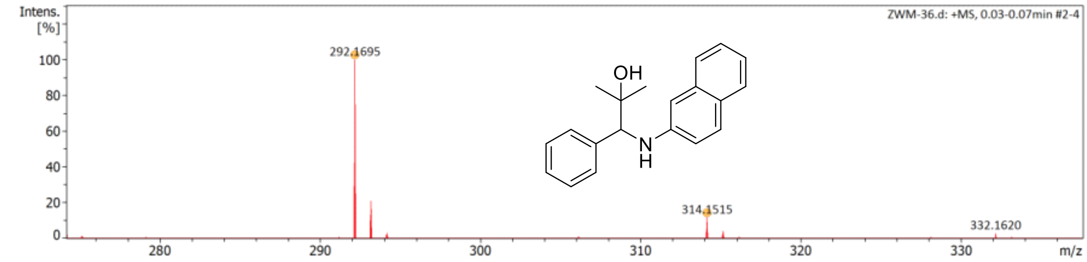
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
290.1305	1	C17H21ClNO	290.1306	M+H	0.2	14.1	100.00	11.0	ok
312.1126	1	C17H20ClNNaO	312.1126	M+Na	0.0	11.7	100.00	11.0	ok

HRMS (ESI) Spectrum of **18**



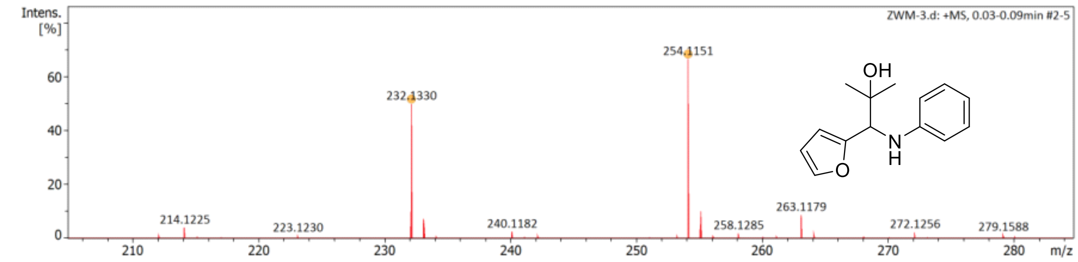
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
292.1695	1	C20H22NO	292.1696	M+H	0.5	2.1	100.00	11.0	ok
314.1514	1	C20H21NNaO	314.1515	M+Na	0.3	17.1	100.00	11.0	ok

HRMS (ESI) Spectrum of **19**



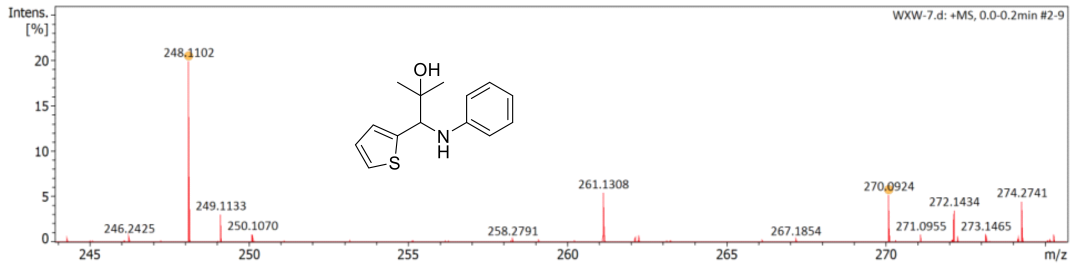
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
292.1695	1	C20H22NO	292.1696	M+H	0.4	7.0	100.00	11.0	ok
314.1515	1	C20H21NNaO	314.1515	M+Na	0.1	76.6	100.00	11.0	ok

HRMS (ESI) Spectrum of **20**



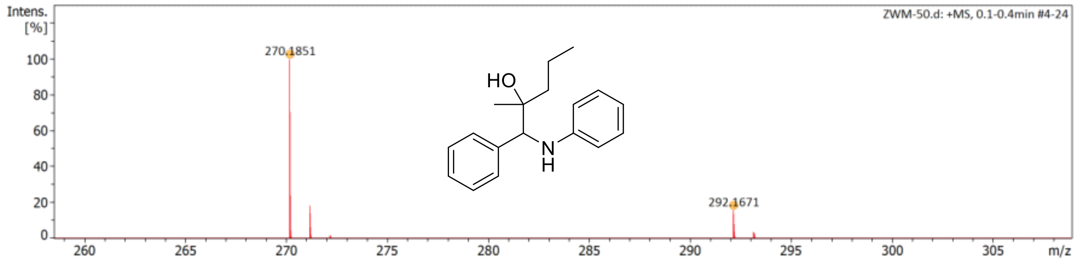
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
232.1330	1	C14H18NO2	232.1332	M+H	0.7	7.2	100.00	7.0	ok
254.1151	1	C14H17NNaO2	254.1151	M+Na	0.3	2.3	100.00	7.0	ok

HRMS (ESI) Spectrum of **21**



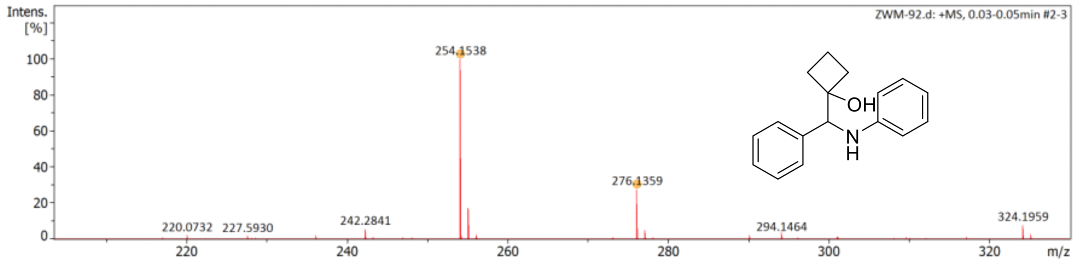
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
248.1102	1	C14H18NOS	248.1104	M+H	0.7	9.8	100.00	9.0	ok
270.0924	1	C14H17NNaOS	270.0923	M+Na	-0.3	9.7	100.00	9.0	ok

HRMS (ESI) Spectrum of **22**



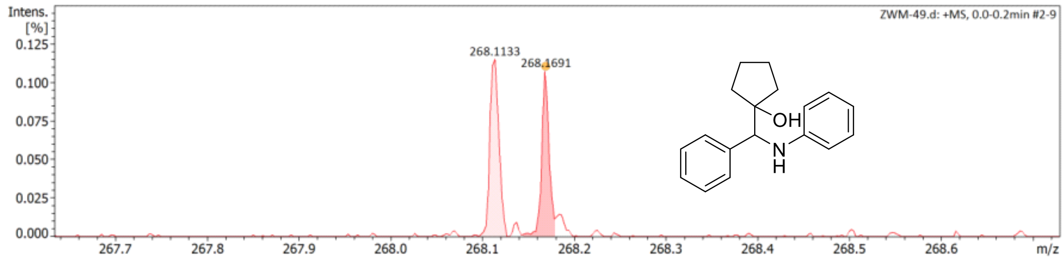
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	e¡¥ Conf
270.1851	1	C18H24NO	270.1852	M+H	0.5	10.0	100.00	8.0	even
292.1671	1	C18H23NNaO	292.1672	M+Na	0.4	1.2	100.00	8.0	even

HRMS (ESI) Spectrum of **23**



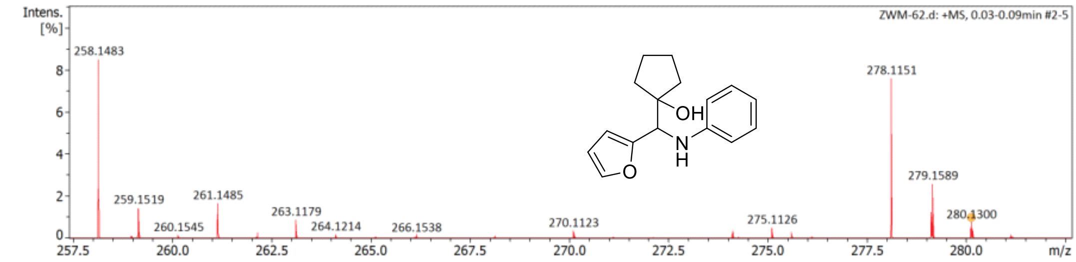
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
254.1538	1	C17H20NO	254.1539	M+H	0.7	7.4	100.00	9.0	ok
276.1359	1	C17H19NNaO	276.1359	M+Na	-0.1	4.9	100.00	9.0	ok

HRMS (ESI) Spectrum of **24**



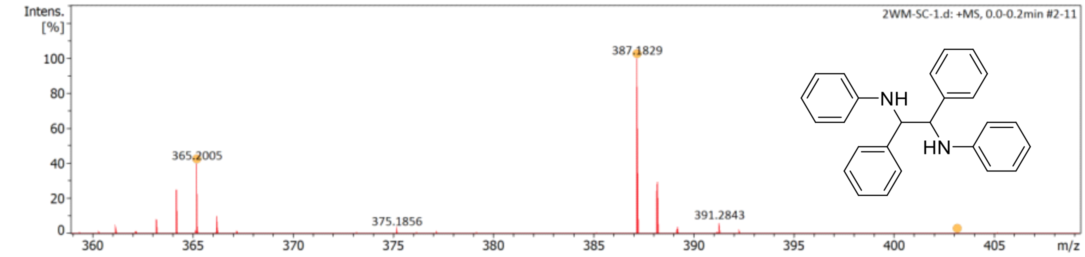
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
268.1691	1	C18H22NO	268.1696	M+H	2.0	n.a.	100.00	9.0	ok

HRMS (ESI) Spectrum of **25**



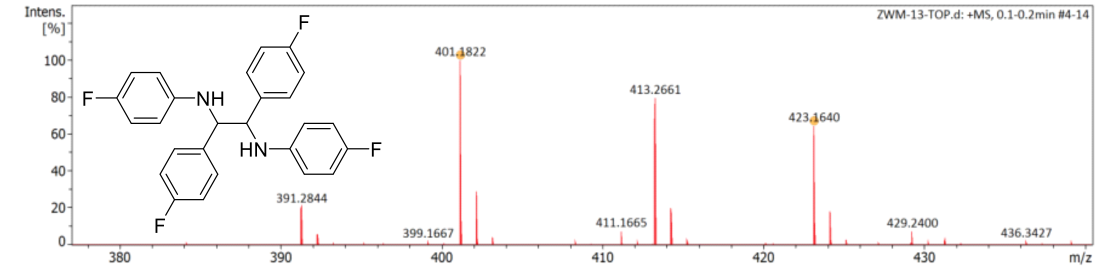
Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
258.1483	1	C16H20NO2	258.1489	M+H	2.3	3.8	100.00	8.0	ok
280.1300	1	C16H19NNaO2	280.1308	M+Na	2.9	13.4	100.00	8.0	ok

HRMS (ESI) Spectrum of **1d**



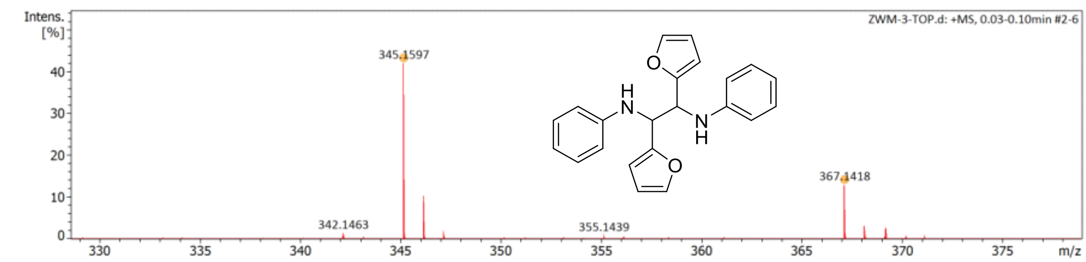
Meas. m/z	#	Ion Formula	Adduct	m/z	err [ppm]	mSigma	Score	rdb	N-Rule
365.2005	1	C26H25N2	M+H	365.2012	2.0	20.5	100.00	16.0	ok
387.1829	1	C26H24N2Na	M+Na	387.1832	0.7	4.0	100.00	16.0	ok
403.1570	1	C26H24KN2	M+K	403.1571	0.1	84.5	100.00	16.0	ok

HRMS (ESI) Spectrum of **9'**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
401.1822	1	C26H23F2N2	401.1824	0.6	1.9	1	100.00	16.0	even	ok
423.1640	1	C26H22F2N2Na	423.1643	0.7	2.2	1	100.00	16.0	even	ok

HRMS (ESI) Spectrum of **20'**



Meas. m/z	#	Ion Formula	m/z	Adduct	err [ppm]	mSigma	Score	rdb	N-Rule
345.1597	1	C22H21N2O2	345.1598	M+H	0.2	1.2	100.00	14.0	ok
367.1418	1	C22H20N2NaO2	367.1417	M+Na	-0.2	4.6	100.00	14.0	ok